Observation of a reversible Isomorphous Phase Transtion and an interplay of "σ-hole" and "π-hole" in Fmoc-Leu-ψ[CH_2-NCS]

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S1. Experimental Methods

Single crystal X-ray diffraction

A good quality Single crystal of size ~ 0.3 mm was chosen using a polarizing microscope and affixed to a Hampton Research Cryoloop using Paratone-N oil. X-ray diffraction data at room temperature (resolution, d=0.77 Å) was collected on an Oxford Xcalibur (Mova) diffractometer equipped with an EOS CCD detector using MoK_α radiation (λ = 0.71073 Å). The crystal to detector distance was fixed at 45 mm and the scan width (Δω) was 1º per frame during the data collection. The crystal was cooled to 100 K with a liquid nitrogen stream using an Oxford Instruments Cryojet-HT nitrogen gas-stream cooling device. A high resolution X-ray data set at 100K of charge density quality (d = 0.45 Å), with high redundancy and completeness of 100% was collected for the low temperature Z'=2 form. Cell refinement, data integration and reduction were carried out using the program CrysAlisPro.[1] Face indexing was done for the accurate numerical absorption correction. Sorting, scaling, and merging of the data sets were carried out using the program SORTAV.[2] The crystal structure was solved by direct methods using SHELXS97 and refined according to spherical-atom approximation (based on F^2) using

SHELXL97 included in the WinGX suite.[3, 4] The hydrogen atoms were fixed stereochemically and the position and isotropic thermal parameters were allowed to refine in the spherical atom model for the room temperature form.

The reversibility of the phase transition was established by determining the unit cell parameters at different temperatures during the heating and cooling cycles from 290-100K in steps of 10K on the same crystal.

Multipole Refinement.

The charge density modeling and multipolar non−spherical atom refinements for Fmoc-Leu-ψ[CH_2-NCS] have been performed with XD2006[5] using the Hansen and Coppens multipole formalism.[6] The function minimized in the least-square procedure was $\Sigma w\{|F_o|^2 - K|F_c|^2\}$, with only those reflections with $I > 3\sigma(I)$. The core and valence scattering factors of all atoms were derived from Su, Coppens and Macchi wave functions.[7, 8] The multipole expansion was truncated at the hexadecapole level for the S atoms, octupole level for the O, N and C atoms and quadrupole level for the H atoms. Initially, the scale factor was refined against the whole resolution range of diffraction data. The scatter plots (Figure S3) showing the dependence of F_{obs}/F_{cal} with $\sin\theta/\lambda$ and the variation of F_{obs} with F_{cal} clearly depicts the quality of the collected data sets. The positional and anisotropic displacement parameters of the non-hydrogen atoms were refined against the reflections with $\sin\theta/\lambda > 0.7$ Å^{-1}. In the next step, the position and displacement parameters of all non-hydrogen atoms were kept fixed to the obtained values and X—H bond lengths were constrained to the values determined by neutron diffraction experiments.[9] The isotropic displacement parameters for H-atoms were refined using reflections

$\sin\theta/\lambda < 0.7$ Å^{-1}. The converged model was used to calculate anisotropic displacement parameters of H-atoms using the SHADE2 analysis.[10, 11] Estimated ADPs for H-atoms were kept fixed during the subsequent multipole refinements and only monopole, bond directed dipole (d_z) and quadrupole (q_{3z^2-1}) components were allowed to refine. For non-hydrogen atoms, the scale, positional and anisotropic displacement parameters, P_{val}, $P_{lm,}$ upto octupole level (l=3), κ and κ' were allowed to refine in a stepwise manner, until the convergence was reached. Two molecules in the asymmetric unit were treated chemically equivalent except the terminal isothiocyanate group during the least-square refinement. Separate κ and κ' were used to define different atom types based on chemical environment. Anharmonic motion for the sulfur atoms was modeled with third and fourth-order Gram-Charlier components.[12] The resultant probability density function (pdf) indicated that this modeling was physically reasonable.

S2. Computational methods:

Two approaches have been considered for theoretical charge density analysis (i) generating theoretical structure factors from CRYSTAL14[13] followed by multipole modelling[6] in XD2006[5] at B3LYP/TZVP level[14, 15] (ii) obtaining topological features directly from wave function analysis using TOPOND program[16] as implemented in CRYSTAL14.

(i) The coordinates from final experimental charge density model was taken as input for periodic quantum mechanical calculations using CRYSTAL14. The single point calculation was performed at the B3LYP/TZVP level of theory. The shrinking factors (IS1, IS2 and IS3) along with the reciprocal lattice vectors were set to 4 (18 k–points in irreducible Brillouin zone). The bi-electronic Coulomb and exchange series values for the truncation parameter were set as ITOL1–ITOL4 = 7 and ITOL5 = 18, respectively. The level shifter was set to 0.7 Hartree/cycle

for better convergence. Upon convergence on energy (~10^{-7} Hartree), the periodic wave functions were obtained and the XFAC keyword was used to generate the theoretical structure factors at the same resolution as observed from the experiments. The atomic positions were held fixed to the values obtained from the experimental charge density during the multipolar refinement with theoretical structure factors. All theoretical structure factors were assigned unit weights during the refinements based on the methodology followed in the literature. The anisotropic displacement parameters were set to zero to consider a static model and multipolar refinements of the theoretical data were carried out up to the same levels as those used for the experimental charge density modelling.

(ii) TOPOND[16] is considerably different from other existing implementations of QTAIM[17] for crystalline systems due to its interface with CRYSTAL package and thus becomes a powerful tool for applying QTAIM to molecules, polymers, surfaces and crystals, exploiting the full symmetry of each of these systems. It calculates full topological features of $\rho(r)$ and $\nabla^2\rho(r)$ scalar fields along with other QTAIM descriptors directly from wave function analysis. The level of theory used is B3LYP/TZVP in our systems.

S3. CSD analysis

A Cambridge Structural Database (CSD v5.35 February 2014) analysis was carried out to investigate the number of reported structures of isothiocyanates and also to find out the propensity of forming the perpendicular N=C=S···N=C=S intermolecular interaction. It has been observed that though isothiocyanates are more common in organometallics, it is relatively rare as organic molecules. (Table S1) Moreover, the perpendicular interaction mode of the NCS groups is sparse (Table S1, Figure S1) .

Table S1. Summary of CSD analysis

	Total No. of hits	No. of hits for specific intermolecular interactions*
N=C=S	5359[a] *400*[b]	154[a] *8*[b]
C– N=C=S	66[a] *51*[b]	1[a] *0*[b]

*The interaction geometry is specified in Figure S1.[a]organics+ organometalics, [b]only organics, given in italics.

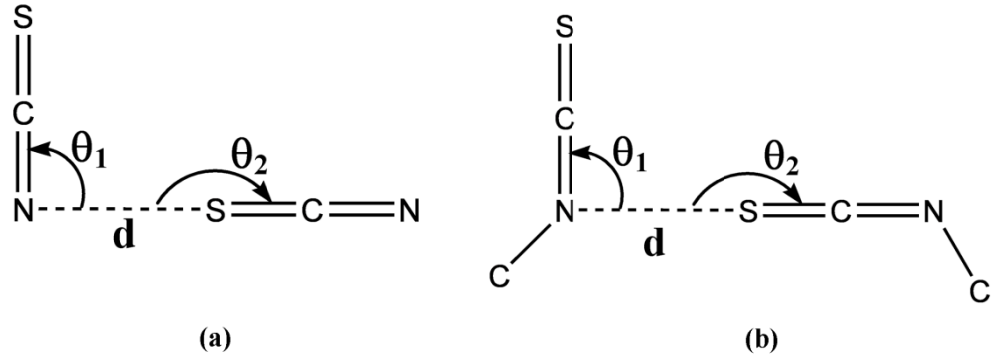

Figure S1. The perpendicular approach of the NCS groups are specified by three parameters, θ_1= 90°±30°, θ_2= 160°±20° and d ≤ sum of van der Waals radii of S and N + 0.3 Å

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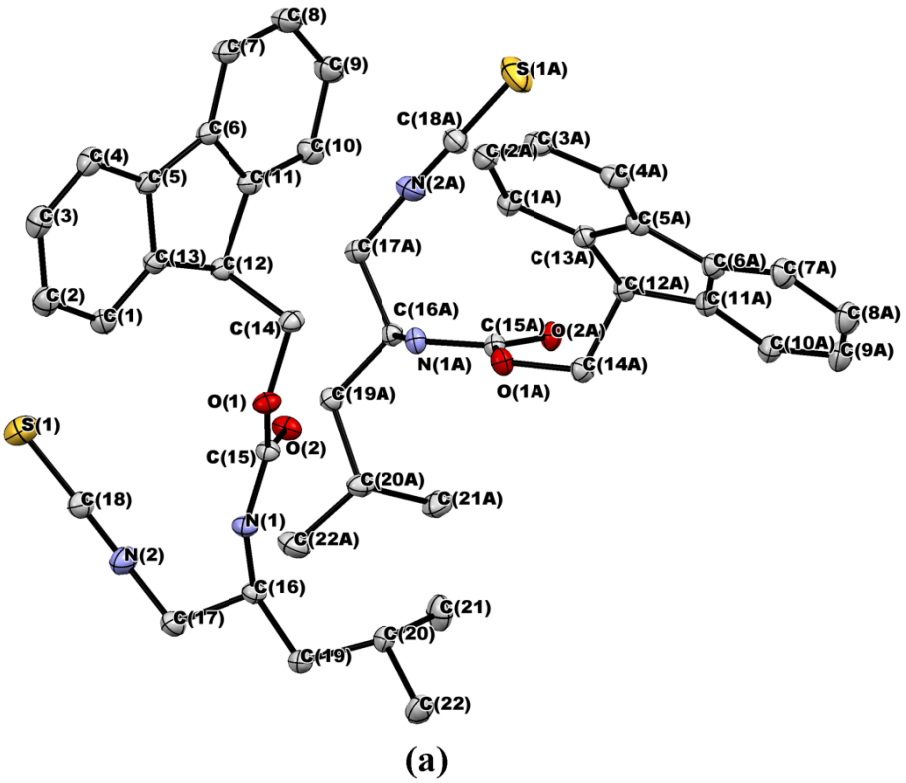

Figure S2a. ORTEP diagram (with 50% probability ellipsoid) of (a) Fmoc–Leu–CH_2NCS

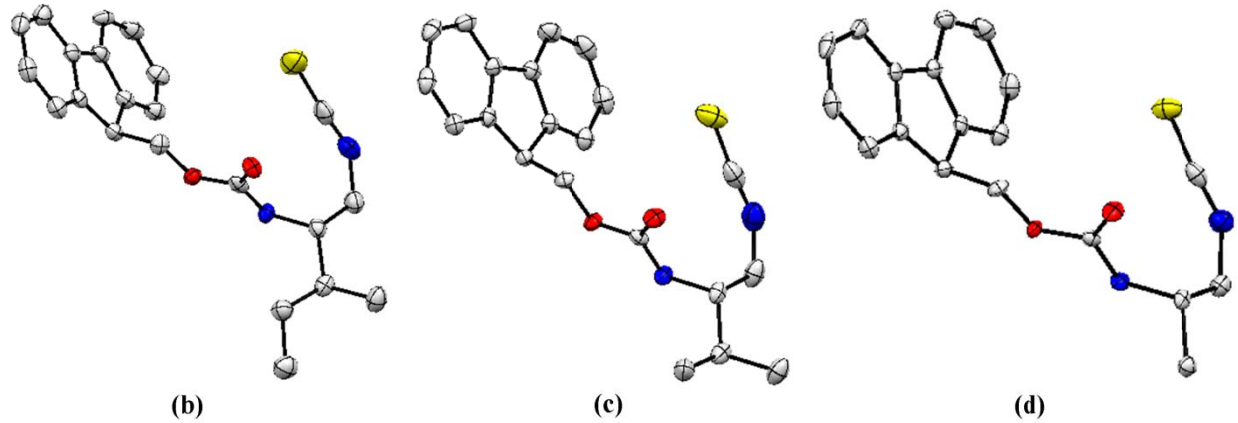

Figure S2b. ORTEP diagram (with 50% probability ellipsoid) of Fmoc–X–CH_2NCS (b) X=Ile, (c) X=Val, (d) X=Ala.

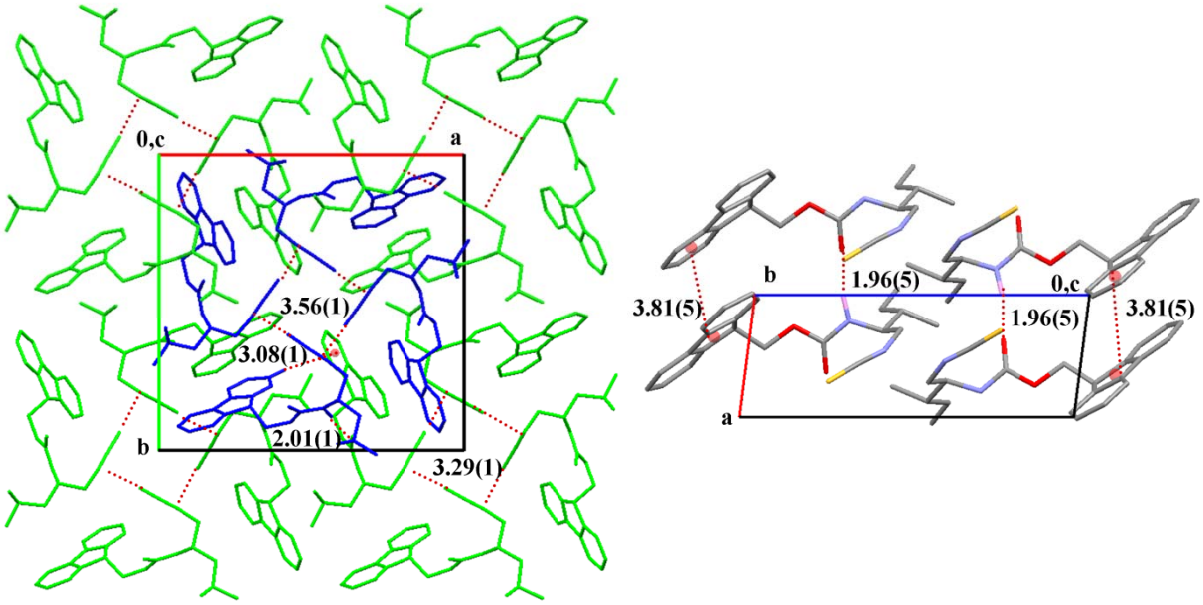

Figure S3. Packing diagrams (a) projection along c axis in Fmoc–Leu–CH_2NCS. The S···N distance is 3.29(1) Å in MOL1 (green) and 3.56(1) Å in MOL2 (blue). The edge to face C–H···π distance involving fluorene moiety is 3.08(1). (b) projection along c axis in Fmoc–Ile–CH_2NCS showing N–H···O hydrogen bonds and face to face π···π interaction involving fluorene moiety.

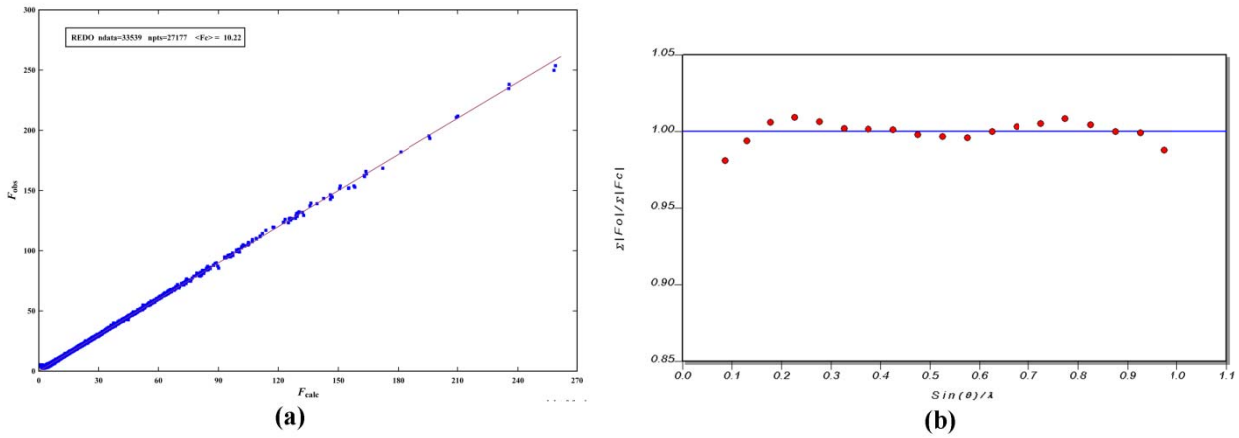

Figure S4. Experimental charge density in Fmoc–Leu–CH_2NCS indicating the quality of the dataset; (a) Scatter plot depicting the variation of F_{obs} with F_{calc} , (b) Variation of F_{obs}/F_{calc} with $\sin\theta/\lambda$

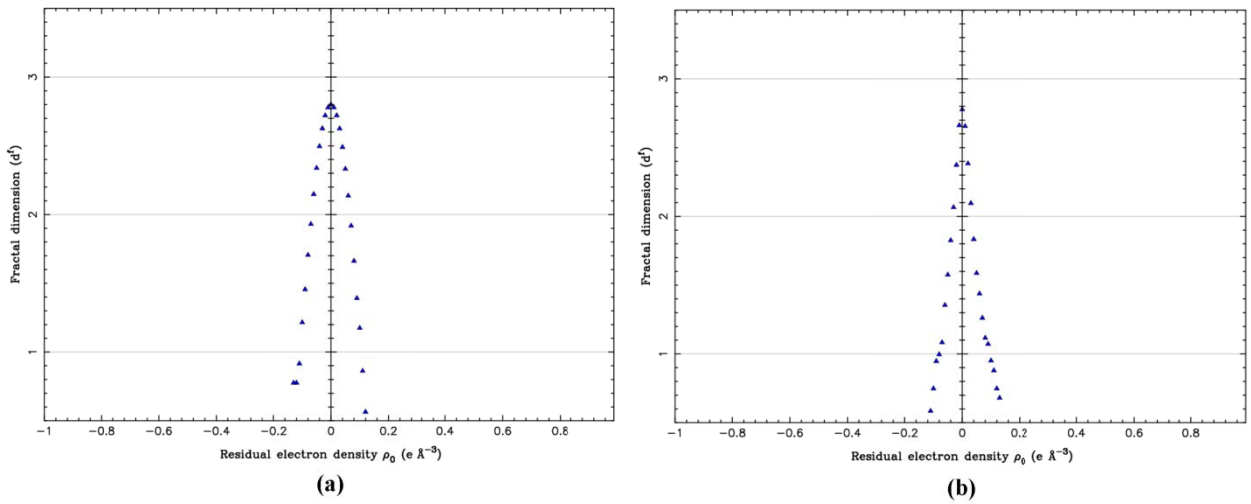

Figure S5. Fractal dimension plot of (a) experimental (b) theoretical multipole model

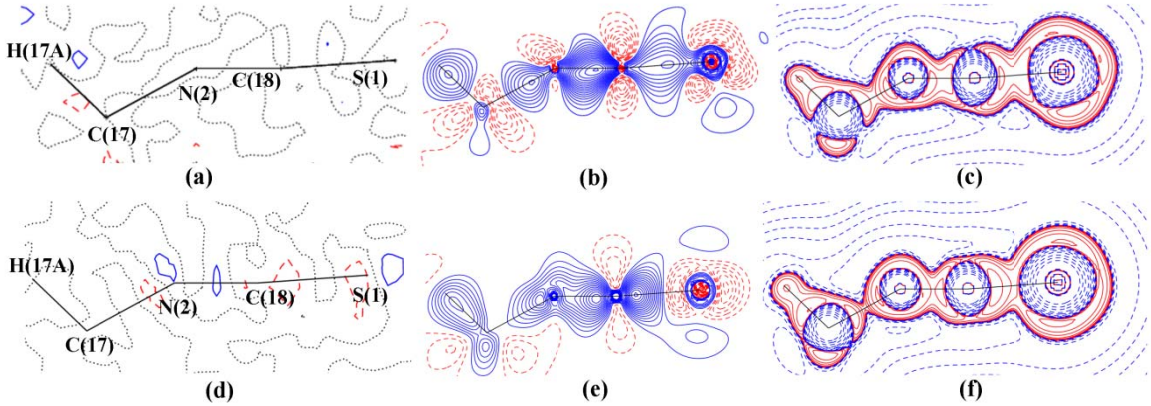

Figure S6a. (a) Residual (b) deformation and (c) Laplacian of the electron density maps of the isothiocyanate group in MOL1 obtained from experimental charge density analysis (1st row); second row depicts (d) residual (e) deformation and (f) Laplacian maps from theoretical multipole model.

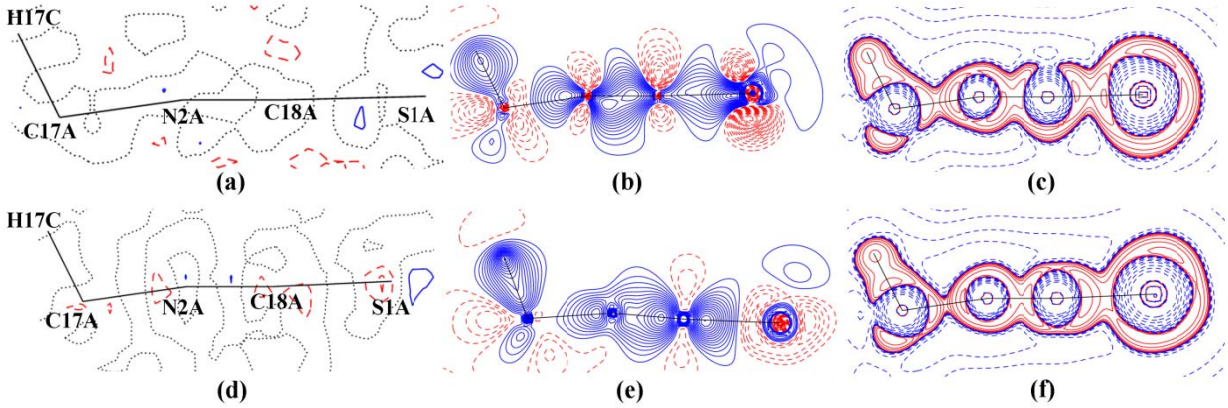

Figure S6b. (a) Residual (b) deformation and (c) Laplacian of the electron density maps of the isothiocyanate group in MOL2 obtained from experimental charge density analysis (1st row); second row depicts (d) residual (e) deformation and (f) Laplacian maps from theoretical multipole model.

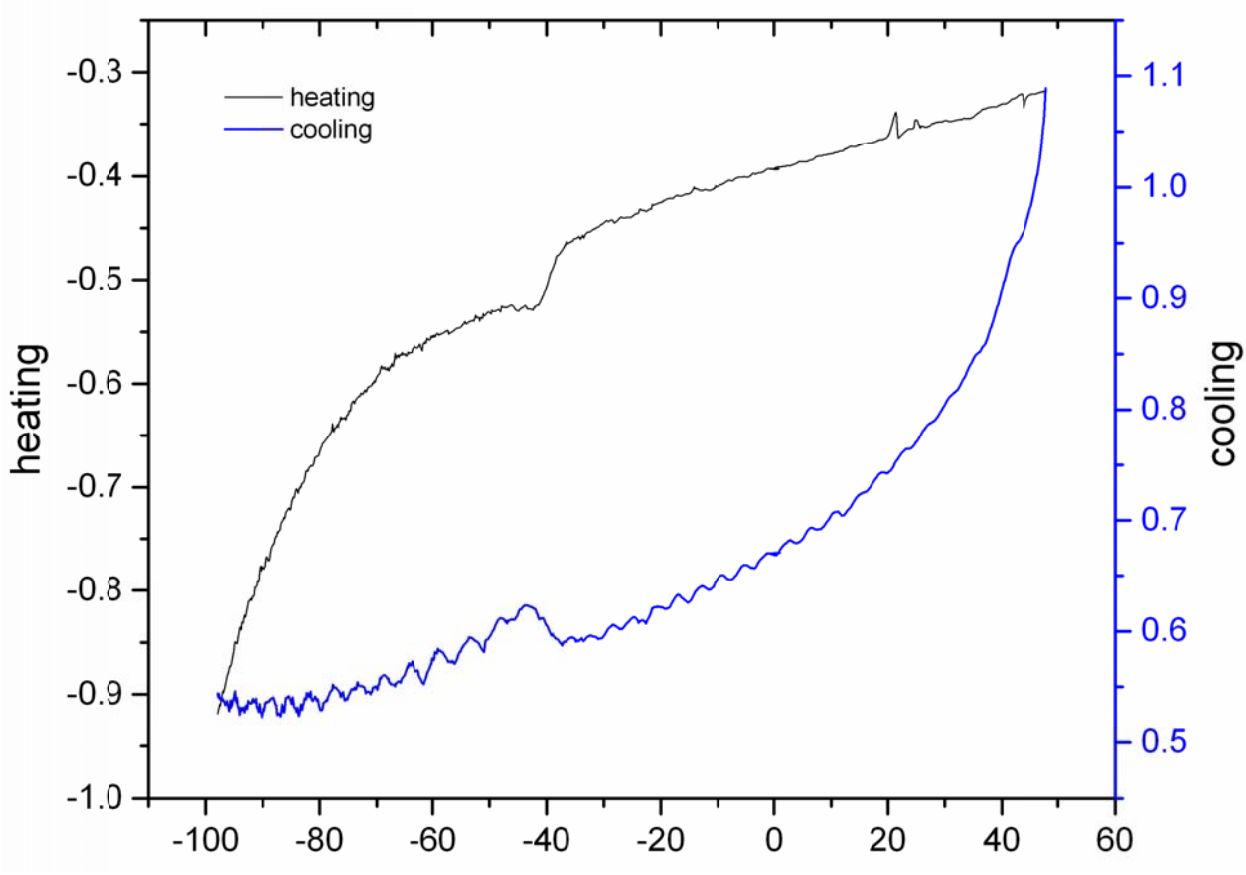

Figure S7. DSC thermograph of Fmoc–Leu–CH_2NCS for heating and cooling cycles.

Table S2a. Crystallographic data of Fmoc–Leu–ψ[CH_2NCS]

CCDC number	1030735	1030363
Empirical Formula	C22 H24 N2 O2 S1	C22 H24 N2 O2 S1
Crystal habit	Block	Block
Crystal size (mm)	0.530 x 0.231 x 0.141	0.599 x 0.310 x 0.256
Crystallizing solvent	Ethyl acetate: hexane (1:1)	Ethyl acetate: hexane (1:1)
Space Group	P 4_1	P 4_1
a(Å)	12.4405(5)	17.4665(1)
c(Å)	13.4141(8)	13.1291(1)
Volume (Å^3)	2076.1(2)	4005.41(4)
Z	4	8
Z'	1	2
Formula weight	380.50	380.50
Calculated density (g/cm^3)	1.217	1.262
F(0 0 0)	808	1616
Radiation	Mo K_α (0.71073 Å)	Mo K_α (0.71073 Å)
Temperature (K)	298 (2)	100(2)
θ range (°)	2.6-26.0	2.6-50.1
Measured reflections	10114	530944
Observed reflection	5371	32688(42280)
	Spherical atom refinement	
R_obs, wR2_obs	0.0596/0.1041	0.0390,0.0969
GoF	1.027	1.0
Max/min Δρ (e/ Å^3)	0.235/-0.167	0.617/-0.529
Data to parameter ratio	5371/250=21.5:1	42280/499=84.7
	Multipole refinement	
Refinement based on		F^2
Observed reflections [I>3σ(I)]		27177
Parameters		940
R(F^2), wR(F^2)		0.023, 0.046
GoF		1.067
Max/min Δρ (e/ Å^3)		-0.141/0.123

Table S2b. Crystallographic data of Fmoc–X–ψ[CH_2NCS], X=Ile, Val and Ala

CCDC number	1030364	1030365	1030366
Empirical Formula	C22 H24 N2 O2 S1	C21 H22 N2 O2 S1	C19 H18 N2 O2 S1
Crystal habit	plate	plate	plate
Crystal size (mm)	0.276 x 0.204 x 0.072	0.257 x 0.239 x 0.048	0.409 x 0.239 x 0.066
Crystallizing solvent	Ethyl acetate: hexane (1:1)	Ethyl acetate: hexane (1:1)	Ethyl acetate: hexane (1:1)
Space Group	P 2_1	P 2_1	P 2_1
a(Å)	4.9386(3)	4.9807(2)	4.9690(2)
b(Å)	15.0974(9)	15.9306(6)	11.3897(4)
c(Å)	13.3932(15)	12.0456(5)	15.0388(5)
β(°)	97.286(7)	99.174(4)	91.707(3)

Volume (Å^3)	990.53(14)	943.54(7)	850.75(5)
Z	2	2	2
Z'	1	1	1
Formula weight	380.50	366.48	338.42
Calculated density (g/cm^3)	1.276	1.290	1.321
F(0 0 0)	404	388	356
Radiation	Mo K_α (0.71073 Å)	Mo K_α (0.71073 Å)	Mo K_α (0.71073 Å)
Temperature (K)	100 (2)	100(2)	100(2)
θ range (°)	2.7-26.0	2.6-26.0	2.7-26.0
Measured reflections	7233	6646	6544
Observed reflection	3881	3702	3343
R_obs/ wR2_obs	0.0613/0.0938	0.0444/0.0812	0.0337/0.0695
GoF	0.983	1.034	1.054
Max/min Δρ (e/ Å^3)	0.234/-0.204	0.189/-0.206	0.196/-0.198
Data to parameter ratio	3881/250=15.5:1	3702/237=15.6:1	3343/222=15.1:1

Table S3. H-bond geometry in Fmoc–Leu–ψ[CH_2NCS]

	D—H···A	D—H (Å)	H···A (Å)	D···A (Å)	∠D—H···A (°)	Symmetry
MOL1	N1—H1N···O2A	0.85(2)	2.17(2)	2.995(1)	164(2)	x,y,z
	C2—H2···Cg9[a]	1.0812	3.314	4.321	155.49	
MOL2	N1A—H1NA ···O2	0.85(2)	2.18(2)	3.007(1)	165(2)	-x+1,-y,+z+1/2
	C2A—H2A···Cg3[a]	1.0824	3.085	4.033	146.68	

[a] Cg9 is the centroid of the 6-membered ring C6A—C7A—C8A—C9A—C10A—C11A. Cg3 is the centroid of the 6-membered ring C6—C7—C8—C9—C10—C11.

Table S4. Topological parameters obtained at the bond critical point (BCP) for NCS moiety in MOL1 and MOL2 of Fmoc–Leu–ψ[CH_2NCS]. r_1 and r_2 are the distances from the BCP to the first atom (A) and second atom (B), respectively. The interaction length, $R_{ij}= (r_1 + r_2)$. [a]

	Atom A	Atom B	R_{ij} (Å) (A–B)	r_1 (Å) (A–CP)	r_2 (Å) (A–CP)	ρ(r) (eÅ^{-3})	$\nabla^2\rho(r)$ (eÅ^{-5})	λ_1	λ_2	λ_3	ε
MOL1	S1	C18	**1.5891**	**0.842**	**0.747**	**1.82**	**-10.9**	**-10.23**	**-8.91**	**8.25**	**0.15**
			1.5930	*0.606*	*0.987*	*1.41*	*14.4*	*-4.39*	*-3.49*	*22.28*	*0.26*
			1.5887	0.627	0.962	1.40	14.4				
	N2	C18	**1.1817**	**0.754**	**0.428**	**3.16**	**-31.8**	**-28.66**	**-26.27**	**23.08**	**0.09**
			1.1833	*0.711*	*0.472*	*2.95*	*-28.2*	*-21.21*	*-20.55*	*13.58*	*0.03*
			1.1812	0.765	0.416	3.00	-14.6				
MOL2	S1A	C18A	**1.5914**	**0.882**	**0.710**	**1.81**	**-8.1**	**-10.59**	**-10.03**	**12.47**	**0.06**
			1.6052	*0.619*	*0.986*	*1.42*	*7.4*	*-4.47*	*-3.90*	*15.73*	*0.15*
			1.5961	0.629	0.967	1.38	13.9				
	N2A	C18A	**1.1685**	**0.7448**	**0.4237**	**3.04**	**-22.8**	**-25.29**	**-23.90**	**26.36**	**0.06**
			1.1700	*0.712*	*0.458*	*3.04*	*-29.8*	*-22.99*	*-21.82*	*14.97*	*0.05*
			1.1669	0.758	0.409	3.02	-7.1				

[a] First/second/third row displays **experimental**/ theoretical multipole/TOPOND calculated values.

Data collection and multipole details of the experimental charge density of Fmoc–Leu–CH_2NCS

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#  Dictionary vers : 2.3
#  Request file    : c:/winxd/lib/xd/xdcif.dat
#  CIF files read  : geo lsm


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#                   UNIT CELL INFORMATION
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_cell_measurement_theta_max     43.8880

#------------------------------------------------------------------------------
#
#                   CRYSTAL INFORMATION
#
#------------------------------------------------------------------------------
#
_exptl_crystal_description       block
_exptl_crystal_colour            colourless

_exptl_crystal_size_max                             0.5992
_exptl_crystal_size_mid                             0.3100
_exptl_crystal_size_min                             0.2556
_exptl_crystal_size_rad          ?
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.262
_exptl_crystal_density_method    'Not Measured'
_exptl_crystal_F_000             1616
_exptl_crystal_density_meas_temp ?

#------------------------------------------------------------------------------
#
#                   ABSORPTION CORRECTION
#
#------------------------------------------------------------------------------
#
 loop_
_exptl_crystal_face_index_h
_exptl_crystal_face_index_k
_exptl_crystal_face_index_l
_exptl_crystal_face_perp_dist
```

```
_exptl_oxdiff_crystal_face_indexfrac_h
_exptl_oxdiff_crystal_face_indexfrac_k
_exptl_oxdiff_crystal_face_indexfrac_l
_exptl_oxdiff_crystal_face_x
_exptl_oxdiff_crystal_face_y
_exptl_oxdiff_crystal_face_z
 -18  -17   -1 0.1676 -17.8258 -16.9032 -1.1698  0.7845 -0.6022  0.1477
 -20  -10    7 0.1522 -19.9993 -10.4895  7.3699  0.7323 -0.5616 -0.3851
   4   17   13 0.1999  4.2840 16.6937 13.2219 -0.4089  0.3148 -0.8566
   9  -13   14 0.1598  9.2059 -13.0523 14.0926 -0.4896 -0.7983 -0.3507
  23    1   -7 0.1637 22.8914  0.8631 -6.7821 -0.8134  0.1948  0.5482
 -24   -4    3 0.1338 -24.0164 -4.2392  2.5160  0.9269 -0.2223 -0.3025
  23    7    2 0.1640 23.4429  7.1527  1.7033 -0.9712  0.2332  0.0488
  22   -9   -4 0.1550 22.4442 -8.8926 -3.6350 -0.7961 -0.2362  0.5572
 -23    8    1 0.1166 -23.2098  8.0058  1.3756  0.8591  0.2548 -0.4439
  14    3   15 0.1961 14.0517  3.0710 15.0244 -0.7587 -0.2242 -0.6116
  24   -7    1 0.1560 23.5989 -6.8018  1.2814 -0.9138 -0.2709  0.3025
   2   -4  -18 0.3395  2.0044 -3.6699 -18.2484  0.1734  0.2816  0.9437
 -14   20   -3 0.1125 -13.6575 20.0534 -3.1609  0.4933  0.8053 -0.3290
 -14   -9  -13 0.2852 -13.9987 -8.9986 -13.0007  0.7551 -0.0401  0.6152
  14  -20    1 0.1327 13.8024 -20.3537  0.9410 -0.4689 -0.7657  0.4403
  10   22   -2 0.1334 10.0752 22.3701 -1.5326 -0.4682  0.8622 -0.1931
  10   23   -1 0.1324  9.8451 22.5184 -1.0849 -0.4656  0.8574 -0.2192
  13   12   13 0.1833 13.0504 12.4330 12.6078 -0.7270  0.1752 -0.6639
 -10  -23    1 0.1932 -9.7533 -22.5720  0.9099  0.4645 -0.8554  0.2293
  -9   -1   17 0.2492 -8.8727 -1.0893 17.2546  0.1287 -0.4367 -0.8904
  19   16    0 0.1348 18.5329 16.1979 -0.1934 -0.7916  0.6076 -0.0641
  -8  -19   10 0.2071 -8.2007 -19.3441  9.6534  0.2768 -0.9352 -0.2207
  13   16  -10 0.1619 13.0018 15.9985 -9.9995 -0.4467  0.8217  0.3435
_exptl_absorpt_coefficient_mu                    0.181
_exptl_absorpt_correction_T_min                  0.859
_exptl_absorpt_correction_T_max                  1.843
_exptl_absorpt_correction_type            'gaussian'
_exptl_absorpt_process_details
;
CrysAlisPro, Agilent Technologies,
Version 1.171.36.28 (release 01-02-2013 CrysAlis171 .NET)
(compiled Feb  1 2013,16:14:44)
Numerical absorption correction based on gaussian integration over
                  a multifaceted crystal model
;

#------------------------------------------------------------------------------
#
#                   DATA COLLECTION
#
#------------------------------------------------------------------------------
#
 _exptl_special_details
;
A nitrogen gas-flow low temperature device was used to cool the crystal.
A face indexed analytical absorption correction was performed.
;
_diffrn_ambient_temperature      100(2)
_diffrn_radiation_wavelength     0.71073
_diffrn_radiation_probe          x-ray
_diffrn_radiation_type           MoK\a
```

```
_diffrn_radiation_source         'Mova (Mo) X-ray Source'
_diffrn_radiation_monochromator  mirror
_diffrn_measurement_device_type  'Xcalibur, Eos, Nova'
_diffrn_detector_area_resol_mean 8.0419
_diffrn_reflns_number 530944
_diffrn_reflns_av_R_equivalents 0.0683
_diffrn_reflns_av_sigmaI/netI 0.0851
_diffrn_reflns_limit_h_min -37
_diffrn_reflns_limit_h_max 37
_diffrn_reflns_limit_k_min -37
_diffrn_reflns_limit_k_max 37
_diffrn_reflns_limit_l_min -28
_diffrn_reflns_limit_l_max 28
_diffrn_reflns_theta_min 2.6076
_diffrn_reflns_theta_max 50.5794
_diffrn_measured_fraction_theta_max 0.9998
_diffrn_reflns_theta_full 26.3154
_diffrn_measured_fraction_theta_full 0.9986
_diffrn_orient_matrix_UB_11      -0.0392178000
_diffrn_orient_matrix_UB_12      -0.0041571000
_diffrn_orient_matrix_UB_13      -0.0129721000
_diffrn_orient_matrix_UB_21       0.0003703000
_diffrn_orient_matrix_UB_22       0.0368155000
_diffrn_orient_matrix_UB_23      -0.0227934000
_diffrn_orient_matrix_UB_31       0.0105873000
_diffrn_orient_matrix_UB_32      -0.0166369000
_diffrn_orient_matrix_UB_33      -0.0472079000
_diffrn_measurement_details
;
#__ type_ start__ end____ width___ exp.time_
  1 omega  -17.00   67.00   1.0000    5.0000
omega____ theta____ kappa____ phi______ frames
    -        0.0000   57.0000   60.0000 84

#__ type_ start__ end____ width___ exp.time_
  2 omega  -44.00   42.00   1.0000    5.0000
omega____ theta____ kappa____ phi______ frames
    -       22.0000  -65.0000  -35.3935 86

#__ type_ start__ end____ width___ exp.time_
  3 omega   -6.00   47.00   1.0000    5.0000
omega____ theta____ kappa____ phi______ frames
    -       22.0000   79.0000 -119.0273 53

#__ type_ start__ end____ width___ exp.time_
  4 omega  -41.00   50.00   1.0000    5.0000
omega____ theta____ kappa____ phi______ frames
    -       26.0000  -72.0000 -112.7324 91

#__ type_ start__ end____ width___ exp.time_
  5 omega  -40.00   46.00   1.0000    5.0000
omega____ theta____ kappa____ phi______ frames
    -       26.0000  -65.0000   93.4368 86

#__ type_ start__ end____ width___ exp.time_
  6 omega    6.00   47.00   1.0000   10.0000
omega____ theta____ kappa____ phi______ frames
```

```
    -       34.0000   79.0000   83.1354 41

#__ type_ start__ end____ width___ exp.time_
  7 omega   10.00   46.00   1.0000   15.0000
omega____ theta____ kappa____ phi______ frames
    -       38.0000   80.0000  100.7223 36

#__ type_ start__ end____ width___ exp.time_
  8 omega   14.00   47.00   1.0000   15.0000
omega____ theta____ kappa____ phi______ frames
    -       42.0000   79.0000  -79.9077 33

#__ type_ start__ end____ width___ exp.time_
  9 omega   14.00   46.00   1.0000   15.0000
omega____ theta____ kappa____ phi______ frames
    -       42.0000   80.0000  -21.9823 32

#__ type_ start__ end____ width___ exp.time_
 10 omega   18.00   46.00   1.0000   20.0000
omega____ theta____ kappa____ phi______ frames
    -       46.0000   80.0000   67.9150 28

#__ type_ start__ end____ width___ exp.time_
 11 omega   18.00   47.00   1.0000   20.0000
omega____ theta____ kappa____ phi______ frames
    -       46.0000   79.0000   21.5631 29

#__ type_ start__ end____ width___ exp.time_
 12 omega   19.00   49.00   1.0000   20.0000
omega____ theta____ kappa____ phi______ frames
    -       46.0000   78.0000 -154.6487 30

#__ type_ start__ end____ width___ exp.time_
 13 omega   19.00   49.00   1.0000   20.0000
omega____ theta____ kappa____ phi______ frames
    -       46.0000   78.0000  136.6745 30

#__ type_ start__ end____ width___ exp.time_
 14 omega   18.00   47.00   1.0000   20.0000
omega____ theta____ kappa____ phi______ frames
    -       46.0000   79.0000 -125.5837 29

#__ type_ start__ end____ width___ exp.time_
 15 omega   23.00   49.00   1.0000   20.0000
omega____ theta____ kappa____ phi______ frames
    -       50.0000   78.0000  154.8597 26

#__ type_ start__ end____ width___ exp.time_
 16 omega   29.00  121.00   1.0000   30.0000
omega____ theta____ kappa____ phi______ frames
    -       54.0000   74.0000  -89.2875 92

#__ type_ start__ end____ width___ exp.time_
 17 omega   27.00  122.00   1.0000   30.0000
omega____ theta____ kappa____ phi______ frames
    -       54.0000   77.0000   39.6605 95
```

```
#__ type_ start__ end____ width___ exp.time_
 18 omega   29.00  121.00   1.0000   30.0000
omega____ theta____ kappa____ phi______ frames
    -       54.0000   74.0000  -38.3141 92

#__ type_ start__ end____ width___ exp.time_
 19 omega   31.00  126.00   1.0000   40.0000
omega____ theta____ kappa____ phi______ frames
    -       58.0000   77.0000    4.2501 95

#__ type_ start__ end____ width___ exp.time_
 20 omega   31.00  126.00   1.0000   40.0000
omega____ theta____ kappa____ phi______ frames
    -       58.0000   77.0000  162.6741 95

#__ type_ start__ end____ width___ exp.time_
 21 omega   32.00  125.00   1.0000   40.0000
omega____ theta____ kappa____ phi______ frames
    -       58.0000   76.0000   95.3589 93

#__ type_ start__ end____ width___ exp.time_
 22 omega   32.00   57.00   1.0000   40.0000
omega____ theta____ kappa____ phi______ frames
    -       58.0000   76.0000 -140.2878 25

#__ type_ start__ end____ width___ exp.time_
 23 omega   79.00  139.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000   60.0000 60

#__ type_ start__ end____ width___ exp.time_
 24 omega   80.00  132.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000  120.0000 52

#__ type_ start__ end____ width___ exp.time_
 25 omega   15.00  100.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591  -80.0000  118.3841 85

#__ type_ start__ end____ width___ exp.time_
 26 omega   45.00   70.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000  120.0000 25

#__ type_ start__ end____ width___ exp.time_
 27 omega   78.00  123.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000  -30.0000 45

#__ type_ start__ end____ width___ exp.time_
 28 omega   45.00   70.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000   60.0000 25

#__ type_ start__ end____ width___ exp.time_
 29 omega   45.00   70.00   1.0000   50.0000
```

```
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000  -30.0000 25

#__ type_ start__ end____ width___ exp.time_
 30 omega    3.00   69.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591  -30.0000  120.0000 66

#__ type_ start__ end____ width___ exp.time_
 31 omega    4.00   95.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591  -80.0000 -129.0744 91

#__ type_ start__ end____ width___ exp.time_
 32 omega   82.00  139.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000  150.0000 57

#__ type_ start__ end____ width___ exp.time_
 33 omega   45.00   70.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000  150.0000 25

#__ type_ start__ end____ width___ exp.time_
 34 omega   63.00   89.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591  -80.0000   45.0689 26

#__ type_ start__ end____ width___ exp.time_
 35 omega   64.00   90.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591  -80.0000  -87.4654 26

#__ type_ start__ end____ width___ exp.time_
 36 omega    4.00   53.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591  -80.0000   45.0689 49

#__ type_ start__ end____ width___ exp.time_
 37 omega   45.00   70.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000  -60.0000 25

#__ type_ start__ end____ width___ exp.time_
 38 omega    8.00   58.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591  -80.0000  -87.4654 50

#__ type_ start__ end____ width___ exp.time_
 39 omega   79.00  137.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000   30.0000 58

#__ type_ start__ end____ width___ exp.time_
 40 omega   45.00   70.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000   30.0000 25
```

```
#__ type_ start__ end____ width___ exp.time_
 41 omega   78.00  139.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000   90.0000 61

#__ type_ start__ end____ width___ exp.time_
 42 omega   45.00   70.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000   90.0000 25

#__ type_ start__ end____ width___ exp.time_
 43 omega   81.00  128.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000    0.0000 47

#__ type_ start__ end____ width___ exp.time_
 44 omega   80.00  131.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000  -60.0000 51

#__ type_ start__ end____ width___ exp.time_
 45 omega   45.00   70.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000 -120.0000 25

#__ type_ start__ end____ width___ exp.time_
 46 omega   81.00  137.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000 -120.0000 56

#__ type_ start__ end____ width___ exp.time_
 47 omega   45.00   78.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000    0.0000 33

#__ type_ start__ end____ width___ exp.time_
 48 omega   80.00  139.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000  -90.0000 59

#__ type_ start__ end____ width___ exp.time_
 49 omega   45.00   70.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000 -180.0000 25

#__ type_ start__ end____ width___ exp.time_
 50 omega   77.00  127.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000 -180.0000 50

#__ type_ start__ end____ width___ exp.time_
 51 omega   75.00  100.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591  -80.0000   92.5700 25

#__ type_ start__ end____ width___ exp.time_
```

```
 52 omega   45.00   70.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000  -90.0000 25

#__ type_ start__ end____ width___ exp.time_
 53 omega   78.00  133.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000 -150.0000 55

#__ type_ start__ end____ width___ exp.time_
 54 omega    4.00   49.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591  -80.0000   92.5700 45

#__ type_ start__ end____ width___ exp.time_
 55 omega   45.00   71.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591   77.0000 -150.0000 26

#__ type_ start__ end____ width___ exp.time_
 56 omega    8.00   99.00   1.0000   50.0000
omega____ theta____ kappa____ phi______ frames
    -       71.8591  -80.0000  -24.4676 91

;
_diffrn_measurement_method '\w scans'

_diffrn_reflns_reduction_process
;
;

# number of unique reflections
_reflns_number_total              42280
_reflns_number_gt                 32688
_reflns_threshold_expression     I>3\s(I)

#-----------------------------------------------------------------------------
#
#                    COMPUTER PROGRAMS USED
#
#-----------------------------------------------------------------------------
#

_computing_data_collection
;
CrysAlisPro, Agilent Technologies,
Version 1.171.36.28 (release 01-02-2013 CrysAlis171 .NET)
(compiled Feb  1 2013,16:14:44)
;
_computing_cell_refinement
;
CrysAlisPro, Agilent Technologies,
Version 1.171.36.28 (release 01-02-2013 CrysAlis171 .NET)
(compiled Feb  1 2013,16:14:44)
;
_computing_data_reduction
;
```

```
CrysAlisPro, Agilent Technologies,
Version 1.171.36.28 (release 01-02-2013 CrysAlis171 .NET)
(compiled Feb  1 2013,16:14:44)
;
_computing_structure_refinement         'Volkov et al, (2006)'
_computing_molecular_graphics           'Volkov et al, (2006)'
_computing_publication_material         'Volkov et al, (2006)'

#------------------------------------------------------------------------------
#
#                   REFINEMENT INFORMATION
#
#------------------------------------------------------------------------------
#

_refine_special_details
;
Reflections were merged with Sortav (Blessing, 1995).
;
_refine_ls_structure_factor_coef        Fsqd
_refine_ls_matrix_type                  full
_refine_ls_weighting_scheme             calc
_refine_ls_weighting_details
;
        calc w2 = 1/[s^2^(Fo^2^)]
;
_refine_ls_extinction_method            none
_refine_ls_number_reflns                27177
_refine_ls_number_parameters            940
_refine_ls_number_restraints            0
_refine_ls_R_factor_all                 0.038
_refine_ls_R_factor_gt                  0.023
_refine_ls_wR_factor_ref                0.046
_refine_ls_goodness_of_fit_ref          1.067
_refine_ls_shift/su_max                 0

#------------------------------------------------------------------------------
#
#                   ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS
#
#------------------------------------------------------------------------------
#

loop_
    _atom_site_label
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
S(1) 0.12844(3) -0.05971(2) 0.705283 0.031 1 4
S(1A) 0.57650(4) -0.38958(5) 0.96607(8) 0.039 1 4
O(1) 0.398795(18) -0.03949(2) 0.64976(5) 0.017 1 4
O(1A) 0.56877(2) -0.095527(18) 0.89331(5) 0.017 1 4
O(2) 0.36753(2) -0.04646(2) 0.81766(5) 0.018 1 4
O(2A) 0.57374(2) -0.14594(2) 1.05290(5) 0.017 1 4
```

N(1) 0.348051(18) 0.06292(2) 0.72383(5) 0.015 1 4
N(1A) 0.461871(19) -0.142435(18) 0.96116(5) 0.015 1 4
N(2) 0.19623(3) 0.06177(4) 0.80636(7) 0.025 1 4
N(2A) 0.44936(4) -0.30259(3) 1.01238(7) 0.026 1 4
C(1) 0.28029(2) -0.11163(2) 0.49703(6) 0.021 1 4
C(1A) 0.63179(2) -0.21712(2) 0.73420(5) 0.02 1 4
C(2) 0.25183(3) -0.11983(3) 0.39784(6) 0.025 1 4
C(2A) 0.63956(3) -0.24551(2) 0.63491(6) 0.023 1 4
C(3) 0.26572(3) -0.18708(3) 0.34261(5) 0.025 1 4
C(3A) 0.70964(3) -0.23982(2) 0.58366(5) 0.022 1 4
C(4) 0.30785(2) -0.24726(3) 0.38495(5) 0.022 1 4
C(4A) 0.77321(3) -0.20575(2) 0.63011(5) 0.02 1 4
C(5) 0.33706(2) -0.23853(2) 0.48336(5) 0.017 1 4
C(5A) 0.76507(2) -0.17675(2) 0.72879(5) 0.016 1 4
C(6) 0.38280(2) -0.29070(2) 0.54672(5) 0.018 1 4
C(6A) 0.82032(2) -0.13785(2) 0.79535(5) 0.017 1 4
C(7) 0.41207(3) -0.36358(3) 0.52645(6) 0.023 1 4
C(7A) 0.89663(3) -0.11734(3) 0.77960(6) 0.023 1 4
C(8) 0.45290(3) -0.40127(3) 0.60321(6) 0.027 1 4
C(8A) 0.93605(3) -0.08028(3) 0.85810(6) 0.027 1 4
C(9) 0.46461(3) -0.36674(3) 0.69834(6) 0.026 1 4
C(9A) 0.89976(3) -0.06359(3) 0.95075(6) 0.026 1 4
C(10) 0.43582(2) -0.29336(3) 0.71811(5) 0.021 1 4
C(10A) 0.82314(2) -0.08406(2) 0.96648(5) 0.021 1 4
C(11) 0.39527(2) -0.25562(2) 0.64183(5) 0.017 1 4
C(11A) 0.78389(2) -0.12127(2) 0.88849(5) 0.016 1 4
C(12) 0.36164(2) -0.17547(2) 0.64266(5) 0.016 1 4
C(12A) 0.70090(2) -0.14705(2) 0.88582(5) 0.015 1 4
C(13) 0.32329(2) -0.17092(2) 0.53900(5) 0.017 1 4
C(13A) 0.69462(2) -0.18246(2) 0.78047(5) 0.016 1 4
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H(22C) 0.559835 0.248579 0.78418 0.04 1 4
H(22E) 0.257133 -0.002969 1.149321 0.042 1 4
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O(2A) 0.01487(12) 0.02401(15) 0.01324(13) 0.00105(12) -0.00125(11) -
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N(2A) 0.0234(2) 0.0188(2) 0.0364(3) -0.0027(2) 0.0007(2) 0.00544(18)
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C(2A) 0.02409(18) 0.02240(16) 0.02147(18) -0.00408(13) -0.00507(15)
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H(19B) 0.036073 0.034062 0.035545 -0.010107 0.004408 -0.000186
H(19D) 0.038001 0.036058 0.032741 0.00312 0.011158 -0.001072
H(19C) 0.035512 0.035554 0.031093 -0.003138 -0.005836 0.001819
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H(21C) 0.04661 0.027666 0.040454 0.00255 -0.006768 -0.009392
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H(22C) 0.026388 0.036701 0.056951 0.001431 -0.000066 -0.000564
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0.000009(7)
-0.000029(9) -0.000012(6) 0.000010(8) -0.000002(4)
S(1A) -0.000004(11) 0.00062(2) -0.00027(5) 0.000026(8) 0.000170(10) -
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-0.000004(3) 0.000002(5) -0.000002(2) -0.000004(4) 0.0000021(12) 0.000011(3)
0.000004(2) -0.0000029(13) -0.0000005(12) -0.0000026(17)
S(1A) 0.000002(4) 0.000013(7) 0.00015(2) 0.000009(2) 0.000004(3) -0.000004(3)
0.000002(8) -0.000008(5) -0.000008(9) -0.000001(2) 0.000007(3) 0.000007(5)
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#-------------------------------------------------------------------------
#
#                    MULTIPOLE PARAMETERS
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    _atom_rho_multipole_radial_slater_zeta4
S(1) 6.75(6) 0 -0.01(2) -0.01(2) 0.03(2) 0.05(2) -0.03(2) -0.03(2) -0.02(2)
0.05(2) 0.147(19) 0.029(16) -0.036(17) 0.021(17) -0.038(17) 0.063(17) -
0.001(17)
0.06(2) -0.016(18) 0.011(19) 0.035(19) 0.020(18) -0.027(19) -0.039(19)
-0.002(19) -0.054(19) 0.946976 1.094612 1.094612 1.094612 1.094612 1.094612 4
3.8512666666667 4 3.8512666666667 4 3.8512666666667 4 3.8512666666667 4
3.8512666666667
S(1A) 6.64(6) 0 0.02(3) -0.10(3) -0.012(19) 0.12(2) -0.05(2) 0.02(2) 0.01(3)
0.09(3) 0.135(19) -0.036(18) 0.050(18) -0.01(2) 0.00(2) -0.03(2) -0.08(2)
```

0.08(2) -0.04(2) -0.03(2) -0.03(2) -0.02(2) 0.02(3) -0.03(3) -0.02(3) -
0.03(3)
0.94767 1.359433 1.359433 1.359433 1.359433 1.359433 4 3.8512666666667 4
3.8512666666667 4 3.8512666666667 4 3.8512666666667 4 3.8512666666667
O(1) 6.000(16) 0 -0.031(9) -0.043(8) 0 0.051(9) 0 0 -0.018(9) 0.034(9) 0
-0.007(6) -0.011(6) 0 0 0.078(6) -0.010(6) 0 0 0 0 0 0 0 0 0 0.988798
1.055753
1.055753 1.055753 1.055753 1.055753 2 4.466 2 4.466 2 4.466 3 4.466 4 4.466
O(1A) 6.0004 0 -0.0309 -0.0427 0 0.0506 0 0 -0.0177 0.0336 0 -0.0074 -0.0114
0 0
0.0777 -0.0102 0 0 0 0 0 0 0 0 0 0.988798 1.055753 1.055753 1.055753 1.055753
1.055753 2 4.466 2 4.466 2 4.466 3 4.466 4 4.466
O(2) 5.976(17) 0 -0.100(11) 0.011(9) -0.018(9) -0.052(10) -0.013(9) 0.019(8)
-0.082(10) 0.009(9) 0.014(7) -0.004(7) -0.003(7) -0.007(7) 0.006(7) 0.031(7)
-0.010(7) 0 0 0 0 0 0 0 0 0 0.985393 0.924662 0.924662 0.924662 0.924662
0.924662 2 4.466 2 4.466 2 4.466 3 4.466 4 4.466
O(2A) 5.9761 0 -0.1001 0.0107 -0.0175 -0.0516 -0.0127 0.0185 -0.0824 0.0092
0.0135 -0.0044 -0.0033 -0.0074 0.0057 0.031 -0.0103 0 0 0 0 0 0 0 0 0
0.985393
0.924662 0.924662 0.924662 0.924662 0.924662 2 4.466 2 4.466 2 4.466 3 4.466
4
4.466
N(1) 4.91(2) 0 0.008(10) 0.032(11) 0 0.007(9) 0 0 0.000(9) -0.018(9) 0 -
0.046(8)
-0.006(7) 0 0 0.166(8) 0.016(8) 0 0 0 0 0 0 0 0 0 0.982488 0.957744 0.957744
0.957744 0.957744 0.957744 2 3.83936 2 3.83936 2 3.83936 3 3.83936 4 3.83936
N(1A) 4.9097 0 0.0078 0.0318 0 0.0069 0 0 0.0003 -0.0181 0 -0.0455 -0.0064 0
0
0.1658 0.0161 0 0 0 0 0 0 0 0 0 0.982488 0.957744 0.957744 0.957744 0.957744
0.957744 2 3.83936 2 3.83936 2 3.83936 3 3.83936 4 3.83936
N(2) 5.05(4) 0 0.043(16) 0.049(14) 0.05(2) 0.10(2) -0.029(17) -0.002(15)
0.009(14) 0.031(14) 0.011(16) 0.081(15) 0.062(14) -0.013(13) -0.028(13)
0.002(12) 0.030(12) 0 0 0 0 0 0 0 0 0 0.981436 0.963224 0.963224 0.963224
0.963224 0.963224 2 3.83936 2 3.83936 2 3.83936 3 3.83936 4 3.83936
N(2A) 5.01(4) 0 0.000(17) 0.049(15) 0.03(2) 0.14(2) 0.027(16) 0.049(15)
-0.021(15) 0.004(15) -0.072(15) 0.019(14) 0.031(13) -0.011(12) 0.003(12)
-0.030(12) -0.003(12) 0 0 0 0 0 0 0 0 0 0.986582 1.00161 1.00161 1.00161
1.00161
1.00161 2 3.83936 2 3.83936 2 3.83936 3 3.83936 4 3.83936
C(1) 4.15(4) 0 0.003(14) -0.023(11) 0 -0.189(11) 0 0 -0.013(12) 0.001(11) 0
-0.010(11) 0.027(9) 0 0 0.238(11) 0.014(11) 0 0 0 0 0 0 0 0 0 0.962175
1.016775
1.016775 1.016775 1.016775 1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(1A) 4.1498 0 0.0028 -0.0227 0 -0.1894 0 0 -0.0128 0.0011 0 -0.0096 0.0269 0
0
0.2376 0.0139 0 0 0 0 0 0 0 0 0 0.962175 1.016775 1.016775 1.016775 1.016775
1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(2) 4.16(3) 0 0.025(14) 0.007(13) 0 -0.183(12) 0 0 0.039(13) -0.017(12) 0
0.031(11) 0.016(10) 0 0 0.245(12) -0.019(12) 0 0 0 0 0 0 0 0 0 0.962175
1.016775
1.016775 1.016775 1.016775 1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(2A) 4.1623 0 0.0248 0.0074 0 -0.1828 0 0 0.0387 -0.0174 0 0.0314 0.0157 0 0
0.2447 -0.0185 0 0 0 0 0 0 0 0 0 0.962175 1.016775 1.016775 1.016775 1.016775
1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(3) 4.15(3) 0 -0.010(14) 0.013(13) 0 -0.198(12) 0 0 0.013(13) -0.022(13) 0

0.016(10) 0.005(10) 0 0 0.269(13) -0.010(12) 0 0 0 0 0 0 0 0 0 0.962175
1.016775
1.016775 1.016775 1.016775 1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(3A) 4.1521 0 -0.01 0.0125 0 -0.1975 0 0 0.0133 -0.0216 0 0.0164 0.0047 0 0
0.2685 -0.0104 0 0 0 0 0 0 0 0 0 0.962175 1.016775 1.016775 1.016775 1.016775
1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(4) 4.15(3) 0 -0.008(13) -0.006(12) 0 -0.175(11) 0 0 -0.004(12) -0.016(12) 0
-0.013(10) 0.036(10) 0 0 0.250(12) 0.004(11) 0 0 0 0 0 0 0 0 0 0.962175
1.016775
1.016775 1.016775 1.016775 1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(4A) 4.1477 0 -0.0078 -0.0061 0 -0.175 0 0 -0.0039 -0.0161 0 -0.0129 0.0363
0 0
0.2503 0.0038 0 0 0 0 0 0 0 0 0 0.962175 1.016775 1.016775 1.016775 1.016775
1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(5) 4.22(3) 0 -0.009(14) 0.044(11) 0 -0.190(10) 0 0 0.041(11) -0.012(11) 0
-0.012(10) 0.000(9) 0 0 0.272(12) -0.040(12) 0 0 0 0 0 0 0 0 0 0.963239
0.990081
0.990081 0.990081 0.990081 0.990081 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(5A) 4.2157 0 -0.0092 0.0437 0 -0.1904 0 0 0.0411 -0.0117 0 -0.0123 0.0004 0
0
0.2717 -0.0401 0 0 0 0 0 0 0 0 0 0.963239 0.990081 0.990081 0.990081 0.990081
0.990081 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(6) 4.11(3) 0 0.012(12) 0.033(13) 0 -0.184(10) 0 0 0.032(11) -0.014(11) 0
0.008(10) 0.006(10) 0 0 0.237(12) -0.050(12) 0 0 0 0 0 0 0 0 0 0.963239
0.990081
0.990081 0.990081 0.990081 0.990081 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(6A) 4.1113 0 0.0119 0.0334 0 -0.1837 0 0 0.0322 -0.0143 0 0.0076 0.006 0 0
0.2373 -0.0496 0 0 0 0 0 0 0 0 0 0.963239 0.990081 0.990081 0.990081 0.990081
0.990081 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(7) 4.20(3) 0 0.003(12) 0.021(14) 0 -0.172(11) 0 0 0.016(12) -0.014(12) 0
0.007(10) 0.038(11) 0 0 0.233(12) -0.039(12) 0 0 0 0 0 0 0 0 0 0.962175
1.016775
1.016775 1.016775 1.016775 1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(7A) 4.2034 0 0.0026 0.0214 0 -0.1715 0 0 0.0155 -0.0144 0 0.007 0.0381 0 0
0.2329 -0.0386 0 0 0 0 0 0 0 0 0 0.962175 1.016775 1.016775 1.016775 1.016775
1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(8) 4.07(3) 0 -0.020(16) -0.018(13) 0 -0.190(13) 0 0 -0.001(13) -0.012(13) 0
0.058(13) -0.009(10) 0 0 0.243(13) 0.023(13) 0 0 0 0 0 0 0 0 0 0.962175
1.016775
1.016775 1.016775 1.016775 1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(8A) 4.0704 0 -0.0202 -0.0175 0 -0.1902 0 0 -0.0009 -0.0124 0 0.0581 -0.0093
0
0 0.2434 0.0227 0 0 0 0 0 0 0 0 0.962175 1.016775 1.016775 1.016775
1.016775
1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(9) 4.22(3) 0 -0.020(13) 0.062(15) 0 -0.202(12) 0 0 0.029(13) -0.015(13) 0
0.028(11) -0.011(12) 0 0 0.253(12) 0.007(12) 0 0 0 0 0 0 0 0 0 0.962175
1.016775
1.016775 1.016775 1.016775 1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762

C(9A) 4.2199 0 -0.0202 0.0624 0 -0.202 0 0 0.0286 -0.0149 0 0.0281 -0.0113 0
0
0.2527 0.0069 0 0 0 0 0 0 0 0 0 0.962175 1.016775 1.016775 1.016775 1.016775
1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(10) 4.12(3) 0 0.043(12) 0.009(13) 0 -0.167(11) 0 0 -0.004(12) 0.002(11) 0
0.016(10) 0.006(10) 0 0 0.248(11) 0.005(11) 0 0 0 0 0 0 0 0 0 0.962175
1.016775
1.016775 1.016775 1.016775 1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(10A) 4.1197 0 0.0432 0.009 0 -0.1667 0 0 -0.0043 0.0022 0 0.0162 0.0062 0 0
0.2479 0.0052 0 0 0 0 0 0 0 0 0 0.962175 1.016775 1.016775 1.016775 1.016775
1.016775 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(11) 4.21(3) 0 0.016(13) 0.014(12) 0 -0.182(11) 0 0 0.022(12) -0.041(11) 0
0.014(10) -0.009(10) 0 0 0.263(11) -0.053(12) 0 0 0 0 0 0 0 0 0 0.963239
0.990081 0.990081 0.990081 0.990081 0.990081 2 3.1762 2 3.1762 2 3.1762 3
3.1762
4 3.1762
C(11A) 4.2051 0 0.0162 0.0142 0 -0.1823 0 0 0.0222 -0.0405 0 0.0143 -0.0092 0
0
0.2625 -0.0525 0 0 0 0 0 0 0 0 0 0.963239 0.990081 0.990081 0.990081 0.990081
0.990081 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(12) 4.13(3) 0 0.010(11) -0.017(13) -0.004(11) -0.001(10) 0.005(9) 0.006(10)
-0.015(10) 0.005(10) 0.022(10) -0.169(10) -0.176(10) 0.002(10) 0.016(10)
0.154(10) -0.070(11) 0 0 0 0 0 0 0 0 0 0.962889 0.969848 0.969848 0.969848
0.969848 0.969848 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(12A) 4.1257 0 0.0103 -0.0168 -0.0035 -0.0007 0.0054 0.0055 -0.0153 0.0045
0.0223 -0.1687 -0.1762 0.0018 0.0155 0.1543 -0.0701 0 0 0 0 0 0 0 0 0
0.962889
0.969848 0.969848 0.969848 0.969848 0.969848 2 3.1762 2 3.1762 2 3.1762 3
3.1762
4 3.1762
C(13) 4.18(3) 0 0.004(12) -0.008(12) 0 -0.172(10) 0 0 0.013(11) -0.011(11) 0
0.014(10) 0.037(10) 0 0 0.264(11) -0.038(11) 0 0 0 0 0 0 0 0 0 0.963239
0.990081
0.990081 0.990081 0.990081 0.990081 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(13A) 4.1826 0 0.0044 -0.0082 0 -0.1717 0 0 0.013 -0.0109 0 0.0138 0.0374 0
0
0.2642 -0.0376 0 0 0 0 0 0 0 0 0 0.963239 0.990081 0.990081 0.990081 0.990081
0.990081 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(14) 4.05(3) 0 -0.002(10) -0.074(10) 0 0.069(10) 0 0 0.032(9) 0.067(9) 0
-0.137(9) -0.187(9) 0 0 0.186(8) -0.058(8) 0 0 0 0 0 0 0 0 0 0.962807
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3.1762
C(14A) 4.0536 0 -0.0022 -0.0735 0 0.0687 0 0 0.0319 0.0671 0 -0.1367 -0.1873
0 0
0.1855 -0.0581 0 0 0 0 0 0 0 0 0 0.962807 1.037883 1.037883 1.037883 1.037883
1.037883 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(15) 4.25(3) 0 0.122(13) -0.017(11) 0 -0.301(11) 0 0 0.104(11) -0.012(11) 0
-0.015(11) 0.024(9) 0 0 0.381(12) 0.035(12) 0 0 0 0 0 0 0 0 0 0.954676
0.975277
0.975277 0.975277 0.975277 0.975277 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(15A) 4.2484 0 0.1224 -0.0165 0 -0.3008 0 0 0.1039 -0.0121 0 -0.0149 0.0239
0 0
0.3812 0.0352 0 0 0 0 0 0 0 0 0 0.954676 0.975277 0.975277 0.975277 0.975277

0.975277 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(16) 4.04(3) 0 -0.034(10) -0.064(10) 0.039(10) 0.078(9) -0.031(9) -0.021(9)
0.024(9) 0.028(9) -0.012(9) -0.128(9) -0.185(9) 0.020(9) 0.021(9) 0.158(9)
-0.046(9) 0 0 0 0 0 0 0 0 0 0.962432 1.02847 1.02847 1.02847 1.02847 1.02847
2
3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(16A) 4.0428 0 -0.0339 -0.0641 0.0391 0.0779 -0.0311 -0.0205 0.024 0.0284
-0.0121 -0.1284 -0.185 0.0201 0.0212 0.1575 -0.0462 0 0 0 0 0 0 0 0 0
0.962432
1.02847 1.02847 1.02847 1.02847 1.02847 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(17) 4.06(4) 0 -0.055(11) -0.006(11) 0 0.013(11) 0 0 -0.084(9) -0.004(9) 0
-0.095(10) -0.139(11) 0 0 0.207(10) -0.038(9) 0 0 0 0 0 0 0 0 0 0.961614
0.998202 0.998202 0.998202 0.998202 0.998202 2 3.1762 2 3.1762 2 3.1762 3
3.1762
4 3.1762
C(17A) 4.0633 0 -0.055 -0.0059 0 0.0126 0 0 -0.0838 -0.0043 0 -0.0954 -0.1392
0
0 0.2065 -0.038 0 0 0 0 0 0 0 0 0 0.961614 0.998202 0.998202 0.998202
0.998202
0.998202 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(18) 4.15(5) 0 0.004(16) 0.010(15) 0.11(3) 0.32(2) 0.009(16) 0.006(16)
0.019(14) 0.014(14) 0.06(2) -0.008(18) -0.010(18) -0.017(14) 0.029(15)
0.012(13)
-0.009(13) 0 0 0 0 0 0 0 0 0 0.970455 0.997343 0.997343 0.997343 0.997343
0.997343 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(18A) 4.19(5) 0 0.010(16) 0.040(16) 0.11(2) 0.30(2) 0.033(16) 0.009(16)
0.015(14) -0.007(14) 0.03(2) 0.049(18) -0.077(18) -0.008(15) -0.025(15)
0.032(14) -0.028(14) 0 0 0 0 0 0 0 0 0 0.971513 0.97515 0.97515 0.97515
0.97515
0.97515 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(19) 4.07(4) 0 -0.029(10) -0.008(10) 0 -0.008(10) 0 0 0.002(9) -0.005(9) 0
-0.112(10) -0.180(10) 0 0 0.190(9) -0.019(9) 0 0 0 0 0 0 0 0 0 0.961614
0.998202
0.998202 0.998202 0.998202 0.998202 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(19A) 4.0667 0 -0.0285 -0.0082 0 -0.0084 0 0 0.002 -0.0048 0 -0.1121 -0.1798
0
0 0.1895 -0.019 0 0 0 0 0 0 0 0 0 0.961614 0.998202 0.998202 0.998202
0.998202
0.998202 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(20) 4.01(3) 0 0.006(10) 0.029(10) -0.016(9) 0.018(10) -0.012(9) 0.003(9)
-0.007(9) 0.009(9) -0.013(11) -0.141(10) -0.169(10) -0.001(10) -0.025(9)
0.160(9) -0.063(9) 0 0 0 0 0 0 0 0 0 0.961614 0.998202 0.998202 0.998202
0.998202 0.998202 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(20A) 4.0149 0 0.0062 0.0291 -0.0161 0.0179 -0.0117 0.0028 -0.0066 0.0086
-0.0126 -0.1413 -0.1688 -0.0007 -0.0248 0.1598 -0.0631 0 0 0 0 0 0 0 0 0
0.961614 0.998202 0.998202 0.998202 0.998202 0.998202 2 3.1762 2 3.1762 2
3.1762
3 3.1762 4 3.1762
C(21) 4.06(4) 0 0.002(12) -0.013(10) -0.019(11) -0.008(11) 0.046(10)
0.018(10)
0.010(10) 0.014(10) -0.048(11) -0.109(10) 0.132(11) -0.048(11) -0.020(10)
0.154(10) 0.052(10) 0 0 0 0 0 0 0 0 0 0.965626 1.038539 1.038539 1.038539
1.038539 1.038539 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(21A) 4.0623 0 0.0023 -0.0128 -0.0194 -0.0083 0.0464 0.018 0.0096 0.014 -
0.0479

-0.1085 0.132 -0.0477 -0.0198 0.1543 0.0519 0 0 0 0 0 0 0 0 0 0.965626
1.038539
1.038539 1.038539 1.038539 1.038539 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
C(22) 4.20(4) 0 -0.053(11) 0.010(11) 0.081(11) 0.008(11) -0.024(10) 0.016(11)
0.005(10) 0.001(10) 0.056(11) -0.136(10) 0.190(12) -0.010(11) -0.012(10)
0.163(10) 0.023(10) 0 0 0 0 0 0 0 0 0 0.965626 1.038539 1.038539 1.038539
1.038539 1.038539 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(22A) 4.2023 0 -0.0533 0.0099 0.0809 0.0075 -0.0241 0.0161 0.0053 0.0009
0.0562
-0.136 0.1897 -0.0095 -0.0117 0.1628 0.023 0 0 0 0 0 0 0 0 0 0.965626
1.038539
1.038539 1.038539 1.038539 1.038539 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4
3.1762
H(1) 0.813(6) 0 0 0 0.118(6) 0.009(7) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(1A) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(1N) 0.895(16) 0 0 0 0.281(14) 0.134(19) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0
0 1.2 1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(2) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(1NA) 0.8949 0 0 0 0.2811 0.1341 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(2A) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(3) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(3A) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(4) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(4A) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(7) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(7A) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(8) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(8A) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(9) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2

H(9A) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(10) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(10A) 0.8129 0 0 0 0.1182 0.0093 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(12) 0.887(9) 0 0 0 0.149(8) 0.066(11) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0
1.2 1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(12A) 0.8865 0 0 0 0.1489 0.0659 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(14A) 0.896(7) 0 0 0 0.147(6) 0.059(8) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0
1.2 1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(14B) 0.8964 0 0 0 0.1469 0.0592 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(14D) 0.8964 0 0 0 0.1469 0.0592 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(14C) 0.8964 0 0 0 0.1469 0.0592 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(16) 0.8865 0 0 0 0.1489 0.0659 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(16A) 0.8865 0 0 0 0.1489 0.0659 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(17A) 0.8964 0 0 0 0.1469 0.0592 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(17B) 0.8964 0 0 0 0.1469 0.0592 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(17D) 0.8964 0 0 0 0.1469 0.0592 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(17C) 0.8964 0 0 0 0.1469 0.0592 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(19A) 0.8964 0 0 0 0.1469 0.0592 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(19B) 0.8964 0 0 0 0.1469 0.0592 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(19D) 0.8964 0 0 0 0.1469 0.0592 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(19C) 0.8964 0 0 0 0.1469 0.0592 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(20) 0.8865 0 0 0 0.1489 0.0659 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2
1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(20A) 0.8865 0 0 0 0.1489 0.0659 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(21A) 0.828(8) 0 0 0 0.115(6) 0.015(7) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0
1.2 1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(21B) 0.8282 0 0 0 0.1151 0.0151 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(21C) 0.8282 0 0 0 0.1151 0.0151 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(21E) 0.8282 0 0 0 0.1151 0.0151 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2

H(21D) 0.8282 0 0 0 0.1151 0.0151 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(21F) 0.8282 0 0 0 0.1151 0.0151 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(22A) 0.8282 0 0 0 0.1151 0.0151 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(22B) 0.8282 0 0 0 0.1151 0.0151 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(22C) 0.8282 0 0 0 0.1151 0.0151 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(22E) 0.8282 0 0 0 0.1151 0.0151 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(22F) 0.8282 0 0 0 0.1151 0.0151 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(22D) 0.8282 0 0 0 0.1151 0.0151 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2
1.2 1.2 1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2

loop_
    _atom_local_axes_atom_label
    _atom_local_axes_atom0
    _atom_local_axes_ax1
    _atom_local_axes_atom1
    _atom_local_axes_atom2
    _atom_local_axes_ax2
S(1) C(18) Z S(1) C(15) Y
S(1A) C(18A) Z S(1A) C(15A) Y
O(1) C(15) X O(1) C(14) Y
O(1A) C(15A) X O(1A) C(14A) Y
O(2) C(15) X O(2) O(1) Y
O(2A) C(15A) X O(2A) O(1A) Y
N(1) C(16) X N(1) C(15) Y
N(1A) C(16A) X N(1A) C(15A) Y
N(2) C(18) Z N(2) N(1) Y
N(2A) C(18A) Z N(2A) N(1A) Y
C(1) C(2) X C(1) C(13) Y
C(1A) C(2A) X C(1A) C(13A) Y
C(2) C(1) X C(2) C(3) Y
C(2A) C(1A) X C(2A) C(3A) Y
C(3) C(4) X C(3) C(2) Y
C(3A) C(4A) X C(3A) C(2A) Y
C(4) C(3) X C(4) C(5) Y
C(4A) C(3A) X C(4A) C(5A) Y
C(5) C(4) X C(5) C(13) Y
C(5A) C(4A) X C(5A) C(13A) Y
C(6) C(7) X C(6) C(11) Y
C(6A) C(7A) X C(6A) C(11A) Y
C(7) C(6) X C(7) C(8) Y
C(7A) C(6A) X C(7A) C(8A) Y
C(8) C(9) X C(8) C(7) Y
C(8A) C(9A) X C(8A) C(7A) Y
C(9) C(10) X C(9) C(8) Y
C(9A) C(10A) X C(9A) C(8A) Y
C(10) C(9) X C(10) C(11) Y
C(10A) C(9A) X C(10A) C(11A) Y
C(11) C(10) X C(11) C(6) Y
C(11A) C(10A) X C(11A) C(6A) Y
C(12) C(11) X C(12) C(13) Y

C(12A) C(11A) X C(12A) C(13A) Y
C(13) C(1) X C(13) C(5) Y
C(13A) C(1A) X C(13A) C(5A) Y
C(14) C(12) X C(14) O(1) Y
C(14A) C(12A) X C(14A) O(1A) Y
C(15) O(2) X C(15) N(1) Y
C(15A) O(2A) X C(15A) N(1A) Y
C(16) C(17) X C(16) N(1) Y
C(16A) C(17A) X C(16A) N(1A) Y
C(17) N(2) X C(17) C(16) Y
C(17A) N(2A) X C(17A) C(16A) Y
C(18) N(2) Z C(18) N(1) Y
C(18A) N(2A) Z C(18A) N(1A) Y
C(19) C(16) X C(19) C(20) Y
C(19A) C(16A) X C(19A) C(20A) Y
C(20) C(19) X C(20) C(21) Y
C(20A) C(19A) X C(20A) C(22A) Y
C(21) C(20) X C(21) C(22) Y
C(21A) C(20A) X C(21A) C(22A) Y
C(22) C(20) X C(22) C(21) Y
C(22A) C(20A) X C(22A) C(21A) Y
H(1) C(1) Z H(1) C(13) Y
H(1A) C(1A) Z H(1A) C(13A) Y
H(1N) N(1) Z H(1N) C(15) Y
H(2) C(2) Z H(2) C(1) Y
H(1NA) N(1A) Z H(1NA) C(15A) Y
H(2A) C(2A) Z H(2A) C(1A) Y
H(3) C(3) Z H(3) C(4) Y
H(3A) C(3A) Z H(3A) C(4A) Y
H(4) C(4) Z H(4) C(3) Y
H(4A) C(4A) Z H(4A) C(3A) Y
H(7) C(7) Z H(7) C(6) Y
H(7A) C(7A) Z H(7A) C(6A) Y
H(8) C(8) Z H(8) C(7) Y
H(8A) C(8A) Z H(8A) C(9A) Y
H(9) C(9) Z H(9) C(8) Y
H(9A) C(9A) Z H(9A) C(8A) Y
H(10) C(10) Z H(10) C(9) Y
H(10A) C(10A) Z H(10A) C(9A) Y
H(12) C(12) Z H(12) C(14) Y
H(12A) C(12A) Z H(12A) C(14A) Y
H(14A) C(14) Z H(14A) O(1) Y
H(14B) C(14) Z H(14B) O(1) Y
H(14D) C(14A) Z H(14D) O(1A) Y
H(14C) C(14A) Z H(14C) O(1A) Y
H(16) C(16) Z H(16) N(1) Y
H(16A) C(16A) Z H(16A) N(1A) Y
H(17A) C(17) Z H(17A) N(2) Y
H(17B) C(17) Z H(17B) N(2) Y
H(17D) C(17A) Z H(17D) N(2A) Y
H(17C) C(17A) Z H(17C) N(2A) Y
H(19A) C(19) Z H(19A) C(16) Y
H(19B) C(19) Z H(19B) C(16) Y
H(19D) C(19A) Z H(19D) C(16A) Y
H(19C) C(19A) Z H(19C) C(16A) Y
H(20) C(20) Z H(20) C(19) Y
H(20A) C(20A) Z H(20A) C(19A) Y

H(21A) C(21) Z H(21A) C(20) Y
H(21B) C(21) Z H(21B) C(20) Y
H(21C) C(21) Z H(21C) C(20) Y
H(21E) C(21A) Z H(21E) C(20A) Y
H(21D) C(21A) Z H(21D) C(20A) Y
H(21F) C(21A) Z H(21F) C(20A) Y
H(22A) C(22) Z H(22A) C(20) Y
H(22B) C(22) Z H(22B) C(20) Y
H(22C) C(22) Z H(22C) C(20) Y
H(22E) C(22A) Z H(22E) C(20A) Y
H(22F) C(22A) Z H(22F) C(20A) Y
H(22D) C(22A) Z H(22D) C(20A) Y