Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.


# Biological halogen bonds in protein-ligand complexes: a combined QTAIM and NCIPlot study in four representative cases

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**Table S1.** List of X-ray structures exhibiting biological HaBs with indication of the Ligand and Protein ID, the HaB donor and acceptor counterparts (Interaction), HaB distance (d in Å) and angle (A in º).

| Ligand ID | PDB ID | Interaction | d | A |
|---|---|---|---|---|
| I7T | 2Y6Q | I···S (MET375) | 2.831 | 176.6 |
| IMM | 1PGF | I···OC(LEU384) | 3.748 | 178.9 |
| IRF | 2J08 | I···OC(GLY342) | 3.351 | 166.8 |
| ISF | 1PGE | I···OC(LEU384) | 3.151 | 177.5 |
| K8Q | 6RLW | I···OC(GLY312) | 3.431 | 176.2 |
| IZG | 3PP1 | I···OC(VAL127) | 3.298 | 178.1 |
| KON | 6RZM | I···OC(GLY182) | 3.249 | 165.9 |
| LCJ | 6NYB | I···OC(VAL127) | 3.607 | 178.4 |
| LSG | 3MBL | I···OC(VAL127) | 3.252 | 176.2 |
| LUG | 3EQB | I···OC(VAL127) | 3.081 | 176.7 |
| M15 | 4LB3 | I···O(THR113) | 2.947 | 167.1 |
| M3K | 4ARK | I···OC(VAL127) | 3.439 | 178.0 |
| MEK | 3DV3 | I···OC(VAL127) | 3.147 | 177.2 |
| P96 | 4AGQ | I···OC(LEU145) | 2.978 | 176.0 |
| P74 | 4AGO | I···OC(LEU145) | 3.000 | 174.7 |
| P51 | 4AGP | I···OC(LEU145) | 2.989 | 175.2 |
| NXG | 4AGN | I···OC(LEU52) | 2.989 | 174.4 |
| PIH | 3DNA | I···SeC(MSE102)<br>I···OC(LEU84) | 3.383<br>3.396 | 170.5<br>164.2 |
| PYZ | 7NQX | I···OC(THR42) | 3.642 | 170.1 |
| Q2J | 6U99 | I···OC(GLY135) | 3.746 | 164.7 |
| Q2A | 6U9A | I···OC(GLY135) | 3.691 | 161.4 |
| Q2A | 6U9B | I···OC(GLY135) | 3.818 | 165.6 |
| Q2D | 6U98 | I···OC(GLY135) | 3.617 | 164.5 |
| QOA | 7M0W | I···OC(VAL127) | 3.561 | 177.1 |
| R22 | 2BE2 | I···OC(TYR188) | 3.372 | 168.5 |
| V04 | 3V04 | I···OC(VAL127) | 3.311 | 176.3 |
| T3W | 7B94 | I···OC(VAL127) | 3.480 | 175.2 |
| VKD | 7JUS | I···OC(VAL127) | 3.644 | 168.9 |
| VRA | 3E8N | I···OC(VAL127) | 3.309 | 176.2 |
| YJ8 | 2YJ8 | I···OC(GLY61) | 3.121 | 176.8 |
| YQY | 4ANB | I···OC(VAL127) | 3.430 | 173.9 |
| 0BT | 4L6C | I···OC(ARG163) | 3.172 | 171.4 |
| 136 | 1GJD | I···OC(VAL41) | 3.418 | 169.9 |
| 1CX | 3DY7 | I···OC(VAL127) | 3.354 | 178.6 |
| 1WW | 4LAZ | I···OC(THR113) | 3.031 | 165.6 |
| 21F | 4LYJ | I···OC(THR58) | 3.276 | 178.3 |
| 21F | 4LYH | I···OC(THR58) | 3.477 | 174.8 |
| 24I | 2C6C | I···OC(ILE456) | 3.767 | 165.4 |
| 2P7 | 4AN9 | I···OC(VAL127) | 3.777 | 172.2 |
| 33E | 4TKI | I···OC(GLY1043) | 2.907 | 179.2 |
| 3AC | 2B5J | I···OC(TYR188) | 3.567 | 169.4 |
| 3BM | 3EQC | I···OC(VAL127) | 3.113 | 178.4 |
| 3OR | 3ORN | I···OC(VAL127) | 3.592 | 179.1 |
| 3V0 | 3V01 | I···OC(VAL127) | 3.281 | 173.9 |
| 3WH | 4X21 | I···SC(MET146) | 3.051 | 173.1 |
| 42F | 4XP5 | I···OC(ASP121) | 3.273 | 165.9 |

| | | | | |
|---|---|---|---|---|
| 4BM | 7JUU | I···OC(VAL127) | 3.543 | 175.4 |
| 4BM | 7JV0 | I···OC(VAL127) | 3.747 | 169.4 |
| 4BM | 7M0X | I···OC(VAL127) | 3.173 | 177.4 |
| 4BM | 3EQG | I···OC(VAL127) | 3.177 | 176.5 |
| 4BM | 3VVH | I···OC(VAL127) | 3.198 | 177.2 |
| 4O9 | 4LBR | I···OC(THR113) | 2.933 | 165.6 |
| 573 | 4MNE | I···OC(VAL127) | 3.423 | 174.0 |
| 5EA | 1S9I | I···OC(VAL131) | 3.165 | 175.6 |
| 5I5 | 2I6A | I···OC(ILE39) | 3.282 | 162.1 |
| 5Y0 | 4AN3 | I···OC(VAL127) | 3.436 | 175.1 |
| 61V | 5HK2 | I···CC(TYR206) | 3.572 | 165.2 |
| 77D | 3SLS | I···OC(VAL127) | 3.130 | 174.8 |
| 7FO | 5TMV | I···OC(GLU419) | 3.175 | 170.8 |
| 7OV | 5U00 | I···OC(TYR827) | 3.062 | 176.1 |
| 9GH | 5O1I | I···OC(LEU145) | 2.887 | 175.0 |
| 9GK | 5O1G | I···OC(LEU145) | 2.919 | 177.1 |
| 9GN | 5O1H | I···OC(LEU145) | 2.921 | 177.4 |
| 9GO | 5O1F | I···OC(LEU145) | 2.929 | 177.6 |
| 9GT | 5O1E | I···OC(LEU145) | 2.913 | 177.5 |
| 9GW | 5O1D | I···OC(LEU145) | 2.944 | 177.1 |
| 9GZ | 5O1C | I···OC(LEU145) | 2.873 | 176.5 |
| BBM | 1S9J | I···OC(VAL127) | 3.134 | 176.1 |
| CZI | 1UHI | I···OC(THR166) | 3.119 | 174.2 |
| DIZ | 1T4E | I···OC(GLN72) | 3.085 | 163.9 |
| ELB | 6G3Y | I···OC(GLY312) | 3.353 | 173.4 |
| EUI | 7JUY | I···OC(VAL127) | 3.861 | 170.8 |
| FIB | 3DN3 | I···SC(MET102) | 2.867 | 172.1 |
| FIB | 3DN8 | I···SeC(MSE102) | 2.989 | 173.9 |
| G9J | 6DFN | I···OC(VAL533) | 3.089 | 173.5 |
| 9H2 | 5O1B | I···OC(LEU145) | 2.895 | 176.8 |
| 9H5 | 5O1A | I···OC(LEU145) | 2.867 | 176.9 |
| DIU | 2BXL | I···OC(ARG257) | 3.469 | 173.3 |
| DIU | 4LUH | I···OC(ASP450) | 3.499 | 170.2 |
| DIU | 5OSW | I···OC(GLU449) | 3.814 | 166.2 |
| P84 | 4AGL | I···OC(LEU145) | 2.980 | 175.3 |
| P86 | 4AGM | I···OC(LEU145) | 2.967 | 174.4 |
| T2B | 3WGW | I···OC(GLY127) | 3.069 | 174.1 |
| Y0V | 5AOJ | I···OC(LEU145) | 2.914 | 172.4 |
| 9ZZ | 5OOH | I···OC(THR177) | 3.390 | 175.1 |
| A0Z | 6SPW | I···OC(ASP237) | 2.888 | 175.1 |
| K8X | 3KXN | I···OC(VAL116) | 2.937 | 168.1 |
| T4A | 1KGI | I···OC(ALA709) | 3.074 | 164.6 |
| T44 | 4LNX | I···OC(PHE218) | 3.060 | 176.0 |
| T44 | 1SN0 | I···OC(LEU109) | 3.295 | 173.7 |
| T44 | 1HK1 | I···OC(ALA406) | 3.516 | 170.0 |
| T44 | 1F86 | I···OC(SER117) | 3.660 | 176.3 |
| T44 | 1ICT | I···OC(SER117) | 3.302 | 171.5 |
| T44 | 1HK2 | I···OC(ALA406) | 3.720 | 169.2 |
| T44 | 1HK3 | I···OC(ALA406) | 3.532 | 169.4 |
| T44 | 1ETB | I···OC(THR109) | 3.227 | 168.5 |
| T44 | 2CEO | I···OC(GLU377) | 3.793 | 162.1 |
| T44 | 1IE4 | I···OC(ALA109) | 3.071 | 167.0 |
| T44 | 5MHE | I···OC(MET111) | 3.700 | 164.8 |

| | | | | |
|---|---|---|---|---|
| 4HY | 2QPY | I···CC(TYR834) | 3.631 | 174.7 |
| 4HY | 3D57 | I···OC(PHE272) | 3.347 | 173.4 |
| 4HY | 3JZC | I···OC(PHE272) | 3.237 | 176.1 |
| 4HY | 3JZB | I···OC(PHE218) | 3.215 | 173.7 |
| 4HY | 2PIN | I···OC(PHE272) | 3.279 | 176.4 |
| 4HY | 2PKL | I···CC(TYR834) | 3.476 | 175.8 |
| 4HY | 2PIU | I···CC(TYR834) | 3.594 | 175.1 |
| 4HY | 2PIT | I···CC(TYR834) | 3.671 | 175.1 |
| 4HY | 1NQ0 | I···OC(PHE272) | 3.329 | 175.8 |
| 4HY | 1NUO | I···OC(PHE272) | 3.691 | 176.1 |
| 4HY | 1NQ2 | I···OC(PHE272) | 3.074 | 174.4 |
| 4QL | 5B34 | I···OC(ILE222) | 3.110 | 177.3 |
| B3I | 1BKE | I···OC(ARG257) | 3.707 | 175.8 |
| I3C | 3E3S | I···OC(GLY20) | 3.486 | 176.2 |
| I3C | 3E79 | I···OC(ALA334) | 3.040 | 161.1 |
| I3C | 3E3D | I···OC(TYR20) | 3.004 | 162.3 |
| I3C | 3E3T | I···OC(LEU141) | 2.829 | 169.4 |
| I3C | 4NC7 | I···OC(GLU34) | 2.110 | 167.7 |
| I3C | 4BVX | I···OC(LEU171) | 3.071 | 168.1 |
| I3C | 3Q7S | I···OC(LEU23) | 2.791 | 177.2 |
| I3C | 5U84 | I···OC(ARG193) | 2.901 | 168.5 |
| I3C | 6EG7 | I···OC(ASP146) | 2.879 | 174.4 |
| I3C | 6MRY | I···OC(GLN3) | 3.122 | 165.2 |
| I3C | 6NQZ | I···OC(THR74) | 3.400 | 170.3 |
| I3C | 6QE4 | I···OC(LEU292) | 3.336 | 166.4 |
| I3C | 7JSY | I···OC(SER312) | 3.309 | 173.8 |
| T3 | 2H77 | I···OC(PHE218) | 3.118 | 176.6 |
| T3 | 4NLW | I···OC(PHE218) | 3.057 | 175.3 |
| T3 | 3VKX | I···OC(GLY127) | 3.068 | 171.1 |
| T3 | 4LNX | I···OC(PHE218) | 3.060 | 176.0 |
| T3 | 1BSX | I···OC(PHE272) | 3.325 | 175.8 |
| T3 | 3GWS | I···OC(PHE272) | 3.101 | 174.5 |
| T3 | 4ZO1 | I···OC(GLY344) | 3.107 | 162.1 |

**Cartesian coordinates of the PDB models**

**3DNA@MSE102**

| | | | |
|---|---|---|---|
| C | 4.1787552 | -0.8318630 | 2.4378021 |
| C | 3.5257552 | 0.4721370 | 1.9648021 |
| O | 3.8027552 | 1.5461370 | 2.5028021 |
| N | 2.6517552 | 0.3701370 | 0.9678021 |
| C | 1.9667552 | 1.5451370 | 0.4348021 |
| C | 1.0867552 | 2.2161370 | 1.4878021 |
| O | 1.1217552 | 3.4381370 | 1.6468021 |
| C | 1.1557552 | 1.1791370 | -0.8091979 |
| C | 2.0227552 | 0.9051370 | -2.0231979 |
| Se | 0.9867552 | 0.7171370 | -3.6481979 |
| C | 0.5617552 | 2.5801370 | -3.9891979 |
| N | 0.3197552 | 1.4121370 | 2.2188021 |
| C | -0.5632448 | 1.9301370 | 3.2678021 |
| C | -3.4772448 | -1.8308630 | -0.1601979 |
| C | -4.3512448 | -2.6668630 | 0.5358021 |
| C | -4.8272448 | -3.8318630 | -0.0721979 |
| C | -4.4292448 | -4.1548630 | -1.3711979 |
| C | -3.5542448 | -3.3138630 | -2.0671979 |
| C | -3.0762448 | -2.1498630 | -1.4591979 |
| I | -1.7582448 | -0.8768630 | -2.4781979 |
| H | 3.9029897 | -0.9927505 | 3.4987171 |
| H | -0.5402563 | 3.0326664 | 3.1935926 |
| H | 2.7194545 | 2.3239439 | 0.1929050 |
| H | 0.4776694 | 0.3236565 | -0.6026147 |
| H | 0.4887488 | 2.0404298 | -1.0228342 |
| H | 2.5924994 | -0.0431694 | -1.9325065 |
| H | 2.7701876 | 1.7107972 | -2.1783501 |
| H | 0.9999209 | 3.2163070 | -3.1956375 |
| H | -0.5345378 | 2.7272104 | -3.9928038 |
| H | 0.9819466 | 2.8871936 | -4.9656326 |
| H | -3.1076213 | -0.9096816 | 0.3169060 |
| H | -4.6629007 | -2.4027683 | 1.5580956 |
| H | -5.5175889 | -4.4945900 | 0.4722953 |
| H | -4.8028117 | -5.0704689 | -1.8551864 |
| H | -3.2460247 | -3.5704564 | -3.0921680 |
| H | 3.9039249 | -1.7336014 | 1.8537916 |
| H | 5.2774618 | -0.7001381 | 2.4066119 |
| H | -1.6021143 | 1.5671126 | 3.1276481 |
| H | -0.2100731 | 1.6327934 | 4.2777114 |
| H | 0.4235798 | 0.4012679 | 2.1144865 |
| H | 2.4908989 | -0.5343602 | 0.5211292 |

**3DNA@LEU84**

| | | | |
|---|---|---|---|
| C | -5.2245734 | 0.2486797 | -0.5622114 |
| C | -3.8505734 | -0.4093203 | -0.6672114 |
| O | -3.5805734 | -1.1363203 | -1.6252114 |
| N | -2.9965734 | -0.1603203 | 0.3247886 |

| | | | |
|---|---|---|---|
| C | -1.6205734 | -0.6603203 | 0.3087886 |
| C | -1.5035734 | -2.1353203 | 0.6897886 |
| O | -0.6675734 | -2.8533203 | 0.1367886 |
| C | -0.7185734 | 0.1846797 | 1.2197886 |
| C | -0.5695734 | 1.6816797 | 0.9207886 |
| C | 0.4784266 | 2.2966797 | 1.8387886 |
| C | -0.2235734 | 1.9296797 | -0.5472114 |
| N | -2.3345734 | -2.5763203 | 1.6317886 |
| C | -2.2595734 | -3.9463203 | 2.1517886 |
| C | 4.5644266 | -0.6023203 | -2.5492114 |
| C | 5.4994266 | 0.3416797 | -2.9792114 |
| C | 5.7134266 | 1.4986797 | -2.2322114 |
| C | 4.9944266 | 1.7136797 | -1.0572114 |
| C | 4.0574266 | 0.7746797 | -0.6272114 |
| C | 3.8424266 | -0.3833203 | -1.3752114 |
| I | 2.4394266 | -1.7933203 | -0.7312114 |
| H | -5.9931096 | -0.5489286 | -0.5783003 |
| H | -1.0527768 | 0.0481420 | 2.2749313 |
| H | 0.2883604 | -0.2843136 | 1.1665743 |
| H | -1.5444100 | 2.1848272 | 1.1305816 |
| H | -0.0566738 | 3.0083103 | -0.7446643 |
| H | 0.7059022 | 1.3877750 | -0.8280049 |
| H | -1.0262507 | 1.5870364 | -1.2311159 |
| H | 0.2468270 | 2.1235437 | 2.9107101 |
| H | 0.5623677 | 3.3916616 | 1.6834282 |
| H | 1.4784194 | 1.8530591 | 1.6418021 |
| H | -1.2574095 | -0.6284703 | -0.7380780 |
| H | -1.3623262 | -4.4133294 | 1.7061111 |
| H | 4.3971476 | -1.5161773 | -3.1384448 |
| H | 6.0637804 | 0.1638336 | -3.9074284 |
| H | 6.4516571 | 2.2431259 | -2.5684549 |
| H | 5.1604494 | 2.6249787 | -0.4620106 |
| H | 3.4914281 | 0.9470214 | 0.3007830 |
| H | -3.1514741 | -4.5411374 | 1.8625522 |
| H | -2.1719155 | -3.9442692 | 3.2576718 |
| H | -5.3843668 | 0.8668435 | -1.4670700 |
| H | -5.3783463 | 0.8796114 | 0.3370006 |
| H | -3.2412128 | 0.5375650 | 1.0297191 |
| H | -3.0782525 | -1.9542698 | 1.9534689 |

**4x21**

| | | | |
|---|---|---|---|
| C | 0.0811085 | -3.3264682 | 5.8894747 |
| C | -0.9528915 | -2.2284682 | 5.7494747 |
| O | -1.3898915 | -1.6334682 | 6.7354747 |
| N | -1.3128915 | -1.9584682 | 4.5194747 |
| C | -2.2318915 | -0.8924682 | 4.2014747 |
| C | -3.3438915 | -1.3844682 | 3.2794747 |
| O | -3.2478915 | -2.4404682 | 2.6844747 |
| C | -1.4798915 | 0.2685318 | 3.5384747 |
| C | -0.2828915 | 0.7855318 | 4.2984747 |
| S | 0.9791085 | 1.5055318 | 3.2874747 |

| | | | |
|---|---|---|---|
| C | 2.1611085 | 0.2255318 | 3.2154747 |
| N | -4.3698915 | -0.5694682 | 3.1264747 |
| C | -5.4278915 | -0.9184682 | 2.2024747 |
| C | -1.3188915 | 0.5095318 | -3.9685253 |
| C | -1.2018915 | 0.1675318 | -6.3755253 |
| N | -1.8708915 | 0.2305318 | -5.1275253 |
| N | -0.0468915 | 0.7905318 | -3.9855253 |
| C | 0.5241085 | 1.0435318 | -2.8055253 |
| C | -0.2398915 | 1.0335318 | -1.6395253 |
| I | 0.4061085 | 1.4105318 | 0.2924747 |
| C | -1.5978915 | 0.7275318 | -1.7565253 |
| N | -2.1298915 | 0.4605318 | -2.9215253 |
| C | 1.9351085 | 1.3585318 | -2.8095253 |
| C | 2.6681085 | 1.9285318 | -1.8215253 |
| N | 3.9661085 | 2.0555318 | -2.1875253 |
| C | 4.0971085 | 1.5795318 | -3.4385253 |
| C | 2.8621085 | 1.1175318 | -3.8775253 |
| C | 2.7411085 | 0.5675318 | -5.1515253 |
| C | 3.8651085 | 0.4805318 | -5.9665253 |
| C | 5.0951085 | 0.9505318 | -5.4995253 |
| C | 5.1931085 | 1.5045318 | -4.2435253 |
| H | 0.2272227 | -3.9374024 | 4.9760613 |
| H | -2.1800779 | 1.0984176 | 3.3068589 |
| H | -1.1430150 | -0.0998405 | 2.5436110 |
| H | -0.5863591 | 1.5413453 | 5.0525482 |
| H | 0.1890787 | -0.0305870 | 4.8832135 |
| H | 1.7548936 | -0.7063154 | 2.7650500 |
| H | 2.5874790 | -0.0123745 | 4.2134341 |
| H | 2.9871706 | 0.5714929 | 2.5627478 |
| H | -2.6541251 | -0.5639771 | 5.1774724 |
| H | -6.0645225 | -1.7412663 | 2.5936429 |
| H | -0.4708992 | -0.6732918 | -6.4299496 |
| H | -2.2538532 | 0.6966625 | -0.8664977 |
| H | 2.3597550 | 2.3494943 | -0.8666861 |
| H | 4.6954598 | 2.5002559 | -1.6344985 |
| H | 1.7550044 | 0.2247044 | -5.4874295 |
| H | 3.7830675 | 0.0457376 | -6.9743434 |
| H | 5.9892539 | 0.8927089 | -6.1389537 |
| H | 6.1687308 | 1.8764824 | -3.8866167 |
| H | -1.9417563 | 0.0289082 | -7.1865486 |
| H | -0.6269405 | 1.0962739 | -6.5817042 |
| H | -4.9914804 | -1.2682791 | 1.2467147 |
| H | -6.0648902 | -0.0344012 | 2.0116838 |
| H | -0.2060516 | -3.9845180 | 6.7310957 |
| H | 1.0528036 | -2.8643807 | 6.1593108 |
| H | -1.1067324 | -2.5994585 | 3.7478094 |
| H | -4.4576699 | 0.2678565 | 3.7023528 |
| H | -2.8607740 | -0.0112111 | -5.0787009 |

**5HK2**

| | | | |
|---|---|---|---|
| C | -5.5883863 | 1.1225453 | -0.3926241 |

| | | | |
|---|---|---|---|
| C | -4.7113863 | 0.2645453 | 0.5133759 |
| O | -5.0433863 | -0.8854547 | 0.7993759 |
| N | -3.5953863 | 0.8265453 | 0.9663759 |
| C | -2.7123863 | 0.1235453 | 1.8883759 |
| C | -3.4203863 | -0.0864547 | 3.2213759 |
| O | -3.3483863 | -1.1654547 | 3.8123759 |
| C | -1.4113863 | 0.8995453 | 2.0973759 |
| C | -0.3233863 | 0.1065453 | 2.7903759 |
| C | -0.3433863 | -1.2834547 | 2.7953759 |
| C | 0.7206137 | 0.7465453 | 3.4473759 |
| C | 0.6496137 | -2.0134547 | 3.4263759 |
| C | 1.7166137 | 0.0245453 | 4.0823759 |
| C | 1.6756137 | -1.3544547 | 4.0683759 |
| O | 2.6626137 | -2.0764547 | 4.6973759 |
| N | -4.1083863 | 0.9565453 | 3.6783759 |
| C | -4.8313863 | 0.9265453 | 4.9463759 |
| C | 5.5476137 | -0.2584547 | -7.5746241 |
| C | 3.8236137 | 0.1025453 | -5.8936241 |
| C | 3.3916137 | -0.1114547 | -4.5936241 |
| C | 2.0976137 | 0.2645453 | -4.2586241 |
| C | 1.6216137 | 0.0635453 | -2.9716241 |
| C | 2.4446137 | -0.5164547 | -2.0186241 |
| C | 3.7406137 | -0.8974547 | -2.3506241 |
| C | 4.2186137 | -0.6964547 | -3.6416241 |
| N | 5.0236137 | -0.4074547 | -6.2106241 |
| O | 3.1116137 | 0.7185453 | -6.6866241 |
| I | 1.7156137 | -0.8114547 | -0.0856241 |
| H | -6.5584034 | 1.2855052 | 0.1183158 |
| H | -1.6193201 | 1.8355404 | 2.6606495 |
| H | -1.0314951 | 1.2143308 | 1.0951845 |
| H | -1.1689792 | -1.8398489 | 2.3363532 |
| H | 0.7564535 | 1.8480917 | 3.4670482 |
| H | 0.6279832 | -3.1123845 | 3.4373551 |
| H | 2.5378423 | 0.5492670 | 4.5982954 |
| H | 3.2931281 | -1.4476017 | 5.0929284 |
| H | -2.5374033 | -0.8882818 | 1.4783534 |
| H | -4.5569103 | -0.0163180 | 5.4554107 |
| H | 4.8642154 | 0.4245214 | -8.1117557 |
| H | 1.4742528 | 0.7218703 | -5.0389664 |
| H | 0.5947294 | 0.3623216 | -2.7132412 |
| H | 4.3933301 | -1.3490817 | -1.5885001 |
| H | 5.2647670 | -0.9669911 | -3.8372187 |
| H | -5.1606641 | 2.1082057 | -0.6677436 |
| H | -5.8040165 | 0.5499255 | -1.3149974 |
| H | -4.5507752 | 1.7888065 | 5.5857823 |
| H | -5.9310092 | 0.9368388 | 4.7902431 |
| H | 6.5710861 | 0.1705512 | -7.5640367 |
| H | 5.5746149 | -1.2310764 | -8.1107782 |
| H | -3.3029193 | 1.7367940 | 0.6055792 |
| H | -4.2322219 | 1.7605381 | 3.0609993 |
| H | 5.5000399 | -1.0533808 | -5.5873484 |

**3PP1**

| | | | |
|---|---|---|---|
| C | -2.2994255 | -4.6424371 | -2.3078033 |
| C | -1.8304255 | -4.6964371 | -0.8718033 |
| O | -2.4734255 | -5.3364371 | -0.0348033 |
| N | -0.7064255 | -4.0364371 | -0.5918033 |
| C | -0.1844255 | -3.9164371 | 0.7721967 |
| C | -1.2204255 | -3.2664371 | 1.6921967 |
| O | -1.8654255 | -2.2724371 | 1.3371967 |
| N | -1.3804255 | -3.8594371 | 2.8681967 |
| C | -2.2964255 | -3.3534371 | 3.8731967 |
| C | 2.4665745 | 6.7955629 | -2.1048033 |
| N | 2.7435745 | 5.8415629 | -1.1388033 |
| C | 2.0235745 | 4.6815629 | -0.8258033 |
| C | 0.8865745 | 4.2695629 | -1.5238033 |
| C | 0.2145745 | 3.1015629 | -1.1608033 |
| C | 0.6445745 | 2.3205629 | -0.0808033 |
| I | -0.4014255 | 0.5535629 | 0.4741967 |
| C | 1.7825745 | 2.7445629 | 0.6151967 |
| C | 2.4735745 | 3.9085629 | 0.2511967 |
| F | 3.5735745 | 4.2915629 | 0.9481967 |
| H | -1.5680117 | -4.2187625 | -3.0254322 |
| H | 0.1254186 | -4.9162077 | 1.1456833 |
| H | -1.8351405 | -3.3929561 | 4.8806649 |
| H | -3.2458109 | -3.9309104 | 3.8894643 |
| H | 0.5209700 | 4.8691915 | -2.3692009 |
| H | -0.6766044 | 2.8023875 | -1.7333398 |
| H | 2.1718261 | 2.1765762 | 1.4739771 |
| H | -2.5379399 | -2.3059660 | 3.6143834 |
| H | -2.5661051 | -5.6687278 | -2.6237856 |
| H | -3.2275792 | -4.0375019 | -2.3509973 |
| H | -0.3210591 | -3.4020918 | -1.2911868 |
| H | -0.9556625 | -4.7756794 | 3.0167521 |
| H | 0.7109617 | -3.2648634 | 0.7410726 |
| H | 3.5208467 | 6.0181558 | -0.5054149 |
| H | 2.4560089 | 6.3838065 | -3.1450675 |
| H | 1.4799488 | 7.3087160 | -1.9671342 |
| H | 3.2409590 | 7.5865750 | -2.0886292 |