

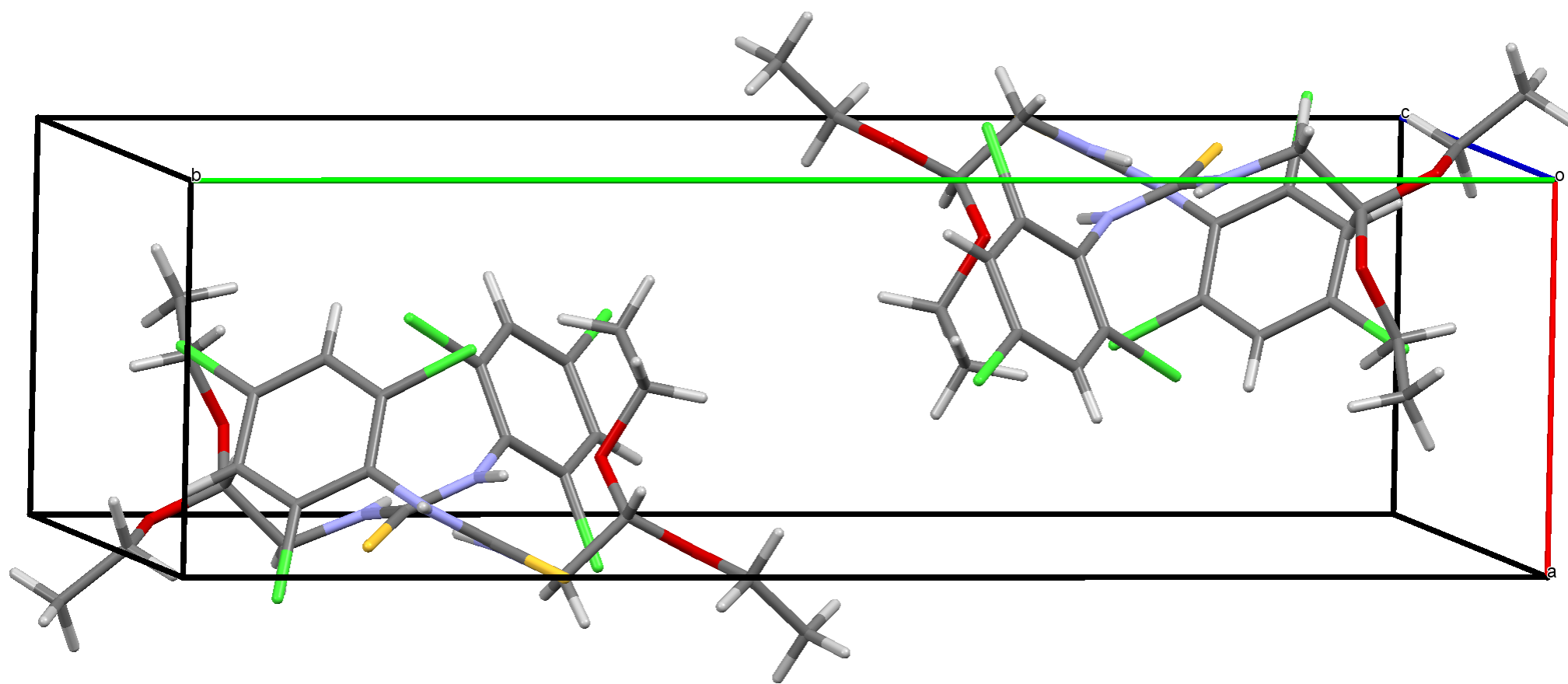
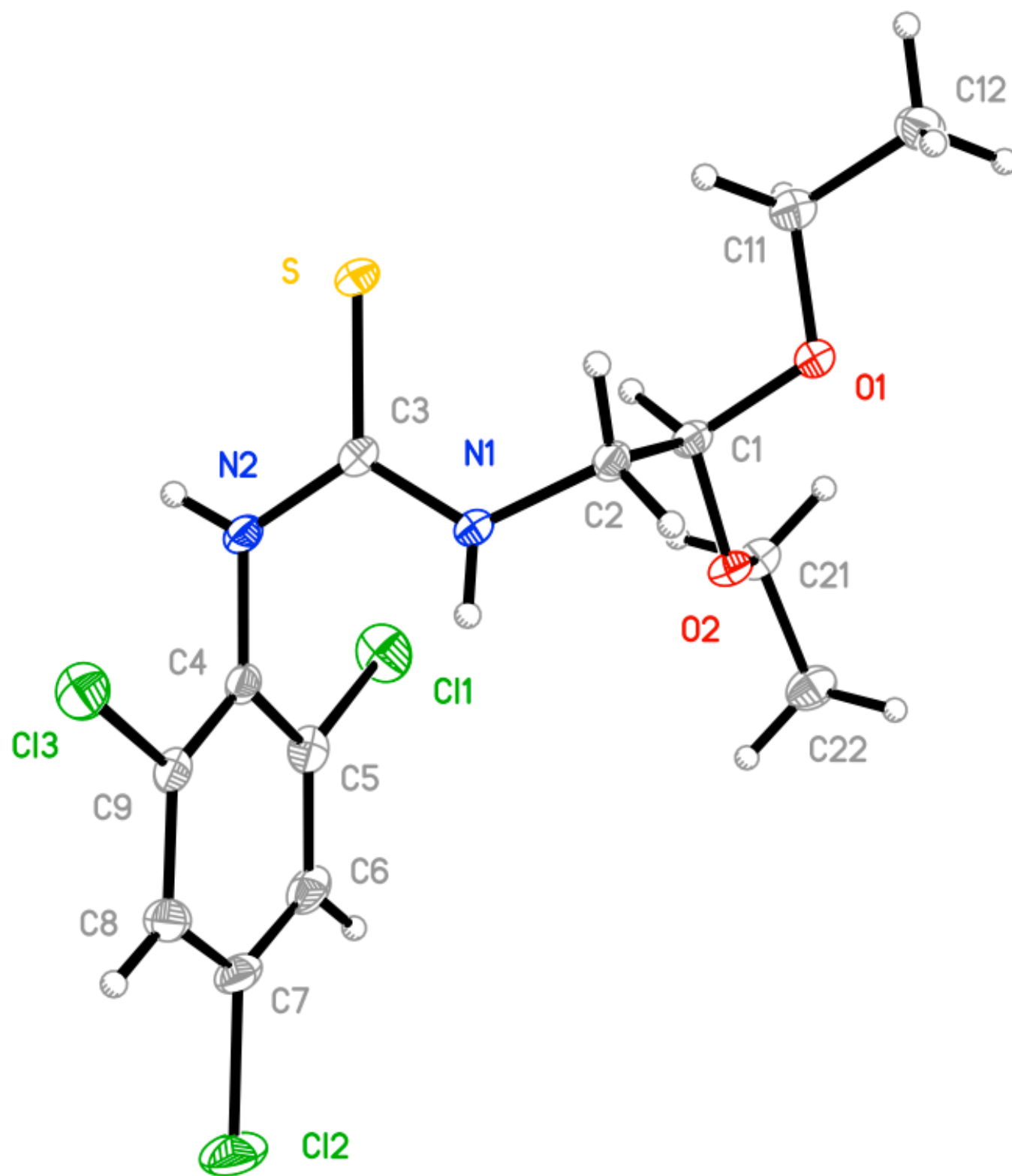
Supporting Information

Synthesis and Structural Characterization of 1-Arylimidazole-2-thiones and *N,N'*-Aryldiethoxyethylthioureas with Electronically Diverse Substituents: A Manifold of Hydrogen Bonding Networks

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 Analysis of Short Intra- and Inter-molecular Contacts , $d(I-J) < R(I) + R(J) + Tolr$, With $Tolr = 0.2$ Ang. $(X - I...J) > 100$. Deg.

Contact Radii : C H Cl N O S
 (Angstrom) 1.70 1.20 1.75 1.55 1.52 1.80

Default Contact Radii are those given by A.Bondi, J.Phys.Chem. (1964),68,441. (or Coval. Rad. + 0.8 Ang. when not given)

* WARNING * : no Far-Reaching Conclusions should be drawn based on the Default Radii Assigned to Metals

Short "INTRA" Distances between two Atoms that are Separated by less than 4 Bonds are NOT Listed (Except for Potential D/A Contacts)

| At(I)[1555.01] | At(J) | [ARU(J)] | D(I-J) | SumRad | Del | Type | X(I) | Y(I) | Z(I) | X(J) | Y(J) | Z(J) | X | X - I...J |
|----------------|-------------|-------------|------------|--------|-------|-------|--------|--------|--------|---------|--------|---------|-------|------------|
| Cl(1) | N(1) | [1455.01] | 3.477(2) | 3.30 | 0.18 | | 0.4785 | 0.7557 | 0.3242 | -0.0220 | 0.7297 | 0.3629 | C(5) | 125.12(8) |
| Cl(1) | N(1) | [] | 3.456(2) | 3.30 | 0.16 | Intra | 0.4785 | 0.7557 | 0.3242 | 0.9780 | 0.7297 | 0.3629 | | |
| Cl(1) | N(2) | [] | 2.986(2)<< | 3.30 | -0.31 | Intra | 0.4785 | 0.7557 | 0.3242 | 0.8642 | 0.7963 | 0.2286 | | |
| Cl(1) | C(2) | [1455.01] | 3.503(3) | 3.45 | 0.05 | | 0.4785 | 0.7557 | 0.3242 | 0.0620 | 0.6764 | 0.3990 | C(5) | 138.44(8) |
| Cl(1) | C(3) | [] | 3.329(2) < | 3.45 | -0.12 | Intra | 0.4785 | 0.7557 | 0.3242 | 0.9511 | 0.7460 | 0.2465 | | |
| Cl(1) | H(2B) | [1455.01] | 3.00 | 2.95 | 0.05 | | 0.4785 | 0.7557 | 0.3242 | 0.1690 | 0.6665 | 0.3418 | C(5) | 153 |
| Cl(1) | H(6A) | [] | 2.80 < | 2.95 | -0.15 | Intra | 0.4785 | 0.7557 | 0.3242 | 0.4027 | 0.8339 | 0.5098 | | |
| Cl(2) | H(6A) | [] | 2.80 < | 2.95 | -0.15 | Intra | 0.5158 | 0.9339 | 0.6250 | 0.4027 | 0.8339 | 0.5098 | | |
| Cl(2) | H(8A) | [] | 2.79 < | 2.95 | -0.16 | Intra | 0.5158 | 0.9339 | 0.6250 | 0.8602 | 0.9427 | 0.4880 | | |
| Cl(2) | C(12) | [4465.01] | 3.509(3) | 3.45 | 0.06 | | 0.5158 | 0.9339 | 0.6250 | 0.1942 | 0.9959 | 0.8359 | C(7) | 164.58(10) |
| Cl(2) | H(11A) | [4465.01] | 3.06 | 2.95 | 0.11 | | 0.5158 | 0.9339 | 0.6250 | 0.1132 | 0.9231 | 0.7467 | C(7) | 129 |
| Cl(2) | H(12A) | [4465.01] | 3.12 | 2.95 | 0.17 | | 0.5158 | 0.9339 | 0.6250 | 0.2317 | 1.0154 | 0.7602 | C(7) | 161 |
| Cl(3) | N(2) | [] | 2.989(2)<< | 3.30 | -0.31 | Intra | 1.1021 | 0.8954 | 0.3101 | 0.8642 | 0.7963 | 0.2286 | | |
| Cl(3) | C(6) | [1655.01] | 3.528(3) | 3.45 | 0.08 | | 1.1021 | 0.8954 | 0.3101 | 1.5222 | 0.8452 | 0.4723 | C(9) | 115.80(8) |
| Cl(3) | H(2) | [] | 3.15(2) | 2.95 | 0.20 | Intra | 1.1021 | 0.8954 | 0.3101 | 0.8490 | 0.8075 | 0.1600 | | |
| Cl(3) | H(8A) | [] | 2.79 < | 2.95 | -0.16 | Intra | 1.1021 | 0.8954 | 0.3101 | 0.8602 | 0.9427 | 0.4880 | | |
| Cl(3) | C(12) | [2755.01] | 3.628(3) | 3.45 | 0.18 | | 1.1021 | 0.8954 | 0.3101 | 0.8058 | 1.0041 | 0.1641 | | |
| Cl(3) | C(22) | [4664.01] | 3.496(3) | 3.45 | 0.05 | | 1.1021 | 0.8954 | 0.3101 | 1.4703 | 0.8830 | 0.0893 | C(9) | 151.10(9) |
| Cl(3) | H(22A) | [4664.01] | 3.04 | 2.95 | 0.09 | | 1.1021 | 0.8954 | 0.3101 | 1.3442 | 0.9025 | 0.0770 | C(9) | 145 |
| S | C(1) | [] | 3.552(2) | 3.50 | 0.05 | Intra | 1.0216 | 0.7061 | 0.1260 | 0.9083 | 0.6303 | 0.3978 | | |
| S | C(2) | [] | 3.050(2)<< | 3.50 | -0.45 | Intra | 1.0216 | 0.7061 | 0.1260 | 1.0620 | 0.6764 | 0.3990 | | |
| S | H(1A) | [] | 3.04 | 3.00 | 0.04 | Intra | 1.0216 | 0.7061 | 0.1260 | 0.8352 | 0.6300 | 0.3168 | | |
| S | H(2) | [] | 2.72(2)<< | 3.00 | -0.28 | Intra | 1.0216 | 0.7061 | 0.1260 | 0.8490 | 0.8075 | 0.1600 | | |
| S | H(2B) | [] | 2.70<< | 3.00 | -0.30 | Intra | 1.0216 | 0.7061 | 0.1260 | 1.1690 | 0.6665 | 0.3418 | | |
| S | N(1) | [4564.01] | 3.246(2) < | 3.35 | -0.10 | | 1.0216 | 0.7061 | 0.1260 | 0.9780 | 0.7703 | -0.1371 | C(3) | 112.87(8) |
| S | C(8) | [4564.01] | 3.618(3) | 3.50 | 0.12 | | 1.0216 | 0.7061 | 0.1260 | 0.7957 | 0.5905 | -0.0395 | C(3) | 133.64(9) |
| S | C(9) | [4564.01] | 3.533(3) | 3.50 | 0.03 | | 1.0216 | 0.7061 | 0.1260 | 0.8769 | 0.6238 | -0.1309 | C(3) | 147.50(8) |
| S | H(1) | [4564.01] | 2.49(2)<< | 3.00 | -0.51 | | 1.0216 | 0.7061 | 0.1260 | 0.9560 | 0.7483 | -0.0810 | C(3) | 114.7(5) |
| S | H(6A) | [4664.01] | 3.04 | 3.00 | 0.04 | | 1.0216 | 0.7061 | 0.1260 | 1.4027 | 0.6661 | 0.0098 | C(3) | 138 |
| O(1) | C(21) | [] | 2.946(3)<< | 3.22 | -0.27 | Intra | 1.0017 | 0.5783 | 0.4174 | 0.5937 | 0.6104 | 0.4762 | C(11) | 122.73(13) |
| O(1) | H(2A) | [] | 2.65 < | 2.72 | -0.07 | Intra | 1.0017 | 0.5783 | 0.4174 | 1.1206 | 0.6797 | 0.4831 | C(11) | 125 |
| O(1) | H(2B) | [] | 2.53 < | 2.72 | -0.19 | Intra | 1.0017 | 0.5783 | 0.4174 | 1.1690 | 0.6665 | 0.3418 | | |
| O(1) | H(12B) | [] | 2.58 < | 2.72 | -0.14 | Intra | 1.0017 | 0.5783 | 0.4174 | 1.1317 | 0.4776 | 0.3921 | C(1) | 164 |

| | | | | | | | | | | | | | | | |
|------|------|--------|------------|------------------|-------|-------|--------|--------|--------|--------|--------|---------|--------|------------|------------|
| O(1) | | H(12C) | [] | 2.57 < 2.72 | -0.15 | Intra | 1.0017 | 0.5783 | 0.4174 | 1.3125 | 0.5200 | 0.3759 | C(1) | 145 | |
| O(1) | | H(21B) | [] | 2.64 < 2.72 | -0.08 | Intra | 1.0017 | 0.5783 | 0.4174 | 0.6207 | 0.5702 | 0.4616 | C(11) | 111 | |
| O(1) | | H(22A) | [1655.01] | 2.91 | 2.72 | 0.19 | 1.0017 | 0.5783 | 0.4174 | 1.3442 | 0.5975 | 0.5770 | C(1) | 108 | |
| | | | | | | | | | | | | | C(11) | 112 | |
| O(1) | | H(12B) | [3766.01] | 2.63 < 2.72 | -0.09 | | 1.0017 | 0.5783 | 0.4174 | 0.8683 | 0.5224 | 0.6079 | C(1) | 114 | |
| | | | | | | | | | | | | | C(11) | 121 | |
| O(2) | | N(1) | [] | 2.922(3) < 3.07 | -0.15 | Intra | 0.7763 | 0.6400 | 0.4942 | 0.9780 | 0.7297 | 0.3629 | C(21) | 134.77(12) | |
| O(2) | | H(2A) | [] | 2.52 << 2.72 | -0.20 | Intra | 0.7763 | 0.6400 | 0.4942 | 1.1206 | 0.6797 | 0.4831 | C(21) | 167 | |
| O(2) | | H(22B) | [] | 2.58 < 2.72 | -0.14 | Intra | 0.7763 | 0.6400 | 0.4942 | 0.4454 | 0.6569 | 0.6039 | C(1) | 159 | |
| O(2) | | H(22C) | [] | 2.60 < 2.72 | -0.12 | Intra | 0.7763 | 0.6400 | 0.4942 | 0.5407 | 0.6011 | 0.6609 | C(1) | 150 | |
| O(2) | | N(2) | [4565.01] | 3.012(2) < 3.07 | -0.06 | | 0.7763 | 0.6400 | 0.4942 | 0.8642 | 0.7037 | 0.7286 | C(1) | 126.25(12) | |
| | | | | | | | | | | | | | C(21) | 121.42(11) | |
| O(2) | | H(2) | [4565.01] | 2.24(2) << 2.72 | -0.48 | | 0.7763 | 0.6400 | 0.4942 | 0.8490 | 0.6925 | 0.6600 | C(1) | 123.7(5) | |
| | | | | | | | | | | | | | C(21) | 124.2(5) | |
| N(1) | | Cl(1) | [] | 3.456(2) | 3.30 | 0.16 | Intra | 0.9780 | 0.7297 | 0.3629 | 0.4785 | 0.7557 | 0.3242 | C(2) | 124.82(13) |
| N(1) | | Cl(1) | [1655.01] | 3.477(2) | 3.30 | 0.18 | 0.9780 | 0.7297 | 0.3629 | 1.4785 | 0.7557 | 0.3242 | | | |
| N(1) | | O(2) | [] | 2.922(3) < 3.07 | -0.15 | Intra | 0.9780 | 0.7297 | 0.3629 | 0.7763 | 0.6400 | 0.4942 | C(3) | 128.21(15) | |
| N(1) | | C(4) | [] | 2.735(3) << 3.25 | -0.52 | Intra | 0.9780 | 0.7297 | 0.3629 | 0.7821 | 0.8285 | 0.3252 | C(2) | 171.17(14) | |
| N(1) | | C(5) | [] | 3.245(3) < 3.25 | -0.01 | Intra | 0.9780 | 0.7297 | 0.3629 | 0.6034 | 0.8140 | 0.3785 | C(2) | 146.81(14) | |
| N(1) | | H(1A) | [] | 2.61 < 2.75 | -0.14 | Intra | 0.9780 | 0.7297 | 0.3629 | 0.8352 | 0.6300 | 0.3168 | H(1) | 131 | |
| N(1) | | S | [4565.01] | 3.246(2) < 3.35 | -0.10 | | 0.9780 | 0.7297 | 0.3629 | 1.0216 | 0.7939 | 0.6260 | C(3) | 134.71(14) | |
| N(2) | | Cl(1) | [] | 2.986(2) << 3.30 | -0.31 | Intra | 0.8642 | 0.7963 | 0.2286 | 0.4785 | 0.7557 | 0.3242 | H(2) | 109.5(15) | |
| N(2) | | Cl(3) | [] | 2.989(2) << 3.30 | -0.31 | Intra | 0.8642 | 0.7963 | 0.2286 | 1.1021 | 0.8954 | 0.3101 | C(3) | 115.56(14) | |
| N(2) | | H(1) | [] | 2.39(2) << 2.75 | -0.36 | Intra | 0.8642 | 0.7963 | 0.2286 | 0.9560 | 0.7517 | 0.4190 | H(2) | 169.4(16) | |
| N(2) | | O(2) | [4564.01] | 3.012(2) < 3.07 | -0.06 | | 0.8642 | 0.7963 | 0.2286 | 0.7763 | 0.8600 | -0.0058 | C(3) | 130.53(13) | |
| | | | | | | | | | | | | | C(4) | 105.82(13) | |
| C(1) | | S | [] | 3.552(2) | 3.50 | 0.05 | Intra | 0.9083 | 0.6303 | 0.3978 | 1.0216 | 0.7061 | 0.1260 | O(1) | 118.19(12) |
| | | | | | | | | | | | | | O(2) | 132.90(13) | |
| C(1) | | C(3) | [] | 3.229(3) < 3.40 | -0.17 | Intra | 0.9083 | 0.6303 | 0.3978 | 0.9511 | 0.7460 | 0.2465 | O(1) | 141.98(13) | |
| | | | | | | | | | | | | | O(2) | 107.42(13) | |
| C(1) | | H(1) | [] | 2.93(2) | 2.90 | 0.03 | Intra | 0.9083 | 0.6303 | 0.3978 | 0.9560 | 0.7517 | 0.4190 | O(1) | 144.4(4) |
| C(1) | | H(11A) | [] | 2.51 << 2.90 | -0.39 | Intra | 0.9083 | 0.6303 | 0.3978 | 1.1132 | 0.5769 | 0.2467 | O(2) | 159 | |
| C(1) | | H(11B) | [] | 2.71 < 2.90 | -0.19 | Intra | 0.9083 | 0.6303 | 0.3978 | 0.9317 | 0.5345 | 0.2645 | O(2) | 125 | |
| | | | | | | | | | | | | | C(2) | 125 | |
| C(1) | | H(21A) | [] | 2.62 << 2.90 | -0.28 | Intra | 0.9083 | 0.6303 | 0.3978 | 0.5218 | 0.6254 | 0.4032 | O(1) | 114 | |
| | | | | | | | | | | | | | C(2) | 136 | |
| C(1) | | H(21B) | [] | 2.52 << 2.90 | -0.38 | Intra | 0.9083 | 0.6303 | 0.3978 | 0.6207 | 0.5702 | 0.4616 | C(2) | 161 | |
| C(2) | | Cl(1) | [1655.01] | 3.503(3) | 3.45 | 0.05 | 1.0620 | 0.6764 | 0.3990 | 1.4785 | 0.7557 | 0.3242 | C(1) | 161.12(13) | |
| C(2) | | S | [] | 3.050(2) << 3.50 | -0.45 | Intra | 1.0620 | 0.6764 | 0.3990 | 1.0216 | 0.7061 | 0.1260 | H(2A) | 154 | |
| C(2) | | C(11) | [] | 3.185(3) << 3.40 | -0.22 | Intra | 1.0620 | 0.6764 | 0.3990 | 1.0521 | 0.5502 | 0.3046 | N(1) | 137.78(14) | |
| | | | | | | | | | | | | | H(2A) | 112 | |
| C(2) | | H(11A) | [] | 2.92 | 2.90 | 0.02 | Intra | 1.0620 | 0.6764 | 0.3990 | 1.1132 | 0.5769 | 0.2467 | N(1) | 128 |
| | | | | | | | | | | | | | H(2A) | 122 | |
| C(3) | | Cl(1) | [] | 3.329(2) < 3.45 | -0.12 | Intra | 0.9511 | 0.7460 | 0.2465 | 0.4785 | 0.7557 | 0.3242 | S | 121.28(10) | |
| C(3) | | C(1) | [] | 3.229(3) < 3.40 | -0.17 | Intra | 0.9511 | 0.7460 | 0.2465 | 0.9083 | 0.6303 | 0.3978 | N(2) | 142.35(15) | |
| C(3) | | C(5) | [] | 3.215(3) < 3.40 | -0.19 | Intra | 0.9511 | 0.7460 | 0.2465 | 0.6034 | 0.8140 | 0.3785 | S | 147.80(11) | |
| C(3) | | C(9) | [] | 3.423(3) | 3.40 | 0.02 | Intra | 0.9511 | 0.7460 | 0.2465 | 0.8769 | 0.8762 | 0.3691 | S | 148.93(11) |
| C(3) | | H(1A) | [] | 2.98 | 2.90 | 0.08 | Intra | 0.9511 | 0.7460 | 0.2465 | 0.8352 | 0.6300 | 0.3168 | N(2) | 138 |

| | | | | | | | | | | | | | | | |
|-------|------|--------|------------|------------|------|-------|-------|--------|--------|--------|--------|--------|--------|--------|------------|
| C(3) | | H(2B) | [] | 2.61<< | 2.90 | -0.29 | Intra | 0.9511 | 0.7460 | 0.2465 | 1.1690 | 0.6665 | 0.3418 | N(2) | 161 |
| C(4) | | N(1) | [] | 2.735(3)<< | 3.25 | -0.52 | Intra | 0.7821 | 0.8285 | 0.3252 | 0.9780 | 0.7297 | 0.3629 | C(9) | 115.93(14) |
| C(4) | | C(7) | [] | 2.770(3)<< | 3.40 | -0.63 | Intra | 0.7821 | 0.8285 | 0.3252 | 0.6188 | 0.8929 | 0.5100 | N(2) | 178.83(15) |
| C(4) | | H(1) | [] | 2.40(2)<< | 2.90 | -0.50 | Intra | 0.7821 | 0.8285 | 0.3252 | 0.9560 | 0.7517 | 0.4190 | C(9) | 105.2(5) |
| C(4) | | C(22) | [4564.01] | 3.535(3) | 3.40 | 0.13 | | 0.7821 | 0.8285 | 0.3252 | 0.4703 | 0.8830 | 0.0893 | C(9) | 102.28(14) |
| C(4) | | H(22C) | [4564.01] | 2.93 | 2.90 | 0.03 | | 0.7821 | 0.8285 | 0.3252 | 0.5407 | 0.8989 | 0.1609 | | |
| C(5) | | N(1) | [] | 3.245(3) < | 3.25 | -0.01 | Intra | 0.6034 | 0.8140 | 0.3785 | 0.9780 | 0.7297 | 0.3629 | C(6) | 133.92(15) |
| C(5) | | C(3) | [] | 3.215(3) < | 3.40 | -0.19 | Intra | 0.6034 | 0.8140 | 0.3785 | 0.9511 | 0.7460 | 0.2465 | C(6) | 154.55(15) |
| C(5) | | C(8) | [] | 2.766(4)<< | 3.40 | -0.63 | Intra | 0.6034 | 0.8140 | 0.3785 | 0.7957 | 0.9095 | 0.4605 | Cl(1) | 178.15(13) |
| C(5) | | H(1) | [] | 2.84(2) < | 2.90 | -0.06 | Intra | 0.6034 | 0.8140 | 0.3785 | 0.9560 | 0.7517 | 0.4190 | C(6) | 120.8(5) |
| C(5) | | H(2) | [] | 2.92(2) | 2.90 | 0.02 | Intra | 0.6034 | 0.8140 | 0.3785 | 0.8490 | 0.8075 | 0.1600 | C(6) | 149.8(5) |
| C(6) | | Cl(3) | [1455.01] | 3.528(3) | 3.45 | 0.08 | | 0.5222 | 0.8452 | 0.4723 | 0.1021 | 0.8954 | 0.3101 | C(7) | 103.96(15) |
| C(6) | | C(9) | [] | 2.767(3)<< | 3.40 | -0.63 | Intra | 0.5222 | 0.8452 | 0.4723 | 0.8769 | 0.8762 | 0.3691 | H(6A) | 178 |
| C(7) | | C(4) | [] | 2.770(3)<< | 3.40 | -0.63 | Intra | 0.6188 | 0.8929 | 0.5100 | 0.7821 | 0.8285 | 0.3252 | Cl(2) | 179.44(14) |
| C(8) | | C(5) | [] | 2.766(4)<< | 3.40 | -0.63 | Intra | 0.7957 | 0.9095 | 0.4605 | 0.6034 | 0.8140 | 0.3785 | H(8A) | 179 |
| C(8) | | H(12A) | [2755.01] | 2.99 | 2.90 | 0.09 | | 0.7957 | 0.9095 | 0.4605 | 0.7683 | 0.9846 | 0.2398 | C(7) | 116 |
| C(8) | | S | [4565.01] | 3.618(3) | 3.50 | 0.12 | | 0.7957 | 0.9095 | 0.4605 | 1.0216 | 0.7939 | 0.6260 | H(8A) | 107 |
| C(9) | | C(3) | [] | 3.423(3) | 3.40 | 0.02 | Intra | 0.8769 | 0.8762 | 0.3691 | 0.9511 | 0.7460 | 0.2465 | C(8) | 149.14(16) |
| C(9) | | C(6) | [] | 2.767(3)<< | 3.40 | -0.63 | Intra | 0.8769 | 0.8762 | 0.3691 | 0.5222 | 0.8452 | 0.4723 | Cl(3) | 177.86(12) |
| C(9) | | H(1) | [] | 3.07(2) | 2.90 | 0.17 | Intra | 0.8769 | 0.8762 | 0.3691 | 0.9560 | 0.7517 | 0.4190 | C(8) | 119.9(4) |
| C(9) | | H(2) | [] | 2.80(2) < | 2.90 | -0.10 | Intra | 0.8769 | 0.8762 | 0.3691 | 0.8490 | 0.8075 | 0.1600 | C(8) | 152.7(4) |
| C(9) | | H(12A) | [2755.01] | 3.03 | 2.90 | 0.13 | | 0.8769 | 0.8762 | 0.3691 | 0.7683 | 0.9846 | 0.2398 | C(4) | 116 |
| C(9) | | S | [4565.01] | 3.533(3) | 3.50 | 0.03 | | 0.8769 | 0.8762 | 0.3691 | 1.0216 | 0.7939 | 0.6260 | Cl(3) | 101.79(9) |
| C(11) | | C(2) | [] | 3.185(3)<< | 3.40 | -0.22 | Intra | 1.0521 | 0.5502 | 0.3046 | 1.0620 | 0.6764 | 0.3990 | C(12) | 127.81(16) |
| | | | | | | | | | | | | | | H(11B) | 121 |
| C(11) | | H(1A) | [] | 2.41<< | 2.90 | -0.49 | Intra | 1.0521 | 0.5502 | 0.3046 | 0.8352 | 0.6300 | 0.3168 | C(12) | 163 |
| C(11) | | H(2B) | [] | 2.92 | 2.90 | 0.02 | Intra | 1.0521 | 0.5502 | 0.3046 | 1.1690 | 0.6665 | 0.3418 | C(12) | 120 |
| | | | | | | | | | | | | | | H(11B) | 130 |
| C(12) | | Cl(3) | [2745.01] | 3.628(3) | 3.45 | 0.18 | | 1.1942 | 0.5041 | 0.3359 | 0.8979 | 0.3954 | 0.1899 | H(12C) | 156 |
| C(12) | | H(21B) | [3766.01] | 3.07 | 2.90 | 0.17 | | 1.1942 | 0.5041 | 0.3359 | 1.3793 | 0.4298 | 0.5384 | C(11) | 147 |
| | | | | | | | | | | | | | | H(12A) | 102 |
| C(12) | | H(22C) | [3766.01] | 3.09 | 2.90 | 0.19 | | 1.1942 | 0.5041 | 0.3359 | 1.4593 | 0.3989 | 0.3391 | C(11) | 166 |
| C(12) | | Cl(2) | [4664.01] | 3.509(3) | 3.45 | 0.06 | | 1.1942 | 0.5041 | 0.3359 | 1.5158 | 0.5661 | 0.1250 | H(12B) | 163 |
| C(21) | | O(1) | [] | 2.946(3)<< | 3.22 | -0.27 | Intra | 0.5937 | 0.6104 | 0.4762 | 1.0017 | 0.5783 | 0.4174 | C(22) | 137.72(14) |
| | | | | | | | | | | | | | | H(21A) | 112 |
| C(21) | | H(1A) | [] | 2.44<< | 2.90 | -0.46 | Intra | 0.5937 | 0.6104 | 0.4762 | 0.8352 | 0.6300 | 0.3168 | C(22) | 161 |
| C(21) | | H(12C) | [1455.01] | 3.06 | 2.90 | 0.16 | | 0.5937 | 0.6104 | 0.4762 | 0.3125 | 0.5200 | 0.3759 | O(2) | 158 |
| C(22) | | H(2A) | [1455.01] | 3.01 | 2.90 | 0.11 | | 0.4703 | 0.6170 | 0.5893 | 0.1206 | 0.6797 | 0.4831 | C(21) | 101 |
| | | | | | | | | | | | | | | H(22C) | 150 |
| C(22) | | Cl(3) | [4465.01] | 3.496(3) | 3.45 | 0.05 | | 0.4703 | 0.6170 | 0.5893 | 0.1021 | 0.6046 | 0.8101 | C(21) | 163.97(15) |
| C(22) | | C(4) | [4565.01] | 3.535(3) | 3.40 | 0.13 | | 0.4703 | 0.6170 | 0.5893 | 0.7821 | 0.6715 | 0.8252 | C(21) | 107.17(13) |
| | | | | | | | | | | | | | | H(22A) | 141 |
| H(1) | | N(2) | [] | 2.39(2)<< | 2.75 | -0.36 | Intra | 0.9560 | 0.7517 | 0.4190 | 0.8642 | 0.7963 | 0.2286 | | |
| H(1) | | C(1) | [] | 2.93(2) | 2.90 | 0.03 | Intra | 0.9560 | 0.7517 | 0.4190 | 0.9083 | 0.6303 | 0.3978 | | |
| H(1) | | C(4) | [] | 2.40(2)<< | 2.90 | -0.50 | Intra | 0.9560 | 0.7517 | 0.4190 | 0.7821 | 0.8285 | 0.3252 | N(1) | 105.7(17) |
| H(1) | | C(5) | [] | 2.84(2) < | 2.90 | -0.06 | Intra | 0.9560 | 0.7517 | 0.4190 | 0.6034 | 0.8140 | 0.3785 | N(1) | 112.6(17) |
| H(1) | | C(9) | [] | 3.07(2) | 2.90 | 0.17 | Intra | 0.9560 | 0.7517 | 0.4190 | 0.8769 | 0.8762 | 0.3691 | N(1) | 121.7(17) |
| H(1) | | H(2A) | [] | 2.16<< | 2.40 | -0.24 | Intra | 0.9560 | 0.7517 | 0.4190 | 1.1206 | 0.6797 | 0.4831 | | |

| | | | | | | | | | | | | | | | |
|--------|------|--------|------------|-----------|------|-------|-------|--------|--------|--------|--------|--------|---------|--------|-----------|
| H(1) | | S | [4565.01] | 2.49(2)<< | 3.00 | -0.51 | | 0.9560 | 0.7517 | 0.4190 | 1.0216 | 0.7939 | 0.6260 | N(1) | 153.6(19) |
| H(1A) | | S | [] | 3.04 | 3.00 | 0.04 | Intra | 0.8352 | 0.6300 | 0.3168 | 1.0216 | 0.7061 | 0.1260 | C(1) | 113 |
| H(1A) | | N(1) | [] | 2.61 | < | 2.75 | -0.14 | Intra | 0.8352 | 0.6300 | 0.3168 | 0.9780 | 0.7297 | 0.3629 | |
| H(1A) | | C(3) | [] | 2.98 | 2.90 | 0.08 | Intra | 0.8352 | 0.6300 | 0.3168 | 0.9511 | 0.7460 | 0.2465 | | |
| H(1A) | | C(11) | [] | 2.41<< | 2.90 | -0.49 | Intra | 0.8352 | 0.6300 | 0.3168 | 1.0521 | 0.5502 | 0.3046 | | |
| H(1A) | | C(21) | [] | 2.44<< | 2.90 | -0.46 | Intra | 0.8352 | 0.6300 | 0.3168 | 0.5937 | 0.6104 | 0.4762 | | |
| H(1A) | | H(2B) | [] | 2.43 | 2.40 | 0.03 | Intra | 0.8352 | 0.6300 | 0.3168 | 1.1690 | 0.6665 | 0.3418 | | |
| H(1A) | | H(11A) | [] | 2.40 | 2.40 | 0.00 | Intra | 0.8352 | 0.6300 | 0.3168 | 1.1132 | 0.5769 | 0.2467 | | |
| H(1A) | | H(11B) | [] | 2.44 | 2.40 | 0.04 | Intra | 0.8352 | 0.6300 | 0.3168 | 0.9317 | 0.5345 | 0.2645 | | |
| H(1A) | | H(21A) | [] | 2.34 | < | 2.40 | -0.06 | Intra | 0.8352 | 0.6300 | 0.3168 | 0.5218 | 0.6254 | 0.4032 | |
| H(1A) | | H(21B) | [] | 2.59 | 2.40 | 0.19 | Intra | 0.8352 | 0.6300 | 0.3168 | 0.6207 | 0.5702 | 0.4616 | | |
| H(2) | | C1(3) | [] | 3.15(2) | 2.95 | 0.20 | Intra | 0.8490 | 0.8075 | 0.1600 | 1.1021 | 0.8954 | 0.3101 | | |
| H(2) | | S | [] | 2.72(2)<< | 3.00 | -0.28 | Intra | 0.8490 | 0.8075 | 0.1600 | 1.0216 | 0.7061 | 0.1260 | | |
| H(2) | | C(5) | [] | 2.92(2) | 2.90 | 0.02 | Intra | 0.8490 | 0.8075 | 0.1600 | 0.6034 | 0.8140 | 0.3785 | | |
| H(2) | | C(9) | [] | 2.80(2) | < | 2.90 | -0.10 | Intra | 0.8490 | 0.8075 | 0.1600 | 0.8769 | 0.8762 | 0.3691 | |
| H(2) | | O(2) | [4564.01] | 2.24(2)<< | 2.72 | -0.48 | | 0.8490 | 0.8075 | 0.1600 | 0.7763 | 0.8600 | -0.0058 | N(2) | 164(2) |
| H(2A) | | O(1) | [] | 2.65 | < | 2.72 | -0.07 | Intra | 1.1206 | 0.6797 | 0.4831 | 1.0017 | 0.5783 | 0.4174 | |
| H(2A) | | O(2) | [] | 2.52<< | 2.72 | -0.20 | Intra | 1.1206 | 0.6797 | 0.4831 | 0.7763 | 0.6400 | 0.4942 | | |
| H(2A) | | C(22) | [1655.01] | 3.01 | 2.90 | 0.11 | | 1.1206 | 0.6797 | 0.4831 | 1.4703 | 0.6170 | 0.5893 | C(2) | 128 |
| H(2A) | | H(1) | [] | 2.16<< | 2.40 | -0.24 | Intra | 1.1206 | 0.6797 | 0.4831 | 0.9560 | 0.7517 | 0.4190 | | |
| H(2A) | | H(22B) | [1655.01] | 2.60 | 2.40 | 0.20 | | 1.1206 | 0.6797 | 0.4831 | 1.4454 | 0.6569 | 0.6039 | C(2) | 140 |
| H(2B) | | C1(1) | [1655.01] | 3.00 | 2.95 | 0.05 | | 1.1690 | 0.6665 | 0.3418 | 1.4785 | 0.7557 | 0.3242 | C(2) | 113 |
| H(2B) | | S | [] | 2.70<< | 3.00 | -0.30 | Intra | 1.1690 | 0.6665 | 0.3418 | 1.0216 | 0.7061 | 0.1260 | C(2) | 101 |
| H(2B) | | O(1) | [] | 2.53 | < | 2.72 | -0.19 | Intra | 1.1690 | 0.6665 | 0.3418 | 1.0017 | 0.5783 | 0.4174 | |
| H(2B) | | C(3) | [] | 2.61<< | 2.90 | -0.29 | Intra | 1.1690 | 0.6665 | 0.3418 | 0.9511 | 0.7460 | 0.2465 | | |
| H(2B) | | C(11) | [] | 2.92 | 2.90 | 0.02 | Intra | 1.1690 | 0.6665 | 0.3418 | 1.0521 | 0.5502 | 0.3046 | | |
| H(2B) | | H(1A) | [] | 2.43 | 2.40 | 0.03 | Intra | 1.1690 | 0.6665 | 0.3418 | 0.8352 | 0.6300 | 0.3168 | | |
| H(2B) | | H(11A) | [] | 2.40 | 2.40 | 0.00 | Intra | 1.1690 | 0.6665 | 0.3418 | 1.1132 | 0.5769 | 0.2467 | C(2) | 112 |
| H(6A) | | C1(1) | [] | 2.80 | < | 2.95 | -0.15 | Intra | 0.4027 | 0.8339 | 0.5098 | 0.4785 | 0.7557 | 0.3242 | |
| H(6A) | | C1(2) | [] | 2.80 | < | 2.95 | -0.15 | Intra | 0.4027 | 0.8339 | 0.5098 | 0.5158 | 0.9339 | 0.6250 | |
| H(6A) | | S | [4465.01] | 3.04 | 3.00 | 0.04 | | 0.4027 | 0.8339 | 0.5098 | 0.0216 | 0.7939 | 0.6260 | C(6) | 178 |
| H(8A) | | C1(2) | [] | 2.79 | < | 2.95 | -0.16 | Intra | 0.8602 | 0.9427 | 0.4880 | 0.5158 | 0.9339 | 0.6250 | |
| H(8A) | | C1(3) | [] | 2.79 | < | 2.95 | -0.16 | Intra | 0.8602 | 0.9427 | 0.4880 | 1.1021 | 0.8954 | 0.3101 | |
| H(11A) | | C(1) | [] | 2.51<< | 2.90 | -0.39 | Intra | 1.1132 | 0.5769 | 0.2467 | 0.9083 | 0.6303 | 0.3978 | | |
| H(11A) | | C(2) | [] | 2.92 | 2.90 | 0.02 | Intra | 1.1132 | 0.5769 | 0.2467 | 1.0620 | 0.6764 | 0.3990 | | |
| H(11A) | | H(1A) | [] | 2.40 | 2.40 | 0.00 | Intra | 1.1132 | 0.5769 | 0.2467 | 0.8352 | 0.6300 | 0.3168 | | |
| H(11A) | | H(2B) | [] | 2.40 | 2.40 | 0.00 | Intra | 1.1132 | 0.5769 | 0.2467 | 1.1690 | 0.6665 | 0.3418 | C(11) | 112 |
| H(11A) | | H(12A) | [] | 2.35 | < | 2.40 | -0.05 | Intra | 1.1132 | 0.5769 | 0.2467 | 1.2317 | 0.4846 | 0.2602 | |
| H(11A) | | H(12C) | [] | 2.36 | < | 2.40 | -0.04 | Intra | 1.1132 | 0.5769 | 0.2467 | 1.3125 | 0.5200 | 0.3759 | |
| H(11A) | | C1(2) | [4664.01] | 3.06 | 2.95 | 0.11 | | 1.1132 | 0.5769 | 0.2467 | 1.5158 | 0.5661 | 0.1250 | C(11) | 127 |
| H(11B) | | C(1) | [] | 2.71 | < | 2.90 | -0.19 | Intra | 0.9317 | 0.5345 | 0.2645 | 0.9083 | 0.6303 | 0.3978 | |
| H(11B) | | H(1A) | [] | 2.44 | 2.40 | 0.04 | Intra | 0.9317 | 0.5345 | 0.2645 | 0.8352 | 0.6300 | 0.3168 | | |
| H(11B) | | H(12A) | [] | 2.36 | < | 2.40 | -0.04 | Intra | 0.9317 | 0.5345 | 0.2645 | 1.2317 | 0.4846 | 0.2602 | |
| H(11B) | | H(12B) | [] | 2.35 | < | 2.40 | -0.05 | Intra | 0.9317 | 0.5345 | 0.2645 | 1.1317 | 0.4776 | 0.3921 | |
| H(12A) | | H(11A) | [] | 2.35 | < | 2.40 | -0.05 | Intra | 1.2317 | 0.4846 | 0.2602 | 1.1132 | 0.5769 | 0.2467 | |
| H(12A) | | H(11B) | [] | 2.36 | < | 2.40 | -0.04 | Intra | 1.2317 | 0.4846 | 0.2602 | 0.9317 | 0.5345 | 0.2645 | |
| H(12A) | | C(8) | [2745.01] | 2.99 | 2.90 | 0.09 | | 1.2317 | 0.4846 | 0.2602 | 1.2043 | 0.4095 | 0.0395 | C(12) | 160 |
| H(12A) | | C(9) | [2745.01] | 3.03 | 2.90 | 0.13 | | 1.2317 | 0.4846 | 0.2602 | 1.1231 | 0.3762 | 0.1309 | C(12) | 137 |

| | | | | | | | | | | | | | | | | |
|--------|------|--------|------------|------|------|------|-------|--------|--------|--------|--------|--------|--------|--------|-------|-----|
| H(12A) | | C1(2) | [4664.01] | 3.12 | 2.95 | 0.17 | | 1.2317 | 0.4846 | 0.2602 | 1.5158 | 0.5661 | 0.1250 | C(12) | 105 | |
| H(12B) | | O(1) | [] | 2.58 | < | 2.72 | -0.14 | Intra | 1.1317 | 0.4776 | 0.3921 | 1.0017 | 0.5783 | 0.4174 | | |
| H(12B) | | H(11B) | [] | 2.35 | < | 2.40 | -0.05 | Intra | 1.1317 | 0.4776 | 0.3921 | 0.9317 | 0.5345 | 0.2645 | | |
| H(12B) | | O(1) | [3766.01] | 2.63 | < | 2.72 | -0.09 | | 1.1317 | 0.4776 | 0.3921 | 0.9983 | 0.4217 | 0.5826 | C(12) | 167 |
| H(12B) | | H(21B) | [3766.01] | 2.56 | | 2.40 | 0.16 | | 1.1317 | 0.4776 | 0.3921 | 1.3793 | 0.4298 | 0.5384 | C(12) | 113 |
| H(12C) | | O(1) | [] | 2.57 | < | 2.72 | -0.15 | Intra | 1.3125 | 0.5200 | 0.3759 | 1.0017 | 0.5783 | 0.4174 | | |
| H(12C) | | C(21) | [1655.01] | 3.06 | | 2.90 | 0.16 | | 1.3125 | 0.5200 | 0.3759 | 1.5937 | 0.6104 | 0.4762 | C(12) | 158 |
| H(12C) | | H(11A) | [] | 2.36 | < | 2.40 | -0.04 | Intra | 1.3125 | 0.5200 | 0.3759 | 1.1132 | 0.5769 | 0.2467 | | |
| H(12C) | | H(21B) | [1655.01] | 2.57 | | 2.40 | 0.17 | | 1.3125 | 0.5200 | 0.3759 | 1.6207 | 0.5702 | 0.4616 | C(12) | 173 |
| H(21A) | | C(1) | [] | 2.62 | << | 2.90 | -0.28 | Intra | 0.5218 | 0.6254 | 0.4032 | 0.9083 | 0.6303 | 0.3978 | | |
| H(21A) | | H(1A) | [] | 2.34 | < | 2.40 | -0.06 | Intra | 0.5218 | 0.6254 | 0.4032 | 0.8352 | 0.6300 | 0.3168 | | |
| H(21A) | | H(22A) | [] | 2.35 | < | 2.40 | -0.05 | Intra | 0.5218 | 0.6254 | 0.4032 | 0.3442 | 0.5975 | 0.5770 | | |
| H(21A) | | H(22B) | [] | 2.37 | < | 2.40 | -0.03 | Intra | 0.5218 | 0.6254 | 0.4032 | 0.4454 | 0.6569 | 0.6039 | | |
| H(21B) | | O(1) | [] | 2.64 | < | 2.72 | -0.08 | Intra | 0.6207 | 0.5702 | 0.4616 | 1.0017 | 0.5783 | 0.4174 | | |
| H(21B) | | C(1) | [] | 2.52 | << | 2.90 | -0.38 | Intra | 0.6207 | 0.5702 | 0.4616 | 0.9083 | 0.6303 | 0.3978 | | |
| H(21B) | | H(1A) | [] | 2.59 | | 2.40 | 0.19 | Intra | 0.6207 | 0.5702 | 0.4616 | 0.8352 | 0.6300 | 0.3168 | | |
| H(21B) | | H(12C) | [1455.01] | 2.57 | | 2.40 | 0.17 | | 0.6207 | 0.5702 | 0.4616 | 0.3125 | 0.5200 | 0.3759 | C(21) | 111 |
| H(21B) | | H(22A) | [] | 2.36 | < | 2.40 | -0.04 | Intra | 0.6207 | 0.5702 | 0.4616 | 0.3442 | 0.5975 | 0.5770 | | |
| H(21B) | | H(22C) | [] | 2.35 | < | 2.40 | -0.05 | Intra | 0.6207 | 0.5702 | 0.4616 | 0.5407 | 0.6011 | 0.6609 | | |
| H(21B) | | C(12) | [3766.01] | 3.07 | | 2.90 | 0.17 | | 0.6207 | 0.5702 | 0.4616 | 0.8058 | 0.4959 | 0.6641 | C(21) | 121 |
| H(21B) | | H(12B) | [3766.01] | 2.56 | | 2.40 | 0.16 | | 0.6207 | 0.5702 | 0.4616 | 0.8683 | 0.5224 | 0.6079 | C(21) | 117 |
| H(22A) | | O(1) | [1455.01] | 2.91 | | 2.72 | 0.19 | | 0.3442 | 0.5975 | 0.5770 | 0.0017 | 0.5783 | 0.4174 | C(22) | 147 |
| H(22A) | | H(21A) | [] | 2.35 | < | 2.40 | -0.05 | Intra | 0.3442 | 0.5975 | 0.5770 | 0.5218 | 0.6254 | 0.4032 | | |
| H(22A) | | H(21B) | [] | 2.36 | < | 2.40 | -0.04 | Intra | 0.3442 | 0.5975 | 0.5770 | 0.6207 | 0.5702 | 0.4616 | | |
| H(22A) | | C1(3) | [4465.01] | 3.04 | | 2.95 | 0.09 | | 0.3442 | 0.5975 | 0.5770 | 0.1021 | 0.6046 | 0.8101 | C(22) | 110 |
| H(22B) | | O(2) | [] | 2.58 | < | 2.72 | -0.14 | Intra | 0.4454 | 0.6569 | 0.6039 | 0.7763 | 0.6400 | 0.4942 | | |
| H(22B) | | H(2A) | [1455.01] | 2.60 | | 2.40 | 0.20 | | 0.4454 | 0.6569 | 0.6039 | 0.1206 | 0.6797 | 0.4831 | C(22) | 106 |
| H(22B) | | H(21A) | [] | 2.37 | < | 2.40 | -0.03 | Intra | 0.4454 | 0.6569 | 0.6039 | 0.5218 | 0.6254 | 0.4032 | | |
| H(22C) | | O(2) | [] | 2.60 | < | 2.72 | -0.12 | Intra | 0.5407 | 0.6011 | 0.6609 | 0.7763 | 0.6400 | 0.4942 | | |
| H(22C) | | H(21B) | [] | 2.35 | < | 2.40 | -0.05 | Intra | 0.5407 | 0.6011 | 0.6609 | 0.6207 | 0.5702 | 0.4616 | | |
| H(22C) | | C(12) | [3766.01] | 3.09 | | 2.90 | 0.19 | | 0.5407 | 0.6011 | 0.6609 | 0.8058 | 0.4959 | 0.6641 | C(22) | 127 |
| H(22C) | | C(4) | [4565.01] | 2.93 | | 2.90 | 0.03 | | 0.5407 | 0.6011 | 0.6609 | 0.7821 | 0.6715 | 0.8252 | C(22) | 121 |

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 1 to Neighbouring ARU'S

| Nr | ARU | Nr.Cont. | d(min) | Del | XHn | X | - At(I) | At(J) | - Y | YHn | Note | Partaking ARU's in Close Contact | Resd. |
|----|------------|----------|--------|-------|-----|-------|--------------|--------|--------|-----|------|----------------------------------|-------|
| 1 | [1455.01] | 9 | 2.5700 | 0.17 | 2 | C(21) | - H(21B) ... | H(12C) | -C(12) | 3 | | 1455.01 | |
| 2 | [4465.01] | 6 | 3.0400 | 0.09 | 3 | C(22) | - H(22A) ... | C1(3) | -C(9) | 0 | | 4465.01 | |
| 3 | [1655.01] | 9 | 2.5700 | 0.17 | 3 | C(12) | - H(12C) ... | H(21B) | -C(21) | 2 | | 1655.01 | |
| 4 | [2755.01] | 3 | 2.9900 | 0.09 | 0 | C(7) | - C(8) ... | H(12A) | -C(12) | 3 | | 2755.01 | |
| 5 | [4664.01] | 6 | 3.0400 | 0.04 | 0 | C(3) | - S ... | H(6A) | -C(6) | 1 | | 4664.01 | |
| 6 | [4564.01] | 8 | 2.2400 | -0.48 | 1 | N(2) | - H(2) ... | O(2) | -C(1) | 1 | << | 4564.01 | |
| 7 | [3766.01] | 8 | 2.5600 | 0.16 | 2 | C(21) | - H(21B) ... | H(12B) | -C(12) | 3 | | 3766.01 | |
| 8 | [4565.01] | 8 | 2.2400 | -0.48 | 1 | C(1) | - O(2) ... | H(2) | -N(2) | 1 | << | 4565.01 | |

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9 [2745.01] 3 2.9900 0.09 3 C(12) - H(12A) ... C(8) -C(7) 0 2745.01

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Asymmetric Residue Unit (= ARU) Code List

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| ARU-CODE | CIF-CODE | Symmetry-Code | sym | TX | TY | TZ | Ires | x(cen) | y(cen) | z(cen) | |
|------------|----------|-------------------|-----|-----|----|----|------|--------|--------|--------|--------|
| [1455.01] | [1_455] | =-1+x,y,z | = | [1 | -1 | 0 | 0 | 1] | -0.170 | 0.697 | 0.398 |
| [4465.01] | [4_476] | =-1+x,3/2-y,1/2+z | = | [4 | -1 | 1 | 0 | 1] | -0.170 | 0.803 | 0.898 |
| [1655.01] | [1_655] | =1+x,y,z | = | [1 | 1 | 0 | 0 | 1] | 1.830 | 0.697 | 0.398 |
| [2755.01] | [2_755] | =2-x,1/2+y,1/2-z | = | [2 | 2 | 0 | 0 | 1] | 1.170 | 1.197 | 0.102 |
| [4664.01] | [4_675] | =1+x,3/2-y,-1/2+z | = | [4 | 1 | 1 | -1 | 1] | 1.830 | 0.803 | -0.102 |
| [4564.01] | [4_575] | =x,3/2-y,-1/2+z | = | [4 | 0 | 1 | -1 | 1] | 0.830 | 0.803 | -0.102 |
| [3766.01] | [3_766] | =2-x,1-y,1-z | = | [3 | 2 | 1 | 1 | 1] | 1.170 | 0.303 | 0.602 |
| [4565.01] | [4_576] | =x,3/2-y,1/2+z | = | [4 | 0 | 1 | 0 | 1] | 0.830 | 0.803 | 0.898 |
| [2745.01] | [2_745] | =2-x,-1/2+y,1/2-z | = | [2 | 2 | -1 | 0 | 1] | 1.170 | 0.197 | 0.102 |

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

X(J) = X(sym) + TX , Y(J) = Y(sym) + TY , Z(J) = Z(sym) + TZ,

SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

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 Analysis of Potential Hydrogen Bonds and Schemes with $d(D...A) < R(D)+R(A)+0.50$, $d(H...A) < R(H)+R(A)-0.12$ Ang., $D-H...A > 100.0$ Deg
 =====

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
 =====

| Nr | Typ | Res | Donor | H...Acceptor | [ARU] | D - H | H...A | D...A | D - H...A | A..H..A* A'..H..A" | Sum(XY,YZ) | Sum(XZ) |
|----|-------|-----|-------|--------------|---------|------------|---------|---------|-----------|--------------------|------------|---------|
| 1 | | 1 | N(1) | --H(1) | ..S | [4565.01] | 0.82(2) | 2.49(2) | 3.246(2) | 153.6(19) | | |
| 2 | | 1 | N(2) | --H(2) | ..O(2) | [4564.01] | 0.80(2) | 2.24(2) | 3.012(2) | 164(2) | | |
| 3 | Intra | 1 | C(2) | --H(2B) | ..S | [] | 0.99 | 2.70 | 3.050(2) | 101 | | |

Translation of ARU-Code to CIF and Equivalent Position Code
 =====

[4564.] = [4_575] =x,3/2-y,-1/2+z
 [4565.] = [4_576] =x,3/2-y,1/2+z

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]

 2-Centre (linear) D-H...X most prob. angle 160 deg - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
 3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg Springer-Verlag, Berlin, 1991, pp 20.
 4-Centre (trifurcated)

Analysis of Potential Donor/Acceptor Atoms -- (Major Disorder Form Only)
 =====

| At.Nr | D/A | #Cov.Bonds | # H | #D-H..A | #A..H | #A..H-C | Sum(A-H) | Sum(A-X) |
|-------|-------|------------|-----|---------|-------|---------|----------|----------|
| 1 | Cl(1) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 2 | Cl(2) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 3 | Cl(3) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 4 | S | 1 | - | 0 | 1 | 1 | 2 | 3 |
| 5 | O(1) | 2 | - | 0 | 0 | 0 | 0 | 2 |
| 6 | O(2) | 2 | - | 0 | 1 | 0 | 1 | 3 |
| 7 | N(1) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 8 | N(2) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |

=====
 Analysis of Hydrogen Bonded Molecular Aggregates (See also Acta Cryst. B36, 1980, 2113 - 2115) -- (Major Disorder Component Only)
 =====

Coordinates of Donor and Acceptor Atoms

Coordinates of D/A-Bonded Atom(s)

| Coordinates of Donor and Acceptor Atoms | | | | | Coordinates of D/A-Bonded Atom(s) | | | | | | | | | |
|---|-------------|--------|--------|--------|-----------------------------------|-------------|--------|--------|--------|--------|--------|--------|--------|---------------|
| D/A I | [ARU] | X | Y | Z | -- D/A J | [ARU] | X | Y | Z | Atom K | X | Y | Z | I..J--K Angle |
| N(1) | [1555.01], | 0.9780 | 0.7297 | 0.3629 | >> S | [4565.01], | 1.0216 | 0.7939 | 0.6260 | C(3) | 0.9511 | 0.7540 | 0.7465 | 112.87(6) |
| S | [1555.01], | 1.0216 | 0.7061 | 0.1260 | << N(1) | [4564.01], | 0.9780 | 0.7703 | 0.1371 | C(2) | 1.0620 | 0.8236 | 0.1010 | 98.55(6) |
| | | | | | | | | | | C(3) | 0.9511 | 0.7540 | 0.2535 | 134.71(7) |
| | | | | | | | | | | H(1) | 0.9560 | 0.7483 | 0.0810 | 19.99(10) |
| N(2) | [1555.01], | 0.8642 | 0.7963 | 0.2286 | >> O(2) | [4564.01], | 0.7763 | 0.8600 | 0.0058 | C(1) | 0.9083 | 0.8697 | 0.1022 | 126.25(7) |
| | | | | | | | | | | C(21) | 0.5937 | 0.8896 | 0.0238 | 121.42(7) |
| O(2) | [1555.01], | 0.7763 | 0.6400 | 0.4942 | << N(2) | [4565.01], | 0.8642 | 0.7037 | 0.7286 | C(3) | 0.9511 | 0.7540 | 0.7465 | 130.53(7) |
| | | | | | | | | | | C(4) | 0.7821 | 0.6715 | 0.8252 | 105.82(7) |
| | | | | | | | | | | H(2) | 0.8490 | 0.6925 | 0.6600 | 11.68(11) |

=====

***** Aggregate = 1 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 4 2 1555.01 -- 4565.01 4564.01T
 4 2 4565.01 -- 1556.01T 1555.01

=====

***** Aggregate = 2 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 4 2 3555.01 -- 2534.01 2535.01T
 4 2 2534.01 -- 3554.01T 3555.01

:: Analysis of H-Bonded Aggregate Type3 Polymeric Structure(s)

:: Resd 0 - Infinite (Type3) 1D-Chain - Base Vector: [0 0 1]

=====
Search for Infinite ARU-Chains (Max = 4)
=====

2-Membered Infinite ARU-Chain (Translation [0 0 1])

1555.01 4565.01 1556.01

2-Membered Infinite ARU-Chain (Translation [0 0 -1])

1555.01 4564.01 1554.01

=====
 Analysis of the (Cooperative) Hydrogen Bond Network (i.e. (In)Finite O-H...O-H...O-H.. Chains and/or Rings (Max = 18 Membered))
 =====

=====
 ***** Network = 1 *****
 =====

| Code | Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|-------|-----|-----------------|--------|--------|--------|---------------|--------|--------|--|
| 1.555 | | N(1) [1555.01] | 0.9780 | 0.7297 | 0.3629 | S [4565.01] | 1.0216 | 0.7939 | 0.6260 |
| | | H(1) | 0.9560 | 0.7517 | 0.4190 | | | | |

=====
 ***** Network = 2 *****
 =====

| Code | Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|-------|-----|-----------------|--------|--------|--------|-----------------|--------|--------|--|
| 2.555 | | N(2) [1555.01] | 0.8642 | 0.7963 | 0.2286 | O(2) [4564.01] | 0.7763 | 0.8600 | -0.0058 |
| | | H(2) | 0.8490 | 0.8075 | 0.1600 | | | | |

 Hydrogen Bonds are Coded as N.IJK Where N = Sequence Number of Hydrogen Bond (NOTE: New Hbond Numbering system)
 I - 5 = Nr of Translation Units Along A-Axis
 J - 5 = Nr of Translation Units Along B-Axis
 K - 5 = Nr of Translation Units Along C-Axis

Ring Closure Links are Indicated with 'R' and Infinite Chain Links With 'T'

=====

3.6 Angstrom Coordination Sphere Around Atom I = Cl(1) [ARU = 1555.01] 0.47855 0.75569 0.32420 3.1813 18.0504 3.5119

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|-----------------|-----------|----------|-------|---------|--------|----------|---------|---------|---------|---------|--------|
| 1 | 1.728(2) | -- | C(5) | | | | Intra | 59.05 | 19.91 | 0.60340 | 0.81401 | 0.37850 | 4.0166 | 19.4434 | 4.1001 |
| 2 | 2.686(3) | << | C(6) | | | | Intra | 82.83 | 36.68 | 0.52220 | 0.84517 | 0.47230 | 3.4502 | 20.1877 | 5.1162 |
| 3 | 2.692(2) | << | C(4) | | | | Intra | 40.26 | 0.23 | 0.78210 | 0.82852 | 0.32519 | 5.2358 | 19.7900 | 3.5226 |
| 4 | 2.986(2) | << | N(2) | | | | Intra | 20.24 | -20.29 | 0.86420 | 0.79626 | 0.22864 | 5.8088 | 19.0195 | 2.4767 |
| 5 | 3.329(2) | .< | C(3) | | | | Intra | -4.13 | -14.65 | 0.95110 | 0.74597 | 0.24647 | 6.3939 | 17.8182 | 2.6699 |
| 6 | 3.456(2) | .. | N(1) | | | | Intra | -10.44 | 6.97 | 0.97800 | 0.72967 | 0.36292 | 6.5551 | 17.4289 | 3.9313 |
| 7 | 3.477(2) | .. | N(1)a | [-1+x,y,z | = | 1455.01] | | -169.63 | 6.93 | -0.02200 | 0.72967 | 0.36292 | -0.2139 | 17.4289 | 3.9313 |
| 8 | 3.503(3) | .. | C(2)a | [-1+x,y,z | = | 1455.01] | | -146.24 | 13.38 | 0.06200 | 0.67641 | 0.39904 | 0.3482 | 16.1567 | 4.3226 |
| 9 | 2.80 | .< | H(6A) | | | | Intra | 106.31 | 45.93 | 0.40270 | 0.83390 | 0.50980 | 2.6346 | 19.9185 | 5.5224 |
| 10 | 3.00 | .. | H(2B)a | [-1+x,y,z | = | 1455.01] | | -134.57 | 3.65 | 0.16900 | 0.66650 | 0.34180 | 1.0828 | 15.9200 | 3.7026 |
| 11 | 3.18 | .. | H(22B)b | [x,3/2-y,-1/2+z | = | 4564.01] | | 95.06 | -48.71 | 0.44540 | 0.84310 | 0.10390 | 2.9963 | 20.1383 | 1.1255 |
| 12 | 3.24 | .. | H(21A) | | | | Intra | -84.88 | 15.32 | 0.52180 | 0.62540 | 0.40320 | 3.4599 | 14.9383 | 4.3677 |
| 13 | 3.34(2) | .. | H(2) | | | | Intra | 26.00 | -32.22 | 0.84900 | 0.80750 | 0.16000 | 5.7182 | 19.2879 | 1.7332 |
| 14 | 3.38(2) | .. | H(1) | | | | Intra | -1.70 | 17.71 | 0.95600 | 0.75170 | 0.41900 | 6.3961 | 17.9551 | 4.5388 |
| 15 | 3.50 | .. | H(2A)a | [-1+x,y,z | = | 1455.01] | | -143.48 | 29.44 | 0.12060 | 0.67970 | 0.48310 | 0.7298 | 16.2353 | 5.2332 |

Angles (Degrees) At1...V...At2 with Vertex V = Cl(1)

| | | | | | | | | | | | | | | | |
|------|---|-------|-----------|------|---|-------|-----------|------|---|-------|-----------|-------|---|-------|-----------|
| C(5) | , | C(6) | 26.69(8) | C(5) | , | C(4) | 26.94(8) | C(5) | , | N(2) | 55.30(8) | C(5) | , | C(3) | 71.08(8) |
| C(5) | , | N(1) | 68.39(8) | C(5) | , | N(1)a | 125.12(8) | C(5) | , | C(2)a | 138.44(8) | C(6) | , | C(4) | 53.63(6) |
| C(6) | , | N(2) | 81.99(6) | C(6) | , | C(3) | 96.31(6) | C(6) | , | N(1) | 88.45(6) | C(6) | , | N(1)a | 99.67(6) |
| C(6) | , | C(2)a | 111.90(6) | C(4) | , | N(2) | 28.36(6) | C(4) | , | C(3) | 46.34(6) | C(4) | , | N(1) | 51.00(6) |
| C(4) | , | N(1)a | 149.34(6) | C(4) | , | C(2)a | 164.94(6) | N(2) | , | C(3) | 23.90(5) | N(2) | , | N(1) | 40.66(5) |
| N(2) | , | N(1)a | 163.57(5) | N(2) | , | C(2)a | 165.35(6) | C(3) | , | N(1) | 22.51(5) | C(3) | , | N(1)a | 163.80(5) |
| C(3) | , | C(2)a | 143.26(6) | N(1) | , | N(1)a | 155.02(5) | N(1) | , | C(2)a | 131.62(5) | N(1)a | , | C(2)a | 23.89(5) |

=====

3.6 Angstrom Coordination Sphere Around Atom I = Cl(3) [ARU = 1555.01] 1.10210 0.89541 0.31011 7.4046 21.3878 3.3593

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|-------------------|-----------|----------|-------|---------|--------|---------|---------|---------|---------|---------|--------|
| 1 | 1.725(2) | -- | C(9) | | | | Intra | -163.38 | 21.74 | 0.87690 | 0.87623 | 0.36907 | 5.8697 | 20.9296 | 3.9980 |
| 2 | 2.680(3) | << | C(8) | | | | Intra | 170.89 | 37.44 | 0.79570 | 0.90952 | 0.46050 | 5.3036 | 21.7248 | 4.9884 |
| 3 | 2.699(2) | << | C(4) | | | | Intra | -143.62 | 3.47 | 0.78210 | 0.82852 | 0.32519 | 5.2358 | 19.7900 | 3.5226 |
| 4 | 2.989(2) | << | N(2) | | | | Intra | -123.97 | -17.17 | 0.86420 | 0.79626 | 0.22864 | 5.8088 | 19.0195 | 2.4767 |
| 5 | 3.496(3) | .. | C(22)c | [1+x,3/2-y,-1/2+z | = | 4664.01] | | -6.70 | -43.18 | 1.47030 | 0.88296 | 0.08930 | 9.9365 | 21.0904 | 0.9673 |
| 6 | 3.528(3) | .. | C(6)a | [1+x,y,z | = | 1655.01] | | -23.09 | 29.86 | 1.52220 | 0.84517 | 0.47230 | 10.2192 | 20.1877 | 5.1162 |
| 7 | 2.79 | < | H(8A) | | | | Intra | 145.91 | 43.71 | 0.86020 | 0.94270 | 0.48800 | 5.7353 | 22.5173 | 5.2863 |
| 8 | 3.04 | .. | H(22A)c | [1+x,3/2-y,-1/2+z | = | 4664.01] | | 5.75 | -56.22 | 1.34420 | 0.90250 | 0.07700 | 9.0851 | 21.5571 | 0.8341 |
| 9 | 3.15(2) | .. | H(2) | | | | Intra | -128.77 | -31.12 | 0.84900 | 0.80750 | 0.16000 | 5.7182 | 19.2879 | 1.7332 |
| 10 | 3.19 | .. | H(12A)b | [2-x,1/2+y,1/2-z | = | 2755.01] | | 136.52 | -13.82 | 0.76830 | 0.98460 | 0.23980 | 5.1577 | 23.5182 | 2.5976 |
| 11 | 3.29 | .. | H(6A)a | [1+x,y,z | = | 1655.01] | | -36.32 | 41.09 | 1.40270 | 0.83390 | 0.50980 | 9.4036 | 19.9185 | 5.5224 |
| 12 | 3.32 | .. | H(12B)b | [2-x,1/2+y,1/2-z | = | 2755.01] | | 128.23 | -41.23 | 0.86830 | 0.97760 | 0.10790 | 5.8582 | 23.3510 | 1.1688 |
| 13 | 3.40 | .. | H(22C)c | [1+x,3/2-y,-1/2+z | = | 4664.01] | | 1.59 | -28.34 | 1.54070 | 0.89890 | 0.16090 | 10.4002 | 21.4711 | 1.7430 |
| 14 | 3.43 | .. | H(11B)b | [2-x,1/2+y,1/2-z | = | 2755.01] | | 93.71 | -13.65 | 1.06830 | 1.03450 | 0.23550 | 7.1892 | 24.7101 | 2.5511 |
| 15 | 3.48 | .. | H(22B)c | [1+x,3/2-y,-1/2+z | = | 4664.01] | | -27.89 | -39.91 | 1.44540 | 0.84310 | 0.10390 | 9.7653 | 20.1383 | 1.1255 |

Angles (Degrees) At1...V...At2 with Vertex V = Cl(3)

| | | | | | | | | | | | | | | | |
|------|---|--------|-----------|------|---|-------|-----------|--------|---|--------|-----------|------|---|--------|-----------|
| C(9) | , | C(8) | 27.18(9) | C(9) | , | C(4) | 26.49(8) | C(9) | , | N(2) | 54.81(8) | C(9) | , | C(22)c | 151.10(9) |
| C(9) | , | C(6)a | 115.80(8) | C(8) | , | C(4) | 53.67(7) | C(8) | , | N(2) | 81.99(7) | C(8) | , | C(22)c | 173.98(7) |
| C(8) | , | C(6)a | 111.44(6) | C(4) | , | N(2) | 28.33(6) | C(4) | , | C(22)c | 124.97(6) | C(4) | , | C(6)a | 114.18(6) |
| N(2) | , | C(22)c | 96.73(6) | N(2) | , | C(6)a | 107.66(6) | C(22)c | , | C(6)a | 74.57(5) | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = O(2) [ARU = 1555.01] 0.77630 0.64000 0.49418 5.1663 15.2870 5.3532

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|----------------|-----------|----------|-------|---------|--------|---------|---------|---------|--------|---------|--------|
| 1 | 1.405(2) | -- | C(1) | | | | Intra | -14.32 | -48.01 | 0.90830 | 0.63027 | 0.39778 | 6.0771 | 15.0546 | 4.3090 |
| 2 | 1.435(3) | -- | C(21) | | | | Intra | -150.12 | -7.78 | 0.59370 | 0.61035 | 0.47625 | 3.9335 | 14.5788 | 5.1590 |
| 3 | 2.288(2) | << | O(1) | | | | Intra | -43.76 | -21.31 | 1.00170 | 0.57829 | 0.41743 | 6.7058 | 13.8130 | 4.5218 |
| 4 | 2.372(3) | << | C(2) | | | | Intra | 24.03 | -25.76 | 1.06200 | 0.67641 | 0.39904 | 7.1172 | 16.1567 | 4.3226 |
| 5 | 2.392(3) | << | C(22) | | | | Intra | -165.29 | 25.51 | 0.47030 | 0.61704 | 0.58930 | 3.0779 | 14.7386 | 6.3836 |
| 6 | 2.922(3) | <. | N(1) | | | | Intra | 57.04 | -29.12 | 0.97800 | 0.72967 | 0.36292 | 6.5551 | 17.4289 | 3.9313 |
| 7 | 3.012(2) | <. | N(2)b | [x,3/2-y,1/2+z | = | 4565.01] | | 70.04 | 57.47 | 0.86420 | 0.70374 | 0.72864 | 5.7193 | 16.8095 | 7.8930 |
| 8 | 3.526(3) | .. | C(11) | | | | Intra | -48.46 | -35.62 | 1.05210 | 0.55017 | 0.30460 | 7.0671 | 13.1414 | 3.2996 |
| 9 | 1.98 | << | H(1A) | | | | Intra | -29.03 | -75.63 | 0.83520 | 0.63000 | 0.31680 | 5.5967 | 15.0482 | 3.4317 |
| 10 | 2.00 | << | H(21B) | | | | Intra | -122.14 | -10.16 | 0.62070 | 0.57020 | 0.46160 | 4.1189 | 13.6198 | 5.0003 |
| 11 | 2.00 | << | H(21A) | | | | Intra | -168.45 | -29.50 | 0.52180 | 0.62540 | 0.40320 | 3.4599 | 14.9383 | 4.3677 |
| 12 | 2.24(2) | << | H(2)b | [x,3/2-y,1/2+z | = | 4565.01] | | 69.76 | 53.35 | 0.84900 | 0.69250 | 0.66000 | 5.6287 | 16.5411 | 7.1495 |
| 13 | 2.52 | << | H(2A) | | | | Intra | 22.12 | -2.73 | 1.12060 | 0.67970 | 0.48310 | 7.4988 | 16.2353 | 5.2332 |
| 14 | 2.58 | <. | H(22B) | | | | Intra | 169.87 | 27.38 | 0.44540 | 0.65690 | 0.60390 | 2.9068 | 15.6907 | 6.5418 |
| 15 | 2.60 | <. | H(22C) | | | | Intra | -150.23 | 43.98 | 0.54070 | 0.60110 | 0.66090 | 3.5417 | 14.3579 | 7.1592 |
| 16 | 3.05(2) | .. | H(1) | | | | Intra | 65.25 | -15.49 | 0.95600 | 0.75170 | 0.41900 | 6.3961 | 17.9551 | 4.5388 |
| 17 | 3.13 | .. | H(12B)a | [2-x,1-y,1-z | = | 3766.01] | | -77.90 | 23.21 | 0.86830 | 0.52240 | 0.60790 | 5.7687 | 12.4780 | 6.5851 |
| 18 | 3.22 | .. | H(2B) | | | | Intra | 13.26 | -30.89 | 1.16900 | 0.66650 | 0.34180 | 7.8518 | 15.9200 | 3.7026 |
| 19 | 3.24 | .. | H(22A) | | | | Intra | -160.95 | 16.09 | 0.34420 | 0.59750 | 0.57700 | 2.2266 | 14.2719 | 6.2504 |

Angles (Degrees) At1...V...At2 with Vertex V = O(2)

| | | | | | | | | | | | | | | | |
|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|
| C(1) | , | C(21) | 112.00(15) | C(1) | , | O(1) | 35.62(10) | C(1) | , | C(2) | 37.29(11) | C(1) | , | C(22) | 148.00(13) |
| C(1) | , | N(1) | 56.73(11) | C(1) | , | N(2)b | 126.25(12) | C(1) | , | C(11) | 28.00(10) | C(21) | , | O(1) | 102.18(12) |
| C(21) | , | C(2) | 145.99(12) | C(21) | , | C(22) | 36.41(11) | C(21) | , | N(1) | 134.77(12) | C(21) | , | N(2)b | 121.42(11) |
| C(21) | , | C(11) | 94.82(12) | O(1) | , | C(2) | 61.63(7) | O(1) | , | C(22) | 126.60(10) | O(1) | , | N(1) | 88.60(7) |
| O(1) | , | N(2)b | 120.56(7) | O(1) | , | C(11) | 14.89(5) | C(2) | , | C(22) | 171.60(11) | C(2) | , | N(1) | 29.40(7) |
| C(2) | , | N(2)b | 91.72(8) | C(2) | , | C(11) | 61.75(7) | C(22) | , | N(1) | 142.42(9) | C(22) | , | N(2)b | 85.01(8) |
| C(22) | , | C(11) | 125.58(9) | N(1) | , | N(2)b | 87.28(6) | N(1) | , | C(11) | 84.63(6) | N(2)b | , | C(11) | 134.40(7) |

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3.6 Angstrom Coordination Sphere Around Atom I = N(2) [ARU = 1555.01] 0.86420 0.79626 0.22864 5.8088 19.0195 2.4767

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|------------|----------------------------|--------|-------|---------|--------|---------|---------|----------|--------|---------|---------|
| 1 | 0.80(2) | -- H(2) | | | Intra | 108.65 | -69.14 | 0.84900 | 0.80750 | 0.16000 | 5.7182 | 19.2879 | 1.7332 |
| 2 | 1.350(3) | -- C(3) | | | Intra | -64.03 | 8.23 | 0.95110 | 0.74597 | 0.24647 | 6.3939 | 17.8182 | 2.6699 |
| 3 | 1.420(3) | -- C(4) | | | Intra | 126.64 | 47.44 | 0.78210 | 0.82852 | 0.32519 | 5.2358 | 19.7900 | 3.5226 |
| 4 | 2.281(3) | << N(1) | | | Intra | -64.86 | 39.62 | 0.97800 | 0.72967 | 0.36292 | 6.5551 | 17.4289 | 3.9313 |
| 5 | 2.443(3) | << C(9) | | | Intra | 88.18 | 38.52 | 0.87690 | 0.87623 | 0.36907 | 5.8697 | 20.9296 | 3.9980 |
| 6 | 2.455(3) | << C(5) | | | Intra | 166.69 | 41.40 | 0.60340 | 0.81401 | 0.37850 | 4.0166 | 19.4434 | 4.1001 |
| 7 | 2.655(2) | << S | | | Intra | -63.28 | -24.76 | 1.02163 | 0.70609 | 0.12598 | 6.8929 | 16.8657 | 1.3647 |
| 8 | 2.986(2) | << Cl(1) | | | Intra | -159.76 | 20.29 | 0.47855 | 0.75569 | 0.32420 | 3.1813 | 18.0504 | 3.5119 |
| 9 | 2.989(2) | << Cl(3) | | | Intra | 56.03 | 17.17 | 1.10210 | 0.89541 | 0.31011 | 7.4046 | 21.3878 | 3.3593 |
| 10 | 3.012(2) | .< O(2)a | [x,3/2-y,-1/2+z = 4564.01] | | | 109.96 | -57.47 | 0.77630 | 0.86000 | -0.00582 | 5.2558 | 20.5420 | -0.0630 |
| 11 | 2.39(2) | << H(1) | | | Intra | -61.11 | 59.48 | 0.95600 | 0.75170 | 0.41900 | 6.3961 | 17.9551 | 4.5388 |
| 12 | 3.25 | .. H(2A)a | [x,3/2-y,-1/2+z = 4564.01] | | | 17.88 | -54.89 | 1.12060 | 0.82030 | -0.01690 | 7.5884 | 19.5937 | -0.1831 |
| 13 | 3.31 | .. H(22B)a | [x,3/2-y,-1/2+z = 4564.01] | | | 158.31 | -24.06 | 0.44540 | 0.84310 | 0.10390 | 2.9963 | 20.1383 | 1.1255 |
| 14 | 3.36 | .. H(22C)a | [x,3/2-y,-1/2+z = 4564.01] | | | 131.61 | -12.61 | 0.54070 | 0.89890 | 0.16090 | 3.6312 | 21.4711 | 1.7430 |

Angles (Degrees) At1...V...At2 with Vertex V = N(2)

| | | | | | | | | | | | | | | | |
|------|---|-------|------------|-------|---|-------|-----------|-------|---|-------|------------|-------|---|-------|------------|
| C(3) | , | C(4) | 123.53(17) | C(3) | , | N(1) | 31.41(10) | C(3) | , | C(9) | 126.58(14) | C(3) | , | C(5) | 112.05(14) |
| C(3) | , | S | 32.99(10) | C(3) | , | Cl(1) | 92.46(13) | C(3) | , | Cl(3) | 115.56(14) | C(3) | , | O(2)a | 130.53(13) |
| C(4) | , | N(1) | 92.34(13) | C(4) | , | C(9) | 29.18(11) | C(4) | , | C(5) | 28.90(11) | C(4) | , | S | 155.99(14) |
| C(4) | , | Cl(1) | 64.25(11) | C(4) | , | Cl(3) | 64.40(11) | C(4) | , | O(2)a | 105.82(13) | N(1) | , | C(9) | 98.05(9) |
| N(1) | , | C(5) | 86.42(9) | N(1) | , | S | 64.40(7) | N(1) | , | Cl(1) | 80.82(8) | N(1) | , | Cl(3) | 100.93(8) |
| N(1) | , | O(2)a | 161.84(10) | C(9) | , | C(5) | 58.08(8) | C(9) | , | S | 152.25(10) | C(9) | , | Cl(1) | 93.43(8) |
| C(9) | , | Cl(3) | 35.24(6) | C(9) | , | O(2)a | 97.72(8) | C(5) | , | S | 135.65(10) | C(5) | , | Cl(1) | 35.35(6) |
| C(5) | , | Cl(3) | 93.31(8) | C(5) | , | O(2)a | 109.65(9) | S | , | Cl(1) | 103.96(7) | S | , | Cl(3) | 123.26(8) |
| S | , | O(2)a | 97.57(6) | Cl(1) | , | Cl(3) | 128.66(7) | Cl(1) | , | O(2)a | 107.15(7) | Cl(3) | , | O(2)a | 86.93(6) |

=====
Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6
=====

van der Waals (or ion) Radii used in the Analysis

=====

C H Cl N O S

1.70 1.20 1.75 1.55 1.52 1.80

:: Grid: X-Axis Step = 0.0278 = Points 36, Angstrom Step = 0.19

:: Grid: Z-Axis Step = 0.0167 = Points 60, Angstrom Step = 0.18

:: Grid: Y-Axis Step = 0.0083 = Points 120, Angstrom Step = 0.20

:: Unit cell Contains NO Residual Solvent Accessible Void.

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

=====
Report Expected Number of Independent Reflections for given Symmetry and Resolution.

:: Hmax = 9 Kmax = 34 Lmax= 15 , Sorting Order : Fast H, Medium K, Slow L

:: Actual Theta-Max: 30.669 Deg. (Applied Theta Limit: 30.670 Deg.)

Space Group H-M: P21/c Laue: 2/m

Space Group Hall: -P 2ybc [Schoenflies: C2h⁵]

Lattice Type: mP, Centric, Monoclinic, Multiplicity: 4(2), No: 14

Nr ***** Symmetry Operation(s) *****

| | | | |
|---|-------|-----------|---------|
| 1 | H , | K , | L |
| 2 | - H , | 1/2 + K , | 1/2 - L |
| 3 | - H , | - K , | - L |
| 4 | H , | 1/2 - K , | 1/2 + L |

:: Number of Independent Type H, K, L Reflections = 5429

Table 0 - Crystal Data and Details of the Structure Determination
 for: tdacl3ph P2(1)/c R = 0.05

Crystal Data

| | | |
|--------------------------|----------|---------------------|
| Formula | | C13 H17 Cl3 N2 O2 S |
| Formula Weight | | 371.71 |
| Crystal System | | monoclinic |
| Space group | | P21/c (No. 14) |
| a, b, c [Angstrom] | 6.769(2) | 23.886(8) 10.834(4) |
| alpha, beta, gamma [deg] | 90 | 90.947(5) 90 |
| V [Ang**3] | | 1751.5(10) |
| Z | | 4 |
| D(calc) [g/cm**3] | | 1.410 |
| Mu(MoKa) [/mm] | | 0.646 |
| F(000) | | 768 |
| Crystal Size [mm] | | 0.07 x 0.23 x 0.29 |

Data Collection

| | | |
|----------------------------------|---------------------------|--------------|
| Temperature (K) | | 150 |
| Radiation [Angstrom] | | MoKa 0.71073 |
| Theta Min-Max [Deg] | | 1.7, 30.7 |
| Dataset | -9: 9 ; -34: 34 ; -15: 15 | |
| Tot., Uniq. Data, R(int) | 27726, 5411, 0.074 | |
| Observed Data [I > 2.0 sigma(I)] | | 3388 |

Refinement

| | | |
|--|--|----------------------|
| Nref, Npar | | 5411, 200 |
| R, wR2, S | | 0.0505, 0.1151, 1.01 |
| w = 1/[\s^2^(Fo^2^)+(0.0457P)^2^+0.3947P] where P=(Fo^2^+2Fc^2^)/3 | | |
| Max. and Av. Shift/Error | | 0.00, 0.00 |
| Min. and Max. Resd. Dens. [e/Ang^3] | | -0.32, 0.41 |

=====

=====

***** N O T I C E *****

=====

- PLATON Reference : Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.
Spek, A.L. (2009). Acta Cryst. D65, 148-155.

- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow

- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)

- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.

- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.

- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@uu.nl

- Recent versions of PLATON may be obtained from <http://www.platonsoft.nl/xraysoft>

- More INFO can be found on <http://http://www.platonsoft.nl/>

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Page 45 --- VOIDS
Page 46 --- EXPECT
Page 47 --- SUMMARY

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR
=====

W: NOMOVE option used.

:: >>> WARNING: 'CONNECTED INPUT SET' is assumed to be TRUE

:: >>> The Network Analysis may be INCORRECT when this assumption is FALSE

=====

:: Input Xtal Data from File tdac13ph.cif - Data Type CIF

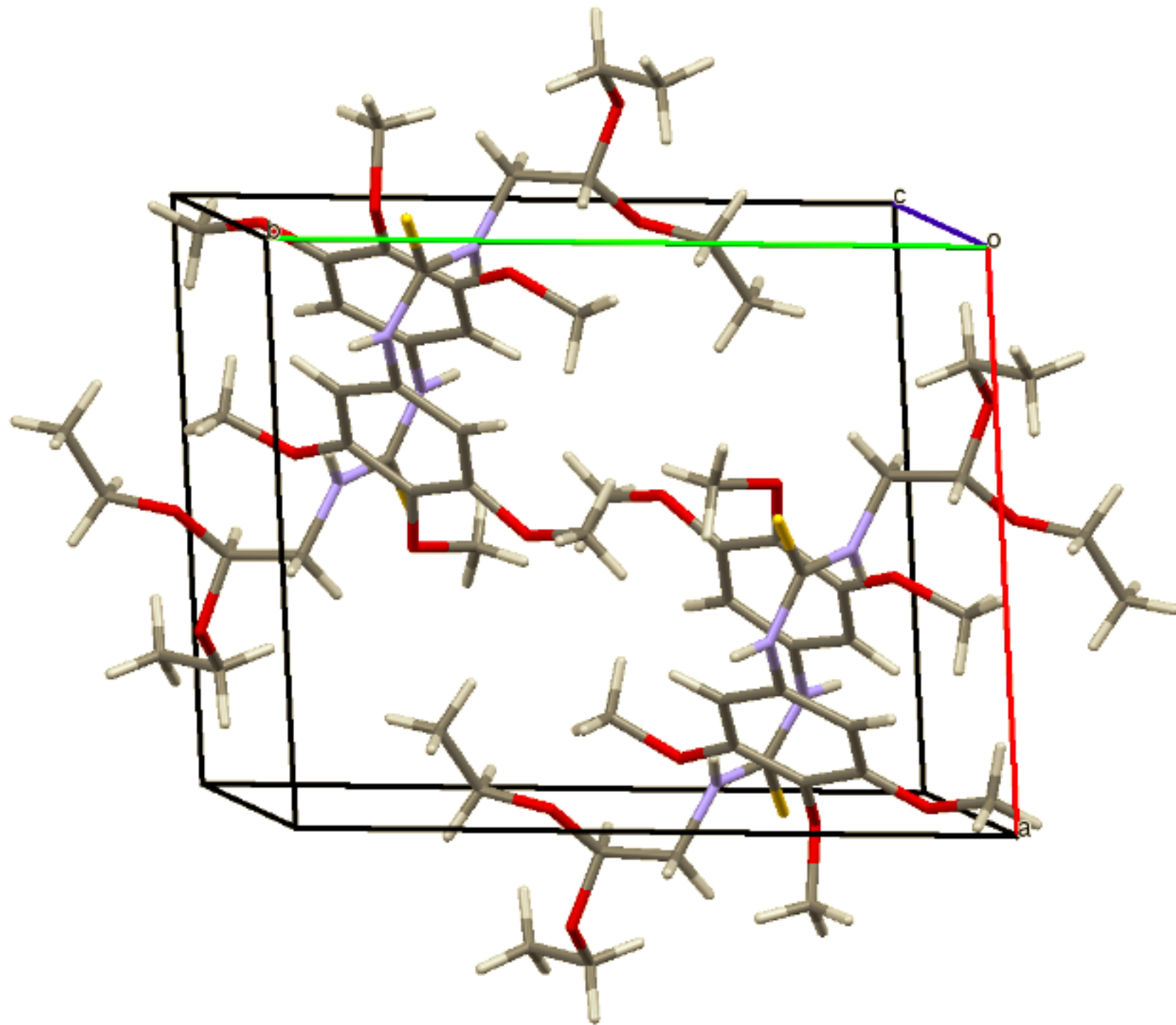
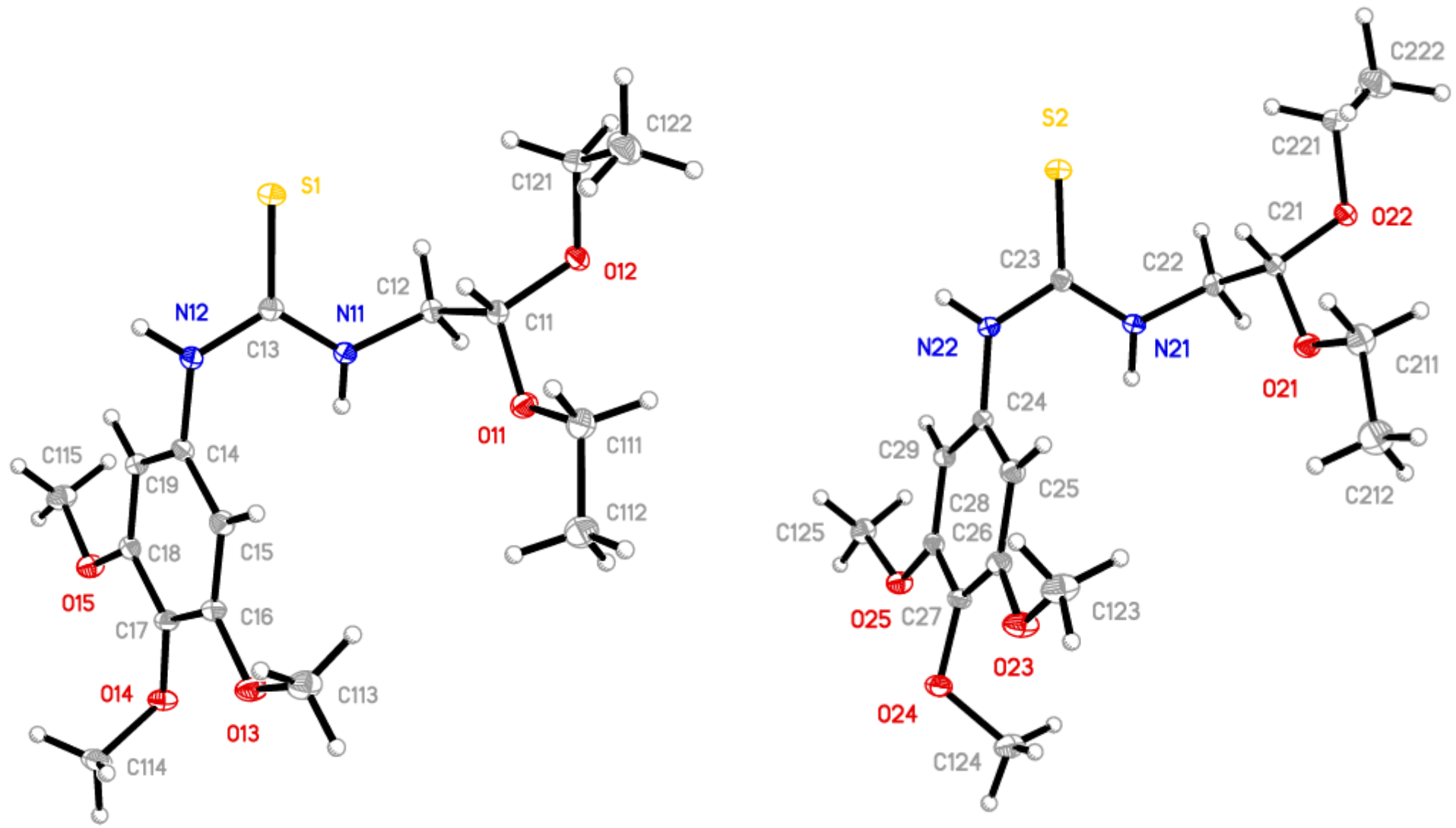
:: NORMAL END of PLATON : 49 Pages on:

:: tdac13ph.lis (ASCII, 132 Characters Wide)

:: tdac13ph.lps (PostScript Version of .lis)

::

H₂detu^{Ar(OMe)₃}



=====
 Analysis of Short Intra- and Inter-molecular Contacts , $d(I-J) < R(I) + R(J) + \text{Tolr}$, With Tolr = 0.2 Ang. ($X - I \dots J$) > 100. Deg.

Contact Radii : C H N O S
 (Angstrom) 1.70 1.20 1.55 1.52 1.80

Default Contact Radii are those given by A.Bondi, J.Phys.Chem. (1964),68,441. (or Coval. Rad. + 0.8 Ang. when not given)

* WARNING * : no Far-Reaching Conclusions should be drawn based on the Default Radii Assigned to Metals

Short "INTRA" Distances between two Atoms that are Separated by less than 4 Bonds are NOT Listed (Except for Potential D/A Contacts)

=====
 ***** ARU = 1555.01 *****
 =====

| At(I)[1555.01] | At(J) | [ARU(J)] | D(I-J) | SumRad | Del | Type | X(I) | Y(I) | Z(I) | X(J) | Y(J) | Z(J) | X | X - I...J |
|----------------|-------------|------------|--------------|--------|-------|-------|---------------|--------|--------|----------------------|--------|--------|--------|------------|
| S(1) | C(11) | [] | 3.640(2) | 3.50 | 0.14 | Intra | 0.4750 | 0.2966 | 0.1056 | 0.4013 | 0.0311 | 0.1586 | | |
| S(1) | C(12) | [] | 3.087(2)<< | 3.50 | -0.41 | Intra | 0.4750 | 0.2966 | 0.1056 | 0.4065 | 0.1238 | 0.2347 | | |
| S(1) | H(11J) | [] | 3.16 | 3.00 | 0.16 | Intra | 0.4750 | 0.2966 | 0.1056 | 0.4354 | 0.0522 | 0.0977 | | |
| S(1) | H(12) | [] | 2.68(2)<< | 3.00 | -0.32 | Intra | 0.4750 | 0.2966 | 0.1056 | 0.7152 | 0.3546 | 0.1920 | | |
| S(1) | H(12A) | [] | 2.71<< | 3.00 | -0.29 | Intra | 0.4750 | 0.2966 | 0.1056 | 0.3412 | 0.1724 | 0.2132 | | |
| O(11) | N(11) | [] | 2.918(2) < | 3.07 | -0.15 | Intra | 0.4772-0.0439 | 0.1981 | | 0.5343 | 0.1784 | 0.2508 | C(111) | 144.54(10) |
| O(11) | H(11N) | [] | 2.57 < | 2.72 | -0.15 | Intra | 0.4772-0.0439 | 0.1981 | | 0.5900-0.2103 | 0.2337 | | C(11) | 166 |
| O(11) | H(110) | [] | 2.60 < | 2.72 | -0.12 | Intra | 0.4772-0.0439 | 0.1981 | | 0.6881-0.1418 | 0.1796 | | C(11) | 143 |
| O(11) | H(12B) | [] | 2.50<< | 2.72 | -0.22 | Intra | 0.4772-0.0439 | 0.1981 | | 0.3836 | 0.0999 | 0.2971 | C(111) | 165 |
| O(11) | H(12H) | [2666.02] | 2.78 | 2.72 | 0.06 | | 0.4772-0.0439 | 0.1981 | | 0.6284-0.0407 | 0.3768 | | C(11) | 131 |
| | | | | | | | | | | | | | C(111) | 114 |
| O(12) | N(22) | [1545.02] | 2.882(2) < | 3.07 | -0.19 | | 0.2697-0.0100 | 0.1377 | | 0.1793-0.1888 | 0.2271 | | C(11) | 120.74(10) |
| | | | | | | | | | | | | | C(121) | 122.78(10) |
| O(12) | C(111) | [] | 2.894(2)<< | 3.22 | -0.33 | Intra | 0.2697-0.0100 | 0.1377 | | 0.4968-0.1305 | 0.1288 | | C(121) | 122.41(10) |
| O(12) | H(11L) | [] | 2.73 | 2.72 | 0.01 | Intra | 0.2697-0.0100 | 0.1377 | | 0.4170-0.1775 | 0.1164 | | C(121) | 119 |
| O(12) | H(12A) | [] | 2.53 < | 2.72 | -0.19 | Intra | 0.2697-0.0100 | 0.1377 | | 0.3412 | 0.1724 | 0.2132 | | |
| O(12) | H(12B) | [] | 2.64 < | 2.72 | -0.08 | Intra | 0.2697-0.0100 | 0.1377 | | 0.3836 | 0.0999 | 0.2971 | C(121) | 129 |
| O(12) | H(12F) | [] | 2.65 < | 2.72 | -0.07 | Intra | 0.2697-0.0100 | 0.1377 | | 0.1825-0.1152-0.0323 | | | C(11) | 122 |
| O(12) | H(12G) | [] | 2.66 < | 2.72 | -0.06 | Intra | 0.2697-0.0100 | 0.1377 | | 0.3087-0.0453-0.0495 | | | | |
| O(12) | H(22) | [1545.02] | 2.060(18)<< | 2.72 | -0.66 | | 0.2697-0.0100 | 0.1377 | | 0.1958-0.1389 | 0.1953 | | C(11) | 124.0(5) |
| | | | | | | | | | | | | | C(121) | 119.4(5) |
| O(13) | O(14) | [] | 2.6876(18)<< | 3.04 | -0.35 | Intra | 0.9830 | 0.0713 | 0.3894 | 1.0218 | 0.2096 | 0.5487 | C(113) | 178.75(11) |
| O(13) | C(114) | [] | 3.103(3) < | 3.22 | -0.12 | Intra | 0.9830 | 0.0713 | 0.3894 | 1.1597 | 0.2223 | 0.5409 | C(113) | 151.98(11) |
| O(13) | H(11F) | [] | 2.58 < | 2.72 | -0.14 | Intra | 0.9830 | 0.0713 | 0.3894 | 1.1809 | 0.1791 | 0.4833 | C(113) | 135 |
| O(13) | H(15A) | [] | 2.67 < | 2.72 | -0.05 | Intra | 0.9830 | 0.0713 | 0.3894 | 0.8226 | 0.1361 | 0.2468 | | |
| O(13) | H(12I) | [2666.02] | 2.68 < | 2.72 | -0.04 | | 0.9830 | 0.0713 | 0.3894 | 0.7521 | 0.0135 | 0.4452 | | |
| O(14) | O(13) | [] | 2.6876(18)<< | 3.04 | -0.35 | Intra | 1.0218 | 0.2096 | 0.5487 | 0.9830 | 0.0713 | 0.3894 | | |

| | | | | | | | | | |
|-------|------|--------|------------|-------------------------|-------|----------------------|----------------------|--------|------------|
| O(14) | | O(15) | [] | 2.6549(19)<< 3.04 -0.39 | Intra | 1.0218 0.2096 0.5487 | 0.9149 0.3917 0.5543 | C(114) | 110.86(10) |
| O(14) | | N(21) | [2666.02] | 3.124(2) 3.07 0.05 | | 1.0218 0.2096 0.5487 | 0.9706 0.3188 0.7514 | C(17) | 118.04(10) |
| | | | | | | | | C(114) | 107.65(10) |
| O(14) | | H(11G) | [2756.01] | 2.70 < 2.72 -0.02 | | 1.0218 0.2096 0.5487 | 0.9969 0.0685 0.6786 | C(17) | 134 |
| | | | | | | | | C(114) | 105 |
| O(14) | | H(21) | [2666.02] | 2.75(2) 2.72 0.03 | | 1.0218 0.2096 0.5487 | 0.9255 0.3277 0.6978 | C(17) | 103.0(4) |
| | | | | | | | | C(114) | 117.4(4) |
| O(15) | | O(14) | [] | 2.6549(19)<< 3.04 -0.39 | Intra | 0.9149 0.3917 0.5543 | 1.0218 0.2096 0.5487 | C(115) | 173.26(11) |
| O(15) | | H(19A) | [] | 2.67 < 2.72 -0.05 | Intra | 0.9149 0.3917 0.5543 | 0.7624 0.4150 0.3912 | | |
| O(15) | | N(21) | [2666.02] | 2.976(2) < 3.07 -0.09 | | 0.9149 0.3917 0.5543 | 0.9706 0.3188 0.7514 | C(18) | 124.63(10) |
| | | | | | | | | C(115) | 108.41(10) |
| O(15) | | C(22) | [2666.02] | 3.371(2) 3.22 0.15 | | 0.9149 0.3917 0.5543 | 1.0964 0.3768 0.7689 | C(18) | 135.33(10) |
| | | | | | | | | C(115) | 107.06(10) |
| O(15) | | H(11C) | [2766.01] | 2.73 2.72 0.01 | | 0.9149 0.3917 0.5543 | 1.1343 0.4712 0.4872 | | |
| O(15) | | H(21) | [2666.02] | 2.21(2)<< 2.72 -0.51 | | 0.9149 0.3917 0.5543 | 0.9255 0.3277 0.6978 | C(18) | 120.6(5) |
| | | | | | | | | C(115) | 106.7(5) |
| O(15) | | H(22B) | [2666.02] | 2.83 2.72 0.11 | | 0.9149 0.3917 0.5543 | 1.1215 0.3984 0.7062 | C(18) | 132 |
| | | | | | | | | C(115) | 110 |
| N(11) | | O(11) | [] | 2.918(2) < 3.07 -0.15 | Intra | 0.5343 0.1784 0.2508 | 0.4772-0.0439 0.1981 | C(13) | 132.25(11) |
| N(11) | | C(14) | [] | 2.784(2)<< 3.25 -0.47 | Intra | 0.5343 0.1784 0.2508 | 0.7786 0.2785 0.3078 | C(12) | 172.37(12) |
| N(11) | | C(15) | [] | 3.151(2) < 3.25 -0.10 | Intra | 0.5343 0.1784 0.2508 | 0.8384 0.1843 0.3035 | C(12) | 151.81(11) |
| N(11) | | H(11J) | [] | 2.63 < 2.75 -0.12 | Intra | 0.5343 0.1784 0.2508 | 0.4354 0.0522 0.0977 | H(11) | 124 |
| N(11) | | O(25) | [2666.02] | 3.014(2) < 3.07 -0.06 | | 0.5343 0.1784 0.2508 | 0.5944 0.0957 0.4462 | C(13) | 141.19(12) |
| N(11) | | C(124) | [2666.02] | 3.299(3) 3.25 0.05 | | 0.5343 0.1784 0.2508 | 0.4397 0.3437 0.4221 | | |
| N(12) | | O(22) | [1655.02] | 2.900(2) < 3.07 -0.17 | | 0.6919 0.3022 0.2261 | 0.7739 0.4845 0.1356 | C(13) | 119.81(11) |
| | | | | | | | | C(14) | 114.70(10) |
| N(12) | | H(11) | [] | 2.42(2)<< 2.75 -0.33 | Intra | 0.6919 0.3022 0.2261 | 0.5836 0.1608 0.2951 | H(12) | 167.2(13) |
| N(12) | | H(12N) | [] | 2.86 2.75 0.11 | | 0.6919 0.3022 0.2261 | 0.5834 0.4950 0.2798 | C(14) | 108 |
| N(12) | | H(15A) | [] | 2.62 < 2.75 -0.13 | Intra | 0.6919 0.3022 0.2261 | 0.8226 0.1361 0.2468 | H(12) | 125 |
| N(12) | | H(19A) | [] | 2.61 < 2.75 -0.14 | Intra | 0.6919 0.3022 0.2261 | 0.7624 0.4150 0.3912 | C(13) | 125 |
| C(11) | | S(1) | [] | 3.640(2) 3.50 0.14 | Intra | 0.4013 0.0311 0.1586 | 0.4750 0.2966 0.1056 | O(11) | 133.05(11) |
| | | | | | | | | O(12) | 117.71(10) |
| C(11) | | C(13) | [] | 3.287(3) < 3.40 -0.11 | Intra | 0.4013 0.0311 0.1586 | 0.5712 0.2554 0.1992 | O(11) | 107.85(10) |
| | | | | | | | | O(12) | 140.34(11) |
| C(11) | | C(122) | [] | 3.217(3) < 3.40 -0.18 | Intra | 0.4013 0.0311 0.1586 | 0.2163-0.0446-0.0395 | O(11) | 116.06(11) |
| | | | | | | | | C(12) | 134.44(12) |
| C(11) | | H(11) | [] | 2.88(2) < 2.90 -0.02 | Intra | 0.4013 0.0311 0.1586 | 0.5836 0.1608 0.2951 | O(12) | 145.3(4) |
| C(11) | | H(11K) | [] | 2.50<< 2.90 -0.40 | Intra | 0.4013 0.0311 0.1586 | 0.5162-0.1053 0.0661 | O(12) | 101 |
| | | | | | | | | C(12) | 150 |
| C(11) | | H(11L) | [] | 2.73 < 2.90 -0.17 | Intra | 0.4013 0.0311 0.1586 | 0.4170-0.1775 0.1164 | C(12) | 149 |
| C(11) | | H(12C) | [] | 2.46<< 2.90 -0.44 | Intra | 0.4013 0.0311 0.1586 | 0.2344 0.0966 0.0438 | O(11) | 156 |
| C(11) | | H(12G) | [] | 3.00 2.90 0.10 | Intra | 0.4013 0.0311 0.1586 | 0.3087-0.0453-0.0495 | O(11) | 108 |
| | | | | | | | | C(12) | 144 |
| C(11) | | H(22) | [1545.02] | 3.092(18) 2.90 0.19 | | 0.4013 0.0311 0.1586 | 0.1958-0.1389 0.1953 | C(12) | 111.3(4) |
| | | | | | | | | H(11J) | 133 |
| C(12) | | S(1) | [] | 3.087(2)<< 3.50 -0.41 | Intra | 0.4065 0.1238 0.2347 | 0.4750 0.2966 0.1056 | H(12B) | 152 |
| C(12) | | C(121) | [] | 3.251(3) < 3.40 -0.15 | Intra | 0.4065 0.1238 0.2347 | 0.2009 0.0252 0.0516 | N(11) | 138.36(12) |
| | | | | | | | | H(12B) | 111 |

| | | | | | | | | | | | | | | | |
|--------|------|--------|------------|------------|--------|-------|-------|--------|---------|--------|--------|---------|--------|--------|------------|
| C(12) | | H(12C) | [] | 3.01 | 2.90 | 0.11 | Intra | 0.4065 | 0.1238 | 0.2347 | 0.2344 | 0.0966 | 0.0438 | N(11) | 125 |
| | | | | | | | | | | | | | | H(12B) | 126 |
| C(12) | | O(25) | [2666.02] | 3.401(2) | 3.22 | 0.18 | | 0.4065 | 0.1238 | 0.2347 | 0.5944 | 0.0957 | 0.4462 | C(11) | 114.10(11) |
| | | | | | | | | | | | | | | H(12A) | 136 |
| C(13) | | C(11) | [] | 3.287(3) | < 3.40 | -0.11 | Intra | 0.5712 | 0.2554 | 0.1992 | 0.4013 | 0.0311 | 0.1586 | N(12) | 144.70(12) |
| C(13) | | C(15) | [] | 3.205(3) | < 3.40 | -0.20 | Intra | 0.5712 | 0.2554 | 0.1992 | 0.8384 | 0.1843 | 0.3035 | S(1) | 154.58(9) |
| C(13) | | C(19) | [] | 3.460(3) | 3.40 | 0.06 | Intra | 0.5712 | 0.2554 | 0.1992 | 0.8025 | 0.3506 | 0.3896 | S(1) | 140.61(9) |
| C(13) | | H(11J) | [] | 3.06 | 2.90 | 0.16 | Intra | 0.5712 | 0.2554 | 0.1992 | 0.4354 | 0.0522 | 0.0977 | N(12) | 141 |
| C(13) | | H(12A) | [] | 2.59<< | 2.90 | -0.31 | Intra | 0.5712 | 0.2554 | 0.1992 | 0.3412 | 0.1724 | 0.2132 | N(12) | 160 |
| C(13) | | H(12M) | [2666.02] | 3.07 | 2.90 | 0.17 | | 0.5712 | 0.2554 | 0.1992 | 0.5259 | 0.3587 | 0.4013 | S(1) | 114 |
| C(14) | | N(11) | [] | 2.784(2)<< | 3.25 | -0.47 | Intra | 0.7786 | 0.2785 | 0.3078 | 0.5343 | 0.1784 | 0.2508 | C(19) | 122.32(12) |
| C(14) | | C(17) | [] | 2.784(2)<< | 3.40 | -0.62 | Intra | 0.7786 | 0.2785 | 0.3078 | 0.9458 | 0.2329 | 0.4669 | N(12) | 179.68(12) |
| C(14) | | H(11) | [] | 2.45(2)<< | 2.90 | -0.45 | Intra | 0.7786 | 0.2785 | 0.3078 | 0.5836 | 0.1608 | 0.2951 | C(19) | 117.9(5) |
| C(15) | | N(11) | [] | 3.151(2) | < 3.25 | -0.10 | Intra | 0.8384 | 0.1843 | 0.3035 | 0.5343 | 0.1784 | 0.2508 | C(16) | 135.47(12) |
| C(15) | | C(13) | [] | 3.205(3) | < 3.40 | -0.20 | Intra | 0.8384 | 0.1843 | 0.3035 | 0.5712 | 0.2554 | 0.1992 | C(16) | 154.29(13) |
| C(15) | | C(18) | [] | 2.793(3)<< | 3.40 | -0.61 | Intra | 0.8384 | 0.1843 | 0.3035 | 0.8856 | 0.3275 | 0.4691 | H(15A) | 179 |
| C(15) | | C(113) | [] | 2.824(3)<< | 3.40 | -0.58 | Intra | 0.8384 | 0.1843 | 0.3035 | 0.9635 | -0.0043 | 0.3054 | C(14) | 177.06(13) |
| C(15) | | H(11) | [] | 2.63(2)<< | 2.90 | -0.27 | Intra | 0.8384 | 0.1843 | 0.3035 | 0.5836 | 0.1608 | 0.2951 | C(16) | 123.1(4) |
| C(15) | | H(11H) | [] | 2.86 | < 2.90 | -0.04 | Intra | 0.8384 | 0.1843 | 0.3035 | 1.0040 | 0.0229 | 0.2511 | C(14) | 162 |
| C(15) | | H(11I) | [] | 2.66<< | 2.90 | -0.24 | Intra | 0.8384 | 0.1843 | 0.3035 | 0.8699 | -0.0189 | 0.2864 | C(14) | 161 |
| C(15) | | H(12) | [] | 3.07(2) | 2.90 | 0.17 | Intra | 0.8384 | 0.1843 | 0.3035 | 0.7152 | 0.3546 | 0.1920 | C(16) | 146.4(4) |
| C(15) | | H(21E) | [1655.02] | 2.97 | 2.90 | 0.07 | | 0.8384 | 0.1843 | 0.3035 | 1.0811 | 0.2880 | 0.2509 | | |
| C(16) | | C(19) | [] | 2.796(3)<< | 3.40 | -0.60 | Intra | 0.9218 | 0.1616 | 0.3837 | 0.8025 | 0.3506 | 0.3896 | O(13) | 175.01(13) |
| C(16) | | C(114) | [] | 3.127(3)<< | 3.40 | -0.27 | Intra | 0.9218 | 0.1616 | 0.3837 | 1.1597 | 0.2223 | 0.5409 | C(15) | 150.75(13) |
| C(16) | | H(11F) | [] | 2.87 | < 2.90 | -0.03 | Intra | 0.9218 | 0.1616 | 0.3837 | 1.1809 | 0.1791 | 0.4833 | C(15) | 148 |
| C(16) | | H(11H) | [] | 2.68<< | 2.90 | -0.22 | Intra | 0.9218 | 0.1616 | 0.3837 | 1.0040 | 0.0229 | 0.2511 | C(17) | 151 |
| C(16) | | H(11I) | [] | 2.59<< | 2.90 | -0.31 | Intra | 0.9218 | 0.1616 | 0.3837 | 0.8699 | -0.0189 | 0.2864 | C(17) | 156 |
| C(16) | | C(125) | [2666.02] | 3.555(3) | 3.40 | 0.15 | | 0.9218 | 0.1616 | 0.3837 | 0.6576 | -0.0009 | 0.4398 | C(17) | 102.96(11) |
| C(16) | | H(12I) | [2666.02] | 2.78 | < 2.90 | -0.12 | | 0.9218 | 0.1616 | 0.3837 | 0.7521 | 0.0135 | 0.4452 | C(17) | 102 |
| C(17) | | C(14) | [] | 2.784(2)<< | 3.40 | -0.62 | Intra | 0.9458 | 0.2329 | 0.4669 | 0.7786 | 0.2785 | 0.3078 | O(14) | 176.43(12) |
| C(17) | | H(11E) | [] | 2.60<< | 2.90 | -0.30 | Intra | 0.9458 | 0.2329 | 0.4669 | 1.1835 | 0.2954 | 0.5344 | C(16) | 120 |
| | | | | | | | | | | | | | | C(18) | 101 |
| C(17) | | H(11F) | [] | 2.56<< | 2.90 | -0.34 | Intra | 0.9458 | 0.2329 | 0.4669 | 1.1809 | 0.1791 | 0.4833 | C(18) | 135 |
| C(17) | | C(29) | [2666.02] | 3.478(3) | 3.40 | 0.08 | | 0.9458 | 0.2329 | 0.4669 | 0.7131 | 0.1408 | 0.6078 | C(16) | 100.21(11) |
| C(18) | | C(15) | [] | 2.793(3)<< | 3.40 | -0.61 | Intra | 0.8856 | 0.3275 | 0.4691 | 0.8384 | 0.1843 | 0.3035 | O(15) | 175.10(12) |
| C(18) | | C(114) | [] | 3.310(3) | < 3.40 | -0.09 | Intra | 0.8856 | 0.3275 | 0.4691 | 1.1597 | 0.2223 | 0.5409 | C(19) | 145.75(12) |
| C(18) | | H(11B) | [] | 2.63<< | 2.90 | -0.27 | Intra | 0.8856 | 0.3275 | 0.4691 | 0.7525 | 0.4673 | 0.5590 | C(17) | 150 |
| C(18) | | H(11C) | [] | 2.64<< | 2.90 | -0.26 | Intra | 0.8856 | 0.3275 | 0.4691 | 0.8657 | 0.5288 | 0.5128 | C(17) | 157 |
| C(18) | | H(11C) | [2766.01] | 3.07 | 2.90 | 0.17 | | 0.8856 | 0.3275 | 0.4691 | 1.1343 | 0.4712 | 0.4872 | C(19) | 109 |
| C(19) | | C(13) | [] | 3.460(3) | 3.40 | 0.06 | Intra | 0.8025 | 0.3506 | 0.3896 | 0.5712 | 0.2554 | 0.1992 | C(18) | 146.50(12) |
| C(19) | | C(16) | [] | 2.796(3)<< | 3.40 | -0.60 | Intra | 0.8025 | 0.3506 | 0.3896 | 0.9218 | 0.1616 | 0.3837 | H(19A) | 180 |
| C(19) | | C(115) | [] | 2.826(3)<< | 3.40 | -0.57 | Intra | 0.8025 | 0.3506 | 0.3896 | 0.8464 | 0.4852 | 0.5645 | C(14) | 175.78(13) |
| C(19) | | H(11B) | [] | 2.77 | < 2.90 | -0.13 | Intra | 0.8025 | 0.3506 | 0.3896 | 0.7525 | 0.4673 | 0.5590 | C(14) | 158 |
| C(19) | | H(11C) | [] | 2.74 | < 2.90 | -0.16 | Intra | 0.8025 | 0.3506 | 0.3896 | 0.8657 | 0.5288 | 0.5128 | C(14) | 164 |
| C(19) | | H(12) | [] | 2.793(19) | < 2.90 | -0.11 | Intra | 0.8025 | 0.3506 | 0.3896 | 0.7152 | 0.3546 | 0.1920 | C(18) | 156.1(4) |
| C(19) | | H(12M) | [2666.02] | 2.89 | < 2.90 | -0.01 | | 0.8025 | 0.3506 | 0.3896 | 0.5259 | 0.3587 | 0.4013 | C(18) | 121 |
| C(111) | | O(12) | [] | 2.894(2)<< | 3.22 | -0.33 | Intra | 0.4968 | -0.1305 | 0.1288 | 0.2697 | -0.0100 | 0.1377 | C(112) | 155.16(14) |
| C(111) | | H(11J) | [] | 2.55<< | 2.90 | -0.35 | Intra | 0.4968 | -0.1305 | 0.1288 | 0.4354 | 0.0522 | 0.0977 | C(112) | 141 |

| | | | | | | | | | | | | | | | |
|--------|------|--------|------------|-------------|------|-------|-------|----------------------|--------|----------------------|---------------|---------------|--------|------------|------------|
| | | | | | | | | | | | H(11L) | 108 | | | |
| C(113) | | C(15) | [] | 2.824(3)<< | 3.40 | -0.58 | Intra | 0.9635-0.0043 | 0.3054 | 0.8384 | 0.1843 | 0.3035 | H(11G) | 167 | |
| C(113) | | C(23) | [1645.02] | 3.549(3) | 3.40 | 0.15 | | 0.9635-0.0043 | 0.3054 | 1.0641-0.2416 | 0.1961 | | O(13) | 145.30(12) | |
| C(113) | | H(15A) | [] | 2.53<< | 2.90 | -0.37 | Intra | 0.9635-0.0043 | 0.3054 | 0.8226 | 0.1361 | 0.2468 | H(11G) | 168 | |
| C(113) | | H(12I) | [2666.02] | 3.06 | 2.90 | 0.16 | | 0.9635-0.0043 | 0.3054 | 0.7521 | 0.0135 | 0.4452 | H(11G) | 102 | |
| | | | | | | | | | | | | | H(11H) | 148 | |
| C(114) | | O(13) | [] | 3.103(3) < | 3.22 | -0.12 | Intra | 1.1597 | 0.2223 | 0.5409 | 0.9830 | 0.0713 | 0.3894 | H(11D) | 124 |
| | | | | | | | | | | | | | H(11E) | 126 | |
| C(114) | | C(16) | [] | 3.127(3)<< | 3.40 | -0.27 | Intra | 1.1597 | 0.2223 | 0.5409 | 0.9218 | 0.1616 | 0.3837 | H(11D) | 144 |
| | | | | | | | | | | | | | H(11E) | 105 | |
| C(114) | | C(18) | [] | 3.310(3) < | 3.40 | -0.09 | Intra | 1.1597 | 0.2223 | 0.5409 | 0.8856 | 0.3275 | 0.4691 | H(11D) | 141 |
| | | | | | | | | | | | | | H(11F) | 105 | |
| C(114) | | C(125) | [1645.02] | 3.532(3) | 3.40 | 0.13 | | 1.1597 | 0.2223 | 0.5409 | 1.3424 | 0.0009 | 0.5602 | O(14) | 117.34(11) |
| | | | | | | | | | | | | | H(11E) | 133 | |
| C(114) | | O(24) | [2766.02] | 3.168(2) < | 3.22 | -0.05 | | 1.1597 | 0.2223 | 0.5409 | 1.4401 | 0.2498 | 0.4699 | O(14) | 166.34(13) |
| C(115) | | C(19) | [] | 2.826(3)<< | 3.40 | -0.57 | Intra | 0.8464 | 0.4852 | 0.5645 | 0.8025 | 0.3506 | 0.3896 | H(11A) | 169 |
| C(115) | | H(19A) | [] | 2.53<< | 2.90 | -0.37 | Intra | 0.8464 | 0.4852 | 0.5645 | 0.7624 | 0.4150 | 0.3912 | H(11A) | 171 |
| C(115) | | H(21) | [2666.02] | 2.97(2) | 2.90 | 0.07 | | 0.8464 | 0.4852 | 0.5645 | 0.9255 | 0.3277 | 0.6978 | H(11C) | 150 |
| C(121) | | C(12) | [] | 3.251(3) < | 3.40 | -0.15 | Intra | 0.2009 | 0.0252 | 0.0516 | 0.4065 | 0.1238 | 0.2347 | C(122) | 132.60(13) |
| | | | | | | | | | | | | | H(12D) | 117 | |
| C(121) | | H(11J) | [] | 2.44<< | 2.90 | -0.46 | Intra | 0.2009 | 0.0252 | 0.0516 | 0.4354 | 0.0522 | 0.0977 | H(12D) | 157 |
| C(121) | | H(12A) | [] | 3.00 | 2.90 | 0.10 | Intra | 0.2009 | 0.0252 | 0.0516 | 0.3412 | 0.1724 | 0.2132 | C(122) | 145 |
| | | | | | | | | | | | | | H(12D) | 106 | |
| C(121) | | H(22) | [1545.02] | 3.043(18) | 2.90 | 0.14 | | 0.2009 | 0.0252 | 0.0516 | 0.1958-0.1389 | 0.1953 | H(12C) | 144 | |
| C(121) | | S(2) | [2565.02] | 3.694(2) | 3.50 | 0.19 | | 0.2009 | 0.0252 | 0.0516 | 0.0290 | 0.2086-0.0973 | O(12) | 156.88(11) | |
| C(122) | | C(11) | [] | 3.217(3) < | 3.40 | -0.18 | Intra | 0.2163-0.0446-0.0395 | | 0.4013 | 0.0311 | 0.1586 | H(12E) | 142 | |
| | | | | | | | | | | | | | H(12F) | 106 | |
| C(122) | | H(11J) | [] | 2.95 | 2.90 | 0.05 | Intra | 0.2163-0.0446-0.0395 | | 0.4354 | 0.0522 | 0.0977 | H(12E) | 131 | |
| | | | | | | | | | | | | | H(12F) | 120 | |
| C(122) | | H(15A) | [2655.01] | 2.97 | 2.90 | 0.07 | | 0.2163-0.0446-0.0395 | | 0.1774-0.1361-0.2468 | | | C(121) | 160 | |
| H(11) | | N(12) | [] | 2.42(2)<< | 2.75 | -0.33 | Intra | 0.5836 | 0.1608 | 0.2951 | 0.6919 | 0.3022 | 0.2261 | | |
| H(11) | | C(11) | [] | 2.88(2) < | 2.90 | -0.02 | Intra | 0.5836 | 0.1608 | 0.2951 | 0.4013 | 0.0311 | 0.1586 | | |
| H(11) | | C(14) | [] | 2.45(2)<< | 2.90 | -0.45 | Intra | 0.5836 | 0.1608 | 0.2951 | 0.7786 | 0.2785 | 0.3078 | N(11) | 106.2(16) |
| H(11) | | C(15) | [] | 2.63(2)<< | 2.90 | -0.27 | Intra | 0.5836 | 0.1608 | 0.2951 | 0.8384 | 0.1843 | 0.3035 | N(11) | 123.7(16) |
| H(11) | | H(12B) | [] | 2.18<< | 2.40 | -0.22 | Intra | 0.5836 | 0.1608 | 0.2951 | 0.3836 | 0.0999 | 0.2971 | | |
| H(11) | | O(25) | [2666.02] | 2.318(19)<< | 2.72 | -0.40 | | 0.5836 | 0.1608 | 0.2951 | 0.5944 | 0.0957 | 0.4462 | N(11) | 144.2(18) |
| H(11) | | C(125) | [2666.02] | 3.099(19) | 2.90 | 0.20 | | 0.5836 | 0.1608 | 0.2951 | 0.6576-0.0009 | 0.4398 | N(11) | 149.3(17) | |
| H(11A) | | O(21) | [2666.02] | 2.62 < | 2.72 | -0.10 | | 0.8742 | 0.5233 | 0.6285 | 1.0207 | 0.5446 | 0.7961 | C(115) | 151 |
| H(11B) | | C(18) | [] | 2.63<< | 2.90 | -0.27 | Intra | 0.7525 | 0.4673 | 0.5590 | 0.8856 | 0.3275 | 0.4691 | | |
| H(11B) | | C(19) | [] | 2.77 < | 2.90 | -0.13 | Intra | 0.7525 | 0.4673 | 0.5590 | 0.8025 | 0.3506 | 0.3896 | | |
| H(11B) | | H(12L) | [] | 2.54 | 2.40 | 0.14 | | 0.7525 | 0.4673 | 0.5590 | 0.5817 | 0.5986 | 0.5325 | C(115) | 123 |
| H(11B) | | H(19A) | [] | 2.37 < | 2.40 | -0.03 | Intra | 0.7525 | 0.4673 | 0.5590 | 0.7624 | 0.4150 | 0.3912 | | |
| H(11B) | | C(26) | [2666.02] | 3.05 | 2.90 | 0.15 | | 0.7525 | 0.4673 | 0.5590 | 0.5594 | 0.3110 | 0.6279 | C(115) | 140 |
| H(11C) | | C(18) | [] | 2.64<< | 2.90 | -0.26 | Intra | 0.8657 | 0.5288 | 0.5128 | 0.8856 | 0.3275 | 0.4691 | | |
| H(11C) | | C(19) | [] | 2.74 < | 2.90 | -0.16 | Intra | 0.8657 | 0.5288 | 0.5128 | 0.8025 | 0.3506 | 0.3896 | | |
| H(11C) | | H(19A) | [] | 2.27 < | 2.40 | -0.13 | Intra | 0.8657 | 0.5288 | 0.5128 | 0.7624 | 0.4150 | 0.3912 | | |
| H(11C) | | O(15) | [2766.01] | 2.73 | 2.72 | 0.01 | | 0.8657 | 0.5288 | 0.5128 | 1.0851 | 0.6083 | 0.4457 | C(115) | 136 |
| H(11C) | | C(18) | [2766.01] | 3.07 | 2.90 | 0.17 | | 0.8657 | 0.5288 | 0.5128 | 1.1144 | 0.6725 | 0.5309 | C(115) | 122 |

| | | | | | | | | | | | | | | | |
|--------|------|--------|------------|-----------|------|-------|-------|---------------|--------|--------|----------------------|---------------|--------|--------|-----------|
| H(11C) | | H(11E) | [2766.01] | 2.49 | 2.40 | 0.09 | | 0.8657 | 0.5288 | 0.5128 | 0.8165 | 0.7046 | 0.4656 | C(115) | 138 |
| H(11D) | | C(125) | [1645.02] | 3.04 | 2.90 | 0.14 | | 1.2082 | 0.2011 | 0.5997 | 1.3424 | 0.0009 | 0.5602 | C(114) | 113 |
| H(11E) | | C(17) | [] | 2.60<< | 2.90 | -0.30 | Intra | 1.1835 | 0.2954 | 0.5344 | 0.9458 | 0.2329 | 0.4669 | | |
| H(11E) | | H(11C) | [2766.01] | 2.49 | 2.40 | 0.09 | | 1.1835 | 0.2954 | 0.5344 | 1.1343 | 0.4712 | 0.4872 | C(114) | 153 |
| H(11F) | | O(13) | [] | 2.58 < | 2.72 | -0.14 | Intra | 1.1809 | 0.1791 | 0.4833 | 0.9830 | 0.0713 | 0.3894 | C(114) | 114 |
| H(11F) | | C(16) | [] | 2.87 < | 2.90 | -0.03 | Intra | 1.1809 | 0.1791 | 0.4833 | 0.9218 | 0.1616 | 0.3837 | | |
| H(11F) | | C(17) | [] | 2.56<< | 2.90 | -0.34 | Intra | 1.1809 | 0.1791 | 0.4833 | 0.9458 | 0.2329 | 0.4669 | | |
| H(11F) | | O(24) | [2766.02] | 2.82 | 2.72 | 0.10 | | 1.1809 | 0.1791 | 0.4833 | 1.4401 | 0.2498 | 0.4699 | C(114) | 102 |
| H(11G) | | N(22) | [1645.02] | 2.80 | 2.75 | 0.05 | | 1.0031-0.0685 | 0.3214 | | 1.1793-0.1888 | 0.2271 | | C(113) | 131 |
| H(11G) | | C(23) | [1645.02] | 2.84 < | 2.90 | -0.06 | | 1.0031-0.0685 | 0.3214 | | 1.0641-0.2416 | 0.1961 | | C(113) | 130 |
| H(11G) | | H(29A) | [1645.02] | 2.55 | 2.40 | 0.15 | | 1.0031-0.0685 | 0.3214 | | 1.2351-0.0825 | 0.3983 | | C(113) | 126 |
| H(11G) | | O(14) | [2756.01] | 2.70 < | 2.72 | -0.02 | | 1.0031-0.0685 | 0.3214 | | 0.9782-0.2096 | 0.4513 | | C(113) | 137 |
| H(11H) | | C(15) | [] | 2.86 < | 2.90 | -0.04 | Intra | 1.0040 | 0.0229 | 0.2511 | 0.8384 | 0.1843 | 0.3035 | | |
| H(11H) | | C(16) | [] | 2.68<< | 2.90 | -0.22 | Intra | 1.0040 | 0.0229 | 0.2511 | 0.9218 | 0.1616 | 0.3837 | | |
| H(11H) | | H(15A) | [] | 2.44 | 2.40 | 0.04 | Intra | 1.0040 | 0.0229 | 0.2511 | 0.8226 | 0.1361 | 0.2468 | | |
| H(11I) | | C(15) | [] | 2.66<< | 2.90 | -0.24 | Intra | 0.8699-0.0189 | 0.2864 | | 0.8384 | 0.1843 | 0.3035 | | |
| H(11I) | | C(16) | [] | 2.59<< | 2.90 | -0.31 | Intra | 0.8699-0.0189 | 0.2864 | | 0.9218 | 0.1616 | 0.3837 | | |
| H(11I) | | H(15A) | [] | 2.20<< | 2.40 | -0.20 | Intra | 0.8699-0.0189 | 0.2864 | | 0.8226 | 0.1361 | 0.2468 | | |
| H(11J) | | S(1) | [] | 3.16 | 3.00 | 0.16 | Intra | 0.4354 | 0.0522 | 0.0977 | 0.4750 | 0.2966 | 0.1056 | C(11) | 111 |
| H(11J) | | N(11) | [] | 2.63 < | 2.75 | -0.12 | Intra | 0.4354 | 0.0522 | 0.0977 | 0.5343 | 0.1784 | 0.2508 | | |
| H(11J) | | C(13) | [] | 3.06 | 2.90 | 0.16 | Intra | 0.4354 | 0.0522 | 0.0977 | 0.5712 | 0.2554 | 0.1992 | | |
| H(11J) | | C(111) | [] | 2.55<< | 2.90 | -0.35 | Intra | 0.4354 | 0.0522 | 0.0977 | 0.4968-0.1305 | 0.1288 | | | |
| H(11J) | | C(121) | [] | 2.44<< | 2.90 | -0.46 | Intra | 0.4354 | 0.0522 | 0.0977 | 0.2009 | 0.0252 | 0.0516 | | |
| H(11J) | | C(122) | [] | 2.95 | 2.90 | 0.05 | Intra | 0.4354 | 0.0522 | 0.0977 | 0.2163-0.0446-0.0395 | | | | |
| H(11J) | | H(11K) | [] | 2.27 < | 2.40 | -0.13 | Intra | 0.4354 | 0.0522 | 0.0977 | 0.5162-0.1053 | 0.0661 | | | |
| H(11J) | | H(12A) | [] | 2.44 | 2.40 | 0.04 | Intra | 0.4354 | 0.0522 | 0.0977 | 0.3412 | 0.1724 | 0.2132 | | |
| H(11J) | | H(12C) | [] | 2.26 < | 2.40 | -0.14 | Intra | 0.4354 | 0.0522 | 0.0977 | 0.2344 | 0.0966 | 0.0438 | | |
| H(11J) | | H(12G) | [] | 2.50 | 2.40 | 0.10 | Intra | 0.4354 | 0.0522 | 0.0977 | 0.3087-0.0453-0.0495 | | | C(11) | 110 |
| H(11J) | | H(11K) | [2655.01] | 2.52 | 2.40 | 0.12 | | 0.4354 | 0.0522 | 0.0977 | 0.4838 | 0.1053-0.0661 | | C(11) | 171 |
| H(11K) | | C(11) | [] | 2.50<< | 2.90 | -0.40 | Intra | 0.5162-0.1053 | 0.0661 | | 0.4013 | 0.0311 | 0.1586 | | |
| H(11K) | | H(11J) | [] | 2.27 < | 2.40 | -0.13 | Intra | 0.5162-0.1053 | 0.0661 | | 0.4354 | 0.0522 | 0.0977 | | |
| H(11K) | | H(11M) | [] | 2.37 < | 2.40 | -0.03 | Intra | 0.5162-0.1053 | 0.0661 | | 0.6209-0.2487 | 0.1254 | | | |
| H(11K) | | H(110) | [] | 2.35 < | 2.40 | -0.05 | Intra | 0.5162-0.1053 | 0.0661 | | 0.6881-0.1418 | 0.1796 | | | |
| H(11K) | | H(11J) | [2655.01] | 2.52 | 2.40 | 0.12 | | 0.5162-0.1053 | 0.0661 | | 0.5646-0.0522-0.0977 | | | C(111) | 177 |
| H(11L) | | O(12) | [] | 2.73 | 2.72 | 0.01 | Intra | 0.4170-0.1775 | 0.1164 | | 0.2697-0.0100 | 0.1377 | | | |
| H(11L) | | C(11) | [] | 2.73 < | 2.90 | -0.17 | Intra | 0.4170-0.1775 | 0.1164 | | 0.4013 | 0.0311 | 0.1586 | | |
| H(11L) | | H(11M) | [] | 2.34 < | 2.40 | -0.06 | Intra | 0.4170-0.1775 | 0.1164 | | 0.6209-0.2487 | 0.1254 | | | |
| H(11L) | | H(11N) | [] | 2.37 < | 2.40 | -0.03 | Intra | 0.4170-0.1775 | 0.1164 | | 0.5900-0.2103 | 0.2337 | | | |
| H(11M) | | H(11K) | [] | 2.37 < | 2.40 | -0.03 | Intra | 0.6209-0.2487 | 0.1254 | | 0.5162-0.1053 | 0.0661 | | | |
| H(11M) | | H(11L) | [] | 2.34 < | 2.40 | -0.06 | Intra | 0.6209-0.2487 | 0.1254 | | 0.4170-0.1775 | 0.1164 | | | |
| H(11N) | | O(11) | [] | 2.57 < | 2.72 | -0.15 | Intra | 0.5900-0.2103 | 0.2337 | | 0.4772-0.0439 | 0.1981 | | | |
| H(11N) | | C(25) | [1545.02] | 2.97 | 2.90 | 0.07 | | 0.5900-0.2103 | 0.2337 | | 0.3441-0.2956 | 0.2977 | | C(112) | 131 |
| H(11N) | | C(26) | [1545.02] | 2.93 | 2.90 | 0.03 | | 0.5900-0.2103 | 0.2337 | | 0.4406-0.3110 | 0.3721 | | C(112) | 157 |
| H(11N) | | H(11L) | [] | 2.37 < | 2.40 | -0.03 | Intra | 0.5900-0.2103 | 0.2337 | | 0.4170-0.1775 | 0.1164 | | | |
| H(110) | | O(11) | [] | 2.60 < | 2.72 | -0.12 | Intra | 0.6881-0.1418 | 0.1796 | | 0.4772-0.0439 | 0.1981 | | | |
| H(110) | | H(11K) | [] | 2.35 < | 2.40 | -0.05 | Intra | 0.6881-0.1418 | 0.1796 | | 0.5162-0.1053 | 0.0661 | | | |
| H(12) | | S(1) | [] | 2.68(2)<< | 3.00 | -0.32 | Intra | 0.7152 | 0.3546 | 0.1920 | 0.4750 | 0.2966 | 0.1056 | | |
| H(12) | | O(22) | [1655.02] | 2.01(2)<< | 2.72 | -0.71 | | 0.7152 | 0.3546 | 0.1920 | 0.7739 | 0.4845 | 0.1356 | N(12) | 171.3(18) |

| | | | | | | | | | | | | | | | |
|--------|------|--------|------------|-----------|--------|-------|-------|--------|---------|---------|--------|---------|---------|--------|-----------|
| H(12) | | C(15) | [] | 3.07(2) | 2.90 | 0.17 | Intra | 0.7152 | 0.3546 | 0.1920 | 0.8384 | 0.1843 | 0.3035 | | |
| H(12) | | C(19) | [] | 2.793(19) | < 2.90 | -0.11 | Intra | 0.7152 | 0.3546 | 0.1920 | 0.8025 | 0.3506 | 0.3896 | | |
| H(12) | | C(21) | [1655.02] | 3.00(2) | 2.90 | 0.10 | | 0.7152 | 0.3546 | 0.1920 | 0.9046 | 0.5277 | 0.1589 | N(12) | 150.5(16) |
| H(12) | | C(221) | [1655.02] | 3.037(19) | 2.90 | 0.14 | | 0.7152 | 0.3546 | 0.1920 | 0.7080 | 0.5184 | 0.0482 | N(12) | 162.3(16) |
| H(12) | | H(21C) | [1655.02] | 2.51 | 2.40 | 0.11 | | 0.7152 | 0.3546 | 0.1920 | 0.9250 | 0.3216 | 0.1207 | N(12) | 111 |
| H(12A) | | S(1) | [] | 2.71<< | 3.00 | -0.29 | Intra | 0.3412 | 0.1724 | 0.2132 | 0.4750 | 0.2966 | 0.1056 | C(12) | 103 |
| H(12A) | | O(12) | [] | 2.53 | < 2.72 | -0.19 | Intra | 0.3412 | 0.1724 | 0.2132 | 0.2697 | -0.0100 | 0.1377 | | |
| H(12A) | | C(13) | [] | 2.59<< | 2.90 | -0.31 | Intra | 0.3412 | 0.1724 | 0.2132 | 0.5712 | 0.2554 | 0.1992 | | |
| H(12A) | | C(121) | [] | 3.00 | 2.90 | 0.10 | Intra | 0.3412 | 0.1724 | 0.2132 | 0.2009 | 0.0252 | 0.0516 | | |
| H(12A) | | C(212) | [] | 3.06 | 2.90 | 0.16 | | 0.3412 | 0.1724 | 0.2132 | 0.1096 | 0.3087 | 0.1896 | C(12) | 166 |
| H(12A) | | H(11J) | [] | 2.44 | 2.40 | 0.04 | Intra | 0.3412 | 0.1724 | 0.2132 | 0.4354 | 0.0522 | 0.0977 | | |
| H(12A) | | H(12C) | [] | 2.57 | 2.40 | 0.17 | Intra | 0.3412 | 0.1724 | 0.2132 | 0.2344 | 0.0966 | 0.0438 | C(12) | 107 |
| H(12A) | | H(21D) | [] | 2.59 | 2.40 | 0.19 | | 0.3412 | 0.1724 | 0.2132 | 0.1255 | 0.2466 | 0.1474 | C(12) | 162 |
| H(12B) | | O(11) | [] | 2.50<< | 2.72 | -0.22 | Intra | 0.3836 | 0.0999 | 0.2971 | 0.4772 | -0.0439 | 0.1981 | | |
| H(12B) | | O(12) | [] | 2.64 | < 2.72 | -0.08 | Intra | 0.3836 | 0.0999 | 0.2971 | 0.2697 | -0.0100 | 0.1377 | | |
| H(12B) | | H(11) | [] | 2.18<< | 2.40 | -0.22 | Intra | 0.3836 | 0.0999 | 0.2971 | 0.5836 | 0.1608 | 0.2951 | | |
| H(12B) | | O(25) | [2666.02] | 2.85 | 2.72 | 0.13 | | 0.3836 | 0.0999 | 0.2971 | 0.5944 | 0.0957 | 0.4462 | C(12) | 116 |
| H(12C) | | C(11) | [] | 2.46<< | 2.90 | -0.44 | Intra | 0.2344 | 0.0966 | 0.0438 | 0.4013 | 0.0311 | 0.1586 | | |
| H(12C) | | C(12) | [] | 3.01 | 2.90 | 0.11 | Intra | 0.2344 | 0.0966 | 0.0438 | 0.4065 | 0.1238 | 0.2347 | | |
| H(12C) | | H(11J) | [] | 2.26 | < 2.40 | -0.14 | Intra | 0.2344 | 0.0966 | 0.0438 | 0.4354 | 0.0522 | 0.0977 | | |
| H(12C) | | H(12A) | [] | 2.57 | 2.40 | 0.17 | Intra | 0.2344 | 0.0966 | 0.0438 | 0.3412 | 0.1724 | 0.2132 | C(121) | 106 |
| H(12C) | | H(12E) | [] | 2.35 | < 2.40 | -0.05 | Intra | 0.2344 | 0.0966 | 0.0438 | 0.1678 | -0.0185 | -0.0959 | | |
| H(12C) | | H(12G) | [] | 2.35 | < 2.40 | -0.05 | Intra | 0.2344 | 0.0966 | 0.0438 | 0.3087 | -0.0453 | -0.0495 | | |
| H(12D) | | H(12E) | [] | 2.34 | < 2.40 | -0.06 | Intra | 0.1073 | 0.0274 | 0.0604 | 0.1678 | -0.0185 | -0.0959 | | |
| H(12D) | | H(12F) | [] | 2.36 | < 2.40 | -0.04 | Intra | 0.1073 | 0.0274 | 0.0604 | 0.1825 | -0.1152 | -0.0323 | | |
| H(12E) | | H(12C) | [] | 2.35 | < 2.40 | -0.05 | Intra | 0.1678 | -0.0185 | -0.0959 | 0.2344 | 0.0966 | 0.0438 | | |
| H(12E) | | H(12D) | [] | 2.34 | < 2.40 | -0.06 | Intra | 0.1678 | -0.0185 | -0.0959 | 0.1073 | 0.0274 | 0.0604 | | |
| H(12E) | | H(15A) | [2655.01] | 2.48 | 2.40 | 0.08 | | 0.1678 | -0.0185 | -0.0959 | 0.1774 | -0.1361 | -0.2468 | C(122) | 111 |
| H(12F) | | O(12) | [] | 2.65 | < 2.72 | -0.07 | Intra | 0.1825 | -0.1152 | -0.0323 | 0.2697 | -0.0100 | 0.1377 | | |
| H(12F) | | H(12D) | [] | 2.36 | < 2.40 | -0.04 | Intra | 0.1825 | -0.1152 | -0.0323 | 0.1073 | 0.0274 | 0.0604 | | |
| H(12G) | | O(12) | [] | 2.66 | < 2.72 | -0.06 | Intra | 0.3087 | -0.0453 | -0.0495 | 0.2697 | -0.0100 | 0.1377 | | |
| H(12G) | | C(11) | [] | 3.00 | 2.90 | 0.10 | Intra | 0.3087 | -0.0453 | -0.0495 | 0.4013 | 0.0311 | 0.1586 | | |
| H(12G) | | H(11J) | [] | 2.50 | 2.40 | 0.10 | Intra | 0.3087 | -0.0453 | -0.0495 | 0.4354 | 0.0522 | 0.0977 | C(122) | 107 |
| H(12G) | | H(12C) | [] | 2.35 | < 2.40 | -0.05 | Intra | 0.3087 | -0.0453 | -0.0495 | 0.2344 | 0.0966 | 0.0438 | | |
| H(15A) | | O(13) | [] | 2.67 | < 2.72 | -0.05 | Intra | 0.8226 | 0.1361 | 0.2468 | 0.9830 | 0.0713 | 0.3894 | | |
| H(15A) | | N(12) | [] | 2.62 | < 2.75 | -0.13 | Intra | 0.8226 | 0.1361 | 0.2468 | 0.6919 | 0.3022 | 0.2261 | | |
| H(15A) | | C(113) | [] | 2.53<< | 2.90 | -0.37 | Intra | 0.8226 | 0.1361 | 0.2468 | 0.9635 | -0.0043 | 0.3054 | | |
| H(15A) | | H(11H) | [] | 2.44 | 2.40 | 0.04 | Intra | 0.8226 | 0.1361 | 0.2468 | 1.0040 | 0.0229 | 0.2511 | C(15) | 106 |
| H(15A) | | H(11I) | [] | 2.20<< | 2.40 | -0.20 | Intra | 0.8226 | 0.1361 | 0.2468 | 0.8699 | -0.0189 | 0.2864 | C(15) | 109 |
| H(15A) | | C(122) | [2655.01] | 2.97 | 2.90 | 0.07 | | 0.8226 | 0.1361 | 0.2468 | 0.7837 | 0.0446 | 0.0395 | C(15) | 162 |
| H(15A) | | H(12E) | [2655.01] | 2.48 | 2.40 | 0.08 | | 0.8226 | 0.1361 | 0.2468 | 0.8322 | 0.0185 | 0.0959 | C(15) | 168 |
| H(19A) | | O(15) | [] | 2.67 | < 2.72 | -0.05 | Intra | 0.7624 | 0.4150 | 0.3912 | 0.9149 | 0.3917 | 0.5543 | | |
| H(19A) | | N(12) | [] | 2.61 | < 2.75 | -0.14 | Intra | 0.7624 | 0.4150 | 0.3912 | 0.6919 | 0.3022 | 0.2261 | | |
| H(19A) | | C(115) | [] | 2.53<< | 2.90 | -0.37 | Intra | 0.7624 | 0.4150 | 0.3912 | 0.8464 | 0.4852 | 0.5645 | | |
| H(19A) | | H(11B) | [] | 2.37 | < 2.40 | -0.03 | Intra | 0.7624 | 0.4150 | 0.3912 | 0.7525 | 0.4673 | 0.5590 | C(19) | 105 |
| H(19A) | | H(11C) | [] | 2.27 | < 2.40 | -0.13 | Intra | 0.7624 | 0.4150 | 0.3912 | 0.8657 | 0.5288 | 0.5128 | C(19) | 110 |
| H(19A) | | H(12M) | [2666.02] | 2.54 | 2.40 | 0.14 | | 0.7624 | 0.4150 | 0.3912 | 0.5259 | 0.3587 | 0.4013 | C(19) | 102 |

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 1 to Neighbouring ARU'S

| Nr | ARU | Nr.Cont. | d(min) | Del | XHn X | - At(I) | At(J) | - Y | YHn | Note | Partaking ARU's in Close Contact | Resd. |
|----|------------|----------|--------|-------|-------|---------------------|----------------|-----|-----|------|----------------------------------|-------|
| 1 | [2666.02] | 24 | 2.2100 | -0.51 | 0 | C(18) - O(15) ... | H(21) -N(21) | | 1 | << | 2666.02 | |
| 2 | [1545.02] | 6 | 2.0600 | -0.66 | 1 | C(11) - O(12) ... | H(22) -N(22) | | 1 | << | 1545.02 | |
| 3 | [2756.01] | 2 | 2.7000 | -0.02 | 3 | C(113) - H(11G) ... | O(14) -C(17) | | 0 | < | 2756.01 | |
| 4 | [2766.01] | 6 | 2.4900 | 0.09 | 3 | C(114) - H(11E) ... | H(11C) -C(115) | | 3 | | 2766.01 | |
| 5 | [1655.02] | 6 | 2.0100 | -0.71 | 1 | N(12) - H(12) ... | O(22) -C(21) | | 1 | << | 1655.02 | |
| 6 | [1555.02] | 4 | 2.5400 | 0.14 | 3 | C(115) - H(11B) ... | H(12L) -C(124) | | 3 | | 1555.02 | |
| 7 | [1645.02] | 6 | 2.5500 | 0.15 | 3 | C(113) - H(11G) ... | H(29A) -C(29) | | 1 | | 1645.02 | |
| 8 | [2766.02] | 2 | 2.8200 | 0.10 | 3 | C(114) - H(11F) ... | O(24) -C(27) | | 0 | | 2766.02 | |
| 9 | [2565.02] | 1 | 3.6940 | 0.19 | 0 | O(12) - C(121) ... | S(2) -C(23) | | 0 | | 2565.02 | |
| 10 | [2655.01] | 6 | 2.4800 | 0.08 | 1 | C(15) - H(15A) ... | H(12E) -C(122) | | 3 | | 2655.01 | |

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

 ***** ARU = 1555.02 *****

| At(I)[1555.02] | At(J) | [ARU(J)] | D(I-J) | SumRad | Del | Type | X(I) | Y(I) | Z(I) | X(J) | Y(J) | Z(J) | X | X - I...J |
|----------------|-------|-------------------|-------------|--------|-------|-------|---------|--------|--------|---------|--------|---------|--------|------------|
| S(2) | | C(21) [] | 3.643(2) | 3.50 | 0.14 | Intra | -0.0290 | 0.7914 | 0.0973 | -0.0953 | 0.5277 | 0.1589 | | |
| S(2) | | C(22) [] | 3.082(2)<< | 3.50 | -0.42 | Intra | -0.0290 | 0.7914 | 0.0973 | -0.0964 | 0.6232 | 0.2311 | | |
| S(2) | | H(21A) [] | 3.17 | 3.00 | 0.17 | Intra | -0.0290 | 0.7914 | 0.0973 | -0.0581 | 0.5465 | 0.0984 | | |
| S(2) | | H(22) [] | 2.640(19)<< | 3.00 | -0.36 | Intra | -0.0290 | 0.7914 | 0.0973 | 0.1958 | 0.8611 | 0.1953 | | |
| S(2) | | H(22A) [] | 2.70<< | 3.00 | -0.30 | Intra | -0.0290 | 0.7914 | 0.0973 | -0.1629 | 0.6690 | 0.2057 | | |
| S(2) | | C(121) [2565.01] | 3.694(2) | 3.50 | 0.19 | | -0.0290 | 0.7914 | 0.0973 | -0.2010 | 0.9748 | -0.0516 | C(23) | 154.40(6) |
| O(21) | | N(21) [] | 2.941(2) < | 3.07 | -0.13 | Intra | -0.0207 | 0.4554 | 0.2039 | 0.0294 | 0.6812 | 0.2486 | C(211) | 143.84(11) |
| O(21) | | H(21E) [] | 2.57 < | 2.72 | -0.15 | Intra | -0.0207 | 0.4554 | 0.2039 | 0.0811 | 0.2880 | 0.2509 | C(21) | 164 |
| O(21) | | H(21F) [] | 2.61 < | 2.72 | -0.11 | Intra | -0.0207 | 0.4554 | 0.2039 | 0.1900 | 0.3533 | 0.2038 | C(21) | 146 |
| O(21) | | H(22B) [] | 2.50<< | 2.72 | -0.22 | Intra | -0.0207 | 0.4554 | 0.2039 | -0.1215 | 0.6016 | 0.2938 | C(211) | 166 |
| O(21) | | H(11A) [2666.01] | 2.62 < | 2.72 | -0.10 | | -0.0207 | 0.4554 | 0.2039 | 0.1258 | 0.4767 | 0.3715 | C(21) | 129 |
| | | | | | | | | | | | | | C(211) | 115 |
| O(22) | | N(12) [1455.01] | 2.900(2) < | 3.07 | -0.17 | | -0.2261 | 0.4845 | 0.1356 | -0.3081 | 0.3022 | 0.2261 | C(21) | 119.08(9) |
| | | | | | | | | | | | | | C(221) | 124.48(10) |
| O(22) | | C(211) [] | 2.898(2)<< | 3.22 | -0.32 | Intra | -0.2261 | 0.4845 | 0.1356 | 0.0053 | 0.3673 | 0.1385 | C(221) | 123.93(10) |
| O(22) | | H(12) [1455.01] | 2.01(2)<< | 2.72 | -0.71 | | -0.2261 | 0.4845 | 0.1356 | -0.2848 | 0.3546 | 0.1920 | C(21) | 120.4(6) |
| | | | | | | | | | | | | | C(221) | 122.4(6) |

| | | | | | | | | | | | | | | | |
|-------|------|--------|------------|--------------------|-------|-------|---------|---------|--------|---------|---------|---------|--------|------------|------------|
| O(22) | | H(21C) | [] | 2.69 < 2.72 | -0.03 | Intra | -0.2261 | 0.4845 | 0.1356 | -0.0750 | 0.3216 | 0.1207 | C(221) | 119 | |
| O(22) | | H(22A) | [] | 2.52 << 2.72 | -0.20 | Intra | -0.2261 | 0.4845 | 0.1356 | -0.1629 | 0.6690 | 0.2057 | | | |
| O(22) | | H(22B) | [] | 2.64 < 2.72 | -0.08 | Intra | -0.2261 | 0.4845 | 0.1356 | -0.1215 | 0.6016 | 0.2938 | C(221) | 127 | |
| O(22) | | H(22F) | [] | 2.67 < 2.72 | -0.05 | Intra | -0.2261 | 0.4845 | 0.1356 | -0.3113 | 0.3780 | -0.0356 | C(21) | 123 | |
| O(22) | | H(22G) | [] | 2.63 < 2.72 | -0.09 | Intra | -0.2261 | 0.4845 | 0.1356 | -0.1794 | 0.4438 | -0.0469 | | | |
| O(23) | | O(24) | [] | 2.7397(19) << 3.04 | -0.30 | Intra | 0.5260 | 0.6113 | 0.3661 | 0.5599 | 0.7502 | 0.5301 | C(123) | 175.35(12) | |
| O(23) | | C(124) | [] | 2.912(2) << 3.22 | -0.31 | Intra | 0.5260 | 0.6113 | 0.3661 | 0.5603 | 0.6563 | 0.5779 | C(123) | 154.30(11) | |
| O(23) | | H(12L) | [] | 2.34 << 2.72 | -0.38 | Intra | 0.5260 | 0.6113 | 0.3661 | 0.5817 | 0.5986 | 0.5325 | C(26) | 100 | |
| | | | | | | | | | | | | | C(123) | 138 | |
| O(23) | | H(25A) | [] | 2.66 < 2.72 | -0.06 | Intra | 0.5260 | 0.6113 | 0.3661 | 0.3294 | 0.6567 | 0.2406 | | | |
| O(24) | | O(23) | [] | 2.7397(19) << 3.04 | -0.30 | Intra | 0.5599 | 0.7502 | 0.5301 | 0.5260 | 0.6113 | 0.3661 | | | |
| O(24) | | O(25) | [] | 2.6377(19) << 3.04 | -0.40 | Intra | 0.5599 | 0.7502 | 0.5301 | 0.4056 | 0.9043 | 0.5538 | C(124) | 127.31(11) | |
| O(24) | | C(114) | [2766.01] | 3.168(2) < 3.22 | -0.05 | | 0.5599 | 0.7502 | 0.5301 | 0.8403 | 0.7777 | 0.4591 | C(27) | 113.88(10) | |
| | | | | | | | | | | | | | C(124) | 105.42(10) | |
| O(24) | | H(11F) | [2766.01] | 2.82 | 2.72 | 0.10 | 0.5599 | 0.7502 | 0.5301 | 0.8191 | 0.8209 | 0.5167 | C(27) | 124 | |
| | | | | | | | | | | | | | C(124) | 109 | |
| O(24) | | H(12J) | [2676.02] | 2.88 | 2.72 | 0.16 | 0.5599 | 0.7502 | 0.5301 | 0.6352 | 0.9587 | 0.4930 | C(124) | 158 | |
| O(25) | | O(24) | [] | 2.6377(19) << 3.04 | -0.40 | Intra | 0.4056 | 0.9043 | 0.5538 | 0.5599 | 0.7502 | 0.5301 | C(125) | 168.39(11) | |
| O(25) | | H(29A) | [] | 2.66 < 2.72 | -0.06 | Intra | 0.4056 | 0.9043 | 0.5538 | 0.2351 | 0.9175 | 0.3983 | | | |
| O(25) | | N(11) | [2666.01] | 3.014(2) < 3.07 | -0.06 | | 0.4056 | 0.9043 | 0.5538 | 0.4657 | 0.8216 | 0.7492 | C(28) | 123.34(10) | |
| | | | | | | | | | | | | | C(125) | 113.29(9) | |
| O(25) | | C(12) | [2666.01] | 3.401(2) | 3.22 | 0.18 | 0.4056 | 0.9043 | 0.5538 | 0.5935 | 0.8762 | 0.7653 | C(28) | 132.00(10) | |
| | | | | | | | | | | | | | C(125) | 111.15(9) | |
| O(25) | | C(125) | [2676.02] | 3.413(2) | 3.22 | 0.19 | 0.4056 | 0.9043 | 0.5538 | 0.6576 | 0.9991 | 0.4398 | | | |
| O(25) | | H(11) | [2666.01] | 2.318(19) << 2.72 | -0.40 | | 0.4056 | 0.9043 | 0.5538 | 0.4164 | 0.8392 | 0.7049 | C(28) | 122.6(5) | |
| | | | | | | | | | | | | | C(125) | 108.9(5) | |
| O(25) | | H(12B) | [2666.01] | 2.85 | 2.72 | 0.13 | 0.4056 | 0.9043 | 0.5538 | 0.6164 | 0.9001 | 0.7029 | C(28) | 128 | |
| | | | | | | | | | | | | | C(125) | 113 | |
| O(25) | | H(12J) | [2676.02] | 2.68 < 2.72 | -0.04 | | 0.4056 | 0.9043 | 0.5538 | 0.6352 | 0.9587 | 0.4930 | C(125) | 103 | |
| N(21) | | O(21) | [] | 2.941(2) < 3.07 | -0.13 | Intra | 0.0294 | 0.6812 | 0.2486 | -0.0207 | 0.4554 | 0.2039 | C(23) | 133.87(11) | |
| N(21) | | C(24) | [] | 2.800(2) << 3.25 | -0.45 | Intra | 0.0294 | 0.6812 | 0.2486 | 0.2696 | 0.7901 | 0.3078 | C(22) | 172.63(12) | |
| N(21) | | C(25) | [] | 3.250(3) | 3.25 | 0.00 | 0.0294 | 0.6812 | 0.2486 | 0.3441 | 0.7044 | 0.2977 | C(22) | 154.13(11) | |
| N(21) | | H(21A) | [] | 2.64 < 2.75 | -0.11 | Intra | 0.0294 | 0.6812 | 0.2486 | -0.0581 | 0.5465 | 0.0984 | H(21) | 130 | |
| N(21) | | O(14) | [2666.01] | 3.124(2) | 3.07 | 0.05 | 0.0294 | 0.6812 | 0.2486 | -0.0218 | 0.7904 | 0.4513 | C(23) | 105.36(10) | |
| N(21) | | O(15) | [2666.01] | 2.976(2) < 3.07 | -0.09 | | 0.0294 | 0.6812 | 0.2486 | 0.0851 | 0.6083 | 0.4457 | C(23) | 140.80(11) | |
| N(22) | | O(12) | [1565.01] | 2.882(2) < 3.07 | -0.19 | | 0.1793 | 0.8112 | 0.2271 | 0.2697 | 0.9900 | 0.1377 | C(23) | 122.42(11) | |
| | | | | | | | | | | | | | C(24) | 111.23(11) | |
| N(22) | | H(11G) | [1465.01] | 2.80 | 2.75 | 0.05 | 0.1793 | 0.8112 | 0.2271 | 0.0031 | 0.9315 | 0.3214 | C(24) | 102 | |
| N(22) | | H(21) | [] | 2.42(2) << 2.75 | -0.33 | Intra | 0.1793 | 0.8112 | 0.2271 | 0.0745 | 0.6723 | 0.3022 | H(22) | 165.2(14) | |
| N(22) | | H(25A) | [] | 2.61 < 2.75 | -0.14 | Intra | 0.1793 | 0.8112 | 0.2271 | 0.3294 | 0.6567 | 0.2406 | C(23) | 100 | |
| | | | | | | | | | | | | | H(22) | 123 | |
| N(22) | | H(29A) | [] | 2.62 < 2.75 | -0.13 | Intra | 0.1793 | 0.8112 | 0.2271 | 0.2351 | 0.9175 | 0.3983 | C(23) | 125 | |
| C(21) | | S(2) | [] | 3.643(2) | 3.50 | 0.14 | Intra | -0.0953 | 0.5277 | 0.1589 | -0.0290 | 0.7914 | 0.0973 | O(21) | 134.32(10) |
| | | | | | | | | | | | | | O(22) | 116.73(9) | |
| C(21) | | C(23) | [] | 3.307(3) < 3.40 | -0.09 | Intra | -0.0953 | 0.5277 | 0.1589 | 0.0641 | 0.7584 | 0.1961 | O(21) | 109.22(10) | |
| | | | | | | | | | | | | | O(22) | 139.00(11) | |
| C(21) | | C(222) | [] | 3.212(3) < 3.40 | -0.19 | Intra | -0.0953 | 0.5277 | 0.1589 | -0.2727 | 0.4476 | -0.0412 | O(21) | 117.34(11) | |
| | | | | | | | | | | | | | C(22) | 132.72(11) | |

| | | | | | | | | | | | | | | | |
|-------|------|--------|------------|------------|------|-------|-------|---------|--------|--------|---------|--------|---------|--------|------------|
| C(21) | | H(12) | [1455.01] | 3.00(2) | 2.90 | 0.10 | | -0.0953 | 0.5277 | 0.1589 | -0.2848 | 0.3546 | 0.1920 | C(22) | 113.5(4) |
| | | | | | | | | | | | | | | H(21A) | 131 |
| C(21) | | H(21) | [] | 2.96(2) | 2.90 | 0.06 | Intra | -0.0953 | 0.5277 | 0.1589 | 0.0745 | 0.6723 | 0.3022 | O(22) | 143.1(4) |
| C(21) | | H(21B) | [] | 2.53<< | 2.90 | -0.37 | Intra | -0.0953 | 0.5277 | 0.1589 | 0.0348 | 0.3911 | 0.0779 | O(22) | 102 |
| | | | | | | | | | | | | | | C(22) | 148 |
| C(21) | | H(21C) | [] | 2.70<< | 2.90 | -0.20 | Intra | -0.0953 | 0.5277 | 0.1589 | -0.0750 | 0.3216 | 0.1207 | C(22) | 151 |
| C(21) | | H(22C) | [] | 2.45<< | 2.90 | -0.45 | Intra | -0.0953 | 0.5277 | 0.1589 | -0.2585 | 0.5898 | 0.0402 | O(21) | 157 |
| C(21) | | H(22G) | [] | 2.97 | 2.90 | 0.07 | Intra | -0.0953 | 0.5277 | 0.1589 | -0.1794 | 0.4438 | -0.0469 | O(21) | 109 |
| | | | | | | | | | | | | | | C(22) | 143 |
| C(22) | | S(2) | [] | 3.082(2)<< | 3.50 | -0.42 | Intra | -0.0964 | 0.6232 | 0.2311 | -0.0290 | 0.7914 | 0.0973 | H(22B) | 152 |
| C(22) | | C(221) | [] | 3.217(3) < | 3.40 | -0.18 | Intra | -0.0964 | 0.6232 | 0.2311 | -0.2920 | 0.5184 | 0.0482 | N(21) | 138.40(11) |
| | | | | | | | | | | | | | | H(22B) | 112 |
| C(22) | | H(22C) | [] | 2.96 | 2.90 | 0.06 | Intra | -0.0964 | 0.6232 | 0.2311 | -0.2585 | 0.5898 | 0.0402 | N(21) | 125 |
| | | | | | | | | | | | | | | H(22B) | 126 |
| C(22) | | O(15) | [2666.01] | 3.371(2) | 3.22 | 0.15 | | -0.0964 | 0.6232 | 0.2311 | 0.0851 | 0.6083 | 0.4457 | C(21) | 113.81(10) |
| | | | | | | | | | | | | | | H(22A) | 136 |
| C(23) | | C(21) | [] | 3.307(3) < | 3.40 | -0.09 | Intra | 0.0641 | 0.7584 | 0.1961 | -0.0953 | 0.5277 | 0.1589 | N(22) | 145.82(12) |
| C(23) | | C(25) | [] | 3.227(3) < | 3.40 | -0.17 | Intra | 0.0641 | 0.7584 | 0.1961 | 0.3441 | 0.7044 | 0.2977 | S(2) | 149.68(9) |
| C(23) | | C(29) | [] | 3.479(3) | 3.40 | 0.08 | Intra | 0.0641 | 0.7584 | 0.1961 | 0.2869 | 0.8592 | 0.3922 | S(2) | 143.04(8) |
| C(23) | | C(113) | [1465.01] | 3.549(3) | 3.40 | 0.15 | | 0.0641 | 0.7584 | 0.1961 | -0.0365 | 0.9957 | 0.3054 | N(21) | 108.81(11) |
| C(23) | | H(11G) | [1465.01] | 2.84 < | 2.90 | -0.06 | | 0.0641 | 0.7584 | 0.1961 | 0.0031 | 0.9315 | 0.3214 | N(21) | 100 |
| C(23) | | H(21A) | [] | 3.09 | 2.90 | 0.19 | Intra | 0.0641 | 0.7584 | 0.1961 | -0.0581 | 0.5465 | 0.0984 | N(22) | 143 |
| C(23) | | H(22A) | [] | 2.58<< | 2.90 | -0.32 | Intra | 0.0641 | 0.7584 | 0.1961 | -0.1629 | 0.6690 | 0.2057 | N(22) | 159 |
| C(24) | | N(21) | [] | 2.800(2)<< | 3.25 | -0.45 | Intra | 0.2696 | 0.7901 | 0.3078 | 0.0294 | 0.6812 | 0.2486 | C(29) | 120.83(12) |
| C(24) | | C(27) | [] | 2.783(2)<< | 3.40 | -0.62 | Intra | 0.2696 | 0.7901 | 0.3078 | 0.4593 | 0.7571 | 0.4577 | N(22) | 175.67(12) |
| C(24) | | H(21) | [] | 2.46(2)<< | 2.90 | -0.44 | Intra | 0.2696 | 0.7901 | 0.3078 | 0.0745 | 0.6723 | 0.3022 | C(29) | 112.2(5) |
| C(25) | | N(21) | [] | 3.250(3) | 3.25 | 0.00 | Intra | 0.3441 | 0.7044 | 0.2977 | 0.0294 | 0.6812 | 0.2486 | C(26) | 140.21(12) |
| C(25) | | C(23) | [] | 3.227(3) < | 3.40 | -0.17 | Intra | 0.3441 | 0.7044 | 0.2977 | 0.0641 | 0.7584 | 0.1961 | C(26) | 158.59(13) |
| C(25) | | C(28) | [] | 2.790(3)<< | 3.40 | -0.61 | Intra | 0.3441 | 0.7044 | 0.2977 | 0.3809 | 0.8419 | 0.4675 | H(25A) | 178 |
| C(25) | | C(123) | [] | 2.807(3)<< | 3.40 | -0.59 | Intra | 0.3441 | 0.7044 | 0.2977 | 0.5149 | 0.5444 | 0.2767 | C(24) | 174.62(13) |
| C(25) | | H(11N) | [1565.01] | 2.97 | 2.90 | 0.07 | | 0.3441 | 0.7044 | 0.2977 | 0.5900 | 0.7897 | 0.2337 | C(24) | 104 |
| C(25) | | H(120) | [] | 2.70<< | 2.90 | -0.20 | Intra | 0.3441 | 0.7044 | 0.2977 | 0.5241 | 0.5861 | 0.2219 | C(24) | 156 |
| C(25) | | H(12P) | [] | 2.77 < | 2.90 | -0.13 | Intra | 0.3441 | 0.7044 | 0.2977 | 0.4294 | 0.5063 | 0.2673 | C(24) | 165 |
| C(25) | | H(21) | [] | 2.81(2) < | 2.90 | -0.09 | Intra | 0.3441 | 0.7044 | 0.2977 | 0.0745 | 0.6723 | 0.3022 | C(26) | 126.4(4) |
| C(25) | | H(22) | [] | 2.982(18) | 2.90 | 0.08 | Intra | 0.3441 | 0.7044 | 0.2977 | 0.1958 | 0.8611 | 0.1953 | C(26) | 145.6(4) |
| C(26) | | C(29) | [] | 2.795(3)<< | 3.40 | -0.61 | Intra | 0.4406 | 0.6890 | 0.3721 | 0.2869 | 0.8592 | 0.3922 | O(23) | 174.68(13) |
| C(26) | | C(124) | [] | 3.059(3)<< | 3.40 | -0.34 | Intra | 0.4406 | 0.6890 | 0.3721 | 0.5603 | 0.6563 | 0.5779 | C(25) | 157.96(13) |
| C(26) | | H(11N) | [1565.01] | 2.93 | 2.90 | 0.03 | | 0.4406 | 0.6890 | 0.3721 | 0.5900 | 0.7897 | 0.2337 | C(27) | 105 |
| C(26) | | H(12L) | [] | 2.90 | 2.90 | 0.00 | Intra | 0.4406 | 0.6890 | 0.3721 | 0.5817 | 0.5986 | 0.5325 | C(25) | 161 |
| C(26) | | H(120) | [] | 2.61<< | 2.90 | -0.29 | Intra | 0.4406 | 0.6890 | 0.3721 | 0.5241 | 0.5861 | 0.2219 | C(27) | 153 |
| C(26) | | H(12P) | [] | 2.65<< | 2.90 | -0.25 | Intra | 0.4406 | 0.6890 | 0.3721 | 0.4294 | 0.5063 | 0.2673 | C(27) | 156 |
| C(26) | | H(11B) | [2666.01] | 3.05 | 2.90 | 0.15 | | 0.4406 | 0.6890 | 0.3721 | 0.2475 | 0.5327 | 0.4410 | | |
| C(27) | | C(24) | [] | 2.783(2)<< | 3.40 | -0.62 | Intra | 0.4593 | 0.7571 | 0.4577 | 0.2696 | 0.7901 | 0.3078 | O(24) | 174.01(12) |
| C(27) | | H(12L) | [] | 2.70<< | 2.90 | -0.20 | Intra | 0.4593 | 0.7571 | 0.4577 | 0.5817 | 0.5986 | 0.5325 | C(28) | 151 |
| C(27) | | H(12M) | [] | 2.56<< | 2.90 | -0.34 | Intra | 0.4593 | 0.7571 | 0.4577 | 0.4741 | 0.6413 | 0.5987 | C(26) | 106 |
| | | | | | | | | | | | | | | C(28) | 116 |
| C(27) | | H(12J) | [2676.02] | 3.07 | 2.90 | 0.17 | | 0.4593 | 0.7571 | 0.4577 | 0.6352 | 0.9587 | 0.4930 | C(26) | 127 |
| C(28) | | C(25) | [] | 2.790(3)<< | 3.40 | -0.61 | Intra | 0.3809 | 0.8419 | 0.4675 | 0.3441 | 0.7044 | 0.2977 | O(25) | 175.58(12) |

| | | | | | | | | | | | | | | | |
|--------|------|--------|------------|-------------|------|-------|-------|---------|---------------|--------|---------|--------|--------|--------|------------|
| C(28) | | C(124) | [] | 3.483(3) | 3.40 | 0.08 | Intra | 0.3809 | 0.8419 | 0.4675 | 0.5603 | 0.6563 | 0.5779 | C(29) | 145.44(12) |
| C(28) | | H(12I) | [] | 2.65<< | 2.90 | -0.25 | Intra | 0.3809 | 0.8419 | 0.4675 | 0.2479 | 0.9865 | 0.5548 | C(27) | 158 |
| C(28) | | H(12J) | [] | 2.61<< | 2.90 | -0.29 | Intra | 0.3809 | 0.8419 | 0.4675 | 0.3648 | 1.0413 | 0.5070 | C(27) | 149 |
| C(28) | | C(125) | [2676.02] | 3.499(3) | 3.40 | 0.10 | | 0.3809 | 0.8419 | 0.4675 | 0.6576 | 0.9991 | 0.4398 | C(29) | 106.56(11) |
| C(28) | | H(12J) | [2676.02] | 2.94 | 2.90 | 0.04 | | 0.3809 | 0.8419 | 0.4675 | 0.6352 | 0.9587 | 0.4930 | C(29) | 121 |
| C(29) | | C(23) | [] | 3.479(3) | 3.40 | 0.08 | Intra | 0.2869 | 0.8592 | 0.3922 | 0.0641 | 0.7584 | 0.1961 | C(28) | 148.81(12) |
| C(29) | | C(26) | [] | 2.795(3)<< | 3.40 | -0.61 | Intra | 0.2869 | 0.8592 | 0.3922 | 0.4406 | 0.6890 | 0.3721 | H(29A) | 179 |
| C(29) | | C(125) | [] | 2.813(3)<< | 3.40 | -0.59 | Intra | 0.2869 | 0.8592 | 0.3922 | 0.3424 | 1.0009 | 0.5602 | C(24) | 175.49(13) |
| C(29) | | H(12I) | [] | 2.74 < | 2.90 | -0.16 | Intra | 0.2869 | 0.8592 | 0.3922 | 0.2479 | 0.9865 | 0.5548 | C(24) | 164 |
| C(29) | | H(12J) | [] | 2.75 < | 2.90 | -0.15 | Intra | 0.2869 | 0.8592 | 0.3922 | 0.3648 | 1.0413 | 0.5070 | C(24) | 157 |
| C(29) | | H(22) | [] | 2.789(18) < | 2.90 | -0.11 | Intra | 0.2869 | 0.8592 | 0.3922 | 0.1958 | 0.8611 | 0.1953 | C(28) | 152.8(4) |
| C(29) | | C(17) | [2666.01] | 3.478(3) | 3.40 | 0.08 | | 0.2869 | 0.8592 | 0.3922 | 0.0542 | 0.7671 | 0.5331 | C(24) | 103.28(11) |
| C(123) | | C(25) | [] | 2.807(3)<< | 3.40 | -0.59 | Intra | 0.5149 | 0.5444 | 0.2767 | 0.3441 | 0.7044 | 0.2977 | H(12N) | 170 |
| C(123) | | H(25A) | [] | 2.51<< | 2.90 | -0.39 | Intra | 0.5149 | 0.5444 | 0.2767 | 0.3294 | 0.6567 | 0.2406 | H(12N) | 170 |
| C(123) | | C(124) | [2666.02] | 3.532(3) | 3.40 | 0.13 | | 0.5149 | 0.5444 | 0.2767 | 0.4397 | 0.3437 | 0.4221 | H(12O) | 164 |
| C(123) | | H(12M) | [2666.02] | 3.09 | 2.90 | 0.19 | | 0.5149 | 0.5444 | 0.2767 | 0.5259 | 0.3587 | 0.4013 | H(12O) | 160 |
| C(123) | | H(22E) | [2565.02] | 3.02 | 2.90 | 0.12 | | 0.5149 | 0.5444 | 0.2767 | 0.3149 | 0.5252 | 0.0995 | O(23) | 131 |
| | | | | | | | | | | | | | | H(12N) | 119 |
| C(124) | | O(23) | [] | 2.912(2)<< | 3.22 | -0.31 | Intra | 0.5603 | 0.6563 | 0.5779 | 0.5260 | 0.6113 | 0.3661 | H(12K) | 144 |
| | | | | | | | | | | | | | | H(12M) | 105 |
| C(124) | | C(26) | [] | 3.059(3)<< | 3.40 | -0.34 | Intra | 0.5603 | 0.6563 | 0.5779 | 0.4406 | 0.6890 | 0.3721 | H(12K) | 157 |
| C(124) | | C(28) | [] | 3.483(3) | 3.40 | 0.08 | Intra | 0.5603 | 0.6563 | 0.5779 | 0.3809 | 0.8419 | 0.4675 | H(12K) | 129 |
| | | | | | | | | | | | | | | H(12L) | 114 |
| C(124) | | N(11) | [2666.01] | 3.299(3) | 3.25 | 0.05 | | 0.5603 | 0.6563 | 0.5779 | 0.4657 | 0.8216 | 0.7492 | H(12L) | 171 |
| C(124) | | C(123) | [2666.02] | 3.532(3) | 3.40 | 0.13 | | 0.5603 | 0.6563 | 0.5779 | 0.4851 | 0.4556 | 0.7233 | O(24) | 163.83(12) |
| C(125) | | C(29) | [] | 2.813(3)<< | 3.40 | -0.59 | Intra | 0.3424 | 1.0009 | 0.5602 | 0.2869 | 0.8592 | 0.3922 | H(12H) | 170 |
| C(125) | | C(114) | [1465.01] | 3.532(3) | 3.40 | 0.13 | | 0.3424 | 1.0009 | 0.5602 | 0.1597 | 1.2223 | 0.5409 | O(25) | 171.03(11) |
| C(125) | | H(11D) | [1465.01] | 3.04 | 2.90 | 0.14 | | 0.3424 | 1.0009 | 0.5602 | 0.2082 | 1.2011 | 0.5997 | O(25) | 173 |
| C(125) | | H(29A) | [] | 2.51<< | 2.90 | -0.39 | Intra | 0.3424 | 1.0009 | 0.5602 | 0.2351 | 0.9175 | 0.3983 | H(12H) | 170 |
| C(125) | | O(25) | [2676.02] | 3.413(2) | 3.22 | 0.19 | | 0.3424 | 1.0009 | 0.5602 | 0.5944 | 1.0957 | 0.4462 | H(12I) | 145 |
| C(125) | | C(16) | [2666.01] | 3.555(3) | 3.40 | 0.15 | | 0.3424 | 1.0009 | 0.5602 | 0.0782 | 0.8384 | 0.6163 | H(12H) | 103 |
| | | | | | | | | | | | | | | H(12J) | 138 |
| C(125) | | C(28) | [2676.02] | 3.499(3) | 3.40 | 0.10 | | 0.3424 | 1.0009 | 0.5602 | 0.6191 | 1.1581 | 0.5325 | H(12I) | 152 |
| C(125) | | H(11) | [2666.01] | 3.099(19) | 2.90 | 0.20 | | 0.3424 | 1.0009 | 0.5602 | 0.4164 | 0.8392 | 0.7049 | H(12J) | 149 |
| C(211) | | O(22) | [] | 2.898(2)<< | 3.22 | -0.32 | Intra | 0.0053 | 0.3673 | 0.1385 | -0.2261 | 0.4845 | 0.1356 | C(212) | 152.40(14) |
| C(211) | | H(21A) | [] | 2.54<< | 2.90 | -0.36 | Intra | 0.0053 | 0.3673 | 0.1385 | -0.0581 | 0.5465 | 0.0984 | C(212) | 144 |
| | | | | | | | | | | | | | | H(21C) | 105 |
| C(212) | | H(12A) | [] | 3.06 | 2.90 | 0.16 | | 0.1096 | 0.3087 | 0.1896 | 0.3412 | 0.1724 | 0.2132 | C(211) | 158 |
| C(221) | | C(22) | [] | 3.217(3) < | 3.40 | -0.18 | Intra | -0.2920 | 0.5184 | 0.0482 | -0.0964 | 0.6232 | 0.2311 | C(222) | 133.02(13) |
| | | | | | | | | | | | | | | H(22D) | 117 |
| C(221) | | H(12) | [1455.01] | 3.037(19) | 2.90 | 0.14 | | -0.2920 | 0.5184 | 0.0482 | -0.2848 | 0.3546 | 0.1920 | H(22C) | 142 |
| C(221) | | H(21A) | [] | 2.45<< | 2.90 | -0.45 | Intra | -0.2920 | 0.5184 | 0.0482 | -0.0581 | 0.5465 | 0.0984 | H(22D) | 157 |
| C(221) | | H(22A) | [] | 2.94 | 2.90 | 0.04 | Intra | -0.2920 | 0.5184 | 0.0482 | -0.1629 | 0.6690 | 0.2057 | C(222) | 145 |
| | | | | | | | | | | | | | | H(22D) | 105 |
| C(222) | | C(21) | [] | 3.212(3) < | 3.40 | -0.19 | Intra | -0.2727 | 0.4476-0.0412 | | -0.0953 | 0.5277 | 0.1589 | H(22E) | 140 |
| | | | | | | | | | | | | | | H(22F) | 109 |
| C(222) | | H(21A) | [] | 2.94 | 2.90 | 0.04 | Intra | -0.2727 | 0.4476-0.0412 | | -0.0581 | 0.5465 | 0.0984 | H(22E) | 128 |
| | | | | | | | | | | | | | | H(22F) | 122 |

| | | | | | | | | | | | | |
|--------|------|--------|------------|-----------|------|-------|---------|-----------------------|---------|---------------|--------|-----------|
| C(222) | | H(25A) | [2565.02] | 2.94 | 2.90 | 0.04 | -0.2727 | 0.4476-0.0412 | -0.3294 | 0.3433-0.2406 | C(221) | 158 |
| H(12H) | | O(11) | [2666.01] | 2.78 | 2.72 | 0.06 | 0.3716 | 1.0407 0.6232 | 0.5228 | 1.0439 0.8019 | C(125) | 146 |
| H(12I) | | C(28) | [] | 2.65<< | 2.90 | -0.25 | Intra | 0.2479 0.9865 0.5548 | 0.3809 | 0.8419 0.4675 | | |
| H(12I) | | C(29) | [] | 2.74 < | 2.90 | -0.16 | Intra | 0.2479 0.9865 0.5548 | 0.2869 | 0.8592 0.3922 | | |
| H(12I) | | H(29A) | [] | 2.25 < | 2.40 | -0.15 | Intra | 0.2479 0.9865 0.5548 | 0.2351 | 0.9175 0.3983 | | |
| H(12I) | | O(13) | [2666.01] | 2.68 < | 2.72 | -0.04 | | 0.2479 0.9865 0.5548 | 0.0170 | 0.9287 0.6106 | C(125) | 158 |
| H(12I) | | C(16) | [2666.01] | 2.78 < | 2.90 | -0.12 | | 0.2479 0.9865 0.5548 | 0.0782 | 0.8384 0.6163 | C(125) | 136 |
| H(12I) | | C(113) | [2666.01] | 3.06 | 2.90 | 0.16 | | 0.2479 0.9865 0.5548 | 0.0365 | 1.0043 0.6946 | C(125) | 136 |
| H(12J) | | C(28) | [] | 2.61<< | 2.90 | -0.29 | Intra | 0.3648 1.0413 0.5070 | 0.3809 | 0.8419 0.4675 | | |
| H(12J) | | C(29) | [] | 2.75 < | 2.90 | -0.15 | Intra | 0.3648 1.0413 0.5070 | 0.2869 | 0.8592 0.3922 | | |
| H(12J) | | H(29A) | [] | 2.35 < | 2.40 | -0.05 | Intra | 0.3648 1.0413 0.5070 | 0.2351 | 0.9175 0.3983 | | |
| H(12J) | | O(24) | [2676.02] | 2.88 | 2.72 | 0.16 | | 0.3648 1.0413 0.5070 | 0.4401 | 1.2498 0.4699 | C(125) | 141 |
| H(12J) | | O(25) | [2676.02] | 2.68 < | 2.72 | -0.04 | | 0.3648 1.0413 0.5070 | 0.5944 | 1.0957 0.4462 | C(125) | 132 |
| H(12J) | | C(27) | [2676.02] | 3.07 | 2.90 | 0.17 | | 0.3648 1.0413 0.5070 | 0.5407 | 1.2429 0.5423 | C(125) | 123 |
| H(12J) | | C(28) | [2676.02] | 2.94 | 2.90 | 0.04 | | 0.3648 1.0413 0.5070 | 0.6191 | 1.1581 0.5325 | C(125) | 117 |
| H(12L) | | O(23) | [] | 2.34<< | 2.72 | -0.38 | Intra | 0.5817 0.5986 0.5325 | 0.5260 | 0.6113 0.3661 | C(124) | 117 |
| H(12L) | | C(26) | [] | 2.90 | 2.90 | 0.00 | Intra | 0.5817 0.5986 0.5325 | 0.4406 | 0.6890 0.3721 | | |
| H(12L) | | C(27) | [] | 2.70<< | 2.90 | -0.20 | Intra | 0.5817 0.5986 0.5325 | 0.4593 | 0.7571 0.4577 | | |
| H(12L) | | H(11B) | [] | 2.54 | 2.40 | 0.14 | | 0.5817 0.5986 0.5325 | 0.7525 | 0.4673 0.5590 | C(124) | 129 |
| H(12M) | | C(27) | [] | 2.56<< | 2.90 | -0.34 | Intra | 0.4741 0.6413 0.5987 | 0.4593 | 0.7571 0.4577 | | |
| H(12M) | | C(13) | [2666.01] | 3.07 | 2.90 | 0.17 | | 0.4741 0.6413 0.5987 | 0.4288 | 0.7446 0.8008 | C(124) | 116 |
| H(12M) | | C(19) | [2666.01] | 2.89 < | 2.90 | -0.01 | | 0.4741 0.6413 0.5987 | 0.1975 | 0.6494 0.6104 | C(124) | 160 |
| H(12M) | | C(123) | [2666.02] | 3.09 | 2.90 | 0.19 | | 0.4741 0.6413 0.5987 | 0.4851 | 0.4556 0.7233 | C(124) | 109 |
| H(12M) | | H(19A) | [2666.01] | 2.54 | 2.40 | 0.14 | | 0.4741 0.6413 0.5987 | 0.2376 | 0.5850 0.6088 | C(124) | 166 |
| H(12N) | | N(12) | [] | 2.86 | 2.75 | 0.11 | | 0.5834 0.4950 0.2798 | 0.6919 | 0.3022 0.2261 | C(123) | 154 |
| H(12O) | | C(25) | [] | 2.70<< | 2.90 | -0.20 | Intra | 0.5241 0.5861 0.2219 | 0.3441 | 0.7044 0.2977 | | |
| H(12O) | | C(26) | [] | 2.61<< | 2.90 | -0.29 | Intra | 0.5241 0.5861 0.2219 | 0.4406 | 0.6890 0.3721 | | |
| H(12O) | | H(25A) | [] | 2.28 < | 2.40 | -0.12 | Intra | 0.5241 0.5861 0.2219 | 0.3294 | 0.6567 0.2406 | | |
| H(12P) | | C(25) | [] | 2.77 < | 2.90 | -0.13 | Intra | 0.4294 0.5063 0.2673 | 0.3441 | 0.7044 0.2977 | | |
| H(12P) | | C(26) | [] | 2.65<< | 2.90 | -0.25 | Intra | 0.4294 0.5063 0.2673 | 0.4406 | 0.6890 0.3721 | | |
| H(12P) | | H(25A) | [] | 2.30 < | 2.40 | -0.10 | Intra | 0.4294 0.5063 0.2673 | 0.3294 | 0.6567 0.2406 | | |
| H(12P) | | H(22E) | [2565.02] | 2.53 | 2.40 | 0.13 | | 0.4294 0.5063 0.2673 | 0.3149 | 0.5252 0.0995 | C(123) | 111 |
| H(21) | | N(22) | [] | 2.42(2)<< | 2.75 | -0.33 | Intra | 0.0745 0.6723 0.3022 | 0.1793 | 0.8112 0.2271 | | |
| H(21) | | C(21) | [] | 2.96(2) | 2.90 | 0.06 | Intra | 0.0745 0.6723 0.3022 | -0.0953 | 0.5277 0.1589 | | |
| H(21) | | C(24) | [] | 2.46(2)<< | 2.90 | -0.44 | Intra | 0.0745 0.6723 0.3022 | 0.2696 | 0.7901 0.3078 | N(21) | 104.8(15) |
| H(21) | | C(25) | [] | 2.81(2) < | 2.90 | -0.09 | Intra | 0.0745 0.6723 0.3022 | 0.3441 | 0.7044 0.2977 | N(21) | 114.1(15) |
| H(21) | | H(22B) | [] | 2.17<< | 2.40 | -0.23 | Intra | 0.0745 0.6723 0.3022 | -0.1215 | 0.6016 0.2938 | | |
| H(21) | | O(14) | [2666.01] | 2.75(2) | 2.72 | 0.03 | | 0.0745 0.6723 0.3022 | -0.0218 | 0.7904 0.4513 | N(21) | 108.2(15) |
| H(21) | | O(15) | [2666.01] | 2.21(2)<< | 2.72 | -0.51 | | 0.0745 0.6723 0.3022 | 0.0851 | 0.6083 0.4457 | N(21) | 148.4(18) |
| H(21) | | C(115) | [2666.01] | 2.97(2) | 2.90 | 0.07 | | 0.0745 0.6723 0.3022 | 0.1536 | 0.5148 0.4355 | N(21) | 143.9(17) |
| H(21A) | | S(2) | [] | 3.17 | 3.00 | 0.17 | Intra | -0.0581 0.5465 0.0984 | -0.0290 | 0.7914 0.0973 | C(21) | 110 |
| H(21A) | | N(21) | [] | 2.64 < | 2.75 | -0.11 | Intra | -0.0581 0.5465 0.0984 | 0.0294 | 0.6812 0.2486 | | |
| H(21A) | | C(23) | [] | 3.09 | 2.90 | 0.19 | Intra | -0.0581 0.5465 0.0984 | 0.0641 | 0.7584 0.1961 | | |
| H(21A) | | C(211) | [] | 2.54<< | 2.90 | -0.36 | Intra | -0.0581 0.5465 0.0984 | 0.0053 | 0.3673 0.1385 | | |
| H(21A) | | C(221) | [] | 2.45<< | 2.90 | -0.45 | Intra | -0.0581 0.5465 0.0984 | -0.2920 | 0.5184 0.0482 | | |
| H(21A) | | C(222) | [] | 2.94 | 2.90 | 0.04 | Intra | -0.0581 0.5465 0.0984 | -0.2727 | 0.4476-0.0412 | | |
| H(21A) | | H(21B) | [] | 2.28 < | 2.40 | -0.12 | Intra | -0.0581 0.5465 0.0984 | 0.0348 | 0.3911 0.0779 | | |
| H(21A) | | H(22A) | [] | 2.44 | 2.40 | 0.04 | Intra | -0.0581 0.5465 0.0984 | -0.1629 | 0.6690 0.2057 | | |

| | | | | | | | | | | | | | | | | | |
|--------|------|--------|---|---------|---|-------------|------|-------|-------|---------|--------|---------|---------|--------|---------|--------|-----------|
| H(21A) | | H(22C) | [| |] | 2.26 < | 2.40 | -0.14 | Intra | -0.0581 | 0.5465 | 0.0984 | -0.2585 | 0.5898 | 0.0402 | | |
| H(21A) | | H(22G) | [| |] | 2.49 | 2.40 | 0.09 | Intra | -0.0581 | 0.5465 | 0.0984 | -0.1794 | 0.4438 | -0.0469 | C(21) | 109 |
| H(21B) | | C(21) | [| |] | 2.53<< | 2.90 | -0.37 | Intra | 0.0348 | 0.3911 | 0.0779 | -0.0953 | 0.5277 | 0.1589 | | |
| H(21B) | | H(21A) | [| |] | 2.28 < | 2.40 | -0.12 | Intra | 0.0348 | 0.3911 | 0.0779 | -0.0581 | 0.5465 | 0.0984 | | |
| H(21B) | | H(21D) | [| |] | 2.37 < | 2.40 | -0.03 | Intra | 0.0348 | 0.3911 | 0.0779 | 0.1255 | 0.2466 | 0.1474 | | |
| H(21B) | | H(21F) | [| |] | 2.35 < | 2.40 | -0.05 | Intra | 0.0348 | 0.3911 | 0.0779 | 0.1900 | 0.3533 | 0.2038 | | |
| H(21C) | | O(22) | [| |] | 2.69 < | 2.72 | -0.03 | Intra | -0.0750 | 0.3216 | 0.1207 | -0.2261 | 0.4845 | 0.1356 | | |
| H(21C) | | C(21) | [| |] | 2.70<< | 2.90 | -0.20 | Intra | -0.0750 | 0.3216 | 0.1207 | -0.0953 | 0.5277 | 0.1589 | | |
| H(21C) | | H(12) | [| 1455.01 |] | 2.51 | 2.40 | 0.11 | | -0.0750 | 0.3216 | 0.1207 | -0.2848 | 0.3546 | 0.1920 | C(211) | 123 |
| H(21C) | | H(21D) | [| |] | 2.35 < | 2.40 | -0.05 | Intra | -0.0750 | 0.3216 | 0.1207 | 0.1255 | 0.2466 | 0.1474 | | |
| H(21C) | | H(21E) | [| |] | 2.38 < | 2.40 | -0.02 | Intra | -0.0750 | 0.3216 | 0.1207 | 0.0811 | 0.2880 | 0.2509 | | |
| H(21D) | | H(12A) | [| |] | 2.59 | 2.40 | 0.19 | | 0.1255 | 0.2466 | 0.1474 | 0.3412 | 0.1724 | 0.2132 | C(212) | 109 |
| H(21D) | | H(21B) | [| |] | 2.37 < | 2.40 | -0.03 | Intra | 0.1255 | 0.2466 | 0.1474 | 0.0348 | 0.3911 | 0.0779 | | |
| H(21D) | | H(21C) | [| |] | 2.35 < | 2.40 | -0.05 | Intra | 0.1255 | 0.2466 | 0.1474 | -0.0750 | 0.3216 | 0.1207 | | |
| H(21E) | | O(21) | [| |] | 2.57 < | 2.72 | -0.15 | Intra | 0.0811 | 0.2880 | 0.2509 | -0.0207 | 0.4554 | 0.2039 | | |
| H(21E) | | C(15) | [| 1455.01 |] | 2.97 | 2.90 | 0.07 | | 0.0811 | 0.2880 | 0.2509 | -0.1616 | 0.1843 | 0.3035 | C(212) | 134 |
| H(21E) | | H(21C) | [| |] | 2.38 < | 2.40 | -0.02 | Intra | 0.0811 | 0.2880 | 0.2509 | -0.0750 | 0.3216 | 0.1207 | | |
| H(21F) | | O(21) | [| |] | 2.61 < | 2.72 | -0.11 | Intra | 0.1900 | 0.3533 | 0.2038 | -0.0207 | 0.4554 | 0.2039 | | |
| H(21F) | | H(21B) | [| |] | 2.35 < | 2.40 | -0.05 | Intra | 0.1900 | 0.3533 | 0.2038 | 0.0348 | 0.3911 | 0.0779 | | |
| H(22) | | S(2) | [| |] | 2.640(19)<< | 3.00 | -0.36 | Intra | 0.1958 | 0.8611 | 0.1953 | -0.0290 | 0.7914 | 0.0973 | | |
| H(22) | | O(12) | [| 1565.01 |] | 2.060(18)<< | 2.72 | -0.66 | | 0.1958 | 0.8611 | 0.1953 | 0.2697 | 0.9900 | 0.1377 | N(22) | 168.2(17) |
| H(22) | | C(11) | [| 1565.01 |] | 3.092(18) | 2.90 | 0.19 | | 0.1958 | 0.8611 | 0.1953 | 0.4013 | 1.0311 | 0.1586 | N(22) | 146.1(16) |
| H(22) | | C(25) | [| |] | 2.982(18) | 2.90 | 0.08 | Intra | 0.1958 | 0.8611 | 0.1953 | 0.3441 | 0.7044 | 0.2977 | | |
| H(22) | | C(29) | [| |] | 2.789(18) < | 2.90 | -0.11 | Intra | 0.1958 | 0.8611 | 0.1953 | 0.2869 | 0.8592 | 0.3922 | | |
| H(22) | | C(121) | [| 1565.01 |] | 3.043(18) | 2.90 | 0.14 | | 0.1958 | 0.8611 | 0.1953 | 0.2010 | 1.0252 | 0.0516 | N(22) | 167.4(17) |
| H(22A) | | S(2) | [| |] | 2.70<< | 3.00 | -0.30 | Intra | -0.1629 | 0.6690 | 0.2057 | -0.0290 | 0.7914 | 0.0973 | C(22) | 103 |
| H(22A) | | O(22) | [| |] | 2.52<< | 2.72 | -0.20 | Intra | -0.1629 | 0.6690 | 0.2057 | -0.2261 | 0.4845 | 0.1356 | | |
| H(22A) | | C(23) | [| |] | 2.58<< | 2.90 | -0.32 | Intra | -0.1629 | 0.6690 | 0.2057 | 0.0641 | 0.7584 | 0.1961 | | |
| H(22A) | | C(221) | [| |] | 2.94 | 2.90 | 0.04 | Intra | -0.1629 | 0.6690 | 0.2057 | -0.2920 | 0.5184 | 0.0482 | | |
| H(22A) | | H(21A) | [| |] | 2.44 | 2.40 | 0.04 | Intra | -0.1629 | 0.6690 | 0.2057 | -0.0581 | 0.5465 | 0.0984 | | |
| H(22A) | | H(22C) | [| |] | 2.50 | 2.40 | 0.10 | Intra | -0.1629 | 0.6690 | 0.2057 | -0.2585 | 0.5898 | 0.0402 | C(22) | 108 |
| H(22B) | | O(21) | [| |] | 2.50<< | 2.72 | -0.22 | Intra | -0.1215 | 0.6016 | 0.2938 | -0.0207 | 0.4554 | 0.2039 | | |
| H(22B) | | O(22) | [| |] | 2.64 < | 2.72 | -0.08 | Intra | -0.1215 | 0.6016 | 0.2938 | -0.2261 | 0.4845 | 0.1356 | | |
| H(22B) | | H(21) | [| |] | 2.17<< | 2.40 | -0.23 | Intra | -0.1215 | 0.6016 | 0.2938 | 0.0745 | 0.6723 | 0.3022 | | |
| H(22B) | | O(15) | [| 2666.01 |] | 2.83 | 2.72 | 0.11 | | -0.1215 | 0.6016 | 0.2938 | 0.0851 | 0.6083 | 0.4457 | C(22) | 115 |
| H(22C) | | C(21) | [| |] | 2.45<< | 2.90 | -0.45 | Intra | -0.2585 | 0.5898 | 0.0402 | -0.0953 | 0.5277 | 0.1589 | | |
| H(22C) | | C(22) | [| |] | 2.96 | 2.90 | 0.06 | Intra | -0.2585 | 0.5898 | 0.0402 | -0.0964 | 0.6232 | 0.2311 | | |
| H(22C) | | H(21A) | [| |] | 2.26 < | 2.40 | -0.14 | Intra | -0.2585 | 0.5898 | 0.0402 | -0.0581 | 0.5465 | 0.0984 | | |
| H(22C) | | H(22A) | [| |] | 2.50 | 2.40 | 0.10 | Intra | -0.2585 | 0.5898 | 0.0402 | -0.1629 | 0.6690 | 0.2057 | C(221) | 107 |
| H(22C) | | H(22E) | [| |] | 2.33 < | 2.40 | -0.07 | Intra | -0.2585 | 0.5898 | 0.0402 | -0.3149 | 0.4748 | -0.0995 | | |
| H(22C) | | H(22G) | [| |] | 2.37 < | 2.40 | -0.03 | Intra | -0.2585 | 0.5898 | 0.0402 | -0.1794 | 0.4438 | -0.0469 | | |
| H(22D) | | H(22E) | [| |] | 2.36 < | 2.40 | -0.04 | Intra | -0.3862 | 0.5203 | 0.0550 | -0.3149 | 0.4748 | -0.0995 | | |
| H(22D) | | H(22F) | [| |] | 2.34 < | 2.40 | -0.06 | Intra | -0.3862 | 0.5203 | 0.0550 | -0.3113 | 0.3780 | -0.0356 | | |
| H(22E) | | H(22C) | [| |] | 2.33 < | 2.40 | -0.07 | Intra | -0.3149 | 0.4748 | -0.0995 | -0.2585 | 0.5898 | 0.0402 | | |
| H(22E) | | H(22D) | [| |] | 2.36 < | 2.40 | -0.04 | Intra | -0.3149 | 0.4748 | -0.0995 | -0.3862 | 0.5203 | 0.0550 | | |
| H(22E) | | C(123) | [| 2565.02 |] | 3.02 | 2.90 | 0.12 | | -0.3149 | 0.4748 | -0.0995 | -0.5149 | 0.4556 | -0.2767 | C(222) | 151 |
| H(22E) | | H(12P) | [| 2565.02 |] | 2.53 | 2.40 | 0.13 | | -0.3149 | 0.4748 | -0.0995 | -0.4294 | 0.4937 | -0.2673 | C(222) | 164 |
| H(22E) | | H(25A) | [| 2565.02 |] | 2.45 | 2.40 | 0.05 | | -0.3149 | 0.4748 | -0.0995 | -0.3294 | 0.3433 | -0.2406 | C(222) | 110 |

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H(22F) .... O(22) [ ] 2.67 < 2.72 -0.05 Intra -0.3113 0.3780-0.0356 -0.2261 0.4845 0.1356
H(22F) .... H(22D) [ ] 2.34 < 2.40 -0.06 Intra -0.3113 0.3780-0.0356 -0.3862 0.5203 0.0550
H(22G) .... O(22) [ ] 2.63 < 2.72 -0.09 Intra -0.1794 0.4438-0.0469 -0.2261 0.4845 0.1356
H(22G) .... C(21) [ ] 2.97 2.90 0.07 Intra -0.1794 0.4438-0.0469 -0.0953 0.5277 0.1589
H(22G) .... H(21A) [ ] 2.49 2.40 0.09 Intra -0.1794 0.4438-0.0469 -0.0581 0.5465 0.0984 C(222) 108
H(22G) .... H(22C) [ ] 2.37 < 2.40 -0.03 Intra -0.1794 0.4438-0.0469 -0.2585 0.5898 0.0402
H(25A) .... O(23) [ ] 2.66 < 2.72 -0.06 Intra 0.3294 0.6567 0.2406 0.5260 0.6113 0.3661
H(25A) .... N(22) [ ] 2.61 < 2.75 -0.14 Intra 0.3294 0.6567 0.2406 0.1793 0.8112 0.2271
H(25A) .... C(123) [ ] 2.51<< 2.90 -0.39 Intra 0.3294 0.6567 0.2406 0.5149 0.5444 0.2767
H(25A) .... H(120) [ ] 2.28 < 2.40 -0.12 Intra 0.3294 0.6567 0.2406 0.5241 0.5861 0.2219 C(25) 106
H(25A) .... H(12P) [ ] 2.30 < 2.40 -0.10 Intra 0.3294 0.6567 0.2406 0.4294 0.5063 0.2673 C(25) 110
H(25A) .... C(222) [ 2565.02] 2.94 2.90 0.04 0.3294 0.6567 0.2406 0.2727 0.5524 0.0412 C(25) 167
H(25A) .... H(22E) [ 2565.02] 2.45 2.40 0.05 0.3294 0.6567 0.2406 0.3149 0.5252 0.0995 C(25) 173
H(29A) .... O(25) [ ] 2.66 < 2.72 -0.06 Intra 0.2351 0.9175 0.3983 0.4056 0.9043 0.5538
H(29A) .... N(22) [ ] 2.62 < 2.75 -0.13 Intra 0.2351 0.9175 0.3983 0.1793 0.8112 0.2271
H(29A) .... C(125) [ ] 2.51<< 2.90 -0.39 Intra 0.2351 0.9175 0.3983 0.3424 1.0009 0.5602
H(29A) .... H(11G) [ 1465.01] 2.55 2.40 0.15 0.2351 0.9175 0.3983 0.0031 0.9315 0.3214 C(29) 127
H(29A) .... H(12I) [ ] 2.25 < 2.40 -0.15 Intra 0.2351 0.9175 0.3983 0.2479 0.9865 0.5548 C(29) 111
H(29A) .... H(12J) [ ] 2.35 < 2.40 -0.05 Intra 0.2351 0.9175 0.3983 0.3648 1.0413 0.5070 C(29) 105
=====

```

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 2 to Neighbouring ARU'S

```

=====
Nr      ARU      Nr.Cont.  d(min)  Del  XHn X      - At(I)      At(J) - Y  YHn Note  Partaking ARU's in Close Contact Resd.
-----
1 [ 2565.01] 1 3.6940 0.19 0 C(23) - S(2) ... C(121) -O(12) 0 2565.01
2 [ 2666.01] 24 2.2100 -0.51 1 N(21) - H(21) ... O(15) -C(18) 0 << 2666.01
3 [ 1455.01] 6 2.0100 -0.71 1 C(21) - O(22) ... H(12) -N(12) 1 << 1455.01
4 [ 2766.01] 2 2.8200 0.10 0 C(27) - O(24) ... H(11F) -C(114) 3 2766.01
5 [ 2676.02] 12 2.6800 -0.04 3 C(125) - H(12J) ... O(25) -C(28) 0 < 2676.02
6 [ 1565.01] 6 2.0600 -0.66 1 N(22) - H(22) ... O(12) -C(11) 1 << 1565.01
7 [ 1465.01] 6 2.5500 0.15 1 C(29) - H(29A) ... H(11G) -C(113) 3 1465.01
8 [ 2666.02] 4 3.0900 0.19 3 C(124) - H(12M) ... C(123) -O(23) 0 2666.02
9 [ 2565.02] 8 2.4500 0.05 1 C(25) - H(25A) ... H(22E) -C(222) 3 2565.02
10 [ 1555.01] 4 2.5400 0.14 3 C(124) - H(12L) ... H(11B) -C(115) 3 1555.01
=====

```

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Asymmetric Residue Unit (= ARU) Code List

=====

```

-----
ARU-CODE      CIF-CODE      Symmetry-Code      sym TX TY TZ Ires      x(cen)      y(cen)      z(cen)
-----

```



```

=====
[ 2666.02] = [ 2_666] =1-x,1-y,1-z           = [ 2 1 1 1 2 ]      0.839   0.372   0.727
[ 1545.02] = [ 1_545] =x,-1+y,z              = [ 1 0 -1 0 2 ]      0.161  -0.372   0.273
[ 2756.01] = [ 2_756] =2-x,-y,1-z           = [ 2 2 0 1 1 ]      1.335  -0.126   0.728
[ 2766.01] = [ 2_766] =2-x,1-y,1-z           = [ 2 2 1 1 1 ]      1.335   0.874   0.728
[ 1655.02] = [ 1_655] =1+x,y,z              = [ 1 1 0 0 2 ]      1.161   0.628   0.273
[ 1645.02] = [ 1_645] =1+x,-1+y,z           = [ 1 1 -1 0 2 ]      1.161  -0.372   0.273
[ 2766.02] = [ 2_766] =2-x,1-y,1-z           = [ 2 2 1 1 2 ]      1.839   0.372   0.727
[ 2565.02] = [ 2_565] =-x,1-y,-z            = [ 2 0 1 0 2 ]      -0.161  0.372  -0.273
[ 2655.01] = [ 2_655] =1-x,-y,-z            = [ 2 1 0 0 1 ]      0.335  -0.126  -0.272
[ 2565.01] = [ 2_565] =-x,1-y,-z            = [ 2 0 1 0 1 ]      -0.665  0.874  -0.272
[ 2666.01] = [ 2_666] =1-x,1-y,1-z           = [ 2 1 1 1 1 ]      0.335  0.874   0.728
[ 1455.01] = [ 1_455] =-1+x,y,z             = [ 1 -1 0 0 1 ]      -0.335  0.126   0.272
[ 2676.02] = [ 2_676] =1-x,2-y,1-z           = [ 2 1 2 1 2 ]      0.839   1.372   0.727
[ 1565.01] = [ 1_565] =x,1+y,z             = [ 1 0 1 0 1 ]      0.665   1.126   0.272
[ 1465.01] = [ 1_465] =-1+x,1+y,z           = [ 1 -1 1 0 1 ]      -0.335  1.126   0.272
=====

```

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

X(J) = X(sym) + TX , Y(J) = Y(sym) + TY , Z(J) = Z(sym) + TZ,
 SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

=====
 Analysis of Potential Hydrogen Bonds and Schemes with $d(D...A) < R(D)+R(A)+0.50$, $d(H...A) < R(H)+R(A)-0.12$ Ang., $D-H...A > 100.0$ Deg
 =====

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
 =====

| Nr | Typ | Res | Donor | H...A | Acceptor | [ARU] | D - H | H...A | D...A | D - H...A | A..H..A* A'..H..A" | Sum(XY,YZ) | Sum(XZ) |
|----|-------|-----|--------|----------|----------|------------|-----------|-----------|----------|-----------|--------------------|------------|---------|
| 1 | | 1 | N(11) | --H(11) | ..O(25) | [2666.02] | 0.81(2) | 2.318(19) | 3.014(2) | 144.2(18) | | | |
| 2 | | 1 | N(12) | --H(12) | ..O(22) | [1655.02] | 0.90(2) | 2.01(2) | 2.900(2) | 171.3(18) | | | |
| 3 | | 2 | N(21) | --H(21) | ..O(15) | [2666.01] | 0.86(2) | 2.21(2) | 2.976(2) | 148.4(18) | | | |
| 4 | | 2 | N(22) | --H(22) | ..O(12) | [1565.01] | 0.834(18) | 2.060(18) | 2.882(2) | 168.2(17) | | | |
| 5 | Intra | 1 | C(114) | --H(11F) | ..O(13) | [] | 0.98 | 2.58 | 3.103(3) | 114 | | | |
| 6 | Intra | 1 | C(12) | --H(12A) | ..S(1) | [] | 0.99 | 2.71 | 3.087(2) | 103 | | | |
| 7 | Intra | 2 | C(124) | --H(12L) | ..O(23) | [] | 0.98 | 2.34 | 2.912(2) | 117 | | | |
| 8 | Intra | 2 | C(22) | --H(22A) | ..S(2) | [] | 0.99 | 2.70 | 3.082(2) | 103 | | | |

Translation of ARU-Code to CIF and Equivalent Position Code
 =====

[2666.] = [2_666] =1-x,1-y,1-z
 [1655.] = [1_655] =1+x,y,z
 [1565.] = [1_565] =x,1+y,z

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]

 2-Centre (linear) D-H...X most prob. angle 160 deg - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
 3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg Springer-Verlag, Berlin, 1991, pp 20.
 4-Centre (trifurcated)

Analysis of Potential Donor/Acceptor Atoms -- (Major Disorder Form Only)
 =====

| At.Nr | D/A | #Cov.Bonds | # H | #D-H..A | #A..H | #A..H-C | Sum(A-H) | Sum(A-X) |
|-------|-------|------------|-----|---------|-------|---------|----------|----------|
| 1 | S(1) | 1 | - | 0 | 0 | 1 | 1 | 2 |
| 2 | S(2) | 1 | - | 0 | 0 | 1 | 1 | 2 |
| 3 | O(11) | 2 | - | 0 | 0 | 0 | 0 | 2 |
| 4 | O(12) | 2 | - | 0 | 1 | 0 | 1 | 3 |
| 5 | O(13) | 2 | - | 0 | 0 | 1 | 1 | 3 |
| 6 | O(14) | 2 | - | 0 | 0 | 0 | 0 | 2 |
| 7 | O(15) | 2 | - | 0 | 1 | 0 | 1 | 3 |
| 8 | O(21) | 2 | - | 0 | 0 | 0 | 0 | 2 |
| 9 | O(22) | 2 | - | 0 | 1 | 0 | 1 | 3 |
| 10 | O(23) | 2 | - | 0 | 0 | 1 | 1 | 3 |
| 11 | O(24) | 2 | - | 0 | 0 | 0 | 0 | 2 |
| 12 | O(25) | 2 | - | 0 | 1 | 0 | 1 | 3 |

```
=====
```

| | | | | | | | | |
|----|-------|---|-----|---|---|---|---|---|
| 13 | N(11) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 14 | N(12) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 15 | N(21) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 16 | N(22) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |

=====
 Analysis of Hydrogen Bonded Molecular Aggregates (See also Acta Cryst. B36, 1980, 2113 - 2115) -- (Major Disorder Component Only)
 =====

Coordinates of Donor and Acceptor Atoms
 =====

Coordinates of D/A-Bonded Atom(s)
 =====

| D/A I | [ARU] | X | Y | Z | -- | D/A J | [ARU] | X | Y | Z | Atom K | X | Y | Z | I..J--K Angle |
|-------|-------------|---------|--------|--------|----|-------|-------------|---------|--------|--------|--------|---------|--------|--------|---------------|
| N(11) | [1555.01], | 0.5343 | 0.1784 | 0.2508 | >> | O(25) | [2666.02], | 0.5944 | 0.0957 | 0.4462 | C(28) | 0.6191 | 0.1581 | 0.5325 | 123.34(8) |
| | | | | | | | | | | | C(125) | 0.6576 | 0.0009 | 0.4398 | 113.29(8) |
| O(25) | [1555.02], | 0.4056 | 0.9043 | 0.5538 | << | N(11) | [2666.01], | 0.4657 | 0.8216 | 0.7492 | C(12) | 0.5935 | 0.8762 | 0.7653 | 92.41(7) |
| | | | | | | | | | | | C(13) | 0.4288 | 0.7446 | 0.8008 | 141.19(9) |
| | | | | | | | | | | | H(11) | 0.4164 | 0.8392 | 0.7049 | 26.75(11) |
| N(12) | [1555.01], | 0.6919 | 0.3022 | 0.2261 | >> | O(22) | [1655.02], | 0.7739 | 0.4845 | 0.1356 | C(21) | 0.9046 | 0.5277 | 0.1589 | 119.08(8) |
| | | | | | | | | | | | C(221) | 0.7080 | 0.5184 | 0.0482 | 124.48(8) |
| O(22) | [1555.02], | -0.2261 | 0.4845 | 0.1356 | << | N(12) | [1455.01], | -0.3081 | 0.3022 | 0.2261 | C(13) | -0.4288 | 0.2554 | 0.1992 | 119.81(8) |
| | | | | | | | | | | | C(14) | -0.2214 | 0.2785 | 0.3078 | 114.70(8) |
| | | | | | | | | | | | H(12) | -0.2848 | 0.3546 | 0.1920 | 6.05(9) |
| N(21) | [1555.02], | 0.0294 | 0.6812 | 0.2486 | >> | O(15) | [2666.01], | 0.0851 | 0.6083 | 0.4457 | C(18) | 0.1144 | 0.6725 | 0.5309 | 124.63(8) |
| | | | | | | | | | | | C(115) | 0.1536 | 0.5148 | 0.4355 | 108.41(8) |
| O(15) | [1555.01], | 0.9149 | 0.3917 | 0.5543 | << | N(21) | [2666.02], | 0.9706 | 0.3188 | 0.7514 | C(22) | 1.0964 | 0.3768 | 0.7689 | 92.59(7) |
| | | | | | | | | | | | C(23) | 0.9359 | 0.2416 | 0.8039 | 140.80(9) |
| | | | | | | | | | | | H(21) | 0.9255 | 0.3277 | 0.6978 | 22.92(10) |
| N(22) | [1555.02], | 0.1793 | 0.8112 | 0.2271 | >> | O(12) | [1565.01], | 0.2697 | 0.9900 | 0.1377 | C(11) | 0.4013 | 1.0311 | 0.1586 | 120.74(8) |
| | | | | | | | | | | | C(121) | 0.2009 | 1.0252 | 0.0516 | 122.78(8) |
| O(12) | [1555.01], | 0.2697 | 0.0100 | 0.1377 | << | N(22) | [1545.02], | 0.1793 | 0.1888 | 0.2271 | C(23) | 0.0641 | 0.2416 | 0.1961 | 122.42(8) |
| | | | | | | | | | | | C(24) | 0.2696 | 0.2099 | 0.3078 | 111.23(8) |
| | | | | | | | | | | | H(22) | 0.1958 | 0.1389 | 0.1953 | 8.41(10) |

=====

***** Aggregate = 1 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

| | | | | | | |
|---|---|---------|----|----------|----------|----------|
| 4 | 3 | 1555.01 | -- | 2666.02 | 1655.02 | 1545.02T |
| 4 | 3 | 2666.02 | -- | 1555.01 | 2656.01 | 2766.01T |
| 4 | 3 | 1655.02 | -- | 2766.01T | 1665.01T | 1555.01 |
| 4 | 3 | 2656.01 | -- | 1545.02T | 2556.02T | 2666.02 |

:: Analysis of H-Bonded Aggregate Type3 Polymeric Structure(s)

:: Resd 0 - Infinite (Type3) 1D-Chain - Base Vector: [1 1 0]

=====
Search for ARU-Circuits (Max = 6 Membered)
=====

4-Membered ARU-Circuit - ResCount - 2, 2,
1555.01 2666.02 2656.01 1545.02 1555.01

4-Membered ARU-Circuit - ResCount - 2, 2,
1555.01 2666.02 2766.01 1655.02 1555.01

=====
Search for Infinite ARU-Chains (Max = 4)
=====

4-Membered Infinite ARU-Chain (Translation [-1 -1 0])
1555.01 2666.02 2656.01 1545.02 1445.01

4-Membered Infinite ARU-Chain (Translation [-1 -1 0])
1555.01 2666.02 2656.01 2556.02 1445.01

4-Membered Infinite ARU-Chain (Translation [1 1 0])
1555.01 2666.02 2766.01 1655.02 1665.01

4-Membered Infinite ARU-Chain (Translation [1 1 0])
1555.01 2666.02 2766.01 2776.02 1665.01

4-Membered Infinite ARU-Chain (Translation [1 1 0])
1555.01 1655.02 2766.01 2776.02 1665.01

2-Membered Infinite ARU-Chain (Translation [1 1 0])
1555.01 1655.02 1665.01

4-Membered Infinite ARU-Chain (Translation [-1 -1 0])
1555.01 1545.02 2656.01 2556.02 1445.01

2-Membered Infinite ARU-Chain (Translation [-1 -1 0])
1555.01 1545.02 1445.01

4-Membered Infinite ARU-Chain (Translation [1 1 0])
2666.02 1555.01 1655.02 2766.01 2776.02

4-Membered Infinite ARU-Chain (Translation [1 1 0])
2666.02 1555.01 1655.02 1665.01 2776.02

4-Membered Infinite ARU-Chain (Translation [-1 -1 0])
2666.02 1555.01 1545.02 2656.01 2556.02

4-Membered Infinite ARU-Chain (Translation [-1 -1 0])
2666.02 1555.01 1545.02 1445.01 2556.02

4-Membered Infinite ARU-Chain (Translation [-1 -1 0])
2666.02 2656.01 1545.02 1445.01 2556.02

2-Membered Infinite ARU-Chain (Translation [-1 -1 0])
2666.02 2656.01 2556.02

4-Membered Infinite ARU-Chain (Translation [1 1 0])
2666.02 2766.01 1655.02 1665.01 2776.02

=====

2-Membered Infinite ARU-Chain (Translation [1 1 0])

2666.02 2766.01 2776.02

=====
 Analysis of the (Cooperative) Hydrogen Bond Network (i.e. (In)Finite O-H...O-H...O-H.. Chains and/or Rings (Max = 18 Membered))
 =====

=====
 ***** Network = 1 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|--------|--------|--------|------------------|--------|--------|--|
| 1.555 | N(11) [1555.01] | 0.5343 | 0.1784 | 0.2508 | O(25) [2666.02] | 0.5944 | 0.0957 | 0.4462 |
| | H(11) | 0.5836 | 0.1608 | 0.2951 | | | | |

=====
 ***** Network = 2 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|--------|--------|--------|------------------|--------|--------|--|
| 2.555 | N(12) [1555.01] | 0.6919 | 0.3022 | 0.2261 | O(22) [1655.02] | 0.7739 | 0.4845 | 0.1356 |
| | H(12) | 0.7152 | 0.3546 | 0.1920 | | | | |

=====
 ***** Network = 3 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|--------|--------|--------|------------------|--------|--------|--|
| 3.555 | N(21) [1555.02] | 0.0294 | 0.6812 | 0.2486 | O(15) [2666.01] | 0.0851 | 0.6083 | 0.4457 |
| | H(21) | 0.0745 | 0.6723 | 0.3022 | | | | |

=====
 ***** Network = 4 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|--------|--------|--------|------------------|--------|--------|--|
| 4.555 | N(22) [1555.02] | 0.1793 | 0.8112 | 0.2271 | O(12) [1565.01] | 0.2697 | 0.9900 | 0.1377 |
| | H(22) | 0.1958 | 0.8611 | 0.1953 | | | | |

Hydrogen Bonds are Coded as N.IJK Where N = Sequence Number of Hydrogen Bond (NOTE: New Hbond Numbering system)
 I - 5 = Nr of Translation Units Along A-Axis
 J - 5 = Nr of Translation Units Along B-Axis
 K - 5 = Nr of Translation Units Along C-Axis

Ring Closure Links are Indicated with 'R' and Infinite Chain Links With 'T'

=====
Analysis of the Coordination Geometry

Distances are calculated from atom I of Unique Molecule Coordinate List to atom J in Asymmetric Residue Unit: ARU.

Phi = Azimuth angle(counter clockwise from XO in XO,YO-Plane), Mu = Angle between D and XO,YO-plane.

'To-Code' : '--' = Bonded atoms, '<<' = .LT. sum vdW-radii - 0.2, '<' = .LT. sum vdW-radii, '..' = .GT. sum vdW-radii.

>>>> NOTICE >>>> : The Symmetry Code Character Added to the Atom Label Applies to the Current Coordination Sphere Only.

>>>>>>>>>>>>>>>>>>>> : Symmetry operations refer to the coordinates listed in the fractional coordinate table given above

The List May be Limited to the Shortest Distances.

=====

3.6 Angstrom Coordination Sphere Around Atom I = S(1) [ARU = 1555.01] 0.47503 0.29658 0.10556 4.5647 3.6920 1.4435

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|-------------------|------------|-----------|--------|-------|---------|--------|---------|---------|----------|--------|--------|---------|
| 1 | 1.6938(18) | -- | C(13) | | | | Intra | -36.54 | 49.11 | 0.57117 | 0.25542 | 0.19920 | 5.4555 | 3.0318 | 2.7239 |
| 2 | 2.6481(18) | << | N(12) | | | | Intra | -2.53 | 38.49 | 0.69194 | 0.30222 | 0.22609 | 6.6353 | 3.6004 | 3.0917 |
| 3 | 2.6772(18) | << | N(11) | | | | Intra | -74.18 | 47.89 | 0.53432 | 0.17837 | 0.25080 | 5.0540 | 1.9648 | 3.4296 |
| 4 | 3.087(2) | << | C(12) | | | | Intra | -107.77 | 34.89 | 0.40654 | 0.12379 | 0.23468 | 3.7918 | 1.2808 | 3.2091 |
| 5 | 2.68(2) | << | H(12) | | | | Intra | 15.23 | 26.14 | 0.71520 | 0.35460 | 0.19200 | 6.8883 | 4.3244 | 2.6255 |
| 6 | 2.71 | << | H(12A) | | | | Intra | -129.62 | 32.89 | 0.34120 | 0.17240 | 0.21320 | 3.1132 | 1.9389 | 2.9154 |
| 7 | 3.16 | .. | H(11J) | | | | Intra | -94.24 | -1.95 | 0.43540 | 0.05220 | 0.09770 | 4.3312 | 0.5418 | 1.3360 |
| 8 | 3.24 | .. | H(11M)b[1-x,-y,-z | = | 2655.01] | | Intra | -154.43 | -77.43 | 0.37910 | 0.24870 | -0.12540 | 3.9292 | 3.3879 | -1.7148 |
| 9 | 3.28 | .. | H(11K)b[1-x,-y,-z | = | 2655.01] | | Intra | -78.36 | -45.75 | 0.48380 | 0.10530 | -0.06610 | 5.0260 | 1.4522 | -0.9039 |
| 10 | 3.29 | .. | H(22F)a[1+x,y,z | = | 1655.02] | | Intra | 27.90 | -35.94 | 0.68870 | 0.37800 | -0.03560 | 6.9180 | 4.9378 | -0.4868 |
| 11 | 3.33 | .. | H(22D)a[1+x,y,z | = | 1655.02] | | Intra | 65.42 | -11.98 | 0.61380 | 0.52030 | 0.05500 | 5.9197 | 6.6546 | 0.7521 |
| 12 | 3.35 | .. | H(22C)c[-x,1-y,-z | = | 2565.02] | | Intra | 141.69 | -36.52 | 0.25850 | 0.41020 | -0.04020 | 2.4527 | 5.3605 | -0.5497 |
| 13 | 3.41 | .. | H(12N) [| = | 02] | | Intra | 72.33 | 44.27 | 0.58340 | 0.49500 | 0.27980 | 5.3066 | 6.0206 | 3.8261 |
| 14 | 3.417(19) | .. | H(11) | | | | Intra | -64.79 | 49.33 | 0.58360 | 0.16080 | 0.29510 | 5.5134 | 1.6770 | 4.0353 |
| 15 | 3.44 | .. | H(12P) [| = | 02] | | Intra | 108.65 | 40.06 | 0.42940 | 0.50630 | 0.26730 | 3.7235 | 6.1838 | 3.6552 |
| 16 | 3.45 | .. | H(21F) [| = | 02] | | Intra | 169.14 | 22.89 | 0.19000 | 0.35330 | 0.20380 | 1.4399 | 4.2915 | 2.7869 |
| 17 | 3.47 | .. | H(22E)c[-x,1-y,-z | = | 2565.02] | | Intra | 121.30 | -1.37 | 0.31490 | 0.52520 | 0.09950 | 2.7620 | 6.6573 | 1.3606 |
| 18 | 3.48 | .. | H(12C) | | | | Intra | -132.17 | -14.04 | 0.23440 | 0.09660 | 0.04380 | 2.2977 | 1.1897 | 0.5989 |
| 19 | 3.49 | .. | H(22D)c[-x,1-y,-z | = | 2565.02] | | Intra | 107.53 | -38.98 | 0.38620 | 0.47970 | -0.05500 | 3.7474 | 6.2797 | -0.7521 |

Angles (Degrees) At1...V...At2 with Vertex V = S(1)

| | | | | | | | |
|---------------|----------|---------------|----------|---------------|----------|---------------|----------|
| C(13) , N(12) | 26.46(7) | C(13) , N(11) | 24.71(7) | C(13) , C(12) | 52.76(7) | N(12) , N(11) | 51.17(5) |
| N(12) , C(12) | 79.21(5) | N(11) , C(12) | 28.05(4) | | | | |

=====

3.6 Angstrom Coordination Sphere Around Atom I = S(2) [ARU = 1555.02] -0.02902 0.79140 0.09734 -0.9726 10.1033 1.3311

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|-------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|---------|
| 1 | 1.6904(18) | -- | C(23) | | | | Intra | -33.56 | 53.05 | 0.06409 | 0.75840 | 0.19613 | -0.1259 | 9.5417 | 2.6820 |
| 2 | 2.6443(18) | << | N(22) | | | | Intra | 2.32 | 42.14 | 0.17929 | 0.81124 | 0.22709 | 0.9864 | 10.1828 | 3.1053 |
| 3 | 2.6749(18) | << | N(21) | | | | Intra | -74.05 | 50.63 | 0.02937 | 0.68124 | 0.24857 | -0.5065 | 8.4721 | 3.3991 |
| 4 | 3.082(2) | << | C(22) | | | | Intra | -108.11 | 36.39 | -0.09644 | 0.62321 | 0.23107 | -1.7440 | 7.7454 | 3.1598 |
| 5 | 2.640(19) | << | H(22) | | | | Intra | 19.73 | 30.50 | 0.19580 | 0.86110 | 0.19530 | 1.1681 | 10.8711 | 2.6706 |
| 6 | 2.70 | << | H(22A) | | | | Intra | -130.03 | 33.24 | -0.16290 | 0.66900 | 0.20570 | -2.4269 | 8.3723 | 2.8128 |
| 7 | 3.17 | .. | H(21A) | | | | Intra | -92.47 | 0.26 | -0.05810 | 0.54650 | 0.09840 | -1.1092 | 6.9343 | 1.3456 |
| 8 | 3.22 | .. | H(21B)d | [-x,1-y,-z | = | 2565.02] | | -81.69 | -48.18 | -0.03480 | 0.60890 | -0.07790 | -0.6627 | 7.9820 | -1.0652 |
| 9 | 3.22 | .. | H(12F)b | [x,1+y,z | = | 1565.01] | | 30.98 | -33.38 | 0.18250 | 0.88480 | -0.03230 | 1.3342 | 11.4884 | -0.4417 |
| 10 | 3.23 | .. | H(12C)c | [-x,1-y,-z | = | 2565.01] | | 140.65 | -36.71 | -0.23440 | 0.90340 | -0.04380 | -2.9747 | 11.7446 | -0.5989 |
| 11 | 3.34 | .. | H(12E)c | [-x,1-y,-z | = | 2565.01] | | 118.37 | -0.34 | -0.16780 | 1.01850 | 0.09590 | -2.5599 | 13.0427 | 1.3114 |
| 12 | 3.37 | .. | H(110)a | [-1+x,1+y,z | = | 1465.01] | | 166.31 | 19.50 | -0.31190 | 0.85820 | 0.17960 | -4.0595 | 10.8551 | 2.4559 |
| 13 | 3.40 | .. | H(12D)b | [x,1+y,z | = | 1565.01] | | 67.23 | -8.54 | 0.10730 | 1.02740 | 0.06040 | 0.3296 | 13.2063 | 0.8259 |
| 14 | 3.41 | .. | H(21D)d | [-x,1-y,-z | = | 2565.02] | | -165.94 | -79.04 | -0.12550 | 0.75340 | -0.14740 | -1.6011 | 9.9459 | -2.0156 |
| 15 | 3.41 | .. | H(22C) | | | | Intra | -130.45 | -13.23 | -0.25850 | 0.58980 | 0.04020 | -3.1297 | 7.5738 | 0.5497 |
| 16 | 3.42 | .. | H(11G)a | [-1+x,1+y,z | = | 1465.01] | | 92.94 | 63.79 | 0.00310 | 0.93150 | 0.32140 | -1.0500 | 11.6096 | 4.3950 |
| 17 | 3.42 | .. | H(12D)c | [-x,1-y,-z | = | 2565.01] | | 105.52 | -39.08 | -0.10730 | 0.97260 | -0.06040 | -1.6835 | 12.6623 | -0.8259 |
| 18 | 3.45(2) | .. | H(21) | | | | Intra | -64.61 | 54.28 | 0.07450 | 0.67230 | 0.30220 | -0.1090 | 8.2832 | 4.1324 |
| 19 | 3.49 | .. | H(11H)a | [-1+x,1+y,z | = | 1465.01] | | 90.64 | 37.06 | 0.00400 | 1.02290 | 0.25110 | -1.0038 | 12.8877 | 3.4337 |
| 20 | 3.52 | .. | H(21C)d | [-x,1-y,-z | = | 2565.02] | | -38.59 | -57.96 | 0.07500 | 0.67840 | -0.12070 | 0.4861 | 8.9394 | -1.6505 |

Angles (Degrees) At1...V...At2 with Vertex V = S(2)

| | | | | | | | |
|---------------|----------|---------------|----------|---------------|----------|---------------|----------|
| C(23) , N(22) | 26.19(6) | C(23) , N(21) | 24.80(6) | C(23) , C(22) | 52.91(6) | N(22) , N(21) | 50.99(5) |
| N(22) , C(22) | 79.07(5) | N(21) , C(22) | 28.16(4) | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = O(11) [ARU = 1555.01] 0.47721 -0.04395 0.19813 4.6877 -0.8389 2.7093

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|--------------|-----------|------------|-------|---------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 1.397(2) | -- | C(11) | | | | Intra | 127.30 | -22.76 | 0.40127 | 0.03112 | 0.15860 | 3.9069 | 0.1860 | 2.1688 |
| 2 | 1.442(2) | -- | C(111) | | | | Intra | -70.73 | -41.11 | 0.49678 | -0.13054 | 0.12882 | 5.0461 | -1.8643 | 1.7615 |
| 3 | 2.3023(18) | << | O(12) | | | | Intra | 165.95 | -21.03 | 0.26970 | -0.00998 | 0.13771 | 2.6031 | -0.3171 | 1.8831 |
| 4 | 2.355(2) | << | C(12) | | | | Intra | 112.91 | 12.25 | 0.40654 | 0.12379 | 0.23468 | 3.7918 | 1.2808 | 3.2091 |
| 5 | 2.389(2) | << | C(112) | | | | Intra | -50.62 | -9.11 | 0.60870 | -0.18780 | 0.17049 | 6.1840 | -2.6618 | 2.3314 |
| 6 | 2.918(2) | <. | N(11) | | | | Intra | 82.56 | 14.29 | 0.53432 | 0.17837 | 0.25080 | 5.0540 | 1.9648 | 3.4296 |
| 7 | 3.509(2) | .. | C(24)a | [x,-1+y,z | | = 1545.02] | | -133.62 | 25.29 | 0.26964 | -0.20995 | 0.30776 | 2.4990 | -3.1356 | 4.2084 |
| 8 | 3.535(2) | .. | C(121) | | | | Intra | 157.92 | -34.52 | 0.20095 | 0.02522 | 0.05163 | 1.9890 | 0.2557 | 0.7060 |
| 9 | 1.98 | << | H(11J) | | | | Intra | 104.48 | -43.92 | 0.43540 | 0.05220 | 0.09770 | 4.3312 | 0.5418 | 1.3360 |
| 10 | 2.01 | << | H(11K) | | | | Intra | -44.22 | -64.03 | 0.51620 | -0.10530 | 0.06610 | 5.3180 | -1.4522 | 0.9039 |
| 11 | 2.01 | << | H(11L) | | | | Intra | -104.49 | -33.81 | 0.41700 | -0.17750 | 0.11640 | 4.2701 | -2.4547 | 1.5917 |
| 12 | 2.50 | << | H(12B) | | | | Intra | 124.92 | 32.74 | 0.38360 | 0.09990 | 0.29710 | 3.4830 | 0.8866 | 4.0627 |
| 13 | 2.57 | <. | H(11N) | | | | Intra | -60.81 | 10.92 | 0.59000 | -0.21030 | 0.23370 | 5.9171 | -3.0391 | 3.1957 |
| 14 | 2.60 | <. | H(110) | | | | Intra | -28.61 | -5.59 | 0.68810 | -0.14180 | 0.17960 | 6.9614 | -2.0792 | 2.4559 |
| 15 | 2.78 | .. | H(12H)c | [1-x,1-y,1-z | | = 2666.02] | | -8.75 | 61.51 | 0.62840 | -0.04070 | 0.37680 | 5.9985 | -1.0407 | 5.1525 |
| 16 | 2.96(2) | .. | H(11) | | | | Intra | 71.83 | 26.60 | 0.58360 | 0.16080 | 0.29510 | 5.5134 | 1.6770 | 4.0353 |
| 17 | 3.095(19) | .. | H(22)a | [x,-1+y,z | | = 1545.02] | | -156.70 | -0.72 | 0.19580 | -0.13890 | 0.19530 | 1.8451 | -2.0632 | 2.6706 |
| 18 | 3.20 | .. | H(12A) | | | | Intra | 119.55 | 3.69 | 0.34120 | 0.17240 | 0.21320 | 3.1132 | 1.9389 | 2.9154 |
| 19 | 3.24 | .. | H(11M) | | | | Intra | -55.88 | -17.90 | 0.62090 | -0.24870 | 0.12540 | 6.4148 | -3.3879 | 1.7148 |
| 20 | 3.40 | .. | H(12G)b | [1-x,-y,-z | | = 2655.01] | | 29.87 | -36.72 | 0.69130 | 0.04530 | 0.04950 | 7.0506 | 0.5184 | 0.6769 |

Angles (Degrees) At1...V...At2 with Vertex V = O(11)

| | | | | | | | | | | | | | | | |
|--------|---|--------|------------|--------|---|--------|------------|--------|---|--------|------------|--------|---|--------|------------|
| C(11) | , | C(111) | 113.98(13) | C(11) | , | O(12) | 35.80(8) | C(11) | , | C(12) | 37.74(9) | C(11) | , | C(112) | 148.07(11) |
| C(11) | , | N(11) | 57.37(9) | C(11) | , | C(24)a | 107.27(10) | C(11) | , | C(121) | 29.18(8) | C(111) | , | O(12) | 98.65(10) |
| C(111) | , | C(12) | 150.97(11) | C(111) | , | C(112) | 36.62(9) | C(111) | , | N(11) | 144.54(10) | C(111) | , | C(24)a | 88.30(9) |
| C(111) | , | C(121) | 92.15(9) | O(12) | , | C(12) | 61.81(6) | O(12) | , | C(112) | 133.11(8) | O(12) | , | N(11) | 89.11(6) |
| O(12) | , | C(24)a | 74.75(5) | O(12) | , | C(121) | 15.23(4) | C(12) | , | C(112) | 163.52(9) | C(12) | , | N(11) | 29.59(5) |
| C(12) | , | C(24)a | 105.14(6) | C(12) | , | C(121) | 63.33(6) | C(112) | , | N(11) | 133.93(8) | C(112) | , | C(24)a | 87.64(7) |
| C(112) | , | C(121) | 128.68(7) | N(11) | , | C(24)a | 127.00(5) | N(11) | , | C(121) | 86.46(5) | C(24)a | , | C(121) | 88.20(5) |

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3.6 Angstrom Coordination Sphere Around Atom I = O(12) [ARU = 1555.01] 0.26970 -0.00998 0.13771 2.6031 -0.3171 1.8831

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|-------------|-----------|------------|-------|---------|--------|---------|----------|----------|---------|---------|---------|
| 1 | 1.426(2) | -- | C(11) | | | | Intra | 21.10 | 11.55 | 0.40127 | 0.03112 | 0.15860 | 3.9069 | 0.1860 | 2.1688 |
| 2 | 1.446(2) | -- | C(121) | | | | Intra | 136.99 | -54.50 | 0.20095 | 0.02522 | 0.05163 | 1.9890 | 0.2557 | 0.7060 |
| 3 | 2.3023(18) | << | O(11) | | | | Intra | -14.05 | 21.03 | 0.47721 | -0.04395 | 0.19813 | 4.6877 | -0.8389 | 2.7093 |
| 4 | 2.393(2) | << | C(12) | | | | Intra | 53.35 | 33.66 | 0.40654 | 0.12379 | 0.23468 | 3.7918 | 1.2808 | 3.2091 |
| 5 | 2.448(2) | << | C(122) | | | | Intra | -143.74 | -81.85 | 0.21630 | -0.04456 | -0.03951 | 2.3231 | -0.5224 | -0.5403 |
| 6 | 2.882(2) | .< | N(22)a | [x, -1+y, z | | = 1545.02] | | -111.11 | 25.10 | 0.17929 | -0.18876 | 0.22709 | 1.6634 | -2.7514 | 3.1053 |
| 7 | 2.894(2) | << | C(111) | | | | Intra | -32.35 | -2.41 | 0.49678 | -0.13054 | 0.12882 | 5.0461 | -1.8643 | 1.7615 |
| 8 | 2.00 | << | H(12C) | | | | Intra | 101.46 | -39.87 | 0.23440 | 0.09660 | 0.04380 | 2.2977 | 1.1897 | 0.5989 |
| 9 | 2.00 | << | H(12D) | | | | Intra | 159.75 | -31.85 | 0.10730 | 0.02740 | 0.06040 | 1.0065 | 0.2720 | 0.8259 |
| 10 | 2.01 | << | H(11J) | | | | Intra | 26.43 | -15.83 | 0.43540 | 0.05220 | 0.09770 | 4.3312 | 0.5418 | 1.3360 |
| 11 | 2.060(18) | << | H(22)a | [x, -1+y, z | | = 1545.02] | | -113.47 | 22.48 | 0.19580 | -0.13890 | 0.19530 | 1.8451 | -2.0632 | 2.6706 |
| 12 | 2.53 | .< | H(12A) | | | | Intra | 77.26 | 24.05 | 0.34120 | 0.17240 | 0.21320 | 3.1132 | 1.9389 | 2.9154 |
| 13 | 2.64 | .< | H(12B) | | | | Intra | 53.83 | 55.62 | 0.38360 | 0.09990 | 0.29710 | 3.4830 | 0.8866 | 4.0627 |
| 14 | 2.65 | .< | H(12F) | | | | Intra | -117.67 | -61.26 | 0.18250 | -0.11520 | -0.03230 | 2.0111 | -1.4459 | -0.4417 |
| 15 | 2.66 | .< | H(12G) | | | | Intra | -16.26 | -74.31 | 0.30870 | -0.04530 | -0.04950 | 3.2934 | -0.5184 | -0.6769 |
| 16 | 2.73 | .. | H(11L) | | | | Intra | -52.05 | -6.14 | 0.41700 | -0.17750 | 0.11640 | 4.2701 | -2.4547 | 1.5917 |
| 17 | 3.10 | .. | H(11K) | | | | Intra | -22.69 | -18.41 | 0.51620 | -0.10530 | 0.06610 | 5.3180 | -1.4522 | 0.9039 |
| 18 | 3.28 | .. | H(12E) | | | | Intra | 163.84 | -76.79 | 0.16780 | -0.01850 | -0.09590 | 1.8830 | -0.1084 | -1.3114 |
| 19 | 3.33 | .. | H(11H)b | [-1+x, y, z | | = 1455.01] | | 174.73 | 27.79 | 0.00400 | 0.02290 | 0.25110 | -0.3268 | -0.0465 | 3.4337 |

Angles (Degrees) At1...V...At2 with Vertex V = O(12)

| | | | | | | | |
|-----------------|------------|-----------------|------------|-----------------|------------|-----------------|------------|
| C(11) , C(121) | 114.30(13) | C(11) , O(11) | 34.96(8) | C(11) , C(12) | 36.81(9) | C(11) , C(122) | 109.41(11) |
| C(11) , N(22)a | 120.74(10) | C(11) , C(111) | 54.93(9) | C(121) , O(11) | 140.04(11) | C(121) , C(12) | 113.43(10) |
| C(121) , C(122) | 34.80(9) | C(121) , N(22)a | 122.78(10) | C(121) , C(111) | 122.41(10) | O(11) , C(12) | 60.17(6) |
| O(11) , C(122) | 116.09(7) | O(11) , N(22)a | 87.22(6) | O(11) , C(111) | 29.50(5) | C(12) , C(122) | 131.41(8) |
| C(12) , N(22)a | 119.42(7) | C(12) , C(111) | 87.76(6) | C(122) , N(22)a | 108.16(7) | C(122) , C(111) | 90.58(7) |
| N(22)a , C(111) | 80.88(6) | | | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = O(13) [ARU = 1555.01] 0.98303 0.07133 0.38936 9.5733 0.3911 5.3243

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------------------|------------|-----------|--------|-------|---------|--------|---------|----------|---------|---------|---------|--------|
| 1 | 1.364(2) | -- | C(16) | | | | Intra | 120.28 | -3.25 | 0.92181 | 0.16164 | 0.38371 | 8.8868 | 1.5669 | 5.2470 |
| 2 | 1.437(2) | -- | C(113) | | | | Intra | -92.18 | -53.03 | 0.96350 | -0.00431 | 0.30538 | 9.5404 | -0.4726 | 4.1759 |
| 3 | 2.330(2) | << | C(17) | | | | Intra | 106.91 | 27.08 | 0.94581 | 0.23294 | 0.46691 | 8.9699 | 2.3756 | 6.3847 |
| 4 | 2.444(2) | << | C(15) | | | | Intra | 132.61 | -28.69 | 0.83843 | 0.18428 | 0.30354 | 8.1216 | 1.9692 | 4.1507 |
| 5 | 2.6876(18) | << | O(14) | | | | Intra | 86.95 | 54.17 | 1.02180 | 0.20960 | 0.54871 | 9.6569 | 1.9621 | 7.5033 |
| 6 | 3.103(3) | .< | C(114) | | | | Intra | 49.11 | 41.89 | 1.15966 | 0.22231 | 0.54087 | 11.0853 | 2.1372 | 7.3961 |
| 7 | 1.99 | << | H(11H) | | | | Intra | -44.60 | -71.75 | 1.00400 | 0.02290 | 0.25110 | 10.0172 | -0.0465 | 3.4337 |
| 8 | 1.99 | << | H(11G) | | | | Intra | -76.95 | -27.82 | 1.00310 | -0.06850 | 0.32140 | 9.9710 | -1.3247 | 4.3950 |
| 9 | 1.99 | << | H(11I) | | | | Intra | -133.22 | -44.99 | 0.86990 | -0.01890 | 0.28640 | 8.6088 | -0.6354 | 3.9164 |
| 10 | 2.58 | .< | H(11F) | | | | Intra | 34.50 | 29.89 | 1.18090 | 0.17910 | 0.48330 | 11.4151 | 1.6568 | 6.6089 |
| 11 | 2.67 | .< | H(15A) | | | | Intra | 145.52 | -46.91 | 0.82260 | 0.13610 | 0.24680 | 8.0702 | 1.4235 | 3.3749 |
| 12 | 2.68 | .< | H(12I)b[1-x,1-y,1-z | = | 2666.02] | | | -161.25 | 16.58 | 0.75210 | 0.01350 | 0.44520 | 7.1452 | -0.4331 | 6.0879 |
| 13 | 3.36 | .. | H(29A)a[1+x,-1+y,z | = | 1645.02] | | | -36.56 | 2.08 | 1.23510 | -0.08250 | 0.39830 | 12.2723 | -1.6107 | 5.4465 |

Angles (Degrees) At1...V...At2 with Vertex V = O(13)

| | | | | | | | |
|-----------------|------------|----------------|------------|----------------|-----------|----------------|------------|
| C(16) , C(113) | 117.47(14) | C(16) , C(17) | 32.96(9) | C(16) , C(15) | 28.02(9) | C(16) , O(14) | 63.74(9) |
| C(16) , C(114) | 78.34(10) | C(113) , C(17) | 150.43(12) | C(113) , C(15) | 89.47(11) | C(113) , O(14) | 178.75(11) |
| C(113) , C(114) | 151.98(11) | C(17) , C(15) | 60.97(6) | C(17) , O(14) | 30.80(5) | C(17) , C(114) | 48.92(6) |
| C(15) , O(14) | 91.74(6) | C(15) , C(114) | 104.28(7) | O(14) , C(114) | 27.69(5) | | |

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3.6 Angstrom Coordination Sphere Around Atom I = O(14) [ARU = 1555.01] 1.02180 0.20960 0.54871 9.6569 1.9621 7.5033

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|--------------|-----------|----------|-------|---------|--------|---------|---------|---------|---------|---------|---------|
| 1 | 1.376(2) | -- | C(17) | | | | Intra | 148.95 | -54.37 | 0.94581 | 0.23294 | 0.46691 | 8.9699 | 2.3756 | 6.3847 |
| 2 | 1.443(2) | -- | C(114) | | | | Intra | 6.99 | -4.26 | 1.15966 | 0.22231 | 0.54087 | 11.0853 | 2.1372 | 7.3961 |
| 3 | 2.398(2) | << | C(18) | | | | Intra | 130.12 | -26.99 | 0.88562 | 0.32751 | 0.46913 | 8.2802 | 3.5958 | 6.4151 |
| 4 | 2.417(2) | << | C(16) | | | | Intra | -152.84 | -69.01 | 0.92181 | 0.16164 | 0.38371 | 8.8868 | 1.5669 | 5.2470 |
| 5 | 2.6549(19) | << | O(15) | | | | Intra | 117.79 | 1.66 | 0.91488 | 0.39171 | 0.55434 | 8.4197 | 4.3098 | 7.5803 |
| 6 | 2.6876(18) | << | O(13) | | | | Intra | -93.05 | -54.17 | 0.98303 | 0.07133 | 0.38936 | 9.5733 | 0.3911 | 5.3243 |
| 7 | 3.124(2) | .. | N(21)a | [1-x,1-y,1-z | = | 2666.02] | | 128.03 | 62.53 | 0.97063 | 0.31876 | 0.75143 | 8.7689 | 3.0973 | 10.2754 |
| 8 | 3.468(2) | .. | C(29)a | [1-x,1-y,1-z | = | 2666.02] | | -163.26 | 13.48 | 0.71314 | 0.14077 | 0.60784 | 6.4276 | 0.9911 | 8.3119 |
| 9 | 3.484(2) | .. | C(113)b | [2-x,-y,1-z | = | 2756.01] | | -88.27 | 34.94 | 1.03650 | 0.00431 | 0.69462 | 9.7430 | -0.8924 | 9.4985 |
| 10 | 3.558(2) | .. | C(22)a | [1-x,1-y,1-z | = | 2666.02] | | 79.37 | 57.83 | 1.09644 | 0.37679 | 0.76893 | 10.0064 | 3.8239 | 10.5147 |
| 11 | 2.00 | << | H(11F) | | | | Intra | -9.85 | -26.62 | 1.18090 | 0.17910 | 0.48330 | 11.4151 | 1.6568 | 6.6089 |
| 12 | 2.00 | << | H(11E) | | | | Intra | 34.64 | -5.62 | 1.18350 | 0.29540 | 0.53440 | 11.2915 | 3.0914 | 7.3076 |
| 13 | 2.00 | << | H(11D) | | | | Intra | -5.51 | 20.44 | 1.20820 | 0.20110 | 0.59970 | 11.5191 | 1.7825 | 8.2006 |
| 14 | 2.70 | < | H(11G)b | [2-x,-y,1-z | = | 2756.01] | | -99.76 | 41.16 | 0.99690 | 0.06850 | 0.67860 | 9.3124 | -0.0403 | 9.2795 |
| 15 | 2.75(2) | .. | H(21)a | [1-x,1-y,1-z | = | 2666.02] | | 134.15 | 47.85 | 0.92550 | 0.32770 | 0.69780 | 8.3714 | 3.2861 | 9.5420 |
| 16 | 3.17 | .. | H(22B)a | [1-x,1-y,1-z | = | 2666.02] | | 72.97 | 42.76 | 1.12150 | 0.39840 | 0.70620 | 10.3392 | 4.1891 | 9.6569 |
| 17 | 3.24 | .. | H(29A)a | [1-x,1-y,1-z | = | 2666.02] | | -147.03 | 12.94 | 0.76490 | 0.08250 | 0.60170 | 7.0111 | 0.2458 | 8.2279 |

Angles (Degrees) At1...V...At2 with Vertex V = O(14)

| | | | | | | | |
|------------------|------------|-----------------|------------|------------------|------------|------------------|------------|
| C(17) , C(114) | 113.41(13) | C(17) , C(18) | 30.66(9) | C(17) , C(16) | 29.68(9) | C(17) , O(15) | 61.66(9) |
| C(17) , O(13) | 60.08(8) | C(17) , N(21)a | 118.04(10) | C(17) , C(29)a | 78.98(9) | C(17) , C(113)b | 136.39(10) |
| C(17) , C(22)a | 125.43(10) | C(114) , C(18) | 116.87(11) | C(114) , C(16) | 105.42(11) | C(114) , O(15) | 110.86(10) |
| C(114) , O(13) | 92.38(10) | C(114) , N(21)a | 107.65(10) | C(114) , C(29)a | 166.67(11) | C(114) , C(113)b | 96.75(10) |
| C(114) , C(22)a | 84.38(10) | C(18) , C(16) | 60.31(6) | C(18) , O(15) | 31.02(5) | C(18) , O(13) | 90.71(6) |
| C(18) , N(21)a | 89.54(6) | C(18) , C(29)a | 76.23(6) | C(18) , C(113)b | 146.35(7) | C(18) , C(22)a | 94.82(6) |
| C(16) , O(15) | 91.33(6) | C(16) , O(13) | 30.40(5) | C(16) , N(21)a | 142.87(7) | C(16) , C(29)a | 82.83(6) |
| C(16) , C(113)b | 114.12(7) | C(16) , C(22)a | 155.12(7) | O(15) , O(13) | 121.73(6) | O(15) , N(21)a | 61.35(4) |
| O(15) , C(29)a | 78.87(5) | O(15) , C(113)b | 136.01(6) | O(15) , C(22)a | 63.80(4) | O(13) , N(21)a | 157.36(6) |
| O(13) , C(29)a | 89.80(5) | O(13) , C(113)b | 89.21(5) | O(13) , C(22)a | 174.41(6) | N(21)a , C(29)a | 68.30(4) |
| N(21)a , C(113)b | 78.26(5) | N(21)a , C(22)a | 24.04(4) | C(29)a , C(113)b | 70.13(5) | C(29)a , C(22)a | 92.33(5) |
| C(113)b , C(22)a | 86.65(5) | | | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = O(15) [ARU = 1555.01] 0.91488 0.39171 0.55434 8.4197 4.3098 7.5803

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|--------------|-----------|----------|-------|---------|--------|---------|---------|---------|---------|--------|---------|
| 1 | 1.374(2) | -- | C(18) | | | | Intra | -101.06 | -58.02 | 0.88562 | 0.32751 | 0.46913 | 8.2802 | 3.5958 | 6.4151 |
| 2 | 1.438(2) | -- | C(115) | | | | Intra | 123.31 | 5.53 | 0.84640 | 0.48523 | 0.56447 | 7.6338 | 5.5056 | 7.7188 |
| 3 | 2.340(2) | << | C(17) | | | | Intra | -74.12 | -30.73 | 0.94581 | 0.23294 | 0.46691 | 8.9699 | 2.3756 | 6.3847 |
| 4 | 2.446(2) | << | C(19) | | | | Intra | -161.23 | -67.05 | 0.80251 | 0.35060 | 0.38962 | 7.5166 | 4.0029 | 5.3278 |
| 5 | 2.6549(19) | << | O(14) | | | | Intra | -62.21 | -1.66 | 1.02180 | 0.20960 | 0.54871 | 9.6569 | 1.9621 | 7.5033 |
| 6 | 2.976(2) | .< | N(21)a | [1-x,1-y,1-z | = | 2666.02] | | -73.93 | 64.91 | 0.97063 | 0.31876 | 0.75143 | 8.7689 | 3.0973 | 10.2754 |
| 7 | 3.371(2) | .. | C(22)a | [1-x,1-y,1-z | = | 2666.02] | | -17.03 | 60.51 | 1.09644 | 0.37679 | 0.76893 | 10.0064 | 3.8239 | 10.5147 |
| 8 | 3.444(2) | .. | C(114) | | | | Intra | -39.18 | -3.07 | 1.15966 | 0.22231 | 0.54087 | 11.0853 | 2.1372 | 7.3961 |
| 9 | 3.498(3) | .. | C(115)b | [2-x,1-y,1-z | = | 2766.01] | | 34.49 | -27.68 | 1.15360 | 0.51477 | 0.43553 | 10.9726 | 6.0637 | 5.9556 |
| 10 | 1.99 | << | H(11B) | | | | Intra | 150.79 | 1.83 | 0.75250 | 0.46730 | 0.55900 | 6.6823 | 5.2812 | 7.6440 |
| 11 | 1.99 | << | H(11C) | | | | Intra | 106.53 | -16.57 | 0.86570 | 0.52880 | 0.51280 | 7.8765 | 6.1397 | 7.0123 |
| 12 | 1.99 | << | H(11A) | | | | Intra | 110.99 | 30.60 | 0.87420 | 0.52330 | 0.62850 | 7.8057 | 5.9106 | 8.5944 |
| 13 | 2.21(2) | << | H(21)a | [1-x,1-y,1-z | = | 2666.02] | | -92.70 | 62.42 | 0.92550 | 0.32770 | 0.69780 | 8.3714 | 3.2861 | 9.5420 |
| 14 | 2.67 | .< | H(19A) | | | | Intra | 158.99 | -56.78 | 0.76240 | 0.41500 | 0.39120 | 7.0558 | 4.8338 | 5.3494 |
| 15 | 2.73 | .. | H(11C)b | [2-x,1-y,1-z | = | 2766.01] | | 25.86 | -19.68 | 1.13430 | 0.47120 | 0.48720 | 10.7299 | 5.4296 | 6.6622 |
| 16 | 2.83 | .. | H(22B)a | [1-x,1-y,1-z | = | 2666.02] | | -3.60 | 47.20 | 1.12150 | 0.39840 | 0.70620 | 10.3392 | 4.1891 | 9.6569 |
| 17 | 3.13 | .. | H(11E) | | | | Intra | -22.99 | -5.00 | 1.18350 | 0.29540 | 0.53440 | 11.2915 | 3.0914 | 7.3076 |

Angles (Degrees) At1...V...At2 with Vertex V = O(15)

| | | | | | | | |
|------------------|------------|-----------------|------------|------------------|------------|------------------|------------|
| C(18) , C(115) | 117.30(13) | C(18) , C(17) | 32.93(9) | C(18) , C(19) | 27.90(9) | C(18) , O(14) | 64.09(9) |
| C(18) , N(21)a | 124.63(10) | C(18) , C(22)a | 135.33(10) | C(18) , C(114) | 72.86(9) | C(18) , C(115)b | 86.61(9) |
| C(115) , C(17) | 149.94(11) | C(115) , C(19) | 89.50(10) | C(115) , O(14) | 173.26(11) | C(115) , N(21)a | 108.41(10) |
| C(115) , C(22)a | 107.06(10) | C(115) , C(114) | 162.37(11) | C(115) , C(115)b | 91.53(10) | C(17) , C(19) | 60.83(6) |
| C(17) , O(14) | 31.18(5) | C(17) , N(21)a | 95.64(6) | C(17) , C(22)a | 102.41(6) | C(17) , C(114) | 43.03(6) |
| C(17) , C(115)b | 90.32(6) | C(19) , O(14) | 91.97(6) | C(19) , N(21)a | 145.71(7) | C(19) , C(22)a | 163.19(7) |
| C(19) , C(114) | 99.06(6) | C(19) , C(115)b | 84.53(6) | O(14) , N(21)a | 67.12(5) | O(14) , C(22)a | 71.24(5) |
| O(14) , C(114) | 23.05(4) | O(14) , C(115)b | 95.16(5) | N(21)a , C(22)a | 25.54(4) | N(21)a , C(114) | 72.58(5) |
| N(21)a , C(115)b | 122.64(6) | C(22)a , C(114) | 65.88(5) | C(22)a , C(115)b | 97.65(5) | C(114) , C(115)b | 74.13(5) |

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3.6 Angstrom Coordination Sphere Around Atom I = O(21) [ARU = 1555.02] -0.02070 0.45537 0.20390 -0.8088 5.6116 2.7882

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|--------------|-----------|----------|-------|---------|--------|----------|---------|---------|---------|--------|--------|
| 1 | 1.396(2) | -- | C(21) | | | | Intra | 127.24 | -26.17 | -0.09535 | 0.52772 | 0.15888 | -1.5667 | 6.6088 | 2.1726 |
| 2 | 1.441(2) | -- | C(211) | | | | Intra | -68.19 | -38.33 | 0.00526 | 0.36732 | 0.13853 | -0.3888 | 4.5619 | 1.8943 |
| 3 | 2.2992(18) | << | O(22) | | | | Intra | 167.09 | -23.95 | -0.22606 | 0.48447 | 0.13564 | -2.8569 | 6.0811 | 1.8548 |
| 4 | 2.359(2) | << | C(22) | | | | Intra | 113.67 | 9.06 | -0.09644 | 0.62321 | 0.23107 | -1.7440 | 7.7454 | 3.1598 |
| 5 | 2.391(3) | << | C(212) | | | | Intra | -52.00 | -4.68 | 0.10960 | 0.30867 | 0.18962 | 0.6584 | 3.7336 | 2.5929 |
| 6 | 2.941(2) | .< | N(21) | | | | Intra | 83.97 | 11.99 | 0.02937 | 0.68124 | 0.24857 | -0.5065 | 8.4721 | 3.3991 |
| 7 | 3.508(3) | .. | C(115)b | [1-x,1-y,1-z | = | 2666.01] | | 17.46 | 64.56 | 0.15360 | 0.51477 | 0.43553 | 0.6286 | 6.0637 | 5.9556 |
| 8 | 3.512(2) | .. | C(14)a | [-1+x,y,z | = | 1455.01] | | -130.87 | 23.85 | -0.22138 | 0.27852 | 0.30776 | -2.9108 | 3.1824 | 4.2084 |
| 9 | 3.537(2) | .. | C(221) | | | | Intra | 158.65 | -37.00 | -0.29201 | 0.51843 | 0.04824 | -3.4393 | 6.6397 | 0.6597 |
| 10 | 3.542(2) | .. | N(12)a | [-1+x,y,z | = | 1455.01] | | -145.26 | 4.91 | -0.30806 | 0.30222 | 0.22609 | -3.7087 | 3.6004 | 3.0917 |
| 11 | 1.98 | << | H(21A) | | | | Intra | 102.79 | -46.77 | -0.05810 | 0.54650 | 0.09840 | -1.1092 | 6.9343 | 1.3456 |
| 12 | 2.01 | << | H(21C) | | | | Intra | -102.36 | -34.51 | -0.07500 | 0.32160 | 0.12070 | -1.1630 | 3.9949 | 1.6505 |
| 13 | 2.01 | << | H(21B) | | | | Intra | -39.68 | -59.07 | 0.03480 | 0.39110 | 0.07790 | -0.0142 | 4.9523 | 1.0652 |
| 14 | 2.50 | << | H(22B) | | | | Intra | 125.64 | 29.46 | -0.12150 | 0.60160 | 0.29380 | -2.0767 | 7.3802 | 4.0176 |
| 15 | 2.57 | .< | H(21E) | | | | Intra | -63.73 | 14.50 | 0.08110 | 0.28800 | 0.25090 | 0.2915 | 3.3826 | 3.4309 |
| 16 | 2.61 | .< | H(21F) | | | | Intra | -30.41 | -0.03 | 0.19000 | 0.35330 | 0.20380 | 1.4399 | 4.2915 | 2.7869 |
| 17 | 2.62 | .< | H(11A)b | [1-x,1-y,1-z | = | 2666.01] | | 2.13 | 61.08 | 0.12580 | 0.47670 | 0.37150 | 0.4568 | 5.6587 | 5.0801 |
| 18 | 2.95(2) | .. | H(12)a | [-1+x,y,z | = | 1455.01] | | -154.07 | -3.16 | -0.28480 | 0.35460 | 0.19200 | -3.4557 | 4.3244 | 2.6255 |
| 19 | 3.07(2) | .. | H(21) | | | | Intra | 75.32 | 25.95 | 0.07450 | 0.67230 | 0.30220 | -0.1090 | 8.2832 | 4.1324 |
| 20 | 3.20 | .. | H(22A) | | | | Intra | 120.37 | 0.44 | -0.16290 | 0.66900 | 0.20570 | -2.4269 | 8.3723 | 2.8128 |
| 21 | 3.24 | .. | H(21D) | | | | Intra | -56.55 | -13.81 | 0.12550 | 0.24660 | 0.14740 | 0.9242 | 2.9884 | 2.0156 |
| 22 | 3.44 | .. | H(22G)c | [-x,1-y,-z | = | 2565.02] | | 34.35 | -38.58 | 0.17940 | 0.55620 | 0.04690 | 1.4133 | 7.1300 | 0.6413 |

Angles (Degrees) At1...V...At2 with Vertex V = O(21)

| | | | | | | | |
|------------------|------------|------------------|------------|-----------------|------------|------------------|------------|
| C(21) , C(211) | 113.89(13) | C(21) , O(22) | 36.03(8) | C(21) , C(22) | 37.62(8) | C(21) , C(212) | 149.13(12) |
| C(21) , N(21) | 56.80(8) | C(21) , C(115)b | 121.92(10) | C(21) , C(14)a | 110.34(10) | C(21) , C(221) | 28.70(8) |
| C(21) , N(12)a | 89.94(9) | C(211) , O(22) | 99.00(10) | C(211) , C(22) | 150.68(11) | C(211) , C(212) | 36.73(10) |
| C(211) , N(21) | 143.84(11) | C(211) , C(115)b | 122.31(10) | C(211) , C(14)a | 85.50(9) | C(211) , C(221) | 93.16(10) |
| C(211) , N(12)a | 83.00(10) | O(22) , C(22) | 61.71(6) | O(22) , C(212) | 132.36(8) | O(22) , N(21) | 88.70(6) |
| O(22) , C(115)b | 134.86(6) | O(22) , C(14)a | 76.84(5) | O(22) , C(221) | 14.92(4) | O(22) , N(12)a | 54.65(5) |
| C(22) , C(212) | 165.12(9) | C(22) , N(21) | 29.33(5) | C(22) , C(115)b | 84.47(6) | C(22) , C(14)a | 108.94(6) |
| C(22) , C(221) | 62.42(6) | C(22) , N(12)a | 100.11(6) | C(212) , N(21) | 135.88(8) | C(212) , C(115)b | 85.61(7) |
| C(212) , C(14)a | 81.78(7) | C(212) , C(221) | 129.46(7) | C(212) , N(12)a | 93.64(7) | N(21) , C(115)b | 69.20(5) |
| N(21) , C(14)a | 130.57(6) | N(21) , C(221) | 85.34(5) | N(21) , N(12)a | 128.22(5) | C(115)b , C(14)a | 88.24(5) |
| C(115)b , C(221) | 144.18(6) | C(115)b , N(12)a | 109.35(5) | C(14)a , C(221) | 89.96(5) | C(14)a , N(12)a | 23.47(4) |
| C(221) , N(12)a | 66.90(4) | | | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = O(22) [ARU = 1555.02] -0.22606 0.48447 0.13564 -2.8569 6.0811 1.8548

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|--------|---------|
| 1 | 1.430(2) | -- | C(21) | | | | Intra | 22.25 | 12.84 | -0.09535 | 0.52772 | 0.15888 | -1.5667 | 6.6088 | 2.1726 |
| 2 | 1.442(2) | -- | C(221) | | | | Intra | 136.20 | -55.97 | -0.29201 | 0.51843 | 0.04824 | -3.4393 | 6.6397 | 0.6597 |
| 3 | 2.2992(18) | << | O(21) | | | | Intra | -12.91 | 23.95 | -0.02070 | 0.45537 | 0.20390 | -0.8088 | 5.6116 | 2.7882 |
| 4 | 2.390(2) | << | C(22) | | | | Intra | 56.23 | 33.10 | -0.09644 | 0.62321 | 0.23107 | -1.7440 | 7.7454 | 3.1598 |
| 5 | 2.439(2) | << | C(222) | | | | Intra | -131.53 | -82.57 | -0.27270 | 0.44756 | -0.04124 | -3.0659 | 5.8452 | -0.5639 |
| 6 | 2.898(2) | << | C(211) | | | | Intra | -31.61 | 0.78 | 0.00526 | 0.36732 | 0.13853 | -0.3888 | 4.5619 | 1.8943 |
| 7 | 2.900(2) | .< | N(12)a | [-1+x,y,z | = | 1455.01] | | -108.95 | 25.25 | -0.30806 | 0.30222 | 0.22609 | -3.7087 | 3.6004 | 3.0917 |
| 8 | 3.547(3) | .. | C(123)b | [-1+x,y,z | = | 1455.02] | | 168.71 | 32.96 | -0.48510 | 0.54439 | 0.27674 | -5.7751 | 6.6636 | 3.7843 |
| 9 | 2.00 | << | H(22D) | | | | Intra | 159.90 | -33.45 | -0.38620 | 0.52030 | 0.05500 | -4.4243 | 6.6546 | 0.7521 |
| 10 | 2.00 | << | H(22C) | | | | Intra | 100.36 | -40.70 | -0.25850 | 0.58980 | 0.04020 | -3.1297 | 7.5738 | 0.5497 |
| 11 | 2.01(2) | << | H(12)a | [-1+x,y,z | = | 1455.01] | | -108.82 | 22.55 | -0.28480 | 0.35460 | 0.19200 | -3.4557 | 4.3244 | 2.6255 |
| 12 | 2.01 | << | H(21A) | | | | Intra | 26.02 | -14.67 | -0.05810 | 0.54650 | 0.09840 | -1.1092 | 6.9343 | 1.3456 |
| 13 | 2.52 | << | H(22A) | | | | Intra | 79.37 | 22.34 | -0.16290 | 0.66900 | 0.20570 | -2.4269 | 8.3723 | 2.8128 |
| 14 | 2.63 | .< | H(22G) | | | | Intra | -19.86 | -71.92 | -0.17940 | 0.44380 | -0.04690 | -2.0903 | 5.8043 | -0.6413 |
| 15 | 2.64 | .< | H(22B) | | | | Intra | 59.01 | 54.98 | -0.12150 | 0.60160 | 0.29380 | -2.0767 | 7.3802 | 4.0176 |
| 16 | 2.67 | .< | H(22F) | | | | Intra | -116.46 | -61.39 | -0.31130 | 0.37800 | -0.03560 | -3.4260 | 4.9378 | -0.4868 |
| 17 | 2.69 | .< | H(21C) | | | | Intra | -50.93 | -4.35 | -0.07500 | 0.32160 | 0.12070 | -1.1630 | 3.9949 | 1.6505 |
| 18 | 2.94 | .. | H(12N)b | [-1+x,y,z | = | 1455.02] | | -178.41 | 42.10 | -0.41660 | 0.49500 | 0.27980 | -5.0374 | 6.0206 | 3.8261 |
| 19 | 3.16 | .. | H(21B) | | | | Intra | -21.66 | -14.47 | 0.03480 | 0.39110 | 0.07790 | -0.0142 | 4.9523 | 1.0652 |
| 20 | 3.24 | .. | H(12O)b | [-1+x,y,z | = | 1455.02] | | 156.67 | 21.33 | -0.47590 | 0.58610 | 0.22190 | -5.6312 | 7.2779 | 3.0344 |
| 21 | 3.27 | .. | H(22E) | | | | Intra | 161.40 | -79.19 | -0.31490 | 0.47480 | -0.09950 | -3.4390 | 6.2770 | -1.3606 |

Angles (Degrees) At1...V...At2 with Vertex V = O(22)

| | | | | | | | | | | | | | | | |
|--------|---|---------|------------|--------|---|---------|-----------|--------|---|---------|------------|--------|---|---------|------------|
| C(21) | , | C(221) | 113.94(13) | C(21) | , | O(21) | 35.04(8) | C(21) | , | C(22) | 37.00(8) | C(21) | , | C(222) | 109.48(10) |
| C(21) | , | C(211) | 54.69(9) | C(21) | , | N(12)a | 119.08(9) | C(21) | , | C(123)b | 124.13(9) | C(221) | , | O(21) | 140.83(11) |
| C(221) | , | C(22) | 111.77(10) | C(221) | , | C(222) | 35.02(9) | C(221) | , | C(211) | 123.93(10) | C(221) | , | N(12)a | 124.48(10) |
| C(221) | , | C(123)b | 93.15(9) | O(21) | , | C(22) | 60.38(6) | O(21) | , | C(222) | 117.33(7) | O(21) | , | C(211) | 29.42(5) |
| O(21) | , | N(12)a | 85.06(5) | O(21) | , | C(123)b | 123.07(6) | C(22) | , | C(222) | 130.45(8) | C(22) | , | C(211) | 87.77(6) |
| C(22) | , | N(12)a | 119.98(6) | C(22) | , | C(123)b | 88.38(6) | C(222) | , | C(211) | 92.05(7) | C(222) | , | N(12)a | 108.36(7) |
| C(222) | , | C(123)b | 119.00(7) | C(211) | , | N(12)a | 78.23(6) | C(211) | , | C(123)b | 141.20(6) | N(12)a | , | C(123)b | 70.53(5) |

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3.6 Angstrom Coordination Sphere Around Atom I = O(23) [ARU = 1555.02] 0.52602 0.61129 0.36606 4.5132 7.4069 5.0057

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------------------|------------|-----------|--------|-------|---------|--------|---------|---------|---------|--------|--------|--------|
| 1 | 1.376(2) | -- | C(26) | | | | Intra | 133.45 | 3.45 | 0.44065 | 0.68900 | 0.37212 | 3.5690 | 8.4038 | 5.0885 |
| 2 | 1.431(2) | -- | C(123) | | | | Intra | -85.71 | -58.60 | 0.51490 | 0.54439 | 0.27674 | 4.5689 | 6.6636 | 3.7843 |
| 3 | 2.348(2) | << | C(27) | | | | Intra | 117.54 | 32.26 | 0.45926 | 0.75706 | 0.45769 | 3.5952 | 9.1673 | 6.2587 |
| 4 | 2.445(2) | << | C(25) | | | | Intra | 144.93 | -22.48 | 0.34410 | 0.70444 | 0.29771 | 2.6643 | 8.7051 | 4.0710 |
| 5 | 2.7397(19) | << | O(24) | | | | Intra | 89.05 | 54.95 | 0.55992 | 0.75024 | 0.53007 | 4.5394 | 8.9803 | 7.2484 |
| 6 | 2.912(2) | << | C(124) | | | | Intra | 84.75 | 84.20 | 0.56034 | 0.65629 | 0.57794 | 4.5401 | 7.6998 | 7.9030 |
| 7 | 1.99 | << | H(120) | | | | Intra | -32.87 | -83.12 | 0.52410 | 0.58610 | 0.22190 | 4.7128 | 7.2779 | 3.0344 |
| 8 | 1.99 | << | H(12N) | | | | Intra | -60.22 | -36.44 | 0.58340 | 0.49500 | 0.27980 | 5.3066 | 6.0206 | 3.8261 |
| 9 | 1.99 | << | H(12P) | | | | Intra | -122.85 | -42.85 | 0.42940 | 0.50630 | 0.26730 | 3.7235 | 6.1838 | 3.6552 |
| 10 | 2.34 | << | H(12L) | | | | Intra | -48.13 | 77.00 | 0.58170 | 0.59860 | 0.53250 | 4.8639 | 7.0156 | 7.2816 |
| 11 | 2.66 | < | H(25A) | | | | Intra | 158.11 | -40.13 | 0.32940 | 0.65670 | 0.24060 | 2.6248 | 8.1655 | 3.2901 |
| 12 | 3.16 | .. | H(11N)a[x,1+y,z | = | 1565.01] | | | 73.71 | -34.92 | 0.59000 | 0.78970 | 0.23370 | 5.2401 | 9.8952 | 3.1957 |
| 13 | 3.29 | .. | H(11E)c[2-x,1-y,1-z | = | 2766.01] | | | 20.92 | 24.41 | 0.81650 | 0.70460 | 0.46560 | 7.3149 | 8.4780 | 6.3668 |
| 14 | 3.30 | .. | H(11B)b[1-x,1-y,1-z | = | 2666.01] | | | -159.12 | 18.08 | 0.24750 | 0.53270 | 0.44100 | 1.5801 | 6.2881 | 6.0304 |
| 15 | 3.30 | .. | H(12M) | | | | Intra | 175.43 | 74.42 | 0.47410 | 0.64130 | 0.59870 | 3.6290 | 7.4776 | 8.1869 |
| 16 | 3.35 | .. | H(12M)d[1-x,1-y,1-z | = | 2666.02] | | | -87.92 | 8.27 | 0.52590 | 0.35870 | 0.40130 | 4.6334 | 4.0918 | 5.4876 |
| 17 | 3.36 | .. | H(12L)d[1-x,1-y,1-z | = | 2666.02] | | | -111.34 | 24.36 | 0.41830 | 0.40140 | 0.46750 | 3.3985 | 4.5537 | 6.3928 |
| 18 | 3.54 | .. | H(11D)c[2-x,1-y,1-z | = | 2766.01] | | | 42.75 | 7.61 | 0.79180 | 0.79890 | 0.40030 | 7.0873 | 9.7868 | 5.4739 |

Angles (Degrees) At1...V...At2 with Vertex V = O(23)

| | | | | | | | |
|-----------------|------------|----------------|------------|----------------|-----------|----------------|------------|
| C(26) , C(123) | 117.04(14) | C(26) , C(27) | 32.44(9) | C(26) , C(25) | 28.25(9) | C(26) , O(24) | 62.68(9) |
| C(26) , C(124) | 82.74(10) | C(123) , C(27) | 149.36(12) | C(123) , C(25) | 88.80(11) | C(123) , O(24) | 175.35(12) |
| C(123) , C(124) | 154.30(11) | C(27) , C(25) | 60.67(7) | C(27) , O(24) | 30.26(5) | C(27) , C(124) | 52.93(6) |
| C(25) , O(24) | 90.88(6) | C(25) , C(124) | 109.51(7) | O(24) , C(124) | 29.28(5) | | |

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3.6 Angstrom Coordination Sphere Around Atom I = O(24) [ARU = 1555.02] 0.55992 0.75024 0.53007 4.5394 8.9803 7.2484

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|--------------|-----------|----------|-------|---------|--------|---------|---------|---------|--------|---------|---------|
| 1 | 1.381(2) | -- | C(27) | | | | Intra | 168.80 | -45.80 | 0.45926 | 0.75706 | 0.45769 | 3.5952 | 9.1673 | 6.2587 |
| 2 | 1.438(2) | -- | C(124) | | | | Intra | -89.97 | 27.08 | 0.56034 | 0.65629 | 0.57794 | 4.5401 | 7.6998 | 7.9030 |
| 3 | 2.384(2) | << | C(28) | | | | Intra | 145.16 | -21.04 | 0.38087 | 0.84192 | 0.46747 | 2.7132 | 10.2516 | 6.3924 |
| 4 | 2.437(2) | << | C(26) | | | | Intra | -149.29 | -62.41 | 0.44065 | 0.68900 | 0.37212 | 3.5690 | 8.4038 | 5.0885 |
| 5 | 2.6377(19) | << | O(25) | | | | Intra | 131.49 | 7.07 | 0.40558 | 0.90434 | 0.55382 | 2.8052 | 10.9411 | 7.5732 |
| 6 | 2.7397(19) | << | O(23) | | | | Intra | -90.95 | -54.95 | 0.52602 | 0.61129 | 0.36606 | 4.5132 | 7.4069 | 5.0057 |
| 7 | 3.168(2) | .< | C(114)b | [2-x,1-y,1-z | = | 2766.01] | | 8.62 | -17.83 | 0.84034 | 0.77769 | 0.45913 | 7.5211 | 9.4322 | 6.2783 |
| 8 | 3.338(2) | .. | N(11)a | [1-x,1-y,1-z | = | 2666.01] | | 154.87 | 63.87 | 0.46568 | 0.82163 | 0.74920 | 3.2084 | 9.6046 | 10.2449 |
| 9 | 3.473(2) | .. | C(12)a | [1-x,1-y,1-z | = | 2666.01] | | 93.01 | 67.84 | 0.59346 | 0.87621 | 0.76532 | 4.4706 | 10.2885 | 10.4653 |
| 10 | 1.99 | << | H(12K) | | | | Intra | -64.72 | 46.21 | 0.62550 | 0.66500 | 0.63520 | 5.1278 | 7.7343 | 8.6860 |
| 11 | 1.99 | << | H(12L) | | | | Intra | -80.62 | 0.96 | 0.58170 | 0.59860 | 0.53250 | 4.8639 | 7.0156 | 7.2816 |
| 12 | 1.99 | << | H(12M) | | | | Intra | -121.21 | 28.11 | 0.47410 | 0.64130 | 0.59870 | 3.6290 | 7.4776 | 8.1869 |
| 13 | 2.82 | .. | H(11F)b | [2-x,1-y,1-z | = | 2766.01] | | 19.37 | -3.72 | 0.81910 | 0.82090 | 0.51670 | 7.1913 | 9.9125 | 7.0656 |
| 14 | 2.88 | .. | H(12J)c | [1-x,2-y,1-z | = | 2676.02] | | 75.91 | -10.15 | 0.63520 | 0.95870 | 0.49300 | 5.2290 | 11.7272 | 6.7415 |
| 15 | 2.92 | .. | H(12B)a | [1-x,1-y,1-z | = | 2666.01] | | 81.97 | 53.97 | 0.61640 | 0.90010 | 0.70290 | 4.7794 | 10.6827 | 9.6118 |
| 16 | 2.96 | .. | H(11E)b | [2-x,1-y,1-z | = | 2766.01] | | -10.26 | -17.36 | 0.81650 | 0.70460 | 0.46560 | 7.3149 | 8.4780 | 6.3668 |
| 17 | 3.123(19) | .. | H(11)a | [1-x,1-y,1-z | = | 2666.01] | | 153.01 | 49.95 | 0.41640 | 0.83920 | 0.70490 | 2.7490 | 9.8923 | 9.6391 |
| 18 | 3.21 | .. | H(11D)b | [2-x,1-y,1-z | = | 2766.01] | | 17.56 | -33.58 | 0.79180 | 0.79890 | 0.40030 | 7.0873 | 9.7868 | 5.4739 |

Angles (Degrees) At1...V...At2 with Vertex V = O(24)

| | | | | | | | | | | | | | | | |
|--------|---|---------|------------|----------|--------|-----------|------------|--------|-----------|---------|------------|--------|----------|---------|------------|
| C(27) | , | C(124) | 116.57(13) | C(27) | , | C(28) | 31.41(9) | C(27) | , | C(26) | 28.88(9) | C(27) | , | O(25) | 62.48(9) |
| C(27) | , | O(23) | 58.96(9) | C(27) | , | C(114)b | 113.88(10) | C(27) | , | N(11)a | 110.22(10) | C(27) | , | C(12)a | 126.83(10) |
| C(124) | , | C(28) | 129.69(11) | C(124) | , | C(26) | 101.13(11) | C(124) | , | O(25) | 127.31(11) | C(124) | , | O(23) | 82.03(10) |
| C(124) | , | C(114)b | 105.42(10) | C(124) | , | N(11)a | 76.00(9) | C(124) | , | C(12)a | 85.06(10) | C(28) | , | C(26) | 60.19(6) |
| C(28) | , | O(25) | 31.15(5) | C(28) | , | O(23) | 90.28(6) | C(28) | , | C(114)b | 122.34(7) | C(28) | , | N(11)a | 85.25(6) |
| C(28) | , | C(12)a | 96.69(6) | C(26) | , | O(25) | 91.33(6) | C(26) | , | O(23) | 30.10(5) | C(26) | , | C(114)b | 97.88(7) |
| C(26) | , | N(11)a | 132.93(7) | C(26) | , | C(12)a | 154.43(7) | O(25) | , | O(23) | 121.43(6) | O(25) | , | C(114)b | 123.40(6) |
| O(25) | , | N(11)a | 59.22(4) | O(25) | , | C(12)a | 65.98(5) | O(23) | , | C(114)b | 80.81(6) | O(23) | , | N(11)a | 146.98(6) |
| O(23) | , | C(12)a | 166.97(6) | C(114)b, | N(11)a | 128.58(6) | C(114)b, | C(12)a | 104.39(6) | N(11)a | , | C(12)a | 24.52(4) | | |

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3.6 Angstrom Coordination Sphere Around Atom I = N(11) [ARU = 1555.01] 0.53432 0.17837 0.25080 5.0540 1.9648 3.4296

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|--------------|-----------|----------|-------|---------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 0.81(2) | -- | H(11) | | | | Intra | -32.06 | 48.18 | 0.58360 | 0.16080 | 0.29510 | 5.5134 | 1.6770 | 4.0353 |
| 2 | 1.341(2) | -- | C(13) | | | | Intra | 69.38 | -31.75 | 0.57117 | 0.25542 | 0.19920 | 5.4555 | 3.0318 | 2.7239 |
| 3 | 1.452(2) | -- | C(12) | | | | Intra | -151.55 | -8.73 | 0.40654 | 0.12379 | 0.23468 | 3.7918 | 1.2808 | 3.2091 |
| 4 | 2.300(2) | << | N(12) | | | | Intra | 45.97 | -8.45 | 0.69194 | 0.30222 | 0.22609 | 6.6353 | 3.6004 | 3.0917 |
| 5 | 2.464(2) | << | C(11) | | | | Intra | -122.82 | -30.78 | 0.40127 | 0.03112 | 0.15860 | 3.9069 | 0.1860 | 2.1688 |
| 6 | 2.6772(18) | << | S(1) | | | | Intra | 105.82 | -47.89 | 0.47503 | 0.29658 | 0.10556 | 4.5647 | 3.6920 | 1.4435 |
| 7 | 2.784(2) | << | C(14) | | | | Intra | 27.10 | 16.25 | 0.77862 | 0.27852 | 0.30776 | 7.4332 | 3.1824 | 4.2084 |
| 8 | 2.918(2) | <. | O(11) | | | | Intra | -97.44 | -14.29 | 0.47721 | -0.04395 | 0.19813 | 4.6877 | -0.8389 | 2.7093 |
| 9 | 3.014(2) | <. | O(25)a | [1-x,1-y,1-z | = | 2666.02] | | -73.21 | 62.41 | 0.59442 | 0.09566 | 0.44618 | 5.4572 | 0.6283 | 6.1013 |
| 10 | 3.151(2) | <. | C(15) | | | | Intra | 0.08 | 13.23 | 0.83843 | 0.18428 | 0.30354 | 8.1216 | 1.9692 | 4.1507 |
| 11 | 3.299(3) | .. | C(124)a | [1-x,1-y,1-z | = | 2666.02] | | 124.96 | 45.22 | 0.43966 | 0.34371 | 0.42206 | 3.7223 | 3.8695 | 5.7714 |
| 12 | 3.338(2) | .. | O(24)a | [1-x,1-y,1-z | = | 2666.02] | | 154.87 | 63.87 | 0.44008 | 0.24976 | 0.46993 | 3.7230 | 2.5890 | 6.4260 |
| 13 | 2.01 | << | H(12B) | | | | Intra | -145.54 | 18.38 | 0.38360 | 0.09990 | 0.29710 | 3.4830 | 0.8866 | 4.0627 |
| 14 | 2.01 | << | H(12A) | | | | Intra | -179.24 | -14.84 | 0.34120 | 0.17240 | 0.21320 | 3.1132 | 1.9389 | 2.9154 |
| 15 | 2.63 | <. | H(11J) | | | | Intra | -116.93 | -52.68 | 0.43540 | 0.05220 | 0.09770 | 4.3312 | 0.5418 | 1.3360 |
| 16 | 2.99 | .. | H(12M)a | [1-x,1-y,1-z | = | 2666.02] | | 101.18 | 43.51 | 0.52590 | 0.35870 | 0.40130 | 4.6334 | 4.0918 | 5.4876 |
| 17 | 3.06 | .. | H(15A) | | | | Intra | -10.17 | -1.02 | 0.82260 | 0.13610 | 0.24680 | 8.0702 | 1.4235 | 3.3749 |
| 18 | 3.10(2) | .. | H(12) | | | | Intra | 52.14 | -15.06 | 0.71520 | 0.35460 | 0.19200 | 6.8883 | 4.3244 | 2.6255 |
| 19 | 3.10 | .. | H(12K)a | [1-x,1-y,1-z | = | 2666.02] | | 135.74 | 30.19 | 0.37450 | 0.33500 | 0.36480 | 3.1346 | 3.8350 | 4.9884 |
| 20 | 3.59 | .. | H(12H)a | [1-x,1-y,1-z | = | 2666.02] | | -72.55 | 28.67 | 0.62840 | -0.04070 | 0.37680 | 5.9985 | -1.0407 | 5.1525 |

Angles (Degrees) At1...V...At2 with Vertex V = N(11)

| | | | | | | | | | | | | | | | |
|-------|---|---------|------------|--------|---|---------|------------|---------|---|---------|------------|--------|---|---------|-----------|
| C(13) | , | C(12) | 123.72(15) | C(13) | , | N(12) | 31.88(9) | C(13) | , | C(11) | 116.40(12) | C(13) | , | S(1) | 31.88(8) |
| C(13) | , | C(14) | 62.82(10) | C(13) | , | O(11) | 132.25(11) | C(13) | , | O(25)a | 141.19(12) | C(13) | , | C(15) | 80.09(10) |
| C(13) | , | C(124)a | 92.00(10) | C(13) | , | O(24)a | 116.30(11) | C(12) | , | N(12) | 155.51(12) | C(12) | , | C(11) | 34.68(9) |
| C(12) | , | S(1) | 91.86(10) | C(12) | , | C(14) | 172.37(12) | C(12) | , | O(11) | 53.20(8) | C(12) | , | O(25)a | 92.41(10) |
| C(12) | , | C(15) | 151.81(11) | C(12) | , | C(124)a | 91.65(10) | C(12) | , | O(24)a | 82.98(9) | N(12) | , | C(11) | 139.32(9) |
| N(12) | , | S(1) | 63.76(5) | N(12) | , | C(14) | 30.96(5) | N(12) | , | O(11) | 137.17(8) | N(12) | , | O(25)a | 110.70(7) |
| N(12) | , | C(15) | 50.46(6) | N(12) | , | C(124)a | 88.35(7) | N(12) | , | O(24)a | 105.85(7) | C(11) | , | S(1) | 90.06(6) |
| C(11) | , | C(14) | 148.97(8) | C(11) | , | O(11) | 28.53(5) | C(11) | , | O(25)a | 101.29(7) | C(11) | , | C(15) | 124.85(7) |
| C(11) | , | C(124)a | 126.31(8) | C(11) | , | O(24)a | 114.13(7) | S(1) | , | C(14) | 94.68(6) | S(1) | , | O(11) | 114.45(6) |
| S(1) | , | O(25)a | 165.47(6) | S(1) | , | C(15) | 110.29(6) | S(1) | , | C(124)a | 94.61(5) | S(1) | , | O(24)a | 118.20(5) |
| C(14) | , | O(11) | 126.63(7) | C(14) | , | O(25)a | 80.31(6) | C(14) | , | C(15) | 26.28(5) | C(14) | , | C(124)a | 83.91(6) |
| C(14) | , | O(24)a | 90.45(6) | O(11) | , | O(25)a | 79.02(5) | O(11) | , | C(15) | 100.37(6) | O(11) | , | C(124)a | 132.79(6) |
| O(11) | , | O(24)a | 110.57(5) | O(25)a | , | C(15) | 70.58(5) | O(25)a | , | C(124)a | 71.39(5) | O(25)a | , | O(24)a | 48.74(4) |
| C(15) | , | C(124)a | 103.28(6) | C(15) | , | O(24)a | 100.51(6) | C(124)a | , | O(24)a | 25.02(4) | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = N(12) [ARU = 1555.01] 0.69194 0.30222 0.22609 6.6353 3.6004 3.0917

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|--------------|-----------|----------|-------|---------|--------|---------|---------|---------|--------|--------|--------|
| 1 | 0.90(2) | -- | H(12) | | | | Intra | 70.74 | -31.29 | 0.71520 | 0.35460 | 0.19200 | 6.8883 | 4.3244 | 2.6255 |
| 2 | 1.360(2) | -- | C(13) | | | | Intra | -154.27 | -15.68 | 0.57117 | 0.25542 | 0.19920 | 5.4555 | 3.0318 | 2.7239 |
| 3 | 1.435(2) | -- | C(14) | | | | Intra | -27.65 | 51.11 | 0.77862 | 0.27852 | 0.30776 | 7.4332 | 3.1824 | 4.2084 |
| 4 | 2.300(2) | << | N(11) | | | | Intra | -134.03 | 8.45 | 0.53432 | 0.17837 | 0.25080 | 5.0540 | 1.9648 | 3.4296 |
| 5 | 2.437(2) | << | C(19) | | | | Intra | 24.55 | 66.57 | 0.80251 | 0.35060 | 0.38962 | 7.5166 | 4.0029 | 5.3278 |
| 6 | 2.448(2) | << | C(15) | | | | Intra | -47.66 | 25.64 | 0.83843 | 0.18428 | 0.30354 | 8.1216 | 1.9692 | 4.1507 |
| 7 | 2.6481(18) | << | S(1) | | | | Intra | 177.47 | -38.49 | 0.47503 | 0.29658 | 0.10556 | 4.5647 | 3.6920 | 1.4435 |
| 8 | 2.900(2) | .< | O(22)a | [1+x,y,z | = | 1655.02] | | 71.05 | -25.25 | 0.77394 | 0.48447 | 0.13564 | 7.4871 | 6.0811 | 1.8548 |
| 9 | 3.542(2) | .. | O(21)a | [1+x,y,z | = | 1655.02] | | 34.74 | -4.91 | 0.97930 | 0.45537 | 0.20390 | 9.5352 | 5.6116 | 2.7882 |
| 10 | 2.42(2) | << | H(11) | | | | Intra | -120.25 | 22.97 | 0.58360 | 0.16080 | 0.29510 | 5.5134 | 1.6770 | 4.0353 |
| 11 | 2.61 | .< | H(19A) | | | | Intra | 71.17 | 60.01 | 0.76240 | 0.41500 | 0.39120 | 7.0558 | 4.8338 | 5.3494 |
| 12 | 2.62 | .< | H(15A) | | | | Intra | -56.61 | 6.20 | 0.82260 | 0.13610 | 0.24680 | 8.0702 | 1.4235 | 3.3749 |
| 13 | 2.86 | .. | H(12N) | [| = | 02] | | 118.77 | 14.90 | 0.58340 | 0.49500 | 0.27980 | 5.3066 | 6.0206 | 3.8261 |
| 14 | 2.95 | .. | H(21C)a | [1+x,y,z | = | 1655.02] | | 8.81 | -29.22 | 0.92500 | 0.32160 | 0.12070 | 9.1810 | 3.9949 | 1.6505 |
| 15 | 3.16 | .. | H(12M)b | [1-x,1-y,1-z | = | 2666.02] | | 166.21 | 49.29 | 0.52590 | 0.35870 | 0.40130 | 4.6334 | 4.0918 | 5.4876 |

Angles (Degrees) At1...V...At2 with Vertex V = N(12)

| | | | | | | | | | | | | | | | |
|-------|---|--------|------------|-------|---|--------|------------|-------|---|--------|------------|--------|---|--------|------------|
| C(13) | , | C(14) | 124.82(15) | C(13) | , | N(11) | 31.37(9) | C(13) | , | C(19) | 129.10(12) | C(13) | , | C(15) | 111.41(12) |
| C(13) | , | S(1) | 33.70(8) | C(13) | , | O(22)a | 119.81(11) | C(13) | , | O(21)a | 157.55(11) | C(14) | , | N(11) | 93.49(11) |
| C(14) | , | C(19) | 29.87(9) | C(14) | , | C(15) | 29.70(9) | C(14) | , | S(1) | 158.34(11) | C(14) | , | O(22)a | 114.70(10) |
| C(14) | , | O(21)a | 77.10(9) | N(11) | , | C(19) | 103.37(8) | N(11) | , | C(15) | 83.11(7) | N(11) | , | S(1) | 65.07(5) |
| N(11) | , | O(22)a | 150.81(8) | N(11) | , | O(21)a | 168.31(7) | C(19) | , | C(15) | 59.57(7) | C(19) | , | S(1) | 148.01(8) |
| C(19) | , | O(22)a | 98.27(7) | C(19) | , | O(21)a | 71.87(6) | C(15) | , | S(1) | 140.10(8) | C(15) | , | O(22)a | 125.19(7) |
| C(15) | , | O(21)a | 85.31(6) | S(1) | , | O(22)a | 86.25(5) | S(1) | , | O(21)a | 124.56(6) | O(22)a | , | O(21)a | 40.29(4) |

=====

3.6 Angstrom Coordination Sphere Around Atom I = N(21) [ARU = 1555.02] 0.02937 0.68124 0.24857 -0.5065 8.4721 3.3991

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|--------------|-----------|----------|-------|---------|--------|----------|---------|---------|---------|---------|--------|
| 1 | 0.86(2) | -- | H(21) | | | | Intra | -25.41 | 59.03 | 0.07450 | 0.67230 | 0.30220 | -0.1090 | 8.2832 | 4.1324 |
| 2 | 1.343(2) | -- | C(23) | | | | Intra | 70.41 | -32.28 | 0.06409 | 0.75840 | 0.19613 | -0.1259 | 9.5417 | 2.6820 |
| 3 | 1.455(2) | -- | C(22) | | | | Intra | -149.58 | -9.47 | -0.09644 | 0.62321 | 0.23107 | -1.7440 | 7.7454 | 3.1598 |
| 4 | 2.290(2) | << | N(22) | | | | Intra | 48.89 | -7.37 | 0.17929 | 0.81124 | 0.22709 | 0.9864 | 10.1828 | 3.1053 |
| 5 | 2.470(2) | << | C(21) | | | | Intra | -119.64 | -29.77 | -0.09535 | 0.52772 | 0.15888 | -1.5667 | 6.6088 | 2.1726 |
| 6 | 2.6749(18) | << | S(2) | | | | Intra | 105.95 | -50.63 | -0.02902 | 0.79140 | 0.09734 | -0.9726 | 10.1033 | 1.3311 |
| 7 | 2.800(2) | << | C(24) | | | | Intra | 29.67 | 16.81 | 0.26964 | 0.79005 | 0.30776 | 1.8220 | 9.7987 | 4.2084 |
| 8 | 2.941(2) | <. | O(21) | | | | Intra | -96.03 | -11.99 | -0.02070 | 0.45537 | 0.20390 | -0.8088 | 5.6116 | 2.7882 |
| 9 | 2.976(2) | <. | O(15)b | [1-x,1-y,1-z | = | 2666.01] | | -73.93 | 64.91 | 0.08512 | 0.60829 | 0.44566 | -0.1573 | 7.2595 | 6.0942 |
| 10 | 3.124(2) | .. | O(14)b | [1-x,1-y,1-z | = | 2666.01] | | 128.03 | 62.53 | -0.02180 | 0.79040 | 0.45129 | -1.3945 | 9.6073 | 6.1711 |
| 11 | 3.250(3) | <. | C(25) | | | | Intra | 4.20 | 11.93 | 0.34410 | 0.70444 | 0.29771 | 2.6643 | 8.7051 | 4.0710 |
| 12 | 2.01 | << | H(22B) | | | | Intra | -145.19 | 17.92 | -0.12150 | 0.60160 | 0.29380 | -2.0767 | 7.3802 | 4.0176 |
| 13 | 2.01 | << | H(22A) | | | | Intra | -177.03 | -16.95 | -0.16290 | 0.66900 | 0.20570 | -2.4269 | 8.3723 | 2.8128 |
| 14 | 2.64 | <. | H(21A) | | | | Intra | -111.40 | -51.19 | -0.05810 | 0.54650 | 0.09840 | -1.1092 | 6.9343 | 1.3456 |
| 15 | 3.015(18) | .. | H(22) | | | | Intra | 55.08 | -13.98 | 0.19580 | 0.86110 | 0.19530 | 1.1681 | 10.8711 | 2.6706 |
| 16 | 3.15 | .. | H(25A) | | | | Intra | -5.59 | -1.98 | 0.32940 | 0.65670 | 0.24060 | 2.6248 | 8.1655 | 3.2901 |
| 17 | 3.34 | .. | H(11G)a | [-1+x,1+y,z | = | 1465.01] | | 99.83 | 17.37 | 0.00310 | 0.93150 | 0.32140 | -1.0500 | 11.6096 | 4.3950 |
| 18 | 3.42 | .. | H(11A)b | [1-x,1-y,1-z | = | 2666.01] | | -71.10 | 29.48 | 0.12580 | 0.47670 | 0.37150 | 0.4568 | 5.6587 | 5.0801 |

Angles (Degrees) At1...V...At2 with Vertex V = N(21)

| | | | | | | | |
|----------------|------------|----------------|------------|-----------------|------------|----------------|------------|
| C(23) , C(22) | 123.44(14) | C(23) , N(22) | 31.95(9) | C(23) , C(21) | 117.22(12) | C(23) , S(2) | 31.87(8) |
| C(23) , C(24) | 62.69(10) | C(23) , O(21) | 133.87(11) | C(23) , O(15)b | 140.80(11) | C(23) , O(14)b | 105.36(10) |
| C(23) , C(25) | 77.10(10) | C(22) , N(22) | 155.06(12) | C(22) , C(21) | 34.55(8) | C(22) , S(2) | 91.67(9) |
| C(22) , C(24) | 172.63(12) | C(22) , O(21) | 52.59(8) | C(22) , O(15)b | 92.59(10) | C(22) , O(14)b | 94.92(10) |
| C(22) , C(25) | 154.13(11) | N(22) , C(21) | 141.25(9) | N(22) , S(2) | 63.82(5) | N(22) , C(24) | 30.75(5) |
| N(22) , O(21) | 140.11(8) | N(22) , O(15)b | 110.13(7) | N(22) , O(14)b | 91.59(6) | N(22) , C(25) | 48.45(6) |
| C(21) , S(2) | 90.08(6) | C(21) , C(24) | 149.11(8) | C(21) , O(21) | 28.22(5) | C(21) , O(15)b | 101.11(7) |
| C(21) , O(14)b | 126.35(7) | C(21) , C(25) | 125.14(7) | S(2) , C(24) | 94.56(6) | S(2) , O(21) | 114.50(6) |
| S(2) , O(15)b | 165.72(6) | S(2) , O(14)b | 114.51(5) | S(2) , C(25) | 106.63(6) | C(24) , O(21) | 127.34(7) |
| C(24) , O(15)b | 80.42(6) | C(24) , O(14)b | 78.91(5) | C(24) , C(25) | 25.13(5) | O(21) , O(15)b | 78.69(5) |
| O(21) , O(14)b | 120.57(6) | O(21) , C(25) | 102.30(6) | O(15)b , O(14)b | 51.53(4) | O(15)b , C(25) | 74.18(5) |
| O(14)b , C(25) | 93.89(5) | | | | | | |

=====

3.6 Angstrom Coordination Sphere Around Atom I = N(22) [ARU = 1555.02] 0.17929 0.81124 0.22709 0.9864 10.1828 3.1053

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|-------------|-----------|----------|-------|---------|--------|----------|---------|---------|---------|---------|--------|
| 1 | 0.834(18) | -- | H(22) | | | | Intra | 75.21 | -31.41 | 0.19580 | 0.86110 | 0.19530 | 1.1681 | 10.8711 | 2.6706 |
| 2 | 1.352(2) | -- | C(23) | | | | Intra | -150.04 | -18.25 | 0.06409 | 0.75840 | 0.19613 | -0.1259 | 9.5417 | 2.6820 |
| 3 | 1.436(2) | -- | C(24) | | | | Intra | -24.69 | 50.18 | 0.26964 | 0.79005 | 0.30776 | 1.8220 | 9.7987 | 4.2084 |
| 4 | 2.290(2) | << | N(21) | | | | Intra | -131.11 | 7.37 | 0.02937 | 0.68124 | 0.24857 | -0.5065 | 8.4721 | 3.3991 |
| 5 | 2.436(2) | << | C(25) | | | | Intra | -41.37 | 23.36 | 0.34410 | 0.70444 | 0.29771 | 2.6643 | 8.7051 | 4.0710 |
| 6 | 2.444(2) | << | C(29) | | | | Intra | 24.99 | 67.48 | 0.28686 | 0.85923 | 0.39216 | 1.8348 | 10.5782 | 5.3626 |
| 7 | 2.6443(18) | << | S(2) | | | | Intra | -177.68 | -42.14 | -0.02902 | 0.79140 | 0.09734 | -0.9726 | 10.1033 | 1.3311 |
| 8 | 2.882(2) | .< | O(12)a | [x,1+y,z | = | 1565.01] | | 68.89 | -25.10 | 0.26970 | 0.99002 | 0.13771 | 1.9261 | 12.6172 | 1.8831 |
| 9 | 3.525(3) | .. | C(113)b | [-1+x,1+y,z | = | 1465.01] | | 137.27 | 17.68 | -0.03650 | 0.99569 | 0.30538 | -1.4805 | 12.4617 | 4.1759 |
| 10 | 2.42(2) | << | H(21) | | | | Intra | -119.97 | 25.10 | 0.07450 | 0.67230 | 0.30220 | -0.1090 | 8.2832 | 4.1324 |
| 11 | 2.61 | .< | H(25A) | | | | Intra | -50.92 | 4.07 | 0.32940 | 0.65670 | 0.24060 | 2.6248 | 8.1655 | 3.2901 |
| 12 | 2.62 | .< | H(29A) | | | | Intra | 76.93 | 63.43 | 0.23510 | 0.91750 | 0.39830 | 1.2513 | 11.3235 | 5.4465 |
| 13 | 2.80 | .. | H(11G)b | [-1+x,1+y,z | = | 1465.01] | | 144.98 | 27.41 | 0.00310 | 0.93150 | 0.32140 | -1.0500 | 11.6096 | 4.3950 |
| 14 | 3.03 | .. | H(11L)a | [x,1+y,z | = | 1565.01] | | 6.49 | -29.98 | 0.41700 | 0.82250 | 0.11640 | 3.5932 | 10.4796 | 1.5917 |
| 15 | 3.37 | .. | H(11H)b | [-1+x,1+y,z | = | 1465.01] | | 126.34 | 5.58 | 0.00400 | 1.02290 | 0.25110 | -1.0038 | 12.8877 | 3.4337 |

Angles (Degrees) At1...V...At2 with Vertex V = N(22)

| | | | | | | | | | | | | | | | |
|-------|---|---------|------------|-------|---|---------|------------|-------|---|---------|------------|--------|---|---------|------------|
| C(23) | , | C(24) | 126.33(15) | C(23) | , | N(21) | 31.71(9) | C(23) | , | C(25) | 113.78(12) | C(23) | , | C(29) | 130.67(12) |
| C(23) | , | S(2) | 33.49(8) | C(23) | , | O(12)a | 122.42(11) | C(23) | , | C(113)b | 79.97(10) | C(24) | , | N(21) | 94.64(11) |
| C(24) | , | C(25) | 29.81(9) | C(24) | , | C(29) | 29.75(8) | C(24) | , | S(2) | 159.78(12) | C(24) | , | O(12)a | 111.23(11) |
| C(24) | , | C(113)b | 110.30(10) | N(21) | , | C(25) | 86.85(8) | N(21) | , | C(29) | 103.23(8) | N(21) | , | S(2) | 65.20(6) |
| N(21) | , | O(12)a | 153.94(8) | N(21) | , | C(113)b | 89.30(7) | C(25) | , | C(29) | 59.52(7) | C(25) | , | S(2) | 139.31(8) |
| C(25) | , | O(12)a | 117.14(7) | C(25) | , | C(113)b | 138.94(8) | C(29) | , | S(2) | 151.87(8) | C(29) | , | O(12)a | 98.16(7) |
| C(29) | , | C(113)b | 81.83(6) | S(2) | , | O(12)a | 88.99(5) | S(2) | , | C(113)b | 72.83(5) | O(12)a | , | C(113)b | 79.10(5) |

=====
Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6
=====

van der Waals (or ion) Radii used in the Analysis

=====
C H N O S

1.70 1.20 1.55 1.52 1.80

:: Grid: X-Axis Step = 0.0208 = Points 48, Angstrom Step = 0.22
:: Grid: Y-Axis Step = 0.0167 = Points 60, Angstrom Step = 0.22
:: Grid: Z-Axis Step = 0.0139 = Points 72, Angstrom Step = 0.19

:: Unit cell Contains NO Residual Solvent Accessible Void.

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

=====
Report Expected Number of Independent Reflections for given Symmetry and Resolution.

:: Hmax = 14 Kmax = 18 Lmax= 19 , Sorting Order : Fast H, Medium K, Slow L

:: Actual Theta-Max: 30.357 Deg. (Applied Theta Limit: 30.360 Deg.)

Space Group H-M: P-1 Laue: -1
Space Group Hall: -P 1 [Schoenflies: Ci^1]
Lattice Type: aP, Centric, Triclinic, Multiplicity: 2(1), No: 2

Nr ***** Symmetry Operation(s) *****

| | | | |
|---|-------|-------|-----|
| 1 | H , | K , | L |
| 2 | - H , | - K , | - L |

:: Number of Independent Type H, K, L Reflections = 11013

Table 0 - Crystal Data and Details of the Structure Determination
for: tdaome3ph P-1 R = 0.05

Crystal Data

| | | | |
|--------------------------|--------------------|-----------|-----------|
| Formula | C16 H26 N2 O5 S | | |
| Formula Weight | 358.46 | | |
| Crystal System | triclinic | | |
| Space group | P-1 | (No. 2) | |
| a, b, c [Angstrom] | 10.344(3) | 12.952(4) | 13.814(4) |
| alpha, beta, gamma [deg] | 95.357(4) | 95.836(4) | 92.996(4) |
| V [Ang**3] | 1829.5(9) | | |
| Z | 4 | | |
| D(calc) [g/cm**3] | 1.301 | | |
| Mu(MoKa) [/mm] | 0.204 | | |
| F(000) | 768 | | |
| Crystal Size [mm] | 0.09 x 0.42 x 0.76 | | |

Data Collection

| | | | |
|----------------------------------|-----------------------------|---------|-------|
| Temperature (K) | 150 | | |
| Radiation [Angstrom] | MoKa | 0.71073 | |
| Theta Min-Max [Deg] | 1.5, 30.4 | | |
| Dataset | -14: 14 ; -18: 18 ; -19: 19 | | |
| Tot., Uniq. Data, R(int) | 28972, | 10893, | 0.055 |
| Observed Data [I > 2.0 sigma(I)] | 6156 | | |

Refinement

| | | | |
|-------------------------------------|--------------------------|--|--|
| Nref, Npar | 10893, 459 | | |
| R, wR2, S | 0.0498, 0.1356, 1.03 | | |
| w = 1/[\s^2^(Fo^2^)+(0.0514P)^2^] | where P=(Fo^2^+2Fc^2^)/3 | | |
| Max. and Av. Shift/Error | 0.00, 0.00 | | |
| Min. and Max. Resd. Dens. [e/Ang^3] | -0.35, 0.35 | | |

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***** N O T I C E *****

=====

- PLATON Reference : Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.
Spek, A.L. (2009). Acta Cryst. D65, 148-155.

- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow

- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)

- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.

- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.

- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@uu.nl

- Recent versions of PLATON may be obtained from <http://www.platonsoft.nl/xraysoft>

- More INFO can be found on <http://http://www.platonsoft.nl/>

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Page 116 --- VOIDS
Page 117 --- EXPECT
Page 118 --- SUMMARY

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR
=====

W: NOMOVE option used.

:: >>> WARNING: 'CONNECTED INPUT SET' is assumed to be TRUE

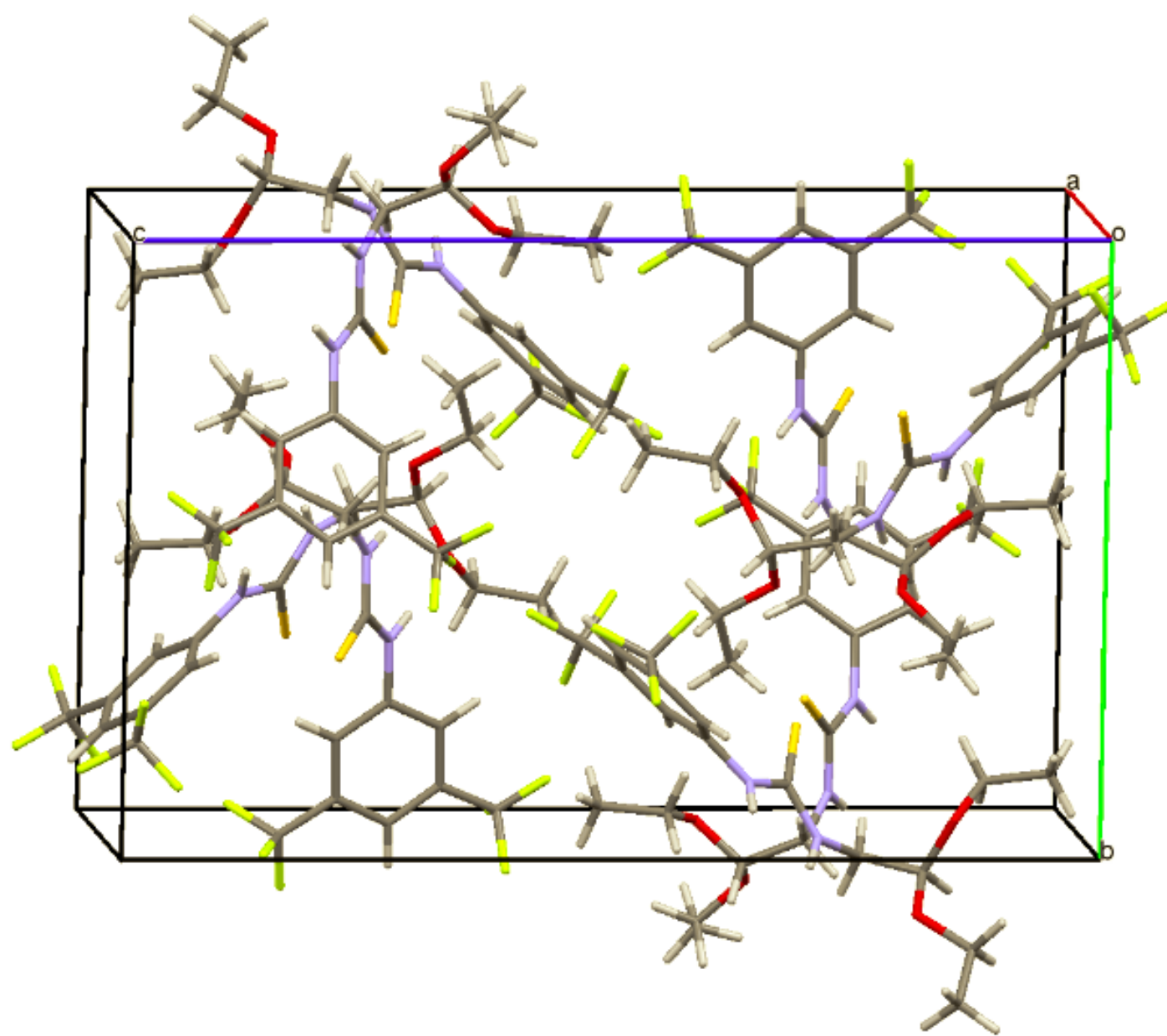
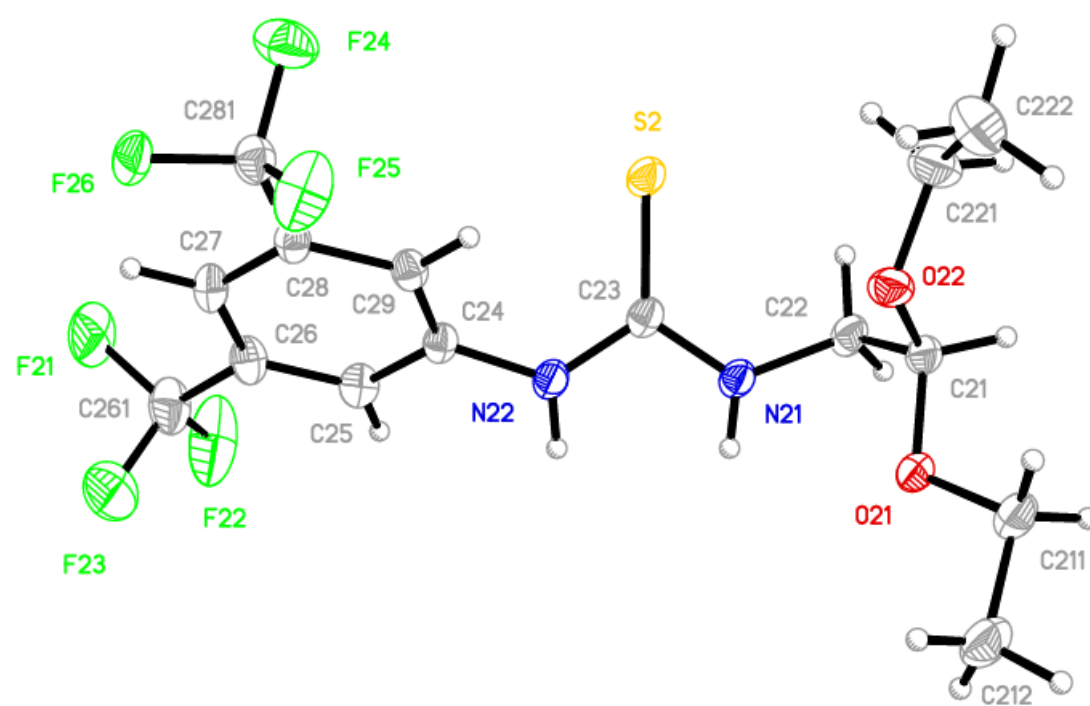
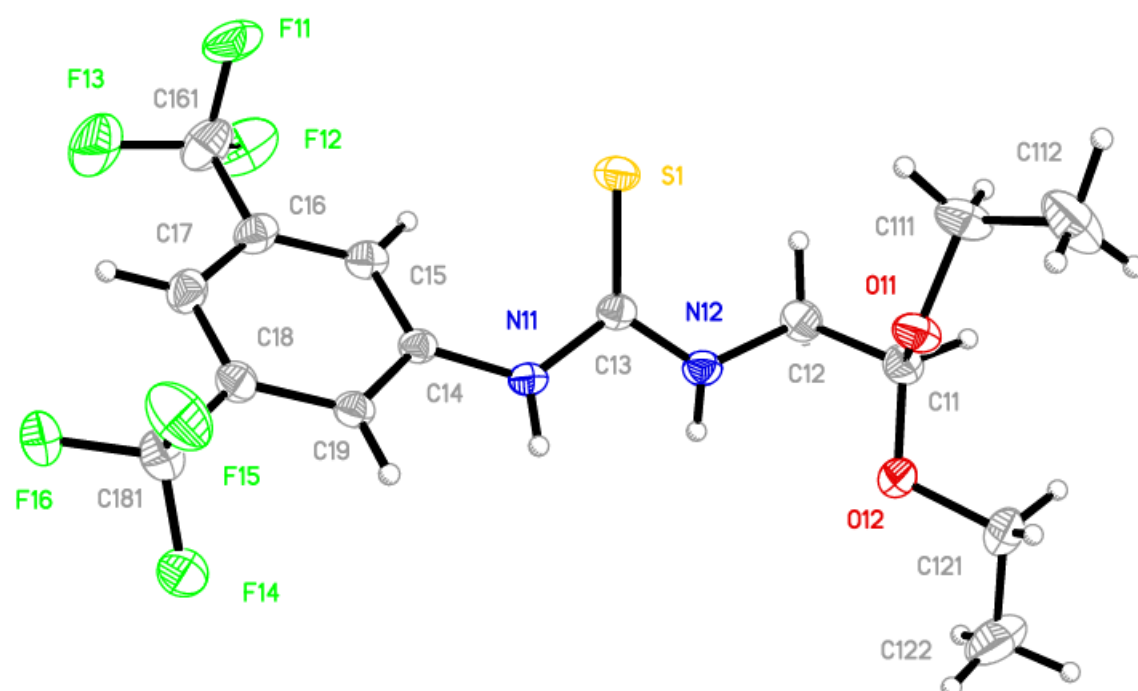
:: >>> The Network Analysis may be INCORRECT when this assumption is FALSE

=====

:: Input Xtal Data from File tdaome3ph.cif - Data Type CIF

:: NORMAL END of PLATON : 120 Pages on:
:: tdaome3ph.lis (ASCII, 132 Characters Wide)
:: tdaome3ph.lps (PostScript Version of .lis)
::

H₂detu^{Ar(CF₃)₂}



=====
 Analysis of Short Intra- and Inter-molecular Contacts , $d(I-J) < R(I) + R(J) + Tolr$, With Tolr = 0.2 Ang. ($X - I...J > 100$. Deg.

Contact Radii : C H F N O S
 (Angstrom) 1.70 1.20 1.47 1.55 1.52 1.80

Default Contact Radii are those given by A.Bondi, J.Phys.Chem. (1964),68,441. (or Coval. Rad. + 0.8 Ang. when not given)

* WARNING * : no Far-Reaching Conclusions should be drawn based on the Default Radii Assigned to Metals

Short "INTRA" Distances between two Atoms that are Separated by less than 4 Bonds are NOT Listed (Except for Potential D/A Contacts)

=====
 ***** ARU = 1555.01 *****
 =====

| At(I)[1555.01] | At(J) | [ARU(J)] | D(I-J) | SumRad | Del | Type | X(I) | Y(I) | Z(I) | X(J) | Y(J) | Z(J) | X | X - I...J |
|----------------|--------------|------------|--------------|--------|-------|-------|--------|--------|---------|--------|---------|---------|--------|------------|
| S(1) | C(12) | [] | 3.114(2)<< | 3.50 | -0.39 | Intra | 0.2650 | 0.3038 | 0.1979 | 0.3024 | 0.5101 | 0.2631 | | |
| S(1) | C(14) | [] | 3.1646(19)<< | 3.50 | -0.34 | Intra | 0.2650 | 0.3038 | 0.1979 | 0.4245 | 0.3069 | 0.0984 | | |
| S(1) | C(15) | [] | 3.204(2)<< | 3.50 | -0.30 | Intra | 0.2650 | 0.3038 | 0.1979 | 0.3300 | 0.2737 | 0.0621 | | |
| S(1) | H(12A) | [] | 2.60<< | 3.00 | -0.40 | Intra | 0.2650 | 0.3038 | 0.1979 | 0.2480 | 0.4585 | 0.2680 | | |
| S(1) | H(15A) | [] | 2.80<< | 3.00 | -0.20 | Intra | 0.2650 | 0.3038 | 0.1979 | 0.2622 | 0.2991 | 0.0689 | | |
| S(1) | <F(21B) | [2555.02] | 3.458(13) | 3.27 | 0.19 | | 0.2650 | 0.3038 | 0.1979 | 0.1235 | 0.4745 | 0.0975 | | |
| >F(14A) | C(19) | [] | 2.895(9)<< | 3.17 | -0.28 | Intra | 0.6943 | 0.2378 | 0.0142 | 0.5225 | 0.2705 | 0.0868 | | |
| >F(14A) | C(222) | [] | 3.290(9) | 3.17 | 0.12 | | 0.6943 | 0.2378 | 0.0142 | 0.6718 | 0.4810 | 0.0255 | C(181) | 132.3(5) |
| >F(14A) | H(19A) | [] | 2.76 | 2.67 | 0.09 | Intra | 0.6943 | 0.2378 | 0.0142 | 0.5876 | 0.2935 | 0.1108 | | |
| >F(14A) | H(22G) | [] | 2.76 | 2.67 | 0.09 | | 0.6943 | 0.2378 | 0.0142 | 0.6161 | 0.4294 | 0.0182 | C(181) | 119 |
| >F(14A) | H(21D) | [3665.02] | 2.76 | 2.67 | 0.09 | | 0.6943 | 0.2378 | 0.0142 | 0.6496 | 0.2439 | -0.1144 | C(181) | 104 |
| >F(14A) | H(11D) | [4554.01] | 2.46<< | 2.67 | -0.21 | | 0.6943 | 0.2378 | 0.0142 | 0.8528 | 0.1757 | -0.0277 | C(181) | 111 |
| >F(15A) | C(19) | [] | 2.925(7)<< | 3.17 | -0.25 | Intra | 0.6923 | 0.1230 | 0.0812 | 0.5225 | 0.2705 | 0.0868 | | |
| >F(15A) | H(19A) | [] | 2.76 | 2.67 | 0.09 | Intra | 0.6923 | 0.1230 | 0.0812 | 0.5876 | 0.2935 | 0.1108 | | |
| >F(15A) | <F(24A) | [] | 2.76(2) < | 2.94 | -0.18 | | 0.6923 | 0.1230 | 0.0812 | 0.5688 | 0.0134 | 0.1513 | C(181) | 112.1(5) |
| >F(15A) | <F(24B) | [] | 2.91(2) < | 2.94 | -0.03 | | 0.6923 | 0.1230 | 0.0812 | 0.5791 | -0.0030 | 0.1591 | C(181) | 116.6(6) |
| >F(15A) | H(12G) | [2645.01] | 2.86 | 2.67 | 0.19 | | 0.6923 | 0.1230 | 0.0812 | 0.8753 | 0.2032 | 0.1609 | C(181) | 130 |
| >F(15A) | <F(11B) | [3655.01] | 2.982(12) | 2.94 | 0.04 | | 0.6923 | 0.1230 | 0.0812 | 0.7550 | -0.0839 | 0.0520 | C(181) | 108.3(5) |
| >F(16A) | C(17) | [] | 2.741(16)<< | 3.17 | -0.43 | Intra | 0.6298 | 0.0944 | -0.0143 | 0.4329 | 0.1658 | 0.0047 | | |
| >F(16A) | H(17A) | [] | 2.43<< | 2.67 | -0.24 | Intra | 0.6298 | 0.0944 | -0.0143 | 0.4354 | 0.1171 | -0.0268 | | |
| >F(16A) | <F(11A) | [3655.01] | 3.128(17) | 2.94 | 0.19 | | 0.6298 | 0.0944 | -0.0143 | 0.7974 | -0.0789 | 0.0112 | C(181) | 115.8(7) |
| >F(16A) | <F(11B) | [3655.01] | 3.094(16) | 2.94 | 0.15 | | 0.6298 | 0.0944 | -0.0143 | 0.7550 | -0.0839 | 0.0520 | C(181) | 103.5(5) |
| O(11) | N(12) | [] | 2.979(2) < | 3.07 | -0.09 | Intra | 0.4162 | 0.4433 | 0.3547 | 0.3678 | 0.4768 | 0.2176 | C(111) | 121.79(13) |
| O(11) | N(22) | [] | 2.956(2) < | 3.07 | -0.11 | | 0.4162 | 0.4433 | 0.3547 | 0.5589 | 0.3192 | 0.2901 | C(111) | 119.73(12) |
| | | | | | | | | | | | | | C(111) | 113.02(13) |
| O(11) | C(121) | [] | 2.911(3)<< | 3.22 | -0.31 | Intra | 0.4162 | 0.4433 | 0.3547 | 0.4996 | 0.6454 | 0.3714 | C(111) | 132.64(15) |
| O(11) | H(11E) | [] | 2.62 < | 2.72 | -0.10 | Intra | 0.4162 | 0.4433 | 0.3547 | 0.4044 | 0.4335 | 0.4740 | C(111) | 114 |

| | | | | | | | | | |
|-------|------|--------|-----|-----------------------|-------|----------------------|----------------------|--------|------------|
| O(11) | | H(11F) | [] | 2.53 < 2.72 -0.19 | Intra | 0.4162 0.4433 0.3547 | 0.4691 0.3404 0.4523 | C(11) | 150 |
| O(11) | | H(12A) | [] | 2.61 < 2.72 -0.11 | Intra | 0.4162 0.4433 0.3547 | 0.2480 0.4585 0.2680 | | |
| O(11) | | H(12D) | [] | 2.74 2.72 0.02 | Intra | 0.4162 0.4433 0.3547 | 0.5467 0.5994 0.3991 | C(111) | 128 |
| O(11) | | H(21) | [] | 2.85(2) 2.72 0.13 | | 0.4162 0.4433 0.3547 | 0.5763 0.4902 0.2798 | C(111) | 160.1(5) |
| O(11) | | H(22) | [] | 2.10(2)<< 2.72 -0.62 | | 0.4162 0.4433 0.3547 | 0.5201 0.3557 0.3105 | C(11) | 120.4(6) |
| | | | | | | | | C(111) | 113.2(6) |
| O(12) | | N(12) | [] | 2.727(2)<< 3.07 -0.34 | Intra | 0.4520 0.5934 0.3160 | 0.3678 0.4768 0.2176 | C(121) | 174.05(15) |
| O(12) | | N(21) | [] | 3.141(2) 3.07 0.07 | | 0.4520 0.5934 0.3160 | 0.6255 0.4650 0.2622 | C(11) | 107.63(12) |
| | | | | | | | | C(121) | 110.85(17) |
| O(12) | | H(12) | [] | 2.53(2) < 2.72 -0.19 | Intra | 0.4520 0.5934 0.3160 | 0.4087 0.5175 0.2085 | C(121) | 165.9(6) |
| O(12) | | H(12B) | [] | 2.61 < 2.72 -0.11 | Intra | 0.4520 0.5934 0.3160 | 0.2635 0.5716 0.2477 | C(121) | 139 |
| O(12) | | H(12F) | [] | 2.48<< 2.72 -0.24 | Intra | 0.4520 0.5934 0.3160 | 0.5170 0.7682 0.3239 | C(11) | 145 |
| O(12) | | H(12G) | [] | 2.61 < 2.72 -0.11 | Intra | 0.4520 0.5934 0.3160 | 0.6247 0.7032 0.3391 | C(11) | 160 |
| O(12) | | H(21) | [] | 2.31(2)<< 2.72 -0.41 | | 0.4520 0.5934 0.3160 | 0.5763 0.4902 0.2798 | C(11) | 104.4(6) |
| | | | | | | | | C(121) | 111.2(6) |
| N(11) | | O(22) | [] | 3.070(2) 3.07 0.00 | | 0.4245 0.3815 0.1437 | 0.6216 0.5074 0.1257 | C(13) | 130.29(12) |
| | | | | | | | | C(14) | 102.49(11) |
| N(11) | | C(23) | [] | 3.388(3) 3.25 0.14 | | 0.4245 0.3815 0.1437 | 0.6343 0.3656 0.2619 | C(14) | 113.72(11) |
| N(11) | | H(12) | [] | 2.33(2)<< 2.75 -0.42 | Intra | 0.4245 0.3815 0.1437 | 0.4087 0.5175 0.2085 | C(14) | 172.1(6) |
| N(11) | | H(15A) | [] | 2.64 < 2.75 -0.11 | Intra | 0.4245 0.3815 0.1437 | 0.2622 0.2991 0.0689 | H(11) | 145 |
| N(11) | | H(19A) | [] | 2.56 < 2.75 -0.19 | Intra | 0.4245 0.3815 0.1437 | 0.5876 0.2935 0.1108 | C(13) | 149 |
| N(12) | | O(11) | [] | 2.979(2) < 3.07 -0.09 | Intra | 0.3678 0.4768 0.2176 | 0.4162 0.4433 0.3547 | C(13) | 112.01(12) |
| | | | | | | | | H(12) | 108.2(16) |
| N(12) | | O(12) | [] | 2.727(2)<< 3.07 -0.34 | Intra | 0.3678 0.4768 0.2176 | 0.4520 0.5934 0.3160 | C(13) | 154.12(13) |
| N(12) | | O(21) | [] | 3.002(2) < 3.07 -0.07 | | 0.3678 0.4768 0.2176 | 0.5387 0.6129 0.1829 | C(12) | 119.03(13) |
| | | | | | | | | C(13) | 115.60(12) |
| N(12) | | N(21) | [] | 3.233(2) 3.10 0.13 | | 0.3678 0.4768 0.2176 | 0.6255 0.4650 0.2622 | C(12) | 117.14(12) |
| N(12) | | C(212) | [] | 3.448(3) 3.25 0.20 | | 0.3678 0.4768 0.2176 | 0.3792 0.7015 0.1420 | C(13) | 121.21(13) |
| N(12) | | H(11) | [] | 2.32(2)<< 2.75 -0.43 | Intra | 0.3678 0.4768 0.2176 | 0.4736 0.4211 0.1457 | C(12) | 179.0(5) |
| N(12) | | H(21) | [] | 2.76(2) 2.75 0.01 | | 0.3678 0.4768 0.2176 | 0.5763 0.4902 0.2798 | C(12) | 103.9(5) |
| | | | | | | | | C(13) | 110.0(5) |
| N(12) | | H(21F) | [] | 2.89 2.75 0.14 | | 0.3678 0.4768 0.2176 | 0.3376 0.6408 0.1304 | C(12) | 100 |
| | | | | | | | | C(13) | 109 |
| C(11) | | C(13) | [] | 3.545(3) 3.40 0.14 | Intra | 0.3690 0.5305 0.3255 | 0.3543 0.3910 0.1858 | H(11A) | 143 |
| C(11) | | C(112) | [] | 3.465(4) 3.40 0.06 | Intra | 0.3690 0.5305 0.3255 | 0.3974 0.3697 0.4518 | O(12) | 120.72(14) |
| | | | | | | | | C(12) | 125.07(15) |
| C(11) | | C(122) | [] | 3.571(4) 3.40 0.17 | Intra | 0.3690 0.5305 0.3255 | 0.5612 0.7275 0.3556 | O(11) | 107.85(13) |
| | | | | | | | | C(12) | 124.44(15) |
| C(11) | | H(11B) | [] | 3.01 2.90 0.11 | Intra | 0.3690 0.5305 0.3255 | 0.3314 0.3209 0.3659 | O(12) | 140 |
| C(11) | | H(11C) | [] | 2.39<< 2.90 -0.51 | Intra | 0.3690 0.5305 0.3255 | 0.2772 0.4214 0.3863 | O(12) | 154 |
| C(11) | | H(12) | [] | 2.67(2)<< 2.90 -0.23 | Intra | 0.3690 0.5305 0.3255 | 0.4087 0.5175 0.2085 | O(11) | 104.2(5) |
| | | | | | | | | H(11A) | 145 |
| C(11) | | H(12C) | [] | 2.47<< 2.90 -0.43 | Intra | 0.3690 0.5305 0.3255 | 0.4421 0.6693 0.3943 | O(11) | 105 |
| | | | | | | | | C(12) | 142 |
| C(11) | | H(12D) | [] | 2.70<< 2.90 -0.20 | Intra | 0.3690 0.5305 0.3255 | 0.5467 0.5994 0.3991 | C(12) | 153 |
| C(11) | | H(21) | [] | 2.98(2) 2.90 0.08 | | 0.3690 0.5305 0.3255 | 0.5763 0.4902 0.2798 | H(11A) | 154 |
| C(11) | | H(22) | [] | 3.07(2) 2.90 0.17 | | 0.3690 0.5305 0.3255 | 0.5201 0.3557 0.3105 | H(11A) | 146 |
| C(12) | | S(1) | [] | 3.114(2)<< 3.50 -0.39 | Intra | 0.3024 0.5101 0.2631 | 0.2650 0.3038 0.1979 | C(11) | 126.60(14) |

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C(12) .... C(111) [      ]      3.140(3)<< 3.40 -0.26 Intra  0.3024 0.5101 0.2631  0.3465 0.3859 0.3870  N(12)  112.16(14)
                                                                    H(12B)  138
C(12) .... H(11C) [      ]      2.99  2.90  0.09 Intra  0.3024 0.5101 0.2631  0.2772 0.4214 0.3863  N(12)  130
                                                                    H(12B)  121
C(12) .... C(27) [ 2555.02]  3.545(3)  3.40  0.14      0.3024 0.5101 0.2631  0.0229 0.5166 0.2040  N(12)  113.15(13)
                                                                    C(11)   134.65(14)
C(13) .... N(22) [      ]      3.294(2)  3.25  0.04      0.3543 0.3910 0.1858  0.5589 0.3192 0.2901
C(13) .... C(11) [      ]      3.545(3)  3.40  0.14 Intra  0.3543 0.3910 0.1858  0.3690 0.5305 0.3255  S(1)   100.58(8)
                                                                    N(11)  131.84(12)
C(13) .... C(15) [      ]      3.089(3)<< 3.40 -0.31 Intra  0.3543 0.3910 0.1858  0.3300 0.2737 0.0621  N(12)  150.93(13)
C(13) .... H(12A) [      ]      2.55<< 2.90 -0.35 Intra  0.3543 0.3910 0.1858  0.2480 0.4585 0.2680  N(11)   164
C(13) .... H(12B) [      ]      3.08  2.90  0.18 Intra  0.3543 0.3910 0.1858  0.2635 0.5716 0.2477  S(1)   100
                                                                    N(11)  133
C(13) .... H(15A) [      ]      2.90  2.90  0.00 Intra  0.3543 0.3910 0.1858  0.2622 0.2991 0.0689  N(12)  145
C(14) .... S(1) [      ]  3.1646(19)<< 3.50 -0.34 Intra  0.4245 0.3069 0.0984  0.2650 0.3038 0.1979  C(19)  142.55(12)
C(14) .... C(17) [      ]      2.794(3)<< 3.40 -0.61 Intra  0.4245 0.3069 0.0984  0.4329 0.1658 0.0047  N(11)  176.52(13)
C(14) .... H(29A) [      ]      2.98  2.90  0.08      0.4245 0.3069 0.0984  0.5450 0.1843 0.2004  C(15)   122
C(14) .... H(22F) [ 3665.02]  3.09  2.90  0.19      0.4245 0.3069 0.0984  0.3586 0.4550-0.0098  C(19)   103
C(15) .... S(1) [      ]      3.204(2)<< 3.50 -0.30 Intra  0.3300 0.2737 0.0621  0.2650 0.3038 0.1979  C(16)  143.05(14)
C(15) .... C(13) [      ]      3.089(3)<< 3.40 -0.31 Intra  0.3300 0.2737 0.0621  0.3543 0.3910 0.1858  C(16)  165.22(15)
C(15) .... C(18) [      ]      2.757(3)<< 3.40 -0.64 Intra  0.3300 0.2737 0.0621  0.5259 0.2003 0.0402  H(15A)  179
C(15) .... H(11) [      ]      3.07(2)  2.90  0.17 Intra  0.3300 0.2737 0.0621  0.4736 0.4211 0.1457  C(16)  140.9(5)
C(15) .... <F(11) [      ]      3.067(8) < 3.17 -0.10 Intra  0.3300 0.2737 0.0621  0.1876 0.0975 0.0110  C(14)  148.2(2)
C(15) .... <F(11A) [      ]  3.338(11)  3.17  0.17 Intra  0.3300 0.2737 0.0621  0.2026 0.0789-0.0112  C(14)  145.5(2)
C(15) .... <F(12) [      ]      2.766(9)<< 3.17 -0.40 Intra  0.3300 0.2737 0.0621  0.1641 0.2387-0.0351  C(14)  164.0(2)
C(15) .... <F(12A) [      ]      2.710(9)<< 3.17 -0.46 Intra  0.3300 0.2737 0.0621  0.1432 0.2253-0.0121  C(14)  175.1(2)
C(15) .... <F(12B) [      ]      2.758(16)<< 3.17 -0.41 Intra  0.3300 0.2737 0.0621  0.1521 0.1697 0.0053  C(14)  167.3(4)
C(15) .... <F(13B) [      ]      3.076(15) < 3.17 -0.09 Intra  0.3300 0.2737 0.0621  0.2142 0.2374-0.0715  C(14)  145.3(3)
C(15) .... H(22F) [ 3665.02]  2.94  2.90  0.04      0.3300 0.2737 0.0621  0.3586 0.4550-0.0098
C(16) .... C(19) [      ]      2.745(3)<< 3.40 -0.66 Intra  0.3355 0.2040 0.0164  0.5225 0.2705 0.0868  C(161) 179.29(17)
C(17) .... >F(16A) [      ]      2.741(16)<< 3.17 -0.43 Intra  0.4329 0.1658 0.0047  0.6298 0.0944-0.0143  C(16)  177.7(2)
C(17) .... C(14) [      ]      2.794(3)<< 3.40 -0.61 Intra  0.4329 0.1658 0.0047  0.4245 0.3069 0.0984  H(17A)  179
C(17) .... <F(11) [      ]      3.235(9)  3.17  0.06 Intra  0.4329 0.1658 0.0047  0.1876 0.0975 0.0110  C(18)  143.34(18)
C(17) .... <F(11A) [      ]      3.086(13) < 3.17 -0.08 Intra  0.4329 0.1658 0.0047  0.2026 0.0789-0.0112  C(18)  152.7(3)
C(17) .... <F(11B) [      ]      2.718(14)<< 3.17 -0.45 Intra  0.4329 0.1658 0.0047  0.2450 0.0839-0.0520  C(18)  172.5(3)
C(17) .... <F(13) [      ]      2.721(8)<< 3.17 -0.45 Intra  0.4329 0.1658 0.0047  0.2488 0.1229-0.0746  C(18)  171.7(2)
C(17) .... <F(13A) [      ]      2.918(8)<< 3.17 -0.25 Intra  0.4329 0.1658 0.0047  0.2326 0.1815-0.0831  C(18)  155.8(3)
C(17) .... <F(13B) [      ]      3.129(16) < 3.17 -0.04 Intra  0.4329 0.1658 0.0047  0.2142 0.2374-0.0715  C(18)  142.3(3)
C(17) .... <F(14B) [      ]      3.00(4) < 3.17 -0.17 Intra  0.4329 0.1658 0.0047  0.6570 0.2040-0.0215  C(16)  148.4(5)
C(17) .... <F(15) [      ]      3.213(12)  3.17  0.04 Intra  0.4329 0.1658 0.0047  0.6649 0.0901 0.0719  C(16)  142.9(2)
C(17) .... <F(16) [      ]      2.69(2)<< 3.17 -0.48 Intra  0.4329 0.1658 0.0047  0.6260 0.1160-0.0258  C(16)  172.0(3)
C(17) .... <F(16B) [      ]      2.79(3)<< 3.17 -0.38 Intra  0.4329 0.1658 0.0047  0.6290 0.0642 0.0200  C(16)  161.4(7)
C(17) .... <F(25) [      ]      3.268(12)  3.17  0.10      0.4329 0.1658 0.0047  0.4302 0.0433 0.1345  H(17A)  106
C(17) .... <F(16B) [ 3655.01]  3.209(17)  3.17  0.04      0.4329 0.1658 0.0047  0.3710-0.0642-0.0200  C(16)  100.9(7)
                                                                    C(18)  125.5(6)
C(18) .... C(15) [      ]      2.757(3)<< 3.40 -0.64 Intra  0.5259 0.2003 0.0402  0.3300 0.2737 0.0621  C(181) 178.47(15)
C(18) .... <F(25) [      ]      3.293(12)  3.17  0.12      0.5259 0.2003 0.0402  0.4302 0.0433 0.1345  C(181) 107.0(2)
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| | | | | | | | | | | | | | | | | |
|--------|------|---------|------------|-------------|------|-------|-------|--------|--------|---------|--------|--------|---------|--------|------------|----------|
| C(19) | | >F(14A) | [] | 2.895(9)<< | 3.17 | -0.28 | Intra | 0.5225 | 0.2705 | 0.0868 | 0.6943 | 0.2378 | 0.0142 | C(14) | 155.7(2) | |
| C(19) | | >F(15A) | [] | 2.925(7)<< | 3.17 | -0.25 | Intra | 0.5225 | 0.2705 | 0.0868 | 0.6923 | 0.1230 | 0.0812 | C(14) | 157.14(18) | |
| C(19) | | C(16) | [] | 2.745(3)<< | 3.40 | -0.66 | Intra | 0.5225 | 0.2705 | 0.0868 | 0.3355 | 0.2040 | 0.0164 | H(19A) | 179 | |
| C(19) | | H(11) | [] | 2.52(2)<< | 2.90 | -0.38 | Intra | 0.5225 | 0.2705 | 0.0868 | 0.4736 | 0.4211 | 0.1457 | C(18) | 162.2(5) | |
| C(19) | | H(22G) | [] | 2.95 | 2.90 | 0.05 | | 0.5225 | 0.2705 | 0.0868 | 0.6161 | 0.4294 | 0.0182 | C(14) | 106 | |
| C(19) | | H(29A) | [] | 2.70<< | 2.90 | -0.20 | | 0.5225 | 0.2705 | 0.0868 | 0.5450 | 0.1843 | 0.2004 | C(18) | 111 | |
| C(19) | | <F(14) | [] | 2.847(15)<< | 3.17 | -0.32 | Intra | 0.5225 | 0.2705 | 0.0868 | 0.7107 | 0.2272 | 0.0335 | C(14) | 164.5(3) | |
| C(19) | | <F(14B) | [] | 3.23(3) | 3.17 | 0.06 | Intra | 0.5225 | 0.2705 | 0.0868 | 0.6570 | 0.2040 | -0.0215 | C(14) | 144.2(6) | |
| C(19) | | <F(15) | [] | 3.057(12) | < | 3.17 | -0.11 | Intra | 0.5225 | 0.2705 | 0.0868 | 0.6649 | 0.0901 | 0.0719 | C(14) | 148.3(3) |
| C(19) | | <F(15B) | [] | 2.74(2)<< | 3.17 | -0.43 | Intra | 0.5225 | 0.2705 | 0.0868 | 0.7138 | 0.1800 | 0.0751 | C(14) | 172.7(5) | |
| C(111) | | C(12) | [] | 3.140(3)<< | 3.40 | -0.26 | Intra | 0.3465 | 0.3859 | 0.3870 | 0.3024 | 0.5101 | 0.2631 | C(112) | 153.1(2) | |
| C(111) | | H(11A) | [] | 2.50<< | 2.90 | -0.40 | Intra | 0.3465 | 0.3859 | 0.3870 | 0.3233 | 0.5636 | 0.3534 | C(112) | 116 | |
| | | | | | | | | | | | | | | H(11B) | 135 | |
| C(111) | | H(12A) | [] | 2.86 | < | 2.90 | -0.04 | Intra | 0.3465 | 0.3859 | 0.3870 | 0.2480 | 0.4585 | 0.2680 | C(112) | 168 |
| C(111) | | H(22) | [] | 2.97(2) | 2.90 | 0.07 | | 0.3465 | 0.3859 | 0.3870 | 0.5201 | 0.3557 | 0.3105 | C(112) | 105.6(4) | |
| | | | | | | | | | | | | | | H(11C) | 141 | |
| C(111) | | H(21D) | [2545.02] | 3.02 | 2.90 | 0.12 | | 0.3465 | 0.3859 | 0.3870 | 0.1496 | 0.2561 | 0.3856 | O(11) | 150 | |
| C(112) | | C(11) | [] | 3.465(4) | 3.40 | 0.06 | Intra | 0.3974 | 0.3697 | 0.4518 | 0.3690 | 0.5305 | 0.3255 | H(11D) | 139 | |
| | | | | | | | | | | | | | | H(11F) | 104 | |
| C(112) | | H(25A) | [] | 3.09 | 2.90 | 0.19 | | 0.3974 | 0.3697 | 0.4518 | 0.5182 | 0.2159 | 0.3821 | H(11E) | 144 | |
| C(112) | | <F(12A) | [4555.01] | 3.318(9) | 3.17 | 0.15 | | 0.3974 | 0.3697 | 0.4518 | 0.6432 | 0.2747 | 0.4879 | C(111) | 122.3(2) | |
| | | | | | | | | | | | | | | H(11D) | 103 | |
| | | | | | | | | | | | | | | H(11E) | 102 | |
| C(112) | | <F(12B) | [4555.01] | 3.271(14) | 3.17 | 0.10 | | 0.3974 | 0.3697 | 0.4518 | 0.6521 | 0.3303 | 0.5053 | C(111) | 128.3(3) | |
| | | | | | | | | | | | | | | H(11D) | 109 | |
| C(112) | | <F(14B) | [4455.01] | 3.31(4) | 3.17 | 0.14 | | 0.3974 | 0.3697 | 0.4518 | 0.1570 | 0.2960 | 0.4785 | H(11E) | 101 | |
| | | | | | | | | | | | | | | H(11F) | 138 | |
| C(121) | | O(11) | [] | 2.911(3)<< | 3.22 | -0.31 | Intra | 0.4996 | 0.6454 | 0.3714 | 0.4162 | 0.4433 | 0.3547 | C(122) | 153.2(2) | |
| C(121) | | H(11A) | [] | 2.45<< | 2.90 | -0.45 | Intra | 0.4996 | 0.6454 | 0.3714 | 0.3233 | 0.5636 | 0.3534 | C(122) | 145 | |
| | | | | | | | | | | | | | | H(12D) | 105 | |
| C(122) | | C(11) | [] | 3.571(4) | 3.40 | 0.17 | Intra | 0.5612 | 0.7275 | 0.3556 | 0.3690 | 0.5305 | 0.3255 | H(12E) | 132 | |
| | | | | | | | | | | | | | | H(12G) | 105 | |
| C(122) | | <F(21) | [1565.02] | 3.320(7) | 3.17 | 0.15 | | 0.5612 | 0.7275 | 0.3556 | 0.4947 | 0.9413 | 0.4164 | C(121) | 113.3(3) | |
| | | | | | | | | | | | | | | H(12G) | 135 | |
| C(122) | | S(2) | [2655.02] | 3.607(4) | 3.50 | 0.11 | | 0.5612 | 0.7275 | 0.3556 | 0.7694 | 0.8049 | 0.2686 | C(121) | 144.8(2) | |
| C(122) | | <F(15B) | [2655.01] | 3.05(2) | < | 3.17 | -0.12 | 0.5612 | 0.7275 | 0.3556 | 0.7862 | 0.6800 | 0.4249 | C(121) | 102.4(5) | |
| | | | | | | | | | | | | | | H(12F) | 147 | |
| C(161) | | H(15A) | [] | 2.62<< | 2.90 | -0.28 | Intra | 0.2337 | 0.1692 | -0.0221 | 0.2622 | 0.2991 | 0.0689 | | | |
| C(161) | | H(17A) | [] | 2.64<< | 2.90 | -0.26 | Intra | 0.2337 | 0.1692 | -0.0221 | 0.4354 | 0.1171 | -0.0268 | | | |
| C(181) | | H(17A) | [] | 2.66<< | 2.90 | -0.24 | Intra | 0.6332 | 0.1615 | 0.0301 | 0.4354 | 0.1171 | -0.0268 | | | |
| C(181) | | H(19A) | [] | 2.62<< | 2.90 | -0.28 | Intra | 0.6332 | 0.1615 | 0.0301 | 0.5876 | 0.2935 | 0.1108 | | | |
| H(11) | | O(21) | [] | 2.78(2) | 2.72 | 0.06 | | 0.4736 | 0.4211 | 0.1457 | 0.5387 | 0.6129 | 0.1829 | N(11) | 144(2) | |
| H(11) | | O(22) | [] | 2.29(2)<< | 2.72 | -0.43 | | 0.4736 | 0.4211 | 0.1457 | 0.6216 | 0.5074 | 0.1257 | N(11) | 163(2) | |
| H(11) | | N(12) | [] | 2.32(2)<< | 2.75 | -0.43 | Intra | 0.4736 | 0.4211 | 0.1457 | 0.3678 | 0.4768 | 0.2176 | | | |
| H(11) | | C(15) | [] | 3.07(2) | 2.90 | 0.17 | Intra | 0.4736 | 0.4211 | 0.1457 | 0.3300 | 0.2737 | 0.0621 | | | |
| H(11) | | C(19) | [] | 2.52(2)<< | 2.90 | -0.38 | Intra | 0.4736 | 0.4211 | 0.1457 | 0.5225 | 0.2705 | 0.0868 | | | |
| H(11) | | C(21) | [] | 2.96(2) | 2.90 | 0.06 | | 0.4736 | 0.4211 | 0.1457 | 0.6403 | 0.5776 | 0.1748 | N(11) | 169.5(19) | |
| H(11) | | C(23) | [] | 3.07(2) | 2.90 | 0.17 | | 0.4736 | 0.4211 | 0.1457 | 0.6343 | 0.3656 | 0.2619 | N(11) | 106.4(17) | |

| | | | | | | | | | | | | | | | |
|--------|------|---------|------------|-----------|------|-------|-------|--------|--------|--------|--------|--------|--------|--------|-----------|
| H(11) | | H(12) | [] | 2.13(3)<< | 2.40 | -0.27 | Intra | 0.4736 | 0.4211 | 0.1457 | 0.4087 | 0.5175 | 0.2085 | | |
| H(11) | | H(19A) | [] | 2.43 | 2.40 | 0.03 | Intra | 0.4736 | 0.4211 | 0.1457 | 0.5876 | 0.2935 | 0.1108 | | |
| H(11A) | | C(111) | [] | 2.50<< | 2.90 | -0.40 | Intra | 0.3233 | 0.5636 | 0.3534 | 0.3465 | 0.3859 | 0.3870 | | |
| H(11A) | | C(121) | [] | 2.45<< | 2.90 | -0.45 | Intra | 0.3233 | 0.5636 | 0.3534 | 0.4996 | 0.6454 | 0.3714 | | |
| H(11A) | | H(11C) | [] | 2.15<< | 2.40 | -0.25 | Intra | 0.3233 | 0.5636 | 0.3534 | 0.2772 | 0.4214 | 0.3863 | | |
| H(11A) | | H(12A) | [] | 2.40 | 2.40 | 0.00 | Intra | 0.3233 | 0.5636 | 0.3534 | 0.2480 | 0.4585 | 0.2680 | | |
| H(11A) | | H(12B) | [] | 2.30 < | 2.40 | -0.10 | Intra | 0.3233 | 0.5636 | 0.3534 | 0.2635 | 0.5716 | 0.2477 | | |
| H(11A) | | H(12C) | [] | 2.15<< | 2.40 | -0.25 | Intra | 0.3233 | 0.5636 | 0.3534 | 0.4421 | 0.6693 | 0.3943 | | |
| H(11A) | | <F(25A) | [2555.02] | 2.86 | 2.67 | 0.19 | | 0.3233 | 0.5636 | 0.3534 | 0.1010 | 0.5178 | 0.3545 | C(11) | 124 |
| H(11B) | | C(11) | [] | 3.01 | 2.90 | 0.11 | Intra | 0.3314 | 0.3209 | 0.3659 | 0.3690 | 0.5305 | 0.3255 | | |
| H(11B) | | C(25) | [] | 3.09 | 2.90 | 0.19 | | 0.3314 | 0.3209 | 0.3659 | 0.5135 | 0.1758 | 0.3457 | C(111) | 122 |
| H(11B) | | H(11D) | [] | 2.28 < | 2.40 | -0.12 | Intra | 0.3314 | 0.3209 | 0.3659 | 0.3528 | 0.3243 | 0.4723 | | |
| H(11B) | | H(11F) | [] | 2.36 < | 2.40 | -0.04 | Intra | 0.3314 | 0.3209 | 0.3659 | 0.4691 | 0.3404 | 0.4523 | | |
| H(11B) | | C(212) | [2545.02] | 3.07 | 2.90 | 0.17 | | 0.3314 | 0.3209 | 0.3659 | 0.1208 | 0.2015 | 0.3580 | C(111) | 126 |
| H(11B) | | H(21D) | [2545.02] | 2.54 | 2.40 | 0.14 | | 0.3314 | 0.3209 | 0.3659 | 0.1496 | 0.2561 | 0.3856 | C(111) | 110 |
| H(11C) | | C(11) | [] | 2.39<< | 2.90 | -0.51 | Intra | 0.2772 | 0.4214 | 0.3863 | 0.3690 | 0.5305 | 0.3255 | | |
| H(11C) | | C(12) | [] | 2.99 | 2.90 | 0.09 | Intra | 0.2772 | 0.4214 | 0.3863 | 0.3024 | 0.5101 | 0.2631 | | |
| H(11C) | | H(11A) | [] | 2.15<< | 2.40 | -0.25 | Intra | 0.2772 | 0.4214 | 0.3863 | 0.3233 | 0.5636 | 0.3534 | | |
| H(11C) | | H(11D) | [] | 2.35 < | 2.40 | -0.05 | Intra | 0.2772 | 0.4214 | 0.3863 | 0.3528 | 0.3243 | 0.4723 | | |
| H(11C) | | H(11E) | [] | 2.29 < | 2.40 | -0.11 | Intra | 0.2772 | 0.4214 | 0.3863 | 0.4044 | 0.4335 | 0.4740 | | |
| H(11C) | | H(12A) | [] | 2.59 | 2.40 | 0.19 | Intra | 0.2772 | 0.4214 | 0.3863 | 0.2480 | 0.4585 | 0.2680 | | |
| H(11C) | | <F(25A) | [2555.02] | 2.56 < | 2.67 | -0.11 | | 0.2772 | 0.4214 | 0.3863 | 0.1010 | 0.5178 | 0.3545 | C(111) | 165 |
| H(11C) | | <F(25B) | [2555.02] | 2.83 | 2.67 | 0.16 | | 0.2772 | 0.4214 | 0.3863 | 0.0870 | 0.5364 | 0.3596 | C(111) | 168 |
| H(11D) | | H(11B) | [] | 2.28 < | 2.40 | -0.12 | Intra | 0.3528 | 0.3243 | 0.4723 | 0.3314 | 0.3209 | 0.3659 | | |
| H(11D) | | H(11C) | [] | 2.35 < | 2.40 | -0.05 | Intra | 0.3528 | 0.3243 | 0.4723 | 0.2772 | 0.4214 | 0.3863 | | |
| H(11D) | | >F(14A) | [4455.01] | 2.46<< | 2.67 | -0.21 | | 0.3528 | 0.3243 | 0.4723 | 0.1943 | 0.2622 | 0.5142 | C(112) | 159 |
| H(11D) | | <F(14) | [4455.01] | 2.48 < | 2.67 | -0.19 | | 0.3528 | 0.3243 | 0.4723 | 0.2107 | 0.2728 | 0.5335 | C(112) | 158 |
| H(11D) | | <F(14B) | [4455.01] | 2.51 < | 2.67 | -0.16 | | 0.3528 | 0.3243 | 0.4723 | 0.1570 | 0.2960 | 0.4785 | C(112) | 139 |
| H(11E) | | O(11) | [] | 2.62 < | 2.72 | -0.10 | Intra | 0.4044 | 0.4335 | 0.4740 | 0.4162 | 0.4433 | 0.3547 | | |
| H(11E) | | H(11C) | [] | 2.29 < | 2.40 | -0.11 | Intra | 0.4044 | 0.4335 | 0.4740 | 0.2772 | 0.4214 | 0.3863 | | |
| H(11E) | | <F(11) | [2555.01] | 2.53 < | 2.67 | -0.14 | | 0.4044 | 0.4335 | 0.4740 | 0.3124 | 0.5975 | 0.4890 | C(112) | 145 |
| H(11E) | | <F(11A) | [2555.01] | 2.57 < | 2.67 | -0.10 | | 0.4044 | 0.4335 | 0.4740 | 0.2974 | 0.5789 | 0.5112 | C(112) | 144 |
| H(11F) | | O(11) | [] | 2.53 < | 2.72 | -0.19 | Intra | 0.4691 | 0.3404 | 0.4523 | 0.4162 | 0.4433 | 0.3547 | | |
| H(11F) | | H(11B) | [] | 2.36 < | 2.40 | -0.04 | Intra | 0.4691 | 0.3404 | 0.4523 | 0.3314 | 0.3209 | 0.3659 | | |
| H(11F) | | H(25A) | [] | 2.41 | 2.40 | 0.01 | | 0.4691 | 0.3404 | 0.4523 | 0.5182 | 0.2159 | 0.3821 | C(112) | 127 |
| H(11F) | | <F(12) | [4555.01] | 2.64 < | 2.67 | -0.03 | | 0.4691 | 0.3404 | 0.4523 | 0.6641 | 0.2613 | 0.4649 | C(112) | 175 |
| H(11F) | | <F(12A) | [4555.01] | 2.37<< | 2.67 | -0.30 | | 0.4691 | 0.3404 | 0.4523 | 0.6432 | 0.2747 | 0.4879 | C(112) | 162 |
| H(11F) | | <F(12B) | [4555.01] | 2.41<< | 2.67 | -0.26 | | 0.4691 | 0.3404 | 0.4523 | 0.6521 | 0.3303 | 0.5053 | C(112) | 146 |
| H(12) | | O(12) | [] | 2.53(2) < | 2.72 | -0.19 | Intra | 0.4087 | 0.5175 | 0.2085 | 0.4520 | 0.5934 | 0.3160 | | |
| H(12) | | O(21) | [] | 2.21(2)<< | 2.72 | -0.51 | | 0.4087 | 0.5175 | 0.2085 | 0.5387 | 0.6129 | 0.1829 | N(12) | 172(2) |
| H(12) | | N(11) | [] | 2.33(2)<< | 2.75 | -0.42 | Intra | 0.4087 | 0.5175 | 0.2085 | 0.4245 | 0.3815 | 0.1437 | | |
| H(12) | | N(21) | [] | 2.88(2) | 2.75 | 0.13 | | 0.4087 | 0.5175 | 0.2085 | 0.6255 | 0.4650 | 0.2622 | N(12) | 109.7(18) |
| H(12) | | C(11) | [] | 2.67(2)<< | 2.90 | -0.23 | Intra | 0.4087 | 0.5175 | 0.2085 | 0.3690 | 0.5305 | 0.3255 | | |
| H(12) | | C(211) | [] | 3.03(2) | 2.90 | 0.13 | | 0.4087 | 0.5175 | 0.2085 | 0.4949 | 0.6841 | 0.1360 | N(12) | 159(2) |
| H(12) | | C(212) | [] | 2.86(2) < | 2.90 | -0.04 | | 0.4087 | 0.5175 | 0.2085 | 0.3792 | 0.7015 | 0.1420 | N(12) | 133(2) |
| H(12) | | H(11) | [] | 2.13(3)<< | 2.40 | -0.27 | Intra | 0.4087 | 0.5175 | 0.2085 | 0.4736 | 0.4211 | 0.1457 | | |
| H(12) | | H(12B) | [] | 2.25 < | 2.40 | -0.15 | Intra | 0.4087 | 0.5175 | 0.2085 | 0.2635 | 0.5716 | 0.2477 | | |
| H(12) | | H(21) | [] | 2.44(3) | 2.40 | 0.04 | | 0.4087 | 0.5175 | 0.2085 | 0.5763 | 0.4902 | 0.2798 | N(12) | 105.4(19) |


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<F(14)  ....  H(19A) [      ]      2.61 < 2.67 -0.06 Intra  0.7107 0.2272 0.0335  0.5876 0.2935 0.1108
<F(14)  ....  H(12E) [ 2645.01]      2.87  2.67  0.20      0.7107 0.2272 0.0335  0.9158 0.2680 0.1072  C(181)      139
<F(14)  ....  H(11D) [ 4554.01]      2.48 < 2.67 -0.19      0.7107 0.2272 0.0335  0.8528 0.1757-0.0277  C(181)      112
<F(14B) ....  C(17)  [      ]      3.00(4) < 3.17 -0.17 Intra  0.6570 0.2040-0.0215  0.4329 0.1658 0.0047
<F(14B) ....  C(19)  [      ]      3.23(3)  3.17  0.06 Intra  0.6570 0.2040-0.0215  0.5225 0.2705 0.0868
<F(14B) ....  C(211) [ 3665.02]      3.26(3)  3.17  0.09      0.6570 0.2040-0.0215  0.5051 0.3159-0.1360  C(181)      131(2)
<F(14B) ....  C(212) [ 3665.02]      2.88(2)<< 3.17 -0.29      0.6570 0.2040-0.0215  0.6208 0.2985-0.1420  C(181)      158(2)
<F(14B) ....  H(21D) [ 3665.02]      2.08<< 2.67 -0.59      0.6570 0.2040-0.0215  0.6496 0.2439-0.1144  C(181)      161
<F(14B) ....  C(112) [ 4554.01]      3.31(4)  3.17  0.14      0.6570 0.2040-0.0215  0.8974 0.1303-0.0482  C(181)     110.4(17)
<F(14B) ....  H(11D) [ 4554.01]      2.51 < 2.67 -0.16      0.6570 0.2040-0.0215  0.8528 0.1757-0.0277  C(181)      109
<F(15)  ....  C(17)  [      ]      3.213(12)  3.17  0.04 Intra  0.6649 0.0901 0.0719  0.4329 0.1658 0.0047
<F(15)  ....  C(19)  [      ]      3.057(12) < 3.17 -0.11 Intra  0.6649 0.0901 0.0719  0.5225 0.2705 0.0868
<F(15B) ....  C(19)  [      ]      2.74(2)<< 3.17 -0.43 Intra  0.7138 0.1800 0.0751  0.5225 0.2705 0.0868
<F(15B) ....  H(19A) [      ]      2.41<< 2.67 -0.26 Intra  0.7138 0.1800 0.0751  0.5876 0.2935 0.1108
<F(15B) ....  C(122) [ 2645.01]      3.05(2) < 3.17 -0.12      0.7138 0.1800 0.0751  0.9388 0.2275 0.1444  C(181)     161.9(15)
<F(15B) ....  H(12E) [ 2645.01]      2.79  2.67  0.12      0.7138 0.1800 0.0751  0.9158 0.2680 0.1072  C(181)      146
<F(15B) ....  H(12G) [ 2645.01]      2.55 < 2.67 -0.12      0.7138 0.1800 0.0751  0.8753 0.2032 0.1609  C(181)      176
<F(16)  ....  C(17)  [      ]      2.69(2)<< 3.17 -0.48 Intra  0.6260 0.1160-0.0258  0.4329 0.1658 0.0047
<F(16)  ....  H(17A) [      ]      2.39<< 2.67 -0.28 Intra  0.6260 0.1160-0.0258  0.4354 0.1171-0.0268
<F(16)  ....  H(21D) [ 3665.02]      2.63 < 2.67 -0.04      0.6260 0.1160-0.0258  0.6496 0.2439-0.1144  C(181)      111
<F(16B) ....  C(17)  [      ]      2.79(3)<< 3.17 -0.38 Intra  0.6290 0.0642 0.0200  0.4329 0.1658 0.0047
<F(16B) ....  H(17A) [      ]      2.58 < 2.67 -0.09 Intra  0.6290 0.0642 0.0200  0.4354 0.1171-0.0268
<F(16B) ....  C(17)  [ 3655.01]      3.209(18)  3.17  0.04      0.6290 0.0642 0.0200  0.5671-0.1658-0.0047  C(181)     168(2)
<F(16B) ....  H(17A) [ 3655.01]      2.58 < 2.67 -0.09      0.6290 0.0642 0.0200  0.5646-0.1171 0.0268  C(181)      158
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Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 1 to Neighbouring ARU'S

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=====
Nr      ARU      Nr.Cont.  d(min)  Del  XHn X      - At(I)      At(J) - Y  YHn Note  Partaking ARU's in Close Contact Resd.
-----
 1 [ 2555.02]      7      2.5600 -0.11  2 C(111) - H(11C) ... *F(25A) -C(281) 0 < 2555.02
 2 [ 1555.02]     41      2.1000 -0.62  1 C(11)  - O(11)  ... H(22) -N(22) 1 << 1555.02
 3 [ 3665.02]      7      2.0800 -0.59  0 C(181) -*F(14B) ... H(21D) -C(212) 3 << 3665.02
 4 [ 4554.01]      4      2.4600 -0.21  0 C(181) -*F(14A) ... H(11D) -C(112) 3 << 4554.01
 5 [ 2645.01]      5      2.5500 -0.12  0 C(181) -*F(15B) ... H(12G) -C(122) 3 < 2645.01
 6 [ 3655.01]     10      2.5800 -0.09  0 C(181) -*F(16B) ... H(17A) -C(17) 1 < 3655.01
 7 [ 2545.02]      3      2.5400  0.14  2 C(111) - H(11B) ... H(21D) -C(212) 3 2545.02
 8 [ 4555.01]      5      2.3700 -0.30  3 C(112) - H(11F) ... *F(12A) -C(161) 0 << 4555.01
 9 [ 4455.01]      4      2.4600 -0.21  3 C(112) - H(11D) ... *F(14A) -C(181) 0 << 4455.01
10 [ 1565.02]      3      2.5700  0.17  3 C(122) - H(12F) ... H(27A) -C(27) 1 1565.02
11 [ 2655.02]      2      2.8900 -0.11  3 C(122) - H(12G) ... S(2) -C(23) 0 < 2655.02
12 [ 2655.01]      5      2.5500 -0.12  3 C(122) - H(12G) ... *F(15B) -C(181) 0 < 2655.01
13 [ 2555.01]      3      2.5300 -0.14  3 C(112) - H(11E) ... *F(11) -C(161) 0 < 2555.01
14 [ 2545.01]      3      2.5300 -0.14  0 C(161) -*F(11)  ... H(11E) -C(112) 3 < 2545.01
15 [ 4454.02]      5      2.4400 -0.23  0 C(161) -*F(12)  ... H(25A) -C(25) 1 << 4454.02
16 [ 4454.01]      5      2.3700 -0.30  0 C(161) -*F(12A) ... H(11F) -C(112) 3 << 4454.01
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 Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

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***** ARU = 1555.02 *****

=====

| At(I)[1555.02] | At(J) | [ARU(J)] | D(I-J) | SumRad | Del | Type | X(I) | Y(I) | Z(I) | X(J) | Y(J) | Z(J) | X | X - I...J |
|----------------|-------|------------|------------|--------------|------|-------|-------|--------|--------|--------|--------|--------|--------|-------------------|
| S(2) | | C(22) | [] | 3.109(2)<< | 3.50 | -0.39 | Intra | 0.7306 | 0.3049 | 0.2314 | 0.6947 | 0.5338 | 0.2356 | |
| S(2) | | C(24) | [] | 3.1576(19)<< | 3.50 | -0.34 | Intra | 0.7306 | 0.3049 | 0.2314 | 0.5369 | 0.2164 | 0.2909 | |
| S(2) | | C(29) | [] | 3.2310(19)<< | 3.50 | -0.27 | Intra | 0.7306 | 0.3049 | 0.2314 | 0.5297 | 0.1571 | 0.2385 | |
| S(2) | | H(19A) | [] | 2.94 < | 3.00 | -0.06 | | 0.7306 | 0.3049 | 0.2314 | 0.5876 | 0.2935 | 0.1108 | |
| S(2) | | H(22A) | [] | 2.63<< | 3.00 | -0.37 | Intra | 0.7306 | 0.3049 | 0.2314 | 0.7610 | 0.4985 | 0.2285 | |
| S(2) | | H(22C) | [] | 3.15 | 3.00 | 0.15 | Intra | 0.7306 | 0.3049 | 0.2314 | 0.7481 | 0.4269 | 0.1093 | C(23) 103 |
| S(2) | | H(29A) | [] | 2.83 < | 3.00 | -0.17 | Intra | 0.7306 | 0.3049 | 0.2314 | 0.5450 | 0.1843 | 0.2004 | |
| S(2) | | C(122) | [2645.01] | 3.607(4) | 3.50 | 0.11 | | 0.7306 | 0.3049 | 0.2314 | 0.9388 | 0.2275 | 0.1444 | C(23) 166.43(8) |
| S(2) | | H(12G) | [2645.01] | 2.89 < | 3.00 | -0.11 | | 0.7306 | 0.3049 | 0.2314 | 0.8753 | 0.2032 | 0.1609 | C(23) 171 |
| S(2) | | H(22B) | [2645.02] | 2.98 < | 3.00 | -0.02 | | 0.7306 | 0.3049 | 0.2314 | 0.7839 | 0.0884 | 0.2344 | C(23) 130 |
| O(21) | | N(12) | [] | 3.002(2) < | 3.07 | -0.07 | | 0.5387 | 0.6129 | 0.1829 | 0.3678 | 0.4768 | 0.2176 | C(21) 121.78(11) |
| | | | | | | | | | | | | | C(211) | 111.81(12) |
| O(21) | | N(21) | [] | 2.741(2)<< | 3.07 | -0.33 | Intra | 0.5387 | 0.6129 | 0.1829 | 0.6255 | 0.4650 | 0.2622 | C(211) 174.09(12) |
| O(21) | | H(11) | [] | 2.78(2) | 2.72 | 0.06 | | 0.5387 | 0.6129 | 0.1829 | 0.4736 | 0.4211 | 0.1457 | C(211) 110.2(5) |
| O(21) | | H(12) | [] | 2.21(2)<< | 2.72 | -0.51 | | 0.5387 | 0.6129 | 0.1829 | 0.4087 | 0.5175 | 0.2085 | C(21) 123.9(6) |
| | | | | | | | | | | | | | C(211) | 110.2(6) |
| O(21) | | H(21) | [] | 2.66(2) < | 2.72 | -0.06 | Intra | 0.5387 | 0.6129 | 0.1829 | 0.5763 | 0.4902 | 0.2798 | C(211) 166.4(5) |
| O(21) | | H(21E) | [] | 2.52<< | 2.72 | -0.20 | Intra | 0.5387 | 0.6129 | 0.1829 | 0.3738 | 0.7190 | 0.1852 | C(21) 164 |
| O(21) | | H(21F) | [] | 2.63 < | 2.72 | -0.09 | Intra | 0.5387 | 0.6129 | 0.1829 | 0.3376 | 0.6408 | 0.1304 | C(21) 146 |
| O(21) | | H(22B) | [] | 2.66 < | 2.72 | -0.06 | Intra | 0.5387 | 0.6129 | 0.1829 | 0.7161 | 0.5884 | 0.2656 | C(211) 138 |
| O(22) | | N(11) | [] | 3.070(2) | 3.07 | 0.00 | | 0.6216 | 0.5074 | 0.1257 | 0.4245 | 0.3815 | 0.1437 | C(21) 108.31(11) |
| | | | | | | | | | | | | | C(221) | 132.67(13) |
| O(22) | | N(21) | [] | 3.010(2) < | 3.07 | -0.06 | Intra | 0.6216 | 0.5074 | 0.1257 | 0.6255 | 0.4650 | 0.2622 | C(221) 123.40(14) |
| O(22) | | C(211) | [] | 2.883(3)<< | 3.22 | -0.34 | Intra | 0.6216 | 0.5074 | 0.1257 | 0.4949 | 0.6841 | 0.1360 | C(221) 131.40(14) |
| O(22) | | H(11) | [] | 2.29(2)<< | 2.72 | -0.43 | | 0.6216 | 0.5074 | 0.1257 | 0.4736 | 0.4211 | 0.1457 | C(21) 103.9(6) |
| | | | | | | | | | | | | | C(221) | 136.8(6) |
| O(22) | | H(19A) | [] | 2.91 | 2.72 | 0.19 | | 0.6216 | 0.5074 | 0.1257 | 0.5876 | 0.2935 | 0.1108 | C(21) 138 |
| O(22) | | H(21B) | [] | 2.56 < | 2.72 | -0.16 | Intra | 0.6216 | 0.5074 | 0.1257 | 0.5004 | 0.6580 | 0.0939 | C(221) 119 |
| O(22) | | H(22A) | [] | 2.62 < | 2.72 | -0.10 | Intra | 0.6216 | 0.5074 | 0.1257 | 0.7610 | 0.4985 | 0.2285 | |
| O(22) | | H(22F) | [] | 2.62 < | 2.72 | -0.10 | Intra | 0.6216 | 0.5074 | 0.1257 | 0.6414 | 0.5450 | 0.0098 | C(21) 125 |
| O(22) | | H(22G) | [] | 2.55 < | 2.72 | -0.17 | Intra | 0.6216 | 0.5074 | 0.1257 | 0.6161 | 0.4294 | 0.0182 | C(21) 160 |
| N(21) | | O(12) | [] | 3.141(2) | 3.07 | 0.07 | | 0.6255 | 0.4650 | 0.2622 | 0.4520 | 0.5934 | 0.3160 | C(22) 106.97(11) |
| | | | | | | | | | | | | | C(23) | 127.67(12) |
| N(21) | | O(21) | [] | 2.741(2)<< | 3.07 | -0.33 | Intra | 0.6255 | 0.4650 | 0.2622 | 0.5387 | 0.6129 | 0.1829 | C(23) 138.13(13) |
| N(21) | | O(22) | [] | 3.010(2) < | 3.07 | -0.06 | Intra | 0.6255 | 0.4650 | 0.2622 | 0.6216 | 0.5074 | 0.1257 | H(21) 117.9(15) |


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N(21) .... N(12) [ ] 3.233(2) 3.10 0.13 0.6255 0.4650 0.2622 0.3678 0.4768 0.2176 C(22) 118.91(12)
N(21) .... H(12) [ ] 2.88(2) 2.75 0.13 0.6255 0.4650 0.2622 0.4087 0.5175 0.2085 C(22) 105.7(5)
                                     C(23) 108.5(5)
N(21) .... H(22) [ ] 2.33(2)<< 2.75 -0.42 Intra 0.6255 0.4650 0.2622 0.5201 0.3557 0.3105 C(22) 176.7(6)
N(22) .... O(11) [ ] 2.956(2) < 3.07 -0.11 0.5589 0.3192 0.2901 0.4162 0.4433 0.3547 C(23) 118.18(12)
                                     C(24) 114.30(12)
N(22) .... C(13) [ ] 3.294(2) 3.25 0.04 0.5589 0.3192 0.2901 0.3543 0.3910 0.1858
N(22) .... H(21) [ ] 2.32(2)<< 2.75 -0.43 Intra 0.5589 0.3192 0.2901 0.5763 0.4902 0.2798 C(24) 173.0(6)
N(22) .... H(25A) [ ] 2.55<< 2.75 -0.20 Intra 0.5589 0.3192 0.2901 0.5182 0.2159 0.3821 C(23) 147
N(22) .... H(29A) [ ] 2.65 < 2.75 -0.10 Intra 0.5589 0.3192 0.2901 0.5450 0.1843 0.2004 H(22) 142
C(21) .... C(23) [ ] 3.425(3) 3.40 0.02 Intra 0.6403 0.5776 0.1748 0.6343 0.3656 0.2619 H(21A) 147
C(21) .... C(222) [ ] 3.569(4) 3.40 0.17 Intra 0.6403 0.5776 0.1748 0.6718 0.4810 0.0255 O(21) 118.03(13)
                                     C(22) 123.66(13)
C(21) .... H(11) [ ] 2.96(2) 2.90 0.06 0.6403 0.5776 0.1748 0.4736 0.4211 0.1457 H(21A) 152
C(21) .... H(21) [ ] 2.79(2) < 2.90 -0.11 Intra 0.6403 0.5776 0.1748 0.5763 0.4902 0.2798 O(22) 107.5(5)
                                     H(21A) 141
C(21) .... H(21B) [ ] 2.53<< 2.90 -0.37 Intra 0.6403 0.5776 0.1748 0.5004 0.6580 0.0939 C(22) 161
C(21) .... H(21C) [ ] 2.67<< 2.90 -0.23 Intra 0.6403 0.5776 0.1748 0.5357 0.7474 0.1419 O(22) 110
                                     C(22) 135
C(21) .... H(22C) [ ] 2.92 2.90 0.02 Intra 0.6403 0.5776 0.1748 0.7481 0.4269 0.1093 O(21) 143
C(21) .... H(22D) [ ] 2.42<< 2.90 -0.48 Intra 0.6403 0.5776 0.1748 0.7638 0.5446 0.1018 O(21) 146
                                     C(22) 105
C(22) .... S(2) [ ] 3.109(2)<< 3.50 -0.39 Intra 0.6947 0.5338 0.2356 0.7306 0.3049 0.2314 C(21) 114.06(12)
                                     H(22B) 136
C(22) .... C(221) [ ] 3.174(4)<< 3.40 -0.23 Intra 0.6947 0.5338 0.2356 0.7113 0.4893 0.0938 N(21) 113.61(13)
                                     H(22B) 137
C(22) .... <F(24) [ 2655.02] 3.365(14) 3.17 0.19 0.6947 0.5338 0.2356 0.9180 0.4739 0.3355 C(21) 151.2(3)
C(23) .... N(11) [ ] 3.388(3) 3.25 0.14 0.6343 0.3656 0.2619 0.4245 0.3815 0.1437 S(2) 104.72(9)
C(23) .... C(21) [ ] 3.425(3) 3.40 0.02 Intra 0.6343 0.3656 0.2619 0.6403 0.5776 0.1748 N(22) 135.04(12)
C(23) .... C(29) [ ] 3.100(3)<< 3.40 -0.30 Intra 0.6343 0.3656 0.2619 0.5297 0.1571 0.2385 N(21) 150.11(13)
C(23) .... H(11) [ ] 3.07(2) 2.90 0.17 0.6343 0.3656 0.2619 0.4736 0.4211 0.1457 S(2) 102.4(4)
C(23) .... H(22A) [ ] 2.57<< 2.90 -0.33 Intra 0.6343 0.3656 0.2619 0.7610 0.4985 0.2285 N(22) 162
C(23) .... H(29A) [ ] 2.92 2.90 0.02 Intra 0.6343 0.3656 0.2619 0.5450 0.1843 0.2004 N(21) 144
C(24) .... S(2) [ ] 3.1576(19)<< 3.50 -0.34 Intra 0.5369 0.2164 0.2909 0.7306 0.3049 0.2314 C(25) 141.34(13)
C(24) .... C(27) [ ] 2.792(3)<< 3.40 -0.61 Intra 0.5369 0.2164 0.2909 0.4771 0.0166 0.2960 N(22) 175.25(13)
C(25) .... C(28) [ ] 2.747(3)<< 3.40 -0.65 Intra 0.5135 0.1758 0.3457 0.5003 0.0581 0.2414 H(25A) 179
C(25) .... H(11B) [ ] 3.09 2.90 0.19 0.5135 0.1758 0.3457 0.3314 0.3209 0.3659 C(26) 113
C(25) .... H(22) [ ] 2.54(2)<< 2.90 -0.36 Intra 0.5135 0.1758 0.3457 0.5201 0.3557 0.3105 C(26) 160.8(5)
C(25) .... <F(22) [ ] 2.715(6)<< 3.17 -0.46 Intra 0.5135 0.1758 0.3457 0.4942 0.0880 0.4561 C(24) 172.7(3)
C(25) .... <F(22A) [ ] 2.847(10)<< 3.17 -0.32 Intra 0.5135 0.1758 0.3457 0.5494 0.0515 0.4532 C(24) 155.5(2)
C(25) .... <F(22B) [ ] 3.175(15) 3.17 0.00 Intra 0.5135 0.1758 0.3457 0.5425-0.0049 0.4412 C(24) 147.8(3)
C(25) .... <F(23) [ ] 3.272(7) 3.17 0.10 Intra 0.5135 0.1758 0.3457 0.3505 0.0261 0.4051 C(24) 144.20(18)
C(25) .... <F(23A) [ ] 2.918(11)<< 3.17 -0.25 Intra 0.5135 0.1758 0.3457 0.3810 0.0797 0.4277 C(24) 156.5(2)
C(25) .... <F(23B) [ ] 2.736(11)<< 3.17 -0.43 Intra 0.5135 0.1758 0.3457 0.4260 0.1101 0.4462 C(24) 168.3(3)
C(25) .... <F(12) [ 4555.01] 3.173(9) 3.17 0.00 0.5135 0.1758 0.3457 0.6641 0.2613 0.4649 C(24) 112.39(19)
                                     C(26) 116.93(18)
C(25) .... <F(13B) [ 4555.01] 3.087(15) < 3.17 -0.08 0.5135 0.1758 0.3457 0.7142 0.2626 0.4285 C(26) 123.2(3)
C(26) .... C(29) [ ] 2.749(3)<< 3.40 -0.65 Intra 0.4834 0.0771 0.3478 0.5297 0.1571 0.2385 C(261) 178.62(16)
    
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<F(22A) .... C(25) [      ] 2.847(10)<< 3.17 -0.32 Intra 0.5494 0.0515 0.4532 0.5135 0.1758 0.3457
<F(22A) .... H(25A) [      ]      2.69  2.67  0.02 Intra 0.5494 0.0515 0.4532 0.5182 0.2159 0.3821
<F(22A) .... H(22D) [ 2645.02]      2.79  2.67  0.12      0.5494 0.0515 0.4532 0.7362 0.0446 0.3982 C(261)      109
<F(22A) .... C(261) [ 3656.02]  3.257(9)  3.17  0.09      0.5494 0.0515 0.4532 0.5404-0.0359 0.5922 C(261)  117.5(5)
<F(22A) .... <F(21A) [ 3656.02]  2.981(16)  2.94  0.04      0.5494 0.0515 0.4532 0.5562 0.0612 0.5909 C(261)  127.7(5)
<F(22A) .... <F(22A) [ 3656.02]  2.892(13) < 2.94 -0.05      0.5494 0.0515 0.4532 0.4506-0.0515 0.5468
<F(22A) .... <F(23A) [ 3656.02]  3.139(15)  2.94  0.20      0.5494 0.0515 0.4532 0.6190-0.0797 0.5723 C(261)  126.1(6)
<F(22B) .... C(25) [      ]  3.175(15)  3.17  0.00 Intra 0.5425-0.0049 0.4412 0.5135 0.1758 0.3457
<F(22B) .... C(27) [      ]  3.146(11) < 3.17 -0.02 Intra 0.5425-0.0049 0.4412 0.4771 0.0166 0.2960
<F(22B) .... C(221) [ 2645.02]  3.296(11)  3.17  0.13      0.5425-0.0049 0.4412 0.7887-0.0107 0.4062 C(261)  125.6(7)
<F(22B) .... H(22D) [ 2645.02]      2.82  2.67  0.15      0.5425-0.0049 0.4412 0.7362 0.0446 0.3982 C(261)      112
<F(22B) .... C(261) [ 3656.02]  3.310(11)  3.17  0.14      0.5425-0.0049 0.4412 0.5404-0.0359 0.5922 C(261)  118.7(6)
<F(22B) .... <F(22B) [ 3656.02]  2.919(15) < 2.94 -0.02      0.5425-0.0049 0.4412 0.4575 0.0049 0.5588
<F(22B) .... <F(23B) [ 3656.02]  2.798(17) < 2.94 -0.14      0.5425-0.0049 0.4412 0.5740-0.1101 0.5538 C(261)  134.1(7)
<F(23) .... C(25) [      ]  3.272(7)  3.17  0.10 Intra 0.3505 0.0261 0.4051 0.5135 0.1758 0.3457
<F(23) .... C(27) [      ]  3.053(7) < 3.17 -0.12 Intra 0.3505 0.0261 0.4051 0.4771 0.0166 0.2960
<F(23) .... H(21F) [ 2545.02]      2.82  2.67  0.15      0.3505 0.0261 0.4051 0.1624 0.1408 0.3696 C(261)      138
<F(23) .... H(22E) [ 4455.02]      2.80  2.67  0.13      0.3505 0.0261 0.4051 0.2320 0.0368 0.5038 C(261)      128
<F(23A) .... C(25) [      ]  2.918(11)<< 3.17 -0.25 Intra 0.3810 0.0797 0.4277 0.5135 0.1758 0.3457
<F(23A) .... H(25A) [      ]      2.80  2.67  0.13 Intra 0.3810 0.0797 0.4277 0.5182 0.2159 0.3821
<F(23A) .... <F(22A) [ 3656.02]  3.139(15)  2.94  0.20      0.3810 0.0797 0.4277 0.4506-0.0515 0.5468
<F(23A) .... H(22E) [ 4455.02]      2.74  2.67  0.07      0.3810 0.0797 0.4277 0.2320 0.0368 0.5038 C(261)      138
<F(23B) .... C(25) [      ]  2.736(11)<< 3.17 -0.43 Intra 0.4260 0.1101 0.4462 0.5135 0.1758 0.3457
<F(23B) .... H(25A) [      ]      2.41<< 2.67 -0.26 Intra 0.4260 0.1101 0.4462 0.5182 0.2159 0.3821
<F(23B) .... <F(22B) [ 3656.02]  2.798(16) < 2.94 -0.14      0.4260 0.1101 0.4462 0.4575 0.0049 0.5588
<F(24) .... C(29) [      ]  3.064(15) < 3.17 -0.11 Intra 0.5820-0.0261 0.1645 0.5297 0.1571 0.2385
<F(24) .... C(22) [ 2645.02]  3.365(14)  3.17  0.19      0.5820-0.0261 0.1645 0.8053 0.0338 0.2644 C(281)  115.3(9)
<F(24) .... H(22A) [ 2645.02]      2.82  2.67  0.15      0.5820-0.0261 0.1645 0.7390-0.0015 0.2715 C(281)      105
<F(24A) .... >F(15A) [      ]      2.76(2) < 2.94 -0.18      0.5688 0.0134 0.1513 0.6923 0.1230 0.0812 C(281)  155.7(12)
<F(24A) .... C(29) [      ]      2.80(2)<< 3.17 -0.37 Intra 0.5688 0.0134 0.1513 0.5297 0.1571 0.2385
<F(24A) .... H(29A) [      ]      2.57 < 2.67 -0.10 Intra 0.5688 0.0134 0.1513 0.5450 0.1843 0.2004
<F(24B) .... >F(15A) [      ]      2.91(2) < 2.94 -0.03      0.5791-0.0030 0.1591 0.6923 0.1230 0.0812 C(281)  138.9(15)
<F(24B) .... C(29) [      ]      2.88(3)<< 3.17 -0.29 Intra 0.5791-0.0030 0.1591 0.5297 0.1571 0.2385
<F(24B) .... H(29A) [      ]      2.73  2.67  0.06 Intra 0.5791-0.0030 0.1591 0.5450 0.1843 0.2004
<F(25) .... C(17) [      ]  3.268(12)  3.17  0.10      0.4302 0.0433 0.1345 0.4329 0.1658 0.0047 C(281)  146.6(6)
<F(25) .... C(18) [      ]  3.293(12)  3.17  0.12      0.4302 0.0433 0.1345 0.5259 0.2003 0.0402 C(281)  125.2(6)
<F(25) .... C(29) [      ]  2.849(12)<< 3.17 -0.32 Intra 0.4302 0.0433 0.1345 0.5297 0.1571 0.2385
<F(25) .... H(29A) [      ]      2.66 < 2.67 -0.01 Intra 0.4302 0.0433 0.1345 0.5450 0.1843 0.2004
<F(25A) .... C(27) [      ]  3.263(19)  3.17  0.09 Intra 0.3990 0.0178 0.1455 0.4771 0.0166 0.2960
<F(25A) .... C(29) [      ]  3.040(17) < 3.17 -0.13 Intra 0.3990 0.0178 0.1455 0.5297 0.1571 0.2385
<F(25A) .... H(11A) [ 2545.01]      2.86  2.67  0.19      0.3990 0.0178 0.1455 0.1767 0.0636 0.1466 C(281)      141
<F(25A) .... H(11C) [ 2545.01]      2.56 < 2.67 -0.11      0.3990 0.0178 0.1455 0.2228-0.0786 0.1137 C(281)      133
<F(25B) .... C(27) [      ]  3.36(2)  3.17  0.19 Intra 0.4130 0.0364 0.1404 0.4771 0.0166 0.2960
<F(25B) .... C(29) [      ]      2.89(2)<< 3.17 -0.28 Intra 0.4130 0.0364 0.1404 0.5297 0.1571 0.2385
<F(25B) .... H(29A) [      ]      2.78  2.67  0.11 Intra 0.4130 0.0364 0.1404 0.5450 0.1843 0.2004
<F(25B) .... H(11C) [ 2545.01]      2.83  2.67  0.16      0.4130 0.0364 0.1404 0.2228-0.0786 0.1137 C(281)      115
<F(26) .... C(27) [      ]  2.699(17)<< 3.17 -0.47 Intra 0.4388-0.0888 0.1890 0.4771 0.0166 0.2960
<F(26) .... C(212) [ 1545.02]  3.049(11) < 3.17 -0.12      0.4388-0.0888 0.1890 0.3792-0.2985 0.1420 C(281)  150.1(11)
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<F(26) .... H(21C) [ 1545.02]      2.78  2.67  0.11      0.4388-0.0888 0.1890  0.5357-0.2526 0.1419  C(281)      115
<F(26) .... H(21D) [ 1545.02]      2.76  2.67  0.09      0.4388-0.0888 0.1890  0.3504-0.2439 0.1144  C(281)      139
<F(26) .... H(21E) [ 1545.02]      2.70  2.67  0.03      0.4388-0.0888 0.1890  0.3738-0.2810 0.1852  C(281)      166
<F(26) .... H(27A) [          ]      2.39<< 2.67 -0.28 Intra 0.4388-0.0888 0.1890  0.4575-0.0515 0.2978
<F(26) .... H(12A) [ 2545.01]      2.73  2.67  0.06      0.4388-0.0888 0.1890  0.2520-0.0415 0.2320  C(281)      106
<F(26A) .... C(27) [          ]      2.690(18)<< 3.17 -0.48 Intra 0.4880-0.0993 0.1961  0.4771 0.0166 0.2960
<F(26A) .... C(211) [ 1545.02]      3.195(13)  3.17  0.02      0.4880-0.0993 0.1961  0.4949-0.3159 0.1360  C(281)      143.4(12)
<F(26A) .... C(212) [ 1545.02]      3.147(14) < 3.17 -0.02      0.4880-0.0993 0.1961  0.3792-0.2985 0.1420  C(281)      140.3(12)
<F(26A) .... H(21C) [ 1545.02]      2.49 < 2.67 -0.18      0.4880-0.0993 0.1961  0.5357-0.2526 0.1419  C(281)      134
<F(26A) .... H(21E) [ 1545.02]      2.82  2.67  0.15      0.4880-0.0993 0.1961  0.3738-0.2810 0.1852  C(281)      148
<F(26A) .... H(27A) [          ]      2.39<< 2.67 -0.28 Intra 0.4880-0.0993 0.1961  0.4575-0.0515 0.2978
<F(26B) .... C(27) [          ]      2.74(2)<< 3.17 -0.43 Intra 0.4620-0.0964 0.1902  0.4771 0.0166 0.2960
<F(26B) .... C(211) [ 1545.02]      3.224(17)  3.17  0.05      0.4620-0.0964 0.1902  0.4949-0.3159 0.1360  C(281)      141.6(15)
<F(26B) .... C(212) [ 1545.02]      3.034(18) < 3.17 -0.14      0.4620-0.0964 0.1902  0.3792-0.2985 0.1420  C(281)      153.6(16)
<F(26B) .... H(21C) [ 1545.02]      2.58 < 2.67 -0.09      0.4620-0.0964 0.1902  0.5357-0.2526 0.1419  C(281)      128
<F(26B) .... H(21D) [ 1545.02]      2.81  2.67  0.14      0.4620-0.0964 0.1902  0.3504-0.2439 0.1144  C(281)      136
<F(26B) .... H(21E) [ 1545.02]      2.71  2.67  0.04      0.4620-0.0964 0.1902  0.3738-0.2810 0.1852  C(281)      168
<F(26B) .... H(27A) [          ]      2.42<< 2.67 -0.25 Intra 0.4620-0.0964 0.1902  0.4575-0.0515 0.2978
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Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 2 to Neighbouring ARU'S

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=====
Nr      ARU      Nr.Cont.  d(min)  Del  XHn X      - At(I)      At(J) - Y  YHn  Note  Partaking ARU's in Close Contact Resd.
-----
1 [ 1555.01]  41      2.1000 -0.62   1 N(22) - H(22) ... O(11) -C(11)  1 << 1555.01
2 [ 2645.01]  2      2.8900 -0.11   0 C(23) - S(2) ... H(12G) -C(122) 3 < 2645.01
3 [ 2645.02]  7      2.7900  0.12   0 C(261) -*F(22A) ... H(22D) -C(221) 2 2645.02
4 [ 2655.02]  7      2.7900  0.12   2 C(221) - H(22D) ... *F(22A) -C(261) 0 2655.02
5 [ 4555.01]  5      2.4400 -0.23   1 C(25) - H(25A) ... *F(12) -C(161) 0 << 4555.01
6 [ 2545.01]  7      2.5600 -0.11   0 C(281) -*F(25A) ... H(11C) -C(111) 2 < 2545.01
7 [ 1565.02]  13     2.4900 -0.18   2 C(211) - H(21C) ... *F(26A) -C(281) 0 < 1565.02
8 [ 3665.01]  7      2.0800 -0.59   3 C(212) - H(21D) ... *F(14B) -C(181) 0 << 3665.01
9 [ 2555.01]  3      2.5400  0.14   3 C(212) - H(21D) ... H(11B) -C(111) 2 2555.01
10 [ 3656.02]  17     2.7790 -0.16   0 C(261) -*F(22) ... *F(21) -C(261) 0 < 3656.02
11 [ 2555.02]  1      2.8200  0.15   3 C(212) - H(21F) ... *F(23) -C(261) 0 2555.02
12 [ 4554.02]  2      2.7400  0.07   3 C(222) - H(22E) ... *F(23A) -C(261) 0 4554.02
13 [ 1545.01]  3      2.5700  0.17   1 C(27) - H(27A) ... H(12F) -C(122) 3 1545.01
14 [ 2545.02]  1      2.8200  0.15   0 C(261) -*F(23) ... H(21F) -C(212) 3 2545.02
15 [ 4455.02]  2      2.7400  0.07   0 C(261) -*F(23A) ... H(22E) -C(222) 3 4455.02
16 [ 1545.02]  13     2.4900 -0.18   0 C(281) -*F(26A) ... H(21C) -C(211) 2 < 1545.02
=====

```

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Asymmetric Residue Unit (= ARU) Code List

=====

| ARU-CODE | CIF-CODE | Symmetry-Code | sym TX TY TZ Ires | x(cen) | y(cen) | z(cen) |
|------------|----------|----------------------|-------------------|--------|--------|--------|
| [2555.02] | [2_555] | =1/2-x,1/2+y,1/2-z | = [2 0 0 0 2] | -0.037 | 0.779 | 0.270 |
| [3665.02] | [3_665] | =1-x,1-y,-z | = [3 1 1 0 2] | 0.463 | 0.721 | -0.230 |
| [4554.01] | [4_665] | =1/2+x,1/2-y,-1/2+z | = [4 0 0 -1 1] | 0.921 | 0.163 | -0.336 |
| [2645.01] | [2_645] | =3/2-x,-1/2+y,1/2-z | = [2 1 -1 0 1] | 1.079 | -0.163 | 0.336 |
| [3655.01] | [3_655] | =1-x,-y,-z | = [3 1 0 0 1] | 0.579 | -0.337 | -0.164 |
| [2545.02] | [2_545] | =1/2-x,-1/2+y,1/2-z | = [2 0 -1 0 2] | -0.037 | -0.221 | 0.270 |
| [4555.01] | [4_666] | =1/2+x,1/2-y,1/2+z | = [4 0 0 0 1] | 0.921 | 0.163 | 0.664 |
| [4455.01] | [4_566] | =-1/2+x,1/2-y,1/2+z | = [4 -1 0 0 1] | -0.079 | 0.163 | 0.664 |
| [1565.02] | [1_565] | =x,1+y,z | = [1 0 1 0 2] | 0.537 | 1.279 | 0.230 |
| [2655.02] | [2_655] | =3/2-x,1/2+y,1/2-z | = [2 1 0 0 2] | 0.963 | 0.779 | 0.270 |
| [2655.01] | [2_655] | =3/2-x,1/2+y,1/2-z | = [2 1 0 0 1] | 1.079 | 0.837 | 0.336 |
| [2555.01] | [2_555] | =1/2-x,1/2+y,1/2-z | = [2 0 0 0 1] | 0.079 | 0.837 | 0.336 |
| [2545.01] | [2_545] | =1/2-x,-1/2+y,1/2-z | = [2 0 -1 0 1] | 0.079 | -0.163 | 0.336 |
| [4454.02] | [4_565] | =-1/2+x,1/2-y,-1/2+z | = [4 -1 0 -1 2] | 0.037 | 0.221 | -0.270 |
| [4454.01] | [4_565] | =-1/2+x,1/2-y,-1/2+z | = [4 -1 0 -1 1] | -0.079 | 0.163 | -0.336 |
| [2645.02] | [2_645] | =3/2-x,-1/2+y,1/2-z | = [2 1 -1 0 2] | 0.963 | -0.221 | 0.270 |
| [3665.01] | [3_665] | =1-x,1-y,-z | = [3 1 1 0 1] | 0.579 | 0.663 | -0.164 |
| [3656.02] | [3_656] | =1-x,-y,1-z | = [3 1 0 1 2] | 0.463 | -0.279 | 0.770 |
| [4554.02] | [4_665] | =1/2+x,1/2-y,-1/2+z | = [4 0 0 -1 2] | 1.037 | 0.221 | -0.270 |
| [1545.01] | [1_545] | =x,-1+y,z | = [1 0 -1 0 1] | 0.421 | -0.663 | 0.164 |
| [4455.02] | [4_566] | =-1/2+x,1/2-y,1/2+z | = [4 -1 0 0 2] | 0.037 | 0.221 | 0.730 |
| [1545.02] | [1_545] | =x,-1+y,z | = [1 0 -1 0 2] | 0.537 | -0.721 | 0.230 |

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

X(J) = X(sym) + TX , Y(J) = Y(sym) + TY , Z(J) = Z(sym) + TZ,
 SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

=====
 Analysis of Potential Hydrogen Bonds and Schemes with $d(D...A) < R(D)+R(A)+0.50$, $d(H...A) < R(H)+R(A)-0.12$ Ang., $D-H...A > 100.0$ Deg
 =====

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
 =====

| Nr | Typ | Res | Donor | H...A | Acceptor | [ARU] | D - H | H...A | D...A | D - H...A | A..H..A* A'..H..A" | Sum(XY,YZ) | Sum(XZ) |
|----|-------|-----|--------|----------|----------|------------|---------|---------|------------|-----------|--------------------|------------|---------|
| 1 | | 1 | N(11) | --H(11) | ..O(22) | [] | 0.81(2) | 2.29(2) | 3.070(2) | 163(2) | | | |
| 2 | | 1 | N(12) | --H(12) | ..O(21) | [] | 0.80(2) | 2.21(2) | 3.002(2) | 172(2) | | | |
| 3 | | 2 | N(21) | --H(21) | ..O(12) | [] | 0.85(2) | 2.31(2) | 3.141(2) | 166(2) | | | |
| 4 | | 2 | N(22) | --H(22) | ..O(11) | [] | 0.86(2) | 2.10(2) | 2.956(2) | 176(2) | | | |
| 5 | | 1 | C(112) | --H(11D) | ..F(14A) | [4455.01] | 0.98 | 2.46 | 3.390(9) | 159 | | | |
| 6 | Intra | 1 | C(12) | --H(12A) | ..S(1) | [] | 0.99 | 2.60 | 3.114(2) | 112 | | | |
| 7 | Intra | 1 | C(15) | --H(15A) | ..S(1) | [] | 0.95 | 2.80 | 3.204(2) | 107 | | | |
| 8 | Intra | 2 | C(22) | --H(22A) | ..S(2) | [] | 0.99 | 2.63 | 3.109(2) | 110 | | | |
| 9 | Intra | 2 | C(29) | --H(29A) | ..S(2) | [] | 0.95 | 2.83 | 3.2310(19) | 106 | | | |

Translation of ARU-Code to CIF and Equivalent Position Code
 =====

$$[4455.] = [4_566] = -1/2+x, 1/2-y, 1/2+z$$

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]
 =====

2-Centre (linear) D-H...X most prob. angle 160 deg - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
 3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg Springer-Verlag, Berlin, 1991, pp 20.
 4-Centre (trifurcated)

Analysis of Potential Donor/Acceptor Atoms -- (Major Disorder Form Only)
 =====

| At.Nr | D/A | #Cov.Bonds | # H | #D-H..A | #A..H | #A..H-C | Sum(A-H) | Sum(A-X) |
|-------|---------|------------|-----|---------|-------|---------|----------|----------|
| 1 | S(1) | 1 | - | 0 | 0 | 2 | 2 | 3 |
| 2 | S(2) | 1 | - | 0 | 0 | 2 | 2 | 3 |
| 3 | >F(14A) | 1 | - | 0 | 0 | 1 | 1 | 2 |
| 4 | >F(15A) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 5 | >F(16A) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 6 | O(11) | 2 | - | 0 | 1 | 0 | 1 | 3 |
| 7 | O(12) | 2 | - | 0 | 1 | 0 | 1 | 3 |
| 8 | O(21) | 2 | - | 0 | 1 | 0 | 1 | 3 |
| 9 | O(22) | 2 | - | 0 | 1 | 0 | 1 | 3 |
| 10 | N(11) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 11 | N(12) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 12 | N(21) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 13 | N(22) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |

=====
 Analysis of Hydrogen Bonded Molecular Aggregates (See also Acta Cryst. B36, 1980, 2113 - 2115) -- (Major Disorder Component Only)
 =====

Coordinates of Donor and Acceptor Atoms
 =====

Coordinates of D/A-Bonded Atom(s)
 =====

| D/A I | [ARU] | X | Y | Z | -- | D/A J | [ARU] | X | Y | Z | Atom K | X | Y | Z | I..J--K Angle |
|-------|-------------|--------|--------|--------|----|-------|-------------|--------|--------|--------|--------|--------|--------|--------|---------------|
| N(11) | [1555.01], | 0.4245 | 0.3815 | 0.1437 | >> | O(22) | [1555.02], | 0.6216 | 0.5074 | 0.1257 | C(21) | 0.6403 | 0.5776 | 0.1748 | 108.3(7) |
| | | | | | | | | | | | C(221) | 0.7113 | 0.4893 | 0.0938 | 132.7(7) |
| O(22) | [1555.02], | 0.6216 | 0.5074 | 0.1257 | << | N(11) | [1555.01], | 0.4245 | 0.3815 | 0.1437 | C(13) | 0.3543 | 0.3910 | 0.1858 | 130.3(7) |
| | | | | | | | | | | | C(14) | 0.4245 | 0.3069 | 0.0984 | 102.5(7) |
| | | | | | | | | | | | H(11) | 0.4736 | 0.4211 | 0.1457 | 12.7(11) |
| N(12) | [1555.01], | 0.3678 | 0.4768 | 0.2176 | >> | O(21) | [1555.02], | 0.5387 | 0.6129 | 0.1829 | C(21) | 0.6403 | 0.5776 | 0.1748 | 121.8(7) |
| | | | | | | | | | | | C(211) | 0.4949 | 0.6841 | 0.1360 | 111.8(7) |
| O(21) | [1555.02], | 0.5387 | 0.6129 | 0.1829 | << | N(12) | [1555.01], | 0.3678 | 0.4768 | 0.2176 | C(12) | 0.3024 | 0.5101 | 0.2631 | 119.0(7) |
| | | | | | | | | | | | C(13) | 0.3543 | 0.3910 | 0.1858 | 115.6(8) |
| | | | | | | | | | | | H(12) | 0.4087 | 0.5175 | 0.2085 | 6.0(11) |
| N(21) | [1555.02], | 0.6255 | 0.4650 | 0.2622 | >> | O(12) | [1555.01], | 0.4520 | 0.5934 | 0.3160 | C(11) | 0.3690 | 0.5305 | 0.3255 | 107.6(7) |
| | | | | | | | | | | | C(121) | 0.4996 | 0.6454 | 0.3714 | 110.9(7) |
| O(12) | [1555.01], | 0.4520 | 0.5934 | 0.3160 | << | N(21) | [1555.02], | 0.6255 | 0.4650 | 0.2622 | C(22) | 0.6947 | 0.5338 | 0.2356 | 107.0(7) |
| | | | | | | | | | | | C(23) | 0.6343 | 0.3656 | 0.2619 | 127.7(8) |
| | | | | | | | | | | | H(21) | 0.5763 | 0.4902 | 0.2798 | 10.1(10) |
| N(22) | [1555.02], | 0.5589 | 0.3192 | 0.2901 | >> | O(11) | [1555.01], | 0.4162 | 0.4433 | 0.3547 | C(11) | 0.3690 | 0.5305 | 0.3255 | 119.7(7) |
| | | | | | | | | | | | C(111) | 0.3465 | 0.3859 | 0.3870 | 113.0(7) |
| O(11) | [1555.01], | 0.4162 | 0.4433 | 0.3547 | << | N(22) | [1555.02], | 0.5589 | 0.3192 | 0.2901 | C(23) | 0.6343 | 0.3656 | 0.2619 | 118.2(7) |
| | | | | | | | | | | | C(24) | 0.5369 | 0.2164 | 0.2909 | 114.3(7) |
| | | | | | | | | | | | H(22) | 0.5201 | 0.3557 | 0.3105 | 3.0(10) |

=====

***** Aggregate = 1 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 4 1 1555.01 -- 1555.02

4 1 1555.02 -- 1555.01

=====

***** Aggregate = 2 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 4 1 2555.01 -- 2555.02

4 1 2555.02 -- 2555.01

=====

=====

***** Aggregate = 3 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

4 1 3555.01 -- 3555.02

4 1 3555.02 -- 3555.01

=====

***** Aggregate = 4 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

4 1 4555.01 -- 4555.02

4 1 4555.02 -- 4555.01

=====
 Analysis of the (Cooperative) Hydrogen Bond Network (i.e. (In)Finite O-H...O-H...O-H.. Chains and/or Rings (Max = 18 Membered))
 =====

=====
 ***** Network = 1 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|--------|--------|--------|------------------|--------|--------|--|
| 1.555 | N(11) [1555.01] | 0.4245 | 0.3815 | 0.1437 | O(22) [1555.02] | 0.6216 | 0.5074 | 0.1257 |
| | H(11) | 0.4736 | 0.4211 | 0.1457 | | | | |

=====
 ***** Network = 2 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|--------|--------|--------|------------------|--------|--------|--|
| 2.555 | N(12) [1555.01] | 0.3678 | 0.4768 | 0.2176 | O(21) [1555.02] | 0.5387 | 0.6129 | 0.1829 |
| | H(12) | 0.4087 | 0.5175 | 0.2085 | | | | |

=====
 ***** Network = 3 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|--------|--------|--------|------------------|--------|--------|--|
| 3.555 | N(21) [1555.02] | 0.6255 | 0.4650 | 0.2622 | O(12) [1555.01] | 0.4520 | 0.5934 | 0.3160 |
| | H(21) | 0.5763 | 0.4902 | 0.2798 | | | | |

=====
 ***** Network = 4 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|--------|--------|--------|------------------|--------|--------|--|
| 4.555 | N(22) [1555.02] | 0.5589 | 0.3192 | 0.2901 | O(11) [1555.01] | 0.4162 | 0.4433 | 0.3547 |
| | H(22) | 0.5201 | 0.3557 | 0.3105 | | | | |

 Hydrogen Bonds are Coded as N.IJK Where N = Sequence Number of Hydrogen Bond (NOTE: New Hbond Numbering system)
 I - 5 = Nr of Translation Units Along A-Axis
 J - 5 = Nr of Translation Units Along B-Axis
 K - 5 = Nr of Translation Units Along C-Axis

Ring Closure Links are Indicated with 'R' and Infinite Chain Links With 'T'

=====

3.6 Angstrom Coordination Sphere Around Atom I = S(1) [ARU = 1555.01] 0.26504 0.30381 0.19786 2.6602 4.0791 4.2446

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|-----------|---------------------------------------|--------|-------|---------|--------|----------|---------|---------|---------|--------|--------|
| 1 | 1.6694(19) | -- | C(13) | | Intra | 45.24 | -8.90 | 0.35434 | 0.39103 | 0.18582 | 3.8216 | 5.2502 | 3.9863 |
| 2 | 2.6591(18) | << | N(12) | | Intra | 62.23 | 9.16 | 0.36780 | 0.47681 | 0.21759 | 3.8835 | 6.4019 | 4.6678 |
| 3 | 2.6846(18) | << | N(11) | | Intra | 25.52 | -25.65 | 0.42452 | 0.38146 | 0.14369 | 4.8442 | 5.1217 | 3.0825 |
| 4 | 3.114(2) | << | C(12) | | Intra | 84.85 | 26.73 | 0.30244 | 0.51013 | 0.26314 | 2.9098 | 6.8493 | 5.6450 |
| 5 | 3.1646(19) | << | C(14) | | Intra | 1.02 | -42.41 | 0.42449 | 0.30692 | 0.09837 | 4.9964 | 4.1209 | 2.1103 |
| 6 | 3.204(2) | << | C(15) | | Intra | -17.62 | -65.36 | 0.33005 | 0.27370 | 0.06209 | 3.9333 | 3.6748 | 1.3320 |
| 7 | 3.458(13) | .. | <F(21B)c[1/2-x,1/2+y,1/2-z = 2555.02] | | | 122.12 | -38.51 | 0.12350 | 0.47450 | 0.09750 | 1.2217 | 6.3709 | 2.0916 |
| 8 | 2.60 | << | H(12A) | | Intra | 102.23 | 35.30 | 0.24800 | 0.45850 | 0.26800 | 2.2102 | 6.1561 | 5.7492 |
| 9 | 2.80 | << | H(15A) | | Intra | -9.02 | -81.70 | 0.26220 | 0.29910 | 0.06890 | 3.0588 | 4.0159 | 1.4781 |
| 10 | 3.37 | .. | H(12B)a[1/2-x,-1/2+y,1/2-z = 2545.01] | | | -99.85 | 20.26 | 0.23650 | 0.07160 | 0.25230 | 2.1187 | 0.9613 | 5.4124 |
| 11 | 3.38(2) | .. | H(12) | | Intra | 58.37 | 3.88 | 0.40870 | 0.51750 | 0.20850 | 4.4274 | 6.9482 | 4.4728 |
| 12 | 3.40(2) | .. | H(11) | | Intra | 29.41 | -19.24 | 0.47360 | 0.42110 | 0.14570 | 5.4534 | 5.6539 | 3.1256 |
| 13 | 3.42 | .. | H(27A)c[1/2-x,1/2+y,1/2-z = 2555.02] | | | 145.32 | 1.56 | 0.04250 | 0.44850 | 0.20220 | -0.1474 | 6.0218 | 4.3377 |
| 14 | 3.49 | .. | H(21E)b[1/2-x,-1/2+y,1/2-z = 2545.02] | | | -151.94 | 46.02 | 0.12620 | 0.21900 | 0.31480 | 0.5240 | 2.9404 | 6.7532 |
| 15 | 3.52 | .. | H(12C)a[1/2-x,-1/2+y,1/2-z = 2545.01] | | | -141.73 | -34.14 | 0.05790 | 0.16930 | 0.10570 | 0.3708 | 2.2731 | 2.2675 |
| 16 | 3.53 | .. | H(12F)a[1/2-x,-1/2+y,1/2-z = 2545.01] | | | -172.15 | -7.60 | -0.01700 | 0.26820 | 0.17610 | -0.8063 | 3.6010 | 3.7778 |
| 17 | 3.53 | .. | H(11A)a[1/2-x,-1/2+y,1/2-z = 2545.01] | | | -106.19 | -18.13 | 0.17670 | 0.06360 | 0.14660 | 1.7241 | 0.8539 | 3.1449 |

Angles (Degrees) At1...V...At2 with Vertex V = S(1)

| | | | | | | | |
|------------------|-----------|------------------|----------|------------------|----------|------------------|-----------|
| C(13) , N(12) | 24.75(7) | C(13) , N(11) | 25.13(7) | C(13) , C(12) | 52.40(7) | C(13) , C(14) | 51.16(7) |
| C(13) , C(15) | 70.82(7) | C(13) , <F(21B)c | 74.2(2) | N(12) , N(11) | 49.87(5) | N(12) , C(12) | 27.69(5) |
| N(12) , C(14) | 75.89(5) | N(12) , C(15) | 94.14(5) | N(12) , <F(21B)c | 73.2(2) | N(11) , C(12) | 77.53(5) |
| N(11) , C(14) | 26.15(5) | N(11) , C(15) | 48.11(5) | N(11) , <F(21B)c | 79.1(2) | C(12) , C(14) | 103.44(5) |
| C(12) , C(15) | 119.29(6) | C(12) , <F(21B)c | 74.0(2) | C(14) , C(15) | 25.22(5) | C(14) , <F(21B)c | 83.0(2) |
| C(15) , <F(21B)c | 71.5(2) | | | | | | |

=====

3.6 Angstrom Coordination Sphere Around Atom I = S(2) [ARU = 1555.02] 0.73064 0.30491 0.23142 8.3908 4.0939 4.9645

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------------------------------------|------------|-----------|--------|-------|---------|--------|---------|---------|---------|---------|--------|--------|
| 1 | 1.6770(19) | -- | C(23) | | | | Intra | 148.14 | 22.98 | 0.63434 | 0.36560 | 0.26194 | 7.0795 | 4.9087 | 5.6192 |
| 2 | 2.6615(17) | << | N(21) | | | | Intra | 123.52 | 14.36 | 0.62546 | 0.46501 | 0.26219 | 6.9672 | 6.2435 | 5.6246 |
| 3 | 2.6749(18) | << | N(22) | | | | Intra | 175.33 | 28.07 | 0.55894 | 0.31921 | 0.29009 | 6.0383 | 4.2859 | 6.2231 |
| 4 | 3.109(2) | << | C(22) | | | | Intra | 98.62 | 1.65 | 0.69466 | 0.53378 | 0.23560 | 7.9252 | 7.1668 | 5.0542 |
| 5 | 3.1576(19) | << | C(24) | | | | Intra | 155.70 | 23.84 | 0.53687 | 0.21640 | 0.29092 | 5.7586 | 2.9055 | 6.2409 |
| 6 | 3.2310(19) | << | C(29) | | | | Intra | 142.06 | 2.68 | 0.52971 | 0.15713 | 0.23846 | 5.8453 | 2.1097 | 5.1155 |
| 7 | 2.63 | << | H(22A) | | | | Intra | 81.45 | -1.37 | 0.76100 | 0.49850 | 0.22850 | 8.7817 | 6.6931 | 4.9019 |
| 8 | 2.83 | .< | H(29A) | | | | Intra | 143.96 | -13.59 | 0.54500 | 0.18430 | 0.20040 | 6.1654 | 2.4745 | 4.2991 |
| 9 | 2.89 | .< | H(12G)a[3/2-x,-1/2+y,1/2-z = 2645.01] | | | | | -33.63 | -31.53 | 0.87530 | 0.20320 | 0.16090 | 10.4439 | 2.7283 | 3.4517 |
| 10 | 2.94 | .< | H(19A) [= 01] | | | | | -173.71 | -61.63 | 0.58760 | 0.29350 | 0.11080 | 7.0017 | 3.9407 | 2.3769 |
| 11 | 2.98 | .< | H(22B)b[3/2-x,-1/2+y,1/2-z = 2645.02] | | | | | -77.24 | 1.23 | 0.78390 | 0.08840 | 0.23440 | 9.0493 | 1.1869 | 5.0284 |
| 12 | 3.15 | .. | H(22C) | | | | Intra | 68.95 | -56.18 | 0.74810 | 0.42690 | 0.10930 | 9.0212 | 5.7318 | 2.3447 |
| 13 | 3.31 | .. | H(21A)b[3/2-x,-1/2+y,1/2-z = 2645.02] | | | | | -72.91 | 43.46 | 0.81540 | 0.13380 | 0.33760 | 9.0971 | 1.7965 | 7.2423 |
| 14 | 3.42(2) | .. | H(21) | | | | Intra | 130.17 | 17.68 | 0.57630 | 0.49020 | 0.27980 | 6.2909 | 6.5817 | 6.0024 |
| 15 | 3.44(2) | .. | H(22) | | | | Intra | 166.81 | 29.59 | 0.52010 | 0.35570 | 0.31050 | 5.4822 | 4.7758 | 6.6610 |
| 16 | 3.59 | .. | H(12F)a[3/2-x,-1/2+y,1/2-z = 2645.01] | | | | | -8.36 | -19.30 | 0.98300 | 0.26820 | 0.17610 | 11.7444 | 3.6010 | 3.7778 |

Angles (Degrees) At1...V...At2 with Vertex V = S(2)

| | | | | | | | |
|---------------|-----------|---------------|-----------|---------------|----------|---------------|----------|
| C(23) , N(21) | 24.83(7) | C(23) , N(22) | 25.00(7) | C(23) , C(22) | 52.51(7) | C(23) , C(24) | 51.18(7) |
| C(23) , C(29) | 70.37(7) | N(21) , N(22) | 49.83(5) | N(21) , C(22) | 27.69(5) | N(21) , C(24) | 75.98(5) |
| N(21) , C(29) | 93.61(5) | N(22) , C(22) | 77.51(5) | N(22) , C(24) | 26.32(5) | N(22) , C(29) | 47.87(5) |
| C(22) , C(24) | 103.62(5) | C(22) , C(29) | 119.18(5) | C(24) , C(29) | 24.94(4) | | |


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<F(16) , C(18)      65.2(7)  <F(16) , <F(15)      57.1(5)  <F(16) , <F(16B)     28.8(8)  <F(16) , C(19)      93.2(7)
<F(16) , C(222)    144.6(7)  <F(16) , C(112)c     77.0(7)  <F(16) , C(17)      52.5(7)  <F(16) , C(212)b    74.6(4)
>F(15A) , >F(16A)   60.1(3)  >F(15A) , C(18)      64.5(3)  >F(15A) , <F(15)    12.8(3)  >F(15A) , <F(16B)   40.9(8)
>F(15A) , C(19)     69.4(3)  >F(15A) , C(222)    131.2(4)  >F(15A) , C(112)c   93.1(3)  >F(15A) , C(17)     73.8(3)
>F(15A) , C(212)b  144.2(4)  >F(16A) , C(18)      63.8(5)  >F(16A) , <F(15)    47.8(4)  >F(16A) , <F(16B)   19.5(8)
>F(16A) , C(19)     90.8(5)  >F(16A) , C(222)    151.7(5)  >F(16A) , C(112)c   77.0(5)  >F(16A) , C(17)     53.7(5)
>F(16A) , C(212)b  84.1(3)  C(18) , <F(15)       58.4(4)  C(18) , <F(16B)     57.6(9)  C(18) , C(19)      28.25(12)
C(18) , C(222)     96.0(3)  C(18) , C(112)c     140.6(3)  C(18) , C(17)      17.69(10)  C(18) , C(212)b    100.0(3)
<F(15) , <F(16B)   28.4(8)  <F(15) , C(19)       69.8(4)  <F(15) , C(222)    139.3(4)  <F(15) , C(112)c   92.5(4)
<F(15) , C(17)     64.7(4)  <F(15) , C(212)b    131.6(4)  <F(16B) , C(19)     80.5(8)  <F(16B) , C(222)   153.6(9)
<F(16B) , C(112)c  84.0(9)  <F(16B) , C(17)      54.0(9)  <F(16B) , C(212)b  103.3(8)  C(19) , C(222)     74.3(2)
C(19) , C(112)c    162.2(3)  C(19) , C(17)       44.13(13)  C(19) , C(212)b   112.9(3)  C(222) , C(112)c   122.1(3)
C(222) , C(17)    101.2(2)  C(222) , C(212)b    80.05(19)  C(112)c, C(17)     129.3(3)  C(112)c, C(212)b   79.15(19)
C(17) , C(212)b    84.3(2)

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3.6 Angstrom Coordination Sphere Around Atom I = F(15A) [ARU = 1555.01] 0.69230 0.12300 0.08120 8.4154 1.6515 1.7419

| Nr | d(I,J) To | Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|--------|----------------------------|------------|-------|---------|--------|---------|----------|----------|---------|---------|---------|
| 1 | 1.340(7) | -- | C(181) | | Intra | 137.80 | -54.98 | 0.63320 | 0.16146 | 0.03006 | 7.8459 | 2.1678 | 0.6449 |
| 2 | 0.577(13) | << | <F(15) | | Intra | -125.28 | -20.24 | 0.66490 | 0.09010 | 0.07190 | 8.1029 | 1.2097 | 1.5424 |
| 3 | 0.83(3) | << | <F(15B) | | Intra | 69.22 | -9.08 | 0.71380 | 0.18000 | 0.07510 | 8.7058 | 2.4168 | 1.6111 |
| 4 | 1.64(3) | << | <F(16B) | | Intra | -126.70 | -53.13 | 0.62900 | 0.06420 | 0.02000 | 7.8271 | 0.8620 | 0.4290 |
| 5 | 1.777(15) | << | <F(14) | | Intra | 74.37 | -35.16 | 0.71070 | 0.22720 | 0.03350 | 8.8070 | 3.0505 | 0.7187 |
| 6 | 2.122(11) | << | >F(14A) | | Intra | 80.76 | -42.63 | 0.69430 | 0.23780 | 0.01420 | 8.6661 | 3.1928 | 0.3046 |
| 7 | 2.135(10) | << | >F(16A) | | Intra | -140.32 | -73.64 | 0.62980 | 0.09440 | -0.01430 | 7.9526 | 1.2675 | -0.3068 |
| 8 | 2.345(13) | << | <F(16) | | Intra | -168.73 | -78.16 | 0.62600 | 0.11600 | -0.02580 | 7.9436 | 1.5575 | -0.5535 |
| 9 | 2.378(7) | << | C(18) | | Intra | 151.98 | -21.70 | 0.52587 | 0.20032 | 0.04020 | 6.4647 | 2.6896 | 0.8624 |
| 10 | 2.46(3) | << | <F(14B) | | Intra | 95.11 | -63.64 | 0.65700 | 0.20400 | -0.02150 | 8.3182 | 2.7390 | -0.4612 |
| 11 | 2.76(2) | < | <F(24A) [| = 02] | | -140.51 | 33.02 | 0.56880 | 0.01340 | 0.15130 | 6.6294 | 0.1799 | 3.2457 |
| 12 | 2.91(2) | < | <F(24B) [| = 02] | | -134.85 | 35.00 | 0.57910 | -0.00300 | 0.15910 | 6.7324 | -0.0403 | 3.4131 |
| 13 | 2.925(7) | << | C(19) | | Intra | 137.35 | 2.37 | 0.52253 | 0.27050 | 0.08683 | 6.2658 | 3.6319 | 1.8627 |
| 14 | 2.982(12) | .. | <F(11B)c[1-x,-y,-z | = 3655.01] | | -72.32 | -12.13 | 0.75500 | -0.08390 | 0.05200 | 9.3007 | -1.1265 | 1.1155 |
| 15 | 3.466(7) | .. | C(17) | | Intra | 169.16 | -28.26 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 16 | 3.467(12) | .. | <F(11A)c[1-x,-y,-z | = 3655.01] | | -60.16 | -25.67 | 0.79740 | -0.07890 | 0.01120 | 9.9702 | -1.0594 | 0.2403 |
| 17 | 3.480(7) | .. | C(122)a[3/2-x,-1/2+y,1/2-z | = 2645.01] | | 25.97 | 22.93 | 0.93880 | 0.22750 | 0.14440 | 11.2964 | 3.0545 | 3.0977 |
| 18 | 2.76 | .. | H(19A) | | Intra | 121.70 | 13.28 | 0.58760 | 0.29350 | 0.11080 | 7.0017 | 3.9407 | 2.3769 |
| 19 | 2.86 | .. | H(12G)a[3/2-x,-1/2+y,1/2-z | = 2645.01] | | 27.96 | 36.67 | 0.87530 | 0.20320 | 0.16090 | 10.4439 | 2.7283 | 3.4517 |
| 20 | 3.25 | .. | H(12D)a[3/2-x,-1/2+y,1/2-z | = 2645.01] | | -5.64 | 7.47 | 0.95330 | 0.09940 | 0.10090 | 11.6248 | 1.3346 | 2.1645 |
| 21 | 3.38 | .. | H(22B)b[3/2-x,-1/2+y,1/2-z | = 2645.02] | | -36.24 | 76.55 | 0.78390 | 0.08840 | 0.23440 | 9.0493 | 1.1869 | 5.0284 |
| 22 | 3.39 | .. | H(12E)a[3/2-x,-1/2+y,1/2-z | = 2645.01] | | 35.62 | 9.47 | 0.91580 | 0.26800 | 0.10720 | 11.1330 | 3.5983 | 2.2997 |
| 23 | 3.41 | .. | H(11D)d[1/2+x,1/2-y,-1/2+z | = 4554.01] | | 16.55 | -43.24 | 0.85280 | 0.17570 | -0.02770 | 10.7965 | 2.3590 | -0.5942 |
| 24 | 3.50 | .. | H(29A) [| = 02] | | 159.91 | 46.86 | 0.54500 | 0.18430 | 0.20040 | 6.1654 | 2.4745 | 4.2991 |

Angles (Degrees) At1...V...At2 with Vertex V = >F(15A)

| | | | | | | | |
|-------------------|----------|--------------------|-----------|-------------------|-----------|--------------------|-----------|
| C(181) , <F(15) | 77.4(13) | C(181) , <F(15B) | 70.4(17) | C(181) , <F(16B) | 51.5(8) | C(181) , <F(14) | 47.1(5) |
| C(181) , >F(14A) | 38.3(3) | C(181) , >F(16A) | 36.0(4) | C(181) , <F(16) | 29.4(5) | C(181) , C(18) | 34.9(2) |
| C(181) , <F(14B) | 22.9(9) | C(181) , <F(24A) | 112.1(5) | C(181) , <F(24B) | 116.6(6) | C(181) , C(19) | 57.4(3) |
| C(181) , <F(11B)c | 108.3(5) | C(181) , C(17) | 35.0(2) | C(181) , <F(11A)c | 97.9(4) | C(181) , C(122)a | 121.0(4) |
| <F(15) , <F(15B) | 147(2) | <F(15) , <F(16B) | 32.9(15) | <F(15) , <F(14) | 121.6(14) | <F(15) , >F(14A) | 112.7(13) |
| <F(15) , >F(16A) | 54.1(12) | <F(15) , <F(16) | 61.4(13) | <F(15) , C(18) | 76.2(13) | <F(15) , <F(14B) | 90.4(14) |
| <F(15) , <F(24A) | 55.2(13) | <F(15) , <F(24B) | 56.0(13) | <F(15) , C(19) | 97.7(14) | <F(15) , <F(11B)c | 51.3(14) |
| <F(15) , C(17) | 59.6(13) | <F(15) , <F(11A)c | 59.6(14) | <F(15) , C(122)a | 153.2(14) | <F(15B) , <F(16B) | 116.3(19) |
| <F(15B) , <F(14) | 26.5(17) | <F(15B) , >F(14A) | 35.0(17) | <F(15B) , >F(16A) | 95.2(17) | <F(15B) , <F(16) | 87.3(18) |
| <F(15B) , C(18) | 80.0(17) | <F(15B) , <F(14B) | 57.6(18) | <F(15B) , <F(24A) | 143.6(18) | <F(15B) , <F(24B) | 146.0(18) |
| <F(15B) , C(19) | 68.8(17) | <F(15B) , <F(11B)c | 136.3(18) | <F(15B) , C(17) | 94.3(17) | <F(15B) , <F(11A)c | 119.8(18) |
| <F(15B) , C(122)a | 53.1(17) | <F(16B) , <F(14) | 89.8(10) | <F(16B) , >F(14A) | 81.4(9) | <F(16B) , >F(16A) | 21.3(9) |
| <F(16B) , <F(16) | 29.0(9) | <F(16B) , C(18) | 67.7(11) | <F(16B) , <F(14B) | 58.8(11) | <F(16B) , <F(24A) | 87.0(12) |

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<F(16B) , <F(24B) 88.4(12) <F(16B) , C(19) 95.5(11) <F(16B) , <F(11B)c 59.4(10) <F(16B) , C(17) 52.5(11)
<F(16B) , <F(11A)c 55.8(11) <F(16B) , C(122)a 143.4(13) <F(14) , >F(14A) 9.0(5) <F(14) , >F(16A) 68.7(6)
<F(14) , <F(16) 60.8(6) <F(14) , C(18) 67.9(5) <F(14) , <F(14B) 31.2(8) <F(14) , <F(24A) 151.2(7)
<F(14) , <F(24B) 156.2(7) <F(14) , C(19) 69.7(5) <F(14) , <F(11B)c 123.2(6) <F(14) , C(17) 77.7(5)
<F(14) , <F(11A)c 105.5(5) <F(14) , C(122)a 74.0(5) >F(14A) , >F(16A) 60.4(4) >F(14A) , <F(16) 52.4(5)
>F(14A) , C(18) 61.9(3) >F(14A) , <F(14B) 22.6(7) >F(14A) , <F(24A) 146.4(5) >F(14A) , <F(24B) 151.5(6)
>F(14A) , C(19) 67.9(3) >F(14A) , <F(11B)c 120.0(4) >F(14A) , C(17) 70.2(3) >F(14A) , <F(11A)c 102.8(4)
>F(14A) , C(122)a 82.7(3) >F(16A) , <F(16) 8.1(4) >F(16A) , C(18) 63.0(4) >F(16A) , <F(14B) 37.9(7)
>F(16A) , <F(24A) 106.7(6) >F(16A) , <F(24B) 108.7(6) >F(16A) , C(19) 90.1(4) >F(16A) , <F(11B)c 72.3(4)
>F(16A) , C(17) 52.3(4) >F(16A) , <F(11A)c 62.7(4) >F(16A) , C(122)a 128.8(5) <F(16) , C(18) 59.4(6)
<F(16) , <F(14B) 29.9(8) <F(16) , <F(24A) 112.4(7) <F(16) , <F(24B) 115.0(7) <F(16) , C(19) 85.4(5)
<F(16) , <F(11B)c 79.4(5) <F(16) , C(17) 50.9(6) <F(16) , <F(11A)c 68.6(5) <F(16) , C(122)a 124.3(6)
C(18) , <F(14B) 56.2(9) C(18) , <F(24A) 84.5(4) C(18) , <F(24B) 89.5(5) C(18) , C(19) 28.00(10)
C(18) , <F(11B)c 124.9(4) C(18) , C(17) 16.87(9) C(18) , <F(11A)c 123.3(3) C(18) , C(122)a 130.3(3)
<F(14B) , <F(24A) 134.3(10) <F(14B) , <F(24B) 138.4(10) <F(14B) , C(19) 73.1(8) <F(14B) , <F(11B)c 103.6(7)
<F(14B) , C(17) 57.9(9) <F(14B) , <F(11A)c 88.6(7) <F(14B) , C(122)a 101.7(8) <F(24A) , <F(24B) 5.1(5)
<F(24A) , C(19) 82.1(4) <F(24A) , <F(11B)c 79.0(5) <F(24A) , C(17) 77.7(4) <F(24A) , <F(11A)c 96.3(5)
<F(24A) , C(122)a 122.6(5) <F(24B) , C(19) 86.8(5) <F(24B) , <F(11B)c 75.6(6) <F(24B) , C(17) 82.4(4)
<F(24B) , <F(11A)c 93.1(6) <F(24B) , C(122)a 119.3(5) C(19) , <F(11B)c 149.0(4) C(19) , C(17) 43.25(10)
C(19) , <F(11A)c 151.3(3) C(19) , C(122)a 108.6(2) <F(11B)c , C(17) 108.2(3) <F(11B)c , <F(11A)c 17.7(3)
<F(11B)c , C(122)a 102.2(3) C(17) , <F(11A)c 108.2(3) C(17) , C(122)a 146.5(2) <F(11A)c , C(122)a 96.5(3)
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3.6 Angstrom Coordination Sphere Around Atom I = F(16A) [ARU = 1555.01] 0.62980 0.09440 -0.01430 7.9526 1.2675 -0.3068

| Nr | d(I,J) To | Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|--------|----------------------------|------------|-------|---------|--------|---------|----------|----------|---------|---------|---------|
| 1 | 1.314(8) | -- | C(181) | | Intra | 96.76 | 46.39 | 0.63320 | 0.16146 | 0.03006 | 7.8459 | 2.1678 | 0.6449 |
| 2 | 0.381(16) | << | <F(16) | | Intra | 91.77 | -40.37 | 0.62600 | 0.11600 | -0.02580 | 7.9436 | 1.5575 | -0.5535 |
| 3 | 0.85(3) | << | <F(16B) | | Intra | -107.20 | 60.02 | 0.62900 | 0.06420 | 0.02000 | 7.8271 | 0.8620 | 0.4290 |
| 4 | 1.52(3) | << | <F(14B) | | Intra | 76.05 | -5.82 | 0.65700 | 0.20400 | -0.02150 | 8.3182 | 2.7390 | -0.4612 |
| 5 | 1.856(13) | << | <F(15) | | Intra | -21.01 | 85.02 | 0.66490 | 0.09010 | 0.07190 | 8.1029 | 1.2097 | 1.5424 |
| 6 | 2.135(10) | << | >F(15A) | | Intra | 39.68 | 73.64 | 0.69230 | 0.12300 | 0.08120 | 8.4154 | 1.6515 | 1.7419 |
| 7 | 2.142(13) | << | >F(14A) | | Intra | 69.66 | 16.58 | 0.69430 | 0.23780 | 0.01420 | 8.6661 | 3.1928 | 0.3046 |
| 8 | 2.227(17) | << | <F(14) | | Intra | 64.40 | 27.41 | 0.71070 | 0.22720 | 0.03350 | 8.8070 | 3.0505 | 0.7187 |
| 9 | 2.36(3) | << | <F(15B) | | Intra | 56.76 | 54.38 | 0.71380 | 0.18000 | 0.07510 | 8.7058 | 2.4168 | 1.6111 |
| 10 | 2.367(12) | << | C(18) | | Intra | 136.29 | 29.60 | 0.52587 | 0.20032 | 0.04020 | 6.4647 | 2.6896 | 0.8624 |
| 11 | 2.741(16) | << | C(17) | | Intra | 159.30 | 8.56 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 12 | 3.094(16) | .. | <F(11B)a[1-x,-y,-z | = 3655.01] | | -60.61 | 27.37 | 0.75500 | -0.08390 | 0.05200 | 9.3007 | -1.1265 | 1.1155 |
| 13 | 3.128(17) | .. | <F(11A)a[1-x,-y,-z | = 3655.01] | | -49.07 | 10.07 | 0.79740 | -0.07890 | 0.01120 | 9.9702 | -1.0594 | 0.2403 |
| 14 | 3.19(2) | .. | <F(25A)c[1-x,-y,-z | = 3655.02] | | -86.95 | -61.81 | 0.60100 | -0.01780 | -0.14550 | 8.0329 | -0.2390 | -3.1213 |
| 15 | 3.23(2) | .. | <F(25B)c[1-x,-y,-z | = 3655.02] | | -93.67 | -56.95 | 0.58700 | -0.03640 | -0.14040 | 7.8400 | -0.4887 | -3.0119 |
| 16 | 3.581(16) | .. | C(112)d[1/2+x,1/2-y,-1/2+z | = 4554.01] | | 7.90 | -11.72 | 0.89740 | 0.13030 | -0.04821 | 11.4253 | 1.7495 | -1.0342 |
| 17 | 3.594(10) | .. | C(17)a [1-x,-y,-z | = 3655.01] | | -103.20 | 3.28 | 0.56710 | -0.16576 | -0.00472 | 7.1334 | -2.2256 | -0.1013 |
| 18 | 2.43 | << | H(17A) | | Intra | 172.76 | -6.33 | 0.43540 | 0.11710 | -0.02680 | 5.5548 | 1.5722 | -0.5749 |
| 19 | 3.00 | .. | H(21D)b[1-x,1-y,-z | = 3665.02] | | 73.74 | -45.76 | 0.64960 | 0.24390 | -0.11440 | 8.5381 | 3.2747 | -2.4542 |
| 20 | 3.06 | .. | H(11D)d[1/2+x,1/2-y,-1/2+z | = 4554.01] | | 21.00 | -5.39 | 0.85280 | 0.17570 | -0.02770 | 10.7965 | 2.3590 | -0.5942 |
| 21 | 3.06 | .. | H(11C)d[1/2+x,1/2-y,-1/2+z | = 4554.01] | | -5.55 | -44.17 | 0.77720 | 0.07860 | -0.11370 | 10.1372 | 1.0553 | -2.4391 |
| 22 | 3.12 | .. | H(17A)a[1-x,-y,-z | = 3655.01] | | -108.62 | 16.40 | 0.56460 | -0.11710 | 0.02680 | 6.9959 | -1.5722 | 0.5749 |
| 23 | 3.51 | .. | H(11E)d[1/2+x,1/2-y,-1/2+z | = 4554.01] | | -6.13 | -4.09 | 0.90440 | 0.06650 | -0.02600 | 11.4384 | 0.8929 | -0.5578 |

Angles (Degrees) At1...V...At2 with Vertex V = >F(16A)

| | | | | | | | |
|--------------------|-----------|--------------------|-----------|--------------------|-----------|--------------------|-----------|
| C(181) , <F(16) | 87(2) | C(181) , <F(16B) | 71.8(14) | C(181) , <F(14B) | 55.4(10) | C(181) , <F(15) | 46.1(4) |
| C(181) , >F(15A) | 36.8(3) | C(181) , >F(14A) | 37.3(4) | C(181) , <F(14) | 31.7(5) | C(181) , <F(15B) | 26.3(7) |
| C(181) , C(18) | 34.9(4) | C(181) , C(17) | 65.0(6) | C(181) , <F(11B)a | 103.5(5) | C(181) , <F(11A)a | 115.8(7) |
| C(181) , <F(25A)c | 164.4(6) | C(181) , <F(25B)c | 167.6(8) | C(181) , C(112)d | 97.7(7) | C(181) , C(17)a | 127.3(5) |
| <F(16) , <F(16B) | 157(4) | <F(16) , <F(14B) | 37(3) | <F(16) , <F(15) | 132(2) | <F(16) , >F(15A) | 119(3) |
| <F(16) , >F(14A) | 61(3) | <F(16) , <F(14) | 72(3) | <F(16) , <F(15B) | 99(3) | <F(16) , C(18) | 81(3) |
| <F(16) , C(17) | 79(4) | <F(16) , <F(11B)a | 154(4) | <F(16) , <F(11A)a | 134(4) | <F(16) , <F(25A)c | 78(2) |
| <F(16) , <F(25B)c | 83(2) | <F(16) , C(112)d | 78(4) | <F(16) , C(17)a | 141(3) | <F(16B) , <F(14B) | 125.7(19) |
| <F(16B) , <F(15) | 30.0(17) | <F(16B) , >F(15A) | 44.5(18) | <F(16B) , >F(14A) | 103.4(17) | <F(16B) , <F(14) | 92.3(18) |
| <F(16B) , <F(15B) | 64.9(19) | <F(16B) , C(18) | 77(2) | <F(16B) , C(17) | 84(3) | <F(16B) , <F(11B)a | 45(2) |
| <F(16B) , <F(11A)a | 66(2) | <F(16B) , <F(25A)c | 122.8(16) | <F(16B) , <F(25B)c | 117.5(16) | <F(16B) , C(112)d | 113(3) |
| <F(16B) , C(17)a | 56.8(15) | <F(14B) , <F(15) | 96.4(11) | <F(14B) , >F(15A) | 82.6(10) | <F(14B) , >F(14A) | 23.3(10) |
| <F(14B) , <F(14) | 35.1(10) | <F(14B) , <F(15B) | 62.3(12) | <F(14B) , C(18) | 67.7(13) | <F(14B) , C(17) | 84.2(15) |
| <F(14B) , <F(11B)a | 133.6(15) | <F(14B) , <F(11A)a | 125.5(16) | <F(14B) , <F(25A)c | 111.1(10) | <F(14B) , <F(25B)c | 116.7(10) |

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<F(14B) , C(112)d  67.5(15)  <F(14B) , C(17)a  177.4(11)  <F(15) , >F(15A)  14.6(4)  <F(15) , >F(14A)  73.5(5)
<F(15) , <F(14)   62.3(5)  <F(15) , <F(15B)  34.9(7)  <F(15) , C(18)    65.0(5)  <F(15) , C(17)    86.4(6)
<F(15) , <F(11B)a  58.9(5)  <F(15) , <F(11A)a  75.6(6)  <F(15) , <F(25A)c  149.5(6)  <F(15) , <F(25B)c  145.2(7)
<F(15) , C(112)d  97.4(7)  <F(15) , C(17)a   86.1(5)  >F(15A) , >F(14A)  59.5(4)  >F(15A) , <F(14)   48.0(4)
>F(15A) , <F(15B)  20.5(7)  >F(15A) , C(18)   63.5(3)  >F(15A) , C(17)   89.7(4)  >F(15A) , <F(11B)a  66.7(4)
>F(15A) , <F(11A)a  80.0(5)  >F(15A) , <F(25A)c  157.7(6)  >F(15A) , <F(25B)c  155.5(6)  >F(15A) , C(112)d  87.7(5)
>F(15A) , C(17)a   99.8(3)  >F(14A) , <F(14)   11.9(4)  >F(14A) , <F(15B)  39.1(7)  >F(14A) , C(18)    61.9(3)
>F(14A) , C(17)    87.2(5)  >F(14A) , <F(11B)a  114.8(6)  >F(14A) , <F(11A)a  113.8(7)  >F(14A) , <F(25A)c  131.8(5)
>F(14A) , <F(25B)c  137.7(6)  >F(14A) , C(112)d  67.3(5)  >F(14A) , C(17)a  158.9(4)  <F(14) , <F(15B)   27.5(7)
<F(14) , C(18)    62.2(4)  <F(14) , C(17)    90.4(5)  <F(14) , <F(11B)a  103.9(6)  <F(14) , <F(11A)a  105.5(7)
<F(14) , <F(25A)c  140.7(6)  <F(14) , <F(25B)c  146.6(7)  <F(14) , C(112)d  67.3(5)  <F(14) , C(17)a  147.1(5)
<F(15B) , C(18)   60.4(6)  <F(15B) , C(17)   90.2(7)  <F(15B) , <F(11B)a  82.2(7)  <F(15B) , <F(11A)a  90.8(8)
<F(15B) , <F(25A)c  159.8(9)  <F(15B) , <F(25B)c  163.3(10)  <F(15B) , C(112)d  77.9(7)  <F(15B) , C(17)a  120.0(7)
C(18) , C(17)     30.1(2)  C(18) , <F(11B)a  120.8(4)  C(18) , <F(11A)a  140.0(4)  C(18) , <F(25A)c  137.3(6)
C(18) , <F(25B)c  136.0(7)  C(18) , C(112)d  129.0(4)  C(18) , C(17)a   114.4(5)  C(17) , <F(11B)a  127.2(5)
C(17) , <F(11A)a  146.2(5)  C(17) , <F(25A)c  108.6(5)  C(17) , <F(25B)c  106.4(5)  C(17) , C(112)d  151.7(3)
C(17) , C(17)a   96.9(4)  <F(11B)a , <F(11A)a  20.4(4)  <F(11B)a , <F(25A)c  91.7(5)  <F(11B)a , <F(25B)c  88.8(5)
<F(11B)a , C(112)d  77.0(4)  <F(11B)a , C(17)a  47.2(3)  <F(11A)a , <F(25A)c  77.7(4)  <F(11A)a , <F(25B)c  76.4(5)
<F(11A)a , C(112)d  60.7(4)  <F(11A)a , C(17)a  54.1(3)  <F(25A)c , <F(25B)c  5.9(5)  <F(25A)c , C(112)d  82.0(4)
<F(25A)c , C(17)a  66.3(3)  <F(25B)c , C(112)d  86.4(4)  <F(25B)c , C(17)a  60.7(4)  C(112)d , C(17)a  111.3(3)
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3.6 Angstrom Coordination Sphere Around Atom I = O(11) [ARU = 1555.01] 0.41615 0.44331 0.35468 4.0288 5.9521 7.6087

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|--------|------------|-----------|--------|-------|---------|--------|---------|---------|---------|--------|--------|---------|
| 1 | 1.417(3) | -- | C(11) | | | | Intra | 112.87 | -26.22 | 0.36896 | 0.53054 | 0.32550 | 3.5347 | 7.1233 | 6.9827 |
| 2 | 1.428(3) | -- | C(111) | | | | Intra | -141.89 | 29.01 | 0.34650 | 0.38590 | 0.38697 | 3.0459 | 5.1813 | 8.3014 |
| 3 | 2.254(2) | << | O(12) | | | | Intra | 73.94 | -21.57 | 0.45200 | 0.59336 | 0.31605 | 4.6088 | 7.9667 | 6.7800 |
| 4 | 2.373(3) | << | C(112) | | | | Intra | -119.64 | 61.37 | 0.39740 | 0.36970 | 0.45179 | 3.4665 | 4.9638 | 9.6920 |
| 5 | 2.432(3) | << | C(12) | | | | Intra | 141.28 | -53.86 | 0.30244 | 0.51013 | 0.26314 | 2.9098 | 6.8493 | 5.6450 |
| 6 | 2.911(3) | << | C(121) | | | | Intra | 69.94 | 7.09 | 0.49960 | 0.64540 | 0.37143 | 5.0197 | 8.6655 | 7.9681 |
| 7 | 2.956(2) | .< | N(22) | [| = | 02] | | -39.66 | -27.96 | 0.55894 | 0.31921 | 0.29009 | 6.0383 | 4.2859 | 6.2231 |
| 8 | 2.979(2) | .< | N(12) | | | | Intra | 107.90 | -80.87 | 0.36780 | 0.47681 | 0.21759 | 3.8835 | 6.4019 | 4.6678 |
| 9 | 3.558(2) | .. | N(21) | [| = | 02] | | 5.66 | -33.90 | 0.62546 | 0.46501 | 0.26219 | 6.9672 | 6.2435 | 5.6246 |
| 10 | 1.99 | << | H(11A) | | | | Intra | 125.71 | -0.79 | 0.32330 | 0.56360 | 0.35340 | 2.8677 | 7.5672 | 7.5813 |
| 11 | 1.99 | << | H(11C) | | | | Intra | -170.97 | 19.90 | 0.27720 | 0.42140 | 0.38630 | 2.1784 | 5.6579 | 8.2871 |
| 12 | 1.99 | << | H(11B) | | | | Intra | -123.83 | 6.94 | 0.33140 | 0.32090 | 0.36590 | 2.9273 | 4.3086 | 7.8494 |
| 13 | 2.10(2) | << | H(22) | [| = | 02] | | -38.98 | -26.88 | 0.52010 | 0.35570 | 0.31050 | 5.4822 | 4.7758 | 6.6610 |
| 14 | 2.53 | .< | H(11F) | | | | Intra | -76.34 | 55.82 | 0.46910 | 0.34040 | 0.45230 | 4.3646 | 4.5704 | 9.7029 |
| 15 | 2.61 | .< | H(12A) | | | | Intra | 173.60 | -45.46 | 0.24800 | 0.45850 | 0.26800 | 2.2102 | 6.1561 | 5.7492 |
| 16 | 2.62 | .< | H(11E) | | | | Intra | -166.51 | 77.56 | 0.40440 | 0.43350 | 0.47400 | 3.4795 | 5.8204 | 10.1684 |
| 17 | 2.74 | .. | H(12D) | | | | Intra | 54.61 | 20.34 | 0.54670 | 0.59940 | 0.39910 | 5.5177 | 8.0478 | 8.5616 |
| 18 | 2.85(2) | .. | H(21) | [| = | 02] | | 15.55 | -34.38 | 0.57630 | 0.49020 | 0.27980 | 6.2909 | 6.5817 | 6.0024 |
| 19 | 3.16 | .. | H(12C) | | | | Intra | 86.37 | 15.62 | 0.44210 | 0.66930 | 0.39430 | 4.2210 | 8.9864 | 8.4587 |
| 20 | 3.22 | .. | H(11D) | | | | Intra | -126.70 | 51.70 | 0.35280 | 0.32430 | 0.47230 | 2.8376 | 4.3542 | 10.1320 |
| 21 | 3.26 | .. | H(12B) | | | | Intra | 132.09 | -44.68 | 0.26350 | 0.57160 | 0.24770 | 2.4731 | 7.6746 | 5.3138 |
| 22 | 3.31(2) | .. | H(12) | | | | Intra | 68.19 | -71.11 | 0.40870 | 0.51750 | 0.20850 | 4.4274 | 6.9482 | 4.4728 |
| 23 | 3.33 | .. | H(25A) | [| = | 02] | | -68.73 | 10.18 | 0.51820 | 0.21590 | 0.38210 | 5.2172 | 2.8988 | 8.1970 |

Angles (Degrees) At1...V...At2 with Vertex V = O(11)

| | | | | | | | | | | | | | | | |
|--------|---|--------|------------|--------|---|--------|------------|--------|---|--------|------------|--------|---|--------|------------|
| C(11) | , | C(111) | 114.86(16) | C(11) | , | O(12) | 35.77(10) | C(11) | , | C(112) | 130.50(15) | C(11) | , | C(12) | 34.70(11) |
| C(11) | , | C(121) | 53.33(12) | C(11) | , | N(22) | 119.73(12) | C(11) | , | N(12) | 54.69(11) | C(11) | , | N(21) | 88.50(11) |
| C(111) | , | O(12) | 146.89(14) | C(111) | , | C(112) | 35.56(13) | C(111) | , | C(12) | 105.91(13) | C(111) | , | C(121) | 132.64(15) |
| C(111) | , | N(22) | 113.02(13) | C(111) | , | N(12) | 121.79(13) | C(111) | , | N(21) | 152.02(13) | O(12) | , | C(112) | 139.09(12) |
| O(12) | , | C(12) | 59.46(7) | O(12) | , | C(121) | 28.93(7) | O(12) | , | N(22) | 99.01(7) | O(12) | , | N(12) | 60.96(6) |
| O(12) | , | N(21) | 60.61(6) | C(112) | , | C(12) | 138.89(10) | C(112) | , | C(121) | 111.13(12) | C(112) | , | N(22) | 109.75(10) |
| C(112) | , | N(12) | 156.63(10) | C(112) | , | N(21) | 136.00(9) | C(12) | , | C(121) | 84.98(9) | C(12) | , | N(22) | 98.18(8) |
| C(12) | , | N(12) | 28.90(6) | C(12) | , | N(21) | 84.23(7) | C(121) | , | N(22) | 110.60(9) | C(121) | , | N(12) | 89.87(7) |
| C(121) | , | N(21) | 73.22(8) | N(22) | , | N(12) | 69.84(6) | N(22) | , | N(21) | 39.02(4) | N(12) | , | N(21) | 58.48(5) |

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3.6 Angstrom Coordination Sphere Around Atom I = O(12) [ARU = 1555.01] 0.45200 0.59336 0.31605 4.6088 7.9667 6.7800

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|--------|------------|-----------|--------|-------|---------|--------|---------|---------|---------|--------|---------|--------|
| 1 | 1.381(3) | -- | C(11) | | | | Intra | -141.86 | 8.44 | 0.36896 | 0.53054 | 0.32550 | 3.5347 | 7.1233 | 6.9827 |
| 2 | 1.438(3) | -- | C(121) | | | | Intra | 59.54 | 55.69 | 0.49960 | 0.64540 | 0.37143 | 5.0197 | 8.6655 | 7.9681 |
| 3 | 2.254(2) | << | O(11) | | | | Intra | -106.06 | 21.57 | 0.41615 | 0.44331 | 0.35468 | 4.0288 | 5.9521 | 7.6087 |
| 4 | 2.329(3) | << | C(12) | | | | Intra | -146.66 | -29.17 | 0.30244 | 0.51013 | 0.26314 | 2.9098 | 6.8493 | 5.6450 |
| 5 | 2.344(4) | << | C(122) | | | | Intra | 55.51 | 21.22 | 0.56120 | 0.72750 | 0.35560 | 5.8461 | 9.7678 | 7.6285 |
| 6 | 2.727(2) | << | N(12) | | | | Intra | -114.87 | -50.77 | 0.36780 | 0.47681 | 0.21759 | 3.8835 | 6.4019 | 4.6678 |
| 7 | 3.141(2) | .. | N(21) | [| = | 02] | | -36.16 | -21.58 | 0.62546 | 0.46501 | 0.26219 | 6.9672 | 6.2435 | 5.6246 |
| 8 | 3.254(2) | .. | O(21) | [| = | 02] | | 9.69 | -61.37 | 0.53873 | 0.61290 | 0.18290 | 6.1456 | 8.2291 | 3.9236 |
| 9 | 3.538(3) | .. | C(111) | | | | Intra | -119.30 | 25.47 | 0.34650 | 0.38590 | 0.38697 | 3.0459 | 5.1813 | 8.3014 |
| 10 | 1.96 | << | H(11A) | | | | Intra | -167.07 | 24.16 | 0.32330 | 0.56360 | 0.35340 | 2.8677 | 7.5672 | 7.5813 |
| 11 | 2.00 | << | H(12D) | | | | Intra | 5.10 | 62.88 | 0.54670 | 0.59940 | 0.39910 | 5.5177 | 8.0478 | 8.5616 |
| 12 | 2.00 | << | H(12C) | | | | Intra | 110.82 | 56.98 | 0.44210 | 0.66930 | 0.39430 | 4.2210 | 8.9864 | 8.4587 |
| 13 | 2.31(2) | << | H(21) | [| = | 02] | | -39.47 | -19.64 | 0.57630 | 0.49020 | 0.27980 | 6.2909 | 6.5817 | 6.0024 |
| 14 | 2.48 | << | H(12F) | | | | Intra | 71.41 | 3.89 | 0.51700 | 0.76820 | 0.32390 | 5.3981 | 10.3142 | 6.9484 |
| 15 | 2.53(2) | <. | H(12) | | | | Intra | -100.09 | -65.85 | 0.40870 | 0.51750 | 0.20850 | 4.4274 | 6.9482 | 4.4728 |
| 16 | 2.61 | <. | H(12G) | | | | Intra | 35.21 | 10.94 | 0.62470 | 0.70320 | 0.33910 | 6.6987 | 9.4415 | 7.2745 |
| 17 | 2.61 | <. | H(12B) | | | | Intra | -172.21 | -34.22 | 0.26350 | 0.57160 | 0.24770 | 2.4731 | 7.6746 | 5.3138 |
| 18 | 3.18 | .. | H(12A) | | | | Intra | -142.95 | -18.93 | 0.24800 | 0.45850 | 0.26800 | 2.2102 | 6.1561 | 5.7492 |
| 19 | 3.19 | .. | H(12E) | | | | Intra | 59.15 | 31.08 | 0.58420 | 0.76800 | 0.39280 | 6.0096 | 10.3116 | 8.4265 |
| 20 | 3.31(2) | .. | H(22) | [| = | 02] | | -74.69 | -2.06 | 0.52010 | 0.35570 | 0.31050 | 5.4822 | 4.7758 | 6.6610 |
| 21 | 3.32 | .. | H(21E) | [| = | 02] | | 107.78 | -57.74 | 0.37380 | 0.71900 | 0.18520 | 4.0679 | 9.6537 | 3.9730 |

Angles (Degrees) At1...V...At2 with Vertex V = O(12)

| | | | | | | | | | | | | | | | |
|--------|---|--------|------------|--------|---|--------|------------|--------|---|--------|------------|--------|---|--------|------------|
| C(11) | , | C(121) | 113.44(19) | C(11) | , | O(11) | 36.86(10) | C(11) | , | C(12) | 37.90(11) | C(11) | , | C(122) | 145.78(16) |
| C(11) | , | N(12) | 63.66(11) | C(11) | , | N(21) | 107.63(12) | C(11) | , | O(21) | 123.06(12) | C(11) | , | C(111) | 27.40(11) |
| C(121) | , | O(11) | 101.77(14) | C(121) | , | C(12) | 147.58(18) | C(121) | , | C(122) | 34.61(15) | C(121) | , | N(12) | 174.05(15) |
| C(121) | , | N(21) | 110.85(17) | C(121) | , | O(21) | 123.43(16) | C(121) | , | C(111) | 98.83(14) | O(11) | , | C(12) | 64.06(8) |
| O(11) | , | C(122) | 133.58(12) | O(11) | , | N(12) | 72.75(7) | O(11) | , | N(21) | 80.68(7) | O(11) | , | O(21) | 121.08(7) |
| O(11) | , | C(111) | 12.74(6) | C(12) | , | C(122) | 158.46(13) | C(12) | , | N(12) | 32.12(7) | C(12) | , | N(21) | 96.04(8) |
| C(12) | , | O(21) | 87.44(7) | C(12) | , | C(111) | 60.63(8) | C(122) | , | N(12) | 149.50(12) | C(122) | , | N(21) | 99.11(11) |
| C(122) | , | O(21) | 90.37(10) | C(122) | , | C(111) | 133.04(11) | N(12) | , | N(21) | 66.42(6) | N(12) | , | O(21) | 59.47(5) |
| N(12) | , | C(111) | 76.34(7) | N(21) | , | O(21) | 50.71(5) | N(21) | , | C(111) | 93.32(6) | O(21) | , | C(111) | 130.51(7) |

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3.6 Angstrom Coordination Sphere Around Atom I = O(22) [ARU = 1555.02] 0.62157 0.50738 0.12574 7.3778 6.8123 2.6974

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|--------|------------|-----------|--------|-------|---------|--------|---------|---------|---------|--------|---------|--------|
| 1 | 1.414(2) | -- | C(21) | | | | Intra | 85.80 | 48.07 | 0.64025 | 0.57758 | 0.17479 | 7.4471 | 7.7549 | 3.7497 |
| 2 | 1.432(3) | -- | C(221) | | | | Intra | -11.13 | -28.57 | 0.71130 | 0.48930 | 0.09383 | 8.6114 | 6.5696 | 2.0129 |
| 3 | 2.2426(19) | << | O(21) | | | | Intra | 131.01 | 33.15 | 0.53873 | 0.61290 | 0.18290 | 6.1456 | 8.2291 | 3.9236 |
| 4 | 2.384(4) | << | C(222) | | | | Intra | -20.10 | -64.38 | 0.67180 | 0.48100 | 0.02554 | 8.3456 | 6.4581 | 0.5479 |
| 5 | 2.445(3) | << | C(22) | | | | Intra | 32.92 | 74.53 | 0.69466 | 0.53378 | 0.23560 | 7.9252 | 7.1668 | 5.0542 |
| 6 | 2.883(3) | << | C(211) | | | | Intra | 124.40 | 4.37 | 0.49490 | 0.68406 | 0.13597 | 5.7535 | 9.1845 | 2.9169 |
| 7 | 3.010(2) | <. | N(21) | | | | Intra | -125.82 | 76.52 | 0.62546 | 0.46501 | 0.26219 | 6.9672 | 6.2435 | 5.6246 |
| 8 | 3.070(2) | <. | N(11) | [| = | 01] | | -146.28 | 7.21 | 0.42452 | 0.38146 | 0.14369 | 4.8442 | 5.1217 | 3.0825 |
| 9 | 3.471(2) | .. | C(19) | [| = | 01] | | -109.27 | -13.91 | 0.52253 | 0.27050 | 0.08683 | 6.2658 | 3.6319 | 1.8627 |
| 10 | 3.500(2) | .. | C(23) | | | | Intra | -98.91 | 56.60 | 0.63434 | 0.36560 | 0.26194 | 7.0795 | 4.9087 | 5.6192 |
| 11 | 1.99 | << | H(21A) | | | | Intra | 68.53 | 23.32 | 0.68460 | 0.63380 | 0.16240 | 8.0454 | 8.5097 | 3.4839 |
| 12 | 2.00 | << | H(22C) | | | | Intra | -33.33 | -10.17 | 0.74810 | 0.42690 | 0.10930 | 9.0212 | 5.7318 | 2.3447 |
| 13 | 2.00 | << | H(22D) | | | | Intra | 14.99 | -14.89 | 0.76380 | 0.54460 | 0.10180 | 9.2435 | 7.3121 | 2.1839 |
| 14 | 2.29(2) | << | H(11) | [| = | 01] | | -148.95 | 10.79 | 0.47360 | 0.42110 | 0.14570 | 5.4534 | 5.6539 | 3.1256 |
| 15 | 2.55 | <. | H(22G) | | | | Intra | -74.34 | -64.76 | 0.61610 | 0.42940 | 0.01820 | 7.6712 | 5.7653 | 0.3904 |
| 16 | 2.56 | <. | H(21B) | | | | Intra | 124.95 | -15.47 | 0.50040 | 0.65800 | 0.09390 | 5.9642 | 8.8346 | 2.0144 |
| 17 | 2.62 | <. | H(22A) | | | | Intra | -4.85 | 57.41 | 0.76100 | 0.49850 | 0.22850 | 8.7817 | 6.6931 | 4.9019 |
| 18 | 2.62 | <. | H(22F) | | | | Intra | 38.31 | -71.86 | 0.64140 | 0.54500 | 0.00980 | 8.0170 | 7.3174 | 0.2102 |
| 19 | 2.91 | .. | H(19A) | [| = | 01] | | -97.46 | -6.31 | 0.58760 | 0.29350 | 0.11080 | 7.0017 | 3.9407 | 2.3769 |
| 20 | 3.23 | .. | H(22E) | | | | Intra | -18.27 | -54.12 | 0.73200 | 0.46320 | 0.00380 | 9.1743 | 6.2192 | 0.0815 |
| 21 | 3.27 | .. | H(22B) | | | | Intra | 56.67 | 66.54 | 0.71610 | 0.58840 | 0.26560 | 8.0933 | 7.9002 | 5.6978 |
| 22 | 3.43 | .. | H(21C) | | | | Intra | 109.36 | 5.80 | 0.53570 | 0.74740 | 0.14190 | 6.2456 | 10.0350 | 3.0441 |
| 23 | 3.45(2) | .. | H(12) | [| = | 01] | | 177.36 | 31.01 | 0.40870 | 0.51750 | 0.20850 | 4.4274 | 6.9482 | 4.4728 |
| 24 | 3.49(2) | .. | H(21) | | | | Intra | -168.02 | 71.42 | 0.57630 | 0.49020 | 0.27980 | 6.2909 | 6.5817 | 6.0024 |

Angles (Degrees) At1...V...At2 with Vertex V = O(22)

| | | | | | | | |
|-----------------|------------|-----------------|------------|-----------------|------------|----------------|------------|
| C(21) , C(221) | 115.25(16) | C(21) , O(21) | 36.78(9) | C(21) , C(222) | 138.59(15) | C(21) , C(22) | 34.45(10) |
| C(21) , C(211) | 54.74(10) | C(21) , N(21) | 53.78(10) | C(21) , N(11) | 108.31(11) | C(21) , C(19) | 143.63(12) |
| C(21) , C(23) | 75.26(10) | C(221) , O(21) | 147.36(14) | C(221) , C(222) | 36.27(15) | C(221) , C(22) | 107.01(14) |
| C(221) , C(211) | 131.40(14) | C(221) , N(21) | 123.40(14) | C(221) , N(11) | 132.67(13) | C(221) , C(19) | 90.33(13) |
| C(221) , C(23) | 112.36(13) | O(21) , C(222) | 144.10(12) | O(21) , C(22) | 60.29(7) | O(21) , C(211) | 29.44(6) |
| O(21) , N(21) | 60.84(6) | O(21) , N(11) | 79.97(6) | O(21) , C(19) | 122.30(7) | O(21) , C(23) | 80.81(6) |
| C(222) , C(22) | 143.10(12) | C(222) , C(211) | 114.81(12) | C(222) , N(21) | 154.71(11) | C(222) , N(11) | 111.49(11) |
| C(222) , C(19) | 77.12(11) | C(222) , C(23) | 134.96(11) | C(22) , C(211) | 86.19(8) | C(22) , N(21) | 28.44(6) |
| C(22) , N(11) | 98.26(7) | C(22) , C(19) | 115.87(7) | C(22) , C(23) | 45.04(6) | C(211) , N(21) | 90.27(7) |
| C(211) , N(11) | 88.78(7) | C(211) , C(19) | 126.28(7) | C(211) , C(23) | 109.63(7) | N(21) , N(11) | 70.21(5) |
| N(21) , C(19) | 90.97(5) | N(21) , C(23) | 22.14(4) | N(11) , C(19) | 42.37(5) | N(11) , C(23) | 61.67(5) |
| C(19) , C(23) | 71.04(5) | | | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = N(11) [ARU = 1555.01] 0.42452 0.38146 0.14369 4.8442 5.1217 3.0825

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|-------------|-----------|----------|-------|---------|--------|---------|---------|----------|--------|--------|---------|
| 1 | 0.81(2) | -- | H(11) | | | | Intra | 41.14 | 3.05 | 0.47360 | 0.42110 | 0.14570 | 5.4534 | 5.6539 | 3.1256 |
| 2 | 1.371(2) | -- | C(13) | | | | Intra | 172.84 | 41.25 | 0.35434 | 0.39103 | 0.18582 | 3.8216 | 5.2502 | 3.9863 |
| 3 | 1.404(2) | -- | C(14) | | | | Intra | -81.35 | -43.84 | 0.42449 | 0.30692 | 0.09837 | 4.9964 | 4.1209 | 2.1103 |
| 4 | 2.253(2) | << | N(12) | | | | Intra | 126.89 | 44.73 | 0.36780 | 0.47681 | 0.21759 | 3.8835 | 6.4019 | 4.6678 |
| 5 | 2.393(2) | << | C(19) | | | | Intra | -46.34 | -30.64 | 0.52253 | 0.27050 | 0.08683 | 6.2658 | 3.6319 | 1.8627 |
| 6 | 2.447(3) | << | C(15) | | | | Intra | -122.19 | -45.68 | 0.33005 | 0.27370 | 0.06209 | 3.9333 | 3.6748 | 1.3320 |
| 7 | 2.6846(18) | << | S(1) | | | | Intra | -154.48 | 25.65 | 0.26504 | 0.30381 | 0.19786 | 2.6602 | 4.0791 | 4.2446 |
| 8 | 3.070(2) | <. | O(22) | [| = | 02] | | 33.72 | -7.21 | 0.62157 | 0.50738 | 0.12574 | 7.3778 | 6.8123 | 2.6974 |
| 9 | 3.388(3) | .. | C(23) | [| = | 02] | | -5.44 | 48.49 | 0.63434 | 0.36560 | 0.26194 | 7.0795 | 4.9087 | 5.6192 |
| 10 | 3.462(2) | .. | N(22) | [| = | 02] | | -34.99 | 65.10 | 0.55894 | 0.31921 | 0.29009 | 6.0383 | 4.2859 | 6.2231 |
| 11 | 3.472(2) | .. | O(21) | [| = | 02] | | 67.28 | 14.02 | 0.53873 | 0.61290 | 0.18290 | 6.1456 | 8.2291 | 3.9236 |
| 12 | 3.497(2) | .. | N(21) | [| = | 02] | | 27.85 | 46.63 | 0.62546 | 0.46501 | 0.26219 | 6.9672 | 6.2435 | 5.6246 |
| 13 | 2.33(2) | << | H(12) | | | | Intra | 102.85 | 36.58 | 0.40870 | 0.51750 | 0.20850 | 4.4274 | 6.9482 | 4.4728 |
| 14 | 2.56 | <. | H(19A) | | | | Intra | -28.70 | -16.01 | 0.58760 | 0.29350 | 0.11080 | 7.0017 | 3.9407 | 2.3769 |
| 15 | 2.64 | <. | H(15A) | | | | Intra | -148.23 | -37.38 | 0.26220 | 0.29910 | 0.06890 | 3.0588 | 4.0159 | 1.4781 |
| 16 | 3.20 | .. | H(29A) | [| = | 02] | | -63.48 | 22.35 | 0.54500 | 0.18430 | 0.20040 | 6.1654 | 2.4745 | 4.2991 |
| 17 | 3.45 | .. | H(22F)a | [1-x,1-y,-z | = | 3665.02] | | 107.46 | -72.55 | 0.35860 | 0.45500 | -0.00980 | 4.5337 | 6.1091 | -0.2102 |
| 18 | 3.57(2) | .. | H(21) | [| = | 02] | | 45.26 | 54.86 | 0.57630 | 0.49020 | 0.27980 | 6.2909 | 6.5817 | 6.0024 |

Angles (Degrees) At1...V...At2 with Vertex V = N(11)

| | | | | | | | | | | | | | | | |
|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|
| C(13) | , | C(14) | 127.19(16) | C(13) | , | N(12) | 33.35(10) | C(13) | , | C(19) | 146.87(14) | C(13) | , | C(15) | 104.44(12) |
| C(13) | , | S(1) | 31.14(9) | C(13) | , | O(22) | 130.29(12) | C(13) | , | C(23) | 90.25(11) | C(13) | , | N(22) | 71.45(10) |
| C(13) | , | O(21) | 92.06(11) | C(13) | , | N(21) | 86.76(11) | C(14) | , | N(12) | 159.87(14) | C(14) | , | C(19) | 30.54(9) |
| C(14) | , | C(15) | 28.74(9) | C(14) | , | S(1) | 96.38(11) | C(14) | , | O(22) | 102.49(11) | C(14) | , | C(23) | 113.72(11) |
| C(14) | , | N(22) | 114.76(11) | C(14) | , | O(21) | 139.93(12) | C(14) | , | N(21) | 131.80(12) | N(12) | , | C(19) | 164.94(10) |
| N(12) | , | C(15) | 132.90(10) | N(12) | , | S(1) | 64.48(6) | N(12) | , | O(22) | 97.31(7) | N(12) | , | C(23) | 77.89(7) |
| N(12) | , | N(22) | 69.26(7) | N(12) | , | O(21) | 58.72(6) | N(12) | , | N(21) | 64.22(6) | C(19) | , | C(15) | 59.23(8) |
| C(19) | , | S(1) | 117.52(8) | C(19) | , | O(22) | 77.80(7) | C(19) | , | C(23) | 87.17(7) | C(19) | , | N(22) | 96.15(7) |
| C(19) | , | O(21) | 117.25(8) | C(19) | , | N(21) | 102.10(7) | C(15) | , | S(1) | 77.13(7) | C(15) | , | O(22) | 122.90(8) |
| C(15) | , | C(23) | 138.09(8) | C(15) | , | N(22) | 129.39(8) | C(15) | , | O(21) | 147.35(8) | C(15) | , | N(21) | 159.35(8) |
| S(1) | , | O(22) | 159.97(7) | S(1) | , | C(23) | 100.85(6) | S(1) | , | N(22) | 78.12(5) | S(1) | , | O(21) | 123.20(6) |
| S(1) | , | N(21) | 107.69(6) | O(22) | , | C(23) | 65.42(5) | O(22) | , | N(22) | 87.83(6) | O(22) | , | O(21) | 39.49(4) |
| O(22) | , | N(21) | 54.09(5) | C(23) | , | N(22) | 22.79(4) | C(23) | , | O(21) | 68.14(5) | C(23) | , | N(21) | 22.37(4) |
| N(22) | , | O(21) | 82.36(5) | N(22) | , | N(21) | 37.69(4) | O(21) | , | N(21) | 46.31(4) | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = N(21) [ARU = 1555.02] 0.62546 0.46501 0.26219 6.9672 6.2435 5.6246

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|--------|------------|-----------|--------|-------|---------|--------|---------|---------|---------|--------|--------|--------|
| 1 | 0.85(2) | -- | H(21) | | | | Intra | 153.43 | 26.55 | 0.57630 | 0.49020 | 0.27980 | 6.2909 | 6.5817 | 6.0024 |
| 2 | 1.340(2) | -- | C(23) | | | | Intra | -85.19 | -0.23 | 0.63434 | 0.36560 | 0.26194 | 7.0795 | 4.9087 | 5.6192 |
| 3 | 1.448(3) | -- | C(22) | | | | Intra | 43.94 | -23.21 | 0.69466 | 0.53378 | 0.23560 | 7.9252 | 7.1668 | 5.0542 |
| 4 | 2.248(2) | << | N(22) | | | | Intra | -115.38 | 15.44 | 0.55894 | 0.31921 | 0.29009 | 6.0383 | 4.2859 | 6.2231 |
| 5 | 2.456(3) | << | C(21) | | | | Intra | 72.38 | -49.78 | 0.64025 | 0.57758 | 0.17479 | 7.4471 | 7.7549 | 3.7497 |
| 6 | 2.6615(17) | << | S(2) | | | | Intra | -56.48 | -14.36 | 0.73064 | 0.30491 | 0.23142 | 8.3908 | 4.0939 | 4.9645 |
| 7 | 2.741(2) | << | O(21) | | | | Intra | 112.48 | -38.36 | 0.53873 | 0.61290 | 0.18290 | 6.1456 | 8.2291 | 3.9236 |
| 8 | 3.010(2) | < | O(22) | | | | Intra | 54.18 | -76.52 | 0.62157 | 0.50738 | 0.12574 | 7.3778 | 6.8123 | 2.6974 |
| 9 | 3.141(2) | .. | O(12) | [| = | 01] | | 143.84 | 21.58 | 0.45200 | 0.59336 | 0.31605 | 4.6088 | 7.9667 | 6.7800 |
| 10 | 3.233(2) | .. | N(12) | [| = | 01] | | 177.06 | -17.22 | 0.36780 | 0.47681 | 0.21759 | 3.8835 | 6.4019 | 4.6678 |
| 11 | 3.497(2) | .. | N(11) | [| = | 01] | | -152.15 | -46.63 | 0.42452 | 0.38146 | 0.14369 | 4.8442 | 5.1217 | 3.0825 |
| 12 | 3.558(2) | .. | O(11) | [| = | 01] | | -174.34 | 33.90 | 0.41615 | 0.44331 | 0.35468 | 4.0288 | 5.9521 | 7.6087 |
| 13 | 2.00 | << | H(22A) | | | | Intra | 13.92 | -21.14 | 0.76100 | 0.49850 | 0.22850 | 8.7817 | 6.6931 | 4.9019 |
| 14 | 2.00 | << | H(22B) | | | | Intra | 55.79 | 2.09 | 0.71610 | 0.58840 | 0.26560 | 8.0933 | 7.9002 | 5.6978 |
| 15 | 2.33(2) | << | H(22) | | | | Intra | -135.34 | 26.40 | 0.52010 | 0.35570 | 0.31050 | 5.4822 | 4.7758 | 6.6610 |
| 16 | 2.88(2) | .. | H(12) | [| = | 01] | | 164.49 | -23.61 | 0.40870 | 0.51750 | 0.20850 | 4.4274 | 6.9482 | 4.4728 |
| 17 | 2.98(2) | .. | H(11) | [| = | 01] | | -158.72 | -56.97 | 0.47360 | 0.42110 | 0.14570 | 5.4534 | 5.6539 | 3.1256 |
| 18 | 3.30 | .. | H(21A) | | | | Intra | 64.56 | -40.46 | 0.68460 | 0.63380 | 0.16240 | 8.0454 | 8.5097 | 3.4839 |

Angles (Degrees) At1...V...At2 with Vertex V = N(21)

| | | | | | | | | | | | | | | | |
|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|
| C(23) | , | C(22) | 125.35(16) | C(23) | , | N(22) | 33.69(10) | C(23) | , | C(21) | 126.43(14) | C(23) | , | S(2) | 31.72(9) |
| C(23) | , | O(21) | 138.13(13) | C(23) | , | O(22) | 99.96(12) | C(23) | , | O(12) | 127.67(12) | C(23) | , | N(12) | 97.33(12) |
| C(23) | , | N(11) | 74.24(11) | C(23) | , | O(11) | 89.42(11) | C(22) | , | N(22) | 159.03(14) | C(22) | , | C(21) | 34.64(10) |
| C(22) | , | S(2) | 93.64(11) | C(22) | , | O(21) | 59.45(10) | C(22) | , | O(22) | 53.56(10) | C(22) | , | O(12) | 106.97(11) |
| C(22) | , | N(12) | 118.91(12) | C(22) | , | N(11) | 108.66(12) | C(22) | , | O(11) | 144.95(12) | N(22) | , | C(21) | 145.09(10) |
| N(22) | , | S(2) | 65.40(6) | N(22) | , | O(21) | 132.25(9) | N(22) | , | O(22) | 118.68(8) | N(22) | , | O(12) | 93.99(7) |
| N(22) | , | N(12) | 74.18(7) | N(22) | , | N(11) | 70.33(7) | N(22) | , | O(11) | 55.87(6) | C(21) | , | S(2) | 101.73(8) |
| C(21) | , | O(21) | 30.54(6) | C(21) | , | O(22) | 27.69(6) | C(21) | , | O(12) | 95.16(7) | C(21) | , | N(12) | 86.00(7) |
| C(21) | , | N(11) | 76.17(7) | C(21) | , | O(11) | 129.62(8) | S(2) | , | O(21) | 126.27(7) | S(2) | , | O(22) | 80.71(5) |
| S(2) | , | O(12) | 159.39(7) | S(2) | , | N(12) | 118.46(6) | S(2) | , | N(11) | 83.42(5) | S(2) | , | O(11) | 120.93(6) |
| O(21) | , | O(22) | 45.61(5) | O(21) | , | O(12) | 66.78(5) | O(21) | , | N(12) | 59.66(5) | O(21) | , | N(11) | 66.37(5) |
| O(21) | , | O(11) | 99.09(6) | O(22) | , | O(12) | 110.88(6) | O(22) | , | N(12) | 80.39(6) | O(22) | , | N(11) | 55.70(5) |
| O(22) | , | O(11) | 132.11(6) | O(12) | , | N(12) | 50.64(5) | O(12) | , | N(11) | 89.29(6) | O(12) | , | O(11) | 38.71(4) |
| N(12) | , | N(11) | 38.87(5) | N(12) | , | O(11) | 51.77(5) | N(11) | , | O(11) | 82.98(5) | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = N(22) [ARU = 1555.02] 0.55894 0.31921 0.29009 6.0383 4.2859 6.2231

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|-----------|----------------------------|------------|-------|--------|--------|---------|---------|---------|--------|--------|--------|
| 1 | 0.86(2) | -- | H(22) | | Intra | 138.62 | 30.57 | 0.52010 | 0.35570 | 0.31050 | 5.4822 | 4.7758 | 6.6610 |
| 2 | 1.355(2) | -- | C(23) | | Intra | 30.89 | -26.46 | 0.63434 | 0.36560 | 0.26194 | 7.0795 | 4.9087 | 5.6192 |
| 3 | 1.409(2) | -- | C(24) | | Intra | 101.46 | 0.72 | 0.53687 | 0.21640 | 0.29092 | 5.7586 | 2.9055 | 6.2409 |
| 4 | 2.248(2) | << | N(21) | | Intra | 64.62 | -15.44 | 0.62546 | 0.46501 | 0.26219 | 6.9672 | 6.2435 | 5.6246 |
| 5 | 2.389(3) | << | C(25) | | Intra | 111.47 | 29.98 | 0.51352 | 0.17580 | 0.34574 | 5.2809 | 2.3604 | 7.4169 |
| 6 | 2.449(2) | << | C(29) | | Intra | -95.07 | -26.88 | 0.52971 | 0.15713 | 0.23846 | 5.8453 | 2.1097 | 5.1155 |
| 7 | 2.6749(18) | << | S(2) | | Intra | -4.67 | -28.07 | 0.73064 | 0.30491 | 0.23142 | 8.3908 | 4.0939 | 4.9645 |
| 8 | 2.956(2) | <. | O(11) [| = 01] | | 140.34 | 27.96 | 0.41615 | 0.44331 | 0.35468 | 4.0288 | 5.9521 | 7.6087 |
| 9 | 3.236(7) | .. | <F(13A)a[1/2+x,1/2-y,1/2+z | = 4555.01] | | -0.31 | 57.21 | 0.73260 | 0.31850 | 0.41690 | 7.7909 | 4.2763 | 8.9435 |
| 10 | 3.294(2) | .. | C(13) [| = 01] | | 156.49 | -42.78 | 0.35434 | 0.39103 | 0.18582 | 3.8216 | 5.2502 | 3.9863 |
| 11 | 3.397(2) | .. | N(12) [| = 01] | | 135.52 | -27.25 | 0.36780 | 0.47681 | 0.21759 | 3.8835 | 6.4019 | 4.6678 |
| 12 | 3.405(15) | .. | <F(13B)a[1/2+x,1/2-y,1/2+z | = 4555.01] | | -27.14 | 60.70 | 0.71420 | 0.26260 | 0.42850 | 7.5209 | 3.5258 | 9.1923 |
| 13 | 3.462(2) | .. | N(11) [| = 01] | | 145.01 | -65.10 | 0.42452 | 0.38146 | 0.14369 | 4.8442 | 5.1217 | 3.0825 |
| 14 | 3.570(7) | .. | <F(13)a [1/2+x,1/2-y,1/2+z | = 4555.01] | | 21.96 | 54.40 | 0.74880 | 0.37710 | 0.42540 | 7.9656 | 5.0631 | 9.1258 |
| 15 | 2.32(2) | << | H(21) | | Intra | 83.72 | -5.46 | 0.57630 | 0.49020 | 0.27980 | 6.2909 | 6.5817 | 6.0024 |
| 16 | 2.55 | << | H(25A) | | Intra | 120.62 | 50.76 | 0.51820 | 0.21590 | 0.38210 | 5.2172 | 2.8988 | 8.1970 |
| 17 | 2.65 | <. | H(29A) | | Intra | -85.99 | -46.66 | 0.54500 | 0.18430 | 0.20040 | 6.1654 | 2.4745 | 4.2991 |
| 18 | 3.44(2) | .. | H(11) [| = 01] | | 113.15 | -64.34 | 0.47360 | 0.42110 | 0.14570 | 5.4534 | 5.6539 | 3.1256 |
| 19 | 3.51 | .. | H(11B) [| = 01] | | 179.58 | 27.60 | 0.33140 | 0.32090 | 0.36590 | 2.9273 | 4.3086 | 7.8494 |
| 20 | 3.57(2) | .. | H(12) [| = 01] | | 121.18 | -29.36 | 0.40870 | 0.51750 | 0.20850 | 4.4274 | 6.9482 | 4.4728 |

Angles (Degrees) At1...V...At2 with Vertex V = N(22)

| | | | | | | | |
|------------------|------------|---------------------|------------|------------------|------------|--------------------|------------|
| C(23) , C(24) | 127.49(16) | C(23) , N(21) | 33.25(9) | C(23) , C(25) | 146.80(14) | C(23) , C(29) | 105.51(12) |
| C(23) , S(2) | 31.54(9) | C(23) , O(11) | 118.18(12) | C(23) , <F(13A)a | 87.7(2) | C(23) , C(13) | 94.58(12) |
| C(23) , N(12) | 89.83(11) | C(23) , <F(13B)a | 99.0(3) | C(23) , N(11) | 75.51(11) | C(23) , <F(13)a | 81.23(16) |
| C(24) , N(21) | 159.86(14) | C(24) , C(25) | 30.77(9) | C(24) , C(29) | 28.29(9) | C(24) , S(2) | 96.33(11) |
| C(24) , O(11) | 114.30(12) | C(24) , <F(13A)a | 95.4(3) | C(24) , C(13) | 99.31(11) | C(24) , N(12) | 119.36(12) |
| C(24) , <F(13B)a | 81.8(2) | C(24) , N(11) | 100.34(11) | C(24) , <F(13)a | 108.08(18) | N(21) , C(25) | 165.02(11) |
| N(21) , C(29) | 133.30(10) | N(21) , S(2) | 64.78(6) | N(21) , O(11) | 85.11(7) | N(21) , <F(13A)a | 90.2(2) |
| N(21) , C(13) | 80.93(7) | N(21) , N(12) | 66.28(6) | N(21) , <F(13B)a | 104.3(2) | N(21) , N(11) | 71.99(7) |
| N(21) , <F(13)a | 78.69(15) | C(25) , C(29) | 58.99(7) | C(25) , S(2) | 117.14(8) | C(25) , O(11) | 90.26(8) |
| C(25) , <F(13A)a | 75.5(2) | C(25) , C(13) | 111.22(8) | C(25) , N(12) | 121.99(8) | C(25) , <F(13B)a | 61.5(2) |
| C(25) , N(11) | 122.58(8) | C(25) , <F(13)a | 86.58(15) | C(29) , S(2) | 78.04(6) | C(29) , O(11) | 131.25(8) |
| C(29) , <F(13A)a | 114.9(2) | C(29) , C(13) | 84.26(7) | C(29) , N(12) | 107.24(7) | C(29) , <F(13B)a | 103.3(2) |
| C(29) , N(11) | 77.12(7) | C(29) , <F(13)a | 127.13(16) | S(2) , O(11) | 149.21(7) | S(2) , <F(13A)a | 85.36(15) |
| S(2) , C(13) | 107.06(6) | S(2) , N(12) | 112.78(6) | S(2) , <F(13B)a | 90.7(3) | S(2) , N(11) | 83.91(5) |
| S(2) , <F(13)a | 85.61(13) | O(11) , <F(13A)a | 88.61(19) | O(11) , C(13) | 72.28(6) | O(11) , N(12) | 55.40(5) |
| O(11) , <F(13B)a | 90.8(3) | O(11) , N(11) | 93.13(6) | O(11) , <F(13)a | 82.13(14) | <F(13A)a , C(13) | 159.4(2) |
| <F(13A)a , N(12) | 136.9(2) | <F(13A)a , <F(13B)a | 14.2(3) | <F(13A)a , N(11) | 161.8(2) | <F(13A)a , <F(13)a | 12.8(3) |
| C(13) , N(12) | 23.04(4) | C(13) , <F(13B)a | 161.9(3) | C(13) , N(11) | 23.24(4) | C(13) , <F(13)a | 148.41(16) |

=====
N(12) , <F(13B)a 144.5(2) N(12) , N(11) 38.33(4) N(12) , <F(13)a 125.39(16) <F(13B)a, N(11) 174.3(3)
<F(13B)a, <F(13)a 26.4(2) N(11) , <F(13)a 150.60(15)

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3.6 Angstrom Coordination Sphere Around Atom I = F(11) [ARU = 1555.01] 0.18760 0.09750 0.01100 2.3175 1.3091 0.2360

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|--|--------|-------|---------|--------|----------|----------|----------|---------|---------|---------|
| 1 | 1.381(8) | -- | C(161) | | Intra | 54.36 | -30.96 | 0.23370 | 0.16920 | -0.02213 | 3.0076 | 2.2718 | -0.4747 |
| 2 | 2.143(10) | << | <F(12) | | Intra | 94.22 | -27.49 | 0.16410 | 0.23870 | -0.03510 | 2.1778 | 3.2049 | -0.7530 |
| 3 | 2.146(10) | << | <F(13) | | Intra | 17.89 | -58.85 | 0.24880 | 0.12290 | -0.07460 | 3.3738 | 1.6501 | -1.6003 |
| 4 | 2.331(8) | << | C(16) | | Intra | 37.88 | 2.83 | 0.33547 | 0.20399 | 0.01637 | 4.1553 | 2.7389 | 0.3512 |
| 5 | 3.067(8) | .< | C(15) | | Intra | 55.67 | 20.93 | 0.33005 | 0.27370 | 0.06209 | 3.9333 | 3.6748 | 1.3320 |
| 6 | 3.235(9) | .. | C(17) | | Intra | 16.47 | -2.39 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 7 | 3.378(8) | .. | C(112)a[1/2-x,-1/2+y,1/2-z = 2545.01] | | | -111.29 | 13.67 | 0.10260 | -0.13030 | 0.04821 | 1.1254 | -1.7495 | 1.0342 |
| 8 | 3.442(15) | .. | >F(16A)b[1-x,-y,-z = 3655.01] | | | -48.49 | 1.18 | 0.37020 | -0.09440 | 0.01430 | 4.5981 | -1.2675 | 0.3068 |
| 9 | 2.53 | .< | H(11E)a[1/2-x,-1/2+y,1/2-z = 2545.01] | | | -118.69 | 7.31 | 0.09560 | -0.06650 | 0.02600 | 1.1123 | -0.8929 | 0.5578 |
| 10 | 2.96 | .. | H(11F)c[-1/2+x,1/2-y,-1/2+z = 4454.01] | | | 161.86 | -25.19 | -0.03090 | 0.15960 | -0.04770 | -0.2272 | 2.1429 | -1.0233 |
| 11 | 2.97 | .. | H(12C)a[1/2-x,-1/2+y,1/2-z = 2545.01] | | | 153.65 | 43.08 | 0.05790 | 0.16930 | 0.10570 | 0.3708 | 2.2731 | 2.2675 |
| 12 | 3.00 | .. | H(11A)a[1/2-x,-1/2+y,1/2-z = 2545.01] | | | -142.51 | 75.58 | 0.17670 | 0.06360 | 0.14660 | 1.7241 | 0.8539 | 3.1449 |
| 13 | 3.07 | .. | H(15A) | | Intra | 74.68 | 23.87 | 0.26220 | 0.29910 | 0.06890 | 3.0588 | 4.0159 | 1.4781 |
| 14 | 3.23 | .. | H(11C)a[1/2-x,-1/2+y,1/2-z = 2545.01] | | | -87.68 | 42.95 | 0.22280 | -0.07860 | 0.11370 | 2.4135 | -1.0553 | 2.4391 |
| 15 | 3.35 | .. | H(17A) | | Intra | 4.65 | -14.02 | 0.43540 | 0.11710 | -0.02680 | 5.5548 | 1.5722 | -0.5749 |
| 16 | 3.54 | .. | H(11E)c[-1/2+x,1/2-y,-1/2+z = 4454.01] | | | -173.08 | -12.94 | -0.09560 | 0.06650 | -0.02600 | -1.1123 | 0.8929 | -0.5578 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(11)

| | | | | | | | |
|-------------------|----------|-------------------|----------|-------------------|-----------|--------------------|-----------|
| C(161) , <F(12) | 34.8(3) | C(161) , <F(13) | 37.2(3) | C(161) , C(16) | 37.3(2) | C(161) , C(15) | 51.9(3) |
| C(161) , C(17) | 45.8(3) | C(161) , C(112)a | 158.3(4) | C(161) , >F(16A)b | 101.6(5) | <F(12) , <F(13) | 59.8(4) |
| <F(12) , C(16) | 62.1(3) | <F(12) , C(15) | 61.1(3) | <F(12) , C(17) | 78.0(3) | <F(12) , C(112)a | 152.5(4) |
| <F(12) , >F(16A)b | 135.7(4) | <F(13) , C(16) | 63.7(3) | <F(13) , C(15) | 85.6(3) | <F(13) , C(17) | 56.5(3) |
| <F(13) , C(112)a | 121.3(4) | <F(13) , >F(16A)b | 79.1(4) | C(16) , C(15) | 25.05(10) | C(16) , C(17) | 22.03(11) |
| C(16) , C(112)a | 145.3(3) | C(16) , >F(16A)b | 86.3(3) | C(15) , C(17) | 44.90(13) | C(15) , C(112)a | 143.1(2) |
| C(15) , >F(16A)b | 102.8(3) | C(17) , C(112)a | 127.2(2) | C(17) , >F(16A)b | 65.0(3) | C(112)a , >F(16A)b | 63.3(3) |

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3.6 Angstrom Coordination Sphere Around Atom I = F(11A) [ARU = 1555.01] 0.20260 0.07890 -0.01120 2.5805 1.0594 -0.2403

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|------------------------|------------|--------|-------|---------|--------|----------|----------|----------|---------|---------|---------|
| 1 | 1.307(9) | -- | C(161) | | | | Intra | 70.59 | -10.34 | 0.23370 | 0.16920 | -0.02213 | 3.0076 | 2.2718 | -0.4747 |
| 2 | 2.101(13) | << | <F(12A) | | | | Intra | 110.69 | -0.53 | 0.14320 | 0.22530 | -0.01210 | 1.8380 | 3.0250 | -0.2596 |
| 3 | 2.159(15) | << | <F(13A) | | | | Intra | 65.82 | -45.61 | 0.23260 | 0.18150 | -0.08310 | 3.1991 | 2.4369 | -1.7827 |
| 4 | 2.377(11) | << | C(16) | | | | Intra | 46.84 | 14.41 | 0.33547 | 0.20399 | 0.01637 | 4.1553 | 2.7389 | 0.3512 |
| 5 | 3.086(13) | < | C(17) | | | | Intra | 22.35 | 6.35 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 6 | 3.128(17) | .. | >F(16A)b | [1-x, -y, -z | = 3655.01] | | | -49.07 | 10.07 | 0.37020 | -0.09440 | 0.01430 | 4.5981 | -1.2675 | 0.3068 |
| 7 | 3.338(11) | .. | C(15) | | | | Intra | 62.65 | 28.10 | 0.33005 | 0.27370 | 0.06209 | 3.9333 | 3.6748 | 1.3320 |
| 8 | 3.410(11) | .. | C(112)a | [1/2-x, -1/2+y, 1/2-z | = 2545.01] | | | -117.39 | 21.94 | 0.10260 | -0.13030 | 0.04821 | 1.1254 | -1.7495 | 1.0342 |
| 9 | 3.467(12) | .. | >F(15A)b | [1-x, -y, -z | = 3655.01] | | | -60.16 | -25.67 | 0.30770 | -0.12300 | -0.08120 | 4.1353 | -1.6515 | -1.7419 |
| 10 | 2.57 | < | H(11E)a | [1/2-x, -1/2+y, 1/2-z | = 2545.01] | | | -126.95 | 18.09 | 0.09560 | -0.06650 | 0.02600 | 1.1123 | -0.8929 | 0.5578 |
| 11 | 3.04 | .. | H(17A) | | | | Intra | 9.78 | -6.33 | 0.43540 | 0.11710 | -0.02680 | 5.5548 | 1.5722 | -0.5749 |
| 12 | 3.11 | .. | H(11F)c | [-1/2+x, 1/2-y, -1/2+z | = 4454.01] | | | 158.90 | -14.58 | -0.03090 | 0.15960 | -0.04770 | -0.2272 | 2.1429 | -1.0233 |
| 13 | 3.42 | .. | H(11C)a | [1/2-x, -1/2+y, 1/2-z | = 2545.01] | | | -94.52 | 51.63 | 0.22280 | -0.07860 | 0.11370 | 2.4135 | -1.0553 | 2.4391 |
| 14 | 3.45 | .. | H(15A) | | | | Intra | 80.81 | 29.84 | 0.26220 | 0.29910 | 0.06890 | 3.0588 | 4.0159 | 1.4781 |
| 15 | 3.49 | .. | H(12D)c | [-1/2+x, 1/2-y, -1/2+z | = 4454.01] | | | -124.65 | -33.47 | 0.04670 | -0.09940 | -0.10090 | 0.9259 | -1.3346 | -2.1645 |
| 16 | 3.50 | .. | H(11A)a | [1/2-x, -1/2+y, 1/2-z | = 2545.01] | | | -166.51 | 75.42 | 0.17670 | 0.06360 | 0.14660 | 1.7241 | 0.8539 | 3.1449 |
| 17 | 3.56 | .. | H(12C)a | [1/2-x, -1/2+y, 1/2-z | = 2545.01] | | | 151.22 | 44.85 | 0.05790 | 0.16930 | 0.10570 | 0.3708 | 2.2731 | 2.2675 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(11A)

| | | | | | | | |
|--------------------|----------|--------------------|-----------|--------------------|----------|--------------------|-----------|
| C(161) , <F(12A) | 41.1(4) | C(161) , <F(13A) | 35.5(5) | C(161) , C(16) | 34.2(4) | C(161) , C(17) | 50.9(5) |
| C(161) , >F(16A)b | 120.7(8) | C(161) , C(15) | 39.2(4) | C(161) , C(112)a | 166.1(8) | C(161) , >F(15A)b | 120.1(7) |
| <F(12A) , <F(13A) | 59.9(5) | <F(12A) , C(16) | 64.9(3) | <F(12A) , C(17) | 88.4(4) | <F(12A) , >F(16A)b | 157.7(7) |
| <F(12A) , C(15) | 54.2(3) | <F(12A) , C(112)a | 128.5(6) | <F(12A) , >F(15A)b | 152.4(6) | <F(13A) , C(16) | 62.4(4) |
| <F(13A) , C(17) | 64.8(4) | <F(13A) , >F(16A)b | 114.5(6) | <F(13A) , C(15) | 73.8(4) | <F(13A) , C(112)a | 156.2(6) |
| <F(13A) , >F(15A)b | 93.5(5) | C(16) , C(17) | 25.38(16) | C(16) , >F(16A)b | 93.1(5) | C(16) , C(15) | 20.07(12) |
| C(16) , C(112)a | 140.5(5) | C(16) , >F(15A)b | 111.3(5) | C(17) , >F(16A)b | 70.7(4) | C(17) , C(15) | 43.89(16) |
| C(17) , C(112)a | 131.5(4) | C(17) , >F(15A)b | 86.1(3) | >F(16A)b, C(15) | 103.8(4) | >F(16A)b, C(112)a | 66.3(3) |
| >F(16A)b, >F(15A)b | 37.3(2) | C(15) , C(112)a | 130.0(4) | C(15) , >F(15A)b | 129.4(4) | C(112)a, >F(15A)b | 73.1(2) |

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3.6 Angstrom Coordination Sphere Around Atom I = F(11B) [ARU = 1555.01] 0.24500 0.08390 -0.05200 3.2500 1.1265 -1.1155

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|-----------------------------|------------|-------|---------|--------|---------|----------|----------|--------|---------|---------|
| 1 | 1.335(11) | -- | C(161) | | Intra | 101.95 | 28.70 | 0.23370 | 0.16920 | -0.02213 | 3.0076 | 2.2718 | -0.4747 |
| 2 | 2.127(15) | << | <F(13B) | | Intra | 98.85 | -11.34 | 0.21420 | 0.23740 | -0.07150 | 2.9291 | 3.1875 | -1.5338 |
| 3 | 2.16(2) | << | <F(12B) | | Intra | 139.71 | 34.61 | 0.15210 | 0.16970 | 0.00530 | 1.8911 | 2.2785 | 0.1137 |
| 4 | 2.360(13) | << | C(16) | | Intra | 60.69 | 38.42 | 0.33547 | 0.20399 | 0.01637 | 4.1553 | 2.7389 | 0.3512 |
| 5 | 2.718(14) | << | C(17) | | Intra | 26.89 | 26.60 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 6 | 2.982(12) | .. | >F(15A)b[1-x,-y,-z | = 3655.01] | | -72.32 | -12.13 | 0.30770 | -0.12300 | -0.08120 | 4.1353 | -1.6515 | -1.7419 |
| 7 | 3.094(16) | .. | >F(16A)b[1-x,-y,-z | = 3655.01] | | -60.61 | 27.37 | 0.37020 | -0.09440 | 0.01430 | 4.5981 | -1.2675 | 0.3068 |
| 8 | 3.599(13) | .. | C(15) | | Intra | 74.99 | 42.85 | 0.33005 | 0.27370 | 0.06209 | 3.9333 | 3.6748 | 1.3320 |
| 9 | 2.41 | << | H(17A) | | Intra | 10.95 | 12.97 | 0.43540 | 0.11710 | -0.02680 | 5.5548 | 1.5722 | -0.5749 |
| 10 | 3.38 | .. | H(11E)a[1/2-x,-1/2+y,1/2-z | = 2545.01] | | -136.63 | 29.64 | 0.09560 | -0.06650 | 0.02600 | 1.1123 | -0.8929 | 0.5578 |
| 11 | 3.54 | .. | H(12D)c[-1/2+x,1/2-y,-1/2+z | = 4454.01] | | -133.36 | -17.22 | 0.04670 | -0.09940 | -0.10090 | 0.9259 | -1.3346 | -2.1645 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(11B)

| | | | | | | | |
|--------------------|-----------|---------------------|-----------|--------------------|-----------|--------------------|----------|
| C(161) , <F(13B) | 40.2(5) | C(161) , <F(12B) | 32.5(6) | C(161) , C(16) | 35.4(4) | C(161) , C(17) | 65.3(5) |
| C(161) , >F(15A)b | 162.6(9) | C(161) , >F(16A)b | 121.5(8) | C(161) , C(15) | 25.9(4) | <F(13B) , <F(12B) | 60.1(7) |
| <F(13B) , C(16) | 61.2(5) | <F(13B) , C(17) | 79.4(6) | <F(13B) , >F(15A)b | 155.0(8) | <F(13B) , >F(16A)b | 154.9(8) |
| <F(13B) , C(15) | 58.4(5) | <F(12B) , C(16) | 61.6(5) | <F(12B) , C(17) | 91.8(6) | <F(12B) , >F(15A)b | 143.3(8) |
| <F(12B) , >F(16A)b | 115.1(8) | <F(12B) , C(15) | 49.9(5) | C(16) , C(17) | 30.64(18) | C(16) , >F(15A)b | 130.8(6) |
| C(16) , >F(16A)b | 94.4(5) | C(16) , C(15) | 11.70(14) | C(17) , >F(15A)b | 103.5(4) | C(17) , >F(16A)b | 76.1(4) |
| C(17) , C(15) | 42.07(19) | >F(15A)b , >F(16A)b | 41.1(2) | >F(15A)b , C(15) | 138.3(5) | >F(16A)b , C(15) | 98.8(4) |

3.6 Angstrom Coordination Sphere Around Atom I = F(12) [ARU = 1555.01] 0.16410 0.23870 -0.03510 2.1778 3.2049 -0.7530

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------|---------------------------------|-------|---------|--------|----------|---------|----------|---------|--------|---------|
| 1 | 1.279(8) | -- | C(161) | | Intra | -48.35 | 12.56 | 0.23370 | 0.16920 | -0.02213 | 3.0076 | 2.2718 | -0.4747 |
| 2 | 2.137(11) | << | <F(13) | | Intra | -52.43 | -23.36 | 0.24880 | 0.12290 | -0.07460 | 3.3738 | 1.6501 | -1.6003 |
| 3 | 2.143(10) | << | <F(11) | | Intra | -85.78 | 27.49 | 0.18760 | 0.09750 | 0.01100 | 2.3175 | 1.3091 | 0.2360 |
| 4 | 2.312(9) | << | C(16) | | Intra | -13.26 | 28.52 | 0.33547 | 0.20399 | 0.01637 | 4.1553 | 2.7389 | 0.3512 |
| 5 | 2.766(9) | << | C(15) | | Intra | 14.99 | 48.92 | 0.33005 | 0.27370 | 0.06209 | 3.9333 | 3.6748 | 1.3320 |
| 6 | 3.173(9) | .. | C(25)b | [-1/2+x,1/2-y,-1/2+z = 4454.02] | | 142.36 | -53.67 | 0.01352 | 0.32420 | -0.15426 | 0.6891 | 4.3529 | -3.3092 |
| 7 | 3.491(9) | .. | C(17) | | Intra | -16.82 | 14.17 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 8 | 2.44 | << | H(25A)b | [-1/2+x,1/2-y,-1/2+z = 4454.02] | | 158.56 | -46.80 | 0.01820 | 0.28410 | -0.11790 | 0.6254 | 3.8145 | -2.5292 |
| 9 | 2.53 | .< | H(15A) | | Intra | 42.63 | 61.78 | 0.26220 | 0.29910 | 0.06890 | 3.0588 | 4.0159 | 1.4781 |
| 10 | 2.64 | .< | H(11F)c | [-1/2+x,1/2-y,-1/2+z = 4454.01] | | -156.17 | -5.87 | -0.03090 | 0.15960 | -0.04770 | -0.2272 | 2.1429 | -1.0233 |
| 11 | 3.43 | .. | H(22D)a | [1-x,1-y,-z = 3665.02] | | 68.78 | -24.63 | 0.23620 | 0.45540 | -0.10180 | 3.3072 | 6.1144 | -2.1839 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(12)

| | | | | | | | |
|-----------------|----------|-----------------|-----------|-----------------|----------|----------------|-----------|
| C(161) , <F(13) | 36.2(3) | C(161) , <F(11) | 38.0(3) | C(161) , C(16) | 36.3(3) | C(161) , C(15) | 63.2(4) |
| C(161) , C(25)b | 138.0(5) | C(161) , C(17) | 30.7(3) | <F(13) , <F(11) | 60.2(3) | <F(13) , C(16) | 64.2(3) |
| <F(13) , C(15) | 93.9(4) | <F(13) , C(25)b | 101.9(4) | <F(13) , C(17) | 51.2(3) | <F(11) , C(16) | 63.0(3) |
| <F(11) , C(15) | 76.2(3) | <F(11) , C(25)b | 136.3(4) | <F(11) , C(17) | 65.1(3) | C(16) , C(15) | 29.71(12) |
| C(16) , C(25)b | 149.2(4) | C(16) , C(17) | 14.73(10) | C(15) , C(25)b | 147.5(3) | C(15) , C(17) | 43.46(14) |
| C(25)b , C(17) | 137.2(3) | | | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(12A) [ARU = 1555.01] 0.14320 0.22530 -0.01210 1.8380 3.0250 -0.2596

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|--------|---------|
| 1 | 1.408(9) | -- | C(161) | | | | Intra | -32.78 | -8.79 | 0.23370 | 0.16920 | -0.02213 | 3.0076 | 2.2718 | -0.4747 |
| 2 | 2.101(13) | << | <F(11A) | | | | Intra | -69.31 | 0.53 | 0.20260 | 0.07890 | -0.01120 | 2.5805 | 1.0594 | -0.2403 |
| 3 | 2.126(12) | << | <F(13A) | | | | Intra | -23.37 | -45.77 | 0.23260 | 0.18150 | -0.08310 | 3.1991 | 2.4369 | -1.7827 |
| 4 | 2.413(9) | << | C(16) | | | | Intra | -7.04 | 14.66 | 0.33547 | 0.20399 | 0.01637 | 4.1553 | 2.7389 | 0.3512 |
| 5 | 2.710(9) | << | C(15) | | | | Intra | 17.23 | 35.96 | 0.33005 | 0.27370 | 0.06209 | 3.9333 | 3.6748 | 1.3320 |
| 6 | 3.318(9) | .. | C(112)c | [-1/2+x, | 1/2-y, | -1/2+z = | | -156.71 | -13.50 | -0.10260 | 0.13030 | -0.04821 | -1.1254 | 1.7495 | -1.0342 |
| 7 | 3.519(9) | .. | C(25)b | [-1/2+x, | 1/2-y, | -1/2+z = | | 130.87 | -60.07 | 0.01352 | 0.32420 | -0.15426 | 0.6891 | 4.3529 | -3.3092 |
| 8 | 2.34 | << | H(15A) | | | | Intra | 39.06 | 47.86 | 0.26220 | 0.29910 | 0.06890 | 3.0588 | 4.0159 | 1.4781 |
| 9 | 2.37 | << | H(11F)c | [-1/2+x, | 1/2-y, | -1/2+z = | | -156.87 | -18.78 | -0.03090 | 0.15960 | -0.04770 | -0.2272 | 2.1429 | -1.0233 |
| 10 | 2.69 | .. | H(25A)b | [-1/2+x, | 1/2-y, | -1/2+z = | | 146.93 | -57.48 | 0.01820 | 0.28410 | -0.11790 | 0.6254 | 3.8145 | -2.5292 |
| 11 | 3.02 | .. | H(12C)a | [1/2-x, | -1/2+y, | 1/2-z = | | -152.87 | 56.88 | 0.05790 | 0.16930 | 0.10570 | 0.3708 | 2.2731 | 2.2675 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(12A)

| | | | | | | | |
|------------------|-----------|-------------------|----------|-------------------|----------|-----------------|-----------|
| C(161) , <F(11A) | 37.6(4) | C(161) , <F(13A) | 37.9(4) | C(161) , C(16) | 34.7(3) | C(161) , C(15) | 64.9(3) |
| C(161) , C(112)c | 120.1(5) | C(161) , C(25)b | 109.9(4) | <F(11A) , <F(13A) | 61.4(6) | <F(11A) , C(16) | 63.1(4) |
| <F(11A) , C(15) | 86.9(5) | <F(11A) , C(112)c | 87.6(5) | <F(11A) , C(25)b | 118.4(5) | <F(13A) , C(16) | 62.2(3) |
| <F(13A) , C(15) | 89.6(4) | <F(13A) , C(112)c | 107.4(4) | <F(13A) , C(25)b | 72.1(3) | C(16) , C(15) | 30.41(12) |
| C(16) , C(112)c | 150.6(4) | C(16) , C(25)b | 125.3(3) | C(15) , C(112)c | 156.9(3) | C(15) , C(25)b | 132.1(3) |
| C(112)c , C(25)b | 69.58(18) | | | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(12B) [ARU = 1555.01] 0.15210 0.16970 0.00530 1.8911 2.2785 0.1137

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|------------|-----------|----------|-------|---------|--------|----------|----------|----------|---------|---------|---------|
| 1 | 1.262(14) | -- | C(161) | | | | Intra | -0.34 | -27.79 | 0.23370 | 0.16920 | -0.02213 | 3.0076 | 2.2718 | -0.4747 |
| 2 | 2.15(2) | << | <F(13B) | | | | Intra | 41.21 | -50.06 | 0.21420 | 0.23740 | -0.07150 | 2.9291 | 3.1875 | -1.5338 |
| 3 | 2.16(2) | << | <F(11B) | | | | Intra | -40.29 | -34.61 | 0.24500 | 0.08390 | -0.05200 | 3.2500 | 1.1265 | -1.1155 |
| 4 | 2.323(13) | << | C(16) | | | | Intra | 11.49 | 5.87 | 0.33547 | 0.20399 | 0.01637 | 4.1553 | 2.7389 | 0.3512 |
| 5 | 2.758(16) | << | C(15) | | | | Intra | 34.36 | 26.22 | 0.33005 | 0.27370 | 0.06209 | 3.9333 | 3.6748 | 1.3320 |
| 6 | 3.271(14) | .. | C(112)b | [-1/2+x, | 1/2-y, | -1/2+z = | | -170.05 | -20.55 | -0.10260 | 0.13030 | -0.04821 | -1.1254 | 1.7495 | -1.0342 |
| 7 | 3.527(13) | .. | C(17) | | | | Intra | -0.86 | -0.20 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 8 | 3.532(15) | .. | C(121)a | [1/2-x, | -1/2+y, | 1/2-z = | | -171.99 | 48.47 | 0.00040 | 0.14540 | 0.12857 | -0.4279 | 1.9522 | 2.7581 |
| 9 | 2.41 | << | H(11F)b | [-1/2+x, | 1/2-y, | -1/2+z = | | -176.34 | -28.18 | -0.03090 | 0.15960 | -0.04770 | -0.2272 | 2.1429 | -1.0233 |
| 10 | 2.50 | .< | H(15A) | | | | Intra | 56.10 | 33.10 | 0.26220 | 0.29910 | 0.06890 | 3.0588 | 4.0159 | 1.4781 |
| 11 | 2.64 | .< | H(12C)a | [1/2-x, | -1/2+y, | 1/2-z = | | -179.80 | 54.78 | 0.05790 | 0.16930 | 0.10570 | 0.3708 | 2.2731 | 2.2675 |
| 12 | 3.30 | .. | H(11E)a | [1/2-x, | -1/2+y, | 1/2-z = | | -103.80 | 7.74 | 0.09560 | -0.06650 | 0.02600 | 1.1123 | -0.8929 | 0.5578 |
| 13 | 3.31 | .. | H(25A)c | [-1/2+x, | 1/2-y, | -1/2+z = | | 129.49 | -53.02 | 0.01820 | 0.28410 | -0.11790 | 0.6254 | 3.8145 | -2.5292 |
| 14 | 3.35 | .. | H(11A)a | [1/2-x, | -1/2+y, | 1/2-z = | | -96.69 | 64.68 | 0.17670 | 0.06360 | 0.14660 | 1.7241 | 0.8539 | 3.1449 |
| 15 | 3.38 | .. | H(11E)b | [-1/2+x, | 1/2-y, | -1/2+z = | | -155.23 | -11.48 | -0.09560 | 0.06650 | -0.02600 | -1.1123 | 0.8929 | -0.5578 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(12B)

| | | | | | | | |
|-------------------|-----------|-------------------|----------|-------------------|----------|-------------------|-----------|
| C(161) , <F(13B) | 38.5(7) | C(161) , <F(11B) | 34.6(7) | C(161) , C(16) | 35.6(4) | C(161) , C(15) | 63.5(7) |
| C(161) , C(112)b | 130.7(9) | C(161) , C(17) | 27.6(5) | C(161) , C(121)a | 158.3(9) | <F(13B) , <F(11B) | 59.1(6) |
| <F(13B) , C(16) | 61.6(6) | <F(13B) , C(15) | 76.5(6) | <F(13B) , C(112)b | 104.2(7) | <F(13B) , C(17) | 61.4(5) |
| <F(13B) , C(121)a | 158.5(9) | <F(11B) , C(16) | 63.4(5) | <F(11B) , C(15) | 93.2(6) | <F(11B) , C(112)b | 107.1(7) |
| <F(11B) , C(17) | 50.4(4) | <F(11B) , C(121)a | 142.0(9) | C(16) , C(15) | 29.8(2) | C(16) , C(112)b | 165.2(6) |
| C(16) , C(17) | 13.75(19) | C(16) , C(121)a | 125.6(6) | C(15) , C(112)b | 156.9(8) | C(15) , C(17) | 43.00(19) |
| C(15) , C(121)a | 101.7(5) | C(112)b , C(17) | 156.7(6) | C(112)b , C(121)a | 69.0(3) | C(17) , C(121)a | 131.1(4) |

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3.6 Angstrom Coordination Sphere Around Atom I = F(13) [ARU = 1555.01] 0.24880 0.12290 -0.07460 3.3738 1.6501 -1.6003

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------|---------------------------------|-------|--------|--------|---------|----------|----------|--------|---------|---------|
| 1 | 1.337(8) | -- | C(161) | | Intra | 120.50 | 57.34 | 0.23370 | 0.16920 | -0.02213 | 3.0076 | 2.2718 | -0.4747 |
| 2 | 2.137(11) | << | <F(12) | | Intra | 127.57 | 23.36 | 0.16410 | 0.23870 | -0.03510 | 2.1778 | 3.2049 | -0.7530 |
| 3 | 2.146(10) | << | <F(11) | | Intra | 162.11 | 58.85 | 0.18760 | 0.09750 | 0.01100 | 2.3175 | 1.3091 | 0.2360 |
| 4 | 2.367(8) | << | C(16) | | Intra | 54.33 | 55.52 | 0.33547 | 0.20399 | 0.01637 | 4.1553 | 2.7389 | 0.3512 |
| 5 | 2.721(8) | << | C(17) | | Intra | 15.73 | 38.71 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 6 | 3.391(11) | .. | >F(15A)a | [1-x,-y,-z = 3655.01] | | -77.01 | -2.39 | 0.30770 | -0.12300 | -0.08120 | 4.1353 | -1.6515 | -1.7419 |
| 7 | 3.570(7) | .. | N(22)b | [-1/2+x,1/2-y,-1/2+z = 4454.02] | | 158.04 | -54.40 | 0.05894 | 0.18079 | -0.20991 | 1.4465 | 2.4274 | -4.5031 |
| 8 | 2.41 | << | H(17A) | | Intra | -2.04 | 25.17 | 0.43540 | 0.11710 | -0.02680 | 5.5548 | 1.5722 | -0.5749 |
| 9 | 3.51(2) | .. | H(22)b | [-1/2+x,1/2-y,-1/2+z = 4454.02] | | 173.40 | -44.59 | 0.02010 | 0.14430 | -0.18950 | 0.8903 | 1.9374 | -4.0652 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(13)

| | | | | | | | |
|-------------------|----------|-------------------|----------|------------------|----------|----------------|-----------|
| C(161) , <F(12) | 34.4(3) | C(161) , <F(11) | 38.6(3) | C(161) , C(16) | 35.2(2) | C(161) , C(17) | 65.2(3) |
| C(161) , >F(15A)a | 123.3(5) | C(161) , N(22)b | 115.8(4) | <F(12) , <F(11) | 60.1(3) | <F(12) , C(16) | 61.5(3) |
| <F(12) , C(17) | 91.1(4) | <F(12) , >F(15A)a | 148.3(4) | <F(12) , N(22)b | 82.1(3) | <F(11) , C(16) | 62.0(3) |
| <F(11) , C(17) | 82.4(3) | <F(11) , >F(15A)a | 89.5(4) | <F(11) , N(22)b | 117.7(4) | C(16) , C(17) | 30.60(11) |
| C(16) , >F(15A)a | 114.1(3) | C(16) , N(22)b | 138.5(4) | C(17) , >F(15A)a | 93.6(3) | C(17) , N(22)b | 150.2(3) |
| >F(15A)a, N(22)b | 107.4(2) | | | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(13A) [ARU = 1555.01] 0.23260 0.18150 -0.08310 3.1991 2.4369 -1.7827

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|-------------------------------|----------|-------|---------|--------|----------|---------|----------|---------|--------|---------|
| 1 | 1.332(7) | -- | C(161) | | Intra | -139.22 | 79.06 | 0.23370 | 0.16920 | -0.02213 | 3.0076 | 2.2718 | -0.4747 |
| 2 | 2.126(12) | << | <F(12A) | | Intra | 156.63 | 45.77 | 0.14320 | 0.22530 | -0.01210 | 1.8380 | 3.0250 | -0.2596 |
| 3 | 2.159(15) | << | <F(11A) | | Intra | -114.18 | 45.61 | 0.20260 | 0.07890 | -0.01120 | 2.5805 | 1.0594 | -0.2403 |
| 4 | 2.358(7) | << | C(16) | | Intra | 17.53 | 64.83 | 0.33547 | 0.20399 | 0.01637 | 4.1553 | 2.7389 | 0.3512 |
| 5 | 2.918(8) | << | C(17) | | Intra | -5.44 | 40.21 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 6 | 3.236(7) | .. | N(22)b [-1/2+x,1/2-y,-1/2+z = | 4454.02] | | -179.69 | -57.21 | 0.05894 | 0.18079 | -0.20991 | 1.4465 | 2.4274 | -4.5031 |
| 7 | 3.431(8) | .. | C(15) | | Intra | 59.33 | 65.20 | 0.33005 | 0.27370 | 0.06209 | 3.9333 | 3.6748 | 1.3320 |
| 8 | 3.458(7) | .. | C(23)b [-1/2+x,1/2-y,-1/2+z = | 4454.02] | | -138.37 | -74.02 | 0.13434 | 0.13440 | -0.23806 | 2.4876 | 1.8045 | -5.1070 |
| 9 | 3.507(10) | .. | C(25)b [-1/2+x,1/2-y,-1/2+z = | 4454.02] | | 142.64 | -25.80 | 0.01352 | 0.32420 | -0.15426 | 0.6891 | 4.3529 | -3.3092 |
| 10 | 2.78 | .. | H(17A) | | Intra | -20.16 | 25.70 | 0.43540 | 0.11710 | -0.02680 | 5.5548 | 1.5722 | -0.5749 |
| 11 | 3.01 | .. | H(25A)b[-1/2+x,1/2-y,-1/2+z = | 4454.02] | | 151.84 | -14.35 | 0.01820 | 0.28410 | -0.11790 | 0.6254 | 3.8145 | -2.5292 |
| 12 | 3.28 | .. | H(21A)a[1-x,1-y,-z = | 3665.02] | | 62.22 | -31.26 | 0.31540 | 0.36620 | -0.16240 | 4.5053 | 4.9168 | -3.4839 |
| 13 | 3.29(2) | .. | H(22)b [-1/2+x,1/2-y,-1/2+z = | 4454.02] | | -167.79 | -44.02 | 0.02010 | 0.14430 | -0.18950 | 0.8903 | 1.9374 | -4.0652 |
| 14 | 3.49 | .. | H(21C)a[1-x,1-y,-z = | 3665.02] | | 17.08 | -21.22 | 0.46430 | 0.25260 | -0.14190 | 6.3051 | 3.3915 | -3.0441 |
| 15 | 3.52 | .. | H(11F)c[-1/2+x,1/2-y,-1/2+z = | 4454.01] | | -175.09 | 12.45 | -0.03090 | 0.15960 | -0.04770 | -0.2272 | 2.1429 | -1.0233 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(13A)

| | | | | | | | |
|-------------------|-----------|------------------|-----------|------------------|----------|------------------|-----------|
| C(161) , <F(12A) | 40.4(4) | C(161) , <F(11A) | 34.7(4) | C(161) , C(16) | 35.5(3) | C(161) , C(17) | 57.8(3) |
| C(161) , N(22)b | 138.3(5) | C(161) , C(15) | 35.3(4) | C(161) , C(23)b | 153.1(7) | C(161) , C(25)b | 113.1(5) |
| <F(12A) , <F(11A) | 58.7(4) | <F(12A) , C(16) | 64.9(3) | <F(12A) , C(17) | 92.5(3) | <F(12A) , N(22)b | 104.9(4) |
| <F(12A) , C(15) | 52.2(3) | <F(12A) , C(23)b | 127.4(4) | <F(12A) , C(25)b | 72.7(4) | <F(11A) , C(16) | 63.3(4) |
| <F(11A) , C(17) | 73.2(4) | <F(11A) , N(22)b | 116.3(5) | <F(11A) , C(15) | 69.1(3) | <F(11A) , C(23)b | 120.8(5) |
| <F(11A) , C(25)b | 117.0(5) | C(16) , C(17) | 27.95(12) | C(16) , N(22)b | 168.8(4) | C(16) , C(15) | 17.34(12) |
| C(16) , C(23)b | 167.7(4) | C(16) , C(25)b | 127.9(4) | C(17) , N(22)b | 162.6(3) | C(17) , C(15) | 43.73(12) |
| C(17) , C(23)b | 139.8(3) | C(17) , C(25)b | 149.8(4) | N(22)b , C(15) | 151.7(4) | N(22)b , C(23)b | 23.05(6) |
| N(22)b , C(25)b | 41.25(11) | C(15) , C(23)b | 169.3(4) | C(15) , C(25)b | 110.6(3) | C(23)b , C(25)b | 62.24(14) |

=====

3.6 Angstrom Coordination Sphere Around Atom I = F(13B) [ARU = 1555.01] 0.21420 0.23740 -0.07150 2.9291 3.1875 -1.5338

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|------------------------|-----------|--------|-------|---------|--------|----------|---------|----------|---------|--------|---------|
| 1 | 1.402(14) | -- | C(161) | | | | Intra | -85.10 | 49.05 | 0.23370 | 0.16920 | -0.02213 | 3.0076 | 2.2718 | -0.4747 |
| 2 | 2.127(15) | << | <F(11B) | | | | Intra | -81.15 | 11.34 | 0.24500 | 0.08390 | -0.05200 | 3.2500 | 1.1265 | -1.1155 |
| 3 | 2.15(2) | << | <F(12B) | | | | Intra | -138.79 | 50.06 | 0.15210 | 0.16970 | 0.00530 | 1.8911 | 2.2785 | 0.1137 |
| 4 | 2.293(15) | << | C(16) | | | | Intra | -20.09 | 55.29 | 0.33547 | 0.20399 | 0.01637 | 4.1553 | 2.7389 | 0.3512 |
| 5 | 3.076(15) | .< | C(15) | | | | Intra | 25.89 | 68.72 | 0.33005 | 0.27370 | 0.06209 | 3.9333 | 3.6748 | 1.3320 |
| 6 | 3.087(15) | .< | C(25)b | [-1/2+x,1/2-y,-1/2+z = | 4454.02] | | | 152.51 | -35.11 | 0.01352 | 0.32420 | -0.15426 | 0.6891 | 4.3529 | -3.3092 |
| 7 | 3.129(16) | .< | C(17) | | | | Intra | -21.14 | 31.51 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 8 | 3.405(15) | .. | N(22)b | [-1/2+x,1/2-y,-1/2+z = | 4454.02] | | | -152.86 | -60.70 | 0.05894 | 0.18079 | -0.20991 | 1.4465 | 2.4274 | -4.5031 |
| 9 | 3.493(15) | .. | C(24)b | [-1/2+x,1/2-y,-1/2+z = | 4454.02] | | | 160.61 | -57.66 | 0.03687 | 0.28360 | -0.20908 | 1.1667 | 3.8078 | -4.4853 |
| 10 | 2.59 | .< | H(25A)b | [-1/2+x,1/2-y,-1/2+z = | 4454.02] | | | 164.77 | -22.63 | 0.01820 | 0.28410 | -0.11790 | 0.6254 | 3.8145 | -2.5292 |
| 11 | 3.02 | .. | H(22D)a | [1-x,1-y,-z = | 3665.02] | | | 82.64 | -12.42 | 0.23620 | 0.45540 | -0.10180 | 3.3072 | 6.1144 | -2.1839 |
| 12 | 3.05 | .. | H(21A)a | [1-x,1-y,-z = | 3665.02] | | | 47.65 | -39.81 | 0.31540 | 0.36620 | -0.16240 | 4.5053 | 4.9168 | -3.4839 |
| 13 | 3.13 | .. | H(15A) | | | | Intra | 81.10 | 74.44 | 0.26220 | 0.29910 | 0.06890 | 3.0588 | 4.0159 | 1.4781 |
| 14 | 3.23 | .. | H(17A) | | | | Intra | -31.60 | 17.28 | 0.43540 | 0.11710 | -0.02680 | 5.5548 | 1.5722 | -0.5749 |
| 15 | 3.36 | .. | H(11F)c | [-1/2+x,1/2-y,-1/2+z = | 4454.01] | | | -161.69 | 8.73 | -0.03090 | 0.15960 | -0.04770 | -0.2272 | 2.1429 | -1.0233 |
| 16 | 3.48(3) | .. | H(22)b | [-1/2+x,1/2-y,-1/2+z = | 4454.02] | | | -148.49 | -46.63 | 0.02010 | 0.14430 | -0.18950 | 0.8903 | 1.9374 | -4.0652 |
| 17 | 3.59 | .. | H(22F)a | [1-x,1-y,-z = | 3665.02] | | | 61.22 | 21.66 | 0.35860 | 0.45500 | -0.00980 | 4.5337 | 6.1091 | -0.2102 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(13B)

| | | | | | | | |
|-------------------|-----------|------------------|-----------|------------------|----------|------------------|-----------|
| C(161) , <F(11B) | 37.9(5) | C(161) , <F(12B) | 34.1(6) | C(161) , C(16) | 38.9(4) | C(161) , C(15) | 51.8(5) |
| C(161) , C(25)b | 136.2(9) | C(161) , C(17) | 50.2(5) | C(161) , N(22)b | 122.5(7) | C(161) , C(24)b | 141.5(8) |
| <F(11B) , <F(12B) | 60.8(8) | <F(11B) , C(16) | 64.4(5) | <F(11B) , C(15) | 85.5(6) | <F(11B) , C(25)b | 126.0(7) |
| <F(11B) , C(17) | 58.6(5) | <F(11B) , N(22)b | 91.2(6) | <F(11B) , C(24)b | 114.5(6) | <F(12B) , C(16) | 63.0(5) |
| <F(12B) , C(15) | 60.7(6) | <F(12B) , C(25)b | 104.5(7) | <F(12B) , C(17) | 81.6(6) | <F(12B) , N(22)b | 111.3(7) |
| <F(12B) , C(24)b | 118.6(7) | C(16) , C(15) | 24.55(17) | C(16) , C(25)b | 159.2(6) | C(16) , C(17) | 23.80(19) |
| C(16) , N(22)b | 155.0(5) | C(16) , C(24)b | 177.6(6) | C(15) , C(25)b | 135.5(5) | C(15) , C(17) | 45.7(2) |
| C(15) , N(22)b | 172.0(5) | C(15) , C(24)b | 157.5(4) | C(25)b , C(17) | 173.6(5) | C(25)b , N(22)b | 42.8(2) |
| C(25)b , C(24)b | 23.20(12) | C(17) , N(22)b | 137.2(4) | C(17) , C(24)b | 153.8(5) | N(22)b , C(24)b | 23.52(11) |

3.6 Angstrom Coordination Sphere Around Atom I = F(14) [ARU = 1555.01] 0.71070 0.22720 0.03350 8.8070 3.0505 0.7187

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|---------------------|-----------|----------|-------|---------|--------|---------|---------|----------|---------|--------|---------|
| 1 | 1.307(15) | -- | C(181) | | | | Intra | -137.44 | -3.24 | 0.63320 | 0.16146 | 0.03006 | 7.8459 | 2.1678 | 0.6449 |
| 2 | 0.460(16) | << | >F(14A) | | | | Intra | 134.70 | -64.19 | 0.69430 | 0.23780 | 0.01420 | 8.6661 | 3.1928 | 0.3046 |
| 3 | 1.777(15) | << | >F(15A) | | | | Intra | -105.63 | 35.16 | 0.69230 | 0.12300 | 0.08120 | 8.4154 | 1.6515 | 1.7419 |
| 4 | 2.136(17) | << | <F(15) | | | | Intra | -110.93 | 22.68 | 0.66490 | 0.09010 | 0.07190 | 8.1029 | 1.2097 | 1.5424 |
| 5 | 2.14(2) | << | <F(16) | | | | Intra | -120.04 | -36.41 | 0.62600 | 0.11600 | -0.02580 | 7.9436 | 1.5575 | -0.5535 |
| 6 | 2.227(17) | << | >F(16A) | | | | Intra | -115.60 | -27.41 | 0.62980 | 0.09440 | -0.01430 | 7.9526 | 1.2675 | -0.3068 |
| 7 | 2.374(15) | << | C(18) | | | | Intra | -171.24 | 3.47 | 0.52587 | 0.20032 | 0.04020 | 6.4647 | 2.6896 | 0.8624 |
| 8 | 2.847(15) | << | C(19) | | | | Intra | 167.11 | 23.69 | 0.52253 | 0.27050 | 0.08683 | 6.2658 | 3.6319 | 1.8627 |
| 9 | 3.409(15) | .. | C(112)c | [1/2+x,1/2-y,-1/2+z | = | 4554.01] | | -26.42 | -30.94 | 0.89740 | 0.13030 | -0.04821 | 11.4253 | 1.7495 | -1.0342 |
| 10 | 3.443(14) | .. | C(222) | [| = | 02] | | 97.71 | -2.84 | 0.67180 | 0.48100 | 0.02554 | 8.3456 | 6.4581 | 0.5479 |
| 11 | 3.443(15) | .. | C(122)a | [3/2-x,-1/2+y,1/2-z | = | 2645.01] | | 0.09 | 43.70 | 0.93880 | 0.22750 | 0.14440 | 11.2964 | 3.0545 | 3.0977 |
| 12 | 3.543(15) | .. | C(17) | | | | Intra | -166.32 | -10.04 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 13 | 2.48 | .< | H(11D)c | [1/2+x,1/2-y,-1/2+z | = | 4554.01] | | -19.17 | -31.94 | 0.85280 | 0.17570 | -0.02770 | 10.7965 | 2.3590 | -0.5942 |
| 14 | 2.61 | .< | H(19A) | | | | Intra | 153.75 | 39.48 | 0.58760 | 0.29350 | 0.11080 | 7.0017 | 3.9407 | 2.3769 |
| 15 | 2.87 | .. | H(12E)a | [3/2-x,-1/2+y,1/2-z | = | 2645.01] | | 13.25 | 33.49 | 0.91580 | 0.26800 | 0.10720 | 11.1330 | 3.5983 | 2.2997 |
| 16 | 2.96 | .. | H(22G) | [| = | 02] | | 112.70 | -6.36 | 0.61610 | 0.42940 | 0.01820 | 7.6712 | 5.7653 | 0.3904 |
| 17 | 3.14 | .. | H(22C) | [| = | 02] | | 85.43 | 31.15 | 0.74810 | 0.42690 | 0.10930 | 9.0212 | 5.7318 | 2.3447 |
| 18 | 3.19 | .. | H(21D)b | [1-x,1-y,-z | = | 3665.02] | | 140.17 | -83.70 | 0.64960 | 0.24390 | -0.11440 | 8.5381 | 3.2747 | -2.4542 |
| 19 | 3.20 | .. | H(12G)a | [3/2-x,-1/2+y,1/2-z | = | 2645.01] | | -11.14 | 58.60 | 0.87530 | 0.20320 | 0.16090 | 10.4439 | 2.7283 | 3.4517 |
| 20 | 3.25 | .. | H(22E) | [| = | 02] | | 83.39 | -11.30 | 0.73200 | 0.46320 | 0.00380 | 9.1743 | 6.2192 | 0.0815 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(14)

| | | | | | | | |
|-------------------|----------|-------------------|----------|-------------------|----------|-------------------|-----------|
| C(181) , >F(14A) | 86(2) | C(181) , >F(15A) | 48.6(5) | C(181) , <F(15) | 36.6(5) | C(181) , <F(16) | 36.9(6) |
| C(181) , >F(16A) | 31.9(5) | C(181) , C(18) | 34.4(4) | C(181) , C(19) | 60.3(6) | C(181) , C(112)c | 106.1(7) |
| C(181) , C(222) | 124.6(8) | C(181) , C(122)a | 124.9(7) | C(181) , C(17) | 29.5(5) | >F(14A) , >F(15A) | 134(2) |
| >F(14A) , <F(15) | 121(2) | >F(14A) , <F(16) | 63.8(19) | >F(14A) , >F(16A) | 73.5(19) | >F(14A) , C(18) | 78(2) |
| >F(14A) , C(19) | 91(2) | >F(14A) , C(112)c | 84(2) | >F(14A) , C(222) | 66.9(19) | >F(14A) , C(122)a | 148(2) |
| >F(14A) , C(17) | 68(2) | >F(15A) , <F(15) | 13.3(4) | >F(15A) , <F(16) | 72.8(6) | >F(15A) , >F(16A) | 63.3(5) |
| >F(15A) , C(18) | 68.2(5) | >F(15A) , C(19) | 74.5(5) | >F(15A) , C(112)c | 99.5(6) | >F(15A) , C(222) | 141.1(7) |
| >F(15A) , C(122)a | 76.3(5) | >F(15A) , C(17) | 72.9(5) | <F(15) , <F(16) | 59.7(6) | <F(15) , >F(16A) | 50.3(5) |
| <F(15) , C(18) | 61.4(5) | <F(15) , C(19) | 74.1(5) | <F(15) , C(112)c | 97.0(6) | <F(15) , C(222) | 145.9(7) |
| <F(15) , C(122)a | 88.5(5) | <F(15) , C(17) | 63.3(5) | <F(16) , >F(16A) | 9.8(4) | <F(16) , C(18) | 62.1(7) |
| <F(16) , C(19) | 91.2(8) | <F(16) , C(112)c | 74.8(7) | <F(16) , C(222) | 127.3(7) | <F(16) , C(122)a | 134.6(8) |
| <F(16) , C(17) | 49.4(7) | >F(16A) , C(18) | 61.8(5) | >F(16A) , C(19) | 90.4(6) | >F(16A) , C(112)c | 75.7(5) |
| >F(16A) , C(222) | 135.9(6) | >F(16A) , C(122)a | 126.6(6) | >F(16A) , C(17) | 50.7(5) | C(18) , C(19) | 29.09(18) |
| C(18) , C(112)c | 137.0(5) | C(18) , C(222) | 91.2(4) | C(18) , C(122)a | 132.2(5) | C(18) , C(17) | 14.37(14) |
| C(19) , C(112)c | 166.0(5) | C(19) , C(222) | 72.4(3) | C(19) , C(122)a | 111.6(4) | C(19) , C(17) | 42.6(2) |
| C(112)c , C(222) | 117.1(4) | C(112)c , C(122)a | 78.5(3) | C(112)c , C(17) | 123.8(4) | C(222) , C(122)a | 97.5(3) |
| C(222) , C(17) | 95.4(4) | C(122)a , C(17) | 144.3(4) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(14B) [ARU = 1555.01] 0.65700 0.20400 -0.02150 8.3182 2.7390 -0.4612

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|---------|----|---------|---------------------|-----------|----------|-------|---------|--------|---------|---------|----------|---------|--------|---------|
| 1 | 1.33(3) | -- | C(181) | | | | Intra | -129.59 | 56.18 | 0.63320 | 0.16146 | 0.03006 | 7.8459 | 2.1678 | 0.6449 |
| 2 | 0.96(3) | << | >F(14A) | | | | Intra | 52.52 | 53.25 | 0.69430 | 0.23780 | 0.01420 | 8.6661 | 3.1928 | 0.3046 |
| 3 | 1.52(3) | << | >F(16A) | | | | Intra | -103.95 | 5.82 | 0.62980 | 0.09440 | -0.01430 | 7.9526 | 1.2675 | -0.3068 |
| 4 | 2.13(3) | << | <F(15B) | | | | Intra | -39.74 | 76.33 | 0.71380 | 0.18000 | 0.07510 | 8.7058 | 2.4168 | 1.6111 |
| 5 | 2.14(3) | << | <F(16B) | | | | Intra | -104.66 | 24.65 | 0.62900 | 0.06420 | 0.02000 | 7.8271 | 0.8620 | 0.4290 |
| 6 | 2.28(3) | << | C(18) | | | | Intra | -178.47 | 35.52 | 0.52587 | 0.20032 | 0.04020 | 6.4647 | 2.6896 | 0.8624 |
| 7 | 2.46(3) | << | >F(15A) | | | | Intra | -84.89 | 63.64 | 0.69230 | 0.12300 | 0.08120 | 8.4154 | 1.6515 | 1.7419 |
| 8 | 2.88(2) | << | C(212)a | [1-x,1-y,-z | = | 3665.02] | | 92.20 | -63.83 | 0.62080 | 0.29852 | -0.14199 | 8.2696 | 4.0081 | -3.0460 |
| 9 | 3.00(4) | .< | C(17) | | | | Intra | -169.96 | 10.81 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 10 | 3.23(3) | .. | C(19) | | | | Intra | 156.49 | 46.08 | 0.52253 | 0.27050 | 0.08683 | 6.2658 | 3.6319 | 1.8627 |
| 11 | 3.26(3) | .. | C(211)a | [1-x,1-y,-z | = | 3665.02] | | 135.34 | -48.95 | 0.50510 | 0.31594 | -0.13597 | 6.7972 | 4.2420 | -2.9169 |
| 12 | 3.31(4) | .. | C(112)b | [1/2+x,1/2-y,-1/2+z | = | 4554.01] | | -17.67 | -9.97 | 0.89740 | 0.13030 | -0.04821 | 11.4253 | 1.7495 | -1.0342 |
| 13 | 3.54(3) | .. | C(111)b | [1/2+x,1/2-y,-1/2+z | = | 4554.01] | | -24.19 | -33.69 | 0.84650 | 0.11410 | -0.11303 | 11.0047 | 1.5320 | -2.4248 |
| 14 | 2.08 | << | H(21D)a | [1-x,1-y,-z | = | 3665.02] | | 67.68 | -73.80 | 0.64960 | 0.24390 | -0.11440 | 8.5381 | 3.2747 | -2.4542 |
| 15 | 2.51 | .< | H(11D)b | [1/2+x,1/2-y,-1/2+z | = | 4554.01] | | -8.72 | -3.04 | 0.85280 | 0.17570 | -0.02770 | 10.7965 | 2.3590 | -0.5942 |
| 16 | 2.97 | .. | H(21B)a | [1-x,1-y,-z | = | 3665.02] | | 133.06 | -31.48 | 0.49960 | 0.34200 | -0.09390 | 6.5865 | 4.5919 | -2.0144 |
| 17 | 3.00 | .. | H(17A) | | | | Intra | -157.11 | -2.17 | 0.43540 | 0.11710 | -0.02680 | 5.5548 | 1.5722 | -0.5749 |
| 18 | 3.16 | .. | H(21F)a | [1-x,1-y,-z | = | 3665.02] | | 78.22 | -47.66 | 0.66240 | 0.35920 | -0.13040 | 8.7526 | 4.8228 | -2.7974 |
| 19 | 3.17 | .. | H(11C)b | [1/2+x,1/2-y,-1/2+z | = | 4554.01] | | -42.79 | -38.59 | 0.77720 | 0.07860 | -0.11370 | 10.1372 | 1.0553 | -2.4391 |
| 20 | 3.21 | .. | H(22G) | [| = | 02] | | 102.07 | 15.39 | 0.61610 | 0.42940 | 0.01820 | 7.6712 | 5.7653 | 0.3904 |
| 21 | 3.34 | .. | H(21C)a | [1-x,1-y,-z | = | 3665.02] | | 162.04 | -50.67 | 0.46430 | 0.25260 | -0.14190 | 6.3051 | 3.3915 | -3.0441 |
| 22 | 3.35 | .. | H(19A) | | | | Intra | 137.61 | 57.87 | 0.58760 | 0.29350 | 0.11080 | 7.0017 | 3.9407 | 2.3769 |
| 23 | 3.54 | .. | H(11B)b | [1/2+x,1/2-y,-1/2+z | = | 4554.01] | | -7.42 | -43.01 | 0.83140 | 0.17910 | -0.13410 | 10.8862 | 2.4047 | -2.8768 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(14B)

| | | | | | | | |
|-------------------|-----------|-------------------|-----------|-------------------|-----------|-------------------|-----------|
| C(181) , >F(14A) | 70.6(16) | C(181) , >F(16A) | 54.3(11) | C(181) , <F(15B) | 36.1(10) | C(181) , <F(16B) | 36.4(11) |
| C(181) , C(18) | 38.7(10) | C(181) , >F(15A) | 23.1(8) | C(181) , C(212)a | 158(2) | C(181) , C(17) | 55.1(13) |
| C(181) , C(19) | 45.2(10) | C(181) , C(211)a | 131(2) | C(181) , C(112)b | 110.4(17) | C(181) , C(111)b | 125.7(17) |
| >F(14A) , >F(16A) | 118(2) | >F(14A) , <F(15B) | 39.4(14) | >F(14A) , <F(16B) | 100(2) | >F(14A) , C(18) | 81(2) |
| >F(14A) , >F(15A) | 58.5(14) | >F(14A) , C(212)a | 121(2) | >F(14A) , C(17) | 106(2) | >F(14A) , C(19) | 61.5(19) |
| >F(14A) , C(211)a | 124(2) | >F(14A) , C(112)b | 87(2) | >F(14A) , C(111)b | 109(3) | >F(16A) , <F(15B) | 78.4(13) |
| >F(16A) , <F(16B) | 18.8(9) | >F(16A) , C(18) | 74.0(14) | >F(16A) , >F(15A) | 59.5(9) | >F(16A) , C(212)a | 120.8(13) |
| >F(16A) , C(17) | 65.4(14) | >F(16A) , C(19) | 92.4(14) | >F(16A) , C(211)a | 114.2(15) | >F(16A) , C(112)b | 87.4(15) |
| >F(16A) , C(111)b | 84.8(13) | <F(15B) , <F(16B) | 60.3(13) | <F(15B) , C(18) | 65.2(10) | <F(15B) , >F(15A) | 19.2(8) |
| <F(15B) , C(212)a | 160.4(15) | <F(15B) , C(17) | 88.2(12) | <F(15B) , C(19) | 57.2(9) | <F(15B) , C(211)a | 152.6(15) |
| <F(15B) , C(112)b | 87.3(13) | <F(15B) , C(111)b | 110.5(14) | <F(16B) , C(18) | 63.4(12) | <F(16B) , >F(15A) | 41.1(10) |
| <F(16B) , C(212)a | 139.3(15) | <F(16B) , C(17) | 63.2(13) | <F(16B) , C(19) | 78.3(12) | <F(16B) , C(211)a | 127.8(17) |
| <F(16B) , C(112)b | 91.5(14) | <F(16B) , C(111)b | 96.1(13) | C(18) , >F(15A) | 60.1(7) | C(18) , C(212)a | 121.2(13) |
| C(18) , C(17) | 25.9(4) | C(18) , C(19) | 21.6(3) | C(18) , C(211)a | 93.9(11) | C(18) , C(112)b | 149.1(11) |

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C(18) , C(111)b 158.8(11) >F(15A) , C(212)a 178.7(17) >F(15A) , C(17) 78.1(9) >F(15A) , C(19) 60.2(6)
>F(15A) , C(211)a 153.9(15) >F(15A) , C(112)b 89.2(10) >F(15A) , C(111)b 108.4(11) C(212)a, C(17) 103.2(10)
C(212)a, C(19) 120.9(11) C(212)a, C(211)a 27.4(3) C(212)a, C(112)b 89.6(8) C(212)a, C(111)b 70.4(6)
C(17) , C(19) 45.3(5) C(17) , C(211)a 76.6(8) C(17) , C(112)b 152.8(10) C(17) , C(111)b 141.2(9)
C(19) , C(211)a 96.8(9) C(19) , C(112)b 143.6(9) C(19) , C(111)b 167.6(10) C(211)a, C(112)b 116.5(8)
C(211)a, C(111)b 95.4(6) C(112)b, C(111)b 24.5(3)

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3.6 Angstrom Coordination Sphere Around Atom I = F(15) [ARU = 1555.01] 0.66490 0.09010 0.07190 8.1029 1.2097 1.5424

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------------|------------|-------|---------|--------|---------|----------|----------|---------|---------|---------|
| 1 | 1.338(11) | -- | C(181) | | Intra | 105.01 | -42.14 | 0.63320 | 0.16146 | 0.03006 | 7.8459 | 2.1678 | 0.6449 |
| 2 | 0.577(13) | << | >F(15A) | | Intra | 54.72 | 20.24 | 0.69230 | 0.12300 | 0.08120 | 8.4154 | 1.6515 | 1.7419 |
| 3 | 1.856(13) | << | >F(16A) | | Intra | 158.99 | -85.02 | 0.62980 | 0.09440 | -0.01430 | 7.9526 | 1.2675 | -0.3068 |
| 4 | 2.131(15) | << | <F(16) | | Intra | 114.61 | -79.66 | 0.62600 | 0.11600 | -0.02580 | 7.9436 | 1.5575 | -0.5535 |
| 5 | 2.136(17) | << | <F(14) | | Intra | 69.07 | -22.68 | 0.71070 | 0.22720 | 0.03350 | 8.8070 | 3.0505 | 0.7187 |
| 6 | 2.310(12) | << | C(18) | | Intra | 137.91 | -17.12 | 0.52587 | 0.20032 | 0.04020 | 6.4647 | 2.6896 | 0.8624 |
| 7 | 2.405(14) | << | >F(14A) | | Intra | 74.14 | -30.98 | 0.69430 | 0.23780 | 0.01420 | 8.6661 | 3.1928 | 0.3046 |
| 8 | 3.057(12) | .< | C(19) | | Intra | 127.18 | 6.01 | 0.52253 | 0.27050 | 0.08683 | 6.2658 | 3.6319 | 1.8627 |
| 9 | 3.213(12) | .. | C(17) | | Intra | 159.28 | -26.65 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 10 | 3.06 | .. | H(19A) | | Intra | 111.96 | 15.82 | 0.58760 | 0.29350 | 0.11080 | 7.0017 | 3.9407 | 2.3769 |
| 11 | 3.15 | .. | H(17A)b[1-x,-y,-z | = 3655.01] | | -111.70 | -17.91 | 0.56460 | -0.11710 | 0.02680 | 6.9959 | -1.5722 | 0.5749 |
| 12 | 3.33 | .. | H(17A) | | Intra | 171.90 | -39.44 | 0.43540 | 0.11710 | -0.02680 | 5.5548 | 1.5722 | -0.5749 |
| 13 | 3.38 | .. | H(12G)a[3/2-x,-1/2+y,1/2-z | = 2645.01] | | 32.97 | 34.38 | 0.87530 | 0.20320 | 0.16090 | 10.4439 | 2.7283 | 3.4517 |
| 14 | 3.58 | .. | H(12D)a[3/2-x,-1/2+y,1/2-z | = 2645.01] | | 2.03 | 10.01 | 0.95330 | 0.09940 | 0.10090 | 11.6248 | 1.3346 | 2.1645 |
| 15 | 3.60 | .. | H(29A) [| = 02] | | 146.86 | 49.99 | 0.54500 | 0.18430 | 0.20040 | 6.1654 | 2.4745 | 4.2991 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(15)

| | | | | | | | |
|-------------------|-----------|------------------|-----------|-------------------|-----------|------------------|-----------|
| C(181) , >F(15A) | 77.7(13) | C(181) , >F(16A) | 45.1(5) | C(181) , <F(16) | 37.7(5) | C(181) , <F(14) | 35.7(5) |
| C(181) , C(18) | 37.6(4) | C(181) , >F(14A) | 27.0(4) | C(181) , C(19) | 52.2(4) | C(181) , C(17) | 46.5(4) |
| >F(15A) , >F(16A) | 111.4(14) | >F(15A) , <F(16) | 104.8(14) | >F(15A) , <F(14) | 45.2(12) | >F(15A) , C(18) | 89.7(13) |
| >F(15A) , >F(14A) | 54.5(12) | >F(15A) , C(19) | 71.5(13) | >F(15A) , C(17) | 111.5(14) | >F(16A) , <F(16) | 7.6(5) |
| >F(16A) , <F(14) | 67.4(6) | >F(16A) , C(18) | 68.3(6) | >F(16A) , >F(14A) | 58.7(5) | >F(16A) , C(19) | 91.8(6) |
| >F(16A) , C(17) | 58.4(6) | <F(16) , <F(14) | 60.3(6) | <F(16) , C(18) | 63.4(7) | <F(16) , >F(14A) | 51.4(5) |
| <F(16) , C(19) | 85.9(6) | <F(16) , C(17) | 56.3(7) | <F(14) , C(18) | 64.4(5) | <F(14) , >F(14A) | 9.5(4) |
| <F(14) , C(19) | 63.6(5) | <F(14) , C(17) | 80.2(5) | C(18) , >F(14A) | 59.1(3) | C(18) , C(19) | 25.45(14) |
| C(18) , C(17) | 21.96(14) | >F(14A) , C(19) | 62.7(3) | >F(14A) , C(17) | 72.8(4) | C(19) , C(17) | 45.10(18) |

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3.6 Angstrom Coordination Sphere Around Atom I = F(15B) [ARU = 1555.01] 0.71380 0.18000 0.07510 8.7058 2.4168 1.6111

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|---------|----|---------|----------------------------------|-----------|--------|-------|---------|--------|---------|---------|----------|---------|--------|---------|
| 1 | 1.32(2) | -- | C(181) | | | | Intra | -163.86 | -47.18 | 0.63320 | 0.16146 | 0.03006 | 7.8459 | 2.1678 | 0.6449 |
| 2 | 0.83(3) | << | >F(15A) | | | | Intra | -110.78 | 9.08 | 0.69230 | 0.12300 | 0.08120 | 8.4154 | 1.6515 | 1.7419 |
| 3 | 1.52(3) | << | >F(14A) | | | | Intra | 92.93 | -59.26 | 0.69430 | 0.23780 | 0.01420 | 8.6661 | 3.1928 | 0.3046 |
| 4 | 2.13(3) | << | <F(14B) | | | | Intra | 140.26 | -76.33 | 0.65700 | 0.20400 | -0.02150 | 8.3182 | 2.7390 | -0.4612 |
| 5 | 2.14(4) | << | <F(16B) | | | | Intra | -119.48 | -33.50 | 0.62900 | 0.06420 | 0.02000 | 7.8271 | 0.8620 | 0.4290 |
| 6 | 2.36(3) | << | >F(16A) | | | | Intra | -123.24 | -54.38 | 0.62980 | 0.09440 | -0.01430 | 7.9526 | 1.2675 | -0.3068 |
| 7 | 2.38(2) | << | C(18) | | | | Intra | 173.06 | -18.35 | 0.52587 | 0.20032 | 0.04020 | 6.4647 | 2.6896 | 0.8624 |
| 8 | 2.74(2) | << | C(19) | | | | Intra | 153.53 | 5.27 | 0.52253 | 0.27050 | 0.08683 | 6.2658 | 3.6319 | 1.8627 |
| 9 | 3.05(2) | .< | C(122)a | [3/2-x, -1/2+y, 1/2-z = 2645.01] | | | | 13.83 | 29.13 | 0.93880 | 0.22750 | 0.14440 | 11.2964 | 3.0545 | 3.0977 |
| 10 | 2.41 | << | H(19A) | | | | Intra | 138.20 | 18.52 | 0.58760 | 0.29350 | 0.11080 | 7.0017 | 3.9407 | 2.3769 |
| 11 | 2.55 | .< | H(12G)a | [3/2-x, -1/2+y, 1/2-z = 2645.01] | | | | 10.16 | 46.19 | 0.87530 | 0.20320 | 0.16090 | 10.4439 | 2.7283 | 3.4517 |
| 12 | 2.79 | .. | H(12E)a | [3/2-x, -1/2+y, 1/2-z = 2645.01] | | | | 25.96 | 14.31 | 0.91580 | 0.26800 | 0.10720 | 11.1330 | 3.5983 | 2.2997 |
| 13 | 3.04 | .. | H(11D)b | [1/2+x, 1/2-y, -1/2+z = 4554.01] | | | | -1.58 | -46.52 | 0.85280 | 0.17570 | -0.02770 | 10.7965 | 2.3590 | -0.5942 |
| 14 | 3.16 | .. | H(12D)a | [3/2-x, -1/2+y, 1/2-z = 2645.01] | | | | -20.34 | 10.08 | 0.95330 | 0.09940 | 0.10090 | 11.6248 | 1.3346 | 2.1645 |
| 15 | 3.41 | .. | H(22C) | [= 02] | | | | 84.57 | 12.43 | 0.74810 | 0.42690 | 0.10930 | 9.0212 | 5.7318 | 2.3447 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(15B)

| | | | | | | | |
|-------------------|-----------|-------------------|-----------|-------------------|-----------|-------------------|-----------|
| C(181) , >F(15A) | 73.3(18) | C(181) , >F(14A) | 56.6(10) | C(181) , <F(14B) | 36.6(12) | C(181) , <F(16B) | 35.9(10) |
| C(181) , >F(16A) | 26.3(7) | C(181) , C(18) | 34.5(7) | C(181) , C(19) | 64.5(10) | C(181) , C(122)a | 161.9(15) |
| >F(15A) , >F(14A) | 127(2) | >F(15A) , <F(14B) | 103(2) | >F(15A) , <F(16B) | 43.4(16) | >F(15A) , >F(16A) | 64.3(16) |
| >F(15A) , C(18) | 80.0(17) | >F(15A) , C(19) | 94.8(18) | >F(15A) , C(122)a | 114.4(19) | >F(14A) , <F(14B) | 23.5(9) |
| >F(14A) , <F(16B) | 83.4(13) | >F(14A) , >F(16A) | 62.7(9) | >F(14A) , C(18) | 69.3(10) | >F(14A) , C(19) | 80.2(11) |
| >F(14A) , C(122)a | 109.5(12) | <F(14B) , <F(16B) | 59.9(12) | <F(14B) , >F(16A) | 39.3(9) | <F(14B) , C(18) | 60.4(12) |
| <F(14B) , C(19) | 82.0(12) | <F(14B) , C(122)a | 126.6(14) | <F(16B) , >F(16A) | 21.1(8) | <F(16B) , C(18) | 61.5(11) |
| <F(16B) , C(19) | 90.4(12) | <F(16B) , C(122)a | 140.2(14) | >F(16A) , C(18) | 60.0(7) | >F(16A) , C(19) | 90.4(9) |
| >F(16A) , C(122)a | 140.2(11) | C(18) , C(19) | 30.5(3) | C(18) , C(122)a | 158.2(11) | C(19) , C(122)a | 128.2(9) |

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3.6 Angstrom Coordination Sphere Around Atom I = F(16) [ARU = 1555.01] 0.62600 0.11600 -0.02580 7.9436 1.5575 -0.5535

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|---------------------|------------|--------|-------|---------|--------|---------|----------|----------|---------|---------|---------|
| 1 | 1.348(12) | -- | C(181) | | | | Intra | 99.10 | 62.71 | 0.63320 | 0.16146 | 0.03006 | 7.8459 | 2.1678 | 0.6449 |
| 2 | 0.381(16) | << | >F(16A) | | | | Intra | -88.23 | 40.37 | 0.62980 | 0.09440 | -0.01430 | 7.9526 | 1.2675 | -0.3068 |
| 3 | 1.983(18) | << | >F(14A) | | | | Intra | 66.16 | 25.64 | 0.69430 | 0.23780 | 0.01420 | 8.6661 | 3.1928 | 0.3046 |
| 4 | 2.131(15) | << | <F(15) | | | | Intra | -65.39 | 79.66 | 0.66490 | 0.09010 | 0.07190 | 8.1029 | 1.2097 | 1.5424 |
| 5 | 2.14(2) | << | <F(14) | | | | Intra | 59.96 | 36.41 | 0.71070 | 0.22720 | 0.03350 | 8.8070 | 3.0505 | 0.7187 |
| 6 | 2.340(19) | << | C(18) | | | | Intra | 142.57 | 37.24 | 0.52587 | 0.20032 | 0.04020 | 6.4647 | 2.6896 | 0.8624 |
| 7 | 2.345(13) | << | >F(15A) | | | | Intra | 11.27 | 78.16 | 0.69230 | 0.12300 | 0.08120 | 8.4154 | 1.6515 | 1.7419 |
| 8 | 2.69(2) | << | C(17) | | | | Intra | 165.19 | 14.07 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 9 | 3.511(13) | .. | C(212)a | [1-x,1-y,-z | = 3665.02] | | | 82.42 | -45.23 | 0.62080 | 0.29852 | -0.14199 | 8.2696 | 4.0081 | -3.0460 |
| 10 | 3.52(3) | .. | C(112)c | [1/2+x,1/2-y,-1/2+z | = 4554.01] | | | 3.16 | -7.85 | 0.89740 | 0.13030 | -0.04821 | 11.4253 | 1.7495 | -1.0342 |
| 11 | 3.59(2) | .. | C(111)c | [1/2+x,1/2-y,-1/2+z | = 4554.01] | | | -0.48 | -31.44 | 0.84650 | 0.11410 | -0.11303 | 11.0047 | 1.5320 | -2.4248 |
| 12 | 3.600(16) | .. | C(19) | | | | Intra | 128.97 | 42.16 | 0.52253 | 0.27050 | 0.08683 | 6.2658 | 3.6319 | 1.8627 |
| 13 | 2.39 | << | H(17A) | | | | Intra | 179.65 | -0.51 | 0.43540 | 0.11710 | -0.02680 | 5.5548 | 1.5722 | -0.5749 |
| 14 | 2.63 | < | H(21D)a | [1-x,1-y,-z | = 3665.02] | | | 70.90 | -46.29 | 0.64960 | 0.24390 | -0.11440 | 8.5381 | 3.2747 | -2.4542 |
| 15 | 2.94 | .. | H(11C)c | [1/2+x,1/2-y,-1/2+z | = 4554.01] | | | -12.89 | -39.96 | 0.77720 | 0.07860 | -0.11370 | 10.1372 | 1.0553 | -2.4391 |
| 16 | 2.96 | .. | H(11D)c | [1/2+x,1/2-y,-1/2+z | = 4554.01] | | | 15.69 | -0.79 | 0.85280 | 0.17570 | -0.02770 | 10.7965 | 2.3590 | -0.5942 |
| 17 | 3.46 | .. | H(17A)b | [1-x,-y,-z | = 3655.01] | | | -106.85 | 19.04 | 0.56460 | -0.11710 | 0.02680 | 6.9959 | -1.5722 | 0.5749 |
| 18 | 3.50 | .. | H(21C)a | [1-x,1-y,-z | = 3665.02] | | | 131.78 | -45.36 | 0.46430 | 0.25260 | -0.14190 | 6.3051 | 3.3915 | -3.0441 |
| 19 | 3.56 | .. | H(11E)c | [1/2+x,1/2-y,-1/2+z | = 4554.01] | | | -10.77 | -0.07 | 0.90440 | 0.06650 | -0.02600 | 11.4384 | 0.8929 | -0.5578 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(16)

| | | | | | | | |
|-------------------|-----------|-------------------|-----------|-------------------|-----------|-------------------|-----------|
| C(181) , >F(16A) | 77(2) | C(181) , >F(14A) | 43.0(5) | C(181) , <F(15) | 37.4(4) | C(181) , <F(14) | 35.5(6) |
| C(181) , C(18) | 36.6(6) | C(181) , >F(15A) | 29.2(4) | C(181) , C(17) | 66.7(9) | C(181) , C(212)a | 108.8(8) |
| C(181) , C(112)c | 99.7(11) | C(181) , C(111)c | 121.9(12) | C(181) , C(19) | 27.0(7) | >F(16A) , >F(14A) | 110(3) |
| >F(16A) , <F(15) | 40(2) | >F(16A) , <F(14) | 98(3) | >F(16A) , C(18) | 90(3) | >F(16A) , >F(15A) | 53(2) |
| >F(16A) , C(17) | 93(4) | >F(16A) , C(212)a | 172(4) | >F(16A) , C(112)c | 96(5) | >F(16A) , C(111)c | 108(4) |
| >F(16A) , C(19) | 91(3) | >F(14A) , <F(15) | 71.4(6) | >F(14A) , <F(14) | 12.0(4) | >F(14A) , C(18) | 64.5(5) |
| >F(14A) , >F(15A) | 58.0(5) | >F(14A) , C(17) | 91.8(7) | >F(14A) , C(212)a | 72.4(5) | >F(14A) , C(112)c | 69.7(7) |
| >F(14A) , C(111)c | 85.5(8) | >F(14A) , C(19) | 53.4(5) | <F(15) , <F(14) | 60.0(6) | <F(15) , C(18) | 62.0(5) |
| <F(15) , >F(15A) | 13.8(4) | <F(15) , C(17) | 82.6(7) | <F(15) , C(212)a | 143.7(7) | <F(15) , C(112)c | 94.0(8) |
| <F(15) , C(111)c | 116.6(10) | <F(15) , C(19) | 57.9(5) | <F(14) , C(18) | 63.8(5) | <F(14) , >F(15A) | 46.4(5) |
| <F(14) , C(17) | 93.5(7) | <F(14) , C(212)a | 84.1(6) | <F(14) , C(112)c | 69.2(8) | <F(14) , C(111)c | 88.3(8) |
| <F(14) , C(19) | 52.3(5) | C(18) , >F(15A) | 61.0(4) | C(18) , C(17) | 30.7(3) | C(18) , C(212)a | 98.7(5) |
| C(18) , C(112)c | 133.0(7) | C(18) , C(111)c | 149.1(7) | C(18) , C(19) | 11.54(17) | >F(15A) , C(17) | 86.6(6) |
| >F(15A) , C(212)a | 130.4(6) | >F(15A) , C(112)c | 86.1(7) | >F(15A) , C(111)c | 109.8(8) | >F(15A) , C(19) | 54.1(3) |
| C(17) , C(212)a | 95.0(5) | C(17) , C(112)c | 161.3(6) | C(17) , C(111)c | 158.2(5) | C(17) , C(19) | 42.0(2) |
| C(212)a , C(112)c | 76.9(4) | C(212)a , C(111)c | 63.6(3) | C(212)a , C(19) | 96.8(4) | C(112)c , C(111)c | 23.83(17) |
| C(112)c , C(19) | 121.4(5) | C(111)c , C(19) | 138.8(5) | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(16B) [ARU = 1555.01] 0.62900 0.06420 0.02000 7.8271 0.8620 0.4290

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|---------------------|-----------|----------|-------|---------|--------|---------|----------|----------|---------|---------|---------|
| 1 | 1.324(16) | -- | C(181) | | | | Intra | 89.17 | 9.38 | 0.63320 | 0.16146 | 0.03006 | 7.8459 | 2.1678 | 0.6449 |
| 2 | 0.85(3) | << | >F(16A) | | | | Intra | 72.80 | -60.02 | 0.62980 | 0.09440 | -0.01430 | 7.9526 | 1.2675 | -0.3068 |
| 3 | 1.64(3) | << | >F(15A) | | | | Intra | 53.30 | 53.13 | 0.69230 | 0.12300 | 0.08120 | 8.4154 | 1.6515 | 1.7419 |
| 4 | 2.14(3) | << | <F(14B) | | | | Intra | 75.34 | -24.65 | 0.65700 | 0.20400 | -0.02150 | 8.3182 | 2.7390 | -0.4612 |
| 5 | 2.14(4) | << | <F(15B) | | | | Intra | 60.52 | 33.50 | 0.71380 | 0.18000 | 0.07510 | 8.7058 | 2.4168 | 1.6111 |
| 6 | 2.32(3) | << | C(18) | | | | Intra | 126.70 | 10.76 | 0.52587 | 0.20032 | 0.04020 | 6.4647 | 2.6896 | 0.8624 |
| 7 | 2.48(2) | << | >F(14A) | | | | Intra | 70.20 | -2.88 | 0.69430 | 0.23780 | 0.01420 | 8.6661 | 3.1928 | 0.3046 |
| 8 | 2.79(3) | << | C(17) | | | | Intra | 150.50 | -6.75 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 9 | 3.209(18) | .. | C(17)a | [1-x,-y,-z | = | 3655.01] | | -102.66 | -9.51 | 0.56710 | -0.16576 | -0.00472 | 7.1334 | -2.2256 | -0.1013 |
| 10 | 3.49(2) | .. | C(19) | | | | Intra | 119.41 | 24.27 | 0.52253 | 0.27050 | 0.08683 | 6.2658 | 3.6319 | 1.8627 |
| 11 | 3.57(2) | .. | C(161)a | [1-x,-y,-z | = | 3655.01] | | -61.29 | 0.73 | 0.76630 | -0.16920 | 0.02213 | 9.5431 | -2.2718 | 0.4747 |
| 12 | 2.58 | .< | H(17A)a | [1-x,-y,-z | = | 3655.01] | | -108.85 | 3.25 | 0.56460 | -0.11710 | 0.02680 | 6.9959 | -1.5722 | 0.5749 |
| 13 | 2.58 | .< | H(17A) | | | | Intra | 162.64 | -22.87 | 0.43540 | 0.11710 | -0.02680 | 5.5548 | 1.5722 | -0.5749 |
| 14 | 3.48 | .. | H(11D)b | [1/2+x,1/2-y,-1/2+z | = | 4554.01] | | 26.76 | -17.10 | 0.85280 | 0.17570 | -0.02770 | 10.7965 | 2.3590 | -0.5942 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(16B)

| | | | | | | | |
|-------------------|-----------|-------------------|-----------|-------------------|-----------|-------------------|-----------|
| C(181) , >F(16A) | 70.6(12) | C(181) , >F(15A) | 52.4(10) | C(181) , <F(14B) | 36.6(10) | C(181) , <F(15B) | 35.7(11) |
| C(181) , C(18) | 37.0(9) | C(181) , >F(14A) | 22.5(8) | C(181) , C(17) | 63.2(13) | C(181) , C(17)a | 168(2) |
| C(181) , C(19) | 32.4(11) | C(181) , C(161)a | 149(2) | >F(16A) , >F(15A) | 114(2) | >F(16A) , <F(14B) | 35.4(12) |
| >F(16A) , <F(15B) | 94.1(19) | >F(16A) , C(18) | 82.7(18) | >F(16A) , >F(14A) | 57.2(13) | >F(16A) , C(17) | 78(2) |
| >F(16A) , C(17)a | 110(2) | >F(16A) , C(19) | 92.5(16) | >F(16A) , C(161)a | 111(2) | >F(15A) , <F(14B) | 80.1(11) |
| >F(15A) , <F(15B) | 20.3(8) | >F(15A) , C(18) | 71.5(9) | >F(15A) , >F(14A) | 57.8(7) | >F(15A) , C(17) | 99.7(12) |
| >F(15A) , C(17)a | 132.3(13) | >F(15A) , C(19) | 56.6(8) | >F(15A) , C(161)a | 103.9(13) | <F(14B) , <F(15B) | 59.8(11) |
| <F(14B) , C(18) | 61.3(10) | <F(14B) , >F(14A) | 22.3(7) | <F(14B) , C(17) | 73.7(12) | <F(14B) , C(17)a | 145.8(15) |
| <F(14B) , C(19) | 64.9(10) | <F(14B) , C(161)a | 131.8(17) | <F(15B) , C(18) | 64.3(9) | <F(15B) , >F(14A) | 37.5(8) |
| <F(15B) , C(17) | 93.7(10) | <F(15B) , C(17)a | 151.5(14) | <F(15B) , C(19) | 51.7(8) | <F(15B) , C(161)a | 115.6(15) |
| C(18) , >F(14A) | 57.9(4) | C(18) , C(17) | 29.5(4) | C(18) , C(17)a | 131.4(14) | C(18) , C(19) | 15.2(3) |
| C(18) , C(161)a | 166.0(13) | >F(14A) , C(17) | 80.0(6) | >F(14A) , C(17)a | 165.7(14) | >F(14A) , C(19) | 55.0(5) |
| >F(14A) , C(161)a | 131.5(14) | C(17) , C(17)a | 105.3(11) | C(17) , C(19) | 43.4(4) | C(17) , C(161)a | 147.7(10) |
| C(17)a , C(19) | 137.3(12) | C(17)a , C(161)a | 42.4(2) | C(19) , C(161)a | 155.0(10) | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(21) [ARU = 1555.02] 0.49470 -0.05870 0.41640 4.8068 -0.7881 8.9328

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------------|------------|-------|---------|--------|---------|----------|---------|--------|---------|---------|
| 1 | 1.348(6) | -- | C(261) | | Intra | 107.96 | -7.90 | 0.45960 | 0.03587 | 0.40777 | 4.3953 | 0.4816 | 8.7476 |
| 2 | 2.120(11) | << | <F(23) | | Intra | 147.27 | -6.57 | 0.35050 | 0.02610 | 0.40510 | 3.0350 | 0.3504 | 8.6904 |
| 3 | 2.151(10) | << | <F(22) | | Intra | 94.06 | 23.33 | 0.49420 | 0.08800 | 0.45610 | 4.6669 | 1.1815 | 9.7844 |
| 4 | 2.346(7) | << | C(26) | | Intra | 87.22 | -38.89 | 0.48335 | 0.07712 | 0.34776 | 4.8955 | 1.0355 | 7.4603 |
| 5 | 2.779(10) | .< | <F(22)c [1-x,-y,1-z | = 3656.02] | | -126.39 | 79.87 | 0.50580 | -0.08800 | 0.54390 | 4.5168 | -1.1815 | 11.6679 |
| 6 | 2.780(8) | << | C(27) | | Intra | 79.65 | -68.30 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 7 | 3.320(7) | .. | C(122)a[x,-1+y,z | = 1545.01] | | -70.10 | -23.13 | 0.56120 | -0.27250 | 0.35560 | 5.8461 | -3.6587 | 7.6285 |
| 8 | 3.526(6) | .. | C(25) | | Intra | 81.44 | -25.46 | 0.51352 | 0.17580 | 0.34574 | 5.2809 | 2.3604 | 7.4169 |
| 9 | 2.55 | .< | H(27A) | | Intra | 124.95 | -87.35 | 0.45750 | -0.05150 | 0.29780 | 4.7392 | -0.6915 | 6.3885 |
| 10 | 2.67 | .< | H(12E)a[x,-1+y,z | = 1545.01] | | -62.67 | -10.94 | 0.58420 | -0.23200 | 0.39280 | 6.0096 | -3.1149 | 8.4265 |
| 11 | 3.11 | .. | H(12F)a[x,-1+y,z | = 1545.01] | | -75.73 | -39.61 | 0.51700 | -0.23180 | 0.32390 | 5.3981 | -3.1123 | 6.9484 |
| 12 | 3.37 | .. | H(22C)b[3/2-x,-1/2+y,1/2-z | = 2645.02] | | -3.34 | -9.43 | 0.75190 | -0.07310 | 0.39070 | 8.1214 | -0.9815 | 8.3814 |
| 13 | 3.41 | .. | H(22D)b[3/2-x,-1/2+y,1/2-z | = 2645.02] | | 24.16 | -6.57 | 0.73620 | 0.04460 | 0.39820 | 7.8991 | 0.5988 | 8.5423 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(21)

| | | | | | | | |
|------------------|----------|------------------|----------|------------------|-----------|-------------------|-----------|
| C(261) , <F(23) | 39.0(3) | C(261) , <F(22) | 34.1(3) | C(261) , C(26) | 36.2(2) | C(261) , <F(22)c | 103.7(5) |
| C(261) , C(27) | 63.3(3) | C(261) , C(122)a | 148.9(5) | C(261) , C(25) | 30.8(3) | <F(23) , <F(22) | 59.9(4) |
| <F(23) , C(26) | 62.8(3) | <F(23) , <F(22)c | 95.8(4) | <F(23) , C(27) | 75.8(3) | <F(23) , C(122)a | 132.9(4) |
| <F(23) , C(25) | 65.4(3) | <F(22) , C(26) | 62.6(2) | <F(22) , <F(22)c | 74.5(3) | <F(22) , C(27) | 92.3(3) |
| <F(22) , C(122)a | 165.5(5) | <F(22) , C(25) | 50.3(2) | C(26) , <F(22)c | 137.1(3) | C(26) , C(27) | 29.71(12) |
| C(26) , C(122)a | 114.4(3) | C(26) , C(25) | 14.28(9) | <F(22)c , C(27) | 166.7(3) | <F(22)c , C(122)a | 107.3(3) |
| <F(22)c , C(25) | 124.3(3) | C(27) , C(122)a | 85.9(2) | C(27) , C(25) | 42.86(10) | C(122)a , C(25) | 124.1(3) |

3.6 Angstrom Coordination Sphere Around Atom I = F(21A) [ARU = 1555.02] 0.44380 -0.06120 0.40910 4.1926 -0.8217 8.7762

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-------------------------------|----------------------|--------|-------|---------|--------|---------|----------|---------|--------|---------|---------|
| 1 | 1.319(10) | -- C(261) | | | Intra | 81.16 | -1.24 | 0.45960 | 0.03587 | 0.40777 | 4.3953 | 0.4816 | 8.7476 |
| 2 | 2.112(17) | << <F(23A) | | | Intra | 114.22 | 10.89 | 0.38100 | 0.07970 | 0.42770 | 3.3417 | 1.0701 | 9.1752 |
| 3 | 2.138(16) | << <F(22A) | | | Intra | 52.13 | 26.27 | 0.54940 | 0.05150 | 0.45320 | 5.3694 | 0.6915 | 9.7222 |
| 4 | 2.382(11) | << C(26) | | | Intra | 69.27 | -33.53 | 0.48335 | 0.07712 | 0.34776 | 4.8955 | 1.0355 | 7.4603 |
| 5 | 2.760(13) | << C(27) | | | Intra | 52.59 | -61.54 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 6 | 2.981(16) | .. <F(22A)c[1-x,-y,1-z | = 3656.02] | | | 161.00 | 82.29 | 0.45060 | -0.05150 | 0.54680 | 3.8143 | -0.6915 | 11.7302 |
| 7 | 3.479(12) | .. C(122)a[x,-1+y,z | = 1545.01] | | | -59.76 | -19.26 | 0.56120 | -0.27250 | 0.35560 | 5.8461 | -3.6587 | 7.6285 |
| 8 | 2.45 | << H(27A) | | | Intra | 13.40 | -76.76 | 0.45750 | -0.05150 | 0.29780 | 4.7392 | -0.6915 | 6.3885 |
| 9 | 2.95 | .. H(12E)a[x,-1+y,z | = 1545.01] | | | -51.61 | -6.82 | 0.58420 | -0.23200 | 0.39280 | 6.0096 | -3.1149 | 8.4265 |
| 10 | 3.17 | .. H(12F)a[x,-1+y,z | = 1545.01] | | | -62.24 | -35.23 | 0.51700 | -0.23180 | 0.32390 | 5.3981 | -3.1123 | 6.9484 |
| 11 | 3.29 | .. H(15A)b[1/2-x,-1/2+y,1/2-z | = 2545.01] | | | -144.81 | 8.25 | 0.23780 | -0.20090 | 0.43110 | 1.5330 | -2.6974 | 9.2481 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(21A)

| | | | | | | | |
|--------------------|----------|--------------------|----------|-------------------|----------|-----------------|-----------|
| C(261) , <F(23A) | 35.0(5) | C(261) , <F(22A) | 39.3(5) | C(261) , C(26) | 34.2(4) | C(261) , C(27) | 64.1(5) |
| C(261) , <F(22A)c | 89.9(6) | C(261) , C(122)a | 136.5(9) | <F(23A) , <F(22A) | 60.3(5) | <F(23A) , C(26) | 61.6(4) |
| <F(23A) , C(27) | 86.8(5) | <F(23A) , <F(22A)c | 73.9(5) | <F(23A) , C(122)a | 169.8(6) | <F(22A) , C(26) | 62.0(4) |
| <F(22A) , C(27) | 87.8(5) | <F(22A) , <F(22A)c | 66.5(4) | <F(22A) , C(122)a | 117.5(7) | C(26) , C(27) | 29.99(17) |
| C(26) , <F(22A)c | 123.4(5) | C(26) , C(122)a | 108.3(5) | C(27) , <F(22A)c | 153.1(5) | C(27) , C(122)a | 83.2(3) |
| <F(22A)c , C(122)a | 115.0(4) | | | | | | |

=====

3.6 Angstrom Coordination Sphere Around Atom I = F(21B) [ARU = 1555.02] 0.37650 -0.02550 0.40250 3.3701 -0.3424 8.6346

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------|----------------------------------|-------|---------|--------|---------|----------|---------|--------|---------|---------|
| 1 | 1.320(14) | -- | C(261) | | Intra | 38.79 | 4.91 | 0.45960 | 0.03587 | 0.40777 | 4.3953 | 0.4816 | 8.7476 |
| 2 | 2.102(16) | << | <F(23B) | | Intra | 75.40 | 26.49 | 0.42600 | 0.11010 | 0.44620 | 3.8442 | 1.4783 | 9.5721 |
| 3 | 2.140(17) | << | <F(22B) | | Intra | 8.06 | 22.82 | 0.54250 | -0.00490 | 0.44120 | 5.3232 | -0.0658 | 9.4648 |
| 4 | 2.367(13) | << | C(26) | | Intra | 42.09 | -29.74 | 0.48335 | 0.07712 | 0.34776 | 4.8955 | 1.0355 | 7.4603 |
| 5 | 2.858(12) | << | C(27) | | Intra | 19.22 | -53.07 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 6 | 3.407(13) | .. | C(13)a | [1/2-x, -1/2+y, 1/2-z = 2545.01] | | -156.68 | -33.79 | 0.14566 | -0.10897 | 0.31418 | 0.7703 | -1.4631 | 6.7399 |
| 7 | 3.413(15) | .. | <F(22B)c | [1-x, -y, 1-z = 3656.02] | | 39.77 | 79.23 | 0.45750 | 0.00490 | 0.55880 | 3.8605 | 0.0658 | 11.9876 |
| 8 | 3.458(13) | .. | S(1)a | [1/2-x, -1/2+y, 1/2-z = 2545.01] | | -122.12 | -38.51 | 0.23496 | -0.19619 | 0.30214 | 1.9316 | -2.6341 | 6.4816 |
| 9 | 3.527(13) | .. | C(25) | | Intra | 54.74 | -20.20 | 0.51352 | 0.17580 | 0.34574 | 5.2809 | 2.3604 | 7.4169 |
| 10 | 2.65 | .< | H(27A) | | Intra | -14.30 | -57.83 | 0.45750 | -0.05150 | 0.29780 | 4.7392 | -0.6915 | 6.3885 |
| 11 | 3.05 | .. | H(15A)a | [1/2-x, -1/2+y, 1/2-z = 2545.01] | | -127.96 | 11.61 | 0.23780 | -0.20090 | 0.43110 | 1.5330 | -2.6974 | 9.2481 |
| 12 | 3.17 | .. | H(22E)d | [-1/2+x, 1/2-y, 1/2+z = 4455.02] | | 158.78 | 43.23 | 0.23200 | 0.03680 | 0.50380 | 1.2155 | 0.4941 | 10.8077 |
| 13 | 3.48 | .. | H(21F)b | [1/2-x, -1/2+y, 1/2-z = 2545.02] | | 139.09 | -11.70 | 0.16240 | 0.14080 | 0.36960 | 0.7938 | 1.8905 | 7.9288 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(21B)

| | | | | | | | |
|--------------------|----------|-------------------|-----------|--------------------|----------|------------------|-----------|
| C(261) , <F(23B) | 41.1(5) | C(261) , <F(22B) | 34.7(6) | C(261) , C(26) | 34.8(3) | C(261) , C(27) | 60.3(5) |
| C(261) , C(13)a | 147.7(7) | C(261) , <F(22B)c | 74.3(5) | C(261) , S(1)a | 142.2(7) | C(261) , C(25) | 29.6(4) |
| <F(23B) , <F(22B) | 60.6(7) | <F(23B) , C(26) | 64.7(5) | <F(23B) , C(27) | 93.3(6) | <F(23B) , C(13)a | 134.8(6) |
| <F(23B) , <F(22B)c | 55.0(5) | <F(23B) , S(1)a | 161.0(6) | <F(23B) , C(25) | 50.8(4) | <F(22B) , C(26) | 61.9(5) |
| <F(22B) , C(27) | 76.5(5) | <F(22B) , C(13)a | 162.7(7) | <F(22B) , <F(22B)c | 58.2(4) | <F(22B) , S(1)a | 135.0(7) |
| <F(22B) , C(25) | 62.6(5) | C(26) , C(27) | 28.70(15) | C(26) , C(13)a | 114.0(4) | C(26) , <F(22B)c | 109.0(5) |
| C(26) , S(1)a | 110.2(4) | C(26) , C(25) | 14.90(14) | C(27) , C(13)a | 93.1(3) | C(27) , <F(22B)c | 132.9(5) |
| C(27) , S(1)a | 82.5(3) | C(27) , C(25) | 42.70(19) | C(13)a , <F(22B)c | 134.1(4) | C(13)a , S(1)a | 28.14(11) |
| C(13)a , C(25) | 118.3(3) | <F(22B)c , S(1)a | 138.7(5) | <F(22B)c , C(25) | 99.8(4) | S(1)a , C(25) | 121.2(3) |

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3.6 Angstrom Coordination Sphere Around Atom I = F(22) [ARU = 1555.02] 0.49420 0.08800 0.45610 4.6669 1.1815 9.7844

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|------------|--------------------------------|--------|-------|---------|--------|---------|----------|---------|--------|---------|---------|
| 1 | 1.280(7) | -- C(261) | | | Intra | -111.20 | -54.09 | 0.45960 | 0.03587 | 0.40777 | 4.3953 | 0.4816 | 8.7476 |
| 2 | 2.133(13) | << <F(23) | | | Intra | -153.01 | -30.86 | 0.35050 | 0.02610 | 0.40510 | 3.0350 | 0.3504 | 8.6904 |
| 3 | 2.151(10) | << <F(21) | | | Intra | -85.94 | -23.33 | 0.49470 | -0.05870 | 0.41640 | 4.8068 | -0.7881 | 8.9328 |
| 4 | 2.340(5) | << C(26) | | | Intra | -32.58 | -83.34 | 0.48335 | 0.07712 | 0.34776 | 4.8955 | 1.0355 | 7.4603 |
| 5 | 2.715(6) | << C(25) | | | Intra | 62.48 | -60.69 | 0.51352 | 0.17580 | 0.34574 | 5.2809 | 2.3604 | 7.4169 |
| 6 | 2.779(10) | .< <F(21)b | [1-x,-y,1-z = 3656.02] | | | -126.39 | 79.87 | 0.50530 | 0.05870 | 0.58360 | 4.3769 | 0.7881 | 12.5196 |
| 7 | 3.026(10) | .. <F(22)b | [1-x,-y,1-z = 3656.02] | | | -93.63 | 38.50 | 0.50580 | -0.08800 | 0.54390 | 4.5168 | -1.1815 | 11.6679 |
| 8 | 3.363(6) | .. C(261)b | [1-x,-y,1-z = 3656.02] | | | -85.82 | 60.27 | 0.54040 | -0.03587 | 0.59223 | 4.7883 | -0.4816 | 12.7047 |
| 9 | 3.581(5) | .. C(27) | | | Intra | -71.30 | -73.58 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 10 | 2.40 | << H(25A) | | | Intra | 72.23 | -41.36 | 0.51820 | 0.21590 | 0.38210 | 5.2172 | 2.8988 | 8.1970 |
| 11 | 3.40 | .. H(11F) | [= 01] | | | 95.10 | -1.37 | 0.46910 | 0.34040 | 0.45230 | 4.3646 | 4.5704 | 9.7029 |
| 12 | 3.51 | .. H(22D)a | [3/2-x,-1/2+y,1/2-z = 2645.02] | | | -10.22 | -20.72 | 0.73620 | 0.04460 | 0.39820 | 7.8991 | 0.5988 | 8.5423 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(22)

| | | | | | | | |
|------------------|----------|-------------------|-----------|-------------------|-----------|-------------------|-----------|
| C(261) , <F(23) | 37.8(4) | C(261) , <F(21) | 36.1(3) | C(261) , C(26) | 35.1(2) | C(261) , C(25) | 65.1(3) |
| C(261) , <F(21)b | 134.3(6) | C(261) , <F(22)b | 93.8(4) | C(261) , C(261)b | 116.1(4) | C(261) , C(27) | 25.3(3) |
| <F(23) , <F(21) | 59.3(4) | <F(23) , C(26) | 62.7(2) | <F(23) , C(25) | 84.0(3) | <F(23) , <F(21)b | 111.7(5) |
| <F(23) , <F(22)b | 88.7(4) | <F(23) , C(261)b | 106.3(4) | <F(23) , C(27) | 58.2(2) | <F(21) , C(26) | 62.8(3) |
| <F(21) , C(25) | 92.2(3) | <F(21) , <F(21)b | 105.5(4) | <F(21) , <F(22)b | 62.3(3) | <F(21) , C(261)b | 83.6(3) |
| <F(21) , C(27) | 50.9(2) | C(26) , C(25) | 30.56(10) | C(26) , <F(21)b | 168.3(4) | C(26) , <F(22)b | 125.1(3) |
| C(26) , C(261)b | 145.9(3) | C(26) , C(27) | 11.96(9) | C(25) , <F(21)b | 160.6(4) | C(25) , <F(22)b | 153.3(4) |
| C(25) , C(261)b | 164.5(5) | C(25) , C(27) | 42.21(9) | <F(21)b , <F(22)b | 43.23(18) | <F(21)b , C(261)b | 22.91(14) |
| <F(21)b , C(27) | 156.3(3) | <F(22)b , C(261)b | 22.32(14) | <F(22)b , C(27) | 113.1(3) | C(261)b , C(27) | 134.2(3) |

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3.6 Angstrom Coordination Sphere Around Atom I = F(22A) [ARU = 1555.02] 0.54940 0.05150 0.45320 5.3694 0.6915 9.7222

| Nr | d(I,J) To | Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|--------|----------------------------|------------|-------|---------|--------|---------|----------|---------|--------|---------|---------|
| 1 | 1.394(9) | -- | C(261) | | Intra | -167.84 | -44.36 | 0.45960 | 0.03587 | 0.40777 | 4.3953 | 0.4816 | 8.7476 |
| 2 | 2.134(13) | << | <F(23A) | | Intra | 169.42 | -14.85 | 0.38100 | 0.07970 | 0.42770 | 3.3417 | 1.0701 | 9.1752 |
| 3 | 2.138(16) | << | <F(21A) | | Intra | -127.87 | -26.27 | 0.44380 | -0.06120 | 0.40910 | 4.1926 | -0.8217 | 8.7762 |
| 4 | 2.337(9) | << | C(26) | | Intra | 144.03 | -75.48 | 0.48335 | 0.07712 | 0.34776 | 4.8955 | 1.0355 | 7.4603 |
| 5 | 2.847(10) | << | C(25) | | Intra | 93.04 | -54.06 | 0.51352 | 0.17580 | 0.34574 | 5.2809 | 2.3604 | 7.4169 |
| 6 | 2.892(13) | <. | <F(22A)b[1-x,-y,1-z | = 3656.02] | | -138.35 | 43.97 | 0.45060 | -0.05150 | 0.54680 | 3.8143 | -0.6915 | 11.7302 |
| 7 | 2.981(16) | .. | <F(21A)b[1-x,-y,1-z | = 3656.02] | | 161.00 | 82.29 | 0.55620 | 0.06120 | 0.59090 | 4.9911 | 0.8217 | 12.6762 |
| 8 | 3.139(15) | .. | <F(23A)b[1-x,-y,1-z | = 3656.02] | | -74.98 | 54.48 | 0.61900 | -0.07970 | 0.57230 | 5.8419 | -1.0701 | 12.2772 |
| 9 | 3.257(9) | .. | C(261)b[1-x,-y,1-z | = 3656.02] | | -116.35 | 66.30 | 0.54040 | -0.03587 | 0.59223 | 4.7883 | -0.4816 | 12.7047 |
| 10 | 3.422(8) | .. | C(221)a[3/2-x,-1/2+y,1/2-z | = 2645.02] | | -14.80 | -17.15 | 0.78870 | -0.01070 | 0.40617 | 8.5312 | -0.1437 | 8.7133 |
| 11 | 3.426(9) | .. | C(27) | | Intra | -128.88 | -79.88 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 12 | 3.585(9) | .. | C(222)a[3/2-x,-1/2+y,1/2-z | = 2645.02] | | -15.44 | 7.31 | 0.82820 | -0.01900 | 0.47446 | 8.7970 | -0.2551 | 10.1783 |
| 13 | 2.69 | .. | H(25A) | | Intra | 93.94 | -34.58 | 0.51820 | 0.21590 | 0.38210 | 5.2172 | 2.8988 | 8.1970 |
| 14 | 2.79 | .. | H(22D)a[3/2-x,-1/2+y,1/2-z | = 2645.02] | | -2.10 | -24.99 | 0.73620 | 0.04460 | 0.39820 | 7.8991 | 0.5988 | 8.5423 |
| 15 | 3.00 | .. | H(22E)a[3/2-x,-1/2+y,1/2-z | = 2645.02] | | -24.52 | 17.90 | 0.76800 | -0.03680 | 0.49620 | 7.9682 | -0.4941 | 10.6447 |
| 16 | 3.49 | .. | H(22C)a[3/2-x,-1/2+y,1/2-z | = 2645.02] | | -31.30 | -22.60 | 0.75190 | -0.07310 | 0.39070 | 8.1214 | -0.9815 | 8.3814 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(22A)

| | | | | | | | |
|--------------------|-----------|---------------------|----------|---------------------|-----------|---------------------|-----------|
| C(261) , <F(23A) | 35.3(4) | C(261) , <F(21A) | 36.8(4) | C(261) , C(26) | 37.2(3) | C(261) , C(25) | 60.0(4) |
| C(261) , <F(22A)b | 92.2(4) | C(261) , <F(21A)b | 127.7(5) | C(261) , <F(23A)b | 126.1(6) | C(261) , C(261)b | 117.5(5) |
| C(261) , C(221)a | 113.8(5) | C(261) , C(27) | 38.2(3) | C(261) , C(222)a | 135.8(5) | <F(23A) , <F(21A) | 59.3(6) |
| <F(23A) , C(26) | 62.2(4) | <F(23A) , C(25) | 70.1(4) | <F(23A) , <F(22A)b | 75.6(4) | <F(23A) , <F(21A)b | 97.2(5) |
| <F(23A) , <F(23A)b | 116.8(5) | <F(23A) , C(261)b | 97.4(4) | <F(23A) , C(221)a | 147.7(5) | <F(23A) , C(27) | 70.6(4) |
| <F(23A) , C(222)a | 171.1(5) | <F(21A) , C(26) | 64.2(4) | <F(21A) , C(25) | 92.3(4) | <F(21A) , <F(22A)b | 70.9(5) |
| <F(21A) , <F(21A)b | 113.6(6) | <F(21A) , <F(23A)b | 92.6(5) | <F(21A) , C(261)b | 93.0(5) | <F(21A) , C(221)a | 101.9(5) |
| <F(21A) , C(27) | 53.6(4) | <F(21A) , C(222)a | 113.3(5) | C(26) , C(25) | 28.79(13) | C(26) , <F(22A)b | 129.3(4) |
| C(26) , <F(21A)b | 158.0(5) | C(26) , <F(23A)b | 154.3(5) | C(26) , C(261)b | 154.6(4) | C(26) , C(221)a | 86.4(2) |
| C(26) , C(27) | 17.21(11) | C(26) , C(222)a | 110.9(3) | C(25) , <F(22A)b | 145.7(3) | C(25) , <F(21A)b | 140.6(4) |
| C(25) , <F(23A)b | 173.0(4) | C(25) , C(261)b | 161.3(4) | C(25) , C(221)a | 86.2(2) | C(25) , C(27) | 43.93(13) |
| C(25) , C(222)a | 106.7(2) | <F(22A)b , <F(21A)b | 42.7(3) | <F(22A)b , <F(23A)b | 41.2(3) | <F(22A)b , C(261)b | 25.32(18) |
| <F(22A)b , C(221)a | 125.8(4) | <F(22A)b , C(27) | 124.0(3) | <F(22A)b , C(222)a | 107.4(3) | <F(21A)b , <F(23A)b | 40.3(3) |
| <F(21A)b , C(261)b | 23.9(2) | <F(21A)b , C(221)a | 114.8(4) | <F(21A)b , C(27) | 165.4(4) | <F(21A)b , C(222)a | 90.4(4) |
| <F(23A)b , C(261)b | 23.0(2) | <F(23A)b , C(221)a | 87.9(3) | <F(23A)b , C(27) | 137.8(4) | <F(23A)b , C(222)a | 66.7(3) |
| C(261)b , C(221)a | 110.3(3) | C(261)b , C(27) | 146.4(3) | C(261)b , C(222)a | 87.7(2) | C(221)a , C(27) | 77.19(19) |
| C(221)a , C(222)a | 24.46(9) | C(27) , C(222)a | 101.2(2) | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(22B) [ARU = 1555.02] 0.54250 -0.00490 0.44120 5.3232 -0.0658 9.4648

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------------------------|------------|-----------|--------|-------|---------|--------|---------|----------|---------|--------|---------|---------|
| 1 | 1.294(12) | -- | C(261) | | | | Intra | 149.46 | -33.65 | 0.45960 | 0.03587 | 0.40777 | 4.3953 | 0.4816 | 8.7476 |
| 2 | 2.140(17) | << | <F(21B) | | | | Intra | -171.94 | -22.82 | 0.37650 | -0.02550 | 0.40250 | 3.3701 | -0.3424 | 8.6346 |
| 3 | 2.141(18) | << | <F(23B) | | | | Intra | 133.77 | 2.87 | 0.42600 | 0.11010 | 0.44620 | 3.8442 | 1.4783 | 9.5721 |
| 4 | 2.327(13) | << | C(26) | | | | Intra | 111.23 | -59.49 | 0.48335 | 0.07712 | 0.34776 | 4.8955 | 1.0355 | 7.4603 |
| 5 | 2.798(17) | .< | <F(23B)c[1-x,-y,1-z | = | 3656.02] | | | -89.34 | 59.68 | 0.57400 | -0.11010 | 0.55380 | 5.3394 | -1.4783 | 11.8803 |
| 6 | 2.919(15) | .< | <F(22B)c[1-x,-y,1-z | = | 3656.02] | | | 174.86 | 59.79 | 0.45750 | 0.00490 | 0.55880 | 3.8605 | 0.0658 | 11.9876 |
| 7 | 3.146(11) | .< | C(27) | | | | Intra | 138.99 | -81.97 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 8 | 3.175(15) | .. | C(25) | | | | Intra | 91.00 | -40.16 | 0.51352 | 0.17580 | 0.34574 | 5.2809 | 2.3604 | 7.4169 |
| 9 | 3.296(11) | .. | C(221)b[3/2-x,-1/2+y,1/2-z | = | 2645.02] | | | -1.39 | -13.18 | 0.78870 | -0.01070 | 0.40617 | 8.5312 | -0.1437 | 8.7133 |
| 10 | 3.310(11) | .. | C(261)c[1-x,-y,1-z | = | 3656.02] | | | -142.14 | 78.19 | 0.54040 | -0.03587 | 0.59223 | 4.7883 | -0.4816 | 12.7047 |
| 11 | 3.413(15) | .. | <F(21B)c[1-x,-y,1-z | = | 3656.02] | | | 39.77 | 79.23 | 0.62350 | 0.02550 | 0.59750 | 5.8136 | 0.3424 | 12.8178 |
| 12 | 3.551(11) | .. | C(222)b[3/2-x,-1/2+y,1/2-z | = | 2645.02] | | | -3.12 | 11.59 | 0.82820 | -0.01900 | 0.47446 | 8.7970 | -0.2551 | 10.1783 |
| 13 | 2.82 | .. | H(22D)b[3/2-x,-1/2+y,1/2-z | = | 2645.02] | | | 14.47 | -19.12 | 0.73620 | 0.04460 | 0.39820 | 7.8991 | 0.5988 | 8.5423 |
| 14 | 2.93 | .. | H(22E)b[3/2-x,-1/2+y,1/2-z | = | 2645.02] | | | -9.20 | 23.77 | 0.76800 | -0.03680 | 0.49620 | 7.9682 | -0.4941 | 10.6447 |
| 15 | 3.14 | .. | H(22C)b[3/2-x,-1/2+y,1/2-z | = | 2645.02] | | | -18.12 | -20.20 | 0.75190 | -0.07310 | 0.39070 | 8.1214 | -0.9815 | 8.3814 |
| 16 | 3.19 | .. | H(27A) | | | | Intra | -133.03 | -74.45 | 0.45750 | -0.05150 | 0.29780 | 4.7392 | -0.6915 | 6.3885 |
| 17 | 3.23 | .. | H(25A) | | | | Intra | 92.05 | -23.14 | 0.51820 | 0.21590 | 0.38210 | 5.2172 | 2.8988 | 8.1970 |
| 18 | 3.29 | .. | H(12E)a[x,-1+y,z | = | 1545.01] | | | -77.31 | -18.38 | 0.58420 | -0.23200 | 0.39280 | 6.0096 | -3.1149 | 8.4265 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(22B)

| | | | | | | | |
|--------------------|-----------|---------------------|-----------|---------------------|-----------|---------------------|-----------|
| C(261) , <F(21B) | 35.5(5) | C(261) , <F(23B) | 39.4(5) | C(261) , C(26) | 36.0(4) | C(261) , <F(23B)c | 134.1(7) |
| C(261) , <F(22B)c | 95.8(6) | C(261) , C(27) | 48.5(4) | C(261) , C(25) | 46.4(5) | C(261) , C(221)b | 125.6(7) |
| C(261) , C(261)c | 118.7(6) | C(261) , <F(21B)c | 126.6(8) | C(261) , C(222)b | 146.6(8) | <F(21B) , <F(23B) | 58.8(6) |
| <F(21B) , C(26) | 63.9(4) | <F(21B) , <F(23B)c | 106.0(6) | <F(21B) , <F(22B)c | 83.3(5) | <F(21B) , C(27) | 62.1(4) |
| <F(21B) , C(25) | 80.6(5) | <F(21B) , C(221)b | 142.8(6) | <F(21B) , C(261)c | 102.5(5) | <F(21B) , <F(21B)c | 121.9(6) |
| <F(21B) , C(222)b | 164.5(7) | <F(23B) , C(26) | 64.8(5) | <F(23B) , <F(23B)c | 109.0(6) | <F(23B) , <F(22B)c | 65.0(5) |
| <F(23B) , C(27) | 84.9(5) | <F(23B) , C(25) | 58.1(5) | <F(23B) , C(221)b | 134.5(7) | <F(23B) , C(261)c | 86.0(5) |
| <F(23B) , <F(21B)c | 87.9(5) | <F(23B) , C(222)b | 134.8(7) | C(26) , <F(23B)c | 169.6(5) | C(26) , <F(22B)c | 129.1(6) |
| C(26) , C(27) | 23.67(14) | C(26) , C(25) | 23.11(19) | C(26) , C(221)b | 89.6(3) | C(26) , C(261)c | 150.8(6) |
| C(26) , <F(21B)c | 144.7(7) | C(26) , C(222)b | 112.2(4) | <F(23B)c , <F(22B)c | 43.9(4) | <F(23B)c , C(27) | 154.4(7) |
| <F(23B)c , C(25) | 160.5(6) | <F(23B)c , C(221)b | 100.3(4) | <F(23B)c , C(261)c | 24.9(2) | <F(23B)c , <F(21B)c | 38.0(3) |
| <F(23B)c , C(222)b | 78.1(4) | <F(22B)c , C(27) | 143.0(4) | <F(22B)c , C(25) | 121.1(6) | <F(22B)c , C(221)b | 133.3(4) |
| <F(22B)c , C(261)c | 22.9(3) | <F(22B)c , <F(21B)c | 38.5(3) | <F(22B)c , C(222)b | 108.6(4) | C(27) , C(25) | 44.76(18) |
| C(27) , C(221)b | 83.1(3) | C(27) , C(261)c | 164.5(4) | C(27) , <F(21B)c | 167.7(6) | C(27) , C(222)b | 107.9(3) |
| C(25) , C(221)b | 83.3(3) | C(25) , C(261)c | 136.5(5) | C(25) , <F(21B)c | 123.0(6) | C(25) , C(222)b | 100.6(3) |
| C(221)b , C(261)c | 112.2(3) | C(221)b , <F(21B)c | 95.0(4) | C(221)b , C(222)b | 24.83(10) | C(261)c , <F(21B)c | 22.6(2) |
| C(261)c , C(222)b | 87.4(3) | <F(21B)c , C(222)b | 70.6(3) | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(23) [ARU = 1555.02] 0.35050 0.02610 0.40510 3.0350 0.3504 8.6904

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------|----------------------------------|-------|---------|--------|---------|----------|---------|--------|---------|---------|
| 1 | 1.368(7) | -- | C(261) | | Intra | 5.51 | 2.40 | 0.45960 | 0.03587 | 0.40777 | 4.3953 | 0.4816 | 8.7476 |
| 2 | 2.120(11) | << | <F(21) | | Intra | -32.73 | 6.57 | 0.49470 | -0.05870 | 0.41640 | 4.8068 | -0.7881 | 8.9328 |
| 3 | 2.133(13) | << | <F(22) | | Intra | 26.99 | 30.86 | 0.49420 | 0.08800 | 0.45610 | 4.6669 | 1.1815 | 9.7844 |
| 4 | 2.333(7) | << | C(26) | | Intra | 20.21 | -31.82 | 0.48335 | 0.07712 | 0.34776 | 4.8955 | 1.0355 | 7.4603 |
| 5 | 3.053(7) | .< | C(27) | | Intra | -3.73 | -50.05 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 6 | 3.272(7) | .. | C(25) | | Intra | 41.83 | -22.90 | 0.51352 | 0.17580 | 0.34574 | 5.2809 | 2.3604 | 7.4169 |
| 7 | 3.496(7) | .. | C(13)a | [1/2-x, -1/2+y, 1/2-z = 2545.01] | | -141.31 | -33.91 | 0.14566 | -0.10897 | 0.31418 | 0.7703 | -1.4631 | 6.7399 |
| 8 | 3.575(7) | .. | N(12)a | [1/2-x, -1/2+y, 1/2-z = 2545.01] | | -164.12 | -47.41 | 0.13220 | -0.02319 | 0.28241 | 0.7083 | -0.3114 | 6.0584 |
| 9 | 2.80 | .. | H(22E)c | [-1/2+x, 1/2-y, 1/2+z = 4455.02] | | 175.49 | 49.24 | 0.23200 | 0.03680 | 0.50380 | 1.2155 | 0.4941 | 10.8077 |
| 10 | 2.82 | .. | H(21F)b | [1/2-x, -1/2+y, 1/2-z = 2545.02] | | 145.51 | -15.64 | 0.16240 | 0.14080 | 0.36960 | 0.7938 | 1.8905 | 7.9288 |
| 11 | 3.05 | .. | H(27A) | | Intra | -31.44 | -49.05 | 0.45750 | -0.05150 | 0.29780 | 4.7392 | -0.6915 | 6.3885 |
| 12 | 3.39 | .. | H(25A) | | Intra | 49.43 | -8.37 | 0.51820 | 0.21590 | 0.38210 | 5.2172 | 2.8988 | 8.1970 |
| 13 | 3.44 | .. | H(15A)a | [1/2-x, -1/2+y, 1/2-z = 2545.01] | | -116.23 | 9.32 | 0.23780 | -0.20090 | 0.43110 | 1.5330 | -2.6974 | 9.2481 |
| 14 | 3.46 | .. | H(12B)a | [1/2-x, -1/2+y, 1/2-z = 2545.01] | | 146.31 | -71.43 | 0.23650 | 0.07160 | 0.25230 | 2.1187 | 0.9613 | 5.4124 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(23)

| | | | | | | | |
|-----------------|-----------|-----------------|----------|-----------------|------------|-----------------|-----------|
| C(261) , <F(21) | 38.3(3) | C(261) , <F(22) | 35.0(3) | C(261) , C(26) | 37.0(2) | C(261) , C(27) | 53.1(2) |
| C(261) , C(25) | 43.5(3) | C(261) , C(13)a | 135.8(4) | C(261) , N(12)a | 134.1(4) | <F(21) , <F(22) | 60.7(4) |
| <F(21) , C(26) | 63.4(3) | <F(21) , C(27) | 61.9(3) | <F(21) , C(25) | 78.5(3) | <F(21) , C(13)a | 109.1(3) |
| <F(21) , N(12)a | 121.9(3) | <F(22) , C(26) | 63.0(3) | <F(22) , C(27) | 85.4(3) | <F(22) , C(25) | 55.6(2) |
| <F(22) , C(13)a | 169.7(4) | <F(22) , N(12)a | 161.4(3) | C(26) , C(27) | 25.47(10) | C(26) , C(25) | 21.11(10) |
| C(26) , C(13)a | 112.0(2) | C(26) , N(12)a | 100.7(2) | C(27) , C(25) | 44.56(11) | C(27) , C(13)a | 88.04(17) |
| C(27) , N(12)a | 81.08(15) | C(25) , C(13)a | 123.1(2) | C(25) , N(12)a | 105.90(18) | C(13)a , N(12)a | 21.81(6) |

3.6 Angstrom Coordination Sphere Around Atom I = F(23A) [ARU = 1555.02] 0.38100 0.07970 0.42770 3.3417 1.0701 9.1752

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-------------------------------|----------------------|--------|-------|---------|--------|---------|----------|---------|--------|---------|---------|
| 1 | 1.280(11) | -- C(261) | | | Intra | -29.19 | -19.51 | 0.45960 | 0.03587 | 0.40777 | 4.3953 | 0.4816 | 8.7476 |
| 2 | 2.112(17) | << <F(21A) | | | Intra | -65.78 | -10.89 | 0.44380 | -0.06120 | 0.40910 | 4.1926 | -0.8217 | 8.7762 |
| 3 | 2.134(13) | << <F(22A) | | | Intra | -10.58 | 14.85 | 0.54940 | 0.05150 | 0.45320 | 5.3694 | 0.6915 | 9.7222 |
| 4 | 2.314(11) | << C(26) | | | Intra | -1.28 | -47.82 | 0.48335 | 0.07712 | 0.34776 | 4.8955 | 1.0355 | 7.4603 |
| 5 | 2.918(11) | << C(25) | | | Intra | 33.64 | -37.05 | 0.51352 | 0.17580 | 0.34574 | 5.2809 | 2.3604 | 7.4169 |
| 6 | 3.139(15) | .. <F(22A)b[1-x,-y,1-z | = 3656.02] | | | -74.98 | 54.48 | 0.45060 | -0.05150 | 0.54680 | 3.8143 | -0.6915 | 11.7302 |
| 7 | 3.380(11) | .. C(27) | | | Intra | -27.19 | -56.72 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 8 | 2.74 | .. H(22E)c[-1/2+x,1/2-y,1/2+z | = 4455.02] | | | -164.84 | 36.54 | 0.23200 | 0.03680 | 0.50380 | 1.2155 | 0.4941 | 10.8077 |
| 9 | 2.80 | .. H(25A) | | | Intra | 44.28 | -20.48 | 0.51820 | 0.21590 | 0.38210 | 5.2172 | 2.8988 | 8.1970 |
| 10 | 2.95 | .. H(21F)a[1/2-x,-1/2+y,1/2-z | = 2545.02] | | | 162.15 | -24.97 | 0.16240 | 0.14080 | 0.36960 | 0.7938 | 1.8905 | 7.9288 |
| 11 | 3.46 | .. H(11D) [| = 01] | | | 98.73 | 16.06 | 0.35280 | 0.32430 | 0.47230 | 2.8376 | 4.3542 | 10.1320 |
| 12 | 3.52 | .. H(11B) [| = 01] | | | 97.29 | -22.10 | 0.33140 | 0.32090 | 0.36590 | 2.9273 | 4.3086 | 7.8494 |
| 13 | 3.58 | .. H(27A) | | | Intra | -51.57 | -51.10 | 0.45750 | -0.05150 | 0.29780 | 4.7392 | -0.6915 | 6.3885 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(23A)

| | | | | | | | |
|-------------------|----------|--------------------|-----------|-------------------|----------|-----------------|-----------|
| C(261) , <F(21A) | 36.3(6) | C(261) , <F(22A) | 38.9(4) | C(261) , C(26) | 36.2(3) | C(261) , C(25) | 57.0(4) |
| C(261) , <F(22A)b | 83.7(6) | C(261) , C(27) | 37.2(4) | <F(21A) , <F(22A) | 60.5(6) | <F(21A) , C(26) | 64.9(5) |
| <F(21A) , C(25) | 90.8(5) | <F(21A) , <F(22A)b | 65.8(5) | <F(21A) , C(27) | 54.6(4) | <F(22A) , C(26) | 63.2(4) |
| <F(22A) , C(25) | 66.5(4) | <F(22A) , <F(22A)b | 63.2(4) | <F(22A) , C(27) | 72.9(4) | C(26) , C(25) | 27.64(15) |
| C(26) , <F(22A)b | 119.6(5) | C(26) , C(27) | 18.03(14) | C(25) , <F(22A)b | 129.7(4) | C(25) , C(27) | 44.18(16) |
| <F(22A)b, C(27) | 117.8(4) | | | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(23B) [ARU = 1555.02] 0.42600 0.11010 0.44620 3.8442 1.4783 9.5721

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-------------------------------|----------------------|----------|-------|---------|--------|---------|----------|---------|--------|---------|---------|
| 1 | 1.406(11) | -- C(261) | | | Intra | -61.06 | -35.90 | 0.45960 | 0.03587 | 0.40777 | 4.3953 | 0.4816 | 8.7476 |
| 2 | 2.102(16) | << <F(21B) | | | Intra | -104.60 | -26.49 | 0.37650 | -0.02550 | 0.40250 | 3.3701 | -0.3424 | 8.6346 |
| 3 | 2.141(18) | << <F(22B) | | | Intra | -46.23 | -2.87 | 0.54250 | -0.00490 | 0.44120 | 5.3232 | -0.0658 | 9.4648 |
| 4 | 2.400(11) | << C(26) | | | Intra | -22.84 | -61.62 | 0.48335 | 0.07712 | 0.34776 | 4.8955 | 1.0355 | 7.4603 |
| 5 | 2.736(11) | << C(25) | | | Intra | 31.55 | -51.96 | 0.51352 | 0.17580 | 0.34574 | 5.2809 | 2.3604 | 7.4169 |
| 6 | 2.798(16) | .< <F(22B)b[1-x,-y,1-z | = | 3656.02] | | -89.34 | 59.68 | 0.45750 | 0.00490 | 0.55880 | 3.8605 | 0.0658 | 11.9876 |
| 7 | 3.508(10) | .. C(112) [| = | 01] | | 96.19 | 1.96 | 0.39740 | 0.36970 | 0.45179 | 3.4665 | 4.9638 | 9.6920 |
| 8 | 2.41 | << H(25A) | | | Intra | 45.97 | -34.84 | 0.51820 | 0.21590 | 0.38210 | 5.2172 | 2.8988 | 8.1970 |
| 9 | 3.07 | .. H(22E)c[-1/2+x,1/2-y,1/2+z | = | 4455.02] | | -159.48 | 23.76 | 0.23200 | 0.03680 | 0.50380 | 1.2155 | 0.4941 | 10.8077 |
| 10 | 3.10 | .. H(11D) [| = | 01] | | 109.29 | 10.41 | 0.35280 | 0.32430 | 0.47230 | 2.8376 | 4.3542 | 10.1320 |
| 11 | 3.14 | .. H(11F) [| = | 01] | | 80.45 | 2.39 | 0.46910 | 0.34040 | 0.45230 | 4.3646 | 4.5704 | 9.7029 |
| 12 | 3.44 | .. H(11B) [| = | 01] | | 107.95 | -30.07 | 0.33140 | 0.32090 | 0.36590 | 2.9273 | 4.3086 | 7.8494 |
| 13 | 3.49 | .. H(21F)a[1/2-x,-1/2+y,1/2-z | = | 2545.02] | | 172.30 | -28.10 | 0.16240 | 0.14080 | 0.36960 | 0.7938 | 1.8905 | 7.9288 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(23B)

| | | | | | | | |
|-------------------|----------|--------------------|----------|-------------------|----------|-----------------|-----------|
| C(261) , <F(21B) | 38.1(5) | C(261) , <F(22B) | 35.8(4) | C(261) , C(26) | 35.1(3) | C(261) , C(25) | 64.0(4) |
| C(261) , <F(22B)b | 98.4(6) | C(261) , C(112) | 140.1(6) | <F(21B) , <F(22B) | 60.6(6) | <F(21B) , C(26) | 63.0(4) |
| <F(21B) , C(25) | 92.7(5) | <F(21B) , <F(22B)b | 87.1(6) | <F(21B) , C(112) | 148.4(6) | <F(22B) , C(26) | 61.3(4) |
| <F(22B) , C(25) | 80.2(5) | <F(22B) , <F(22B)b | 71.1(5) | <F(22B) , C(112) | 142.4(6) | C(26) , C(25) | 30.29(15) |
| C(26) , <F(22B)b | 131.6(5) | C(26) , C(112) | 105.1(3) | C(25) , <F(22B)b | 147.1(5) | C(25) , C(112) | 76.3(2) |
| <F(22B)b, C(112) | 118.2(5) | | | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(24) [ARU = 1555.02] 0.58200 -0.02610 0.16450 6.7506 -0.3504 3.5289

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|------------------------------|------------|-------|---------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 1.337(12) | -- | C(281) | | Intra | 165.56 | 17.57 | 0.48874 | -0.00243 | 0.18331 | 5.5168 | -0.0326 | 3.9324 |
| 2 | 2.126(17) | << | <F(26) | | Intra | 155.87 | 14.32 | 0.43880 | -0.08880 | 0.18900 | 4.8709 | -1.1923 | 4.0545 |
| 3 | 2.130(16) | << | <F(25) | | Intra | 152.69 | -17.59 | 0.43020 | 0.04330 | 0.13450 | 4.9464 | 0.5814 | 2.8853 |
| 4 | 2.376(15) | << | C(28) | | Intra | 138.65 | 43.95 | 0.50031 | 0.05807 | 0.24136 | 5.4666 | 0.7797 | 5.1777 |
| 5 | 3.064(15) | .< | C(29) | | Intra | 110.20 | 31.18 | 0.52971 | 0.15713 | 0.23846 | 5.8453 | 2.1097 | 5.1155 |
| 6 | 3.158(16) | .. | >F(15A) [| = 01] | | 50.25 | -34.46 | 0.69230 | 0.12300 | 0.08120 | 8.4154 | 1.6515 | 1.7419 |
| 7 | 3.365(14) | .. | C(22)b [3/2-x, -1/2+y, 1/2-z | = 2645.02] | | 18.05 | 39.56 | 0.80534 | 0.03378 | 0.26440 | 9.2173 | 0.4535 | 5.6720 |
| 8 | 3.374(16) | .. | C(27) | | Intra | 161.95 | 56.74 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 9 | 2.82 | .. | H(22A)b[3/2-x, -1/2+y, 1/2-z | = 2645.02] | | 11.59 | 54.39 | 0.73900 | -0.00150 | 0.27150 | 8.3608 | -0.0201 | 5.8243 |
| 10 | 2.99 | .. | H(29A) | | Intra | 101.70 | 14.95 | 0.54500 | 0.18430 | 0.20040 | 6.1654 | 2.4745 | 4.2991 |
| 11 | 3.12 | .. | H(21C)a[x, -1+y, z | = 1545.02] | | -99.43 | -8.94 | 0.53570 | -0.25260 | 0.14190 | 6.2456 | -3.3915 | 3.0441 |
| 12 | 3.15 | .. | H(22B)b[3/2-x, -1/2+y, 1/2-z | = 2645.02] | | 33.77 | 28.47 | 0.78390 | 0.08840 | 0.23440 | 9.0493 | 1.1869 | 5.0284 |
| 13 | 3.21 | .. | H(17A)c[1-x, -y, -z | = 3655.01] | | -78.65 | -67.13 | 0.56460 | -0.11710 | 0.02680 | 6.9959 | -1.5722 | 0.5749 |
| 14 | 3.51 | .. | H(27A) | | Intra | -170.38 | 54.50 | 0.45750 | -0.05150 | 0.29780 | 4.7392 | -0.6915 | 6.3885 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(24)

| | | | | | | | |
|------------------|----------|------------------|-----------|------------------|-----------|------------------|----------|
| C(281) , <F(26) | 37.2(4) | C(281) , <F(25) | 37.4(5) | C(281) , C(28) | 34.8(5) | C(281) , C(29) | 51.7(5) |
| C(281) , >F(15A) | 120.5(8) | C(281) , C(22)b | 115.3(9) | C(281) , C(27) | 39.3(6) | <F(26) , <F(25) | 59.9(6) |
| <F(26) , C(28) | 62.5(5) | <F(26) , C(29) | 85.9(6) | <F(26) , >F(15A) | 149.0(8) | <F(26) , C(22)b | 125.8(8) |
| <F(26) , C(27) | 53.1(6) | <F(25) , C(28) | 62.9(4) | <F(25) , C(29) | 63.6(5) | <F(25) , >F(15A) | 89.9(6) |
| <F(25) , C(22)b | 135.1(7) | <F(25) , C(27) | 74.7(5) | C(28) , C(29) | 25.72(17) | C(28) , >F(15A) | 112.1(5) |
| C(28) , C(22)b | 80.8(4) | C(28) , C(27) | 19.45(17) | C(29) , >F(15A) | 86.6(4) | C(29) , C(22)b | 72.2(3) |
| C(29) , C(27) | 43.7(2) | >F(15A) , C(22)b | 79.8(3) | >F(15A) , C(27) | 129.8(5) | C(22)b , C(27) | 79.0(4) |

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3.6 Angstrom Coordination Sphere Around Atom I = F(24A) [ARU = 1555.02] 0.56880 0.01340 0.15130 6.6294 0.1799 3.2457

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|---------------------|-----------|----------|-------|--------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 1.325(18) | -- | C(281) | | | | Intra | 169.18 | 31.23 | 0.48874 | -0.00243 | 0.18331 | 5.5168 | -0.0326 | 3.9324 |
| 2 | 2.116(19) | << | <F(25A) | | | | Intra | 178.40 | -3.37 | 0.39900 | 0.01780 | 0.14550 | 4.5178 | 0.2390 | 3.1213 |
| 3 | 2.14(2) | << | <F(26A) | | | | Intra | 127.59 | 26.71 | 0.48800 | -0.09930 | 0.19610 | 5.4645 | -1.3333 | 4.2068 |
| 4 | 2.33(2) | << | C(28) | | | | Intra | 152.72 | 55.89 | 0.50031 | 0.05807 | 0.24136 | 5.4666 | 0.7797 | 5.1777 |
| 5 | 2.76(2) | < | >F(15A) | [| = | 01] | | 39.49 | -33.02 | 0.69230 | 0.12300 | 0.08120 | 8.4154 | 1.6515 | 1.7419 |
| 6 | 2.80(2) | << | C(29) | | | | Intra | 112.11 | 41.91 | 0.52971 | 0.15713 | 0.23846 | 5.8453 | 2.1097 | 5.1155 |
| 7 | 3.47(2) | .. | C(18) | [| = | 01] | | 93.76 | -43.46 | 0.52587 | 0.20032 | 0.04020 | 6.4647 | 2.6896 | 0.8624 |
| 8 | 3.49(2) | .. | C(181) | [| = | 01] | | 58.54 | -48.14 | 0.63320 | 0.16146 | 0.03006 | 7.8459 | 2.1678 | 0.6449 |
| 9 | 3.51(2) | .. | C(27) | | | | Intra | 178.50 | 62.17 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 10 | 3.558(19) | .. | C(22)b | [3/2-x,-1/2+y,1/2-z | = | 2645.02] | | 6.04 | 42.99 | 0.80534 | 0.03378 | 0.26440 | 9.2173 | 0.4535 | 5.6720 |
| 11 | 2.57 | < | H(29A) | | | | Intra | 101.43 | 24.22 | 0.54500 | 0.18430 | 0.20040 | 6.1654 | 2.4745 | 4.2991 |
| 12 | 3.11 | .. | H(22A)b | [3/2-x,-1/2+y,1/2-z | = | 2645.02] | | -6.59 | 55.94 | 0.73900 | -0.00150 | 0.27150 | 8.3608 | -0.0201 | 5.8243 |
| 13 | 3.17 | .. | H(22B)b | [3/2-x,-1/2+y,1/2-z | = | 2645.02] | | 22.59 | 34.22 | 0.78390 | 0.08840 | 0.23440 | 9.0493 | 1.1869 | 5.0284 |
| 14 | 3.22 | .. | H(17A)c | [1-x,-y,-z | = | 3655.01] | | -78.19 | -56.17 | 0.56460 | -0.11710 | 0.02680 | 6.9959 | -1.5722 | 0.5749 |
| 15 | 3.60 | .. | H(21C)a | [x,-1+y,z | = | 1545.02] | | -96.13 | -3.21 | 0.53570 | -0.25260 | 0.14190 | 6.2456 | -3.3915 | 3.0441 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(24A)

| | | | | | | | |
|------------------|-----------|-------------------|-----------|-------------------|-----------|-------------------|-----------|
| C(281) , <F(25A) | 36.6(7) | C(281) , <F(26A) | 36.5(7) | C(281) , C(28) | 36.2(6) | C(281) , >F(15A) | 155.7(12) |
| C(281) , C(29) | 61.9(8) | C(281) , C(18) | 115.7(10) | C(281) , C(181) | 140.4(11) | C(281) , C(27) | 32.0(7) |
| C(281) , C(22)b | 105.7(12) | <F(25A) , <F(26A) | 60.2(8) | <F(25A) , C(28) | 62.9(7) | <F(25A) , >F(15A) | 126.8(10) |
| <F(25A) , C(29) | 75.0(7) | <F(25A) , C(18) | 83.8(8) | <F(25A) , C(181) | 106.7(9) | <F(25A) , C(27) | 65.5(7) |
| <F(25A) , C(22)b | 139.8(11) | <F(26A) , C(28) | 62.5(7) | <F(26A) , >F(15A) | 167.2(10) | <F(26A) , C(29) | 92.0(9) |
| <F(26A) , C(18) | 142.8(8) | <F(26A) , C(181) | 158.1(11) | <F(26A) , C(27) | 50.0(7) | <F(26A) , C(22)b | 98.3(9) |
| C(28) , >F(15A) | 129.5(8) | C(28) , C(29) | 29.6(3) | C(28) , C(18) | 111.1(7) | C(28) , C(181) | 130.1(8) |
| C(28) , C(27) | 14.6(2) | C(28) , C(22)b | 77.2(6) | >F(15A) , C(29) | 100.2(6) | >F(15A) , C(18) | 43.1(3) |
| >F(15A) , C(181) | 20.8(2) | >F(15A) , C(27) | 141.0(7) | >F(15A) , C(22)b | 81.9(4) | C(29) , C(18) | 87.0(5) |
| C(29) , C(181) | 101.7(6) | C(29) , C(27) | 43.1(3) | C(29) , C(22)b | 72.3(5) | C(18) , C(181) | 24.77(16) |
| C(18) , C(27) | 125.3(5) | C(18) , C(22)b | 116.6(5) | C(181) , C(27) | 144.5(6) | C(181) , C(22)b | 102.2(4) |
| C(27) , C(22)b | 74.7(5) | | | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(24B) [ARU = 1555.02] 0.57910 -0.00300 0.15910 6.7324 -0.0403 3.4131

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|------------------------------|------------|-------|--------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 1.322(18) | -- | C(281) | | Intra | 179.64 | 23.13 | 0.48874 | -0.00243 | 0.18331 | 5.5168 | -0.0326 | 3.9324 |
| 2 | 2.12(3) | << | <F(26B) | | Intra | 141.46 | 18.34 | 0.46200 | -0.09640 | 0.19020 | 5.1580 | -1.2943 | 4.0802 |
| 3 | 2.13(3) | << | <F(25B) | | Intra | 165.34 | -10.87 | 0.41300 | 0.03640 | 0.14040 | 4.7107 | 0.4887 | 3.0119 |
| 4 | 2.32(2) | << | C(28) | | Intra | 147.07 | 49.48 | 0.50031 | 0.05807 | 0.24136 | 5.4666 | 0.7797 | 5.1777 |
| 5 | 2.88(3) | << | C(29) | | Intra | 112.42 | 36.20 | 0.52971 | 0.15713 | 0.23846 | 5.8453 | 2.1097 | 5.1155 |
| 6 | 2.91(2) | .< | >F(15A) [| = 01] | | 45.15 | -35.00 | 0.69230 | 0.12300 | 0.08120 | 8.4154 | 1.6515 | 1.7419 |
| 7 | 3.39(2) | .. | C(22)b [3/2-x, -1/2+y, 1/2-z | = 2645.02] | | 11.24 | 41.72 | 0.80534 | 0.03378 | 0.26440 | 9.2173 | 0.4535 | 5.6720 |
| 8 | 3.42(2) | .. | C(27) | | Intra | 171.41 | 59.06 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 9 | 2.73 | .. | H(29A) | | Intra | 102.71 | 18.97 | 0.54500 | 0.18430 | 0.20040 | 6.1654 | 2.4745 | 4.2991 |
| 10 | 2.91 | .. | H(22A)b[3/2-x, -1/2+y, 1/2-z | = 2645.02] | | 0.71 | 55.97 | 0.73900 | -0.00150 | 0.27150 | 8.3608 | -0.0201 | 5.8243 |
| 11 | 3.08 | .. | H(22B)b[3/2-x, -1/2+y, 1/2-z | = 2645.02] | | 27.91 | 31.64 | 0.78390 | 0.08840 | 0.23440 | 9.0493 | 1.1869 | 5.0284 |
| 12 | 3.24 | .. | H(17A)c[1-x, -y, -z | = 3655.01] | | -80.24 | -61.29 | 0.56460 | -0.11710 | 0.02680 | 6.9959 | -1.5722 | 0.5749 |
| 13 | 3.41 | .. | H(21C)a[x, -1+y, z | = 1545.02] | | -98.26 | -6.22 | 0.53570 | -0.25260 | 0.14190 | 6.2456 | -3.3915 | 3.0441 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(24B)

| | | | | | | | |
|------------------|-----------|------------------|-----------|-------------------|-----------|-------------------|-----------|
| C(281) , <F(26B) | 36.6(8) | C(281) , <F(25B) | 36.8(8) | C(281) , C(28) | 36.7(7) | C(281) , C(29) | 58.7(10) |
| C(281) , >F(15A) | 138.9(15) | C(281) , C(22)b | 114.3(14) | C(281) , C(27) | 36.4(8) | <F(26B) , <F(25B) | 60.1(10) |
| <F(26B) , C(28) | 64.2(8) | <F(26B) , C(29) | 91.5(9) | <F(26B) , >F(15A) | 162.3(13) | <F(26B) , C(22)b | 114.9(12) |
| <F(26B) , C(27) | 53.0(8) | <F(25B) , C(28) | 62.5(8) | <F(25B) , C(29) | 68.5(9) | <F(25B) , >F(15A) | 107.2(12) |
| <F(25B) , C(22)b | 141.7(12) | <F(25B) , C(27) | 70.1(8) | C(28) , C(29) | 28.3(3) | C(28) , >F(15A) | 123.1(11) |
| C(28) , C(22)b | 80.9(7) | C(28) , C(27) | 17.0(3) | C(29) , >F(15A) | 94.8(8) | C(29) , C(22)b | 74.0(6) |
| C(29) , C(27) | 43.9(3) | >F(15A) , C(22)b | 82.8(5) | >F(15A) , C(27) | 137.8(9) | C(22)b , C(27) | 77.9(5) |

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3.6 Angstrom Coordination Sphere Around Atom I = F(25) [ARU = 1555.02] 0.43020 0.04330 0.13450 4.9464 0.5814 2.8853

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------------|------------|-------|---------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 1.341(11) | -- | C(281) | | Intra | -47.11 | 51.33 | 0.48874 | -0.00243 | 0.18331 | 5.5168 | -0.0326 | 3.9324 |
| 2 | 2.126(18) | << | <F(26) | | Intra | -92.44 | 33.37 | 0.43880 | -0.08880 | 0.18900 | 4.8709 | -1.1923 | 4.0545 |
| 3 | 2.130(16) | << | <F(24) | | Intra | -27.31 | 17.59 | 0.58200 | -0.02610 | 0.16450 | 6.7506 | -0.3504 | 3.5289 |
| 4 | 2.359(11) | << | C(28) | | Intra | 20.87 | 76.35 | 0.50031 | 0.05807 | 0.24136 | 5.4666 | 0.7797 | 5.1777 |
| 5 | 2.849(12) | << | C(29) | | Intra | 59.54 | 51.51 | 0.52971 | 0.15713 | 0.23846 | 5.8453 | 2.1097 | 5.1155 |
| 6 | 3.192(14) | .. | >F(16A)b[1-x,-y,-z | = 3655.01] | | -100.67 | -53.89 | 0.37020 | -0.09440 | 0.01430 | 4.5981 | -1.2675 | 0.3068 |
| 7 | 3.268(12) | .. | C(17) [| = 01] | | 74.02 | -58.44 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 8 | 3.293(12) | .. | C(18) [| = 01] | | 54.24 | -37.91 | 0.52587 | 0.20032 | 0.04020 | 6.4647 | 2.6896 | 0.8624 |
| 9 | 3.421(12) | .. | C(16) [| = 01] | | 110.14 | -47.80 | 0.33547 | 0.20399 | 0.01637 | 4.1553 | 2.7389 | 0.3512 |
| 10 | 3.477(13) | .. | C(19) [| = 01] | | 66.61 | -17.10 | 0.52253 | 0.27050 | 0.08683 | 6.2658 | 3.6319 | 1.8627 |
| 11 | 3.483(11) | .. | C(27) | | Intra | -82.85 | 84.04 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 12 | 2.66 | .< | H(29A) | | Intra | 57.22 | 32.12 | 0.54500 | 0.18430 | 0.20040 | 6.1654 | 2.4745 | 4.2991 |
| 13 | 3.05 | .. | H(11C)a[1/2-x,-1/2+y,1/2-z | = 2545.01] | | -147.13 | -8.42 | 0.22280 | -0.07860 | 0.11370 | 2.4135 | -1.0553 | 2.4391 |
| 14 | 3.24 | .. | H(11A)a[1/2-x,-1/2+y,1/2-z | = 2545.01] | | 175.17 | 4.59 | 0.17670 | 0.06360 | 0.14660 | 1.7241 | 0.8539 | 3.1449 |
| 15 | 3.50 | .. | H(12A)a[1/2-x,-1/2+y,1/2-z | = 2545.01] | | -156.06 | 36.70 | 0.25200 | -0.04150 | 0.23200 | 2.3816 | -0.5572 | 4.9770 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(25)

| | | | | | | | |
|-------------------|-----------|-------------------|-----------|------------------|-----------|-----------------|-----------|
| C(281) , <F(26) | 37.2(5) | C(281) , <F(24) | 37.2(5) | C(281) , C(28) | 35.5(3) | C(281) , C(29) | 60.0(4) |
| C(281) , >F(16A)b | 114.3(7) | C(281) , C(17) | 146.6(6) | C(281) , C(18) | 125.2(6) | C(281) , C(16) | 164.9(7) |
| C(281) , C(19) | 118.0(6) | C(281) , C(27) | 34.0(3) | <F(26) , <F(24) | 59.9(6) | <F(26) , C(28) | 62.8(5) |
| <F(26) , C(29) | 91.6(6) | <F(26) , >F(16A)b | 87.5(6) | <F(26) , C(17) | 153.3(7) | <F(26) , C(18) | 152.7(6) |
| <F(26) , C(16) | 157.7(6) | <F(26) , C(19) | 155.1(6) | <F(26) , C(27) | 50.8(5) | <F(24) , C(28) | 63.7(5) |
| <F(24) , C(29) | 74.4(5) | <F(24) , >F(16A)b | 94.8(7) | <F(24) , C(17) | 110.8(6) | <F(24) , C(18) | 94.3(5) |
| <F(24) , C(16) | 134.1(6) | <F(24) , C(19) | 98.7(5) | <F(24) , C(27) | 69.1(5) | C(28) , C(29) | 28.92(15) |
| C(28) , >F(16A)b | 149.1(6) | C(28) , C(17) | 138.9(5) | C(28) , C(18) | 116.2(4) | C(28) , C(16) | 135.9(5) |
| C(28) , C(19) | 97.4(4) | C(28) , C(27) | 16.12(12) | C(29) , >F(16A)b | 167.8(5) | C(29) , C(17) | 110.6(4) |
| C(29) , C(18) | 89.5(3) | C(29) , C(16) | 108.3(4) | C(29) , C(19) | 68.9(3) | C(29) , C(27) | 43.33(16) |
| >F(16A)b, C(17) | 67.6(3) | >F(16A)b, C(18) | 85.7(3) | >F(16A)b, C(16) | 75.0(3) | >F(16A)b, C(19) | 108.2(4) |
| >F(16A)b, C(27) | 138.2(5) | C(17) , C(18) | 24.20(10) | C(17) , C(16) | 23.76(10) | C(17) , C(19) | 41.70(16) |
| C(17) , C(27) | 153.8(4) | C(18) , C(16) | 41.21(15) | C(18) , C(19) | 23.47(10) | C(18) , C(27) | 132.2(4) |
| C(16) , C(19) | 46.89(17) | C(16) , C(27) | 143.6(4) | C(19) , C(27) | 112.2(3) | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(25A) [ARU = 1555.02] 0.39900 0.01780 0.14550 4.5178 0.2390 3.1213

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|---------------------|------------|--------|-------|---------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 1.315(16) | -- | C(281) | | | | Intra | -15.21 | 38.08 | 0.48874 | -0.00243 | 0.18331 | 5.5168 | -0.0326 | 3.9324 |
| 2 | 2.116(19) | << | <F(24A) | | | | Intra | -1.60 | 3.37 | 0.56880 | 0.01340 | 0.15130 | 6.6294 | 0.1799 | 3.2457 |
| 3 | 2.13(2) | << | <F(26A) | | | | Intra | -58.95 | 30.60 | 0.48800 | -0.09930 | 0.19610 | 5.4645 | -1.3333 | 4.2068 |
| 4 | 2.328(18) | << | C(28) | | | | Intra | 29.68 | 62.03 | 0.50031 | 0.05807 | 0.24136 | 5.4666 | 0.7797 | 5.1777 |
| 5 | 3.040(17) | .< | C(29) | | | | Intra | 54.64 | 41.00 | 0.52971 | 0.15713 | 0.23846 | 5.8453 | 2.1097 | 5.1155 |
| 6 | 3.19(2) | .. | >F(16A)b | [1-x,-y,-z | = 3655.01] | | | -86.95 | -61.81 | 0.37020 | -0.09440 | 0.01430 | 4.5981 | -1.2675 | 0.3068 |
| 7 | 3.263(19) | .. | C(27) | | | | Intra | -1.96 | 81.65 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 8 | 3.449(15) | .. | C(12)a | [1/2-x,-1/2+y,1/2-z | = 2545.01] | | | -177.92 | 34.63 | 0.19756 | 0.01013 | 0.23686 | 1.6820 | 0.1360 | 5.0812 |
| 9 | 3.520(13) | .. | C(11)a | [1/2-x,-1/2+y,1/2-z | = 2545.01] | | | 177.17 | 10.18 | 0.13104 | 0.03054 | 0.17450 | 1.0571 | 0.4100 | 3.7434 |
| 10 | 3.529(14) | .. | C(111)a | [1/2-x,-1/2+y,1/2-z | = 2545.01] | | | -149.21 | -11.38 | 0.15350 | -0.11410 | 0.11303 | 1.5460 | -1.5320 | 2.4248 |
| 11 | 2.56 | .< | H(11C)a | [1/2-x,-1/2+y,1/2-z | = 2545.01] | | | -148.41 | -15.44 | 0.22280 | -0.07860 | 0.11370 | 2.4135 | -1.0553 | 2.4391 |
| 12 | 2.86 | .. | H(11A)a | [1/2-x,-1/2+y,1/2-z | = 2545.01] | | | 167.59 | 0.47 | 0.17670 | 0.06360 | 0.14660 | 1.7241 | 0.8539 | 3.1449 |
| 13 | 2.94 | .. | H(12A)a | [1/2-x,-1/2+y,1/2-z | = 2545.01] | | | -159.56 | 39.14 | 0.25200 | -0.04150 | 0.23200 | 2.3816 | -0.5572 | 4.9770 |
| 14 | 3.02 | .. | H(29A) | | | | Intra | 53.61 | 22.98 | 0.54500 | 0.18430 | 0.20040 | 6.1654 | 2.4745 | 4.2991 |
| 15 | 3.40 | .. | H(12B)a | [1/2-x,-1/2+y,1/2-z | = 2545.01] | | | 163.24 | 42.44 | 0.23650 | 0.07160 | 0.25230 | 2.1187 | 0.9613 | 5.4124 |
| 16 | 3.40 | .. | H(27A) | | | | Intra | -76.61 | 73.68 | 0.45750 | -0.05150 | 0.29780 | 4.7392 | -0.6915 | 6.3885 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(25A)

| | | | | | | | |
|--------------------|-----------|-------------------|----------|-------------------|-----------|--------------------|-----------|
| C(281) , <F(24A) | 36.9(7) | C(281) , <F(26A) | 36.5(6) | C(281) , C(28) | 36.3(5) | C(281) , C(29) | 52.5(6) |
| C(281) , >F(16A)b | 115.3(9) | C(281) , C(27) | 43.8(6) | C(281) , C(12)a | 105.5(9) | C(281) , C(11)a | 130.4(10) |
| C(281) , C(111)a | 131.1(9) | <F(24A) , <F(26A) | 60.4(8) | <F(24A) , C(28) | 63.1(8) | <F(24A) , C(29) | 62.8(7) |
| <F(24A) , >F(16A)b | 90.8(9) | <F(24A) , C(27) | 78.3(8) | <F(24A) , C(12)a | 141.8(10) | <F(24A) , C(11)a | 166.4(10) |
| <F(24A) , C(111)a | 146.9(9) | <F(26A) , C(28) | 62.7(7) | <F(26A) , C(29) | 85.8(7) | <F(26A) , >F(16A)b | 95.2(8) |
| <F(26A) , C(27) | 55.1(7) | <F(26A) , C(12)a | 93.1(8) | <F(26A) , C(11)a | 112.5(7) | <F(26A) , C(111)a | 96.0(6) |
| C(28) , C(29) | 25.80(19) | C(28) , >F(16A)b | 151.4(6) | C(28) , C(27) | 21.3(2) | C(28) , C(12)a | 80.8(5) |
| C(28) , C(11)a | 103.5(6) | C(28) , C(111)a | 129.4(6) | C(29) , >F(16A)b | 149.1(6) | C(29) , C(27) | 44.8(3) |
| C(29) , C(12)a | 90.3(5) | C(29) , C(11)a | 106.5(5) | C(29) , C(111)a | 143.7(6) | >F(16A)b, C(27) | 150.0(6) |
| >F(16A)b, C(12)a | 120.5(5) | >F(16A)b, C(11)a | 101.7(5) | >F(16A)b, C(111)a | 67.1(4) | C(27) , C(12)a | 63.7(3) |
| C(27) , C(11)a | 88.2(4) | C(27) , C(111)a | 108.4(5) | C(12)a , C(11)a | 24.86(11) | C(12)a , C(111)a | 53.5(2) |
| C(11)a , C(111)a | 39.77(15) | | | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(25B) [ARU = 1555.02] 0.41300 0.03640 0.14040 4.7107 0.4887 3.0119

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|---------|-------------------------------|----------------------|----------|-------|---------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 1.33(2) | -- C(281) | | | Intra | -32.89 | 43.80 | 0.48874 | -0.00243 | 0.18331 | 5.5168 | -0.0326 | 3.9324 |
| 2 | 2.13(3) | << <F(26B) | | | Intra | -75.92 | 30.16 | 0.46200 | -0.09640 | 0.19020 | 5.1580 | -1.2943 | 4.0802 |
| 3 | 2.13(3) | << <F(24B) | | | Intra | -14.66 | 10.87 | 0.57910 | -0.00300 | 0.15910 | 6.7324 | -0.0403 | 3.4131 |
| 4 | 2.31(2) | << C(28) | | | Intra | 21.05 | 69.50 | 0.50031 | 0.05807 | 0.24136 | 5.4666 | 0.7797 | 5.1777 |
| 5 | 2.89(2) | << C(29) | | | Intra | 55.01 | 46.75 | 0.52971 | 0.15713 | 0.23846 | 5.8453 | 2.1097 | 5.1155 |
| 6 | 3.23(2) | .. >F(16A)b[1-x,-y,-z | = | 3655.01] | | -93.67 | -56.95 | 0.37020 | -0.09440 | 0.01430 | 4.5981 | -1.2675 | 0.3068 |
| 7 | 3.36(2) | .. C(27) | | | Intra | -43.46 | 83.39 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 8 | 3.46(2) | .. C(17) [| = | 01] | | 67.86 | -57.21 | 0.43290 | 0.16576 | 0.00472 | 5.4173 | 2.2256 | 0.1013 |
| 9 | 3.53(2) | .. C(16) [| = | 01] | | 103.87 | -48.94 | 0.33547 | 0.20399 | 0.01637 | 4.1553 | 2.7389 | 0.3512 |
| 10 | 3.54(2) | .. C(18) [| = | 01] | | 51.45 | -37.37 | 0.52587 | 0.20032 | 0.04020 | 6.4647 | 2.6896 | 0.8624 |
| 11 | 2.78 | .. H(29A) | | | Intra | 53.78 | 27.60 | 0.54500 | 0.18430 | 0.20040 | 6.1654 | 2.4745 | 4.2991 |
| 12 | 2.83 | .. H(11C)a[1/2-x,-1/2+y,1/2-z | = | 2545.01] | | -146.09 | -11.69 | 0.22280 | -0.07860 | 0.11370 | 2.4135 | -1.0553 | 2.4391 |
| 13 | 3.01 | .. H(11A)a[1/2-x,-1/2+y,1/2-z | = | 2545.01] | | 173.03 | 2.53 | 0.17670 | 0.06360 | 0.14660 | 1.7241 | 0.8539 | 3.1449 |
| 14 | 3.22 | .. H(12A)a[1/2-x,-1/2+y,1/2-z | = | 2545.01] | | -155.82 | 37.58 | 0.25200 | -0.04150 | 0.23200 | 2.3816 | -0.5572 | 4.9770 |
| 15 | 3.56 | .. H(12B)a[1/2-x,-1/2+y,1/2-z | = | 2545.01] | | 169.67 | 42.34 | 0.23650 | 0.07160 | 0.25230 | 2.1187 | 0.9613 | 5.4124 |
| 16 | 3.58 | .. H(27A) | | | Intra | -88.61 | 70.73 | 0.45750 | -0.05150 | 0.29780 | 4.7392 | -0.6915 | 6.3885 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(25B)

| | | | | | | | |
|--------------------|-----------|-------------------|----------|------------------|-----------|--------------------|-----------|
| C(281) , <F(26B) | 36.5(9) | C(281) , <F(24B) | 36.5(9) | C(281) , C(28) | 37.2(7) | C(281) , C(29) | 58.5(8) |
| C(281) , >F(16A)b | 112.8(12) | C(281) , C(27) | 39.7(7) | C(281) , C(17) | 130.9(11) | C(281) , C(16) | 150.1(12) |
| C(281) , C(18) | 111.3(10) | <F(26B) , <F(24B) | 59.8(11) | <F(26B) , C(28) | 64.3(9) | <F(26B) , C(29) | 91.3(10) |
| <F(26B) , >F(16A)b | 88.4(9) | <F(26B) , C(27) | 54.3(8) | <F(26B) , C(17) | 143.1(11) | <F(26B) , C(16) | 161.2(12) |
| <F(26B) , C(18) | 136.2(10) | <F(24B) , C(28) | 62.9(9) | <F(24B) , C(29) | 68.2(9) | <F(24B) , >F(16A)b | 93.2(10) |
| <F(24B) , C(27) | 73.4(9) | <F(24B) , C(17) | 95.1(10) | <F(24B) , C(16) | 116.8(11) | <F(24B) , C(18) | 78.4(9) |
| C(28) , C(29) | 28.2(3) | C(28) , >F(16A)b | 149.9(9) | C(28) , C(27) | 18.6(2) | C(28) , C(17) | 131.1(8) |
| C(28) , C(16) | 132.7(8) | C(28) , C(18) | 109.2(7) | C(29) , >F(16A)b | 158.4(8) | C(29) , C(27) | 44.6(3) |
| C(29) , C(17) | 104.5(6) | C(29) , C(16) | 104.7(6) | C(29) , C(18) | 84.2(5) | >F(16A)b , C(27) | 142.4(7) |
| >F(16A)b , C(17) | 64.9(5) | >F(16A)b , C(16) | 73.1(5) | >F(16A)b , C(18) | 81.2(5) | C(27) , C(17) | 149.1(7) |
| C(27) , C(16) | 144.4(7) | C(27) , C(18) | 127.7(6) | C(17) , C(16) | 22.83(16) | C(17) , C(18) | 22.61(15) |
| C(16) , C(18) | 39.1(2) | | | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(26) [ARU = 1555.02] 0.43880 -0.08880 0.18900 4.8709 -1.1923 4.0545

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-------------------------------|----------------------|--------|-------|---------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 1.333(11) | -- C(281) | | | Intra | 60.88 | -5.25 | 0.48874 | -0.00243 | 0.18331 | 5.5168 | -0.0326 | 3.9324 |
| 2 | 2.126(17) | << <F(24) | | | Intra | 24.13 | -14.32 | 0.58200 | -0.02610 | 0.16450 | 6.7506 | -0.3504 | 3.5289 |
| 3 | 2.126(18) | << <F(25) | | | Intra | 87.56 | -33.37 | 0.43020 | 0.04330 | 0.13450 | 4.9464 | 0.5814 | 2.8853 |
| 4 | 2.346(13) | << C(28) | | | Intra | 73.19 | 28.60 | 0.50031 | 0.05807 | 0.24136 | 5.4666 | 0.7797 | 5.1777 |
| 5 | 2.699(17) | << C(27) | | | Intra | 85.13 | 58.26 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 6 | 3.049(11) | .< C(212)a[x,-1+y,z | = 1545.02] | | | -101.83 | -19.32 | 0.37920 | -0.29852 | 0.14199 | 4.2811 | -4.0081 | 3.0460 |
| 7 | 3.373(11) | .. C(211)a[x,-1+y,z | = 1545.02] | | | -73.86 | -19.71 | 0.49490 | -0.31594 | 0.13597 | 5.7535 | -4.2420 | 2.9169 |
| 8 | 2.39 | << H(27A) | | | Intra | 104.73 | 77.49 | 0.45750 | -0.05150 | 0.29780 | 4.7392 | -0.6915 | 6.3885 |
| 9 | 2.70 | .. H(21E)a[x,-1+y,z | = 1545.02] | | | -107.28 | -1.73 | 0.37380 | -0.28100 | 0.18520 | 4.0679 | -3.7728 | 3.9730 |
| 10 | 2.73 | .. H(12A)c[1/2-x,-1/2+y,1/2-z | = 2545.01] | | | 165.69 | 19.75 | 0.25200 | -0.04150 | 0.23200 | 2.3816 | -0.5572 | 4.9770 |
| 11 | 2.76 | .. H(21D)a[x,-1+y,z | = 1545.02] | | | -112.40 | -35.39 | 0.35040 | -0.24390 | 0.11440 | 4.0126 | -3.2747 | 2.4542 |
| 12 | 2.78 | .. H(21C)a[x,-1+y,z | = 1545.02] | | | -57.99 | -21.28 | 0.53570 | -0.25260 | 0.14190 | 6.2456 | -3.3915 | 3.0441 |
| 13 | 2.94 | .. H(11C)c[1/2-x,-1/2+y,1/2-z | = 2545.01] | | | 176.81 | -33.28 | 0.22280 | -0.07860 | 0.11370 | 2.4135 | -1.0553 | 2.4391 |
| 14 | 3.51 | .. H(12F)b[x,-1+y,z | = 1545.01] | | | -74.64 | 55.47 | 0.51700 | -0.23180 | 0.32390 | 5.3981 | -3.1123 | 6.9484 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(26)

| | | | | | | | |
|-------------------|-----------|------------------|----------|------------------|----------|-----------------|----------|
| C(281) , <F(24) | 37.3(5) | C(281) , <F(25) | 37.5(5) | C(281) , C(28) | 35.9(4) | C(281) , C(27) | 66.4(7) |
| C(281) , C(212)a | 150.1(11) | C(281) , C(211)a | 129.0(8) | <F(24) , <F(25) | 60.1(6) | <F(24) , C(28) | 64.0(5) |
| <F(24) , C(27) | 87.9(6) | <F(24) , C(212)a | 117.1(7) | <F(24) , C(211)a | 92.5(6) | <F(25) , C(28) | 63.5(4) |
| <F(25) , C(27) | 91.7(5) | <F(25) , C(212)a | 126.6(8) | <F(25) , C(211)a | 124.0(8) | C(28) , C(27) | 30.8(2) |
| C(28) , C(212)a | 169.7(7) | C(28) , C(211)a | 148.8(5) | C(27) , C(212)a | 140.7(6) | C(27) , C(211)a | 138.5(6) |
| C(212)a , C(211)a | 26.34(11) | | | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(26A) [ARU = 1555.02] 0.48800 -0.09930 0.19610 5.4645 -1.3333 4.2068

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|-----------------------|-----------|----------|-------|---------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 1.330(12) | -- | C(281) | | | | Intra | 87.70 | -11.90 | 0.48874 | -0.00243 | 0.18331 | 5.5168 | -0.0326 | 3.9324 |
| 2 | 2.13(2) | << | <F(25A) | | | | Intra | 121.05 | -30.60 | 0.39900 | 0.01780 | 0.14550 | 4.5178 | 0.2390 | 3.1213 |
| 3 | 2.14(2) | << | <F(24A) | | | | Intra | 52.41 | -26.71 | 0.56880 | 0.01340 | 0.15130 | 6.6294 | 0.1799 | 3.2457 |
| 4 | 2.325(13) | << | C(28) | | | | Intra | 89.94 | 24.68 | 0.50031 | 0.05807 | 0.24136 | 5.4666 | 0.7797 | 5.1777 |
| 5 | 2.690(18) | << | C(27) | | | | Intra | 106.91 | 52.81 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 6 | 3.147(14) | .< | C(212)a | [x, -1+y, z | = | 1545.02] | | -113.86 | -21.65 | 0.37920 | -0.29852 | 0.14199 | 4.2811 | -4.0081 | 3.0460 |
| 7 | 3.195(13) | .. | C(211)a | [x, -1+y, z | = | 1545.02] | | -84.32 | -23.81 | 0.49490 | -0.31594 | 0.13597 | 5.7535 | -4.2420 | 2.9169 |
| 8 | 3.581(12) | .. | C(29) | | | | Intra | 83.69 | 14.70 | 0.52971 | 0.15713 | 0.23846 | 5.8453 | 2.1097 | 5.1155 |
| 9 | 2.39 | << | H(27A) | | | | Intra | 138.49 | 66.06 | 0.45750 | -0.05150 | 0.29780 | 4.7392 | -0.6915 | 6.3885 |
| 10 | 2.49 | .< | H(21C)a | [x, -1+y, z | = | 1545.02] | | -69.22 | -27.84 | 0.53570 | -0.25260 | 0.14190 | 6.2456 | -3.3915 | 3.0441 |
| 11 | 2.82 | .. | H(21E)a | [x, -1+y, z | = | 1545.02] | | -119.79 | -4.76 | 0.37380 | -0.28100 | 0.18520 | 4.0679 | -3.7728 | 3.9730 |
| 12 | 2.99 | .. | H(21D)a | [x, -1+y, z | = | 1545.02] | | -126.79 | -35.87 | 0.35040 | -0.24390 | 0.11440 | 4.0126 | -3.2747 | 2.4542 |
| 13 | 3.27 | .. | H(12F)b | [x, -1+y, z | = | 1545.01] | | -92.14 | 57.00 | 0.51700 | -0.23180 | 0.32390 | 5.3981 | -3.1123 | 6.9484 |
| 14 | 3.27 | .. | H(12A)c | [1/2-x, -1/2+y, 1/2-z | = | 2545.01] | | 165.87 | 13.62 | 0.25200 | -0.04150 | 0.23200 | 2.3816 | -0.5572 | 4.9770 |
| 15 | 3.54 | .. | H(11C)c | [1/2-x, -1/2+y, 1/2-z | = | 2545.01] | | 174.80 | -29.98 | 0.22280 | -0.07860 | 0.11370 | 2.4135 | -1.0553 | 2.4391 |
| 16 | 3.57 | .. | H(22A)d | [3/2-x, -1/2+y, 1/2-z | = | 2645.02] | | 24.39 | 26.96 | 0.73900 | -0.00150 | 0.27150 | 8.3608 | -0.0201 | 5.8243 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(26A)

| | | | | | | | |
|-------------------|-----------|-------------------|-----------|-------------------|----------|-------------------|-----------|
| C(281) , <F(25A) | 36.1(6) | C(281) , <F(24A) | 36.3(7) | C(281) , C(28) | 36.7(5) | C(281) , C(27) | 66.8(7) |
| C(281) , C(212)a | 140.3(12) | C(281) , C(211)a | 143.4(12) | C(281) , C(29) | 26.9(6) | <F(25A) , <F(24A) | 59.4(7) |
| <F(25A) , C(28) | 62.8(6) | <F(25A) , C(27) | 84.3(7) | <F(25A) , C(212)a | 105.8(8) | <F(25A) , C(211)a | 120.4(9) |
| <F(25A) , C(29) | 57.8(5) | <F(24A) , C(28) | 62.9(7) | <F(24A) , C(27) | 92.6(7) | <F(24A) , C(212)a | 129.9(10) |
| <F(24A) , C(211)a | 114.4(9) | <F(24A) , C(29) | 51.4(6) | C(28) , C(27) | 30.9(2) | C(28) , C(212)a | 157.9(7) |
| C(28) , C(211)a | 174.7(7) | C(28) , C(29) | 11.58(17) | C(27) , C(212)a | 136.0(6) | C(27) , C(211)a | 149.8(7) |
| C(27) , C(29) | 42.31(18) | C(212)a , C(211)a | 27.28(13) | C(212)a , C(29) | 162.0(6) | C(211)a , C(29) | 165.5(6) |

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3.6 Angstrom Coordination Sphere Around Atom I = F(26B) [ARU = 1555.02] 0.46200 -0.09640 0.19020 5.1580 -1.2943 4.0802

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|-----------------------|-----------|----------|-------|---------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 1.320(16) | -- | C(281) | | | | Intra | 74.13 | -6.43 | 0.48874 | -0.00243 | 0.18331 | 5.5168 | -0.0326 | 3.9324 |
| 2 | 2.12(3) | << | <F(24B) | | | | Intra | 38.54 | -18.34 | 0.57910 | -0.00300 | 0.15910 | 6.7324 | -0.0403 | 3.4131 |
| 3 | 2.13(3) | << | <F(25B) | | | | Intra | 104.08 | -30.16 | 0.41300 | 0.03640 | 0.14040 | 4.7107 | 0.4887 | 3.0119 |
| 4 | 2.367(18) | << | C(28) | | | | Intra | 81.54 | 27.63 | 0.50031 | 0.05807 | 0.24136 | 5.4666 | 0.7797 | 5.1777 |
| 5 | 2.74(2) | << | C(27) | | | | Intra | 96.27 | 56.08 | 0.47711 | 0.01659 | 0.29600 | 4.9914 | 0.2227 | 6.3499 |
| 6 | 3.034(18) | .< | C(212)a | [x, -1+y, z | = | 1545.02] | | -107.91 | -19.93 | 0.37920 | -0.29852 | 0.14199 | 4.2811 | -4.0081 | 3.0460 |
| 7 | 3.224(17) | .. | C(211)a | [x, -1+y, z | = | 1545.02] | | -78.58 | -21.15 | 0.49490 | -0.31594 | 0.13597 | 5.7535 | -4.2420 | 2.9169 |
| 8 | 2.42 | << | H(27A) | | | | Intra | 124.79 | 72.36 | 0.45750 | -0.05150 | 0.29780 | 4.7392 | -0.6915 | 6.3885 |
| 9 | 2.58 | .< | H(21C)a | [x, -1+y, z | = | 1545.02] | | -62.59 | -23.68 | 0.53570 | -0.25260 | 0.14190 | 6.2456 | -3.3915 | 3.0441 |
| 10 | 2.71 | .. | H(21E)a | [x, -1+y, z | = | 1545.02] | | -113.74 | -2.27 | 0.37380 | -0.28100 | 0.18520 | 4.0679 | -3.7728 | 3.9730 |
| 11 | 2.81 | .. | H(21D)a | [x, -1+y, z | = | 1545.02] | | -120.04 | -35.40 | 0.35040 | -0.24390 | 0.11440 | 4.0126 | -3.2747 | 2.4542 |
| 12 | 3.01 | .. | H(12A)c | [1/2-x, -1/2+y, 1/2-z | = | 2545.01] | | 165.13 | 17.34 | 0.25200 | -0.04150 | 0.23200 | 2.3816 | -0.5572 | 4.9770 |
| 13 | 3.21 | .. | H(11C)c | [1/2-x, -1/2+y, 1/2-z | = | 2545.01] | | 175.02 | -30.78 | 0.22280 | -0.07860 | 0.11370 | 2.4135 | -1.0553 | 2.4391 |
| 14 | 3.40 | .. | H(12F)b | [x, -1+y, z | = | 1545.01] | | -82.48 | 57.41 | 0.51700 | -0.23180 | 0.32390 | 5.3981 | -3.1123 | 6.9484 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(26B)

| | | | | | | | |
|-------------------|-----------|-------------------|-----------|-------------------|-----------|-----------------|----------|
| C(281) , <F(24B) | 36.7(9) | C(281) , <F(25B) | 36.8(8) | C(281) , C(28) | 34.8(6) | C(281) , C(27) | 65.1(9) |
| C(281) , C(212)a | 153.6(16) | C(281) , C(211)a | 141.6(15) | <F(24B) , <F(25B) | 60.1(10) | <F(24B) , C(28) | 62.0(8) |
| <F(24B) , C(27) | 88.8(10) | <F(24B) , C(212)a | 129.5(12) | <F(24B) , C(211)a | 106.9(11) | <F(25B) , C(28) | 61.7(7) |
| <F(25B) , C(27) | 86.5(8) | <F(25B) , C(212)a | 121.2(12) | <F(25B) , C(211)a | 128.6(12) | C(28) , C(27) | 30.4(3) |
| C(28) , C(212)a | 168.4(11) | C(28) , C(211)a | 160.8(10) | C(27) , C(212)a | 139.6(9) | C(27) , C(211)a | 144.9(8) |
| C(212)a , C(211)a | 27.45(16) | | | | | | |

=====
Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6
=====

van der Waals (or ion) Radii used in the Analysis

=====

C H F N O S

1.70 1.20 1.47 1.55 1.52 1.80

:: Grid: X-Axis Step = 0.0167 = Points 60, Angstrom Step = 0.21

:: Grid: Y-Axis Step = 0.0139 = Points 72, Angstrom Step = 0.19

:: Grid: Z-Axis Step = 0.0093 = Points 108, Angstrom Step = 0.20

:: Unit cell Contains NO Residual Solvent Accessible Void.

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

=====
Report Expected Number of Independent Reflections for given Symmetry and Resolution.

:: Hmax = 17 Kmax = 18 Lmax= 30 , Sorting Order : Fast H, Medium K, Slow L

:: Actual Theta-Max: 30.032 Deg. (Applied Theta Limit: 30.032 Deg.)

Space Group H-M: P21/n Laue: 2/m
Space Group Hall: -P 2yn [Schoenflies: C2h^5]
Lattice Type: mP, Centric, Monoclinic, Multiplicity: 4(2), No: 14

Nr ***** Symmetry Operation(s) *****

| | | | |
|---|-----------|-----------|---------|
| 1 | H , | K , | L |
| 2 | 1/2 - H , | 1/2 + K , | 1/2 - L |
| 3 | - H , | - K , | - L |
| 4 | 1/2 + H , | 1/2 - K , | 1/2 + L |

:: Number of Independent Type H, K, L Reflections = 10562

Table 0 - Crystal Data and Details of the Structure Determination
for: tdacf30514P 21/n R = 0.05

Crystal Data

| | | | |
|--------------------------|--------------------|-------------|-----------|
| Formula | C15 H18 F6 N2 O2 S | | |
| Formula Weight | 404.38 | | |
| Crystal System | monoclinic | | |
| Space group | P21/n | (No. 14) | |
| a, b, c [Angstrom] | 12.5507(13) | 13.4265(14) | 21.715(2) |
| alpha, beta, gamma [deg] | 90 | 98.920(2) | 90 |
| V [Ang**3] | 3615.0(6) | | |
| Z | 8 | | |
| D(calc) [g/cm**3] | 1.486 | | |
| Mu(MoKa) [/mm] | 0.250 | | |
| F(000) | 1664 | | |
| Crystal Size [mm] | 0.68 x 0.78 x 1.20 | | |

Data Collection

| | | | |
|----------------------------------|-----------------------------|---------|-------|
| Temperature (K) | 150 | | |
| Radiation [Angstrom] | MoKa | 0.71073 | |
| Theta Min-Max [Deg] | 1.8, 30.0 | | |
| Dataset | -17: 17 ; -18: 18 ; -30: 30 | | |
| Tot., Uniq. Data, R(int) | 55289, | 10539, | 0.041 |
| Observed Data [I > 2.0 sigma(I)] | 7066 | | |

Refinement

| | | | |
|--|----------------------|--|--|
| Nref, Npar | 10539, 713 | | |
| R, wR2, S | 0.0509, 0.1331, 1.02 | | |
| w = ^2^(FO^2^)+(0.0496P)^2^+1.9419P] WHERE P=(FO^2^+2FC^2^)/3' | | | |
| Max. and Av. Shift/Error | 0.00, 0.00 | | |
| Min. and Max. Resd. Dens. [e/Ang^3] | -0.31, 0.48 | | |

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***** N O T I C E *****

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- PLATON Reference : Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.
Spek, A.L. (2009). Acta Cryst. D65, 148-155.

- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow

- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)

- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.

- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.

- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@uu.nl

- Recent versions of PLATON may be obtained from <http://www.platonsoft.nl/xraysoft>

- More INFO can be found on <http://http://www.platonsoft.nl/>

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Page 8 --- MOLSYM
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Page 49 --- INTER
Page 66 --- H-BONDS
Page 70 --- COORDN
Page 122 --- VOIDS
Page 123 --- EXPECT
Page 124 --- SUMMARY

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR
=====

W: NOMOVE option used.

:: >>> WARNING: 'CONNECTED INPUT SET' is assumed to be TRUE

:: >>> The Network Analysis may be INCORRECT when this assumption is FALSE

N: DISORDERED structure - ATOMS with Pop. .LT. 1.0 are not moved or as a group.

W: Structure contains 3 Intra H..H contacts < Sum(vdW-rad) -0.25 A (max -0.31)
=====

:: Input Xtal Data from File tdacf30514.cif - Data Type CIF13

:: NORMAL END of PLATON : 126 Pages on:

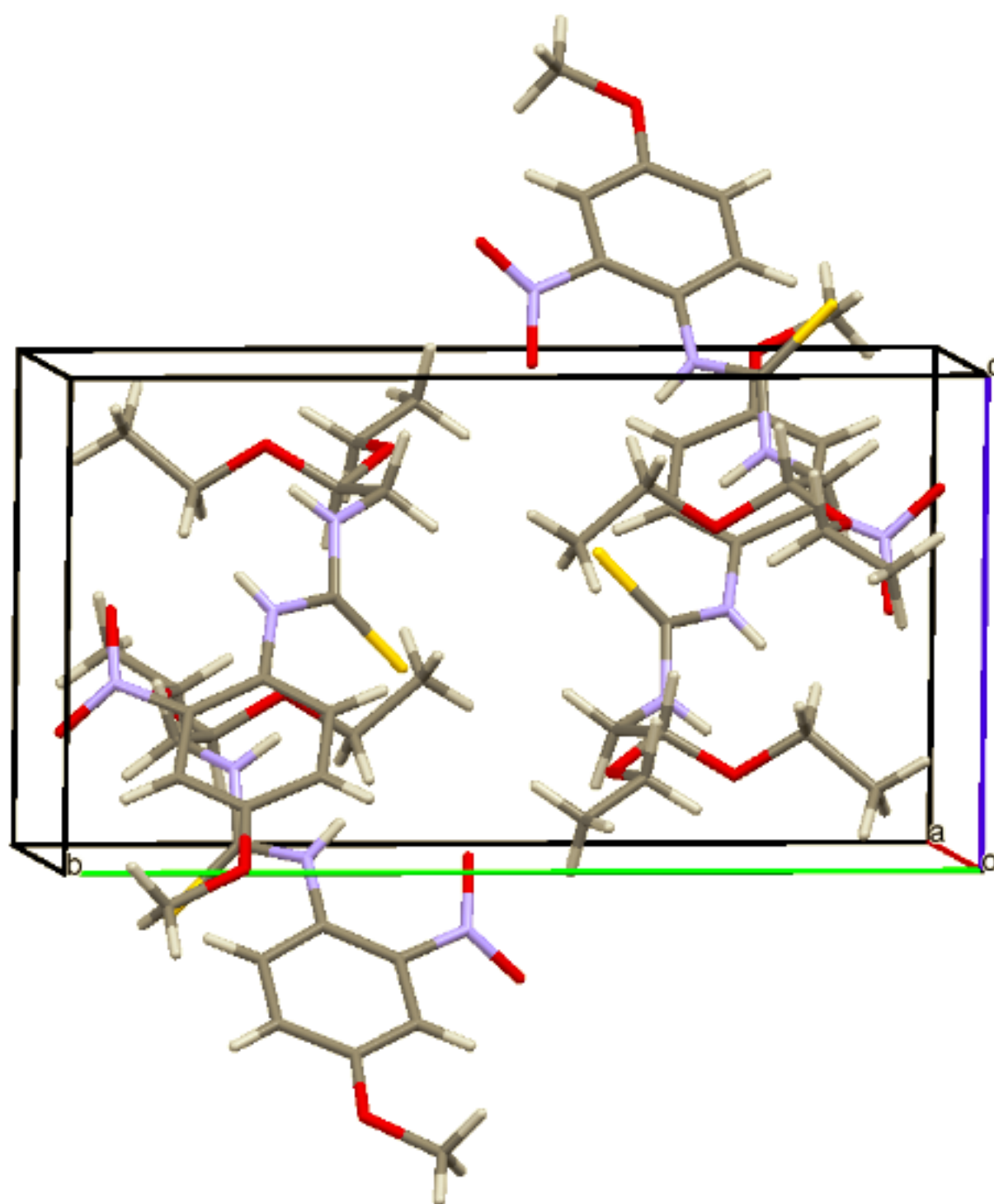
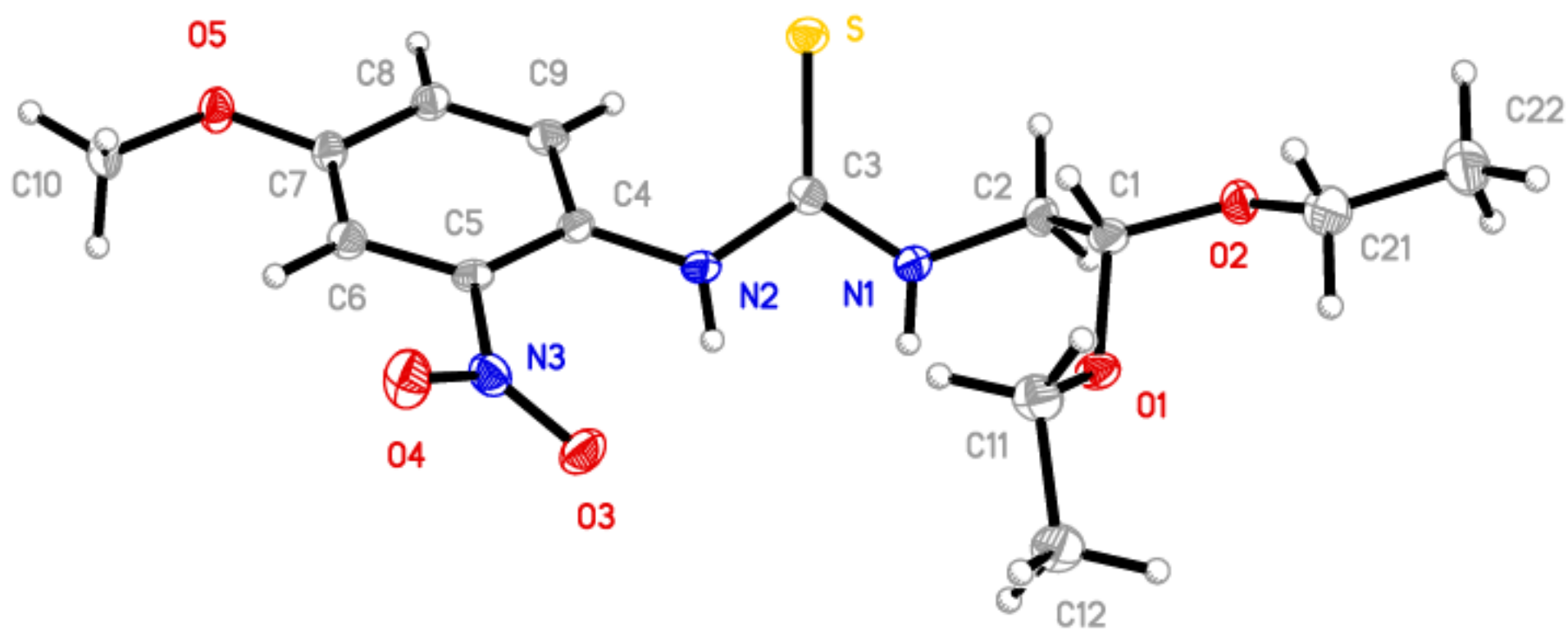
:: tdacf30514.lis (ASCII, 132 Characters Wide)

:: tdacf30514.lps (PostScript Version of .lis)

::.lps (PostScript Version of .lis)

::

H₂detu^{ArOMe,NO₂}



=====
 Analysis of Short Intra- and Inter-molecular Contacts , $d(I-J) < R(I) + R(J) + \text{Tolr}$, With Tolr = 0.2 Ang. ($X - I \dots J$) > 100. Deg.

Contact Radii : C H N O S
 (Angstrom) 1.70 1.20 1.55 1.52 1.80

Default Contact Radii are those given by A.Bondi, J.Phys.Chem. (1964),68,441. (or Coval. Rad. + 0.8 Ang. when not given)

* WARNING * : no Far-Reaching Conclusions should be drawn based on the Default Radii Assigned to Metals

Short "INTRA" Distances between two Atoms that are Separated by less than 4 Bonds are NOT Listed (Except for Potential D/A Contacts)

| At(I)[1555.01] | At(J) | [ARU(J)] | D(I-J) | SumRad | Del | Type | X(I) | Y(I) | Z(I) | X(J) | Y(J) | Z(J) | X | X - I...J | |
|----------------|-------|------------|------------|------------|------|-------|-------|--------|---------------|----------------------|----------------------|---------------|--------|------------|------------|
| S | | C(2) | [] | 3.124(3)<< | 3.50 | -0.38 | Intra | 0.8119 | 0.1243 | 0.0969 | 0.6784 | 0.1372-0.2518 | | | |
| S | | C(4) | [] | 3.177(3)<< | 3.50 | -0.32 | Intra | 0.8119 | 0.1243 | 0.0969 | 0.9690 | 0.2836 | 0.1083 | | |
| S | | C(9) | [] | 3.181(3)<< | 3.50 | -0.32 | Intra | 0.8119 | 0.1243 | 0.0969 | 1.0327 | 0.2147 | 0.1739 | | |
| S | | H(2A) | [] | 2.66<< | 3.00 | -0.34 | Intra | 0.8119 | 0.1243 | 0.0969 | 0.6849 | 0.0849-0.1800 | | | |
| S | | H(9A) | [] | 2.74<< | 3.00 | -0.26 | Intra | 0.8119 | 0.1243 | 0.0969 | 1.0187 | 0.1569 | 0.1317 | | |
| S | | C(10) | [2745.01] | 3.642(3) | 3.50 | 0.14 | | 0.8119 | 0.1243 | 0.0969 | 0.7523-0.0988-0.0525 | | C(3) | 115.09(10) | |
| S | | H(6A) | [2745.01] | 3.09 | 3.00 | 0.09 | | 0.8119 | 0.1243 | 0.0969 | 0.9101-0.0608 | 0.1556 | C(3) | 130 | |
| S | | H(10C) | [2745.01] | 2.97 < | 3.00 | -0.03 | | 0.8119 | 0.1243 | 0.0969 | 0.7335-0.0583 | 0.0279 | C(3) | 124 | |
| S | | O(3) | [4555.01] | 3.334(3) | 3.32 | 0.01 | | 0.8119 | 0.1243 | 0.0969 | 0.8857 | 0.0533 | 0.4770 | C(3) | 149.12(10) |
| S | | N(1) | [4555.01] | 3.348(3) < | 3.35 | 0.00 | | 0.8119 | 0.1243 | 0.0969 | 0.7634 | 0.3032 | 0.3036 | | |
| S | | N(2) | [4555.01] | 3.541(3) | 3.35 | 0.19 | | 0.8119 | 0.1243 | 0.0969 | 0.8863 | 0.2299 | 0.4773 | C(3) | 107.15(10) |
| S | | H(1) | [4555.01] | 2.52(3)<< | 3.00 | -0.48 | | 0.8119 | 0.1243 | 0.0969 | 0.7640 | 0.2589 | 0.2420 | | |
| S | | H(2) | [4555.01] | 2.80(3)<< | 3.00 | -0.20 | | 0.8119 | 0.1243 | 0.0969 | 0.8770 | 0.1943 | 0.4080 | C(3) | 111.2(5) |
| S | | H(12C) | [4555.01] | 3.03 | 3.00 | 0.03 | | 0.8119 | 0.1243 | 0.0969 | 0.5895 | 0.0729 | 0.0873 | C(3) | 111 |
| O(1) | | N(1) | [] | 2.776(3)<< | 3.07 | -0.29 | Intra | 0.5716 | 0.2620-0.3396 | 0.7634 | 0.1968-0.1964 | | C(11) | 107.86(16) | |
| O(1) | | C(21) | [] | 2.831(3)<< | 3.22 | -0.39 | Intra | 0.5716 | 0.2620-0.3396 | 0.3980 | 0.1540-0.3337 | | C(11) | 103.26(16) | |
| O(1) | | H(1) | [] | 2.53(3) < | 2.72 | -0.19 | Intra | 0.5716 | 0.2620-0.3396 | 0.7640 | 0.2411-0.2580 | | C(11) | 103.7(6) | |
| O(1) | | H(2B) | [] | 2.66 < | 2.72 | -0.06 | Intra | 0.5716 | 0.2620-0.3396 | 0.6811 | 0.1169-0.3629 | | C(11) | 150 | |
| O(1) | | H(12B) | [] | 2.54 < | 2.72 | -0.18 | Intra | 0.5716 | 0.2620-0.3396 | 0.4712 | 0.3980-0.4537 | | C(1) | 149 | |
| O(1) | | H(12C) | [] | 2.60 < | 2.72 | -0.12 | Intra | 0.5716 | 0.2620-0.3396 | 0.5895 | 0.4271-0.4127 | | C(1) | 162 | |
| O(1) | | H(21A) | [] | 2.53 < | 2.72 | -0.19 | Intra | 0.5716 | 0.2620-0.3396 | 0.3868 | 0.2096-0.3963 | | | | |
| O(1) | | H(1A) | [4554.01] | 2.58 < | 2.72 | -0.14 | | 0.5716 | 0.2620-0.3396 | 0.5674 | 0.3062-0.6379 | | C(1) | 136 | |
| | | | | | | | | | | | | | C(11) | 109 | |
| O(2) | | C(11) | [] | 3.367(4) | 3.22 | 0.15 | Intra | 0.5008 | 0.1234-0.3277 | 0.5518 | 0.3384-0.2508 | | | | |
| O(2) | | H(2A) | [] | 2.58 < | 2.72 | -0.14 | Intra | 0.5008 | 0.1234-0.3277 | 0.6849 | 0.0849-0.1800 | | C(21) | 154 | |
| O(2) | | H(2B) | [] | 2.46<< | 2.72 | -0.26 | Intra | 0.5008 | 0.1234-0.3277 | 0.6811 | 0.1169-0.3629 | | C(21) | 161 | |
| O(2) | | H(22B) | [] | 2.61 < | 2.72 | -0.11 | Intra | 0.5008 | 0.1234-0.3277 | 0.3320 | 0.0316-0.3455 | | C(1) | 153 | |
| O(2) | | H(22C) | [] | 2.55 < | 2.72 | -0.17 | Intra | 0.5008 | 0.1234-0.3277 | 0.3394 | 0.0707-0.5199 | | C(1) | 158 | |
| O(2) | | H(12A) | [2644.01] | 2.67 < | 2.72 | -0.05 | | 0.5008 | 0.1234-0.3277 | 0.4899-0.0343-0.1912 | | | C(1) | 118 | |
| | | | | | | | | | | | | | C(21) | 100 | |
| O(3) | | N(2) | [] | 2.677(3)<< | 3.07 | -0.39 | Intra | 0.8857 | 0.4466-0.0230 | 0.8863 | 0.2701-0.0227 | | | | |
| O(3) | | C(4) | [] | 2.842(4)<< | 3.22 | -0.38 | Intra | 0.8857 | 0.4466-0.0230 | 0.9690 | 0.2836 | 0.1083 | | | |
| O(3) | | H(2) | [] | 2.21(3)<< | 2.72 | -0.51 | Intra | 0.8857 | 0.4466-0.0230 | 0.8770 | 0.3057-0.0920 | | N(3) | 102.0(7) | |

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O(3) .... N(3) [ 3765.01]  3.200(3)  3.07  0.13      0.8857 0.4466-0.0230  1.0712 0.5566-0.1200
O(3) .... S   [ 4554.01]  3.334(3)  3.32  0.01      0.8857 0.4466-0.0230  0.8119 0.3756-0.4032  N(3)  156.90(17)
O(4) .... C(6) [         ]  2.720(4)<< 3.22 -0.50 Intra  0.9225 0.5018 0.2185  1.0762 0.3817 0.3006
O(4) .... H(6A) [         ]      2.46<< 2.72 -0.26 Intra  0.9225 0.5018 0.2185  1.0899 0.4392 0.3444
O(4) .... C(9) [ 2755.01]  3.373(4)  3.22  0.15      0.9225 0.5018 0.2185  0.9673 0.7147 0.3261  N(3)  147.26(19)
O(4) .... H(8A) [ 2755.01]      2.89  2.72  0.17      0.9225 0.5018 0.2185  0.8438 0.6788 0.1595  N(3)  129
O(4) .... H(9A) [ 2755.01]      2.71 < 2.72 -0.01      0.9225 0.5018 0.2185  0.9813 0.6569 0.3683  N(3)  153
O(4) .... H(10B) [ 3766.01]      2.61 < 2.72 -0.11      0.9225 0.5018 0.2185  0.8123 0.5755 0.4085  N(3)  147
O(5) .... H(6A) [         ]      2.66 < 2.72 -0.06 Intra  1.2232 0.3169 0.4799  1.0899 0.4392 0.3444
O(5) .... H(8A) [         ]      2.48<< 2.72 -0.24 Intra  1.2232 0.3169 0.4799  1.1562 0.1788 0.3405  C(10) 172
O(5) .... H(21A) [ 1656.01]      2.75  2.72  0.03      1.2232 0.3169 0.4799  1.3868 0.2096 0.6037  C(7)  136
                                            C(10)  106

O(5) .... C(8) [ 4555.01]  3.326(3)  3.22  0.11      1.2232 0.3169 0.4799  1.1149 0.2724 0.7971
O(5) .... C(9) [ 4555.01]  3.289(3)  3.22  0.07      1.2232 0.3169 0.4799  1.0327 0.2853 0.6739
N(1) .... O(1) [         ]  2.776(3)<< 3.07 -0.29 Intra  0.7634 0.1968-0.1964  0.5716 0.2620-0.3396  C(3)  134.7(2)
N(1) .... H(1A) [         ]      2.73 < 2.75 -0.02 Intra  0.7634 0.1968-0.1964  0.5674 0.1938-0.1379  C(3)  103
                                            H(1)  104

N(1) .... H(2) [         ]      2.29(3)<< 2.75 -0.46 Intra  0.7634 0.1968-0.1964  0.8770 0.3057-0.0920  C(2)  170.0(7)
N(1) .... S   [ 4554.01]  3.348(3) < 3.35  0.00      0.7634 0.1968-0.1964  0.8119 0.3756-0.4032  C(2)  123.53(16)
                                            C(3)  109.13(18)

N(1) .... C(4) [ 4554.01]  3.449(4)  3.25  0.20      0.7634 0.1968-0.1964  0.9690 0.2164-0.3917  C(2)  122.44(17)
N(2) .... O(3) [         ]  2.677(3)<< 3.07 -0.39 Intra  0.8863 0.2701-0.0227  0.8857 0.4466-0.0230  C(3)  141.2(2)
N(2) .... N(3) [         ]  2.898(4)<< 3.10 -0.20 Intra  0.8863 0.2701-0.0227  0.9288 0.4434 0.1200  C(3)  146.9(2)
N(2) .... H(1) [         ]      2.35(3)<< 2.75 -0.40 Intra  0.8863 0.2701-0.0227  0.7640 0.2411-0.2580  C(4)  173.0(7)
N(2) .... H(9A) [         ]      2.61 < 2.75 -0.14 Intra  0.8863 0.2701-0.0227  1.0187 0.1569 0.1317  H(2)  144
N(2) .... S   [ 4554.01]  3.541(3)  3.35  0.19      0.8863 0.2701-0.0227  0.8119 0.3756-0.4032  C(4)  132.72(17)
N(3) .... N(2) [         ]  2.898(4)<< 3.10 -0.20 Intra  0.9288 0.4434 0.1200  0.8863 0.2701-0.0227  O(4)  154.4(2)
N(3) .... H(2) [         ]      2.74(3) < 2.75 -0.01 Intra  0.9288 0.4434 0.1200  0.8770 0.3057-0.0920  O(4)  161.2(6)
N(3) .... H(6A) [         ]      2.56 < 2.75 -0.19 Intra  0.9288 0.4434 0.1200  1.0899 0.4392 0.3444  O(3)  152
N(3) .... O(3) [ 3765.01]  3.200(3)  3.07  0.13      0.9288 0.4434 0.1200  1.1143 0.5533 0.0230
C(1) .... C(3) [         ]  3.377(4) < 3.40 -0.02 Intra  0.5761 0.1821-0.2517  0.8209 0.1998-0.0470  O(2)  144.60(18)
C(1) .... H(1) [         ]      2.65(3)<< 2.90 -0.25 Intra  0.5761 0.1821-0.2517  0.7640 0.2411-0.2580  O(2)  142.7(6)
                                            H(1A)  104

C(1) .... H(11A) [         ]      2.70<< 2.90 -0.20 Intra  0.5761 0.1821-0.2517  0.6127 0.3523-0.1662  O(2)  144
                                            C(2)  108

C(1) .... H(11B) [         ]      2.55<< 2.90 -0.35 Intra  0.5761 0.1821-0.2517  0.4926 0.3275-0.1971  O(2)  110
                                            C(2)  144

C(1) .... H(21A) [         ]      2.60<< 2.90 -0.30 Intra  0.5761 0.1821-0.2517  0.3868 0.2096-0.3963  C(2)  149
C(1) .... H(21B) [         ]      2.58<< 2.90 -0.32 Intra  0.5761 0.1821-0.2517  0.3866 0.1656-0.2225  O(1)  101
                                            C(2)  147

C(2) .... S   [         ]  3.124(3)<< 3.50 -0.38 Intra  0.6784 0.1372-0.2518  0.8119 0.1243 0.0969  C(1)  111.92(15)
                                            H(2B)  138

C(2) .... C(11) [         ]  3.481(4)  3.40  0.08 Intra  0.6784 0.1372-0.2518  0.5518 0.3384-0.2508  H(2A)  133
                                            H(2B)  112

C(3) .... C(1) [         ]  3.377(4) < 3.40 -0.02 Intra  0.8209 0.1998-0.0470  0.5761 0.1821-0.2517  N(2)  131.16(19)
C(3) .... C(9) [         ]  3.061(4)<< 3.40 -0.34 Intra  0.8209 0.1998-0.0470  1.0327 0.2147 0.1739  N(1)  149.5(2)
C(3) .... H(2A) [         ]      2.60<< 2.90 -0.30 Intra  0.8209 0.1998-0.0470  0.6849 0.0849-0.1800  N(2)  163
C(3) .... H(9A) [         ]      2.83 < 2.90 -0.07 Intra  0.8209 0.1998-0.0470  1.0187 0.1569 0.1317  N(1)  142

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C(3)   .... H(1)   [ 4555.01]   2.82(3) < 2.90 -0.08   0.8209 0.1998-0.0470   0.7640 0.2589 0.2420   N(1)   128.3(6)
C(4)   .... S     [       ]   3.177(3)<< 3.50 -0.32 Intra 0.9690 0.2836 0.1083   0.8119 0.1243 0.0969   C(5)   142.86(19)
C(4)   .... O(3)  [       ]   2.842(4)<< 3.22 -0.38 Intra 0.9690 0.2836 0.1083   0.8857 0.4466-0.0230   C(9)   165.8(2)
C(4)   .... C(7)  [       ]   2.804(4)<< 3.40 -0.60 Intra 0.9690 0.2836 0.1083   1.1386 0.3114 0.3595   N(2)   177.7(2)
C(4)   .... N(1)  [ 4555.01]   3.449(4)   3.25  0.20   0.9690 0.2836 0.1083   0.7634 0.3032 0.3036   C(9)   110.54(17)
C(4)   .... C(8)  [ 4554.01]   3.538(4)   3.40  0.14   0.9690 0.2836 0.1083   1.1149 0.2724-0.2029   C(5)   103.29(17)
C(5)   .... C(8)  [       ]   2.725(4)<< 3.40 -0.68 Intra 0.9931 0.3662 0.1758   1.1149 0.2276 0.2971   N(3)   176.59(19)
C(5)   .... H(2)  [       ]   2.64(3)<< 2.90 -0.26 Intra 0.9931 0.3662 0.1758   0.8770 0.3057-0.0920   C(6)   162.4(6)
C(6)   .... O(4)  [       ]   2.720(4)<< 3.22 -0.50 Intra 1.0762 0.3817 0.3006   0.9225 0.5018 0.2185   C(7)   167.2(2)
C(6)   .... C(9)  [       ]   2.764(4)<< 3.40 -0.64 Intra 1.0762 0.3817 0.3006   1.0327 0.2147 0.1739   H(6A)   179
C(6)   .... C(10) [       ]   2.808(4)<< 3.40 -0.59 Intra 1.0762 0.3817 0.3006   1.2477 0.4012 0.5525   C(5)   176.2(2)
C(6)   .... H(10B) [       ]   2.68<< 2.90 -0.22 Intra 1.0762 0.3817 0.3006   1.1877 0.4245 0.5915   C(5)   162
C(6)   .... H(10C) [       ]   2.80 < 2.90 -0.10 Intra 1.0762 0.3817 0.3006   1.2665 0.4417 0.4721   C(5)   161
C(6)   .... H(9A)  [ 4555.01]   3.08   2.90  0.18   1.0762 0.3817 0.3006   1.0187 0.3431 0.6317   C(5)   111
C(7)   .... C(4)  [       ]   2.804(4)<< 3.40 -0.60 Intra 1.1386 0.3114 0.3595   0.9690 0.2836 0.1083   O(5)   174.7(2)
C(7)   .... H(10B) [       ]   2.58<< 2.90 -0.32 Intra 1.1386 0.3114 0.3595   1.1877 0.4245 0.5915   C(8)   154
C(7)   .... H(10C) [       ]   2.66<< 2.90 -0.24 Intra 1.1386 0.3114 0.3595   1.2665 0.4417 0.4721   C(8)   154
C(7)   .... C(9)  [ 4555.01]   3.242(4) < 3.40 -0.16   1.1386 0.3114 0.3595   1.0327 0.2853 0.6739
C(7)   .... H(9A)  [ 4555.01]   3.06   2.90  0.16   1.1386 0.3114 0.3595   1.0187 0.3431 0.6317   C(8)   108
C(8)   .... C(5)  [       ]   2.725(4)<< 3.40 -0.68 Intra 1.1149 0.2276 0.2971   0.9931 0.3662 0.1758   H(8A)   179
C(8)   .... O(5)  [ 4554.01]   3.326(3)   3.22  0.11   1.1149 0.2276 0.2971   1.2232 0.1831-0.0201   C(7)   112.77(17)
C(8)   .... C(4)  [ 4555.01]   3.538(4)   3.40  0.14   1.1149 0.2276 0.2971   0.9690 0.2164 0.6083
C(8)   .... C(10) [ 4554.01]   3.536(4)   3.40  0.14   1.1149 0.2276 0.2971   1.2477 0.0988 0.0525   C(7)   128.56(18)
C(9)   .... S     [       ]   3.181(3)<< 3.50 -0.32 Intra 1.0327 0.2147 0.1739   0.8119 0.1243 0.0969   C(8)   141.69(18)
C(9)   .... C(3)  [       ]   3.061(4)<< 3.40 -0.34 Intra 1.0327 0.2147 0.1739   0.8209 0.1998-0.0470   C(8)   167.3(2)
C(9)   .... C(6)  [       ]   2.764(4)<< 3.40 -0.64 Intra 1.0327 0.2147 0.1739   1.0762 0.3817 0.3006   H(9A)   179
C(9)   .... H(2)  [       ]   3.06(3)   2.90  0.16 Intra 1.0327 0.2147 0.1739   0.8770 0.3057-0.0920   C(8)   144.7(5)
C(9)   .... O(4)  [ 2745.01]   3.373(4)   3.22  0.15   1.0327 0.2147 0.1739   1.0775 0.0018 0.2815   C(4)   152.68(19)
C(9)   .... O(5)  [ 4554.01]   3.289(3)   3.22  0.07   1.0327 0.2147 0.1739   1.2232 0.1831-0.0201   C(4)   112.21(17)
C(9)   .... C(7)  [ 4554.01]   3.242(4) < 3.40 -0.16   1.0327 0.2147 0.1739   1.1386 0.1886-0.1405   C(8)   103.21(18)
C(10)  .... C(6)  [       ]   2.808(4)<< 3.40 -0.59 Intra 1.2477 0.4012 0.5525   1.0762 0.3817 0.3006   H(10A)   168
C(10)  .... H(6A)  [       ]   2.52<< 2.90 -0.38 Intra 1.2477 0.4012 0.5525   1.0899 0.4392 0.3444   H(10A)   170
C(10)  .... H(12B) [ 1656.01]   2.97   2.90  0.07   1.2477 0.4012 0.5525   1.4712 0.3980 0.5463   H(10B)   152
C(10)  .... S     [ 2755.01]   3.642(3)   3.50  0.14   1.2477 0.4012 0.5525   1.1881 0.6244 0.4031   O(5)   131.94(15)
                                           H(10A)   116
C(10)  .... H(2A) [ 2755.01]   3.06   2.90  0.16   1.2477 0.4012 0.5525   1.3151 0.5849 0.6800   O(5)   174
C(10)  .... C(8)  [ 4555.01]   3.536(4)   3.40  0.14   1.2477 0.4012 0.5525   1.1149 0.2724 0.7971   H(10C)   165
C(11)  .... O(2)  [       ]   3.367(4)   3.22  0.15 Intra 0.5518 0.3384-0.2508   0.5008 0.1234-0.3277   C(12)   127.42(19)
                                           H(11A)   117
C(11)  .... C(2)  [       ]   3.481(4)   3.40  0.08 Intra 0.5518 0.3384-0.2508   0.6784 0.1372-0.2518   C(12)   135.07(19)
                                           H(11B)   106
C(11)  .... C(21) [       ]   3.451(4)   3.40  0.05 Intra 0.5518 0.3384-0.2508   0.3980 0.1540-0.3337   C(12)   116.69(19)
                                           H(11A)   133
C(11)  .... H(1A) [       ]   2.38<< 2.90 -0.52 Intra 0.5518 0.3384-0.2508   0.5674 0.1938-0.1379   C(12)   163
C(11)  .... H(21A) [       ]   3.01   2.90  0.11 Intra 0.5518 0.3384-0.2508   0.3868 0.2096-0.3963   C(12)   101
                                           H(11A)   149
C(12)  .... H(10A) [ 1454.01]   2.99   2.90  0.09   0.5287 0.4138-0.3664   0.3055 0.3953-0.3560   H(12C)   157
C(12)  .... H(22B) [ 2654.01]   2.92   2.90  0.02   0.5287 0.4138-0.3664   0.6680 0.5316-0.1545   H(12B)   156
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H(6A)  .... S    [ 2755.01]      3.09  3.00  0.09      1.0899 0.4392 0.3444  1.1881 0.6244 0.4031  C(6)      160
H(8A)  .... O(5)  [          ]      2.48<< 2.72 -0.24 Intra  1.1562 0.1788 0.3405  1.2232 0.3169 0.4799
H(8A)  .... C(22) [ 1656.01]      3.09  2.90  0.19      1.1562 0.1788 0.3405  1.3245 0.0848 0.5870  C(8)      155
H(8A)  .... H(9A) [          ]      2.30 < 2.40 -0.10 Intra  1.1562 0.1788 0.3405  1.0187 0.1569 0.1317
H(8A)  .... H(22A) [ 1656.01]      2.40  2.40  0.00      1.1562 0.1788 0.3405  1.2539 0.1070 0.5746  C(8)      148
H(8A)  .... O(4)  [ 2745.01]      2.89  2.72  0.17      1.1562 0.1788 0.3405  1.0775 0.0018 0.2815  C(8)      120
H(9A)  .... S    [          ]      2.74<< 3.00 -0.26 Intra  1.0187 0.1569 0.1317  0.8119 0.1243 0.0969  C(9)      109
H(9A)  .... N(2)  [          ]      2.61 < 2.75 -0.14 Intra  1.0187 0.1569 0.1317  0.8863 0.2701-0.0227
H(9A)  .... C(3)  [          ]      2.83 < 2.90 -0.07 Intra  1.0187 0.1569 0.1317  0.8209 0.1998-0.0470
H(9A)  .... H(8A) [          ]      2.30 < 2.40 -0.10 Intra  1.0187 0.1569 0.1317  1.1562 0.1788 0.3405
H(9A)  .... O(4)  [ 2745.01]      2.71 < 2.72 -0.01      1.0187 0.1569 0.1317  1.0775 0.0018 0.2815  C(9)      127
H(9A)  .... C(6)  [ 4554.01]      3.08  2.90  0.18      1.0187 0.1569 0.1317  1.0762 0.1183-0.1994  C(9)      117
H(9A)  .... C(7)  [ 4554.01]      3.06  2.90  0.16      1.0187 0.1569 0.1317  1.1386 0.1886-0.1405
H(10A) .... C(12) [ 1656.01]      2.99  2.90  0.09      1.3055 0.3953 0.6440  1.5287 0.4138 0.6336  C(10)     127
H(10A) .... H(12B) [ 1656.01]      2.49  2.40  0.09      1.3055 0.3953 0.6440  1.4712 0.3980 0.5463  C(10)     110
H(10B) .... C(6)  [          ]      2.68<< 2.90 -0.22 Intra  1.1877 0.4245 0.5915  1.0762 0.3817 0.3006
H(10B) .... C(7)  [          ]      2.58<< 2.90 -0.32 Intra  1.1877 0.4245 0.5915  1.1386 0.3114 0.3595
H(10B) .... H(6A) [          ]      2.24 < 2.40 -0.16 Intra  1.1877 0.4245 0.5915  1.0899 0.4392 0.3444
H(10B) .... O(4)  [ 3766.01]      2.61 < 2.72 -0.11      1.1877 0.4245 0.5915  1.0775 0.4982 0.7815  C(10)     160
H(10C) .... C(6)  [          ]      2.80 < 2.90 -0.10 Intra  1.2665 0.4417 0.4721  1.0762 0.3817 0.3006
H(10C) .... C(7)  [          ]      2.66<< 2.90 -0.24 Intra  1.2665 0.4417 0.4721  1.1386 0.3114 0.3595
H(10C) .... H(6A) [          ]      2.38 < 2.40 -0.02 Intra  1.2665 0.4417 0.4721  1.0899 0.4392 0.3444
H(10C) .... S    [ 2755.01]      2.97 < 3.00 -0.03      1.2665 0.4417 0.4721  1.1881 0.6244 0.4031  C(10)     126
H(11A) .... C(1)  [          ]      2.70<< 2.90 -0.20 Intra  0.6127 0.3523-0.1662  0.5761 0.1821-0.2517
H(11A) .... H(1A) [          ]      2.50  2.40  0.10 Intra  0.6127 0.3523-0.1662  0.5674 0.1938-0.1379
H(11A) .... H(12A) [          ]      2.37 < 2.40 -0.03 Intra  0.6127 0.3523-0.1662  0.5101 0.4657-0.3088
H(11A) .... H(12C) [          ]      2.33 < 2.40 -0.07 Intra  0.6127 0.3523-0.1662  0.5895 0.4271-0.4127
H(11A) .... H(2B) [ 4555.01]      2.58  2.40  0.18      0.6127 0.3523-0.1662  0.6811 0.3831 0.1371  C(11)     146
H(11B) .... C(1)  [          ]      2.55<< 2.90 -0.35 Intra  0.4926 0.3275-0.1971  0.5761 0.1821-0.2517
H(11B) .... C(21) [          ]      3.04  2.90  0.14 Intra  0.4926 0.3275-0.1971  0.3980 0.1540-0.3337  C(11)     106
H(11B) .... H(1A) [          ]      2.27 < 2.40 -0.13 Intra  0.4926 0.3275-0.1971  0.5674 0.1938-0.1379
H(11B) .... H(12A) [          ]      2.33 < 2.40 -0.07 Intra  0.4926 0.3275-0.1971  0.5101 0.4657-0.3088
H(11B) .... H(12B) [          ]      2.37 < 2.40 -0.03 Intra  0.4926 0.3275-0.1971  0.4712 0.3980-0.4537
H(12A) .... H(11A) [          ]      2.37 < 2.40 -0.03 Intra  0.5101 0.4657-0.3088  0.6127 0.3523-0.1662
H(12A) .... H(11B) [          ]      2.33 < 2.40 -0.07 Intra  0.5101 0.4657-0.3088  0.4926 0.3275-0.1971
H(12A) .... O(2)  [ 2654.01]      2.67 < 2.72 -0.05      0.5101 0.4657-0.3088  0.4992 0.6234-0.1723  C(12)     166
H(12A) .... H(22B) [ 2654.01]      2.45  2.40  0.05      0.5101 0.4657-0.3088  0.6680 0.5316-0.1545  C(12)     109
H(12B) .... O(1)  [          ]      2.54 < 2.72 -0.18 Intra  0.4712 0.3980-0.4537  0.5716 0.2620-0.3396
H(12B) .... C(10) [ 1454.01]      2.97  2.90  0.07      0.4712 0.3980-0.4537  0.2477 0.4012-0.4475  C(12)     128
H(12B) .... H(10A) [ 1454.01]      2.49  2.40  0.09      0.4712 0.3980-0.4537  0.3055 0.3953-0.3560  C(12)     111
H(12B) .... H(11B) [          ]      2.37 < 2.40 -0.03 Intra  0.4712 0.3980-0.4537  0.4926 0.3275-0.1971
H(12B) .... H(1A) [ 4554.01]      2.59  2.40  0.19      0.4712 0.3980-0.4537  0.5674 0.3062-0.6379  C(12)     100
H(12B) .... H(21B) [ 4554.01]      2.51  2.40  0.11      0.4712 0.3980-0.4537  0.3866 0.3344-0.7225  C(12)     156
H(12C) .... O(1)  [          ]      2.60 < 2.72 -0.12 Intra  0.5895 0.4271-0.4127  0.5716 0.2620-0.3396
H(12C) .... H(11A) [          ]      2.33 < 2.40 -0.07 Intra  0.5895 0.4271-0.4127  0.6127 0.3523-0.1662
H(12C) .... S    [ 4554.01]      3.03  3.00  0.03      0.5895 0.4271-0.4127  0.8119 0.3756-0.4032  C(12)     144
H(21A) .... O(1)  [          ]      2.53 < 2.72 -0.19 Intra  0.3868 0.2096-0.3963  0.5716 0.2620-0.3396
H(21A) .... O(5)  [ 1454.01]      2.75  2.72  0.03      0.3868 0.2096-0.3963  0.2232 0.3169-0.5201  C(21)     137
=====

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=====
H(21A) .... C(1) [ ] 2.60<< 2.90 -0.30 Intra 0.3868 0.2096-0.3963 0.5761 0.1821-0.2517
H(21A) .... C(11) [ ] 3.01 2.90 0.11 Intra 0.3868 0.2096-0.3963 0.5518 0.3384-0.2508 C(21) 108
H(21A) .... H(22A) [ ] 2.33 < 2.40 -0.07 Intra 0.3868 0.2096-0.3963 0.2539 0.1070-0.4254
H(21A) .... H(22C) [ ] 2.38 < 2.40 -0.02 Intra 0.3868 0.2096-0.3963 0.3394 0.0707-0.5199
H(21B) .... C(1) [ ] 2.58<< 2.90 -0.32 Intra 0.3866 0.1656-0.2225 0.5761 0.1821-0.2517
H(21B) .... H(1A) [ ] 2.40 2.40 0.00 Intra 0.3866 0.1656-0.2225 0.5674 0.1938-0.1379
H(21B) .... H(22A) [ ] 2.37 < 2.40 -0.03 Intra 0.3866 0.1656-0.2225 0.2539 0.1070-0.4254
H(21B) .... H(22B) [ ] 2.33 < 2.40 -0.07 Intra 0.3866 0.1656-0.2225 0.3320 0.0316-0.3455
H(21B) .... H(12B) [ 4555.01] 2.51 2.40 0.11 0.3866 0.1656-0.2225 0.4712 0.1020 0.0463 C(21) 131
H(22A) .... H(8A) [ 1454.01] 2.40 2.40 0.00 0.2539 0.1070-0.4254 0.1562 0.1788-0.6595 C(22) 127
H(22A) .... H(21A) [ ] 2.33 < 2.40 -0.07 Intra 0.2539 0.1070-0.4254 0.3868 0.2096-0.3963
H(22A) .... H(21B) [ ] 2.37 < 2.40 -0.03 Intra 0.2539 0.1070-0.4254 0.3866 0.1656-0.2225
H(22B) .... O(2) [ ] 2.61 < 2.72 -0.11 Intra 0.3320 0.0316-0.3455 0.5008 0.1234-0.3277
H(22B) .... H(21B) [ ] 2.33 < 2.40 -0.07 Intra 0.3320 0.0316-0.3455 0.3866 0.1656-0.2225
H(22B) .... C(12) [ 2644.01] 2.92 2.90 0.02 0.3320 0.0316-0.3455 0.4713-0.0862-0.1336 C(22) 147
H(22B) .... H(12A) [ 2644.01] 2.45 2.40 0.05 0.3320 0.0316-0.3455 0.4899-0.0343-0.1912 C(22) 129
H(22C) .... O(2) [ ] 2.55 < 2.72 -0.17 Intra 0.3394 0.0707-0.5199 0.5008 0.1234-0.3277
H(22C) .... H(21A) [ ] 2.38 < 2.40 -0.02 Intra 0.3394 0.0707-0.5199 0.3868 0.2096-0.3963
=====

```

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 1 to Neighbouring ARU'S

```

=====
Nr      ARU      Nr.Cont.  d(min)  Del  XHn X      - At(I)      At(J) - Y      YHn  Note  Partaking ARU's in Close Contact Resd.
-----
1 [ 2745.01] 7 2.7100 -0.01 1 C(9) - H(9A) ... O(4) -N(3) 0 < 2745.01
2 [ 4555.01] 20 2.5100 0.11 2 C(21) - H(21B) ... H(12B) -C(12) 3 4555.01
3 [ 4554.01] 20 2.5100 0.11 3 C(12) - H(12B) ... H(21B) -C(21) 2 4554.01
4 [ 2644.01] 3 2.4500 0.05 3 C(22) - H(22B) ... H(12A) -C(12) 3 2644.01
5 [ 3765.01] 2 3.2000 0.13 0 O(3) - N(3) ... O(3) -N(3) 0 3765.01
6 [ 2755.01] 7 2.7100 -0.01 0 N(3) - O(4) ... H(9A) -C(9) 1 < 2755.01
7 [ 3766.01] 2 2.6100 -0.11 3 C(10) - H(10B) ... O(4) -N(3) 0 < 3766.01
8 [ 1656.01] 6 2.4000 0.00 1 C(8) - H(8A) ... H(22A) -C(22) 3 1656.01
9 [ 1454.01] 6 2.4000 0.00 3 C(22) - H(22A) ... H(8A) -C(8) 1 1454.01
10 [ 2654.01] 3 2.4500 0.05 3 C(12) - H(12A) ... H(22B) -C(22) 3 2654.01
11 [ 3664.01] 1 3.4350 0.03 2 C(11) - C(12) ... C(12) -C(11) 2 3664.01
=====

```

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Asymmetric Residue Unit (= ARU) Code List

=====

```

-----
ARU-CODE      CIF-CODE      Symmetry-Code      sym TX TY TZ Ires      x(cen)      y(cen)      z(cen)
-----

```

```

=====
[ 2745.01] = [ 2_745] =2-x, -1/2+y, 1/2-z          = [ 2 2 -1 0 1 ]      1.229   -0.229   0.543
[ 4555.01] = [ 4_566] =x, 1/2-y, 1/2+z            = [ 4 0 0 0 1 ]      0.771    0.229   0.457
[ 4554.01] = [ 4_565] =x, 1/2-y, -1/2+z          = [ 4 0 0 -1 1 ]     0.771    0.229  -0.543
[ 2644.01] = [ 2_644] =1-x, -1/2+y, -1/2-z       = [ 2 1 -1 -1 1 ]     0.229   -0.229  -0.457
[ 3765.01] = [ 3_765] =2-x, 1-y, -z              = [ 3 2 1 0 1 ]      1.229    0.729   0.043
[ 2755.01] = [ 2_755] =2-x, 1/2+y, 1/2-z         = [ 2 2 0 0 1 ]      1.229    0.771   0.543
[ 3766.01] = [ 3_766] =2-x, 1-y, 1-z             = [ 3 2 1 1 1 ]      1.229    0.729   1.043
[ 1656.01] = [ 1_656] =1+x, y, 1+z               = [ 1 1 0 1 1 ]      1.771    0.271   0.957
[ 1454.01] = [ 1_454] =-1+x, y, -1+z             = [ 1 -1 0 -1 1 ]    -0.229   0.271  -1.043
[ 2654.01] = [ 2_654] =1-x, 1/2+y, -1/2-z       = [ 2 1 0 -1 1 ]     0.229    0.771  -0.457
[ 3664.01] = [ 3_664] =1-x, 1-y, -1-z           = [ 3 1 1 -1 1 ]     0.229    0.729  -0.957
=====

```

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

$X(J) = X(sym) + TX$, $Y(J) = Y(sym) + TY$, $Z(J) = Z(sym) + TZ$,
 SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

=====
 Analysis of Potential Hydrogen Bonds and Schemes with $d(D...A) < R(D)+R(A)+0.50$, $d(H...A) < R(H)+R(A)-0.12$ Ang., $D-H...A > 100.0$ Deg
 =====

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
 =====

| Nr | Typ | Res | Donor | H...A | Acceptor | [ARU] | D - H | H...A | D...A | D - H...A | A..H..A* | A'..H..A" | Sum(XY,YZ) | Sum(XZ) |
|----|-------|-----|-------|---------|----------|------------|---------|---------|----------|-----------|----------|-----------|------------|---------|
| 1 | | 1 | N(1) | --H(1) | ..S | [4554.01] | 0.85(3) | 2.52(3) | 3.348(3) | 166(2) | | | | |
| 2 | Intra | 1 | N(2) | --H(2) | ..O(3) | [] | 0.79(3) | 2.21(3) | 2.677(3) | 119(2) | | | | |
| 3 | | 1 | N(2) | --H(2) | ..S | [4554.01] | 0.79(3) | 2.80(2) | 3.541(3) | 158(2)' | 82.5(8)' | | 360(3) | |
| 4 | | 1 | C(1) | --H(1A) | ..O(1) | [4555.01] | 1.00 | 2.58 | 3.574(3) | 171 | | | | |
| 5 | Intra | 1 | C(2) | --H(2A) | ..S | [] | 0.99 | 2.66 | 3.124(3) | 109 | | | | |
| 6 | Intra | 1 | C(9) | --H(9A) | ..S | [] | 0.95 | 2.74 | 3.181(3) | 109 | | | | |

Translation of ARU-Code to CIF and Equivalent Position Code
 =====

[4555.] = [4_566] =x,1/2-y,1/2+z
 [4554.] = [4_565] =x,1/2-y,-1/2+z

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]
 =====

2-Centre (linear) D-H...X most prob. angle 160 deg - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
 3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg Springer-Verlag, Berlin, 1991, pp 20.
 4-Centre (trifurcated)

Analysis of Potential Donor/Acceptor Atoms -- (Major Disorder Form Only)
 =====

| At.Nr | D/A | #Cov.Bonds | # H | #D-H..A | #A..H | #A..H-C | Sum(A-H) | Sum(A-X) |
|-------|------|------------|-----|---------|-------|---------|----------|----------|
| 1 | S | 1 | - | 0 | 2 | 2 | 4 | 5 |
| 2 | O(1) | 2 | - | 0 | 0 | 1 | 1 | 3 |
| 3 | O(2) | 2 | - | 0 | 0 | 0 | 0 | 2 |
| 4 | O(3) | 1 | - | 0 | 1 | 0 | 1 | 2 |
| 5 | O(4) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 6 | O(5) | 2 | - | 0 | 0 | 0 | 0 | 2 |
| 7 | N(1) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 8 | N(2) | 3 | 1 H | 2 | 0 | 0 | 2 | 4 |
| 9 | N(3) | 3 | - | 0 | 0 | 0 | 0 | 3 |

=====
 Analysis of Hydrogen Bonded Molecular Aggregates (See also Acta Cryst. B36, 1980, 2113 - 2115) -- (Major Disorder Component Only)
 =====

Coordinates of Donor and Acceptor Atoms
 =====

Coordinates of D/A-Bonded Atom(s)
 =====

| D/A I | [ARU] | X | Y | Z | -- | D/A J | [ARU] | X | Y | Z | Atom K | X | Y | Z | I..J--K Angle |
|-------|-------------|--------|--------|--------|----|-------|-------------|--------|--------|--------|--------|--------|--------|--------|---------------|
| N(1) | [1555.01], | 0.7634 | 0.1968 | 0.1964 | >> | S | [4554.01], | 0.8119 | 0.3756 | 0.4031 | C(3) | 0.8209 | 0.3002 | 0.5470 | 82.47(8) |
| S | [1555.01], | 0.8119 | 0.1243 | 0.0969 | << | N(1) | [4555.01], | 0.7634 | 0.3032 | 0.3036 | C(2) | 0.6784 | 0.3628 | 0.2482 | 123.53(8) |
| | | | | | | | | | | | C(3) | 0.8209 | 0.3002 | 0.4530 | 109.13(9) |
| | | | | | | | | | | | H(1) | 0.7640 | 0.2589 | 0.2420 | 10.82(13) |
| N(2) | [1555.01], | 0.8863 | 0.2701 | 0.0227 | >> | O(3) | [1555.01], | 0.8857 | 0.4466 | 0.0230 | N(3) | 0.9288 | 0.4434 | 0.1200 | 87.60(11) |
| O(3) | [1555.01], | 0.8857 | 0.4466 | 0.0230 | << | N(2) | [1555.01], | 0.8863 | 0.2701 | 0.0227 | C(3) | 0.8209 | 0.1998 | 0.0470 | 141.23(10) |
| | | | | | | | | | | | C(4) | 0.9690 | 0.2836 | 0.1083 | 81.78(10) |
| | | | | | | | | | | | H(2) | 0.8770 | 0.3057 | 0.0920 | 46.56(14) |
| N(2) | [1555.01], | 0.8863 | 0.2701 | 0.0227 | >> | S | [4554.01], | 0.8119 | 0.3756 | 0.4031 | C(3) | 0.8209 | 0.3002 | 0.5470 | 107.15(8) |
| S | [1555.01], | 0.8119 | 0.1243 | 0.0969 | << | N(2) | [4555.01], | 0.8863 | 0.2299 | 0.4773 | C(3) | 0.8209 | 0.3002 | 0.4530 | 99.15(8) |
| | | | | | | | | | | | C(4) | 0.9690 | 0.2164 | 0.6083 | 132.72(8) |
| | | | | | | | | | | | H(2) | 0.8770 | 0.1943 | 0.4080 | 17.13(14) |

=====

***** Aggregate = 1 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 4 2 1555.01 -- 4554.01 4555.01T
 4 2 4554.01 -- 1554.01T 1555.01

=====

***** Aggregate = 2 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 4 2 3555.01 -- 2545.01 2544.01T
 4 2 2545.01 -- 3556.01T 3555.01

:: Analysis of H-Bonded Aggregate Type3 Polymeric Structure(s)

:: Resd 0 - Infinite (Type3) 1D-Chain - Base Vector: [0 0 1]

=====
Search for Infinite ARU-Chains (Max = 4)
=====

2-Membered Infinite ARU-Chain (Translation [0 0 -1])

1555.01 4554.01 1554.01

2-Membered Infinite ARU-Chain (Translation [0 0 1])

1555.01 4555.01 1556.01

=====
 Analysis of the (Cooperative) Hydrogen Bond Network (i.e. (In)Finite O-H...O-H...O-H.. Chains and/or Rings (Max = 18 Membered))
 =====

=====
 ***** Network = 1 *****
 =====

| Code | Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|-------|-----|-----------------|--------|--------|---------|-----------------|--------|--------|--|
| 1.555 | | N(1) [1555.01] | 0.7634 | 0.1968 | -0.1964 | S [4554.01] | 0.8119 | 0.3756 | -0.4032 |
| | | H(1) | 0.7640 | 0.2411 | -0.2580 | | | | |
| 2.555 | | N(2) [1555.01] | 0.8863 | 0.2701 | -0.0227 | S [4554.01] | 0.8119 | 0.3756 | -0.4032 |
| | | H(2) | 0.8770 | 0.3057 | -0.0920 | | | | |
| 3.555 | | N(2) [1555.01] | 0.8863 | 0.2701 | -0.0227 | O(3) [1555.01] | 0.8857 | 0.4466 | -0.0230 |
| | | H(2) | 0.8770 | 0.3057 | -0.0920 | | | | |

 Hydrogen Bonds are Coded as N.IJK Where N = Sequence Number of Hydrogen Bond (NOTE: New Hbond Numbering system)
 I - 5 = Nr of Translation Units Along A-Axis
 J - 5 = Nr of Translation Units Along B-Axis
 K - 5 = Nr of Translation Units Along C-Axis

Ring Closure Links are Indicated with 'R' and Infinite Chain Links With 'T'

=====

3.6 Angstrom Coordination Sphere Around Atom I = S [ARU = 1555.01] 0.81190 0.12435 0.09685 10.5950 1.8851 0.7984

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|-------------------|-----------|----------|-------|---------|--------|---------|----------|----------|---------|---------|---------|
| 1 | 1.684(3) | -- | C(3) | | | | Intra | 72.98 | -44.77 | 0.82090 | 0.19976 | -0.04700 | 10.9449 | 3.0284 | -0.3874 |
| 2 | 2.661(3) | << | N(1) | | | | Intra | 98.90 | -65.31 | 0.76340 | 0.19677 | -0.19640 | 10.4231 | 2.9830 | -1.6190 |
| 3 | 2.690(3) | << | N(2) | | | | Intra | 61.96 | -21.49 | 0.88630 | 0.27008 | -0.02270 | 11.7719 | 4.0944 | -0.1871 |
| 4 | 3.124(3) | << | C(2) | | | | Intra | 170.82 | -66.93 | 0.67840 | 0.13724 | -0.25180 | 9.3865 | 2.0806 | -2.0757 |
| 5 | 3.177(3) | << | C(4) | | | | Intra | 49.51 | 1.70 | 0.96900 | 0.28363 | 0.10830 | 12.6568 | 4.2998 | 0.8928 |
| 6 | 3.181(3) | << | C(9) | | | | Intra | 26.06 | 11.52 | 1.03270 | 0.21467 | 0.17390 | 13.3951 | 3.2544 | 1.4335 |
| 7 | 3.334(3) | .. | O(3)b | [x,1/2-y,1/2+z | = | 4555.01] | | -71.16 | 70.05 | 0.88568 | 0.05335 | 0.47700 | 10.9623 | 0.8088 | 3.9321 |
| 8 | 3.348(3) | < | N(1)b | [x,1/2-y,1/2+z | = | 4555.01] | | 109.75 | 30.60 | 0.76340 | 0.30323 | 0.30360 | 9.6213 | 4.5970 | 2.5027 |
| 9 | 3.541(3) | .. | N(2)b | [x,1/2-y,1/2+z | = | 4555.01] | | 76.81 | 62.34 | 0.88630 | 0.22992 | 0.47730 | 10.9700 | 3.4856 | 3.9346 |
| 10 | 2.52(3) | << | H(1)b | [x,1/2-y,1/2+z | = | 4555.01] | | 113.03 | 28.36 | 0.76400 | 0.25890 | 0.24200 | 9.7280 | 3.9249 | 1.9949 |
| 11 | 2.66 | << | H(2A) | | | | Intra | -154.21 | -58.94 | 0.68490 | 0.08490 | -0.18000 | 9.3574 | 1.2871 | -1.4838 |
| 12 | 2.74 | << | H(9A) | | | | Intra | 10.42 | 6.01 | 1.01870 | 0.15690 | 0.13170 | 13.2774 | 2.3786 | 1.0857 |
| 13 | 2.80(3) | << | H(2)b | [x,1/2-y,1/2+z | = | 4555.01] | | 71.10 | 66.40 | 0.87700 | 0.19430 | 0.40800 | 10.9580 | 2.9456 | 3.3633 |
| 14 | 2.97 | < | H(10C)a | [2-x,-1/2+y,1/2-z | = | 2745.01] | | -108.52 | -11.01 | 0.73350 | -0.05830 | 0.02790 | 9.6675 | -0.8838 | 0.2300 |
| 15 | 3.03 | .. | H(12C)b | [x,1/2-y,1/2+z | = | 4555.01] | | -165.09 | -1.49 | 0.58950 | 0.07290 | 0.08730 | 7.6656 | 1.1052 | 0.7197 |
| 16 | 3.09 | .. | H(6A)a | [2-x,-1/2+y,1/2-z | = | 2745.01] | | -66.75 | 9.01 | 0.91010 | -0.06080 | 0.15560 | 11.8011 | -0.9217 | 1.2827 |
| 17 | 3.37(3) | .. | H(2) | | | | Intra | 67.04 | -27.54 | 0.87700 | 0.30570 | -0.09200 | 11.7599 | 4.6344 | -0.7584 |
| 18 | 3.42 | .. | H(10B)a | [2-x,-1/2+y,1/2-z | = | 2745.01] | | -84.21 | -27.02 | 0.81230 | -0.07550 | -0.09150 | 10.9024 | -1.1446 | -0.7543 |
| 19 | 3.42(3) | .. | H(1) | | | | Intra | 92.11 | -58.81 | 0.76400 | 0.24110 | -0.25800 | 10.5299 | 3.6551 | -2.1268 |

Angles (Degrees) At1...V...At2 with Vertex V = S

| | | | | | | | | | | | | | | | |
|------|---|-------|-----------|-------|---|-------|------------|-------|---|-------|-----------|-------|---|-------|------------|
| C(3) | , | N(1) | 24.96(11) | C(3) | , | N(2) | 24.99(10) | C(3) | , | C(2) | 52.41(10) | C(3) | , | C(4) | 50.95(10) |
| C(3) | , | C(9) | 70.46(10) | C(3) | , | O(3)b | 149.12(10) | C(3) | , | N(1)b | 82.47(10) | C(3) | , | N(2)b | 107.15(10) |
| N(1) | , | N(2) | 49.95(8) | N(1) | , | C(2) | 27.54(8) | N(1) | , | C(4) | 75.83(7) | N(1) | , | C(9) | 93.48(8) |
| N(1) | , | O(3)b | 173.95(7) | N(1) | , | N(1)b | 96.29(7) | N(1) | , | N(2)b | 128.69(7) | N(2) | , | C(2) | 77.34(8) |
| N(2) | , | C(4) | 26.19(7) | N(2) | , | C(9) | 48.29(7) | N(2) | , | O(3)b | 124.15(7) | N(2) | , | N(1)b | 69.42(7) |
| N(2) | , | N(2)b | 84.66(7) | C(2) | , | C(4) | 103.35(7) | C(2) | , | C(9) | 119.82(7) | C(2) | , | O(3)b | 158.07(7) |
| C(2) | , | N(1)b | 107.77(7) | C(2) | , | N(2)b | 145.85(7) | C(4) | , | C(9) | 25.25(7) | C(4) | , | O(3)b | 98.40(6) |
| C(4) | , | N(1)b | 63.76(7) | C(4) | , | N(2)b | 63.98(6) | C(9) | , | O(3)b | 81.62(6) | C(9) | , | N(1)b | 78.80(7) |
| C(9) | , | N(2)b | 62.31(6) | O(3)b | , | N(1)b | 79.34(6) | O(3)b | , | N(2)b | 45.71(5) | N(1)b | , | N(2)b | 38.16(6) |

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3.6 Angstrom Coordination Sphere Around Atom I = O(1) [ARU = 1555.01] 0.57160 0.26204 -0.33960 8.1132 3.9725 -2.7995

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|-----------------|-----------|----------|-------|---------|--------|---------|---------|----------|---------|--------|---------|
| 1 | 1.414(3) | -- | C(1) | | | | Intra | -93.84 | 30.83 | 0.57610 | 0.18214 | -0.25170 | 8.0318 | 2.7612 | -2.0749 |
| 2 | 1.429(3) | -- | C(11) | | | | Intra | 109.26 | 30.83 | 0.55180 | 0.33843 | -0.25080 | 7.7086 | 5.1306 | -2.0675 |
| 3 | 2.312(3) | << | O(2) | | | | Intra | -114.49 | 2.43 | 0.50075 | 0.12340 | -0.32770 | 7.1560 | 1.8707 | -2.7014 |
| 4 | 2.370(3) | << | C(12) | | | | Intra | 102.86 | -5.35 | 0.52870 | 0.41377 | -0.36640 | 7.5881 | 6.2728 | -3.0204 |
| 5 | 2.393(3) | << | C(2) | | | | Intra | -56.06 | 17.61 | 0.67840 | 0.13724 | -0.25180 | 9.3865 | 2.0806 | -2.0757 |
| 6 | 2.776(3) | << | N(1) | | | | Intra | -23.19 | 25.16 | 0.76340 | 0.19677 | -0.19640 | 10.4231 | 2.9830 | -1.6190 |
| 7 | 2.831(3) | << | C(21) | | | | Intra | -144.64 | 0.98 | 0.39800 | 0.15400 | -0.33370 | 5.8051 | 2.3346 | -2.7508 |
| 8 | 3.574(3) | .. | C(1)a | [x,1/2-y,-1/2+z | = | 4554.01] | | 49.59 | -71.88 | 0.57610 | 0.31786 | -0.75170 | 8.8336 | 4.8188 | -6.1966 |
| 9 | 1.99 | << | H(1A) | | | | Intra | -110.12 | 56.47 | 0.56740 | 0.19380 | -0.13790 | 7.7341 | 2.9380 | -1.1368 |
| 10 | 2.00 | << | H(11A) | | | | Intra | 78.99 | 45.72 | 0.61270 | 0.35230 | -0.16620 | 8.3793 | 5.3409 | -1.3701 |
| 11 | 2.00 | << | H(11B) | | | | Intra | 142.10 | 36.03 | 0.49260 | 0.32750 | -0.19710 | 6.8386 | 4.9649 | -1.6248 |
| 12 | 2.53(3) | .< | H(1) | | | | Intra | -7.48 | 15.43 | 0.76400 | 0.24110 | -0.25800 | 10.5299 | 3.6551 | -2.1268 |
| 13 | 2.53 | .< | H(21A) | | | | Intra | -161.35 | -10.65 | 0.38680 | 0.20960 | -0.39630 | 5.7572 | 3.1775 | -3.2669 |
| 14 | 2.54 | .< | H(12B) | | | | Intra | 119.08 | -21.74 | 0.47120 | 0.39800 | -0.45370 | 6.9668 | 6.0337 | -3.7401 |
| 15 | 2.58 | .< | H(1A)a | [x,1/2-y,-1/2+z | = | 4554.01] | | 57.73 | -72.15 | 0.56740 | 0.30620 | -0.63790 | 8.5359 | 4.6420 | -5.2585 |
| 16 | 2.60 | .< | H(12C) | | | | Intra | 81.94 | -13.41 | 0.58950 | 0.42710 | -0.41270 | 8.4674 | 6.4748 | -3.4021 |
| 17 | 2.66 | .< | H(2B) | | | | Intra | -55.94 | -4.14 | 0.68110 | 0.11690 | -0.36290 | 9.6004 | 1.7722 | -2.9915 |
| 18 | 3.17 | .. | H(21B) | | | | Intra | -151.00 | 17.75 | 0.38660 | 0.16560 | -0.22250 | 5.4758 | 2.5105 | -1.8342 |
| 19 | 3.22 | .. | H(12A) | | | | Intra | 105.63 | 4.53 | 0.51010 | 0.46570 | -0.30880 | 7.2495 | 7.0600 | -2.5456 |
| 20 | 3.24 | .. | H(2A) | | | | Intra | -65.14 | 23.97 | 0.68490 | 0.08490 | -0.18000 | 9.3574 | 1.2871 | -1.4838 |
| 21 | 3.28 | .. | H(11B)a | [x,1/2-y,-1/2+z | = | 4554.01] | | -109.20 | -64.00 | 0.49260 | 0.17250 | -0.69710 | 7.6405 | 2.6151 | -5.7465 |
| 22 | 3.38 | .. | H(11A)a | [x,1/2-y,-1/2+z | = | 4554.01] | | -58.36 | -52.90 | 0.61270 | 0.14770 | -0.66620 | 9.1812 | 2.2391 | -5.4918 |

Angles (Degrees) At1...V...At2 with Vertex V = O(1)

| | | | | | | | | | | | | | | | |
|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|
| C(1) | , | C(11) | 114.6(2) | C(1) | , | O(2) | 34.45(12) | C(1) | , | C(12) | 150.07(16) | C(1) | , | C(2) | 36.69(13) |
| C(1) | , | N(1) | 61.62(14) | C(1) | , | C(21) | 56.53(14) | C(1) | , | C(1)a | 134.55(15) | C(11) | , | O(2) | 126.73(16) |
| C(11) | , | C(12) | 36.69(15) | C(11) | , | C(2) | 129.55(17) | C(11) | , | N(1) | 107.86(16) | C(11) | , | C(21) | 103.26(16) |
| C(11) | , | C(1)a | 110.62(16) | O(2) | , | C(12) | 142.64(12) | O(2) | , | C(2) | 59.24(9) | O(2) | , | N(1) | 90.14(9) |
| O(2) | , | C(21) | 30.17(8) | O(2) | , | C(1)a | 109.82(8) | C(12) | , | C(2) | 156.02(12) | C(12) | , | N(1) | 124.75(11) |
| C(12) | , | C(21) | 112.50(11) | C(12) | , | C(1)a | 74.11(9) | C(2) | , | N(1) | 31.44(9) | C(2) | , | C(21) | 88.35(10) |
| C(2) | , | C(1)a | 111.56(9) | N(1) | , | C(21) | 117.70(10) | N(1) | , | C(1)a | 108.71(9) | C(21) | , | C(1)a | 108.52(9) |

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3.6 Angstrom Coordination Sphere Around Atom I = O(2) [ARU = 1555.01] 0.50075 0.12340 -0.32770 7.1560 1.8707 -2.7014

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|----------------------|------------|--------|-------|---------|--------|---------|----------|----------|--------|---------|---------|
| 1 | 1.397(3) | -- | C(1) | | | | Intra | 45.48 | 26.64 | 0.57610 | 0.18214 | -0.25170 | 8.0318 | 2.7612 | -2.0749 |
| 2 | 1.429(3) | -- | C(21) | | | | Intra | 161.05 | -1.98 | 0.39800 | 0.15400 | -0.33370 | 5.8051 | 2.3346 | -2.7508 |
| 3 | 2.312(3) | << | O(1) | | | | Intra | 65.51 | -2.43 | 0.57160 | 0.26204 | -0.33960 | 8.1132 | 3.9725 | -2.7995 |
| 4 | 2.326(3) | << | C(2) | | | | Intra | 5.37 | 15.60 | 0.67840 | 0.13724 | -0.25180 | 9.3865 | 2.0806 | -2.0757 |
| 5 | 2.380(4) | << | C(22) | | | | Intra | 165.08 | -17.19 | 0.32450 | 0.08480 | -0.41300 | 4.9590 | 1.2856 | -3.4045 |
| 6 | 3.367(4) | .. | C(11) | | | | Intra | 80.38 | 10.85 | 0.55180 | 0.33843 | -0.25080 | 7.7086 | 5.1306 | -2.0675 |
| 7 | 1.98 | << | H(1A) | | | | Intra | 61.56 | 52.20 | 0.56740 | 0.19380 | -0.13790 | 7.7341 | 2.9380 | -1.1368 |
| 8 | 2.00 | << | H(21A) | | | | Intra | 136.95 | -16.46 | 0.38680 | 0.20960 | -0.39630 | 5.7572 | 3.1775 | -3.2669 |
| 9 | 2.00 | << | H(21B) | | | | Intra | 159.15 | 25.75 | 0.38660 | 0.16560 | -0.22250 | 5.4758 | 2.5105 | -1.8342 |
| 10 | 2.46 | << | H(2B) | | | | Intra | -2.31 | -6.76 | 0.68110 | 0.11690 | -0.36290 | 9.6004 | 1.7722 | -2.9915 |
| 11 | 2.55 | .< | H(22C) | | | | Intra | 156.39 | -38.45 | 0.33940 | 0.07070 | -0.51990 | 5.3278 | 1.0718 | -4.2858 |
| 12 | 2.58 | .< | H(2A) | | | | Intra | -14.85 | 28.13 | 0.68490 | 0.08490 | -0.18000 | 9.3574 | 1.2871 | -1.4838 |
| 13 | 2.61 | .< | H(22B) | | | | Intra | 147.75 | -3.22 | 0.33200 | 0.03160 | -0.34550 | 4.9501 | 0.4791 | -2.8481 |
| 14 | 2.67 | .< | H(12A)a | [1-x, -1/2+y, -1/2-z | = 2644.01] | | | -98.62 | 24.95 | 0.48990 | -0.03430 | -0.19120 | 6.7934 | -0.5200 | -1.5761 |
| 15 | 3.17 | .. | H(11B)b | [x, 1/2-y, -1/2+z | = 4554.01] | | | 56.94 | -73.74 | 0.49260 | 0.17250 | -0.69710 | 7.6405 | 2.6151 | -5.7465 |
| 16 | 3.22 | .. | H(22A) | | | | Intra | 175.43 | -14.47 | 0.25390 | 0.10700 | -0.42540 | 4.0441 | 1.6221 | -3.5068 |
| 17 | 3.25 | .. | H(12B)c | [x, 1/2-y, 1/2+z | = 4555.01] | | | -161.87 | 71.31 | 0.47120 | 0.10200 | 0.04630 | 6.1649 | 1.5463 | 0.3817 |
| 18 | 3.29 | .. | H(11B) | | | | Intra | 95.86 | 19.09 | 0.49260 | 0.32750 | -0.19710 | 6.8386 | 4.9649 | -1.6248 |
| 19 | 3.47 | .. | H(11A)b | [x, 1/2-y, -1/2+z | = 4554.01] | | | 10.31 | -53.58 | 0.61270 | 0.14770 | -0.66620 | 9.1812 | 2.2391 | -5.4918 |
| 20 | 3.54 | .. | H(12C)c | [x, 1/2-y, 1/2+z | = 4555.01] | | | -56.35 | 74.95 | 0.58950 | 0.07290 | 0.08730 | 7.6656 | 1.1052 | 0.7197 |

Angles (Degrees) At1...V...At2 with Vertex V = O(2)

| | | | | | | | | | | | | | | | |
|-------|---|-------|------------|-------|---|-------|-----------|-------|---|-------|------------|-------|---|-------|------------|
| C(1) | , | C(21) | 113.7(2) | C(1) | , | O(1) | 34.92(12) | C(1) | , | C(2) | 38.82(14) | C(1) | , | C(22) | 150.20(18) |
| C(1) | , | C(11) | 36.45(13) | C(21) | , | O(1) | 95.44(16) | C(21) | , | C(2) | 152.43(18) | C(21) | , | C(22) | 36.58(15) |
| C(21) | , | C(11) | 81.22(15) | O(1) | , | C(2) | 62.12(10) | O(1) | , | C(22) | 126.39(12) | O(1) | , | C(11) | 19.88(7) |
| C(2) | , | C(22) | 170.71(14) | C(2) | , | C(11) | 72.82(10) | C(22) | , | C(11) | 116.44(11) | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = O(4) [ARU = 1555.01] 0.92252 0.50180 0.21850 11.8647 7.6073 1.8012

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|-------------------|-----------|----------|-------|--------|--------|---------|---------|----------|---------|---------|---------|
| 1 | 1.225(3) | -- | N(3) | | | | Intra | -74.78 | -41.50 | 0.92879 | 0.44339 | 0.12000 | 12.1057 | 6.7218 | 0.9892 |
| 2 | 2.162(3) | << | O(3) | | | | Intra | -96.85 | -67.07 | 0.88568 | 0.44665 | -0.02300 | 11.7642 | 6.7712 | -0.1896 |
| 3 | 2.314(3) | << | C(5) | | | | Intra | -63.99 | -8.75 | 0.99310 | 0.36619 | 0.17580 | 12.8677 | 5.5514 | 1.4492 |
| 4 | 2.720(4) | << | C(6) | | | | Intra | -43.74 | 14.41 | 1.07620 | 0.38168 | 0.30060 | 13.7679 | 5.7863 | 2.4780 |
| 5 | 3.369(3) | .. | O(3)c | [2-x,1-y,-z | = | 3765.01] | | 15.32 | -28.58 | 1.11432 | 0.55335 | 0.02300 | 14.7178 | 8.3888 | 0.1896 |
| 6 | 3.373(4) | .. | C(9)a | [2-x,1/2+y,1/2-z | = | 2755.01] | | 82.58 | 15.25 | 0.96730 | 0.71467 | 0.32610 | 12.2851 | 10.8344 | 2.6882 |
| 7 | 3.457(4) | .. | C(8)a | [2-x,1/2+y,1/2-z | = | 2755.01] | | 97.83 | -2.13 | 0.88510 | 0.72757 | 0.20290 | 11.3942 | 11.0300 | 1.6726 |
| 8 | 3.520(4) | .. | C(4) | | | | Intra | -76.53 | -14.95 | 0.96900 | 0.28363 | 0.10830 | 12.6568 | 4.2998 | 0.8928 |
| 9 | 3.549(4) | .. | C(10)d | [2-x,1-y,1-z | = | 3766.01] | | 150.70 | 32.13 | 0.75230 | 0.59883 | 0.44750 | 9.2435 | 9.0783 | 3.6889 |
| 10 | 2.46 | << | H(6A) | | | | Intra | -25.23 | 24.99 | 1.08990 | 0.43920 | 0.34440 | 13.8790 | 6.6583 | 2.8390 |
| 11 | 2.61 | .< | H(10B)d | [2-x,1-y,1-z | = | 3766.01] | | 147.65 | 36.87 | 0.81230 | 0.57550 | 0.40850 | 10.1005 | 8.7246 | 3.3675 |
| 12 | 2.71 | .< | H(9A)a | [2-x,1/2+y,1/2-z | = | 2755.01] | | 77.11 | 27.11 | 0.98130 | 0.65690 | 0.36830 | 12.4027 | 9.9586 | 3.0361 |
| 13 | 2.89 | .. | H(8A)a | [2-x,1/2+y,1/2-z | = | 2755.01] | | 109.45 | -9.70 | 0.84380 | 0.67880 | 0.15950 | 10.9170 | 10.2906 | 1.3148 |
| 14 | 3.44 | .. | H(22A)b | [1-x,1/2+y,-1/2-z | = | 2654.01] | | 139.48 | -44.55 | 0.74610 | 0.60700 | -0.07460 | 9.9987 | 9.2021 | -0.6150 |

Angles (Degrees) At1...V...At2 with Vertex V = O(4)

| | | | | | | | | | | | | | | | |
|-------|---|--------|------------|-------|---|--------|------------|-------|---|--------|------------|-------|---|--------|------------|
| N(3) | , | O(3) | 28.28(14) | N(3) | , | C(5) | 34.11(15) | N(3) | , | C(6) | 62.83(16) | N(3) | , | O(3)c | 71.58(16) |
| N(3) | , | C(9)a | 147.26(19) | N(3) | , | C(8)a | 135.85(19) | N(3) | , | C(4) | 26.59(14) | N(3) | , | C(10)d | 142.86(18) |
| O(3) | , | C(5) | 62.39(10) | O(3) | , | C(6) | 90.16(11) | O(3) | , | O(3)c | 71.85(9) | O(3) | , | C(9)a | 128.17(11) |
| O(3) | , | C(8)a | 110.02(11) | O(3) | , | C(4) | 53.80(8) | O(3) | , | C(10)d | 128.01(11) | C(5) | , | C(6) | 30.66(9) |
| C(5) | , | O(3)c | 76.48(9) | C(5) | , | C(9)a | 146.70(12) | C(5) | , | C(8)a | 158.86(12) | C(5) | , | C(4) | 13.74(8) |
| C(5) | , | C(10)d | 140.27(11) | C(6) | , | O(3)c | 71.44(8) | C(6) | , | C(9)a | 119.21(10) | C(6) | , | C(8)a | 140.12(11) |
| C(6) | , | C(4) | 43.75(8) | C(6) | , | C(10)d | 131.45(11) | O(3)c | , | C(9)a | 78.36(7) | O(3)c | , | C(8)a | 82.40(7) |
| O(3)c | , | C(4) | 84.49(7) | O(3)c | , | C(10)d | 141.61(8) | C(9)a | , | C(8)a | 23.01(6) | C(9)a | , | C(4) | 159.84(10) |
| C(9)a | , | C(10)d | 63.62(7) | C(8)a | , | C(4) | 162.02(10) | C(8)a | , | C(10)d | 60.59(7) | C(4) | , | C(10)d | 133.85(9) |

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3.6 Angstrom Coordination Sphere Around Atom I = O(5) [ARU = 1555.01] 1.22319 0.31689 0.47990 15.4266 4.8041 3.9560

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|------------------|-----------|----------|-------|---------|--------|---------|---------|---------|---------|--------|--------|
| 1 | 1.361(3) | -- | C(7) | | | | Intra | -174.87 | -46.84 | 1.13860 | 0.31140 | 0.35950 | 14.4997 | 4.7208 | 2.9635 |
| 2 | 1.426(3) | -- | C(10) | | | | Intra | 80.75 | 24.81 | 1.24770 | 0.40117 | 0.55250 | 15.6347 | 6.0817 | 4.5545 |
| 3 | 2.325(3) | << | C(8) | | | | Intra | -130.11 | -40.40 | 1.11490 | 0.22757 | 0.29710 | 14.2859 | 3.4500 | 2.4491 |
| 4 | 2.429(3) | << | C(6) | | | | Intra | 149.37 | -37.48 | 1.07620 | 0.38168 | 0.30060 | 13.7679 | 5.7863 | 2.4780 |
| 5 | 3.289(3) | .. | C(9)b | [x,1/2-y,1/2+z | = | 4555.01] | | -170.42 | 29.10 | 1.03270 | 0.28533 | 0.67390 | 12.5932 | 4.3256 | 5.5553 |
| 6 | 3.326(3) | .. | C(8)b | [x,1/2-y,1/2+z | = | 4555.01] | | -160.86 | 51.82 | 1.11490 | 0.27243 | 0.79710 | 13.4841 | 4.1300 | 6.5709 |
| 7 | 3.539(4) | .. | C(21)a | [1+x,y,1+z | = | 1656.01] | | -50.78 | 25.74 | 1.39800 | 0.15400 | 0.66630 | 17.4424 | 2.3346 | 5.4926 |
| 8 | 3.591(3) | .. | C(9) | | | | Intra | -142.66 | -44.63 | 1.03270 | 0.21467 | 0.17390 | 13.3951 | 3.2544 | 1.4335 |
| 9 | 1.98 | << | H(10A) | | | | Intra | 55.18 | 43.05 | 1.30550 | 0.39530 | 0.64400 | 16.2533 | 5.9927 | 5.3088 |
| 10 | 1.98 | << | H(10C) | | | | Intra | 72.79 | -1.86 | 1.26650 | 0.44170 | 0.47210 | 16.0126 | 6.6962 | 3.8917 |
| 11 | 1.98 | << | H(10B) | | | | Intra | 111.69 | 27.65 | 1.18770 | 0.42450 | 0.59150 | 14.7777 | 6.4354 | 4.8760 |
| 12 | 2.48 | << | H(8A) | | | | Intra | -107.58 | -27.62 | 1.15620 | 0.17880 | 0.34050 | 14.7632 | 2.7106 | 2.8069 |
| 13 | 2.66 | < | H(6A) | | | | Intra | 129.85 | -24.82 | 1.08990 | 0.43920 | 0.34440 | 13.8790 | 6.6583 | 2.8390 |
| 14 | 2.75 | .. | H(21A)a | [1+x,y,1+z | = | 1656.01] | | -39.58 | 21.79 | 1.38680 | 0.20960 | 0.60370 | 17.3945 | 3.1775 | 4.9766 |
| 15 | 3.01 | .. | H(21B)c | [1+x,1/2-y,1/2+z | = | 4655.01] | | 6.09 | -33.69 | 1.38660 | 0.33440 | 0.27750 | 17.9149 | 5.0695 | 2.2876 |
| 16 | 3.23 | .. | H(9A)b | [x,1/2-y,1/2+z | = | 4555.01] | | 172.33 | 22.79 | 1.01870 | 0.34310 | 0.63170 | 12.4755 | 5.2014 | 5.2074 |
| 17 | 3.29 | .. | H(22A)a | [1+x,y,1+z | = | 1656.01] | | -85.42 | 13.74 | 1.25390 | 0.10700 | 0.57460 | 15.6814 | 1.6221 | 4.7367 |
| 18 | 3.31 | .. | H(8A)b | [x,1/2-y,1/2+z | = | 4555.01] | | 177.45 | 63.74 | 1.15620 | 0.32120 | 0.84050 | 13.9613 | 4.8694 | 6.9286 |
| 19 | 3.45 | .. | H(12B)a | [1+x,y,1+z | = | 1656.01] | | 21.16 | 9.13 | 1.47120 | 0.39800 | 0.54630 | 18.6041 | 6.0337 | 4.5034 |

Angles (Degrees) At1...V...At2 with Vertex V = O(5)

| | | | | | | | | | | | | | | | |
|-------|---|--------|------------|-------|---|--------|------------|-------|---|-------|-----------|--------|---|--------|------------|
| C(7) | , | C(10) | 117.4(2) | C(7) | , | C(8) | 32.58(15) | C(7) | , | C(6) | 27.83(15) | C(7) | , | C(9)b | 76.05(14) |
| C(7) | , | C(8)b | 99.39(15) | C(7) | , | C(21)a | 131.46(17) | C(7) | , | C(9) | 22.43(14) | C(10) | , | C(8) | 149.92(17) |
| C(10) | , | C(6) | 89.58(15) | C(10) | , | C(9)b | 92.98(14) | C(10) | , | C(8)b | 86.38(13) | C(10) | , | C(21)a | 111.09(14) |
| C(10) | , | C(9) | 139.82(15) | C(8) | , | C(6) | 60.40(10) | C(8) | , | C(9)b | 78.92(9) | C(8) | , | C(8)b | 96.03(10) |
| C(8) | , | C(21)a | 98.89(10) | C(8) | , | C(9) | 10.16(8) | C(6) | , | C(9)b | 76.49(9) | C(6) | , | C(8)b | 99.29(10) |
| C(6) | , | C(21)a | 159.28(11) | C(6) | , | C(9) | 50.26(9) | C(9)b | , | C(8)b | 23.81(6) | C(9)b | , | C(21)a | 100.26(8) |
| C(9)b | , | C(9) | 77.96(7) | C(8)b | , | C(21)a | 81.37(8) | C(8)b | , | C(9) | 97.72(8) | C(21)a | , | C(9) | 109.04(8) |

=====

3.6 Angstrom Coordination Sphere Around Atom I = N(3) [ARU = 1555.01] 0.92879 0.44339 0.12000 12.1057 6.7218 0.9892

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|--------|----------------|-----------|----------|-------|---------|--------|---------|---------|----------|---------|--------|---------|
| 1 | 1.225(3) | -- | O(4) | | | | Intra | 105.22 | 41.50 | 0.92252 | 0.50180 | 0.21850 | 11.8647 | 7.6073 | 1.8012 |
| 2 | 1.228(4) | -- | O(3) | | | | Intra | 171.77 | -73.68 | 0.88568 | 0.44665 | -0.02300 | 11.7642 | 6.7712 | -0.1896 |
| 3 | 1.470(4) | -- | C(5) | | | | Intra | -56.93 | 18.23 | 0.99310 | 0.36619 | 0.17580 | 12.8677 | 5.5514 | 1.4492 |
| 4 | 2.420(4) | << | C(6) | | | | Intra | -29.37 | 37.97 | 1.07620 | 0.38168 | 0.30060 | 13.7679 | 5.7863 | 2.4780 |
| 5 | 2.486(4) | << | C(4) | | | | Intra | -77.18 | -2.22 | 0.96900 | 0.28363 | 0.10830 | 12.6568 | 4.2998 | 0.8928 |
| 6 | 2.898(4) | << | N(2) | | | | Intra | -97.24 | -23.95 | 0.88630 | 0.27008 | -0.02270 | 11.7719 | 4.0944 | -0.1871 |
| 7 | 3.200(3) | .. | O(3)a | [2-x,1-y,-z | = | 3765.01] | | 32.54 | -14.47 | 1.11432 | 0.55335 | 0.02300 | 14.7178 | 8.3888 | 0.1896 |
| 8 | 3.466(4) | .. | N(3)a | [2-x,1-y,-z | = | 3765.01] | | 37.09 | -34.80 | 1.07121 | 0.55661 | -0.12000 | 14.3763 | 8.4382 | -0.9892 |
| 9 | 2.56 | .< | H(6A) | | | | Intra | -2.05 | 46.19 | 1.08990 | 0.43920 | 0.34440 | 13.8790 | 6.6583 | 2.8390 |
| 10 | 2.74(3) | .< | H(2) | | | | Intra | -99.41 | -39.56 | 0.87700 | 0.30570 | -0.09200 | 11.7599 | 4.6344 | -0.7584 |
| 11 | 3.43 | .. | H(2B)b | [x,1/2-y,1/2+z | = | 4555.01] | | -164.55 | 2.35 | 0.68110 | 0.38310 | 0.13710 | 8.7986 | 5.8078 | 1.1302 |

Angles (Degrees) At1...V...At2 with Vertex V = N(3)

| | | | | | | | | | | | | | | | |
|------|---|-------|------------|------|---|-------|------------|------|---|-------|------------|-------|---|-------|------------|
| O(4) | , | O(3) | 123.5(2) | O(4) | , | C(5) | 118.0(2) | O(4) | , | C(6) | 90.39(18) | O(4) | , | C(4) | 140.7(2) |
| O(4) | , | N(2) | 154.4(2) | O(4) | , | O(3)a | 87.12(16) | O(4) | , | N(3)a | 98.58(17) | O(3) | , | C(5) | 118.5(2) |
| O(3) | , | C(6) | 142.9(2) | O(3) | , | C(4) | 93.65(17) | O(3) | , | N(2) | 67.35(15) | O(3) | , | O(3)a | 88.06(16) |
| O(3) | , | N(3)a | 67.32(15) | C(5) | , | C(6) | 31.10(13) | C(5) | , | C(4) | 28.56(13) | C(5) | , | N(2) | 57.66(14) |
| C(5) | , | O(3)a | 94.00(16) | C(5) | , | N(3)a | 103.48(16) | C(6) | , | C(4) | 59.66(11) | C(6) | , | N(2) | 88.76(11) |
| C(6) | , | O(3)a | 78.14(10) | C(6) | , | N(3)a | 95.31(11) | C(4) | , | N(2) | 29.12(8) | C(4) | , | O(3)a | 108.47(11) |
| C(4) | , | N(3)a | 108.36(11) | N(2) | , | O(3)a | 117.70(10) | N(2) | , | N(3)a | 107.02(10) | O(3)a | , | N(3)a | 20.74(6) |

=====
Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6
=====

van der Waals (or ion) Radii used in the Analysis

=====
C H N O S

1.70 1.20 1.55 1.52 1.80

:: Grid: Z-Axis Step = 0.0278 = Points 36, Angstrom Step = 0.23
:: Grid: X-Axis Step = 0.0139 = Points 72, Angstrom Step = 0.18
:: Grid: Y-Axis Step = 0.0139 = Points 72, Angstrom Step = 0.21

:: Unit cell Contains NO Residual Solvent Accessible Void.

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

=====
Report Expected Number of Independent Reflections for given Symmetry and Resolution.

:: Hmax = 17 Kmax = 20 Lmax= 11 , Sorting Order : Fast H, Medium K, Slow L

:: Actual Theta-Max: 28.280 Deg. (Applied Theta Limit: 28.280 Deg.)

Space Group H-M: P21/c Laue: 2/m
Space Group Hall: -P 2ybc [Schoenflies: C2h⁵]
Lattice Type: mP, Centric, Monoclinic, Multiplicity: 4(2), No: 14

Nr ***** Symmetry Operation(s) *****

| | | | |
|---|-------|-----------|---------|
| 1 | H , | K , | L |
| 2 | - H , | 1/2 + K , | 1/2 - L |
| 3 | - H , | - K , | - L |
| 4 | H , | 1/2 - K , | 1/2 + L |

:: Number of Independent Type H, K, L Reflections = 4102

Table 0 - Crystal Data and Details of the Structure Determination
for: tdaomeno2pP2(1)/c R = 0.06

Crystal Data

| | | | |
|--------------------------|--------------------|------------|----------|
| Formula | C14 H21 N3 O5 S | | |
| Formula Weight | 343.41 | | |
| Crystal System | monoclinic | | |
| Space group | P21/c | (No. 14) | |
| a, b, c [Angstrom] | 13.241(4) | 15.160(4) | 8.398(2) |
| alpha, beta, gamma [deg] | 90 | 101.009(4) | 90 |
| V [Ang**3] | 1654.7(8) | | |
| Z | 4 | | |
| D(calc) [g/cm**3] | 1.378 | | |
| Mu(MoKa) [/mm] | 0.224 | | |
| F(000) | 728 | | |
| Crystal Size [mm] | 0.04 x 0.08 x 0.17 | | |

Data Collection

| | | | |
|----------------------------------|---------------------------|---------|-------|
| Temperature (K) | 150 | | |
| Radiation [Angstrom] | MoKa | 0.71073 | |
| Theta Min-Max [Deg] | 1.6, 28.3 | | |
| Dataset | 0: 17 ; -20: 20 ; -11: 10 | | |
| Tot., Uniq. Data, R(int) | 8040, | 4104, | 0.112 |
| Observed Data [I > 2.0 sigma(I)] | 1820 | | |

Refinement

| | | | |
|-------------------------------------|--------------------------|--|--|
| Nref, Npar | 4104, 219 | | |
| R, wR2, S | 0.0558, 0.0834, 1.00 | | |
| w = 1/[\s^2^(Fo^2^)+(0.0000P)^2^] | where P=(Fo^2^+2Fc^2^)/3 | | |
| Max. and Av. Shift/Error | 0.00, 0.00 | | |
| Min. and Max. Resd. Dens. [e/Ang^3] | -0.31, 0.27 | | |

=====

=====

***** N O T I C E *****

=====

- PLATON Reference : Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.
Spek, A.L. (2009). Acta Cryst. D65, 148-155.

- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow

- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)

- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.

- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.

- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@uu.nl

- Recent versions of PLATON may be obtained from <http://www.platonsoft.nl/xraysoft>

- More INFO can be found on <http://http://www.platonsoft.nl/>

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Page - Index
=====

Page 1 --- GENERAL
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Page 3 --- GEOMETRY
Page 6 --- MOLSYM
Page 8 --- NONSYM
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Page 17 --- GEOMETRY
Page 28 --- INTER
Page 35 --- H-BONDS
Page 39 --- COORDN
Page 49 --- VOIDS
Page 50 --- EXPECT
Page 51 --- SUMMARY

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR
=====

W: NOMOVE option used.

:: >>> WARNING: 'CONNECTED INPUT SET' is assumed to be TRUE

:: >>> The Network Analysis may be INCORRECT when this assumption is FALSE

W: Structure contains 1 Intra H..H contacts < Sum(vdW-rad) -0.25 A (max -0.32)
=====

:: Input Xtal Data from File tdaomeno2ph.cif - Data Type CIF

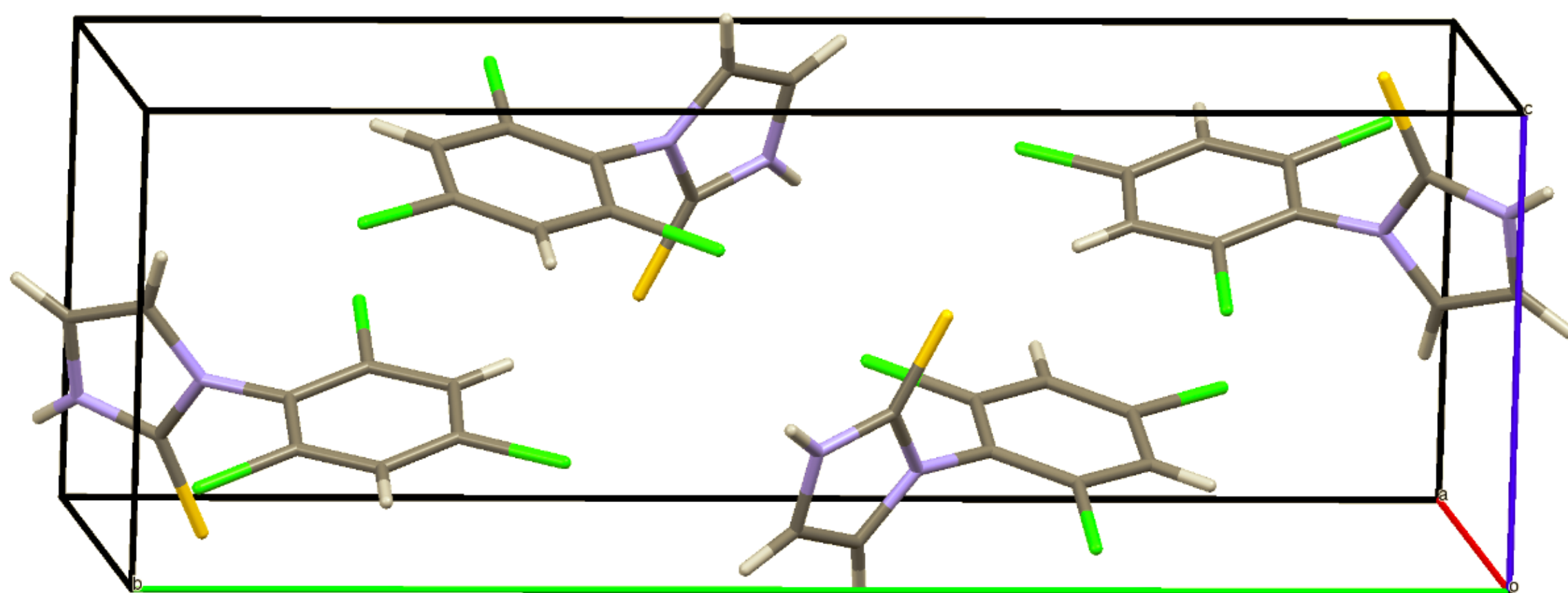
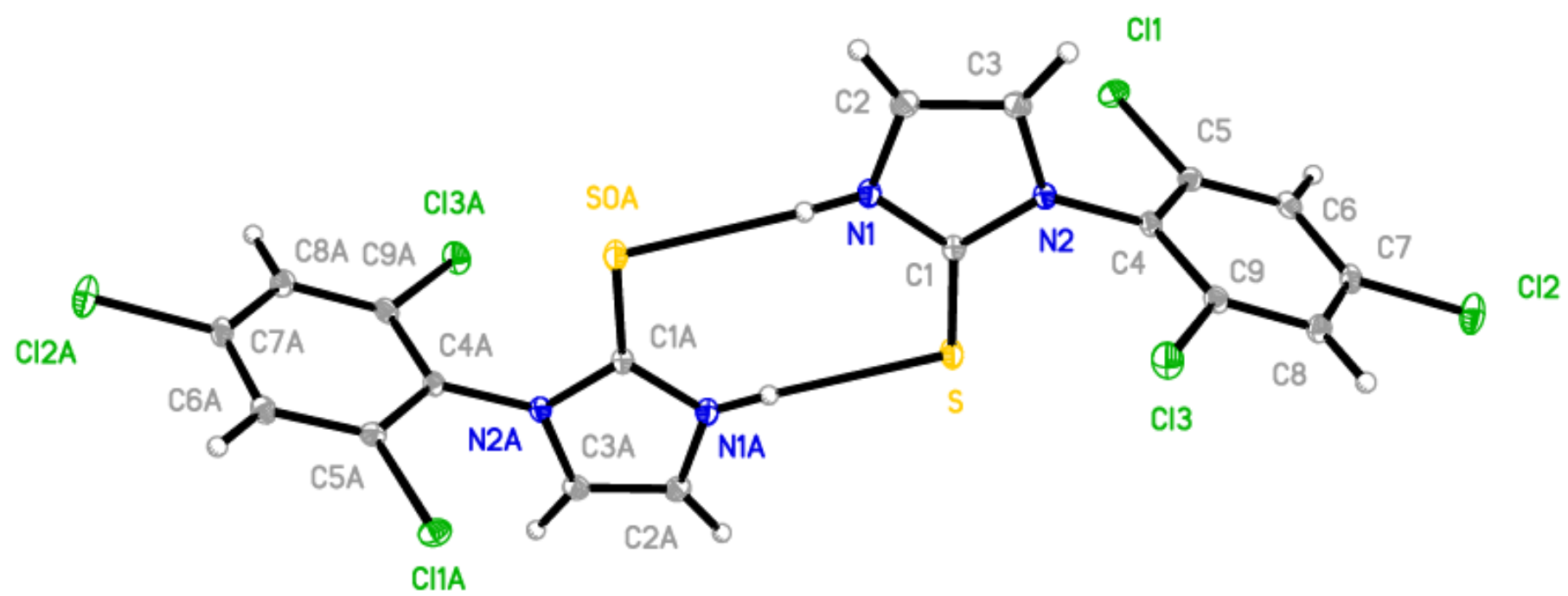
:: NORMAL END of PLATON : 53 Pages on:

:: tdaomeno2ph.lis (ASCII, 132 Characters Wide)

:: tdaomeno2ph.lps (PostScript Version of .lis)

::

Hmim^{ArCl₃}



=====
 Analysis of the IntraMolecular Geometry in Terms of Unique Molecule(s)/Ions, with Bond Criterium: $d(i-j) < R(i) + R(j) + Tol$

-- Tol = 0.40 Ang. for Normal Bonds + 0.70 for (Earth)alkali-NonMetal Contacts and adjusted by -.40 Ang. for Metal-Metal Distances

-- The Bond Distance and Angle su's have been Incremented to Include the Effect of the Unit-cell su.

(Rel.Error in Dist. 0.0001 Ang. , Abs. Angle Error 0.001 Deg.)

-- Bonds below with '>' or '<' Substituted for '-' have Distances that Deviate from Expected Values(Based on the hybridisations).

Bond Lengths (Angstrom). - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().
 =====

| | | | | | | | |
|--------------|------------|--------------|------------|--------------|------------|--------------|------------|
| C1(1) - C(5) | 1.7258(13) | C1(2) - C(7) | 1.7351(13) | C1(3) - C(9) | 1.7248(12) | S - C(1) | 1.6881(12) |
| N(1) - C(1) | 1.3504(16) | N(1) - C(2) | 1.3845(16) | N(2) - C(1) | 1.3677(15) | N(2) - C(3) | 1.3960(16) |
| N(2) - C(4) | 1.4166(16) | C(2) - C(3) | 1.3487(17) | C(4) - C(5) | 1.3958(16) | C(4) - C(9) | 1.3953(17) |
| C(5) - C(6) | 1.3900(17) | C(6) - C(7) | 1.3869(17) | C(7) - C(8) | 1.3901(18) | C(8) - C(9) | 1.3887(17) |
| N(1) - H(1) | 0.838(18) | C(2) - H(2A) | 0.95 | C(3) - H(3A) | 0.95 | C(6) - H(6A) | 0.95 |
| C(8) - H(8A) | 0.95 | | | | | | |

Bond/Valence Angles (Degrees) - (Angles are ordered on the middle label, left to right and top to bottom) - su in last digit in ().
 =====

| | | | | | |
|---------------------|------------|---------------------|------------|---------------------|------------|
| C(1) - N(1) - C(2) | 110.91(10) | C(1) - N(2) - C(3) | 110.37(10) | C(1) - N(2) - C(4) | 123.65(10) |
| C(3) - N(2) - C(4) | 125.87(10) | S - C(1) - N(1) | 128.95(9) | S - C(1) - N(2) | 126.08(9) |
| N(1) - C(1) - N(2) | 104.96(10) | N(1) - C(2) - C(3) | 107.36(11) | N(2) - C(3) - C(2) | 106.40(10) |
| N(2) - C(4) - C(5) | 120.16(11) | N(2) - C(4) - C(9) | 120.96(10) | C(5) - C(4) - C(9) | 118.89(11) |
| C1(1) - C(5) - C(4) | 118.75(9) | C1(1) - C(5) - C(6) | 119.92(9) | C(4) - C(5) - C(6) | 121.34(11) |
| C(5) - C(6) - C(7) | 117.73(11) | C1(2) - C(7) - C(6) | 118.73(10) | C1(2) - C(7) - C(8) | 118.32(9) |
| C(6) - C(7) - C(8) | 122.95(11) | C(7) - C(8) - C(9) | 117.80(11) | C1(3) - C(9) - C(4) | 119.11(9) |
| C1(3) - C(9) - C(8) | 119.61(9) | C(4) - C(9) - C(8) | 121.27(11) | | |
| C(1) - N(1) - H(1) | 123.2(14) | C(2) - N(1) - H(1) | 125.9(14) | N(1) - C(2) - H(2A) | 126 |
| C(3) - C(2) - H(2A) | 126 | N(2) - C(3) - H(3A) | 127 | C(2) - C(3) - H(3A) | 127 |
| C(5) - C(6) - H(6A) | 121 | C(7) - C(6) - H(6A) | 121 | C(7) - C(8) - H(8A) | 121 |
| C(9) - C(8) - H(8A) | 121 | | | | |

Torsion/Dihedral Angles (Deg.) - Klyne & Prelog Convention (Dunitz, p241) - (Excl. Minor Disorder & Embedded Bond Angl. > 160. Deg.)
 =====

| | | | | | |
|----------------------|-------------|----------------------|------------|----------------------|------------|
| C(2) N(1) C(1) S | -179.29(10) | C(2) N(1) C(1) N(2) | 0.42(13) | C(1) N(1) C(2) C(3) | -0.52(14) |
| C(3) N(2) C(1) S | 179.55(9) | C(3) N(2) C(1) N(1) | -0.17(13) | C(4) N(2) C(1) S | 3.22(17) |
| C(4) N(2) C(1) N(1) | -176.50(10) | C(1) N(2) C(3) C(2) | -0.14(13) | C(4) N(2) C(3) C(2) | 176.09(11) |
| C(1) N(2) C(4) C(5) | 88.57(14) | C(1) N(2) C(4) C(9) | -91.45(14) | C(3) N(2) C(4) C(5) | -87.18(14) |
| C(3) N(2) C(4) C(9) | 92.81(14) | N(1) C(2) C(3) N(2) | 0.39(13) | N(2) C(4) C(5) C1(1) | 0.00(16) |
| N(2) C(4) C(5) C(6) | -179.79(10) | C(9) C(4) C(5) C1(1) | 180.00(8) | C(9) C(4) C(5) C(6) | 0.23(17) |
| N(2) C(4) C(9) C1(3) | -1.71(15) | N(2) C(4) C(9) C(8) | 178.86(11) | C(5) C(4) C(9) C1(3) | 178.27(9) |
| C(5) C(4) C(9) C(8) | -1.16(17) | C1(1) C(5) C(6) C(7) | -178.78(9) | C(4) C(5) C(6) C(7) | 0.99(17) |
| C(5) C(6) C(7) C1(2) | 178.45(9) | C(5) C(6) C(7) C(8) | -1.37(18) | C1(2) C(7) C(8) C(9) | -179.33(9) |
| C(6) C(7) C(8) C(9) | 0.49(18) | C(7) C(8) C(9) C1(3) | -178.62(9) | C(7) C(8) C(9) C(4) | 0.81(18) |
| H(1) N(1) C(1) S | 2.5(14) | H(1) N(1) C(1) N(2) | -177.8(14) | C(1) N(1) C(2) H(2A) | 180 |

```

=====
H(1)  N(1)  C(2)  C(3)      177.6(14)  H(1)  N(1)  C(2)  H(2A)      -2  C(1)  N(2)  C(3)  H(3A)      180
C(4)  N(2)  C(3)  H(3A)      -4  N(1)  C(2)  C(3)  H(3A)     -180  H(2A)  C(2)  C(3)  N(2)     -180
H(2A) C(2)  C(3)  H(3A)       0  Cl(1) C(5)  C(6)  H(6A)       1  C(4)  C(5)  C(6)  H(6A)    -179
H(6A) C(6)  C(7)  Cl(2)      -2  H(6A) C(6)  C(7)  C(8)     179  Cl(2) C(7)  C(8)  H(8A)       1
C(6)  C(7)  C(8)  H(8A)    -180  H(8A) C(8)  C(9)  Cl(3)       1  H(8A) C(8)  C(9)  C(4)    -179
=====

```


Automatic Search for Rings (3 to 24-Membered) and Planes Determined by 4 or More Connected Atoms (with Deviation < 0.10 Ang.)

Least-Squares Planes - P*X+Q*Y+R*Z=S :: First Line Orthogonal(XO,YO,ZO), Second Line Fractional(X,Y,Z)

Ring/Plan/Resd/Lspl N Indicates that the Ring/Plane/Residue Involves N Atoms

Sigref - R.M.S-Error of the Contributing Atoms

The Deviation D of an Atom with Sigpln - Sqrt(Sum(j=1:N)(D(j)**2)/(N-3))

Chisq - Chi-Squared = Sum(j=1:N)(D(j)**2)/Sigref**2

Fractional Coordinates X,Y,Z may be Pl.Hyp. - Result of the Chi.Sq. Test for Planarity (See Stout & Jensen, p424)

Calculated via Substitution in

**** - Atoms Deviating by More Than 1.5 Angstrom and Hydrogen Atoms are NOT Listed

D = P*X + Q*Y + R*Z - S (2nd Line) Note - Weights : UNIT

- Deviations from planes are in Angstrom Units

- The Plane determining Atoms have been Marked #

- DISTANCES TO PLANES ROUNDED TO 3 DECIMALS !!(Use Graphical Interface for more)

| Nr | 1 | P | Q | R | S | Sigref | 0.001 | Sigpln | 0.003 | Chisq | 18.2 | Pl.Hyp. | P<5 |
|------|---|-----------|-----------|-----------|-----------|--------|-----------|--------|-----------|-------|-----------|---------|-----------|
| Ring | | 0.7832(4) | 0.4838(5) | 0.3907(6) | 12.018(4) | #N(1) | 0.003(1) | #N(2) | 0.000(1) | #C(1) | -0.002(1) | #C(2) | -0.003(1) |
| A 5 | | 5.828(3) | 9.895(11) | 2.701(4) | 12.018(4) | #C(3) | 0.002(1) | Cl(2) | -0.343(1) | S | -0.015(1) | C(4) | -0.075(1) |
| | | | | | | C(5) | -1.318(1) | C(6) | -1.420(1) | C(7) | -0.244(1) | C(8) | 1.015(1) |
| | | | | | | C(9) | 1.082(1) | | | | | | |

| Nr | 2 | P | Q | R | S | Sigref | 0.001 | Sigpln | 0.008 | Chisq | 131.4 | Pl.Hyp. | P<5 |
|------|---|------------|------------|------------|----------|--------|-----------|--------|-----------|-------|-----------|---------|-----------|
| Ring | | -0.3676(5) | -0.1183(5) | 0.9224(2) | 2.058(8) | #C(4) | -0.005(1) | #C(5) | -0.002(1) | #C(6) | 0.008(1) | #C(7) | -0.006(1) |
| A 6 | | -2.735(3) | -2.420(10) | 6.6660(14) | 2.058(8) | #C(8) | -0.002(1) | #C(9) | 0.007(1) | Cl(1) | -0.018(1) | Cl(2) | -0.035(1) |
| | | | | | | Cl(3) | 0.049(1) | N(1) | -0.747(1) | N(2) | -0.020(1) | C(1) | -1.166(1) |
| | | | | | | C(2) | 0.636(1) | C(3) | 1.101(1) | | | | |

| Nr | 3 | P | Q | R | S | Sigref | 0.001 | Sigpln | 0.923 | Chisq | 999999.9 | Pl.Hyp. | P<5 |
|------|---|------------|------------|------------|----------|--------|-----------|--------|-----------|--------|-----------|---------|-----------|
| Resd | | -0.3298(3) | -0.1695(2) | 0.9287(1) | 1.397(5) | #Cl(1) | 0.172(1) | #Cl(2) | -0.134(1) | #Cl(3) | 0.257(1) | #S | -2.450(1) |
| A 15 | | -2.454(2) | -3.468(5) | 6.7060(11) | 1.397(5) | #N(1) | -0.338(1) | #N(2) | 0.259(1) | #C(1) | -0.838(1) | #C(2) | 1.046(1) |
| | | | | | | #C(3) | 1.430(1) | #C(4) | 0.183(1) | #C(5) | 0.137(1) | #C(6) | 0.058(1) |
| | | | | | | #C(7) | 0.006(1) | #C(8) | 0.057(1) | #C(9) | 0.155(1) | | |

| Nr | 4 | P | Q | R | S | Sigref | 0.001 | Sigpln | 0.021 | Chisq | 1608.5 | Pl.Hyp. | P<5 |
|------|---|------------|-----------|------------|-----------|--------|-----------|--------|-----------|-------|-----------|---------|-----------|
| Plan | | 0.7732(2) | 0.4992(3) | 0.3911(2) | 12.129(3) | #S | 0.002(1) | #N(1) | -0.011(1) | #N(2) | 0.025(1) | #C(1) | 0.007(1) |
| A 7 | | 5.7532(17) | 10.211(7) | 2.7055(17) | 12.129(3) | #C(2) | -0.014(1) | #C(3) | 0.014(1) | #C(4) | -0.024(1) | Cl(2) | -0.210(1) |
| | | | | | | C(5) | -1.255(1) | C(6) | -1.332(1) | C(7) | -0.142(1) | C(8) | 1.106(1) |
| | | | | | | C(9) | 1.147(1) | | | | | | |

| Nr | 5 | P | Q | R | S | Sigref | 0.001 | Sigpln | 0.019 | Chisq | 2516.4 | Pl.Hyp. | P<5 |
|------|---|-------------|------------|-----------|----------|--------|-----------|--------|-----------|--------|----------|---------|-----------|
| Plan | | -0.3765(1) | -0.1198(2) | 0.9187(1) | 1.981(2) | #Cl(1) | 0.003(1) | #Cl(2) | -0.019(1) | #Cl(3) | 0.023(1) | #N(2) | -0.028(1) |
| A 10 | | -2.8011(11) | -2.450(3) | 6.6400(4) | 1.981(2) | #C(4) | -0.007(1) | #C(5) | 0.009(1) | #C(6) | 0.025(1) | #C(7) | 0.003(1) |

```

=====
#C(8)  -0.006(1) #C(9)  -0.003(1) N(1)  -0.762(1) C(1)  -1.177(1)
C(2)   0.621(1) C(3)   1.091(1)

```

(Acute) Angles (Degrees) Between Planes (Numbers I,J from List Above)

```

-----
1, 2=  89.13(6)  1, 3=  88.71(6)  1, 4=   1.05(6)  1, 5=  89.65(5)  2, 3=   3.66(5)  2, 4=  89.00(5)  2, 5=   0.56(4)
3, 4=  88.65(4)  3, 5=   3.95(3)  4, 5=  89.52(3)

```

(Acute) Angles (Degrees) Between Axes, Lines, and Bonds with L.S.-Planes

```

-----
Bond / Plane NM --> M      1      2      3      4      5      6      7      8      9     10
-----
Axes 0 --->a / OM =  51.55(5), 21.57(4), 19.26(2), 50.64(3), 22.11(1),
      b / OM =  28.93(5),  6.80(4),  9.76(2), 29.95(3),  6.88(1),
      c / OM =  22.11(5), 68.27(4), 69.15(2), 22.15(3), 67.72(1),
      a* / OM =  52.20(5), 20.54(4), 18.24(2), 51.28(3), 21.09(1),
      b* / OM =  28.93(5),  6.80(4),  9.76(2), 29.95(3),  6.88(1),
      c* / OM =  23.00(5), 67.28(4), 68.23(2), 23.02(3), 66.73(1),
C1(1) -C(5) / OM =  55.85(7),  0.51(6),  1.18(5), 56.90(5),  0.19(4),
C1(2) -C(7) / OM =   3.27(7),  0.96(6),  4.62(5),  2.22(5),  0.73(4),
C1(3) -C(9) / OM =  63.12(6),  1.40(6),  3.41(5), 62.07(5),  0.84(4),
S     -C(1) / OM =   0.44(6), 69.14(6), 72.76(5),  0.19(5), 68.95(4),
N(1)  -C(1) / OM =   0.18(8), 18.10(8), 21.74(7),  0.77(7), 17.90(7),
      -C(2) / OM =   0.21(8), 86.98(8), 88.29(7),  0.14(7), 86.94(7),
N(2)  -C(1) / OM =   0.07(8), 56.93(7), 53.28(7),  0.75(7), 57.14(6),
      -C(3) / OM =   0.06(8), 53.42(8), 57.05(7),  0.46(7), 53.23(7),
      -C(4) / OM =   3.05(8),  0.61(8),  3.05(7),  2.00(7),  0.83(7),
C(2)  -C(3) / OM =   0.17(9), 20.18(8), 16.54(8),  1.20(8), 20.37(7),
C(4)  -C(5) / OM =  62.88(8),  0.12(8),  1.91(7), 61.83(7),  0.67(7),
      -C(9) / OM =  55.99(9),  0.51(8),  1.18(7), 57.04(7),  0.19(7),
C(5)  -C(6) / OM =   4.23(9),  0.42(8),  3.24(7),  3.18(8),  0.65(7),
C(6)  -C(7) / OM =  57.99(9),  0.58(8),  2.15(7), 59.03(8),  0.92(7),
C(7)  -C(8) / OM =  64.93(9),  0.18(8),  2.10(8), 63.88(8),  0.37(8),
C(8)  -C(9) / OM =   2.73(9),  0.37(8),  4.02(7),  1.69(8),  0.15(7),

```

=====
 Ring Puckering Analysis (Cremer & Pople) - (e.s.d. following Norrestam, Acta Cryst. (1981), A37, 764-765)

Symmetrical Forms

References

| | |
|---|---|
| <p>-----</p> <p>5-Membered Rings : E : Envelope - $\Phi = k \times 36$ T : Half Chair- $\Phi = k \times 36 + 18$</p> <p>6-Membered Rings : C : Chair - $\Theta = 0.0$ H : Half-Chair- $\Theta = 50.8$; $\Phi = k \times 60 + 30$ E : Envelope - $\Theta = 54.7$; $\Phi = k \times 60$ S : Screw-Boat- $\Theta = 67.5$; $\Phi = k \times 60 + 30$ B : Boat - $\Theta = 90.0$; $\Phi = k \times 60$ T : Twist-Boat- $\Theta = 90.0$; $\Phi = k \times 60 + 30$</p> | <p>-----</p> <p>D. Cremer & J.A. Pople, J.Amer.Chem.Soc., 97,(1975),1354-1358</p> <p>J.C.A. Boeyens, J.Cryst.Mol.Struct. 8,(1978),317-320</p> |
|---|---|

Definitions (All Values Rounded on Esd)

Dev - Deviation of Atom I from Cremer&Pople Plane (Defined Differently from Least-Squares Plane)
 Cs(I),C2(I) - Mirror Plane and 2-Axis Asym. Par. for Atom I (See Duax et al., Topics in Stereochemistry,V-9, (1976) pp.271-383)
 Cs(I-J),C2(I-J)- Asymmetry Parameters for Bond I-J
 Tors(I-J) - Torsion Angle for Bond I-J

Descriptors for Torsion Angles

Descriptors for Ring Substituents (J.Appl.Cryst.,1983,16,431)

| Torsion Angle Range | | | Full Descriptor | Short Descriptor | Angle Range of Subst. | | | Full Descriptor | Short Descriptor |
|---------------------|----|--------|-------------------|------------------|-----------------------|----|---------|-----------------|------------------|
| ----- | | | ----- | ----- | ----- | | | ----- | ----- |
| 0 | TO | 30 Deg | + Syn-Periplanar | +sp | 0 | TO | 30 Deg. | Axial | ax |
| 30 | to | 90 | + Syn-Clinal | +sc | 30 | to | 60 | Bisectional | bi |
| 90 | to | 150 | + Anti-Clinal | +ac | 60 | to | 90 | Equatorial | eq |
| 150 | to | 180 | + Anti-Periplanar | +ap | | | | | |
| 0 | to | -30 | - Syn-Periplanar | -sp | | | | | |
| -30 | to | -90 | - Syn-Clinal | -sc | | | | | |
| -90 | to | -150 | - Anti-Clinal | -ac | | | | | |
| -150 | to | -180 | - Anti-Periplanar | -ap | | | | | |

*** NOTE *** - For Ring Puckering Comparisons: Make Sure that the Absolute Configuration, Pivot Atom and Cyclic Sense Agree.
 - The "RING AT1 AT2 AT3 ... ATn" Instruction Gives the User Explicit Choice of Pivot Atom (AT1) and Sense (AT2).
 - Use TRNS Instructions to Obtain the Required Absolute Configuration.
 - The Values of Theta and Phi [= Phi(2)] Depend on the Abs. Conf. and the Choice of the First and Second Ring Atom.
 - Alternatively, Appropriate Phase Shifts may be Applied to the Same Effect (see Below)

For Correct Usage of C&P Puckering Parameters see also: D. Cremer, Acta Cryst. (1984). B40, 498-500.

```

=====
5-Membered Ring ( 1)  N(1)  -->  C(1)  -->  N(2)  -->  C(3)  -->  C(2)  -->
-----

```

| | sp2 | sp2 | sp2 | sp2 | sp2 |
|--------------------------|-------------|------------|-------------|-------------|------------|
| Dev. (Ang) | -0.0026(11) | 0.0017(13) | -0.0001(11) | -0.0015(13) | 0.0025(13) |
| Cs(I)-Asym-Par (Deg) | 0.17(13) | 0.50(13) | 0.61(13) | 0.52(13) | 0.22(13) |
| C2(I)-Asym-Par (Deg) | 0.77(13) | 0.50(13) | 0.03(13) | 0.45(13) | 0.76(13) |
| Ring Bond Angle(Deg) | 110.91(10) | 104.96(10) | 110.37(10) | 106.40(10) | 107.36(11) |
| Tors(I-J) (Deg) | 0.42(13) | -0.17(13) | -0.14(13) | 0.39(13) | -0.52(14) |
| Cs(I-J)-Asym-Par (Deg) | 0.52(13) | 0.22(13) | 0.17(13) | 0.50(13) | 0.61(13) |
| C2(I-J)-Asym-Par (Deg) | 0.45(13) | 0.76(13) | 0.77(13) | 0.50(13) | 0.03(13) |
| Ring Bond Distance (Ang) | 1.3504(16) | 1.3677(15) | 1.3960(16) | 1.3487(17) | 1.3845(16) |

Weighted Average Ring Bond Distance = 1.3699(7, 91) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 0.32(6, 7) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since $\langle \tau \rangle = 0.3 < 5.0$ Deg.

| | | | |
|--------------------------|------------|------------|------------|
| Centroid Cg(1) : x ,y ,z | 0.77539(7) | 0.53536(3) | 0.81536(7) |
| X0,Y0,Z0 | 5.6636(5) | 10.9502(5) | 5.8500(5) |


```

=====
6-Membered Ring ( 2)  C(4)  -->  C(5)  -->  C(6)  -->  C(7)  -->  C(8)  -->  C(9)  -->
-----

```

| | sp2 | sp2 | sp2 | sp2 | sp2 | sp2 |
|--------------------------|-------------|-------------|------------|-------------|-------------|------------|
| Dev. (Ang) | -0.0053(12) | -0.0023(13) | 0.0080(13) | -0.0060(13) | -0.0016(13) | 0.0072(13) |
| Cs(I)-Asym-Par (Deg) | 1.28(14) | 1.79(14) | 0.51(14) | 1.28(14) | 1.79(14) | 0.51(14) |
| C2(I)-Asym-Par (Deg) | 1.35(14) | 0.49(14) | 1.78(14) | 1.35(14) | 0.49(14) | 1.78(14) |
| Ring Bond Angle(Deg) | 118.89(11) | 121.34(11) | 117.73(11) | 122.95(11) | 117.80(11) | 121.27(11) |
| Tors(I-J) (Deg) | 0.23(17) | 0.99(17) | -1.37(18) | 0.49(18) | 0.81(18) | -1.16(17) |
| Cs(I-J)-Asym-Par (Deg) | 0.41(18) | 0.94(18) | 1.28(18) | 0.41(18) | 0.94(18) | 1.28(18) |
| C2(I-J)-Asym-Par (Deg) | 2.17(18) | 1.63(18) | 0.54(18) | 2.17(18) | 1.63(18) | 0.54(18) |
| Ring Bond Distance (Ang) | 1.3958(16) | 1.3900(17) | 1.3869(17) | 1.3901(18) | 1.3887(17) | 1.3953(17) |

Weighted Average Ring Bond Distance = 1.3913(7, 15) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 0.84(7, 17) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since $\langle \tau \rangle = 0.8 < 5.0$ Deg.

| | | | |
|--------------------------|------------|------------|------------|
| Centroid Cg(2) : x ,y ,z | 0.49414(6) | 0.69855(2) | 0.76512(7) |
| X0,Y0,Z0 | 3.5774(5) | 14.2881(5) | 5.4895(5) |

=====
 Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0Deg.
 =====

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

| Cg(I) | Res(I) | Cg(J) | [ARU(J)] | Cg-Cg | Transformed | J-Plane | P, Q, R, S | Alpha | Beta | Gamma | CgI_Perp | CgJ_Perp | Slippage | |
|------------|--------|----------|------------|-----------|-------------|---------|------------------|-------|------|-------|------------|------------|----------|--|
| Cg(1) | [1] | -> Cg(1) | [3667.01] | 5.1287(9) | -0.7832 | -0.4838 | -0.3907 -9.1062 | 0 | 55.4 | 55.4 | -2.9119(5) | -2.9119(5) | 4.222 | |
| Cg(1) | [1] | -> Cg(1) | [3767.01] | 4.4683(9) | -0.7832 | -0.4838 | -0.3907 -14.9337 | 0 | 49.3 | 49.3 | 2.9155(5) | 2.9155(5) | 3.386 | |
| Cg(2) | [1] | -> Cg(2) | [4564.01] | 4.1597(8) | -0.3676 | 0.1183 | 0.9224 2.3552 | 14 | 30.6 | 42.2 | 3.0839(5) | -3.5820(5) | | |
| Cg(2) | [1] | -> Cg(2) | [4565.01] | 4.1598(8) | -0.3676 | 0.1183 | 0.9224 9.0211 | 14 | 42.2 | 30.6 | -3.5820(5) | 3.0840(5) | | |
| ----- | | | | | | | | | | | | | | |
| Min or Max | | | | | | | | 4.160 | 0.0 | 30.6 | 55.4 | -3.582 | -3.582 | |

- [3667] = 1-X,1-Y,2-Z
- [3767] = 2-X,1-Y,2-Z
- [4564] = X,3/2-Y,-1/2+Z
- [4565] = X,3/2-Y,1/2+Z

=====
 Analysis of Y-X...Cg(Pi-Ring) Interactions (X..Cg < 4.0 Ang. - Gamma < 30.0 Deg)
 =====

| Y--X(I) | Res(I) | Cg(J) | [ARU(J)] | X..Cg | Transformed | J-Plane | P, Q, R, S | X-Perp | Gamma | Y-X..Cg | Y..Cg | Y-X,Pi | |
|---------|--------|----------|------------------|-----------|-------------|---------|------------|--------|-------|---------|----------|------------|-------|
| C(7) | -Cl(2) | [1] -> | Cg(2) [4564.01] | 3.6860(7) | -0.3676 | 0.1183 | 0.9224 | 2.3552 | 3.663 | 6.37 | 75.36(4) | 3.6556(14) | 10.48 |
| | | | | ----- | | | | | | | | | |
| | | | Min or Max | 3.686 | | | | | 3.663 | 6.4 | 75.36 | 3.656 | 10.48 |

[4564] = X,3/2-Y,-1/2+Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

| Cg(I) | x | y | z | Xo | Yo | Zo |
|-------|------------|------------|------------|-----------|------------|-----------|
| Cg(1) | 0.77539(7) | 0.53536(3) | 0.81536(7) | 5.6636(5) | 10.9502(5) | 5.8500(5) |
| Cg(2) | 0.49414(6) | 0.69855(2) | 0.76512(7) | 3.5774(5) | 14.2881(5) | 5.4895(5) |

=====
 Analysis of Short Intra- and Inter-molecular Contacts , $d(I-J) < R(I) + R(J) + Tolr$, With Tolr = 0.2 Ang. ($X - I...J > 100$. Deg.

Contact Radii : C H Cl N S
 (Angstrom) 1.70 1.20 1.75 1.55 1.80

Default Contact Radii are those given by A.Bondi, J.Phys.Chem. (1964),68,441. (or Coval. Rad. + 0.8 Ang. when not given)

* WARNING * : no Far-Reaching Conclusions should be drawn based on the Default Radii Assigned to Metals

Short "INTRA" Distances between two Atoms that are Separated by less than 4 Bonds are NOT Listed (Except for Potential D/A Contacts)

| At(I)[1555.01] | At(J) | [ARU(J)] | D(I-J) | SumRad | Del | Type | X(I) | Y(I) | Z(I) | X(J) | Y(J) | Z(J) | X | X - I...J |
|----------------|------------|------------|--------------|--------|-------|-------|--------|--------|--------|---------|--------|--------|------|-----------|
| Cl(1) | N(2) | [] | 2.9516(11)<< | 3.30 | -0.35 | Intra | 0.3331 | 0.5641 | 0.6476 | 0.6987 | 0.5836 | 0.8043 | | |
| Cl(1) | C(1) | [] | 3.5055(12) | 3.45 | 0.06 | Intra | 0.3331 | 0.5641 | 0.6476 | 0.8040 | 0.5590 | 0.6666 | | |
| Cl(1) | C(3) | [] | 3.5170(13) | 3.45 | 0.07 | Intra | 0.3331 | 0.5641 | 0.6476 | 0.6994 | 0.5415 | 0.9574 | | |
| Cl(1) | H(6A) | [] | 2.83 < | 2.95 | -0.12 | Intra | 0.3331 | 0.5641 | 0.6476 | 0.1974 | 0.6932 | 0.6450 | | |
| Cl(1) | S | [3666.01] | 3.5527(6) | 3.55 | 0.00 | | 0.3331 | 0.5641 | 0.6476 | 0.1604 | 0.4062 | 0.5428 | C(5) | 176.20(4) |
| Cl(1) | N(1) | [3666.01] | 3.3936(11) | 3.30 | 0.09 | | 0.3331 | 0.5641 | 0.6476 | 0.1308 | 0.4979 | 0.2643 | C(5) | 137.30(4) |
| Cl(1) | C(1) | [3666.01] | 3.5187(13) | 3.45 | 0.07 | | 0.3331 | 0.5641 | 0.6476 | 0.1960 | 0.4410 | 0.3334 | C(5) | 155.92(5) |
| Cl(1) | C(2) | [3667.01] | 3.5202(13) | 3.45 | 0.07 | | 0.3331 | 0.5641 | 0.6476 | 0.1943 | 0.5094 | 1.0872 | | |
| Cl(1) | C(3) | [3667.01] | 3.5756(13) | 3.45 | 0.13 | | 0.3331 | 0.5641 | 0.6476 | 0.3006 | 0.4585 | 1.0426 | C(5) | 110.54(4) |
| Cl(1) | H(2A) | [3667.01] | 2.93 < | 2.95 | -0.02 | | 0.3331 | 0.5641 | 0.6476 | 0.1678 | 0.5462 | 1.0111 | | |
| Cl(1) | H(3A) | [3667.01] | 3.06 | 2.95 | 0.11 | | 0.3331 | 0.5641 | 0.6476 | 0.3627 | 0.4525 | 0.9293 | C(5) | 117 |
| Cl(2) | H(6A) | [] | 2.80 < | 2.95 | -0.15 | Intra | 0.2708 | 0.8255 | 0.7143 | 0.1974 | 0.6932 | 0.6450 | | |
| Cl(2) | H(8A) | [] | 2.80 < | 2.95 | -0.15 | Intra | 0.2708 | 0.8255 | 0.7143 | 0.6179 | 0.8004 | 0.8522 | | |
| Cl(2) | C(2) | [2656.01] | 3.5427(13) | 3.45 | 0.09 | | 0.2708 | 0.8255 | 0.7143 | 0.1943 | 0.9906 | 0.5872 | C(7) | 156.10(5) |
| Cl(2) | H(2A) | [2656.01] | 3.09 | 2.95 | 0.14 | | 0.2708 | 0.8255 | 0.7143 | 0.1678 | 0.9538 | 0.5111 | C(7) | 154 |
| Cl(2) | Cl(3) | [4464.01] | 3.5530(6) | 3.50 | 0.05 | | 0.2708 | 0.8255 | 0.7143 | -0.1185 | 0.7947 | 0.4339 | C(7) | 110.33(4) |
| Cl(2) | C(6) | [4565.01] | 3.4685(13) | 3.45 | 0.02 | | 0.2708 | 0.8255 | 0.7143 | 0.3173 | 0.8048 | 1.1925 | | |
| Cl(3) | N(2) | [] | 2.9777(11)<< | 3.30 | -0.32 | Intra | 0.8815 | 0.7053 | 0.9339 | 0.6987 | 0.5836 | 0.8043 | | |
| Cl(3) | C(1) | [] | 3.5953(13) | 3.45 | 0.15 | Intra | 0.8815 | 0.7053 | 0.9339 | 0.8040 | 0.5590 | 0.6666 | | |
| Cl(3) | C(3) | [] | 3.6188(13) | 3.45 | 0.17 | Intra | 0.8815 | 0.7053 | 0.9339 | 0.6994 | 0.5415 | 0.9574 | | |
| Cl(3) | H(8A) | [] | 2.82 < | 2.95 | -0.13 | Intra | 0.8815 | 0.7053 | 0.9339 | 0.6179 | 0.8004 | 0.8522 | | |
| Cl(3) | Cl(2) | [4665.01] | 3.5530(6) | 3.50 | 0.05 | | 0.8815 | 0.7053 | 0.9339 | 1.2708 | 0.6745 | 1.2143 | C(9) | 162.97(4) |
| S | C(4) | [] | 3.1532(12)<< | 3.50 | -0.35 | Intra | 0.8396 | 0.5938 | 0.4572 | 0.5960 | 0.6416 | 0.7854 | | |
| S | H(1) | [] | 2.936(19) < | 3.00 | -0.06 | Intra | 0.8396 | 0.5938 | 0.4572 | 0.9410 | 0.4783 | 0.6780 | | |
| S | Cl(1) | [3666.01] | 3.5527(6) | 3.55 | 0.00 | | 0.8396 | 0.5938 | 0.4572 | 0.6669 | 0.4359 | 0.3524 | | |
| S | N(1) | [3766.01] | 3.2512(11) < | 3.35 | -0.10 | | 0.8396 | 0.5938 | 0.4572 | 1.1308 | 0.4979 | 0.2643 | C(1) | 103.93(5) |
| S | H(1) | [3766.01] | 2.416(17)<< | 3.00 | -0.58 | | 0.8396 | 0.5938 | 0.4572 | 1.0590 | 0.5217 | 0.3220 | C(1) | 102.6(5) |
| S | H(8A) | [4564.01] | 2.82 < | 3.00 | -0.18 | | 0.8396 | 0.5938 | 0.4572 | 0.6179 | 0.6996 | 0.3522 | C(1) | 118 |
| N(1) | C(3) | [] | 2.2022(16)<< | 3.25 | -1.05 | Intra | 0.8692 | 0.5021 | 0.7357 | 0.6994 | 0.5415 | 0.9574 | H(1) | 161.5(14) |
| N(1) | Cl(1) | [3666.01] | 3.3936(11) | 3.30 | 0.09 | | 0.8692 | 0.5021 | 0.7357 | 0.6669 | 0.4359 | 0.3524 | C(2) | 121.51(7) |
| N(1) | S | [3766.01] | 3.2512(11) < | 3.35 | -0.10 | | 0.8692 | 0.5021 | 0.7357 | 1.1604 | 0.4062 | 0.5428 | C(1) | 126.96(7) |
| | | | | | | | | | | | | | C(2) | 121.97(7) |
| N(2) | Cl(1) | [] | 2.9516(11)<< | 3.30 | -0.35 | Intra | 0.6987 | 0.5836 | 0.8043 | 0.3331 | 0.5641 | 0.6476 | C(1) | 102.20(7) |

```

=====
                C(3)      101.96(7)
N(2)  .... C1(3) [      ]  2.9777(11)<< 3.30 -0.32 Intra  0.6987 0.5836 0.8043  0.8815 0.7053 0.9339  C(1)      105.59(7)
                                          C(3)      105.92(7)
N(2)  .... C(2)  [      ]  2.1978(16)<< 3.25 -1.05 Intra  0.6987 0.5836 0.8043  0.8057 0.4906 0.9128  C(4)      161.73(9)
C(1)  .... C1(1) [      ]  3.5055(12)   3.45  0.06 Intra  0.8040 0.5590 0.6666  0.3331 0.5641 0.6476  N(1)      113.12(7)
C(1)  .... C1(3) [      ]  3.5953(13)   3.45  0.15 Intra  0.8040 0.5590 0.6666  0.8815 0.7053 0.9339  N(1)      117.87(7)
C(1)  .... C(3)  [      ]  2.2690(17)<< 3.40 -1.13 Intra  0.8040 0.5590 0.6666  0.6994 0.5415 0.9574  S          161.30(8)
C(1)  .... C(5)  [      ]  3.3097(17) < 3.40 -0.09 Intra  0.8040 0.5590 0.6666  0.4208 0.6390 0.7130  N(1)      133.89(8)
C(1)  .... C(9)  [      ]  3.3409(18) < 3.40 -0.06 Intra  0.8040 0.5590 0.6666  0.6673 0.7020 0.8385  N(1)      136.73(8)
C(1)  .... C1(1) [ 3666.01] 3.5187(13)   3.45  0.07           0.8040 0.5590 0.6666  0.6669 0.4359 0.3524  N(2)      124.26(7)
C(2)  .... N(2)  [      ]  2.1978(16)<< 3.25 -1.05 Intra  0.8057 0.4906 0.9128  0.6987 0.5836 0.8043  H(2A)       164
C(2)  .... C(4)  [      ]  3.5708(18)   3.40  0.17 Intra  0.8057 0.4906 0.9128  0.5960 0.6416 0.7854  H(2A)       157
C(2)  .... C1(2) [ 2646.01] 3.5426(14)   3.45  0.09           0.8057 0.4906 0.9128  0.7292 0.3255 0.7857  C(3)      134.76(9)
C(2)  .... C1(1) [ 3667.01] 3.5202(13)   3.45  0.07           0.8057 0.4906 0.9128  0.6669 0.4359 1.3524  N(1)      170.96(8)
C(2)  .... C(2)  [ 3767.01] 3.1529(18)<< 3.40 -0.25           0.8057 0.4906 0.9128  1.1943 0.5094 1.0872  C(3)      110.48(8)
C(2)  .... H(2A) [ 3767.01]      3.00   2.90  0.10           0.8057 0.4906 0.9128  1.1678 0.5462 1.0111  C(3)       100
C(3)  .... C1(1) [      ]  3.5170(13)   3.45  0.07 Intra  0.6994 0.5415 0.9574  0.3331 0.5641 0.6476  C(2)      113.75(8)
C(3)  .... C1(3) [      ]  3.6188(13)   3.45  0.17 Intra  0.6994 0.5415 0.9574  0.8815 0.7053 0.9339  C(2)      118.75(8)
C(3)  .... N(1)  [      ]  2.2022(16)<< 3.25 -1.05 Intra  0.6994 0.5415 0.9574  0.8692 0.5021 0.7357  H(3A)       164
C(3)  .... C(5)  [      ]  3.3497(17) < 3.40 -0.05 Intra  0.6994 0.5415 0.9574  0.4208 0.6390 0.7130  C(2)      134.02(9)
C(3)  .... C(9)  [      ]  3.3999(18) < 3.40  0.00 Intra  0.6994 0.5415 0.9574  0.6673 0.7020 0.8385  C(2)      136.38(9)
C(3)  .... H(1)  [      ]  3.009(19)    2.90  0.11 Intra  0.6994 0.5415 0.9574  0.9410 0.4783 0.6780  H(3A)       159
C(3)  .... C1(1) [ 3667.01] 3.5756(13)   3.45  0.13           0.6994 0.5415 0.9574  0.6669 0.4359 1.3524  N(2)      175.84(8)
C(3)  .... C(3)  [ 3667.01] 3.4817(17)   3.40  0.08           0.6994 0.5415 0.9574  0.3006 0.4585 1.0426  N(2)      116.59(8)
C(4)  .... S      [      ]  3.1532(12)<< 3.50 -0.35 Intra  0.5960 0.6416 0.7854  0.8396 0.5938 0.4572  C(5)      104.83(7)
                                          C(9)      104.92(7)
C(4)  .... C(2)  [      ]  3.5708(18)   3.40  0.17 Intra  0.5960 0.6416 0.7854  0.8057 0.4906 0.9128  C(5)      117.61(8)
                                          C(9)      122.27(8)
C(4)  .... C(7)  [      ]  2.7616(17)<< 3.40 -0.64 Intra  0.5960 0.6416 0.7854  0.3950 0.7543 0.7438  N(2)      179.23(8)
C(4)  .... H(3A) [      ]      2.82 < 2.90 -0.08 Intra  0.5960 0.6416 0.7854  0.6373 0.5475 1.0707  C(5)       109
                                          C(9)      112
C(5)  .... C(1)  [      ]  3.3097(17) < 3.40 -0.09 Intra  0.4208 0.6390 0.7130  0.8040 0.5590 0.6666  C(6)      151.04(9)
C(5)  .... C(3)  [      ]  3.3497(17) < 3.40 -0.05 Intra  0.4208 0.6390 0.7130  0.6994 0.5415 0.9574  C(6)      152.17(8)
C(5)  .... C(8)  [      ]  2.7908(18)<< 3.40 -0.61 Intra  0.4208 0.6390 0.7130  0.5685 0.7592 0.8174  C1(1)     179.00(7)
C(6)  .... C(9)  [      ]  2.7930(17)<< 3.40 -0.61 Intra  0.3173 0.6952 0.6925  0.6673 0.7020 0.8385  H(6A)       179
C(6)  .... C1(2) [ 4564.01] 3.4685(13)   3.45  0.02           0.3173 0.6952 0.6925  0.2708 0.6745 0.2143  C(7)      113.72(8)
C(6)  .... C(7)  [ 4564.01] 3.4407(17)   3.40  0.04           0.3173 0.6952 0.6925  0.3950 0.7457 0.2438  C(5)      104.20(8)
C(6)  .... C(8)  [ 4564.01] 3.4338(17)   3.40  0.03           0.3173 0.6952 0.6925  0.5685 0.7408 0.3174  H(6A)       105
C(7)  .... C(4)  [      ]  2.7616(17)<< 3.40 -0.64 Intra  0.3950 0.7543 0.7438  0.5960 0.6416 0.7854  C1(2)     179.03(7)
C(7)  .... C(6)  [ 4565.01] 3.4407(17)   3.40  0.04           0.3950 0.7543 0.7438  0.3173 0.8048 1.1925  C(6)      115.70(8)
C(7)  .... C(7)  [ 4564.01] 3.5923(18)   3.40  0.19           0.3950 0.7543 0.7438  0.3950 0.7457 0.2438  C(8)      111.51(8)
C(7)  .... C(7)  [ 4565.01] 3.5923(18)   3.40  0.19           0.3950 0.7543 0.7438  0.3950 0.7457 1.2438  C(6)      102.39(8)
C(7)  .... C(8)  [ 4564.01] 3.3536(18) < 3.40 -0.05           0.3950 0.7543 0.7438  0.5685 0.7408 0.3174
C(8)  .... C(5)  [      ]  2.7908(18)<< 3.40 -0.61 Intra  0.5685 0.7592 0.8174  0.4208 0.6390 0.7130  H(8A)       179
C(8)  .... C(6)  [ 4565.01] 3.4338(17)   3.40  0.03           0.5685 0.7592 0.8174  0.3173 0.8048 1.1925  C(9)      115.97(8)
C(8)  .... C(7)  [ 4565.01] 3.3536(18) < 3.40 -0.05           0.5685 0.7592 0.8174  0.3950 0.7457 1.2438
C(9)  .... C(1)  [      ]  3.3409(18) < 3.40 -0.06 Intra  0.6673 0.7020 0.8385  0.8040 0.5590 0.6666  C(8)      149.52(9)
C(9)  .... C(3)  [      ]  3.3999(18) < 3.40  0.00 Intra  0.6673 0.7020 0.8385  0.6994 0.5415 0.9574  C(8)      151.15(9)
=====
    
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| | | | | | | | | | | | | | | | |
|-------|------|-------|------------|--------------|------|-------|-------|--------|--------|--------|--------|--------|--------|-------|-----------|
| C(9) | | C(6) | [] | 2.7930(17)<< | 3.40 | -0.61 | Intra | 0.6673 | 0.7020 | 0.8385 | 0.3173 | 0.6952 | 0.6925 | C1(3) | 178.51(7) |
| H(1) | | S | [] | 2.936(19) < | 3.00 | -0.06 | Intra | 0.9410 | 0.4783 | 0.6780 | 0.8396 | 0.5938 | 0.4572 | | |
| H(1) | | C(3) | [] | 3.009(19) | 2.90 | 0.11 | Intra | 0.9410 | 0.4783 | 0.6780 | 0.6994 | 0.5415 | 0.9574 | | |
| H(1) | | H(2A) | [] | 2.44 | 2.40 | 0.04 | Intra | 0.9410 | 0.4783 | 0.6780 | 0.8322 | 0.4538 | 0.9889 | | |
| H(1) | | S | [3766.01] | 2.416(18)<< | 3.00 | -0.58 | | 0.9410 | 0.4783 | 0.6780 | 1.1604 | 0.4062 | 0.5428 | N(1) | 174.1(19) |
| H(2A) | | H(1) | [] | 2.44 | 2.40 | 0.04 | Intra | 0.8322 | 0.4538 | 0.9889 | 0.9410 | 0.4783 | 0.6780 | | |
| H(2A) | | H(3A) | [] | 2.48 | 2.40 | 0.08 | Intra | 0.8322 | 0.4538 | 0.9889 | 0.6373 | 0.5475 | 1.0707 | | |
| H(2A) | | C1(2) | [2646.01] | 3.09 | 2.95 | 0.14 | | 0.8322 | 0.4538 | 0.9889 | 0.7292 | 0.3255 | 0.7857 | C(2) | 111 |
| H(2A) | | C1(1) | [3667.01] | 2.93 < | 2.95 | -0.02 | | 0.8322 | 0.4538 | 0.9889 | 0.6669 | 0.4359 | 1.3524 | C(2) | 122 |
| H(2A) | | C(2) | [3767.01] | 3.00 | 2.90 | 0.10 | | 0.8322 | 0.4538 | 0.9889 | 1.1943 | 0.5094 | 1.0872 | | |
| H(3A) | | C(4) | [] | 2.82 < | 2.90 | -0.08 | Intra | 0.6373 | 0.5475 | 1.0707 | 0.5960 | 0.6416 | 0.7854 | | |
| H(3A) | | H(2A) | [] | 2.48 | 2.40 | 0.08 | Intra | 0.6373 | 0.5475 | 1.0707 | 0.8322 | 0.4538 | 0.9889 | | |
| H(3A) | | C1(1) | [3667.01] | 3.06 | 2.95 | 0.11 | | 0.6373 | 0.5475 | 1.0707 | 0.6669 | 0.4359 | 1.3524 | C(3) | 116 |
| H(6A) | | C1(1) | [] | 2.83 < | 2.95 | -0.12 | Intra | 0.1974 | 0.6932 | 0.6450 | 0.3331 | 0.5641 | 0.6476 | | |
| H(6A) | | C1(2) | [] | 2.80 < | 2.95 | -0.15 | Intra | 0.1974 | 0.6932 | 0.6450 | 0.2708 | 0.8255 | 0.7143 | | |
| H(8A) | | C1(2) | [] | 2.80 < | 2.95 | -0.15 | Intra | 0.6179 | 0.8004 | 0.8522 | 0.2708 | 0.8255 | 0.7143 | | |
| H(8A) | | C1(3) | [] | 2.82 < | 2.95 | -0.13 | Intra | 0.6179 | 0.8004 | 0.8522 | 0.8815 | 0.7053 | 0.9339 | | |
| H(8A) | | S | [4565.01] | 2.82 < | 3.00 | -0.18 | | 0.6179 | 0.8004 | 0.8522 | 0.8396 | 0.9062 | 0.9572 | C(8) | 167 |

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 1 to Neighbouring ARU'S

| Nr | ARU | Nr.Cont. | d(min) | Del | XHn | X | - At(I) | At(J) | - Y | YHn | Note | Partaking ARU's in Close Contact | Resd. |
|----|------------|----------|--------|-------|-----|------|---------|-----------|-------|-----|------|----------------------------------|-------|
| 1 | [3666.01] | 6 | 3.3936 | 0.09 | 0 | C(1) | - N(1) | ... C1(1) | -C(5) | 0 | | 3666.01 | |
| 2 | [3667.01] | 9 | 2.9300 | -0.02 | 1 | C(2) | - H(2A) | ... C1(1) | -C(5) | 0 | < | 3667.01 | |
| 3 | [2656.01] | 2 | 3.0900 | 0.14 | 0 | C(7) | - C1(2) | ... H(2A) | -C(2) | 1 | | 2656.01 | |
| 4 | [4464.01] | 1 | 3.5530 | 0.05 | 0 | C(7) | - C1(2) | ... C1(3) | -C(9) | 0 | | 4464.01 | |
| 5 | [4565.01] | 6 | 2.8200 | -0.18 | 1 | C(8) | - H(8A) | ... S | -C(1) | 0 | < | 4565.01 | |
| 6 | [4665.01] | 1 | 3.5530 | 0.05 | 0 | C(9) | - C1(3) | ... C1(2) | -C(7) | 0 | | 4665.01 | |
| 7 | [3766.01] | 4 | 2.4160 | -0.58 | 1 | N(1) | - H(1) | ... S | -C(1) | 0 | << | 3766.01 | |
| 8 | [4564.01] | 6 | 2.8200 | -0.18 | 0 | C(1) | - S | ... H(8A) | -C(8) | 1 | < | 4564.01 | |
| 9 | [2646.01] | 2 | 3.0900 | 0.14 | 1 | C(2) | - H(2A) | ... C1(2) | -C(7) | 0 | | 2646.01 | |
| 10 | [3767.01] | 3 | 3.0000 | 0.10 | 1 | C(2) | - H(2A) | ... C(2) | -N(1) | 1 | | 3767.01 | |

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Asymmetric Residue Unit (= ARU) Code List

=====

| ARU-CODE | CIF-CODE | Symmetry-Code | sym | TX | TY | TZ | Ires | x(cen) | y(cen) | z(cen) | |
|------------|----------|---------------|-----|-----|----|----|------|--------|--------|--------|-------|
| [3666.01] | [3_666] | =1-x,1-y,1-z | = | [3 | 1 | 1 | 1 | 1] | 0.380 | 0.374 | 0.217 |

```

=====
[ 3667.01] = [ 3_667] =1-x,1-y,2-z           = [ 3 1 1 2 1 ]      0.380   0.374   1.217
[ 2656.01] = [ 2_656] =1-x,1/2+y,3/2-z       = [ 2 1 0 1 1 ]      0.380   1.126   0.717
[ 4464.01] = [ 4_475] =-1+x,3/2-y,-1/2+z     = [ 4 -1 1 -1 1 ]    -0.380   0.874   0.283
[ 4565.01] = [ 4_576] =x,3/2-y,1/2+z         = [ 4 0 1 0 1 ]      0.620   0.874   1.283
[ 4665.01] = [ 4_676] =1+x,3/2-y,1/2+z       = [ 4 1 1 0 1 ]      1.620   0.874   1.283
[ 3766.01] = [ 3_766] =2-x,1-y,1-z           = [ 3 2 1 1 1 ]      1.380   0.374   0.217
[ 4564.01] = [ 4_575] =x,3/2-y,-1/2+z       = [ 4 0 1 -1 1 ]     0.620   0.874   0.283
[ 2646.01] = [ 2_646] =1-x,-1/2+y,3/2-z     = [ 2 1 -1 1 1 ]     0.380   0.126   0.717
[ 3767.01] = [ 3_767] =2-x,1-y,2-z           = [ 3 2 1 2 1 ]      1.380   0.374   1.217

```

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

$X(J) = X(sym) + TX$, $Y(J) = Y(sym) + TY$, $Z(J) = Z(sym) + TZ$,
 SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

=====
 Analysis of Short Non-Hydrogen Inter-Molecular Contacts For Inter-Molecular Clusters and/or Networks (Minor Disorder Excluded)
 =====

Contact-Nr Atom I[ARU] Atom J[ARU] d(I-J) Del

 1 C(2) [1555.01] ... C(2) [3767.01] = 3.153 -0.25

=====
 ***** Cluster = 1 *****
 =====

(N:M) : ARU -- Connected with (N) Interactions to/from (M) ARU(S). T = Translated Molecule (Infinite chain etc.)

 1 1 1555.01 -- 3767.01
 1 1 3767.01 -- 1555.01

=====
 ***** Cluster = 2 *****
 =====

(N:M) : ARU -- Connected with (N) Interactions to/from (M) ARU(S). T = Translated Molecule (Infinite chain etc.)

 1 1 2555.01 -- 4363.01
 1 1 4363.01 -- 2555.01

=====
 Analysis of Potential Hydrogen Bonds and Schemes with $d(D...A) < R(D)+R(A)+0.50$, $d(H...A) < R(H)+R(A)-0.12$ Ang., $D-H...A > 100.0$ Deg
 =====

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
 =====

| Nr | Typ | Res | Donor | H...A | Acceptor | [ARU] | D - H | H...A | D...A | D - H...A | A..H..A* A'..H..A" | Sum(XY,YZ) | Sum(XZ) |
|----|-----|-----|-------|---------|----------|------------|-----------|-----------|------------|-----------|--------------------|------------|---------|
| 1 | | 1 | N(1) | --H(1) | ..S | [3766.01] | 0.838(18) | 2.416(18) | 3.2512(11) | 174.1(19) | | | |
| 2 | | 1 | C(8) | --H(8A) | ..S | [4565.01] | 0.95 | 2.82 | 3.7468(14) | 167 | | | |

Translation of ARU-Code to CIF and Equivalent Position Code
 =====

[4565.] = [4_576] =x,3/2-y,1/2+z
 [3766.] = [3_766] =2-x,1-y,1-z

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]

2-Centre (linear) D-H...X most prob. angle 160 deg - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
 3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg Springer-Verlag, Berlin, 1991, pp 20.
 4-Centre (trifurcated)

Analysis of Potential Donor/Acceptor Atoms -- (Major Disorder Form Only)
 =====

| At.Nr | D/A | #Cov.Bonds | # H | #D-H..A | #A..H | #A..H-C | Sum(A-H) | Sum(A-X) |
|-------|-------|------------|-----|---------|-------|---------|----------|----------|
| 1 | Cl(1) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 2 | Cl(2) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 3 | Cl(3) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 4 | S | 1 | - | 0 | 1 | 1 | 2 | 3 |
| 5 | N(1) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 6 | N(2) | 3 | - | 0 | 0 | 0 | 0 | 3 |

=====
 Analysis of Hydrogen Bonded Molecular Aggregates (See also Acta Cryst. B36, 1980, 2113 - 2115) -- (Major Disorder Component Only)
 =====

Coordinates of Donor and Acceptor Atoms
 =====

Coordinates of D/A-Bonded Atom(s)
 =====

| D/A I | [ARU] | X | Y | Z | -- | D/A J | [ARU] | X | Y | Z | Atom K | X | Y | Z | I..J--K Angle |
|-------|-------------|--------|--------|--------|----|-------|-------------|--------|--------|--------|--------|--------|--------|--------|---------------|
| N(1) | [1555.01], | 0.8692 | 0.5021 | 0.7357 | >> | S | [3766.01], | 1.1604 | 0.4062 | 0.5428 | C(1) | 1.1960 | 0.4410 | 0.3334 | 103.93(3) |
| S | [1555.01], | 0.8396 | 0.5938 | 0.4572 | << | N(1) | [3766.01], | 1.1308 | 0.4979 | 0.2643 | C(1) | 1.1960 | 0.4410 | 0.3334 | 126.96(2) |
| | | | | | | | | | | | C(2) | 1.1943 | 0.5094 | 0.0872 | 121.97(3) |
| | | | | | | | | | | | H(1) | 1.0590 | 0.5217 | 0.3220 | 4.38(3) |

=====

***** Aggregate = 1 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 2 1 1555.01 -- 3766.01
 2 1 3766.01 -- 1555.01

=====

***** Aggregate = 2 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 2 1 2555.01 -- 4364.01
 2 1 4364.01 -- 2555.01

=====
 Analysis of the (Cooperative) Hydrogen Bond Network (i.e. (In)Finite O-H...O-H...O-H.. Chains and/or Rings (Max = 18 Membered))
 =====

=====
 ***** Network = 1 *****
 =====

| Code | Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|-------|-----|-----------------|--------|--------|--------|---------------|--------|--------|--|
| 1.555 | | N(1) [1555.01] | 0.8692 | 0.5021 | 0.7357 | S [3766.01] | 1.1604 | 0.4062 | 0.5428 |
| | | H(1) | 0.9410 | 0.4783 | 0.6780 | | | | |

 Hydrogen Bonds are Coded as N.IJK Where N = Sequence Number of Hydrogen Bond (NOTE: New Hbond Numbering system)
 I - 5 = Nr of Translation Units Along A-Axis
 J - 5 = Nr of Translation Units Along B-Axis
 K - 5 = Nr of Translation Units Along C-Axis

Ring Closure Links are Indicated with 'R' and Infinite Chain Links With 'T'

3.6 Angstrom Coordination Sphere Around Atom I = Cl(1) [ARU = 1555.01] 0.33309 0.56415 0.64757 2.3943 11.5391 4.6461

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|--------|--------------|-----------|----------|-------|---------|--------|----------|---------|---------|---------|---------|--------|
| 1 | 1.7258(13) | -- | C(5) | | | | Intra | 67.19 | 15.79 | 0.42077 | 0.63899 | 0.71304 | 3.0382 | 13.0699 | 5.1159 |
| 2 | 2.6915(12) | << | C(4) | | | | Intra | 39.25 | 21.56 | 0.59600 | 0.64158 | 0.78545 | 4.3327 | 13.1229 | 5.6354 |
| 3 | 2.7024(13) | << | C(6) | | | | Intra | 92.64 | 6.85 | 0.31728 | 0.69519 | 0.69251 | 2.2708 | 14.2194 | 4.9686 |
| 4 | 2.9516(11) | << | N(2) | | | | Intra | 8.36 | 22.39 | 0.69870 | 0.58356 | 0.80428 | 5.0944 | 11.9361 | 5.7705 |
| 5 | 3.3936(11) | .. | N(1)b | [1-x,1-y,1-z | = | 3666.01] | | -137.03 | -54.12 | 0.13081 | 0.49786 | 0.26435 | 0.9390 | 10.1832 | 1.8966 |
| 6 | 3.5055(12) | .. | C(1) | | | | Intra | -1.73 | 2.23 | 0.80397 | 0.55897 | 0.66660 | 5.8956 | 11.4332 | 4.7827 |
| 7 | 3.5170(13) | .. | C(3) | | | | Intra | -9.80 | 39.21 | 0.69939 | 0.54148 | 0.95745 | 5.0796 | 11.0754 | 6.8694 |
| 8 | 3.5187(13) | .. | C(1)b | [1-x,1-y,1-z | = | 3666.01] | | -111.24 | -39.84 | 0.19603 | 0.44103 | 0.33340 | 1.4153 | 9.0208 | 2.3921 |
| 9 | 3.5202(13) | .. | C(2)c | [1-x,1-y,2-z | = | 3667.01] | | -134.20 | 63.63 | 0.19429 | 0.50936 | 1.08717 | 1.3044 | 10.4184 | 7.8001 |
| 10 | 3.5527(6) | .. | S_b | [1-x,1-y,1-z | = | 3666.01] | | -111.48 | -12.22 | 0.16036 | 0.40619 | 0.54276 | 1.1227 | 8.3082 | 3.8942 |
| 11 | 3.5756(13) | .. | C(3)c | [1-x,1-y,2-z | = | 3667.01] | | -97.72 | 52.43 | 0.30061 | 0.45852 | 1.04255 | 2.1013 | 9.3786 | 7.4800 |
| 12 | 2.83 | < | H(6A) | | | | Intra | 110.93 | -0.37 | 0.19740 | 0.69320 | 0.64500 | 1.3850 | 14.1787 | 4.6277 |
| 13 | 2.93 | < | H(2A)c | [1-x,1-y,2-z | = | 3667.01] | | -163.96 | 63.00 | 0.16780 | 0.54620 | 1.01110 | 1.1172 | 11.1720 | 7.2544 |
| 14 | 3.06 | .. | H(3A)c | [1-x,1-y,2-z | = | 3667.01] | | -85.40 | 41.42 | 0.36270 | 0.45250 | 0.92930 | 2.5780 | 9.2554 | 6.6675 |
| 15 | 3.194(19) | .. | H(1)b | [1-x,1-y,1-z | = | 3666.01] | | -156.50 | -47.01 | 0.05900 | 0.52170 | 0.32200 | 0.3972 | 10.6709 | 2.3103 |
| 16 | 3.416(16) | .. | H(1)a | [-1+x,y,z | = | 1455.01] | | -148.99 | 3.66 | -0.05900 | 0.47830 | 0.67800 | -0.5271 | 9.7831 | 4.8645 |

Angles (Degrees) At1...V...At2 with Vertex V = Cl(1)

| | | | | | | | | | | | | | | | |
|-------|---|-------|-----------|-------|---|-------|-----------|-------|---|-------|-----------|-------|---|-------|-----------|
| C(5) | , | C(4) | 27.04(5) | C(5) | , | C(6) | 26.48(5) | C(5) | , | N(2) | 55.65(4) | C(5) | , | N(1)b | 137.30(4) |
| C(5) | , | C(1) | 69.12(4) | C(5) | , | C(3) | 70.12(4) | C(5) | , | C(1)b | 155.92(5) | C(5) | , | C(2)c | 98.86(4) |
| C(5) | , | S_b | 176.20(4) | C(5) | , | C(3)c | 110.54(4) | C(4) | , | C(6) | 53.52(4) | C(4) | , | N(2) | 28.60(3) |
| C(4) | , | N(1)b | 147.33(3) | C(4) | , | C(1) | 44.29(3) | C(4) | , | C(3) | 45.20(3) | C(4) | , | C(1)b | 148.98(3) |
| C(4) | , | C(2)c | 94.65(3) | C(4) | , | S_b | 150.54(3) | C(4) | , | C(3)c | 97.08(3) | C(6) | , | N(2) | 82.12(3) |
| C(6) | , | N(1)b | 118.25(3) | C(6) | , | C(1) | 94.07(3) | C(6) | , | C(3) | 95.18(3) | C(6) | , | C(1)b | 140.67(3) |
| C(6) | , | C(2)c | 101.23(3) | C(6) | , | S_b | 155.63(3) | C(6) | , | C(3)c | 120.07(3) | N(2) | , | N(1)b | 139.00(3) |
| N(2) | , | C(1) | 22.42(3) | N(2) | , | C(3) | 22.85(3) | N(2) | , | C(1)b | 126.50(3) | N(2) | , | C(2)c | 89.13(3) |
| N(2) | , | S_b | 122.03(2) | N(2) | , | C(3)c | 81.62(3) | N(1)b | , | C(1) | 116.60(3) | N(1)b | , | C(3) | 141.90(3) |
| N(1)b | , | C(1)b | 22.44(3) | N(1)b | , | C(2)c | 117.77(3) | N(1)b | , | S_b | 46.50(2) | N(1)b | , | C(3)c | 111.44(3) |
| C(1) | , | C(3) | 37.70(3) | C(1) | , | C(1)b | 106.33(3) | C(1) | , | C(2)c | 105.35(3) | C(1) | , | S_b | 109.77(2) |
| C(1) | , | C(3)c | 91.87(3) | C(3) | , | C(1)b | 121.54(3) | C(3) | , | C(2)c | 68.16(3) | C(3) | , | S_b | 106.69(2) |
| C(3) | , | C(3)c | 58.79(3) | C(1)b | , | C(2)c | 105.07(3) | C(1)b | , | S_b | 27.62(2) | C(1)b | , | C(3)c | 93.01(3) |
| C(2)c | , | S_b | 77.84(2) | C(2)c | , | C(3)c | 21.90(3) | S_b | , | C(3)c | 65.73(2) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = Cl(2) [ARU = 1555.01] 0.27082 0.82548 0.71431 1.9223 16.8843 5.1250

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|--------|--------------------|-----------|----------|-------|---------|--------|----------|---------|---------|---------|---------|--------|
| 1 | 1.7351(13) | -- | C(7) | | | | Intra | -57.71 | 6.99 | 0.39498 | 0.75430 | 0.74376 | 2.8423 | 15.4285 | 5.3363 |
| 2 | 2.6891(13) | << | C(8) | | | | Intra | -31.61 | 15.97 | 0.56853 | 0.75923 | 0.81743 | 4.1241 | 15.5293 | 5.8648 |
| 3 | 2.6921(13) | << | C(6) | | | | Intra | -82.55 | -3.33 | 0.31728 | 0.69519 | 0.69251 | 2.2708 | 14.2194 | 4.9686 |
| 4 | 3.4685(13) | .. | C(6)c | [x,3/2-y,1/2+z | = | 4565.01] | | -56.14 | 81.56 | 0.31728 | 0.80481 | 1.19251 | 2.2059 | 16.4616 | 8.5559 |
| 5 | 3.5427(13) | .. | C(2)a | [1-x,1/2+y,3/2-z | = | 2656.01] | | 99.30 | -14.92 | 0.19429 | 0.99064 | 0.58717 | 1.3694 | 20.2626 | 4.2128 |
| 6 | 3.5530(6) | .. | Cl(3)b | [-1+x,3/2-y,-1/2+z | = | 4464.01] | | -167.60 | -34.49 | -0.11848 | 0.79474 | 0.43391 | -0.9380 | 16.2556 | 3.1132 |
| 7 | 2.80 | .< | H(8A) | | | | Intra | -11.31 | 20.72 | 0.61790 | 0.80040 | 0.85220 | 4.4869 | 16.3714 | 6.1143 |
| 8 | 2.80 | .< | H(6A) | | | | Intra | -101.23 | -10.22 | 0.19740 | 0.69320 | 0.64500 | 1.3850 | 14.1787 | 4.6277 |
| 9 | 3.09 | .. | H(2A)a | [1-x,1/2+y,3/2-z | = | 2656.01] | | 105.75 | -28.13 | 0.16780 | 0.95380 | 0.51110 | 1.1822 | 19.5090 | 3.6670 |
| 10 | 3.17 | .. | H(6A)c | [x,3/2-y,1/2+z | = | 4565.01] | | -147.62 | 77.00 | 0.19740 | 0.80680 | 1.14500 | 1.3200 | 16.5023 | 8.2151 |
| 11 | 3.591(18) | .. | H(1)a | [1-x,1/2+y,3/2-z | = | 2656.01] | | 116.96 | 12.42 | 0.05900 | 0.97830 | 0.82200 | 0.3322 | 20.0101 | 5.8976 |

Angles (Degrees) At1...V...At2 with Vertex V = Cl(2)

| | | | | | | | | | | | | | | | |
|-------|---|--------|-----------|-------|---|--------|-----------|-------|---|--------|-----------|------|---|--------|-----------|
| C(7) | , | C(8) | 27.07(5) | C(7) | , | C(6) | 26.86(5) | C(7) | , | C(6)c | 74.57(5) | C(7) | , | C(2)a | 156.10(5) |
| C(7) | , | Cl(3)b | 110.33(4) | C(8) | , | C(6) | 53.93(4) | C(8) | , | C(6)c | 66.39(3) | C(8) | , | C(2)a | 132.78(4) |
| C(8) | , | Cl(3)b | 136.53(3) | C(6) | , | C(6)c | 85.77(3) | C(6) | , | C(2)a | 161.66(3) | C(6) | , | Cl(3)b | 84.04(3) |
| C(6)c | , | C(2)a | 112.56(3) | C(6)c | , | Cl(3)b | 127.18(2) | C(2)a | , | Cl(3)b | 84.10(2) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = Cl(3) [ARU = 1555.01] 0.88152 0.70526 0.93391 6.4379 14.4254 6.7005

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|-----------|----------------------|------------|-------|---------|--------|---------|---------|---------|--------|---------|--------|
| 1 | 1.7248(12) | -- C(9) | | | Intra | -177.59 | -23.38 | 0.66728 | 0.70201 | 0.83851 | 4.8561 | 14.3589 | 6.0161 |
| 2 | 2.6950(12) | << C(4) | | | Intra | -148.25 | -23.28 | 0.59600 | 0.64158 | 0.78545 | 4.3327 | 13.1229 | 5.6354 |
| 3 | 2.6964(13) | << C(8) | | | Intra | 154.49 | -18.06 | 0.56853 | 0.75923 | 0.81743 | 4.1241 | 15.5293 | 5.8648 |
| 4 | 2.9777(11) | << N(2) | | | Intra | -118.36 | -18.20 | 0.69870 | 0.58356 | 0.80428 | 5.0944 | 11.9361 | 5.7705 |
| 5 | 3.5530(6) | .. Cl(2)b | [1+x,3/2-y,1/2+z | = 4665.01] | | -12.40 | 34.49 | 1.27082 | 0.67452 | 1.21431 | 9.2981 | 13.7966 | 8.7123 |
| 6 | 3.5953(13) | .. C(1) | | | Intra | -100.27 | -32.24 | 0.80397 | 0.55897 | 0.66660 | 5.8956 | 11.4332 | 4.7827 |
| 7 | 2.82 | .< H(8A) | | | Intra | 135.07 | -12.01 | 0.61790 | 0.80040 | 0.85220 | 4.4869 | 16.3714 | 6.1143 |
| 8 | 3.17 | .. H(6A)a | [1+x,y,z | = 1655.01] | | -5.90 | -40.81 | 1.19740 | 0.69320 | 0.64500 | 8.8258 | 14.1787 | 4.6277 |
| 9 | 3.46 | .. H(6A)b | [1+x,3/2-y,1/2+z | = 4665.01] | | 41.80 | 25.92 | 1.19740 | 0.80680 | 1.14500 | 8.7608 | 16.5023 | 8.2151 |

Angles (Degrees) At1...V...At2 with Vertex V = Cl(3)

| | | | | | | | | | | | | | | | |
|------|---|--------|-----------|------|---|------|----------|--------|---|--------|-----------|------|---|--------|-----------|
| C(9) | , | C(4) | 26.89(5) | C(9) | , | C(8) | 26.60(5) | C(9) | , | N(2) | 55.25(5) | C(9) | , | Cl(2)b | 162.97(4) |
| C(9) | , | C(1) | 67.54(5) | C(4) | , | C(8) | 53.49(4) | C(4) | , | N(2) | 28.37(3) | C(4) | , | Cl(2)b | 140.10(3) |
| C(4) | , | C(1) | 43.04(3) | C(8) | , | N(2) | 81.85(3) | C(8) | , | Cl(2)b | 159.84(3) | C(8) | , | C(1) | 92.63(3) |
| N(2) | , | Cl(2)b | 113.09(2) | N(2) | , | C(1) | 21.50(3) | Cl(2)b | , | C(1) | 106.03(2) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = S [ARU = 1555.01] 0.83964 0.59381 0.45724 6.1882 12.1458 3.2806

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|--------|-----------------|-----------|----------|-------|---------|--------|---------|---------|---------|--------|---------|--------|
| 1 | 1.6881(12) | -- | C(1) | | | | Intra | -112.32 | 62.85 | 0.80397 | 0.55897 | 0.66660 | 5.8956 | 11.4332 | 4.7827 |
| 2 | 2.7277(11) | << | N(2) | | | | Intra | -169.15 | 65.90 | 0.69870 | 0.58356 | 0.80428 | 5.0944 | 11.9361 | 5.7705 |
| 3 | 2.7458(11) | << | N(1) | | | | Intra | -84.40 | 46.67 | 0.86919 | 0.50214 | 0.73565 | 6.3719 | 10.2708 | 5.2781 |
| 4 | 3.1532(12) | << | C(4) | | | | Intra | 152.23 | 48.31 | 0.59600 | 0.64158 | 0.78545 | 4.3327 | 13.1229 | 5.6354 |
| 5 | 3.2512(11) | .< | N(1)d | [2-x,1-y,1-z | = | 3766.01] | | -41.84 | -25.19 | 1.13081 | 0.49786 | 0.26435 | 8.3798 | 10.1832 | 1.8966 |
| 6 | 3.5527(6) | .. | Cl(1)c | [1-x,1-y,1-z | = | 3666.01] | | -111.48 | -12.22 | 0.66691 | 0.43585 | 0.35243 | 4.9165 | 8.9149 | 2.5286 |
| 7 | 2.416(17) | << | H(1)d | [2-x,1-y,1-z | = | 3766.01] | | -41.80 | -23.68 | 1.05900 | 0.52170 | 0.32200 | 7.8380 | 10.6709 | 2.3103 |
| 8 | 2.82 | .< | H(8A)e | [x,3/2-y,-1/2+z | = | 4564.01] | | 127.10 | -15.53 | 0.61790 | 0.69960 | 0.35220 | 4.5519 | 14.3096 | 2.5269 |
| 9 | 2.936(19) | .< | H(1) | | | | Intra | -72.93 | 32.65 | 0.94100 | 0.47830 | 0.67800 | 6.9137 | 9.7831 | 4.8645 |
| 10 | 3.27 | .. | H(3A)a | [x,y,-1+z | = | 1554.01] | | -146.94 | -57.95 | 0.63730 | 0.54750 | 0.07070 | 4.7328 | 11.1986 | 0.5073 |
| 11 | 3.59 | .. | H(6A)b | [1+x,y,z | = | 1655.01] | | 37.62 | 22.02 | 1.19740 | 0.69320 | 0.64500 | 8.8258 | 14.1787 | 4.6277 |

Angles (Degrees) At1...V...At2 with Vertex V = S

| | | | | | | | | | | | | | | | |
|------|---|--------|-----------|------|---|--------|-----------|-------|---|--------|----------|------|---|--------|-----------|
| C(1) | , | N(2) | 23.91(5) | C(1) | , | N(1) | 22.49(5) | C(1) | , | C(4) | 50.53(5) | C(1) | , | N(1)d | 103.93(5) |
| C(1) | , | Cl(1)c | 75.07(4) | N(2) | , | N(1) | 46.39(3) | N(2) | , | C(4) | 26.64(3) | N(2) | , | N(1)d | 127.77(3) |
| N(2) | , | Cl(1)c | 88.84(2) | N(1) | , | C(4) | 73.00(3) | N(1) | , | N(1)d | 81.51(3) | N(1) | , | Cl(1)c | 63.70(2) |
| C(4) | , | N(1)d | 154.37(3) | C(4) | , | Cl(1)c | 103.25(2) | N(1)d | , | Cl(1)c | 66.56(2) | | | | |

=====
 3.6 Angstrom Coordination Sphere Around Atom I = N(1) [ARU = 1555.01] 0.86919 0.50214 0.73565 6.3719 10.2708 5.2781
 =====

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|--------|--------------|-----------|----------|-------|---------|--------|---------|---------|---------|--------|---------|--------|
| 1 | 0.838(18) | -- | H(1) | | | | Intra | -41.99 | -29.57 | 0.94100 | 0.47830 | 0.67800 | 6.9137 | 9.7831 | 4.8645 |
| 2 | 1.3504(16) | -- | C(1) | | | | Intra | 112.28 | -21.52 | 0.80397 | 0.55897 | 0.66660 | 5.8956 | 11.4332 | 4.7827 |
| 3 | 1.3845(16) | -- | C(2) | | | | Intra | -154.60 | 66.67 | 0.80571 | 0.49064 | 0.91283 | 5.8765 | 10.0356 | 6.5493 |
| 4 | 2.1559(15) | << | N(2) | | | | Intra | 127.49 | 13.20 | 0.69870 | 0.58356 | 0.80428 | 5.0944 | 11.9361 | 5.7705 |
| 5 | 2.2022(16) | << | C(3) | | | | Intra | 148.09 | 46.27 | 0.69939 | 0.54148 | 0.95745 | 5.0796 | 11.0754 | 6.8694 |
| 6 | 2.7458(11) | << | S | | | | Intra | 95.60 | -46.67 | 0.83964 | 0.59381 | 0.45724 | 6.1882 | 12.1458 | 3.2806 |
| 7 | 3.2512(11) | .< | S_b | [2-x,1-y,1-z | = | 3766.01] | | -41.84 | -25.19 | 1.16036 | 0.40619 | 0.54276 | 8.5635 | 8.3082 | 3.8942 |
| 8 | 3.3936(11) | .. | Cl(1)a | [1-x,1-y,1-z | = | 3666.01] | | -137.03 | -54.12 | 0.66691 | 0.43585 | 0.35243 | 4.9165 | 8.9149 | 2.5286 |
| 9 | 3.4663(17) | .. | C(2)c | [2-x,1-y,2-z | = | 3767.01] | | 3.56 | 46.68 | 1.19429 | 0.50936 | 1.08717 | 8.7452 | 10.4184 | 7.8001 |
| 10 | 3.5243(16) | .. | C(4) | | | | Intra | 125.56 | 5.82 | 0.59600 | 0.64158 | 0.78545 | 4.3327 | 13.1229 | 5.6354 |
| 11 | 2.09 | << | H(2A) | | | | Intra | -107.31 | 60.32 | 0.83220 | 0.45380 | 0.98890 | 6.0637 | 9.2820 | 7.0951 |
| 12 | 3.08 | .. | H(2A)c | [2-x,1-y,2-z | = | 3767.01] | | 22.40 | 39.89 | 1.16780 | 0.54620 | 1.01110 | 8.5580 | 11.1720 | 7.2544 |
| 13 | 3.13 | .. | H(3A) | | | | Intra | 152.32 | 50.27 | 0.63730 | 0.54750 | 1.07070 | 4.6029 | 11.1986 | 7.6820 |
| 14 | 3.33(2) | .. | H(1)b | [2-x,1-y,1-z | = | 3766.01] | | 15.26 | -62.88 | 1.05900 | 0.52170 | 0.32200 | 7.8380 | 10.6709 | 2.3103 |

Angles (Degrees) At1...V...At2 with Vertex V = N(1)

| | | | | | | | | | | | | | | | |
|------|---|--------|------------|--------|---|--------|-----------|--------|---|--------|-----------|-------|---|--------|-----------|
| C(1) | , | C(2) | 110.91(10) | C(1) | , | N(2) | 37.80(6) | C(1) | , | C(3) | 75.14(7) | C(1) | , | S | 28.56(6) |
| C(1) | , | S_b | 126.96(7) | C(1) | , | Cl(1)a | 84.00(7) | C(1) | , | C(2)c | 118.15(8) | C(1) | , | C(4) | 30.29(6) |
| C(2) | , | N(2) | 73.11(7) | C(2) | , | C(3) | 35.77(7) | C(2) | , | S | 139.47(8) | C(2) | , | S_b | 121.97(7) |
| C(2) | , | Cl(1)a | 121.51(7) | C(2) | , | C(2)c | 65.43(7) | C(2) | , | C(4) | 80.64(7) | N(2) | , | C(3) | 37.35(5) |
| N(2) | , | S | 66.36(4) | N(2) | , | S_b | 164.36(5) | N(2) | , | Cl(1)a | 103.86(4) | N(2) | , | C(2)c | 101.93(5) |
| N(2) | , | C(4) | 7.62(3) | C(3) | , | S | 103.70(5) | C(3) | , | S_b | 157.48(5) | C(3) | , | Cl(1)a | 118.67(5) |
| C(3) | , | C(2)c | 81.98(5) | C(3) | , | C(4) | 44.89(4) | S | , | S_b | 98.49(3) | S | , | Cl(1)a | 69.80(2) |
| S | , | C(2)c | 123.09(4) | S | , | C(4) | 58.83(3) | S_b | , | Cl(1)a | 72.72(2) | S_b | , | C(2)c | 82.76(3) |
| S_b | , | C(4) | 157.18(4) | Cl(1)a | , | C(2)c | 154.18(4) | Cl(1)a | , | C(4) | 99.05(3) | C(2)c | , | C(4) | 106.73(4) |

=====
Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6
=====

van der Waals (or ion) Radii used in the Analysis

=====
C H Cl N S

1.70 1.20 1.75 1.55 1.80

:: Grid: Z-Axis Step = 0.0278 = Points 36, Angstrom Step = 0.20
:: Grid: X-Axis Step = 0.0278 = Points 36, Angstrom Step = 0.21
:: Grid: Y-Axis Step = 0.0093 = Points 108, Angstrom Step = 0.19

:: Unit cell Contains NO Residual Solvent Accessible Void.

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

=====
Report Expected Number of Independent Reflections for given Symmetry and Resolution.

:: Hmax = 10 Kmax = 29 Lmax= 10 , Sorting Order : Fast H, Medium K, Slow L

:: Actual Theta-Max: 30.506 Deg. (Applied Theta Limit: 30.510 Deg.)

Space Group H-M: P21/c Laue: 2/m
Space Group Hall: -P 2ybc [Schoenflies: C2h⁵]
Lattice Type: mP, Centric, Monoclinic, Multiplicity: 4(2), No: 14

Nr ***** Symmetry Operation(s) *****

| | | | |
|---|-------|-----------|---------|
| 1 | H , | K , | L |
| 2 | - H , | 1/2 + K , | 1/2 - L |
| 3 | - H , | - K , | - L |
| 4 | H , | 1/2 - K , | 1/2 + L |

:: Number of Independent Type H, K, L Reflections = 3342

Table 0 - Crystal Data and Details of the Structure Determination

for: hmimc13 P2(1)/c R = 0.03

Crystal Data

| | | | |
|--------------------------|--------------------|-------------|-----------|
| Formula | C9 H5 Cl3 N2 S | | |
| Formula Weight | 279.57 | | |
| Crystal System | monoclinic | | |
| Space group | P21/c | (No. 14) | |
| a, b, c [Angstrom] | 7.4408(8) | 20.454(2) | 7.1759(8) |
| alpha, beta, gamma [deg] | 90 | 91.0376(14) | 90 |
| V [Ang**3] | 1092.0(2) | | |
| Z | 4 | | |
| D(calc) [g/cm**3] | 1.701 | | |
| Mu(MoKa) [/mm] | 0.993 | | |
| F(000) | 560 | | |
| Crystal Size [mm] | 0.14 x 0.45 x 0.66 | | |

Data Collection

| | | | |
|----------------------------------|-----------------------------|---------|-------|
| Temperature (K) | 130 | | |
| Radiation [Angstrom] | MoKa | 0.71073 | |
| Theta Min-Max [Deg] | 2.0, 30.5 | | |
| Dataset | -10: 10 ; -29: 29 ; -10: 10 | | |
| Tot., Uniq. Data, R(int) | 17407, | 3337, | 0.033 |
| Observed Data [I > 2.0 sigma(I)] | 3242 | | |

Refinement

| | | | |
|--|----------------------|--|--|
| Nref, Npar | 3337, 139 | | |
| R, wR2, S | 0.0276, 0.0728, 1.13 | | |
| w = 1/[\s^2^(Fo^2^)+(0.0305P)^2^+0.6285P] where P=(Fo^2^+2Fc^2^)/3 | | | |
| Max. and Av. Shift/Error | 0.00, 0.00 | | |
| Min. and Max. Resd. Dens. [e/Ang^3] | -0.39, 0.56 | | |

=====

=====

***** N O T I C E *****

=====

- PLATON Reference : Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.
Spek, A.L. (2009). Acta Cryst. D65, 148-155.

- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow

- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)

- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.

- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.

- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@uu.nl

- Recent versions of PLATON may be obtained from <http://www.platonsoft.nl/xraysoft>

- More INFO can be found on <http://http://www.platonsoft.nl/>

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Page 41 --- VOIDS
Page 42 --- EXPECT
Page 43 --- SUMMARY

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR
=====

W: NOMOVE option used.

:: >>> WARNING: 'CONNECTED INPUT SET' is assumed to be TRUE

:: >>> The Network Analysis may be INCORRECT when this assumption is FALSE

=====

:: Input Xtal Data from File hmimc13.cif - Data Type CIF

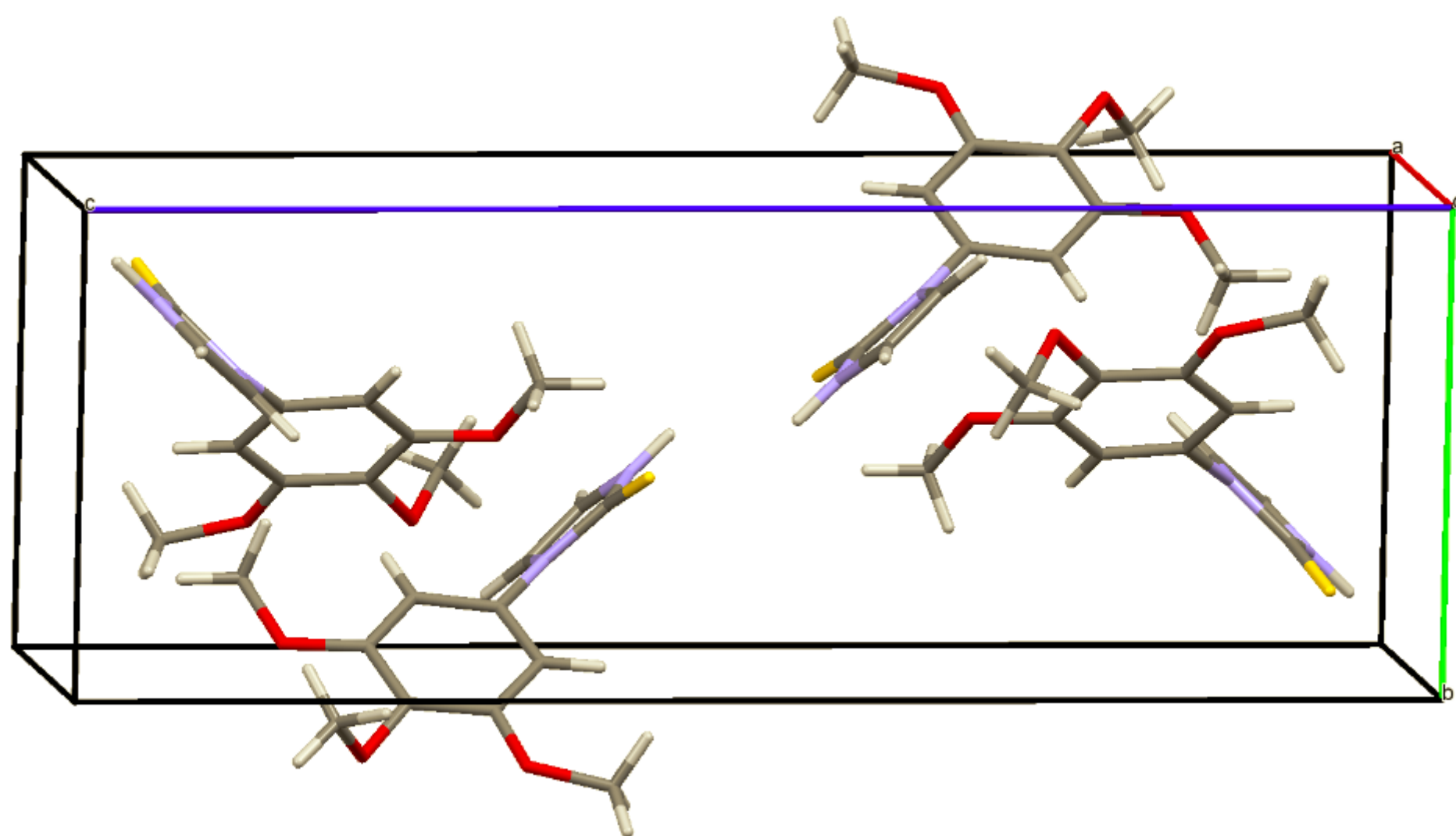
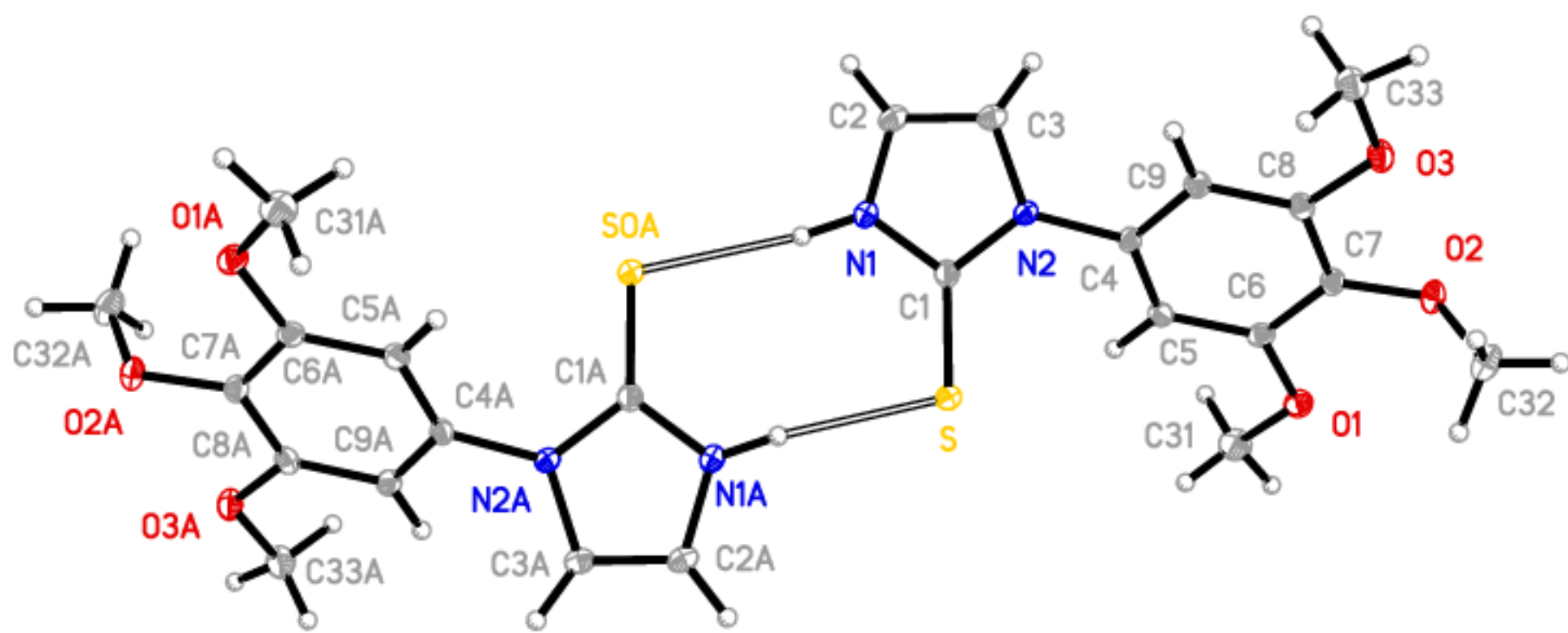
:: NORMAL END of PLATON : 45 Pages on:

:: hmimc13.lis (ASCII, 132 Characters Wide)

:: hmimc13.lps (PostScript Version of .lis)

::

Hmim^{Ar(OMe)₃}



=====
 Analysis of Short Intra- and Inter-molecular Contacts , $d(I-J) < R(I) + R(J) + \text{Tolr}$, With Tolr = 0.2 Ang. ($X - I \dots J$) > 100. Deg.

Contact Radii : C H N O S
 (Angstrom) 1.70 1.20 1.55 1.52 1.80

Default Contact Radii are those given by A.Bondi, J.Phys.Chem. (1964),68,441. (or Coval. Rad. + 0.8 Ang. when not given)

* WARNING * : no Far-Reaching Conclusions should be drawn based on the Default Radii Assigned to Metals

Short "INTRA" Distances between two Atoms that are Separated by less than 4 Bonds are NOT Listed (Except for Potential D/A Contacts)

| At(I)[1555.01] | At(J) | [ARU(J)] | D(I-J) | SumRad | Del | Type | X(I) | Y(I) | Z(I) | X(J) | Y(J) | Z(J) | X | X - I...J |
|----------------|-------------|-------------|--------------|--------|-------|-------|---------------|--------|---------------|---------------|--------|--------|-------|------------|
| S | C(2) | [1655.01] | 3.6876(16) | 3.50 | 0.19 | | 0.2224 | 0.3659 | 0.4513 | 0.7034 | 0.2467 | 0.4246 | C(1) | 135.37(6) |
| S | C(4) | [] | 3.2635(16)<< | 3.50 | -0.24 | Intra | 0.2224 | 0.3659 | 0.4513 | 0.0914 | 0.0893 | 0.3497 | | |
| S | C(5) | [] | 3.4215(16) < | 3.50 | -0.08 | Intra | 0.2224 | 0.3659 | 0.4513 | 0.2354-0.0065 | 0.3747 | | | |
| S | H(1) | [] | 2.93(2) < | 3.00 | -0.07 | Intra | 0.2224 | 0.3659 | 0.4513 | -0.1620 | 0.4110 | 0.4828 | | |
| S | H(2A) | [1655.01] | 2.76<< | 3.00 | -0.24 | | 0.2224 | 0.3659 | 0.4513 | 0.5760 | 0.2570 | 0.4323 | C(1) | 133 |
| S | H(5A) | [] | 3.13 | 3.00 | 0.13 | Intra | 0.2224 | 0.3659 | 0.4513 | 0.2565-0.0140 | 0.4170 | | | |
| S | H(31B) | [1565.01] | 3.15 | 3.00 | 0.15 | | 0.2224 | 0.3659 | 0.4513 | 0.4042 | 0.7201 | 0.4303 | C(1) | 132 |
| S | N(1) | [3566.01] | 3.2662(15) < | 3.35 | -0.08 | | 0.2224 | 0.3659 | 0.4513 | 0.1515 | 0.6677 | 0.5467 | C(1) | 105.80(6) |
| S | C(31) | [3656.01] | 3.5763(19) | 3.50 | 0.08 | | 0.2224 | 0.3659 | 0.4513 | 0.4820 | 0.2288 | 0.5832 | C(1) | 122.46(7) |
| S | H(1) | [3566.01] | 2.36(2)<< | 3.00 | -0.64 | | 0.2224 | 0.3659 | 0.4513 | 0.1620 | 0.5890 | 0.5172 | C(1) | 104.3(5) |
| S | H(31A) | [3656.01] | 3.00 | 3.00 | 0.00 | | 0.2224 | 0.3659 | 0.4513 | 0.3792 | 0.3082 | 0.5768 | C(1) | 119 |
| O(1) | O(2) | [] | 2.6487(16)<< | 3.04 | -0.39 | Intra | 0.4948-0.1891 | 0.3546 | 0.4157-0.1784 | 0.2374 | | | C(31) | 167.76(10) |
| O(1) | C(3) | [1655.01] | 3.398(2) | 3.22 | 0.18 | | 0.4948-0.1891 | 0.3546 | 0.7762 | 0.1464 | 0.3840 | | | |
| O(1) | C(32) | [] | 3.352(2) | 3.22 | 0.13 | Intra | 0.4948-0.1891 | 0.3546 | 0.5650-0.0924 | 0.2114 | | | C(31) | 164.54(11) |
| O(1) | H(3A) | [1655.01] | 2.60 < | 2.72 | -0.12 | | 0.4948-0.1891 | 0.3546 | 0.7101 | 0.0723 | 0.3572 | | | |
| O(1) | H(5A) | [] | 2.67 < | 2.72 | -0.05 | Intra | 0.4948-0.1891 | 0.3546 | 0.2565-0.0140 | 0.4170 | | | | |
| O(1) | H(32C) | [2645.01] | 2.60 < | 2.72 | -0.12 | | 0.4948-0.1891 | 0.3546 | 0.4813-0.4891 | 0.3081 | | | C(6) | 113 |
| | | | | | | | | | | | | | C(31) | 101 |
| O(2) | O(1) | [] | 2.6487(16)<< | 3.04 | -0.39 | Intra | 0.4157-0.1784 | 0.2374 | 0.4948-0.1891 | 0.3546 | | | C(32) | 106.77(10) |
| O(2) | O(3) | [] | 2.6704(16)<< | 3.04 | -0.37 | Intra | 0.4157-0.1784 | 0.2374 | 0.1511 | 0.0223 | 0.1896 | | | |
| O(2) | C(3) | [2545.01] | 3.288(2) | 3.22 | 0.07 | | 0.4157-0.1784 | 0.2374 | 0.2238-0.3536 | 0.1160 | | | C(7) | 121.30(9) |
| O(3) | O(2) | [] | 2.6704(16)<< | 3.04 | -0.37 | Intra | 0.1511 | 0.0223 | 0.1896 | 0.4157-0.1784 | 0.2374 | | C(33) | 174.16(11) |
| O(3) | C(32) | [] | 3.1445(19) < | 3.22 | -0.08 | Intra | 0.1511 | 0.0223 | 0.1896 | 0.5650-0.0924 | 0.2114 | | C(33) | 147.65(11) |
| O(3) | H(9A) | [] | 2.67 < | 2.72 | -0.05 | Intra | 0.1511 | 0.0223 | 0.1896 | -0.0422 | 0.1734 | 0.2726 | | |
| O(3) | H(32C) | [] | 2.66 < | 2.72 | -0.06 | Intra | 0.1511 | 0.0223 | 0.1896 | 0.5187 | 0.0109 | 0.1919 | C(33) | 131 |
| N(1) | C(3) | [] | 2.182(2)<< | 3.25 | -1.07 | Intra | -0.1515 | 0.3323 | 0.4533 | -0.2238 | 0.1464 | 0.3840 | H(1) | 161.4(14) |
| N(1) | S | [3566.01] | 3.2662(15) < | 3.35 | -0.08 | | -0.1515 | 0.3323 | 0.4533 | -0.2224 | 0.6341 | 0.5487 | C(1) | 127.05(10) |
| | | | | | | | | | | | | | C(2) | 121.46(10) |
| N(2) | C(2) | [] | 2.194(2)<< | 3.25 | -1.06 | Intra | -0.0336 | 0.1707 | 0.3882 | -0.2966 | 0.2467 | 0.4246 | C(4) | 158.93(11) |
| N(2) | H(5A) | [] | 2.61 < | 2.75 | -0.14 | Intra | -0.0336 | 0.1707 | 0.3882 | 0.2565-0.0140 | 0.4170 | | C(3) | 136 |
| N(2) | H(9A) | [] | 2.58 < | 2.75 | -0.17 | Intra | -0.0336 | 0.1707 | 0.3882 | -0.0422 | 0.1734 | 0.2726 | C(1) | 134 |
| C(1) | C(3) | [] | 2.251(2)<< | 3.40 | -1.15 | Intra | 0.0110 | 0.2879 | 0.4311 | -0.2238 | 0.1464 | 0.3840 | S | 163.42(10) |
| C(1) | C(5) | [] | 3.148(2)<< | 3.40 | -0.25 | Intra | 0.0110 | 0.2879 | 0.4311 | 0.2354-0.0065 | 0.3747 | | N(1) | 145.14(11) |

| | | | | | | | | | | | | | | | |
|--------|------|--------|---|----------|-------------|-------|-------|---------------|--------|---------------|----------------|--------|-----------|-----------|--|
| H(5A) | | H(31B) | [|] | 2.38 < 2.40 | -0.02 | Intra | 0.2565-0.0140 | 0.4170 | 0.4042-0.2799 | 0.4303 | C(5) | 103 | | |
| H(5A) | | H(31C) | [|] | 2.30 < 2.40 | -0.10 | Intra | 0.2565-0.0140 | 0.4170 | 0.5450-0.1257 | 0.4397 | C(5) | 110 | | |
| H(9A) | | O(3) | [|] | 2.67 < 2.72 | -0.05 | Intra | -0.0422 | 0.1734 | 0.2726 | 0.1511 | 0.0223 | 0.1896 | | |
| H(9A) | | N(2) | [|] | 2.58 < 2.75 | -0.17 | Intra | -0.0422 | 0.1734 | 0.2726 | -0.0336 | 0.1707 | 0.3882 | | |
| H(9A) | | C(3) | [|] | 2.88 < 2.90 | -0.02 | Intra | -0.0422 | 0.1734 | 0.2726 | -0.2238 | 0.1464 | 0.3840 | | |
| H(9A) | | C(33) | [|] | 2.52<< 2.90 | -0.38 | Intra | -0.0422 | 0.1734 | 0.2726 | 0.0244 | 0.1417 | 0.1635 | | |
| H(9A) | | H(33B) | [|] | 2.33 < 2.40 | -0.07 | Intra | -0.0422 | 0.1734 | 0.2726 | 0.0558 | 0.2542 | 0.1789 | C(9) 103 | |
| H(9A) | | H(33C) | [|] | 2.27 < 2.40 | -0.13 | Intra | -0.0422 | 0.1734 | 0.2726 | -0.1015 | 0.1126 | 0.1739 | C(9) 110 | |
| H(9A) | | C(7) | [| 2555.01] | 2.93 | 2.90 | 0.03 | -0.0422 | 0.1734 | 0.2726 | -0.3148 | 0.4190 | 0.2257 | C(9) 173 | |
| H(9A) | | C(8) | [| 2555.01] | 2.94 | 2.90 | 0.04 | -0.0422 | 0.1734 | 0.2726 | -0.1708 | 0.5192 | 0.2496 | C(9) 145 | |
| H(31A) | | S | [| 3656.01] | 3.00 | 3.00 | 0.00 | 0.6208-0.3082 | 0.4232 | 0.7776-0.3659 | 0.5487 | C(31) | 119 | | |
| H(31B) | | S | [| 1545.01] | 3.15 | 3.00 | 0.15 | 0.4042-0.2799 | 0.4303 | 0.2224-0.6341 | 0.4513 | C(31) | 141 | | |
| H(31B) | | C(5) | [|] | 2.75 < 2.90 | -0.15 | Intra | 0.4042-0.2799 | 0.4303 | 0.2354-0.0065 | 0.3747 | | | | |
| H(31B) | | C(6) | [|] | 2.59<< 2.90 | -0.31 | Intra | 0.4042-0.2799 | 0.4303 | 0.3483-0.0913 | 0.3363 | | | | |
| H(31B) | | H(5A) | [|] | 2.38 < 2.40 | -0.02 | Intra | 0.4042-0.2799 | 0.4303 | 0.2565-0.0140 | 0.4170 | | | | |
| H(31C) | | C(3) | [| 1655.01] | 3.04 | 2.90 | 0.14 | 0.5450-0.1257 | 0.4397 | 0.7762 | 0.1464 | 0.3840 | C(31) | 119 | |
| H(31C) | | C(5) | [|] | 2.77 < 2.90 | -0.13 | Intra | 0.5450-0.1257 | 0.4397 | 0.2354-0.0065 | 0.3747 | | | | |
| H(31C) | | C(6) | [|] | 2.66<< 2.90 | -0.24 | Intra | 0.5450-0.1257 | 0.4397 | 0.3483-0.0913 | 0.3363 | | | | |
| H(31C) | | H(5A) | [|] | 2.30 < 2.40 | -0.10 | Intra | 0.5450-0.1257 | 0.4397 | 0.2565-0.0140 | 0.4170 | | | | |
| H(32A) | | C(4) | [| 2645.01] | 2.97 | 2.90 | 0.07 | 0.6193-0.1653 | 0.1816 | 0.9086-0.4107 | 0.1503 | C(32) | 149 | | |
| H(32A) | | C(9) | [| 2645.01] | 3.02 | 2.90 | 0.12 | 0.6193-0.1653 | 0.1816 | 0.9432-0.3946 | 0.2116 | C(32) | 123 | | |
| H(32B) | | C(7) | [|] | 2.63<< 2.90 | -0.27 | Intra | 0.6594-0.0638 | 0.2429 | 0.3148-0.0810 | 0.2743 | | | | |
| H(32C) | | O(3) | [|] | 2.66 < 2.72 | -0.06 | Intra | 0.5187 | 0.0109 | 0.1919 | 0.1511 | 0.0223 | 0.1896 | C(32) 111 | |
| H(32C) | | C(7) | [|] | 2.53<< 2.90 | -0.37 | Intra | 0.5187 | 0.0109 | 0.1919 | 0.3148-0.0810 | 0.2743 | | | |
| H(32C) | | C(8) | [|] | 2.90 | 2.90 | 0.00 | Intra | 0.5187 | 0.0109 | 0.1919 | 0.1708 | 0.0192 | 0.2504 | |
| H(32C) | | O(1) | [| 2655.01] | 2.60 < 2.72 | -0.12 | | 0.5187 | 0.0109 | 0.1919 | 0.5052 | 0.3109 | 0.1454 | C(32) 162 | |
| H(33A) | | C(1) | [| 2545.01] | 3.03 | 2.90 | 0.13 | 0.0317 | 0.1406 | 0.1198 | -0.0110-0.2121 | 0.0689 | C(33) | 112 | |
| H(33B) | | C(8) | [|] | 2.57<< 2.90 | -0.33 | Intra | 0.0558 | 0.2542 | 0.1789 | 0.1708 | 0.0192 | 0.2504 | | |
| H(33B) | | C(9) | [|] | 2.72 < 2.90 | -0.18 | Intra | 0.0558 | 0.2542 | 0.1789 | 0.0568 | 0.1054 | 0.2884 | | |
| H(33B) | | H(9A) | [|] | 2.33 < 2.40 | -0.07 | Intra | 0.0558 | 0.2542 | 0.1789 | -0.0422 | 0.1734 | 0.2726 | | |
| H(33B) | | C(4) | [| 2555.01] | 2.93 | 2.90 | 0.03 | 0.0558 | 0.2542 | 0.1789 | -0.0914 | 0.5893 | 0.1503 | C(33) 133 | |
| H(33B) | | C(5) | [| 2555.01] | 3.04 | 2.90 | 0.14 | 0.0558 | 0.2542 | 0.1789 | -0.2354 | 0.4935 | 0.1253 | C(33) 107 | |
| H(33B) | | C(9) | [| 2555.01] | 3.01 | 2.90 | 0.11 | 0.0558 | 0.2542 | 0.1789 | -0.0568 | 0.6054 | 0.2116 | C(33) 151 | |
| H(33C) | | C(8) | [|] | 2.64<< 2.90 | -0.26 | Intra | -0.1015 | 0.1126 | 0.1739 | 0.1708 | 0.0192 | 0.2504 | | |
| H(33C) | | C(9) | [|] | 2.75 < 2.90 | -0.15 | Intra | -0.1015 | 0.1126 | 0.1739 | 0.0568 | 0.1054 | 0.2884 | | |
| H(33C) | | C(32) | [| 1455.01] | 3.07 | 2.90 | 0.17 | -0.1015 | 0.1126 | 0.1739 | -0.4350-0.0924 | 0.2114 | C(33) 161 | | |
| H(33C) | | H(9A) | [|] | 2.27 < 2.40 | -0.13 | Intra | -0.1015 | 0.1126 | 0.1739 | -0.0422 | 0.1734 | 0.2726 | | |
| H(33C) | | C(6) | [| 2555.01] | 2.96 | 2.90 | 0.06 | -0.1015 | 0.1126 | 0.1739 | -0.3483 | 0.4087 | 0.1637 | C(33) 111 | |

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 1 to Neighbouring ARU'S

| Nr | ARU | Nr.Cont. | d(min) | Del | XHn | X | - At(I) | At(J) | - Y | YHn | Note | Partaking ARU's in Close Contact | Resd. |
|----|------------|----------|--------|-------|-----|------|---------|-------|--------|--------|------|----------------------------------|---------|
| 1 | [1655.01] | 7 | 2.6000 | -0.12 | 0 | C(6) | - O(1) | ... | H(3A) | -C(3) | 1 | < | 1655.01 |
| 2 | [1565.01] | 1 | 3.1500 | 0.15 | 0 | C(1) | - S | ... | H(31B) | -C(31) | 3 | | 1565.01 |

```

=====
 3 [ 3566.01]    4    2.3600 -0.64    1 N(1)  - H(1)  ... S   -C(1)  0  << 3566.01
 4 [ 3656.01]    4    3.0000  0.00    3 C(31) - H(31A) ... S   -C(1)  0    3656.01
 5 [ 2645.01]    3    2.6000 -0.12    0 C(6)  - O(1)  ... H(32C) -C(32) 3   < 2645.01
 6 [ 2545.01]   11    2.9300  0.03    0 O(2)  - C(7)  ... H(9A) -C(9)  1    2545.01
 7 [ 2555.01]   11    2.9300  0.03    3 C(33) - H(33B) ... C(4)  -N(2)  0    2555.01
 8 [ 1455.01]    7    2.6000 -0.12    1 C(3)  - H(3A)  ... O(1)  -C(6)  0   < 1455.01
 9 [ 2655.01]    3    2.6000 -0.12    3 C(32) - H(32C) ... O(1)  -C(6)  0   < 2655.01
10 [ 1545.01]    1    3.1500  0.15    3 C(31) - H(31B) ... S   -C(1)  0    1545.01
=====

```

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Asymmetric Residue Unit (= ARU) Code List

=====

| ARU-CODE | CIF-CODE | Symmetry-Code | sym | TX | TY | TZ | Ires | x(cen) | y(cen) | z(cen) | |
|------------|----------|-------------------|-----|-----|----|----|------|--------|--------|--------|-------|
| [1655.01] | [1_655] | =1+x,y,z | = | [1 | 1 | 0 | 0 | 1 | 1.175 | 0.048 | 0.323 |
| [1565.01] | [1_565] | =x,1+y,z | = | [1 | 0 | 1 | 0 | 1 | 0.175 | 1.048 | 0.323 |
| [3566.01] | [3_566] | =-x,1-y,1-z | = | [3 | 0 | 1 | 1 | 1 | -0.175 | 0.952 | 0.677 |
| [3656.01] | [3_656] | =1-x,-y,1-z | = | [3 | 1 | 0 | 1 | 1 | 0.825 | -0.048 | 0.677 |
| [2645.01] | [2_645] | =1-x,-1/2+y,1/2-z | = | [2 | 1 | -1 | 0 | 1 | 0.825 | -0.452 | 0.177 |
| [2545.01] | [2_545] | =-x,-1/2+y,1/2-z | = | [2 | 0 | -1 | 0 | 1 | -0.175 | -0.452 | 0.177 |
| [2555.01] | [2_555] | =-x,1/2+y,1/2-z | = | [2 | 0 | 0 | 0 | 1 | -0.175 | 0.548 | 0.177 |
| [1455.01] | [1_455] | =-1+x,y,z | = | [1 | -1 | 0 | 0 | 1 | -0.825 | 0.048 | 0.323 |
| [2655.01] | [2_655] | =1-x,1/2+y,1/2-z | = | [2 | 1 | 0 | 0 | 1 | 0.825 | 0.548 | 0.177 |
| [1545.01] | [1_545] | =x,-1+y,z | = | [1 | 0 | -1 | 0 | 1 | 0.175 | -0.952 | 0.323 |

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

X(J) = X(sym) + TX , Y(J) = Y(sym) + TY , Z(J) = Z(sym) + TZ,
 SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

=====
 Analysis of Potential Hydrogen Bonds and Schemes with $d(D...A) < R(D)+R(A)+0.50$, $d(H...A) < R(H)+R(A)-0.12$ Ang., $D-H...A > 100.0$ Deg
 =====

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
 =====

| Nr | Typ | Res | Donor | H...A | Acceptor | [ARU] | D - H | H...A | D...A | D - H...A | A..H..A* A'..H..A" | Sum(XY,YZ) | Sum(XZ) |
|----|-----|-----|-------|----------|----------|------------|---------|---------|------------|-----------|--------------------|------------|---------|
| 1 | | 1 | N(1) | --H(1) | ..S | [3566.01] | 0.92(2) | 2.36(2) | 3.2662(15) | 171.2(19) | | | |
| 2 | | 1 | C(2) | --H(2A) | ..S | [1455.01] | 0.95 | 2.76 | 3.6876(16) | 167 | | | |
| 3 | | 1 | C(3) | --H(3A) | ..O(1) | [1455.01] | 0.95 | 2.60 | 3.398(2) | 142 | | | |
| 4 | | 1 | C(32) | --H(32C) | ..O(1) | [2655.01] | 0.98 | 2.60 | 3.544(2) | 162 | | | |

Translation of ARU-Code to CIF and Equivalent Position Code
 =====

[3566.] = [3_566] = -x,1-y,1-z
 [1455.] = [1_455] = -1+x,y,z
 [2655.] = [2_655] = 1-x,1/2+y,1/2-z

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]

2-Centre (linear) D-H...X most prob. angle 160 deg - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
 3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg Springer-Verlag, Berlin, 1991, pp 20.
 4-Centre (trifurcated)

Analysis of Potential Donor/Acceptor Atoms -- (Major Disorder Form Only)
 =====

| At.Nr | D/A | #Cov.Bonds | # H | #D-H..A | #A..H | #A..H-C | Sum(A-H) | Sum(A-X) |
|-------|------|------------|-----|---------|-------|---------|----------|----------|
| 1 | S | 1 | - | 0 | 1 | 1 | 2 | 3 |
| 2 | O(1) | 2 | - | 0 | 0 | 2 | 2 | 4 |
| 3 | O(2) | 2 | - | 0 | 0 | 0 | 0 | 2 |
| 4 | O(3) | 2 | - | 0 | 0 | 0 | 0 | 2 |
| 5 | N(1) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 6 | N(2) | 3 | - | 0 | 0 | 0 | 0 | 3 |

=====
 Analysis of Hydrogen Bonded Molecular Aggregates (See also Acta Cryst. B36, 1980, 2113 - 2115) -- (Major Disorder Component Only)
 =====

Coordinates of Donor and Acceptor Atoms
 =====

Coordinates of D/A-Bonded Atom(s)
 =====

| D/A I | [ARU] | X | Y | Z | -- | D/A J | [ARU] | X | Y | Z | Atom K | X | Y | Z | I..J--K Angle |
|-------|-------------|---------|--------|--------|----|-------|-------------|---------|--------|--------|--------|---------|--------|--------|---------------|
| N(1) | [1555.01], | -0.1515 | 0.3323 | 0.4533 | >> | S | [3566.01], | -0.2224 | 0.6341 | 0.5487 | C(1) | -0.0110 | 0.7121 | 0.5689 | 105.80(3) |
| S | [1555.01], | 0.2224 | 0.3659 | 0.4513 | << | N(1) | [3566.01], | 0.1515 | 0.6677 | 0.5467 | C(1) | -0.0110 | 0.7121 | 0.5689 | 127.05(3) |
| | | | | | | | | | | | C(2) | 0.2966 | 0.7533 | 0.5754 | 121.46(3) |
| | | | | | | | | | | | H(1) | 0.1620 | 0.5890 | 0.5172 | 6.33(4) |

=====

***** Aggregate = 1 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 2 1 1555.01 -- 3566.01
 2 1 3566.01 -- 1555.01

=====

***** Aggregate = 2 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 2 1 2555.01 -- 4564.01
 2 1 4564.01 -- 2555.01

=====
 Analysis of the (Cooperative) Hydrogen Bond Network (i.e. (In)Finite O-H...O-H...O-H.. Chains and/or Rings (Max = 18 Membered))
 =====

=====
 ***** Network = 1 *****
 =====

| Code | Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|-------|-----|-----------------|---------|--------|--------|---------------|---------|--------|--|
| 1.555 | | N(1) [1555.01] | -0.1515 | 0.3323 | 0.4533 | S [3566.01] | -0.2224 | 0.6341 | 0.5487 |
| | | H(1) | -0.1620 | 0.4110 | 0.4828 | | | | |

 Hydrogen Bonds are Coded as N.IJK Where N = Sequence Number of Hydrogen Bond (NOTE: New Hbond Numbering system)
 I - 5 = Nr of Translation Units Along A-Axis
 J - 5 = Nr of Translation Units Along B-Axis
 K - 5 = Nr of Translation Units Along C-Axis

Ring Closure Links are Indicated with 'R' and Infinite Chain Links With 'T'

3.6 Angstrom Coordination Sphere Around Atom I = O(1) [ARU = 1555.01] 0.49482 -0.18911 0.35457 3.1570 -1.5026 7.9040

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|-------------------|-----------|----------|-------|---------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 1.3598(19) | -- | C(6) | | | | Intra | 143.18 | -17.42 | 0.34830 | -0.09126 | 0.33631 | 2.1184 | -0.7251 | 7.4970 |
| 2 | 1.426(2) | -- | C(31) | | | | Intra | -73.53 | 76.67 | 0.51800 | -0.22880 | 0.41683 | 3.2503 | -1.8180 | 9.2919 |
| 3 | 2.3237(19) | << | C(7) | | | | Intra | 144.55 | -50.39 | 0.31480 | -0.08098 | 0.27426 | 1.9502 | -0.6435 | 6.1138 |
| 4 | 2.4341(19) | << | C(5) | | | | Intra | 142.66 | 10.64 | 0.23540 | -0.00648 | 0.37473 | 1.2551 | -0.0515 | 8.3534 |
| 5 | 2.6487(16) | << | O(2) | | | | Intra | 168.84 | -80.42 | 0.41567 | -0.17837 | 0.23741 | 2.7244 | -1.4173 | 5.2923 |
| 6 | 3.352(2) | .. | C(32) | | | | Intra | 48.52 | -72.18 | 0.56500 | -0.09240 | 0.21140 | 3.8365 | -0.7342 | 4.7125 |
| 7 | 3.398(2) | .. | C(3)a | [1+x,y,z | = | 1655.01] | | 53.10 | 11.13 | 0.77620 | 0.14640 | 0.38399 | 5.1585 | 1.1633 | 8.5598 |
| 8 | 3.544(2) | .. | C(32)b | [1-x,-1/2+y,1/2-z | = | 2645.01] | | -96.30 | -24.52 | 0.43500 | -0.59240 | 0.28860 | 2.8031 | -4.7072 | 6.4334 |
| 9 | 1.98 | << | H(31C) | | | | Intra | 62.59 | 73.35 | 0.54500 | -0.12570 | 0.43970 | 3.4183 | -0.9988 | 9.8017 |
| 10 | 1.98 | << | H(31A) | | | | Intra | -48.76 | 50.56 | 0.62080 | -0.30820 | 0.42320 | 3.9867 | -2.4489 | 9.4339 |
| 11 | 1.98 | << | H(31B) | | | | Intra | -135.98 | 58.41 | 0.40420 | -0.27990 | 0.43030 | 2.4104 | -2.2241 | 9.5922 |
| 12 | 2.60 | .< | H(3A)a | [1+x,y,z | = | 1655.01] | | 53.18 | 1.29 | 0.71010 | 0.07230 | 0.35720 | 4.7122 | 0.5745 | 7.9627 |
| 13 | 2.60 | .< | H(32C)b | [1-x,-1/2+y,1/2-z | = | 2645.01] | | -91.01 | -23.49 | 0.48130 | -0.48910 | 0.30810 | 3.1148 | -3.8863 | 6.8681 |
| 14 | 2.67 | .< | H(5A) | | | | Intra | 142.29 | 31.46 | 0.25650 | -0.01400 | 0.41700 | 1.3573 | -0.1112 | 9.2957 |
| 15 | 2.99 | .. | H(32B) | | | | Intra | 36.92 | -56.34 | 0.65940 | -0.06380 | 0.24290 | 4.4821 | -0.5069 | 5.4147 |
| 16 | 3.29 | .. | H(33C)c | [-x,-1/2+y,1/2-z | = | 2545.01] | | -150.75 | -11.14 | 0.10150 | -0.38740 | 0.32610 | 0.3442 | -3.0782 | 7.2694 |
| 17 | 3.41 | .. | H(33B)b | [1-x,-1/2+y,1/2-z | = | 2645.01] | | -7.79 | -12.65 | 0.94420 | -0.24580 | 0.32110 | 6.4499 | -1.9531 | 7.1579 |

Angles (Degrees) At1...V...At2 with Vertex V = O(1)

| | | | | | | | | | | | | | | | |
|-------|---|--------|------------|-------|---|--------|------------|-------|---|--------|------------|-------|---|--------|------------|
| C(6) | , | C(31) | 117.88(13) | C(6) | , | C(7) | 32.99(8) | C(6) | , | C(5) | 28.06(8) | C(6) | , | O(2) | 64.00(8) |
| C(6) | , | C(32) | 74.86(8) | C(6) | , | C(3)a | 93.39(9) | C(6) | , | C(32)b | 108.45(9) | C(31) | , | C(7) | 149.92(12) |
| C(31) | , | C(5) | 90.19(10) | C(31) | , | O(2) | 167.76(10) | C(31) | , | C(32) | 164.54(11) | C(31) | , | C(3)a | 86.97(9) |
| C(31) | , | C(32)b | 102.15(9) | C(7) | , | C(5) | 61.05(6) | C(7) | , | O(2) | 31.08(5) | C(7) | , | C(32) | 44.52(5) |
| C(7) | , | C(3)a | 99.47(6) | C(7) | , | C(32)b | 87.87(6) | C(5) | , | O(2) | 92.02(6) | C(5) | , | C(32) | 101.39(6) |
| C(5) | , | C(3)a | 87.53(5) | C(5) | , | C(32)b | 122.53(6) | O(2) | , | C(32) | 24.07(4) | O(2) | , | C(3)a | 105.15(5) |
| O(2) | , | C(32)b | 66.65(5) | C(32) | , | C(3)a | 83.37(5) | C(32) | , | C(32)b | 80.35(5) | C(3)a | , | C(32)b | 148.05(5) |

3.6 Angstrom Coordination Sphere Around Atom I = O(2) [ARU = 1555.01] 0.41567 -0.17837 0.23741 2.7244 -1.4173 5.2923

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|---------------------|-----------|----------|-------|---------|--------|---------|----------|---------|--------|---------|--------|
| 1 | 1.3686(19) | -- | C(7) | | | | Intra | 135.01 | 36.88 | 0.31480 | -0.08098 | 0.27426 | 1.9502 | -0.6435 | 6.1138 |
| 2 | 1.428(2) | -- | C(32) | | | | Intra | 31.56 | -23.95 | 0.56500 | -0.09240 | 0.21140 | 3.8365 | -0.7342 | 4.7125 |
| 3 | 2.3889(19) | << | C(6) | | | | Intra | 131.21 | 67.35 | 0.34830 | -0.09126 | 0.33631 | 2.1184 | -0.7251 | 7.4970 |
| 4 | 2.3971(19) | << | C(8) | | | | Intra | 138.72 | 6.95 | 0.17080 | 0.01921 | 0.25043 | 0.9364 | 0.1526 | 5.5825 |
| 5 | 2.6487(16) | << | O(1) | | | | Intra | -11.16 | 80.42 | 0.49482 | -0.18911 | 0.35457 | 3.1570 | -1.5026 | 7.9040 |
| 6 | 2.6704(16) | << | O(3) | | | | Intra | 139.37 | -23.54 | 0.15106 | 0.02225 | 0.18957 | 0.8664 | 0.1768 | 4.2259 |
| 7 | 3.288(2) | .. | C(3)a | [-x, -1/2+y, 1/2-z | = | 2545.01] | | -131.77 | -55.40 | 0.22380 | -0.35360 | 0.11601 | 1.4810 | -2.8097 | 2.5861 |
| 8 | 3.483(2) | .. | C(32)b | [1-x, -1/2+y, 1/2-z | = | 2645.01] | | -88.63 | 19.12 | 0.43500 | -0.59240 | 0.28860 | 2.8031 | -4.7072 | 6.4334 |
| 9 | 1.98 | << | H(32C) | | | | Intra | 61.98 | -30.77 | 0.51870 | 0.01090 | 0.19190 | 3.5247 | 0.0866 | 4.2778 |
| 10 | 1.98 | << | H(32A) | | | | Intra | 3.86 | -38.86 | 0.61930 | -0.16530 | 0.18160 | 4.2652 | -1.3135 | 4.0482 |
| 11 | 1.98 | << | H(32B) | | | | Intra | 27.38 | 3.54 | 0.65940 | -0.06380 | 0.24290 | 4.4821 | -0.5069 | 5.4147 |
| 12 | 2.95 | .. | H(9A)a | [-x, -1/2+y, 1/2-z | = | 2545.01] | | -156.36 | -4.34 | 0.04220 | -0.32660 | 0.22740 | 0.0331 | -2.5951 | 5.0692 |
| 13 | 2.95 | .. | H(32C)b | [1-x, -1/2+y, 1/2-z | = | 2645.01] | | -81.01 | 32.23 | 0.48130 | -0.48910 | 0.30810 | 3.1148 | -3.8863 | 6.8681 |
| 14 | 3.00 | .. | H(3A)a | [-x, -1/2+y, 1/2-z | = | 2545.01] | | -111.92 | -44.64 | 0.28990 | -0.42770 | 0.14280 | 1.9274 | -3.3985 | 3.1833 |
| 15 | 3.15 | .. | H(32B)b | [1-x, -1/2+y, 1/2-z | = | 2645.01] | | -100.49 | 8.02 | 0.34060 | -0.56380 | 0.25710 | 2.1575 | -4.4799 | 5.7312 |
| 16 | 3.51 | .. | H(33C)a | [-x, -1/2+y, 1/2-z | = | 2545.01] | | -145.09 | 34.26 | 0.10150 | -0.38740 | 0.32610 | 0.3442 | -3.0782 | 7.2694 |

Angles (Degrees) At1...V...At2 with Vertex V = O(2)

| | | | | | | | | | | | | | | | |
|-------|---|--------|------------|-------|---|--------|------------|-------|---|--------|-----------|-------|---|--------|------------|
| C(7) | , | C(32) | 114.44(12) | C(7) | , | C(6) | 30.54(8) | C(7) | , | C(8) | 30.12(8) | C(7) | , | O(1) | 61.24(8) |
| C(7) | , | O(3) | 60.56(8) | C(7) | , | C(3)a | 121.30(9) | C(7) | , | C(32)b | 110.50(9) | C(32) | , | C(6) | 115.70(10) |
| C(32) | , | C(8) | 108.46(9) | C(32) | , | O(1) | 106.77(10) | C(32) | , | O(3) | 95.40(9) | C(32) | , | C(3)a | 99.38(10) |
| C(32) | , | C(32)b | 124.56(9) | C(6) | , | C(8) | 60.61(6) | C(6) | , | O(1) | 30.77(5) | C(6) | , | O(3) | 91.09(6) |
| C(6) | , | C(3)a | 141.85(6) | C(6) | , | C(32)b | 88.69(6) | C(8) | , | O(1) | 91.35(6) | C(8) | , | O(3) | 30.50(5) |
| C(8) | , | C(3)a | 95.45(6) | C(8) | , | C(32)b | 126.57(6) | O(1) | , | O(3) | 121.78(5) | O(1) | , | C(3)a | 149.29(6) |
| O(1) | , | C(32)b | 69.07(5) | O(3) | , | C(3)a | 70.18(4) | O(3) | , | C(32)b | 135.27(5) | C(3)a | , | C(32)b | 83.00(5) |

3.6 Angstrom Coordination Sphere Around Atom I = O(3) [ARU = 1555.01] 0.15106 0.02225 0.18957 0.8664 0.1768 4.2259

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|--------------------|------------|--------|-------|---------|--------|----------|----------|---------|---------|---------|--------|
| 1 | 1.3587(19) | -- | C(8) | | | | Intra | -19.04 | 86.88 | 0.17080 | 0.01921 | 0.25043 | 0.9364 | 0.1526 | 5.5825 |
| 2 | 1.422(2) | -- | C(33) | | | | Intra | 133.02 | -24.10 | 0.02440 | 0.14170 | 0.16352 | -0.0192 | 1.1259 | 3.6452 |
| 3 | 2.3263(19) | << | C(7) | | | | Intra | -37.12 | 54.25 | 0.31480 | -0.08098 | 0.27426 | 1.9502 | -0.6435 | 6.1138 |
| 4 | 2.4359(19) | << | C(9) | | | | Intra | 140.49 | 64.78 | 0.05680 | 0.10535 | 0.28843 | 0.0657 | 0.8371 | 6.4296 |
| 5 | 2.6704(16) | << | O(2) | | | | Intra | -40.63 | 23.54 | 0.41567 | -0.17837 | 0.23741 | 2.7244 | -1.4173 | 5.2923 |
| 6 | 3.1445(19) | .< | C(32) | | | | Intra | -17.05 | 8.90 | 0.56500 | -0.09240 | 0.21140 | 3.8365 | -0.7342 | 4.7125 |
| 7 | 3.3741(17) | .. | N(2)a | [-x, -1/2+y, 1/2-z | = 2545.01] | | | -105.16 | -30.93 | 0.03361 | -0.32932 | 0.11177 | 0.1094 | -2.6167 | 2.4916 |
| 8 | 3.4290(19) | .. | C(1)a | [-x, -1/2+y, 1/2-z | = 2545.01] | | | -118.91 | -51.65 | -0.01100 | -0.21210 | 0.06893 | -0.1622 | -1.6853 | 1.5366 |
| 9 | 3.462(2) | .. | C(3)a | [-x, -1/2+y, 1/2-z | = 2545.01] | | | -78.37 | -28.27 | 0.22380 | -0.35360 | 0.11601 | 1.4810 | -2.8097 | 2.5861 |
| 10 | 3.5280(18) | .. | N(1)a | [-x, -1/2+y, 1/2-z | = 2545.01] | | | -83.41 | -64.49 | 0.15151 | -0.16772 | 0.04674 | 1.0407 | -1.3327 | 1.0419 |
| 11 | 3.563(2) | .. | C(2)a | [-x, -1/2+y, 1/2-z | = 2545.01] | | | -61.47 | -45.61 | 0.29660 | -0.25330 | 0.07536 | 2.0566 | -2.0127 | 1.6799 |
| 12 | 1.98 | << | H(33C) | | | | Intra | 158.36 | -10.17 | -0.10150 | 0.11260 | 0.17390 | -0.9429 | 0.8947 | 3.8766 |
| 13 | 1.98 | << | H(33B) | | | | Intra | 110.16 | -6.91 | 0.05580 | 0.25420 | 0.17890 | 0.1897 | 2.0198 | 3.9880 |
| 14 | 1.98 | << | H(33A) | | | | Intra | 129.69 | -51.84 | 0.03170 | 0.14060 | 0.11980 | 0.0860 | 1.1172 | 2.6706 |
| 15 | 2.66 | .< | H(32C) | | | | Intra | -1.94 | 1.12 | 0.51870 | 0.01090 | 0.19190 | 3.5247 | 0.0866 | 4.2778 |
| 16 | 2.67 | .< | H(9A) | | | | Intra | 141.28 | 43.95 | -0.04220 | 0.17340 | 0.27260 | -0.6319 | 1.3778 | 6.0768 |
| 17 | 3.01 | .. | H(9A)a | [-x, -1/2+y, 1/2-z | = 2545.01] | | | -106.73 | 16.24 | 0.04220 | -0.32660 | 0.22740 | 0.0331 | -2.5951 | 5.0692 |
| 18 | 3.37 | .. | H(31A)b | [1-x, 1/2+y, 1/2-z | = 2655.01] | | | 37.02 | -48.33 | 0.37920 | 0.19180 | 0.07680 | 2.6528 | 1.5240 | 1.7120 |

Angles (Degrees) At1...V...At2 with Vertex V = O(3)

| | | | | | | | | | | | | | | | |
|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|-----------|
| C(8) | , | C(33) | 116.85(12) | C(8) | , | C(7) | 32.79(8) | C(8) | , | C(9) | 28.16(8) | C(8) | , | O(2) | 63.56(8) |
| C(8) | , | C(32) | 77.98(9) | C(8) | , | N(2)a | 120.67(9) | C(8) | , | C(1)a | 142.09(9) | C(8) | , | C(3)a | 116.65(9) |
| C(8) | , | N(1)a | 153.00(9) | C(8) | , | C(2)a | 133.27(9) | C(33) | , | C(7) | 148.97(11) | C(33) | , | C(9) | 89.07(10) |
| C(33) | , | O(2) | 174.16(11) | C(33) | , | C(32) | 147.65(11) | C(33) | , | N(2)a | 101.71(9) | C(33) | , | C(1)a | 81.69(9) |
| C(33) | , | C(3)a | 119.53(9) | C(33) | , | N(1)a | 87.01(9) | C(33) | , | C(2)a | 109.05(9) | C(7) | , | C(9) | 60.96(6) |
| C(7) | , | O(2) | 30.82(5) | C(7) | , | C(32) | 48.10(6) | C(7) | , | N(2)a | 103.28(6) | C(7) | , | C(1)a | 125.79(6) |
| C(7) | , | C(3)a | 89.86(6) | C(7) | , | N(1)a | 123.96(6) | C(7) | , | C(2)a | 101.98(6) | C(9) | , | O(2) | 91.67(6) |
| C(9) | , | C(32) | 104.42(6) | C(9) | , | N(2)a | 128.00(6) | C(9) | , | C(1)a | 139.30(6) | C(9) | , | C(3)a | 136.11(6) |
| C(9) | , | N(1)a | 161.57(6) | C(9) | , | C(2)a | 157.36(6) | O(2) | , | C(32) | 26.88(4) | O(2) | , | N(2)a | 82.36(4) |
| O(2) | , | C(1)a | 101.41(5) | O(2) | , | C(3)a | 63.30(4) | O(2) | , | N(1)a | 94.05(5) | O(2) | , | C(2)a | 71.70(4) |
| C(32) | , | N(2)a | 92.96(5) | C(32) | , | C(1)a | 104.32(5) | C(32) | , | C(3)a | 69.86(5) | C(32) | , | N(1)a | 88.23(5) |
| C(32) | , | C(2)a | 67.48(5) | N(2)a | , | C(1)a | 23.07(4) | N(2)a | , | C(3)a | 23.39(3) | N(2)a | , | N(1)a | 36.19(3) |
| N(2)a | , | C(2)a | 36.76(3) | C(1)a | , | C(3)a | 38.12(4) | C(1)a | , | N(1)a | 22.28(3) | C(1)a | , | C(2)a | 37.44(4) |
| C(3)a | , | N(1)a | 36.36(4) | C(3)a | , | C(2)a | 21.88(4) | N(1)a | , | C(2)a | 22.42(3) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = N(1) [ARU = 1555.01] -0.15151 0.33228 0.45326 -1.6395 2.6403 10.1040

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|-----------------|-----------|----------|-------|---------|--------|----------|---------|---------|---------|--------|---------|
| 1 | 0.92(2) | -- | H(1) | | | | Intra | 100.09 | 46.03 | -0.16200 | 0.41100 | 0.48280 | -1.7508 | 3.2658 | 10.7625 |
| 2 | 1.348(2) | -- | C(1) | | | | Intra | -16.34 | -21.54 | 0.01100 | 0.28790 | 0.43107 | -0.4366 | 2.2876 | 9.6094 |
| 3 | 1.379(2) | -- | C(2) | | | | Intra | -146.20 | -27.56 | -0.29660 | 0.24670 | 0.42464 | -2.6554 | 1.9603 | 9.4660 |
| 4 | 2.1488(19) | << | N(2) | | | | Intra | -54.05 | -42.42 | -0.03361 | 0.17068 | 0.38823 | -0.7082 | 1.3562 | 8.6544 |
| 5 | 2.182(2) | << | C(3) | | | | Intra | -106.60 | -45.05 | -0.22380 | 0.14640 | 0.38399 | -2.0798 | 1.1633 | 8.5598 |
| 6 | 2.7220(14) | << | S | | | | Intra | 5.64 | -0.91 | 0.22236 | 0.36594 | 0.45132 | 1.0690 | 2.9077 | 10.0608 |
| 7 | 3.2662(15) | < | S_c | [-x,1-y,1-z | = | 3566.01] | | 104.66 | 40.64 | -0.22236 | 0.63406 | 0.54868 | -2.2666 | 5.0382 | 12.2311 |
| 8 | 3.5280(18) | .. | O(3)b | [-x,1/2+y,1/2-z | = | 2555.01] | | 83.41 | -64.49 | -0.15106 | 0.52225 | 0.31043 | -1.4652 | 4.1497 | 6.9201 |
| 9 | 3.550(2) | .. | C(4) | | | | Intra | -45.73 | -40.57 | 0.09140 | 0.08927 | 0.34967 | 0.2428 | 0.7093 | 7.7948 |
| 10 | 2.09 | << | H(2A) | | | | Intra | -162.92 | -12.92 | -0.42400 | 0.25700 | 0.43230 | -3.5867 | 2.0421 | 9.6368 |
| 11 | 3.09 | .. | H(33A)b | [-x,1/2+y,1/2-z | = | 2555.01] | | 68.71 | -31.77 | -0.03170 | 0.64060 | 0.38020 | -0.6848 | 5.0901 | 8.4754 |
| 12 | 3.10 | .. | H(3A) | | | | Intra | -113.23 | -43.61 | -0.28990 | 0.07230 | 0.35720 | -2.5261 | 0.5745 | 7.9627 |
| 13 | 3.28 | .. | H(31B)d | [-x,-y,1-z | = | 3556.01] | | -168.06 | 52.22 | -0.40420 | 0.27990 | 0.56970 | -3.6080 | 2.2241 | 12.6997 |
| 14 | 3.32(2) | .. | H(1)c | [-x,1-y,1-z | = | 3566.01] | | 42.93 | 25.45 | 0.16200 | 0.58900 | 0.51720 | 0.5532 | 4.6801 | 11.5293 |
| 15 | 3.35 | .. | H(31A)a | [-1+x,1+y,z | = | 1465.01] | | 119.44 | -11.55 | -0.37920 | 0.69180 | 0.42320 | -3.2516 | 5.4970 | 9.4339 |

Angles (Degrees) At1...V...At2 with Vertex V = N(1)

| | | | | | | | | | | | | | | | |
|------|---|-------|------------|------|---|-------|------------|------|---|------|------------|-------|---|-------|-----------|
| C(1) | , | C(2) | 111.02(13) | C(1) | , | N(2) | 37.74(8) | C(1) | , | C(3) | 75.12(10) | C(1) | , | S | 29.74(8) |
| C(1) | , | S_c | 127.05(10) | C(1) | , | O(3)b | 74.73(9) | C(1) | , | C(4) | 31.31(8) | C(2) | , | N(2) | 73.29(9) |
| C(2) | , | C(3) | 35.91(8) | C(2) | , | S | 140.73(11) | C(2) | , | S_c | 121.46(10) | C(2) | , | O(3)b | 80.20(9) |
| C(2) | , | C(4) | 79.72(9) | N(2) | , | C(3) | 37.39(6) | N(2) | , | S | 67.47(5) | N(2) | , | S_c | 164.00(7) |
| N(2) | , | O(3)b | 68.00(5) | N(2) | , | C(4) | 6.50(4) | C(3) | , | S | 104.84(6) | C(3) | , | S_c | 156.81(7) |
| C(3) | , | O(3)b | 70.18(6) | C(3) | , | C(4) | 43.82(5) | S | , | S_c | 97.43(4) | S | , | O(3)b | 83.94(4) |
| S | , | C(4) | 61.02(4) | S_c | , | O(3)b | 106.45(4) | S_c | , | C(4) | 157.62(5) | O(3)b | , | C(4) | 67.64(4) |

3.6 Angstrom Coordination Sphere Around Atom I = N(2) [ARU = 1555.01] -0.03361 0.17068 0.38823 -0.7082 1.3562 8.6544

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|--------|-----------------|-----------|----------|-------|---------|--------|----------|----------|---------|---------|---------|---------|
| 1 | 1.361(2) | -- | C(1) | | | | Intra | 73.74 | 44.55 | 0.01100 | 0.28790 | 0.43107 | -0.4366 | 2.2876 | 9.6094 |
| 2 | 1.3883(19) | -- | C(3) | | | | Intra | -171.99 | -3.90 | -0.22380 | 0.14640 | 0.38399 | -2.0798 | 1.1633 | 8.5598 |
| 3 | 1.436(2) | -- | C(4) | | | | Intra | -34.22 | -36.77 | 0.09140 | 0.08927 | 0.34967 | 0.2428 | 0.7093 | 7.7948 |
| 4 | 2.1488(19) | << | N(1) | | | | Intra | 125.95 | 42.42 | -0.15151 | 0.33228 | 0.45326 | -1.6395 | 2.6403 | 10.1040 |
| 5 | 2.194(2) | << | C(2) | | | | Intra | 162.77 | 21.71 | -0.29660 | 0.24670 | 0.42464 | -2.6554 | 1.9603 | 9.4660 |
| 6 | 2.412(2) | << | C(9) | | | | Intra | -33.85 | -67.27 | 0.05680 | 0.10535 | 0.28843 | 0.0657 | 0.8371 | 6.4296 |
| 7 | 2.4345(19) | << | C(5) | | | | Intra | -35.64 | -7.10 | 0.23540 | -0.00648 | 0.37473 | 1.2551 | -0.0515 | 8.3534 |
| 8 | 2.7466(14) | << | S | | | | Intra | 41.12 | 30.80 | 0.22236 | 0.36594 | 0.45132 | 1.0690 | 2.9077 | 10.0608 |
| 9 | 3.3741(17) | .. | O(3)a | [-x,1/2+y,1/2-z | = | 2555.01] | | 105.16 | -30.93 | -0.15106 | 0.52225 | 0.31043 | -1.4652 | 4.1497 | 6.9201 |
| 10 | 2.10 | << | H(3A) | | | | Intra | -156.73 | -19.27 | -0.28990 | 0.07230 | 0.35720 | -2.5261 | 0.5745 | 7.9627 |
| 11 | 2.58 | .< | H(9A) | | | | Intra | 0.00 | -90.00 | -0.04220 | 0.17340 | 0.27260 | -0.6319 | 1.3778 | 6.0768 |
| 12 | 2.61 | .< | H(5A) | | | | Intra | -35.39 | 14.20 | 0.25650 | -0.01400 | 0.41700 | 1.3573 | -0.1112 | 9.2957 |
| 13 | 3.03(2) | .. | H(1) | | | | Intra | 118.63 | 44.10 | -0.16200 | 0.41100 | 0.48280 | -1.7508 | 3.2658 | 10.7625 |
| 14 | 3.12 | .. | H(2A) | | | | Intra | 166.60 | 18.37 | -0.42400 | 0.25700 | 0.43230 | -3.5867 | 2.0421 | 9.6368 |

Angles (Degrees) At1...V...At2 with Vertex V = N(2)

| | | | | | | | | | | | | | | | |
|------|---|-------|------------|------|---|-------|------------|------|---|-------|-----------|------|---|-------|------------|
| C(1) | , | C(3) | 109.87(13) | C(1) | , | C(4) | 126.59(12) | C(1) | , | N(1) | 37.29(8) | C(1) | , | C(2) | 74.29(9) |
| C(1) | , | C(9) | 136.91(11) | C(1) | , | C(5) | 108.75(10) | C(1) | , | S | 28.98(7) | C(1) | , | O(3)a | 80.73(9) |
| C(3) | , | C(4) | 123.44(13) | C(3) | , | N(1) | 72.59(9) | C(3) | , | C(2) | 35.59(9) | C(3) | , | C(9) | 102.96(11) |
| C(3) | , | C(5) | 135.07(11) | C(3) | , | S | 138.82(10) | C(3) | , | O(3)a | 81.86(9) | C(4) | , | N(1) | 163.76(11) |
| C(4) | , | C(2) | 158.93(11) | C(4) | , | C(9) | 30.50(8) | C(4) | , | C(5) | 29.70(8) | C(4) | , | S | 97.61(8) |
| C(4) | , | O(3)a | 102.35(9) | N(1) | , | C(2) | 37.01(6) | N(1) | , | C(9) | 152.86(8) | N(1) | , | C(5) | 141.12(8) |
| N(1) | , | S | 66.26(5) | N(1) | , | O(3)a | 75.81(5) | C(2) | , | C(9) | 133.25(8) | C(2) | , | C(5) | 157.00(8) |
| C(2) | , | S | 103.26(7) | C(2) | , | O(3)a | 76.30(6) | C(9) | , | C(5) | 60.18(6) | C(9) | , | S | 112.72(6) |
| C(9) | , | O(3)a | 77.06(5) | C(5) | , | S | 82.42(5) | C(5) | , | O(3)a | 126.59(6) | S | , | O(3)a | 86.60(4) |

=====
Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6
=====

van der Waals (or ion) Radii used in the Analysis

=====
C H N O S

1.70 1.20 1.55 1.52 1.80

:: Grid: X-Axis Step = 0.0278 = Points 36, Angstrom Step = 0.20
:: Grid: Y-Axis Step = 0.0278 = Points 36, Angstrom Step = 0.22
:: Grid: Z-Axis Step = 0.0093 = Points 108, Angstrom Step = 0.21

:: Unit cell Contains NO Residual Solvent Accessible Void.

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

=====
Report Expected Number of Independent Reflections for given Symmetry and Resolution.

:: Hmax = 10 Kmax = 11 Lmax= 31 , Sorting Order : Fast H, Medium K, Slow L

:: Actual Theta-Max: 30.609 Deg. (Applied Theta Limit: 30.610 Deg.)

Space Group H-M: P21/c Laue: 2/m
Space Group Hall: -P 2ybc [Schoenflies: C2h^5]
Lattice Type: mP, Centric, Monoclinic, Multiplicity: 4(2), No: 14

Nr ***** Symmetry Operation(s) *****

| | | | |
|---|-------|-----------|---------|
| 1 | H , | K , | L |
| 2 | - H , | 1/2 + K , | 1/2 - L |
| 3 | - H , | - K , | - L |
| 4 | H , | 1/2 - K , | 1/2 + L |

:: Number of Independent Type H, K, L Reflections = 3948

Table 0 - Crystal Data and Details of the Structure Determination
 for: hmimome3phP2(1)/c R = 0.04

Crystal Data

| | | | |
|--------------------------|--------------------|-----------|-----------|
| Formula | C12 H14 N2 O3 S | | |
| Formula Weight | 266.32 | | |
| Crystal System | monoclinic | | |
| Space group | P21/c | (No. 14) | |
| a, b, c [Angstrom] | 7.2383(6) | 7.9459(7) | 22.324(2) |
| alpha, beta, gamma [deg] | 90 | 93.075(1) | 90 |
| V [Ang**3] | 1282.11(19) | | |
| Z | 4 | | |
| D(calc) [g/cm**3] | 1.380 | | |
| Mu(MoKa) [/mm] | 0.254 | | |
| F(000) | 560 | | |
| Crystal Size [mm] | 0.04 x 0.13 x 0.15 | | |

Data Collection

| | | | |
|----------------------------------|---------------------------|---------|-------|
| Temperature (K) | 150 | | |
| Radiation [Angstrom] | MoKa | 0.71073 | |
| Theta Min-Max [Deg] | 1.8, 30.6 | | |
| Dataset | -10: 10 ; -11: 11 ; 0: 31 | | |
| Tot., Uniq. Data, R(int) | 7575, | 3945, | 0.042 |
| Observed Data [I > 2.0 sigma(I)] | 2649 | | |

Refinement

| | | | |
|--|----------------------|--|--|
| Nref, Npar | 3945, 170 | | |
| R, wR2, S | 0.0426, 0.1042, 1.05 | | |
| w = 1/[\s^2^(Fo^2^)+(0.0417P)^2^+0.1422P] where P=(Fo^2^+2Fc^2^)/3 | | | |
| Max. and Av. Shift/Error | 0.00, 0.00 | | |
| Min. and Max. Resd. Dens. [e/Ang^3] | -0.28, 0.33 | | |

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***** N O T I C E *****

=====

- PLATON Reference : Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.
Spek, A.L. (2009). Acta Cryst. D65, 148-155.

- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow

- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)

- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.

- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.

- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@uu.nl

- Recent versions of PLATON may be obtained from <http://www.platonsoft.nl/xraysoft>

- More INFO can be found on <http://http://www.platonsoft.nl/>

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Page 49 --- EXPECT
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Summary and Remarks : N = NOTE, W = WARNING, E = ERROR
=====

W: NOMOVE option used.

:: >>> WARNING: 'CONNECTED INPUT SET' is assumed to be TRUE

:: >>> The Network Analysis may be INCORRECT when this assumption is FALSE

=====

:: Input Xtal Data from File hmimome3ph.cif - Data Type CIF

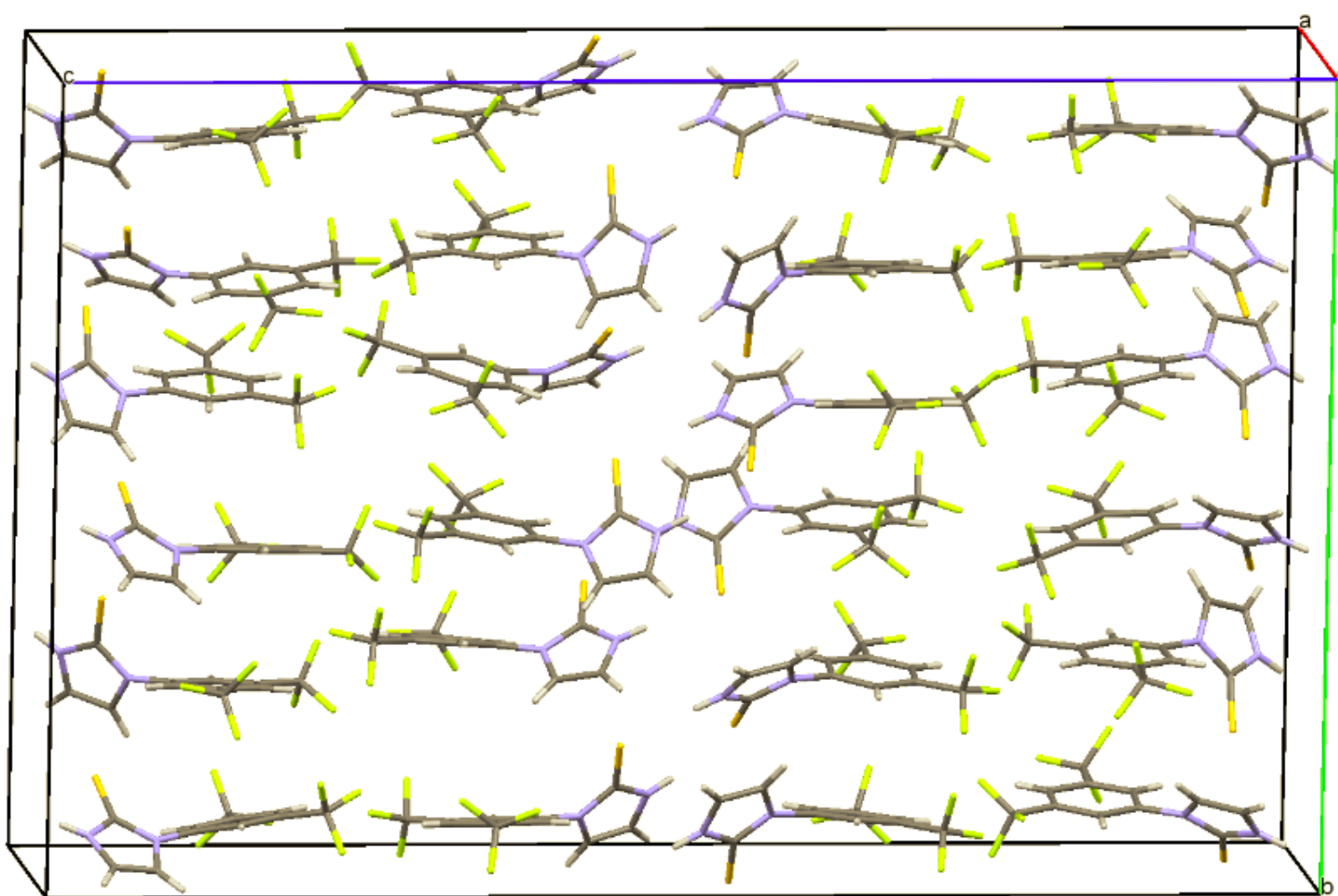
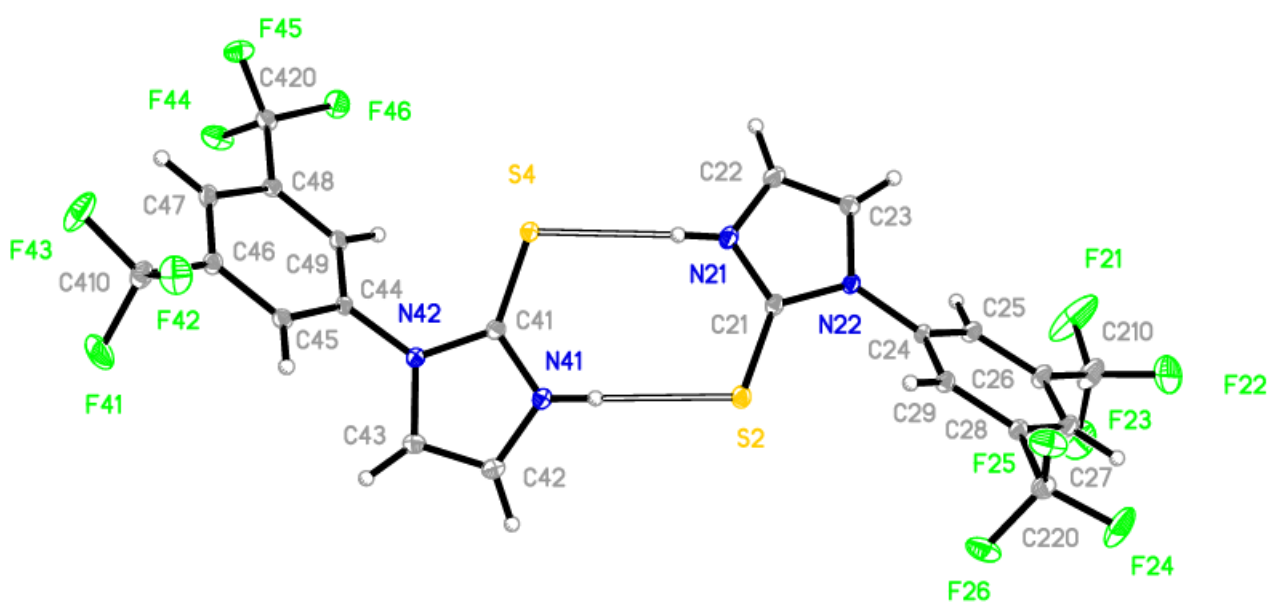
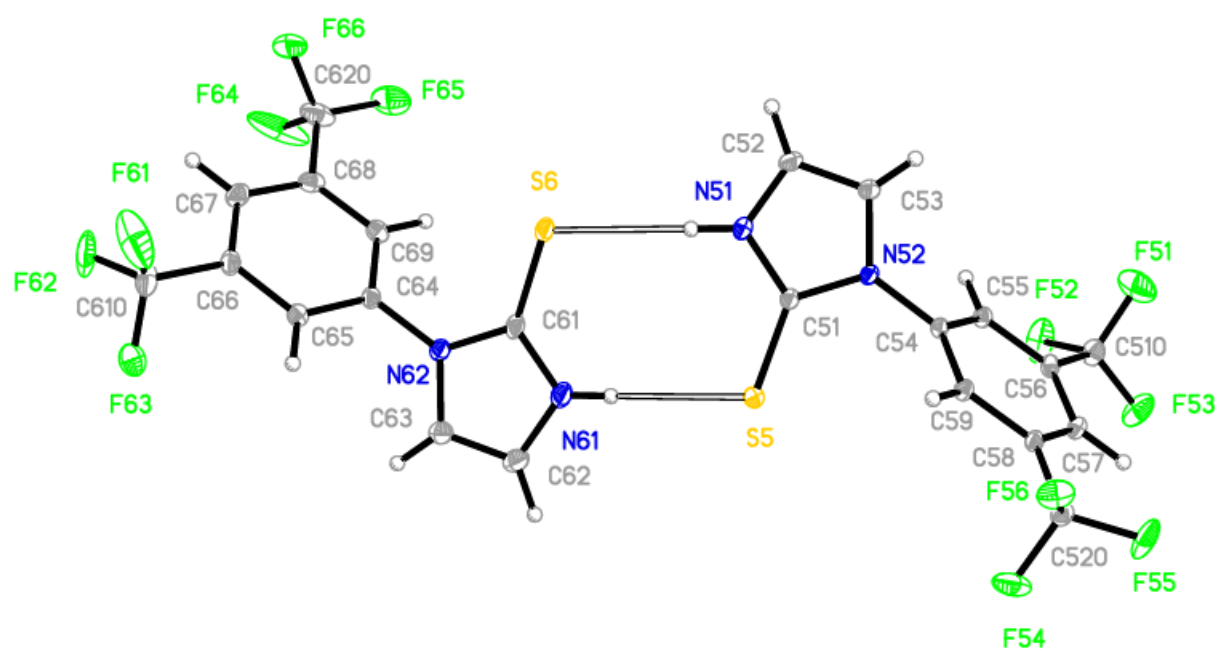
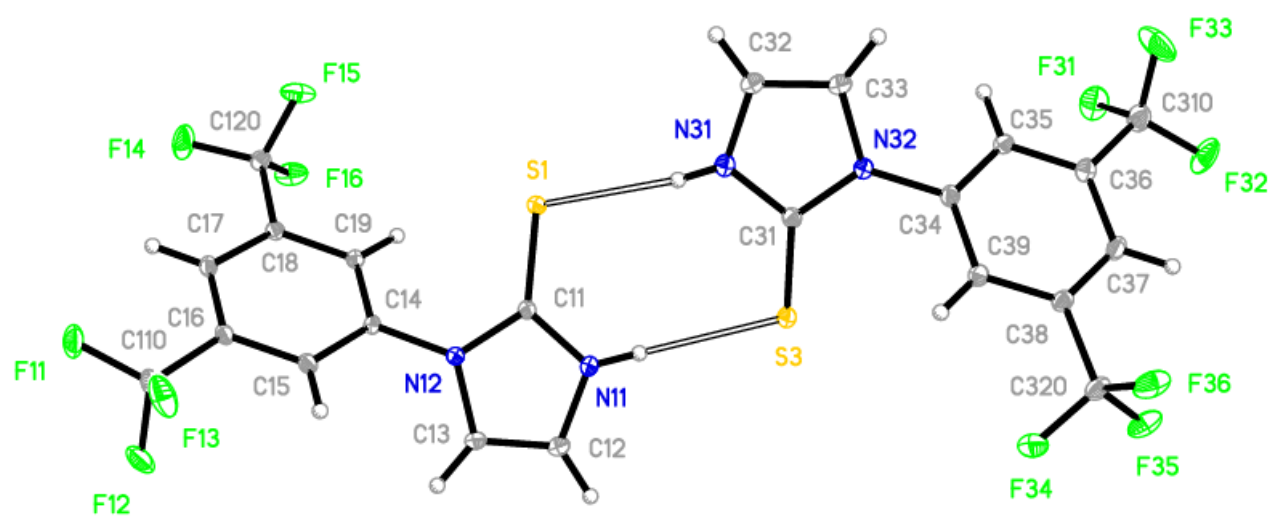
:: NORMAL END of PLATON : 52 Pages on:

:: hmimome3ph.lis (ASCII, 132 Characters Wide)

:: hmimome3ph.lps (PostScript Version of .lis)

::

Hmim^{Ar(CF₃)₂}



=====
 Analysis of Short Intra- and Inter-molecular Contacts , $d(I-J) < R(I) + R(J) + \text{Tolr}$, With $\text{Tolr} = 0.2 \text{ Ang.}$ ($X - I \dots J$) $> 100. \text{ Deg.}$

Contact Radii : C H F N S
 (Angstrom) 1.70 1.20 1.47 1.55 1.80

Default Contact Radii are those given by A.Bondi, J.Phys.Chem. (1964),68,441. (or Coval. Rad. + 0.8 Ang. when not given)

* WARNING * : no Far-Reaching Conclusions should be drawn based on the Default Radii Assigned to Metals

Short "INTRA" Distances between two Atoms that are Separated by less than 4 Bonds are NOT Listed (Except for Potential D/A Contacts)

=====
 ***** ARU = 1555.01 *****
 =====

| At(I)[1555.01] | At(J) | [ARU(J)] | D(I-J) | SumRad | Del | Type | X(I) | Y(I) | Z(I) | X(J) | Y(J) | Z(J) | X | X - I...J |
|----------------|--------------|------------|----------|---------|-------|-------|---------|--------|---------|---------|--------|---------|--------|------------|
| S(3) | N(11) | [] | 3.284(2) | < 3.35 | -0.07 | | -0.3034 | 0.6716 | -0.5461 | -0.2811 | 0.7314 | -0.4656 | C(31) | 107.31(8) |
| S(3) | C(34) | [] | 3.269(2) | << 3.50 | -0.23 | Intra | -0.3034 | 0.6716 | -0.5461 | -0.2236 | 0.5771 | -0.6081 | | |
| S(3) | C(39) | [] | 3.259(2) | << 3.50 | -0.24 | Intra | -0.3034 | 0.6716 | -0.5461 | -0.3864 | 0.5844 | -0.6119 | | |
| S(3) | H(11) | [] | 2.45(3) | << 3.00 | -0.55 | | -0.3034 | 0.6716 | -0.5461 | -0.2840 | 0.7169 | -0.4863 | C(31) | 107.3(8) |
| S(3) | H(31) | [] | 2.85(3) | < 3.00 | -0.15 | Intra | -0.3034 | 0.6716 | -0.5461 | -0.0810 | 0.6167 | -0.4995 | | |
| S(3) | H(39A) | [] | 2.87 | < 3.00 | -0.13 | Intra | -0.3034 | 0.6716 | -0.5461 | -0.4526 | 0.5879 | -0.5910 | | |
| S(3) | C(19) | [3464.05] | 3.678(2) | 3.50 | 0.18 | | -0.3034 | 0.6716 | -0.5461 | -0.4667 | 0.7455 | -0.6258 | C(31) | 128.37(8) |
| S(3) | H(12A) | [3564.05] | 2.91 | < 3.00 | -0.09 | | -0.3034 | 0.6716 | -0.5461 | 0.0079 | 0.7224 | -0.5377 | | |
| S(3) | H(19A) | [3464.05] | 2.81 | < 3.00 | -0.19 | | -0.3034 | 0.6716 | -0.5461 | -0.4076 | 0.7394 | -0.6041 | C(31) | 131 |
| F(34) | C(39) | [] | 2.751(3) | << 3.17 | -0.42 | Intra | -0.6960 | 0.6168 | -0.6227 | -0.3864 | 0.5844 | -0.6119 | | |
| F(34) | H(39A) | [] | 2.46 | << 2.67 | -0.21 | Intra | -0.6960 | 0.6168 | -0.6227 | -0.4526 | 0.5879 | -0.5910 | | |
| F(34) | C(13) | [3464.05] | 3.230(3) | 3.17 | 0.06 | | -0.6960 | 0.6168 | -0.6227 | -0.8557 | 0.7249 | -0.5842 | C(320) | 149.31(16) |
| F(34) | C(14) | [3464.05] | 3.299(3) | 3.17 | 0.13 | | -0.6960 | 0.6168 | -0.6227 | -0.6304 | 0.7534 | -0.6245 | C(320) | 108.34(14) |
| F(34) | H(13A) | [3464.05] | 2.86 | 2.67 | 0.19 | | -0.6960 | 0.6168 | -0.6227 | -0.9128 | 0.7030 | -0.6015 | C(320) | 143 |
| F(35) | C(37) | [] | 2.791(3) | << 3.17 | -0.38 | Intra | -0.6585 | 0.6273 | -0.6801 | -0.3549 | 0.5807 | -0.6776 | | |
| F(35) | H(37A) | [] | 2.55 | < 2.67 | -0.12 | Intra | -0.6585 | 0.6273 | -0.6801 | -0.3999 | 0.5824 | -0.7013 | | |
| F(35) | <F(31) | [1455.01] | 2.787(8) | < 2.94 | -0.15 | | -0.6585 | 0.6273 | -0.6801 | -0.9694 | 0.6088 | -0.7030 | C(320) | 109.4(2) |
| F(35) | <F(33A) | [1455.01] | 2.87(2) | < 2.94 | -0.07 | | -0.6585 | 0.6273 | -0.6801 | -0.9412 | 0.5675 | -0.7003 | | |
| F(35) | >F(53) | [3464.03] | 3.084(7) | 2.94 | 0.14 | | -0.6585 | 0.6273 | -0.6801 | -0.5199 | 0.6298 | -0.7580 | C(320) | 130.6(3) |
| F(35) | C(15) | [3464.05] | 3.350(3) | 3.17 | 0.18 | | -0.6585 | 0.6273 | -0.6801 | -0.7181 | 0.7614 | -0.6563 | C(320) | 113.40(15) |
| F(35) | C(16) | [3464.05] | 3.195(3) | 3.17 | 0.02 | | -0.6585 | 0.6273 | -0.6801 | -0.6403 | 0.7605 | -0.6897 | C(320) | 131.91(15) |
| F(36) | C(27) | [] | 3.343(3) | 3.17 | 0.17 | | -0.6992 | 0.5449 | -0.6579 | -0.6864 | 0.4159 | -0.6936 | C(320) | 148.28(16) |
| F(36) | C(28) | [] | 3.198(3) | 3.17 | 0.03 | | -0.6992 | 0.5449 | -0.6579 | -0.7650 | 0.4127 | -0.6605 | C(320) | 160.50(16) |
| F(36) | C(29) | [] | 3.242(3) | 3.17 | 0.07 | | -0.6992 | 0.5449 | -0.6579 | -0.6848 | 0.4172 | -0.6275 | C(320) | 137.99(16) |
| F(36) | C(37) | [] | 3.111(3) | < 3.17 | -0.06 | Intra | -0.6992 | 0.5449 | -0.6579 | -0.3549 | 0.5807 | -0.6776 | | |
| F(36) | C(39) | [] | 3.268(3) | 3.17 | 0.10 | Intra | -0.6992 | 0.5449 | -0.6579 | -0.3864 | 0.5844 | -0.6119 | | |
| F(36) | H(35A) | [1455.01] | 2.83 | 2.67 | 0.16 | | -0.6992 | 0.5449 | -0.6579 | -1.0152 | 0.5657 | -0.6354 | C(320) | 104 |

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F(36)    .... <F(33A) [ 1455.01]   2.621(17)<< 2.94 -0.32      -0.6992 0.5449-0.6579 -0.9412 0.5675-0.7003  C(320)   106.2(7)
F(36)    .... <F(33B) [ 1455.01]   2.854(13) < 2.94 -0.09      -0.6992 0.5449-0.6579 -0.9729 0.5303-0.7027  C(320)   125.1(3)
N(31)    .... S(1)  [          ]   3.278(2) < 3.35 -0.07      -0.0879 0.5988-0.5175 -0.0037 0.6795-0.4477  C(31)   123.57(14)
                                            C(32)   123.32(13)
N(31)    .... C(33) [          ]   2.203(3)<< 3.25 -1.05 Intra -0.0879 0.5988-0.5175 -0.0389 0.5380-0.5614  H(31)   162(2)
N(32)    .... C(32) [          ]   2.201(3)<< 3.25 -1.05 Intra -0.1544 0.5764-0.5725  0.0006 0.5519-0.5269  C(34)  159.95(16)
N(32)    .... H(31) [          ]   2.91(3)  2.75  0.16 Intra -0.1544 0.5764-0.5725 -0.0810 0.6167-0.4995  C(34)  157.3(7)
N(32)    .... H(35A) [          ]   2.60 < 2.75 -0.15 Intra -0.1544 0.5764-0.5725 -0.0152 0.5657-0.6354  C(31)   142
N(32)    .... H(39A) [          ]   2.62 < 2.75 -0.13 Intra -0.1544 0.5764-0.5725 -0.4526 0.5879-0.5910  C(33)   145
C(31)    .... C(33) [          ]   2.272(3)<< 3.40 -1.13 Intra -0.1831 0.6147-0.5453 -0.0389 0.5380-0.5614  S(3)   163.70(13)
C(31)    .... C(35) [          ]   3.599(3)  3.40  0.20 Intra -0.1831 0.6147-0.5453 -0.1262 0.5710-0.6383  S(3)   107.19(9)
                                            N(31)  123.68(15)
C(31)    .... C(39) [          ]   3.069(3)<< 3.40 -0.33 Intra -0.1831 0.6147-0.5453 -0.3864 0.5844-0.6119  N(31)  149.94(16)
C(31)    .... H(39A) [          ]   2.89 < 2.90 -0.01 Intra -0.1831 0.6147-0.5453 -0.4526 0.5879-0.5910  N(31)   147
C(31)    .... H(12A) [ 3564.05]   3.04  2.90  0.14      -0.1831 0.6147-0.5453  0.0079 0.7224-0.5377  N(32)   122
C(32)    .... S(2)  [ 1655.02]   3.444(3) < 3.50 -0.06      0.0006 0.5519-0.5269  0.3577 0.4982-0.5563  N(31)  147.92(16)
C(32)    .... N(32) [          ]   2.201(3)<< 3.25 -1.05 Intra  0.0006 0.5519-0.5269 -0.1544 0.5764-0.5725  H(32A)  164
C(32)    .... C(34) [          ]   3.578(3)  3.40  0.18 Intra  0.0006 0.5519-0.5269 -0.2236 0.5771-0.6081  H(32A)  156
C(33)    .... S(2)  [ 1655.02]   3.480(3) < 3.50 -0.02      -0.0389 0.5380-0.5614  0.3577 0.4982-0.5563  N(32)  149.76(16)
C(33)    .... N(31) [          ]   2.203(3)<< 3.25 -1.05 Intra -0.0389 0.5380-0.5614 -0.0879 0.5988-0.5175  H(33A)  164
C(33)    .... C(22) [          ]   3.428(4)  3.40  0.03      -0.0389 0.5380-0.5614 -0.2451 0.4144-0.5544  N(32)  103.27(15)
                                            C(32)  105.43(17)
C(33)    .... C(35) [          ]   3.020(3)<< 3.40 -0.38 Intra -0.0389 0.5380-0.5614 -0.1262 0.5710-0.6383  C(32)  150.74(18)
C(33)    .... H(31) [          ]   2.96(3)  2.90  0.06 Intra -0.0389 0.5380-0.5614 -0.0810 0.6167-0.4995  H(33A)  159
C(33)    .... H(35A) [          ]   2.80 < 2.90 -0.10 Intra -0.0389 0.5380-0.5614 -0.0152 0.5657-0.6354  C(32)   146
C(34)    .... S(3)  [          ]   3.269(2)<< 3.50 -0.23 Intra -0.2236 0.5771-0.6081 -0.3034 0.6716-0.5461  C(35)  138.59(15)
C(34)    .... C(32) [          ]   3.578(3)  3.40  0.18 Intra -0.2236 0.5771-0.6081  0.0006 0.5519-0.5269  C(35)  109.55(16)
                                            C(39)  128.67(15)
C(34)    .... C(37) [          ]   2.780(3)<< 3.40 -0.62 Intra -0.2236 0.5771-0.6081 -0.3549 0.5807-0.6776  N(32)  178.76(16)
C(34)    .... H(33A) [          ]   2.80 < 2.90 -0.10 Intra -0.2236 0.5771-0.6081  0.0037 0.5080-0.5753  C(39)   142
C(34)    .... F(16) [ 3464.05]   3.124(3) < 3.17 -0.05      -0.2236 0.5771-0.6081 -0.1647 0.6956-0.6420  N(32)  108.01(14)
C(35)    .... F(26) [ 1655.02]   3.075(3) < 3.17 -0.10      -0.1262 0.5710-0.6383 -0.0156 0.4482-0.6438  C(34)  109.37(14)
C(35)    .... C(31) [          ]   3.599(3)  3.40  0.20 Intra -0.1262 0.5710-0.6383 -0.1831 0.6147-0.5453  C(36)  143.54(17)
C(35)    .... C(33) [          ]   3.020(3)<< 3.40 -0.38 Intra -0.1262 0.5710-0.6383 -0.0389 0.5380-0.5614  C(36)  163.74(17)
C(35)    .... C(38) [          ]   2.771(4)<< 3.40 -0.63 Intra -0.1262 0.5710-0.6383 -0.4499 0.5864-0.6468  H(35A)  180
C(35)    .... H(33A) [          ]   2.96  2.90  0.06 Intra -0.1262 0.5710-0.6383  0.0037 0.5080-0.5753  C(36)   151
C(35)    .... <F(31) [          ]   2.860(8)<< 3.17 -0.31 Intra -0.1262 0.5710-0.6383  0.0306 0.6088-0.7030  C(34)  154.5(2)
C(35)    .... <F(31B) [          ]   3.095(11) < 3.17 -0.08 Intra -0.1262 0.5710-0.6383 -0.0120 0.6161-0.7130  C(34)  148.7(3)
C(35)    .... <F(32A) [          ]   3.37(2)  3.17  0.20 Intra -0.1262 0.5710-0.6383 -0.1300 0.5206-0.7242  C(34)  141.1(5)
C(35)    .... <F(33) [          ]   2.975(14) < 3.17 -0.20 Intra -0.1262 0.5710-0.6383 -0.0114 0.5215-0.7080  C(34)  157.0(3)
C(35)    .... <F(33A) [          ]   2.757(17)<< 3.17 -0.41 Intra -0.1262 0.5710-0.6383  0.0588 0.5675-0.7003  C(34)  175.2(6)
C(35)    .... <F(33B) [          ]   2.860(14)<< 3.17 -0.31 Intra -0.1262 0.5710-0.6383  0.0271 0.5303-0.7027  C(34)  164.3(3)
C(35)    .... F(16) [ 3464.05]   2.990(3) < 3.17 -0.18      -0.1262 0.5710-0.6383 -0.1647 0.6956-0.6420  H(35A)  104
C(36)    .... C(39) [          ]   2.787(3)<< 3.40 -0.61 Intra -0.1931 0.5726-0.6731 -0.3864 0.5844-0.6119  C(310)  177.45(18)
C(36)    .... F(16) [ 3464.05]   3.153(3) < 3.17 -0.02      -0.1931 0.5726-0.6731 -0.1647 0.6956-0.6420  C(310)  107.32(16)
C(37)    .... F(35) [          ]   2.791(3)<< 3.17 -0.38 Intra -0.3549 0.5807-0.6776 -0.6585 0.6273-0.6801  C(36)  163.90(18)
C(37)    .... F(36) [          ]   3.111(3) < 3.17 -0.06 Intra -0.3549 0.5807-0.6776 -0.6992 0.5449-0.6579  C(36)  148.32(17)
C(37)    .... C(34) [          ]   2.780(3)<< 3.40 -0.62 Intra -0.3549 0.5807-0.6776 -0.2236 0.5771-0.6081  H(37A)  179
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| | | | | | | | | | | |
|--------|-------------------------|------------|------|-------|---------|-----------------------|---------|---------------|--------|------------|
| C(37) | <F(21A) [] | 3.352(15) | 3.17 | 0.18 | -0.3549 | 0.5807-0.6776 | -0.3930 | 0.4773-0.7390 | C(38) | 124.1(4) |
| C(37) | <F(31A) [] | 2.77(2)<< | 3.17 | -0.40 | Intra | -0.3549 0.5807-0.6776 | -0.1290 | 0.6100-0.7289 | C(38) | 157.5(4) |
| C(37) | <F(31B) [] | 3.279(12) | 3.17 | 0.11 | Intra | -0.3549 0.5807-0.6776 | -0.0120 | 0.6161-0.7130 | C(38) | 143.5(2) |
| C(37) | <F(32) [] | 2.702(8)<< | 3.17 | -0.47 | Intra | -0.3549 0.5807-0.6776 | -0.1599 | 0.5811-0.7361 | C(38) | 173.9(3) |
| C(37) | <F(32A) [] | 2.93(2)<< | 3.17 | -0.24 | Intra | -0.3549 0.5807-0.6776 | -0.1300 | 0.5206-0.7242 | C(38) | 153.4(5) |
| C(37) | <F(32B) [] | 2.766(9)<< | 3.17 | -0.40 | Intra | -0.3549 0.5807-0.6776 | -0.1663 | 0.5531-0.7367 | C(38) | 171.8(3) |
| C(38) | C(35) [] | 2.771(4)<< | 3.40 | -0.63 | Intra | -0.4499 0.5864-0.6468 | -0.1262 | 0.5710-0.6383 | C(320) | 178.90(16) |
| C(39) | S(2) [] | 3.608(2) | 3.50 | 0.11 | | -0.3864 0.5844-0.6119 | -0.6423 | 0.4982-0.5563 | C(34) | 117.61(14) |
| | | | | | | | | | C(38) | 108.06(15) |
| C(39) | S(3) [] | 3.259(2)<< | 3.50 | -0.24 | Intra | -0.3864 0.5844-0.6119 | -0.3034 | 0.6716-0.5461 | C(38) | 137.99(15) |
| C(39) | F(34) [] | 2.751(3)<< | 3.17 | -0.42 | Intra | -0.3864 0.5844-0.6119 | -0.6960 | 0.6168-0.6227 | C(34) | 170.40(17) |
| C(39) | F(36) [] | 3.268(3) | 3.17 | 0.10 | Intra | -0.3864 0.5844-0.6119 | -0.6992 | 0.5449-0.6579 | C(34) | 144.28(16) |
| C(39) | C(21) [] | 3.582(3) | 3.40 | 0.18 | | -0.3864 0.5844-0.6119 | -0.4797 | 0.4580-0.5634 | C(38) | 113.71(15) |
| C(39) | C(31) [] | 3.069(3)<< | 3.40 | -0.33 | Intra | -0.3864 0.5844-0.6119 | -0.1831 | 0.6147-0.5453 | C(38) | 160.13(17) |
| C(39) | C(36) [] | 2.787(3)<< | 3.40 | -0.61 | Intra | -0.3864 0.5844-0.6119 | -0.1931 | 0.5726-0.6731 | H(39A) | 179 |
| C(310) | H(35A) [] | 2.66<< | 2.90 | -0.24 | Intra | -0.0869 0.5690-0.7060 | -0.0152 | 0.5657-0.6354 | | |
| C(310) | H(37A) [] | 2.66<< | 2.90 | -0.24 | Intra | -0.0869 0.5690-0.7060 | -0.3999 | 0.5824-0.7013 | | |
| C(320) | H(37A) [] | 2.64<< | 2.90 | -0.26 | Intra | -0.6259 0.5938-0.6519 | -0.3999 | 0.5824-0.7013 | F(34) | 155 |
| C(320) | H(39A) [] | 2.67<< | 2.90 | -0.23 | Intra | -0.6259 0.5938-0.6519 | -0.4526 | 0.5879-0.5910 | F(35) | 142 |
| | | | | | | | | | F(36) | 110 |
| C(320) | <F(33A) [1455.01] | 3.257(16) | 3.17 | 0.09 | | -0.6259 0.5938-0.6519 | -0.9412 | 0.5675-0.7003 | C(38) | 148.1(4) |
| H(31) | S(1) [] | 2.50(3)<< | 3.00 | -0.50 | | -0.0810 0.6167-0.4995 | -0.0037 | 0.6795-0.4477 | N(31) | 168(3) |
| H(31) | S(3) [] | 2.85(3) < | 3.00 | -0.15 | Intra | -0.0810 0.6167-0.4995 | -0.3034 | 0.6716-0.5461 | | |
| H(31) | N(32) [] | 2.91(3) | 2.75 | 0.16 | Intra | -0.0810 0.6167-0.4995 | -0.1544 | 0.5764-0.5725 | | |
| H(31) | C(33) [] | 2.96(3) | 2.90 | 0.06 | Intra | -0.0810 0.6167-0.4995 | -0.0389 | 0.5380-0.5614 | | |
| H(31) | H(32A) [] | 2.43 | 2.40 | 0.03 | Intra | -0.0810 0.6167-0.4995 | 0.0751 | 0.5331-0.5118 | | |
| H(32A) | S(2) [1655.02] | 3.00 | 3.00 | 0.00 | | 0.0751 0.5331-0.5118 | 0.3577 | 0.4982-0.5563 | C(32) | 110 |
| H(32A) | H(31) [] | 2.43 | 2.40 | 0.03 | Intra | 0.0751 0.5331-0.5118 | -0.0810 | 0.6167-0.4995 | | |
| H(32A) | H(33A) [] | 2.48 | 2.40 | 0.08 | Intra | 0.0751 0.5331-0.5118 | 0.0037 | 0.5080-0.5753 | | |
| H(33A) | S(2) [1655.02] | 3.07 | 3.00 | 0.07 | | 0.0037 0.5080-0.5753 | 0.3577 | 0.4982-0.5563 | C(33) | 108 |
| H(33A) | C(34) [] | 2.80 < | 2.90 | -0.10 | Intra | 0.0037 0.5080-0.5753 | -0.2236 | 0.5771-0.6081 | | |
| H(33A) | C(35) [] | 2.96 | 2.90 | 0.06 | Intra | 0.0037 0.5080-0.5753 | -0.1262 | 0.5710-0.6383 | | |
| H(33A) | H(32A) [] | 2.48 | 2.40 | 0.08 | Intra | 0.0037 0.5080-0.5753 | 0.0751 | 0.5331-0.5118 | | |
| H(35A) | F(26) [1655.02] | 2.82 | 2.67 | 0.15 | | -0.0152 0.5657-0.6354 | -0.0156 | 0.4482-0.6438 | | |
| H(35A) | F(36) [1655.01] | 2.83 | 2.67 | 0.16 | | -0.0152 0.5657-0.6354 | 0.3008 | 0.5449-0.6579 | C(35) | 156 |
| H(35A) | N(32) [] | 2.60 < | 2.75 | -0.15 | Intra | -0.0152 0.5657-0.6354 | -0.1544 | 0.5764-0.5725 | | |
| H(35A) | C(33) [] | 2.80 < | 2.90 | -0.10 | Intra | -0.0152 0.5657-0.6354 | -0.0389 | 0.5380-0.5614 | | |
| H(35A) | C(310) [] | 2.66<< | 2.90 | -0.24 | Intra | -0.0152 0.5657-0.6354 | -0.0869 | 0.5690-0.7060 | | |
| H(35A) | <F(31) [] | 2.71 | 2.67 | 0.04 | Intra | -0.0152 0.5657-0.6354 | 0.0306 | 0.6088-0.7030 | | |
| H(35A) | <F(33) [] | 2.86 | 2.67 | 0.19 | Intra | -0.0152 0.5657-0.6354 | -0.0114 | 0.5215-0.7080 | | |
| H(35A) | <F(33A) [] | 2.46<< | 2.67 | -0.21 | Intra | -0.0152 0.5657-0.6354 | 0.0588 | 0.5675-0.7003 | | |
| H(35A) | <F(33B) [] | 2.63 < | 2.67 | -0.04 | Intra | -0.0152 0.5657-0.6354 | 0.0271 | 0.5303-0.7027 | | |
| H(37A) | F(35) [] | 2.55 < | 2.67 | -0.12 | Intra | -0.3999 0.5824-0.7013 | -0.6585 | 0.6273-0.6801 | | |
| H(37A) | C(310) [] | 2.66<< | 2.90 | -0.24 | Intra | -0.3999 0.5824-0.7013 | -0.0869 | 0.5690-0.7060 | | |
| H(37A) | C(320) [] | 2.64<< | 2.90 | -0.26 | Intra | -0.3999 0.5824-0.7013 | -0.6259 | 0.5938-0.6519 | | |
| H(37A) | <F(21A) [] | 2.86 | 2.67 | 0.19 | | -0.3999 0.5824-0.7013 | -0.3930 | 0.4773-0.7390 | C(37) | 113 |
| H(37A) | <F(31A) [] | 2.58 < | 2.67 | -0.09 | Intra | -0.3999 0.5824-0.7013 | -0.1290 | 0.6100-0.7289 | | |
| H(37A) | <F(32) [] | 2.39<< | 2.67 | -0.28 | Intra | -0.3999 0.5824-0.7013 | -0.1599 | 0.5811-0.7361 | | |


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H(37A) .... <F(32A) [      ]      2.84  2.67  0.17 Intra -0.3999 0.5824-0.7013 -0.1300 0.5206-0.7242
H(37A) .... <F(32B) [      ]      2.46<< 2.67 -0.21 Intra -0.3999 0.5824-0.7013 -0.1663 0.5531-0.7367
H(37A) .... >F(53)  [ 3464.03]      2.57 < 2.67 -0.10      -0.3999 0.5824-0.7013 -0.5199 0.6298-0.7580 C(37)      156
H(37A) .... <F(51A) [ 3464.03]      2.85  2.67  0.18      -0.3999 0.5824-0.7013 -0.6050 0.5676-0.7625 C(37)      163
H(39A) .... S(2)   [      ]      2.96 < 3.00 -0.04      -0.4526 0.5879-0.5910 -0.6423 0.4982-0.5563 C(39)      127
H(39A) .... S(3)   [      ]      2.87 < 3.00 -0.13 Intra -0.4526 0.5879-0.5910 -0.3034 0.6716-0.5461 C(39)      105
H(39A) .... F(34)   [      ]      2.46<< 2.67 -0.21 Intra -0.4526 0.5879-0.5910 -0.6960 0.6168-0.6227
H(39A) .... N(32)  [      ]      2.62 < 2.75 -0.13 Intra -0.4526 0.5879-0.5910 -0.1544 0.5764-0.5725
H(39A) .... C(31)  [      ]      2.89 < 2.90 -0.01 Intra -0.4526 0.5879-0.5910 -0.1831 0.6147-0.5453
H(39A) .... C(320) [      ]      2.67<< 2.90 -0.23 Intra -0.4526 0.5879-0.5910 -0.6259 0.5938-0.6519
<F(31) .... F(35)  [ 1655.01]      2.787(8) < 2.94 -0.15      0.0306 0.6088-0.7030 0.3415 0.6273-0.6801 C(310)     144.1(5)
<F(31) .... C(35)  [      ]      2.860(8)<< 3.17 -0.31 Intra 0.0306 0.6088-0.7030 -0.1262 0.5710-0.6383
<F(31) .... H(35A) [      ]      2.71  2.67  0.04 Intra 0.0306 0.6088-0.7030 -0.0152 0.5657-0.6354
<F(31) .... F(12)  [ 3564.05]      3.040(9)  2.94  0.10      0.0306 0.6088-0.7030 0.1727 0.7193-0.7287 C(310)     148.8(5)
<F(31A) .... >F(62A) [ 1554.04]      2.73(2)<< 2.94 -0.21      -0.1290 0.6100-0.7289 -0.1675 0.6969-0.7766 C(310)     171.4(16)
<F(31A) .... C(37)  [      ]      2.77(2)<< 3.17 -0.40 Intra -0.1290 0.6100-0.7289 -0.3549 0.5807-0.6776
<F(31A) .... H(37A) [      ]      2.58 < 2.67 -0.09 Intra -0.1290 0.6100-0.7289 -0.3999 0.5824-0.7013
<F(31A) .... H(57A) [ 3464.03]      2.73  2.67  0.06      -0.1290 0.6100-0.7289 -0.2898 0.5970-0.7929 C(310)     126
<F(31B) .... C(35)  [      ]      3.095(11) < 3.17 -0.08 Intra -0.0120 0.6161-0.7130 -0.1262 0.5710-0.6383
<F(31B) .... C(37)  [      ]      3.279(12)  3.17  0.11 Intra -0.0120 0.6161-0.7130 -0.3549 0.5807-0.6776
<F(31B) .... F(12)  [ 3564.05]      2.965(10)  2.94  0.02      -0.0120 0.6161-0.7130 0.1727 0.7193-0.7287 C(310)     177.1(7)
<F(32) .... >F(62A) [ 1554.04]      3.132(10)  2.94  0.19      -0.1599 0.5811-0.7361 -0.1675 0.6969-0.7766 C(310)     127.6(6)
<F(32) .... C(37)  [      ]      2.702(8)<< 3.17 -0.47 Intra -0.1599 0.5811-0.7361 -0.3549 0.5807-0.6776
<F(32) .... H(37A) [      ]      2.39<< 2.67 -0.28 Intra -0.1599 0.5811-0.7361 -0.3999 0.5824-0.7013
<F(32) .... F(55)  [ 3464.03]      3.011(8)  2.94  0.07      -0.1599 0.5811-0.7361 -0.0283 0.5620-0.8114 C(310)     124.9(5)
<F(32) .... C(57)  [ 3464.03]      3.311(8)  3.17  0.14      -0.1599 0.5811-0.7361 -0.3415 0.5928-0.8158 C(310)     171.8(6)
<F(32) .... H(57A) [ 3464.03]      2.38<< 2.67 -0.29      -0.1599 0.5811-0.7361 -0.2898 0.5970-0.7929 C(310)     176
<F(32A) .... >F(21) [      ]      2.64(3)<< 2.94 -0.30      -0.1300 0.5206-0.7242 -0.2832 0.4240-0.7265 C(310)     150.7(16)
<F(32A) .... >F(23) [      ]      3.08(3)  2.94  0.14      -0.1300 0.5206-0.7242 -0.4649 0.4796-0.7440 C(310)     128.4(13)
<F(32A) .... C(35)  [      ]      3.37(2)  3.17  0.20 Intra -0.1300 0.5206-0.7242 -0.1262 0.5710-0.6383
<F(32A) .... C(37)  [      ]      2.93(2)<< 3.17 -0.24 Intra -0.1300 0.5206-0.7242 -0.3549 0.5807-0.6776
<F(32A) .... H(37A) [      ]      2.84  2.67  0.17 Intra -0.1300 0.5206-0.7242 -0.3999 0.5824-0.7013
<F(32A) .... F(43)  [ 2464.06]      2.98(2)  2.94  0.04      -0.1300 0.5206-0.7242 0.0045 0.4267-0.7683 C(310)     142.0(15)
<F(32B) .... >F(23) [      ]      3.078(14)  2.94  0.14      -0.1663 0.5531-0.7367 -0.4649 0.4796-0.7440 C(310)     129.1(5)
<F(32B) .... C(37)  [      ]      2.766(9)<< 3.17 -0.40 Intra -0.1663 0.5531-0.7367 -0.3549 0.5807-0.6776
<F(32B) .... H(37A) [      ]      2.46<< 2.67 -0.21 Intra -0.1663 0.5531-0.7367 -0.3999 0.5824-0.7013
<F(32B) .... F(55)  [ 3464.03]      2.984(8)  2.94  0.04      -0.1663 0.5531-0.7367 -0.0283 0.5620-0.8114 C(310)     123.2(6)
<F(32B) .... H(57A) [ 3464.03]      2.53 < 2.67 -0.14      -0.1663 0.5531-0.7367 -0.2898 0.5970-0.7929 C(310)     139
<F(33) .... F(24)  [ 1655.02]      3.039(12)  2.94  0.10      -0.0114 0.5215-0.7080 -0.0061 0.3964-0.6916 C(310)     148.1(8)
<F(33) .... F(26)  [ 1655.02]      2.931(14) < 2.94 -0.01      -0.0114 0.5215-0.7080 -0.0156 0.4482-0.6438 C(310)     117.8(8)
<F(33) .... C(35)  [      ]      2.975(14) < 3.17 -0.20 Intra -0.0114 0.5215-0.7080 -0.1262 0.5710-0.6383
<F(33) .... H(35A) [      ]      2.86  2.67  0.19 Intra -0.0114 0.5215-0.7080 -0.0152 0.5657-0.6354
<F(33A) .... F(35)  [ 1655.01]      2.87(2) < 2.94 -0.07      0.0588 0.5675-0.7003 0.3415 0.6273-0.6801 C(310)     147.8(19)
<F(33A) .... F(36)  [ 1655.01]      2.621(17)<< 2.94 -0.32      0.0588 0.5675-0.7003 0.3008 0.5449-0.6579 C(310)     150.7(14)
<F(33A) .... C(35)  [      ]      2.757(17)<< 3.17 -0.41 Intra 0.0588 0.5675-0.7003 -0.1262 0.5710-0.6383
<F(33A) .... C(320) [ 1655.01]      3.257(16)  3.17  0.09      0.0588 0.5675-0.7003 0.3741 0.5938-0.6519 C(310)     152.9(13)
<F(33A) .... H(35A) [      ]      2.46<< 2.67 -0.21 Intra 0.0588 0.5675-0.7003 -0.0152 0.5657-0.6354
<F(33B) .... F(26)  [ 1655.02]      2.936(14) < 2.94  0.00      0.0271 0.5303-0.7027 -0.0156 0.4482-0.6438 C(310)     115.9(7)
=====

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<F(33B) .... F(36) [ 1655.01] 2.854(13) < 2.94 -0.09 0.0271 0.5303-0.7027 0.3008 0.5449-0.6579 C(310) 123.3(7)
<F(33B) .... C(35) [ ] 2.860(14)<< 3.17 -0.31 Intra 0.0271 0.5303-0.7027 -0.1262 0.5710-0.6383
<F(33B) .... H(35A) [ ] 2.63 < 2.67 -0.04 Intra 0.0271 0.5303-0.7027 -0.0152 0.5657-0.6354
=====

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Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 1 to Neighbouring ARU'S

```

=====
Nr      ARU      Nr.Cont.  d(min)  Del  XHn X      - At(I)      At(J) - Y  YHn Note  Partaking ARU's in Close Contact Resd.
-----
1 [ 1555.05] 4 2.4500 -0.55 0 C(31) - S(3) ... H(11) -N(11) 1 << 1555.05
2 [ 3464.05] 10 2.8100 -0.19 0 C(31) - S(3) ... H(19A) -C(19) 1 < 3464.05
3 [ 3564.05] 4 2.9100 -0.09 0 C(31) - S(3) ... H(12A) -C(12) 1 < 3564.05
4 [ 1455.01] 6 2.6210 -0.32 0 C(320) - F(36) ... *F(33A) -C(310) 0 << 1455.01
5 [ 3464.03] 9 2.3800 -0.29 0 C(310) -*F(32) ... H(57A) -C(57) 1 << 3464.03
6 [ 1555.02] 12 2.6400 -0.30 0 C(310) -*F(32A) ... *F(21) -C(210) 0 << 1555.02
7 [ 1655.02] 9 2.8200 0.15 1 C(35) - H(35A) ... F(26) -C(220) 0 1655.02
8 [ 1655.01] 6 2.6210 -0.32 0 C(310) -*F(33A) ... F(36) -C(320) 0 << 1655.01
9 [ 1554.04] 2 2.7300 -0.21 0 C(310) -*F(31A) ... *F(62A) -C(610) 0 << 1554.04
10 [ 2464.06] 1 2.9800 0.04 0 C(310) -*F(32A) ... F(43) -C(410) 0 2464.06
=====

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Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

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=====
***** ARU = 1555.02 *****
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-----
At(I)[1555.02] At(J) [ ARU(J) ]      D(I-J) SumRad Del Type  X(I)  Y(I)  Z(I)  X(J)  Y(J)  Z(J)  X      X - I...J
-----
S(2) .... N(41) [ ] 3.291(2) < 3.35 -0.06 -0.6423 0.4982-0.5563 -0.5517 0.5818-0.4879 C(21) 105.71(8)
S(2) .... C(24) [ ] 3.291(2)<< 3.50 -0.21 Intra -0.6423 0.4982-0.5563 -0.5221 0.4265-0.6279
S(2) .... C(29) [ ] 3.265(2)<< 3.50 -0.23 Intra -0.6423 0.4982-0.5563 -0.6848 0.4172-0.6275
S(2) .... C(32) [ 1455.01] 3.444(3) < 3.50 -0.06 -0.6423 0.4982-0.5563 -0.9994 0.5519-0.5269 C(21) 165.10(9)
S(2) .... C(33) [ 1455.01] 3.480(3) < 3.50 -0.02 -0.6423 0.4982-0.5563 -1.0389 0.5380-0.5614 C(21) 157.58(9)
S(2) .... C(39) [ ] 3.608(2) 3.50 0.11 -0.6423 0.4982-0.5563 -0.3864 0.5844-0.6119
S(2) .... H(21) [ ] 2.92(3) < 3.00 -0.08 Intra -0.6423 0.4982-0.5563 -0.3550 0.4623-0.5187
S(2) .... H(29A) [ ] 2.81 < 3.00 -0.19 Intra -0.6423 0.4982-0.5563 -0.7403 0.4139-0.6050
S(2) .... H(32A) [ 1455.01] 3.00 3.00 0.00 -0.6423 0.4982-0.5563 -0.9249 0.5331-0.5118 C(21) 152
S(2) .... H(33A) [ 1455.01] 3.07 3.00 0.07 -0.6423 0.4982-0.5563 -0.9963 0.5080-0.5753 C(21) 143
S(2) .... H(39A) [ ] 2.96 < 3.00 -0.04 -0.6423 0.4982-0.5563 -0.4526 0.5879-0.5910
S(2) .... H(41) [ ] 2.46(3)<< 3.00 -0.54 -0.6423 0.4982-0.5563 -0.5570 0.5647-0.5089 C(21) 103.6(8)
S(2) .... S(6) [ 4444.04] 3.7777(9) 3.60 0.18 -0.6423 0.4982-0.5563 -0.7846 0.3484-0.5473
>F(21) .... F(24) [ 1655.02] 2.743(8) < 2.94 -0.20 -0.2832 0.4240-0.7265 -0.0061 0.3964-0.6916 C(210) 153.9(6)

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>F(21) .... C(25) [ ] 2.752(7)<< 3.17 -0.42 Intra -0.2832 0.4240-0.7265 -0.4398 0.4302-0.6608
>F(21) .... H(25A) [ ] 2.45<< 2.67 -0.22 Intra -0.2832 0.4240-0.7265 -0.3287 0.4367-0.6610
>F(21) .... <F(32A) [ ] 2.64(3)<< 2.94 -0.30 -0.2832 0.4240-0.7265 -0.1300 0.5206-0.7242 C(210) 114.7(12)
>F(21) .... F(43) [ 2464.06] 2.870(7) < 2.94 -0.07 -0.2832 0.4240-0.7265 0.0045 0.4267-0.7683 C(210) 143.3(5)
>F(21) .... H(47A) [ 2464.06] 2.81 2.67 0.14 -0.2832 0.4240-0.7265 -0.2368 0.4250-0.8025
>F(22) .... C(27) [ ] 2.789(11)<< 3.17 -0.38 Intra -0.4910 0.3920-0.7530 -0.6864 0.4159-0.6936
>F(22) .... H(27A) [ ] 2.56 < 2.67 -0.11 Intra -0.4910 0.3920-0.7530 -0.7424 0.4124-0.7160
>F(22) .... F(11) [ 2464.05] 3.125(10) 2.94 0.18 -0.4910 0.3920-0.7530 -0.3497 0.2711-0.7463 C(210) 114.9(6)
>F(23) .... C(25) [ ] 3.278(7) 3.17 0.11 Intra -0.4649 0.4796-0.7440 -0.4398 0.4302-0.6608
>F(23) .... C(27) [ ] 3.034(8) < 3.17 -0.14 Intra -0.4649 0.4796-0.7440 -0.6864 0.4159-0.6936
>F(23) .... <F(32A) [ ] 3.08(3) 2.94 0.14 -0.4649 0.4796-0.7440 -0.1300 0.5206-0.7242
>F(23) .... F(45) [ 2464.06] 3.036(7) 2.94 0.10 -0.4649 0.4796-0.7440 -0.4996 0.4651-0.8259 C(210) 108.5(4)
>F(23) .... >F(51) [ 3464.03] 3.012(12) 2.94 0.07 -0.4649 0.4796-0.7440 -0.6862 0.5671-0.7745 C(210) 151.5(6)
F(24) .... >F(21) [ 1455.02] 2.743(8) < 2.94 -0.20 -1.0061 0.3964-0.6916 -1.2832 0.4240-0.7265 C(220) 137.9(3)
F(24) .... C(27) [ ] 2.736(3)<< 3.17 -0.43 Intra -1.0061 0.3964-0.6916 -0.6864 0.4159-0.6936
F(24) .... H(27A) [ ] 2.43<< 2.67 -0.24 Intra -1.0061 0.3964-0.6916 -0.7424 0.4124-0.7160
F(24) .... <F(22A) [ 1455.02] 2.768(11) < 2.94 -0.17 -1.0061 0.3964-0.6916 -1.2990 0.3984-0.7257 C(220) 140.8(3)
F(24) .... <F(33) [ 1455.01] 3.039(12) 2.94 0.10 -1.0061 0.3964-0.6916 -1.0114 0.5215-0.7080
F(24) .... F(43) [ 2364.06] 2.905(2) < 2.94 -0.04 -1.0061 0.3964-0.6916 -0.9955 0.4267-0.7683 C(220) 145.59(18)
F(24) .... <F(61) [ 4444.04] 2.996(10) 2.94 0.06 -1.0061 0.3964-0.6916 -0.8690 0.2884-0.7192 C(220) 105.0(3)
F(25) .... C(23) [ 1455.02] 3.341(3) 3.17 0.17 -0.9812 0.3598-0.6384 -1.2904 0.4031-0.5889 C(220) 105.35(14)
F(25) .... C(29) [ ] 2.876(3)<< 3.17 -0.29 Intra -0.9812 0.3598-0.6384 -0.6848 0.4172-0.6275
F(25) .... H(23A) [ 1455.02] 2.49 < 2.67 -0.18 -0.9812 0.3598-0.6384 -1.2339 0.3811-0.6061 C(220) 109
F(25) .... H(29A) [ ] 2.70 2.67 0.03 Intra -0.9812 0.3598-0.6384 -0.7403 0.4139-0.6050
F(25) .... F(66) [ 4344.04] 3.075(3) 2.94 0.13 -0.9812 0.3598-0.6384 -1.2967 0.2989-0.6529 C(220) 119.37(15)
F(25) .... C(65) [ 4444.04] 2.974(3) < 3.17 -0.20 -0.9812 0.3598-0.6384 -0.8571 0.2429-0.6382 C(220) 130.20(15)
F(26) .... C(23) [ 1455.02] 3.252(3) 3.17 0.08 -1.0156 0.4482-0.6438 -1.2904 0.4031-0.5889 C(220) 109.40(15)
F(26) .... C(29) [ ] 2.946(3)<< 3.17 -0.22 Intra -1.0156 0.4482-0.6438 -0.6848 0.4172-0.6275
F(26) .... C(35) [ 1455.01] 3.075(3) < 3.17 -0.10 -1.0156 0.4482-0.6438 -1.1262 0.5710-0.6383 C(220) 155.57(16)
F(26) .... H(23A) [ 1455.02] 2.80 2.67 0.13 -1.0156 0.4482-0.6438 -1.2339 0.3811-0.6061
F(26) .... H(25A) [ 1455.02] 2.73 2.67 0.06 -1.0156 0.4482-0.6438 -1.3287 0.4367-0.6610 C(220) 106
F(26) .... H(29A) [ ] 2.84 2.67 0.17 Intra -1.0156 0.4482-0.6438 -0.7403 0.4139-0.6050
F(26) .... H(35A) [ 1455.01] 2.82 2.67 0.15 -1.0156 0.4482-0.6438 -1.0152 0.5657-0.6354 C(220) 145
F(26) .... <F(33) [ 1455.01] 2.931(14) < 2.94 -0.01 -1.0156 0.4482-0.6438 -1.0114 0.5215-0.7080
F(26) .... <F(33B) [ 1455.01] 2.936(14) < 2.94 0.00 -1.0156 0.4482-0.6438 -0.9729 0.5303-0.7027
N(21) .... S(4) [ ] 3.260(2) < 3.35 -0.09 -0.3619 0.4478-0.5393 -0.3346 0.5085-0.4598 C(21) 123.78(14)
C(22) 124.28(14)
N(21) .... C(23) [ ] 2.191(3)<< 3.25 -1.06 Intra -0.3619 0.4478-0.5393 -0.2904 0.4031-0.5889 H(21) 159(2)
N(22) .... C(22) [ ] 2.210(3)<< 3.25 -1.04 Intra -0.4359 0.4298-0.5945 -0.2451 0.4144-0.5544 C(24) 158.95(16)
N(22) .... H(25A) [ ] 2.61 < 2.75 -0.14 Intra -0.4359 0.4298-0.5945 -0.3287 0.4367-0.6610 C(21) 147
N(22) .... H(29A) [ ] 2.62 < 2.75 -0.13 Intra -0.4359 0.4298-0.5945 -0.7403 0.4139-0.6050 C(23) 145
C(21) .... C(23) [ ] 2.265(3)<< 3.40 -1.13 Intra -0.4797 0.4580-0.5634 -0.2904 0.4031-0.5889 S(2) 163.91(13)
C(21) .... C(29) [ ] 3.075(3)<< 3.40 -0.33 Intra -0.4797 0.4580-0.5634 -0.6848 0.4172-0.6275 N(21) 148.80(16)
C(21) .... C(39) [ ] 3.582(3) 3.40 0.18 -0.4797 0.4580-0.5634 -0.3864 0.5844-0.6119 N(21) 108.39(15)
C(21) .... H(29A) [ ] 2.87 < 2.90 -0.03 Intra -0.4797 0.4580-0.5634 -0.7403 0.4139-0.6050 N(21) 147
C(22) .... N(22) [ ] 2.210(3)<< 3.25 -1.04 Intra -0.2451 0.4144-0.5544 -0.4359 0.4298-0.5945 H(22A) 164
C(22) .... C(24) [ ] 3.578(3) 3.40 0.18 Intra -0.2451 0.4144-0.5544 -0.5221 0.4265-0.6279 H(22A) 156
C(22) .... C(33) [ ] 3.428(4) 3.40 0.03 -0.2451 0.4144-0.5544 -0.0389 0.5380-0.5614 C(23) 104.19(17)
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| | | | | | | | | | | | | | |
|--------|------|---------|------------|-------------|------|-------|---------|---------------|---------------|---------------|---------------|------------|------------|
| C(23) | | F(25) | [1655.02] | 3.341(3) | 3.17 | 0.17 | -0.2904 | 0.4031-0.5889 | 0.0188 | 0.3598-0.6384 | N(22) | 138.21(15) | |
| | | | | | | | | | | | C(22) | 110.55(17) | |
| C(23) | | F(26) | [1655.02] | 3.252(3) | 3.17 | 0.08 | -0.2904 | 0.4031-0.5889 | -0.0156 | 0.4482-0.6438 | N(22) | 112.61(14) | |
| | | | | | | | | | | | C(22) | 108.26(17) | |
| C(23) | | N(21) | [] | 2.191(3)<< | 3.25 | -1.06 | Intra | -0.2904 | 0.4031-0.5889 | -0.3619 | 0.4478-0.5393 | H(23A) | 163 |
| C(23) | | C(25) | [] | 2.992(3)<< | 3.40 | -0.41 | Intra | -0.2904 | 0.4031-0.5889 | -0.4398 | 0.4302-0.6608 | C(22) | 154.51(19) |
| C(23) | | H(21) | [] | 2.98(3) | 2.90 | 0.08 | Intra | -0.2904 | 0.4031-0.5889 | -0.3550 | 0.4623-0.5187 | H(23A) | 158 |
| C(23) | | H(25A) | [] | 2.78 < | 2.90 | -0.12 | Intra | -0.2904 | 0.4031-0.5889 | -0.3287 | 0.4367-0.6610 | C(22) | 150 |
| C(23) | | F(65) | [4444.04] | 3.143(3) < | 3.17 | -0.03 | | -0.2904 | 0.4031-0.5889 | -0.3020 | 0.2719-0.5974 | N(22) | 114.21(15) |
| | | | | | | | | | | | C(22) | 107.53(17) | |
| C(24) | | S(2) | [] | 3.291(2)<< | 3.50 | -0.21 | Intra | -0.5221 | 0.4265-0.6279 | -0.6423 | 0.4982-0.5563 | C(25) | 144.11(16) |
| C(24) | | C(22) | [] | 3.578(3) | 3.40 | 0.18 | Intra | -0.5221 | 0.4265-0.6279 | -0.2451 | 0.4144-0.5544 | C(25) | 109.39(16) |
| | | | | | | | | | | | C(29) | 128.57(14) | |
| C(24) | | C(27) | [] | 2.792(3)<< | 3.40 | -0.61 | Intra | -0.5221 | 0.4265-0.6279 | -0.6864 | 0.4159-0.6936 | N(22) | 177.78(16) |
| C(24) | | H(23A) | [] | 2.78 < | 2.90 | -0.12 | Intra | -0.5221 | 0.4265-0.6279 | -0.2339 | 0.3811-0.6061 | C(29) | 143 |
| C(25) | | >F(21) | [] | 2.752(7)<< | 3.17 | -0.42 | Intra | -0.4398 | 0.4302-0.6608 | -0.2832 | 0.4240-0.7265 | C(24) | 173.2(4) |
| C(25) | | >F(23) | [] | 3.278(7) | 3.17 | 0.11 | Intra | -0.4398 | 0.4302-0.6608 | -0.4649 | 0.4796-0.7440 | C(24) | 142.8(2) |
| C(25) | | C(23) | [] | 2.992(3)<< | 3.40 | -0.41 | Intra | -0.4398 | 0.4302-0.6608 | -0.2904 | 0.4031-0.5889 | C(26) | 160.93(18) |
| C(25) | | C(28) | [] | 2.773(4)<< | 3.40 | -0.63 | Intra | -0.4398 | 0.4302-0.6608 | -0.7650 | 0.4127-0.6605 | H(25A) | 179 |
| C(25) | | H(23A) | [] | 2.90 | 2.90 | 0.00 | Intra | -0.4398 | 0.4302-0.6608 | -0.2339 | 0.3811-0.6061 | C(26) | 149 |
| C(25) | | <F(21A) | [] | 3.105(18) < | 3.17 | -0.07 | Intra | -0.4398 | 0.4302-0.6608 | -0.3930 | 0.4773-0.7390 | C(24) | 152.3(4) |
| C(25) | | <F(22A) | [] | 2.766(11)<< | 3.17 | -0.40 | Intra | -0.4398 | 0.4302-0.6608 | -0.2990 | 0.3984-0.7257 | C(24) | 160.2(3) |
| C(25) | | F(66) | [4444.04] | 3.365(3) | 3.17 | 0.19 | | -0.4398 | 0.4302-0.6608 | -0.2967 | 0.2989-0.6529 | | |
| C(26) | | C(29) | [] | 2.772(3)<< | 3.40 | -0.63 | Intra | -0.5237 | 0.4242-0.6932 | -0.6848 | 0.4172-0.6275 | C(210) | 179.6(2) |
| C(27) | | >F(22) | [] | 2.789(11)<< | 3.17 | -0.38 | Intra | -0.6864 | 0.4159-0.6936 | -0.4910 | 0.3920-0.7530 | C(28) | 162.9(3) |
| C(27) | | >F(23) | [] | 3.034(8) < | 3.17 | -0.14 | Intra | -0.6864 | 0.4159-0.6936 | -0.4649 | 0.4796-0.7440 | C(28) | 148.8(2) |
| C(27) | | F(24) | [] | 2.736(3)<< | 3.17 | -0.43 | Intra | -0.6864 | 0.4159-0.6936 | -1.0061 | 0.3964-0.6916 | C(26) | 177.33(18) |
| C(27) | | F(36) | [] | 3.343(3) | 3.17 | 0.17 | | -0.6864 | 0.4159-0.6936 | -0.6992 | 0.5449-0.6579 | H(27A) | 114 |
| C(27) | | C(24) | [] | 2.792(3)<< | 3.40 | -0.61 | Intra | -0.6864 | 0.4159-0.6936 | -0.5221 | 0.4265-0.6279 | H(27A) | 180 |
| C(27) | | <F(21A) | [] | 3.32(2) | 3.17 | 0.15 | Intra | -0.6864 | 0.4159-0.6936 | -0.3930 | 0.4773-0.7390 | C(28) | 145.0(3) |
| C(27) | | <F(23A) | [] | 2.749(14)<< | 3.17 | -0.42 | Intra | -0.6864 | 0.4159-0.6936 | -0.5117 | 0.4031-0.7564 | C(28) | 169.7(5) |
| C(28) | | F(36) | [] | 3.198(3) | 3.17 | 0.03 | | -0.7650 | 0.4127-0.6605 | -0.6992 | 0.5449-0.6579 | C(220) | 108.04(15) |
| C(28) | | C(25) | [] | 2.773(4)<< | 3.40 | -0.63 | Intra | -0.7650 | 0.4127-0.6605 | -0.4398 | 0.4302-0.6608 | C(220) | 178.30(17) |
| C(29) | | S(2) | [] | 3.265(2)<< | 3.50 | -0.23 | Intra | -0.6848 | 0.4172-0.6275 | -0.6423 | 0.4982-0.5563 | C(28) | 142.55(16) |
| C(29) | | F(25) | [] | 2.876(3)<< | 3.17 | -0.29 | Intra | -0.6848 | 0.4172-0.6275 | -0.9812 | 0.3598-0.6384 | C(24) | 158.76(16) |
| C(29) | | F(26) | [] | 2.946(3)<< | 3.17 | -0.22 | Intra | -0.6848 | 0.4172-0.6275 | -1.0156 | 0.4482-0.6438 | C(24) | 153.12(16) |
| C(29) | | F(36) | [] | 3.242(3) | 3.17 | 0.07 | | -0.6848 | 0.4172-0.6275 | -0.6992 | 0.5449-0.6579 | H(29A) | 111 |
| C(29) | | C(21) | [] | 3.075(3)<< | 3.40 | -0.33 | Intra | -0.6848 | 0.4172-0.6275 | -0.4797 | 0.4580-0.5634 | C(28) | 164.26(16) |
| C(29) | | C(26) | [] | 2.772(3)<< | 3.40 | -0.63 | Intra | -0.6848 | 0.4172-0.6275 | -0.5237 | 0.4242-0.6932 | H(29A) | 179 |
| C(29) | | S(6) | [4444.04] | 3.468(2) < | 3.50 | -0.03 | | -0.6848 | 0.4172-0.6275 | -0.7846 | 0.3484-0.5473 | C(24) | 108.91(14) |
| | | | | | | | | | | | C(28) | 125.74(16) | |
| C(210) | | H(25A) | [] | 2.66<< | 2.90 | -0.24 | Intra | -0.4369 | 0.4284-0.7289 | -0.3287 | 0.4367-0.6610 | >F(22) | 143 |
| | | | | | | | | | | | >F(23) | 112 | |
| | | | | | | | | | | | <F(23A) | 155 | |
| C(210) | | H(27A) | [] | 2.65<< | 2.90 | -0.25 | Intra | -0.4369 | 0.4284-0.7289 | -0.7424 | 0.4124-0.7160 | >F(21) | 161 |
| | | | | | | | | | | | <F(21A) | 118 | |
| | | | | | | | | | | | <F(22A) | 137 | |
| C(220) | | H(27A) | [] | 2.68<< | 2.90 | -0.22 | Intra | -0.9410 | 0.4038-0.6592 | -0.7424 | 0.4124-0.7160 | F(25) | 131 |

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F(26) 124
C(220) .... H(29A) [ ] 2.62<< 2.90 -0.28 Intra -0.9410 0.4038-0.6592 -0.7403 0.4139-0.6050 F(24) 164
H(21) .... S(2) [ ] 2.92(3) < 3.00 -0.08 Intra -0.3550 0.4623-0.5187 -0.6423 0.4982-0.5563
H(21) .... S(4) [ ] 2.43(3)<< 3.00 -0.57 -0.3550 0.4623-0.5187 -0.3346 0.5085-0.4598 N(21) 178(3)
H(21) .... C(23) [ ] 2.98(3) 2.90 0.08 Intra -0.3550 0.4623-0.5187 -0.2904 0.4031-0.5889
H(21) .... H(22A) [ ] 2.41 2.40 0.01 Intra -0.3550 0.4623-0.5187 -0.1510 0.4019-0.5427
H(22A) .... H(21) [ ] 2.41 2.40 0.01 Intra -0.1510 0.4019-0.5427 -0.3550 0.4623-0.5187
H(22A) .... H(23A) [ ] 2.48 2.40 0.08 Intra -0.1510 0.4019-0.5427 -0.2339 0.3811-0.6061
H(23A) .... F(25) [ 1655.02] 2.49 < 2.67 -0.18 -0.2339 0.3811-0.6061 0.0188 0.3598-0.6384 C(23) 149
H(23A) .... F(26) [ 1655.02] 2.80 2.67 0.13 -0.2339 0.3811-0.6061 -0.0156 0.4482-0.6438 C(23) 110
H(23A) .... C(24) [ ] 2.78 < 2.90 -0.12 Intra -0.2339 0.3811-0.6061 -0.5221 0.4265-0.6279
H(23A) .... C(25) [ ] 2.90 2.90 0.00 Intra -0.2339 0.3811-0.6061 -0.4398 0.4302-0.6608
H(23A) .... H(22A) [ ] 2.48 2.40 0.08 Intra -0.2339 0.3811-0.6061 -0.1510 0.4019-0.5427
H(23A) .... H(25A) [ ] 2.54 2.40 0.14 Intra -0.2339 0.3811-0.6061 -0.3287 0.4367-0.6610
H(23A) .... F(65) [ 4444.04] 2.68 2.67 0.01 -0.2339 0.3811-0.6061 -0.3020 0.2719-0.5974 C(23) 110
H(23A) .... F(66) [ 4444.04] 2.66 < 2.67 -0.01 -0.2339 0.3811-0.6061 -0.2967 0.2989-0.6529 C(23) 137
H(25A) .... >F(21) [ ] 2.45<< 2.67 -0.22 Intra -0.3287 0.4367-0.6610 -0.2832 0.4240-0.7265
H(25A) .... F(26) [ 1655.02] 2.73 2.67 0.06 -0.3287 0.4367-0.6610 -0.0156 0.4482-0.6438 C(25) 166
H(25A) .... N(22) [ ] 2.61 < 2.75 -0.14 Intra -0.3287 0.4367-0.6610 -0.4359 0.4298-0.5945
H(25A) .... C(23) [ ] 2.78 < 2.90 -0.12 Intra -0.3287 0.4367-0.6610 -0.2904 0.4031-0.5889
H(25A) .... C(210) [ ] 2.66<< 2.90 -0.24 Intra -0.3287 0.4367-0.6610 -0.4369 0.4284-0.7289
H(25A) .... H(23A) [ ] 2.54 2.40 0.14 Intra -0.3287 0.4367-0.6610 -0.2339 0.3811-0.6061 C(25) 103
H(25A) .... <F(22A) [ ] 2.55 < 2.67 -0.12 Intra -0.3287 0.4367-0.6610 -0.2990 0.3984-0.7257
H(27A) .... >F(22) [ ] 2.56 < 2.67 -0.11 Intra -0.7424 0.4124-0.7160 -0.4910 0.3920-0.7530
H(27A) .... F(24) [ ] 2.43<< 2.67 -0.24 Intra -0.7424 0.4124-0.7160 -1.0061 0.3964-0.6916
H(27A) .... C(210) [ ] 2.65<< 2.90 -0.25 Intra -0.7424 0.4124-0.7160 -0.4369 0.4284-0.7289
H(27A) .... C(220) [ ] 2.68<< 2.90 -0.22 Intra -0.7424 0.4124-0.7160 -0.9410 0.4038-0.6592
H(27A) .... <F(23A) [ ] 2.45<< 2.67 -0.22 Intra -0.7424 0.4124-0.7160 -0.5117 0.4031-0.7564
H(29A) .... S(2) [ ] 2.81 < 3.00 -0.19 Intra -0.7403 0.4139-0.6050 -0.6423 0.4982-0.5563 C(29) 110
H(29A) .... F(25) [ ] 2.70 2.67 0.03 Intra -0.7403 0.4139-0.6050 -0.9812 0.3598-0.6384
H(29A) .... F(26) [ ] 2.84 2.67 0.17 Intra -0.7403 0.4139-0.6050 -1.0156 0.4482-0.6438
H(29A) .... N(22) [ ] 2.62 < 2.75 -0.13 Intra -0.7403 0.4139-0.6050 -0.4359 0.4298-0.5945
H(29A) .... C(21) [ ] 2.87 < 2.90 -0.03 Intra -0.7403 0.4139-0.6050 -0.4797 0.4580-0.5634
H(29A) .... C(220) [ ] 2.62<< 2.90 -0.28 Intra -0.7403 0.4139-0.6050 -0.9410 0.4038-0.6592
H(29A) .... S(6) [ 4444.04] 2.65<< 3.00 -0.35 -0.7403 0.4139-0.6050 -0.7846 0.3484-0.5473 C(29) 144
<F(21A) .... C(25) [ ] 3.105(18) < 3.17 -0.07 Intra -0.3930 0.4773-0.7390 -0.4398 0.4302-0.6608
<F(21A) .... C(27) [ ] 3.32(2) 3.17 0.15 Intra -0.3930 0.4773-0.7390 -0.6864 0.4159-0.6936
<F(21A) .... C(37) [ ] 3.352(15) 3.17 0.18 -0.3930 0.4773-0.7390 -0.3549 0.5807-0.6776 C(210) 120.2(10)
<F(21A) .... H(37A) [ ] 2.86 2.67 0.19 -0.3930 0.4773-0.7390 -0.3999 0.5824-0.7013 C(210) 131
<F(22A) .... F(24) [ 1655.02] 2.768(11) < 2.94 -0.17 -0.2990 0.3984-0.7257 -0.0061 0.3964-0.6916 C(210) 143.6(8)
<F(22A) .... C(25) [ ] 2.766(11)<< 3.17 -0.40 Intra -0.2990 0.3984-0.7257 -0.4398 0.4302-0.6608
<F(22A) .... H(25A) [ ] 2.55 < 2.67 -0.12 Intra -0.2990 0.3984-0.7257 -0.3287 0.4367-0.6610
<F(22A) .... F(13) [ 2464.05] 3.087(13) 2.94 0.15 -0.2990 0.3984-0.7257 -0.1614 0.3086-0.7775 C(210) 128.9(6)
<F(22A) .... F(43) [ 2464.06] 3.073(11) 2.94 0.13 -0.2990 0.3984-0.7257 0.0045 0.4267-0.7683 C(210) 123.2(7)
<F(23A) .... C(27) [ ] 2.749(14)<< 3.17 -0.42 Intra -0.5117 0.4031-0.7564 -0.6864 0.4159-0.6936
<F(23A) .... H(27A) [ ] 2.45<< 2.67 -0.22 Intra -0.5117 0.4031-0.7564 -0.7424 0.4124-0.7160
<F(23A) .... F(44) [ 2464.06] 3.119(15) 2.94 0.18 -0.5117 0.4031-0.7564 -0.5407 0.3788-0.8397 C(210) 149.5(9)
<F(23A) .... F(45) [ 2464.06] 2.947(17) 2.94 0.01 -0.5117 0.4031-0.7564 -0.4996 0.4651-0.8259 C(210) 114.2(11)
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Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 2 to Neighbouring ARU'S

| Nr | ARU | Nr.Cont. | d(min) | Del | XHn | X | - At(I) | At(J) | - Y | YHn | Note | Partaking ARU's in Close Contact | Resd. |
|----|------------|----------|--------|-------|-----|--------|---------------------|---------|-----|-----|------|----------------------------------|-------|
| 1 | [1555.06] | 4 | 2.4300 | -0.57 | 1 | N(21) | - H(21) ... S(4) | -C(41) | 0 | << | | 1555.06 | |
| 2 | [1455.01] | 9 | 2.8200 | 0.15 | 0 | C(220) | - F(26) ... H(35A) | -C(35) | 1 | | | 1455.01 | |
| 3 | [1555.01] | 11 | 2.6400 | -0.30 | 0 | C(210) | -*F(21) ... *F(32A) | -C(310) | 0 | << | | 1555.01 | |
| 4 | [4444.04] | 9 | 2.6500 | -0.35 | 1 | C(29) | - H(29A) ... S(6) | -C(61) | 0 | << | | 4444.04 | |
| 5 | [1655.02] | 7 | 2.4900 | -0.18 | 1 | C(23) | - H(23A) ... F(25) | -C(220) | 0 | < | | 1655.02 | |
| 6 | [2464.06] | 6 | 2.8100 | 0.14 | 0 | C(210) | -*F(21) ... H(47A) | -C(47) | 1 | | | 2464.06 | |
| 7 | [2464.05] | 2 | 3.0870 | 0.15 | 0 | C(210) | -*F(22A) ... F(13) | -C(110) | 0 | | | 2464.05 | |
| 8 | [3464.03] | 1 | 3.0120 | 0.07 | 0 | C(210) | -*F(23) ... *F(51) | -C(510) | 0 | | | 3464.03 | |
| 9 | [1455.02] | 7 | 2.4900 | -0.18 | 0 | C(220) | - F(25) ... H(23A) | -C(23) | 1 | < | | 1455.02 | |
| 10 | [2364.06] | 1 | 2.9050 | -0.04 | 0 | C(220) | - F(24) ... F(43) | -C(410) | 0 | < | | 2364.06 | |
| 11 | [4344.04] | 1 | 3.0750 | 0.13 | 0 | C(220) | - F(25) ... F(66) | -C(620) | 0 | | | 4344.04 | |

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

***** ARU = 1555.03 *****

| At(I)[1555.03] | At(J) | [ARU(J)] | D(I-J) | SumRad | Del | Type | X(I) | Y(I) | Z(I) | X(J) | Y(J) | Z(J) | X | X - I...J |
|----------------|-------|-------------------|-------------|--------|-------|-------|---------|---------------|---------|---------------|--------|-------|-----------|-----------|
| S(5) | | N(61) [] | 3.370(2) | 3.35 | 0.02 | | 0.1298 | 0.8614-0.0406 | -0.0074 | 0.7699 | 0.0220 | C(51) | 103.36(9) | |
| S(5) | | C(54) [] | 3.284(2)<< | 3.50 | -0.22 | Intra | 0.1298 | 0.8614-0.0406 | 0.0085 | 0.9190-0.1170 | | | | |
| S(5) | | C(59) [] | 3.288(2)<< | 3.50 | -0.21 | Intra | 0.1298 | 0.8614-0.0406 | 0.1719 | 0.9261-0.1192 | | | | |
| S(5) | | H(51) [] | 2.87(5) < | 3.00 | -0.13 | Intra | 0.1298 | 0.8614-0.0406 | -0.1560 | 0.9009-0.0066 | | | | |
| S(5) | | H(59A) [] | 2.88 < | 3.00 | -0.12 | Intra | 0.1298 | 0.8614-0.0406 | 0.2324 | 0.9351-0.0981 | | | | |
| S(5) | | H(61) [] | 2.54(3)<< | 3.00 | -0.46 | | 0.1298 | 0.8614-0.0406 | 0.0200 | 0.7901 | 0.0043 | C(51) | 102.7(8) | |
| S(5) | | N(62) [3565.04] | 3.495(2) | 3.35 | 0.14 | | 0.1298 | 0.8614-0.0406 | 0.3791 | 0.7548-0.0724 | | | C(51) | 144.47(9) |
| S(5) | | C(63) [3565.04] | 3.441(3) < | 3.50 | -0.06 | | 0.1298 | 0.8614-0.0406 | 0.4834 | 0.7977-0.0626 | | | C(51) | 152.81(9) |
| S(5) | | C(69) [3565.04] | 3.508(3) | 3.50 | 0.01 | | 0.1298 | 0.8614-0.0406 | 0.1204 | 0.7480-0.1016 | | | C(51) | 105.73(9) |
| S(5) | | H(69A) [3565.04] | 3.13 | 3.00 | 0.13 | | 0.1298 | 0.8614-0.0406 | 0.0708 | 0.7456-0.0784 | | | C(51) | 105 |
| >F(51) | | C(55) [] | 3.052(11) < | 3.17 | -0.12 | Intra | -0.1862 | 0.9329-0.2255 | -0.0803 | 0.9063-0.1478 | | | | |
| >F(51) | | C(57) [] | 3.334(11) | 3.17 | 0.16 | Intra | -0.1862 | 0.9329-0.2255 | 0.1585 | 0.9072-0.1842 | | | | |
| >F(51) | | >F(23) [3564.02] | 3.012(12) | 2.94 | 0.07 | | -0.1862 | 0.9329-0.2255 | 0.0351 | 1.0204-0.2560 | | | C(510) | 109.0(6) |
| >F(51) | | F(42) [4454.06] | 3.063(8) | 2.94 | 0.12 | | -0.1862 | 0.9329-0.2255 | -0.3129 | 1.0443-0.1956 | | | C(510) | 140.2(6) |
| >F(52) | | F(12) [] | 3.030(9) | 2.94 | 0.09 | | -0.2112 | 0.8489-0.2068 | -0.3273 | 0.7807-0.2713 | | | C(510) | 115.1(4) |
| >F(52) | | C(55) [] | 2.787(9)<< | 3.17 | -0.38 | Intra | -0.2112 | 0.8489-0.2068 | -0.0803 | 0.9063-0.1478 | | | | |

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>F(52)  ....  H(55A) [      ]      2.56 < 2.67 -0.11 Intra -0.2112 0.8489-0.2068 -0.1918 0.9014-0.1460
>F(52)  ....  F(64)  [ 3565.04]    2.828(9) < 2.94 -0.11      -0.2112 0.8489-0.2068 -0.2186 0.7887-0.1403  C(510)  123.7(5)
>F(52)  ....  <F(63) [ 3465.04]    3.077(15)  2.94  0.14      -0.2112 0.8489-0.2068 -0.5387 0.7919-0.2055  C(510)  157.7(6)
>F(53)  ....  C(57)  [      ]      2.745(8)<< 3.17 -0.43 Intra -0.0199 0.8702-0.2420  0.1585 0.9072-0.1842
>F(53)  ....  H(57A) [      ]      2.45<< 2.67 -0.22 Intra -0.0199 0.8702-0.2420  0.2102 0.9030-0.2071
>F(53)  ....  F(35)  [ 3564.01]    3.084(7)  2.94  0.14      -0.0199 0.8702-0.2420 -0.1585 0.8727-0.3199  C(510)  120.6(5)
>F(53)  ....  H(37A) [ 3564.01]    2.57 < 2.67 -0.10      -0.0199 0.8702-0.2420  0.1001 0.9176-0.2987  C(510)    134
>F(53)  ....  <F(62) [ 3565.04]    3.023(15)  2.94  0.08      -0.0199 0.8702-0.2420  0.2404 0.7852-0.2291  C(510)  119.4(5)
F(54)  ....  C(57)  [      ]      3.269(3)  3.17  0.10 Intra  0.4967 0.8785-0.1448  0.1585 0.9072-0.1842
F(54)  ....  C(59)  [      ]      3.108(3) < 3.17 -0.06 Intra  0.4967 0.8785-0.1448  0.1719 0.9261-0.1192
F(54)  ....  H(55A) [ 1655.03]    2.68  2.67  0.01      0.4967 0.8785-0.1448  0.8082 0.9014-0.1460  C(520)    107
F(54)  ....  C(65)  [ 3565.04]    3.131(3) < 3.17 -0.04      0.4967 0.8785-0.1448  0.3571 0.7571-0.1382  C(520)  128.00(15)
F(54)  ....  H(63A) [ 3565.04]    2.77  2.67  0.10      0.4967 0.8785-0.1448  0.5016 0.8315-0.0757  C(520)    127
F(54)  ....  H(65A) [ 3565.04]    2.81  2.67  0.14      0.4967 0.8785-0.1448  0.4690 0.7610-0.1399  C(520)    144
F(54)  ....  <F(63) [ 3565.04]    3.049(11)  2.94  0.11      0.4967 0.8785-0.1448  0.4613 0.7919-0.2055  C(520)  108.0(3)
F(55)  ....  C(57)  [      ]      2.745(3)<< 3.17 -0.43 Intra  0.4717 0.9380-0.1886  0.1585 0.9072-0.1842
F(55)  ....  H(57A) [      ]      2.45<< 2.67 -0.22 Intra  0.4717 0.9380-0.1886  0.2102 0.9030-0.2071
F(55)  ....  <F(52A) [ 1655.03]    3.003(10)  2.94  0.06      0.4717 0.9380-0.1886  0.7574 0.8699-0.2095  C(520)  111.7(3)
F(55)  ....  <F(32)  [ 3564.01]    3.011(8)  2.94  0.07      0.4717 0.9380-0.1886  0.3401 0.9189-0.2639  C(520)  134.0(2)
F(55)  ....  <F(32B) [ 3564.01]    2.984(8)  2.94  0.04      0.4717 0.9380-0.1886  0.3337 0.9469-0.2633  C(520)  137.5(3)
F(55)  ....  F(42)  [ 4554.06]    3.127(3)  2.94  0.19      0.4717 0.9380-0.1886  0.6871 1.0443-0.1956  C(520)  116.20(16)
F(56)  ....  C(53)  [ 1655.03]    3.262(3)  3.17  0.09      0.4768 0.9660-0.1335  0.7819 0.9527-0.0794  C(520)  124.65(15)
F(56)  ....  C(59)  [      ]      2.789(3)<< 3.17 -0.38 Intra  0.4768 0.9660-0.1335  0.1719 0.9261-0.1192
F(56)  ....  H(53A) [ 1655.03]    2.48 < 2.67 -0.19      0.4768 0.9660-0.1335  0.7269 0.9727-0.0979  C(520)    131
F(56)  ....  H(59A) [      ]      2.54 < 2.67 -0.13 Intra  0.4768 0.9660-0.1335  0.2324 0.9351-0.0981
F(56)  ....  C(44)  [ 4554.06]    3.303(3)  3.17  0.13      0.4768 0.9660-0.1335  0.4279 1.0960-0.1041  C(520)  145.82(15)
F(56)  ....  C(45)  [ 4554.06]    3.113(3) < 3.17 -0.06      0.4768 0.9660-0.1335  0.5300 1.0953-0.1338  C(520)  139.54(16)
F(56)  ....  C(46)  [ 4554.06]    3.177(3)  3.17  0.01      0.4768 0.9660-0.1335  0.4670 1.0878-0.1686  C(520)  113.95(15)
N(51)  ....  S(6)  [      ]      3.206(2) < 3.35 -0.14      -0.1497 0.9144-0.0274 -0.2154 0.8484 0.0473  C(51)  123.29(15)
                                           C(52)  122.05(16)
N(51)  ....  C(53)  [      ]      2.191(3)<< 3.25 -1.06 Intra -0.1497 0.9144-0.0274 -0.2181 0.9527-0.0794  H(51)    161(4)
N(52)  ....  C(52)  [      ]      2.215(3)<< 3.25 -1.04 Intra -0.0721 0.9252-0.0832 -0.2661 0.9455-0.0446  C(54)  158.70(16)
N(52)  ....  H(55A) [      ]      2.58 < 2.75 -0.17 Intra -0.0721 0.9252-0.0832 -0.1918 0.9014-0.1460  C(51)    142
N(52)  ....  H(59A) [      ]      2.64 < 2.75 -0.11 Intra -0.0721 0.9252-0.0832  0.2324 0.9351-0.0981  C(53)    147
C(51)  ....  C(53)  [      ]      2.263(3)<< 3.40 -1.14 Intra -0.0313 0.9008-0.0506 -0.2181 0.9527-0.0794  S(5)  164.34(15)
C(51)  ....  C(55)  [      ]      3.591(3)  3.40  0.19 Intra -0.0313 0.9008-0.0506 -0.0803 0.9063-0.1478  S(5)  109.12(11)
                                           N(51)  122.09(16)
C(51)  ....  C(59)  [      ]      3.103(3)<< 3.40 -0.30 Intra -0.0313 0.9008-0.0506  0.1719 0.9261-0.1192  N(51)  150.74(16)
C(51)  ....  H(59A) [      ]      2.94  2.90  0.04 Intra -0.0313 0.9008-0.0506  0.2324 0.9351-0.0981  N(51)    150
C(52)  ....  N(52)  [      ]      2.215(3)<< 3.25 -1.04 Intra -0.2661 0.9455-0.0446 -0.0721 0.9252-0.0832  H(52A)  164
C(52)  ....  C(54)  [      ]      3.578(3)  3.40  0.18 Intra -0.2661 0.9455-0.0446  0.0085 0.9190-0.1170  H(52A)  156
C(52)  ....  S(4)  [ 4454.06]    3.689(3)  3.50  0.19      -0.2661 0.9455-0.0446 -0.6654 1.0085-0.0402  N(51)  147.71(17)
                                           C(53)  105.33(17)
C(53)  ....  F(56)  [ 1455.03]    3.262(3)  3.17  0.09      -0.2181 0.9527-0.0794 -0.5232 0.9660-0.1335  N(52)  132.73(15)
                                           C(52)  110.48(17)
C(53)  ....  N(51)  [      ]      2.191(3)<< 3.25 -1.06 Intra -0.2181 0.9527-0.0794 -0.1497 0.9144-0.0274  H(53A)  163
C(53)  ....  C(55)  [      ]      2.976(3)<< 3.40 -0.42 Intra -0.2181 0.9527-0.0794 -0.0803 0.9063-0.1478  C(52)  150.1(2)
C(53)  ....  H(51)  [      ]      2.99(4)  2.90  0.09 Intra -0.2181 0.9527-0.0794 -0.1560 0.9009-0.0066  H(53A)  159
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C(53) .... H(55A) [ ] 2.74 < 2.90 -0.16 Intra -0.2181 0.9527-0.0794 -0.1918 0.9014-0.1460 C(52) 144
C(53) .... F(46) [ 4554.06] 3.236(3) 3.17 0.07 -0.2181 0.9527-0.0794 -0.0441 1.0578-0.1185 C(52) 130.74(18)
C(54) .... S(5) [ ] 3.284(2)<< 3.50 -0.22 Intra 0.0085 0.9190-0.1170 0.1298 0.8614-0.0406 C(55) 140.43(15)
C(54) .... C(52) [ ] 3.578(3) 3.40 0.18 Intra 0.0085 0.9190-0.1170 -0.2661 0.9455-0.0446 C(55) 107.03(16)
C(54) .....
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H(51)  ....  S(6)  [      ]  2.39(4)<< 3.00 -0.61      -0.1560 0.9009-0.0066 -0.2154 0.8484 0.0473  N(51)      167(5)
H(51)  ....  C(53) [      ]  2.99(4)   2.90  0.09 Intra -0.1560 0.9009-0.0066 -0.2181 0.9527-0.0794
H(51)  ....  H(52A) [      ]  2.44    2.40  0.04 Intra -0.1560 0.9009-0.0066 -0.3614 0.9592-0.0340
H(52A) ....  H(51)  [      ]  2.44    2.40  0.04 Intra -0.3614 0.9592-0.0340 -0.1560 0.9009-0.0066
H(52A) ....  H(53A) [      ]  2.48    2.40  0.08 Intra -0.3614 0.9592-0.0340 -0.2731 0.9727-0.0979
H(52A) ....  S(4)  [ 4454.06]  2.83 < 3.00 -0.17      -0.3614 0.9592-0.0340 -0.6654 1.0085-0.0402  C(52)      151
H(52A) ....  C(41) [ 4454.06]  2.94    2.90  0.04      -0.3614 0.9592-0.0340 -0.5418 1.0643-0.0399  C(52)      134
H(53A) ....  F(56) [ 1455.03]  2.48 < 2.67 -0.19      -0.2731 0.9727-0.0979 -0.5232 0.9660-0.1335  C(53)      139
H(53A) ....  C(54) [      ]  2.79 < 2.90 -0.11 Intra -0.2731 0.9727-0.0979  0.0085 0.9190-0.1170
H(53A) ....  C(55) [      ]  2.91    2.90  0.01 Intra -0.2731 0.9727-0.0979 -0.0803 0.9063-0.1478
H(53A) ....  H(52A) [      ]  2.48    2.40  0.08 Intra -0.2731 0.9727-0.0979 -0.3614 0.9592-0.0340
H(53A) ....  H(55A) [      ]  2.54    2.40  0.14 Intra -0.2731 0.9727-0.0979 -0.1918 0.9014-0.1460
H(55A) ....  >F(52) [      ]  2.56 < 2.67 -0.11 Intra -0.1918 0.9014-0.1460 -0.2112 0.8489-0.2068
H(55A) ....  F(54) [ 1455.03]  2.68    2.67  0.01      -0.1918 0.9014-0.1460 -0.5033 0.8785-0.1448  C(55)      174
H(55A) ....  N(52) [      ]  2.58 < 2.75 -0.17 Intra -0.1918 0.9014-0.1460 -0.0721 0.9252-0.0832
H(55A) ....  C(53) [      ]  2.74 < 2.90 -0.16 Intra -0.1918 0.9014-0.1460 -0.2181 0.9527-0.0794
H(55A) ....  C(510) [      ]  2.65<< 2.90 -0.25 Intra -0.1918 0.9014-0.1460 -0.1014 0.8884-0.2148
H(55A) ....  H(53A) [      ]  2.54    2.40  0.14 Intra -0.1918 0.9014-0.1460 -0.2731 0.9727-0.0979  C(55)      103
H(55A) ....  <F(52A) [      ]  2.48 < 2.67 -0.19 Intra -0.1918 0.9014-0.1460 -0.2426 0.8699-0.2095
H(55A) ....  F(64) [ 3565.04]  2.70    2.67  0.03      -0.1918 0.9014-0.1460 -0.2186 0.7887-0.1403  C(55)      102
H(57A) ....  >F(53) [      ]  2.45<< 2.67 -0.22 Intra  0.2102 0.9030-0.2071 -0.0199 0.8702-0.2420
H(57A) ....  F(55) [      ]  2.45<< 2.67 -0.22 Intra  0.2102 0.9030-0.2071  0.4717 0.9380-0.1886
H(57A) ....  C(510) [      ]  2.66<< 2.90 -0.24 Intra  0.2102 0.9030-0.2071 -0.1014 0.8884-0.2148
H(57A) ....  C(520) [      ]  2.66<< 2.90 -0.24 Intra  0.2102 0.9030-0.2071  0.4217 0.9256-0.1553
H(57A) ....  <F(53A) [      ]  2.59 < 2.67 -0.08 Intra  0.2102 0.9030-0.2071 -0.0246 0.8481-0.2355
H(57A) ....  >F(62A) [ 3565.04]  2.66 < 2.67 -0.01      0.2102 0.9030-0.2071  0.3325 0.8031-0.2234  C(57)      118
H(57A) ....  <F(31A) [ 3564.01]  2.73    2.67  0.06      0.2102 0.9030-0.2071  0.3710 0.8900-0.2711  C(57)      177
H(57A) ....  <F(32)  [ 3564.01]  2.38<< 2.67 -0.29      0.2102 0.9030-0.2071  0.3401 0.9189-0.2639  C(57)      165
H(57A) ....  <F(32B) [ 3564.01]  2.53 < 2.67 -0.14      0.2102 0.9030-0.2071  0.3337 0.9469-0.2633  C(57)      150
H(59A) ....  S(5)  [      ]  2.88 < 3.00 -0.12 Intra  0.2324 0.9351-0.0981  0.1298 0.8614-0.0406  C(59)      107
H(59A) ....  F(56) [      ]  2.54 < 2.67 -0.13 Intra  0.2324 0.9351-0.0981  0.4768 0.9660-0.1335
H(59A) ....  N(52) [      ]  2.64 < 2.75 -0.11 Intra  0.2324 0.9351-0.0981 -0.0721 0.9252-0.0832
H(59A) ....  C(51) [      ]  2.94    2.90  0.04 Intra  0.2324 0.9351-0.0981 -0.0313 0.9008-0.0506
H(59A) ....  C(520) [      ]  2.65<< 2.90 -0.25 Intra  0.2324 0.9351-0.0981  0.4217 0.9256-0.1553
H(59A) ....  S(4)  [ 4554.06]  2.88 < 3.00 -0.12      0.2324 0.9351-0.0981  0.3346 1.0085-0.0402  C(59)      154
<F(51A) ....  C(55) [      ]  3.353(8)  3.17  0.18 Intra -0.1050 0.9324-0.2375 -0.0803 0.9063-0.1478
<F(51A) ....  C(57) [      ]  3.019(14) < 3.17 -0.15 Intra -0.1050 0.9324-0.2375  0.1585 0.9072-0.1842
<F(51A) ....  >F(23) [ 3564.02]  2.499(13)<< 2.94 -0.44      -0.1050 0.9324-0.2375  0.0351 1.0204-0.2560  C(510)     144.5(9)
<F(51A) ....  H(37A) [ 3564.01]  2.85    2.67  0.18      -0.1050 0.9324-0.2375  0.1001 0.9176-0.2987  C(510)     112
<F(52A) ....  F(55) [ 1455.03]  3.003(10)  2.94  0.06      -0.2426 0.8699-0.2095 -0.5283 0.9380-0.1886  C(510)     126.7(8)
<F(52A) ....  C(55) [      ]  2.782(11)<< 3.17 -0.39 Intra -0.2426 0.8699-0.2095 -0.0803 0.9063-0.1478
<F(52A) ....  H(55A) [      ]  2.48 < 2.67 -0.19 Intra -0.2426 0.8699-0.2095 -0.1918 0.9014-0.1460
<F(53A) ....  F(11) [      ]  3.057(12)  2.94  0.12      -0.0246 0.8481-0.2355 -0.1503 0.7289-0.2463  C(510)     123.6(6)
<F(53A) ....  C(57) [      ]  2.811(11)<< 3.17 -0.36 Intra -0.0246 0.8481-0.2355  0.1585 0.9072-0.1842
<F(53A) ....  H(57A) [      ]  2.59 < 2.67 -0.08 Intra -0.0246 0.8481-0.2355  0.2102 0.9030-0.2071
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Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 3 to Neighbouring ARU'S

| Nr | ARU | Nr.Cont. | d(min) | Del | XHn X | - At(I) | At(J) | - Y | YHn | Note | Partaking ARU's in Close Contact | Resd. |
|----|------------|----------|--------|-------|----------|--------------|---------|---------|-----|------|----------------------------------|-------|
| 1 | [1555.04] | 4 | 2.3900 | -0.61 | 1 N(51) | - H(51) ... | S(6) | -C(61) | 0 | << | 1555.04 | |
| 2 | [3565.04] | 14 | 2.6600 | -0.01 | 1 C(57) | - H(57A) ... | *F(62A) | -C(610) | 0 | < | 3565.04 | |
| 3 | [3564.02] | 2 | 2.4990 | -0.44 | 0 C(510) | -*F(51A) ... | *F(23) | -C(210) | 0 | << | 3564.02 | |
| 4 | [4454.06] | 4 | 2.8300 | -0.17 | 1 C(52) | - H(52A) ... | S(4) | -C(41) | 0 | < | 4454.06 | |
| 5 | [1555.05] | 2 | 3.0300 | 0.09 | 0 C(510) | -*F(52) ... | F(12) | -C(110) | 0 | | 1555.05 | |
| 6 | [3465.04] | 1 | 3.0770 | 0.14 | 0 C(510) | -*F(52) ... | *F(63) | -C(610) | 0 | | 3465.04 | |
| 7 | [3564.01] | 9 | 2.3800 | -0.29 | 1 C(57) | - H(57A) ... | *F(32) | -C(310) | 0 | << | 3564.01 | |
| 8 | [1655.03] | 4 | 2.4800 | -0.19 | 0 C(520) | - F(56) ... | H(53A) | -C(53) | 1 | < | 1655.03 | |
| 9 | [4554.06] | 10 | 2.8800 | -0.12 | 1 C(59) | - H(59A) ... | S(4) | -C(41) | 0 | < | 4554.06 | |
| 10 | [1455.03] | 4 | 2.4800 | -0.19 | 1 C(53) | - H(53A) ... | F(56) | -C(520) | 0 | < | 1455.03 | |

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

 ***** ARU = 1555.04 *****

| At(I)[1555.04] | At(J) | [ARU(J)] | D(I-J) | SumRad | Del | Type | X(I) | Y(I) | Z(I) | X(J) | Y(J) | Z(J) | X | X - I...J |
|----------------|-------|--------------------|-----------|---------|-------|-------|---------|--------|--------|---------|--------|---------|--------|-----------|
| S(6) | | N(51) [] | 3.206(2) | < 3.35 | -0.14 | | -0.2154 | 0.8484 | 0.0473 | -0.1497 | 0.9144 | -0.0274 | C(61) | 109.23(9) |
| S(6) | | C(64) [] | 3.209(2) | << 3.50 | -0.29 | Intra | -0.2154 | 0.8484 | 0.0473 | -0.2159 | 0.7465 | 0.1045 | | |
| S(6) | | C(69) [] | 3.341(3) | < 3.50 | -0.16 | Intra | -0.2154 | 0.8484 | 0.0473 | -0.3796 | 0.7520 | 0.1016 | | |
| S(6) | | H(51) [] | 2.39(4) | << 3.00 | -0.61 | | -0.2154 | 0.8484 | 0.0473 | -0.1560 | 0.9009 | -0.0066 | C(61) | 109.8(11) |
| S(6) | | H(61) [] | 2.89(3) | < 3.00 | -0.11 | Intra | -0.2154 | 0.8484 | 0.0473 | 0.0200 | 0.7901 | 0.0043 | | |
| S(6) | | H(69A) [] | 3.09 | 3.00 | 0.09 | Intra | -0.2154 | 0.8484 | 0.0473 | -0.4292 | 0.7544 | 0.0784 | | |
| S(6) | | H(62A) [3465.04] | 2.93 | < 3.00 | -0.07 | | -0.2154 | 0.8484 | 0.0473 | -0.3697 | 0.8030 | -0.0180 | | |
| S(6) | | S(2) [4454.02] | 3.7777(9) | 3.60 | 0.18 | | -0.2154 | 0.8484 | 0.0473 | -0.3577 | 0.9982 | 0.0563 | C(61) | 167.21(9) |
| S(6) | | C(29) [4454.02] | 3.468(2) | < 3.50 | -0.03 | | -0.2154 | 0.8484 | 0.0473 | -0.3152 | 0.9172 | 0.1275 | C(61) | 122.32(9) |
| S(6) | | H(29A) [4454.02] | 2.65 | << 3.00 | -0.35 | | -0.2154 | 0.8484 | 0.0473 | -0.2597 | 0.9139 | 0.1050 | C(61) | 126 |
| >F(61A) | | C(67) [] | 2.857(7) | << 3.17 | -0.31 | Intra | -0.2127 | 0.7830 | 0.2291 | -0.3989 | 0.7507 | 0.1675 | | |
| >F(61A) | | H(67A) [] | 2.66 | < 2.67 | -0.01 | Intra | -0.2127 | 0.7830 | 0.2291 | -0.4615 | 0.7523 | 0.1890 | | |
| >F(61A) | | F(14) [3465.05] | 3.064(6) | 2.94 | 0.12 | | -0.2127 | 0.7830 | 0.2291 | -0.1556 | 0.7382 | 0.3064 | C(610) | 105.6(4) |
| >F(61A) | | H(17A) [3465.05] | 2.81 | 2.67 | 0.14 | | -0.2127 | 0.7830 | 0.2291 | -0.4241 | 0.7544 | 0.2853 | C(610) | 120 |
| >F(62A) | | C(65) [] | 3.317(6) | 3.17 | 0.15 | Intra | -0.1675 | 0.6969 | 0.2234 | -0.1429 | 0.7429 | 0.1382 | | |
| >F(62A) | | C(67) [] | 3.106(8) | < 3.17 | -0.06 | Intra | -0.1675 | 0.6969 | 0.2234 | -0.3989 | 0.7507 | 0.1675 | | |
| >F(62A) | | <F(31A) [1556.01] | 2.73(2) | << 2.94 | -0.21 | | -0.1675 | 0.6969 | 0.2234 | -0.1290 | 0.6100 | 0.2711 | C(610) | 164.5(7) |

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>F(62A) .... C(57) [ 3465.03] 3.218(6) 3.17 0.05 -0.1675 0.6969 0.2234 -0.3415 0.5928 0.1842 C(610) 119.0(4)
>F(62A) .... H(57A) [ 3465.03] 2.66 < 2.67 -0.01 -0.1675 0.6969 0.2234 -0.2898 0.5970 0.2071 C(610) 134
>F(63A) .... C(65) [ ] 2.744(4)<< 3.17 -0.43 Intra -0.0002 0.7564 0.2049 -0.1429 0.7429 0.1382
>F(63A) .... H(65A) [ ] 2.43<< 2.67 -0.24 Intra -0.0002 0.7564 0.2049 -0.0310 0.7390 0.1399
>F(63A) .... F(12) [ 3565.05] 2.972(4) 2.94 0.03 -0.0002 0.7564 0.2049 0.1727 0.7193 0.2713 C(610) 111.8(3)
F(64) .... C(67) [ ] 3.024(4) < 3.17 -0.15 Intra -0.7186 0.7113 0.1403 -0.3989 0.7507 0.1675
F(64) .... C(69) [ ] 3.335(4) 3.17 0.16 Intra -0.7186 0.7113 0.1403 -0.3796 0.7520 0.1016
F(64) .... H(65A) [ 1455.04] 2.72 2.67 0.05 -0.7186 0.7113 0.1403 -1.0310 0.7390 0.1399 C(620) 103
F(64) .... >F(52) [ 3465.03] 2.828(9) < 2.94 -0.11 -0.7186 0.7113 0.1403 -0.7112 0.6511 0.2068 C(620) 130.2(3)
F(64) .... C(55) [ 3465.03] 3.045(3) < 3.17 -0.13 -0.7186 0.7113 0.1403 -0.5803 0.5937 0.1478 C(620) 129.3(2)
F(64) .... H(55A) [ 3465.03] 2.70 2.67 0.03 -0.7186 0.7113 0.1403 -0.6918 0.5986 0.1460 C(620) 146
F(65) .... C(69) [ ] 2.730(3)<< 3.17 -0.44 Intra -0.6980 0.7719 0.0974 -0.3796 0.7520 0.1016
F(65) .... H(69A) [ ] 2.41<< 2.67 -0.26 Intra -0.6980 0.7719 0.0974 -0.4292 0.7544 0.0784
F(65) .... C(23) [ 4454.02] 3.143(3) < 3.17 -0.03 -0.6980 0.7719 0.0974 -0.7096 0.9031 0.0889 C(620) 109.89(19)
F(65) .... H(23A) [ 4454.02] 2.68 2.67 0.01 -0.6980 0.7719 0.0974 -0.7661 0.8811 0.1061 C(620) 101
F(66) .... C(67) [ ] 2.862(4)<< 3.17 -0.31 Intra -0.7033 0.7989 0.1529 -0.3989 0.7507 0.1675
F(66) .... H(67A) [ ] 2.67 2.67 0.00 Intra -0.7033 0.7989 0.1529 -0.4615 0.7523 0.1890
F(66) .... F(25) [ 4354.02] 3.075(3) 2.94 0.13 -0.7033 0.7989 0.1529 -1.0188 0.8598 0.1384 C(620) 122.6(2)
F(66) .... C(25) [ 4454.02] 3.365(3) 3.17 0.19 -0.7033 0.7989 0.1529 -0.5602 0.9302 0.1608 C(620) 126.6(2)
F(66) .... H(23A) [ 4454.02] 2.66 < 2.67 -0.01 -0.7033 0.7989 0.1529 -0.7661 0.8811 0.1061 C(620) 102
N(61) .... S(5) [ ] 3.370(2) 3.35 0.02 -0.0074 0.7699 0.0220 0.1298 0.8614-0.0406 C(61) 119.56(15)
C(62) .... S(5) [ ] 3.370(2) 3.35 0.02 -0.0074 0.7699 0.0220 0.1298 0.8614-0.0406 C(62) 128.29(17)
N(61) .... C(63) [ ] 2.195(3)<< 3.25 -1.06 Intra -0.0074 0.7699 0.0220 -0.0166 0.7023 0.0627 H(61) 163(2)
N(62) .... C(62) [ ] 2.204(3)<< 3.25 -1.05 Intra -0.1209 0.7452 0.0724 0.0535 0.7178 0.0313 C(64) 161.17(17)
N(62) .... H(65A) [ ] 2.59 < 2.75 -0.16 Intra -0.1209 0.7452 0.0724 -0.0310 0.7390 0.1399 C(61) 133
N(62) .... H(69A) [ ] 2.62 < 2.75 -0.13 Intra -0.1209 0.7452 0.0724 -0.4292 0.7544 0.0784 C(63) 135
N(62) .... S(5) [ 3465.03] 3.495(2) 3.35 0.14 -0.1209 0.7452 0.0724 -0.3702 0.6386 0.0406 C(61) 109.45(13)
C(61) .... C(63) [ ] 2.256(4)<< 3.40 -1.14 Intra -0.1136 0.7873 0.0471 -0.0166 0.7023 0.0627 S(6) 162.81(15)
C(61) .... C(65) [ ] 3.514(3) 3.40 0.11 Intra -0.1136 0.7873 0.0471 -0.1429 0.7429 0.1382 S(6) 102.59(10)
C(61) .... C(65) [ ] 3.514(3) 3.40 0.11 Intra -0.1136 0.7873 0.0471 -0.1429 0.7429 0.1382 N(61) 127.07(16)
C(61) .... C(69) [ ] 3.121(3)<< 3.40 -0.28 Intra -0.1136 0.7873 0.0471 -0.3796 0.7520 0.1016 N(61) 146.24(17)
C(61) .... H(69A) [ ] 3.00 2.90 0.10 Intra -0.1136 0.7873 0.0471 -0.4292 0.7544 0.0784 N(61) 140
C(62) .... N(62) [ ] 2.204(3)<< 3.25 -1.05 Intra 0.0535 0.7178 0.0313 -0.1209 0.7452 0.0724 H(62A) 164
C(62) .... C(64) [ ] 3.583(4) 3.40 0.18 Intra 0.0535 0.7178 0.0313 -0.2159 0.7465 0.1045 H(62A) 156
C(63) .... N(61) [ ] 2.195(3)<< 3.25 -1.06 Intra -0.0166 0.7023 0.0627 -0.0074 0.7699 0.0220 H(63A) 163
C(63) .... C(65) [ ] 3.122(3)<< 3.40 -0.28 Intra -0.0166 0.7023 0.0627 -0.1429 0.7429 0.1382 C(62) 145.5(2)
C(63) .... C(69) [ ] 3.579(4) 3.40 0.18 Intra -0.0166 0.7023 0.0627 -0.3796 0.7520 0.1016 C(62) 128.83(18)
C(63) .... C(69) [ ] 3.579(4) 3.40 0.18 Intra -0.0166 0.7023 0.0627 -0.3796 0.7520 0.1016 H(63A) 103
C(63) .... H(61) [ ] 3.01(3) 2.90 0.11 Intra -0.0166 0.7023 0.0627 0.0200 0.7901 0.0043 H(63A) 159
C(63) .... H(65A) [ ] 2.97 2.90 0.07 Intra -0.0166 0.7023 0.0627 -0.0310 0.7390 0.1399 C(62) 139
C(63) .... S(5) [ 3465.03] 3.441(3) < 3.50 -0.06 -0.0166 0.7023 0.0627 -0.3702 0.6386 0.0406 C(62) 107.49(17)
C(64) .... S(6) [ ] 3.209(2)<< 3.50 -0.29 Intra -0.2159 0.7465 0.1045 -0.2154 0.8484 0.0473 C(65) 129.02(15)
C(64) .... C(62) [ ] 3.583(4) 3.40 0.18 Intra -0.2159 0.7465 0.1045 0.0535 0.7178 0.0313 C(65) 112.07(17)
C(64) .... C(62) [ ] 3.583(4) 3.40 0.18 Intra -0.2159 0.7465 0.1045 0.0535 0.7178 0.0313 C(69) 126.14(16)
C(64) .... C(67) [ ] 2.779(3)<< 3.40 -0.62 Intra -0.2159 0.7465 0.1045 -0.3989 0.7507 0.1675 N(62) 179.03(16)
C(64) .... H(63A) [ ] 2.82 < 2.90 -0.08 Intra -0.2159 0.7465 0.1045 0.0016 0.6685 0.0757 C(69) 133
C(65) .... >F(62A) [ ] 3.317(6) 3.17 0.15 Intra -0.1429 0.7429 0.1382 -0.1675 0.6969 0.2234 C(64) 146.5(2)
C(65) .... >F(63A) [ ] 2.744(4)<< 3.17 -0.43 Intra -0.1429 0.7429 0.1382 -0.0002 0.7564 0.2049 C(64) 169.8(2)
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C(65)  ....  C(61)  [      ]  3.514(3)  3.40  0.11  Intra  -0.1429  0.7429  0.1382  -0.1136  0.7873  0.0471  C(66)  144.54(17)
C(65)  ....  C(63)  [      ]  3.122(3)<< 3.40 -0.28  Intra  -0.1429  0.7429  0.1382  -0.0166  0.7023  0.0627  C(66)  159.62(18)
C(65)  ....  C(68)  [      ]  2.766(4)<< 3.40 -0.63  Intra  -0.1429  0.7429  0.1382  -0.4689  0.7539  0.1334  H(65A)   180
C(65)  .... <F(61) [      ]  3.163(11) < 3.17 -0.01  Intra  -0.1429  0.7429  0.1382  -0.1310  0.7884  0.2192  C(64)  146.3(3)
C(65)  .... <F(63) [      ]  2.746(8)<< 3.17 -0.42  Intra  -0.1429  0.7429  0.1382  -0.0387  0.7081  0.2055  C(64)  164.4(3)
C(65)  ....  F(54)  [ 3465.03]  3.131(3) < 3.17 -0.04        -0.1429  0.7429  0.1382  -0.0033  0.6215  0.1448  C(64)  106.99(15)
                                           C(66)  100.55(15)

C(65)  ....  F(25)  [ 4454.02]  2.974(3) < 3.17 -0.20        -0.1429  0.7429  0.1382  -0.0188  0.8598  0.1384
C(66)  ....  C(69)  [      ]  2.776(3)<< 3.40 -0.62  Intra  -0.2353  0.7452  0.1696  -0.3796  0.7520  0.1016  C(610)  178.6(2)
C(67)  .... >F(61A) [      ]  2.857(7)<< 3.17 -0.31  Intra  -0.3989  0.7507  0.1675  -0.2127  0.7830  0.2291  C(68)  159.0(2)
C(67)  .... >F(62A) [      ]  3.106(8) < 3.17 -0.06  Intra  -0.3989  0.7507  0.1675  -0.1675  0.6969  0.2234  C(68)  152.4(2)
C(67)  ....  F(64)  [      ]  3.024(4) < 3.17 -0.15  Intra  -0.3989  0.7507  0.1675  -0.7186  0.7113  0.1403  C(66)  150.97(19)
C(67)  ....  F(66)  [      ]  2.862(4)<< 3.17 -0.31  Intra  -0.3989  0.7507  0.1675  -0.7033  0.7989  0.1529  C(66)  160.0(2)
C(67)  ....  C(64)  [      ]  2.779(3)<< 3.40 -0.62  Intra  -0.3989  0.7507  0.1675  -0.2159  0.7465  0.1045  H(67A)   180
C(67)  .... <F(61) [      ]  3.082(14) < 3.17 -0.09  Intra  -0.3989  0.7507  0.1675  -0.1310  0.7884  0.2192  C(68)  148.4(3)
C(67)  .... <F(62) [      ]  2.685(9)<< 3.17 -0.49  Intra  -0.3989  0.7507  0.1675  -0.2596  0.7148  0.2291  C(68)  164.4(3)
C(68)  ....  C(65)  [      ]  2.766(4)<< 3.40 -0.63  Intra  -0.4689  0.7539  0.1334  -0.1429  0.7429  0.1382  C(620)  178.57(19)
C(69)  ....  S(6)  [      ]  3.341(3) < 3.50 -0.16  Intra  -0.3796  0.7520  0.1016  -0.2154  0.8484  0.0473  C(68)  134.62(16)
C(69)  ....  F(64)  [      ]  3.335(4)  3.17  0.16  Intra  -0.3796  0.7520  0.1016  -0.7186  0.7113  0.1403  C(64)  142.24(18)
C(69)  ....  F(65)  [      ]  2.730(3)<< 3.17 -0.44  Intra  -0.3796  0.7520  0.1016  -0.6980  0.7719  0.0974  C(64)  175.29(18)
C(69)  ....  C(61)  [      ]  3.121(3)<< 3.40 -0.28  Intra  -0.3796  0.7520  0.1016  -0.1136  0.7873  0.0471  C(68)  156.79(18)
C(69)  ....  C(63)  [      ]  3.579(4)  3.40  0.18  Intra  -0.3796  0.7520  0.1016  -0.0166  0.7023  0.0627  C(68)  144.11(18)
C(69)  ....  C(66)  [      ]  2.776(3)<< 3.40 -0.62  Intra  -0.3796  0.7520  0.1016  -0.2353  0.7452  0.1696  H(69A)   180
C(69)  ....  S(5)  [ 3465.03]  3.508(3)  3.50  0.01        -0.3796  0.7520  0.1016  -0.3702  0.6386  0.0406  C(68)  124.99(16)
C(610)  .... H(65A) [      ]  2.66<< 2.90 -0.24  Intra  -0.1558  0.7430  0.2064  -0.0310  0.7390  0.1399 >F(61A)  137
                                           >F(62A)  117
                                           <F(61)   109
                                           <F(62)   142

C(610)  .... H(67A) [      ]  2.66<< 2.90 -0.24  Intra  -0.1558  0.7430  0.2064  -0.4615  0.7523  0.1890 >F(63A)  155
                                           <F(61)   101
                                           <F(63)   142

C(620)  .... H(67A) [      ]  2.65<< 2.90 -0.25  Intra  -0.6477  0.7584  0.1310  -0.4615  0.7523  0.1890  F(65)   160
C(620)  .... H(69A) [      ]  2.67<< 2.90 -0.23  Intra  -0.6477  0.7584  0.1310  -0.4292  0.7544  0.0784  F(64)   118
                                           F(66)   134

H(61)  ....  S(5)  [      ]  2.54(3)<< 3.00 -0.46        0.0200  0.7901  0.0043  0.1298  0.8614-0.0406  N(61)  170(3)
H(61)  ....  S(6)  [      ]  2.89(3) < 3.00 -0.11  Intra  0.0200  0.7901  0.0043  -0.2154  0.8484  0.0473
H(61)  ....  C(63)  [      ]  3.01(3)  2.90  0.11  Intra  0.0200  0.7901  0.0043  -0.0166  0.7023  0.0627
H(61)  .... H(62A) [      ]  2.46  2.40  0.06  Intra  0.0200  0.7901  0.0043  0.1303  0.6970  0.0180
H(62A)  .... H(61) [      ]  2.46  2.40  0.06  Intra  0.1303  0.6970  0.0180  0.0200  0.7901  0.0043
H(62A)  .... H(63A) [      ]  2.47  2.40  0.07  Intra  0.1303  0.6970  0.0180  0.0016  0.6685  0.0757
H(62A)  ....  S(6)  [ 3565.04]  2.93 < 3.00 -0.07        0.1303  0.6970  0.0180  0.2846  0.6516-0.0473  C(62)  156
H(63A)  ....  C(64)  [      ]  2.82 < 2.90 -0.08  Intra  0.0016  0.6685  0.0757  -0.2159  0.7465  0.1045
H(63A)  .... H(62A) [      ]  2.47  2.40  0.07  Intra  0.0016  0.6685  0.0757  0.1303  0.6970  0.0180
H(63A)  ....  F(54)  [ 3465.03]  2.77  2.67  0.10        0.0016  0.6685  0.0757  -0.0033  0.6215  0.1448  C(63)  143
H(65A)  .... >F(63A) [      ]  2.43<< 2.67 -0.24  Intra  -0.0310  0.7390  0.1399  -0.0002  0.7564  0.2049
H(65A)  ....  F(64)  [ 1655.04]  2.72  2.67  0.05        -0.0310  0.7390  0.1399  0.2814  0.7113  0.1403  C(65)  171
H(65A)  ....  N(62)  [      ]  2.59 < 2.75 -0.16  Intra  -0.0310  0.7390  0.1399  -0.1209  0.7452  0.0724
H(65A)  ....  C(63)  [      ]  2.97  2.90  0.07  Intra  -0.0310  0.7390  0.1399  -0.0166  0.7023  0.0627
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H(65A) .... C(610) [      ]      2.66<< 2.90 -0.24 Intra -0.0310 0.7390 0.1399 -0.1558 0.7430 0.2064
H(65A) .... <F(63) [      ]      2.52 < 2.67 -0.15 Intra -0.0310 0.7390 0.1399 -0.0387 0.7081 0.2055
H(65A) .... F(54) [ 3465.03]      2.81  2.67  0.14      -0.0310 0.7390 0.1399 -0.0033 0.6215 0.1448 C(65)      101
H(67A) .... >F(61A) [      ]      2.66 < 2.67 -0.01 Intra -0.4615 0.7523 0.1890 -0.2127 0.7830 0.2291
H(67A) .... F(66) [      ]      2.67  2.67  0.00 Intra -0.4615 0.7523 0.1890 -0.7033 0.7989 0.1529
H(67A) .... C(610) [      ]      2.66<< 2.90 -0.24 Intra -0.4615 0.7523 0.1890 -0.1558 0.7430 0.2064
H(67A) .... C(620) [      ]      2.65<< 2.90 -0.25 Intra -0.4615 0.7523 0.1890 -0.6477 0.7584 0.1310
H(67A) .... <F(62) [      ]      2.42<< 2.67 -0.25 Intra -0.4615 0.7523 0.1890 -0.2596 0.7148 0.2291
H(67A) .... F(11) [ 3465.05]      2.67  2.67  0.00      -0.4615 0.7523 0.1890 -0.6503 0.7711 0.2463 C(67)      172
H(69A) .... S(6) [      ]      3.09  3.00  0.09 Intra -0.4292 0.7544 0.0784 -0.2154 0.8484 0.0473
H(69A) .... F(65) [      ]      2.41<< 2.67 -0.26 Intra -0.4292 0.7544 0.0784 -0.6980 0.7719 0.0974
H(69A) .... N(62) [      ]      2.62 < 2.75 -0.13 Intra -0.4292 0.7544 0.0784 -0.1209 0.7452 0.0724
H(69A) .... C(61) [      ]      3.00  2.90  0.10 Intra -0.4292 0.7544 0.0784 -0.1136 0.7873 0.0471
H(69A) .... C(620) [      ]      2.67<< 2.90 -0.23 Intra -0.4292 0.7544 0.0784 -0.6477 0.7584 0.1310
H(69A) .... S(5) [ 3465.03]      3.13  3.00  0.13      -0.4292 0.7544 0.0784 -0.3702 0.6386 0.0406 C(69)      106
<F(61) .... C(65) [      ]      3.163(11) < 3.17 -0.01 Intra -0.1310 0.7884 0.2192 -0.1429 0.7429 0.1382
<F(61) .... C(67) [      ]      3.082(14) < 3.17 -0.09 Intra -0.1310 0.7884 0.2192 -0.3989 0.7507 0.1675
<F(61) .... F(24) [ 4454.02]      2.996(10)  2.94  0.06      -0.1310 0.7884 0.2192  0.0061 0.8964 0.1916 C(610)    135.3(7)
<F(62) .... C(67) [      ]      2.685(9)<< 3.17 -0.49 Intra -0.2596 0.7148 0.2291 -0.3989 0.7507 0.1675
<F(62) .... H(67A) [      ]      2.42<< 2.67 -0.25 Intra -0.2596 0.7148 0.2291 -0.4615 0.7523 0.1890
<F(62) .... F(14) [ 3465.05]      3.017(8)  2.94  0.08      -0.2596 0.7148 0.2291 -0.1556 0.7382 0.3064 C(610)    106.9(5)
<F(62) .... >F(53) [ 3465.03]      3.023(15)  2.94  0.08      -0.2596 0.7148 0.2291 -0.5199 0.6298 0.2420 C(610)    151.7(5)
<F(62) .... H(17A) [ 3465.05]      2.66 < 2.67 -0.01      -0.2596 0.7148 0.2291 -0.4241 0.7544 0.2853 C(610)    129
<F(63) .... C(65) [      ]      2.746(8)<< 3.17 -0.42 Intra -0.0387 0.7081 0.2055 -0.1429 0.7429 0.1382
<F(63) .... H(65A) [      ]      2.52 < 2.67 -0.15 Intra -0.0387 0.7081 0.2055 -0.0310 0.7390 0.1399
<F(63) .... F(12) [ 3565.05]      3.012(8)  2.94  0.07      -0.0387 0.7081 0.2055  0.1727 0.7193 0.2713 C(610)    112.0(5)
<F(63) .... >F(52) [ 3565.03]      3.077(15)  2.94  0.14      -0.0387 0.7081 0.2055  0.2888 0.6511 0.2068 C(610)    165.9(8)
<F(63) .... F(54) [ 3465.03]      3.049(11)  2.94  0.11      -0.0387 0.7081 0.2055 -0.0033 0.6215 0.1448 C(610)    122.0(5)
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Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 4 to Neighbouring ARU'S

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=====
Nr      ARU      Nr.Cont.  d(min)  Del  XHn X      - At(I)      At(J) - Y  YHn Note  Partaking ARU's in Close Contact Resd.
-----
1 [ 1555.03]      4      2.3900 -0.61  0 C(61) - S(6) ... H(51) -N(51)  1 << 1555.03
2 [ 3465.04]      1      2.9300 -0.07  0 C(61) - S(6) ... H(62A) -C(62)  1 < 3465.04
3 [ 4454.02]      9      2.6500 -0.35  0 C(61) - S(6) ... H(29A) -C(29)  1 << 4454.02
4 [ 3465.05]      5      2.6600 -0.01  0 C(610) -*F(62) ... H(17A) -C(17)  1 < 3465.05
5 [ 1556.01]      1      2.7300 -0.21  0 C(610) -*F(62A) ... *F(31A) -C(310)  0 << 1556.01
6 [ 3465.03]     14      2.6600 -0.01  0 C(610) -*F(62A) ... H(57A) -C(57)  1 < 3465.03
7 [ 3565.05]      2      2.9720  0.03  0 C(610) -*F(63A) ... F(12) -C(110)  0      3565.05
8 [ 1455.04]      1      2.7200  0.05  0 C(620) - F(64) ... H(65A) -C(65)  1      1455.04
9 [ 4354.02]      1      3.0750  0.13  0 C(620) - F(66) ... F(25) -C(220)  0      4354.02
10 [ 3565.04]      1      2.9300 -0.07  1 C(62) - H(62A) ... S(6) -C(61)  0 < 3565.04
11 [ 1655.04]      1      2.7200  0.05  1 C(65) - H(65A) ... F(64) -C(620)  0      1655.04
12 [ 3565.03]      1      3.0770  0.14  0 C(610) -*F(63) ... *F(52) -C(510)  0      3565.03
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Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

***** ARU = 1555.05 *****

Table with columns: At(I)[1555.05], At(J), [ARU(J)], D(I-J), SumRad, Del, Type, X(I), Y(I), Z(I), X(J), Y(J), Z(J), X, X - I...J. Rows include contact details for atoms S(1), F(11), F(12), and F(13) with various neighbor types and distances.

| | | | | | | | | | | | | | |
|-------|------|--------------------|--|------------|------|-------|-------|---------|---------------|---------|---------------|--------|------------|
| F(14) | | H(17A) [] | | 2.42<< | 2.67 | -0.25 | Intra | 0.3444 | 0.7618-0.3064 | 0.0759 | 0.7456-0.2853 | | |
| F(14) | | >F(61A) [3565.04] | | 3.064(6) | 2.94 | 0.12 | | 0.3444 | 0.7618-0.3064 | 0.2873 | 0.7170-0.2292 | C(120) | 141.1(2) |
| F(14) | | <F(62) [3565.04] | | 3.017(8) | 2.94 | 0.08 | | 0.3444 | 0.7618-0.3064 | 0.2404 | 0.7852-0.2291 | C(120) | 140.1(2) |
| F(15) | | F(41) [1655.06] | | 3.008(3) | 2.94 | 0.07 | | 0.3574 | 0.7154-0.3563 | 0.3401 | 0.6321-0.2947 | | |
| F(15) | | C(19) [] | | 2.961(2)<< | 3.17 | -0.21 | Intra | 0.3574 | 0.7154-0.3563 | 0.0333 | 0.7545-0.3742 | | |
| F(15) | | C(45) [1655.06] | | 3.035(3) < | 3.17 | -0.13 | | 0.3574 | 0.7154-0.3563 | 0.4700 | 0.5953-0.3662 | C(120) | 157.18(15) |
| F(15) | | H(15A) [1655.05] | | 2.70 | 2.67 | 0.03 | | 0.3574 | 0.7154-0.3563 | 0.6706 | 0.7326-0.3449 | C(120) | 105 |
| F(15) | | H(43A) [1655.06] | | 2.87 | 2.67 | 0.20 | | 0.3574 | 0.7154-0.3563 | 0.3475 | 0.6681-0.4282 | C(120) | 135 |
| F(15) | | H(45A) [1655.06] | | 2.79 | 2.67 | 0.12 | | 0.3574 | 0.7154-0.3563 | 0.3590 | 0.5999-0.3696 | C(120) | 147 |
| F(16) | | C(19) [] | | 2.871(2)<< | 3.17 | -0.30 | Intra | 0.3353 | 0.8044-0.3580 | 0.0333 | 0.7545-0.3742 | | |
| F(16) | | H(13A) [1655.05] | | 2.60 < | 2.67 | -0.07 | | 0.3353 | 0.8044-0.3580 | 0.5872 | 0.7970-0.3985 | C(120) | 119 |
| F(16) | | H(19A) [] | | 2.69 | 2.67 | 0.02 | Intra | 0.3353 | 0.8044-0.3580 | 0.0924 | 0.7606-0.3959 | | |
| F(16) | | C(34) [3564.01] | | 3.124(3) < | 3.17 | -0.05 | | 0.3353 | 0.8044-0.3580 | 0.2764 | 0.9229-0.3919 | C(120) | 151.32(15) |
| F(16) | | C(35) [3564.01] | | 2.990(3) < | 3.17 | -0.18 | | 0.3353 | 0.8044-0.3580 | 0.3738 | 0.9290-0.3617 | C(120) | 148.93(15) |
| F(16) | | C(36) [3564.01] | | 3.153(3) < | 3.17 | -0.02 | | 0.3353 | 0.8044-0.3580 | 0.3069 | 0.9274-0.3269 | C(120) | 122.89(14) |
| N(11) | | S(3) [] | | 3.284(2) < | 3.35 | -0.07 | | -0.2811 | 0.7314-0.4656 | -0.3034 | 0.6716-0.5461 | C(11) | 123.58(13) |
| | | | | | | | | | | | | C(12) | 124.60(14) |
| N(11) | | C(13) [] | | 2.194(3)<< | 3.25 | -1.06 | Intra | -0.2811 | 0.7314-0.4656 | -0.3557 | 0.7751-0.4158 | H(11) | 161(2) |
| N(12) | | C(12) [] | | 2.212(3)<< | 3.25 | -1.04 | Intra | -0.2109 | 0.7477-0.4098 | -0.3987 | 0.7646-0.4504 | C(14) | 159.38(16) |
| N(12) | | H(15A) [] | | 2.60 < | 2.75 | -0.15 | Intra | -0.2109 | 0.7477-0.4098 | -0.3294 | 0.7326-0.3449 | C(11) | 143 |
| N(12) | | H(19A) [] | | 2.63 < | 2.75 | -0.12 | Intra | -0.2109 | 0.7477-0.4098 | 0.0924 | 0.7606-0.3959 | C(13) | 145 |
| C(11) | | C(13) [] | | 2.266(3)<< | 3.40 | -1.13 | Intra | -0.1661 | 0.7200-0.4410 | -0.3557 | 0.7751-0.4158 | S(1) | 163.68(12) |
| C(11) | | C(19) [] | | 3.083(3)<< | 3.40 | -0.32 | Intra | -0.1661 | 0.7200-0.4410 | 0.0333 | 0.7545-0.3742 | N(11) | 150.17(16) |
| C(11) | | H(19A) [] | | 2.90 | 2.90 | 0.00 | Intra | -0.1661 | 0.7200-0.4410 | 0.0924 | 0.7606-0.3959 | N(11) | 148 |
| C(12) | | N(12) [] | | 2.212(3)<< | 3.25 | -1.04 | Intra | -0.3987 | 0.7646-0.4504 | -0.2109 | 0.7477-0.4098 | H(12A) | 164 |
| C(12) | | C(14) [] | | 3.585(3) | 3.40 | 0.18 | Intra | -0.3987 | 0.7646-0.4504 | -0.1304 | 0.7466-0.3755 | H(12A) | 156 |
| C(12) | | C(43) [] | | 3.480(3) | 3.40 | 0.08 | | -0.3987 | 0.7646-0.4504 | -0.6074 | 0.6392-0.4427 | C(13) | 102.61(16) |
| C(13) | | N(11) [] | | 2.194(3)<< | 3.25 | -1.06 | Intra | -0.3557 | 0.7751-0.4158 | -0.2811 | 0.7314-0.4656 | H(13A) | 164 |
| C(13) | | C(15) [] | | 3.012(3)<< | 3.40 | -0.39 | Intra | -0.3557 | 0.7751-0.4158 | -0.2181 | 0.7386-0.3438 | C(12) | 151.53(18) |
| C(13) | | H(11) [] | | 3.00(3) | 2.90 | 0.10 | Intra | -0.3557 | 0.7751-0.4158 | -0.2840 | 0.7169-0.4863 | H(13A) | 158 |
| C(13) | | H(15A) [] | | 2.80 < | 2.90 | -0.10 | Intra | -0.3557 | 0.7751-0.4158 | -0.3294 | 0.7326-0.3449 | C(12) | 146 |
| C(13) | | F(34) [3564.01] | | 3.230(3) | 3.17 | 0.06 | | -0.3557 | 0.7751-0.4158 | -0.1960 | 0.8832-0.3773 | C(12) | 132.27(17) |
| C(14) | | S(1) [] | | 3.273(2)<< | 3.50 | -0.23 | Intra | -0.1304 | 0.7466-0.3755 | -0.0037 | 0.6795-0.4477 | C(15) | 141.54(15) |
| C(14) | | C(12) [] | | 3.585(3) | 3.40 | 0.18 | Intra | -0.1304 | 0.7466-0.3755 | -0.3987 | 0.7646-0.4504 | C(15) | 108.78(16) |
| | | | | | | | | | | | | C(19) | 129.33(13) |
| C(14) | | C(17) [] | | 2.786(3)<< | 3.40 | -0.61 | Intra | -0.1304 | 0.7466-0.3755 | 0.0231 | 0.7460-0.3082 | N(12) | 179.04(16) |
| C(14) | | H(13A) [] | | 2.80 < | 2.90 | -0.10 | Intra | -0.1304 | 0.7466-0.3755 | -0.4128 | 0.7970-0.3985 | C(19) | 143 |
| C(14) | | F(34) [3564.01] | | 3.299(3) | 3.17 | 0.13 | | -0.1304 | 0.7466-0.3755 | -0.1960 | 0.8832-0.3773 | | |
| C(15) | | F(12) [] | | 2.986(3) < | 3.17 | -0.18 | Intra | -0.2181 | 0.7386-0.3438 | -0.3273 | 0.7807-0.2713 | C(14) | 149.49(16) |
| C(15) | | F(13) [] | | 2.863(3)<< | 3.17 | -0.31 | Intra | -0.2181 | 0.7386-0.3438 | -0.3386 | 0.6914-0.2775 | C(14) | 162.14(17) |
| C(15) | | C(13) [] | | 3.012(3)<< | 3.40 | -0.39 | Intra | -0.2181 | 0.7386-0.3438 | -0.3557 | 0.7751-0.4158 | C(16) | 161.79(16) |
| C(15) | | C(18) [] | | 2.771(3)<< | 3.40 | -0.63 | Intra | -0.2181 | 0.7386-0.3438 | 0.1077 | 0.7532-0.3404 | H(15A) | 179 |
| C(15) | | H(13A) [] | | 2.94 | 2.90 | 0.04 | Intra | -0.2181 | 0.7386-0.3438 | -0.4128 | 0.7970-0.3985 | C(16) | 149 |
| C(15) | | F(35) [3564.01] | | 3.350(3) | 3.17 | 0.18 | | -0.2181 | 0.7386-0.3438 | -0.1585 | 0.8727-0.3199 | H(15A) | 108 |
| C(16) | | C(19) [] | | 2.786(3)<< | 3.40 | -0.61 | Intra | -0.1403 | 0.7395-0.3103 | 0.0333 | 0.7545-0.3742 | C(110) | 176.48(17) |
| C(16) | | F(35) [3564.01] | | 3.195(3) | 3.17 | 0.02 | | -0.1403 | 0.7395-0.3103 | -0.1585 | 0.8727-0.3199 | | |
| C(17) | | F(11) [] | | 2.730(3)<< | 3.17 | -0.44 | Intra | 0.0231 | 0.7460-0.3082 | -0.1503 | 0.7289-0.2463 | C(18) | 177.69(17) |
| C(17) | | F(12) [] | | 3.352(3) | 3.17 | 0.18 | Intra | 0.0231 | 0.7460-0.3082 | -0.3273 | 0.7807-0.2713 | C(18) | 139.83(15) |

| | | | | | | | | | | | | | | |
|--------|------|---------|------------|------------|------|-------|-------|---------|---------------|---------------|---------------|---------------|------------|-----|
| ===== | | | | | | | | | | | | | | |
| C(17) | | F(14) | [] | 2.735(3)<< | 3.17 | -0.44 | Intra | 0.0231 | 0.7460-0.3082 | 0.3444 | 0.7618-0.3064 | C(16) | 177.65(16) | |
| C(17) | | F(44) | [] | 3.194(3) | 3.17 | 0.02 | | 0.0231 | 0.7460-0.3082 | 0.0407 | 0.6212-0.3397 | H(17A) | 107 | |
| C(17) | | C(14) | [] | 2.786(3)<< | 3.40 | -0.61 | Intra | 0.0231 | 0.7460-0.3082 | -0.1304 | 0.7466-0.3755 | H(17A) | 180 | |
| C(18) | | F(44) | [] | 3.195(3) | 3.17 | 0.02 | | 0.1077 | 0.7532-0.3404 | 0.0407 | 0.6212-0.3397 | C(120) | 105.57(13) | |
| C(18) | | C(15) | [] | 2.771(3)<< | 3.40 | -0.63 | Intra | 0.1077 | 0.7532-0.3404 | -0.2181 | 0.7386-0.3438 | C(120) | 177.68(16) | |
| C(19) | | S(1) | [] | 3.249(2)<< | 3.50 | -0.25 | Intra | 0.0333 | 0.7545-0.3742 | -0.0037 | 0.6795-0.4477 | C(18) | 140.45(14) | |
| C(19) | | F(15) | [] | 2.961(2)<< | 3.17 | -0.21 | Intra | 0.0333 | 0.7545-0.3742 | 0.3574 | 0.7154-0.3563 | C(14) | 151.47(15) | |
| C(19) | | F(16) | [] | 2.871(2)<< | 3.17 | -0.30 | Intra | 0.0333 | 0.7545-0.3742 | 0.3353 | 0.8044-0.3580 | C(14) | 160.17(15) | |
| C(19) | | C(11) | [] | 3.083(3)<< | 3.40 | -0.32 | Intra | 0.0333 | 0.7545-0.3742 | -0.1661 | 0.7200-0.4410 | C(18) | 161.64(16) | |
| C(19) | | C(16) | [] | 2.786(3)<< | 3.40 | -0.61 | Intra | 0.0333 | 0.7545-0.3742 | -0.1403 | 0.7395-0.3103 | H(19A) | 179 | |
| C(19) | | S(3) | [3564.01] | 3.678(2) | 3.50 | 0.18 | | 0.0333 | 0.7545-0.3742 | 0.1966 | 0.8284-0.4539 | C(14) | 114.15(12) | |
| | | | | | | | | | | | | C(18) | 123.39(12) | |
| C(110) | | H(15A) | [] | 2.63<< | 2.90 | -0.27 | Intra | -0.2386 | 0.7349-0.2763 | -0.3294 | 0.7326-0.3449 | F(11) | 161 | |
| C(110) | | H(17A) | [] | 2.68<< | 2.90 | -0.22 | Intra | -0.2386 | 0.7349-0.2763 | 0.0759 | 0.7456-0.2853 | F(12) | 119 | |
| | | | | | | | | | | | | F(13) | 134 | |
| C(120) | | H(17A) | [] | 2.68<< | 2.90 | -0.22 | Intra | 0.2853 | 0.7592-0.3397 | 0.0759 | 0.7456-0.2853 | F(15) | 123 | |
| | | | | | | | | | | | | F(16) | 133 | |
| C(120) | | H(19A) | [] | 2.63<< | 2.90 | -0.27 | Intra | 0.2853 | 0.7592-0.3397 | 0.0924 | 0.7606-0.3959 | F(14) | 164 | |
| H(11) | | S(1) | [] | 2.89(3) | < | 3.00 | -0.11 | Intra | -0.2840 | 0.7169-0.4863 | -0.0037 | 0.6795-0.4477 | | |
| H(11) | | S(3) | [] | 2.45(3)<< | 3.00 | -0.55 | | -0.2840 | 0.7169-0.4863 | -0.3034 | 0.6716-0.5461 | N(11) | 177(4) | |
| H(11) | | C(13) | [] | 3.00(3) | 2.90 | 0.10 | Intra | -0.2840 | 0.7169-0.4863 | -0.3557 | 0.7751-0.4158 | | | |
| H(11) | | H(12A) | [] | 2.44 | 2.40 | 0.04 | Intra | -0.2840 | 0.7169-0.4863 | -0.4921 | 0.7776-0.4623 | | | |
| H(12A) | | H(11) | [] | 2.44 | 2.40 | 0.04 | Intra | -0.4921 | 0.7776-0.4623 | -0.2840 | 0.7169-0.4863 | | | |
| H(12A) | | H(13A) | [] | 2.48 | 2.40 | 0.08 | Intra | -0.4921 | 0.7776-0.4623 | -0.4128 | 0.7970-0.3985 | | | |
| H(12A) | | S(3) | [3464.01] | 2.91 | < | 3.00 | -0.09 | | -0.4921 | 0.7776-0.4623 | -0.8034 | 0.8284-0.4539 | C(12) | 147 |
| H(12A) | | C(31) | [3464.01] | 3.04 | 2.90 | 0.14 | | -0.4921 | 0.7776-0.4623 | -0.6831 | 0.8853-0.4547 | C(12) | 132 | |
| H(13A) | | F(16) | [1455.05] | 2.60 | < | 2.67 | -0.07 | | -0.4128 | 0.7970-0.3985 | -0.6647 | 0.8044-0.3580 | C(13) | 146 |
| H(13A) | | C(14) | [] | 2.80 | < | 2.90 | -0.10 | Intra | -0.4128 | 0.7970-0.3985 | -0.1304 | 0.7466-0.3755 | | |
| H(13A) | | C(15) | [] | 2.94 | 2.90 | 0.04 | Intra | -0.4128 | 0.7970-0.3985 | -0.2181 | 0.7386-0.3438 | | | |
| H(13A) | | H(12A) | [] | 2.48 | 2.40 | 0.08 | Intra | -0.4128 | 0.7970-0.3985 | -0.4921 | 0.7776-0.4623 | | | |
| H(13A) | | H(15A) | [] | 2.59 | 2.40 | 0.19 | Intra | -0.4128 | 0.7970-0.3985 | -0.3294 | 0.7326-0.3449 | | | |
| H(13A) | | F(34) | [3564.01] | 2.86 | 2.67 | 0.19 | | -0.4128 | 0.7970-0.3985 | -0.1960 | 0.8832-0.3773 | C(13) | 105 | |
| H(15A) | | F(13) | [] | 2.66 | < | 2.67 | -0.01 | Intra | -0.3294 | 0.7326-0.3449 | -0.3386 | 0.6914-0.2775 | | |
| H(15A) | | F(15) | [1455.05] | 2.70 | 2.67 | 0.03 | | -0.3294 | 0.7326-0.3449 | -0.6426 | 0.7154-0.3563 | C(15) | 174 | |
| H(15A) | | N(12) | [] | 2.60 | < | 2.75 | -0.15 | Intra | -0.3294 | 0.7326-0.3449 | -0.2109 | 0.7477-0.4098 | | |
| H(15A) | | C(13) | [] | 2.80 | < | 2.90 | -0.10 | Intra | -0.3294 | 0.7326-0.3449 | -0.3557 | 0.7751-0.4158 | | |
| H(15A) | | C(110) | [] | 2.63<< | 2.90 | -0.27 | Intra | -0.3294 | 0.7326-0.3449 | -0.2386 | 0.7349-0.2763 | | | |
| H(15A) | | H(13A) | [] | 2.59 | 2.40 | 0.19 | Intra | -0.3294 | 0.7326-0.3449 | -0.4128 | 0.7970-0.3985 | C(15) | 102 | |
| H(17A) | | F(11) | [] | 2.42<< | 2.67 | -0.25 | Intra | 0.0759 | 0.7456-0.2853 | -0.1503 | 0.7289-0.2463 | | | |
| H(17A) | | F(14) | [] | 2.42<< | 2.67 | -0.25 | Intra | 0.0759 | 0.7456-0.2853 | 0.3444 | 0.7618-0.3064 | | | |
| H(17A) | | C(110) | [] | 2.68<< | 2.90 | -0.22 | Intra | 0.0759 | 0.7456-0.2853 | -0.2386 | 0.7349-0.2763 | | | |
| H(17A) | | C(120) | [] | 2.68<< | 2.90 | -0.22 | Intra | 0.0759 | 0.7456-0.2853 | 0.2853 | 0.7592-0.3397 | | | |
| H(17A) | | >F(61A) | [3565.04] | 2.81 | 2.67 | 0.14 | | 0.0759 | 0.7456-0.2853 | 0.2873 | 0.7170-0.2292 | C(17) | 161 | |
| H(17A) | | <F(62) | [3565.04] | 2.66 | < | 2.67 | -0.01 | | 0.0759 | 0.7456-0.2853 | 0.2404 | 0.7852-0.2291 | C(17) | 158 |
| H(19A) | | S(1) | [] | 2.83 | < | 3.00 | -0.17 | Intra | 0.0924 | 0.7606-0.3959 | -0.0037 | 0.6795-0.4477 | C(19) | 108 |
| H(19A) | | F(16) | [] | 2.69 | 2.67 | 0.02 | Intra | 0.0924 | 0.7606-0.3959 | 0.3353 | 0.8044-0.3580 | | | |
| H(19A) | | N(12) | [] | 2.63 | < | 2.75 | -0.12 | Intra | 0.0924 | 0.7606-0.3959 | -0.2109 | 0.7477-0.4098 | | |
| H(19A) | | C(11) | [] | 2.90 | 2.90 | 0.00 | Intra | 0.0924 | 0.7606-0.3959 | -0.1661 | 0.7200-0.4410 | | | |


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H(19A) .... C(120) [          ]      2.63<< 2.90 -0.27 Intra  0.0924 0.7606-0.3959  0.2853 0.7592-0.3397
H(19A) .... S(3)  [ 3564.01]      2.81 < 3.00 -0.19      0.0924 0.7606-0.3959  0.1966 0.8284-0.4539  C(19)      152
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Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 5 to Neighbouring ARU'S

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=====
Nr      ARU      Nr.Cont.  d(min)  Del  XHn X      - At(I)      At(J) - Y  YHn Note  Partaking ARU's in Close Contact Resd.
-----
1 [ 1555.01]      4      2.4500 -0.55   1 N(11) - H(11) ... S(3) -C(31)  0 << 1555.01
2 [ 1655.06]      9      2.7900  0.12   0 C(120) - F(15) ... H(45A) -C(45)  1      1655.06
3 [ 1555.06]      9      2.9500 -0.05   0 C(11) - S(1) ... H(49A) -C(49)  1 < 1555.06
4 [ 1555.03]      2      3.0300  0.09   0 C(110) - F(12) ... *F(52) -C(510)  0      1555.03
5 [ 2465.02]      2      3.0870  0.15   0 C(110) - F(13) ... *F(22A) -C(210)  0      2465.02
6 [ 3565.04]      5      2.6600 -0.01   1 C(17) - H(17A) ... *F(62) -C(610)  0 < 3565.04
7 [ 1455.05]      3      2.6000 -0.07   1 C(13) - H(13A) ... F(16) -C(120)  0 < 1455.05
8 [ 3465.04]      2      2.9720  0.03   0 C(110) - F(12) ... *F(63A) -C(610)  0      3465.04
9 [ 3464.01]      4      2.9100 -0.09   1 C(12) - H(12A) ... S(3) -C(31)  0 < 3464.01
10 [ 1655.05]      3      2.6000 -0.07   0 C(120) - F(16) ... H(13A) -C(13)  1 < 1655.05
11 [ 3564.01]     10      2.8100 -0.19   1 C(19) - H(19A) ... S(3) -C(31)  0 < 3564.01
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Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

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***** ARU = 1555.06 *****
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At(I)[1555.06] At(J) [ ARU(J) ]      D(I-J) SumRad Del Type  X(I)  Y(I)  Z(I)  X(J)  Y(J)  Z(J)  X      X - I...J
-----
S(4) .... N(21) [          ]      3.260(2) < 3.35 -0.09      -0.3346 0.5085-0.4598 -0.3619 0.4478-0.5393  C(41)      107.54(9)
S(4) .... C(44) [          ]      3.234(2)<< 3.50 -0.27 Intra -0.3346 0.5085-0.4598 -0.4279 0.5960-0.3959
S(4) .... C(49) [          ]      3.223(2)<< 3.50 -0.28 Intra -0.3346 0.5085-0.4598 -0.2645 0.5901-0.3916
S(4) .... H(21) [          ]      2.43(3)<< 3.00 -0.57      -0.3346 0.5085-0.4598 -0.3550 0.4623-0.5187  C(41)      108.0(8)
S(4) .... H(41) [          ]      2.92(3) < 3.00 -0.08 Intra -0.3346 0.5085-0.4598 -0.5570 0.5647-0.5089
S(4) .... H(49A) [          ]      2.89 < 3.00 -0.11 Intra -0.3346 0.5085-0.4598 -0.1954 0.5917-0.4120
S(4) .... C(52) [ 4444.03]      3.689(3)  3.50  0.19      -0.3346 0.5085-0.4598 -0.7339 0.4455-0.4554
S(4) .... H(52A) [ 4444.03]      2.83 < 3.00 -0.17      -0.3346 0.5085-0.4598 -0.6386 0.4592-0.4660
S(4) .... H(59A) [ 4544.03]      2.88 < 3.00 -0.12      -0.3346 0.5085-0.4598 -0.2324 0.4351-0.4019  C(41)      132
F(41) .... F(13) [          ]      3.120(2)  2.94  0.18      -0.6599 0.6321-0.2947 -0.3386 0.6914-0.2775
F(41) .... F(14) [ 1455.05]      3.119(3)  2.94  0.18      -0.6599 0.6321-0.2947 -0.6556 0.7618-0.3064  C(410)     144.65(15)
F(41) .... F(15) [ 1455.05]      3.008(3)  2.94  0.07      -0.6599 0.6321-0.2947 -0.6426 0.7154-0.3563  C(410)     115.86(14)
F(41) .... F(44) [ 1455.06]      3.027(2)  2.94  0.09      -0.6599 0.6321-0.2947 -0.9593 0.6212-0.3397  C(410)     106.57(14)
F(41) .... C(45) [          ]      2.974(3) < 3.17 -0.20 Intra -0.6599 0.6321-0.2947 -0.5300 0.5953-0.3662
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| | | | | | | | | | | | | | |
|-------|------|---------|------------|-----------|---------|-------|-------|---------|---------------|---------|---------------|--------|------------|
| F(41) | | H(45A) | [] | 2.86 | 2.67 | 0.19 | Intra | -0.6599 | 0.6321-0.2947 | -0.6410 | 0.5999-0.3696 | | |
| F(42) | | F(45) | [1455.06] | 2.766(2) | < 2.94 | -0.17 | | -0.6871 | 0.5443-0.3044 | -1.0004 | 0.5349-0.3259 | C(410) | 138.67(16) |
| F(42) | | C(45) | [] | 2.893(3) | << 3.17 | -0.28 | Intra | -0.6871 | 0.5443-0.3044 | -0.5300 | 0.5953-0.3662 | | |
| F(42) | | H(45A) | [] | 2.76 | 2.67 | 0.09 | Intra | -0.6871 | 0.5443-0.3044 | -0.6410 | 0.5999-0.3696 | | |
| F(42) | | >F(51) | [4444.03] | 3.063(8) | 2.94 | 0.12 | | -0.6871 | 0.5443-0.3044 | -0.8138 | 0.4329-0.2745 | C(410) | 144.1(3) |
| F(42) | | F(55) | [4544.03] | 3.127(3) | 2.94 | 0.19 | | -0.6871 | 0.5443-0.3044 | -0.4717 | 0.4380-0.3114 | C(410) | 101.11(15) |
| F(43) | | C(47) | [] | 2.713(3) | << 3.17 | -0.46 | Intra | -0.5045 | 0.5733-0.2683 | -0.3052 | 0.5806-0.3262 | | |
| F(43) | | H(47A) | [] | 2.39 | << 2.67 | -0.28 | Intra | -0.5045 | 0.5733-0.2683 | -0.2632 | 0.5750-0.3025 | | |
| F(43) | | >F(21) | [2465.02] | 2.870(7) | < 2.94 | -0.07 | | -0.5045 | 0.5733-0.2683 | -0.2168 | 0.5760-0.2265 | C(410) | 148.3(3) |
| F(43) | | F(24) | [2365.02] | 2.905(2) | < 2.94 | -0.04 | | -0.5045 | 0.5733-0.2683 | -0.4939 | 0.6036-0.1916 | C(410) | 142.86(18) |
| F(43) | | <F(22A) | [2465.02] | 3.073(11) | 2.94 | 0.13 | | -0.5045 | 0.5733-0.2683 | -0.2010 | 0.6016-0.2257 | C(410) | 141.6(3) |
| F(43) | | <F(32A) | [2465.01] | 2.98(2) | 2.94 | 0.04 | | -0.5045 | 0.5733-0.2683 | -0.3700 | 0.4794-0.2242 | C(410) | 142.7(5) |
| F(44) | | F(41) | [1655.06] | 3.027(2) | 2.94 | 0.09 | | 0.0407 | 0.6212-0.3397 | 0.3401 | 0.6321-0.2947 | C(420) | 127.85(14) |
| F(44) | | C(17) | [] | 3.194(3) | 3.17 | 0.02 | | 0.0407 | 0.6212-0.3397 | 0.0231 | 0.7460-0.3082 | C(420) | 150.71(15) |
| F(44) | | C(18) | [] | 3.195(3) | 3.17 | 0.02 | | 0.0407 | 0.6212-0.3397 | 0.1077 | 0.7532-0.3404 | C(420) | 154.51(15) |
| F(44) | | C(47) | [] | 3.112(3) | < 3.17 | -0.06 | Intra | 0.0407 | 0.6212-0.3397 | -0.3052 | 0.5806-0.3262 | | |
| F(44) | | C(49) | [] | 3.285(3) | 3.17 | 0.12 | Intra | 0.0407 | 0.6212-0.3397 | -0.2645 | 0.5901-0.3916 | | |
| F(44) | | <F(23A) | [2465.02] | 3.119(15) | 2.94 | 0.18 | | 0.0407 | 0.6212-0.3397 | 0.0117 | 0.5969-0.2564 | | |
| F(45) | | F(42) | [1655.06] | 2.766(2) | < 2.94 | -0.17 | | -0.0004 | 0.5349-0.3259 | 0.3129 | 0.5443-0.3044 | C(420) | 108.58(14) |
| F(45) | | C(47) | [] | 2.790(3) | << 3.17 | -0.38 | Intra | -0.0004 | 0.5349-0.3259 | -0.3052 | 0.5806-0.3262 | | |
| F(45) | | H(47A) | [] | 2.56 | < 2.67 | -0.11 | Intra | -0.0004 | 0.5349-0.3259 | -0.2632 | 0.5750-0.3025 | | |
| F(45) | | >F(23) | [2465.02] | 3.036(7) | 2.94 | 0.10 | | -0.0004 | 0.5349-0.3259 | -0.0351 | 0.5204-0.2440 | C(420) | 137.9(2) |
| F(45) | | <F(23A) | [2465.02] | 2.947(17) | 2.94 | 0.01 | | -0.0004 | 0.5349-0.3259 | 0.0117 | 0.5969-0.2564 | C(420) | 104.5(4) |
| F(45) | | C(55) | [4544.03] | 3.282(3) | 3.17 | 0.11 | | -0.0004 | 0.5349-0.3259 | 0.0803 | 0.4063-0.3522 | C(420) | 119.41(13) |
| F(45) | | C(56) | [4544.03] | 3.204(3) | 3.17 | 0.03 | | -0.0004 | 0.5349-0.3259 | 0.0048 | 0.4009-0.3186 | C(420) | 139.34(14) |
| F(45) | | C(57) | [4544.03] | 3.342(3) | 3.17 | 0.17 | | -0.0004 | 0.5349-0.3259 | -0.1585 | 0.4072-0.3158 | C(420) | 129.77(14) |
| F(46) | | C(49) | [] | 2.738(2) | << 3.17 | -0.43 | Intra | 0.0441 | 0.5578-0.3815 | -0.2645 | 0.5901-0.3916 | | |
| F(46) | | H(49A) | [] | 2.45 | << 2.67 | -0.22 | Intra | 0.0441 | 0.5578-0.3815 | -0.1954 | 0.5917-0.4120 | | |
| F(46) | | C(53) | [4544.03] | 3.236(3) | 3.17 | 0.07 | | 0.0441 | 0.5578-0.3815 | 0.2181 | 0.4527-0.4206 | C(420) | 143.75(15) |
| F(46) | | C(54) | [4544.03] | 3.334(3) | 3.17 | 0.16 | | 0.0441 | 0.5578-0.3815 | -0.0085 | 0.4190-0.3830 | C(420) | 103.89(14) |
| N(41) | | S(2) | [] | 3.291(2) | < 3.35 | -0.06 | | -0.5517 | 0.5818-0.4879 | -0.6423 | 0.4982-0.5563 | C(41) | 121.60(14) |
| | | | | | | | | | | | | C(42) | 123.60(13) |
| N(41) | | C(43) | [] | 2.199(3) | << 3.25 | -1.05 | Intra | -0.5517 | 0.5818-0.4879 | -0.6074 | 0.6392-0.4427 | H(41) | 161(2) |
| N(42) | | C(42) | [] | 2.202(3) | << 3.25 | -1.05 | Intra | -0.4915 | 0.6008-0.4319 | -0.6430 | 0.6274-0.4776 | C(44) | 160.82(15) |
| N(42) | | H(45A) | [] | 2.61 | < 2.75 | -0.14 | Intra | -0.4915 | 0.6008-0.4319 | -0.6410 | 0.5999-0.3696 | C(41) | 139 |
| N(42) | | H(49A) | [] | 2.61 | < 2.75 | -0.14 | Intra | -0.4915 | 0.6008-0.4319 | -0.1954 | 0.5917-0.4120 | C(43) | 143 |
| C(41) | | C(43) | [] | 2.272(3) | << 3.40 | -1.13 | Intra | -0.4582 | 0.5643-0.4601 | -0.6074 | 0.6392-0.4427 | S(4) | 163.23(14) |
| C(41) | | C(45) | [] | 3.570(3) | 3.40 | 0.17 | Intra | -0.4582 | 0.5643-0.4601 | -0.5300 | 0.5953-0.3662 | S(4) | 105.21(10) |
| | | | | | | | | | | | | N(41) | 124.38(13) |
| C(41) | | C(49) | [] | 3.057(3) | << 3.40 | -0.34 | Intra | -0.4582 | 0.5643-0.4601 | -0.2645 | 0.5901-0.3916 | N(41) | 150.24(16) |
| C(41) | | H(49A) | [] | 2.90 | 2.90 | 0.00 | Intra | -0.4582 | 0.5643-0.4601 | -0.1954 | 0.5917-0.4120 | N(41) | 146 |
| C(41) | | H(52A) | [4444.03] | 2.94 | 2.90 | 0.04 | | -0.4582 | 0.5643-0.4601 | -0.6386 | 0.4592-0.4660 | N(42) | 119 |
| C(42) | | S(1) | [1455.05] | 3.463(3) | < 3.50 | -0.04 | | -0.6430 | 0.6274-0.4776 | -1.0037 | 0.6795-0.4477 | N(41) | 148.93(16) |
| C(42) | | N(42) | [] | 2.202(3) | << 3.25 | -1.05 | Intra | -0.6430 | 0.6274-0.4776 | -0.4915 | 0.6008-0.4319 | H(42A) | 164 |
| C(42) | | C(44) | [] | 3.583(3) | 3.40 | 0.18 | Intra | -0.6430 | 0.6274-0.4776 | -0.4279 | 0.5960-0.3959 | H(42A) | 156 |
| C(43) | | S(1) | [1455.05] | 3.482(3) | < 3.50 | -0.02 | | -0.6074 | 0.6392-0.4427 | -1.0037 | 0.6795-0.4477 | N(42) | 150.17(15) |
| C(43) | | N(41) | [] | 2.199(3) | << 3.25 | -1.05 | Intra | -0.6074 | 0.6392-0.4427 | -0.5517 | 0.5818-0.4879 | H(43A) | 163 |
| C(43) | | C(12) | [] | 3.480(3) | 3.40 | 0.08 | | -0.6074 | 0.6392-0.4427 | -0.3987 | 0.7646-0.4504 | N(42) | 103.40(15) |

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C(42) 102.41(16)
C(43) .... C(45) [ ] 3.063(3)<< 3.40 -0.34 Intra -0.6074 0.6392-0.4427 -0.5300 0.5953-0.3662 C(42) 148.01(18)
C(43) .... H(41) [ ] 3.04(3) 2.90 0.14 Intra -0.6074 0.6392-0.4427 -0.5570 0.5647-0.5089 H(43A) 158
C(43) .... H(45A) [ ] 2.85 < 2.90 -0.05 Intra -0.6074 0.6392-0.4427 -0.6410 0.5999-0.3696 C(42) 144
C(44) .... S(4) [ ] 3.234(2)<< 3.50 -0.27 Intra -0.4279 0.5960-0.3959 -0.3346 0.5085-0.4598 C(45) 135.41(15)
C(44) .... C(42) [ ] 3.583(3) 3.40 0.18 Intra -0.4279 0.5960-0.3959 -0.6430 0.6274-0.4776 C(45) 110.13(14)
C(44) .... C(47) [ ] 2.780(3)<< 3.40 -0.62 Intra -0.4279 0.5960-0.3959 -0.3052 0.5806-0.3262 C(49) 128.01(15)
C(44) .... H(43A) [ ] 2.82 < 2.90 -0.08 Intra -0.4279 0.5960-0.3959 -0.6525 0.6681-0.4282 N(42) 177.04(16)
C(44) .... F(56) [ 4544.03] 3.303(3) 3.17 0.13 -0.4279 0.5960-0.3959 -0.4768 0.4660-0.3665 C(49) 141
C(45) .... F(15) [ 1455.05] 3.035(3) < 3.17 -0.13 -0.5300 0.5953-0.3662 -0.6426 0.7154-0.3563 N(42) 109.20(13)
C(45) .... F(41) [ ] 2.974(3) < 3.17 -0.20 Intra -0.5300 0.5953-0.3662 -0.6426 0.7154-0.3563 C(44) 106.14(14)
C(45) .... F(42) [ ] 2.893(3)<< 3.17 -0.28 Intra -0.5300 0.5953-0.3662 -0.6599 0.6321-0.2947 C(44) 156.43(16)
C(45) .... C(41) [ ] 2.893(3)<< 3.17 -0.28 Intra -0.5300 0.5953-0.3662 -0.6871 0.5443-0.3044 C(44) 154.59(16)
C(45) .... C(43) [ ] 3.570(3) 3.40 0.17 Intra -0.5300 0.5953-0.3662 -0.4582 0.5643-0.4601 C(46) 142.34(17)
C(45) .... C(48) [ ] 3.063(3)<< 3.40 -0.34 Intra -0.5300 0.5953-0.3662 -0.6074 0.6392-0.4427 C(46) 164.39(17)
C(45) .... H(43A) [ ] 2.780(4)<< 3.40 -0.62 Intra -0.5300 0.5953-0.3662 -0.2052 0.5818-0.3566 H(45A) 180
C(45) .... F(56) [ 4544.03] 3.04 2.90 0.14 Intra -0.5300 0.5953-0.3662 -0.6525 0.6681-0.4282 C(46) 152
C(45) .... F(13) [ ] 3.113(3) < 3.17 -0.06 -0.5300 0.5953-0.3662 -0.4768 0.4660-0.3665 C(46) 152
C(46) .... C(49) [ ] 3.342(3) 3.17 0.17 -0.4670 0.5878-0.3314 -0.6525 0.6681-0.4282 H(45A) 105
C(46) .... F(56) [ 4544.03] 3.177(3) 3.17 0.01 -0.4670 0.5878-0.3314 -0.3386 0.6914-0.2775 C(45) 124.83(15)
C(47) .... F(13) [ ] 2.791(3)<< 3.40 -0.61 Intra -0.4670 0.5878-0.3314 -0.2645 0.5901-0.3916 C(410) 177.84(17)
C(47) .... F(43) [ ] 3.200(3) 3.17 0.03 -0.4670 0.5878-0.3314 -0.4768 0.4660-0.3665 C(410) 104.57(15)
C(47) .... F(44) [ ] 3.177(3) 3.17 0.01 -0.4670 0.5878-0.3314 -0.4768 0.4660-0.3665 C(48) 118.80(15)
C(47) .... F(45) [ ] 2.713(3)<< 3.17 -0.46 Intra -0.3052 0.5806-0.3262 -0.3386 0.6914-0.2775 C(48) 177.18(17)
C(47) .... C(44) [ ] 3.112(3) < 3.17 -0.06 Intra -0.3052 0.5806-0.3262 0.0407 0.6212-0.3397 C(46) 149.42(16)
C(47) .... C(45) [ ] 2.790(3)<< 3.17 -0.38 Intra -0.3052 0.5806-0.3262 -0.0004 0.5349-0.3259 C(46) 162.53(16)
C(48) .... C(42) [ ] 2.780(3)<< 3.40 -0.62 Intra -0.3052 0.5806-0.3262 -0.4279 0.5960-0.3959 H(47A) 179
C(48) .... S(1) [ ] 2.780(4)<< 3.40 -0.62 Intra -0.2052 0.5818-0.3566 -0.5300 0.5953-0.3662 C(420) 179.36(16)
C(49) .... S(4) [ ] 3.689(2) 3.50 0.19 -0.2645 0.5901-0.3916 -0.0037 0.6795-0.4477 C(44) 117.92(14)
C(49) .... F(44) [ ] 3.177(3) 3.17 0.01 -0.4670 0.5878-0.3314 -0.4768 0.4660-0.3665 C(48) 112.51(13)
C(49) .... F(46) [ ] 2.738(2)<< 3.17 -0.43 Intra -0.2645 0.5901-0.3916 -0.3346 0.5085-0.4598 C(48) 134.14(15)
C(49) .... C(41) [ ] 3.057(3)<< 3.40 -0.34 Intra -0.2645 0.5901-0.3916 0.0407 0.6212-0.3397 C(44) 144.81(15)
C(49) .... C(46) [ ] 2.791(3)<< 3.40 -0.61 Intra -0.2645 0.5901-0.3916 0.0441 0.5578-0.3815 C(44) 169.32(16)
C(410) .... F(13) [ ] 3.350(3) 3.17 0.18 -0.5783 0.5845-0.2995 -0.4582 0.5643-0.4601 C(44) 157.05(16)
C(410) .... H(45A) [ ] 2.65<< 2.90 -0.25 Intra -0.2645 0.5901-0.3916 -0.4670 0.5878-0.3314 H(49A) 179
C(410) .... H(47A) [ ] 2.67<< 2.90 -0.23 Intra -0.5783 0.5845-0.2995 -0.3386 0.6914-0.2775 F(42) 171.94(17)
C(410) .... H(42A) [ ] 2.45 2.40 0.05 Intra -0.5783 0.5845-0.2995 -0.6410 0.5999-0.3696 F(43) 163
C(420) .... H(47A) [ ] 2.65<< 2.90 -0.25 Intra -0.0301 0.5742-0.3509 -0.2632 0.5750-0.3025 F(41) 126
C(420) .... H(49A) [ ] 2.67<< 2.90 -0.23 Intra -0.0301 0.5742-0.3509 -0.2632 0.5750-0.3025 F(42) 128
C(420) .... H(49A) [ ] 2.65<< 2.90 -0.25 Intra -0.0301 0.5742-0.3509 -0.1954 0.5917-0.4120 F(46) 155
C(420) .... H(49A) [ ] 2.67<< 2.90 -0.23 Intra -0.0301 0.5742-0.3509 -0.1954 0.5917-0.4120 F(44) 111
C(420) .... H(49A) [ ] 2.65<< 2.90 -0.25 Intra -0.0301 0.5742-0.3509 -0.1954 0.5917-0.4120 F(45) 142
H(41) .... S(2) [ ] 2.46(3)<< 3.00 -0.54 -0.5570 0.5647-0.5089 -0.6423 0.4982-0.5563 N(41) 160(3)
H(41) .... S(4) [ ] 2.92(3) < 3.00 -0.08 Intra -0.5570 0.5647-0.5089 -0.6423 0.4982-0.5563
H(41) .... C(43) [ ] 3.04(3) 2.90 0.14 Intra -0.5570 0.5647-0.5089 -0.3346 0.5085-0.4598
H(41) .... H(42A) [ ] 2.45 2.40 0.05 Intra -0.5570 0.5647-0.5089 -0.7173 0.6468-0.4925
H(42A) .... S(1) [ 1455.05] 3.02 3.00 0.02 -0.7173 0.6468-0.4925 -1.0037 0.6795-0.4477 C(42) 110
H(42A) .... H(41) [ ] 2.45 2.40 0.05 Intra -0.7173 0.6468-0.4925 -0.5570 0.5647-0.5089
H(42A) .... H(43A) [ ] 2.47 2.40 0.07 Intra -0.7173 0.6468-0.4925 -0.6525 0.6681-0.4282
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H(43A) .... S(1) [ 1455.05]      3.06  3.00  0.06      -0.6525 0.6681-0.4282 -1.0037 0.6795-0.4477 C(43)      109
H(43A) .... F(15) [ 1455.05]     2.87  2.67  0.20      -0.6525 0.6681-0.4282 -0.6426 0.7154-0.3563 C(43)      142
H(43A) .... C(44) [          ]     2.82 < 2.90 -0.08 Intra -0.6525 0.6681-0.4282 -0.4279 0.5960-0.3959
H(43A) .... C(45) [          ]     3.04  2.90  0.14 Intra -0.6525 0.6681-0.4282 -0.5300 0.5953-0.3662
H(43A) .... H(42A) [          ]     2.47  2.40  0.07 Intra -0.6525 0.6681-0.4282 -0.7173 0.6468-0.4925
H(45A) .... F(15) [ 1455.05]     2.79  2.67  0.12      -0.6410 0.5999-0.3696 -0.6426 0.7154-0.3563
H(45A) .... F(41) [          ]     2.86  2.67  0.19 Intra -0.6410 0.5999-0.3696 -0.6599 0.6321-0.2947
H(45A) .... F(42) [          ]     2.76  2.67  0.09 Intra -0.6410 0.5999-0.3696 -0.6871 0.5443-0.3044
H(45A) .... N(42) [          ]     2.61 < 2.75 -0.14 Intra -0.6410 0.5999-0.3696 -0.4915 0.6008-0.4319
H(45A) .... C(43) [          ]     2.85 < 2.90 -0.05 Intra -0.6410 0.5999-0.3696 -0.6074 0.6392-0.4427
H(45A) .... C(410) [          ]     2.65<< 2.90 -0.25 Intra -0.6410 0.5999-0.3696 -0.5783 0.5845-0.2995
H(47A) .... F(43) [          ]     2.39<< 2.67 -0.28 Intra -0.2632 0.5750-0.3025 -0.5045 0.5733-0.2683 C(47)      100
H(47A) .... F(45) [          ]     2.56 < 2.67 -0.11 Intra -0.2632 0.5750-0.3025 -0.0004 0.5349-0.3259
H(47A) .... C(410) [          ]     2.67<< 2.90 -0.23 Intra -0.2632 0.5750-0.3025 -0.5783 0.5845-0.2995
H(47A) .... C(420) [          ]     2.65<< 2.90 -0.25 Intra -0.2632 0.5750-0.3025 -0.0301 0.5742-0.3509
H(47A) .... >F(21) [ 2465.02]     2.81  2.67  0.14      -0.2632 0.5750-0.3025 -0.2168 0.5760-0.2265 C(47)      163
H(49A) .... S(1) [          ]     2.95 < 3.00 -0.05      -0.1954 0.5917-0.4120 -0.0037 0.6795-0.4477 C(49)      136
H(49A) .... S(4) [          ]     2.89 < 3.00 -0.11 Intra -0.1954 0.5917-0.4120 -0.3346 0.5085-0.4598 C(49)      102
H(49A) .... F(46) [          ]     2.45<< 2.67 -0.22 Intra -0.1954 0.5917-0.4120  0.0441 0.5578-0.3815
H(49A) .... N(42) [          ]     2.61 < 2.75 -0.14 Intra -0.1954 0.5917-0.4120 -0.4915 0.6008-0.4319
H(49A) .... C(41) [          ]     2.90  2.90  0.00 Intra -0.1954 0.5917-0.4120 -0.4582 0.5643-0.4601
H(49A) .... C(420) [          ]     2.67<< 2.90 -0.23 Intra -0.1954 0.5917-0.4120 -0.0301 0.5742-0.3509
=====

```

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 6 to Neighbouring ARU'S

```

=====
Nr      ARU      Nr.Cont.  d(min)  Del  XHn X      - At(I)      At(J) - Y  YHn  Note  Partaking ARU's in Close Contact Resd.
-----
1 [ 1555.02]      4      2.4300 -0.57   0 C(41) - S(4) ... H(21) -N(21)  1 << 1555.02
2 [ 4444.03]      4      2.8300 -0.17   0 C(41) - S(4) ... H(52A) -C(52)  1 < 4444.03
3 [ 4544.03]     10      2.8800 -0.12   0 C(41) - S(4) ... H(59A) -C(59)  1 < 4544.03
4 [ 1555.05]      9      2.9500 -0.05   1 C(49) - H(49A) ... S(1) -C(11)  0 < 1555.05
5 [ 1455.05]      9      2.7900  0.12   1 C(45) - H(45A) ... F(15) -C(120)  0 1455.05
6 [ 1455.06]      2      2.7660 -0.17   0 C(410) - F(42) ... F(45) -C(420)  0 < 1455.06
7 [ 2465.02]      6      2.8100  0.14   1 C(47) - H(47A) ... *F(21) -C(210)  0 2465.02
8 [ 2365.02]      1      2.9050 -0.04   0 C(410) - F(43) ... F(24) -C(220)  0 < 2365.02
9 [ 2465.01]      1      2.9800  0.04   0 C(410) - F(43) ... *F(32A) -C(310)  0 2465.01
10 [ 1655.06]      2      2.7660 -0.17   0 C(420) - F(45) ... F(42) -C(410)  0 < 1655.06
=====

```

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Asymmetric Residue Unit (= ARU) Code List

=====

| ARU-CODE | CIF-CODE | Symmetry-Code | sym TX TY TZ Ires | x(cen) | y(cen) | z(cen) |
|------------|----------|---------------------|--------------------|--------|--------|--------|
| [3464.05] | [4_464] | =-1/2+x,3/2-y,-1-z | = [3 -1 1 -1 5] | -0.489 | 0.588 | -0.862 |
| [3564.05] | [4_564] | =1/2+x,3/2-y,-1-z | = [3 0 1 -1 5] | 0.511 | 0.588 | -0.862 |
| [1455.01] | [1_455] | =-1+x,y,z | = [1 -1 0 0 1] | -1.109 | 0.746 | -0.365 |
| [3464.03] | [4_464] | =-1/2+x,3/2-y,-1-z | = [3 -1 1 -1 3] | -0.707 | 0.923 | -0.362 |
| [1655.02] | [1_655] | =1+x,y,z | = [1 1 0 0 2] | 0.467 | 0.424 | -0.649 |
| [1655.01] | [1_655] | =1+x,y,z | = [1 1 0 0 1] | 0.891 | 0.746 | -0.365 |
| [1554.04] | [1_554] | =x,y,-1+z | = [1 0 0 -1 4] | -0.411 | 0.589 | -1.385 |
| [2464.06] | [2_464] | =-1/2-x,1-y,-1/2+z | = [2 -1 1 -1 6] | -0.267 | 0.252 | -0.374 |
| [4444.04] | [3_444] | =-1-x,-1/2+y,-1/2-z | = [4 -1 -1 -1 4] | -0.589 | 0.089 | -0.115 |
| [2464.05] | [2_464] | =-1/2-x,1-y,-1/2+z | = [2 -1 1 -1 5] | -0.511 | 0.088 | -0.638 |
| [1455.02] | [1_455] | =-1+x,y,z | = [1 -1 0 0 2] | -1.533 | 0.424 | -0.649 |
| [2364.06] | [2_364] | =-3/2-x,1-y,-1/2+z | = [2 -2 1 -1 6] | -1.267 | 0.252 | -0.374 |
| [4344.04] | [3_344] | =-2-x,-1/2+y,-1/2-z | = [4 -2 -1 -1 4] | -1.589 | 0.089 | -0.115 |
| [3565.04] | [4_565] | =1/2+x,3/2-y,-z | = [3 0 1 0 4] | 0.089 | 0.911 | 0.385 |
| [3564.02] | [4_564] | =1/2+x,3/2-y,-1-z | = [3 0 1 -1 2] | -0.033 | 1.076 | -0.351 |
| [4454.06] | [3_454] | =-1-x,1/2+y,-1/2-z | = [4 -1 0 -1 6] | -0.767 | 1.248 | -0.626 |
| [3465.04] | [4_465] | =-1/2+x,3/2-y,-z | = [3 -1 1 0 4] | -0.911 | 0.911 | 0.385 |
| [3564.01] | [4_564] | =1/2+x,3/2-y,-1-z | = [3 0 1 -1 1] | 0.391 | 0.754 | -0.635 |
| [1655.03] | [1_655] | =1+x,y,z | = [1 1 0 0 3] | 0.793 | 0.577 | -0.638 |
| [4554.06] | [3_554] | =-x,1/2+y,-1/2-z | = [4 0 0 -1 6] | 0.233 | 1.248 | -0.626 |
| [1455.03] | [1_455] | =-1+x,y,z | = [1 -1 0 0 3] | -1.207 | 0.577 | -0.638 |
| [4454.02] | [3_454] | =-1-x,1/2+y,-1/2-z | = [4 -1 0 -1 2] | -0.467 | 0.924 | 0.149 |
| [3465.05] | [4_465] | =-1/2+x,3/2-y,-z | = [3 -1 1 0 5] | -0.489 | 0.588 | 0.138 |
| [1556.01] | [1_556] | =x,y,1+z | = [1 0 0 1 1] | -0.109 | 0.746 | 0.635 |
| [3465.03] | [4_465] | =-1/2+x,3/2-y,-z | = [3 -1 1 0 3] | -0.707 | 0.923 | 0.638 |
| [3565.05] | [4_565] | =1/2+x,3/2-y,-z | = [3 0 1 0 5] | 0.511 | 0.588 | 0.138 |
| [1455.04] | [1_455] | =-1+x,y,z | = [1 -1 0 0 4] | -1.411 | 0.589 | -0.385 |
| [4354.02] | [3_354] | =-2-x,1/2+y,-1/2-z | = [4 -2 0 -1 2] | -1.467 | 0.924 | 0.149 |
| [1655.04] | [1_655] | =1+x,y,z | = [1 1 0 0 4] | 0.589 | 0.589 | -0.385 |
| [3565.03] | [4_565] | =1/2+x,3/2-y,-z | = [3 0 1 0 3] | 0.293 | 0.923 | 0.638 |
| [1655.06] | [1_655] | =1+x,y,z | = [1 1 0 0 6] | 0.767 | 0.748 | 0.126 |
| [2465.02] | [2_465] | =-1/2-x,1-y,1/2+z | = [2 -1 1 0 2] | 0.033 | 0.576 | -0.149 |
| [1455.05] | [1_455] | =-1+x,y,z | = [1 -1 0 0 5] | -0.989 | 0.912 | -0.138 |
| [3464.01] | [4_464] | =-1/2+x,3/2-y,-1-z | = [3 -1 1 -1 1] | -0.609 | 0.754 | -0.635 |
| [1655.05] | [1_655] | =1+x,y,z | = [1 1 0 0 5] | 1.011 | 0.912 | -0.138 |
| [4444.03] | [3_444] | =-1-x,-1/2+y,-1/2-z | = [4 -1 -1 -1 3] | -0.793 | 0.077 | 0.138 |
| [4544.03] | [3_544] | =-x,-1/2+y,-1/2-z | = [4 0 -1 -1 3] | 0.207 | 0.077 | 0.138 |
| [1455.06] | [1_455] | =-1+x,y,z | = [1 -1 0 0 6] | -1.233 | 0.748 | 0.126 |
| [2365.02] | [2_365] | =-3/2-x,1-y,1/2+z | = [2 -2 1 0 2] | -0.967 | 0.576 | -0.149 |
| [2465.01] | [2_465] | =-1/2-x,1-y,1/2+z | = [2 -1 1 0 1] | -0.391 | 0.254 | 0.135 |

=====
Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

$X(J) = X(\text{sym}) + TX$, $Y(J) = Y(\text{sym}) + TY$, $Z(J) = Z(\text{sym}) + TZ$,
SYM - Number of the Symmetry Operator.
Ires - Residue Number.
TX, TY, TZ - Unit Cell Translations.

=====
 Analysis of Potential Hydrogen Bonds and Schemes with $d(D...A) < R(D)+R(A)+0.50$, $d(H...A) < R(H)+R(A)-0.12$ Ang., $D-H...A > 100.0$ Deg
 =====

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
 =====

| Nr | Typ | Res | Donor | H...A | Acceptor | [ARU] | D - H | H...A | D...A | D - H...A | A..H..A* | A'..H..A" | Sum(XY,YZ) | Sum(XZ) |
|----|-------|-----|-------|----------|----------|------------|---------|---------|----------|-----------|----------|-----------|------------|---------|
| 1 | | 5 | N(11) | --H(11) | ..S(3) | [] | 0.84(3) | 2.45(3) | 3.284(2) | 177(4) | | | | |
| 2 | | 2 | N(21) | --H(21) | ..S(4) | [] | 0.83(3) | 2.43(3) | 3.260(2) | 178(3) | | | | |
| 3 | | 1 | N(31) | --H(31) | ..S(1) | [] | 0.79(3) | 2.50(3) | 3.278(2) | 168(3) | | | | |
| 4 | | 6 | N(41) | --H(41) | ..S(2) | [] | 0.87(3) | 2.46(3) | 3.291(2) | 160(3) | | | | |
| 5 | | 3 | N(51) | --H(51) | ..S(6) | [] | 0.83(4) | 2.39(4) | 3.206(2) | 167(5) | | | | |
| 6 | | 4 | N(61) | --H(61) | ..S(5) | [] | 0.84(3) | 2.54(3) | 3.370(2) | 170(3) | | | | |
| 7 | Intra | 5 | C(19) | --H(19A) | ..S(1) | [] | 0.95 | 2.83 | 3.249(2) | 108 | | | | |
| 8 | | 5 | C(19) | --H(19A) | ..S(3) | [3564.01] | 0.95 | 2.81 | 3.678(2) | 152' | 88' | | 348 | |
| 9 | | 2 | C(23) | --H(23A) | ..F(25) | [1655.02] | 0.95 | 2.49 | 3.341(3) | 149 | | | | |
| 10 | Intra | 2 | C(29) | --H(29A) | ..S(2) | [] | 0.95 | 2.81 | 3.265(2) | 110 | | | | |
| 11 | | 2 | C(29) | --H(29A) | ..S(6) | [4444.04] | 0.95 | 2.65 | 3.468(2) | 144' | 87' | | 341 | |
| 12 | Intra | 1 | C(39) | --H(39A) | ..S(3) | [] | 0.95 | 2.87 | 3.259(2) | 105 | | | | |
| 13 | Intra | 6 | C(47) | --H(47A) | ..F(43) | [] | 0.95 | 2.39 | 2.713(3) | 100 | | | | |
| 14 | | 3 | C(52) | --H(52A) | ..S(4) | [4454.06] | 0.95 | 2.83 | 3.689(3) | 151 | | | | |
| 15 | | 3 | C(53) | --H(53A) | ..F(56) | [1455.03] | 0.95 | 2.48 | 3.262(3) | 139 | | | | |

Translation of ARU-Code to CIF and Equivalent Position Code

=====
 [1655.] = [1_655] =1+x,y,z
 [4444.] = [3_444] =-1-x,-1/2+y,-1/2-z
 [4454.] = [3_454] =-1-x,1/2+y,-1/2-z
 [3564.] = [4_564] =1/2+x,3/2-y,-1-z
 [1455.] = [1_455] =-1+x,y,z

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]

 2-Centre (linear) D-H...X most prob. angle 160 deg - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
 3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg Springer-Verlag, Berlin, 1991, pp 20.
 4-Centre (trifurcated)

Analysis of Potential Donor/Acceptor Atoms -- (Major Disorder Form Only)

=====
 At.Nr D/A #Cov.Bonds # H #D-H..A #A..H #A..H-C Sum(A-H) Sum(A-X)

| | | | | | | | | |
|---|------|---|---|---|---|---|---|---|
| 1 | S(1) | 1 | - | 0 | 1 | 1 | 2 | 3 |
| 2 | S(2) | 1 | - | 0 | 1 | 1 | 2 | 3 |
| 3 | S(3) | 1 | - | 0 | 1 | 2 | 3 | 4 |

| | | | | | | | | |
|----|---------|---|-----|---|---|---|---|---|
| 4 | S(4) | 1 | - | 0 | 1 | 1 | 2 | 3 |
| 5 | S(5) | 1 | - | 0 | 1 | 0 | 1 | 2 |
| 6 | S(6) | 1 | - | 0 | 1 | 1 | 2 | 3 |
| 7 | F(11) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 8 | F(12) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 9 | F(13) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 10 | F(14) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 11 | F(15) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 12 | F(16) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 13 | >F(21) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 14 | >F(22) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 15 | >F(23) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 16 | F(24) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 17 | F(25) | 1 | - | 0 | 0 | 1 | 1 | 2 |
| 18 | F(26) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 19 | F(34) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 20 | F(35) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 21 | F(36) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 22 | F(41) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 23 | F(42) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 24 | F(43) | 1 | - | 0 | 0 | 1 | 1 | 2 |
| 25 | F(44) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 26 | F(45) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 27 | F(46) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 28 | >F(51) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 29 | >F(52) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 30 | >F(53) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 31 | F(54) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 32 | F(55) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 33 | F(56) | 1 | - | 0 | 0 | 1 | 1 | 2 |
| 34 | >F(61A) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 35 | >F(62A) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 36 | >F(63A) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 37 | F(64) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 38 | F(65) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 39 | F(66) | 1 | - | 0 | 0 | 0 | 0 | 1 |
| 40 | N(11) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 41 | N(12) | 3 | - | 0 | 0 | 0 | 0 | 3 |
| 42 | N(21) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 43 | N(22) | 3 | - | 0 | 0 | 0 | 0 | 3 |
| 44 | N(31) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 45 | N(32) | 3 | - | 0 | 0 | 0 | 0 | 3 |
| 46 | N(41) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 47 | N(42) | 3 | - | 0 | 0 | 0 | 0 | 3 |
| 48 | N(51) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 49 | N(52) | 3 | - | 0 | 0 | 0 | 0 | 3 |
| 50 | N(61) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 51 | N(62) | 3 | - | 0 | 0 | 0 | 0 | 3 |

=====
 Analysis of Hydrogen Bonded Molecular Aggregates (See also Acta Cryst. B36, 1980, 2113 - 2115) -- (Major Disorder Component Only)
 =====

Coordinates of Donor and Acceptor Atoms
 =====

Coordinates of D/A-Bonded Atom(s)
 =====

| D/A I | [ARU] | X | Y | Z | -- | D/A J | [ARU] | X | Y | Z | Atom K | X | Y | Z | I..J--K Angle |
|-------|------------|---------|--------|---------|----|-------|------------|---------|--------|---------|--------|---------|--------|---------|---------------|
| N(11) | [1555.05] | -0.2811 | 0.7314 | -0.4656 | >> | S(3) | [1555.01] | -0.3034 | 0.6716 | -0.5461 | C(31) | -0.1831 | 0.6147 | -0.5453 | 107.31(9) |
| S(3) | [1555.01] | -0.3034 | 0.6716 | -0.5461 | << | N(11) | [1555.05] | -0.2811 | 0.7314 | -0.4656 | C(11) | -0.1661 | 0.7200 | -0.4410 | 123.58(10) |
| | | | | | | | | | | | C(12) | -0.3987 | 0.7646 | -0.4504 | 124.60(10) |
| | | | | | | | | | | | H(11) | -0.2840 | 0.7169 | -0.4863 | 2.06(10) |
| N(21) | [1555.02] | -0.3619 | 0.4478 | -0.5393 | >> | S(4) | [1555.06] | -0.3346 | 0.5085 | -0.4598 | C(41) | -0.4582 | 0.5643 | -0.4601 | 107.54(9) |
| S(4) | [1555.06] | -0.3346 | 0.5085 | -0.4598 | << | N(21) | [1555.02] | -0.3619 | 0.4478 | -0.5393 | C(21) | -0.4797 | 0.4580 | -0.5634 | 123.78(10) |
| | | | | | | | | | | | C(22) | -0.2451 | 0.4144 | -0.5544 | 124.28(10) |
| | | | | | | | | | | | H(21) | -0.3550 | 0.4623 | -0.5187 | 1.73(10) |
| N(31) | [1555.01] | -0.0879 | 0.5988 | -0.5175 | >> | S(1) | [1555.05] | -0.0037 | 0.6795 | -0.4477 | C(11) | -0.1661 | 0.7200 | -0.4410 | 105.79(8) |
| S(1) | [1555.05] | -0.0037 | 0.6795 | -0.4477 | << | N(31) | [1555.01] | -0.0879 | 0.5988 | -0.5175 | C(31) | -0.1831 | 0.6147 | -0.5453 | 123.57(10) |
| | | | | | | | | | | | C(32) | 0.0006 | 0.5519 | -0.5269 | 123.32(10) |
| | | | | | | | | | | | H(31) | -0.0810 | 0.6167 | -0.4995 | 9.21(11) |
| N(41) | [1555.06] | -0.5517 | 0.5818 | -0.4879 | >> | S(2) | [1555.02] | -0.6423 | 0.4982 | -0.5563 | C(21) | -0.4797 | 0.4580 | -0.5634 | 105.71(8) |
| S(2) | [1555.02] | -0.6423 | 0.4982 | -0.5563 | << | N(41) | [1555.06] | -0.5517 | 0.5818 | -0.4879 | C(41) | -0.4582 | 0.5643 | -0.4601 | 121.60(9) |
| | | | | | | | | | | | C(42) | -0.6430 | 0.6274 | -0.4776 | 123.60(10) |
| | | | | | | | | | | | H(41) | -0.5570 | 0.5647 | -0.5089 | 14.79(10) |
| N(51) | [1555.03] | -0.1497 | 0.9144 | -0.0274 | >> | S(6) | [1555.04] | -0.2154 | 0.8484 | 0.0473 | C(61) | -0.1136 | 0.7873 | 0.0471 | 109.23(9) |
| S(6) | [1555.04] | -0.2154 | 0.8484 | 0.0473 | << | N(51) | [1555.03] | -0.1497 | 0.9144 | -0.0274 | C(51) | -0.0313 | 0.9008 | -0.0506 | 123.29(10) |
| | | | | | | | | | | | C(52) | -0.2661 | 0.9455 | -0.0446 | 122.05(10) |
| | | | | | | | | | | | H(51) | -0.1560 | 0.9009 | -0.0066 | 9.38(10) |
| N(61) | [1555.04] | -0.0074 | 0.7699 | 0.0220 | >> | S(5) | [1555.03] | 0.1298 | 0.8614 | -0.0406 | C(51) | -0.0313 | 0.9008 | -0.0506 | 103.36(8) |
| S(5) | [1555.03] | 0.1298 | 0.8614 | -0.0406 | << | N(61) | [1555.04] | -0.0074 | 0.7699 | 0.0220 | C(61) | -0.1136 | 0.7873 | 0.0471 | 119.56(9) |
| | | | | | | | | | | | C(62) | 0.0535 | 0.7178 | 0.0313 | 128.29(10) |
| | | | | | | | | | | | H(61) | 0.0200 | 0.7901 | 0.0043 | 7.75(10) |

=====

***** Aggregate = 1 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 2 1 1555.01 -- 1555.05
 2 1 1555.05 -- 1555.01

=====

Aggregate = 2 *****

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

2 1 1555.03 -- 1555.04
2 1 1555.04 -- 1555.03

Aggregate = 3 *****

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

2 1 1555.02 -- 1555.06
2 1 1555.06 -- 1555.02

Aggregate = 4 *****

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

2 1 2555.01 -- 2555.05
2 1 2555.05 -- 2555.01

Aggregate = 5 *****

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

2 1 2555.03 -- 2555.04
2 1 2555.04 -- 2555.03

Aggregate = 6 *****

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

2 1 2555.02 -- 2555.06
2 1 2555.06 -- 2555.02

=====

Aggregate = 7 *****

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

2 1 3555.01 -- 3555.05
2 1 3555.05 -- 3555.01

Aggregate = 8 *****

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

2 1 3555.03 -- 3555.04
2 1 3555.04 -- 3555.03

Aggregate = 9 *****

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

2 1 3555.02 -- 3555.06
2 1 3555.06 -- 3555.02

Aggregate = 10 *****

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

2 1 4555.01 -- 4555.05
2 1 4555.05 -- 4555.01

Aggregate = 11 *****

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

2 1 4555.03 -- 4555.04
2 1 4555.04 -- 4555.03

=====

=====

***** Aggregate = 12 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

2 1 4555.02 -- 4555.06

2 1 4555.06 -- 4555.02

=====
 Analysis of the (Cooperative) Hydrogen Bond Network (i.e. (In)Finite O-H...O-H...O-H.. Chains and/or Rings (Max = 18 Membered))
 =====

=====
 ***** Network = 1 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|---------|--------|---------|-----------------|---------|--------|--|
| 1.555 | N(11) [1555.05] | -0.2811 | 0.7314 | -0.4656 | S(3) [1555.01] | -0.3034 | 0.6716 | -0.5461 |
| | H(11) | -0.2840 | 0.7169 | -0.4863 | | | | |

=====
 ***** Network = 2 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|---------|--------|---------|-----------------|---------|--------|--|
| 2.555 | N(21) [1555.02] | -0.3619 | 0.4478 | -0.5393 | S(4) [1555.06] | -0.3346 | 0.5085 | -0.4598 |
| | H(21) | -0.3550 | 0.4623 | -0.5187 | | | | |

=====
 ***** Network = 3 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|---------|--------|---------|-----------------|---------|--------|--|
| 3.555 | N(31) [1555.01] | -0.0879 | 0.5988 | -0.5175 | S(1) [1555.05] | -0.0037 | 0.6795 | -0.4477 |
| | H(31) | -0.0810 | 0.6167 | -0.4995 | | | | |

=====
 ***** Network = 4 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|---------|--------|---------|-----------------|---------|--------|--|
| 4.555 | N(41) [1555.06] | -0.5517 | 0.5818 | -0.4879 | S(2) [1555.02] | -0.6423 | 0.4982 | -0.5563 |
| | H(41) | -0.5570 | 0.5647 | -0.5089 | | | | |

=====
 ***** Network = 5 *****
 =====

| Code Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|----------|------------------|---------|--------|---------|-----------------|---------|--------|--|
| 5.555 | N(51) [1555.03] | -0.1497 | 0.9144 | -0.0274 | S(6) [1555.04] | -0.2154 | 0.8484 | 0.0473 |
| | H(51) | -0.1560 | 0.9009 | -0.0066 | | | | |

=====

=====

***** Network = 6 *****

=====

| Code | Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|-------|-----|------------------|---------|--------|--------|-----------------|--------|--------|--|
| 6.555 | | N(61) [1555.04] | -0.0074 | 0.7699 | 0.0220 | S(5) [1555.03] | 0.1298 | 0.8614 | -0.0406 |
| | | H(61) | 0.0200 | 0.7901 | 0.0043 | | | | |

Hydrogen Bonds are Coded as N.IJK Where N = Sequence Number of Hydrogen Bond (NOTE: New Hbond Numbering system)

I - 5 = Nr of Translation Units Along A-Axis

J - 5 = Nr of Translation Units Along B-Axis

K - 5 = Nr of Translation Units Along C-Axis

Ring Closure Links are Indicated with 'R' and Infinite Chain Links With 'T'

=====
Analysis of the Coordination Geometry

Distances are calculated from atom I of Unique Molecule Coordinate List to atom J in Asymmetric Residue Unit: ARU.

Phi = Azimuth angle(counter clockwise from X0 in X0,Y0-Plane), Mu = Angle between D and X0,Y0-plane.

'To-Code' : '--' = Bonded atoms, '<<' = .LT. sum vdW-radii - 0.2, '<' = .LT. sum vdW-radii, '..' = .GT. sum vdW-radii.

>>>> NOTICE >>>> : The Symmetry Code Character Added to the Atom Label Applies to the Current Coordination Sphere Only.

>>>>>>>>>>>>>>>>>> : Symmetry operations refer to the coordinates listed in the fractional coordinate table given above

The List May be Limited to the Shortest Distances.

3.6 Angstrom Coordination Sphere Around Atom I = S(1) [ARU = 1555.05] -0.00373 0.67954 -0.44773 -0.0314 16.1834-16.4165

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|-------------------|------------|--------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.6921(19) | -- | C(11) | | | | Intra | 144.84 | 8.34 | -0.16610 | 0.72002 | -0.44104 | -1.4003 | 17.1474 | -16.1712 |
| 2 | 2.7244(19) | << | N(11) | | | | Intra | 152.15 | -13.90 | -0.28110 | 0.73142 | -0.46558 | -2.3697 | 17.4189 | -17.0710 |
| 3 | 2.7602(19) | << | N(12) | | | | Intra | 137.12 | 30.28 | -0.21090 | 0.74765 | -0.40977 | -1.7779 | 17.8054 | -15.0246 |
| 4 | 3.249(2) | << | C(19) | | | | Intra | 80.08 | 56.08 | 0.03330 | 0.75452 | -0.37421 | 0.2807 | 17.9690 | -13.7208 |
| 5 | 3.273(2) | << | C(14) | | | | Intra | 123.76 | 54.05 | -0.13040 | 0.74662 | -0.37546 | -1.0993 | 17.7809 | -13.7666 |
| 6 | 3.278(2) | .< | N(31) | [| = 01] | | | -110.26 | -51.31 | -0.08790 | 0.59883 | -0.51751 | -0.7410 | 14.2613 | -18.9750 |
| 7 | 3.463(3) | .< | C(42)a | [1+x,y,z | = 1655.06] | | | -22.22 | -18.46 | 0.35700 | 0.62737 | -0.47764 | 3.0096 | 14.9409 | -17.5131 |
| 8 | 3.482(3) | .< | C(43)a | [1+x,y,z | = 1655.06] | | | -16.06 | 3.02 | 0.39260 | 0.63916 | -0.44272 | 3.3097 | 15.2217 | -16.2328 |
| 9 | 2.50(3) | << | H(31) | [| = 01] | | | -113.52 | -49.31 | -0.08100 | 0.61670 | -0.49950 | -0.6828 | 14.6868 | -18.3147 |
| 10 | 2.83 | .< | H(19A) | | | | Intra | 67.23 | 42.23 | 0.09240 | 0.76060 | -0.39590 | 0.7790 | 18.1138 | -14.5161 |
| 11 | 2.89(3) | .< | H(11) | | | | Intra | 159.37 | -29.26 | -0.28400 | 0.71690 | -0.48630 | -2.3942 | 17.0731 | -17.8307 |
| 12 | 2.95 | .< | H(49A) | [| = 06] | | | -127.68 | 26.36 | -0.19540 | 0.59170 | -0.41200 | -1.6473 | 14.0915 | -15.1064 |
| 13 | 3.02 | .. | H(42A)a | [1+x,y,z | = 1655.06] | | | -17.90 | -32.90 | 0.28270 | 0.64680 | -0.49250 | 2.3832 | 15.4037 | -18.0580 |
| 14 | 3.06 | .. | H(43A)a | [1+x,y,z | = 1655.06] | | | -5.26 | 13.54 | 0.34750 | 0.66810 | -0.42820 | 2.9295 | 15.9109 | -15.7004 |
| 15 | 3.45 | .. | H(12A)b | [1/2+x,3/2-y,-1-z | = 3564.05] | | | 84.51 | -72.73 | 0.00790 | 0.72240 | -0.53770 | 0.0666 | 17.2041 | -19.7153 |

Angles (Degrees) At1...V...At2 with Vertex V = S(1)

| | | | | | | | | | | | | | | | |
|-------|---|--------|-----------|-------|---|--------|-----------|-------|---|--------|-----------|--------|---|--------|-----------|
| C(11) | , | N(11) | 23.39(7) | C(11) | , | N(12) | 23.11(7) | C(11) | , | C(19) | 69.16(7) | C(11) | , | C(14) | 48.75(8) |
| C(11) | , | N(31) | 105.79(8) | C(11) | , | C(42)a | 163.87(8) | C(11) | , | C(43)a | 157.82(8) | N(11) | , | N(12) | 46.49(5) |
| N(11) | , | C(19) | 91.87(5) | N(11) | , | C(14) | 72.13(6) | N(11) | , | N(31) | 83.84(5) | N(11) | , | C(42)a | 147.17(6) |
| N(11) | , | C(43)a | 164.07(6) | N(12) | , | C(19) | 47.10(5) | N(12) | , | C(14) | 25.65(6) | N(12) | , | N(31) | 126.96(5) |
| N(12) | , | C(42)a | 157.84(6) | N(12) | , | C(43)a | 137.98(6) | C(19) | , | C(14) | 24.67(5) | C(19) | , | N(31) | 172.25(5) |
| C(19) | , | C(42)a | 112.06(5) | C(19) | , | C(43)a | 90.91(5) | C(14) | , | N(31) | 147.94(6) | C(14) | , | C(42)a | 135.88(6) |
| C(14) | , | C(43)a | 113.90(6) | N(31) | , | C(42)a | 74.49(5) | N(31) | , | C(43)a | 94.99(5) | C(42)a | , | C(43)a | 22.33(5) |

3.6 Angstrom Coordination Sphere Around Atom I = S(2) [ARU = 1555.02] -0.64233 0.49822 -0.55631 -5.4150 11.8652-20.3977

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|---------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.692(2) | -- | C(21) | | | | Intra | -34.91 | -8.83 | -0.47970 | 0.45804 | -0.56339 | -4.0440 | 10.9083 | -20.6573 |
| 2 | 2.7247(19) | << | N(21) | | | | Intra | -26.95 | 13.26 | -0.36190 | 0.44776 | -0.53926 | -3.0509 | 10.6635 | -19.7725 |
| 3 | 2.7646(19) | << | N(22) | | | | Intra | -43.12 | -30.41 | -0.43590 | 0.42978 | -0.59447 | -3.6747 | 10.2353 | -21.7968 |
| 4 | 3.265(2) | << | C(29) | | | | Intra | -100.51 | -53.04 | -0.68480 | 0.41717 | -0.62747 | -5.7730 | 9.9350 | -23.0068 |
| 5 | 3.291(2) | .< | N(41) | [| = | 06] | | 69.00 | 49.62 | -0.55170 | 0.58178 | -0.48794 | -4.6509 | 13.8552 | -17.8908 |
| 6 | 3.291(2) | << | C(24) | | | | Intra | -59.31 | -52.88 | -0.52210 | 0.42651 | -0.62787 | -4.4014 | 10.1574 | -23.0215 |
| 7 | 3.444(3) | .< | C(32)a | [-1+x,y,z | = | 1455.01] | | 156.97 | 18.26 | -0.99940 | 0.55195 | -0.52688 | -8.4251 | 13.1448 | -19.3186 |
| 8 | 3.480(3) | .< | C(33)a | [-1+x,y,z | = | 1455.01] | | 164.16 | -3.05 | -1.03890 | 0.53804 | -0.56136 | -8.7581 | 12.8135 | -20.5828 |
| 9 | 2.46(3) | << | H(41) | [| = | 06] | | 65.57 | 44.99 | -0.55700 | 0.56470 | -0.50890 | -4.6956 | 13.4484 | -18.6593 |
| 10 | 2.81 | .< | H(29A) | | | | Intra | -112.36 | -39.43 | -0.74030 | 0.41390 | -0.60500 | -6.2409 | 9.8571 | -22.1829 |
| 11 | 2.92(3) | .< | H(21) | | | | Intra | -19.45 | 28.23 | -0.35500 | 0.46230 | -0.51870 | -2.9927 | 11.0098 | -19.0187 |
| 12 | 2.96 | .< | H(39A) | [| = | 01] | | 53.17 | -25.49 | -0.45260 | 0.58790 | -0.59100 | -3.8155 | 14.0010 | -21.6696 |
| 13 | 3.00 | .< | H(32A)a | [-1+x,y,z | = | 1455.01] | | 160.78 | 32.90 | -0.92490 | 0.53310 | -0.51180 | -7.7971 | 12.6959 | -18.7657 |
| 14 | 3.07 | .. | H(33A)a | [-1+x,y,z | = | 1455.01] | | 175.54 | -13.10 | -0.99630 | 0.50800 | -0.57530 | -8.3990 | 12.0981 | -21.0939 |
| 15 | 3.44 | .. | H(52A)b | [-1-x,-1/2+y,-1/2-z | = | 4444.03] | | -88.06 | 74.32 | -0.63860 | 0.45920 | -0.46600 | -5.3835 | 10.9359 | -17.0864 |

Angles (Degrees) At1...V...At2 with Vertex V = S(2)

| | | | | | | | | | | | | | | | |
|-------|---|--------|-----------|-------|---|--------|-----------|-------|---|--------|-----------|--------|---|--------|-----------|
| C(21) | , | N(21) | 23.46(8) | C(21) | , | N(22) | 22.90(8) | C(21) | , | C(29) | 68.40(8) | C(21) | , | N(41) | 105.71(8) |
| C(21) | , | C(24) | 48.28(8) | C(21) | , | C(32)a | 165.10(9) | C(21) | , | C(33)a | 157.58(9) | N(21) | , | N(22) | 46.36(5) |
| N(21) | , | C(29) | 91.02(6) | N(21) | , | N(41) | 83.71(5) | N(21) | , | C(24) | 71.75(6) | N(21) | , | C(32)a | 148.24(6) |
| N(21) | , | C(33)a | 165.00(6) | N(22) | , | C(29) | 46.85(6) | N(22) | , | N(41) | 126.58(5) | N(22) | , | C(24) | 25.39(6) |
| N(22) | , | C(32)a | 158.09(6) | N(22) | , | C(33)a | 137.60(6) | C(29) | , | N(41) | 172.62(6) | C(29) | , | C(24) | 24.47(6) |
| C(29) | , | C(32)a | 111.97(6) | C(29) | , | C(33)a | 90.76(6) | N(41) | , | C(24) | 148.19(6) | N(41) | , | C(32)a | 74.91(5) |
| N(41) | , | C(33)a | 95.67(5) | C(24) | , | C(32)a | 135.38(6) | C(24) | , | C(33)a | 113.26(6) | C(32)a | , | C(33)a | 22.46(6) |

3.6 Angstrom Coordination Sphere Around Atom I = S(3) [ARU = 1555.01] -0.30343 0.67159 -0.54610 -2.5580 15.9941-20.0233

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 | |
|----|------------|----|--------|------------|-----------|--------|-------|----------|--------|----------|----------|----------|----------|---------|----------|----------|
| 1 | 1.692(2) | -- | C(31) | | | | Intra | -53.16 | 0.98 | -0.18310 | 0.61473 | -0.54531 | -1.5436 | 14.6399 | -19.9943 | |
| 2 | 2.721(2) | << | N(31) | | | | Intra | -43.64 | 22.66 | -0.08790 | 0.59883 | -0.51751 | -0.7410 | 14.2613 | -18.9750 | |
| 3 | 2.7677(19) | << | N(32) | | | | Intra | -61.02 | -20.49 | -0.15440 | 0.57636 | -0.57252 | -1.3016 | 13.7261 | -20.9920 | |
| 4 | 3.259(2) | << | C(39) | | | | Intra | -108.61 | -47.74 | -0.38640 | 0.58437 | -0.61188 | -3.2574 | 13.9169 | -22.4352 | |
| 5 | 3.269(2) | << | C(34) | | | | Intra | -73.35 | -44.07 | -0.22360 | 0.57709 | -0.60812 | -1.8850 | 13.7435 | -22.2973 | |
| 6 | 3.284(2) | .< | N(11) | [| = | 05] | | 82.47 | 64.04 | -0.28110 | 0.73142 | -0.46558 | -2.3697 | 17.4189 | -17.0710 | |
| 7 | 2.45(3) | << | H(11) | [| = | 05] | | 81.37 | 63.54 | -0.28400 | 0.71690 | -0.48630 | -2.3942 | 17.0731 | -17.8307 | |
| 8 | 2.81 | .< | H(19A) | b[-1/2+x, | 3/2-y, | -1-z | = | 3464.05] | 118.54 | -49.16 | -0.40760 | 0.73940 | -0.60410 | -3.4361 | 17.6090 | -22.1499 |
| 9 | 2.85(3) | .< | H(31) | | | | Intra | -34.88 | 36.78 | -0.08100 | 0.61670 | -0.49950 | -0.6828 | 14.6868 | -18.3147 | |
| 10 | 2.87 | .< | H(39A) | | | | Intra | -122.25 | -34.94 | -0.45260 | 0.58790 | -0.59100 | -3.8155 | 14.0010 | -21.6696 | |
| 11 | 2.91 | .< | H(12A) | a[1/2+x, | 3/2-y, | -1-z | = | 3564.05] | 24.75 | 6.08 | 0.00790 | 0.72240 | -0.53770 | 0.0666 | 17.2041 | -19.7153 |
| 12 | 3.59(3) | .. | H(41) | [| = | 06] | | -130.02 | 22.31 | -0.55700 | 0.56470 | -0.50890 | -4.6956 | 13.4484 | -18.6593 | |

Angles (Degrees) At1...V...At2 with Vertex V = S(3)

| | | | | | | | | | | | | | | | |
|-------|---|-------|-----------|-------|---|-------|-----------|-------|---|-------|-----------|-------|---|-------|-----------|
| C(31) | , | N(31) | 23.57(8) | C(31) | , | N(32) | 22.80(8) | C(31) | , | C(39) | 68.36(8) | C(31) | , | C(34) | 48.52(8) |
| C(31) | , | N(11) | 107.31(8) | N(31) | , | N(32) | 46.36(6) | N(31) | , | C(39) | 91.29(6) | N(31) | , | C(34) | 72.07(6) |
| N(31) | , | N(11) | 83.78(6) | N(32) | , | C(39) | 46.85(6) | N(32) | , | C(34) | 25.72(6) | N(32) | , | N(11) | 130.11(6) |
| C(39) | , | C(34) | 24.59(6) | C(39) | , | N(11) | 162.61(6) | C(34) | , | N(11) | 155.82(6) | | | | |

=====

3.6 Angstrom Coordination Sphere Around Atom I = S(4) [ARU = 1555.06] -0.33464 0.50849 -0.45983 -2.8211 12.1098-16.8601

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 | | |
|----|------------|----|---------|------------|-----------|--------|-------|----------|--------|----------|---------|----------|---------|----------|----------|---------|----------|
| 1 | 1.689(2) | -- | C(41) | | | | Intra | 128.07 | -0.29 | -0.45820 | 0.56434 | -0.46006 | -3.8627 | 13.4399 | -16.8686 | | |
| 2 | 2.7308(19) | << | N(41) | | | | Intra | 136.35 | -22.17 | -0.55170 | 0.58178 | -0.48794 | -4.6509 | 13.8552 | -17.8908 | | |
| 3 | 2.7623(19) | << | N(42) | | | | Intra | 121.04 | 21.79 | -0.49150 | 0.60077 | -0.43186 | -4.1434 | 14.3075 | -15.8346 | | |
| 4 | 3.223(2) | << | C(49) | | | | Intra | 73.08 | 50.93 | -0.26450 | 0.59010 | -0.39159 | -2.2298 | 14.0533 | -14.3580 | | |
| 5 | 3.234(2) | << | C(44) | | | | Intra | 110.68 | 46.48 | -0.42790 | 0.59597 | -0.39588 | -3.6073 | 14.1931 | -14.5153 | | |
| 6 | 3.260(2) | .< | N(21) | [| = | 02] | | -99.03 | -63.31 | -0.36190 | 0.44776 | -0.53926 | -3.0509 | 10.6635 | -19.7725 | | |
| 7 | 2.43(3) | << | H(21) | [| = | 02] | | -98.87 | -62.72 | -0.35500 | 0.46230 | -0.51870 | -2.9927 | 11.0098 | -19.0187 | | |
| 8 | 2.83 | .< | H(52A)a | [-1-x, | -1/2+y, | -1/2-z | = | 4444.03] | | -155.39 | -4.59 | -0.63860 | 0.45920 | -0.46600 | -5.3835 | 10.9359 | -17.0864 |
| 9 | 2.88 | .< | H(59A)b | [-x, | -1/2+y, | -1/2-z | = | 4544.03] | | -63.75 | 47.46 | -0.23240 | 0.43510 | -0.40190 | -1.9592 | 10.3620 | -14.7361 |
| 10 | 2.89 | .< | H(49A) | | | | Intra | 59.36 | 37.29 | -0.19540 | 0.59170 | -0.41200 | -1.6473 | 14.0915 | -15.1064 | | |
| 11 | 2.92(3) | .< | H(41) | | | | Intra | 144.47 | -37.99 | -0.55700 | 0.56470 | -0.50890 | -4.6956 | 13.4484 | -18.6593 | | |

Angles (Degrees) At1...V...At2 with Vertex V = S(4)

| | | | | | | | | | | | | | | | |
|-------|---|-------|-----------|-------|---|-------|-----------|-------|---|-------|-----------|-------|---|-------|-----------|
| C(41) | , | N(41) | 23.33(8) | C(41) | , | N(42) | 23.12(8) | C(41) | , | C(49) | 69.04(8) | C(41) | , | C(44) | 49.19(8) |
| C(41) | , | N(21) | 107.54(9) | N(41) | , | N(42) | 46.44(5) | N(41) | , | C(49) | 91.75(5) | N(41) | , | C(44) | 72.48(5) |
| N(41) | , | N(21) | 84.21(5) | N(42) | , | C(49) | 47.14(5) | N(42) | , | C(44) | 26.08(5) | N(42) | , | N(21) | 130.61(5) |
| C(49) | , | C(44) | 24.93(4) | C(49) | , | N(21) | 166.92(5) | C(44) | , | N(21) | 156.43(5) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = S(5) [ARU = 1555.03] 0.12980 0.86139 -0.04060 1.0942 20.5142 -1.4886

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|---------|------------------|------------|--------|-------|---------|--------|----------|---------|----------|---------|---------|---------|
| 1 | 1.691(2) | -- | C(51) | | | | Intra | 145.33 | -12.51 | -0.03130 | 0.90083 | -0.05059 | -0.2639 | 21.4534 | -1.8549 |
| 2 | 2.716(3) | << | N(51) | | | | Intra | 151.84 | 10.26 | -0.14970 | 0.91436 | -0.02741 | -1.2620 | 21.7757 | -1.0050 |
| 3 | 2.7642(19) | << | N(52) | | | | Intra | 138.25 | -34.37 | -0.07210 | 0.92519 | -0.08316 | -0.6078 | 22.0336 | -3.0491 |
| 4 | 3.284(2) | << | C(54) | | | | Intra | 126.68 | -58.58 | 0.00850 | 0.91903 | -0.11702 | 0.0717 | 21.8869 | -4.2907 |
| 5 | 3.288(2) | << | C(59) | | | | Intra | 77.03 | -61.24 | 0.17190 | 0.92612 | -0.11920 | 1.4492 | 22.0557 | -4.3706 |
| 6 | 3.370(2) | .. | N(61) | [| = 04] | | | -117.95 | 42.92 | -0.00740 | 0.76987 | 0.02198 | -0.0624 | 18.3346 | 0.8059 |
| 7 | 3.441(3) | .< | C(63)a | [1/2+x,3/2-y,-z | = 3565.04] | | | -26.98 | -13.59 | 0.48340 | 0.79768 | -0.06265 | 4.0752 | 18.9969 | -2.2971 |
| 8 | 3.495(2) | .. | N(62)a | [1/2+x,3/2-y,-z | = 3565.04] | | | -50.38 | -19.47 | 0.37910 | 0.75481 | -0.07238 | 3.1959 | 17.9760 | -2.6539 |
| 9 | 3.508(3) | .. | C(69)a | [1/2+x,3/2-y,-z | = 3565.04] | | | -91.68 | -39.64 | 0.12040 | 0.74801 | -0.10164 | 1.0150 | 17.8140 | -3.7267 |
| 10 | 2.54(3) | << | H(61) | [| = 04] | | | -118.60 | 40.41 | 0.02000 | 0.79010 | 0.00430 | 0.1686 | 18.8164 | 0.1577 |
| 11 | 2.87(5) | .< | H(51) | | | | Intra | 158.67 | 25.73 | -0.15600 | 0.90090 | -0.00660 | -1.3151 | 21.4551 | -0.2420 |
| 12 | 2.88 | .< | H(59A) | | | | Intra | 63.77 | -47.13 | 0.23240 | 0.93510 | -0.09810 | 1.9592 | 22.2696 | -3.5969 |
| 13 | 3.13 | .. | H(69A)a | [1/2+x,3/2-y,-z | = 3565.04] | | | -100.22 | -26.32 | 0.07080 | 0.74560 | -0.07840 | 0.5969 | 17.7566 | -2.8746 |
| 14 | 3.21 | .. | H(22A)b | [-x,1/2+y,-1/2-z | = 4554.02] | | | 79.50 | 72.19 | 0.15100 | 0.90190 | 0.04270 | 1.2730 | 21.4789 | 1.5656 |
| 15 | 3.46 | .. | H(63A)a | [1/2+x,3/2-y,-z | = 3565.04] | | | -12.80 | -21.82 | 0.50160 | 0.83150 | -0.07570 | 4.2286 | 19.8023 | -2.7756 |

Angles (Degrees) At1...V...At2 with Vertex V = S(5)

| | | | | | | | | | | | | | | | |
|-------|---|--------|-----------|--------|---|--------|-----------|--------|---|--------|-----------|--------|---|--------|-----------|
| C(51) | , | N(51) | 23.66(9) | C(51) | , | N(52) | 22.79(9) | C(51) | , | C(54) | 48.16(9) | C(51) | , | C(59) | 68.68(9) |
| C(51) | , | N(61) | 103.36(9) | C(51) | , | C(63)a | 152.81(9) | C(51) | , | N(62)a | 144.47(9) | C(51) | , | C(69)a | 105.73(9) |
| N(51) | , | N(52) | 46.45(6) | N(51) | , | C(54) | 71.80(6) | N(51) | , | C(59) | 91.83(6) | N(51) | , | N(61) | 83.19(6) |
| N(51) | , | C(63)a | 176.47(6) | N(51) | , | N(62)a | 156.67(6) | N(51) | , | C(69)a | 116.84(6) | N(52) | , | C(54) | 25.40(6) |
| N(52) | , | C(59) | 46.67(6) | N(52) | , | N(61) | 121.91(6) | N(52) | , | C(63)a | 130.03(6) | N(52) | , | N(62)a | 125.54(5) |
| N(52) | , | C(69)a | 92.81(6) | C(54) | , | C(59) | 24.43(6) | C(54) | , | N(61) | 138.13(6) | C(54) | , | C(63)a | 104.69(6) |
| C(54) | , | N(62)a | 101.91(5) | C(54) | , | C(69)a | 76.72(6) | C(59) | , | N(61) | 159.61(6) | C(59) | , | C(63)a | 84.68(6) |
| C(59) | , | N(62)a | 89.05(5) | C(59) | , | C(69)a | 78.70(6) | N(61) | , | C(63)a | 99.91(6) | N(61) | , | N(62)a | 87.92(5) |
| N(61) | , | C(69)a | 85.92(6) | C(63)a | , | N(62)a | 23.17(5) | C(63)a | , | C(69)a | 61.99(6) | N(62)a | , | C(69)a | 40.71(5) |

=====

3.6 Angstrom Coordination Sphere Around Atom I = F(11) [ARU = 1555.05] -0.15030 0.72885 -0.24630 -1.2671 17.3577 -9.0308

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|-------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.335(3) | -- | C(110) | | | | Intra | 169.06 | -55.40 | -0.23860 | 0.73489 | -0.27627 | -2.0114 | 17.5016 | -10.1297 |
| 2 | 2.143(3) | << | F(12) | | | | Intra | 140.36 | -25.31 | -0.32730 | 0.78075 | -0.27129 | -2.7592 | 18.5937 | -9.9471 |
| 3 | 2.149(2) | << | F(13) | | | | Intra | 150.70 | -32.12 | -0.33860 | 0.69145 | -0.27747 | -2.8545 | 16.4670 | -10.1737 |
| 4 | 2.361(2) | << | C(16) | | | | Intra | 71.68 | -83.48 | -0.14030 | 0.73954 | -0.31028 | -1.1828 | 17.6123 | -11.3767 |
| 5 | 2.730(3) | << | C(17) | | | | Intra | 15.64 | -56.21 | 0.02310 | 0.74603 | -0.30817 | 0.1947 | 17.7669 | -11.2994 |
| 6 | 3.057(12) | .. | <F(53A) | [| = | 03] | | 69.54 | 7.44 | -0.02460 | 0.84810 | -0.23550 | -0.2074 | 20.1977 | -8.6348 |
| 7 | 3.125(10) | .. | >F(22)a | [-1/2-x,1-y,1/2+z | = | 2465.02] | | -67.52 | -4.51 | -0.00900 | 0.60800 | -0.25300 | -0.0759 | 14.4796 | -9.2765 |
| 8 | 3.152(14) | .. | <F(22A)a | [-1/2-x,1-y,1/2+z | = | 2465.02] | | -98.03 | 13.86 | -0.20100 | 0.60160 | -0.22570 | -1.6945 | 14.3272 | -8.2755 |
| 9 | 3.246(9) | .. | >F(52) | [| = | 03] | | 100.18 | 26.50 | -0.21120 | 0.84890 | -0.20680 | -1.7805 | 20.2167 | -7.5825 |
| 10 | 3.336(4) | .. | >F(63A)b | [-1/2+x,3/2-y,-z | = | 3465.04] | | 173.21 | 27.07 | -0.50020 | 0.74360 | -0.20490 | -4.2168 | 17.7090 | -7.5129 |
| 11 | 3.45(2) | .. | <F(23A)a | [-1/2-x,1-y,1/2+z | = | 2465.02] | | -66.51 | -6.17 | 0.01170 | 0.59690 | -0.25640 | 0.0986 | 14.2153 | -9.4012 |
| 12 | 3.518(3) | .. | F(66)c | [1/2+x,3/2-y,-z | = | 3565.04] | | -124.07 | 76.90 | -0.20330 | 0.70111 | -0.15286 | -1.7139 | 16.6971 | -5.6048 |
| 13 | 3.545(14) | .. | >F(53) | [| = | 03] | | 71.91 | 2.53 | -0.01990 | 0.87020 | -0.24204 | -0.1678 | 20.7240 | -8.8746 |
| 14 | 2.42 | << | H(17A) | | | | Intra | 11.82 | -36.28 | 0.07590 | 0.74560 | -0.28530 | 0.6399 | 17.7566 | -10.4608 |
| 15 | 2.67 | < | H(67A)c | [1/2+x,3/2-y,-z | = | 3565.04] | | 15.75 | 51.79 | 0.03850 | 0.74770 | -0.18900 | 0.3246 | 17.8066 | -6.9299 |

Angles (Degrees) At1...V...At2 with Vertex V = F(11)

| | | | | | | | |
|---------------------|------------|---------------------|------------|--------------------|------------|--------------------|-----------|
| C(110) , F(12) | 36.66(13) | C(110) , F(13) | 36.40(13) | C(110) , C(16) | 35.95(13) | C(110) , C(17) | 66.32(13) |
| C(110) , <F(53A) | 101.5(3) | C(110) , >F(22)a | 104.3(3) | C(110) , <F(22A)a | 103.0(3) | C(110) , >F(52) | 100.6(2) |
| C(110) , >F(63A)b | 82.54(14) | C(110) , <F(23A)a | 103.3(3) | C(110) , F(66)c | 138.68(15) | C(110) , >F(53) | 96.14(19) |
| F(12) , F(13) | 59.83(8) | F(12) , C(16) | 62.48(8) | F(12) , C(17) | 86.05(8) | F(12) , <F(53A) | 76.2(2) |
| F(12) , >F(22)a | 139.7(2) | F(12) , <F(22A)a | 124.2(2) | F(12) , >F(52) | 64.70(18) | F(12) , >F(63A)b | 61.20(11) |
| F(12) , <F(23A)a | 139.1(3) | F(12) , F(66)c | 115.87(8) | F(12) , >F(53) | 71.77(15) | F(13) , C(16) | 62.79(9) |
| F(13) , C(17) | 90.90(9) | F(13) , <F(53A) | 135.2(2) | F(13) , >F(22)a | 81.8(2) | F(13) , <F(22A)a | 68.2(2) |
| F(13) , >F(52) | 119.0(2) | F(13) , >F(63A)b | 68.44(10) | F(13) , <F(23A)a | 81.8(2) | F(13) , F(66)c | 110.26(9) |
| F(13) , >F(53) | 130.24(15) | C(16) , C(17) | 30.57(8) | C(16) , <F(53A) | 90.9(2) | C(16) , >F(22)a | 90.4(2) |
| C(16) , <F(22A)a | 110.3(2) | C(16) , >F(52) | 110.73(16) | C(16) , >F(63A)b | 118.18(11) | C(16) , <F(23A)a | 88.7(3) |
| C(16) , F(66)c | 172.95(10) | C(16) , >F(53) | 86.00(13) | C(17) , <F(53A) | 77.5(2) | C(17) , >F(22)a | 82.5(2) |
| C(17) , <F(22A)a | 114.6(2) | C(17) , >F(52) | 108.88(18) | C(17) , >F(63A)b | 146.71(11) | C(17) , <F(23A)a | 80.5(3) |
| C(17) , F(66)c | 154.91(9) | C(17) , >F(53) | 74.23(13) | <F(53A) , >F(22)a | 137.2(3) | <F(53A) , <F(22A)a | 155.4(3) |
| <F(53A) , >F(52) | 34.8(3) | <F(53A) , >F(63A)b | 98.6(2) | <F(53A) , <F(23A)a | 136.4(3) | <F(53A) , F(66)c | 95.3(2) |
| <F(53A) , >F(53) | 5.5(2) | >F(22)a , <F(22A)a | 35.4(3) | >F(22)a , >F(52) | 155.1(3) | >F(22)a , >F(63A)b | 118.0(2) |
| >F(22)a , <F(23A)a | 1.9(3) | >F(22)a , F(66)c | 87.3(2) | >F(22)a , >F(53) | 139.5(2) | <F(22A)a , >F(52) | 135.9(3) |
| <F(22A)a , >F(63A)b | 82.7(2) | <F(22A)a , <F(23A)a | 37.2(3) | <F(22A)a , F(66)c | 64.5(2) | <F(22A)a , >F(53) | 160.8(2) |
| >F(52) , >F(63A)b | 64.2(2) | >F(52) , <F(23A)a | 156.0(3) | >F(52) , F(66)c | 73.19(15) | >F(52) , >F(53) | 36.2(2) |
| >F(63A)b , <F(23A)a | 119.7(3) | >F(63A)b , F(66)c | 57.61(8) | >F(63A)b , >F(53) | 98.87(18) | <F(23A)a , F(66)c | 89.1(3) |
| <F(23A)a , >F(53) | 138.4(3) | F(66)c , >F(53) | 100.07(12) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(12) [ARU = 1555.05] -0.32730 0.78075 -0.27129 -2.7592 18.5937 -9.9471

| Nr | d(I,J) | To Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|------------|--------------------|------------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.336(3) | -- | C(110) | | | Intra | -55.60 | -7.85 | -0.23860 | 0.73489 | -0.27627 | -2.0114 | 17.5016 | -10.1297 |
| 2 | 2.141(3) | << | F(13) | | | Intra | -92.56 | -6.08 | -0.33860 | 0.69145 | -0.27747 | -2.8545 | 16.4670 | -10.1737 |
| 3 | 2.143(3) | << | F(11) | | | Intra | -39.64 | 25.31 | -0.15030 | 0.72885 | -0.24630 | -1.2671 | 17.3577 | -9.0308 |
| 4 | 2.344(3) | << | C(16) | | | Intra | -31.90 | -37.59 | -0.14030 | 0.73954 | -0.31028 | -1.1828 | 17.6123 | -11.3767 |
| 5 | 2.965(10) | .. | <F(31B)d | [-1/2+x,3/2-y,-1-z | = 3464.01] | | 122.37 | -11.20 | -0.51200 | 0.88390 | -0.28700 | -4.3163 | 21.0503 | -10.5231 |
| 6 | 2.972(4) | .. | >F(63A)c | [-1/2+x,3/2-y,-z | = 3465.04] | | -148.74 | 54.99 | -0.50020 | 0.74360 | -0.20490 | -4.2168 | 17.7090 | -7.5129 |
| 7 | 2.986(3) | < | C(15) | | | Intra | -47.48 | -62.86 | -0.21810 | 0.73860 | -0.34375 | -1.8386 | 17.5899 | -12.6039 |
| 8 | 3.012(8) | .. | <F(63)c | [-1/2+x,3/2-y,-z | = 3465.04] | | 171.53 | 53.25 | -0.53870 | 0.79190 | -0.20547 | -4.5413 | 18.8593 | -7.5338 |
| 9 | 3.030(9) | .. | >F(52) | [| = 03] | | 58.91 | 51.29 | -0.21120 | 0.84890 | -0.20680 | -1.7805 | 20.2167 | -7.5825 |
| 10 | 3.040(9) | .. | <F(31)d | [-1/2+x,3/2-y,-1-z | = 3464.01] | | 114.49 | -18.06 | -0.46940 | 0.89120 | -0.29700 | -3.9571 | 21.2241 | -10.8898 |
| 11 | 3.085(2) | .. | F(14)a | [-1+x,y,z | = 1455.05] | | -170.75 | -24.63 | -0.65560 | 0.76183 | -0.30636 | -5.5268 | 18.1431 | -11.2330 |
| 12 | 3.162(3) | .. | F(35)b | [1/2+x,3/2-y,-1-z | = 3564.01] | | 56.99 | -34.28 | -0.15850 | 0.87273 | -0.31986 | -1.3362 | 20.7842 | -11.7280 |
| 13 | 3.186(13) | .. | <F(52A) | [| = 03] | | 71.41 | 45.33 | -0.24260 | 0.86990 | -0.20950 | -2.0452 | 20.7168 | -7.6815 |
| 14 | 3.287(10) | .. | <F(53A) | [| = 03] | | 32.15 | 23.53 | -0.02460 | 0.84810 | -0.23550 | -0.2074 | 20.1977 | -8.6348 |
| 15 | 3.352(3) | .. | C(17) | | | Intra | -15.64 | -23.79 | 0.02310 | 0.74603 | -0.30817 | 0.1947 | 17.7669 | -11.2994 |
| 16 | 3.405(8) | .. | >F(62A)c | [-1/2+x,3/2-y,-z | = 3465.04] | | 169.46 | 31.05 | -0.66750 | 0.80315 | -0.22340 | -5.6272 | 19.1272 | -8.1912 |
| 17 | 3.522(11) | .. | >F(53) | [| = 03] | | 39.42 | 17.73 | -0.01990 | 0.87020 | -0.24204 | -0.1678 | 20.7240 | -8.8746 |
| 18 | 3.594(13) | .. | <F(61)c | [-1/2+x,3/2-y,-z | = 3465.04] | | -147.25 | 32.10 | -0.63100 | 0.71160 | -0.21920 | -5.3195 | 16.9469 | -8.0372 |
| 19 | 2.93 | .. | H(15A) | | | Intra | -90.88 | -66.98 | -0.32940 | 0.73260 | -0.34490 | -2.7769 | 17.4470 | -12.6461 |
| 20 | 3.54 | .. | H(17A) | | | Intra | -13.84 | -8.35 | 0.07590 | 0.74560 | -0.28530 | 0.6399 | 17.7566 | -10.4608 |

Angles (Degrees) At1...V...At2 with Vertex V = F(12)

| | | | | | | | |
|-------------------|------------|-------------------|------------|--------------------|------------|-------------------|------------|
| C(110) , F(13) | 36.72(13) | C(110) , F(11) | 36.62(12) | C(110) , C(16) | 36.67(12) | C(110) , <F(31B)d | 160.8(3) |
| C(110) , >F(63A)c | 98.23(18) | C(110) , C(15) | 55.32(12) | C(110) , <F(63)c | 120.9(3) | C(110) , >F(52) | 111.3(2) |
| C(110) , <F(31)d | 152.30(19) | C(110) , F(14)a | 109.01(15) | C(110) , F(35)b | 103.74(14) | C(110) , <F(52A) | 121.1(2) |
| C(110) , <F(53A) | 91.1(2) | C(110) , C(17) | 41.42(12) | C(110) , >F(62A)c | 132.06(16) | C(110) , >F(53) | 97.1(2) |
| C(110) , <F(61)c | 95.6(2) | F(13) , F(11) | 60.22(9) | F(13) , C(16) | 63.22(9) | F(13) , <F(31B)d | 141.2(2) |
| F(13) , >F(63A)c | 76.65(15) | F(13) , C(15) | 65.52(8) | F(13) , <F(63)c | 98.4(3) | F(13) , >F(52) | 128.98(19) |
| F(13) , <F(31)d | 144.01(17) | F(13) , F(14)a | 76.75(8) | F(13) , F(35)b | 130.44(9) | F(13) , <F(52A) | 138.4(2) |
| F(13) , <F(53A) | 124.2(2) | F(13) , C(17) | 75.61(8) | F(13) , >F(62A)c | 99.95(11) | F(13) , >F(53) | 131.8(2) |
| F(13) , <F(61)c | 64.49(15) | F(11) , C(16) | 63.32(8) | F(11) , <F(31B)d | 157.9(2) | F(11) , >F(63A)c | 79.61(12) |
| F(11) , C(15) | 88.39(8) | F(11) , <F(63)c | 96.9(2) | F(11) , >F(52) | 75.6(2) | F(11) , <F(31)d | 154.94(18) |
| F(11) , F(14)a | 135.94(11) | F(11) , F(35)b | 109.09(8) | F(11) , <F(52A) | 85.7(2) | F(11) , <F(53A) | 64.6(2) |
| F(11) , C(17) | 54.32(7) | F(11) , >F(62A)c | 117.15(12) | F(11) , >F(53) | 72.9(2) | F(11) , <F(61)c | 90.3(2) |
| C(16) , <F(31B)d | 125.6(2) | C(16) , >F(63A)c | 134.82(16) | C(16) , C(15) | 26.99(7) | C(16) , <F(63)c | 157.5(3) |
| C(16) , >F(52) | 118.9(2) | C(16) , <F(31)d | 115.99(16) | C(16) , F(14)a | 106.74(9) | C(16) , F(35)b | 69.13(7) |
| C(16) , <F(52A) | 124.20(15) | C(16) , <F(53A) | 85.7(2) | C(16) , C(17) | 19.59(7) | C(16) , >F(62A)c | 161.23(13) |
| C(16) , >F(53) | 86.80(17) | C(16) , <F(61)c | 127.70(17) | <F(31B)d, >F(63A)c | 98.5(3) | <F(31B)d, C(15) | 105.5(2) |
| <F(31B)d, <F(63)c | 76.8(3) | <F(31B)d, >F(52) | 83.0(3) | <F(31B)d, <F(31)d | 10.3(3) | <F(31B)d, F(14)a | 64.5(2) |
| <F(31B)d, F(35)b | 63.4(2) | <F(31B)d, <F(52A) | 72.8(3) | <F(31B)d, <F(53A) | 94.6(3) | <F(31B)d, C(17) | 126.1(2) |

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<F(31B)d, >F(62A)c    61.8(2)  <F(31B)d, >F(53)    86.8(3)  <F(31B)d, <F(61)c    96.3(3)  >F(63A)c, C(15)    141.26(15)
>F(63A)c, <F(63)c    23.0(3)  >F(63A)c, >F(52)    71.3(2)  >F(63A)c, <F(31)d  108.56(19) >F(63A)c, F(14)a    81.83(9)
>F(63A)c, F(35)b    152.67(15) >F(63A)c, <F(52A)    74.1(2)  >F(63A)c, <F(53A)    101.5(2)  >F(63A)c, C(17)    133.56(13)
>F(63A)c, >F(62A)c    37.92(14) >F(63A)c, >F(53)    106.95(15) >F(63A)c, <F(61)c    22.9(2)  C(15) , <F(63)c    157.7(2)
C(15) , >F(52)    140.8(2)  C(15) , <F(31)d    97.84(15)  C(15) , F(14)a    81.76(7)  C(15) , F(35)b    65.98(6)
C(15) , <F(52A)    141.98(18) C(15) , <F(53A)    106.3(2)  C(15) , C(17)    44.47(7)  C(15) , >F(62A)c  140.47(13)
C(15) , >F(53)    104.33(14) C(15) , <F(61)c    122.58(17) <F(63)c , >F(52)    61.2(3)  <F(63)c , <F(31)d    86.5(3)
<F(63)c , F(14)a    79.40(18) <F(63)c , F(35)b    131.0(3)  <F(63)c , <F(52A)    60.3(3)  <F(63)c , <F(53A)    95.5(3)
<F(63)c , C(17)    150.04(19) <F(63)c , >F(62A)c    22.3(2)  <F(63)c , >F(53)    97.9(3)  <F(63)c , <F(61)c    36.2(3)
>F(52) , <F(31)d    84.6(2)  >F(52) , F(14)a    133.9(2)  >F(52) , F(35)b    85.59(18) >F(52) , <F(52A)    10.2(3)
>F(52) , <F(53A)    34.6(3)  >F(52) , C(17)    99.3(2)  >F(52) , >F(62A)c    77.6(2)  >F(52) , >F(53)    37.0(2)
>F(52) , <F(61)c    93.5(3)  <F(31)d , F(14)a    69.12(16) <F(31)d , F(35)b    53.36(15) <F(31)d , <F(52A)    74.5(3)
<F(31)d , <F(53A)    90.4(3)  <F(31)d , C(17)    115.82(16) <F(31)d , >F(62A)c    72.09(17) <F(31)d , >F(53)    82.0(3)
<F(31)d , <F(61)c    106.3(2)  F(14)a , F(35)b    105.68(7)  F(14)a , <F(52A)    126.50(16) F(14)a , <F(53A)    159.1(2)
F(14)a , C(17)    125.90(7)  F(14)a , >F(62A)c    58.81(12)  F(14)a , >F(53)    151.1(2)  F(14)a , <F(61)c    61.0(2)
F(35)b , <F(52A)    80.7(2)  F(35)b , <F(53A)    62.4(2)  F(35)b , C(17)    63.07(6)  F(35)b , >F(62A)c  124.13(10)
F(35)b , >F(53)    54.64(14)  F(35)b , <F(61)c    159.7(2)  <F(52A) , <F(53A)    38.5(2)  <F(52A) , C(17)    104.70(14)
<F(52A) , >F(62A)c    73.60(17) <F(52A) , >F(53)    38.32(19) <F(52A) , <F(61)c    95.0(2)  <F(53A) , C(17)    66.26(19)
<F(53A) , >F(62A)c    111.8(2)  <F(53A) , >F(53)    8.9(3)  <F(53A) , <F(61)c    124.4(3)  C(17) , >F(62A)c  171.45(12)
C(17) , >F(53)    67.89(16)  C(17) , <F(61)c    136.81(18) >F(62A)c, >F(53)    111.59(18) >F(62A)c, <F(61)c    36.64(17)
>F(53) , <F(61)c    129.8(2)
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3.6 Angstrom Coordination Sphere Around Atom I = F(13) [ARU = 1555.05] -0.33860 0.69145 -0.27747 -2.8545 16.4670-10.1737

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|-------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.335(3) | -- | C(110) | | | | Intra | 50.82 | 1.89 | -0.23860 | 0.73489 | -0.27627 | -2.0114 | 17.5016 | -10.1297 |
| 2 | 2.141(3) | << | F(12) | | | | Intra | 87.44 | 6.08 | -0.32730 | 0.78075 | -0.27129 | -2.7592 | 18.5937 | -9.9471 |
| 3 | 2.149(2) | << | F(11) | | | | Intra | 29.30 | 32.12 | -0.15030 | 0.72885 | -0.24630 | -1.2671 | 17.3577 | -9.0308 |
| 4 | 2.357(3) | << | C(16) | | | | Intra | 34.41 | -30.70 | -0.14030 | 0.73954 | -0.31028 | -1.1828 | 17.6123 | -11.3767 |
| 5 | 2.863(3) | << | C(15) | | | | Intra | 47.87 | -58.07 | -0.21810 | 0.73860 | -0.34375 | -1.8386 | 17.5899 | -12.6039 |
| 6 | 3.087(13) | .. | <F(22A)b | [-1/2-x,1-y,1/2+z | = | 2465.02] | | -61.54 | 37.95 | -0.20100 | 0.60160 | -0.22570 | -1.6945 | 14.3272 | -8.2755 |
| 7 | 3.120(2) | .. | F(41) | [| = | 06] | | -152.44 | -11.68 | -0.65990 | 0.63209 | -0.29470 | -5.5631 | 15.0533 | -10.8055 |
| 8 | 3.160(3) | .. | F(43) | [| = | 06] | | -116.43 | 6.09 | -0.50450 | 0.57329 | -0.26832 | -4.2530 | 13.6530 | -9.8382 |
| 9 | 3.200(3) | .. | C(47) | [| = | 06] | | -83.91 | -33.96 | -0.30520 | 0.58063 | -0.32622 | -2.5729 | 13.8278 | -11.9612 |
| 10 | 3.237(5) | .. | >F(63A)c | [-1/2+x,3/2-y,-z | = | 3465.04] | | 137.65 | 55.29 | -0.50020 | 0.74360 | -0.20490 | -4.2168 | 17.7090 | -7.5129 |
| 11 | 3.297(14) | .. | <F(61)c | [-1/2+x,3/2-y,-z | = | 3465.04] | | 168.98 | 40.39 | -0.63100 | 0.71160 | -0.21920 | -5.3195 | 16.9469 | -8.0372 |
| 12 | 3.328(3) | .. | F(14)a | [-1+x,y,z | = | 1455.05] | | 147.90 | -18.56 | -0.65560 | 0.76183 | -0.30636 | -5.5268 | 18.1431 | -11.2330 |
| 13 | 3.342(3) | .. | C(46) | [| = | 06] | | -113.69 | -36.28 | -0.46700 | 0.58785 | -0.33140 | -3.9369 | 13.9998 | -12.1511 |
| 14 | 3.350(3) | .. | C(410) | [| = | 06] | | -128.43 | -13.92 | -0.57830 | 0.58451 | -0.29945 | -4.8752 | 13.9202 | -10.9796 |
| 15 | 3.479(16) | .. | >F(21)b | [-1/2-x,1-y,1/2+z | = | 2465.02] | | -69.52 | 32.49 | -0.21680 | 0.57600 | -0.22650 | -1.8277 | 13.7176 | -8.3049 |
| 16 | 3.501(3) | .. | C(17) | | | | Intra | 23.09 | -18.76 | 0.02310 | 0.74603 | -0.30817 | 0.1947 | 17.7669 | -11.2994 |
| 17 | 3.532(11) | .. | >F(22)b | [-1/2-x,1-y,1/2+z | = | 2465.02] | | -35.57 | 14.72 | -0.00900 | 0.60800 | -0.25300 | -0.0759 | 14.4796 | -9.2765 |
| 18 | 2.66 | .< | H(15A) | | | | Intra | 85.47 | -68.32 | -0.32940 | 0.73260 | -0.34490 | -2.7769 | 17.4470 | -12.6461 |
| 19 | 2.99 | .. | H(47A) | [| = | 06] | | -77.09 | -17.88 | -0.26320 | 0.57500 | -0.30250 | -2.2188 | 13.6937 | -11.0915 |

Angles (Degrees) At1...V...At2 with Vertex V = F(13)

| | | | | | | | |
|-------------------|------------|--------------------|------------|-------------------|------------|------------------|------------|
| C(110) , F(12) | 36.75(13) | C(110) , F(11) | 36.40(12) | C(110) , C(16) | 36.14(12) | C(110) , C(15) | 60.01(12) |
| C(110) , <F(22A)b | 106.2(3) | C(110) , F(41) | 154.94(16) | C(110) , F(43) | 164.98(15) | C(110) , C(47) | 127.00(15) |
| C(110) , >F(63A)c | 86.64(17) | C(110) , <F(61)c | 109.8(2) | C(110) , F(14)a | 97.31(15) | C(110) , C(46) | 142.75(15) |
| C(110) , C(410) | 167.94(15) | C(110) , >F(21)b | 114.1(2) | C(110) , C(17) | 34.20(12) | C(110) , >F(22)b | 86.0(2) |
| F(12) , F(11) | 59.95(9) | F(12) , C(16) | 62.59(8) | F(12) , C(15) | 71.61(8) | F(12) , <F(22A)b | 127.4(3) |
| F(12) , F(41) | 120.68(9) | F(12) , F(43) | 153.25(9) | F(12) , C(47) | 150.99(10) | F(12) , >F(63A)c | 63.29(13) |
| F(12) , <F(61)c | 79.64(15) | F(12) , F(14)a | 64.47(7) | F(12) , C(46) | 144.14(9) | F(12) , C(410) | 143.87(10) |
| F(12) , >F(21)b | 135.6(2) | F(12) , C(17) | 68.06(7) | F(12) , >F(22)b | 119.81(18) | F(11) , C(16) | 63.01(8) |
| F(11) , C(15) | 91.53(9) | F(11) , <F(22A)b | 71.5(2) | F(11) , F(41) | 159.50(10) | F(11) , F(43) | 129.75(10) |
| F(11) , C(47) | 125.02(10) | F(11) , >F(63A)c | 73.43(10) | F(11) , <F(61)c | 98.5(2) | F(11) , F(14)a | 123.62(10) |
| F(11) , C(46) | 149.29(10) | F(11) , C(410) | 152.70(10) | F(11) , >F(21)b | 79.9(2) | F(11) , C(17) | 51.23(7) |
| F(11) , >F(22)b | 61.12(18) | C(16) , C(15) | 28.89(7) | C(16) , <F(22A)b | 112.6(2) | C(16) , F(41) | 137.11(9) |
| C(16) , F(43) | 143.21(10) | C(16) , C(47) | 93.05(9) | C(16) , >F(63A)c | 122.12(14) | C(16) , <F(61)c | 142.22(16) |
| C(16) , F(14)a | 99.35(9) | C(16) , C(46) | 106.65(9) | C(16) , C(410) | 132.43(9) | C(16) , >F(21)b | 116.67(14) |
| C(16) , C(17) | 15.74(7) | C(16) , >F(22)b | 81.09(19) | C(15) , <F(22A)b | 131.3(2) | C(15) , F(41) | 108.29(8) |
| C(15) , F(43) | 126.61(8) | C(15) , C(47) | 79.52(7) | C(15) , >F(63A)c | 134.15(14) | C(15) , <F(61)c | 139.30(19) |
| C(15) , F(14)a | 79.47(7) | C(15) , C(46) | 84.39(7) | C(15) , C(410) | 107.94(8) | C(15) , >F(21)b | 131.38(14) |
| C(15) , C(17) | 43.32(7) | C(15) , >F(22)b | 99.04(19) | <F(22A)b, F(41) | 97.9(2) | <F(22A)b, F(43) | 58.9(2) |
| <F(22A)b, C(47) | 74.9(2) | <F(22A)b, >F(63A)c | 85.3(2) | <F(22A)b, <F(61)c | 89.1(3) | <F(22A)b, F(14)a | 147.9(2) |

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<F(22A)b, C(46)      88.5(2)  <F(22A)b, C(410)    81.2(2)  <F(22A)b, >F(21)b    8.5(3)  <F(22A)b, C(17)     97.3(2)
<F(22A)b, >F(22)b   32.7(3)  F(41) , F(43)      39.99(5)  F(41) , C(47)       65.77(7)  F(41) , >F(63A)c   88.56(10)
F(41) , <F(61)c    63.1(2)  F(41) , F(14)a     57.76(6)  F(41) , C(46)       42.65(6)  F(41) , C(410)     23.51(6)
F(41) , >F(21)b    90.40(18)  F(41) , C(17)     149.24(8)  F(41) , >F(22)b    118.65(18)  F(43) , C(47)      50.49(6)
F(43) , >F(63A)c   93.91(13)  F(43) , <F(61)c    74.33(15)  F(43) , F(14)a      97.29(7)  F(43) , C(46)      42.45(5)
F(43) , C(410)     23.29(5)  F(43) , >F(21)b    50.95(19)  F(43) , C(17)      138.61(8)  F(43) , >F(22)b    79.64(17)
C(47) , >F(63A)c   144.35(14)  C(47) , <F(61)c    123.22(18)  C(47) , F(14)a     107.96(8)  C(47) , C(46)      24.37(6)
C(47) , C(410)     44.89(7)  C(47) , >F(21)b    67.8(2)   C(47) , C(17)      92.87(7)   C(47) , >F(22)b    66.96(18)
>F(63A)c, <F(61)c   25.4(2)   >F(63A)c, F(14)a    74.36(10)  >F(63A)c, C(46)     129.29(12)  >F(63A)c, C(410)   103.63(12)
>F(63A)c, >F(21)b   89.2(2)   >F(63A)c, C(17)    119.24(12)  >F(63A)c, >F(22)b   109.8(2)   <F(61)c , F(14)a    62.1(2)
<F(61)c , C(46)    104.4(2)  <F(61)c , C(410)   79.37(19)  <F(61)c , >F(21)b   89.3(2)   <F(61)c , C(17)    143.66(19)
<F(61)c , >F(22)b   120.4(3)  F(14)a , C(46)     85.61(7)   F(14)a , C(410)     79.74(7)   F(14)a , >F(21)b   143.71(14)
F(14)a , C(17)     114.21(7)  F(14)a , >F(22)b   174.91(18)  C(46) , C(410)     25.96(6)   C(46) , >F(21)b    80.2(2)
C(46) , C(17)      111.47(7)  C(46) , >F(22)b    89.41(18)  C(410) , >F(21)b    72.9(2)   C(410) , C(17)    136.93(8)
C(410) , >F(22)b   96.19(18)  >F(21)b , C(17)    102.07(13)  >F(21)b , >F(22)b   35.6(2)   C(17) , >F(22)b    66.76(18)
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3.6 Angstrom Coordination Sphere Around Atom I = F(14) [ARU = 1555.05] 0.34440 0.76183 -0.30636 2.9034 18.1431-11.2330

| Nr | d(I,J) To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------------|---------------------------|------------|--------|---------|--------|---------|---------|----------|--------|---------|----------|
| 1 | 1.321(3) -- | C(120) | | Intra- | 172.70 | -67.64 | 0.28530 | 0.75915 | -0.33967 | 2.4051 | 18.0793 | -12.4543 |
| 2 | 2.141(3) << | F(15) | | Intra- | -84.36 | -58.72 | 0.35737 | 0.71538 | -0.35626 | 3.0127 | 17.0369 | -13.0626 |
| 3 | 2.149(3) << | F(16) | | Intra | 94.33 | -61.78 | 0.33530 | 0.80437 | -0.35799 | 2.8266 | 19.1562 | -13.1261 |
| 4 | 2.363(3) << | C(18) | | Intra- | 174.12 | -31.91 | 0.10770 | 0.75320 | -0.34043 | 0.9079 | 17.9376 | -12.4822 |
| 5 | 2.735(3) << | C(17) | | Intra- | 172.09 | -1.39 | 0.02310 | 0.74603 | -0.30817 | 0.1947 | 17.7669 | -11.2994 |
| 6 | 3.017(8) .. | <F(62)c [1/2+x,3/2-y,-z | = 3565.04] | | 147.59 | 69.87 | 0.24040 | 0.78520 | -0.22910 | 2.0266 | 18.6997 | -8.4002 |
| 7 | 3.064(6) .. | >F(61A)c[1/2+x,3/2-y,-z | = 3565.04] | | -114.27 | 67.53 | 0.28730 | 0.71700 | -0.22915 | 2.4220 | 17.0755 | -8.4020 |
| 8 | 3.085(2) .. | F(12)a [1+x,y,z | = 1655.05] | | 9.25 | 24.63 | 0.67270 | 0.78075 | -0.27129 | 5.6710 | 18.5937 | -9.9471 |
| 9 | 3.119(3) .. | F(41)b [1+x,y,z | = 1655.06] | | -90.67 | 7.88 | 0.34010 | 0.63209 | -0.29470 | 2.8671 | 15.0533 | -10.8055 |
| 10 | 3.199(6) .. | >F(62A)c[1/2+x,3/2-y,-z | = 3565.04] | | 95.82 | 71.99 | 0.33250 | 0.80315 | -0.22340 | 2.8030 | 19.1272 | -8.1912 |
| 11 | 3.228(10) .. | <F(31B)d[1/2+x,3/2-y,-1-z | = 3564.01] | | 67.39 | 12.70 | 0.48800 | 0.88390 | -0.28700 | 4.1139 | 21.0503 | -10.5231 |
| 12 | 3.323(19) .. | <F(31A)d[1/2+x,3/2-y,-1-z | = 3564.01] | | 85.80 | 22.90 | 0.37100 | 0.89000 | -0.27110 | 3.1276 | 21.1955 | -9.9402 |
| 13 | 3.328(3) .. | F(13)a [1+x,y,z | = 1655.05] | | -32.10 | 18.56 | 0.66140 | 0.69145 | -0.27747 | 5.5757 | 16.4670 | -10.1737 |
| 14 | 3.419(11) .. | <F(61)c [1/2+x,3/2-y,-z | = 3565.04] | | -80.16 | 69.20 | 0.36900 | 0.71160 | -0.21920 | 3.1107 | 16.9469 | -8.0372 |
| 15 | 3.475(9) .. | <F(31)d [1/2+x,3/2-y,-1-z | = 3564.01] | | 63.00 | 5.67 | 0.53060 | 0.89120 | -0.29700 | 4.4731 | 21.2241 | -10.8898 |
| 16 | 2.42 << | H(17A) | | Intra- | 170.31 | 18.59 | 0.07590 | 0.74560 | -0.28530 | 0.6399 | 17.7566 | -10.4608 |
| 17 | 3.17 .. | H(15A)a[1+x,y,z | = 1655.05] | | -14.21 | -26.48 | 0.67060 | 0.73260 | -0.34490 | 5.6533 | 17.4470 | -12.6461 |

Angles (Degrees) At1...V...At2 with Vertex V = F(14)

| | | | | | | | |
|---------------------|------------|---------------------|------------|-------------------|------------|---------------------|------------|
| C(120) , F(15) | 37.24(13) | C(120) , F(16) | 36.33(13) | C(120) , C(18) | 35.74(13) | C(120) , C(17) | 66.26(14) |
| C(120) , <F(62)c | 140.1(2) | C(120) , >F(61A)c | 141.1(2) | C(120) , F(12)a | 136.97(15) | C(120) , F(41)b | 94.27(16) |
| C(120) , >F(62A)c | 152.0(2) | C(120) , <F(31B)d | 112.9(3) | C(120) , <F(31A)d | 115.5(4) | C(120) , F(13)a | 124.96(16) |
| C(120) , <F(61)c | 150.5(3) | C(120) , <F(31)d | 107.7(2) | F(15) , F(16) | 59.50(8) | F(15) , C(18) | 63.03(8) |
| F(15) , C(17) | 87.64(9) | F(15) , <F(62)c | 155.9(2) | F(15) , >F(61A)c | 128.15(17) | F(15) , F(12)a | 112.70(9) |
| F(15) , F(41)b | 66.79(8) | F(15) , >F(62A)c | 166.73(14) | F(15) , <F(31B)d | 129.4(2) | F(15) , <F(31A)d | 143.5(3) |
| F(15) , F(13)a | 88.33(8) | F(15) , <F(61)c | 127.95(17) | F(15) , <F(31)d | 121.30(15) | F(16) , C(18) | 62.94(8) |
| F(16) , C(17) | 90.47(9) | F(16) , <F(62)c | 136.9(2) | F(16) , >F(61A)c | 166.64(17) | F(16) , F(12)a | 109.30(9) |
| F(16) , F(41)b | 125.97(10) | F(16) , >F(62A)c | 133.77(13) | F(16) , <F(31B)d | 77.4(2) | F(16) , <F(31A)d | 85.0(3) |
| F(16) , F(13)a | 123.14(9) | F(16) , <F(61)c | 172.24(17) | F(16) , <F(31)d | 71.64(14) | C(18) , C(17) | 30.58(7) |
| C(18) , <F(62)c | 105.49(19) | C(18) , >F(61A)c | 109.00(16) | C(18) , F(12)a | 172.14(10) | C(18) , F(41)b | 88.65(9) |
| C(18) , >F(62A)c | 120.20(18) | C(18) , <F(31B)d | 120.8(2) | C(18) , <F(31A)d | 110.0(4) | C(18) , F(13)a | 143.38(11) |
| C(18) , <F(61)c | 121.0(3) | C(18) , <F(31)d | 120.72(16) | C(17) , <F(62)c | 76.14(19) | C(17) , >F(61A)c | 79.57(16) |
| C(17) , F(12)a | 156.72(9) | C(17) , F(41)b | 81.70(8) | C(17) , >F(62A)c | 91.97(18) | C(17) , <F(31B)d | 120.0(2) |
| C(17) , <F(31A)d | 101.7(4) | C(17) , F(13)a | 137.19(10) | C(17) , <F(61)c | 92.0(3) | C(17) , <F(31)d | 124.87(16) |
| <F(62)c , >F(61A)c | 31.9(3) | <F(62)c , F(12)a | 80.93(18) | <F(62)c , F(41)b | 92.9(2) | <F(62)c , >F(62A)c | 16.5(2) |
| <F(62)c , <F(31B)d | 74.7(3) | <F(62)c , <F(31A)d | 59.0(4) | <F(62)c , F(13)a | 91.57(19) | <F(62)c , <F(61)c | 37.3(3) |
| <F(62)c , <F(31)d | 82.8(3) | >F(61A)c , F(12)a | 78.85(15) | >F(61A)c , F(41)b | 61.73(14) | >F(61A)c , >F(62A)c | 39.06(16) |
| >F(61A)c , <F(31B)d | 99.8(2) | >F(61A)c , <F(31A)d | 88.4(3) | >F(61A)c , F(13)a | 69.91(15) | >F(61A)c , <F(61)c | 12.5(3) |
| >F(61A)c , <F(31)d | 106.78(19) | F(12)a , F(41)b | 95.62(7) | F(12)a , >F(62A)c | 65.59(17) | F(12)a , <F(31B)d | 56.0(2) |
| F(12)a , <F(31A)d | 69.1(4) | F(12)a , F(13)a | 38.77(5) | F(12)a , <F(61)c | 66.9(3) | F(12)a , <F(31)d | 54.83(14) |

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=====
F(41)b , >F(62A)c 100.02(11)   F(41)b , <F(31B)d 150.0(2)   F(41)b , <F(31A)d 149.0(3)   F(41)b , F(13)a 57.78(6)
F(41)b , <F(61)c 61.71(14)   F(41)b , <F(31)d 150.45(15)   >F(62A)c, <F(31B)d 61.7(2)   >F(62A)c, <F(31A)d 49.4(3)
>F(62A)c, F(13)a 82.96(15)   >F(62A)c, <F(61)c 38.79(16)   >F(62A)c, <F(31)d 69.36(17)   <F(31B)d, <F(31A)d 20.2(5)
<F(31B)d, F(13)a 94.7(2)   <F(31B)d, <F(61)c 95.0(3)   <F(31B)d, <F(31)d 8.3(2)   <F(31A)d, F(13)a 106.5(4)
<F(31A)d, <F(61)c 87.3(3)   <F(31A)d, <F(31)d 27.9(4)   F(13)a , <F(61)c 58.5(3)   F(13)a , <F(31)d 93.00(14)
<F(61)c , <F(31)d 101.0(2)

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3.6 Angstrom Coordination Sphere Around Atom I = F(15) [ARU = 1555.05] 0.35737 0.71538 -0.35626 3.0127 17.0369-13.0626

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|------------|-----------|----------|-------|---------|--------|---------|---------|----------|--------|---------|----------|
| 1 | 1.351(3) | -- | C(120) | | | | Intra | 120.24 | 26.76 | 0.28530 | 0.75915 | -0.33967 | 2.4051 | 18.0793 | -12.4543 |
| 2 | 2.128(2) | << | F(16) | | | | Intra | 95.02 | -1.71 | 0.33530 | 0.80437 | -0.35799 | 2.8266 | 19.1562 | -13.1261 |
| 3 | 2.141(3) | << | F(14) | | | | Intra | 95.64 | 58.72 | 0.34440 | 0.76183 | -0.30636 | 2.9034 | 18.1431 | -11.2330 |
| 4 | 2.362(2) | << | C(18) | | | | Intra | 156.83 | 14.23 | 0.10770 | 0.75320 | -0.34043 | 0.9079 | 17.9376 | -12.4822 |
| 5 | 2.961(2) | << | C(19) | | | | Intra | 161.16 | -12.84 | 0.03330 | 0.75452 | -0.37421 | 0.2807 | 17.9690 | -13.7208 |
| 6 | 3.008(3) | .. | F(41)a | [1+x,y,z | = | 1655.06] | | -94.20 | 48.61 | 0.34010 | 0.63209 | -0.29470 | 2.8671 | 15.0533 | -10.8055 |
| 7 | 3.035(3) | < | C(45)a | [1+x,y,z | = | 1655.06] | | -71.63 | -6.92 | 0.47000 | 0.59531 | -0.36623 | 3.9622 | 14.1774 | -13.4282 |
| 8 | 3.403(3) | .. | C(17) | | | | Intra | 165.48 | 31.20 | 0.02310 | 0.74603 | -0.30817 | 0.1947 | 17.7669 | -11.2994 |
| 9 | 3.500(3) | .. | C(46)a | [1+x,y,z | = | 1655.06] | | -64.01 | 15.10 | 0.53300 | 0.58785 | -0.33140 | 4.4933 | 13.9998 | -12.1511 |
| 10 | 3.539(2) | .. | F(44) | [| = | 06] | | -139.95 | 9.87 | 0.04074 | 0.62118 | -0.33971 | 0.3434 | 14.7935 | -12.4558 |
| 11 | 3.554(3) | .. | C(13)b | [1+x,y,z | = | 1655.05] | | 30.45 | -37.87 | 0.64430 | 0.77508 | -0.41576 | 5.4316 | 18.4587 | -15.2443 |
| 12 | 2.70 | .. | H(15A)b | [1+x,y,z | = | 1655.05] | | 8.83 | 8.86 | 0.67060 | 0.73260 | -0.34490 | 5.6533 | 17.4470 | -12.6461 |
| 13 | 2.79 | .. | H(45A)a | [1+x,y,z | = | 1655.06] | | -89.71 | -10.08 | 0.35900 | 0.59990 | -0.36960 | 3.0264 | 14.2867 | -13.5518 |
| 14 | 2.87 | .. | H(43A)a | [1+x,y,z | = | 1655.06] | | -94.23 | -66.83 | 0.34750 | 0.66810 | -0.42820 | 2.9295 | 15.9109 | -15.7004 |
| 15 | 2.87 | .. | H(19A) | | | | Intra | 154.26 | -30.38 | 0.09240 | 0.76060 | -0.39590 | 0.7790 | 18.1138 | -14.5161 |
| 16 | 3.15 | .. | H(13A)b | [1+x,y,z | = | 1655.05] | | 45.09 | -29.44 | 0.58720 | 0.79700 | -0.39850 | 4.9502 | 18.9807 | -14.6114 |
| 17 | 3.59 | .. | H(17A) | | | | Intra | 163.13 | 46.38 | 0.07590 | 0.74560 | -0.28530 | 0.6399 | 17.7566 | -10.4608 |

Angles (Degrees) At1...V...At2 with Vertex V = F(15)

| | | | | | | | |
|-----------------|-----------|-----------------|------------|-----------------|------------|-----------------|------------|
| C(120) , F(16) | 37.43(12) | C(120) , F(14) | 36.26(12) | C(120) , C(18) | 36.34(12) | C(120) , C(19) | 56.10(12) |
| C(120) , F(41)a | 98.58(14) | C(120) , C(45)a | 157.18(15) | C(120) , C(17) | 39.56(12) | C(120) , C(46)a | 137.94(14) |
| C(120) , F(44) | 94.17(13) | C(120) , C(13)b | 105.89(14) | F(16) , F(14) | 60.43(9) | F(16) , C(18) | 63.24(8) |
| F(16) , C(19) | 66.37(7) | F(16) , F(41)a | 132.43(10) | F(16) , C(45)a | 164.13(10) | F(16) , C(17) | 74.31(7) |
| F(16) , C(46)a | 155.35(9) | F(16) , F(44) | 124.77(8) | F(16) , C(13)b | 69.08(7) | F(14) , C(18) | 63.09(8) |
| F(14) , C(19) | 88.86(8) | F(14) , F(41)a | 72.36(9) | F(14) , C(45)a | 127.28(10) | F(14) , C(17) | 53.42(7) |
| F(14) , C(46)a | 104.33(9) | F(14) , F(44) | 98.19(8) | F(14) , C(13)b | 110.65(9) | C(18) , C(19) | 27.41(7) |
| C(18) , F(41)a | 91.37(8) | C(18) , C(45)a | 131.89(9) | C(18) , C(17) | 18.74(7) | C(18) , C(46)a | 130.09(9) |
| C(18) , F(44) | 61.80(7) | C(18) , C(13)b | 127.22(9) | C(19) , F(41)a | 109.25(7) | C(19) , C(45)a | 123.95(8) |
| C(19) , C(17) | 44.24(6) | C(19) , C(46)a | 136.18(8) | C(19) , F(44) | 62.73(6) | C(19) , C(13)b | 111.45(7) |
| F(41)a , C(45)a | 58.96(6) | F(41)a , C(17) | 73.30(6) | F(41)a , C(46)a | 41.66(6) | F(41)a , F(44) | 54.33(5) |
| F(41)a , C(13)b | 139.22(7) | C(45)a , C(17) | 121.57(8) | C(45)a , C(46)a | 23.28(6) | C(45)a , F(44) | 70.09(6) |
| C(45)a , C(13)b | 95.17(7) | C(17) , C(46)a | 113.67(7) | C(17) , F(44) | 54.74(5) | C(17) , C(13)b | 142.73(7) |
| C(46)a , F(44) | 74.00(6) | C(46)a , C(13)b | 102.66(7) | F(44) , C(13)b | 150.70(7) | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(16) [ARU = 1555.05] 0.33530 0.80437 -0.35799 2.8266 19.1562-13.1261

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|-------------------|------------|--------|-------|---------|--------|---------|---------|----------|--------|---------|----------|
| 1 | 1.337(3) | -- | C(120) | | | | Intra | -111.38 | 30.15 | 0.28530 | 0.75915 | -0.33967 | 2.4051 | 18.0793 | -12.4543 |
| 2 | 2.128(2) | << | F(15) | | | | Intra | -84.98 | 1.71 | 0.35737 | 0.71538 | -0.35626 | 3.0127 | 17.0369 | -13.0626 |
| 3 | 2.149(3) | << | F(14) | | | | Intra | -85.67 | 61.78 | 0.34440 | 0.76183 | -0.30636 | 2.9034 | 18.1431 | -11.2330 |
| 4 | 2.362(2) | << | C(18) | | | | Intra | -147.58 | 15.82 | 0.10770 | 0.75320 | -0.34043 | 0.9079 | 17.9376 | -12.4822 |
| 5 | 2.871(2) | << | C(19) | | | | Intra | -155.00 | -11.95 | 0.03330 | 0.75452 | -0.37421 | 0.2807 | 17.9690 | -13.7208 |
| 6 | 2.990(3) | <. | C(35)b | [1/2+x,3/2-y,-1-z | = 3564.01] | | | 83.76 | -2.59 | 0.37380 | 0.92904 | -0.36167 | 3.1512 | 22.1253 | -13.2610 |
| 7 | 3.124(3) | <. | C(34)b | [1/2+x,3/2-y,-1-z | = 3564.01] | | | 99.98 | -23.44 | 0.27640 | 0.92291 | -0.39188 | 2.3301 | 21.9793 | -14.3687 |
| 8 | 3.153(3) | <. | C(36)b | [1/2+x,3/2-y,-1-z | = 3564.01] | | | 94.67 | 21.18 | 0.30690 | 0.92740 | -0.32693 | 2.5872 | 22.0862 | -11.9872 |
| 9 | 3.426(3) | .. | C(39)b | [1/2+x,3/2-y,-1-z | = 3564.01] | | | 125.20 | -18.81 | 0.11360 | 0.91563 | -0.38812 | 0.9577 | 21.8059 | -14.2308 |
| 10 | 3.429(3) | .. | C(13)a | [1+x,y,z | = 1655.05] | | | -14.99 | -38.15 | 0.64430 | 0.77508 | -0.41576 | 5.4316 | 18.4587 | -15.2443 |
| 11 | 3.430(3) | .. | C(37)b | [1/2+x,3/2-y,-1-z | = 3564.01] | | | 120.37 | 22.37 | 0.14510 | 0.91928 | -0.32238 | 1.2232 | 21.8928 | -11.8204 |
| 12 | 3.462(8) | .. | <F(31)b | [1/2+x,3/2-y,-1-z | = 3564.01] | | | 51.47 | 40.23 | 0.53060 | 0.89120 | -0.29700 | 4.4731 | 21.2241 | -10.8898 |
| 13 | 3.467(11) | .. | <F(31B)b | [1/2+x,3/2-y,-1-z | = 3564.01] | | | 55.80 | 48.66 | 0.48800 | 0.88390 | -0.28700 | 4.1139 | 21.0503 | -10.5231 |
| 14 | 3.492(3) | .. | C(17) | | | | Intra | -152.17 | 31.54 | 0.02310 | 0.74603 | -0.30817 | 0.1947 | 17.7669 | -11.2994 |
| 15 | 3.547(3) | .. | C(38)b | [1/2+x,3/2-y,-1-z | = 3564.01] | | | 132.74 | 2.85 | 0.05010 | 0.91361 | -0.35318 | 0.4224 | 21.7578 | -12.9497 |
| 16 | 2.60 | <. | H(13A)a | [1+x,y,z | = 1655.05] | | | -4.72 | -34.88 | 0.58720 | 0.79700 | -0.39850 | 4.9502 | 18.9807 | -14.6114 |
| 17 | 2.69 | .. | H(19A) | | | | Intra | -153.02 | -31.17 | 0.09240 | 0.76060 | -0.39590 | 0.7790 | 18.1138 | -14.5161 |
| 18 | 3.34 | .. | H(15A)a | [1+x,y,z | = 1655.05] | | | -31.16 | 8.27 | 0.67060 | 0.73260 | -0.34490 | 5.6533 | 17.4470 | -12.6461 |
| 19 | 3.35 | .. | H(35A)b | [1/2+x,3/2-y,-1-z | = 3564.01] | | | 67.84 | -4.15 | 0.48480 | 0.93430 | -0.36460 | 4.0870 | 22.2505 | -13.3684 |

Angles (Degrees) At1...V...At2 with Vertex V = F(16)

| | | | | | | | |
|------------------|------------|------------------|------------|-------------------|------------|-------------------|------------|
| C(120) , F(15) | 37.89(12) | C(120) , F(14) | 35.81(12) | C(120) , C(18) | 36.08(13) | C(120) , C(19) | 59.45(13) |
| C(120) , C(35)b | 148.93(15) | C(120) , C(34)b | 151.32(15) | C(120) , C(36)b | 122.89(14) | C(120) , C(39)b | 127.80(14) |
| C(120) , C(13)a | 112.70(14) | C(120) , C(37)b | 107.69(14) | C(120) , <F(31)b | 107.84(19) | C(120) , <F(31B)b | 100.4(2) |
| C(120) , C(17) | 34.85(12) | C(120) , C(38)b | 110.61(14) | F(15) , F(14) | 60.07(9) | F(15) , C(18) | 63.21(8) |
| F(15) , C(19) | 70.85(7) | F(15) , C(35)b | 168.72(10) | F(15) , C(34)b | 157.75(10) | F(15) , C(36)b | 157.11(10) |
| F(15) , C(39)b | 145.84(9) | F(15) , C(13)a | 75.49(8) | F(15) , C(37)b | 145.48(9) | F(15) , <F(31)b | 122.27(17) |
| F(15) , <F(31B)b | 119.28(19) | F(15) , C(17) | 69.77(7) | F(15) , C(38)b | 142.01(9) | F(14) , C(18) | 62.98(8) |
| F(14) , C(19) | 91.10(8) | F(14) , C(35)b | 120.28(10) | F(14) , C(34)b | 141.47(10) | F(14) , C(36)b | 97.05(9) |
| F(14) , C(39)b | 131.94(9) | F(14) , C(13)a | 114.91(8) | F(14) , C(37)b | 93.30(9) | F(14) , <F(31)b | 72.28(16) |
| F(14) , <F(31B)b | 65.34(18) | F(14) , C(17) | 51.57(7) | F(14) , C(38)b | 109.04(9) | C(18) , C(19) | 28.72(7) |
| C(18) , C(35)b | 127.79(9) | C(18) , C(34)b | 116.45(9) | C(18) , C(36)b | 108.62(9) | C(18) , C(39)b | 92.51(8) |
| C(18) , C(13)a | 132.87(9) | C(18) , C(37)b | 85.88(8) | C(18) , <F(31)b | 121.22(15) | C(18) , <F(31B)b | 112.3(2) |
| C(18) , C(17) | 16.27(7) | C(18) , C(38)b | 79.30(7) | C(19) , C(35)b | 119.83(8) | C(19) , C(34)b | 98.65(8) |
| C(19) , C(36)b | 113.06(8) | C(19) , C(39)b | 76.66(7) | C(19) , C(13)a | 117.48(8) | C(19) , C(37)b | 89.67(7) |
| C(19) , <F(31)b | 143.35(14) | C(19) , <F(31B)b | 135.3(2) | C(19) , C(17) | 43.58(6) | C(19) , C(38)b | 73.29(7) |
| C(35)b , C(34)b | 26.10(6) | C(35)b , C(36)b | 26.05(6) | C(35)b , C(39)b | 43.66(6) | C(35)b , C(13)a | 95.26(7) |
| C(35)b , C(37)b | 43.58(6) | C(35)b , <F(31)b | 52.01(15) | C(35)b , <F(31B)b | 56.71(17) | C(35)b , C(17) | 120.04(8) |
| C(35)b , C(38)b | 49.26(7) | C(34)b , C(36)b | 44.91(6) | C(34)b , C(39)b | 23.94(6) | C(34)b , C(13)a | 93.37(7) |
| C(34)b , C(37)b | 49.92(6) | C(34)b , <F(31)b | 78.04(15) | C(34)b , <F(31B)b | 82.18(17) | C(34)b , C(17) | 116.60(8) |

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C(34)b , C(38)b    41.34(6)   C(36)b , C(39)b    49.92(6)   C(36)b , C(13)a   118.03(8)   C(36)b , C(37)b    23.86(6)
C(36)b , <F(31)b  41.21(15)  C(36)b , <F(31B)b  41.35(18)  C(36)b , C(17)    97.10(7)   C(36)b , C(38)b    41.31(6)
C(39)b , C(13)a   111.88(7)  C(39)b , C(37)b    41.46(6)   C(39)b , <F(31)b  90.33(15)  C(39)b , <F(31B)b  91.27(18)
C(39)b , C(17)    93.74(7)   C(39)b , C(38)b    22.90(5)   C(13)a , C(37)b   138.81(7)  C(13)a , <F(31)b   99.16(14)
C(13)a , <F(31B)b 107.0(2)   C(13)a , C(17)    144.56(7)  C(13)a , C(38)b   134.02(7)  C(37)b , <F(31)b   59.99(15)
C(37)b , <F(31B)b 56.76(19)  C(37)b , C(17)    76.47(6)   C(37)b , C(38)b   22.92(5)   <F(31)b , <F(31B)b  9.0(2)
<F(31)b , C(17)  104.96(14) <F(31)b , C(38)b  81.50(15)  <F(31B)b, C(17)   96.00(19)  <F(31B)b, C(38)b  79.26(19)
C(17) , C(38)b   75.81(6)

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3.6 Angstrom Coordination Sphere Around Atom I = F(21) [ARU = 1555.02] -0.28320 0.42400 -0.72650 -2.3874 10.0976-26.6378

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|---------------------------|------------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.303(7) | -- | C(210) | | Intra | 175.33 | -3.90 | -0.43690 | 0.42844 | -0.72892 | -3.6832 | 10.2034 | -26.7266 |
| 2 | 2.124(15) | << | >F(23) | | Intra | 139.16 | -17.61 | -0.46490 | 0.47960 | -0.74403 | -3.9192 | 11.4218 | -27.2806 |
| 3 | 2.143(14) | << | >F(22) | | Intra | -156.49 | -26.96 | -0.49100 | 0.39200 | -0.75300 | -4.1392 | 9.3356 | -27.6095 |
| 4 | 2.367(7) | << | C(26) | | Intra | 179.86 | 31.05 | -0.52370 | 0.42421 | -0.69321 | -4.4149 | 10.1026 | -25.4172 |
| 5 | 2.64(3) | << | <F(32A) [| = 01] | | 60.69 | 1.83 | -0.13000 | 0.52060 | -0.72420 | -1.0959 | 12.3982 | -26.5535 |
| 6 | 2.743(8) | .< | F(24)a [1+x,y,z | = 1655.02] | | -15.70 | 27.80 | -0.00610 | 0.39642 | -0.69160 | -0.0514 | 9.4408 | -25.3582 |
| 7 | 2.752(7) | << | C(25) | | Intra | 173.60 | 61.14 | -0.43980 | 0.43022 | -0.66077 | -3.7076 | 10.2458 | -24.2278 |
| 8 | 2.870(7) | .< | F(43)c [-1/2-x,1-y,-1/2+z | = 2464.06] | | 1.52 | -32.29 | 0.00450 | 0.42671 | -0.76832 | 0.0379 | 10.1622 | -28.1712 |
| 9 | 3.479(16) | .. | F(13)b [-1/2-x,1-y,-1/2+z | = 2464.05] | | -69.52 | -32.49 | -0.16140 | 0.30855 | -0.77747 | -1.3606 | 7.3482 | -28.5067 |
| 10 | 2.45 | << | H(25A) | | Intra | 141.74 | 78.50 | -0.32870 | 0.43670 | -0.66100 | -2.7710 | 10.4001 | -24.2362 |
| 11 | 2.81 | .. | H(47A)c[-1/2-x,1-y,-1/2+z | = 2464.06] | | 3.48 | -81.99 | -0.23680 | 0.42500 | -0.80250 | -1.9963 | 10.1215 | -29.4245 |

Angles (Degrees) At1...V...At2 with Vertex V = >F(21)

| | | | | | | | |
|------------------|----------|------------------|----------|------------------|----------|------------------|-----------|
| C(210) , >F(23) | 38.0(5) | C(210) , >F(22) | 35.4(5) | C(210) , C(26) | 35.2(2) | C(210) , <F(32A) | 114.7(12) |
| C(210) , F(24)a | 153.9(6) | C(210) , C(25) | 65.1(3) | C(210) , F(43)c | 143.3(5) | C(210) , F(13)b | 108.7(8) |
| >F(23) , >F(22) | 59.7(4) | >F(23) , C(26) | 62.4(3) | >F(23) , <F(32A) | 79.6(8) | >F(23) , F(24)a | 154.7(8) |
| >F(23) , C(25) | 83.4(4) | >F(23) , F(43)c | 115.7(5) | >F(23) , F(13)b | 122.9(4) | >F(22) , C(26) | 62.3(3) |
| >F(22) , <F(32A) | 136.4(9) | >F(22) , F(24)a | 145.3(9) | >F(22) , C(25) | 91.4(4) | >F(22) , F(43)c | 117.2(5) |
| >F(22) , F(13)b | 73.5(5) | C(26) , <F(32A) | 113.6(8) | C(26) , F(24)a | 119.3(3) | C(26) , C(25) | 30.37(12) |
| C(26) , F(43)c | 178.1(6) | C(26) , F(13)b | 122.1(6) | <F(32A) , F(24)a | 77.1(6) | <F(32A) , C(25) | 99.2(7) |
| <F(32A) , F(43)c | 65.4(6) | <F(32A) , F(13)b | 124.2(6) | F(24)a , C(25) | 90.7(2) | F(24)a , F(43)c | 62.29(14) |
| F(24)a , F(13)b | 79.1(3) | C(25) , F(43)c | 150.7(3) | C(25) , F(13)b | 130.9(6) | F(43)c , F(13)b | 58.8(2) |

3.6 Angstrom Coordination Sphere Around Atom I = F(22) [ARU = 1555.02] -0.49100 0.39200 -0.75300 -4.1392 9.3356-27.6095

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|--------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.319(11) | -- | C(210) | | | | Intra | 62.28 | 42.01 | -0.43690 | 0.42844 | -0.72892 | -3.6832 | 10.2034 | -26.7266 |
| 2 | 2.123(12) | << | >F(23) | | | | Intra | 83.98 | 8.91 | -0.46490 | 0.47960 | -0.74403 | -3.9192 | 11.4218 | -27.2806 |
| 3 | 2.143(14) | << | >F(21) | | | | Intra | 23.51 | 26.96 | -0.28320 | 0.42400 | -0.72650 | -2.3874 | 10.0976 | -26.6378 |
| 4 | 2.339(11) | << | C(26) | | | | Intra | 109.77 | 69.60 | -0.52370 | 0.42421 | -0.69321 | -4.4149 | 10.1026 | -25.4172 |
| 5 | 2.789(11) | << | C(27) | | | | Intra | 160.95 | 51.32 | -0.68640 | 0.41588 | -0.69363 | -5.7865 | 9.9043 | -25.4326 |
| 6 | 3.125(10) | .. | F(11)a | [-1/2-x,1-y,-1/2+z | = | 2464.05] | | -67.52 | 4.51 | -0.34970 | 0.27115 | -0.74630 | -2.9480 | 6.4575 | -27.3638 |
| 7 | 3.190(11) | .. | F(45)c | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | 92.37 | -56.91 | -0.49956 | 0.46507 | -0.82590 | -4.2114 | 11.0757 | -30.2824 |
| 8 | 3.222(11) | .. | F(44)c | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | -143.18 | -80.64 | -0.54074 | 0.37882 | -0.83971 | -4.5585 | 9.0217 | -30.7888 |
| 9 | 3.366(11) | .. | F(41)b | [-3/2-x,1-y,-1/2+z | = | 2364.06] | | -168.97 | -27.02 | -0.84010 | 0.36791 | -0.79470 | -7.0822 | 8.7619 | -29.1385 |
| 10 | 3.529(11) | .. | C(25) | | | | Intra | 64.63 | 73.41 | -0.43980 | 0.43022 | -0.66077 | -3.7076 | 10.2458 | -24.2278 |
| 11 | 3.532(11) | .. | F(13)a | [-1/2-x,1-y,-1/2+z | = | 2464.05] | | -35.57 | -14.72 | -0.16140 | 0.30855 | -0.77747 | -1.3606 | 7.3482 | -28.5067 |
| 12 | 2.56 | .< | H(27A) | | | | Intra | 167.09 | 31.96 | -0.74240 | 0.41240 | -0.71600 | -6.2586 | 9.8214 | -26.2529 |
| 13 | 2.92 | .. | H(47A)c | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | 20.14 | -38.49 | -0.23680 | 0.42500 | -0.80250 | -1.9963 | 10.1215 | -29.4245 |
| 14 | 3.56 | .. | H(17A)a | [-1/2-x,1-y,-1/2+z | = | 2464.05] | | -102.32 | -19.45 | -0.57590 | 0.25440 | -0.78530 | -4.8550 | 6.0586 | -28.7938 |

Angles (Degrees) At1...V...At2 with Vertex V = >F(22)

| | | | | | | | |
|-----------------|-----------|-----------------|-----------|-----------------|-----------|-----------------|-----------|
| C(210) , >F(23) | 38.2(4) | C(210) , >F(21) | 34.9(5) | C(210) , C(26) | 36.7(3) | C(210) , C(27) | 63.1(4) |
| C(210) , F(11)a | 114.9(6) | C(210) , F(45)c | 102.1(5) | C(210) , F(44)c | 140.3(6) | C(210) , F(41)b | 135.9(6) |
| C(210) , C(25) | 31.4(4) | C(210) , F(13)a | 105.6(6) | >F(23) , >F(21) | 59.7(6) | >F(23) , C(26) | 62.9(3) |
| >F(23) , C(27) | 74.9(4) | >F(23) , F(11)a | 148.6(5) | >F(23) , F(45)c | 66.2(3) | >F(23) , F(44)c | 105.2(4) |
| >F(23) , F(41)b | 109.2(5) | >F(23) , C(25) | 65.5(3) | >F(23) , F(13)a | 120.7(5) | >F(21) , C(26) | 63.6(4) |
| >F(21) , C(27) | 93.2(4) | >F(21) , F(11)a | 88.9(6) | >F(21) , F(45)c | 101.8(5) | >F(21) , F(44)c | 126.0(5) |
| >F(21) , F(41)b | 168.9(6) | >F(21) , C(25) | 51.2(3) | >F(21) , F(13)a | 70.9(5) | C(26) , C(27) | 29.75(16) |
| C(26) , F(11)a | 105.9(4) | C(26) , F(45)c | 127.1(4) | C(26) , F(44)c | 160.3(4) | C(26) , F(41)b | 112.3(4) |
| C(26) , C(25) | 14.42(13) | C(26) , F(13)a | 121.0(4) | C(27) , F(11)a | 110.6(3) | C(27) , F(45)c | 122.0(3) |
| C(27) , F(44)c | 135.5(4) | C(27) , F(41)b | 82.7(3) | C(27) , C(25) | 43.24(17) | C(27) , F(13)a | 141.1(4) |
| F(11)a , F(45)c | 125.2(3) | F(11)a , F(44)c | 92.2(3) | F(11)a , F(41)b | 102.2(3) | F(11)a , C(25) | 96.6(3) |
| F(11)a , F(13)a | 37.04(12) | F(45)c , F(44)c | 39.06(14) | F(45)c , F(41)b | 72.1(2) | F(45)c , C(25) | 131.7(3) |
| F(45)c , F(13)a | 96.4(3) | F(44)c , F(41)b | 54.65(18) | F(44)c , C(25) | 170.6(3) | F(44)c , F(13)a | 78.3(2) |
| F(41)b , C(25) | 125.9(3) | F(41)b , F(13)a | 118.5(3) | C(25) , F(13)a | 107.0(3) | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(23) [ARU = 1555.02] -0.46490 0.47960 -0.74403 -3.9192 11.4218-27.2806

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|--------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.359(8) | -- | C(210) | | | | Intra | -79.04 | 24.06 | -0.43690 | 0.42844 | -0.72892 | -3.6832 | 10.2034 | -26.7266 |
| 2 | 2.123(12) | << | >F(22) | | | | Intra | -96.02 | -8.91 | -0.49100 | 0.39200 | -0.75300 | -4.1392 | 9.3356 | -27.6095 |
| 3 | 2.124(15) | << | >F(21) | | | | Intra | -40.84 | 17.61 | -0.28320 | 0.42400 | -0.72650 | -2.3874 | 10.0976 | -26.6378 |
| 4 | 2.336(7) | << | C(26) | | | | Intra | -110.60 | 52.90 | -0.52370 | 0.42421 | -0.69321 | -4.4149 | 10.1026 | -25.4172 |
| 5 | 3.012(12) | .. | >F(51)b | [-1/2+x,3/2-y,-1-z | = | 3464.03] | | 131.84 | -21.77 | -0.68620 | 0.56710 | -0.77450 | -5.7848 | 13.5056 | -28.3978 |
| 6 | 3.034(8) | < | C(27) | | | | Intra | -140.90 | 37.52 | -0.68640 | 0.41588 | -0.69363 | -5.7865 | 9.9043 | -25.4326 |
| 7 | 3.036(7) | .. | F(45)a | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | -130.18 | -81.42 | -0.49956 | 0.46507 | -0.82590 | -4.2114 | 11.0757 | -30.2824 |
| 8 | 3.08(3) | .. | <F(32A) | [| = | 01] | | 19.08 | 13.68 | -0.13000 | 0.52060 | -0.72420 | -1.0959 | 12.3982 | -26.5535 |
| 9 | 3.278(7) | .. | C(25) | | | | Intra | -79.80 | 68.62 | -0.43980 | 0.43022 | -0.66077 | -3.7076 | 10.2458 | -24.2278 |
| 10 | 3.548(7) | .. | C(37) | [| = | 01] | | 68.94 | 43.34 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 11 | 2.96 | .. | H(37A) | [| = | 01] | | 77.38 | 31.98 | -0.39990 | 0.58240 | -0.70130 | -3.3712 | 13.8700 | -25.7139 |
| 12 | 3.01 | .. | H(27A) | | | | Intra | -145.62 | 19.93 | -0.74240 | 0.41240 | -0.71600 | -6.2586 | 9.8214 | -26.2529 |
| 13 | 3.16 | .. | H(47A)a | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | -34.07 | -42.72 | -0.23680 | 0.42500 | -0.80250 | -1.9963 | 10.1215 | -29.4245 |
| 14 | 3.41 | .. | H(25A) | | | | Intra | -41.66 | 63.21 | -0.32870 | 0.43670 | -0.66100 | -2.7710 | 10.4001 | -24.2362 |

Angles (Degrees) At1...V...At2 with Vertex V = >F(23)

| | | | | | | | |
|-------------------|-----------|------------------|-----------|------------------|-----------|------------------|----------|
| C(210) , >F(22) | 36.9(4) | C(210) , >F(21) | 36.2(4) | C(210) , C(26) | 37.4(2) | C(210) , >F(51)b | 151.5(6) |
| C(210) , C(27) | 53.9(3) | C(210) , F(45)a | 108.5(4) | C(210) , <F(32A) | 91.7(6) | C(210) , C(25) | 44.6(2) |
| C(210) , C(37) | 106.5(4) | >F(22) , >F(21) | 60.6(5) | >F(22) , C(26) | 63.1(4) | >F(22) , >F(51)b | 123.9(5) |
| >F(22) , C(27) | 62.6(4) | >F(22) , F(45)a | 74.0(4) | >F(22) , <F(32A) | 116.4(6) | >F(22) , C(25) | 78.4(4) |
| >F(22) , C(37) | 143.2(4) | >F(21) , C(26) | 63.9(3) | >F(21) , >F(51)b | 172.0(5) | >F(21) , C(27) | 87.0(4) |
| >F(21) , F(45)a | 107.3(4) | >F(21) , <F(32A) | 57.6(6) | >F(21) , C(25) | 56.5(2) | >F(21) , C(37) | 91.6(4) |
| C(26) , >F(51)b | 123.7(4) | C(26) , C(27) | 26.00(12) | C(26) , F(45)a | 134.7(3) | C(26) , <F(32A) | 100.7(5) |
| C(26) , C(25) | 21.32(11) | C(26) , C(37) | 83.8(2) | >F(51)b , C(27) | 101.0(3) | >F(51)b , F(45)a | 69.7(3) |
| >F(51)b , <F(32A) | 115.9(5) | >F(51)b , C(25) | 129.3(3) | >F(51)b , C(37) | 87.0(3) | C(27) , F(45)a | 119.1(3) |
| C(27) , <F(32A) | 125.5(5) | C(27) , C(25) | 45.02(11) | C(27) , C(37) | 94.72(18) | F(45)a , <F(32A) | 111.0(5) |
| F(45)a , C(25) | 152.4(3) | F(45)a , C(37) | 141.4(2) | <F(32A) , C(25) | 80.5(5) | <F(32A) , C(37) | 51.8(5) |
| C(25) , C(37) | 65.64(14) | | | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(24) [ARU = 1555.02] -1.00610 0.39642 -0.69160 -8.4816 9.4408-25.3582

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------|--------------------------------|-------|--------|--------|----------|---------|----------|----------|---------|----------|
| 1 | 1.321(3) | -- | C(220) | | Intra | 17.85 | 64.11 | -0.94100 | 0.40384 | -0.65920 | -7.9328 | 9.6175 | -24.1702 |
| 2 | 2.144(3) | << | F(26) | | Intra | 93.72 | 54.82 | -1.01560 | 0.44819 | -0.64380 | -8.5617 | 10.6737 | -23.6056 |
| 3 | 2.146(3) | << | F(25) | | Intra | -76.47 | 65.29 | -0.98121 | 0.35980 | -0.63844 | -8.2718 | 8.5687 | -23.4090 |
| 4 | 2.363(3) | << | C(28) | | Intra | 10.82 | 28.86 | -0.76500 | 0.41273 | -0.66050 | -6.4491 | 9.8292 | -24.2179 |
| 5 | 2.736(3) | << | C(27) | | Intra | 9.76 | -1.56 | -0.68640 | 0.41588 | -0.69363 | -5.7865 | 9.9043 | -25.4326 |
| 6 | 2.743(8) | <. | >F(21)a | [-1+x,y,z = 1455.02] | | 164.30 | -27.80 | -1.28320 | 0.42400 | -0.72650 | -10.8176 | 10.0976 | -26.6378 |
| 7 | 2.768(11) | <. | <F(22A)a | [-1+x,y,z = 1455.02] | | 178.91 | -26.85 | -1.29900 | 0.39840 | -0.72570 | -10.9508 | 9.4880 | -26.6085 |
| 8 | 2.905(2) | <. | F(43)c | [-3/2-x,1-y,-1/2+z = 2364.06] | | 82.94 | -75.51 | -0.99550 | 0.42671 | -0.76832 | -8.3923 | 10.1622 | -28.1712 |
| 9 | 2.996(10) | .. | <F(61)d | [-1-x,-1/2+y,-1/2-z = 4444.04] | | -65.81 | -19.74 | -0.86900 | 0.28840 | -0.71920 | -7.3258 | 6.8683 | -26.3702 |
| 10 | 3.039(12) | .. | <F(33)b | [-1+x,y,z = 1455.01] | | 90.86 | -11.41 | -1.01140 | 0.52150 | -0.70800 | -8.5263 | 12.4196 | -25.9595 |
| 11 | 3.226(12) | .. | <F(33B)b | [-1+x,y,z = 1455.01] | | 84.98 | -7.25 | -0.97290 | 0.53030 | -0.70270 | -8.2017 | 12.6292 | -25.7652 |
| 12 | 3.36(2) | .. | <F(32A)b | [-1+x,y,z = 1455.01] | | 109.45 | -20.86 | -1.13000 | 0.52060 | -0.72420 | -9.5261 | 12.3982 | -26.5535 |
| 13 | 3.371(8) | .. | >F(63A)d | [-1-x,-1/2+y,-1/2-z = 4444.04] | | -89.09 | -8.32 | -0.99980 | 0.25640 | -0.70490 | -8.4285 | 6.1062 | -25.8459 |
| 14 | 3.549(7) | .. | >F(61A)d | [-1-x,-1/2+y,-1/2-z = 4444.04] | | -55.67 | -22.83 | -0.78730 | 0.28300 | -0.72915 | -6.6371 | 6.7397 | -26.7350 |
| 15 | 2.43 | << | H(27A) | | Intra | 9.71 | -21.64 | -0.74240 | 0.41240 | -0.71600 | -6.2586 | 9.8214 | -26.2529 |
| 16 | 3.09 | .. | H(25A)a | [-1+x,y,z = 1455.02] | | 160.57 | 21.26 | -1.32870 | 0.43670 | -0.66100 | -11.2012 | 10.4001 | -24.2362 |

Angles (Degrees) At1...V...At2 with Vertex V = F(24)

| | | | | | | | |
|---------------------|------------|---------------------|------------|---------------------|------------|---------------------|------------|
| C(220) , F(26) | 37.18(14) | C(220) , F(25) | 36.53(13) | C(220) , C(28) | 35.54(13) | C(220) , C(27) | 65.94(14) |
| C(220) , >F(21)a | 137.9(3) | C(220) , <F(22A)a | 140.8(3) | C(220) , F(43)c | 145.59(18) | C(220) , <F(61)d | 105.0(3) |
| C(220) , <F(33)b | 93.0(3) | C(220) , <F(33B)b | 86.9(3) | C(220) , <F(32A)b | 109.4(5) | C(220) , >F(63A)d | 104.83(18) |
| C(220) , >F(61A)d | 103.58(18) | F(26) , F(25) | 59.66(8) | F(26) , C(28) | 62.82(9) | F(26) , C(27) | 87.80(9) |
| F(26) , >F(21)a | 102.2(3) | F(26) , <F(22A)a | 109.0(3) | F(26) , F(43)c | 130.52(13) | F(26) , <F(61)d | 141.6(2) |
| F(26) , <F(33)b | 66.3(3) | F(26) , <F(33B)b | 62.5(3) | F(26) , <F(32A)b | 76.9(4) | F(26) , >F(63A)d | 133.45(11) |
| F(26) , >F(61A)d | 140.73(13) | F(25) , C(28) | 62.89(8) | F(25) , C(27) | 89.84(9) | F(25) , >F(21)a | 127.2(2) |
| F(25) , <F(22A)a | 120.3(3) | F(25) , F(43)c | 167.81(12) | F(25) , <F(61)d | 85.4(2) | F(25) , <F(33)b | 125.4(3) |
| F(25) , <F(33B)b | 120.5(3) | F(25) , <F(32A)b | 135.4(4) | F(25) , >F(63A)d | 74.20(10) | F(25) , >F(61A)d | 89.56(13) |
| C(28) , C(27) | 30.43(7) | C(28) , >F(21)a | 156.7(4) | C(28) , <F(22A)a | 169.3(3) | C(28) , F(43)c | 113.58(10) |
| C(28) , <F(61)d | 88.4(3) | C(28) , <F(33)b | 87.0(3) | C(28) , <F(33B)b | 79.9(2) | C(28) , <F(32A)b | 107.1(4) |
| C(28) , >F(63A)d | 102.65(11) | C(28) , >F(61A)d | 82.26(14) | C(27) , >F(21)a | 141.8(3) | C(27) , <F(22A)a | 149.7(3) |
| C(27) , F(43)c | 84.34(8) | C(27) , <F(61)d | 75.9(3) | C(27) , <F(33)b | 81.0(3) | C(27) , <F(33B)b | 75.2(2) |
| C(27) , <F(32A)b | 98.5(4) | C(27) , >F(63A)d | 98.52(11) | C(27) , >F(61A)d | 66.82(14) | >F(21)a , <F(22A)a | 13.0(5) |
| >F(21)a , F(43)c | 61.00(16) | >F(21)a , <F(61)d | 112.1(4) | >F(21)a , <F(33)b | 70.2(5) | >F(21)a , <F(33B)b | 77.2(4) |
| >F(21)a , <F(32A)b | 50.1(6) | >F(21)a , >F(63A)d | 100.5(4) | >F(21)a , >F(61A)d | 116.4(3) | <F(22A)a , F(43)c | 65.5(2) |
| <F(22A)a , <F(61)d | 101.9(4) | <F(22A)a , <F(33)b | 83.2(4) | <F(22A)a , <F(33B)b | 90.2(4) | <F(22A)a , <F(32A)b | 63.0(5) |
| <F(22A)a , >F(63A)d | 88.0(3) | <F(22A)a , >F(61A)d | 107.5(3) | F(43)c , <F(61)d | 82.8(2) | F(43)c , <F(33)b | 64.3(3) |
| F(43)c , <F(33B)b | 68.3(3) | F(43)c , <F(32A)b | 56.4(4) | F(43)c , >F(63A)d | 96.03(10) | F(43)c , >F(61A)d | 78.31(11) |
| <F(61)d , <F(33)b | 141.3(4) | <F(61)d , <F(33B)b | 140.6(3) | <F(61)d , <F(32A)b | 139.1(5) | <F(61)d , >F(63A)d | 25.3(3) |
| <F(61)d , >F(61A)d | 9.9(3) | <F(33)b , <F(33B)b | 7.1(3) | <F(33)b , <F(32A)b | 20.2(5) | <F(33)b , >F(63A)d | 160.3(3) |
| <F(33)b , >F(61A)d | 132.6(3) | <F(33B)b , <F(32A)b | 27.3(5) | <F(33B)b , >F(63A)d | 163.4(3) | <F(33B)b , >F(61A)d | 131.2(3) |

=====

<F(32A)b, >F(63A)d 145.6(4) <F(32A)b, >F(61A)d 134.0(4) >F(63A)d, >F(61A)d 35.18(14)

3.6 Angstrom Coordination Sphere Around Atom I = F(25) [ARU = 1555.02] -0.98121 0.35980 -0.63844 -8.2718 8.5687-23.4090

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|----------------------------------|-----------|--------|-------|---------|--------|----------|---------|----------|----------|---------|----------|
| 1 | 1.340(3) | -- | C(220) | | | | Intra | 72.09 | -34.63 | -0.94100 | 0.40384 | -0.65920 | -7.9328 | 9.6175 | -24.1702 |
| 2 | 2.134(2) | << | F(26) | | | | Intra | 97.84 | -5.28 | -1.01560 | 0.44819 | -0.64380 | -8.5617 | 10.6737 | -23.6056 |
| 3 | 2.146(3) | << | F(24) | | | | Intra | 103.53 | -65.29 | -1.00610 | 0.39642 | -0.69160 | -8.4816 | 9.4408 | -25.3582 |
| 4 | 2.359(3) | << | C(28) | | | | Intra | 34.67 | -20.05 | -0.76500 | 0.41273 | -0.66050 | -6.4491 | 9.8292 | -24.2179 |
| 5 | 2.876(3) | << | C(29) | | | | Intra | 28.67 | 8.04 | -0.68480 | 0.41717 | -0.62747 | -5.7730 | 9.9350 | -23.0068 |
| 6 | 2.974(3) | < | C(65)b | [-1-x, -1/2+y, -1/2-z = 4444.04] | | | | -69.40 | 0.16 | -0.85710 | 0.24293 | -0.63821 | -7.2255 | 5.7854 | -23.4006 |
| 7 | 3.075(3) | .. | F(66)c | [-2-x, -1/2+y, -1/2-z = 4344.04] | | | | -151.39 | -9.90 | -1.29670 | 0.29889 | -0.65286 | -10.9314 | 7.1181 | -23.9378 |
| 8 | 3.341(3) | .. | C(23)a | [-1+x, y, z = 1455.02] | | | | 158.40 | 32.96 | -1.29040 | 0.40313 | -0.58886 | -10.8783 | 9.6006 | -21.5911 |
| 9 | 3.405(3) | .. | C(64)b | [-1-x, -1/2+y, -1/2-z = 4444.04] | | | | -58.38 | 21.41 | -0.78410 | 0.24647 | -0.60454 | -6.6101 | 5.8697 | -22.1661 |
| 10 | 3.468(6) | .. | >F(63A)b | [-1-x, -1/2+y, -1/2-z = 4444.04] | | | | -93.64 | -44.64 | -0.99980 | 0.25640 | -0.70490 | -8.4285 | 6.1062 | -25.8459 |
| 11 | 3.472(3) | .. | C(27) | | | | Intra | 28.25 | -35.65 | -0.68640 | 0.41588 | -0.69363 | -5.7865 | 9.9043 | -25.4326 |
| 12 | 3.476(3) | .. | C(66)b | [-1-x, -1/2+y, -1/2-z = 4444.04] | | | | -56.23 | -19.16 | -0.76470 | 0.24520 | -0.66956 | -6.4466 | 5.8395 | -24.5501 |
| 13 | 3.543(11) | .. | <F(61)b | [-1-x, -1/2+y, -1/2-z = 4444.04] | | | | -60.91 | -56.69 | -0.86900 | 0.28840 | -0.71920 | -7.3258 | 6.8683 | -26.3702 |
| 14 | 2.49 | < | H(23A)a | [-1+x, y, z = 1455.02] | | | | 166.61 | 28.44 | -1.23390 | 0.38110 | -0.60610 | -10.4020 | 9.0760 | -22.2233 |
| 15 | 2.70 | .. | H(29A) | | | | Intra | 32.39 | 27.01 | -0.74030 | 0.41390 | -0.60500 | -6.2409 | 9.8571 | -22.1829 |
| 16 | 2.88 | .. | H(65A)b | [-1-x, -1/2+y, -1/2-z = 4444.04] | | | | -87.95 | -1.07 | -0.96900 | 0.23900 | -0.63990 | -8.1689 | 5.6918 | -23.4626 |
| 17 | 3.55 | .. | H(25A)a | [-1+x, y, z = 1455.02] | | | | 147.99 | -13.46 | -1.32870 | 0.43670 | -0.66100 | -11.2012 | 10.4001 | -24.2362 |

Angles (Degrees) At1...V...At2 with Vertex V = F(25)

| | | | | | | | |
|-------------------|------------|-------------------|------------|--------------------|------------|-------------------|------------|
| C(220) , F(26) | 37.79(13) | C(220) , F(24) | 35.93(13) | C(220) , C(28) | 36.03(13) | C(220) , C(29) | 59.18(13) |
| C(220) , C(65)b | 130.20(15) | C(220) , F(66)c | 119.37(15) | C(220) , C(23)a | 105.35(14) | C(220) , C(64)b | 134.80(15) |
| C(220) , >F(63A)b | 99.68(17) | C(220) , C(27) | 35.56(13) | C(220) , C(66)b | 107.18(15) | C(220) , <F(61)b | 80.40(19) |
| F(26) , F(24) | 60.14(9) | F(26) , C(28) | 63.02(8) | F(26) , C(29) | 70.27(8) | F(26) , C(65)b | 166.27(10) |
| F(26) , F(66)c | 109.39(9) | F(26) , C(23)a | 68.87(8) | F(26) , C(64)b | 151.88(9) | F(26) , >F(63A)b | 129.02(13) |
| F(26) , C(27) | 70.38(8) | F(26) , C(66)b | 144.65(9) | F(26) , <F(61)b | 115.64(16) | F(24) , C(28) | 63.06(9) |
| F(24) , C(29) | 91.08(9) | F(24) , C(65)b | 114.67(10) | F(24) , F(66)c | 87.19(9) | F(24) , C(23)a | 107.00(9) |
| F(24) , C(64)b | 134.56(10) | F(24) , >F(63A)b | 69.26(12) | F(24) , C(27) | 51.99(7) | F(24) , C(66)b | 94.15(9) |
| F(24) , <F(61)b | 57.45(17) | C(28) , C(29) | 28.70(7) | C(28) , C(65)b | 103.25(9) | C(28) , F(66)c | 149.46(10) |
| C(28) , C(23)a | 128.63(9) | C(28) , C(64)b | 99.89(9) | C(28) , >F(63A)b | 99.99(11) | C(28) , C(27) | 16.59(7) |
| C(28) , C(66)b | 84.34(8) | C(28) , <F(61)b | 76.3(2) | C(29) , C(65)b | 97.96(8) | C(29) , F(66)c | 178.14(9) |
| C(29) , C(23)a | 117.06(8) | C(29) , C(64)b | 84.35(7) | C(29) , >F(63A)b | 118.35(10) | C(29) , C(27) | 43.69(6) |
| C(29) , C(66)b | 87.86(7) | C(29) , <F(61)b | 96.5(2) | C(65)b , F(66)c | 82.14(8) | C(65)b , C(23)a | 124.20(8) |
| C(65)b , C(64)b | 23.82(6) | C(65)b , >F(63A)b | 49.70(10) | C(65)b , C(27) | 96.31(8) | C(65)b , C(66)b | 23.25(6) |
| C(65)b , <F(61)b | 57.26(16) | F(66)c , C(23)a | 64.19(7) | F(66)c , C(64)b | 96.37(7) | F(66)c , >F(63A)b | 60.34(9) |
| F(66)c , C(27) | 134.45(8) | F(66)c , C(66)b | 91.57(7) | F(66)c , <F(61)b | 82.0(2) | C(23)a , C(64)b | 115.28(8) |
| C(23)a , >F(63A)b | 124.50(9) | C(23)a , C(27) | 139.18(8) | C(23)a , C(66)b | 146.18(8) | C(23)a , <F(61)b | 144.2(3) |
| C(64)b , >F(63A)b | 73.48(10) | C(64)b , C(27) | 99.69(7) | C(64)b , C(66)b | 40.63(6) | C(64)b , <F(61)b | 78.13(18) |
| >F(63A)b , C(27) | 84.03(10) | >F(63A)b , C(66)b | 40.14(9) | >F(63A)b , <F(61)b | 23.7(2) | C(27) , C(66)b | 74.62(7) |
| C(27) , <F(61)b | 60.4(2) | C(66)b , <F(61)b | 37.69(19) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(26) [ARU = 1555.02] -1.01560 0.44819 -0.64380 -8.5617 10.6737-23.6056

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------|------------|-------|---------|--------|----------|---------|----------|----------|---------|----------|
| 1 | 1.353(3) | -- | C(220) | | Intra | -59.23 | -24.67 | -0.94100 | 0.40384 | -0.65920 | -7.9328 | 9.6175 | -24.1702 |
| 2 | 2.134(2) | << | F(25) | | Intra | -82.16 | 5.28 | -0.98121 | 0.35980 | -0.63844 | -8.2718 | 8.5687 | -23.4090 |
| 3 | 2.144(3) | << | F(24) | | Intra | -86.28 | -54.82 | -1.00610 | 0.39642 | -0.69160 | -8.4816 | 9.4408 | -25.3582 |
| 4 | 2.356(3) | << | C(28) | | Intra | -21.79 | -15.06 | -0.76500 | 0.41273 | -0.66050 | -6.4491 | 9.8292 | -24.2179 |
| 5 | 2.931(14) | <. | <F(33)b [-1+x,y,z | = 1455.01] | | 88.84 | -53.43 | -1.01140 | 0.52150 | -0.70800 | -8.5263 | 12.4196 | -25.9595 |
| 6 | 2.936(14) | <. | <F(33B)b[-1+x,y,z | = 1455.01] | | 79.57 | -47.36 | -0.97290 | 0.53030 | -0.70270 | -8.2017 | 12.6292 | -25.7652 |
| 7 | 2.946(3) | << | C(29) | | Intra | -14.84 | 11.73 | -0.68480 | 0.41717 | -0.62747 | -5.7730 | 9.9350 | -23.0068 |
| 8 | 3.075(3) | <. | C(35)b [-1+x,y,z | = 1455.01] | | 107.69 | 3.74 | -1.12620 | 0.57096 | -0.63833 | -9.4941 | 13.5975 | -23.4050 |
| 9 | 3.252(3) | .. | C(23)a [-1+x,y,z | = 1455.02] | | -155.15 | 38.27 | -1.29040 | 0.40313 | -0.58886 | -10.8783 | 9.6006 | -21.5911 |
| 10 | 3.411(3) | .. | C(27) | | Intra | -15.50 | -32.39 | -0.68640 | 0.41588 | -0.69363 | -5.7865 | 9.9043 | -25.4326 |
| 11 | 3.489(3) | .. | C(36)b [-1+x,y,z | = 1455.01] | | 116.80 | -17.92 | -1.19310 | 0.57260 | -0.67307 | -10.0581 | 13.6366 | -24.6788 |
| 12 | 3.55(2) | .. | <F(32A)b[-1+x,y,z | = 1455.01] | | 119.22 | -56.17 | -1.13000 | 0.52060 | -0.72420 | -9.5261 | 12.3982 | -26.5535 |
| 13 | 3.562(2) | .. | F(36) [| = 01] | | 40.81 | -8.33 | -0.69920 | 0.54491 | -0.65788 | -5.8944 | 12.9771 | -24.1218 |
| 14 | 3.57(3) | .. | <F(33A)b[-1+x,y,z | = 1455.01] | | 77.55 | -35.45 | -0.94120 | 0.56750 | -0.70030 | -7.9345 | 13.5151 | -25.6772 |
| 15 | 2.73 | .. | H(25A)a[-1+x,y,z | = 1455.02] | | -174.08 | -13.37 | -1.32870 | 0.43670 | -0.66100 | -11.2012 | 10.4001 | -24.2362 |
| 16 | 2.80 | .. | H(23A)a[-1+x,y,z | = 1455.02] | | -139.04 | 29.56 | -1.23390 | 0.38110 | -0.60610 | -10.4020 | 9.0760 | -22.2233 |
| 17 | 2.82 | .. | H(35A)b[-1+x,y,z | = 1455.01] | | 89.93 | 6.28 | -1.01520 | 0.56570 | -0.63540 | -8.5583 | 13.4723 | -23.2976 |
| 18 | 2.84 | .. | H(29A) | | Intra | -19.39 | 30.04 | -0.74030 | 0.41390 | -0.60500 | -6.2409 | 9.8571 | -22.1829 |
| 19 | 2.89 | .. | H(33A)b[-1+x,y,z | = 1455.01] | | 83.48 | 60.28 | -0.99630 | 0.50800 | -0.57530 | -8.3990 | 12.0981 | -21.0939 |

Angles (Degrees) At1...V...At2 with Vertex V = F(26)

| | | | | | | | |
|---------------------|-----------|-------------------|------------|---------------------|------------|-------------------|------------|
| C(220) , F(25) | 37.35(13) | C(220) , F(24) | 36.15(13) | C(220) , C(28) | 36.37(13) | C(220) , <F(33)b | 97.1(3) |
| C(220) , <F(33B)b | 99.0(3) | C(220) , C(29) | 56.57(13) | C(220) , C(35)b | 155.57(16) | C(220) , C(23)a | 109.40(15) |
| C(220) , C(27) | 38.92(13) | C(220) , C(36)b | 137.24(15) | C(220) , <F(32A)b | 99.2(4) | C(220) , F(36) | 95.53(14) |
| C(220) , <F(33A)b | 107.3(4) | F(25) , F(24) | 60.20(9) | F(25) , C(28) | 63.16(8) | F(25) , <F(33)b | 131.3(3) |
| F(25) , <F(33B)b | 135.1(3) | F(25) , C(29) | 66.76(7) | F(25) , C(35)b | 166.65(10) | F(25) , C(23)a | 73.40(8) |
| F(25) , C(27) | 73.52(8) | F(25) , C(36)b | 157.58(10) | F(25) , <F(32A)b | 126.4(3) | F(25) , F(36) | 123.34(8) |
| F(25) , <F(33A)b | 144.5(4) | F(24) , C(28) | 63.13(8) | F(24) , <F(33)b | 71.7(3) | F(24) , <F(33B)b | 77.1(3) |
| F(24) , C(29) | 89.23(8) | F(24) , C(35)b | 127.68(10) | F(24) , C(23)a | 110.07(9) | F(24) , C(27) | 53.28(7) |
| F(24) , C(36)b | 104.65(9) | F(24) , <F(32A)b | 67.1(4) | F(24) , F(36) | 103.03(9) | F(24) , <F(33A)b | 88.7(4) |
| C(28) , <F(33)b | 89.7(3) | C(28) , <F(33B)b | 86.4(2) | C(28) , C(29) | 27.66(7) | C(28) , C(35)b | 129.02(10) |
| C(28) , C(23)a | 132.96(9) | C(28) , C(27) | 18.25(7) | C(28) , C(36)b | 127.52(9) | C(28) , <F(32A)b | 101.7(4) |
| C(28) , F(36) | 61.49(7) | C(28) , <F(33A)b | 88.7(3) | <F(33)b , <F(33B)b | 8.5(4) | <F(33)b , C(29) | 107.5(3) |
| <F(33)b , C(35)b | 59.3(3) | <F(33)b , C(23)a | 134.6(3) | <F(33)b , C(27) | 72.2(3) | <F(33)b , C(36)b | 41.6(3) |
| <F(33)b , <F(32A)b | 17.6(5) | <F(33)b , F(36) | 59.3(3) | <F(33)b , <F(33A)b | 19.7(4) | <F(33B)b , C(29) | 101.6(2) |
| <F(33B)b , C(35)b | 56.8(3) | <F(33B)b , C(23)a | 139.7(2) | <F(33B)b , C(27) | 69.9(2) | <F(33B)b , C(36)b | 42.3(2) |
| <F(33B)b , <F(32A)b | 25.7(5) | <F(33B)b , F(36) | 51.0(2) | <F(33B)b , <F(33A)b | 12.0(4) | C(29) , C(35)b | 120.80(8) |
| C(29) , C(23)a | 117.75(8) | C(29) , C(27) | 44.12(6) | C(29) , C(36)b | 132.96(8) | C(29) , <F(32A)b | 123.2(4) |
| C(29) , F(36) | 58.86(6) | C(29) , <F(33A)b | 98.7(2) | C(35)b , C(23)a | 93.29(8) | C(35)b , C(27) | 119.74(8) |
| C(35)b , C(36)b | 23.45(6) | C(35)b , <F(32A)b | 60.7(4) | C(35)b , F(36) | 67.77(6) | C(35)b , <F(33A)b | 48.3(4) |

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C(23)a , C(27)      146.83(8)   C(23)a , C(36)b    99.51(7)   C(23)a , <F(32A)b  118.8(4)   C(23)a , F(36)     146.78(8)
C(23)a , <F(33A)b   138.3(3)   C(27) , C(36)b    112.08(7)  C(27) , <F(32A)b   83.4(4)   C(27) , F(36)     57.24(6)
C(27) , <F(33A)b    74.1(3)   C(36)b , <F(32A)b  38.3(4)   C(36)b , F(36)     74.18(6)  C(36)b , <F(33A)b  38.9(3)
<F(32A)b, F(36)    76.6(4)   <F(32A)b, <F(33A)b 34.9(5)   F(36) , <F(33A)b   43.1(2)

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3.6 Angstrom Coordination Sphere Around Atom I = F(34) [ARU = 1555.01] -0.69600 0.61683 -0.62274 -5.8674 14.6899-22.8334

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|--------------------|------------|--------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.338(3) | -- | C(320) | | | | Intra | -42.91 | -52.92 | -0.62590 | 0.59376 | -0.65186 | -5.2765 | 14.1405 | -23.9011 |
| 2 | 2.143(3) | << | F(35) | | | | Intra | 38.18 | -79.18 | -0.65850 | 0.62727 | -0.68014 | -5.5513 | 14.9386 | -24.9380 |
| 3 | 2.144(3) | << | F(36) | | | | Intra | -90.90 | -36.95 | -0.69920 | 0.54491 | -0.65788 | -5.8944 | 12.9771 | -24.1218 |
| 4 | 2.368(3) | << | C(38) | | | | Intra | -19.26 | -21.89 | -0.44990 | 0.58639 | -0.64682 | -3.7927 | 13.9650 | -23.7163 |
| 5 | 2.751(3) | << | C(39) | | | | Intra | -16.50 | 8.32 | -0.38640 | 0.58437 | -0.61188 | -3.2574 | 13.9169 | -22.4352 |
| 6 | 3.230(3) | .. | C(13)b | [-1/2+x,3/2-y,-1-z | = 3464.05] | | | 117.61 | 25.92 | -0.85570 | 0.72492 | -0.58424 | -7.2137 | 17.2641 | -21.4217 |
| 7 | 3.299(3) | .. | C(14)b | [-1/2+x,3/2-y,-1-z | = 3464.05] | | | 80.35 | -1.15 | -0.63040 | 0.75338 | -0.62454 | -5.3144 | 17.9419 | -22.8994 |
| 8 | 3.443(3) | .. | N(12)b | [-1/2+x,3/2-y,-1-z | = 3464.05] | | | 92.23 | 20.26 | -0.71090 | 0.75235 | -0.59023 | -5.9930 | 17.9174 | -21.6414 |
| 9 | 2.46 | << | H(39A) | | | | Intra | -18.56 | 28.27 | -0.45260 | 0.58790 | -0.59100 | -3.8155 | 14.0010 | -21.6696 |
| 10 | 2.86 | .. | H(13A)b | [-1/2+x,3/2-y,-1-z | = 3464.05] | | | 131.69 | 15.82 | -0.91280 | 0.70300 | -0.60150 | -7.6951 | 16.7421 | -22.0546 |
| 11 | 2.99 | .. | H(35A)a | [-1+x,y,z | = 1455.01] | | | -155.65 | -8.93 | -1.01520 | 0.56570 | -0.63540 | -8.5583 | 13.4723 | -23.2976 |

Angles (Degrees) At1...V...At2 with Vertex V = F(34)

| | | | | | | | |
|-----------------|------------|-----------------|------------|-----------------|------------|-----------------|------------|
| C(320) , F(35) | 36.76(13) | C(320) , F(36) | 36.67(13) | C(320) , C(38) | 35.92(13) | C(320) , C(39) | 65.24(14) |
| C(320) , C(13)b | 149.31(16) | C(320) , C(14)b | 108.34(14) | C(320) , N(12)b | 132.62(15) | F(35) , F(36) | 60.28(9) |
| F(35) , C(38) | 62.62(9) | F(35) , C(39) | 91.99(9) | F(35) , C(13)b | 113.47(10) | F(35) , C(14)b | 80.87(8) |
| F(35) , N(12)b | 103.69(9) | F(36) , C(38) | 62.77(9) | F(36) , C(39) | 82.79(9) | F(36) , C(13)b | 153.42(10) |
| F(36) , C(14)b | 141.05(10) | F(36) , N(12)b | 163.09(10) | C(38) , C(39) | 30.33(7) | C(38) , C(13)b | 140.54(10) |
| C(38) , C(14)b | 98.48(9) | C(38) , N(12)b | 116.61(9) | C(39) , C(13)b | 123.79(9) | C(39) , C(14)b | 96.94(8) |
| C(39) , N(12)b | 104.35(8) | C(13)b , C(14)b | 45.01(6) | C(13)b , N(12)b | 23.98(5) | C(14)b , N(12)b | 24.36(5) |

3.6 Angstrom Coordination Sphere Around Atom I = F(35) [ARU = 1555.01] -0.65850 0.62727 -0.68014 -5.5513 14.9386-24.9380

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-------------|-------------------------------|--------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.337(3) | -- C(320) | | | Intra | -71.00 | 50.85 | -0.62590 | 0.59376 | -0.65186 | -5.2765 | 14.1405 | -23.9011 |
| 2 | 2.143(3) | << F(34) | | | Intra | -141.82 | 79.18 | -0.69600 | 0.61683 | -0.62274 | -5.8674 | 14.6899 | -22.8334 |
| 3 | 2.152(3) | << F(36) | | | Intra | -99.92 | 22.29 | -0.69920 | 0.54491 | -0.65788 | -5.8944 | 12.9771 | -24.1218 |
| 4 | 2.352(3) | << C(38) | | | Intra | -28.97 | 31.29 | -0.44990 | 0.58639 | -0.64682 | -3.7927 | 13.9650 | -23.7163 |
| 5 | 2.787(8) | <. <F(31)a | [-1+x,y,z = 1455.01] | | | -170.47 | -17.50 | -0.96940 | 0.60880 | -0.70300 | -8.1722 | 14.4987 | -25.7762 |
| 6 | 2.791(3) | << C(37) | | | Intra | -23.42 | 1.90 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 7 | 2.87(2) | <. <F(33A)a | [-1+x,y,z = 1455.01] | | | -149.15 | -14.91 | -0.94120 | 0.56750 | -0.70030 | -7.9345 | 13.5151 | -25.6772 |
| 8 | 3.084(7) | >. >F(53)c | [-1/2+x,3/2-y,-1-z = 3464.03] | | | 2.95 | -67.70 | -0.51990 | 0.62980 | -0.75796 | -4.3829 | 14.9988 | -27.7914 |
| 9 | 3.162(3) | >. F(12)b | [-1/2+x,3/2-y,-1-z = 3464.05] | | | 123.01 | -34.28 | -0.82730 | 0.71925 | -0.72871 | -6.9743 | 17.1291 | -26.7189 |
| 10 | 3.195(3) | >. C(16)b | [-1/2+x,3/2-y,-1-z = 3464.05] | | | 87.23 | -6.31 | -0.64030 | 0.76046 | -0.68972 | -5.3979 | 18.1105 | -25.2893 |
| 11 | 3.225(12) | >. <F(31B)a | [-1+x,y,z = 1455.01] | | | -174.90 | -21.93 | -1.01200 | 0.61610 | -0.71300 | -8.5314 | 14.6725 | -26.1429 |
| 12 | 3.345(11) | >. <F(53A)c | [-1/2+x,3/2-y,-1-z = 3464.03] | | | 27.46 | -67.64 | -0.52460 | 0.65190 | -0.76450 | -4.4225 | 15.5251 | -28.0312 |
| 13 | 3.350(3) | >. C(15)b | [-1/2+x,3/2-y,-1-z = 3464.05] | | | 98.94 | 15.16 | -0.71810 | 0.76140 | -0.65625 | -6.0537 | 18.1329 | -24.0621 |
| 14 | 3.368(8) | >. <F(51A)c | [-1/2+x,3/2-y,-1-z = 3464.03] | | | -72.39 | -63.72 | -0.60500 | 0.56760 | -0.76250 | -5.1003 | 13.5175 | -27.9578 |
| 15 | 3.411(3) | >. C(17)b | [-1/2+x,3/2-y,-1-z = 3464.05] | | | 63.10 | -7.22 | -0.47690 | 0.75397 | -0.69183 | -4.0204 | 17.9559 | -25.3666 |
| 16 | 3.545(3) | >. C(39) | | | Intra | -24.01 | 44.91 | -0.38640 | 0.58437 | -0.61188 | -3.2574 | 13.9169 | -22.4352 |
| 17 | 2.55 | <. H(37A) | | | Intra | -26.11 | -17.72 | -0.39990 | 0.58240 | -0.70130 | -3.3712 | 13.8700 | -25.7139 |

Angles (Degrees) At1...V...At2 with Vertex V = F(35)

| | | | | | | | |
|--------------------|------------|---------------------|------------|---------------------|------------|---------------------|------------|
| C(320) , F(34) | 36.80(13) | C(320) , F(36) | 36.35(13) | C(320) , C(38) | 36.53(13) | C(320) , <F(31)a | 109.4(2) |
| C(320) , C(37) | 63.17(14) | C(320) , <F(33A)a | 94.3(5) | C(320) , >F(53)c | 130.6(3) | C(320) , F(12)b | 160.56(15) |
| C(320) , C(16)b | 131.91(15) | C(320) , <F(31B)a | 115.5(2) | C(320) , <F(53A)c | 138.8(2) | C(320) , C(15)b | 113.40(15) |
| C(320) , <F(51A)c | 114.6(2) | C(320) , C(17)b | 122.23(15) | C(320) , C(39) | 31.52(12) | F(34) , F(36) | 59.88(9) |
| F(34) , C(38) | 63.39(9) | F(34) , <F(31)a | 97.95(17) | F(34) , C(37) | 93.25(9) | F(34) , <F(33A)a | 94.2(4) |
| F(34) , >F(53)c | 165.23(19) | F(34) , F(12)b | 124.56(9) | F(34) , C(16)b | 103.31(9) | F(34) , <F(31B)a | 102.8(2) |
| F(34) , <F(53A)c | 168.11(19) | F(34) , C(15)b | 80.31(8) | F(34) , <F(51A)c | 148.38(16) | F(34) , C(17)b | 107.00(9) |
| F(34) , C(39) | 50.85(7) | F(36) , C(38) | 62.93(9) | F(36) , <F(31)a | 79.7(2) | F(36) , C(37) | 76.80(9) |
| F(36) , <F(33A)a | 60.9(5) | F(36) , >F(53)c | 115.4(3) | F(36) , F(12)b | 140.66(9) | F(36) , C(16)b | 162.60(10) |
| F(36) , <F(31B)a | 85.37(19) | F(36) , <F(53A)c | 124.4(2) | F(36) , C(15)b | 138.24(10) | F(36) , <F(51A)c | 88.67(15) |
| F(36) , C(17)b | 157.76(10) | F(36) , C(39) | 64.71(8) | C(38) , <F(31)a | 142.6(2) | C(38) , C(37) | 29.86(7) |
| C(38) , <F(33A)a | 123.3(6) | C(38) , >F(53)c | 101.85(19) | C(38) , F(12)b | 156.33(10) | C(38) , C(16)b | 115.60(9) |
| C(38) , <F(31B)a | 148.3(2) | C(38) , <F(53A)c | 107.50(19) | C(38) , C(15)b | 111.78(9) | C(38) , <F(51A)c | 101.0(3) |
| C(38) , C(17)b | 95.50(9) | C(38) , C(39) | 14.16(7) | <F(31)a , C(37) | 144.1(2) | <F(31)a , <F(33A)a | 20.6(6) |
| <F(31)a , >F(53)c | 94.7(2) | <F(31)a , F(12)b | 61.09(19) | <F(31)a , C(16)b | 99.7(2) | <F(31)a , <F(31B)a | 6.1(3) |
| <F(31)a , <F(53A)c | 93.8(2) | <F(31)a , C(15)b | 95.1(2) | <F(31)a , <F(51A)c | 77.9(3) | <F(31)a , C(17)b | 121.6(2) |
| <F(31)a , C(39) | 140.84(19) | C(37) , <F(33A)a | 124.9(5) | C(37) , >F(53)c | 72.00(18) | C(37) , F(12)b | 134.97(8) |
| C(37) , C(16)b | 110.73(9) | C(37) , <F(31B)a | 145.8(2) | C(37) , <F(53A)c | 77.92(18) | C(37) , C(15)b | 120.51(9) |
| C(37) , <F(51A)c | 74.9(3) | C(37) , C(17)b | 86.79(8) | C(37) , C(39) | 43.01(6) | <F(33A)a , >F(53)c | 94.9(4) |
| <F(33A)a , F(12)b | 79.9(5) | <F(33A)a , C(16)b | 120.2(6) | <F(33A)a , <F(31B)a | 25.4(6) | <F(33A)a , <F(53A)c | 97.4(4) |
| <F(33A)a , C(15)b | 114.5(5) | <F(33A)a , <F(51A)c | 70.8(5) | <F(33A)a , C(17)b | 141.1(5) | <F(33A)a , C(39) | 125.1(5) |

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>F(53)c , F(12)b      68.6(2)  >F(53)c , C(16)b      82.0(3)  >F(53)c , <F(31B)a    90.4(2)  >F(53)c , <F(53A)c     9.3(3)
>F(53)c , C(15)b     106.3(3) >F(53)c , <F(51A)c    29.3(3)  >F(53)c , C(17)b      72.3(3)  >F(53)c , C(39)     114.44(17)
F(12)b , C(16)b      43.27(6)  F(12)b , <F(31B)a    55.31(18) F(12)b , <F(53A)c    60.62(19) F(12)b , C(15)b     54.49(6)
F(12)b , <F(51A)c    81.23(18) F(12)b , C(17)b      61.20(6)  F(12)b , C(39)     152.69(8)  C(16)b , <F(31B)a    94.89(18)
C(16)b , <F(53A)c     73.0(2)  C(16)b , C(15)b      24.40(5)  C(16)b , <F(51A)c   108.29(14) C(16)b , C(17)b     23.98(6)
C(16)b , C(39)      109.43(7) <F(31B)a, <F(53A)c    88.9(3)  <F(31B)a, C(15)b     92.16(18) <F(31B)a, <F(51A)c    75.8(3)
<F(31B)a, C(17)b    116.15(19) <F(31B)a, C(39)     146.9(2)  <F(53A)c, C(15)b     97.2(2)  <F(53A)c, <F(51A)c    36.8(3)
<F(53A)c, C(17)b     65.0(2)  <F(53A)c, C(39)    119.02(18) C(15)b , <F(51A)c   131.06(14) C(15)b , C(17)b     41.98(6)
C(15)b , C(39)      100.79(7) <F(51A)c, C(17)b    101.57(19) <F(51A)c, C(39)     115.1(2)  C(17)b , C(39)     93.05(7)
=====

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3.6 Angstrom Coordination Sphere Around Atom I = F(36) [ARU = 1555.01] -0.69920 0.54491 -0.65788 -5.8944 12.9771-24.1218

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.336(3) | -- | C(320) | | | | Intra | 62.02 | 9.51 | -0.62590 | 0.59376 | -0.65186 | -5.2765 | 14.1405 | -23.9011 |
| 2 | 2.144(3) | << | F(34) | | | | Intra | 89.10 | 36.95 | -0.69600 | 0.61683 | -0.62274 | -5.8674 | 14.6899 | -22.8334 |
| 3 | 2.152(3) | << | F(35) | | | | Intra | 80.08 | -22.29 | -0.65850 | 0.62727 | -0.68014 | -5.5513 | 14.9386 | -24.9380 |
| 4 | 2.357(3) | << | C(38) | | | | Intra | 25.18 | 9.91 | -0.44990 | 0.58639 | -0.64682 | -3.7927 | 13.9650 | -23.7163 |
| 5 | 2.621(17) | << | <F(33A)a | [-1+x,y,z | = | 1455.01] | | 165.23 | -36.40 | -0.94120 | 0.56750 | -0.70030 | -7.9345 | 13.5151 | -25.6772 |
| 6 | 2.854(13) | <. | <F(33B)a | [-1+x,y,z | = | 1455.01] | | -171.42 | -35.16 | -0.97290 | 0.53030 | -0.70270 | -8.2017 | 12.6292 | -25.7652 |
| 7 | 3.111(3) | <. | C(37) | | | | Intra | 16.37 | -13.46 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 8 | 3.198(3) | .. | C(28) | [| = | 02] | | -99.99 | -1.72 | -0.76500 | 0.41273 | -0.66050 | -6.4491 | 9.8292 | -24.2179 |
| 9 | 3.200(8) | .. | <F(31)a | [-1+x,y,z | = | 1455.01] | | 146.26 | -31.13 | -0.96940 | 0.60880 | -0.70300 | -8.1722 | 14.4987 | -25.7762 |
| 10 | 3.242(3) | .. | C(29) | [| = | 02] | | -87.71 | 20.11 | -0.68480 | 0.41717 | -0.62747 | -5.7730 | 9.9350 | -23.0068 |
| 11 | 3.258(14) | .. | <F(33)a | [-1+x,y,z | = | 1455.01] | | -168.04 | -34.34 | -1.01140 | 0.52150 | -0.70800 | -8.5263 | 12.4196 | -25.9595 |
| 12 | 3.268(3) | .. | C(39) | | | | Intra | 19.61 | 31.07 | -0.38640 | 0.58437 | -0.61188 | -3.2574 | 13.9169 | -22.4352 |
| 13 | 3.343(3) | .. | C(27) | [| = | 02] | | -87.99 | -23.09 | -0.68640 | 0.41588 | -0.69363 | -5.7865 | 9.9043 | -25.4326 |
| 14 | 3.375(3) | .. | C(24) | [| = | 02] | | -62.10 | 19.03 | -0.52210 | 0.42651 | -0.62787 | -4.4014 | 10.1574 | -23.0215 |
| 15 | 3.483(3) | .. | C(26) | [| = | 02] | | -62.77 | -21.84 | -0.52370 | 0.42421 | -0.69321 | -4.4149 | 10.1026 | -25.4172 |
| 16 | 3.501(3) | .. | C(25) | [| = | 02] | | -51.32 | -1.73 | -0.43980 | 0.43022 | -0.66077 | -3.7076 | 10.2458 | -24.2278 |
| 17 | 3.562(2) | .. | F(26) | [| = | 02] | | -139.19 | 8.33 | -1.01560 | 0.44819 | -0.64380 | -8.5617 | 10.6737 | -23.6056 |
| 18 | 2.83 | .. | H(35A)a | [-1+x,y,z | = | 1455.01] | | 169.47 | 16.92 | -1.01520 | 0.56570 | -0.63540 | -8.5583 | 13.4723 | -23.2976 |
| 19 | 3.11 | .. | H(37A) | | | | Intra | 19.49 | -30.75 | -0.39990 | 0.58240 | -0.70130 | -3.3712 | 13.8700 | -25.7139 |
| 20 | 3.37 | .. | H(39A) | | | | Intra | 26.22 | 46.62 | -0.45260 | 0.58790 | -0.59100 | -3.8155 | 14.0010 | -21.6696 |

Angles (Degrees) At1...V...At2 with Vertex V = F(36)

| | | | | | | | |
|-------------------|------------|--------------------|------------|---------------------|------------|--------------------|------------|
| C(320) , F(34) | 36.76(13) | C(320) , F(35) | 36.39(13) | C(320) , C(38) | 36.31(13) | C(320) , <F(33A)a | 106.2(7) |
| C(320) , <F(33B)a | 125.1(3) | C(320) , C(37) | 50.80(13) | C(320) , C(28) | 160.50(16) | C(320) , <F(31)a | 90.0(2) |
| C(320) , C(29) | 137.99(16) | C(320) , <F(33)a | 128.0(3) | C(320) , C(39) | 44.85(13) | C(320) , C(27) | 148.28(16) |
| C(320) , C(24) | 117.98(15) | C(320) , C(26) | 125.72(15) | C(320) , C(25) | 113.30(14) | C(320) , F(26) | 152.35(16) |
| F(34) , F(35) | 59.85(8) | F(34) , C(38) | 63.29(9) | F(34) , <F(33A)a | 101.7(6) | F(34) , <F(33B)a | 117.0(3) |
| F(34) , C(37) | 84.78(8) | F(34) , C(28) | 143.79(11) | F(34) , <F(31)a | 86.55(17) | F(34) , C(29) | 122.86(11) |
| F(34) , <F(33)a | 119.1(2) | F(34) , C(39) | 56.62(7) | F(34) , C(27) | 165.92(11) | F(34) , C(24) | 117.78(10) |
| F(34) , C(26) | 151.37(10) | F(34) , C(25) | 129.33(10) | F(34) , F(26) | 116.04(9) | F(35) , C(38) | 62.69(8) |
| F(35) , <F(33A)a | 73.3(6) | F(35) , <F(33B)a | 91.2(3) | F(35) , C(37) | 60.86(8) | F(35) , C(28) | 155.99(11) |
| F(35) , <F(31)a | 58.94(17) | F(35) , C(29) | 168.42(10) | F(35) , <F(33)a | 94.1(2) | F(35) , C(39) | 78.76(8) |
| F(35) , C(27) | 133.16(11) | F(35) , C(24) | 144.55(9) | F(35) , C(26) | 122.92(10) | F(35) , C(25) | 126.88(9) |
| F(35) , F(26) | 139.80(9) | C(38) , <F(33A)a | 135.2(6) | C(38) , <F(33B)a | 150.6(3) | C(38) , C(37) | 24.94(7) |
| C(38) , C(28) | 124.91(9) | C(38) , <F(31)a | 121.62(18) | C(38) , C(29) | 107.50(9) | C(38) , <F(33)a | 152.7(3) |
| C(38) , C(39) | 21.79(7) | C(38) , C(27) | 115.08(9) | C(38) , C(24) | 84.24(8) | C(38) , C(26) | 91.78(9) |
| C(38) , C(25) | 77.01(8) | C(38) , F(26) | 156.02(10) | <F(33A)a , <F(33B)a | 18.9(7) | <F(33A)a , C(37) | 122.1(4) |
| <F(33A)a , C(28) | 92.8(7) | <F(33A)a , <F(31)a | 16.6(7) | <F(33A)a , C(29) | 115.2(6) | <F(33A)a , <F(33)a | 21.8(7) |
| <F(33A)a , C(39) | 151.1(7) | <F(33A)a , C(27) | 88.9(6) | <F(33A)a , C(24) | 135.2(7) | <F(33A)a , C(26) | 106.2(6) |
| <F(33A)a , C(25) | 128.9(6) | <F(33A)a , F(26) | 68.7(6) | <F(33B)a , C(37) | 130.8(3) | <F(33B)a , C(28) | 73.9(2) |

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<F(33B)a, <F(31)a    35.4(3)  <F(33B)a, C(29)    96.5(3)  <F(33B)a, <F(33)a    2.9(3)  <F(33B)a, C(39)    169.9(3)
<F(33B)a, C(27)      71.8(2)  <F(33B)a, C(24)   116.3(2)  <F(33B)a, C(26)    91.6(3)  <F(33B)a, C(25)   113.1(3)
<F(33B)a, F(26)      53.1(3)  C(37) , C(28)   115.14(8)  C(37) , <F(31)a  114.43(16)  C(37) , C(29)   107.60(8)
C(37) , <F(33)a     132.0(3)  C(37) , C(39)   44.63(6)  C(37) , C(27)    97.51(8)  C(37) , C(24)   83.81(7)
C(37) , C(26)       75.13(7)  C(37) , C(25)   67.91(7)  C(37) , F(26)   155.48(8)  C(28) , <F(31)a  109.21(18)
C(28) , C(29)       24.94(6)  C(28) , <F(33)a  71.0(2)   C(28) , C(39)   116.01(8)  C(28) , C(27)   24.34(6)
C(28) , C(24)       42.62(6)  C(28) , C(26)   41.42(6)  C(28) , C(25)   48.65(7)  C(28) , F(26)   40.35(6)
<F(31)a , C(29)    130.58(18)  <F(31)a , <F(33)a  38.3(3)   <F(31)a , C(39)  134.78(18)  <F(31)a , C(27)  104.91(17)
<F(31)a , C(24)    151.72(18)  <F(31)a , C(26)  120.17(17)  <F(31)a , C(25)  143.13(17)  <F(31)a , F(26)   81.34(16)
C(29) , <F(33)a     93.7(2)   C(29) , C(39)   93.56(8)  C(29) , C(27)   43.20(6)  C(29) , C(24)   24.14(6)
C(29) , C(26)       48.52(6)  C(29) , C(25)   41.83(6)  C(29) , F(26)   51.06(6)  <F(33)a , C(39)  172.8(2)
<F(33)a , C(27)     69.4(2)   <F(33)a , C(24)  113.5(2)   <F(33)a , C(26)   89.6(2)   <F(33)a , C(25)  110.7(2)
<F(33)a , F(26)     50.7(2)   C(39) , C(27)   116.15(8)  C(39) , C(24)   73.45(7)   C(39) , C(26)   94.96(7)
C(39) , C(25)       74.69(7)  C(39) , F(26)  135.67(8)  C(27) , C(24)   49.12(6)   C(27) , C(26)   23.32(6)
C(27) , C(25)       41.46(6)  C(27) , F(26)   59.10(6)  C(24) , C(26)   40.87(5)   C(24) , C(25)   23.31(5)
C(24) , F(26)       75.15(6)  C(26) , C(25)   22.98(5)  C(26) , F(26)   80.69(6)   C(25) , F(26)   88.14(6)
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3.6 Angstrom Coordination Sphere Around Atom I = F(41) [ARU = 1555.06] -0.65990 0.63209 -0.29470 -5.5631 15.0533-10.8055

| Nr | d(I,J) | To Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|------------|-------------------|------------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.337(3) | -- | C(410) | | | Intra | -58.74 | -7.48 | -0.57830 | 0.58451 | -0.29945 | -4.8752 | 13.9202 | -10.9796 |
| 2 | 2.133(3) | << | F(42) | | | Intra | -96.26 | -9.60 | -0.68710 | 0.54430 | -0.30440 | -5.7924 | 12.9626 | -11.1611 |
| 3 | 2.148(3) | << | F(43) | | | Intra | -46.91 | 26.77 | -0.50450 | 0.57329 | -0.26832 | -4.2530 | 13.6530 | -9.8382 |
| 4 | 2.359(3) | << | C(46) | | | Intra | -32.94 | -34.78 | -0.46700 | 0.58785 | -0.33140 | -3.9369 | 13.9998 | -12.1511 |
| 5 | 2.974(3) | < | C(45) | | | Intra | -38.66 | -61.87 | -0.53000 | 0.59531 | -0.36623 | -4.4680 | 14.1774 | -13.4282 |
| 6 | 3.008(3) | .. | F(15)a | [-1+x,y,z | = 1455.05] | | 85.80 | -48.61 | -0.64263 | 0.71538 | -0.35626 | -5.4175 | 17.0369 | -13.0626 |
| 7 | 3.027(2) | .. | F(44)b | [-1+x,y,z | = 1455.06] | | -174.12 | -33.04 | -0.95926 | 0.62118 | -0.33971 | -8.0868 | 14.7935 | -12.4558 |
| 8 | 3.119(3) | .. | F(14)a | [-1+x,y,z | = 1455.05] | | 89.33 | -7.88 | -0.65560 | 0.76183 | -0.30636 | -5.5268 | 18.1431 | -11.2330 |
| 9 | 3.120(2) | .. | F(13) | [| = 05] | | 27.56 | 11.68 | -0.33860 | 0.69145 | -0.27747 | -2.8545 | 16.4670 | -10.1737 |
| 10 | 3.172(7) | .. | >F(61A)d | [-1/2+x,3/2-y,-z | = 3465.04] | | 102.41 | 49.26 | -0.71270 | 0.71700 | -0.22915 | -6.0082 | 17.0755 | -8.4020 |
| 11 | 3.215(14) | .. | <F(23A)c | [-3/2-x,1-y,1/2+z | = 2365.02] | | -163.16 | 25.90 | -0.98830 | 0.59690 | -0.25640 | -8.3316 | 14.2153 | -9.4012 |
| 12 | 3.363(10) | .. | <F(61)d | [-1/2+x,3/2-y,-z | = 3465.04] | | 82.67 | 55.41 | -0.63100 | 0.71160 | -0.21920 | -5.3195 | 16.9469 | -8.0372 |
| 13 | 3.366(11) | .. | >F(22)c | [-3/2-x,1-y,1/2+z | = 2365.02] | | -168.97 | 27.02 | -1.00900 | 0.60800 | -0.25300 | -8.5061 | 14.4796 | -9.2765 |
| 14 | 3.432(3) | .. | C(47) | | | Intra | -22.29 | -19.68 | -0.30520 | 0.58063 | -0.32622 | -2.5729 | 13.8278 | -11.9612 |
| 15 | 3.477(3) | .. | C(120)a | [-1+x,y,z | = 1455.05] | | 98.68 | -28.31 | -0.71470 | 0.75915 | -0.33967 | -6.0251 | 18.0793 | -12.4543 |
| 16 | 2.86 | .. | H(45A) | | | Intra | -78.26 | -74.09 | -0.64100 | 0.59990 | -0.36960 | -5.4038 | 14.2867 | -13.5518 |
| 17 | 3.18 | .. | H(27A)c | [-3/2-x,1-y,1/2+z | = 2365.02] | | -127.86 | 65.06 | -0.75760 | 0.58760 | -0.21600 | -6.3867 | 13.9938 | -7.9199 |
| 18 | 3.52 | .. | H(17A)a | [-1+x,y,z | = 1455.05] | | 129.49 | 5.62 | -0.92410 | 0.74560 | -0.28530 | -7.7903 | 17.7566 | -10.4608 |

Angles (Degrees) At1...V...At2 with Vertex V = F(41)

| | | | | | | | |
|-------------------|------------|-------------------|------------|-------------------|------------|-------------------|------------|
| C(410) , F(42) | 37.15(13) | C(410) , F(43) | 36.12(12) | C(410) , C(46) | 36.15(12) | C(410) , C(45) | 56.36(12) |
| C(410) , F(15)a | 115.86(14) | C(410) , F(44)b | 106.57(14) | C(410) , F(14)a | 144.65(15) | C(410) , F(13) | 87.92(14) |
| C(410) , >F(61A)d | 135.33(19) | C(410) , <F(23A)c | 106.2(4) | C(410) , <F(61)d | 123.2(3) | C(410) , >F(22)c | 111.4(2) |
| C(410) , C(47) | 37.37(13) | C(410) , C(120)a | 138.09(15) | F(42) , F(43) | 60.11(9) | F(42) , C(46) | 62.69(9) |
| F(42) , C(45) | 66.66(8) | F(42) , F(15)a | 121.76(9) | F(42) , F(44)b | 74.65(8) | F(42) , F(14)a | 161.66(10) |
| F(42) , F(13) | 124.83(9) | F(42) , >F(61A)d | 137.39(15) | F(42) , <F(23A)c | 74.0(4) | F(42) , <F(61)d | 134.18(17) |
| F(42) , >F(22)c | 79.32(18) | F(42) , C(47) | 71.79(8) | F(42) , C(120)a | 139.43(10) | F(43) , C(46) | 62.95(8) |
| F(43) , C(45) | 88.88(9) | F(43) , F(15)a | 137.59(9) | F(43) , F(44)b | 134.28(10) | F(43) , F(14)a | 134.46(10) |
| F(43) , F(13) | 71.02(8) | F(43) , >F(61A)d | 99.21(15) | F(43) , <F(23A)c | 99.1(3) | F(43) , <F(61)d | 87.3(2) |
| F(43) , >F(22)c | 102.57(19) | F(43) , C(47) | 52.22(7) | F(43) , C(120)a | 149.55(10) | C(46) , C(45) | 27.33(8) |
| C(46) , F(15)a | 80.40(8) | C(46) , F(44)b | 103.03(9) | C(46) , F(14)a | 110.87(9) | C(46) , F(13) | 73.71(8) |
| C(46) , >F(61A)d | 144.45(16) | C(46) , <F(23A)c | 136.6(4) | C(46) , <F(61)d | 132.2(3) | C(46) , >F(22)c | 141.79(19) |
| C(46) , C(47) | 17.80(7) | C(46) , C(120)a | 102.11(9) | C(45) , F(15)a | 60.97(6) | C(45) , F(44)b | 78.51(7) |
| C(45) , F(14)a | 99.59(8) | C(45) , F(13) | 89.56(7) | C(45) , >F(61A)d | 155.17(15) | C(45) , <F(23A)c | 128.7(3) |
| C(45) , <F(61)d | 149.9(3) | C(45) , >F(22)c | 132.3(2) | C(45) , C(47) | 43.70(6) | C(45) , C(120)a | 83.51(7) |
| F(15)a , F(44)b | 71.81(6) | F(15)a , F(14)a | 40.85(5) | F(15)a , F(13) | 79.12(6) | F(15)a , >F(61A)d | 98.91(13) |
| F(15)a , <F(23A)c | 122.8(3) | F(15)a , <F(61)d | 104.06(16) | F(15)a , >F(22)c | 119.71(19) | F(15)a , C(47) | 86.60(6) |
| F(15)a , C(120)a | 22.60(5) | F(44)b , F(14)a | 91.15(7) | F(44)b , F(13) | 150.84(8) | F(44)b , >F(61A)d | 110.54(15) |
| F(44)b , <F(23A)c | 59.9(3) | F(44)b , <F(61)d | 123.9(3) | F(44)b , >F(22)c | 60.26(19) | F(44)b , C(47) | 120.81(8) |
| F(44)b , C(120)a | 72.86(6) | F(14)a , F(13) | 64.46(6) | F(14)a , >F(61A)d | 58.27(13) | F(14)a , <F(23A)c | 109.2(4) |

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F(14)a , <F(61)d 63.53(15)  F(14)a , >F(22)c 103.96(17)  F(14)a , C(47) 107.30(7)  F(14)a , C(120)a 22.26(5)
F(13) , >F(61A)d 71.31(15)  F(13) , <F(23A)c 141.0(3)  F(13) , <F(61)d 61.0(3)  F(13) , >F(22)c 138.11(19)
F(13) , C(47) 58.24(6)  F(13) , C(120)a 79.46(7)  >F(61A)d, <F(23A)c 73.4(4)  >F(61A)d, <F(61)d 13.5(3)
>F(61A)d, >F(22)c 69.0(2)  >F(61A)d, C(47) 127.23(15)  >F(61A)d, C(120)a 77.64(13)  <F(23A)c, <F(61)d 81.4(4)
<F(23A)c, >F(22)c 5.3(4)  <F(23A)c, C(47) 143.5(4)  <F(23A)c, C(120)a 108.6(4)  <F(61)d , >F(22)c 77.6(3)
<F(61)d , C(47) 114.5(3)  <F(61)d , C(120)a 84.83(16)  >F(22)c , C(47) 148.64(18)  >F(22)c , C(120)a 104.34(18)
C(47) , C(120)a 105.48(7)

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3.6 Angstrom Coordination Sphere Around Atom I = F(42) [ARU = 1555.06] -0.68710 0.54430 -0.30440 -5.7924 12.9626-11.1611

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|---------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.338(3) | -- | C(410) | | | | Intra | 46.23 | 7.79 | -0.57830 | 0.58451 | -0.29945 | -4.8752 | 13.9202 | -10.9796 |
| 2 | 2.133(3) | << | F(41) | | | | Intra | 83.74 | 9.60 | -0.65990 | 0.63209 | -0.29470 | -5.5631 | 15.0533 | -10.8055 |
| 3 | 2.144(2) | << | F(43) | | | | Intra | 24.16 | 38.10 | -0.50450 | 0.57329 | -0.26832 | -4.2530 | 13.6530 | -9.8382 |
| 4 | 2.345(3) | << | C(46) | | | | Intra | 29.20 | -24.97 | -0.46700 | 0.58785 | -0.33140 | -3.9369 | 13.9998 | -12.1511 |
| 5 | 2.766(2) | < | F(45)a | [-1+x,y,z | = | 1455.06] | | -175.17 | -16.56 | -1.00044 | 0.53493 | -0.32590 | -8.4339 | 12.7395 | -11.9494 |
| 6 | 2.893(3) | << | C(45) | | | | Intra | 42.53 | -51.60 | -0.53000 | 0.59531 | -0.36623 | -4.4680 | 14.1774 | -13.4282 |
| 7 | 3.063(8) | .. | >F(51)c | [-1-x,-1/2+y,-1/2-z | = | 4444.03] | | -111.93 | 20.97 | -0.81380 | 0.43290 | -0.27450 | -6.8605 | 10.3096 | -10.0648 |
| 8 | 3.127(3) | .. | F(55)d | [-x,-1/2+y,-1/2-z | = | 4544.03] | | -54.36 | -4.73 | -0.47170 | 0.43797 | -0.31143 | -3.9765 | 10.4303 | -11.4189 |
| 9 | 3.208(2) | .. | F(44)a | [-1+x,y,z | = | 1455.06] | | 141.41 | -23.80 | -0.95926 | 0.62118 | -0.33971 | -8.0868 | 14.7935 | -12.4558 |
| 10 | 3.334(15) | .. | <F(23A)b | [-3/2-x,1-y,1/2+z | = | 2365.02] | | 153.74 | 31.86 | -0.98830 | 0.59690 | -0.25640 | -8.3316 | 14.2153 | -9.4012 |
| 11 | 3.428(3) | .. | C(47) | | | | Intra | 15.04 | -13.50 | -0.30520 | 0.58063 | -0.32622 | -2.5729 | 13.8278 | -11.9612 |
| 12 | 3.432(3) | .. | C(420)a | [-1+x,y,z | = | 1455.06] | | 166.17 | -29.80 | -1.03010 | 0.57418 | -0.35092 | -8.6839 | 13.6742 | -12.8668 |
| 13 | 3.437(3) | .. | F(56)d | [-x,-1/2+y,-1/2-z | = | 4544.03] | | -46.45 | -41.53 | -0.47680 | 0.46598 | -0.36655 | -4.0195 | 11.0974 | -13.4399 |
| 14 | 3.540(11) | .. | <F(51A)c | [-1-x,-1/2+y,-1/2-z | = | 4444.03] | | -123.33 | 25.72 | -0.89500 | 0.43240 | -0.26250 | -7.5450 | 10.2977 | -9.6248 |
| 15 | 2.76 | .. | H(45A) | | | | Intra | 73.64 | -60.00 | -0.64100 | 0.59990 | -0.36960 | -5.4038 | 14.2867 | -13.5518 |
| 16 | 3.45 | .. | H(27A)b | [-3/2-x,1-y,1/2+z | = | 2365.02] | | 119.96 | 69.84 | -0.75760 | 0.58760 | -0.21600 | -6.3867 | 13.9938 | -7.9199 |

Angles (Degrees) At1...V...At2 with Vertex V = F(42)

| | | | | | | | |
|---------------------|------------|--------------------|------------|--------------------|------------|-------------------|------------|
| C(410) , F(41) | 37.10(13) | C(410) , F(43) | 36.28(13) | C(410) , C(46) | 36.73(12) | C(410) , F(45)a | 138.67(16) |
| C(410) , C(45) | 59.48(12) | C(410) , >F(51)c | 144.1(3) | C(410) , F(55)d | 101.11(15) | C(410) , F(44)a | 97.85(15) |
| C(410) , <F(23A)b | 100.5(4) | C(410) , C(47) | 37.58(13) | C(410) , C(420)a | 119.77(15) | C(410) , F(56)d | 97.16(14) |
| C(410) , <F(51A)c | 145.0(2) | F(41) , F(43) | 60.28(10) | F(41) , C(46) | 63.37(9) | F(41) , F(45)a | 103.26(9) |
| F(41) , C(45) | 70.72(8) | F(41) , >F(51)c | 145.8(2) | F(41) , F(55)d | 138.17(9) | F(41) , F(44)a | 65.47(7) |
| F(41) , <F(23A)b | 68.0(4) | F(41) , C(47) | 71.98(7) | F(41) , C(420)a | 88.29(8) | F(41) , F(56)d | 125.94(9) |
| F(41) , <F(51A)c | 135.94(17) | F(43) , C(46) | 63.25(9) | F(43) , F(45)a | 152.58(10) | F(43) , C(45) | 91.12(9) |
| F(43) , >F(51)c | 108.0(2) | F(43) , F(55)d | 83.96(9) | F(43) , F(44)a | 125.36(11) | F(43) , <F(23A)b | 95.8(3) |
| F(43) , C(47) | 52.30(7) | F(43) , C(420)a | 147.66(11) | F(43) , F(56)d | 102.33(8) | F(43) , <F(51A)c | 109.3(2) |
| C(46) , F(45)a | 132.15(10) | C(46) , C(45) | 28.50(8) | C(46) , >F(51)c | 144.1(2) | C(46) , F(55)d | 82.18(8) |
| C(46) , F(44)a | 98.23(9) | C(46) , <F(23A)b | 131.3(4) | C(46) , C(47) | 17.60(7) | C(46) , C(420)a | 111.42(9) |
| C(46) , F(56)d | 63.38(7) | C(46) , <F(51A)c | 155.2(3) | F(45)a , C(45) | 104.35(8) | F(45)a , >F(51)c | 72.5(2) |
| F(45)a , F(55)d | 117.77(8) | F(45)a , F(44)a | 41.23(5) | F(45)a , <F(23A)b | 56.9(3) | F(45)a , C(47) | 148.30(8) |
| F(45)a , C(420)a | 21.61(5) | F(45)a , F(56)d | 105.06(7) | F(45)a , <F(51A)c | 65.8(2) | C(45) , >F(51)c | 143.5(2) |
| C(45) , F(55)d | 90.55(7) | C(45) , F(44)a | 76.79(7) | C(45) , <F(23A)b | 127.2(3) | C(45) , C(47) | 44.05(7) |
| C(45) , C(420)a | 84.79(8) | C(45) , F(56)d | 58.14(6) | C(45) , <F(51A)c | 151.98(14) | >F(51)c , F(55)d | 62.0(2) |
| >F(51)c , F(44)a | 112.9(2) | >F(51)c , <F(23A)b | 82.6(4) | >F(51)c , C(47) | 129.0(2) | >F(51)c , C(420)a | 93.7(2) |
| >F(51)c , F(56)d | 87.0(2) | >F(51)c , <F(51A)c | 11.5(3) | F(55)d , F(44)a | 147.59(8) | F(55)d , <F(23A)b | 142.2(3) |
| F(55)d , C(47) | 68.89(6) | F(55)d , C(420)a | 128.05(8) | F(55)d , F(56)d | 37.47(5) | F(55)d , <F(51A)c | 73.4(2) |
| F(44)a , <F(23A)b | 56.9(3) | F(44)a , C(47) | 115.68(7) | F(44)a , C(420)a | 22.85(5) | F(44)a , F(56)d | 114.27(7) |
| F(44)a , <F(51A)c | 104.5(3) | <F(23A)b , C(47) | 138.0(3) | <F(23A)b , C(420)a | 62.8(2) | <F(23A)b , F(56)d | 161.2(3) |
| <F(23A)b , <F(51A)c | 71.1(4) | C(47) , C(420)a | 128.53(8) | C(47) , F(56)d | 59.86(5) | C(47) , <F(51A)c | 139.1(3) |

=====
C(420)a, F(56)d 102.57(7) C(420)a, <F(51A)c 87.4(2) F(56)d , <F(51A)c 97.73(17)

3.6 Angstrom Coordination Sphere Around Atom I = F(43) [ARU = 1555.06] -0.50450 0.57329 -0.26832 -4.2530 13.6530 -9.8382

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------|------------------------------|-------|--------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.327(3) | -- | C(410) | | Intra | 156.76 | -59.32 | -0.57830 | 0.58451 | -0.29945 | -4.8752 | 13.9202 | -10.9796 |
| 2 | 2.144(2) | << | F(42) | | Intra | 155.84 | -38.10 | -0.68710 | 0.54430 | -0.30440 | -5.7924 | 12.9626 | -11.1611 |
| 3 | 2.148(3) | << | F(41) | | Intra | 133.09 | -26.77 | -0.65990 | 0.63209 | -0.29470 | -5.5631 | 15.0533 | -10.8055 |
| 4 | 2.360(3) | << | C(46) | | Intra | 47.64 | -78.53 | -0.46700 | 0.58785 | -0.33140 | -3.9369 | 13.9998 | -12.1511 |
| 5 | 2.713(3) | << | C(47) | | Intra | 5.94 | -51.49 | -0.30520 | 0.58063 | -0.32622 | -2.5729 | 13.8278 | -11.9612 |
| 6 | 2.870(7) | <. | >F(21)a | [-1/2-x,1-y,1/2+z = 2465.02] | | 1.52 | 32.29 | -0.21680 | 0.57600 | -0.22650 | -1.8277 | 13.7176 | -8.3049 |
| 7 | 2.905(2) | <. | F(24)b | [-3/2-x,1-y,1/2+z = 2365.02] | | 82.94 | 75.51 | -0.49390 | 0.60358 | -0.19160 | -4.1637 | 14.3744 | -7.0252 |
| 8 | 2.98(2) | .. | <F(32A)c | [-1/2-x,1-y,1/2+z = 2465.01] | | -63.11 | 32.83 | -0.37000 | 0.47940 | -0.22420 | -3.1192 | 11.4170 | -8.2205 |
| 9 | 3.073(11) | .. | <F(22A)a | [-1/2-x,1-y,1/2+z = 2465.02] | | 14.76 | 30.57 | -0.20100 | 0.60160 | -0.22570 | -1.6945 | 14.3272 | -8.2755 |
| 10 | 3.160(3) | .. | F(13) | [= 05] | | 63.57 | -6.09 | -0.33860 | 0.69145 | -0.27747 | -2.8545 | 16.4670 | -10.1737 |
| 11 | 3.163(14) | .. | <F(33)c | [-1/2-x,1-y,1/2+z = 2465.01] | | -86.60 | 44.36 | -0.48860 | 0.47850 | -0.20800 | -4.1190 | 11.3956 | -7.6265 |
| 12 | 3.451(13) | .. | <F(33B)c | [-1/2-x,1-y,1/2+z = 2465.01] | | -94.42 | 44.20 | -0.52710 | 0.46970 | -0.20270 | -4.4436 | 11.1860 | -7.4322 |
| 13 | 3.532(12) | .. | <F(32B)c | [-1/2-x,1-y,1/2+z = 2465.01] | | -64.44 | 19.16 | -0.33370 | 0.44690 | -0.23670 | -2.8132 | 10.6430 | -8.6788 |
| 14 | 2.39 | << | H(47A) | | Intra | 1.15 | -31.63 | -0.26320 | 0.57500 | -0.30250 | -2.2188 | 13.6937 | -11.0915 |
| 15 | 2.89 | .. | H(27A)b | [-3/2-x,1-y,1/2+z = 2365.02] | | 170.93 | 41.60 | -0.75760 | 0.58760 | -0.21600 | -6.3867 | 13.9938 | -7.9199 |

Angles (Degrees) At1...V...At2 with Vertex V = F(43)

| | | | | | | | |
|--------------------|-----------|---------------------|------------|---------------------|------------|---------------------|------------|
| C(410) , F(42) | 36.63(14) | C(410) , F(41) | 36.43(14) | C(410) , C(46) | 35.94(13) | C(410) , C(47) | 66.69(13) |
| C(410) , >F(21)a | 148.3(3) | C(410) , F(24)b | 142.86(18) | C(410) , <F(32A)c | 142.7(5) | C(410) , <F(22A)a | 141.6(3) |
| C(410) , F(13) | 86.38(17) | C(410) , <F(33)c | 139.9(3) | C(410) , <F(33B)c | 135.9(3) | C(410) , <F(32B)c | 130.2(2) |
| F(42) , F(41) | 59.61(8) | F(42) , C(46) | 62.53(9) | F(42) , C(47) | 89.00(9) | F(42) , >F(21)a | 160.7(4) |
| F(42) , F(24)b | 134.38(9) | F(42) , <F(32A)c | 111.5(5) | F(42) , <F(22A)a | 169.2(2) | F(42) , F(13) | 122.62(10) |
| F(42) , <F(33)c | 103.4(3) | F(42) , <F(33B)c | 99.2(2) | F(42) , <F(32B)c | 102.8(2) | F(41) , C(46) | 62.91(9) |
| F(41) , C(47) | 89.05(9) | F(41) , >F(21)a | 137.9(4) | F(41) , F(24)b | 107.03(11) | F(41) , <F(32A)c | 164.7(5) |
| F(41) , <F(22A)a | 126.4(3) | F(41) , F(13) | 69.00(9) | F(41) , <F(33)c | 143.7(3) | F(41) , <F(33B)c | 138.3(2) |
| F(41) , <F(32B)c | 162.2(2) | C(46) , C(47) | 30.76(8) | C(46) , >F(21)a | 114.02(18) | C(46) , F(24)b | 155.27(13) |
| C(46) , <F(32A)c | 126.2(5) | C(46) , <F(22A)a | 110.8(2) | C(46) , F(13) | 72.89(9) | C(46) , <F(33)c | 141.7(3) |
| C(46) , <F(33B)c | 142.7(2) | C(46) , <F(32B)c | 113.10(16) | C(47) , >F(21)a | 83.87(16) | C(47) , F(24)b | 136.27(9) |
| C(47) , <F(32A)c | 103.7(5) | C(47) , <F(22A)a | 82.4(2) | C(47) , F(13) | 65.51(7) | C(47) , <F(33)c | 124.5(3) |
| C(47) , <F(33B)c | 128.7(2) | C(47) , <F(32B)c | 93.40(16) | >F(21)a , F(24)b | 56.71(18) | >F(21)a , <F(32A)c | 53.6(6) |
| >F(21)a , <F(22A)a | 11.4(5) | >F(21)a , F(13) | 70.3(4) | >F(21)a , <F(33)c | 66.8(4) | >F(21)a , <F(33B)c | 72.0(4) |
| >F(21)a , <F(32B)c | 60.0(4) | F(24)b , <F(32A)c | 69.5(5) | F(24)b , <F(22A)a | 55.1(2) | F(24)b , F(13) | 82.42(8) |
| F(24)b , <F(33)c | 59.9(2) | F(24)b , <F(33B)c | 60.3(2) | F(24)b , <F(32B)c | 83.18(15) | <F(32A)c , <F(22A)a | 64.7(5) |
| <F(32A)c , F(13) | 123.8(5) | <F(32A)c , <F(33)c | 21.6(5) | <F(32A)c , <F(33B)c | 26.8(5) | <F(32A)c , <F(32B)c | 13.7(5) |
| <F(22A)a , F(13) | 59.4(3) | <F(22A)a , <F(33)c | 76.5(3) | <F(22A)a , <F(33B)c | 81.3(3) | <F(22A)a , <F(32B)c | 71.4(3) |
| F(13) , <F(33)c | 133.7(3) | F(13) , <F(33B)c | 137.3(2) | F(13) , <F(32B)c | 127.82(19) | <F(33)c , <F(33B)c | 5.6(3) |
| <F(33)c , <F(32B)c | 31.3(3) | <F(33B)c , <F(32B)c | 35.4(3) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(44) [ARU = 1555.06] 0.04074 0.62118 -0.33971 0.3434 14.7935-12.4558

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|-------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.334(3) | -- | C(420) | | | | Intra | -118.08 | -17.95 | -0.03010 | 0.57418 | -0.35092 | -0.2537 | 13.6742 | -12.8668 |
| 2 | 2.144(2) | << | F(45) | | | | Intra | -99.59 | 13.66 | -0.00044 | 0.53493 | -0.32590 | -0.0037 | 12.7395 | -11.9494 |
| 3 | 2.151(3) | << | F(46) | | | | Intra | -88.93 | -45.42 | 0.04410 | 0.55778 | -0.38150 | 0.3718 | 13.2836 | -13.9881 |
| 4 | 2.358(3) | << | C(48) | | | | Intra | -155.66 | -15.18 | -0.20520 | 0.58180 | -0.35655 | -1.7299 | 13.8557 | -13.0733 |
| 5 | 3.027(2) | .. | F(41)a | [1+x,y,z | = | 1655.06] | | 5.88 | 33.04 | 0.34010 | 0.63209 | -0.29470 | 2.8671 | 15.0533 | -10.8055 |
| 6 | 3.112(3) | < | C(47) | | | | Intra | -161.68 | 9.15 | -0.30520 | 0.58063 | -0.32622 | -2.5729 | 13.8278 | -11.9612 |
| 7 | 3.119(15) | .. | <F(23A)b | [-1/2-x,1-y,1/2+z | = | 2465.02] | | -112.95 | 78.38 | 0.01170 | 0.59690 | -0.25640 | 0.0986 | 14.2153 | -9.4012 |
| 8 | 3.194(3) | .. | C(17) | [| = | 05] | | 92.86 | 21.23 | 0.02310 | 0.74603 | -0.30817 | 0.1947 | 17.7669 | -11.2994 |
| 9 | 3.195(3) | .. | C(18) | [| = | 05] | | 79.82 | -0.47 | 0.10770 | 0.75320 | -0.34043 | 0.9079 | 17.9376 | -12.4822 |
| 10 | 3.208(2) | .. | F(42)a | [1+x,y,z | = | 1655.06] | | -38.59 | 23.80 | 0.31290 | 0.54430 | -0.30440 | 2.6378 | 12.9626 | -11.1611 |
| 11 | 3.222(11) | .. | >F(22)b | [-1/2-x,1-y,1/2+z | = | 2465.02] | | -143.18 | 80.64 | -0.00900 | 0.60800 | -0.25300 | -0.0759 | 14.4796 | -9.2765 |
| 12 | 3.285(3) | .. | C(49) | | | | Intra | -163.95 | -35.39 | -0.26450 | 0.59010 | -0.39159 | -2.2298 | 14.0533 | -14.3580 |
| 13 | 3.382(3) | .. | C(16) | [| = | 05] | | 118.43 | 18.61 | -0.14030 | 0.73954 | -0.31028 | -1.1828 | 17.6123 | -11.3767 |
| 14 | 3.419(3) | .. | C(19) | [| = | 05] | | 91.13 | -21.72 | 0.03330 | 0.75452 | -0.37421 | 0.2807 | 17.9690 | -13.7208 |
| 15 | 3.539(2) | .. | F(15) | [| = | 05] | | 40.05 | -9.87 | 0.35737 | 0.71538 | -0.35626 | 3.0127 | 17.0369 | -13.0626 |
| 16 | 3.550(3) | .. | C(15) | [| = | 05] | | 127.97 | -2.39 | -0.21810 | 0.73860 | -0.34375 | -1.8386 | 17.5899 | -12.6039 |
| 17 | 3.567(3) | .. | C(14) | [| = | 05] | | 115.78 | -21.56 | -0.13040 | 0.74662 | -0.37546 | -1.0993 | 17.7809 | -13.7666 |
| 18 | 2.94 | .. | H(45A)a | [1+x,y,z | = | 1655.06] | | -10.70 | -21.87 | 0.35900 | 0.59990 | -0.36960 | 3.0264 | 14.2867 | -13.5518 |
| 19 | 3.10 | .. | H(47A) | | | | Intra | -156.77 | 26.07 | -0.26320 | 0.57500 | -0.30250 | -2.2188 | 13.6937 | -11.0915 |
| 20 | 3.39 | .. | H(49A) | | | | Intra | -160.57 | -51.47 | -0.19540 | 0.59170 | -0.41200 | -1.6473 | 14.0915 | -15.1064 |
| 21 | 3.58 | .. | H(17A) | [| = | 05] | | 84.29 | 33.82 | 0.07590 | 0.74560 | -0.28530 | 0.6399 | 17.7566 | -10.4608 |

Angles (Degrees) At1...V...At2 with Vertex V = F(44)

| | | | | | | | |
|------------------|------------|-------------------|------------|------------------|------------|-------------------|------------|
| C(420) , F(45) | 36.50(12) | C(420) , F(46) | 36.61(12) | C(420) , C(48) | 36.07(13) | C(420) , F(41)a | 127.85(14) |
| C(420) , C(47) | 50.86(12) | C(420) , <F(23A)b | 96.4(4) | C(420) , C(17) | 150.71(15) | C(420) , C(18) | 154.51(15) |
| C(420) , F(42)a | 88.03(13) | C(420) , >F(22)b | 99.4(2) | C(420) , C(49) | 44.07(12) | C(420) , C(16) | 126.57(14) |
| C(420) , C(19) | 131.10(14) | C(420) , F(15) | 144.78(14) | C(420) , C(15) | 111.90(14) | C(420) , C(14) | 114.11(14) |
| F(45) , F(46) | 59.86(8) | F(45) , C(48) | 62.51(8) | F(45) , F(41)a | 95.08(8) | F(45) , C(47) | 60.88(7) |
| F(45) , <F(23A)b | 65.1(4) | F(45) , C(17) | 143.03(10) | F(45) , C(18) | 166.80(10) | F(45) , F(42)a | 58.24(7) |
| F(45) , >F(22)b | 69.67(18) | F(45) , C(49) | 78.11(7) | F(45) , C(16) | 130.55(9) | F(45) , C(19) | 167.00(9) |
| F(45) , F(15) | 140.35(8) | F(45) , C(15) | 131.68(8) | F(45) , C(14) | 145.46(9) | F(46) , C(48) | 62.99(8) |
| F(46) , F(41)a | 115.95(8) | F(46) , C(47) | 84.71(8) | F(46) , <F(23A)b | 124.7(4) | F(46) , C(17) | 155.77(10) |
| F(46) , C(18) | 133.04(10) | F(46) , F(42)a | 82.96(8) | F(46) , >F(22)b | 129.50(19) | F(46) , C(49) | 55.92(7) |
| F(46) , C(16) | 144.89(9) | F(46) , C(19) | 112.87(9) | F(46) , F(15) | 108.23(8) | F(46) , C(15) | 122.09(9) |
| F(46) , C(14) | 109.35(9) | C(48) , F(41)a | 155.53(10) | C(48) , C(47) | 25.05(7) | C(48) , <F(23A)b | 96.5(3) |
| C(48) , C(17) | 115.10(9) | C(48) , C(18) | 123.00(9) | C(48) , F(42)a | 120.50(9) | C(48) , >F(22)b | 96.0(2) |
| C(48) , C(49) | 21.53(7) | C(48) , C(16) | 91.05(8) | C(48) , C(19) | 104.86(8) | C(48) , F(15) | 150.51(9) |
| C(48) , C(15) | 76.23(8) | C(48) , C(14) | 83.18(8) | F(41)a , C(47) | 136.18(8) | F(41)a , <F(23A)b | 63.1(2) |
| F(41)a , C(17) | 76.20(7) | F(41)a , C(18) | 76.86(6) | F(41)a , F(42)a | 39.88(5) | F(41)a , >F(22)b | 65.1(2) |
| F(41)a , C(49) | 171.27(8) | F(41)a , C(16) | 97.51(7) | F(41)a , C(19) | 97.89(6) | F(41)a , F(15) | 53.86(5) |

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F(41)a , C(15) 117.88(7) F(41)a , C(14) 117.76(7) C(47) , <F(23A)b 73.3(3) C(47) , C(17) 100.82(8)
C(47) , C(18) 118.19(7) C(47) , F(42)a 115.40(7) C(47) , >F(22)b 72.0(2) C(47) , C(49) 44.59(6)
C(47) , C(16) 77.59(7) C(47) , C(19) 109.26(7) C(47) , F(15) 158.57(7) C(47) , C(15) 71.04(6)
C(47) , C(14) 86.52(7) <F(23A)b, C(17) 79.3(4) <F(23A)b, C(18) 101.8(4) <F(23A)b, F(42)a 63.6(3)
<F(23A)b, >F(22)b 5.9(4) <F(23A)b, C(49) 117.7(3) <F(23A)b, C(16) 78.9(4) <F(23A)b, C(19) 122.2(4)
<F(23A)b, F(15) 110.2(3) <F(23A)b, C(15) 98.0(3) <F(23A)b, C(14) 118.9(4) C(17) , C(18) 25.17(6)
C(17) , F(42)a 114.74(7) C(17) , >F(22)b 74.18(18) C(17) , C(49) 112.52(7) C(17) , C(16) 24.16(6)
C(17) , C(19) 42.98(5) C(17) , F(15) 60.47(6) C(17) , C(15) 41.68(6) C(17) , C(14) 48.28(6)
C(18) , F(42)a 116.02(7) C(18) , >F(22)b 97.30(18) C(18) , C(49) 110.82(7) C(18) , C(16) 42.45(6)
C(18) , C(19) 23.93(5) C(18) , F(15) 40.66(5) C(18) , C(15) 48.16(5) C(18) , C(14) 40.90(5)
F(42)a , >F(22)b 68.86(19) F(42)a , C(49) 131.71(7) F(42)a , C(16) 132.04(7) F(42)a , C(19) 133.83(7)
F(42)a , F(15) 83.78(5) F(42)a , C(15) 154.95(8) F(42)a , C(14) 156.28(7) >F(22)b , C(49) 116.6(2)
>F(22)b , C(16) 73.00(18) >F(22)b , C(19) 116.95(18) >F(22)b , F(15) 109.21(19) >F(22)b , C(15) 92.17(19)
>F(22)b , C(14) 113.05(18) C(49) , C(16) 91.09(7) C(49) , C(19) 88.89(6) C(49) , F(15) 129.38(7)
C(49) , C(15) 70.84(6) C(49) , C(14) 70.06(6) C(16) , C(19) 48.37(5) C(16) , F(15) 82.34(6)
C(16) , C(15) 23.00(5) C(16) , C(14) 40.25(5) C(19) , F(15) 50.33(5) C(19) , C(15) 40.68(5)
C(19) , C(14) 22.89(5) F(15) , C(15) 87.54(6) F(15) , C(14) 73.21(6) C(15) , C(14) 22.54(5)
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3.6 Angstrom Coordination Sphere Around Atom I = F(45) [ARU = 1555.06] -0.00044 0.53493 -0.32590 -0.0037 12.7395-11.9494

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|-------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.333(3) | -- | C(420) | | | | Intra | 104.98 | -43.47 | -0.03010 | 0.57418 | -0.35092 | -0.2537 | 13.6742 | -12.8668 |
| 2 | 2.143(2) | << | F(46) | | | | Intra | 55.39 | -72.03 | 0.04410 | 0.55778 | -0.38150 | 0.3718 | 13.2836 | -13.9881 |
| 3 | 2.144(2) | << | F(44) | | | | Intra | 80.41 | -13.66 | 0.04074 | 0.62118 | -0.33971 | 0.3434 | 14.7935 | -12.4558 |
| 4 | 2.343(3) | << | C(48) | | | | Intra | 147.11 | -28.67 | -0.20520 | 0.58180 | -0.35655 | -1.7299 | 13.8557 | -13.0733 |
| 5 | 2.766(2) | <. | F(42)a | [1+x,y,z | = | 1655.06] | | 4.83 | 16.56 | 0.31290 | 0.54430 | -0.30440 | 2.6378 | 12.9626 | -11.1611 |
| 6 | 2.790(3) | << | C(47) | | | | Intra | 157.04 | -0.24 | -0.30520 | 0.58063 | -0.32622 | -2.5729 | 13.8278 | -11.9612 |
| 7 | 2.947(17) | .. | <F(23A)b | [-1/2-x,1-y,1/2+z | = | 2465.02] | | 86.03 | 59.86 | 0.01170 | 0.59690 | -0.25640 | 0.0986 | 14.2153 | -9.4012 |
| 8 | 3.036(7) | .. | >F(23)b | [-1/2-x,1-y,1/2+z | = | 2465.02] | | -130.18 | 81.42 | -0.03510 | 0.52040 | -0.24403 | -0.2959 | 12.3934 | -8.9476 |
| 9 | 3.190(11) | .. | >F(22)b | [-1/2-x,1-y,1/2+z | = | 2465.02] | | 92.37 | 56.91 | -0.00900 | 0.60800 | -0.25300 | -0.0759 | 14.4796 | -9.2765 |
| 10 | 3.204(3) | .. | C(56)c | [-x,-1/2+y,-1/2-z | = | 4544.03] | | -89.21 | 4.79 | 0.00480 | 0.40086 | -0.31860 | 0.0405 | 9.5466 | -11.6818 |
| 11 | 3.282(3) | .. | C(55)c | [-x,-1/2+y,-1/2-z | = | 4544.03] | | -77.47 | -17.08 | 0.08030 | 0.40632 | -0.35219 | 0.6769 | 9.6766 | -12.9134 |
| 12 | 3.323(19) | .. | <F(21A)b | [-1/2-x,1-y,1/2+z | = | 2465.02] | | -162.04 | 73.49 | -0.10700 | 0.52270 | -0.23900 | -0.9020 | 12.4482 | -8.7632 |
| 13 | 3.342(3) | .. | C(57)c | [-x,-1/2+y,-1/2-z | = | 4544.03] | | -113.65 | 6.36 | -0.15850 | 0.40719 | -0.31580 | -1.3362 | 9.6973 | -11.5791 |
| 14 | 3.454(9) | .. | >F(51)c | [-x,-1/2+y,-1/2-z | = | 4544.03] | | -57.08 | 33.07 | 0.18620 | 0.43290 | -0.27450 | 1.5697 | 10.3096 | -10.0648 |
| 15 | 3.465(3) | .. | C(54)c | [-x,-1/2+y,-1/2-z | = | 4544.03] | | -91.41 | -37.16 | -0.00850 | 0.41903 | -0.38298 | -0.0717 | 9.9793 | -14.0423 |
| 16 | 3.487(8) | .. | <F(51A)c | [-x,-1/2+y,-1/2-z | = | 4544.03] | | -70.00 | 41.82 | 0.10500 | 0.43240 | -0.26250 | 0.8852 | 10.2977 | -9.6248 |
| 17 | 3.518(3) | .. | C(58)c | [-x,-1/2+y,-1/2-z | = | 4544.03] | | -126.90 | -12.67 | -0.24490 | 0.41967 | -0.34694 | -2.0646 | 9.9945 | -12.7209 |
| 18 | 3.533(3) | .. | C(49) | | | | Intra | 149.45 | -42.98 | -0.26450 | 0.59010 | -0.39159 | -2.2298 | 14.0533 | -14.3580 |
| 19 | 3.586(3) | .. | C(59)c | [-x,-1/2+y,-1/2-z | = | 4544.03] | | -119.15 | -34.15 | -0.17190 | 0.42612 | -0.38080 | -1.4492 | 10.1481 | -13.9624 |
| 20 | 2.56 | <. | H(47A) | | | | Intra | 156.69 | 19.58 | -0.26320 | 0.57500 | -0.30250 | -2.2188 | 13.6937 | -11.0915 |

Angles (Degrees) At1...V...At2 with Vertex V = F(45)

| | | | | | | | |
|------------------|------------|-------------------|------------|-------------------|------------|-------------------|------------|
| C(420) , F(46) | 36.91(12) | C(420) , F(44) | 36.50(12) | C(420) , C(48) | 36.66(13) | C(420) , F(42)a | 108.58(14) |
| C(420) , C(47) | 63.32(13) | C(420) , <F(23A)b | 104.5(4) | C(420) , >F(23)b | 137.9(2) | C(420) , >F(22)b | 100.9(2) |
| C(420) , C(56)c | 139.34(14) | C(420) , C(55)c | 119.41(13) | C(420) , <F(21A)b | 132.1(3) | C(420) , C(57)c | 129.77(14) |
| C(420) , >F(51)c | 162.5(2) | C(420) , C(54)c | 98.00(13) | C(420) , <F(51A)c | 176.0(3) | C(420) , C(58)c | 106.63(13) |
| C(420) , C(49) | 32.02(12) | C(420) , C(59)c | 92.57(13) | F(46) , F(44) | 60.24(8) | F(46) , C(48) | 63.37(8) |
| F(46) , F(42)a | 94.78(8) | F(46) , C(47) | 93.34(8) | F(46) , <F(23A)b | 133.6(4) | F(46) , >F(23)b | 170.54(17) |
| F(46) , >F(22)b | 131.5(2) | F(46) , C(56)c | 109.27(9) | F(46) , C(55)c | 85.48(8) | F(46) , <F(21A)b | 169.0(3) |
| F(46) , C(57)c | 113.98(9) | F(46) , >F(51)c | 128.2(2) | F(46) , C(54)c | 68.35(7) | F(46) , <F(51A)c | 140.1(2) |
| F(46) , C(58)c | 95.29(8) | F(46) , C(49) | 50.77(6) | F(46) , C(59)c | 73.75(7) | F(44) , C(48) | 63.23(8) |
| F(44) , F(42)a | 80.52(8) | F(44) , C(47) | 76.96(8) | F(44) , <F(23A)b | 73.7(4) | F(44) , >F(23)b | 111.00(16) |
| F(44) , >F(22)b | 71.27(19) | F(44) , C(56)c | 166.45(9) | F(44) , C(55)c | 142.29(9) | F(44) , <F(21A)b | 110.74(19) |
| F(44) , C(57)c | 164.36(9) | F(44) , >F(51)c | 136.81(18) | F(44) , C(54)c | 128.60(8) | F(44) , <F(51A)c | 141.9(2) |
| F(44) , C(58)c | 142.24(9) | F(44) , C(49) | 65.46(7) | F(44) , C(59)c | 128.69(8) | C(48) , F(42)a | 143.32(10) |
| C(48) , C(47) | 29.97(8) | C(48) , <F(23A)b | 101.6(3) | C(48) , >F(23)b | 117.24(19) | C(48) , >F(22)b | 97.2(2) |
| C(48) , C(56)c | 121.67(9) | C(48) , C(55)c | 117.16(9) | C(48) , <F(21A)b | 107.6(4) | C(48) , C(57)c | 101.13(9) |
| C(48) , >F(51)c | 158.83(19) | C(48) , C(54)c | 94.32(8) | C(48) , <F(51A)c | 147.3(3) | C(48) , C(58)c | 80.50(8) |
| C(48) , C(49) | 14.44(7) | C(48) , C(59)c | 77.17(8) | F(42)a , C(47) | 148.12(9) | F(42)a , <F(23A)b | 71.3(3) |
| F(42)a , >F(23)b | 79.59(18) | F(42)a , >F(22)b | 74.9(2) | F(42)a , C(56)c | 92.49(8) | F(42)a , C(55)c | 87.76(7) |

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F(42)a , <F(21A)b      89.5(4)   F(42)a , C(57)c      115.01(8)   F(42)a , >F(51)c     57.74(17)   F(42)a , C(54)c      104.79(7)
F(42)a , <F(51A)c      67.9(3)   F(42)a , C(58)c      133.23(8)   F(42)a , C(49)       140.00(7)   F(42)a , C(59)c      127.11(8)
C(47) , <F(23A)b       80.8(3)   C(47) , >F(23)b      87.71(18)   C(47) , >F(22)b       76.7(2)     C(47) , C(56)c       113.69(8)
C(47) , C(55)c         123.62(8)  C(47) , <F(21A)b     77.8(4)     C(47) , C(57)c       89.34(8)    C(47) , >F(51)c     134.12(19)
C(47) , C(54)c         106.87(8)  C(47) , <F(51A)c     120.7(3)    C(47) , C(58)c       76.35(7)    C(47) , C(49)       43.28(6)
C(47) , C(59)c         84.74(7)   <F(23A)b, >F(23)b    37.4(4)     <F(23A)b, >F(22)b     4.4(4)      <F(23A)b, C(56)c     115.2(4)
<F(23A)b, C(55)c       135.6(4)   <F(23A)b, <F(21A)b   39.1(4)     <F(23A)b, C(57)c     112.0(4)    <F(23A)b, >F(51)c     82.2(4)
<F(23A)b, C(54)c       157.2(4)   <F(23A)b, <F(51A)c   76.4(4)     <F(23A)b, C(58)c     126.9(3)    <F(23A)b, C(49)     115.2(3)
<F(23A)b, C(59)c       149.5(3)   >F(23)b , >F(22)b    39.8(2)     >F(23)b , C(56)c     78.76(15)   >F(23)b , C(55)c    101.77(15)
>F(23)b , <F(21A)b     10.3(5)    >F(23)b , C(57)c     75.42(15)   >F(23)b , >F(51)c     54.8(2)     >F(23)b , C(54)c    120.31(15)
>F(23)b , <F(51A)c     44.4(2)    >F(23)b , C(58)c     94.10(16)   >F(23)b , C(49)     130.98(18)   >F(23)b , C(59)c    115.72(16)
>F(22)b , C(56)c       118.28(19) >F(22)b , C(55)c     139.44(19)   >F(22)b , <F(21A)b   40.4(3)     >F(22)b , C(57)c    113.25(19)
>F(22)b , >F(51)c       86.4(2)    >F(22)b , C(54)c     160.09(19)   >F(22)b , <F(51A)c   80.2(2)     >F(22)b , C(58)c    126.6(2)
>F(22)b , C(49)        110.7(2)   >F(22)b , C(59)c     148.8(2)    C(56)c , C(55)c      24.75(6)    C(56)c , <F(21A)b   80.58(18)
C(56)c , C(57)c         24.38(6)   C(56)c , >F(51)c     41.17(16)   C(56)c , C(54)c      42.00(5)    C(56)c , <F(51A)c   40.80(14)
C(56)c , C(58)c         41.32(6)   C(56)c , C(49)       115.86(7)    C(56)c , C(59)c      48.11(6)    C(55)c , <F(21A)b  104.82(18)
C(55)c , C(57)c         42.76(6)   C(55)c , >F(51)c     53.80(17)   C(55)c , C(54)c      23.54(5)    C(55)c , <F(51A)c   59.30(13)
C(55)c , C(58)c         47.86(6)   C(55)c , C(49)       106.11(7)    C(55)c , C(59)c      40.92(6)    <F(21A)b, C(57)c    72.9(2)
<F(21A)b, >F(51)c       62.5(4)    <F(21A)b, C(54)c     120.27(19)   <F(21A)b, <F(51A)c   50.8(3)     <F(21A)b, C(58)c    89.1(3)
<F(21A)b, C(49)        121.1(4)   <F(21A)b, C(59)c     111.5(3)     C(57)c , >F(51)c     58.72(17)   C(57)c , C(54)c     48.23(6)
C(57)c , <F(51A)c       52.4(2)    C(57)c , C(58)c      23.14(5)     C(57)c , C(49)       99.37(7)    C(57)c , C(59)c     40.85(5)
>F(51)c , C(54)c        77.18(17)   >F(51)c , <F(51A)c    13.5(3)     >F(51)c , C(58)c     80.66(16)   >F(51)c , C(49)     157.00(17)
>F(51)c , C(59)c        88.94(16)   C(54)c , <F(51A)c    81.36(13)    C(54)c , C(58)c      40.04(6)    C(54)c , C(49)      82.65(6)
C(54)c , C(59)c         22.66(6)   <F(51A)c, C(58)c     75.5(2)     <F(51A)c, C(49)     151.1(2)    <F(51A)c, C(59)c    88.34(17)
C(58)c , C(49)         76.80(6)   C(58)c , C(59)c      22.61(5)     C(49) , C(59)c      68.41(6)
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3.6 Angstrom Coordination Sphere Around Atom I = F(46) [ARU = 1555.06] 0.04410 0.55778 -0.38150 0.3718 13.2836-13.9881

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|---------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.342(3) | -- | C(420) | | | | Intra | 148.02 | 56.67 | -0.03010 | 0.57418 | -0.35092 | -0.2537 | 13.6742 | -12.8668 |
| 2 | 2.143(2) | << | F(45) | | | | Intra | -124.61 | 72.03 | -0.00044 | 0.53493 | -0.32590 | -0.0037 | 12.7395 | -11.9494 |
| 3 | 2.151(3) | << | F(44) | | | | Intra | 91.07 | 45.42 | 0.04074 | 0.62118 | -0.33971 | 0.3434 | 14.7935 | -12.4558 |
| 4 | 2.362(3) | << | C(48) | | | | Intra | 164.77 | 22.78 | -0.20520 | 0.58180 | -0.35655 | -1.7299 | 13.8557 | -13.0733 |
| 5 | 2.738(2) | << | C(49) | | | | Intra | 163.52 | -7.77 | -0.26450 | 0.59010 | -0.39159 | -2.2298 | 14.0533 | -14.3580 |
| 6 | 3.236(3) | .. | C(53)b | [-x, -1/2+y, -1/2-z | = | 4544.03] | | -59.63 | -26.29 | 0.21810 | 0.45268 | -0.42059 | 1.8386 | 10.7807 | -15.4214 |
| 7 | 3.334(3) | .. | C(54)b | [-x, -1/2+y, -1/2-z | = | 4544.03] | | -97.64 | -0.93 | -0.00850 | 0.41903 | -0.38298 | -0.0717 | 9.9793 | -14.0423 |
| 8 | 3.421(3) | .. | N(52)b | [-x, -1/2+y, -1/2-z | = | 4544.03] | | -85.72 | -22.26 | 0.07210 | 0.42519 | -0.41684 | 0.6078 | 10.1260 | -15.2839 |
| 9 | 2.45 | << | H(49A) | | | | Intra | 158.19 | -27.21 | -0.19540 | 0.59170 | -0.41200 | -1.6473 | 14.0915 | -15.1064 |
| 10 | 2.87 | .. | H(45A)a | [1+x,y,z | = | 1655.06] | | 20.70 | 8.74 | 0.35900 | 0.59990 | -0.36960 | 3.0264 | 14.2867 | -13.5518 |
| 11 | 2.90 | .. | H(53A)b | [-x, -1/2+y, -1/2-z | = | 4544.03] | | -46.39 | -15.10 | 0.27310 | 0.47270 | -0.40210 | 2.3023 | 11.2574 | -14.7434 |

Angles (Degrees) At1...V...At2 with Vertex V = F(46)

| | | | | | | | |
|-----------------|------------|-----------------|------------|-----------------|------------|-----------------|------------|
| C(420) , F(45) | 36.63(12) | C(420) , F(44) | 36.35(12) | C(420) , C(48) | 36.04(13) | C(420) , C(49) | 65.68(13) |
| C(420) , C(53)b | 143.75(15) | C(420) , C(54)b | 103.89(14) | C(420) , N(52)b | 128.11(15) | F(45) , F(44) | 59.89(8) |
| F(45) , C(48) | 62.44(8) | F(45) , C(49) | 91.92(8) | F(45) , C(53)b | 107.72(9) | F(45) , C(54)b | 74.96(8) |
| F(45) , N(52)b | 97.93(8) | F(44) , C(48) | 62.78(8) | F(44) , C(49) | 83.48(8) | F(44) , C(53)b | 149.80(9) |
| F(44) , C(54)b | 134.86(9) | F(44) , N(52)b | 156.69(10) | C(48) , C(49) | 30.57(7) | C(48) , C(53)b | 139.65(10) |
| C(48) , C(54)b | 97.35(9) | C(48) , N(52)b | 115.56(9) | C(49) , C(53)b | 126.04(9) | C(49) , C(54)b | 98.63(8) |
| C(49) , N(52)b | 105.89(7) | C(53)b , C(54)b | 44.48(6) | C(53)b , N(52)b | 24.09(6) | C(54)b , N(52)b | 24.27(5) |

3.6 Angstrom Coordination Sphere Around Atom I = F(51) [ARU = 1555.03] -0.18620 0.93290 -0.22550 -1.5697 22.2172 -8.2682

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|--------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.338(9) | -- | C(510) | | | | Intra | -56.02 | 17.04 | -0.10140 | 0.88836 | -0.21481 | -0.8548 | 21.1565 | -7.8762 |
| 2 | 2.125(12) | << | >F(52) | | | | Intra | -96.01 | 18.82 | -0.21120 | 0.84890 | -0.20680 | -1.7805 | 20.2167 | -7.5825 |
| 3 | 2.136(15) | << | >F(53) | | | | Intra | -46.81 | -16.49 | -0.01990 | 0.87020 | -0.24204 | -0.1678 | 20.7240 | -8.8746 |
| 4 | 2.353(11) | << | C(56) | | | | Intra | -26.52 | 43.41 | -0.00480 | 0.90086 | -0.18140 | -0.0405 | 21.4542 | -6.6512 |
| 5 | 3.012(12) | .. | >F(23)b | [1/2+x,3/2-y,-1-z | = | 3564.02] | | 48.16 | -21.77 | 0.03510 | 1.02040 | -0.25597 | 0.2959 | 24.3010 | -9.3854 |
| 6 | 3.052(11) | < | C(55) | | | | Intra | -35.34 | 68.98 | -0.08030 | 0.90632 | -0.14781 | -0.6769 | 21.5842 | -5.4196 |
| 7 | 3.063(8) | .. | F(42)d | [-1-x,1/2+y,-1/2-z | = | 4454.06] | | 111.93 | 20.97 | -0.31290 | 1.04430 | -0.19560 | -2.6378 | 24.8702 | -7.1719 |
| 8 | 3.188(11) | .. | F(55)a | [-1+x,y,z | = | 1455.03] | | 177.60 | 25.13 | -0.52830 | 0.93797 | -0.18857 | -4.4537 | 22.3379 | -6.9141 |
| 9 | 3.334(11) | .. | C(57) | | | | Intra | -11.90 | 27.02 | 0.15850 | 0.90719 | -0.18420 | 1.3362 | 21.6049 | -6.7539 |
| 10 | 3.454(9) | .. | F(45)e | [-x,1/2+y,-1/2-z | = | 4554.06] | | 57.08 | 33.07 | 0.00044 | 1.03493 | -0.17410 | 0.0037 | 24.6471 | -6.3836 |
| 11 | 3.47(2) | .. | <F(33A)c | [-1/2+x,3/2-y,-1-z | = | 3464.01] | | -179.75 | -51.69 | -0.44120 | 0.93250 | -0.29970 | -3.7194 | 22.2077 | -10.9888 |
| 12 | 3.52(2) | .. | <F(21A)b | [1/2+x,3/2-y,-1-z | = | 3564.02] | | 40.87 | -21.71 | 0.10700 | 1.02270 | -0.26100 | 0.9020 | 24.3558 | -9.5698 |
| 13 | 3.01 | .. | H(55A) | | | | Intra | -93.60 | 75.54 | -0.19180 | 0.90140 | -0.14600 | -1.6169 | 21.4670 | -5.3532 |
| 14 | 3.48 | .. | H(57A) | | | | Intra | -12.03 | 11.17 | 0.21020 | 0.90300 | -0.20710 | 1.7720 | 21.5051 | -7.5935 |

Angles (Degrees) At1...V...At2 with Vertex V = >F(51)

| | | | | | | | |
|--------------------|-----------|---------------------|-----------|-------------------|-----------|--------------------|-----------|
| C(510) , >F(52) | 38.0(4) | C(510) , >F(53) | 34.7(4) | C(510) , C(56) | 36.3(3) | C(510) , >F(23)b | 109.0(6) |
| C(510) , C(55) | 53.5(4) | C(510) , F(42)d | 140.2(6) | C(510) , F(55)a | 112.9(5) | C(510) , C(57) | 41.9(4) |
| C(510) , F(45)e | 98.9(5) | C(510) , <F(33A)c | 124.0(7) | C(510) , <F(21A)b | 102.4(6) | >F(52) , >F(53) | 59.9(5) |
| >F(52) , C(56) | 62.5(4) | >F(52) , >F(23)b | 146.4(6) | >F(52) , C(55) | 62.1(3) | >F(52) , F(42)d | 131.7(5) |
| >F(52) , F(55)a | 79.0(4) | >F(52) , C(57) | 76.5(4) | >F(52) , F(45)e | 122.1(5) | >F(52) , <F(33A)c | 100.9(6) |
| >F(52) , <F(21A)b | 139.6(6) | >F(53) , C(56) | 62.7(3) | >F(53) , >F(23)b | 88.4(5) | >F(53) , C(55) | 85.9(4) |
| >F(53) , F(42)d | 159.4(5) | >F(53) , F(55)a | 137.8(5) | >F(53) , C(57) | 55.1(3) | >F(53) , F(45)e | 110.4(5) |
| >F(53) , <F(33A)c | 100.5(6) | >F(53) , <F(21A)b | 81.9(5) | C(56) , >F(23)b | 94.4(4) | C(56) , C(55) | 25.98(14) |
| C(56) , F(42)d | 105.2(4) | C(56) , F(55)a | 108.0(4) | C(56) , C(57) | 20.22(13) | C(56) , F(45)e | 63.7(2) |
| C(56) , <F(33A)c | 160.3(6) | C(56) , <F(21A)b | 89.7(5) | >F(23)b , C(55) | 108.0(4) | >F(23)b , F(42)d | 75.5(2) |
| >F(23)b , F(55)a | 133.8(3) | >F(23)b , C(57) | 75.9(3) | >F(23)b , F(45)e | 55.5(2) | >F(23)b , <F(33A)c | 95.4(5) |
| >F(23)b , <F(21A)b | 6.8(3) | C(55) , F(42)d | 87.0(3) | C(55) , F(55)a | 82.9(3) | C(55) , C(57) | 44.18(16) |
| C(55) , F(45)e | 60.22(19) | C(55) , <F(33A)c | 156.0(5) | C(55) , <F(21A)b | 105.4(4) | F(42)d , F(55)a | 59.98(19) |
| F(42)d , C(57) | 107.5(3) | F(42)d , F(45)e | 49.78(13) | F(42)d , <F(33A)c | 93.8(5) | F(42)d , <F(21A)b | 81.4(3) |
| F(55)a , C(57) | 127.1(3) | F(55)a , F(45)e | 98.8(3) | F(55)a , <F(33A)c | 76.9(4) | F(55)a , <F(21A)b | 140.3(4) |
| C(57) , F(45)e | 58.96(18) | C(57) , <F(33A)c | 153.7(5) | C(57) , <F(21A)b | 70.6(4) | F(45)e , <F(33A)c | 135.4(6) |
| F(45)e , <F(21A)b | 56.9(3) | <F(33A)c , <F(21A)b | 98.5(6) | | | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(52) [ARU = 1555.03] -0.21120 0.84890 -0.20680 -1.7805 20.2167 -7.5825

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|---------|
| 1 | 1.351(10) | -- | C(510) | | | | Intra | 45.43 | -12.55 | -0.10140 | 0.88836 | -0.21481 | -0.8548 | 21.1565 | -7.8762 |
| 2 | 2.125(12) | << | >F(51) | | | | Intra | 83.99 | -18.82 | -0.18620 | 0.93290 | -0.22550 | -1.5697 | 22.2172 | -8.2682 |
| 3 | 2.128(12) | << | >F(53) | | | | Intra | 17.46 | -37.39 | -0.01990 | 0.87020 | -0.24204 | -0.1678 | 20.7240 | -8.8746 |
| 4 | 2.329(10) | << | C(56) | | | | Intra | 35.42 | 23.57 | -0.00480 | 0.90086 | -0.18140 | -0.0405 | 21.4542 | -6.6512 |
| 5 | 2.787(9) | << | C(55) | | | | Intra | 51.10 | 50.91 | -0.08030 | 0.90632 | -0.14781 | -0.6769 | 21.5842 | -5.4196 |
| 6 | 2.828(9) | .< | F(64)c | [1/2+x,3/2-y,-z | = | 3565.04] | | -92.49 | 59.53 | -0.21860 | 0.78875 | -0.14032 | -1.8428 | 18.7842 | -5.1450 |
| 7 | 3.030(9) | .. | F(12) | [| = | 05] | | -121.09 | -51.29 | -0.32730 | 0.78075 | -0.27129 | -2.7592 | 18.5937 | -9.9471 |
| 8 | 3.077(15) | .. | <F(63)b | [-1/2+x,3/2-y,-z | = | 3465.04] | | -153.82 | 0.91 | -0.53870 | 0.79190 | -0.20547 | -4.5413 | 18.8593 | -7.5338 |
| 9 | 3.246(9) | .. | F(11) | [| = | 05] | | -79.82 | -26.50 | -0.15030 | 0.72885 | -0.24630 | -1.2671 | 17.3577 | -9.0308 |
| 10 | 3.426(10) | .. | F(54)a | [-1+x,y,z | = | 1455.03] | | 164.03 | 41.61 | -0.50330 | 0.87850 | -0.14476 | -4.2429 | 20.9217 | -5.3078 |
| 11 | 3.477(11) | .. | F(55)a | [-1+x,y,z | = | 1455.03] | | 141.57 | 11.08 | -0.52830 | 0.93797 | -0.18857 | -4.4537 | 22.3379 | -6.9141 |
| 12 | 3.497(12) | .. | >F(63A)b | [-1/2+x,3/2-y,-z | = | 3465.04] | | -134.17 | 1.14 | -0.50020 | 0.74360 | -0.20490 | -4.2168 | 17.7090 | -7.5129 |
| 13 | 3.511(11) | .. | C(57) | | | | Intra | 24.01 | 13.65 | 0.15850 | 0.90719 | -0.18420 | 1.3362 | 21.6049 | -6.7539 |
| 14 | 2.56 | .< | H(55A) | | | | Intra | 82.55 | 60.51 | -0.19180 | 0.90140 | -0.14600 | -1.6169 | 21.4670 | -5.3532 |
| 15 | 3.27 | .. | H(67A)c | [1/2+x,3/2-y,-z | = | 3565.04] | | -48.87 | 11.53 | 0.03850 | 0.74770 | -0.18900 | 0.3246 | 17.8066 | -6.9299 |

Angles (Degrees) At1...V...At2 with Vertex V = >F(52)

| | | | | | | | |
|------------------|-----------|-------------------|-----------|--------------------|-----------|-------------------|----------|
| C(510) , >F(51) | 37.6(4) | C(510) , >F(53) | 35.2(4) | C(510) , C(56) | 37.4(3) | C(510) , C(55) | 63.7(3) |
| C(510) , F(64)c | 123.7(5) | C(510) , F(12) | 115.1(4) | C(510) , <F(63)b | 157.7(6) | C(510) , F(11) | 114.0(5) |
| C(510) , F(54)a | 119.6(5) | C(510) , F(55)a | 98.3(5) | C(510) , >F(63A)b | 168.6(5) | C(510) , C(57) | 33.7(3) |
| >F(51) , >F(53) | 60.3(5) | >F(51) , C(56) | 63.6(4) | >F(51) , C(55) | 75.5(4) | >F(51) , F(64)c | 139.2(5) |
| >F(51) , F(12) | 106.5(4) | >F(51) , <F(63)b | 120.6(6) | >F(51) , F(11) | 132.0(4) | >F(51) , F(54)a | 95.3(4) |
| >F(51) , F(55)a | 64.2(4) | >F(51) , >F(63A)b | 138.6(5) | >F(51) , C(57) | 67.4(4) | >F(53) , C(56) | 63.3(4) |
| >F(53) , C(55) | 93.1(4) | >F(53) , F(64)c | 131.4(5) | >F(53) , F(12) | 84.2(4) | >F(53) , <F(63)b | 142.6(4) |
| >F(53) , F(11) | 79.6(5) | >F(53) , F(54)a | 154.0(5) | >F(53) , F(55)a | 123.6(5) | >F(53) , >F(63A)b | 135.3(5) |
| >F(53) , C(57) | 51.4(3) | C(56) , C(55) | 29.92(13) | C(56) , F(64)c | 86.6(3) | C(56) , F(12) | 146.9(4) |
| C(56) , <F(63)b | 153.9(4) | C(56) , F(11) | 121.9(4) | C(56) , F(54)a | 99.3(3) | C(56) , F(55)a | 100.0(3) |
| C(56) , >F(63A)b | 153.3(3) | C(56) , C(57) | 14.66(12) | C(55) , F(64)c | 65.69(18) | C(55) , F(12) | 175.1(4) |
| C(55) , <F(63)b | 124.0(3) | C(55) , F(11) | 135.7(4) | C(55) , F(54)a | 70.63(19) | C(55) , F(55)a | 81.7(2) |
| C(55) , >F(63A)b | 127.8(3) | C(55) , C(57) | 43.22(16) | F(64)c , F(12) | 113.2(3) | F(64)c , <F(63)b | 75.1(3) |
| F(64)c , F(11) | 86.7(3) | F(64)c , F(54)a | 61.05(17) | F(64)c , F(55)a | 97.3(3) | F(64)c , >F(63A)b | 66.7(2) |
| F(64)c , C(57) | 90.9(2) | F(12) , <F(63)b | 59.1(2) | F(12) , F(11) | 39.75(12) | F(12) , F(54)a | 113.3(3) |
| F(12) , F(55)a | 103.2(3) | F(12) , >F(63A)b | 53.59(17) | F(12) , C(57) | 133.1(3) | <F(63)b , F(11) | 76.1(3) |
| <F(63)b , F(54)a | 55.6(2) | <F(63)b , F(55)a | 64.9(3) | <F(63)b , >F(63A)b | 19.6(3) | <F(63)b , C(57) | 165.3(3) |
| F(11) , F(54)a | 126.3(3) | F(11) , F(55)a | 138.1(3) | F(11) , >F(63A)b | 59.17(19) | F(11) , C(57) | 108.3(3) |
| F(54)a , F(55)a | 36.32(11) | F(54)a , >F(63A)b | 68.5(2) | F(54)a , C(57) | 113.6(2) | F(55)a , >F(63A)b | 84.2(3) |
| F(55)a , C(57) | 113.3(3) | >F(63A)b , C(57) | 153.8(3) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(53) [ARU = 1555.03] -0.01990 0.87020 -0.24204 -0.1678 20.7240 -8.8746

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|-------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.287(8) | -- | C(510) | | | | Intra | 147.81 | 50.88 | -0.10140 | 0.88836 | -0.21481 | -0.8548 | 21.1565 | -7.8762 |
| 2 | 2.128(12) | << | >F(52) | | | | Intra | 162.54 | 37.39 | -0.21120 | 0.84890 | -0.20680 | -1.7805 | 20.2167 | -7.5825 |
| 3 | 2.136(15) | << | >F(51) | | | | Intra | 133.19 | 16.49 | -0.18620 | 0.93290 | -0.22550 | -1.5697 | 22.2172 | -8.2682 |
| 4 | 2.344(8) | << | C(56) | | | | Intra | 80.11 | 71.56 | -0.00480 | 0.90086 | -0.18140 | -0.0405 | 21.4542 | -6.6512 |
| 5 | 2.745(8) | << | C(57) | | | | Intra | 30.36 | 50.58 | 0.15850 | 0.90719 | -0.18420 | 1.3362 | 21.6049 | -6.7539 |
| 6 | 3.023(15) | .. | <F(62)b | [1/2+x,3/2-y,-z | = | 3565.04] | | -42.69 | 9.03 | 0.24040 | 0.78520 | -0.22910 | 2.0266 | 18.6997 | -8.4002 |
| 7 | 3.084(7) | .. | F(35)a | [1/2+x,3/2-y,-1-z | = | 3564.01] | | 177.05 | -67.70 | -0.15850 | 0.87273 | -0.31986 | -1.3362 | 20.7842 | -11.7280 |
| 8 | 3.441(13) | .. | >F(62A)b | [1/2+x,3/2-y,-z | = | 3565.04] | | -28.26 | 11.46 | 0.33250 | 0.80315 | -0.22340 | 2.8030 | 19.1272 | -8.1912 |
| 9 | 3.461(8) | .. | C(37)a | [1/2+x,3/2-y,-1-z | = | 3564.01] | | 40.04 | -58.33 | 0.14510 | 0.91928 | -0.32238 | 1.2232 | 21.8928 | -11.8204 |
| 10 | 3.50(3) | .. | <F(31A)a | [1/2+x,3/2-y,-1-z | = | 3564.01] | | 8.14 | -17.75 | 0.37100 | 0.89000 | -0.27110 | 3.1276 | 21.1955 | -9.9402 |
| 11 | 3.522(11) | .. | F(12) | [| = | 05] | | -140.58 | -17.73 | -0.32730 | 0.78075 | -0.27129 | -2.7592 | 18.5937 | -9.9471 |
| 12 | 3.545(14) | .. | F(11) | [| = | 05] | | -108.09 | -2.53 | -0.15030 | 0.72885 | -0.24630 | -1.2671 | 17.3577 | -9.0308 |
| 13 | 3.582(15) | .. | <F(32B)a | [1/2+x,3/2-y,-1-z | = | 3564.01] | | 31.50 | -12.57 | 0.33370 | 0.94690 | -0.26330 | 2.8132 | 22.5506 | -9.6542 |
| 14 | 3.597(8) | .. | C(55) | | | | Intra | 120.62 | 73.86 | -0.08030 | 0.90632 | -0.14781 | -0.6769 | 21.5842 | -5.4196 |
| 15 | 2.45 | << | H(57A) | | | | Intra | 21.93 | 31.49 | 0.21020 | 0.90300 | -0.20710 | 1.7720 | 21.5051 | -7.5935 |
| 16 | 2.57 | < | H(37A)a | [1/2+x,3/2-y,-1-z | = | 3564.01] | | 48.13 | -53.88 | 0.10010 | 0.91760 | -0.29870 | 0.8439 | 21.8528 | -10.9521 |
| 17 | 3.46 | .. | H(17A) | [| = | 05] | | -74.77 | -27.28 | 0.07590 | 0.74560 | -0.28530 | 0.6399 | 17.7566 | -10.4608 |
| 18 | 3.54 | .. | H(67A)b | [1/2+x,3/2-y,-z | = | 3565.04] | | -80.42 | 33.32 | 0.03850 | 0.74770 | -0.18900 | 0.3246 | 17.8066 | -6.9299 |

Angles (Degrees) At1...V...At2 with Vertex V = >F(53)

| | | | | | | | |
|--------------------|-----------|--------------------|------------|---------------------|-----------|---------------------|-----------|
| C(510) , >F(52) | 37.3(4) | C(510) , >F(51) | 36.3(5) | C(510) , C(56) | 35.7(2) | C(510) , C(57) | 65.5(3) |
| C(510) , <F(62)b | 119.4(5) | C(510) , F(35)a | 120.6(5) | C(510) , >F(62A)b | 117.6(4) | C(510) , C(37)a | 139.6(8) |
| C(510) , <F(31A)a | 134.0(7) | C(510) , F(12) | 92.7(5) | C(510) , F(11) | 100.8(6) | C(510) , <F(32B)a | 116.2(7) |
| C(510) , C(55) | 25.7(2) | >F(52) , >F(51) | 59.8(4) | >F(52) , C(56) | 62.6(3) | >F(52) , C(57) | 91.3(3) |
| >F(52) , <F(62)b | 107.2(5) | >F(52) , F(35)a | 106.2(4) | >F(52) , >F(62A)b | 115.0(5) | >F(52) , C(37)a | 154.4(4) |
| >F(52) , <F(31A)a | 158.7(5) | >F(52) , F(12) | 58.9(3) | >F(52) , F(11) | 64.2(4) | >F(52) , <F(32B)a | 152.2(5) |
| >F(52) , C(55) | 50.7(3) | >F(51) , C(56) | 63.2(4) | >F(51) , C(57) | 85.2(5) | >F(51) , <F(62)b | 154.2(4) |
| >F(51) , F(35)a | 90.0(4) | >F(51) , >F(62A)b | 146.6(5) | >F(51) , C(37)a | 105.6(5) | >F(51) , <F(31A)a | 127.7(7) |
| >F(51) , F(12) | 91.5(4) | >F(51) , F(11) | 118.2(4) | >F(51) , <F(32B)a | 104.6(6) | >F(51) , C(55) | 57.8(3) |
| C(56) , C(57) | 30.39(13) | C(56) , <F(62)b | 91.2(3) | C(56) , F(35)a | 153.2(5) | C(56) , >F(62A)b | 84.8(2) |
| C(56) , C(37)a | 132.9(5) | C(56) , <F(31A)a | 101.3(4) | C(56) , F(12) | 121.2(3) | C(56) , F(11) | 110.8(4) |
| C(56) , <F(32B)a | 90.1(3) | C(56) , C(55) | 12.01(10) | C(57) , <F(62)b | 72.3(3) | C(57) , F(35)a | 156.4(5) |
| C(57) , >F(62A)b | 61.48(18) | C(57) , C(37)a | 109.2(3) | C(57) , <F(31A)a | 71.1(4) | C(57) , F(12) | 146.4(3) |
| C(57) , F(11) | 120.6(4) | C(57) , <F(32B)a | 63.2(2) | C(57) , C(55) | 42.16(12) | <F(62)b , F(35)a | 115.7(4) |
| <F(62)b , >F(62A)b | 14.4(2) | <F(62)b , C(37)a | 93.9(3) | <F(62)b , <F(31A)a | 56.9(4) | <F(62)b , F(12) | 100.2(4) |
| <F(62)b , F(11) | 66.2(3) | <F(62)b , <F(32B)a | 76.8(3) | <F(62)b , C(55) | 96.4(2) | F(35)a , >F(62A)b | 121.3(3) |
| F(35)a , C(37)a | 50.07(12) | F(35)a , <F(31A)a | 94.2(4) | F(35)a , F(12) | 56.72(15) | F(35)a , F(11) | 82.0(3) |
| F(35)a , <F(32B)a | 96.0(3) | F(35)a , C(55) | 146.2(3) | >F(62A)b , C(37)a | 88.8(2) | >F(62A)b , <F(31A)a | 46.3(4) |
| >F(62A)b , F(12) | 114.5(4) | >F(62A)b , F(11) | 80.6(3) | >F(62A)b , <F(32B)a | 64.0(2) | >F(62A)b , C(55) | 92.4(2) |
| C(37)a , <F(31A)a | 46.9(3) | C(37)a , F(12) | 103.94(19) | C(37)a , F(11) | 114.1(3) | C(37)a , <F(32B)a | 46.22(17) |

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| | | | | | | | |
|------------------|----------|-----------------|-----------|------------------|----------|--------------------|----------|
| C(37)a , C(55) | 142.5(4) | <F(31A)a, F(12) | 133.0(4) | <F(31A)a, F(11) | 114.0(4) | <F(31A)a, <F(32B)a | 23.1(4) |
| <F(31A)a, C(55) | 113.2(4) | F(12) , F(11) | 35.31(13) | F(12) , <F(32B)a | 148.7(3) | F(12) , C(55) | 109.5(2) |
| F(11) , <F(32B)a | 137.1(4) | F(11) , C(55) | 103.0(3) | <F(32B)a, C(55) | 101.8(3) | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(54) [ARU = 1555.03] 0.49670 0.87850 -0.14476 4.1873 20.9217 -5.3078

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|-----------------|-----------|----------|-------|---------|--------|---------|---------|----------|--------|---------|---------|
| 1 | 1.344(3) | -- | C(520) | | | | Intra | 119.42 | -16.71 | 0.42170 | 0.92557 | -0.15530 | 3.5550 | 22.0426 | -5.6942 |
| 2 | 2.131(2) | << | F(56) | | | | Intra | 94.60 | 11.22 | 0.47680 | 0.96598 | -0.13345 | 4.0195 | 23.0050 | -4.8931 |
| 3 | 2.152(3) | << | F(55) | | | | Intra | 98.46 | -48.29 | 0.47170 | 0.93797 | -0.18857 | 3.9765 | 22.3379 | -6.9141 |
| 4 | 2.358(3) | << | C(58) | | | | Intra | 155.21 | -7.42 | 0.24490 | 0.91967 | -0.15306 | 2.0646 | 21.9021 | -5.6121 |
| 5 | 3.049(11) | .. | <F(63)c | [1/2+x,3/2-y,-z | = | 3565.04] | | -98.23 | -46.89 | 0.46130 | 0.79190 | -0.20547 | 3.8889 | 18.8593 | -7.5338 |
| 6 | 3.108(3) | < | C(59) | | | | Intra | 157.50 | 17.55 | 0.17190 | 0.92612 | -0.11920 | 1.4492 | 22.0557 | -4.3706 |
| 7 | 3.131(3) | < | C(65)c | [1/2+x,3/2-y,-z | = | 3565.04] | | -112.14 | 4.40 | 0.35710 | 0.75707 | -0.13821 | 3.0104 | 18.0298 | -5.0676 |
| 8 | 3.218(3) | .. | F(64)b | [3/2+x,3/2-y,-z | = | 3665.04] | | -41.69 | 2.90 | 0.78140 | 0.78875 | -0.14032 | 6.5874 | 18.7842 | -5.1450 |
| 9 | 3.241(10) | .. | <F(52A)a | [1+x,y,z | = | 1655.03] | | -5.32 | -47.08 | 0.75740 | 0.86990 | -0.20950 | 6.3850 | 20.7168 | -7.6815 |
| 10 | 3.269(3) | .. | C(57) | | | | Intra | 166.52 | -26.25 | 0.15850 | 0.90719 | -0.18420 | 1.3362 | 21.6049 | -6.7539 |
| 11 | 3.426(10) | .. | >F(52)a | [1+x,y,z | = | 1655.03] | | -15.97 | -41.61 | 0.78880 | 0.84890 | -0.20680 | 6.6497 | 20.2167 | -7.5825 |
| 12 | 3.575(3) | .. | C(63)c | [1/2+x,3/2-y,-z | = | 3565.04] | | -93.33 | 57.36 | 0.48340 | 0.79768 | -0.06265 | 4.0752 | 18.9969 | -2.2971 |
| 13 | 2.68 | .. | H(55A)a | [1+x,y,z | = | 1655.03] | | 11.73 | -0.97 | 0.80820 | 0.90140 | -0.14600 | 6.8133 | 21.4670 | -5.3532 |
| 14 | 2.77 | .. | H(63A)c | [1/2+x,3/2-y,-z | = | 3565.04] | | -87.89 | 66.14 | 0.50160 | 0.83150 | -0.07570 | 4.2286 | 19.8023 | -2.7756 |
| 15 | 2.81 | .. | H(65A)c | [1/2+x,3/2-y,-z | = | 3565.04] | | -94.77 | 3.63 | 0.46900 | 0.76100 | -0.13990 | 3.9538 | 18.1234 | -5.1296 |
| 16 | 3.12 | .. | H(59A) | | | | Intra | 148.83 | 33.30 | 0.23240 | 0.93510 | -0.09810 | 1.9592 | 22.2696 | -3.5969 |
| 17 | 3.38 | .. | H(57A) | | | | Intra | 166.42 | -42.61 | 0.21020 | 0.90300 | -0.20710 | 1.7720 | 21.5051 | -7.5935 |
| 18 | 3.43 | .. | H(53A)a | [1+x,y,z | = | 1655.03] | | 49.14 | 30.08 | 0.72690 | 0.97270 | -0.09790 | 6.1279 | 23.1650 | -3.5896 |

Angles (Degrees) At1...V...At2 with Vertex V = F(54)

| | | | | | | | |
|-------------------|------------|--------------------|------------|-------------------|------------|-------------------|------------|
| C(520) , F(56) | 37.19(13) | C(520) , F(55) | 35.92(13) | C(520) , C(58) | 36.14(13) | C(520) , <F(63)c | 108.0(3) |
| C(520) , C(59) | 50.79(13) | C(520) , C(65)c | 128.00(15) | C(520) , F(64)b | 156.86(17) | C(520) , <F(52A)a | 99.3(3) |
| C(520) , C(57) | 44.61(13) | C(520) , >F(52)a | 108.6(2) | C(520) , C(63)c | 132.58(16) | F(56) , F(55) | 59.61(9) |
| F(56) , C(58) | 63.11(8) | F(56) , <F(63)c | 142.7(2) | F(56) , C(59) | 61.00(7) | F(56) , C(65)c | 149.14(10) |
| F(56) , F(64)b | 134.29(10) | F(56) , <F(52A)a | 104.9(3) | F(56) , C(57) | 79.23(8) | F(56) , >F(52)a | 112.77(18) |
| F(56) , C(63)c | 111.10(10) | F(55) , C(58) | 62.73(9) | F(55) , <F(63)c | 83.7(2) | F(55) , C(59) | 84.18(8) |
| F(55) , C(65)c | 128.92(11) | F(55) , F(64)b | 123.23(11) | F(55) , <F(52A)a | 64.0(2) | F(55) , C(57) | 56.41(7) |
| F(55) , >F(52)a | 73.15(17) | F(55) , C(63)c | 168.49(10) | C(58) , <F(63)c | 95.7(2) | C(58) , C(59) | 25.07(7) |
| C(58) , C(65)c | 93.19(9) | C(58) , F(64)b | 162.58(10) | C(58) , <F(52A)a | 122.8(2) | C(58) , C(57) | 21.70(7) |
| C(58) , >F(52)a | 130.32(18) | C(58) , C(63)c | 107.72(9) | <F(63)c , C(59) | 112.4(2) | <F(63)c , C(65)c | 52.7(2) |
| <F(63)c , F(64)b | 70.2(2) | <F(63)c , <F(52A)a | 59.3(3) | <F(63)c , C(57) | 74.5(2) | <F(63)c , >F(52)a | 56.4(3) |
| <F(63)c , C(63)c | 104.3(2) | C(59) , C(65)c | 89.01(7) | C(59) , F(64)b | 152.14(10) | C(59) , <F(52A)a | 147.3(2) |
| C(59) , C(57) | 44.67(6) | C(59) , >F(52)a | 155.30(17) | C(59) , C(63)c | 85.12(7) | C(65)c , F(64)b | 70.31(7) |
| C(65)c , <F(52A)a | 104.6(3) | C(65)c , C(57) | 84.21(7) | C(65)c , >F(52)a | 97.53(17) | C(65)c , C(63)c | 55.00(7) |
| F(64)b , <F(52A)a | 59.3(2) | F(64)b , C(57) | 144.26(10) | F(64)b , >F(52)a | 50.27(17) | F(64)b , C(63)c | 67.86(9) |
| <F(52A)a , C(57) | 106.30(18) | <F(52A)a , >F(52)a | 9.4(3) | <F(52A)a , C(63)c | 127.2(2) | C(57) , >F(52)a | 112.10(17) |
| C(57) , C(63)c | 117.24(8) | >F(52)a , C(63)c | 118.10(16) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(55) [ARU = 1555.03] 0.47170 0.93797 -0.18857 3.9765 22.3379 -6.9141

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|------------------------------|----------------------|--------|-------|---------|--------|---------|---------|----------|--------|---------|----------|
| 1 | 1.324(3) | -- C(520) | | | Intra | -144.99 | 67.13 | 0.42170 | 0.92557 | -0.15530 | 3.5550 | 22.0426 | -5.6942 |
| 2 | 2.129(3) | << F(56) | | | Intra | 86.31 | 71.70 | 0.47680 | 0.96598 | -0.13345 | 4.0195 | 23.0050 | -4.8931 |
| 3 | 2.152(3) | << F(54) | | | Intra | -81.54 | 48.29 | 0.49670 | 0.87850 | -0.14476 | 4.1873 | 20.9217 | -5.3078 |
| 4 | 2.354(3) | << C(58) | | | Intra | -167.16 | 33.58 | 0.24490 | 0.91967 | -0.15306 | 2.0646 | 21.9021 | -5.6121 |
| 5 | 2.745(3) | << C(57) | | | Intra | -164.48 | 3.35 | 0.15850 | 0.90719 | -0.18420 | 1.3362 | 21.6049 | -6.7539 |
| 6 | 2.984(8) | .. <F(32B)b[1/2+x,3/2-y,-1-z | = 3564.01] | | | 169.64 | -66.65 | 0.33370 | 0.94690 | -0.26330 | 2.8132 | 22.5506 | -9.6542 |
| 7 | 3.003(10) | .. <F(52A)a[1+x,y,z | = 1655.03] | | | -33.94 | -14.81 | 0.75740 | 0.86990 | -0.20950 | 6.3850 | 20.7168 | -7.6815 |
| 8 | 3.011(8) | .. <F(32)b [1/2+x,3/2-y,-1-z | = 3564.01] | | | -157.74 | -66.54 | 0.34010 | 0.91890 | -0.26390 | 2.8671 | 21.8838 | -9.6762 |
| 9 | 3.127(3) | .. F(42)d [-x,1/2+y,-1/2-z | = 4554.06] | | | 54.36 | -4.73 | 0.68710 | 1.04430 | -0.19560 | 5.7924 | 24.8702 | -7.1719 |
| 10 | 3.188(11) | .. >F(51)a [1+x,y,z | = 1655.03] | | | -2.40 | -25.13 | 0.81380 | 0.93290 | -0.22550 | 6.8605 | 22.2172 | -8.2682 |
| 11 | 3.344(19) | .. <F(31A)b[1/2+x,3/2-y,-1-z | = 3564.01] | | | -126.62 | -64.81 | 0.37100 | 0.89000 | -0.27110 | 3.1276 | 21.1955 | -9.9402 |
| 12 | 3.46(3) | .. <F(32A)b[1/2+x,3/2-y,-1-z | = 3564.01] | | | 130.99 | -67.77 | 0.37000 | 0.97940 | -0.27580 | 3.1192 | 23.3246 | -10.1125 |
| 13 | 3.477(11) | .. >F(52)a [1+x,y,z | = 1655.03] | | | -38.43 | -11.08 | 0.78880 | 0.84890 | -0.20680 | 6.6497 | 20.2167 | -7.5825 |
| 14 | 3.535(14) | .. <F(63)c [1/2+x,3/2-y,-z | = 3565.04] | | | -91.44 | -10.10 | 0.46130 | 0.79190 | -0.20547 | 3.8889 | 18.8593 | -7.5338 |
| 15 | 3.597(3) | .. C(59) | | | Intra | -173.63 | 45.00 | 0.17190 | 0.92612 | -0.11920 | 1.4492 | 22.0557 | -4.3706 |
| 16 | 2.45 | << H(57A) | | | Intra | -159.30 | -16.08 | 0.21020 | 0.90300 | -0.20710 | 1.7720 | 21.5051 | -7.5935 |
| 17 | 3.35 | .. H(55A)a[1+x,y,z | = 1655.03] | | | -17.07 | 27.74 | 0.80820 | 0.90140 | -0.14600 | 6.8133 | 21.4670 | -5.3532 |

Angles (Degrees) At1...V...At2 with Vertex V = F(55)

| | | | | | | | |
|--------------------|------------|--------------------|------------|-------------------|------------|--------------------|------------|
| C(520) , F(56) | 37.02(13) | C(520) , F(54) | 36.55(14) | C(520) , C(58) | 35.95(13) | C(520) , C(57) | 65.19(14) |
| C(520) , <F(32B)b | 137.5(3) | C(520) , <F(52A)a | 111.7(3) | C(520) , <F(32)b | 134.0(2) | C(520) , F(42)d | 116.20(16) |
| C(520) , >F(51)a | 132.1(2) | C(520) , <F(31A)b | 132.6(4) | C(520) , <F(32A)b | 146.9(4) | C(520) , >F(52)a | 106.6(2) |
| C(520) , <F(63)c | 86.22(19) | C(520) , C(59) | 26.78(13) | F(56) , F(54) | 59.71(8) | F(56) , C(58) | 63.21(9) |
| F(56) , C(57) | 92.73(9) | F(56) , <F(32B)b | 149.0(2) | F(56) , <F(52A)a | 113.3(2) | F(56) , <F(32)b | 157.8(2) |
| F(56) , F(42)d | 79.21(9) | F(56) , >F(51)a | 113.4(2) | F(56) , <F(31A)b | 166.2(4) | F(56) , <F(32A)b | 142.6(4) |
| F(56) , >F(52)a | 110.99(15) | F(56) , <F(63)c | 118.38(14) | F(56) , C(59) | 50.76(7) | F(54) , C(58) | 62.92(9) |
| F(54) , C(57) | 82.81(9) | F(54) , <F(32B)b | 140.4(3) | F(54) , <F(52A)a | 75.9(2) | F(54) , <F(32)b | 128.4(2) |
| F(54) , F(42)d | 122.53(9) | F(54) , >F(51)a | 101.74(19) | F(54) , <F(31A)b | 118.4(3) | F(54) , <F(32A)b | 154.6(3) |
| F(54) , >F(52)a | 70.53(15) | F(54) , <F(63)c | 59.04(13) | F(54) , C(59) | 59.29(7) | C(58) , C(57) | 30.34(8) |
| C(58) , <F(32B)b | 101.8(2) | C(58) , <F(52A)a | 133.9(3) | C(58) , <F(32)b | 100.38(19) | C(58) , F(42)d | 131.86(11) |
| C(58) , >F(51)a | 164.29(19) | C(58) , <F(31A)b | 103.4(4) | C(58) , <F(32A)b | 111.3(4) | C(58) , >F(52)a | 128.16(18) |
| C(58) , <F(63)c | 83.95(17) | C(58) , C(59) | 12.46(7) | C(57) , <F(32B)b | 72.4(2) | C(57) , <F(52A)a | 130.0(3) |
| C(57) , <F(32)b | 70.05(18) | C(57) , F(42)d | 141.24(10) | C(57) , >F(51)a | 152.22(19) | C(57) , <F(31A)b | 73.6(4) |
| C(57) , <F(32A)b | 83.8(4) | C(57) , >F(52)a | 126.00(19) | C(57) , <F(63)c | 73.95(18) | C(57) , C(59) | 42.43(6) |
| <F(32B)b, <F(52A)a | 96.7(3) | <F(32B)b, <F(32)b | 12.8(3) | <F(32B)b, F(42)d | 95.3(2) | <F(32B)b, >F(51)a | 88.0(3) |
| <F(32B)b, <F(31A)b | 25.1(4) | <F(32B)b, <F(32A)b | 14.8(4) | <F(32B)b, >F(52)a | 99.6(3) | <F(32B)b, <F(63)c | 84.2(3) |
| <F(32B)b, C(59) | 112.4(2) | <F(52A)a, <F(32)b | 88.8(3) | <F(52A)a, F(42)d | 87.2(2) | <F(52A)a, >F(51)a | 31.3(3) |
| <F(52A)a, <F(31A)b | 77.8(5) | <F(52A)a, <F(32A)b | 96.7(5) | <F(52A)a, >F(52)a | 5.7(3) | <F(52A)a, <F(63)c | 56.2(3) |
| <F(52A)a, C(59) | 134.6(2) | <F(32)b , F(42)d | 105.10(19) | <F(32)b , >F(51)a | 86.4(3) | <F(32)b , <F(31A)b | 12.8(4) |
| <F(32)b , <F(32A)b | 26.2(4) | <F(32)b , >F(52)a | 90.9(2) | <F(32)b , <F(63)c | 71.4(2) | <F(32)b , C(59) | 112.21(18) |

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=====
F(42)d , >F(51)a  58.02(14)  F(42)d , <F(31A)b  110.5(4)  F(42)d , <F(32A)b  80.6(4)  F(42)d , >F(52)a  91.82(17)
F(42)d , <F(63)c  142.85(17)  F(42)d , C(59)  122.00(8)  >F(51)a , <F(31A)b  80.4(5)  >F(51)a , <F(32A)b  80.9(5)
>F(51)a , >F(52)a  36.9(2)  >F(51)a , <F(63)c  84.9(2)  >F(51)a , C(59)  158.9(2)  <F(31A)b, <F(32A)b  36.6(5)
<F(31A)b, >F(52)a  79.2(4)  <F(31A)b, <F(63)c  59.9(3)  <F(31A)b, C(59)  115.8(4)  <F(32A)b, >F(52)a  100.8(4)
<F(32A)b, <F(63)c  96.5(3)  <F(32A)b, C(59)  120.2(4)  >F(52)a , <F(63)c  52.1(2)  >F(52)a , C(59)  128.92(16)
<F(63)c , C(59)  91.68(15)

```

3.6 Angstrom Coordination Sphere Around Atom I = F(56) [ARU = 1555.03] 0.47680 0.96598 -0.13345 4.0195 23.0050 -4.8931

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|------------------|------------|--------|-------|---------|--------|---------|---------|----------|--------|---------|---------|
| 1 | 1.336(3) | -- | C(520) | | | | Intra | -115.77 | -36.86 | 0.42170 | 0.92557 | -0.15530 | 3.5550 | 22.0426 | -5.6942 |
| 2 | 2.129(3) | << | F(55) | | | | Intra | -93.69 | -71.70 | 0.47170 | 0.93797 | -0.18857 | 3.9765 | 22.3379 | -6.9141 |
| 3 | 2.131(2) | << | F(54) | | | | Intra | -85.40 | -11.22 | 0.49670 | 0.87850 | -0.14476 | 4.1873 | 20.9217 | -5.3078 |
| 4 | 2.357(3) | << | C(58) | | | | Intra | -150.57 | -17.76 | 0.24490 | 0.91967 | -0.15306 | 2.0646 | 21.9021 | -5.6121 |
| 5 | 2.789(3) | << | C(59) | | | | Intra | -159.73 | 10.80 | 0.17190 | 0.92612 | -0.11920 | 1.4492 | 22.0557 | -4.3706 |
| 6 | 3.113(3) | .< | C(45)b | [-x,1/2+y,-1/2-z | = 4554.06] | | | 81.72 | -0.22 | 0.53000 | 1.09531 | -0.13377 | 4.4680 | 26.0850 | -4.9048 |
| 7 | 3.177(3) | .. | C(46)b | [-x,1/2+y,-1/2-z | = 4554.06] | | | 91.63 | -23.94 | 0.46700 | 1.08785 | -0.16860 | 3.9369 | 25.9074 | -6.1819 |
| 8 | 3.262(3) | .. | C(53)a | [1+x,y,z | = 1655.03] | | | -7.02 | 37.40 | 0.78190 | 0.95268 | -0.07941 | 6.5916 | 22.6883 | -2.9116 |
| 9 | 3.303(3) | .. | C(44)b | [-x,1/2+y,-1/2-z | = 4554.06] | | | 97.59 | 19.00 | 0.42790 | 1.09597 | -0.10412 | 3.6073 | 26.1007 | -3.8177 |
| 10 | 3.426(3) | .. | C(47)b | [-x,1/2+y,-1/2-z | = 4554.06] | | | 117.92 | -25.57 | 0.30520 | 1.08063 | -0.17378 | 2.5729 | 25.7354 | -6.3718 |
| 11 | 3.437(3) | .. | F(42)b | [-x,1/2+y,-1/2-z | = 4554.06] | | | 46.45 | -41.53 | 0.68710 | 1.04430 | -0.19560 | 5.7924 | 24.8702 | -7.1719 |
| 12 | 3.553(3) | .. | C(57) | | | | Intra | -152.45 | -31.58 | 0.15850 | 0.90719 | -0.18420 | 1.3362 | 21.6049 | -6.7539 |
| 13 | 3.575(3) | .. | C(49)b | [-x,1/2+y,-1/2-z | = 4554.06] | | | 121.19 | 14.88 | 0.26450 | 1.09010 | -0.10841 | 2.2298 | 25.9610 | -3.9750 |
| 14 | 2.48 | .< | H(53A)a | [1+x,y,z | = 1655.03] | | | 4.34 | 31.65 | 0.72690 | 0.97270 | -0.09790 | 6.1279 | 23.1650 | -3.5896 |
| 15 | 2.54 | .< | H(59A) | | | | Intra | -160.36 | 30.65 | 0.23240 | 0.93510 | -0.09810 | 1.9592 | 22.2696 | -3.5969 |
| 16 | 3.22 | .. | H(55A)a | [1+x,y,z | = 1655.03] | | | -28.83 | -8.21 | 0.80820 | 0.90140 | -0.14600 | 6.8133 | 21.4670 | -5.3532 |
| 17 | 3.48 | .. | H(45A)b | [-x,1/2+y,-1/2-z | = 4554.06] | | | 66.54 | 1.84 | 0.64100 | 1.09990 | -0.13040 | 5.4038 | 26.1943 | -4.7812 |

Angles (Degrees) At1...V...At2 with Vertex V = F(56)

| | | | | | | | |
|-----------------|------------|-----------------|------------|-----------------|------------|-----------------|------------|
| C(520) , F(55) | 36.65(13) | C(520) , F(54) | 37.45(13) | C(520) , C(58) | 36.04(13) | C(520) , C(59) | 63.04(13) |
| C(520) , C(45)b | 139.54(16) | C(520) , C(46)b | 113.95(15) | C(520) , C(53)a | 124.65(15) | C(520) , C(44)b | 145.82(15) |
| C(520) , C(47)b | 99.70(14) | C(520) , F(42)b | 99.95(14) | C(520) , C(57) | 30.59(13) | C(520) , C(49)b | 125.15(14) |
| F(55) , F(54) | 60.69(10) | F(55) , C(58) | 63.06(9) | F(55) , C(59) | 93.01(9) | F(55) , C(45)b | 108.03(10) |
| F(55) , C(46)b | 84.30(9) | F(55) , C(53)a | 124.21(9) | F(55) , C(44)b | 126.89(10) | F(55) , C(47)b | 80.29(9) |
| F(55) , F(42)b | 63.32(8) | F(55) , C(57) | 50.51(7) | F(55) , C(49)b | 119.52(9) | F(54) , C(58) | 63.16(8) |
| F(54) , C(59) | 77.07(8) | F(54) , C(45)b | 162.83(10) | F(54) , C(46)b | 144.72(11) | F(54) , C(53)a | 87.78(9) |
| F(54) , C(44)b | 171.71(10) | F(54) , C(47)b | 136.76(10) | F(54) , F(42)b | 111.16(9) | F(54) , C(57) | 64.68(7) |
| F(54) , C(49)b | 153.86(9) | C(58) , C(59) | 29.96(7) | C(58) , C(45)b | 125.55(9) | C(58) , C(46)b | 106.39(9) |
| C(58) , C(53)a | 142.55(10) | C(58) , C(44)b | 115.75(8) | C(58) , C(47)b | 83.74(8) | C(58) , F(42)b | 118.65(9) |
| C(58) , C(57) | 13.93(7) | C(58) , C(49)b | 92.87(8) | C(59) , C(45)b | 118.05(8) | C(59) , C(46)b | 111.28(8) |
| C(59) , C(53)a | 125.43(9) | C(59) , C(44)b | 98.22(7) | C(59) , C(47)b | 87.88(7) | C(59) , F(42)b | 141.64(8) |
| C(59) , C(57) | 42.95(6) | C(59) , C(49)b | 76.82(7) | C(45)b , C(46)b | 25.59(6) | C(45)b , C(53)a | 89.13(8) |
| C(45)b , C(44)b | 24.74(6) | C(45)b , C(47)b | 43.15(6) | C(45)b , F(42)b | 52.14(6) | C(45)b , C(57) | 119.79(8) |
| C(45)b , C(49)b | 41.84(6) | C(46)b , C(53)a | 110.83(8) | C(46)b , C(44)b | 43.33(6) | C(46)b , C(47)b | 23.89(6) |
| C(46)b , F(42)b | 41.30(6) | C(46)b , C(57) | 97.35(7) | C(46)b , C(49)b | 48.38(6) | C(53)a , C(44)b | 89.52(7) |
| C(53)a , C(47)b | 132.26(8) | C(53)a , F(42)b | 92.79(7) | C(53)a , C(57) | 151.08(8) | C(53)a , C(49)b | 108.60(7) |
| C(44)b , C(47)b | 48.76(6) | C(44)b , F(42)b | 76.80(6) | C(44)b , C(57) | 116.46(7) | C(44)b , C(49)b | 22.94(4) |
| C(47)b , F(42)b | 59.94(6) | C(47)b , C(57) | 76.65(6) | C(47)b , C(49)b | 40.58(5) | F(42)b , C(57) | 104.84(7) |
| F(42)b , C(49)b | 88.84(6) | C(57) , C(49)b | 94.72(6) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(61A) [ARU = 1555.04] -0.21270 0.78300 0.22915 -1.7931 18.6473 8.4020

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|-----------|----------------------|-------------------------------|-------|---------|--------|----------|---------|---------|---------|---------|---------|
| 1 | 1.353(7) | -- | C(610) | | Intra | -63.26 | -38.00 | -0.15580 | 0.74302 | 0.20643 | -1.3134 | 17.6952 | 7.5690 |
| 2 | 2.097(9) | << | >F(62A) | | Intra | -79.48 | -5.77 | -0.16750 | 0.69685 | 0.22340 | -1.4121 | 16.5956 | 8.1912 |
| 3 | 2.098(8) | << | >F(63A) | | Intra | -19.47 | -25.08 | -0.00020 | 0.75640 | 0.20490 | -0.0017 | 18.0138 | 7.5129 |
| 4 | 2.371(6) | << | C(66) | | Intra | -101.95 | -67.16 | -0.23530 | 0.74520 | 0.16956 | -1.9836 | 17.7471 | 6.2171 |
| 5 | 2.857(7) | << | C(67) | | Intra | -153.91 | -52.28 | -0.39890 | 0.75072 | 0.16752 | -3.3628 | 17.8785 | 6.1423 |
| 6 | 3.064(6) | .. | F(14)a | [-1/2+x,3/2-y,-z = 3465.05] | | -65.73 | 67.53 | -0.15560 | 0.73817 | 0.30636 | -1.3117 | 17.5797 | 11.2330 |
| 7 | 3.172(7) | .. | F(41)b | [1/2+x,3/2-y,-z = 3565.06] | | 77.59 | 49.26 | -0.15990 | 0.86791 | 0.29470 | -1.3480 | 20.6695 | 10.8055 |
| 8 | 3.518(6) | .. | C(65) | | Intra | -58.34 | -71.42 | -0.14290 | 0.74293 | 0.13821 | -1.2047 | 17.6930 | 5.0676 |
| 9 | 3.526(7) | .. | C(27)c | [-1-x,1/2+y,-1/2-z = 4454.02] | | 105.05 | -21.68 | -0.31360 | 0.91588 | 0.19363 | -2.6437 | 21.8119 | 7.0996 |
| 10 | 3.549(7) | .. | F(24)c | [-1-x,1/2+y,-1/2-z = 4454.02] | | 55.67 | -22.83 | 0.00610 | 0.89642 | 0.19160 | 0.0514 | 21.3484 | 7.0252 |
| 11 | 2.66 | .< | H(67A) | | Intra | -160.78 | -33.54 | -0.46150 | 0.75230 | 0.18900 | -3.8905 | 17.9162 | 6.9299 |
| 12 | 2.81 | .. | H(17A)a | [-1/2+x,3/2-y,-z = 3465.05] | | -159.08 | 47.18 | -0.42410 | 0.75440 | 0.28530 | -3.5752 | 17.9662 | 10.4608 |
| 13 | 3.14 | .. | H(27A)c | [-1-x,1/2+y,-1/2-z = 4454.02] | | 97.00 | -8.83 | -0.25760 | 0.91240 | 0.21600 | -2.1716 | 21.7290 | 7.9199 |

Angles (Degrees) At1...V...At2 with Vertex V = >F(61A)

| | | | | | | | |
|------------------|-----------|-------------------|-----------|------------------|------------|------------------|-----------|
| C(610) , >F(62A) | 35.4(3) | C(610) , >F(63A) | 39.1(3) | C(610) , C(66) | 36.3(2) | C(610) , C(67) | 61.2(3) |
| C(610) , F(14)a | 105.6(4) | C(610) , F(41)b | 149.9(5) | C(610) , C(65) | 33.5(2) | C(610) , C(27)c | 119.3(3) |
| C(610) , F(24)c | 96.5(3) | >F(62A) , >F(63A) | 60.5(4) | >F(62A) , C(66) | 63.3(2) | >F(62A) , C(67) | 75.9(3) |
| >F(62A) , F(14)a | 74.0(2) | >F(62A) , F(41)b | 132.4(3) | >F(62A) , C(65) | 67.0(2) | >F(62A) , C(27)c | 152.2(3) |
| >F(62A) , F(24)c | 127.7(4) | >F(63A) , C(66) | 64.1(2) | >F(63A) , C(67) | 93.0(2) | >F(63A) , F(14)a | 98.8(3) |
| >F(63A) , F(41)b | 113.2(3) | >F(63A) , C(65) | 51.21(16) | >F(63A) , C(27)c | 108.7(3) | >F(63A) , F(24)c | 67.8(3) |
| C(66) , C(67) | 28.92(11) | C(66) , F(14)a | 137.1(3) | C(66) , F(41)b | 162.1(3) | C(66) , C(65) | 15.61(10) |
| C(66) , C(27)c | 88.91(19) | C(66) , F(24)c | 88.47(19) | C(67) , F(14)a | 136.3(3) | C(67) , F(41)b | 148.0(3) |
| C(67) , C(65) | 43.04(10) | C(67) , C(27)c | 79.44(16) | C(67) , F(24)c | 100.58(17) | F(14)a , F(41)b | 60.00(12) |
| F(14)a , C(65) | 139.0(2) | F(14)a , C(27)c | 133.8(2) | F(14)a , F(24)c | 122.8(2) | F(41)b , C(65) | 150.2(2) |
| F(41)b , C(27)c | 75.03(16) | F(41)b , F(24)c | 74.68(16) | C(65) , C(27)c | 86.20(14) | C(65) , F(24)c | 75.63(13) |
| C(27)c , F(24)c | 45.49(10) | | | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(62A) [ARU = 1555.04] -0.16750 0.69685 0.22340 -1.4121 16.5956 8.1912

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|------------------|-----------|----------|-------|---------|--------|----------|---------|---------|---------|---------|---------|
| 1 | 1.267(6) | -- | C(610) | | | | Intra | 84.87 | -29.41 | -0.15580 | 0.74302 | 0.20643 | -1.3134 | 17.6952 | 7.5690 |
| 2 | 2.097(9) | << | >F(61A) | | | | Intra | 100.52 | 5.77 | -0.21270 | 0.78300 | 0.22915 | -1.7931 | 18.6473 | 8.4020 |
| 3 | 2.112(9) | << | >F(63A) | | | | Intra | 45.16 | -18.73 | -0.00020 | 0.75640 | 0.20490 | -0.0017 | 18.0138 | 7.5129 |
| 4 | 2.356(6) | << | C(66) | | | | Intra | 116.40 | -56.93 | -0.23530 | 0.74520 | 0.16956 | -1.9836 | 17.7471 | 6.2171 |
| 5 | 2.73(2) | << | <F(31A)a | [x,y,1+z | = | 1556.01] | | -81.08 | 39.87 | -0.12900 | 0.61000 | 0.27110 | -1.0875 | 14.5273 | 9.9402 |
| 6 | 3.106(8) | .< | C(67) | | | | Intra | 146.67 | -41.27 | -0.39890 | 0.75072 | 0.16752 | -3.3628 | 17.8785 | 6.1423 |
| 7 | 3.199(6) | .. | F(14)c | [-1/2+x,3/2-y,-z | = | 3465.05] | | 84.18 | 71.99 | -0.15560 | 0.73817 | 0.30636 | -1.3117 | 17.5797 | 11.2330 |
| 8 | 3.218(6) | .. | C(57)d | [-1/2+x,3/2-y,-z | = | 3465.03] | | -120.63 | -26.53 | -0.34150 | 0.59281 | 0.18420 | -2.8789 | 14.1179 | 6.7539 |
| 9 | 3.317(6) | .. | C(65) | | | | Intra | 79.30 | -70.33 | -0.14290 | 0.74293 | 0.13821 | -1.2047 | 17.6930 | 5.0676 |
| 10 | 3.405(8) | .. | F(12)b | [1/2+x,3/2-y,-z | = | 3565.05] | | 10.54 | 31.05 | 0.17270 | 0.71925 | 0.27129 | 1.4559 | 17.1291 | 9.9471 |
| 11 | 3.441(13) | .. | >F(53)d | [-1/2+x,3/2-y,-z | = | 3465.03] | | -151.74 | 11.46 | -0.51990 | 0.62980 | 0.24204 | -4.3829 | 14.9988 | 8.8746 |
| 12 | 2.66 | .< | H(57A)d | [-1/2+x,3/2-y,-z | = | 3465.03] | | -113.44 | -12.98 | -0.28980 | 0.59700 | 0.20710 | -2.4431 | 14.2177 | 7.5935 |
| 13 | 3.08 | .. | H(67A) | | | | Intra | 151.95 | -24.19 | -0.46150 | 0.75230 | 0.18900 | -3.8905 | 17.9162 | 6.9299 |
| 14 | 3.42 | .. | H(65A) | | | | Intra | 41.10 | -63.49 | -0.03100 | 0.73900 | 0.13990 | -0.2613 | 17.5994 | 5.1296 |
| 15 | 3.42 | .. | H(17A)c | [-1/2+x,3/2-y,-z | = | 3465.05] | | 147.64 | 41.55 | -0.42410 | 0.75440 | 0.28530 | -3.5752 | 17.9662 | 10.4608 |

Angles (Degrees) At1...V...At2 with Vertex V = >F(62A)

| | | | | | | | |
|--------------------|-----------|------------------|-----------|-------------------|------------|--------------------|------------|
| C(610) , >F(61A) | 38.3(3) | C(610) , >F(63A) | 37.6(3) | C(610) , C(66) | 35.3(2) | C(610) , <F(31A)a | 164.5(7) |
| C(610) , C(67) | 50.7(3) | C(610) , F(14)c | 101.4(3) | C(610) , C(57)d | 119.0(4) | C(610) , C(65) | 41.0(2) |
| C(610) , F(12)b | 93.0(4) | C(610) , >F(53)d | 124.6(6) | >F(61A) , >F(63A) | 59.8(3) | >F(61A) , C(66) | 64.0(2) |
| >F(61A) , <F(31A)a | 134.3(5) | >F(61A) , C(67) | 63.1(2) | >F(61A) , F(14)c | 67.0(2) | >F(61A) , C(57)d | 135.7(4) |
| >F(61A) , C(65) | 77.4(2) | >F(61A) , F(12)b | 87.0(3) | >F(61A) , >F(53)d | 106.1(4) | >F(63A) , C(66) | 64.19(19) |
| >F(63A) , <F(31A)a | 129.5(7) | >F(63A) , C(67) | 86.0(2) | >F(63A) , F(14)c | 94.5(2) | >F(63A) , C(57)d | 132.7(3) |
| >F(63A) , C(65) | 55.51(16) | >F(63A) , F(12)b | 59.9(2) | >F(63A) , >F(53)d | 162.2(4) | C(66) , <F(31A)a | 159.5(5) |
| C(66) , C(67) | 24.91(12) | C(66) , F(14)c | 130.9(2) | C(66) , C(57)d | 83.8(2) | C(66) , C(65) | 20.68(10) |
| C(66) , F(12)b | 124.1(3) | C(66) , >F(53)d | 100.6(3) | <F(31A)a , C(67) | 144.2(6) | <F(31A)a , F(14)c | 67.7(4) |
| <F(31A)a , C(57)d | 75.9(4) | <F(31A)a , C(65) | 147.9(5) | <F(31A)a , F(12)b | 71.8(5) | <F(31A)a , >F(53)d | 67.9(6) |
| C(67) , F(14)c | 121.3(2) | C(67) , C(57)d | 74.76(18) | C(67) , C(65) | 44.07(10) | C(67) , F(12)b | 143.55(19) |
| C(67) , >F(53)d | 77.3(3) | F(14)c , C(57)d | 132.5(2) | F(14)c , C(65) | 142.35(17) | F(14)c , F(12)b | 55.59(12) |
| F(14)c , >F(53)d | 88.9(2) | C(57)d , C(65) | 82.11(14) | C(57)d , F(12)b | 137.3(2) | C(57)d , >F(53)d | 48.5(2) |
| C(65) , F(12)b | 112.4(2) | C(65) , >F(53)d | 113.2(3) | F(12)b , >F(53)d | 134.2(2) | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(63A) [ARU = 1555.04] -0.00020 0.75640 0.20490 -0.0017 18.0138 7.5129

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|--------------------|------------|--------|--------------|--------|----------|----------|---------|---------|---------|---------|---------|
| 1 | 1.351(6) | -- | C(610) | | | | Intra-166.35 | 2.38 | -0.15580 | 0.74302 | 0.20643 | -1.3134 | 17.6952 | 7.5690 | |
| 2 | 2.098(8) | << | >F(61A) | | | | Intra 160.53 | 25.08 | -0.21270 | 0.78300 | 0.22915 | -1.7931 | 18.6473 | 8.4020 | |
| 3 | 2.112(9) | << | >F(62A) | | | | Intra-134.84 | 18.73 | -0.16750 | 0.69685 | 0.22340 | -1.4121 | 16.5956 | 8.1912 | |
| 4 | 2.383(5) | << | C(66) | | | | Intra-172.34 | -32.94 | -0.23530 | 0.74520 | 0.16956 | -1.9836 | 17.7471 | 6.2171 | |
| 5 | 2.744(4) | << | C(65) | | | | Intra-165.07 | -63.02 | -0.14290 | 0.74293 | 0.13821 | -1.2047 | 17.6930 | 5.0676 | |
| 6 | 2.972(4) | .. | F(12)b | [1/2+x,3/2-y,-z | = 3565.05] | | | -31.26 | 54.99 | 0.17270 | 0.71925 | 0.27129 | 1.4559 | 17.1291 | 9.9471 |
| 7 | 3.237(5) | .. | F(13)b | [1/2+x,3/2-y,-z | = 3565.05] | | | 42.35 | 55.29 | 0.16140 | 0.80855 | 0.27747 | 1.3606 | 19.2558 | 10.1737 |
| 8 | 3.306(5) | .. | F(66)a | [1+x,y,z | = 1655.04] | | | 22.01 | -35.25 | 0.29670 | 0.79889 | 0.15286 | 2.5012 | 19.0257 | 5.6048 |
| 9 | 3.336(4) | .. | F(11)b | [1/2+x,3/2-y,-z | = 3565.05] | | | 6.79 | 27.07 | 0.34970 | 0.77115 | 0.24630 | 2.9480 | 18.3651 | 9.0308 |
| 10 | 3.371(8) | .. | F(24)d | [-1-x,1/2+y,-1/2-z | = 4454.02] | | | 89.09 | -8.32 | 0.00610 | 0.89642 | 0.19160 | 0.0514 | 21.3484 | 7.0252 |
| 11 | 3.429(4) | .. | C(110)b | [1/2+x,3/2-y,-z | = 3565.05] | | | 5.37 | 49.75 | 0.26140 | 0.76511 | 0.27627 | 2.2037 | 18.2212 | 10.1297 |
| 12 | 3.468(6) | .. | F(25)d | [-1-x,1/2+y,-1/2-z | = 4454.02] | | | 93.64 | -44.64 | -0.01879 | 0.85980 | 0.13844 | -0.1584 | 20.4763 | 5.0760 |
| 13 | 3.497(12) | .. | >F(52)c | [1/2+x,3/2-y,-z | = 3565.03] | | | -45.83 | 1.14 | 0.28880 | 0.65110 | 0.20680 | 2.4346 | 15.5061 | 7.5825 |
| 14 | 3.521(5) | .. | F(64)a | [1+x,y,z | = 1655.04] | | | -24.37 | -42.26 | 0.28140 | 0.71125 | 0.14032 | 2.3723 | 16.9386 | 5.1450 |
| 15 | 2.43 | << | H(65A) | | | | Intra-122.07 | -78.40 | -0.03100 | 0.73900 | 0.13990 | -0.2613 | 17.5994 | 5.1296 | |

Angles (Degrees) At1...V...At2 with Vertex V = >F(63A)

| | | | | | | | |
|-------------------|------------|-------------------|------------|-------------------|------------|-------------------|------------|
| C(610) , >F(61A) | 39.2(3) | C(610) , >F(62A) | 34.9(3) | C(610) , C(66) | 35.77(16) | C(610) , C(65) | 65.40(19) |
| C(610) , F(12)b | 111.8(3) | C(610) , F(13)b | 117.7(2) | C(610) , F(66)a | 146.2(2) | C(610) , F(11)b | 149.8(2) |
| C(610) , F(24)d | 104.8(3) | C(610) , C(110)b | 127.4(2) | C(610) , F(25)d | 98.8(3) | C(610) , >F(52)c | 120.4(4) |
| C(610) , F(64)a | 127.6(3) | >F(61A) , >F(62A) | 59.8(3) | >F(61A) , C(66) | 63.5(2) | >F(61A) , C(65) | 92.2(2) |
| >F(61A) , F(12)b | 99.3(2) | >F(61A) , F(13)b | 84.0(2) | >F(61A) , F(66)a | 143.0(4) | >F(61A) , F(11)b | 122.0(2) |
| >F(61A) , F(24)d | 77.1(3) | >F(61A) , C(110)b | 102.0(2) | >F(61A) , F(25)d | 92.6(3) | >F(61A) , >F(52)c | 143.4(3) |
| >F(61A) , F(64)a | 162.4(2) | >F(62A) , C(66) | 62.9(2) | >F(62A) , C(65) | 85.1(2) | >F(62A) , F(12)b | 82.2(2) |
| >F(62A) , F(13)b | 105.9(2) | >F(62A) , F(66)a | 153.7(3) | >F(62A) , F(11)b | 121.0(3) | >F(62A) , F(24)d | 136.2(3) |
| >F(62A) , C(110)b | 103.0(2) | >F(62A) , F(25)d | 132.3(3) | >F(62A) , >F(52)c | 88.7(3) | >F(62A) , F(64)a | 117.5(3) |
| C(66) , C(65) | 30.42(9) | C(66) , F(12)b | 145.1(2) | C(66) , F(13)b | 147.1(2) | C(66) , F(66)a | 110.49(14) |
| C(66) , F(11)b | 174.08(16) | C(66) , F(24)d | 92.59(19) | C(66) , C(110)b | 163.10(17) | C(66) , F(25)d | 70.11(13) |
| C(66) , >F(52)c | 120.7(3) | C(66) , F(64)a | 99.26(15) | C(65) , F(12)b | 155.5(3) | C(65) , F(13)b | 164.1(3) |
| C(65) , F(66)a | 81.57(11) | C(65) , F(11)b | 143.66(15) | C(65) , F(24)d | 89.64(16) | C(65) , C(110)b | 165.76(17) |
| C(65) , F(25)d | 55.74(10) | C(65) , >F(52)c | 103.9(2) | C(65) , F(64)a | 70.16(11) | F(12)b , F(13)b | 40.05(7) |
| F(12)b , F(66)a | 101.10(13) | F(12)b , F(11)b | 39.19(7) | F(12)b , F(24)d | 113.91(17) | F(12)b , C(110)b | 22.69(6) |
| F(12)b , F(25)d | 144.0(2) | F(12)b , >F(52)c | 55.15(16) | F(12)b , F(64)a | 97.43(15) | F(13)b , F(66)a | 92.20(14) |
| F(13)b , F(11)b | 38.13(6) | F(13)b , F(24)d | 74.50(14) | F(13)b , C(110)b | 22.88(6) | F(13)b , F(25)d | 108.9(2) |
| F(13)b , >F(52)c | 88.03(17) | F(13)b , F(64)a | 112.72(13) | F(66)a , F(11)b | 63.96(9) | F(66)a , F(24)d | 66.53(13) |
| F(66)a , C(110)b | 86.27(12) | F(66)a , F(25)d | 53.94(9) | F(66)a , >F(52)c | 72.76(18) | F(66)a , F(64)a | 36.38(7) |
| F(11)b , F(24)d | 87.00(15) | F(11)b , C(110)b | 22.71(5) | F(11)b , F(25)d | 106.56(16) | F(11)b , >F(52)c | 56.66(18) |
| F(11)b , F(64)a | 75.05(11) | F(24)d , C(110)b | 92.32(15) | F(24)d , F(25)d | 36.54(8) | F(24)d , >F(52)c | 134.5(2) |
| F(24)d , F(64)a | 101.20(14) | C(110)b , F(25)d | 121.50(19) | C(110)b , >F(52)c | 65.17(17) | C(110)b , F(64)a | 95.63(13) |
| F(25)d , >F(52)c | 123.69(18) | F(25)d , F(64)a | 76.98(10) | >F(52)c , F(64)a | 47.52(16) | | |

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3.6 Angstrom Coordination Sphere Around Atom I = F(64) [ARU = 1555.04] -0.71860 0.71125 0.14032 -6.0579 16.9386 5.1450

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|------------------|------------|--------|-------|---------|--------|----------|---------|---------|---------|---------|--------|
| 1 | 1.317(4) | -- | C(620) | | | | Intra | 61.97 | -15.09 | -0.64770 | 0.75839 | 0.13097 | -5.4602 | 18.0612 | 4.8021 |
| 2 | 2.141(3) | << | F(66) | | | | Intra | 86.46 | 12.40 | -0.70330 | 0.79889 | 0.15286 | -5.9290 | 19.0257 | 5.6048 |
| 3 | 2.143(4) | << | F(65) | | | | Intra | 83.14 | -47.24 | -0.69800 | 0.77190 | 0.09742 | -5.8843 | 18.3830 | 3.5720 |
| 4 | 2.351(4) | << | C(68) | | | | Intra | 25.77 | -6.19 | -0.46890 | 0.75393 | 0.13341 | -3.9529 | 17.9550 | 4.8916 |
| 5 | 2.828(9) | <. | >F(52)b | [-1/2+x,3/2-y,-z | = 3465.03] | | | -87.51 | 59.53 | -0.71120 | 0.65110 | 0.20680 | -5.9956 | 15.5061 | 7.5825 |
| 6 | 3.024(4) | <. | C(67) | | | | Intra | 19.23 | 19.26 | -0.39890 | 0.75072 | 0.16752 | -3.3628 | 17.8785 | 6.1423 |
| 7 | 3.045(3) | <. | C(55)b | [-1/2+x,3/2-y,-z | = 3465.03] | | | -67.39 | 5.17 | -0.58030 | 0.59368 | 0.14781 | -4.8920 | 14.1386 | 5.4196 |
| 8 | 3.195(13) | .. | <F(52A)b | [-1/2+x,3/2-y,-z | = 3465.03] | | | -95.98 | 52.55 | -0.74260 | 0.63010 | 0.20950 | -6.2603 | 15.0060 | 7.6815 |
| 9 | 3.218(3) | .. | F(54)c | [-3/2+x,3/2-y,-z | = 3365.03] | | | -138.31 | 2.90 | -1.00330 | 0.62150 | 0.14476 | -8.4580 | 14.8011 | 5.3078 |
| 10 | 3.335(4) | .. | C(69) | | | | Intra | 18.75 | -25.17 | -0.37960 | 0.75199 | 0.10164 | -3.2001 | 17.9088 | 3.7267 |
| 11 | 3.521(5) | .. | >F(63A)a | [-1+x,y,z | = 1455.04] | | | 155.63 | 42.26 | -1.00020 | 0.75640 | 0.20490 | -8.4319 | 18.0138 | 7.5129 |
| 12 | 3.556(4) | .. | C(56)b | [-1/2+x,3/2-y,-z | = 3465.03] | | | -55.98 | 25.06 | -0.50480 | 0.59914 | 0.18140 | -4.2556 | 14.2686 | 6.6512 |
| 13 | 2.70 | .. | H(55A)b | [-1/2+x,3/2-y,-z | = 3465.03] | | | -85.19 | 4.42 | -0.69180 | 0.59860 | 0.14600 | -5.8320 | 14.2558 | 5.3532 |
| 14 | 2.72 | .. | H(65A)a | [-1+x,y,z | = 1455.04] | | | 165.91 | -0.32 | -1.03100 | 0.73900 | 0.13990 | -8.6915 | 17.5994 | 5.1296 |
| 15 | 2.97 | .. | H(67A) | | | | Intra | 24.28 | 36.90 | -0.46150 | 0.75230 | 0.18900 | -3.8905 | 17.9162 | 6.9299 |
| 16 | 3.49 | .. | H(69A) | | | | Intra | 22.84 | -40.62 | -0.42920 | 0.75440 | 0.07840 | -3.6182 | 17.9662 | 2.8746 |
| 17 | 3.49 | .. | H(63A)a | [-1+x,y,z | = 1455.04] | | | -156.65 | -42.68 | -0.99840 | 0.66850 | 0.07570 | -8.4167 | 15.9205 | 2.7756 |

Angles (Degrees) At1...V...At2 with Vertex V = F(64)

| | | | | | | | |
|--------------------|------------|-------------------|------------|---------------------|------------|--------------------|------------|
| C(620) , F(66) | 36.65(19) | C(620) , F(65) | 36.6(2) | C(620) , C(68) | 36.61(17) | C(620) , >F(52)b | 130.2(3) |
| C(620) , C(67) | 54.3(2) | C(620) , C(55)b | 129.3(2) | C(620) , <F(52A)b | 138.7(3) | C(620) , F(54)c | 156.6(2) |
| C(620) , C(69) | 41.62(18) | C(620) , >F(63A)a | 102.8(2) | C(620) , C(56)b | 121.3(2) | F(66) , F(65) | 59.71(11) |
| F(66) , C(68) | 63.12(11) | F(66) , >F(52)b | 107.9(3) | F(66) , C(67) | 64.69(11) | F(66) , C(55)b | 148.63(16) |
| F(66) , <F(52A)b | 115.0(3) | F(66) , F(54)c | 132.96(14) | F(66) , C(69) | 75.88(11) | F(66) , >F(63A)a | 66.33(15) |
| F(66) , C(56)b | 127.62(16) | F(65) , C(68) | 63.70(11) | F(65) , >F(52)b | 166.5(3) | F(65) , C(67) | 87.73(11) |
| F(65) , C(55)b | 130.92(17) | F(65) , <F(52A)b | 174.7(3) | F(65) , F(54)c | 123.05(15) | F(65) , C(69) | 54.70(9) |
| F(65) , >F(63A)a | 110.03(15) | F(65) , C(56)b | 140.90(13) | C(68) , >F(52)b | 107.0(3) | C(68) , C(67) | 26.25(9) |
| C(68) , C(55)b | 93.69(11) | C(68) , <F(52A)b | 113.8(2) | C(68) , F(54)c | 163.80(13) | C(68) , C(69) | 20.14(9) |
| C(68) , >F(63A)a | 122.96(17) | C(68) , C(56)b | 85.21(11) | >F(52)b , C(67) | 81.6(2) | >F(52)b , C(55)b | 56.5(2) |
| >F(52)b , <F(52A)b | 8.4(3) | >F(52)b , F(54)c | 68.7(2) | >F(52)b , C(69) | 119.7(2) | >F(52)b , >F(63A)a | 65.8(2) |
| >F(52)b , C(56)b | 40.8(2) | C(67) , C(55)b | 85.11(10) | C(67) , <F(52A)b | 89.01(19) | C(67) , F(54)c | 148.72(14) |
| C(67) , C(69) | 44.43(7) | C(67) , >F(63A)a | 106.51(14) | C(67) , C(56)b | 69.02(9) | C(55)b , <F(52A)b | 52.9(2) |
| C(55)b , F(54)c | 70.75(8) | C(55)b , C(69) | 88.73(9) | C(55)b , >F(63A)a | 118.57(16) | C(55)b , C(56)b | 22.70(6) |
| <F(52A)b , F(54)c | 60.72(18) | <F(52A)b , C(69) | 124.60(16) | <F(52A)b , >F(63A)a | 66.9(2) | <F(52A)b , C(56)b | 40.69(17) |
| F(54)c , C(69) | 148.64(13) | F(54)c , >F(63A)a | 70.49(12) | F(54)c , C(56)b | 81.83(8) | C(69) , >F(63A)a | 140.80(14) |
| C(69) , C(56)b | 87.95(8) | >F(63A)a , C(56)b | 106.63(15) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(65) [ARU = 1555.04] -0.69800 0.77190 0.09742 -5.8843 18.3830 3.5720

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|-----------|----------------------|-------------------------------|-------|---------|--------|----------|---------|---------|---------|---------|--------|
| 1 | 1.340(5) | -- | C(620) | | Intra | -37.19 | 66.60 | -0.64770 | 0.75839 | 0.13097 | -5.4602 | 18.0612 | 4.8021 |
| 2 | 2.132(3) | << | F(66) | | Intra | 93.98 | 72.41 | -0.70330 | 0.79889 | 0.15286 | -5.9290 | 19.0257 | 5.6048 |
| 3 | 2.143(4) | << | F(64) | | Intra | -96.86 | 47.24 | -0.71860 | 0.71125 | 0.14032 | -6.0579 | 16.9386 | 5.1450 |
| 4 | 2.378(3) | << | C(68) | | Intra | -12.49 | 33.71 | -0.46890 | 0.75393 | 0.13341 | -3.9529 | 17.9550 | 4.8916 |
| 5 | 2.730(3) | << | C(69) | | Intra | -10.02 | 3.25 | -0.37960 | 0.75199 | 0.10164 | -3.2001 | 17.9088 | 3.7267 |
| 6 | 3.143(3) | .< | C(23)b | [-1-x,1/2+y,-1/2-z = 4454.02] | | 91.79 | -5.73 | -0.70960 | 0.90313 | 0.08886 | -5.9821 | 21.5082 | 3.2581 |
| 7 | 3.404(3) | .. | C(63)a | [-1+x,y,z = 1455.04] | | -148.33 | -22.00 | -1.01660 | 0.70232 | 0.06265 | -8.5701 | 16.7259 | 2.2971 |
| 8 | 3.454(4) | .. | C(62)a | [-1+x,y,z = 1455.04] | | -148.40 | -44.60 | -0.94650 | 0.71779 | 0.03128 | -7.9792 | 17.0943 | 1.1469 |
| 9 | 2.41 | << | H(69A) | | Intra | -10.42 | -16.84 | -0.42920 | 0.75440 | 0.07840 | -3.6182 | 17.9662 | 2.8746 |
| 10 | 2.68 | .. | H(23A)b | [-1-x,1/2+y,-1/2-z = 4454.02] | | 102.45 | 6.81 | -0.76610 | 0.88110 | 0.10610 | -6.4584 | 20.9836 | 3.8903 |
| 11 | 3.30 | .. | H(65A)a | [-1+x,y,z = 1455.04] | | -164.41 | 28.12 | -1.03100 | 0.73900 | 0.13990 | -8.6915 | 17.5994 | 5.1296 |

Angles (Degrees) At1...V...At2 with Vertex V = F(65)

| | | | | | | | |
|-----------------|------------|-----------------|------------|-----------------|------------|-----------------|------------|
| C(620) , F(66) | 37.26(17) | C(620) , F(64) | 35.91(17) | C(620) , C(68) | 35.96(17) | C(620) , C(69) | 66.13(17) |
| C(620) , C(23)b | 109.89(19) | C(620) , C(63)a | 118.46(19) | C(620) , C(62)a | 138.30(19) | F(66) , F(64) | 60.11(13) |
| F(66) , C(68) | 62.76(11) | F(66) , C(69) | 91.08(11) | F(66) , C(23)b | 78.16(10) | F(66) , C(63)a | 119.16(11) |
| F(66) , C(62)a | 140.27(11) | F(64) , C(68) | 62.43(11) | F(64) , C(69) | 85.47(11) | F(64) , C(23)b | 137.84(15) |
| F(64) , C(63)a | 83.27(11) | F(64) , C(62)a | 102.40(12) | C(68) , C(69) | 30.55(9) | C(68) , C(23)b | 105.05(10) |
| C(68) , C(63)a | 139.57(12) | C(68) , C(62)a | 144.60(12) | C(69) , C(23)b | 102.06(9) | C(69) , C(63)a | 135.44(11) |
| C(69) , C(62)a | 124.84(11) | C(23)b , C(63)a | 114.97(9) | C(23)b , C(62)a | 106.38(9) | C(63)a , C(62)a | 22.60(6) |

3.6 Angstrom Coordination Sphere Around Atom I = F(66) [ARU = 1555.04] -0.70330 0.79889 0.15286 -5.9290 19.0257 5.6048

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------|-------------------------------|-------|---------|--------|----------|---------|---------|---------|---------|--------|
| 1 | 1.340(4) | -- | C(620) | | Intra | -64.08 | -36.81 | -0.64770 | 0.75839 | 0.13097 | -5.4602 | 18.0612 | 4.8021 |
| 2 | 2.132(3) | << | F(65) | | Intra | -86.02 | -72.41 | -0.69800 | 0.77190 | 0.09742 | -5.8843 | 18.3830 | 3.5720 |
| 3 | 2.141(3) | << | F(64) | | Intra | -93.54 | -12.40 | -0.71860 | 0.71125 | 0.14032 | -6.0579 | 16.9386 | 5.1450 |
| 4 | 2.358(4) | << | C(68) | | Intra | -28.45 | -17.60 | -0.46890 | 0.75393 | 0.13341 | -3.9529 | 17.9550 | 4.8916 |
| 5 | 2.862(4) | << | C(67) | | Intra | -24.09 | 10.83 | -0.39890 | 0.75072 | 0.16752 | -3.3628 | 17.8785 | 6.1423 |
| 6 | 3.075(3) | .. | F(25)c | [-2-x,1/2+y,-1/2-z = 4354.02] | | 151.39 | -9.90 | -1.01879 | 0.85980 | 0.13844 | -8.5886 | 20.4763 | 5.0760 |
| 7 | 3.306(5) | .. | >F(63A)a | [-1+x,y,z = 1455.04] | | -157.99 | 35.25 | -1.00020 | 0.75640 | 0.20490 | -8.4319 | 18.0138 | 7.5129 |
| 8 | 3.365(3) | .. | C(25)d | [-1-x,1/2+y,-1/2-z = 4454.02] | | 68.91 | 4.94 | -0.56020 | 0.93022 | 0.16077 | -4.7226 | 22.1534 | 5.8948 |
| 9 | 3.417(3) | .. | C(23)d | [-1-x,1/2+y,-1/2-z = 4454.02] | | 91.23 | -43.38 | -0.70960 | 0.90313 | 0.08886 | -5.9821 | 21.5082 | 3.2581 |
| 10 | 3.496(4) | .. | C(69) | | Intra | -22.26 | -32.49 | -0.37960 | 0.75199 | 0.10164 | -3.2001 | 17.9088 | 3.7267 |
| 11 | 3.518(3) | .. | F(11)b | [-1/2+x,3/2-y,-z = 3465.05] | | -55.93 | 76.90 | -0.65030 | 0.77115 | 0.24630 | -5.4822 | 18.3651 | 9.0308 |
| 12 | 3.571(13) | .. | <F(22A)d | [-1-x,1/2+y,-1/2-z = 4454.02] | | 89.53 | 48.42 | -0.70100 | 0.89840 | 0.22570 | -5.9096 | 21.3956 | 8.2755 |
| 13 | 2.66 | < | H(23A)d | [-1-x,1/2+y,-1/2-z = 4454.02] | | 105.13 | -40.21 | -0.76610 | 0.88110 | 0.10610 | -6.4584 | 20.9836 | 3.8903 |
| 14 | 2.67 | < | H(67A) | | Intra | -28.56 | 29.72 | -0.46150 | 0.75230 | 0.18900 | -3.8905 | 17.9162 | 6.9299 |
| 15 | 3.15 | .. | H(65A)a | [-1+x,y,z = 1455.04] | | -152.69 | -8.69 | -1.03100 | 0.73900 | 0.13990 | -8.6915 | 17.5994 | 5.1296 |
| 16 | 3.31 | .. | H(25A)d | [-1-x,1/2+y,-1/2-z = 4454.02] | | 85.30 | 5.18 | -0.67130 | 0.93670 | 0.16100 | -5.6592 | 22.3077 | 5.9032 |

Angles (Degrees) At1...V...At2 with Vertex V = F(66)

| | | | | | | | |
|-------------------|------------|-------------------|------------|-------------------|------------|---------------------|------------|
| C(620) , F(65) | 37.29(18) | C(620) , F(64) | 35.95(19) | C(620) , C(68) | 36.73(17) | C(620) , C(67) | 60.67(19) |
| C(620) , F(25)c | 122.6(2) | C(620) , >F(63A)a | 113.0(2) | C(620) , C(25)d | 126.6(2) | C(620) , C(23)d | 96.72(19) |
| C(620) , C(69) | 34.40(17) | C(620) , F(11)b | 113.8(2) | C(620) , <F(22A)d | 157.6(3) | F(65) , F(64) | 60.18(15) |
| F(65) , C(68) | 63.72(11) | F(65) , C(67) | 92.26(11) | F(65) , F(25)c | 89.79(10) | F(65) , >F(63A)a | 118.28(13) |
| F(65) , C(25)d | 110.78(11) | F(65) , C(23)d | 64.19(9) | F(65) , C(69) | 51.34(8) | F(65) , F(11)b | 150.36(12) |
| F(65) , <F(22A)d | 155.9(2) | F(64) , C(68) | 62.80(11) | F(64) , C(67) | 72.76(11) | F(64) , F(25)c | 111.76(12) |
| F(64) , >F(63A)a | 77.29(16) | F(64) , C(25)d | 161.13(14) | F(64) , C(23)d | 124.05(15) | F(64) , C(69) | 67.68(11) |
| F(64) , F(11)b | 91.93(14) | F(64) , <F(22A)d | 143.9(3) | C(68) , C(67) | 28.76(9) | C(68) , F(25)c | 152.50(12) |
| C(68) , >F(63A)a | 132.07(16) | C(68) , C(25)d | 98.49(11) | C(68) , C(23)d | 97.77(11) | C(68) , C(69) | 15.90(8) |
| C(68) , F(11)b | 95.90(11) | C(68) , <F(22A)d | 121.5(2) | C(67) , F(25)c | 175.46(11) | C(67) , >F(63A)a | 116.60(13) |
| C(67) , C(25)d | 92.00(9) | C(67) , C(23)d | 115.74(10) | C(67) , C(69) | 43.36(7) | C(67) , F(11)b | 68.15(8) |
| C(67) , <F(22A)d | 96.9(2) | F(25)c , >F(63A)a | 65.72(11) | F(25)c , C(25)d | 83.48(8) | F(25)c , C(23)d | 61.69(7) |
| F(25)c , C(69) | 137.18(9) | F(25)c , F(11)b | 111.46(8) | F(25)c , <F(22A)d | 79.64(19) | >F(63A)a , C(25)d | 120.41(14) |
| >F(63A)a , C(23)d | 127.38(13) | >F(63A)a , C(69) | 143.44(15) | >F(63A)a , F(11)b | 58.44(8) | >F(63A)a , <F(22A)d | 77.0(2) |
| C(25)d , C(23)d | 52.36(7) | C(25)d , C(69) | 93.64(8) | C(25)d , F(11)b | 92.58(7) | C(25)d , <F(22A)d | 46.9(2) |
| C(23)d , C(69) | 82.84(8) | C(23)d , F(11)b | 143.84(9) | C(23)d , <F(22A)d | 91.8(2) | C(69) , F(11)b | 111.35(8) |
| C(69) , <F(22A)d | 127.6(2) | F(11)b , <F(22A)d | 52.8(2) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = N(12) [ARU = 1555.05] -0.21090 0.74765 -0.40977 -1.7779 17.8054-15.0246

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|--------|------------|------------|------------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.375(3) | -- | C(11) | | | | Intra | -60.15 | -56.51 | -0.16610 | 0.72002 | -0.44104 | -1.4003 | 17.1474 | -16.1712 |
| 2 | 1.402(3) | -- | C(13) | | | | Intra | 151.85 | -9.01 | -0.35570 | 0.77508 | -0.41576 | -2.9986 | 18.4587 | -15.2443 |
| 3 | 1.430(3) | -- | C(14) | | | | Intra | -2.07 | 61.64 | -0.13040 | 0.74662 | -0.37546 | -1.0993 | 17.7809 | -13.7666 |
| 4 | 2.165(3) | << | N(11) | | | | Intra | -146.85 | -70.94 | -0.28110 | 0.73142 | -0.46558 | -2.3697 | 17.4189 | -17.0710 |
| 5 | 2.212(3) | << | C(12) | | | | Intra | 165.66 | -42.37 | -0.39870 | 0.76465 | -0.45042 | -3.3611 | 18.2103 | -16.5151 |
| 6 | 2.431(3) | << | C(15) | | | | Intra | -105.73 | 84.72 | -0.21810 | 0.73860 | -0.34375 | -1.8386 | 17.5899 | -12.6039 |
| 7 | 2.442(2) | << | C(19) | | | | Intra | 4.54 | 32.27 | 0.03330 | 0.75452 | -0.37421 | 0.2807 | 17.9690 | -13.7208 |
| 8 | 2.7602(19) | << | S(1) | | | | Intra | -42.88 | -30.28 | -0.00373 | 0.67954 | -0.44773 | -0.0314 | 16.1834 | -16.4165 |
| 9 | 3.443(3) | .. | F(34)a | [1/2+x, | 3/2-y,-1-z | = 3564.01] | | 87.77 | 20.26 | -0.19600 | 0.88317 | -0.37726 | -1.6523 | 21.0329 | -13.8326 |
| 10 | 2.11 | << | H(13A) | | | | Intra | 145.37 | 11.30 | -0.41280 | 0.79700 | -0.39850 | -3.4800 | 18.9807 | -14.6114 |
| 11 | 2.60 | .< | H(15A) | | | | Intra | -160.26 | 65.95 | -0.32940 | 0.73260 | -0.34490 | -2.7769 | 17.4470 | -12.6461 |
| 12 | 2.63 | .< | H(19A) | | | | Intra | 6.88 | 11.17 | 0.09240 | 0.76060 | -0.39590 | 0.7790 | 18.1138 | -14.5161 |
| 13 | 2.97(3) | .. | H(11) | | | | Intra | -130.08 | -71.17 | -0.28400 | 0.71690 | -0.48630 | -2.3942 | 17.0731 | -17.8307 |
| 14 | 3.14 | .. | H(12A) | | | | Intra | 163.25 | -37.88 | -0.49210 | 0.77760 | -0.46230 | -4.1485 | 18.5187 | -16.9507 |

Angles (Degrees) At1...V...At2 with Vertex V = N(12)

| | | | | | | | | | | | | | | | |
|-------|---|--------|------------|-------|---|--------|------------|-------|---|--------|------------|-------|---|--------|------------|
| C(11) | , | C(13) | 109.37(17) | C(11) | , | C(14) | 126.53(17) | C(11) | , | N(11) | 37.00(10) | C(11) | , | C(12) | 73.88(12) |
| C(11) | , | C(15) | 142.64(15) | C(11) | , | C(19) | 104.22(12) | C(11) | , | S(1) | 28.88(9) | C(11) | , | F(34)a | 136.67(14) |
| C(13) | , | C(14) | 124.00(18) | C(13) | , | N(11) | 72.37(13) | C(13) | , | C(12) | 35.49(12) | C(13) | , | C(15) | 100.11(14) |
| C(13) | , | C(19) | 141.85(16) | C(13) | , | S(1) | 138.23(14) | C(13) | , | F(34)a | 69.46(12) | C(14) | , | N(11) | 163.43(16) |
| C(14) | , | C(12) | 159.38(16) | C(14) | , | C(15) | 30.01(12) | C(14) | , | C(19) | 29.68(11) | C(14) | , | S(1) | 97.66(13) |
| C(14) | , | F(34)a | 72.19(12) | N(11) | , | C(12) | 36.88(9) | N(11) | , | C(15) | 156.71(12) | N(11) | , | C(19) | 138.33(10) |
| N(11) | , | S(1) | 65.88(7) | N(11) | , | F(34)a | 120.31(10) | C(12) | , | C(15) | 132.02(12) | C(12) | , | C(19) | 161.96(12) |
| C(12) | , | S(1) | 102.75(9) | C(12) | , | F(34)a | 95.04(9) | C(15) | , | C(19) | 59.70(8) | C(15) | , | S(1) | 117.76(9) |
| C(15) | , | F(34)a | 74.89(8) | C(19) | , | S(1) | 77.01(7) | C(19) | , | F(34)a | 73.84(7) | S(1) | , | F(34)a | 134.62(7) |

3.6 Angstrom Coordination Sphere Around Atom I = N(21) [ARU = 1555.02] -0.36190 0.44776 -0.53926 -3.0509 10.6635-19.7725

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|--|----------------------|--------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 0.83(3) | -- H(21) | | | Intra | 80.46 | 65.03 | -0.35500 | 0.46230 | -0.51870 | -2.9927 | 11.0098 | -19.0187 |
| 2 | 1.352(3) | -- C(21) | | | Intra | 166.15 | -40.86 | -0.47970 | 0.45804 | -0.56339 | -4.0440 | 10.9083 | -20.6573 |
| 3 | 1.381(3) | -- C(22) | | | Intra | -38.87 | -23.66 | -0.24510 | 0.41444 | -0.55437 | -2.0662 | 9.8700 | -20.3265 |
| 4 | 2.161(3) | << N(22) | | | Intra | -145.53 | -69.51 | -0.43590 | 0.42978 | -0.59447 | -3.6747 | 10.2353 | -21.7968 |
| 5 | 2.191(3) | << C(23) | | | Intra | -60.44 | -56.10 | -0.29040 | 0.40313 | -0.58886 | -2.4481 | 9.6006 | -21.5911 |
| 6 | 2.7247(19) | << S(2) | | | Intra | 153.05 | -13.26 | -0.64233 | 0.49822 | -0.55631 | -5.4150 | 11.8652 | -20.3977 |
| 7 | 3.260(2) | .< S(4) [| = | 06] | | 80.97 | 63.31 | -0.33464 | 0.50849 | -0.45983 | -2.8211 | 12.1098 | -16.8601 |
| 8 | 3.555(3) | .. C(24) | | | Intra | -159.46 | -66.06 | -0.52210 | 0.42651 | -0.62787 | -4.4014 | 10.1574 | -23.0215 |
| 9 | 3.563(3) | .. C(33) [| = | 01] | | 38.29 | -13.15 | -0.03890 | 0.53804 | -0.56136 | -0.3279 | 12.8135 | -20.5828 |
| 10 | 2.09 | << H(22A) | | | Intra | -31.56 | -3.46 | -0.15100 | 0.40190 | -0.54270 | -1.2730 | 9.5713 | -19.8986 |
| 11 | 3.11 | .. H(23A) | | | Intra | -55.80 | -51.93 | -0.23390 | 0.38110 | -0.60610 | -1.9718 | 9.0760 | -22.2233 |
| 12 | 3.42(3) | .. H(41) [| = | 06] | | 120.57 | 18.99 | -0.55700 | 0.56470 | -0.50890 | -4.6956 | 13.4484 | -18.6593 |
| 13 | 3.57 | .. H(52A)a[-1-x,-1/2+y,-1/2-z = 4444.03] | | | | 173.34 | 48.84 | -0.63860 | 0.45920 | -0.46600 | -5.3835 | 10.9359 | -17.0864 |

Angles (Degrees) At1...V...At2 with Vertex V = N(21)

| | | | | | | | | | | | | | | | |
|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|
| C(21) | , | C(22) | 111.42(19) | C(21) | , | N(22) | 37.92(11) | C(21) | , | C(23) | 75.33(14) | C(21) | , | S(2) | 29.88(10) |
| C(21) | , | S(4) | 123.78(14) | C(21) | , | C(24) | 31.66(11) | C(21) | , | C(33) | 107.65(14) | C(22) | , | N(22) | 73.51(14) |
| C(22) | , | C(23) | 36.09(13) | C(22) | , | S(2) | 141.28(15) | C(22) | , | S(4) | 124.28(14) | C(22) | , | C(24) | 79.77(14) |
| C(22) | , | C(33) | 73.17(14) | N(22) | , | C(23) | 37.42(9) | N(22) | , | S(2) | 67.79(7) | N(22) | , | S(4) | 160.93(10) |
| N(22) | , | C(24) | 6.27(6) | N(22) | , | C(33) | 97.31(9) | C(23) | , | S(2) | 105.20(9) | C(23) | , | S(4) | 159.62(10) |
| C(23) | , | C(24) | 43.68(8) | C(23) | , | C(33) | 83.90(9) | S(2) | , | S(4) | 94.04(6) | S(2) | , | C(24) | 61.54(5) |
| S(2) | , | C(33) | 110.17(8) | S(4) | , | C(24) | 155.03(7) | S(4) | , | C(33) | 83.20(6) | C(24) | , | C(33) | 99.70(7) |

3.6 Angstrom Coordination Sphere Around Atom I = N(22) [ARU = 1555.02] -0.43590 0.42978 -0.59447 -3.6747 10.2353-21.7968

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|--------|------------|-----------|--------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.374(3) | -- | C(21) | | | | Intra | 118.75 | 56.03 | -0.47970 | 0.45804 | -0.56339 | -4.0440 | 10.9083 | -20.6573 |
| 2 | 1.396(3) | -- | C(23) | | | | Intra | -27.36 | 8.47 | -0.29040 | 0.40313 | -0.58886 | -2.4481 | 9.6006 | -21.5911 |
| 3 | 1.426(3) | -- | C(24) | | | | Intra | -173.88 | -59.17 | -0.52210 | 0.42651 | -0.62787 | -4.4014 | 10.1574 | -23.0215 |
| 4 | 2.161(3) | << | N(21) | | | | Intra | 34.47 | 69.51 | -0.36190 | 0.44776 | -0.53926 | -3.0509 | 10.6635 | -19.7725 |
| 5 | 2.210(3) | << | C(22) | | | | Intra | -12.80 | 41.71 | -0.24510 | 0.41444 | -0.55437 | -2.0662 | 9.8700 | -20.3265 |
| 6 | 2.431(3) | << | C(25) | | | | Intra | 0.00 | -90.00 | -0.43980 | 0.43022 | -0.66077 | -3.7076 | 10.2458 | -24.2278 |
| 7 | 2.441(3) | << | C(29) | | | | Intra | -171.85 | -29.72 | -0.68480 | 0.41717 | -0.62747 | -5.7730 | 9.9350 | -23.0068 |
| 8 | 2.7646(19) | << | S(2) | | | | Intra | 136.88 | 30.41 | -0.64233 | 0.49822 | -0.55631 | -5.4150 | 11.8652 | -20.3977 |
| 9 | 2.10 | << | H(23A) | | | | Intra | -34.25 | -11.69 | -0.23390 | 0.38110 | -0.60610 | -1.9718 | 9.0760 | -22.2233 |
| 10 | 2.61 | .< | H(25A) | | | | Intra | 10.33 | -69.36 | -0.32870 | 0.43670 | -0.66100 | -2.7710 | 10.4001 | -24.2362 |
| 11 | 2.62 | .< | H(29A) | | | | Intra | -171.62 | -8.47 | -0.74030 | 0.41390 | -0.60500 | -6.2409 | 9.8571 | -22.1829 |
| 12 | 2.96(3) | .. | H(21) | | | | Intra | 48.63 | 69.62 | -0.35500 | 0.46230 | -0.51870 | -2.9927 | 11.0098 | -19.0187 |
| 13 | 3.13 | .. | H(22A) | | | | Intra | -15.45 | 37.30 | -0.15100 | 0.40190 | -0.54270 | -1.2730 | 9.5713 | -19.8986 |

Angles (Degrees) At1...V...At2 with Vertex V = N(22)

| | | | | | | | | | | | | | | | |
|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|
| C(21) | , | C(23) | 109.67(18) | C(21) | , | C(24) | 127.01(19) | C(21) | , | N(21) | 37.22(12) | C(21) | , | C(22) | 74.02(14) |
| C(21) | , | C(25) | 145.44(16) | C(21) | , | C(29) | 103.91(15) | C(21) | , | S(2) | 28.63(11) | C(23) | , | C(24) | 123.32(18) |
| C(23) | , | N(21) | 72.45(13) | C(23) | , | C(22) | 35.65(12) | C(23) | , | C(25) | 99.27(14) | C(23) | , | C(29) | 140.56(16) |
| C(23) | , | S(2) | 138.28(14) | C(24) | , | N(21) | 164.21(16) | C(24) | , | C(22) | 158.95(16) | C(24) | , | C(25) | 30.09(12) |
| C(24) | , | C(29) | 29.49(12) | C(24) | , | S(2) | 98.40(13) | N(21) | , | C(22) | 36.81(9) | N(21) | , | C(25) | 160.00(12) |
| N(21) | , | C(29) | 137.47(11) | N(21) | , | S(2) | 65.85(7) | C(22) | , | C(25) | 132.52(12) | C(22) | , | C(29) | 159.28(12) |
| C(22) | , | S(2) | 102.65(10) | C(25) | , | C(29) | 59.55(9) | C(25) | , | S(2) | 119.67(9) | C(29) | , | S(2) | 77.43(7) |

3.6 Angstrom Coordination Sphere Around Atom I = N(32) [ARU = 1555.01] -0.15440 0.57636 -0.57252 -1.3016 13.7261-20.9920

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|--------|------------|-----------|--------|-------|--------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.374(3) | -- | C(31) | | | | Intra | 104.83 | 46.54 | -0.18310 | 0.61473 | -0.54531 | -1.5436 | 14.6399 | -19.9943 |
| 2 | 1.396(3) | -- | C(33) | | | | Intra | -43.15 | 17.05 | -0.03890 | 0.53804 | -0.56136 | -0.3279 | 12.8135 | -20.5828 |
| 3 | 1.430(3) | -- | C(34) | | | | Intra | 178.29 | -65.91 | -0.22360 | 0.57709 | -0.60812 | -1.8850 | 13.7435 | -22.2973 |
| 4 | 2.161(3) | << | N(31) | | | | Intra | 43.67 | 68.98 | -0.08790 | 0.59883 | -0.51751 | -0.7410 | 14.2613 | -18.9750 |
| 5 | 2.201(3) | << | C(32) | | | | Intra | -23.98 | 49.48 | 0.00060 | 0.55195 | -0.52688 | 0.0051 | 13.1448 | -19.3186 |
| 6 | 2.428(3) | << | C(35) | | | | Intra | -28.41 | -83.61 | -0.12620 | 0.57096 | -0.63833 | -1.0639 | 13.5975 | -23.4050 |
| 7 | 2.438(3) | << | C(39) | | | | Intra | 174.43 | -36.29 | -0.38640 | 0.58437 | -0.61188 | -3.2574 | 13.9169 | -22.4352 |
| 8 | 2.7677(19) | << | S(3) | | | | Intra | 118.98 | 20.49 | -0.30343 | 0.67159 | -0.54610 | -2.5580 | 15.9941 | -20.0233 |
| 9 | 2.11 | << | H(33A) | | | | Intra | -50.69 | -2.77 | 0.00370 | 0.50800 | -0.57530 | 0.0312 | 12.0981 | -21.0939 |
| 10 | 2.60 | .< | H(35A) | | | | Intra | -12.21 | -62.49 | -0.01520 | 0.56570 | -0.63540 | -0.1281 | 13.4723 | -23.2976 |
| 11 | 2.62 | .< | H(39A) | | | | Intra | 173.76 | -15.00 | -0.45260 | 0.58790 | -0.59100 | -3.8155 | 14.0010 | -21.6696 |
| 12 | 2.91(3) | .. | H(31) | | | | Intra | 57.21 | 66.89 | -0.08100 | 0.61670 | -0.49950 | -0.6828 | 14.6868 | -18.3147 |
| 13 | 3.12 | .. | H(32A) | | | | Intra | -28.04 | 45.45 | 0.07510 | 0.53310 | -0.51180 | 0.6331 | 12.6959 | -18.7657 |

Angles (Degrees) At1...V...At2 with Vertex V = N(32)

| | | | | | | | | | | | | | | | |
|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|
| C(31) | , | C(33) | 110.16(19) | C(31) | , | C(34) | 125.65(18) | C(31) | , | N(31) | 37.19(12) | C(31) | , | C(32) | 74.23(14) |
| C(31) | , | C(35) | 140.70(15) | C(31) | , | C(39) | 103.68(15) | C(31) | , | S(3) | 28.50(10) | C(33) | , | C(34) | 124.07(19) |
| C(33) | , | N(31) | 72.98(14) | C(33) | , | C(32) | 35.94(13) | C(33) | , | C(35) | 100.86(15) | C(33) | , | C(39) | 141.65(16) |
| C(33) | , | S(3) | 138.57(15) | C(34) | , | N(31) | 162.75(16) | C(34) | , | C(32) | 159.95(16) | C(34) | , | C(35) | 29.93(12) |
| C(34) | , | C(39) | 29.70(12) | C(34) | , | S(3) | 97.14(13) | N(31) | , | C(32) | 37.04(9) | N(31) | , | C(35) | 156.26(11) |
| N(31) | , | C(39) | 137.84(11) | N(31) | , | S(3) | 65.68(7) | C(32) | , | C(35) | 133.11(12) | C(32) | , | C(39) | 161.23(12) |
| C(32) | , | S(3) | 102.70(9) | C(35) | , | C(39) | 59.63(9) | C(35) | , | S(3) | 115.83(9) | C(39) | , | S(3) | 77.23(7) |

3.6 Angstrom Coordination Sphere Around Atom I = N(42) [ARU = 1555.06] -0.49150 0.60077 -0.43186 -4.1434 14.3075-15.8346

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|--------|------------|-----------|--------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.379(3) | -- | C(41) | | | | Intra | -72.07 | -48.59 | -0.45820 | 0.56434 | -0.46006 | -3.8627 | 13.4399 | -16.8686 |
| 2 | 1.396(3) | -- | C(43) | | | | Intra | 136.90 | -16.57 | -0.60740 | 0.63916 | -0.44272 | -5.1205 | 15.2217 | -16.2328 |
| 3 | 1.429(3) | -- | C(44) | | | | Intra | -12.04 | 67.43 | -0.42790 | 0.59597 | -0.39588 | -3.6073 | 14.1931 | -14.5153 |
| 4 | 2.166(3) | << | N(41) | | | | Intra | -138.29 | -71.71 | -0.55170 | 0.58178 | -0.48794 | -4.6509 | 13.8552 | -17.8908 |
| 5 | 2.202(3) | << | C(42) | | | | Intra | 153.62 | -49.66 | -0.64300 | 0.62737 | -0.47764 | -5.4206 | 14.9409 | -17.5131 |
| 6 | 2.430(3) | << | C(49) | | | | Intra | -7.56 | 37.41 | -0.26450 | 0.59010 | -0.39159 | -2.2298 | 14.0533 | -14.3580 |
| 7 | 2.432(3) | << | C(45) | | | | Intra | -158.17 | 81.73 | -0.53000 | 0.59531 | -0.36623 | -4.4680 | 14.1774 | -13.4282 |
| 8 | 2.7623(19) | << | S(4) | | | | Intra | -58.96 | -21.79 | -0.33464 | 0.50849 | -0.45983 | -2.8211 | 12.1098 | -16.8601 |
| 9 | 2.11 | << | H(43A) | | | | Intra | 130.25 | 3.66 | -0.65250 | 0.66810 | -0.42820 | -5.5007 | 15.9109 | -15.7004 |
| 10 | 2.61 | .< | H(45A) | | | | Intra | -179.06 | 61.09 | -0.64100 | 0.59990 | -0.36960 | -5.4038 | 14.2867 | -13.5518 |
| 11 | 2.61 | .< | H(49A) | | | | Intra | -4.95 | 16.21 | -0.19540 | 0.59170 | -0.41200 | -1.6473 | 14.0915 | -15.1064 |
| 12 | 3.00(3) | .. | H(41) | | | | Intra | -122.73 | -70.12 | -0.55700 | 0.56470 | -0.50890 | -4.6956 | 13.4484 | -18.6593 |
| 13 | 3.13 | .. | H(42A) | | | | Intra | 150.06 | -45.35 | -0.71730 | 0.64680 | -0.49250 | -6.0470 | 15.4037 | -18.0580 |

Angles (Degrees) At1...V...At2 with Vertex V = N(42)

| | | | | | | | | | | | | | | | |
|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|
| C(41) | , | C(43) | 109.92(17) | C(41) | , | C(44) | 124.46(18) | C(41) | , | N(41) | 37.27(11) | C(41) | , | C(42) | 74.19(13) |
| C(41) | , | C(49) | 103.27(13) | C(41) | , | C(45) | 137.37(15) | C(41) | , | S(4) | 28.76(10) | C(43) | , | C(44) | 125.34(18) |
| C(43) | , | N(41) | 72.66(13) | C(43) | , | C(42) | 35.75(12) | C(43) | , | C(49) | 142.45(16) | C(43) | , | C(45) | 102.94(14) |
| C(43) | , | S(4) | 138.60(14) | C(44) | , | N(41) | 161.44(16) | C(44) | , | C(42) | 160.82(15) | C(44) | , | C(49) | 30.13(9) |
| C(44) | , | C(45) | 29.77(10) | C(44) | , | S(4) | 95.71(12) | N(41) | , | C(42) | 36.92(8) | N(41) | , | C(49) | 137.69(11) |
| N(41) | , | C(45) | 153.79(11) | N(41) | , | S(4) | 66.02(7) | C(42) | , | C(49) | 161.76(12) | C(42) | , | C(45) | 133.81(12) |
| C(42) | , | S(4) | 102.92(9) | C(49) | , | C(45) | 59.89(9) | C(49) | , | S(4) | 76.43(7) | C(45) | , | S(4) | 112.88(9) |

3.6 Angstrom Coordination Sphere Around Atom I = N(52) [ARU = 1555.03] -0.07210 0.92519 -0.08316 -0.6078 22.0336 -3.0491

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|------------|----|--------|------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|---------|
| 1 | 1.372(3) | -- | C(51) | | | | Intra | -59.34 | 60.54 | -0.03130 | 0.90083 | -0.05059 | -0.2639 | 21.4534 | -1.8549 |
| 2 | 1.401(3) | -- | C(53) | | | | Intra | 151.99 | 5.63 | -0.21810 | 0.95268 | -0.07941 | -1.8386 | 22.6883 | -2.9116 |
| 3 | 1.423(3) | -- | C(54) | | | | Intra | -12.18 | -60.76 | 0.00850 | 0.91903 | -0.11702 | 0.0717 | 21.8869 | -4.2907 |
| 4 | 2.162(3) | << | N(51) | | | | Intra | -158.48 | 71.02 | -0.14970 | 0.91436 | -0.02741 | -1.2620 | 21.7757 | -1.0050 |
| 5 | 2.215(3) | << | C(52) | | | | Intra | 163.51 | 39.63 | -0.26610 | 0.94552 | -0.04464 | -2.2433 | 22.5177 | -1.6368 |
| 6 | 2.414(3) | << | C(55) | | | | Intra | -98.74 | -79.14 | -0.08030 | 0.90632 | -0.14781 | -0.6769 | 21.5842 | -5.4196 |
| 7 | 2.445(3) | << | C(59) | | | | Intra | 0.62 | -32.72 | 0.17190 | 0.92612 | -0.11920 | 1.4492 | 22.0557 | -4.3706 |
| 8 | 2.7642(19) | << | S(5) | | | | Intra | -41.75 | 34.37 | 0.12980 | 0.86139 | -0.04060 | 1.0942 | 20.5142 | -1.4886 |
| 9 | 3.421(3) | .. | F(46)a | [-x,1/2+y,-1/2-z | = | 4554.06] | | 85.72 | -22.26 | -0.04410 | 1.05778 | -0.11850 | -0.3718 | 25.1912 | -4.3449 |
| 10 | 2.11 | << | H(53A) | | | | Intra | 146.27 | -14.86 | -0.27310 | 0.97270 | -0.09790 | -2.3023 | 23.1650 | -3.5896 |
| 11 | 2.58 | .< | H(55A) | | | | Intra | -150.69 | -63.33 | -0.19180 | 0.90140 | -0.14600 | -1.6169 | 21.4670 | -5.3532 |
| 12 | 2.64 | .< | H(59A) | | | | Intra | 5.25 | -12.00 | 0.23240 | 0.93510 | -0.09810 | 1.9592 | 22.2696 | -3.5969 |
| 13 | 2.95(4) | .. | H(51) | | | | Intra | -140.72 | 71.97 | -0.15600 | 0.90090 | -0.00660 | -1.3151 | 21.4551 | -0.2420 |
| 14 | 3.14 | .. | H(52A) | | | | Intra | 161.63 | 35.05 | -0.36140 | 0.95920 | -0.03400 | -3.0467 | 22.8435 | -1.2466 |

Angles (Degrees) At1...V...At2 with Vertex V = N(52)

| | | | | | | | | | | | | | | | |
|-------|---|--------|------------|-------|---|--------|------------|-------|---|--------|------------|-------|---|--------|------------|
| C(51) | , | C(53) | 109.42(18) | C(51) | , | C(54) | 126.61(19) | C(51) | , | N(51) | 37.07(13) | C(51) | , | C(52) | 73.88(14) |
| C(51) | , | C(55) | 141.59(16) | C(51) | , | C(59) | 105.28(15) | C(51) | , | S(5) | 28.54(11) | C(51) | , | F(46)a | 134.66(14) |
| C(53) | , | C(54) | 123.60(18) | C(53) | , | N(51) | 72.37(13) | C(53) | , | C(52) | 35.55(12) | C(53) | , | C(55) | 99.11(14) |
| C(53) | , | C(59) | 142.00(16) | C(53) | , | S(5) | 137.94(14) | C(53) | , | F(46)a | 70.52(13) | C(54) | , | N(51) | 163.20(16) |
| C(54) | , | C(52) | 158.70(16) | C(54) | , | C(55) | 30.41(12) | C(54) | , | C(59) | 29.26(12) | C(54) | , | S(5) | 98.16(13) |
| C(54) | , | F(46)a | 74.44(12) | N(51) | , | C(52) | 36.82(10) | N(51) | , | C(55) | 153.87(12) | N(51) | , | C(59) | 140.06(12) |
| N(51) | , | S(5) | 65.60(8) | N(51) | , | F(46)a | 119.28(10) | C(52) | , | C(55) | 130.24(12) | C(52) | , | C(59) | 164.59(12) |
| C(52) | , | S(5) | 102.41(10) | C(52) | , | F(46)a | 95.21(9) | C(55) | , | C(59) | 59.67(9) | C(55) | , | S(5) | 118.02(9) |
| C(55) | , | F(46)a | 78.57(8) | C(59) | , | S(5) | 78.00(7) | C(59) | , | F(46)a | 74.27(7) | S(5) | , | F(46)a | 132.74(7) |

3.6 Angstrom Coordination Sphere Around Atom I = N(61) [ARU = 1555.04] -0.00740 0.76987 0.02198 -0.0624 18.3346 0.8059

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----------------------------|----------------------|----------|-------|---------|--------|----------|---------|----------|---------|---------|---------|
| 1 | 0.84(3) | -- H(61) | | | Intra | 64.38 | -50.50 | 0.02000 | 0.79010 | 0.00430 | 0.1686 | 18.8164 | 0.1577 |
| 2 | 1.349(3) | -- C(61) | | | Intra | 155.15 | 42.99 | -0.11360 | 0.78728 | 0.04706 | -0.9577 | 18.7492 | 1.7255 |
| 3 | 1.385(4) | -- C(62) | | | Intra | -67.51 | 14.25 | 0.05350 | 0.71779 | 0.03128 | 0.4510 | 17.0943 | 1.1469 |
| 4 | 2.162(3) | << N(62) | | | Intra | -148.44 | 58.71 | -0.12090 | 0.74519 | 0.07238 | -1.0192 | 17.7469 | 2.6539 |
| 5 | 2.195(3) | << C(63) | | | Intra | -92.76 | 42.80 | -0.01660 | 0.70232 | 0.06265 | -0.1399 | 16.7259 | 2.2971 |
| 6 | 2.727(2) | << S(6) | | | Intra | 133.14 | 19.92 | -0.21538 | 0.84844 | 0.04732 | -1.8157 | 20.2058 | 1.7350 |
| 7 | 3.370(2) | .. S(5) [| = | 03] | | 62.05 | -42.92 | 0.12980 | 0.86139 | -0.04060 | 1.0942 | 20.5142 | -1.4886 |
| 8 | 3.545(3) | .. C(64) | | | Intra | -162.41 | 58.65 | -0.21590 | 0.74647 | 0.10454 | -1.8201 | 17.7773 | 3.8331 |
| 9 | 2.09 | << H(62A) | | | Intra | -56.22 | -4.00 | 0.13030 | 0.69700 | 0.01800 | 1.0985 | 16.5992 | 0.6600 |
| 10 | 3.12 | .. H(63A) | | | Intra | -88.20 | 39.20 | 0.00160 | 0.66850 | 0.07570 | 0.0135 | 15.9205 | 2.7756 |
| 11 | 3.48 | .. H(62A)a[-1/2+x,3/2-y,-z | = | 3465.04] | | 165.52 | -24.92 | -0.36970 | 0.80300 | -0.01800 | -3.1166 | 19.1236 | -0.6600 |
| 12 | 3.50 | .. H(22A)b[-x,1/2+y,-1/2-z | = | 4554.02] | | 66.99 | 12.54 | 0.15100 | 0.90190 | 0.04270 | 1.2730 | 21.4789 | 1.5656 |
| 13 | 3.52(4) | .. H(51) [| = | 03] | | 111.87 | -17.31 | -0.15600 | 0.90090 | -0.00660 | -1.3151 | 21.4551 | -0.2420 |

Angles (Degrees) At1...V...At2 with Vertex V = N(61)

| | | | | | | | |
|---------------|------------|---------------|------------|---------------|-----------|---------------|------------|
| C(61) , C(62) | 110.7(2) | C(61) , N(62) | 37.55(13) | C(61) , C(63) | 74.85(15) | C(61) , S(6) | 29.55(12) |
| C(61) , S(5) | 119.56(15) | C(61) , C(64) | 30.33(12) | C(62) , N(62) | 73.15(16) | C(62) , C(63) | 35.85(15) |
| C(62) , S(6) | 140.25(18) | C(62) , S(5) | 128.29(17) | C(62) , C(64) | 80.37(15) | N(62) , C(63) | 37.30(9) |
| N(62) , S(6) | 67.10(8) | N(62) , S(5) | 155.46(11) | N(62) , C(64) | 7.25(7) | C(63) , S(6) | 104.40(11) |
| C(63) , S(5) | 161.60(13) | C(63) , C(64) | 44.52(9) | S(6) , S(5) | 90.51(6) | S(6) , C(64) | 59.88(6) |
| S(5) , C(64) | 148.60(8) | | | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = N(62) [ARU = 1555.04] -0.12090 0.74519 0.07238 -1.0192 17.7469 2.6539

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|--------|------------|-----------|------------|-------|---------|--------|----------|---------|---------|---------|---------|--------|
| 1 | 1.368(3) | -- | C(61) | | | | Intra | 86.49 | -42.75 | -0.11360 | 0.78728 | 0.04706 | -0.9577 | 18.7492 | 1.7255 |
| 2 | 1.394(3) | -- | C(63) | | | | Intra | -49.26 | -14.83 | -0.01660 | 0.70232 | 0.06265 | -0.1399 | 16.7259 | 2.2971 |
| 3 | 1.426(3) | -- | C(64) | | | | Intra | 177.82 | 55.80 | -0.21590 | 0.74647 | 0.10454 | -1.8201 | 17.7773 | 3.8331 |
| 4 | 2.162(3) | << | N(61) | | | | Intra | 31.56 | -58.71 | -0.00740 | 0.76987 | 0.02198 | -0.0624 | 18.3346 | 0.8059 |
| 5 | 2.204(3) | << | C(62) | | | | Intra | -23.93 | -43.13 | 0.05350 | 0.71779 | 0.03128 | 0.4510 | 17.0943 | 1.1469 |
| 6 | 2.421(3) | << | C(65) | | | | Intra | -163.82 | 85.43 | -0.14290 | 0.74293 | 0.13821 | -1.2047 | 17.6930 | 5.0676 |
| 7 | 2.436(3) | << | C(69) | | | | Intra | 175.75 | 26.13 | -0.37960 | 0.75199 | 0.10164 | -3.2001 | 17.9088 | 3.7267 |
| 8 | 2.743(2) | << | S(6) | | | | Intra | 107.95 | -19.57 | -0.21538 | 0.84844 | 0.04732 | -1.8157 | 20.2058 | 1.7350 |
| 9 | 3.495(2) | .. | S(5)a | [-1/2+x, | 3/2-y,-z | = 3465.03] | | -129.62 | -19.47 | -0.37020 | 0.63861 | 0.04060 | -3.1209 | 15.2086 | 1.4886 |
| 10 | 2.10 | << | H(63A) | | | | Intra | -60.51 | 3.32 | 0.00160 | 0.66850 | 0.07570 | 0.0135 | 15.9205 | 2.7756 |
| 11 | 2.59 | .< | H(65A) | | | | Intra | -11.01 | 72.68 | -0.03100 | 0.73900 | 0.13990 | -0.2613 | 17.5994 | 5.1296 |
| 12 | 2.62 | .< | H(69A) | | | | Intra | 175.18 | 4.84 | -0.42920 | 0.75440 | 0.07840 | -3.6182 | 17.9662 | 2.8746 |
| 13 | 2.96(3) | .. | H(61) | | | | Intra | 42.00 | -57.37 | 0.02000 | 0.79010 | 0.00430 | 0.1686 | 18.8164 | 0.1577 |
| 14 | 3.13 | .. | H(62A) | | | | Intra | -28.46 | -39.62 | 0.13030 | 0.69700 | 0.01800 | 1.0985 | 16.5992 | 0.6600 |

Angles (Degrees) At1...V...At2 with Vertex V = N(62)

| | | | | | | | | | | | | | | | |
|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|-------|---|-------|------------|
| C(61) | , | C(63) | 109.56(19) | C(61) | , | C(64) | 124.82(19) | C(61) | , | N(61) | 36.94(13) | C(61) | , | C(62) | 73.91(15) |
| C(61) | , | C(65) | 134.14(16) | C(61) | , | C(69) | 106.89(15) | C(61) | , | S(6) | 29.39(11) | C(61) | , | S(5)a | 109.45(13) |
| C(63) | , | C(64) | 125.57(19) | C(63) | , | N(61) | 72.62(14) | C(63) | , | C(62) | 35.65(14) | C(63) | , | C(65) | 106.69(15) |
| C(63) | , | C(69) | 136.57(16) | C(63) | , | S(6) | 138.94(15) | C(63) | , | S(5)a | 76.24(13) | C(64) | , | N(61) | 161.72(16) |
| C(64) | , | C(62) | 161.17(17) | C(64) | , | C(65) | 29.89(12) | C(64) | , | C(69) | 29.70(12) | C(64) | , | S(6) | 95.44(12) |
| C(64) | , | S(5)a | 87.34(12) | N(61) | , | C(62) | 36.97(10) | N(61) | , | C(65) | 153.10(12) | N(61) | , | C(69) | 138.98(12) |
| N(61) | , | S(6) | 66.33(8) | N(61) | , | S(5)a | 100.29(9) | C(62) | , | C(65) | 136.55(12) | C(62) | , | C(69) | 156.64(13) |
| C(62) | , | S(6) | 103.30(10) | C(62) | , | S(5)a | 87.60(9) | C(65) | , | C(69) | 59.59(9) | C(65) | , | S(6) | 109.37(9) |
| C(65) | , | S(5)a | 105.67(8) | C(69) | , | S(6) | 80.10(8) | C(69) | , | S(5)a | 69.93(7) | S(6) | , | S(5)a | 111.39(6) |

3.6 Angstrom Coordination Sphere Around Atom I = F(21A) [ARU = 1555.02] -0.39300 0.47730 -0.73900 -3.3131 11.3670-27.0962

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|--------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.276(13) | -- | C(210) | | | | Intra | -107.64 | 16.84 | -0.43690 | 0.42844 | -0.72892 | -3.6832 | 10.2034 | -26.7266 |
| 2 | 0.64(3) | << | >F(23) | | | | Intra | 174.84 | -16.86 | -0.46490 | 0.47960 | -0.74403 | -3.9192 | 11.4218 | -27.2806 |
| 3 | 1.64(2) | << | >F(21) | | | | Intra | -53.90 | 16.26 | -0.28320 | 0.42400 | -0.72650 | -2.3874 | 10.0976 | -26.6378 |
| 4 | 2.097(19) | << | <F(22A) | | | | Intra | -67.13 | 13.45 | -0.29900 | 0.39840 | -0.72570 | -2.5206 | 9.4880 | -26.6085 |
| 5 | 2.13(2) | << | <F(23A) | | | | Intra | -119.52 | -17.44 | -0.51170 | 0.40310 | -0.75640 | -4.3137 | 9.5999 | -27.7342 |
| 6 | 2.252(17) | << | >F(22) | | | | Intra | -112.13 | -13.17 | -0.49100 | 0.39200 | -0.75300 | -4.1392 | 9.3356 | -27.6095 |
| 7 | 2.373(18) | << | C(26) | | | | Intra | -131.07 | 45.03 | -0.52370 | 0.42421 | -0.69321 | -4.4149 | 10.1026 | -25.4172 |
| 8 | 3.105(18) | .< | C(25) | | | | Intra | -109.39 | 67.49 | -0.43980 | 0.43022 | -0.66077 | -3.7076 | 10.2458 | -24.2278 |
| 9 | 3.32(2) | .. | C(27) | | | | Intra | -149.40 | 30.07 | -0.68640 | 0.41588 | -0.69363 | -5.7865 | 9.9043 | -25.4326 |
| 10 | 3.323(19) | .. | F(45)a | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | -162.04 | -73.49 | -0.49956 | 0.46507 | -0.82590 | -4.2114 | 11.0757 | -30.2824 |
| 11 | 3.352(15) | .. | C(37) | [| = | 01] | | 82.57 | 42.18 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 12 | 3.52(2) | .. | >F(51)b | [-1/2+x,3/2-y,-1-z | = | 3464.03] | | 139.13 | -21.71 | -0.68620 | 0.56710 | -0.77450 | -5.7848 | 13.5056 | -28.3978 |
| 13 | 3.59(2) | .. | C(310) | [| = | 01] | | 40.23 | 19.71 | -0.08690 | 0.56898 | -0.70598 | -0.7326 | 13.5504 | -25.8855 |
| 14 | 2.86 | .. | H(37A) | [| = | 01] | | 91.33 | 28.90 | -0.39990 | 0.58240 | -0.70130 | -3.3712 | 13.8700 | -25.7139 |
| 15 | 2.95 | .. | H(47A)a | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | -43.41 | -52.10 | -0.23680 | 0.42500 | -0.80250 | -1.9963 | 10.1215 | -29.4245 |
| 16 | 3.07 | .. | H(25A) | | | | Intra | -60.72 | 68.81 | -0.32870 | 0.43670 | -0.66100 | -2.7710 | 10.4001 | -24.2362 |
| 17 | 3.43 | .. | H(27A) | | | | Intra | -152.31 | 14.23 | -0.74240 | 0.41240 | -0.71600 | -6.2586 | 9.8214 | -26.2529 |
| 18 | 3.58 | .. | H(57A)b | [-1/2+x,3/2-y,-1-z | = | 3464.03] | | 73.03 | -33.55 | -0.28980 | 0.59700 | -0.79290 | -2.4431 | 14.2177 | -29.0725 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(21A)

| | | | | | | | |
|-------------------|-----------|-------------------|-----------|------------------|-----------|------------------|-----------|
| C(210) , >F(23) | 83.5(18) | C(210) , >F(21) | 51.4(7) | C(210) , <F(22A) | 39.2(6) | C(210) , <F(23A) | 36.2(7) |
| C(210) , >F(22) | 30.3(5) | C(210) , C(26) | 34.4(6) | C(210) , C(25) | 50.7(7) | C(210) , C(27) | 40.3(8) |
| C(210) , F(45)a | 96.9(9) | C(210) , C(37) | 120.2(10) | C(210) , >F(51)b | 117.3(14) | C(210) , C(310) | 131.7(12) |
| >F(23) , >F(21) | 133.4(16) | >F(23) , <F(22A) | 120.3(15) | >F(23) , <F(23A) | 62.4(13) | >F(23) , >F(22) | 70.2(13) |
| >F(23) , C(26) | 79.0(18) | >F(23) , C(25) | 100.3(19) | >F(23) , C(27) | 58.2(16) | >F(23) , F(45)a | 58.1(16) |
| >F(23) , C(37) | 102.9(15) | >F(23) , >F(51)b | 34.0(10) | >F(23) , C(310) | 136.9(12) | >F(21) , <F(22A) | 13.1(6) |
| >F(21) , <F(23A) | 72.9(7) | >F(21) , >F(22) | 64.6(6) | >F(21) , C(26) | 69.6(6) | >F(21) , C(25) | 62.2(6) |
| >F(21) , C(27) | 86.5(7) | >F(21) , F(45)a | 110.7(8) | >F(21) , C(37) | 109.1(10) | >F(21) , >F(51)b | 166.5(11) |
| >F(21) , C(310) | 88.3(10) | <F(22A) , <F(23A) | 60.2(6) | <F(22A) , >F(22) | 51.9(5) | <F(22A) , C(26) | 62.2(5) |
| <F(22A) , C(25) | 60.6(5) | <F(22A) , C(27) | 76.7(6) | <F(22A) , F(45)a | 104.3(6) | <F(22A) , C(37) | 117.8(8) |
| <F(22A) , >F(51)b | 153.7(9) | <F(22A) , C(310) | 101.2(9) | <F(23A) , >F(22) | 8.3(5) | <F(23A) , C(26) | 63.4(6) |
| <F(23A) , C(25) | 85.3(6) | <F(23A) , C(27) | 55.6(6) | <F(23A) , F(45)a | 60.8(6) | <F(23A) , C(37) | 148.9(10) |
| <F(23A) , >F(51)b | 93.6(9) | <F(23A) , C(310) | 160.7(10) | >F(22) , C(26) | 60.7(5) | >F(22) , C(25) | 80.7(5) |
| >F(22) , C(27) | 56.2(5) | >F(22) , F(45)a | 66.6(5) | >F(22) , C(37) | 148.3(9) | >F(22) , >F(51)b | 101.9(8) |
| >F(22) , C(310) | 152.7(9) | C(26) , C(25) | 25.2(2) | C(26) , C(27) | 20.8(3) | C(26) , F(45)a | 120.4(7) |
| C(26) , C(37) | 87.8(5) | C(26) , >F(51)b | 105.0(8) | C(26) , C(310) | 114.8(7) | C(25) , C(27) | 44.2(3) |
| C(25) , F(45)a | 145.1(6) | C(25) , C(37) | 70.0(4) | C(25) , >F(51)b | 118.2(7) | C(25) , C(310) | 90.0(5) |
| C(27) , F(45)a | 103.9(6) | C(27) , C(37) | 93.4(5) | C(27) , >F(51)b | 86.0(6) | C(27) , C(310) | 129.4(5) |
| F(45)a , C(37) | 137.2(4) | F(45)a , >F(51)b | 60.6(4) | F(45)a , C(310) | 124.8(5) | C(37) , >F(51)b | 82.5(3) |

=====
C(37) , C(310) 42.1(2) >F(51)b , C(310) 105.1(3)

3.6 Angstrom Coordination Sphere Around Atom I = F(22A) [ARU = 1555.02] -0.29900 0.39840 -0.72570 -2.5206 9.4880-26.6085

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|---------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.370(12) | -- | C(210) | | | | Intra | 148.39 | -4.94 | -0.43690 | 0.42844 | -0.72892 | -3.6832 | 10.2034 | -26.7266 |
| 2 | 0.63(2) | << | >F(21) | | | | Intra | 77.68 | -2.69 | -0.28320 | 0.42400 | -0.72650 | -2.3874 | 10.0976 | -26.6378 |
| 3 | 1.909(16) | << | >F(22) | | | | Intra | -174.62 | -31.62 | -0.49100 | 0.39200 | -0.75300 | -4.1392 | 9.3356 | -27.6095 |
| 4 | 2.097(19) | << | <F(21A) | | | | Intra | 112.87 | -13.45 | -0.39300 | 0.47730 | -0.73900 | -3.3131 | 11.3670 | -27.0962 |
| 5 | 2.120(17) | << | <F(23A) | | | | Intra | 176.43 | -32.07 | -0.51170 | 0.40310 | -0.75640 | -4.3137 | 9.5999 | -27.7342 |
| 6 | 2.321(11) | << | C(26) | | | | Intra | 162.02 | 30.89 | -0.52370 | 0.42421 | -0.69321 | -4.4149 | 10.1026 | -25.4172 |
| 7 | 2.479(15) | << | >F(23) | | | | Intra | 125.88 | -15.73 | -0.46490 | 0.47960 | -0.74403 | -3.9192 | 11.4218 | -27.2806 |
| 8 | 2.766(11) | << | C(25) | | | | Intra | 147.44 | 59.39 | -0.43980 | 0.43022 | -0.66077 | -3.7076 | 10.2458 | -24.2278 |
| 9 | 2.768(11) | < | F(24)a | [1+x,y,z | = | 1655.02] | | -1.09 | 26.85 | -0.00610 | 0.39642 | -0.69160 | -0.0514 | 9.4408 | -25.3582 |
| 10 | 3.073(11) | .. | F(43)c | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | 14.76 | -30.57 | 0.00450 | 0.42671 | -0.76832 | 0.0379 | 10.1622 | -28.1712 |
| 11 | 3.087(13) | .. | F(13)b | [-1/2-x,1-y,-1/2+z | = | 2464.05] | | -61.54 | -37.95 | -0.16140 | 0.30855 | -0.77747 | -1.3606 | 7.3482 | -28.5067 |
| 12 | 3.152(14) | .. | F(11)b | [-1/2-x,1-y,-1/2+z | = | 2464.05] | | -98.03 | -13.86 | -0.34970 | 0.27115 | -0.74630 | -2.9480 | 6.4575 | -27.3638 |
| 13 | 3.496(11) | .. | C(27) | | | | Intra | 172.74 | 19.65 | -0.68640 | 0.41588 | -0.69363 | -5.7865 | 9.9043 | -25.4326 |
| 14 | 3.571(13) | .. | F(66)d | [-1-x,-1/2+y,-1/2-z | = | 4444.04] | | -89.53 | 48.42 | -0.29670 | 0.29889 | -0.65286 | -2.5012 | 7.1181 | -23.9378 |
| 15 | 2.55 | < | H(25A) | | | | Intra | 105.35 | 68.26 | -0.32870 | 0.43670 | -0.66100 | -2.7710 | 10.4001 | -24.2362 |
| 16 | 2.93 | .. | H(47A)c | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | 50.38 | -73.72 | -0.23680 | 0.42500 | -0.80250 | -1.9963 | 10.1215 | -29.4245 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(22A)

| | | | | | | | |
|-------------------|-----------|------------------|-----------|------------------|-----------|------------------|----------|
| C(210) , >F(21) | 70.6(13) | C(210) , >F(22) | 43.7(5) | C(210) , <F(21A) | 36.0(8) | C(210) , <F(23A) | 37.7(6) |
| C(210) , C(26) | 38.1(3) | C(210) , >F(23) | 24.6(4) | C(210) , C(25) | 64.3(4) | C(210) , F(24)a | 143.6(8) |
| C(210) , F(43)c | 123.2(7) | C(210) , F(13)b | 128.9(6) | C(210) , F(11)b | 111.5(7) | C(210) , C(27) | 34.3(4) |
| C(210) , F(66)d | 114.6(6) | >F(21) , >F(22) | 103.5(14) | >F(21) , <F(21A) | 36.4(12) | >F(21) , <F(23A) | 96.0(14) |
| >F(21) , C(26) | 86.5(13) | >F(21) , >F(23) | 49.2(11) | >F(21) , C(25) | 82.2(13) | >F(21) , F(24)a | 81.2(12) |
| >F(21) , F(43)c | 65.5(12) | >F(21) , F(13)b | 124.6(13) | >F(21) , F(11)b | 162.9(14) | >F(21) , C(27) | 95.7(13) |
| >F(21) , F(66)d | 133.0(13) | >F(22) , <F(21A) | 68.2(8) | >F(22) , <F(23A) | 7.6(6) | >F(22) , C(26) | 66.3(5) |
| >F(22) , >F(23) | 56.1(5) | >F(22) , C(25) | 96.3(5) | >F(22) , F(24)a | 172.6(7) | >F(22) , F(43)c | 117.2(6) |
| >F(22) , F(13)b | 86.6(5) | >F(22) , F(11)b | 71.5(5) | >F(22) , C(27) | 52.7(4) | >F(22) , F(66)d | 110.1(6) |
| <F(21A) , <F(23A) | 60.6(9) | <F(21A) , C(26) | 64.8(7) | <F(21A) , >F(23) | 12.8(7) | <F(21A) , C(25) | 78.0(7) |
| <F(21A) , F(24)a | 117.2(8) | <F(21A) , F(43)c | 90.0(8) | <F(21A) , F(13)b | 128.3(7) | <F(21A) , F(11)b | 139.0(7) |
| <F(21A) , C(27) | 67.6(7) | <F(21A) , F(66)d | 140.4(7) | <F(23A) , C(26) | 64.4(5) | <F(23A) , >F(23) | 48.5(7) |
| <F(23A) , C(25) | 94.6(6) | <F(23A) , F(24)a | 174.4(7) | <F(23A) , F(43)c | 115.0(6) | <F(23A) , F(13)b | 91.6(6) |
| <F(23A) , F(11)b | 79.0(7) | <F(23A) , C(27) | 51.8(5) | <F(23A) , F(66)d | 115.9(7) | C(26) , >F(23) | 58.1(3) |
| C(26) , C(25) | 30.15(16) | C(26) , F(24)a | 120.1(4) | C(26) , F(43)c | 152.0(6) | C(26) , F(13)b | 143.7(5) |
| C(26) , F(11)b | 105.5(4) | C(26) , C(27) | 14.82(13) | C(26) , F(66)d | 78.2(3) | >F(23) , C(25) | 77.2(4) |
| >F(23) , F(24)a | 129.7(6) | >F(23) , F(43)c | 99.3(5) | >F(23) , F(13)b | 125.9(4) | >F(23) , F(11)b | 127.5(5) |
| >F(23) , C(27) | 58.1(3) | >F(23) , F(66)d | 136.3(4) | C(25) , F(24)a | 89.9(3) | C(25) , F(43)c | 137.3(5) |
| C(25) , F(13)b | 151.7(5) | C(25) , F(11)b | 114.3(4) | C(25) , C(27) | 43.70(17) | C(25) , F(66)d | 62.6(2) |
| F(24)a , F(43)c | 59.4(2) | F(24)a , F(13)b | 86.0(3) | F(24)a , F(11)b | 102.3(4) | F(24)a , C(27) | 133.1(4) |
| F(24)a , F(66)d | 69.3(3) | F(43)c , F(13)b | 61.7(2) | F(43)c , F(11)b | 101.7(4) | F(43)c , C(27) | 157.3(5) |

=====
F(43)c , F(66)d 121.4(4) F(13)b , F(11)b 40.28(18) F(13)b , C(27) 129.8(4) F(13)b , F(66)d 89.9(3)
F(11)b , C(27) 93.9(3) F(11)b , F(66)d 62.7(3) C(27) , F(66)d 80.4(2)

3.6 Angstrom Coordination Sphere Around Atom I = F(23A) [ARU = 1555.02] -0.51170 0.40310 -0.75640 -4.3137 9.5999-27.7342

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|--------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.333(16) | -- | C(210) | | | | Intra | 43.74 | 49.10 | -0.43690 | 0.42844 | -0.72892 | -3.6832 | 10.2034 | -26.7266 |
| 2 | 0.34(2) | << | >F(22) | | | | Intra | -56.57 | 21.48 | -0.49100 | 0.39200 | -0.75300 | -4.1392 | 9.3356 | -27.6095 |
| 3 | 1.92(2) | << | >F(23) | | | | Intra | 77.78 | 13.68 | -0.46490 | 0.47960 | -0.74403 | -3.9192 | 11.4218 | -27.2806 |
| 4 | 2.120(17) | << | <F(22A) | | | | Intra | -3.57 | 32.07 | -0.29900 | 0.39840 | -0.72570 | -2.5206 | 9.4880 | -26.6085 |
| 5 | 2.13(2) | << | <F(21A) | | | | Intra | 60.48 | 17.44 | -0.39300 | 0.47730 | -0.73900 | -3.3131 | 11.3670 | -27.0962 |
| 6 | 2.272(16) | << | >F(21) | | | | Intra | 14.49 | 28.86 | -0.28320 | 0.42400 | -0.72650 | -2.3874 | 10.0976 | -26.6378 |
| 7 | 2.373(15) | << | C(26) | | | | Intra | 101.38 | 77.52 | -0.52370 | 0.42421 | -0.69321 | -4.4149 | 10.1026 | -25.4172 |
| 8 | 2.749(14) | << | C(27) | | | | Intra | 168.32 | 56.84 | -0.68640 | 0.41588 | -0.69363 | -5.7865 | 9.9043 | -25.4326 |
| 9 | 2.947(17) | .. | F(45)c | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | 86.03 | -59.86 | -0.49956 | 0.46507 | -0.82590 | -4.2114 | 11.0757 | -30.2824 |
| 10 | 3.119(15) | .. | F(44)c | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | -112.95 | -78.38 | -0.54074 | 0.37882 | -0.83971 | -4.5585 | 9.0217 | -30.7888 |
| 11 | 3.215(14) | .. | F(41)b | [-3/2-x,1-y,-1/2+z | = | 2364.06] | | -163.16 | -25.90 | -0.84010 | 0.36791 | -0.79470 | -7.0822 | 8.7619 | -29.1385 |
| 12 | 3.334(15) | .. | F(42)b | [-3/2-x,1-y,-1/2+z | = | 2364.06] | | 153.74 | -31.86 | -0.81290 | 0.45570 | -0.80440 | -6.8529 | 10.8526 | -29.4941 |
| 13 | 3.45(2) | .. | F(11)a | [-1/2-x,1-y,-1/2+z | = | 2464.05] | | -66.51 | 6.17 | -0.34970 | 0.27115 | -0.74630 | -2.9480 | 6.4575 | -27.3638 |
| 14 | 3.525(15) | .. | C(420)c | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | 56.93 | -79.45 | -0.46990 | 0.42582 | -0.85092 | -3.9614 | 10.1410 | -31.1998 |
| 15 | 2.45 | << | H(27A) | | | | Intra | 173.50 | 37.12 | -0.74240 | 0.41240 | -0.71600 | -6.2586 | 9.8214 | -26.2529 |
| 16 | 2.92 | .. | H(47A)c | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | 12.68 | -35.43 | -0.23680 | 0.42500 | -0.80250 | -1.9963 | 10.1215 | -29.4245 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(23A)

| | | | | | | | |
|-------------------|-----------|-------------------|----------|-------------------|-----------|------------------|-----------|
| C(210) , >F(22) | 80(3) | C(210) , >F(23) | 45.1(7) | C(210) , <F(22A) | 39.0(5) | C(210) , <F(21A) | 34.4(7) |
| C(210) , >F(21) | 30.1(4) | C(210) , C(26) | 35.5(4) | C(210) , C(27) | 64.6(6) | C(210) , F(45)c | 114.2(11) |
| C(210) , F(44)c | 149.5(9) | C(210) , F(41)b | 148.8(8) | C(210) , F(42)b | 126.1(11) | C(210) , F(11)a | 98.3(9) |
| C(210) , C(420)c | 128.8(10) | >F(22) , >F(23) | 123(3) | >F(22) , <F(22A) | 48(3) | >F(22) , <F(21A) | 107(3) |
| >F(22) , >F(21) | 64(3) | >F(22) , C(26) | 80(3) | >F(22) , C(27) | 93(3) | >F(22) , F(45)c | 134(3) |
| >F(22) , F(44)c | 105(3) | >F(22) , F(41)b | 114(3) | >F(22) , F(42)b | 151(4) | >F(22) , F(11)a | 18(3) |
| >F(22) , C(420)c | 115(3) | >F(23) , <F(22A) | 75.6(7) | >F(23) , <F(21A) | 17.1(7) | >F(23) , >F(21) | 60.2(7) |
| >F(23) , C(26) | 65.0(5) | >F(23) , C(27) | 78.9(6) | >F(23) , F(45)c | 73.8(6) | >F(23) , F(44)c | 115.1(7) |
| >F(23) , F(41)b | 121.9(7) | >F(23) , F(42)b | 85.7(7) | >F(23) , F(11)a | 139.4(6) | >F(23) , C(420)c | 93.8(6) |
| <F(22A) , <F(21A) | 59.1(8) | <F(22A) , >F(21) | 15.9(6) | <F(22A) , C(26) | 61.9(5) | <F(22A) , C(27) | 90.8(6) |
| <F(22A) , F(45)c | 117.1(7) | <F(22A) , F(44)c | 125.2(7) | <F(22A) , F(41)b | 161.1(10) | <F(22A) , F(42)b | 160.8(10) |
| <F(22A) , F(11)a | 63.9(6) | <F(22A) , C(420)c | 116.5(6) | <F(21A) , >F(21) | 43.5(8) | <F(21A) , C(26) | 63.4(7) |
| <F(21A) , C(27) | 84.8(8) | <F(21A) , F(45)c | 80.0(8) | <F(21A) , F(44)c | 119.0(8) | <F(21A) , F(41)b | 138.8(10) |
| <F(21A) , F(42)b | 101.8(9) | <F(21A) , F(11)a | 122.6(8) | <F(21A) , C(420)c | 96.9(8) | >F(21) , C(26) | 61.2(4) |
| >F(21) , C(27) | 91.5(5) | >F(21) , F(45)c | 106.2(7) | >F(21) , F(44)c | 125.5(6) | >F(21) , F(41)b | 176.4(9) |
| >F(21) , F(42)b | 144.9(10) | >F(21) , F(11)a | 79.2(7) | >F(21) , C(420)c | 110.9(5) | C(26) , C(27) | 30.27(19) |
| C(26) , F(45)c | 137.7(9) | C(26) , F(44)c | 172.9(5) | C(26) , F(41)b | 116.4(5) | C(26) , F(42)b | 113.8(6) |
| C(26) , F(11)a | 96.0(5) | C(26) , C(420)c | 158.7(8) | C(27) , F(45)c | 133.4(7) | C(27) , F(44)c | 143.0(5) |
| C(27) , F(41)b | 86.2(3) | C(27) , F(42)b | 89.6(4) | C(27) , F(11)a | 102.9(5) | C(27) , C(420)c | 149.3(6) |
| F(45)c , F(44)c | 41.3(2) | F(45)c , F(41)b | 77.5(3) | F(45)c , F(42)b | 51.8(3) | F(45)c , F(11)a | 122.4(5) |
| F(45)c , C(420)c | 21.48(12) | F(44)c , F(41)b | 57.1(3) | F(44)c , F(42)b | 59.5(3) | F(44)c , F(11)a | 88.1(5) |

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F(44)c , C(420)c 22.08(12) F(41)b , F(42)b 37.96(16) F(41)b , F(11)a 98.7(5) F(41)b , C(420)c 72.3(3)
F(42)b , F(11)a 134.5(6) F(42)b , C(420)c 60.0(3) F(11)a , C(420)c 101.9(4)

3.6 Angstrom Coordination Sphere Around Atom I = F(31) [ARU = 1555.01] 0.03060 0.60880 -0.70300 0.2580 14.4987-25.7762

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|--------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.376(9) | -- | C(310) | | | | Intra | -136.25 | -4.56 | -0.08690 | 0.56898 | -0.70598 | -0.7326 | 13.5504 | -25.8855 |
| 2 | 2.117(15) | << | <F(33) | | | | Intra | -99.66 | -4.97 | -0.01140 | 0.52150 | -0.70800 | -0.0961 | 12.4196 | -25.9595 |
| 3 | 2.118(12) | << | <F(32) | | | | Intra | -157.67 | -34.95 | -0.15990 | 0.58110 | -0.73610 | -1.3480 | 13.8390 | -26.9898 |
| 4 | 2.346(8) | << | C(36) | | | | Intra | -155.43 | 27.89 | -0.19310 | 0.57260 | -0.67307 | -1.6279 | 13.6366 | -24.6788 |
| 5 | 2.787(8) | <. | F(35)a | [1+x,y,z | = | 1655.01] | | 9.53 | 17.50 | 0.34150 | 0.62727 | -0.68014 | 2.8789 | 14.9386 | -24.9380 |
| 6 | 2.860(8) | << | C(35) | | | | Intra | -145.72 | 55.99 | -0.12620 | 0.57096 | -0.63833 | -1.0639 | 13.5975 | -23.4050 |
| 7 | 3.040(9) | .. | F(12)b | [1/2+x,3/2-y,-1-z | = | 3564.05] | | 65.51 | -18.06 | 0.17270 | 0.71925 | -0.72871 | 1.4559 | 17.1291 | -26.7189 |
| 8 | 3.200(8) | .. | F(36)a | [1+x,y,z | = | 1655.01] | | -33.74 | 31.13 | 0.30080 | 0.54491 | -0.65788 | 2.5358 | 12.9771 | -24.1218 |
| 9 | 3.446(8) | .. | C(37) | | | | Intra | -168.37 | 15.67 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 10 | 3.462(8) | .. | F(16)c | [-1/2+x,3/2-y,-1-z | = | 3464.05] | | 128.53 | 40.23 | -0.16470 | 0.69563 | -0.64201 | -1.3885 | 16.5666 | -23.5399 |
| 11 | 3.468(8) | .. | C(320)a | [1+x,y,z | = | 1655.01] | | -7.05 | 32.73 | 0.37410 | 0.59376 | -0.65186 | 3.1537 | 14.1405 | -23.9011 |
| 12 | 3.475(9) | .. | F(14)c | [-1/2+x,3/2-y,-1-z | = | 3464.05] | | 117.00 | 5.67 | -0.15560 | 0.73817 | -0.69364 | -1.3117 | 17.5797 | -25.4330 |
| 13 | 2.71 | .. | H(35A) | | | | Intra | -110.61 | 66.13 | -0.01520 | 0.56570 | -0.63540 | -0.1281 | 13.4723 | -23.2976 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(31)

| | | | | | | | |
|------------------|-----------|------------------|----------|------------------|-----------|------------------|-----------|
| C(310) , <F(33) | 36.5(5) | C(310) , <F(32) | 36.3(3) | C(310) , C(36) | 37.4(2) | C(310) , F(35)a | 144.1(5) |
| C(310) , C(35) | 61.1(3) | C(310) , F(12)b | 148.8(5) | C(310) , F(36)a | 103.1(5) | C(310) , C(37) | 37.7(3) |
| C(310) , F(16)c | 96.9(4) | C(310) , C(320)a | 125.0(5) | C(310) , F(14)c | 107.1(4) | <F(33) , <F(32) | 61.2(5) |
| <F(33) , C(36) | 63.0(4) | <F(33) , F(35)a | 109.8(5) | <F(33) , C(35) | 71.6(5) | <F(33) , F(12)b | 152.7(5) |
| <F(33) , F(36)a | 72.4(4) | <F(33) , C(37) | 71.0(4) | <F(33) , F(16)c | 124.3(5) | <F(33) , C(320)a | 94.9(5) |
| <F(33) , F(14)c | 143.5(5) | <F(32) , C(36) | 62.9(3) | <F(32) , F(35)a | 159.2(4) | <F(32) , C(35) | 91.5(4) |
| <F(32) , F(12)b | 113.0(4) | <F(32) , F(36)a | 133.5(5) | <F(32) , C(37) | 51.6(3) | <F(32) , F(16)c | 101.3(4) |
| <F(32) , C(320)a | 155.6(5) | <F(32) , F(14)c | 89.4(4) | C(36) , F(35)a | 132.3(3) | C(36) , C(35) | 28.95(12) |
| C(36) , F(12)b | 141.2(4) | C(36) , F(36)a | 99.0(3) | C(36) , C(37) | 17.11(10) | C(36) , F(16)c | 62.30(18) |
| C(36) , C(320)a | 112.4(3) | C(36) , F(14)c | 85.2(2) | F(35)a , C(35) | 103.6(2) | F(35)a , F(12)b | 65.55(19) |
| F(35)a , F(36)a | 41.42(12) | F(35)a , C(37) | 146.8(3) | F(35)a , F(16)c | 99.1(2) | F(35)a , C(320)a | 21.32(8) |
| F(35)a , F(14)c | 104.8(3) | C(35) , F(12)b | 135.4(3) | C(35) , F(36)a | 75.6(2) | C(35) , C(37) | 43.88(12) |
| C(35) , F(16)c | 55.46(14) | C(35) , C(320)a | 84.6(2) | C(35) , F(14)c | 89.4(2) | F(12)b , F(36)a | 106.9(2) |
| F(12)b , C(37) | 128.6(3) | F(12)b , F(16)c | 82.6(2) | F(12)b , C(320)a | 85.9(2) | F(12)b , F(14)c | 56.05(17) |
| F(36)a , C(37) | 116.1(2) | F(36)a , F(16)c | 106.8(2) | F(36)a , C(320)a | 22.65(7) | F(36)a , F(14)c | 133.8(3) |
| C(37) , F(16)c | 59.54(13) | C(37) , C(320)a | 128.4(2) | C(37) , F(14)c | 73.70(17) | F(16)c , C(320)a | 96.3(2) |
| F(16)c , F(14)c | 36.08(10) | C(320)a , F(14)c | 114.5(2) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(31A) [ARU = 1555.01] -0.12900 0.61000 -0.72890 -1.0875 14.5273-26.7258

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|----------|--------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.337(19) | -- | C(310) | | | | Intra | -70.03 | 38.96 | -0.08690 | 0.56898 | -0.70598 | -0.7326 | 13.5504 | -25.8855 |
| 2 | 2.14(3) | << | <F(32A) | | | | Intra | -90.23 | 4.63 | -0.13000 | 0.52060 | -0.72420 | -1.0959 | 12.3982 | -26.5535 |
| 3 | 2.15(3) | << | <F(33A) | | | | Intra | -32.59 | 29.16 | 0.05880 | 0.56750 | -0.70030 | 0.4957 | 13.5151 | -25.6772 |
| 4 | 2.297(19) | << | C(36) | | | | Intra | -121.24 | 63.03 | -0.19310 | 0.57260 | -0.67307 | -1.6279 | 13.6366 | -24.6788 |
| 5 | 2.73(2) | << | >F(62A)a | [x,y,-1+z | = | 1554.04] | | 98.92 | -39.87 | -0.16750 | 0.69685 | -0.77660 | -1.4121 | 16.5956 | -28.4748 |
| 6 | 2.77(2) | << | C(37) | | | | Intra | -159.89 | 42.83 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 7 | 3.323(19) | .. | F(14)b | [-1/2+x,3/2-y,-1-z | = | 3464.05] | | 94.20 | 22.90 | -0.15560 | 0.73817 | -0.69364 | -1.3117 | 17.5797 | -25.4330 |
| 8 | 3.344(19) | .. | F(55)c | [-1/2+x,3/2-y,-1-z | = | 3464.03] | | -53.38 | -64.81 | -0.02830 | 0.56203 | -0.81143 | -0.2386 | 13.3849 | -29.7519 |
| 9 | 3.449(19) | .. | C(35) | | | | Intra | -88.55 | 74.35 | -0.12620 | 0.57096 | -0.63833 | -1.0639 | 13.5975 | -23.4050 |
| 10 | 3.50(3) | .. | >F(53)c | [-1/2+x,3/2-y,-1-z | = | 3464.03] | | 171.86 | -17.75 | -0.51990 | 0.62980 | -0.75796 | -4.3829 | 14.9988 | -27.7914 |
| 11 | 2.58 | .< | H(37A) | | | | Intra | -163.94 | 23.07 | -0.39990 | 0.58240 | -0.70130 | -3.3712 | 13.8700 | -25.7139 |
| 12 | 2.73 | .. | H(57A)c | [-1/2+x,3/2-y,-1-z | = | 3464.03] | | -167.13 | -59.35 | -0.28980 | 0.59700 | -0.79290 | -2.4431 | 14.2177 | -29.0725 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(31A)

| | | | | | | | |
|-------------------|-----------|-------------------|-----------|--------------------|-----------|--------------------|-----------|
| C(310) , <F(32A) | 38.9(9) | C(310) , <F(33A) | 32.3(9) | C(310) , C(36) | 38.6(6) | C(310) , >F(62A)a | 171.4(16) |
| C(310) , C(37) | 64.6(9) | C(310) , F(14)b | 116.4(10) | C(310) , F(55)c | 104.6(10) | C(310) , C(35) | 36.5(6) |
| C(310) , >F(53)c | 122.7(13) | <F(32A) , <F(33A) | 59.7(11) | <F(32A) , C(36) | 62.7(9) | <F(32A) , >F(62A)a | 143.8(11) |
| <F(32A) , C(37) | 72.0(9) | <F(32A) , F(14)b | 152.1(11) | <F(32A) , F(55)c | 74.5(9) | <F(32A) , C(35) | 69.7(8) |
| <F(32A) , >F(53)c | 98.9(11) | <F(33A) , C(36) | 63.7(7) | <F(33A) , >F(62A)a | 139.2(12) | <F(33A) , C(37) | 93.3(8) |
| <F(33A) , F(14)b | 107.0(10) | <F(33A) , F(55)c | 95.4(9) | <F(33A) , C(35) | 53.1(6) | <F(33A) , >F(53)c | 154.9(11) |
| C(36) , >F(62A)a | 146.9(10) | C(36) , C(37) | 30.0(3) | C(36) , F(14)b | 89.6(6) | C(36) , F(55)c | 137.2(7) |
| C(36) , C(35) | 16.0(2) | C(36) , >F(53)c | 95.9(8) | >F(62A)a , C(37) | 123.0(9) | >F(62A)a , F(14)b | 62.9(4) |
| >F(62A)a , F(55)c | 73.1(4) | >F(62A)a , C(35) | 145.3(7) | >F(62A)a , >F(53)c | 65.8(5) | C(37) , F(14)b | 85.5(5) |
| C(37) , F(55)c | 134.7(7) | C(37) , C(35) | 44.1(3) | C(37) , >F(53)c | 65.9(5) | F(14)b , F(55)c | 133.1(6) |
| F(14)b , C(35) | 82.7(4) | F(14)b , >F(53)c | 86.1(6) | F(55)c , C(35) | 141.0(6) | F(55)c , >F(53)c | 90.6(5) |
| C(35) , >F(53)c | 109.7(6) | | | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(31B) [ARU = 1555.01] -0.01200 0.61610 -0.71300 -0.1012 14.6725-26.1429

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------|-------------------------------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.313(11) | -- | C(310) | | Intra | -119.37 | 11.30 | -0.08690 | 0.56898 | -0.70598 | -0.7326 | 13.5504 | -25.8855 |
| 2 | 2.104(15) | << | <F(33B) | | Intra | -80.84 | 10.34 | 0.02710 | 0.53030 | -0.70270 | 0.2285 | 12.6292 | -25.7652 |
| 3 | 2.168(15) | << | <F(32B) | | Intra | -130.92 | -23.63 | -0.16630 | 0.55310 | -0.73670 | -1.4019 | 13.1722 | -27.0118 |
| 4 | 2.355(11) | << | C(36) | | Intra | -145.84 | 38.43 | -0.19310 | 0.57260 | -0.67307 | -1.6279 | 13.6366 | -24.6788 |
| 5 | 2.965(10) | .. | F(12)c | [1/2+x,3/2-y,-1-z = 3564.05] | | 57.63 | -11.20 | 0.17270 | 0.71925 | -0.72871 | 1.4559 | 17.1291 | -26.7189 |
| 6 | 3.095(11) | < | C(35) | | Intra | -131.85 | 62.21 | -0.12620 | 0.57096 | -0.63833 | -1.0639 | 13.5975 | -23.4050 |
| 7 | 3.225(12) | .. | F(35)a | [1+x,y,z = 1655.01] | | 5.10 | 21.93 | 0.34150 | 0.62727 | -0.68014 | 2.8789 | 14.9386 | -24.9380 |
| 8 | 3.228(10) | .. | F(14)d | [-1/2+x,3/2-y,-1-z = 3464.05] | | 112.61 | 12.70 | -0.15560 | 0.73817 | -0.69364 | -1.3117 | 17.5797 | -25.4330 |
| 9 | 3.279(12) | .. | C(37) | | Intra | -163.75 | 23.31 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 10 | 3.295(12) | .. | >F(62A)b | [x,y,-1+z = 1554.04] | | 124.28 | -45.06 | -0.16750 | 0.69685 | -0.77660 | -1.4121 | 16.5956 | -28.4748 |
| 11 | 3.467(11) | .. | F(16)d | [-1/2+x,3/2-y,-1-z = 3464.05] | | 124.20 | 48.66 | -0.16470 | 0.69563 | -0.64201 | -1.3885 | 16.5666 | -23.5399 |
| 12 | 3.09 | .. | H(35A) | | Intra | -91.29 | 67.12 | -0.01520 | 0.56570 | -0.63540 | -0.1281 | 13.4723 | -23.2976 |
| 13 | 3.39 | .. | H(37A) | | Intra | -166.21 | 7.26 | -0.39990 | 0.58240 | -0.70130 | -3.3712 | 13.8700 | -25.7139 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(31B)

| | | | | | | | |
|-------------------|-----------|--------------------|----------|-------------------|-----------|-------------------|-----------|
| C(310) , <F(33B) | 37.8(4) | C(310) , <F(32B) | 36.7(4) | C(310) , C(36) | 36.0(3) | C(310) , F(12)c | 177.1(7) |
| C(310) , C(35) | 51.7(4) | C(310) , F(35)a | 116.2(6) | C(310) , F(14)d | 123.1(6) | C(310) , C(37) | 43.9(4) |
| C(310) , >F(62A)b | 116.5(6) | C(310) , F(16)d | 98.1(6) | <F(33B) , <F(32B) | 59.6(5) | <F(33B) , C(36) | 64.1(5) |
| <F(33B) , F(12)c | 139.2(6) | <F(33B) , C(35) | 63.4(5) | <F(33B) , F(35)a | 82.4(5) | <F(33B) , F(14)d | 153.4(6) |
| <F(33B) , C(37) | 79.5(5) | <F(33B) , >F(62A)b | 139.1(6) | <F(33B) , F(16)d | 117.0(6) | <F(32B) , C(36) | 63.6(4) |
| <F(32B) , F(12)c | 144.2(5) | <F(32B) , C(35) | 85.8(4) | <F(32B) , F(35)a | 139.6(5) | <F(32B) , F(14)d | 119.1(5) |
| <F(32B) , C(37) | 56.7(4) | <F(32B) , >F(62A)b | 83.2(4) | <F(32B) , F(16)d | 117.2(5) | C(36) , F(12)c | 145.7(4) |
| C(36) , C(35) | 25.27(14) | C(36) , F(35)a | 113.8(4) | C(36) , F(14)d | 90.9(3) | C(36) , C(37) | 21.49(14) |
| C(36) , >F(62A)b | 116.0(4) | C(36) , F(16)d | 62.2(3) | F(12)c , C(35) | 128.5(4) | F(12)c , F(35)a | 61.3(2) |
| F(12)c , F(14)d | 59.57(18) | F(12)c , C(37) | 138.8(4) | F(12)c , >F(62A)b | 65.7(2) | F(12)c , F(16)d | 83.6(2) |
| C(35) , F(35)a | 89.2(3) | C(35) , F(14)d | 90.1(3) | C(35) , C(37) | 44.47(17) | C(35) , >F(62A)b | 134.8(4) |
| C(35) , F(16)d | 53.85(18) | F(35)a , F(14)d | 101.0(3) | F(35)a , C(37) | 133.5(4) | F(35)a , >F(62A)b | 125.7(4) |
| F(35)a , F(16)d | 91.0(3) | F(14)d , C(37) | 79.3(3) | F(14)d , >F(62A)b | 58.7(2) | F(14)d , F(16)d | 37.22(12) |
| C(37) , >F(62A)b | 94.6(3) | C(37) , F(16)d | 61.1(2) | >F(62A)b , F(16)d | 93.7(3) | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(32) [ARU = 1555.01] -0.15990 0.58110 -0.73610 -1.3480 13.8390-26.9898

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------------|------------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.297(8) | -- | C(310) | | Intra | -25.13 | 58.39 | -0.08690 | 0.56898 | -0.70598 | -0.7326 | 13.5504 | -25.8855 |
| 2 | 2.118(12) | << | <F(31) | | Intra | 22.33 | 34.96 | 0.03060 | 0.60880 | -0.70300 | 0.2580 | 14.4987 | -25.7762 |
| 3 | 2.155(16) | << | <F(33) | | Intra | -48.59 | 28.56 | -0.01140 | 0.52150 | -0.70800 | -0.0961 | 12.4196 | -25.9595 |
| 4 | 2.337(8) | << | C(36) | | Intra | -144.12 | 81.50 | -0.19310 | 0.57260 | -0.67307 | -1.6279 | 13.6366 | -24.6788 |
| 5 | 2.702(8) | << | C(37) | | Intra | -179.68 | 52.52 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 6 | 3.011(8) | .. | F(55)b [-1/2+x,3/2-y,-1-z | = 3464.03] | | -22.26 | -66.54 | -0.02830 | 0.56203 | -0.81143 | -0.2386 | 13.3849 | -29.7519 |
| 7 | 3.132(10) | .. | >F(62A)a[x,y,-1+z | = 1554.04] | | 91.33 | -28.30 | -0.16750 | 0.69685 | -0.77660 | -1.4121 | 16.5956 | -28.4748 |
| 8 | 3.311(8) | .. | C(57)b [-1/2+x,3/2-y,-1-z | = 3464.03] | | 169.68 | -61.96 | -0.34150 | 0.59281 | -0.81580 | -2.8789 | 14.1179 | -29.9121 |
| 9 | 3.346(13) | .. | >F(53)b [-1/2+x,3/2-y,-1-z | = 3464.03] | | 159.09 | -13.86 | -0.51990 | 0.62980 | -0.75796 | -4.3829 | 14.9988 | -27.7914 |
| 10 | 3.541(13) | .. | >F(23) [| = 02] | | -136.77 | -4.71 | -0.46490 | 0.47960 | -0.74403 | -3.9192 | 11.4218 | -27.2806 |
| 11 | 2.38 | << | H(57A)b[-1/2+x,3/2-y,-1-z | = 3464.03] | | 160.93 | -60.91 | -0.28980 | 0.59700 | -0.79290 | -2.4431 | 14.2177 | -29.0725 |
| 12 | 2.39 | << | H(37A) | | Intra | 179.12 | 32.23 | -0.39990 | 0.58240 | -0.70130 | -3.3712 | 13.8700 | -25.7139 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(32)

| | | | | | | | |
|--------------------|-----------|-------------------|----------|------------------|-----------|-------------------|-----------|
| C(310) , <F(31) | 38.9(4) | C(310) , <F(33) | 34.0(5) | C(310) , C(36) | 36.4(3) | C(310) , C(37) | 67.2(3) |
| C(310) , F(55)b | 124.9(5) | C(310) , >F(62A)a | 127.6(6) | C(310) , C(57)b | 171.8(6) | C(310) , >F(53)b | 135.4(5) |
| C(310) , >F(23) | 105.2(5) | <F(31) , <F(33) | 59.4(5) | <F(31) , C(36) | 63.3(3) | <F(31) , C(37) | 90.4(3) |
| <F(31) , F(55)b | 107.1(4) | <F(31) , >F(62A)a | 90.8(4) | <F(31) , C(57)b | 146.1(4) | <F(31) , >F(53)b | 135.8(5) |
| <F(31) , >F(23) | 144.1(4) | <F(33) , C(36) | 62.6(4) | <F(33) , C(37) | 88.4(5) | <F(33) , F(55)b | 97.2(5) |
| <F(33) , >F(62A)a | 144.9(6) | <F(33) , C(57)b | 138.3(5) | <F(33) , >F(53)b | 150.4(6) | <F(33) , >F(23) | 90.7(5) |
| C(36) , C(37) | 30.90(13) | C(36) , F(55)b | 159.8(4) | C(36) , >F(62A)a | 122.9(4) | C(36) , C(57)b | 145.6(4) |
| C(36) , >F(53)b | 99.1(3) | C(36) , >F(23) | 86.3(3) | C(37) , F(55)b | 162.1(4) | C(37) , >F(62A)a | 111.5(3) |
| C(37) , C(57)b | 114.8(3) | C(37) , >F(53)b | 68.9(2) | C(37) , >F(23) | 67.7(2) | F(55)b , >F(62A)a | 72.9(2) |
| F(55)b , C(57)b | 51.20(13) | F(55)b , >F(53)b | 99.6(2) | F(55)b , >F(23) | 95.1(3) | >F(62A)a , C(57)b | 59.86(19) |
| >F(62A)a , >F(53)b | 64.1(3) | >F(62A)a , >F(23) | 123.2(3) | C(57)b , >F(53)b | 48.70(18) | C(57)b , >F(23) | 69.5(2) |
| >F(53)b , >F(23) | 63.8(3) | | | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(32A) [ARU = 1555.01] -0.13000 0.52060 -0.72420 -1.0959 12.3982-26.5535

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|---------|----|---------|--------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.38(2) | -- | C(310) | | | | Intra | 72.50 | 28.94 | -0.08690 | 0.56898 | -0.70598 | -0.7326 | 13.5504 | -25.8855 |
| 2 | 2.13(3) | << | <F(33A) | | | | Intra | 35.06 | 24.26 | 0.05880 | 0.56750 | -0.70030 | 0.4957 | 13.5151 | -25.6772 |
| 3 | 2.14(3) | << | <F(31A) | | | | Intra | 89.77 | -4.63 | -0.12900 | 0.61000 | -0.72890 | -1.0875 | 14.5273 | -26.7258 |
| 4 | 2.31(2) | << | C(36) | | | | Intra | 113.25 | 54.29 | -0.19310 | 0.57260 | -0.67307 | -1.6279 | 13.6366 | -24.6788 |
| 5 | 2.64(3) | << | >F(21) | [| = | 02] | | -119.31 | -1.83 | -0.28320 | 0.42400 | -0.72650 | -2.3874 | 10.0976 | -26.6378 |
| 6 | 2.93(2) | << | C(37) | | | | Intra | 142.94 | 35.71 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 7 | 2.98(2) | .. | F(43)b | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | -63.11 | -32.83 | 0.00450 | 0.42671 | -0.76832 | 0.0379 | 10.1622 | -28.1712 |
| 8 | 3.08(3) | .. | >F(23) | [| = | 02] | | -160.92 | -13.68 | -0.46490 | 0.47960 | -0.74403 | -3.9192 | 11.4218 | -27.2806 |
| 9 | 3.36(2) | .. | F(24)a | [1+x,y,z | = | 1655.02] | | -70.55 | 20.86 | -0.00610 | 0.39642 | -0.69160 | -0.0514 | 9.4408 | -25.3582 |
| 10 | 3.37(2) | .. | C(35) | | | | Intra | 88.47 | 69.14 | -0.12620 | 0.57096 | -0.63833 | -1.0639 | 13.5975 | -23.4050 |
| 11 | 3.40(2) | .. | C(210) | [| = | 02] | | -139.69 | -2.92 | -0.43690 | 0.42844 | -0.72892 | -3.6832 | 10.2034 | -26.7266 |
| 12 | 3.46(3) | .. | F(55)c | [-1/2+x,3/2-y,-1-z | = | 3464.03] | | 49.01 | -67.77 | -0.02830 | 0.56203 | -0.81143 | -0.2386 | 13.3849 | -29.7519 |
| 13 | 3.55(2) | .. | F(26)a | [1+x,y,z | = | 1655.02] | | -60.78 | 56.17 | -0.01560 | 0.44819 | -0.64380 | -0.1315 | 10.6737 | -23.6056 |
| 14 | 2.84 | .. | H(37A) | | | | Intra | 147.10 | 17.22 | -0.39990 | 0.58240 | -0.70130 | -3.3712 | 13.8700 | -25.7139 |
| 15 | 3.39 | .. | H(57A)c | [-1/2+x,3/2-y,-1-z | = | 3464.03] | | 126.52 | -48.05 | -0.28980 | 0.59700 | -0.79290 | -2.4431 | 14.2177 | -29.0725 |
| 16 | 3.49 | .. | H(25A) | [| = | 02] | | -129.97 | 41.63 | -0.32870 | 0.43670 | -0.66100 | -2.7710 | 10.4001 | -24.2362 |
| 17 | 3.56 | .. | H(35A) | | | | Intra | 47.98 | 66.06 | -0.01520 | 0.56570 | -0.63540 | -0.1281 | 13.4723 | -23.2976 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(32A)

| | | | | | | | |
|-------------------|-----------|------------------|-----------|------------------|-----------|------------------|-----------|
| C(310) , <F(33A) | 33.7(9) | C(310) , <F(31A) | 37.5(8) | C(310) , C(36) | 38.8(7) | C(310) , >F(21) | 150.7(16) |
| C(310) , C(37) | 58.7(9) | C(310) , F(43)b | 142.0(15) | C(310) , >F(23) | 128.4(13) | C(310) , F(24)a | 118.8(13) |
| C(310) , C(35) | 41.3(8) | C(310) , C(210) | 139.8(14) | C(310) , F(55)c | 98.3(11) | C(310) , F(26)a | 86.1(11) |
| <F(33A) , <F(31A) | 60.5(11) | <F(33A) , C(36) | 63.7(8) | <F(33A) , >F(21) | 146.6(13) | <F(33A) , C(37) | 89.3(9) |
| <F(33A) , F(43)b | 109.4(11) | <F(33A) , >F(23) | 161.6(12) | <F(33A) , F(24)a | 94.8(11) | <F(33A) , C(35) | 54.7(7) |
| <F(33A) , C(210) | 158.1(12) | <F(33A) , F(55)c | 92.6(9) | <F(33A) , F(26)a | 73.2(10) | <F(31A) , C(36) | 62.1(8) |
| <F(31A) , >F(21) | 150.2(14) | <F(31A) , C(37) | 64.0(8) | <F(31A) , F(43)b | 134.6(12) | <F(31A) , >F(23) | 107.5(11) |
| <F(31A) , F(24)a | 154.9(12) | <F(31A) , C(35) | 73.8(8) | <F(31A) , C(210) | 130.0(12) | <F(31A) , F(55)c | 68.9(8) |
| <F(31A) , F(26)a | 123.4(11) | C(36) , >F(21) | 112.4(10) | C(36) , C(37) | 27.7(3) | C(36) , F(43)b | 158.4(10) |
| C(36) , >F(23) | 98.7(8) | C(36) , F(24)a | 104.8(8) | C(36) , C(35) | 18.7(3) | C(36) , C(210) | 102.3(8) |
| C(36) , F(55)c | 131.0(7) | C(36) , F(26)a | 69.4(6) | >F(21) , C(37) | 97.4(8) | >F(21) , F(43)b | 61.0(5) |
| >F(21) , >F(23) | 42.8(4) | >F(21) , F(24)a | 52.8(4) | >F(21) , C(35) | 110.2(8) | >F(21) , C(210) | 20.4(3) |
| >F(21) , F(55)c | 109.9(8) | >F(21) , F(26)a | 74.7(5) | C(37) , F(43)b | 158.3(9) | C(37) , >F(23) | 72.5(6) |
| C(37) , F(24)a | 115.2(8) | C(37) , C(35) | 44.5(4) | C(37) , C(210) | 81.5(6) | C(37) , F(55)c | 124.2(7) |
| C(37) , F(26)a | 85.9(6) | F(43)b , >F(23) | 89.0(6) | F(43)b , F(24)a | 54.2(3) | F(43)b , C(35) | 140.3(8) |
| F(43)b , C(210) | 77.2(5) | F(43)b , F(55)c | 67.5(5) | F(43)b , F(26)a | 89.0(5) | >F(23) , F(24)a | 95.2(6) |
| >F(23) , C(35) | 110.1(8) | >F(23) , C(210) | 23.6(2) | >F(23) , F(55)c | 95.7(7) | >F(23) , F(26)a | 107.0(6) |
| F(24)a , C(35) | 88.7(6) | F(24)a , C(210) | 71.7(4) | F(24)a , F(55)c | 120.3(7) | F(24)a , F(26)a | 36.1(2) |
| C(35) , C(210) | 106.6(7) | C(35) , F(55)c | 139.6(6) | C(35) , F(26)a | 52.7(4) | C(210) , F(55)c | 109.1(7) |
| C(210) , F(26)a | 86.3(5) | F(55)c , F(26)a | 147.2(8) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(32B) [ARU = 1555.01] -0.16630 0.55310 -0.73670 -1.4019 13.1722-27.0118

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|-----------|----------------------------|------------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.364(9) | -- | C(310) | | Intra | 29.47 | 55.68 | -0.08690 | 0.56898 | -0.70598 | -0.7326 | 13.5504 | -25.8855 |
| 2 | 2.123(16) | << | <F(33B) | | Intra | -18.42 | 35.96 | 0.02710 | 0.53030 | -0.70270 | 0.2285 | 12.6292 | -25.7652 |
| 3 | 2.168(15) | << | <F(31B) | | Intra | 49.08 | 23.63 | -0.01200 | 0.61610 | -0.71300 | -0.1012 | 14.6725 | -26.1429 |
| 4 | 2.390(8) | << | C(36) | | Intra | 115.94 | 77.52 | -0.19310 | 0.57260 | -0.67307 | -1.6279 | 13.6366 | -24.6788 |
| 5 | 2.766(9) | << | C(37) | | Intra | 157.52 | 51.54 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 6 | 2.984(8) | .. | F(55)b [-1/2+x,3/2-y,-1-z | = 3464.03] | | 10.36 | -66.65 | -0.02830 | 0.56203 | -0.81143 | -0.2386 | 13.3849 | -29.7519 |
| 7 | 3.078(14) | .. | >F(23) [| = 02] | | -145.19 | -5.01 | -0.46490 | 0.47960 | -0.74403 | -3.9192 | 11.4218 | -27.2806 |
| 8 | 3.25(2) | .. | >F(21) [| = 02] | | -107.77 | 6.61 | -0.28320 | 0.42400 | -0.72650 | -2.3874 | 10.0976 | -26.6378 |
| 9 | 3.389(9) | .. | C(57)b [-1/2+x,3/2-y,-1-z | = 3464.03] | | 147.37 | -58.84 | -0.34150 | 0.59281 | -0.81580 | -2.8789 | 14.1179 | -29.9121 |
| 10 | 3.532(12) | .. | F(43)a [-1/2-x,1-y,-1/2+z | = 2464.06] | | -64.44 | -19.16 | 0.00450 | 0.42671 | -0.76832 | 0.0379 | 10.1622 | -28.1712 |
| 11 | 3.582(15) | .. | >F(53)b [-1/2+x,3/2-y,-1-z | = 3464.03] | | 148.50 | -12.57 | -0.51990 | 0.62980 | -0.75796 | -4.3829 | 14.9988 | -27.7914 |
| 12 | 2.46 | << | H(37A) | | Intra | 160.49 | 31.85 | -0.39990 | 0.58240 | -0.70130 | -3.3712 | 13.8700 | -25.7139 |
| 13 | 2.53 | < | H(57A)b[-1/2+x,3/2-y,-1-z | = 3464.03] | | 134.88 | -54.40 | -0.28980 | 0.59700 | -0.79290 | -2.4431 | 14.2177 | -29.0725 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(32B)

| | | | | | | | |
|------------------|----------|------------------|-----------|-------------------|-----------|------------------|-----------|
| C(310) , <F(33B) | 37.7(5) | C(310) , <F(31B) | 35.2(4) | C(310) , C(36) | 35.5(3) | C(310) , C(37) | 64.5(4) |
| C(310) , F(55)b | 123.2(6) | C(310) , >F(23) | 129.1(5) | C(310) , >F(21) | 108.4(5) | C(310) , C(57)b | 147.5(7) |
| C(310) , F(43)a | 107.9(6) | C(310) , >F(53)b | 116.5(6) | <F(33B) , <F(31B) | 58.7(5) | <F(33B) , C(36) | 63.2(4) |
| <F(33B) , C(37) | 92.4(5) | <F(33B) , F(55)b | 105.0(5) | <F(33B) , >F(23) | 122.3(6) | <F(33B) , >F(21) | 85.6(5) |
| <F(33B) , C(57)b | 155.3(6) | <F(33B) , F(43)a | 70.2(5) | <F(33B) , >F(53)b | 153.8(5) | <F(31B) , C(36) | 62.0(4) |
| <F(31B) , C(37) | 82.3(4) | <F(31B) , F(55)b | 94.9(5) | <F(31B) , >F(23) | 156.9(5) | <F(31B) , >F(21) | 142.2(5) |
| <F(31B) , C(57)b | 114.3(5) | <F(31B) , F(43)a | 118.5(5) | <F(31B) , >F(53)b | 103.5(5) | C(36) , C(37) | 30.11(13) |
| C(36) , F(55)b | 156.8(5) | C(36) , >F(23) | 96.8(3) | C(36) , >F(21) | 92.5(3) | C(36) , C(57)b | 137.7(4) |
| C(36) , F(43)a | 121.6(4) | C(36) , >F(53)b | 92.0(3) | C(37) , F(55)b | 157.8(4) | C(37) , >F(23) | 74.6(3) |
| C(37) , >F(21) | 87.7(3) | C(37) , C(57)b | 110.7(3) | C(37) , F(43)a | 133.9(4) | C(37) , >F(53)b | 64.6(3) |
| F(55)b , >F(23) | 106.2(3) | F(55)b , >F(21) | 106.9(3) | F(55)b , C(57)b | 50.53(13) | F(55)b , F(43)a | 66.5(2) |
| F(55)b , >F(53)b | 95.1(3) | >F(23) , >F(21) | 39.1(2) | >F(23) , C(57)b | 74.2(2) | >F(23) , F(43)a | 79.6(3) |
| >F(23) , >F(53)b | 65.8(3) | >F(21) , C(57)b | 103.3(3) | >F(21) , F(43)a | 49.9(2) | >F(21) , >F(53)b | 104.8(4) |
| C(57)b , F(43)a | 97.7(2) | C(57)b , >F(53)b | 46.28(18) | F(43)a , >F(53)b | 134.6(3) | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(33) [ARU = 1555.01] -0.01140 0.52150 -0.70800 -0.0961 12.4196-25.9595

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|--------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.300(13) | -- | C(310) | | | | Intra | 119.37 | 3.27 | -0.08690 | 0.56898 | -0.70598 | -0.7326 | 13.5504 | -25.8855 |
| 2 | 2.117(15) | << | <F(31) | | | | Intra | 80.34 | 4.97 | 0.03060 | 0.60880 | -0.70300 | 0.2580 | 14.4987 | -25.7762 |
| 3 | 2.155(16) | << | <F(32) | | | | Intra | 131.41 | -28.56 | -0.15990 | 0.58110 | -0.73610 | -1.3480 | 13.8390 | -26.9898 |
| 4 | 2.338(14) | << | C(36) | | | | Intra | 141.53 | 33.21 | -0.19310 | 0.57260 | -0.67307 | -1.6279 | 13.6366 | -24.6788 |
| 5 | 2.931(14) | .< | F(26)a | [1+x,y,z | = | 1655.02] | | -91.16 | 53.43 | -0.01560 | 0.44819 | -0.64380 | -0.1315 | 10.6737 | -23.6056 |
| 6 | 2.975(14) | .< | C(35) | | | | Intra | 129.41 | 59.17 | -0.12620 | 0.57096 | -0.63833 | -1.0639 | 13.5975 | -23.4050 |
| 7 | 3.039(12) | .. | F(24)a | [1+x,y,z | = | 1655.02] | | -89.14 | 11.41 | -0.00610 | 0.39642 | -0.69160 | -0.0514 | 9.4408 | -25.3582 |
| 8 | 3.163(14) | .. | F(43)c | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | -86.60 | -44.36 | 0.00450 | 0.42671 | -0.76832 | 0.0379 | 10.1622 | -28.1712 |
| 9 | 3.258(14) | .. | F(36)b | [1+x,y,z | = | 1655.01] | | 11.96 | 34.34 | 0.30080 | 0.54491 | -0.65788 | 2.5358 | 12.9771 | -24.1218 |
| 10 | 3.332(19) | .. | >F(21) | [| = | 02] | | -134.62 | -11.75 | -0.28320 | 0.42400 | -0.72650 | -2.3874 | 10.0976 | -26.6378 |
| 11 | 3.377(13) | .. | C(220)a | [1+x,y,z | = | 1655.02] | | -78.04 | 31.99 | 0.05900 | 0.40384 | -0.65920 | 0.4974 | 9.6175 | -24.1702 |
| 12 | 3.408(14) | .. | C(37) | | | | Intra | 154.03 | 19.08 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 13 | 2.86 | .. | H(35A) | | | | Intra | 91.74 | 68.42 | -0.01520 | 0.56570 | -0.63540 | -0.1281 | 13.4723 | -23.2976 |
| 14 | 3.46 | .. | H(27A)a | [1+x,y,z | = | 1655.02] | | -48.89 | -4.86 | 0.25760 | 0.41240 | -0.71600 | 2.1716 | 9.8214 | -26.2529 |
| 15 | 3.59 | .. | H(37A) | | | | Intra | 156.11 | 3.92 | -0.39990 | 0.58240 | -0.70130 | -3.3712 | 13.8700 | -25.7139 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(33)

| | | | | | | | |
|------------------|----------|------------------|-----------|------------------|-----------|------------------|-----------|
| C(310) , <F(31) | 39.0(4) | C(310) , <F(32) | 33.9(4) | C(310) , C(36) | 36.4(4) | C(310) , F(26)a | 117.8(8) |
| C(310) , C(35) | 56.4(5) | C(310) , F(24)a | 148.1(8) | C(310) , F(43)c | 133.0(8) | C(310) , F(36)b | 102.4(7) |
| C(310) , >F(21) | 106.3(7) | C(310) , C(220)a | 141.1(9) | C(310) , C(37) | 37.4(5) | <F(31) , <F(32) | 59.5(5) |
| <F(31) , C(36) | 63.3(4) | <F(31) , F(26)a | 121.2(6) | <F(31) , C(35) | 65.9(4) | <F(31) , F(24)a | 160.6(7) |
| <F(31) , F(43)c | 139.0(6) | <F(31) , F(36)b | 69.4(4) | <F(31) , >F(21) | 144.8(6) | <F(31) , C(220)a | 137.7(6) |
| <F(31) , C(37) | 73.0(4) | <F(32) , C(36) | 62.5(4) | <F(32) , F(26)a | 140.3(6) | <F(32) , C(35) | 87.8(5) |
| <F(32) , F(24)a | 138.5(6) | <F(32) , F(43)c | 99.2(5) | <F(32) , F(36)b | 128.8(5) | <F(32) , >F(21) | 87.8(5) |
| <F(32) , C(220)a | 154.4(6) | <F(32) , C(37) | 52.4(4) | C(36) , F(26)a | 82.1(4) | C(36) , C(35) | 27.19(18) |
| C(36) , F(24)a | 114.3(5) | C(36) , F(43)c | 141.5(5) | C(36) , F(36)b | 97.5(5) | C(36) , >F(21) | 91.4(5) |
| C(36) , C(220)a | 104.9(5) | C(36) , C(37) | 18.01(15) | F(26)a , C(35) | 62.8(3) | F(26)a , F(24)a | 42.05(18) |
| F(26)a , F(43)c | 97.9(3) | F(26)a , F(36)b | 70.0(3) | F(26)a , >F(21) | 74.9(3) | F(26)a , C(220)a | 23.42(11) |
| F(26)a , C(37) | 88.5(4) | C(35) , F(24)a | 102.9(4) | C(35) , F(43)c | 153.7(5) | C(35) , F(36)b | 73.2(3) |
| C(35) , >F(21) | 103.1(4) | C(35) , C(220)a | 86.0(4) | C(35) , C(37) | 43.87(19) | F(24)a , F(43)c | 55.8(2) |
| F(24)a , F(36)b | 92.5(4) | F(24)a , >F(21) | 50.8(3) | F(24)a , C(220)a | 22.98(11) | F(24)a , C(37) | 110.7(4) |
| F(43)c , F(36)b | 118.8(4) | F(43)c , >F(21) | 52.4(3) | F(43)c , C(220)a | 76.8(3) | F(43)c , C(37) | 124.1(4) |
| F(36)b , >F(21) | 142.2(5) | F(36)b , C(220)a | 72.6(3) | F(36)b , C(37) | 115.5(4) | >F(21) , C(220)a | 69.5(3) |
| >F(21) , C(37) | 76.7(4) | C(220)a , C(37) | 108.6(4) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(33A) [ARU = 1555.01] 0.05880 0.56750 -0.70030 0.4957 13.5151-25.6772

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|-------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.246(14) | -- | C(310) | | | | Intra | 178.36 | -9.62 | -0.08690 | 0.56898 | -0.70598 | -0.7326 | 13.5504 | -25.8855 |
| 2 | 2.13(3) | << | <F(32A) | | | | Intra | -144.94 | -24.26 | -0.13000 | 0.52060 | -0.72420 | -1.0959 | 12.3982 | -26.5535 |
| 3 | 2.15(3) | << | <F(31A) | | | | Intra | 147.41 | -29.16 | -0.12900 | 0.61000 | -0.72890 | -1.0875 | 14.5273 | -26.7258 |
| 4 | 2.350(15) | << | C(36) | | | | Intra | 176.73 | 25.14 | -0.19310 | 0.57260 | -0.67307 | -1.6279 | 13.6366 | -24.6788 |
| 5 | 2.621(17) | << | F(36)b | [1+x,y,z | = | 1655.01] | | -14.77 | 36.40 | 0.30080 | 0.54491 | -0.65788 | 2.5358 | 12.9771 | -24.1218 |
| 6 | 2.757(17) | << | C(35) | | | | Intra | 176.98 | 55.50 | -0.12620 | 0.57096 | -0.63833 | -1.0639 | 13.5975 | -23.4050 |
| 7 | 2.87(2) | < | F(35)b | [1+x,y,z | = | 1655.01] | | 30.85 | 14.91 | 0.34150 | 0.62727 | -0.68014 | 2.8789 | 14.9386 | -24.9380 |
| 8 | 3.257(16) | .. | C(320)b | [1+x,y,z | = | 1655.01] | | 13.24 | 33.04 | 0.37410 | 0.59376 | -0.65186 | 3.1537 | 14.1405 | -23.9011 |
| 9 | 3.47(2) | .. | >F(51)c | [1/2+x,3/2-y,-1-z | = | 3564.03] | | -0.25 | -51.69 | 0.31380 | 0.56710 | -0.77450 | 2.6454 | 13.5056 | -28.3978 |
| 10 | 3.57(3) | .. | F(26)a | [1+x,y,z | = | 1655.02] | | -102.45 | 35.45 | -0.01560 | 0.44819 | -0.64380 | -0.1315 | 10.6737 | -23.6056 |
| 11 | 3.599(14) | .. | C(37) | | | | Intra | 174.84 | 13.36 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 12 | 2.46 | << | H(35A) | | | | Intra | -176.07 | 75.28 | -0.01520 | 0.56570 | -0.63540 | -0.1281 | 13.4723 | -23.2976 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(33A)

| | | | | | | | |
|-------------------|-----------|-------------------|-----------|-------------------|-----------|-------------------|-----------|
| C(310) , <F(32A) | 37.9(10) | C(310) , <F(31A) | 34.9(9) | C(310) , C(36) | 34.8(5) | C(310) , F(36)b | 150.7(14) |
| C(310) , C(35) | 65.1(7) | C(310) , F(35)b | 147.8(19) | C(310) , C(320)b | 152.9(13) | C(310) , >F(51)c | 118.7(10) |
| C(310) , F(26)a | 86.9(12) | C(310) , C(37) | 23.2(6) | <F(32A) , <F(31A) | 59.8(9) | <F(32A) , C(36) | 61.8(8) |
| <F(32A) , F(36)b | 135.8(15) | <F(32A) , C(35) | 86.1(9) | <F(32A) , F(35)b | 169.9(11) | <F(32A) , C(320)b | 159.0(14) |
| <F(32A) , >F(51)c | 98.0(10) | <F(32A) , F(26)a | 72.0(10) | <F(32A) , C(37) | 54.4(7) | <F(31A) , C(36) | 61.2(7) |
| <F(31A) , F(36)b | 163.4(15) | <F(31A) , C(35) | 88.4(8) | <F(31A) , F(35)b | 120.2(14) | <F(31A) , C(320)b | 140.9(14) |
| <F(31A) , >F(51)c | 94.3(9) | <F(31A) , F(26)a | 121.8(9) | <F(31A) , C(37) | 50.1(6) | C(36) , F(36)b | 117.5(7) |
| C(36) , C(35) | 30.4(2) | C(36) , F(35)b | 127.9(10) | C(36) , C(320)b | 119.7(7) | C(36) , >F(51)c | 153.4(7) |
| C(36) , F(26)a | 68.7(6) | C(36) , C(37) | 11.92(17) | F(36)b , C(35) | 87.6(6) | F(36)b , F(35)b | 45.8(3) |
| F(36)b , C(320)b | 23.19(18) | F(36)b , >F(51)c | 89.0(4) | F(36)b , F(26)a | 68.2(6) | F(36)b , C(37) | 129.4(6) |
| C(35) , F(35)b | 104.0(7) | C(35) , C(320)b | 90.4(5) | C(35) , >F(51)c | 175.9(6) | C(35) , F(26)a | 56.4(4) |
| C(35) , C(37) | 42.2(2) | F(35)b , C(320)b | 24.16(14) | F(35)b , >F(51)c | 71.9(4) | F(35)b , F(26)a | 113.0(6) |
| F(35)b , C(37) | 134.5(9) | C(320)b , >F(51)c | 85.6(4) | C(320)b , F(26)a | 88.8(5) | C(320)b , C(37) | 130.4(6) |
| >F(51)c , F(26)a | 124.2(8) | >F(51)c , C(37) | 141.5(6) | F(26)a , C(37) | 76.4(4) | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(33B) [ARU = 1555.01] 0.02710 0.53030 -0.70270 0.2285 12.6292-25.7652

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|--------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.337(12) | -- | C(310) | | | | Intra | 136.21 | -5.16 | -0.08690 | 0.56898 | -0.70598 | -0.7326 | 13.5504 | -25.8855 |
| 2 | 2.104(15) | << | <F(31B) | | | | Intra | 99.16 | -10.34 | -0.01200 | 0.61610 | -0.71300 | -0.1012 | 14.6725 | -26.1429 |
| 3 | 2.123(16) | << | <F(32B) | | | | Intra | 161.58 | -35.96 | -0.16630 | 0.55310 | -0.73670 | -1.4019 | 13.1722 | -27.0118 |
| 4 | 2.375(13) | << | C(36) | | | | Intra | 151.51 | 27.22 | -0.19310 | 0.57260 | -0.67307 | -1.6279 | 13.6366 | -24.6788 |
| 5 | 2.854(13) | .< | F(36)b | [1+x,y,z | = | 1655.01] | | 8.58 | 35.16 | 0.30080 | 0.54491 | -0.65788 | 2.5358 | 12.9771 | -24.1218 |
| 6 | 2.860(14) | << | C(35) | | | | Intra | 143.16 | 55.62 | -0.12620 | 0.57096 | -0.63833 | -1.0639 | 13.5975 | -23.4050 |
| 7 | 2.936(14) | .< | F(26)a | [1+x,y,z | = | 1655.02] | | -100.43 | 47.36 | -0.01560 | 0.44819 | -0.64380 | -0.1315 | 10.6737 | -23.6056 |
| 8 | 3.226(12) | .. | F(24)a | [1+x,y,z | = | 1655.02] | | -95.02 | 7.25 | -0.00610 | 0.39642 | -0.69160 | -0.0514 | 9.4408 | -25.3582 |
| 9 | 3.419(13) | .. | C(220)a | [1+x,y,z | = | 1655.02] | | -84.90 | 27.81 | 0.05900 | 0.40384 | -0.65920 | 0.4974 | 9.6175 | -24.1702 |
| 10 | 3.451(14) | .. | F(43)c | [-1/2-x,1-y,-1/2+z | = | 2464.06] | | -94.42 | -44.20 | 0.00450 | 0.42671 | -0.76832 | 0.0379 | 10.1622 | -28.1712 |
| 11 | 3.558(12) | .. | C(37) | | | | Intra | 159.55 | 14.98 | -0.35490 | 0.58072 | -0.67762 | -2.9919 | 13.8300 | -24.8456 |
| 12 | 2.63 | .< | H(35A) | | | | Intra | 112.93 | 69.65 | -0.01520 | 0.56570 | -0.63540 | -0.1281 | 13.4723 | -23.2976 |
| 13 | 3.45 | .. | H(27A)a | [1+x,y,z | = | 1655.02] | | -55.31 | -8.13 | 0.25760 | 0.41240 | -0.71600 | 2.1716 | 9.8214 | -26.2529 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(33B)

| | | | | | | | |
|-------------------|-----------|------------------|-----------|-------------------|-----------|------------------|----------|
| C(310) , <F(31B) | 37.1(5) | C(310) , <F(32B) | 38.6(5) | C(310) , C(36) | 35.6(4) | C(310) , F(36)b | 123.3(7) |
| C(310) , C(35) | 61.1(5) | C(310) , F(26)a | 115.9(7) | C(310) , F(24)a | 129.1(7) | C(310) , C(220)a | 134.9(7) |
| C(310) , F(43)c | 113.0(7) | C(310) , C(37) | 30.7(4) | <F(31B) , <F(32B) | 61.7(6) | <F(31B) , C(36) | 63.1(5) |
| <F(31B) , F(36)b | 96.4(5) | <F(31B) , C(35) | 75.4(5) | <F(31B) , F(26)a | 139.5(7) | <F(31B) , F(24)a | 165.7(6) |
| <F(31B) , C(220)a | 162.1(7) | <F(31B) , F(43)c | 124.1(6) | <F(31B) , C(37) | 65.0(4) | <F(32B) , C(36) | 63.9(4) |
| <F(32B) , F(36)b | 158.1(6) | <F(32B) , C(35) | 92.9(5) | <F(32B) , F(26)a | 120.5(6) | <F(32B) , F(24)a | 105.1(5) |
| <F(32B) , C(220)a | 124.0(6) | <F(32B) , F(43)c | 74.4(5) | <F(32B) , C(37) | 51.0(3) | C(36) , F(36)b | 108.5(5) |
| C(36) , C(35) | 29.03(18) | C(36) , F(26)a | 81.4(4) | C(36) , F(24)a | 107.1(4) | C(36) , C(220)a | 102.8(4) |
| C(36) , F(43)c | 125.4(4) | C(36) , C(37) | 14.35(14) | F(36)b , C(35) | 81.3(4) | F(36)b , F(26)a | 75.9(3) |
| F(36)b , F(24)a | 96.8(4) | F(36)b , C(220)a | 77.0(3) | F(36)b , F(43)c | 122.2(4) | F(36)b , C(37) | 122.8(4) |
| C(35) , F(26)a | 64.1(3) | C(35) , F(24)a | 101.0(4) | C(35) , C(220)a | 87.1(4) | C(35) , F(43)c | 142.4(4) |
| C(35) , C(37) | 42.56(18) | F(26)a , F(24)a | 40.38(17) | F(26)a , C(220)a | 23.01(11) | F(26)a , F(43)c | 91.7(3) |
| F(26)a , C(37) | 85.6(3) | F(24)a , C(220)a | 22.69(10) | F(24)a , F(43)c | 51.45(19) | F(24)a , C(37) | 102.9(3) |
| C(220)a , F(43)c | 72.5(2) | C(220)a , C(37) | 104.4(3) | F(43)c , C(37) | 111.8(3) | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(51A) [ARU = 1555.03] -0.10500 0.93240 -0.23750 -0.8852 22.2053 -8.7082

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|--------------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.339(8) | -- | C(510) | | | | Intra | -88.34 | 38.41 | -0.10140 | 0.88836 | -0.21481 | -0.8548 | 21.1565 | -7.8762 |
| 2 | 0.814(18) | << | >F(51) | | | | Intra | 179.00 | 32.73 | -0.18620 | 0.93290 | -0.22550 | -1.5697 | 22.2172 | -8.2682 |
| 3 | 1.654(16) | << | >F(53) | | | | Intra | -64.16 | -5.78 | -0.01990 | 0.87020 | -0.24204 | -0.1678 | 20.7240 | -8.8746 |
| 4 | 2.120(15) | << | <F(53A) | | | | Intra | -71.34 | 1.98 | -0.02460 | 0.84810 | -0.23550 | -0.2074 | 20.1977 | -8.6348 |
| 5 | 2.148(16) | << | <F(52A) | | | | Intra | -127.93 | 28.55 | -0.24260 | 0.86990 | -0.20950 | -2.0452 | 20.7168 | -7.6815 |
| 6 | 2.347(9) | << | C(56) | | | | Intra | -41.64 | 61.21 | -0.00480 | 0.90086 | -0.18140 | -0.0405 | 21.4542 | -6.6512 |
| 7 | 2.454(13) | << | >F(52) | | | | Intra | -114.24 | 27.30 | -0.21120 | 0.84890 | -0.20680 | -1.7805 | 20.2167 | -7.5825 |
| 8 | 2.499(13) | << | >F(23)a | [1/2+x,3/2-y,-1-z | = | 3564.02] | | 60.60 | -15.72 | 0.03510 | 1.02040 | -0.25597 | 0.2959 | 24.3010 | -9.3854 |
| 9 | 3.019(14) | < | C(57) | | | | Intra | -15.12 | 40.34 | 0.15850 | 0.90719 | -0.18420 | 1.3362 | 21.6049 | -6.7539 |
| 10 | 3.353(8) | .. | C(55) | | | | Intra | -71.47 | 78.73 | -0.08030 | 0.90632 | -0.14781 | -0.6769 | 21.5842 | -5.4196 |
| 11 | 3.368(8) | .. | F(35)b | [1/2+x,3/2-y,-1-z | = | 3564.01] | | -107.61 | -63.72 | -0.15850 | 0.87273 | -0.31986 | -1.3362 | 20.7842 | -11.7280 |
| 12 | 3.487(8) | .. | F(45)d | [-x,1/2+y,-1/2-z | = | 4554.06] | | 70.00 | 41.82 | 0.00044 | 1.03493 | -0.17410 | 0.0037 | 24.6471 | -6.3836 |
| 13 | 3.540(11) | .. | F(42)c | [-1-x,1/2+y,-1/2-z | = | 4454.06] | | 123.33 | 25.72 | -0.31290 | 1.04430 | -0.19560 | -2.6378 | 24.8702 | -7.1719 |
| 14 | 2.85 | .. | H(37A)b | [1/2+x,3/2-y,-1-z | = | 3564.01] | | -11.52 | -51.82 | 0.10010 | 0.91760 | -0.29870 | 0.8439 | 21.8528 | -10.9521 |
| 15 | 2.97 | .. | H(57A) | | | | Intra | -14.76 | 22.08 | 0.21020 | 0.90300 | -0.20710 | 1.7720 | 21.5051 | -7.5935 |
| 16 | 3.51 | .. | H(55A) | | | | Intra | -134.75 | 72.79 | -0.19180 | 0.90140 | -0.14600 | -1.6169 | 21.4670 | -5.3532 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(51A)

| | | | | | | | |
|-------------------|-----------|-------------------|-----------|------------------|-----------|------------------|----------|
| C(510) , >F(51) | 72.2(8) | C(510) , >F(53) | 49.6(4) | C(510) , <F(53A) | 39.6(4) | C(510) , <F(52A) | 34.2(4) |
| C(510) , C(56) | 36.6(3) | C(510) , >F(52) | 24.3(4) | C(510) , >F(23)a | 144.5(9) | C(510) , C(57) | 54.9(5) |
| C(510) , C(55) | 40.9(3) | C(510) , F(35)b | 103.3(4) | C(510) , F(45)d | 97.4(4) | C(510) , F(42)c | 109.3(5) |
| >F(51) , >F(53) | 115.6(9) | >F(51) , <F(53A) | 105.3(9) | >F(51) , <F(52A) | 45.4(7) | >F(51) , C(56) | 80.4(9) |
| >F(51) , >F(52) | 57.1(7) | >F(51) , >F(23)a | 122.1(8) | >F(51) , C(57) | 105.8(10) | >F(51) , C(55) | 61.6(9) |
| >F(51) , F(35)b | 112.2(12) | >F(51) , F(45)d | 81.0(8) | >F(51) , F(42)c | 48.6(7) | >F(53) , <F(53A) | 10.6(4) |
| >F(53) , <F(52A) | 70.2(5) | >F(53) , C(56) | 69.2(4) | >F(53) , >F(52) | 58.6(5) | >F(53) , >F(23)a | 121.2(9) |
| >F(53) , C(57) | 64.4(5) | >F(53) , C(55) | 84.6(4) | >F(53) , F(35)b | 65.8(3) | >F(53) , F(45)d | 125.7(7) |
| >F(53) , F(42)c | 158.8(5) | <F(53A) , <F(52A) | 60.0(5) | <F(53A) , C(56) | 63.4(4) | <F(53A) , >F(52) | 48.2(4) |
| <F(53A) , >F(23)a | 130.7(8) | <F(53A) , C(57) | 63.5(4) | <F(53A) , C(55) | 76.8(4) | <F(53A) , F(35)b | 71.0(4) |
| <F(53A) , F(45)d | 124.0(5) | <F(53A) , F(42)c | 148.9(5) | <F(52A) , C(56) | 63.5(3) | <F(52A) , >F(52) | 12.2(4) |
| <F(52A) , >F(23)a | 165.0(6) | <F(52A) , C(57) | 87.1(4) | <F(52A) , C(55) | 55.7(3) | <F(52A) , F(35)b | 93.7(4) |
| <F(52A) , F(45)d | 107.7(4) | <F(52A) , F(42)c | 92.7(5) | C(56) , >F(52) | 58.0(3) | C(56) , >F(23)a | 109.6(5) |
| C(56) , C(57) | 26.39(19) | C(56) , C(55) | 19.76(13) | C(56) , F(35)b | 134.4(3) | C(56) , F(45)d | 63.1(2) |
| C(56) , F(42)c | 92.2(2) | >F(52) , >F(23)a | 167.5(5) | >F(52) , C(57) | 79.1(3) | >F(52) , C(55) | 54.7(2) |
| >F(52) , F(35)b | 91.2(3) | >F(52) , F(45)d | 110.8(3) | >F(52) , F(42)c | 103.3(5) | >F(23)a , C(57) | 89.7(5) |
| >F(23)a , C(55) | 113.1(4) | >F(23)a , F(35)b | 100.0(3) | >F(23)a , F(45)d | 58.2(2) | >F(23)a , F(42)c | 73.8(3) |
| C(57) , C(55) | 44.16(13) | C(57) , F(35)b | 126.5(4) | C(57) , F(45)d | 61.3(2) | C(57) , F(42)c | 103.5(2) |
| C(55) , F(35)b | 144.1(2) | C(55) , F(45)d | 57.32(13) | C(55) , F(42)c | 75.20(18) | F(35)b , F(45)d | 158.1(3) |
| F(35)b , F(42)c | 129.8(4) | F(45)d , F(42)c | 46.35(10) | | | | |

=====

3.6 Angstrom Coordination Sphere Around Atom I = F(52A) [ARU = 1555.03] -0.24260 0.86990 -0.20950 -2.0452 20.7168 -7.6815

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|-----------------|-----------|----------|-------|---------|--------|----------|---------|----------|---------|---------|---------|
| 1 | 1.284(8) | -- | C(510) | | | | Intra | 20.27 | -8.72 | -0.10140 | 0.88836 | -0.21481 | -0.8548 | 21.1565 | -7.8762 |
| 2 | 0.574(16) | << | >F(52) | | | | Intra | -62.11 | 9.92 | -0.21120 | 0.84890 | -0.20680 | -1.7805 | 20.2167 | -7.5825 |
| 3 | 1.680(16) | << | >F(51) | | | | Intra | 72.42 | -20.44 | -0.18620 | 0.93290 | -0.22550 | -1.5697 | 22.2172 | -8.2682 |
| 4 | 2.134(13) | << | <F(53A) | | | | Intra | -15.77 | -26.53 | -0.02460 | 0.84810 | -0.23550 | -0.2074 | 20.1977 | -8.6348 |
| 5 | 2.148(16) | << | <F(51A) | | | | Intra | 52.07 | -28.55 | -0.10500 | 0.93240 | -0.23750 | -0.8852 | 22.2053 | -8.7082 |
| 6 | 2.225(11) | << | >F(53) | | | | Intra | 0.22 | -32.44 | -0.01990 | 0.87020 | -0.24204 | -0.1678 | 20.7240 | -8.8746 |
| 7 | 2.372(9) | << | C(56) | | | | Intra | 20.19 | 25.75 | -0.00480 | 0.90086 | -0.18140 | -0.0405 | 21.4542 | -6.6512 |
| 8 | 2.782(11) | << | C(55) | | | | Intra | 32.37 | 54.39 | -0.08030 | 0.90632 | -0.14781 | -0.6769 | 21.5842 | -5.4196 |
| 9 | 3.003(10) | .. | F(55)a | [-1+x,y,z | = | 1455.03] | | 146.06 | 14.81 | -0.52830 | 0.93797 | -0.18857 | -4.4537 | 22.3379 | -6.9141 |
| 10 | 3.186(13) | .. | F(12) | [| = | 05] | | -108.59 | -45.33 | -0.32730 | 0.78075 | -0.27129 | -2.7592 | 18.5937 | -9.9471 |
| 11 | 3.195(13) | .. | F(64)b | [1/2+x,3/2-y,-z | = | 3565.04] | | -84.02 | 52.55 | -0.21860 | 0.78875 | -0.14032 | -1.8428 | 18.7842 | -5.1450 |
| 12 | 3.241(10) | .. | F(54)a | [-1+x,y,z | = | 1455.03] | | 174.68 | 47.08 | -0.50330 | 0.87850 | -0.14476 | -4.2429 | 20.9217 | -5.3078 |
| 13 | 2.48 | .< | H(55A) | | | | Intra | 60.28 | 69.64 | -0.19180 | 0.90140 | -0.14600 | -1.6169 | 21.4670 | -5.3532 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(52A)

| | | | | | | | |
|------------------|-----------|------------------|-----------|-------------------|-----------|------------------|-----------|
| C(510) , >F(52) | 84.1(13) | C(510) , >F(51) | 51.6(6) | C(510) , <F(53A) | 38.5(4) | C(510) , <F(51A) | 35.9(5) |
| C(510) , >F(53) | 30.1(4) | C(510) , C(56) | 34.5(3) | C(510) , C(55) | 63.9(4) | C(510) , F(55)a | 126.7(8) |
| C(510) , F(12) | 109.2(6) | C(510) , F(64)b | 105.6(6) | C(510) , F(54)a | 135.9(7) | >F(52) , >F(51) | 135.0(15) |
| >F(52) , <F(53A) | 57.9(12) | >F(52) , <F(51A) | 115.9(14) | >F(52) , >F(53) | 72.9(13) | >F(52) , C(56) | 78.8(13) |
| >F(52) , C(55) | 84.5(13) | >F(52) , F(55)a | 142.7(15) | >F(52) , F(12) | 69.3(14) | >F(52) , F(64)b | 46.2(12) |
| >F(52) , F(54)a | 104.0(14) | >F(51) , <F(53A) | 79.5(6) | >F(51) , <F(51A) | 20.2(5) | >F(51) , >F(53) | 64.6(6) |
| >F(51) , C(56) | 68.6(5) | >F(51) , C(55) | 82.3(6) | >F(51) , F(55)a | 80.5(6) | >F(51) , F(12) | 114.2(6) |
| >F(51) , F(64)b | 143.1(6) | >F(51) , F(54)a | 113.0(6) | <F(53A) , <F(51A) | 59.4(5) | <F(53A) , >F(53) | 15.1(5) |
| <F(53A) , C(56) | 62.7(3) | <F(53A) , C(55) | 90.9(4) | <F(53A) , F(55)a | 159.4(7) | <F(53A) , F(12) | 73.3(5) |
| <F(53A) , F(64)b | 98.8(5) | <F(53A) , F(54)a | 157.9(6) | <F(51A) , >F(53) | 44.4(5) | <F(51A) , C(56) | 62.3(4) |
| <F(51A) , C(55) | 84.7(4) | <F(51A) , F(55)a | 100.4(6) | <F(51A) , F(12) | 104.1(4) | <F(51A) , F(64)b | 139.8(5) |
| <F(51A) , F(54)a | 132.3(6) | >F(53) , C(56) | 61.2(3) | >F(53) , C(55) | 91.2(3) | >F(53) , F(55)a | 144.3(7) |
| >F(53) , F(12) | 79.0(4) | >F(53) , F(64)b | 112.0(5) | >F(53) , F(54)a | 164.8(5) | C(56) , C(55) | 30.02(15) |
| C(56) , F(55)a | 113.5(5) | C(56) , F(12) | 134.9(4) | C(56) , F(64)b | 77.9(3) | C(56) , F(54)a | 103.6(4) |
| C(55) , F(55)a | 91.1(3) | C(55) , F(12) | 153.7(5) | C(55) , F(64)b | 60.8(2) | C(55) , F(54)a | 73.6(3) |
| F(55)a , F(12) | 111.2(2) | F(55)a , F(64)b | 100.1(3) | F(55)a , F(54)a | 40.09(12) | F(12) , F(64)b | 100.1(4) |
| F(12) , F(54)a | 114.3(3) | F(64)b , F(54)a | 60.0(2) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(53A) [ARU = 1555.03] -0.02460 0.84810 -0.23550 -0.2074 20.1977 -8.6348

| Nr | d(I,J) To | Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|--------|--------------------------|------------|-------|---------|--------|----------|---------|----------|---------|---------|----------|
| 1 | 1.384(11) | -- | C(510) | | Intra | 124.03 | 33.25 | -0.10140 | 0.88836 | -0.21481 | -0.8548 | 21.1565 | -7.8762 |
| 2 | 0.580(18) | << | >F(53) | | Intra | 85.69 | -24.43 | -0.01990 | 0.87020 | -0.24204 | -0.1678 | 20.7240 | -8.8746 |
| 3 | 1.893(14) | << | >F(52) | | Intra | 179.31 | 33.78 | -0.21120 | 0.84890 | -0.20680 | -1.7805 | 20.2167 | -7.5825 |
| 4 | 2.120(15) | << | <F(51A) | | Intra | 108.66 | -1.98 | -0.10500 | 0.93240 | -0.23750 | -0.8852 | 22.2053 | -8.7082 |
| 5 | 2.134(13) | << | <F(52A) | | Intra | 164.23 | 26.53 | -0.24260 | 0.86990 | -0.20950 | -2.0452 | 20.7168 | -7.6815 |
| 6 | 2.354(11) | << | C(56) | | Intra | 82.43 | 57.42 | -0.00480 | 0.90086 | -0.18140 | -0.0405 | 21.4542 | -6.6512 |
| 7 | 2.464(14) | << | >F(51) | | Intra | 124.00 | 8.56 | -0.18620 | 0.93290 | -0.22550 | -1.5697 | 22.2172 | -8.2682 |
| 8 | 2.811(11) | << | C(57) | | Intra | 42.35 | 42.00 | 0.15850 | 0.90719 | -0.18420 | 1.3362 | 21.6049 | -6.7539 |
| 9 | 3.057(12) | .. | F(11) [| = 05] | | -110.46 | -7.44 | -0.15030 | 0.72885 | -0.24630 | -1.2671 | 17.3577 | -9.0308 |
| 10 | 3.226(13) | .. | >F(62A)b[1/2+x,3/2-y,-z | = 3565.04] | | -19.58 | 7.91 | 0.33250 | 0.80315 | -0.22340 | 2.8030 | 19.1272 | -8.1912 |
| 11 | 3.287(10) | .. | F(12) [| = 05] | | -147.85 | -23.53 | -0.32730 | 0.78075 | -0.27129 | -2.7592 | 18.5937 | -9.9471 |
| 12 | 3.345(11) | .. | F(35)a [1/2+x,3/2-y,-1-z | = 3564.01] | | 152.54 | -67.64 | -0.15850 | 0.87273 | -0.31986 | -1.3362 | 20.7842 | -11.7280 |
| 13 | 3.533(11) | .. | C(55) | | Intra | 108.71 | 65.52 | -0.08030 | 0.90632 | -0.14781 | -0.6769 | 21.5842 | -5.4196 |
| 14 | 3.572(11) | .. | C(110) [| = 05] | | -123.79 | -24.74 | -0.23860 | 0.73489 | -0.27627 | -2.0114 | 17.5016 | -10.1297 |
| 15 | 3.588(12) | .. | C(67)b [1/2+x,3/2-y,-z | = 3565.04] | | -65.76 | 44.00 | 0.10110 | 0.74928 | -0.16752 | 0.8523 | 17.8443 | -6.1423 |
| 16 | 2.59 | < | H(57A) | | Intra | 33.45 | 23.70 | 0.21020 | 0.90300 | -0.20710 | 1.7720 | 21.5051 | -7.5935 |
| 17 | 2.98 | .. | H(67A)b[1/2+x,3/2-y,-z | = 3565.04] | | -77.46 | 34.84 | 0.03850 | 0.74770 | -0.18900 | 0.3246 | 17.8066 | -6.9299 |
| 18 | 3.04 | .. | H(37A)a[1/2+x,3/2-y,-1-z | = 3564.01] | | 57.58 | -49.76 | 0.10010 | 0.91760 | -0.29870 | 0.8439 | 21.8528 | -10.9521 |
| 19 | 3.16 | .. | H(17A) [| = 05] | | -70.86 | -35.25 | 0.07590 | 0.74560 | -0.28530 | 0.6399 | 17.7566 | -10.4608 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(53A)

| | | | | | | | |
|--------------------|-----------|-------------------|-----------|--------------------|-----------|-------------------|----------|
| C(510) , >F(53) | 68.3(13) | C(510) , >F(52) | 45.5(4) | C(510) , <F(51A) | 38.1(4) | C(510) , <F(52A) | 35.3(4) |
| C(510) , C(56) | 37.0(3) | C(510) , >F(51) | 24.7(4) | C(510) , C(57) | 62.8(4) | C(510) , F(11) | 123.6(6) |
| C(510) , >F(62A)b | 126.3(6) | C(510) , F(12) | 101.2(5) | C(510) , F(35)a | 103.2(5) | C(510) , C(55) | 33.6(3) |
| C(510) , C(110) | 121.1(5) | C(510) , C(67)b | 102.2(5) | >F(53) , >F(52) | 106.1(14) | >F(53) , <F(51A) | 31.6(12) |
| >F(53) , <F(52A) | 91.3(14) | >F(53) , C(56) | 81.9(14) | >F(53) , >F(51) | 49.8(12) | >F(53) , C(57) | 77.6(13) |
| >F(53) , F(11) | 144.4(15) | >F(53) , >F(62A)b | 107.1(12) | >F(53) , F(12) | 109.3(13) | >F(53) , F(35)a | 58.8(13) |
| >F(53) , C(55) | 91.7(14) | >F(53) , C(110) | 123.1(14) | >F(53) , C(67)b | 149.6(14) | >F(52) , <F(51A) | 75.2(6) |
| >F(52) , <F(52A) | 14.9(5) | >F(52) , C(56) | 65.5(4) | >F(52) , >F(51) | 56.6(5) | >F(52) , C(57) | 94.6(5) |
| >F(52) , F(11) | 78.1(5) | >F(52) , >F(62A)b | 134.6(6) | >F(52) , F(12) | 65.3(4) | >F(52) , F(35)a | 103.4(5) |
| >F(52) , C(55) | 51.7(4) | >F(52) , C(110) | 79.7(4) | >F(52) , C(67)b | 82.3(5) | <F(51A) , <F(52A) | 60.7(6) |
| <F(51A) , C(56) | 63.0(4) | <F(51A) , >F(51) | 18.6(5) | <F(51A) , C(57) | 74.0(5) | <F(51A) , F(11) | 139.9(6) |
| <F(51A) , >F(62A)b | 128.1(6) | <F(51A) , F(12) | 101.5(5) | <F(51A) , F(35)a | 72.2(4) | <F(51A) , C(55) | 67.5(4) |
| <F(51A) , C(110) | 122.6(5) | <F(51A) , C(67)b | 137.7(5) | <F(52A) , C(56) | 63.6(4) | <F(52A) , >F(51) | 42.1(5) |
| <F(52A) , C(57) | 93.0(5) | <F(52A) , F(11) | 89.2(5) | <F(52A) , >F(62A)b | 145.4(6) | <F(52A) , F(12) | 68.2(4) |
| <F(52A) , F(35)a | 94.6(4) | <F(52A) , C(55) | 52.0(4) | <F(52A) , C(110) | 86.3(5) | <F(52A) , C(67)b | 95.9(5) |
| C(56) , >F(51) | 58.4(4) | C(56) , C(57) | 29.54(15) | C(56) , F(11) | 129.0(4) | C(56) , >F(62A)b | 89.7(3) |
| C(56) , F(12) | 130.7(4) | C(56) , F(35)a | 135.2(4) | C(56) , C(55) | 14.77(12) | C(56) , C(110) | 142.3(4) |
| C(56) , C(67)b | 75.2(3) | >F(51) , C(57) | 78.1(4) | >F(51) , F(11) | 126.1(4) | >F(51) , >F(62A)b | 140.2(5) |

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>F(51) , F(12)      91.7(4)  >F(51) , F(35)a    78.9(4)  >F(51) , C(55)     58.0(3)  >F(51) , C(110)    113.7(4)
>F(51) , C(67)b    126.7(5)  C(57) , F(11)     137.9(4)  C(57) , >F(62A)b  64.0(2)  C(57) , F(12)     159.7(4)
C(57) , F(35)a    135.8(4)  C(57) , C(55)     42.90(17) C(57) , C(110)    159.3(4)  C(57) , C(67)b     72.6(2)
F(11) , >F(62A)b   91.9(3)   F(11) , F(12)     39.28(14) F(11) , F(35)a    85.8(3)  F(11) , C(55)     115.9(3)
F(11) , C(110)    21.48(9)  F(11) , C(67)b    65.4(2)   >F(62A)b, F(12)   128.1(4)  >F(62A)b, F(35)a   120.0(3)
>F(62A)b, C(55)   97.4(3)   >F(62A)b, C(110)  106.2(3)  >F(62A)b, C(67)b  53.9(2)   F(12) , F(35)a    56.93(18)
F(12) , C(55)    116.9(3)  F(12) , C(110)    21.96(9)  F(12) , C(67)b    100.8(3)  F(35)a , C(55)    136.7(3)
F(35)a , C(110)   64.8(2)   F(35)a , C(67)b   149.0(4)  C(55) , C(110)    127.6(3)  C(55) , C(67)b    70.4(2)
C(110) , C(67)b   86.8(3)

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3.6 Angstrom Coordination Sphere Around Atom I = F(61) [ARU = 1555.04] -0.13100 0.78840 0.21920 -1.1044 18.7759 8.0372

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|--------------------|-----------|----------|-------|---------|--------|----------|---------|---------|---------|---------|---------|
| 1 | 1.196(9) | -- | C(610) | | | | Intra | 100.95 | -23.04 | -0.15580 | 0.74302 | 0.20643 | -1.3134 | 17.6952 | 7.5690 |
| 2 | 0.790(17) | << | >F(61A) | | | | Intra | 169.42 | 27.51 | -0.21270 | 0.78300 | 0.22915 | -1.7931 | 18.6473 | 8.4020 |
| 3 | 1.439(14) | << | >F(63A) | | | | Intra | -34.65 | -21.36 | -0.00020 | 0.75640 | 0.20490 | -0.0017 | 18.0138 | 7.5129 |
| 4 | 2.093(15) | << | <F(62) | | | | Intra | 121.74 | 9.99 | -0.25960 | 0.71480 | 0.22910 | -2.1885 | 17.0231 | 8.4002 |
| 5 | 2.125(16) | << | <F(63) | | | | Intra | -67.86 | -13.70 | -0.03870 | 0.70810 | 0.20547 | -0.3262 | 16.8635 | 7.5338 |
| 6 | 2.207(9) | << | >F(62A) | | | | Intra | -98.03 | 4.00 | -0.16750 | 0.69685 | 0.22340 | -1.4121 | 16.5956 | 8.1912 |
| 7 | 2.268(12) | << | C(66) | | | | Intra | 130.52 | -53.37 | -0.23530 | 0.74520 | 0.16956 | -1.9836 | 17.7471 | 6.2171 |
| 8 | 2.996(10) | .. | F(24)d | [-1-x,1/2+y,-1/2-z | = | 4454.02] | | 65.81 | -19.74 | 0.00610 | 0.89642 | 0.19160 | 0.0514 | 21.3484 | 7.0252 |
| 9 | 3.082(14) | < | C(67) | | | | Intra | 158.33 | -37.94 | -0.39890 | 0.75072 | 0.16752 | -3.3628 | 17.8785 | 6.1423 |
| 10 | 3.163(11) | < | C(65) | | | | Intra | -95.29 | -69.89 | -0.14290 | 0.74293 | 0.13821 | -1.2047 | 17.6930 | 5.0676 |
| 11 | 3.297(14) | .. | F(13)a | [1/2+x,3/2-y,-z | = | 3565.05] | | 11.02 | 40.39 | 0.16140 | 0.80855 | 0.27747 | 1.3606 | 19.2558 | 10.1737 |
| 12 | 3.363(10) | .. | F(41)c | [1/2+x,3/2-y,-z | = | 3565.06] | | 97.33 | 55.41 | -0.15990 | 0.86791 | 0.29470 | -1.3480 | 20.6695 | 10.8055 |
| 13 | 3.419(11) | .. | F(14)b | [-1/2+x,3/2-y,-z | = | 3465.05] | | -99.84 | 69.20 | -0.15560 | 0.73817 | 0.30636 | -1.3117 | 17.5797 | 11.2330 |
| 14 | 3.531(10) | .. | C(27)d | [-1-x,1/2+y,-1/2-z | = | 4454.02] | | 116.89 | -15.40 | -0.31360 | 0.91588 | 0.19363 | -2.6437 | 21.8119 | 7.0996 |
| 15 | 3.543(11) | .. | F(25)d | [-1-x,1/2+y,-1/2-z | = | 4454.02] | | 60.91 | -56.69 | -0.01879 | 0.85980 | 0.13844 | -0.1584 | 20.4763 | 5.0760 |
| 16 | 3.573(9) | .. | C(220)d | [-1-x,1/2+y,-1/2-z | = | 4454.02] | | 77.55 | -38.00 | -0.05900 | 0.90384 | 0.15920 | -0.4974 | 21.5251 | 5.8372 |
| 17 | 3.594(13) | .. | F(12)a | [1/2+x,3/2-y,-z | = | 3565.05] | | -32.75 | 32.10 | 0.17270 | 0.71925 | 0.27129 | 1.4559 | 17.1291 | 9.9471 |
| 18 | 3.12 | .. | H(67A) | | | | Intra | 162.85 | -20.79 | -0.46150 | 0.75230 | 0.18900 | -3.8905 | 17.9162 | 6.9299 |
| 19 | 3.14 | .. | H(27A)d | [-1-x,1/2+y,-1/2-z | = | 4454.02] | | 109.87 | -2.14 | -0.25760 | 0.91240 | 0.21600 | -2.1716 | 21.7290 | 7.9199 |
| 20 | 3.25 | .. | H(65A) | | | | Intra | -54.38 | -63.54 | -0.03100 | 0.73900 | 0.13990 | -0.2613 | 17.5994 | 5.1296 |
| 21 | 3.55 | .. | H(17A)b | [-1/2+x,3/2-y,-z | = | 3465.05] | | -161.86 | 42.99 | -0.42410 | 0.75440 | 0.28530 | -3.5752 | 17.9662 | 10.4608 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(61)

| | | | | | | | |
|-------------------|-----------|-------------------|-----------|------------------|-----------|-------------------|-----------|
| C(610) , >F(61A) | 83.2(10) | C(610) , >F(63A) | 60.9(6) | C(610) , <F(62) | 38.8(5) | C(610) , <F(63) | 32.7(5) |
| C(610) , >F(62A) | 27.2(3) | C(610) , C(66) | 37.7(4) | C(610) , F(24)d | 135.3(7) | C(610) , C(67) | 50.8(6) |
| C(610) , C(65) | 47.0(4) | C(610) , F(13)a | 121.1(8) | C(610) , F(41)c | 144.9(7) | C(610) , F(14)b | 92.3(5) |
| C(610) , C(27)d | 126.6(8) | C(610) , F(25)d | 98.8(6) | C(610) , C(220)d | 118.9(6) | C(610) , F(12)a | 85.3(6) |
| >F(61A) , >F(63A) | 138.6(10) | >F(61A) , <F(62) | 48.1(7) | >F(61A) , <F(63) | 106.4(9) | >F(61A) , >F(62A) | 71.7(8) |
| >F(61A) , C(66) | 87.6(11) | >F(61A) , F(24)d | 129.2(9) | >F(61A) , C(67) | 66.3(10) | >F(61A) , C(65) | 110.5(11) |
| >F(61A) , F(13)a | 112.1(10) | >F(61A) , F(41)c | 69.4(8) | >F(61A) , F(14)b | 57.2(9) | >F(61A) , C(27)d | 83.3(9) |
| >F(61A) , F(25)d | 134.2(11) | >F(61A) , C(220)d | 123.9(10) | >F(61A) , F(12)a | 107.5(10) | >F(63A) , <F(62) | 91.0(5) |
| >F(63A) , <F(63) | 32.5(4) | >F(63A) , >F(62A) | 67.0(4) | >F(63A) , C(66) | 76.4(4) | >F(63A) , F(24)d | 92.1(6) |
| >F(63A) , C(67) | 100.6(5) | >F(63A) , C(65) | 60.1(4) | >F(63A) , F(13)a | 75.0(6) | >F(63A) , F(41)c | 130.8(7) |
| >F(63A) , F(14)b | 101.6(5) | >F(63A) , C(27)d | 133.8(6) | >F(63A) , F(25)d | 75.2(5) | >F(63A) , C(220)d | 93.0(6) |
| >F(63A) , F(12)a | 53.5(4) | <F(62) , <F(63) | 58.5(4) | <F(62) , >F(62A) | 24.3(4) | <F(62) , C(66) | 63.8(4) |
| <F(62) , F(24)d | 167.8(7) | <F(62) , C(67) | 58.9(4) | <F(62) , C(65) | 81.9(4) | <F(62) , F(13)a | 113.4(5) |
| <F(62) , F(41)c | 106.9(5) | <F(62) , F(14)b | 60.9(3) | <F(62) , C(27)d | 122.7(7) | <F(62) , F(25)d | 133.3(5) |
| <F(62) , C(220)d | 147.1(6) | <F(62) , F(12)a | 83.9(4) | <F(63) , >F(62A) | 34.8(4) | <F(63) , C(66) | 62.9(3) |
| <F(63) , F(24)d | 123.5(6) | <F(63) , C(67) | 82.0(4) | <F(63) , C(65) | 58.7(3) | <F(63) , F(13)a | 90.6(5) |

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<F(63) , F(41)c 136.7(5) <F(63) , F(14)b 85.9(3) <F(63) , C(27)d 150.5(5) <F(63) , F(25)d 97.8(5)
<F(63) , C(220)d 119.0(5) <F(63) , F(12)a 56.8(4) >F(62A) , C(66) 63.5(3) >F(62A) , F(24)d 157.7(6)
>F(62A) , C(67) 69.7(4) >F(62A) , C(65) 73.9(3) >F(62A) , F(13)a 101.7(5) >F(62A) , F(41)c 119.3(4)
>F(62A) , F(14)b 65.2(3) >F(62A) , C(27)d 143.8(7) >F(62A) , F(25)d 124.7(4) >F(62A) , C(220)d 145.8(5)
>F(62A) , F(12)a 67.0(4) C(66) , F(24)d 105.5(4) C(66) , C(67) 24.55(19) C(66) , C(65) 22.91(15)
C(66) , F(13)a 151.1(5) C(66) , F(41)c 152.6(6) C(66) , F(14)b 124.6(4) C(66) , C(27)d 90.5(4)
C(66) , F(25)d 69.6(3) C(66) , C(220)d 85.5(3) C(66) , F(12)a 119.7(3) F(24)d , C(67) 109.0(3)
F(24)d , C(65) 89.4(3) F(24)d , F(13)a 78.8(3) F(24)d , F(41)c 79.8(2) F(24)d , F(14)b 129.8(4)
F(24)d , C(27)d 48.72(13) F(24)d , F(25)d 37.13(13) F(24)d , C(220)d 20.92(9) F(24)d , F(12)a 107.4(4)
C(67) , C(65) 45.54(18) C(67) , F(13)a 171.4(3) C(67) , F(41)c 128.1(5) C(67) , F(14)b 115.4(4)
C(67) , C(27)d 76.6(3) C(67) , F(25)d 79.7(3) C(67) , C(220)d 88.3(3) C(67) , F(12)a 135.7(2)
C(65) , F(13)a 133.0(5) C(65) , F(41)c 164.5(3) C(65) , F(14)b 139.1(2) C(65) , C(27)d 91.8(3)
C(65) , F(25)d 52.27(17) C(65) , C(220)d 72.0(2) C(65) , F(12)a 111.4(3) F(13)a , F(41)c 55.86(19)
F(13)a , F(14)b 59.4(2) F(13)a , C(27)d 111.9(2) F(13)a , F(25)d 105.8(4) F(13)a , C(220)d 99.2(3)
F(13)a , F(12)a 35.87(15) F(41)c , F(14)b 54.77(18) F(41)c , C(27)d 72.71(18) F(41)c , F(25)d 115.9(2)
F(41)c , C(220)d 94.93(19) F(41)c , F(12)a 82.7(3) F(14)b , C(27)d 121.5(3) F(14)b , F(25)d 164.9(4)
F(14)b , C(220)d 148.8(3) F(14)b , F(12)a 52.12(17) C(27)d , F(25)d 58.79(15) C(27)d , C(220)d 41.32(11)
C(27)d , F(12)a 147.8(3) F(25)d , C(220)d 21.69(8) F(25)d , F(12)a 118.3(4) C(220)d , F(12)a 124.0(4)
=====

```

3.6 Angstrom Coordination Sphere Around Atom I = F(62) [ARU = 1555.04] -0.25960 0.71480 0.22910 -2.1885 17.0231 8.4002

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|------------------|-----------|----------|-------|---------|--------|----------|---------|---------|---------|---------|---------|
| 1 | 1.381(10) | -- | C(610) | | | | Intra | 37.53 | -36.99 | -0.15580 | 0.74302 | 0.20643 | -1.3134 | 17.6952 | 7.5690 |
| 2 | 0.911(13) | << | >F(62A) | | | | Intra | -28.84 | -13.27 | -0.16750 | 0.69685 | 0.22340 | -1.4121 | 16.5956 | 8.1912 |
| 3 | 1.672(14) | << | >F(61A) | | | | Intra | 76.32 | 0.06 | -0.21270 | 0.78300 | 0.22915 | -1.7931 | 18.6473 | 8.4020 |
| 4 | 2.060(13) | << | <F(63) | | | | Intra | -4.90 | -24.87 | -0.03870 | 0.70810 | 0.20547 | -0.3262 | 16.8635 | 7.5338 |
| 5 | 2.093(15) | << | <F(61) | | | | Intra | 58.26 | -9.99 | -0.13100 | 0.78840 | 0.21920 | -1.1044 | 18.7759 | 8.0372 |
| 6 | 2.309(8) | << | C(66) | | | | Intra | 74.20 | -70.98 | -0.23530 | 0.74520 | 0.16956 | -1.9836 | 17.7471 | 6.2171 |
| 7 | 2.560(11) | << | >F(63A) | | | | Intra | 24.37 | -20.28 | -0.00020 | 0.75640 | 0.20490 | -0.0017 | 18.0138 | 7.5129 |
| 8 | 2.685(9) | << | C(67) | | | | Intra | 143.93 | -57.24 | -0.39890 | 0.75072 | 0.16752 | -3.3628 | 17.8785 | 6.1423 |
| 9 | 3.017(8) | .. | F(14)a | [-1/2+x,3/2-y,-z | = | 3465.05] | | 32.41 | 69.87 | -0.15560 | 0.73817 | 0.30636 | -1.3117 | 17.5797 | 11.2330 |
| 10 | 3.023(15) | .. | >F(53)b | [-1/2+x,3/2-y,-z | = | 3465.03] | | -137.31 | 9.03 | -0.51990 | 0.62980 | 0.24204 | -4.3829 | 14.9988 | 8.8746 |
| 11 | 3.410(11) | .. | C(57)b | [-1/2+x,3/2-y,-z | = | 3465.03] | | -103.37 | -28.87 | -0.34150 | 0.59281 | 0.18420 | -2.8789 | 14.1179 | 6.7539 |
| 12 | 3.539(8) | .. | C(65) | | | | Intra | 34.25 | -70.35 | -0.14290 | 0.74293 | 0.13821 | -1.2047 | 17.6930 | 5.0676 |
| 13 | 3.554(9) | .. | C(17)a | [-1/2+x,3/2-y,-z | = | 3465.05] | | 153.01 | 54.66 | -0.47690 | 0.75397 | 0.30817 | -4.0204 | 17.9559 | 11.2994 |
| 14 | 2.42 | << | H(67A) | | | | Intra | 152.31 | -37.41 | -0.46150 | 0.75230 | 0.18900 | -3.8905 | 17.9162 | 6.9299 |
| 15 | 2.66 | < | H(17A)a | [-1/2+x,3/2-y,-z | = | 3465.05] | | 145.78 | 50.86 | -0.42410 | 0.75440 | 0.28530 | -3.5752 | 17.9662 | 10.4608 |
| 16 | 2.93 | .. | H(57A)b | [-1/2+x,3/2-y,-z | = | 3465.03] | | -95.19 | -15.98 | -0.28980 | 0.59700 | 0.20710 | -2.4431 | 14.2177 | 7.5935 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(62)

| | | | | | | | |
|-------------------|----------|-------------------|-----------|-------------------|-----------|-------------------|-----------|
| C(610) , >F(62A) | 63.3(6) | C(610) , >F(61A) | 51.6(5) | C(610) , <F(63) | 38.0(5) | C(610) , <F(61) | 32.9(4) |
| C(610) , C(66) | 39.0(2) | C(610) , >F(63A) | 20.3(3) | C(610) , C(67) | 67.4(3) | C(610) , F(14)a | 106.9(5) |
| C(610) , >F(53)b | 151.7(5) | C(610) , C(57)b | 104.6(5) | C(610) , C(65) | 33.4(3) | C(610) , C(17)a | 133.6(6) |
| >F(62A) , >F(61A) | 104.8(9) | >F(62A) , <F(63) | 25.4(6) | >F(62A) , <F(61) | 84.9(9) | >F(62A) , C(66) | 81.6(6) |
| >F(62A) , >F(63A) | 51.2(7) | >F(62A) , C(67) | 109.2(6) | >F(62A) , F(14)a | 93.1(7) | >F(62A) , >F(53)b | 109.9(9) |
| >F(62A) , C(57)b | 70.2(8) | >F(62A) , C(65) | 68.6(6) | >F(62A) , C(17)a | 138.6(7) | >F(61A) , <F(63) | 82.1(6) |
| >F(61A) , <F(61) | 20.6(4) | >F(61A) , C(66) | 71.1(4) | >F(61A) , >F(63A) | 54.7(4) | >F(61A) , C(67) | 78.2(4) |
| >F(61A) , F(14)a | 75.6(4) | >F(61A) , >F(53)b | 145.3(6) | >F(61A) , C(57)b | 151.2(4) | >F(61A) , C(65) | 75.6(3) |
| >F(61A) , C(17)a | 82.3(4) | <F(63) , <F(61) | 61.6(6) | <F(63) , C(66) | 63.0(3) | <F(63) , >F(63A) | 27.4(4) |
| <F(63) , C(67) | 93.8(4) | <F(63) , F(14)a | 98.4(4) | <F(63) , >F(53)b | 132.1(7) | <F(63) , C(57)b | 85.1(5) |
| <F(63) , C(65) | 50.8(3) | <F(63) , C(17)a | 146.0(4) | <F(61) , C(66) | 61.8(4) | <F(61) , >F(63A) | 34.2(4) |
| <F(61) , C(67) | 79.3(5) | <F(61) , F(14)a | 81.8(4) | <F(61) , >F(53)b | 164.6(7) | <F(61) , C(57)b | 137.3(4) |
| <F(61) , C(65) | 62.2(4) | <F(61) , C(17)a | 100.9(5) | C(66) , >F(63A) | 58.3(2) | C(66) , C(67) | 31.11(13) |
| C(66) , F(14)a | 143.5(5) | C(66) , >F(53)b | 115.0(4) | C(66) , C(57)b | 80.1(3) | C(66) , C(65) | 13.00(12) |
| C(66) , C(17)a | 137.3(4) | >F(63A) , C(67) | 87.6(3) | >F(63A) , F(14)a | 90.3(3) | >F(63A) , >F(53)b | 159.0(5) |
| >F(63A) , C(57)b | 109.6(3) | >F(63A) , C(65) | 50.41(16) | >F(63A) , C(17)a | 128.4(4) | C(67) , F(14)a | 149.1(5) |
| C(67) , >F(53)b | 91.6(3) | C(67) , C(57)b | 77.1(2) | C(67) , C(65) | 43.06(13) | C(67) , C(17)a | 112.1(3) |
| F(14)a , >F(53)b | 100.8(3) | F(14)a , C(57)b | 132.0(4) | F(14)a , C(65) | 140.2(3) | F(14)a , C(17)a | 48.35(13) |
| >F(53)b , C(57)b | 50.1(3) | >F(53)b , C(65) | 118.5(3) | >F(53)b , C(17)a | 71.0(3) | C(57)b , C(65) | 76.29(18) |
| C(57)b , C(17)a | 120.9(3) | C(65) , C(17)a | 149.5(4) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = F(63) [ARU = 1555.04] -0.03870 0.70810 0.20547 -0.3262 16.8635 7.5338

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|-----------|----|---------|------------------|-----------|----------|-------|---------|--------|----------|---------|---------|---------|---------|--------|
| 1 | 1.291(12) | -- | C(610) | | | | Intra | 139.89 | 1.56 | -0.15580 | 0.74302 | 0.20643 | -1.3134 | 17.6952 | 7.5690 |
| 2 | 1.195(16) | << | >F(63A) | | | | Intra | 74.24 | -1.00 | -0.00020 | 0.75640 | 0.20490 | -0.0017 | 18.0138 | 7.5129 |
| 3 | 1.297(13) | << | >F(62A) | | | | Intra | -166.14 | 30.45 | -0.16750 | 0.69685 | 0.22340 | -1.4121 | 16.5956 | 8.1912 |
| 4 | 2.060(13) | << | <F(62) | | | | Intra | 175.10 | 24.87 | -0.25960 | 0.71480 | 0.22910 | -2.1885 | 17.0231 | 8.4002 |
| 5 | 2.125(16) | << | <F(61) | | | | Intra | 112.14 | 13.70 | -0.13100 | 0.78840 | 0.21920 | -1.1044 | 18.7759 | 8.0372 |
| 6 | 2.294(10) | << | C(66) | | | | Intra | 151.94 | -35.03 | -0.23530 | 0.74520 | 0.16956 | -1.9836 | 17.7471 | 6.2171 |
| 7 | 2.467(14) | << | >F(61A) | | | | Intra | 129.43 | 20.60 | -0.21270 | 0.78300 | 0.22915 | -1.7931 | 18.6473 | 8.4020 |
| 8 | 2.746(8) | << | C(65) | | | | Intra | 136.64 | -63.90 | -0.14290 | 0.74293 | 0.13821 | -1.2047 | 17.6930 | 5.0676 |
| 9 | 3.012(8) | .. | F(12)a | [1/2+x,3/2-y,-z | = | 3565.05] | | 8.47 | 53.25 | 0.17270 | 0.71925 | 0.27129 | 1.4559 | 17.1291 | 9.9471 |
| 10 | 3.049(11) | .. | F(54)c | [-1/2+x,3/2-y,-z | = | 3465.03] | | -81.77 | -46.89 | -0.00330 | 0.62150 | 0.14476 | -0.0278 | 14.8011 | 5.3078 |
| 11 | 3.077(15) | .. | >F(52)b | [1/2+x,3/2-y,-z | = | 3565.03] | | -26.18 | 0.91 | 0.28880 | 0.65110 | 0.20680 | 2.4346 | 15.5061 | 7.5825 |
| 12 | 3.491(10) | .. | C(67) | | | | Intra | 161.52 | -23.49 | -0.39890 | 0.75072 | 0.16752 | -3.3628 | 17.8785 | 6.1423 |
| 13 | 3.535(14) | .. | F(55)c | [-1/2+x,3/2-y,-z | = | 3465.03] | | -88.56 | -10.10 | -0.02830 | 0.56203 | 0.18857 | -0.2386 | 13.3849 | 6.9141 |
| 14 | 2.52 | .< | H(65A) | | | | Intra | 84.96 | -72.92 | -0.03100 | 0.73900 | 0.13990 | -0.2613 | 17.5994 | 5.1296 |
| 15 | 3.39 | .. | H(57A)c | [-1/2+x,3/2-y,-z | = | 3465.03] | | -128.66 | 1.01 | -0.28980 | 0.59700 | 0.20710 | -2.4431 | 14.2177 | 7.5935 |

Angles (Degrees) At1...V...At2 with Vertex V = <F(63)

| | | | | | | | |
|-------------------|-----------|------------------|----------|-------------------|-----------|------------------|-----------|
| C(610) , >F(63A) | 65.7(7) | C(610) , >F(62A) | 58.6(5) | C(610) , <F(62) | 41.2(4) | C(610) , <F(61) | 30.0(5) |
| C(610) , C(66) | 38.3(3) | C(610) , >F(61A) | 21.6(3) | C(610) , C(65) | 65.5(4) | C(610) , F(12)a | 112.0(5) |
| C(610) , F(54)c | 122.0(5) | C(610) , >F(52)b | 165.9(8) | C(610) , C(67) | 32.7(3) | C(610) , F(55)c | 131.1(7) |
| >F(63A) , >F(62A) | 115.8(10) | >F(63A) , <F(62) | 100.3(8) | >F(63A) , <F(61) | 40.3(6) | >F(63A) , C(66) | 79.4(6) |
| >F(63A) , >F(61A) | 58.1(6) | >F(63A) , C(65) | 77.3(5) | >F(63A) , F(12)a | 76.6(4) | >F(63A) , F(54)c | 127.7(5) |
| >F(63A) , >F(52)b | 100.4(6) | >F(63A) , C(67) | 87.1(6) | >F(63A) , F(55)c | 159.6(6) | >F(62A) , <F(62) | 17.5(5) |
| >F(62A) , <F(61) | 76.1(7) | >F(62A) , C(66) | 76.5(5) | >F(62A) , >F(61A) | 58.2(5) | >F(62A) , C(65) | 104.5(6) |
| >F(62A) , F(12)a | 96.2(4) | >F(62A) , F(54)c | 108.2(7) | >F(62A) , >F(52)b | 130.7(8) | >F(62A) , C(67) | 62.2(5) |
| >F(62A) , F(55)c | 84.6(7) | <F(62) , <F(61) | 60.0(6) | <F(62) , C(66) | 63.8(4) | <F(62) , >F(61A) | 42.2(4) |
| <F(62) , C(65) | 93.7(4) | <F(62) , F(12)a | 101.0(3) | <F(62) , F(54)c | 116.6(5) | <F(62) , >F(52)b | 147.0(6) |
| <F(62) , C(67) | 50.1(3) | <F(62) , F(55)c | 99.9(6) | <F(61) , C(66) | 61.6(5) | <F(61) , >F(61A) | 17.9(4) |
| <F(61) , C(65) | 79.9(5) | <F(61) , F(12)a | 87.0(5) | <F(61) , F(54)c | 144.8(5) | <F(61) , >F(52)b | 136.2(7) |
| <F(61) , C(67) | 60.9(5) | <F(61) , F(55)c | 159.4(6) | C(66) , >F(61A) | 59.6(3) | C(66) , C(65) | 30.35(12) |
| C(66) , F(12)a | 148.6(6) | C(66) , F(54)c | 85.0(2) | C(66) , >F(52)b | 145.8(3) | C(66) , C(67) | 14.23(12) |
| C(66) , F(55)c | 107.2(4) | >F(61A) , C(65) | 84.7(4) | >F(61A) , F(12)a | 90.4(3) | >F(61A) , F(54)c | 143.5(4) |
| >F(61A) , >F(52)b | 147.9(5) | >F(61A) , C(67) | 54.1(3) | >F(61A) , F(55)c | 142.0(4) | C(65) , F(12)a | 151.9(5) |
| C(65) , F(54)c | 65.17(17) | C(65) , >F(52)b | 115.8(3) | C(65) , C(67) | 43.62(16) | C(65) , F(55)c | 98.5(3) |
| F(12)a , F(54)c | 125.9(4) | F(12)a , >F(52)b | 59.7(2) | F(12)a , C(67) | 144.0(4) | F(12)a , F(55)c | 102.3(3) |
| F(54)c , >F(52)b | 68.0(3) | F(54)c , C(67) | 89.5(2) | F(54)c , F(55)c | 37.24(16) | >F(52)b , C(67) | 156.2(3) |
| >F(52)b , F(55)c | 63.0(3) | C(67) , F(55)c | 103.8(3) | | | | |

=====
Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6
=====

van der Waals (or ion) Radii used in the Analysis

=====
C H F N S

1.70 1.20 1.47 1.55 1.80

:: Grid: X-Axis Step = 0.0208 = Points 48, Angstrom Step = 0.18
:: Grid: Z-Axis Step = 0.0056 = Points 180, Angstrom Step = 0.20
:: Grid: Y-Axis Step = 0.0083 = Points 120, Angstrom Step = 0.20

:: Unit cell Contains NO Residual Solvent Accessible Void.

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

Report Expected Number of Independent Reflections for given Symmetry and Resolution.

:: Hmax = 12 Kmax = 34 Lmax= 52 , Sorting Order : Fast H, Medium K, Slow L

:: Actual Theta-Max: 30.508 Deg. (Applied Theta Limit: 30.508 Deg.)

Space Group H-M: P212121 Laue: mmm
 Space Group Hall: P 2ac 2ab [Schoenflies: D2^4]
 Lattice Type: oP, Acentric, Orthorhombic, Multiplicity: 4(4), No: 19

CHIRAL - See P.G. Jones, Acta Cryst. (1986), A42, 57.

Nr ***** Symmetry Operation(s) *****

| | | | |
|---|-----------|-----------|---------|
| 1 | H , | K , | L |
| 2 | 1/2 - H , | - K , | 1/2 + L |
| 3 | 1/2 + H , | 1/2 - K , | - L |
| 4 | - H , | 1/2 + K , | 1/2 - L |

:: Number of Independent Type H, K, L Reflections = 12300

:: Number of Independent Type -H,-K,-L Reflections = 10136

Table 0 - Crystal Data and Details of the Structure Determination
for: hmimcf3051P 21 21 21 R = 0.04

Crystal Data

| | |
|--------------------|---------------------------------|
| Formula | C11 H6 F6 N2 S |
| Formula Weight | 312.25 |
| Crystal System | orthorhombic |
| Space group | P212121 (No. 19) |
| a, b, c [Angstrom] | 8.4302(5) 23.8152(15) 36.666(2) |
| V [Ang**3] | 7361.3(8) |
| Z | 24 |
| D(calc) [g/cm**3] | 1.691 |
| Mu(MoKa) [/mm] | 0.329 |
| F(000) | 3744 |
| Crystal Size [mm] | 0.07 x 0.18 x 0.66 |

Data Collection

| | |
|----------------------------------|-----------------------------|
| Temperature (K) | 130 |
| Radiation [Angstrom] | MoKa 0.71073 |
| Theta Min-Max [Deg] | 1.4, 30.5 |
| Dataset | -12: 12 ; -34: 34 ; -52: 52 |
| Tot., Uniq. Data, R(int) | 117976, 22429, 0.026 |
| Observed Data [I > 2.0 sigma(I)] | 21428 |

Refinement

| | |
|--|----------------------|
| Nref, Npar | 22429, 1247 |
| R, wR2, S | 0.0358, 0.0882, 1.08 |
| w = $\frac{1}{\sigma^2(F_o^2) + (0.0420P)^2 + 3.1799P}$ WHERE $P = \frac{(F_o^2 + 2F_c^2)}{3}$ | |
| Max. and Av. Shift/Error | 0.00, 0.00 |
| Flack x | 0.34(4) |
| Min. and Max. Resd. Dens. [e/Ang^3] | -0.31, 0.45 |

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***** N O T I C E *****

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- PLATON Reference : Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.
 Spek, A.L. (2009). Acta Cryst. D65, 148-155.

- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow

- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)

- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.

- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.

- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@uu.nl

- Recent versions of PLATON may be obtained from <http://www.platonsoft.nl/xraysoft>

- More INFO can be found on <http://http://www.platonsoft.nl/>

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Summary and Remarks : N = NOTE, W = WARNING, E = ERROR
=====

W: NOMOVE option used.

:: >>> WARNING: 'CONNECTED INPUT SET' is assumed to be TRUE

:: >>> The Network Analysis may be INCORRECT when this assumption is FALSE

N: DISORDERED structure - ATOMS with Pop. .LT. 1.0 are not moved or as a group.

W: Number of unusual anisotropic displacement parameters 7
=====

:: Input Xtal Data from File hmimcf30514.cif - Data Type CIF13

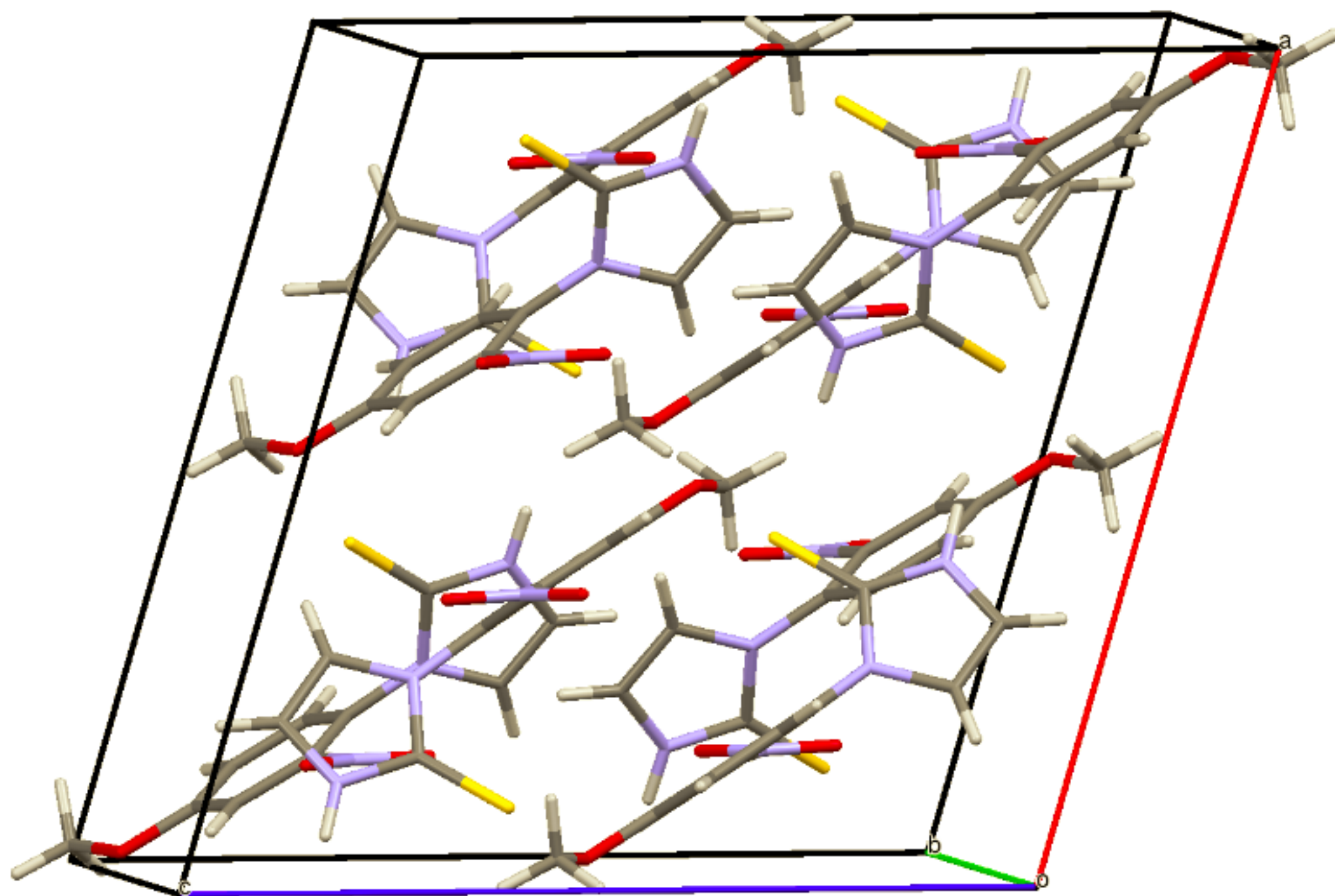
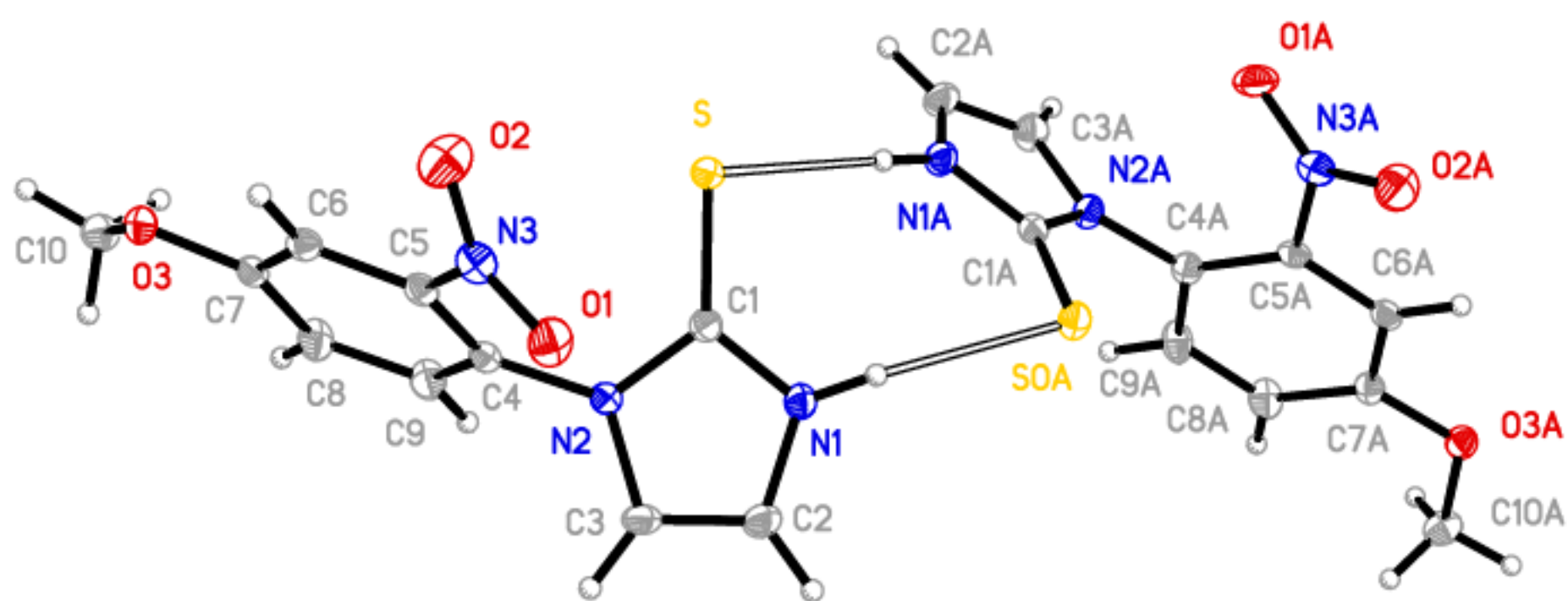
:: NORMAL END of PLATON : 231 Pages on:

:: hmimcf30514.lis (ASCII, 132 Characters Wide)

:: hmimcf30514.lps (PostScript Version of .lis)

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Hmim^{ArOMe,NO₂}



=====
 Analysis of Short Intra- and Inter-molecular Contacts , $d(I-J) < R(I) + R(J) + \text{Tolr}$, With Tolr = 0.2 Ang. ($X - I \dots J$) > 100. Deg.

Contact Radii : C H N O S
 (Angstrom) 1.70 1.20 1.55 1.52 1.80

Default Contact Radii are those given by A.Bondi, J.Phys.Chem. (1964),68,441. (or Coval. Rad. + 0.8 Ang. when not given)

* WARNING * : no Far-Reaching Conclusions should be drawn based on the Default Radii Assigned to Metals

Short "INTRA" Distances between two Atoms that are Separated by less than 4 Bonds are NOT Listed (Except for Potential D/A Contacts)

| At(I)[1555.01] | At(J) | [ARU(J)] | D(I-J) | SumRad | Del | Type | X(I) | Y(I) | Z(I) | X(J) | Y(J) | Z(J) | X | X - I...J |
|----------------|-------|------------|------------|------------|------|-------|-------|--------|--------|--------|---------|--------|--------|-------------------------------------|
| S | | N(3) | [] | 3.481(3) | 3.35 | 0.13 | Intra | 0.1016 | 0.9788 | 0.6474 | 0.3582 | 0.9144 | 0.7135 | |
| S | | C(4) | [] | 3.220(3)<< | 3.50 | -0.28 | Intra | 0.1016 | 0.9788 | 0.6474 | 0.3130 | 1.1059 | 0.7193 | |
| S | | C(5) | [] | 3.516(3) | 3.50 | 0.02 | Intra | 0.1016 | 0.9788 | 0.6474 | 0.3609 | 1.0256 | 0.6800 | |
| S | | H(1) | [] | 2.92(3) < | 3.00 | -0.08 | Intra | 0.1016 | 0.9788 | 0.6474 | 0.0680 | 1.0150 | 0.8470 | |
| S | | N(1) | [2556.01] | 3.292(3) < | 3.35 | -0.06 | | 0.1016 | 0.9788 | 0.6474 | -0.1304 | 1.0370 | 0.6524 | |
| S | | H(1) | [2556.01] | 2.40(3)<< | 3.00 | -0.60 | | 0.1016 | 0.9788 | 0.6474 | -0.0680 | 1.0150 | 0.6530 | |
| S | | H(2A) | [4574.01] | 2.93 < | 3.00 | -0.07 | | 0.1016 | 0.9788 | 0.6474 | 0.1966 | 0.9010 | 0.4941 | C(1) 127 |
| S | | H(10B) | [5445.01] | 2.79<< | 3.00 | -0.21 | | 0.1016 | 0.9788 | 0.6474 | 0.0041 | 0.8192 | 0.5141 | C(1) 157 |
| S | | C(10) | [7576.01] | 3.567(3) | 3.50 | 0.07 | | 0.1016 | 0.9788 | 0.6474 | 0.0289 | 1.2334 | 0.5375 | |
| S | | H(10C) | [7576.01] | 3.16 | 3.00 | 0.16 | | 0.1016 | 0.9788 | 0.6474 | 0.1002 | 1.2139 | 0.5674 | |
| O(1) | | N(2) | [] | 2.738(3)<< | 3.07 | -0.33 | Intra | 0.3541 | 0.8983 | 0.8008 | 0.2527 | 1.0867 | 0.7875 | |
| O(1) | | C(1) | [] | 3.082(3) < | 3.22 | -0.14 | Intra | 0.3541 | 0.8983 | 0.8008 | 0.1611 | 1.0350 | 0.7619 | |
| O(1) | | C(3) | [] | 3.327(3) | 3.22 | 0.11 | Intra | 0.3541 | 0.8983 | 0.8008 | 0.2772 | 1.1186 | 0.8901 | N(3) 108.87(16) |
| O(1) | | C(4) | [] | 2.841(3)<< | 3.22 | -0.38 | Intra | 0.3541 | 0.8983 | 0.8008 | 0.3130 | 1.1059 | 0.7193 | |
| O(1) | | O(3) | [4575.01] | 2.975(3) < | 3.04 | -0.07 | | 0.3541 | 0.8983 | 0.8008 | 0.4768 | 0.8365 | 1.0099 | N(3) 143.60(17) |
| O(1) | | C(10) | [4575.01] | 3.125(3) < | 3.22 | -0.10 | | 0.3541 | 0.8983 | 0.8008 | 0.4711 | 0.7334 | 0.9625 | N(3) 129.78(17) |
| O(1) | | H(10C) | [4575.01] | 2.90 | 2.72 | 0.18 | | 0.3541 | 0.8983 | 0.8008 | 0.3998 | 0.7139 | 0.9326 | N(3) 132 |
| O(1) | | H(9A) | [6546.01] | 2.57 < | 2.72 | -0.15 | | 0.3541 | 0.8983 | 0.8008 | 0.2091 | 0.7652 | 0.7861 | N(3) 106 |
| O(2) | | C(6) | [] | 2.759(3)<< | 3.22 | -0.46 | Intra | 0.3614 | 0.8437 | 0.6520 | 0.4146 | 1.0459 | 0.6100 | |
| O(2) | | H(6A) | [] | 2.49<< | 2.72 | -0.23 | Intra | 0.3614 | 0.8437 | 0.6520 | 0.4455 | 0.9897 | 0.5834 | |
| O(2) | | H(10A) | [3676.01] | 2.60 < | 2.72 | -0.12 | | 0.3614 | 0.8437 | 0.6520 | 0.4946 | 0.7356 | 0.5914 | N(3) 139 |
| O(2) | | C(2) | [4574.01] | 3.346(4) | 3.22 | 0.13 | | 0.3614 | 0.8437 | 0.6520 | 0.2012 | 0.9121 | 0.4266 | N(3) 107.22(16) |
| O(2) | | H(2A) | [4574.01] | 2.74 | 2.72 | 0.02 | | 0.3614 | 0.8437 | 0.6520 | 0.1966 | 0.9010 | 0.4941 | |
| O(2) | | C(3) | [6546.01] | 3.379(4) | 3.22 | 0.16 | | 0.3614 | 0.8437 | 0.6520 | 0.2228 | 0.6186 | 0.6099 | N(3) 126.63(18) |
| O(3) | | H(6A) | [] | 2.50<< | 2.72 | -0.22 | Intra | 0.4768 | 1.1635 | 0.5099 | 0.4455 | 0.9897 | 0.5834 | C(10) 167 |
| O(3) | | H(8A) | [] | 2.67 < | 2.72 | -0.05 | Intra | 0.4768 | 1.1635 | 0.5099 | 0.3847 | 1.3033 | 0.6005 | |
| O(3) | | C(3) | [2656.01] | 3.317(3) | 3.22 | 0.10 | | 0.4768 | 1.1635 | 0.5099 | 0.7228 | 1.1186 | 0.6099 | C(7) 112.74(14) C(10) 104.89(15) |
| O(3) | | H(3A) | [2656.01] | 2.46<< | 2.72 | -0.26 | | 0.4768 | 1.1635 | 0.5099 | 0.6632 | 1.1552 | 0.5732 | C(7) 118 |
| O(3) | | H(6A) | [3676.01] | 2.70 < | 2.72 | -0.02 | | 0.4768 | 1.1635 | 0.5099 | 0.5545 | 1.0103 | 0.4166 | C(7) 127 C(10) 114 |
| O(3) | | O(1) | [4574.01] | 2.975(3) < | 3.04 | -0.07 | | 0.4768 | 1.1635 | 0.5099 | 0.3541 | 1.1017 | 0.3008 | C(7) 111.01(14) |
| N(1) | | C(3) | [] | 2.193(4)<< | 3.25 | -1.06 | Intra | 0.1304 | 1.0370 | 0.8476 | 0.2772 | 1.1186 | 0.8901 | H(1) 162.1(17) |

| | | | | | | | | |
|------|------|--------|------------|-----------------------------|----------------------|-----------------------|-------|------------|
| N(1) | | S | [2556.01] | 3.292(3) < 3.35 -0.06 | 0.1304 1.0370 0.8476 | -0.1016 0.9788 0.8526 | C(1) | 123.83(16) |
| | | | | | | | C(2) | 123.89(16) |
| N(2) | | O(1) | [] | 2.738(3)<< 3.07 -0.33 Intra | 0.2527 1.0867 0.7875 | 0.3541 0.8983 0.8008 | C(3) | 102.13(15) |
| N(2) | | N(3) | [] | 2.948(3) < 3.10 -0.15 Intra | 0.2527 1.0867 0.7875 | 0.3582 0.9144 0.7135 | C(3) | 123.47(16) |
| N(2) | | C(2) | [] | 2.204(3)<< 3.25 -1.05 Intra | 0.2527 1.0867 0.7875 | 0.2012 1.0879 0.9266 | C(4) | 160.78(18) |
| N(2) | | H(9A) | [] | 2.58 < 2.75 -0.17 Intra | 0.2527 1.0867 0.7875 | 0.2909 1.2652 0.7139 | C(1) | 126 |
| N(3) | | S | [] | 3.481(3) 3.35 0.13 Intra | 0.3582 0.9144 0.7135 | 0.1016 0.9788 0.6474 | O(2) | 102.84(16) |
| N(3) | | N(2) | [] | 2.948(3) < 3.10 -0.15 Intra | 0.3582 0.9144 0.7135 | 0.2527 1.0867 0.7875 | O(2) | 151.95(18) |
| N(3) | | C(1) | [] | 3.334(4) 3.25 0.08 Intra | 0.3582 0.9144 0.7135 | 0.1611 1.0350 0.7619 | O(2) | 130.75(18) |
| N(3) | | H(6A) | [] | 2.59 < 2.75 -0.16 Intra | 0.3582 0.9144 0.7135 | 0.4455 0.9897 0.5834 | O(1) | 152 |
| C(1) | | O(1) | [] | 3.082(3) < 3.22 -0.14 Intra | 0.1611 1.0350 0.7619 | 0.3541 0.8983 0.8008 | N(1) | 109.08(16) |
| C(1) | | N(3) | [] | 3.334(4) 3.25 0.08 Intra | 0.1611 1.0350 0.7619 | 0.3582 0.9144 0.7135 | N(1) | 130.64(16) |
| C(1) | | C(3) | [] | 2.265(4)<< 3.40 -1.13 Intra | 0.1611 1.0350 0.7619 | 0.2772 1.1186 0.8901 | S | 162.54(16) |
| C(1) | | C(5) | [] | 3.247(4) < 3.40 -0.15 Intra | 0.1611 1.0350 0.7619 | 0.3609 1.0256 0.6800 | N(1) | 143.22(17) |
| C(1) | | C(9) | [] | 3.471(4) 3.40 0.07 Intra | 0.1611 1.0350 0.7619 | 0.3226 1.2092 0.6880 | S | 100.33(10) |
| | | | | | | | N(1) | 128.48(16) |
| C(1) | | H(1) | [2556.01] | 3.09(3) 2.90 0.19 | 0.1611 1.0350 0.7619 | -0.0680 1.0150 0.6530 | N(2) | 153.9(5) |
| C(2) | | N(2) | [] | 2.204(3)<< 3.25 -1.05 Intra | 0.2012 1.0879 0.9266 | 0.2527 1.0867 0.7875 | H(2A) | 164 |
| C(2) | | C(4) | [] | 3.587(4) 3.40 0.19 Intra | 0.2012 1.0879 0.9266 | 0.3130 1.1059 0.7193 | H(2A) | 156 |
| C(2) | | O(2) | [4575.01] | 3.346(4) 3.22 0.13 | 0.2012 1.0879 0.9266 | 0.3614 1.1563 1.1520 | N(1) | 165.07(18) |
| C(3) | | O(1) | [] | 3.327(3) 3.22 0.11 Intra | 0.2772 1.1186 0.8901 | 0.3541 0.8983 0.8008 | C(2) | 104.90(17) |
| | | | | | | | H(3A) | 106 |
| C(3) | | N(1) | [] | 2.193(4)<< 3.25 -1.06 Intra | 0.2772 1.1186 0.8901 | 0.1304 1.0370 0.8476 | H(3A) | 164 |
| C(3) | | C(5) | [] | 3.574(4) 3.40 0.17 Intra | 0.2772 1.1186 0.8901 | 0.3609 1.0256 0.6800 | C(2) | 131.85(18) |
| C(3) | | C(9) | [] | 3.203(4) < 3.40 -0.20 Intra | 0.2772 1.1186 0.8901 | 0.3226 1.2092 0.6880 | C(2) | 142.01(19) |
| C(3) | | H(1) | [] | 3.06(3) 2.90 0.16 Intra | 0.2772 1.1186 0.8901 | 0.0680 1.0150 0.8470 | H(3A) | 159 |
| C(3) | | H(9A) | [] | 3.08 2.90 0.18 Intra | 0.2772 1.1186 0.8901 | 0.2909 1.2652 0.7139 | C(2) | 134 |
| C(3) | | O(3) | [2656.01] | 3.317(3) 3.22 0.10 | 0.2772 1.1186 0.8901 | 0.5232 1.1635 0.9901 | N(2) | 112.83(17) |
| | | | | | | | C(2) | 135.25(18) |
| C(3) | | O(2) | [6556.01] | 3.379(4) 3.22 0.16 | 0.2772 1.1186 0.8901 | 0.1386 1.3437 0.8480 | | |
| C(4) | | S | [] | 3.220(3)<< 3.50 -0.28 Intra | 0.3130 1.1059 0.7193 | 0.1016 0.9788 0.6474 | C(9) | 122.00(17) |
| C(4) | | O(1) | [] | 2.841(3)<< 3.22 -0.38 Intra | 0.3130 1.1059 0.7193 | 0.3541 0.8983 0.8008 | C(9) | 163.81(19) |
| C(4) | | C(2) | [] | 3.587(4) 3.40 0.19 Intra | 0.3130 1.1059 0.7193 | 0.2012 1.0879 0.9266 | C(5) | 127.63(16) |
| | | | | | | | C(9) | 113.64(17) |
| C(4) | | C(7) | [] | 2.807(4)<< 3.40 -0.59 Intra | 0.3130 1.1059 0.7193 | 0.4227 1.1505 0.5791 | N(2) | 176.86(17) |
| C(4) | | H(3A) | [] | 2.82 < 2.90 -0.08 Intra | 0.3130 1.1059 0.7193 | 0.3368 1.1552 0.9268 | C(5) | 128 |
| C(5) | | S | [] | 3.516(3) 3.50 0.02 Intra | 0.3609 1.0256 0.6800 | 0.1016 0.9788 0.6474 | C(6) | 131.54(16) |
| C(5) | | C(1) | [] | 3.247(4) < 3.40 -0.15 Intra | 0.3609 1.0256 0.6800 | 0.1611 1.0350 0.7619 | C(6) | 153.84(17) |
| C(5) | | C(3) | [] | 3.574(4) 3.40 0.17 Intra | 0.3609 1.0256 0.6800 | 0.2772 1.1186 0.8901 | C(6) | 147.84(17) |
| C(5) | | C(8) | [] | 2.762(4)<< 3.40 -0.64 Intra | 0.3609 1.0256 0.6800 | 0.3777 1.2320 0.6197 | N(3) | 176.77(18) |
| C(5) | | C(6) | [2656.01] | 3.573(4) 3.40 0.17 | 0.3609 1.0256 0.6800 | 0.5854 1.0459 0.8900 | | |
| C(6) | | O(2) | [] | 2.759(3)<< 3.22 -0.46 Intra | 0.4146 1.0459 0.6100 | 0.3614 0.8437 0.6520 | C(7) | 169.46(18) |
| C(6) | | C(9) | [] | 2.784(4)<< 3.40 -0.62 Intra | 0.4146 1.0459 0.6100 | 0.3226 1.2092 0.6880 | H(6A) | 179 |
| C(6) | | C(5) | [2656.01] | 3.573(4) 3.40 0.17 | 0.4146 1.0459 0.6100 | 0.6391 1.0256 0.8200 | C(7) | 100.63(15) |
| C(7) | | C(4) | [] | 2.807(4)<< 3.40 -0.59 Intra | 0.4227 1.1505 0.5791 | 0.3130 1.1059 0.7193 | O(3) | 175.37(17) |
| C(7) | | H(10B) | [] | 2.67<< 2.90 -0.23 Intra | 0.4227 1.1505 0.5791 | 0.5041 1.3192 0.5141 | C(6) | 158 |
| C(7) | | H(10C) | [] | 2.58<< 2.90 -0.32 Intra | 0.4227 1.1505 0.5791 | 0.3998 1.2861 0.4326 | C(6) | 149 |
| C(8) | | C(5) | [] | 2.762(4)<< 3.40 -0.64 Intra | 0.3777 1.2320 0.6197 | 0.3609 1.0256 0.6800 | H(8A) | 179 |

| | | | | | | | | | | | | | | | | |
|--------|------|--------|---|----------|------------|------|-------|-------|--------|--------|--------|---------|--------|--------|--------|------------|
| C(8) | | C(10) | [|] | 2.827(4)<< | 3.40 | -0.57 | Intra | 0.3777 | 1.2320 | 0.6197 | 0.4711 | 1.2666 | 0.4625 | C(9) | 173.2(2) |
| C(8) | | H(10B) | [|] | 2.78 < | 2.90 | -0.12 | Intra | 0.3777 | 1.2320 | 0.6197 | 0.5041 | 1.3192 | 0.5141 | C(9) | 166 |
| C(8) | | H(10C) | [|] | 2.74 < | 2.90 | -0.16 | Intra | 0.3777 | 1.2320 | 0.6197 | 0.3998 | 1.2861 | 0.4326 | C(9) | 155 |
| C(9) | | C(1) | [|] | 3.471(4) | 3.40 | 0.07 | Intra | 0.3226 | 1.2092 | 0.6880 | 0.1611 | 1.0350 | 0.7619 | C(8) | 147.39(18) |
| C(9) | | C(3) | [|] | 3.203(4) < | 3.40 | -0.20 | Intra | 0.3226 | 1.2092 | 0.6880 | 0.2772 | 1.1186 | 0.8901 | C(8) | 158.2(2) |
| C(9) | | C(6) | [|] | 2.784(4)<< | 3.40 | -0.62 | Intra | 0.3226 | 1.2092 | 0.6880 | 0.4146 | 1.0459 | 0.6100 | H(9A) | 179 |
| C(9) | | H(10C) | [| 7576.01] | 3.03 | 2.90 | 0.13 | | 0.3226 | 1.2092 | 0.6880 | 0.1002 | 1.2139 | 0.5674 | C(8) | 107 |
| C(10) | | C(8) | [|] | 2.827(4)<< | 3.40 | -0.57 | Intra | 0.4711 | 1.2666 | 0.4625 | 0.3777 | 1.2320 | 0.6197 | H(10A) | 169 |
| C(10) | | H(8A) | [|] | 2.54<< | 2.90 | -0.36 | Intra | 0.4711 | 1.2666 | 0.4625 | 0.3847 | 1.3033 | 0.6005 | H(10A) | 171 |
| C(10) | | H(3A) | [| 2656.01] | 2.99 | 2.90 | 0.09 | | 0.4711 | 1.2666 | 0.4625 | 0.6632 | 1.1552 | 0.5732 | H(10C) | 164 |
| C(10) | | O(1) | [| 4574.01] | 3.125(3) < | 3.22 | -0.10 | | 0.4711 | 1.2666 | 0.4625 | 0.3541 | 1.1017 | 0.3008 | H(10B) | 177 |
| C(10) | | S | [| 7576.01] | 3.567(3) | 3.50 | 0.07 | | 0.4711 | 1.2666 | 0.4625 | 0.3984 | 1.5212 | 0.3526 | O(3) | 166.48(17) |
| H(1) | | S | [|] | 2.92(3) < | 3.00 | -0.08 | Intra | 0.0680 | 1.0150 | 0.8470 | 0.1016 | 0.9788 | 0.6474 | | |
| H(1) | | C(3) | [|] | 3.06(3) | 2.90 | 0.16 | Intra | 0.0680 | 1.0150 | 0.8470 | 0.2772 | 1.1186 | 0.8901 | | |
| H(1) | | H(2A) | [|] | 2.50 | 2.40 | 0.10 | Intra | 0.0680 | 1.0150 | 0.8470 | 0.1966 | 1.0990 | 0.9941 | | |
| H(1) | | S | [| 2556.01] | 2.40(3)<< | 3.00 | -0.60 | | 0.0680 | 1.0150 | 0.8470 | -0.1016 | 0.9788 | 0.8526 | N(1) | 173(2) |
| H(1) | | C(1) | [| 2556.01] | 3.09(3) | 2.90 | 0.19 | | 0.0680 | 1.0150 | 0.8470 | -0.1611 | 1.0350 | 0.7381 | N(1) | 145(2) |
| H(2A) | | H(1) | [|] | 2.50 | 2.40 | 0.10 | Intra | 0.1966 | 1.0990 | 0.9941 | 0.0680 | 1.0150 | 0.8470 | | |
| H(2A) | | H(3A) | [|] | 2.46 | 2.40 | 0.06 | Intra | 0.1966 | 1.0990 | 0.9941 | 0.3368 | 1.1552 | 0.9268 | | |
| H(2A) | | S | [| 4575.01] | 2.93 < | 3.00 | -0.07 | | 0.1966 | 1.0990 | 0.9941 | 0.1016 | 1.0212 | 1.1474 | C(2) | 144 |
| H(2A) | | O(2) | [| 4575.01] | 2.74 | 2.72 | 0.02 | | 0.1966 | 1.0990 | 0.9941 | 0.3614 | 1.1563 | 1.1520 | C(2) | 122 |
| H(3A) | | C(4) | [|] | 2.82 < | 2.90 | -0.08 | Intra | 0.3368 | 1.1552 | 0.9268 | 0.3130 | 1.1059 | 0.7193 | | |
| H(3A) | | H(2A) | [|] | 2.46 | 2.40 | 0.06 | Intra | 0.3368 | 1.1552 | 0.9268 | 0.1966 | 1.0990 | 0.9941 | | |
| H(3A) | | O(3) | [| 2656.01] | 2.46<< | 2.72 | -0.26 | | 0.3368 | 1.1552 | 0.9268 | 0.5232 | 1.1635 | 0.9901 | C(3) | 149 |
| H(3A) | | C(10) | [| 2656.01] | 2.99 | 2.90 | 0.09 | | 0.3368 | 1.1552 | 0.9268 | 0.5289 | 1.2666 | 1.0375 | C(3) | 178 |
| H(6A) | | O(2) | [|] | 2.49<< | 2.72 | -0.23 | Intra | 0.4455 | 0.9897 | 0.5834 | 0.3614 | 0.8437 | 0.6520 | | |
| H(6A) | | O(3) | [|] | 2.50<< | 2.72 | -0.22 | Intra | 0.4455 | 0.9897 | 0.5834 | 0.4768 | 1.1635 | 0.5099 | | |
| H(6A) | | N(3) | [|] | 2.59 < | 2.75 | -0.16 | Intra | 0.4455 | 0.9897 | 0.5834 | 0.3582 | 0.9144 | 0.7135 | | |
| H(6A) | | O(3) | [| 3676.01] | 2.70 < | 2.72 | -0.02 | | 0.4455 | 0.9897 | 0.5834 | 0.5232 | 0.8365 | 0.4901 | C(6) | 175 |
| H(8A) | | O(3) | [|] | 2.67 < | 2.72 | -0.05 | Intra | 0.3847 | 1.3033 | 0.6005 | 0.4768 | 1.1635 | 0.5099 | | |
| H(8A) | | C(10) | [|] | 2.54<< | 2.90 | -0.36 | Intra | 0.3847 | 1.3033 | 0.6005 | 0.4711 | 1.2666 | 0.4625 | | |
| H(8A) | | H(9A) | [|] | 2.33 < | 2.40 | -0.07 | Intra | 0.3847 | 1.3033 | 0.6005 | 0.2909 | 1.2652 | 0.7139 | | |
| H(8A) | | H(10B) | [|] | 2.28 < | 2.40 | -0.12 | Intra | 0.3847 | 1.3033 | 0.6005 | 0.5041 | 1.3192 | 0.5141 | C(8) | 112 |
| H(8A) | | H(10C) | [|] | 2.37 < | 2.40 | -0.03 | Intra | 0.3847 | 1.3033 | 0.6005 | 0.3998 | 1.2861 | 0.4326 | C(8) | 103 |
| H(9A) | | N(2) | [|] | 2.58 < | 2.75 | -0.17 | Intra | 0.2909 | 1.2652 | 0.7139 | 0.2527 | 1.0867 | 0.7875 | | |
| H(9A) | | C(3) | [|] | 3.08 | 2.90 | 0.18 | Intra | 0.2909 | 1.2652 | 0.7139 | 0.2772 | 1.1186 | 0.8901 | | |
| H(9A) | | H(8A) | [|] | 2.33 < | 2.40 | -0.07 | Intra | 0.2909 | 1.2652 | 0.7139 | 0.3847 | 1.3033 | 0.6005 | | |
| H(9A) | | O(1) | [| 6556.01] | 2.57 < | 2.72 | -0.15 | | 0.2909 | 1.2652 | 0.7139 | 0.1459 | 1.3983 | 0.6992 | C(9) | 152 |
| H(10A) | | O(2) | [| 3676.01] | 2.60 < | 2.72 | -0.12 | | 0.5054 | 1.2644 | 0.4086 | 0.6386 | 1.1563 | 0.3480 | C(10) | 142 |
| H(10B) | | C(7) | [|] | 2.67<< | 2.90 | -0.23 | Intra | 0.5041 | 1.3192 | 0.5141 | 0.4227 | 1.1505 | 0.5791 | | |
| H(10B) | | C(8) | [|] | 2.78 < | 2.90 | -0.12 | Intra | 0.5041 | 1.3192 | 0.5141 | 0.3777 | 1.2320 | 0.6197 | | |
| H(10B) | | H(8A) | [|] | 2.28 < | 2.40 | -0.12 | Intra | 0.5041 | 1.3192 | 0.5141 | 0.3847 | 1.3033 | 0.6005 | | |
| H(10B) | | S | [| 5555.01] | 2.79<< | 3.00 | -0.21 | | 0.5041 | 1.3192 | 0.5141 | 0.6016 | 1.4788 | 0.6474 | C(10) | 175 |
| H(10C) | | C(7) | [|] | 2.58<< | 2.90 | -0.32 | Intra | 0.3998 | 1.2861 | 0.4326 | 0.4227 | 1.1505 | 0.5791 | | |
| H(10C) | | C(8) | [|] | 2.74 < | 2.90 | -0.16 | Intra | 0.3998 | 1.2861 | 0.4326 | 0.3777 | 1.2320 | 0.6197 | | |
| H(10C) | | H(8A) | [|] | 2.37 < | 2.40 | -0.03 | Intra | 0.3998 | 1.2861 | 0.4326 | 0.3847 | 1.3033 | 0.6005 | | |
| H(10C) | | O(1) | [| 4574.01] | 2.90 | 2.72 | 0.18 | | 0.3998 | 1.2861 | 0.4326 | 0.3541 | 1.1017 | 0.3008 | | |
| H(10C) | | S | [| 7576.01] | 3.16 | 3.00 | 0.16 | | 0.3998 | 1.2861 | 0.4326 | 0.3984 | 1.5212 | 0.3526 | C(10) | 107 |

H(10C) C(9) [7576.01] 3.03 2.90 0.13 0.3998 1.2861 0.4326 0.1774 1.2908 0.3120 C(10) 165

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 1 to Neighbouring ARU'S

| Nr | ARU | Nr.Cont. | d(min) | Del | XHn X | - At(I) | At(J) | - Y | YHn | Note | Partaking ARU's in Close Contact | Resd. |
|----|------------|----------|--------|-------|---------|----------|------------|--------|-----|------|----------------------------------|-------|
| 1 | [2556.01] | 6 | 2.4000 | -0.60 | 1 N(1) | - H(1) | ... S | -C(1) | 0 | << | 2556.01 | |
| 2 | [4574.01] | 6 | 2.7400 | 0.02 | 0 N(3) | - O(2) | ... H(2A) | -C(2) | 1 | | 4574.01 | |
| 3 | [5445.01] | 1 | 2.7900 | -0.21 | 0 C(1) | - S | ... H(10B) | -C(10) | 3 | << | 5445.01 | |
| 4 | [7576.01] | 6 | 3.0300 | 0.13 | 3 C(10) | - H(10C) | ... C(9) | -C(4) | 0 | | 7576.01 | |
| 5 | [4575.01] | 6 | 2.7400 | 0.02 | 1 C(2) | - H(2A) | ... O(2) | -N(3) | 0 | | 4575.01 | |
| 6 | [6546.01] | 2 | 2.5700 | -0.15 | 0 N(3) | - O(1) | ... H(9A) | -C(9) | 1 | < | 6546.01 | |
| 7 | [3676.01] | 4 | 2.6000 | -0.12 | 3 C(10) | - H(10A) | ... O(2) | -N(3) | 0 | < | 3676.01 | |
| 8 | [2656.01] | 8 | 2.4600 | -0.26 | 1 C(3) | - H(3A) | ... O(3) | -C(7) | 0 | << | 2656.01 | |
| 9 | [6556.01] | 2 | 2.5700 | -0.15 | 1 C(9) | - H(9A) | ... O(1) | -N(3) | 0 | < | 6556.01 | |
| 10 | [5555.01] | 1 | 2.7900 | -0.21 | 3 C(10) | - H(10B) | ... S | -C(1) | 0 | << | 5555.01 | |

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Asymmetric Residue Unit (= ARU) Code List

| ARU-CODE | CIF-CODE | Symmetry-Code | sym | TX | TY | TZ | Ires | x(cen) | y(cen) | z(cen) |
|------------|----------|---------------------|-----|-----|----|----|--------|--------|--------|--------|
| [2556.01] | [2_556] | =-x,y,3/2-z | = | [2 | 0 | 0 | 1 1] | -0.327 | 1.111 | 0.811 |
| [4574.01] | [6_575] | =x,2-y,-1/2+z | = | [4 | 0 | 2 | -1 1] | 0.327 | 0.889 | 0.189 |
| [5445.01] | [3_445] | =-1/2+x,-1/2+y,z | = | [5 | -1 | -1 | 0 1] | -0.173 | 0.611 | 0.689 |
| [7576.01] | [7_576] | =1/2-x,5/2-y,1-z | = | [7 | 0 | 2 | 1 1] | 0.173 | 1.389 | 0.311 |
| [4575.01] | [6_576] | =x,2-y,1/2+z | = | [4 | 0 | 2 | 0 1] | 0.327 | 0.889 | 1.189 |
| [6546.01] | [4_546] | =1/2-x,-1/2+y,3/2-z | = | [6 | 0 | -1 | 1 1] | 0.173 | 0.611 | 0.811 |
| [3676.01] | [5_676] | =1-x,2-y,1-z | = | [3 | 1 | 2 | 1 1] | 0.673 | 0.889 | 0.311 |
| [2656.01] | [2_656] | =1-x,y,3/2-z | = | [2 | 1 | 0 | 1 1] | 0.673 | 1.111 | 0.811 |
| [6556.01] | [4_556] | =1/2-x,1/2+y,3/2-z | = | [6 | 0 | 0 | 1 1] | 0.173 | 1.611 | 0.811 |
| [5555.01] | [3_555] | =1/2+x,1/2+y,z | = | [5 | 0 | 0 | 0 1] | 0.827 | 1.611 | 0.689 |

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

X(J) = X(sym) + TX , Y(J) = Y(sym) + TY , Z(J) = Z(sym) + TZ,
 SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

=====
 Analysis of Potential Hydrogen Bonds and Schemes with $d(D...A) < R(D)+R(A)+0.50$, $d(H...A) < R(H)+R(A)-0.12$ Ang., $D-H...A > 100.0$ Deg
 =====

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
 =====

| Nr | Typ | Res | Donor | --- H...Acceptor | [ARU] | D - H | H...A | D...A | D - H...A | A..H..A* A'..H..A" | Sum(XY,YZ) | Sum(XZ) |
|----|-----|-----|-------|------------------|---------|------------|---------|---------|-----------|--------------------|------------|---------|
| 1 | | 1 | N(1) | --H(1) | ..S | [2556.01] | 0.90(3) | 2.40(3) | 3.292(3) | 173(2) | | |
| 2 | | 1 | C(3) | --H(3A) | ..O(3) | [2656.01] | 0.95 | 2.46 | 3.317(3) | 149 | | |
| 3 | | 1 | C(9) | --H(9A) | ..O(1) | [6556.01] | 0.95 | 2.57 | 3.440(4) | 152 | | |
| 4 | | 1 | C(10) | --H(10A) | ..O(2) | [3676.01] | 0.98 | 2.60 | 3.423(4) | 142 | | |
| 5 | | 1 | C(10) | --H(10B) | ..S | [5555.01] | 0.98 | 2.79 | 3.766(3) | 175 | | |

Translation of ARU-Code to CIF and Equivalent Position Code
 =====

- [2556.] = [2_556] = -x,y,3/2-z
- [3676.] = [5_676] = 1-x,2-y,1-z
- [2656.] = [2_656] = 1-x,y,3/2-z
- [6556.] = [4_556] = 1/2-x,1/2+y,3/2-z
- [5555.] = [3_555] = 1/2+x,1/2+y,z

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]
 =====

- 2-Centre (linear) D-H...X most prob. angle 160 deg - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
- 3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg Springer-Verlag, Berlin, 1991, pp 20.
- 4-Centre (trifurcated)

Analysis of Potential Donor/Acceptor Atoms -- (Major Disorder Form Only)
 =====

| At.Nr | D/A | #Cov.Bonds | # H | #D-H..A | #A..H | #A..H-C | Sum(A-H) | Sum(A-X) |
|-------|------|------------|-----|---------|-------|---------|----------|----------|
| 1 | S | 1 | - | 0 | 1 | 1 | 2 | 3 |
| 2 | O(1) | 1 | - | 0 | 0 | 1 | 1 | 2 |
| 3 | O(2) | 1 | - | 0 | 0 | 1 | 1 | 2 |
| 4 | O(3) | 2 | - | 0 | 0 | 1 | 1 | 3 |
| 5 | N(1) | 3 | 1 H | 1 | 0 | 0 | 1 | 3 |
| 6 | N(2) | 3 | - | 0 | 0 | 0 | 0 | 3 |
| 7 | N(3) | 3 | - | 0 | 0 | 0 | 0 | 3 |

=====
 Analysis of Hydrogen Bonded Molecular Aggregates (See also Acta Cryst. B36, 1980, 2113 - 2115) -- (Major Disorder Component Only)
 =====

Coordinates of Donor and Acceptor Atoms
 =====

Coordinates of D/A-Bonded Atom(s)
 =====

| D/A I | [ARU] | X | Y | Z | -- | D/A J | [ARU] | X | Y | Z | Atom K | X | Y | Z | I..J--K Angle |
|-------|-------------|--------|--------|--------|----|-------|-------------|---------|--------|--------|--------|---------|--------|--------|---------------|
| N(1) | [1555.01], | 0.1304 | 1.0370 | 0.8476 | >> | S | [2556.01], | -0.1016 | 0.9788 | 0.8526 | C(1) | -0.1611 | 1.0350 | 0.7381 | 96.01(7) |
| S | [1555.01], | 0.1016 | 0.9788 | 0.6474 | << | N(1) | [2556.01], | -0.1304 | 1.0370 | 0.6524 | C(1) | -0.1611 | 1.0350 | 0.7381 | 123.83(8) |
| | | | | | | | | | | | C(2) | -0.2012 | 1.0879 | 0.5734 | 123.89(8) |
| | | | | | | | | | | | H(1) | -0.0680 | 1.0150 | 0.6530 | 5.37(11) |

=====

***** Aggregate = 1 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 2 1 1555.01 -- 2556.01
 2 1 2556.01 -- 1555.01

=====

***** Aggregate = 2 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 2 1 3555.01 -- 4553.01
 2 1 4553.01 -- 3555.01

=====

***** Aggregate = 3 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

 2 1 5555.01 -- 6556.01
 2 1 6556.01 -- 5555.01

=====

***** Aggregate = 4 *****

=====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

=====

| | | | | |
|---|---|---------|----|---------|
| 2 | 1 | 7555.01 | -- | 8553.01 |
|---|---|---------|----|---------|

| | | | | |
|---|---|---------|----|---------|
| 2 | 1 | 8553.01 | -- | 7555.01 |
|---|---|---------|----|---------|

=====
 Analysis of the (Cooperative) Hydrogen Bond Network (i.e. (In)Finite O-H...O-H...O-H.. Chains and/or Rings (Max = 18 Membered))
 =====

=====
 ***** Network = 1 *****
 =====

| Code | Acc | Donor Atom | X | Y | Z | Acceptor Atom | X | Y | Z up to BondCode(s) of Forward Link(s) |
|-------|-----|-----------------|--------|--------|--------|---------------|---------|--------|--|
| 1.555 | | N(1) [1555.01] | 0.1304 | 1.0370 | 0.8476 | S [2556.01] | -0.1016 | 0.9788 | 0.8526 |
| | | H(1) | 0.0680 | 1.0150 | 0.8470 | | | | |

 Hydrogen Bonds are Coded as N.IJK Where N = Sequence Number of Hydrogen Bond (NOTE: New Hbond Numbering system)
 I - 5 = Nr of Translation Units Along A-Axis
 J - 5 = Nr of Translation Units Along B-Axis
 K - 5 = Nr of Translation Units Along C-Axis

Ring Closure Links are Indicated with 'R' and Infinite Chain Links With 'T'

3.6 Angstrom Coordination Sphere Around Atom I = S [ARU = 1555.01] 0.10157 0.97882 0.64738 -1.1096 12.3576 8.4618

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|---------------------|-----------|----------|-------|---------|--------|----------|---------|---------|---------|---------|---------|
| 1 | 1.698(2) | -- | C(1) | | | | Intra | 62.11 | 61.78 | 0.16113 | 1.03503 | 0.76187 | -0.7340 | 13.0673 | 9.9583 |
| 2 | 2.745(2) | << | N(1) | | | | Intra | 117.30 | 72.47 | 0.13036 | 1.03702 | 0.84760 | -1.4888 | 13.0924 | 11.0789 |
| 3 | 2.751(2) | << | N(2) | | | | Intra | 41.59 | 41.76 | 0.25266 | 1.08671 | 0.78755 | 0.4249 | 13.7197 | 10.2940 |
| 4 | 3.220(3) | << | C(4) | | | | Intra | 31.41 | 16.99 | 0.31304 | 1.10594 | 0.71935 | 1.5189 | 13.9625 | 9.4026 |
| 5 | 3.292(3) | .< | N(1)a | [-x,y,3/2-z | = | 2556.01] | | 167.10 | 1.14 | -0.13036 | 1.03702 | 0.65240 | -4.3174 | 13.0924 | 8.5275 |
| 6 | 3.481(3) | .. | N(3) | | | | Intra | -13.95 | 14.37 | 0.35825 | 0.91443 | 0.71347 | 2.1632 | 11.5447 | 9.3257 |
| 7 | 3.516(3) | .. | C(5) | | | | Intra | 9.74 | 6.97 | 0.36095 | 1.02558 | 0.68001 | 2.3298 | 12.9479 | 8.8883 |
| 8 | 3.567(3) | .. | C(10)e | [1/2-x,5/2-y,1-z | = | 7576.01] | | 100.12 | -23.74 | 0.02890 | 1.23340 | 0.53750 | -1.6833 | 15.5717 | 7.0256 |
| 9 | 2.40(3) | << | H(1)a | [-x,y,3/2-z | = | 2556.01] | | 169.01 | 1.76 | -0.06800 | 1.01500 | 0.65300 | -3.4624 | 12.8144 | 8.5353 |
| 10 | 2.79 | << | H(10B)c | [-1/2+x,-1/2+y,z | = | 5445.01] | | -112.24 | -38.67 | 0.00410 | 0.81920 | 0.51410 | -1.9336 | 10.3424 | 6.7198 |
| 11 | 2.92(3) | .< | H(1) | | | | Intra | 159.69 | 63.24 | 0.06800 | 1.01500 | 0.84700 | -2.3438 | 12.8144 | 11.0711 |
| 12 | 2.93 | .< | H(2A)b | [x,2-y,-1/2+z | = | 4574.01] | | -27.35 | -43.13 | 0.19660 | 0.90100 | 0.49410 | 0.7901 | 11.3751 | 6.4583 |
| 13 | 3.16 | .. | H(10C)e | [1/2-x,5/2-y,1-z | = | 7576.01] | | 84.40 | -19.32 | 0.10020 | 1.21390 | 0.56740 | -0.8188 | 15.3255 | 7.4164 |
| 14 | 3.38 | .. | H(9A)d | [1/2-x,-1/2+y,3/2-z | = | 6546.01] | | -70.76 | 32.41 | 0.20910 | 0.76520 | 0.78610 | -0.1683 | 9.6607 | 10.2750 |
| 15 | 3.41 | .. | H(10B)e | [1/2-x,5/2-y,1-z | = | 7576.01] | | 107.98 | -38.21 | -0.00410 | 1.18080 | 0.48590 | -1.9372 | 14.9076 | 6.3512 |
| 16 | 3.55 | .. | H(10A)e | [1/2-x,5/2-y,1-z | = | 7576.01] | | 111.14 | -11.89 | -0.00540 | 1.23560 | 0.59140 | -2.3634 | 15.5995 | 7.7301 |

Angles (Degrees) At1...V...At2 with Vertex V = S

| | | | | | | | | | | | | | | | |
|-------|---|--------|----------|------|---|--------|----------|-------|---|--------|-----------|-------|---|--------|-----------|
| C(1) | , | N(1) | 22.85(9) | C(1) | , | N(2) | 23.48(9) | C(1) | , | C(4) | 49.74(9) | C(1) | , | N(1)a | 96.01(9) |
| C(1) | , | N(3) | 70.79(9) | C(1) | , | C(5) | 66.83(9) | C(1) | , | C(10)e | 90.79(9) | N(1) | , | N(2) | 46.32(7) |
| N(1) | , | C(4) | 72.59(7) | N(1) | , | N(1)a | 77.68(6) | N(1) | , | N(3) | 87.47(6) | N(1) | , | C(5) | 88.54(6) |
| N(1) | , | C(10)e | 96.92(7) | N(2) | , | C(4) | 26.27(6) | N(2) | , | N(1)a | 114.82(6) | N(2) | , | N(3) | 54.96(6) |
| N(2) | , | C(5) | 44.79(6) | N(2) | , | C(10)e | 84.94(6) | C(4) | , | N(1)a | 132.72(6) | C(4) | , | N(3) | 43.66(6) |
| C(4) | , | C(5) | 23.41(6) | C(4) | , | C(10)e | 78.45(6) | N(1)a | , | N(3) | 164.46(6) | N(1)a | , | C(5) | 156.00(6) |
| N(1)a | , | C(10)e | 69.52(6) | N(3) | , | C(5) | 24.41(5) | N(3) | , | C(10)e | 117.49(6) | C(5) | , | C(10)e | 93.15(6) |

3.6 Angstrom Coordination Sphere Around Atom I = O(2) [ARU = 1555.01] 0.36145 0.84373 0.65199 2.4451 10.6521 8.5221

| Nr | d(I,J) | To | Atom J | Symm_Oper. | on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|----|---------|---------------------|-----------|----------|-------|---------|--------|---------|---------|---------|---------|---------|---------|
| 1 | 1.234(3) | -- | N(3) | | | | Intra | 107.53 | 40.65 | 0.35825 | 0.91443 | 0.71347 | 2.1632 | 11.5447 | 9.3257 |
| 2 | 2.172(3) | << | O(1) | | | | Intra | 134.52 | 63.60 | 0.35411 | 0.89826 | 0.80081 | 1.7682 | 11.3405 | 10.4673 |
| 3 | 2.328(3) | << | C(5) | | | | Intra | 92.88 | 9.05 | 0.36095 | 1.02558 | 0.68001 | 2.3298 | 12.9479 | 8.8883 |
| 4 | 2.759(3) | << | C(6) | | | | Intra | 70.70 | -11.48 | 0.41464 | 1.04586 | 0.60999 | 3.3389 | 13.2040 | 7.9731 |
| 5 | 3.346(4) | .. | C(2)b | [x,2-y,-1/2+z | = | 4574.01] | | 147.03 | -61.70 | 0.20120 | 0.91210 | 0.42662 | 1.1145 | 11.5153 | 5.5763 |
| 6 | 3.379(4) | .. | C(3)c | [1/2-x,-1/2+y,3/2-z | = | 6546.01] | | -121.52 | -9.36 | 0.22280 | 0.61860 | 0.60994 | 0.7019 | 7.8098 | 7.9725 |
| 7 | 3.423(4) | .. | C(10)a | [1-x,2-y,1-z | = | 3676.01] | | -26.90 | -25.93 | 0.52890 | 0.73340 | 0.53750 | 5.1902 | 9.2592 | 7.0256 |
| 8 | 3.435(3) | .. | C(2)c | [1/2-x,-1/2+y,3/2-z | = | 6546.01] | | -99.78 | -17.41 | 0.29880 | 0.58790 | 0.57338 | 1.8882 | 7.4222 | 7.4946 |
| 9 | 3.460(3) | .. | C(3)b | [x,2-y,-1/2+z | = | 4574.01] | | 106.88 | -81.74 | 0.27720 | 0.88140 | 0.39006 | 2.3008 | 11.1277 | 5.0984 |
| 10 | 3.549(3) | .. | C(4) | | | | Intra | 105.63 | 14.37 | 0.31304 | 1.10594 | 0.71935 | 1.5189 | 13.9625 | 9.4026 |
| 11 | 3.552(3) | .. | O(3)a | [1-x,2-y,1-z | = | 3676.01] | | -1.84 | -36.58 | 0.52323 | 0.83648 | 0.49008 | 5.2958 | 10.5606 | 6.4058 |
| 12 | 2.49 | << | H(6A) | | | | Intra | 52.37 | -21.07 | 0.44550 | 0.98970 | 0.58340 | 3.8661 | 12.4950 | 7.6256 |
| 13 | 2.60 | < | H(10A)a | [1-x,2-y,1-z | = | 3676.01] | | -33.47 | -17.74 | 0.49460 | 0.73560 | 0.59140 | 4.5101 | 9.2870 | 7.7301 |
| 14 | 2.74 | .. | H(2A)b | [x,2-y,-1/2+z | = | 4574.01] | | 156.40 | -48.81 | 0.19660 | 0.90100 | 0.49410 | 0.7901 | 11.3751 | 6.4583 |
| 15 | 2.99 | .. | H(3A)b | [x,2-y,-1/2+z | = | 4574.01] | | 1.45 | -79.74 | 0.33680 | 0.84480 | 0.42680 | 2.9779 | 10.6656 | 5.5787 |
| 16 | 3.30 | .. | H(9A)c | [1/2-x,-1/2+y,3/2-z | = | 6546.01] | | -159.23 | 32.09 | 0.20910 | 0.76520 | 0.78610 | -0.1683 | 9.6607 | 10.2750 |
| 17 | 3.55 | .. | H(3A)c | [1/2-x,-1/2+y,3/2-z | = | 6546.01] | | -135.48 | -16.88 | 0.16320 | 0.65520 | 0.57320 | 0.0248 | 8.2719 | 7.4922 |

Angles (Degrees) At1...V...At2 with Vertex V = O(2)

| | | | | | | | | | | | | | | | |
|--------|---|--------|------------|--------|---|--------|------------|--------|---|--------|------------|--------|---|--------|------------|
| N(3) | , | O(1) | 27.86(13) | N(3) | , | C(5) | 34.17(13) | N(3) | , | C(6) | 62.26(14) | N(3) | , | C(2)b | 107.22(16) |
| N(3) | , | C(3)c | 126.63(18) | N(3) | , | C(10)a | 139.69(18) | N(3) | , | C(2)c | 146.94(18) | N(3) | , | C(3)b | 122.39(16) |
| N(3) | , | C(4) | 26.33(13) | N(3) | , | O(3)a | 126.17(17) | O(1) | , | C(5) | 62.03(10) | O(1) | , | C(6) | 89.20(10) |
| O(1) | , | C(2)b | 125.66(11) | O(1) | , | C(3)c | 104.57(10) | O(1) | , | C(10)a | 140.41(12) | O(1) | , | C(2)c | 121.03(11) |
| O(1) | , | C(3)b | 146.08(11) | O(1) | , | C(4) | 53.18(8) | O(1) | , | O(3)a | 142.38(11) | C(5) | , | C(6) | 30.13(8) |
| C(5) | , | C(2)b | 82.21(9) | C(5) | , | C(3)c | 146.06(12) | C(5) | , | C(10)a | 120.66(11) | C(5) | , | C(2)c | 165.12(12) |
| C(5) | , | C(3)b | 91.03(9) | C(5) | , | C(4) | 13.57(7) | C(5) | , | O(3)a | 99.15(10) | C(6) | , | C(2)b | 73.44(8) |
| C(6) | , | C(3)c | 155.88(10) | C(6) | , | C(10)a | 91.70(9) | C(6) | , | C(2)c | 149.63(10) | C(6) | , | C(3)b | 71.91(8) |
| C(6) | , | C(4) | 43.20(7) | C(6) | , | O(3)a | 69.22(7) | C(2)b | , | C(3)c | 82.45(8) | C(2)b | , | C(10)a | 92.24(8) |
| C(2)b | , | C(2)c | 85.11(8) | C(2)b | , | C(3)b | 22.57(7) | C(2)b | , | C(4) | 82.76(7) | C(2)b | , | O(3)a | 78.53(7) |
| C(3)c | , | C(10)a | 90.02(8) | C(3)c | , | C(2)c | 22.60(7) | C(3)c | , | C(3)b | 86.17(8) | C(3)c | , | C(4) | 133.66(10) |
| C(3)c | , | O(3)a | 107.19(8) | C(10)a | , | C(2)c | 67.46(8) | C(10)a | , | C(3)b | 69.92(8) | C(10)a | , | C(4) | 134.23(9) |
| C(10)a | , | O(3)a | 23.83(5) | C(2)c | , | C(3)b | 80.01(7) | C(2)c | , | C(4) | 155.39(10) | C(2)c | , | O(3)a | 85.85(7) |
| C(3)b | , | C(4) | 96.11(8) | C(3)b | , | O(3)a | 56.45(6) | C(4) | , | O(3)a | 112.42(7) | | | | |

3.6 Angstrom Coordination Sphere Around Atom I = N(3) [ARU = 1555.01] 0.35825 0.91443 0.71347 2.1632 11.5447 9.3257

| Nr | d(I,J) | To Atom J | Symm_Oper. on Atom J | ARU(J) | Type | Phi | Mu | X | Y | Z | X0 | Y0 | Z0 |
|----|----------|---------------------------------|----------------------|--------|-------|---------|--------|---------|---------|---------|---------|---------|---------|
| 1 | 1.225(3) | -- O(1) | | | Intra | -152.67 | 68.72 | 0.35411 | 0.89826 | 0.80081 | 1.7682 | 11.3405 | 10.4673 |
| 2 | 1.234(3) | -- O(2) | | | Intra | -72.47 | -40.65 | 0.36145 | 0.84373 | 0.65199 | 2.4451 | 10.6521 | 8.5221 |
| 3 | 1.479(3) | -- C(5) | | | Intra | 83.23 | -17.20 | 0.36095 | 1.02558 | 0.68001 | 2.3298 | 12.9479 | 8.8883 |
| 4 | 2.442(3) | << C(6) | | | Intra | 54.68 | -33.63 | 0.41464 | 1.04586 | 0.60999 | 3.3389 | 13.2040 | 7.9731 |
| 5 | 2.503(3) | << C(4) | | | Intra | 104.92 | 1.76 | 0.31304 | 1.10594 | 0.71935 | 1.5189 | 13.9625 | 9.4026 |
| 6 | 2.948(3) | .< N(2) | | | Intra | 128.63 | 19.18 | 0.25266 | 1.08671 | 0.78755 | 0.4249 | 13.7197 | 10.2940 |
| 7 | 3.334(4) | .. C(1) | | | Intra | 152.28 | 10.94 | 0.16113 | 1.03503 | 0.76187 | -0.7340 | 13.0673 | 9.9583 |
| 8 | 3.481(3) | .. S | | | Intra | 166.05 | -14.37 | 0.10157 | 0.97882 | 0.64738 | -1.1096 | 12.3576 | 8.4618 |
| 9 | 2.59 | .< H(6A) | | | Intra | 29.16 | -41.08 | 0.44550 | 0.98970 | 0.58340 | 3.8661 | 12.4950 | 7.6256 |
| 10 | 3.14 | .. H(9A)c [1/2-x, -1/2+y, 3/2-z | = 6546.01] | | | -141.06 | 17.57 | 0.20910 | 0.76520 | 0.78610 | -0.1683 | 9.6607 | 10.2750 |
| 11 | 3.18 | .. H(2A)b [x, 2-y, -1/2+z | = 4574.01] | | | -172.96 | -64.24 | 0.19660 | 0.90100 | 0.49410 | 0.7901 | 11.3751 | 6.4583 |
| 12 | 3.41 | .. H(6A)a [1-x, y, 3/2-z | = 2656.01] | | | 26.43 | 51.20 | 0.55450 | 0.98970 | 0.91660 | 4.0747 | 12.4950 | 11.9808 |

Angles (Degrees) At1...V...At2 with Vertex V = N(3)

| | | | | | | | | | | | | | | | |
|------|---|------|------------|------|---|------|------------|------|---|------|------------|------|---|------|------------|
| O(1) | , | O(2) | 124.1(2) | O(1) | , | C(5) | 118.0(2) | O(1) | , | C(6) | 141.67(18) | O(1) | , | C(4) | 92.83(16) |
| O(1) | , | N(2) | 68.08(14) | O(1) | , | C(1) | 67.61(14) | O(1) | , | S | 88.11(15) | O(2) | , | C(5) | 117.9(2) |
| O(2) | , | C(6) | 91.19(16) | O(2) | , | C(4) | 141.04(18) | O(2) | , | N(2) | 151.95(18) | O(2) | , | C(1) | 130.75(18) |
| O(2) | , | S | 102.84(16) | C(5) | , | C(6) | 30.41(12) | C(5) | , | C(4) | 28.58(12) | C(5) | , | N(2) | 57.56(12) |
| C(5) | , | C(1) | 73.78(13) | C(5) | , | S | 79.11(13) | C(6) | , | C(4) | 58.98(9) | C(6) | , | N(2) | 87.97(9) |
| C(6) | , | C(1) | 102.31(10) | C(6) | , | S | 99.00(9) | C(4) | , | N(2) | 29.02(7) | C(4) | , | C(1) | 47.88(8) |
| C(4) | , | S | 62.62(7) | N(2) | , | C(1) | 24.24(6) | N(2) | , | S | 49.82(5) | C(1) | , | S | 28.76(4) |

=====
Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6
=====

van der Waals (or ion) Radii used in the Analysis

=====
C H N O S

1.70 1.20 1.55 1.52 1.80

:: Grid: Y-Axis Step = 0.0167 = Points 60, Angstrom Step = 0.21
:: Grid: Z-Axis Step = 0.0139 = Points 72, Angstrom Step = 0.19
:: Grid: X-Axis Step = 0.0139 = Points 72, Angstrom Step = 0.19

:: Unit cell Contains NO Residual Solvent Accessible Void.

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

=====
Report Expected Number of Independent Reflections for given Symmetry and Resolution.

:: Hmax = 17 Kmax = 15 Lmax= 17 , Sorting Order : Fast H, Medium K, Slow L

:: Actual Theta-Max: 26.370 Deg. (Applied Theta Limit: 26.370 Deg.)

Space Group H-M: C2/c Laue: 2/m
Space Group Hall: -C 2yc [Schoenflies: C2h^6]
Lattice Type: mC, Centric, Monoclinic, Multiplicity: 4(2), No: 15

Nr ***** Symmetry Operation(s) *****

| | | | |
|---|-------|-------|---------|
| 1 | H , | K , | L |
| 2 | - H , | K , | 1/2 - L |
| 3 | - H , | - K , | - L |
| 4 | H , | - K , | 1/2 + L |

:: Number of Independent Type H, K, L Reflections = 2330

Table 0 - Crystal Data and Details of the Structure Determination
for: hmimomeno2C2/c R = 0.04

Crystal Data

| | | | |
|--------------------------|--------------------|------------|-----------|
| Formula | C10 H9 N3 O3 S | | |
| Formula Weight | 251.27 | | |
| Crystal System | monoclinic | | |
| Space group | C2/c | (No. 15) | |
| a, b, c [Angstrom] | 13.747(5) | 12.625(4) | 13.632(5) |
| alpha, beta, gamma [deg] | 90 | 106.496(5) | 90 |
| V [Ang**3] | 2268.5(14) | | |
| Z | 8 | | |
| D(calc) [g/cm**3] | 1.472 | | |
| Mu(MoKa) [/mm] | 0.285 | | |
| F(000) | 1040 | | |
| Crystal Size [mm] | 0.18 x 0.27 x 0.40 | | |

Data Collection

| | | | |
|----------------------------------|-----------------------------|---------|-------|
| Temperature (K) | 130 | | |
| Radiation [Angstrom] | MoKa | 0.71073 | |
| Theta Min-Max [Deg] | 2.2, 26.4 | | |
| Dataset | -17: 17 ; -15: 15 ; -17: 17 | | |
| Tot., Uniq. Data, R(int) | 12681, | 2330, | 0.067 |
| Observed Data [I > 2.0 sigma(I)] | 1962 | | |

Refinement

| | | | |
|--|----------------------|--|--|
| Nref, Npar | 2330, 158 | | |
| R, wR2, S | 0.0449, 0.1182, 1.12 | | |
| w = 1/[\s^2^(Fo^2^)+(0.0257P)^2^+4.8130P] where P=(Fo^2^+2Fc^2^)/3 | | | |
| Max. and Av. Shift/Error | 0.00, 0.00 | | |
| Min. and Max. Resd. Dens. [e/Ang^3] | -0.26, 0.36 | | |

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***** N O T I C E *****

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- PLATON Reference : Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.
 Spek, A.L. (2009). Acta Cryst. D65, 148-155.

- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow

- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)

- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.

- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.

- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@uu.nl

- Recent versions of PLATON may be obtained from <http://www.platonsoft.nl/xraysoft>

- More INFO can be found on <http://http://www.platonsoft.nl/>

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Page 44 --- SUMMARY

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR
=====

W: NOMOVE option used.

:: >>> WARNING: 'CONNECTED INPUT SET' is assumed to be TRUE

:: >>> The Network Analysis may be INCORRECT when this assumption is FALSE

=====

:: Input Xtal Data from File hmimomeno2ph.cif - Data Type CIF

:: NORMAL END of PLATON : 46 Pages on:

:: hmimomeno2ph.lis (ASCII, 132 Characters Wide)

:: hmimomeno2ph.lps (PostScript Version of .lis)

::