Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 03:07 PM JST

PDB ID	:	5XIC
Title	:	Crystal Structure of HasAp with Fe-5,10,15-triphenylporphyrin
Authors	:	Shoji, O.; Uehara, H.; Sugimoto, H.; Shiro, Y.; Watanabe, Y.
Deposited on	:	2017-04-26
Resolution	:	1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

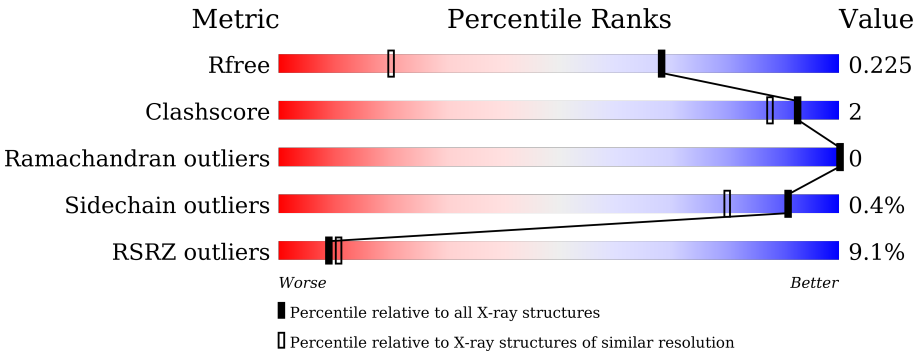
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	184	7% 96% .
1	B	184	10% 98% .
1	C	184	10% 96% .
1	D	184	10% 97% .

2 Entry composition

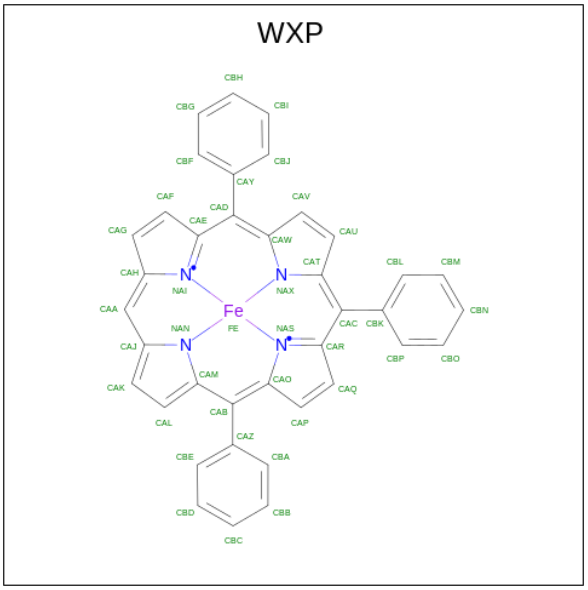
There are 4 unique types of molecules in this entry. The entry contains 6343 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Heme acquisition protein HasAp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	7	0
			1385	864	227	292	2			
1	B	184	Total	C	N	O	S	0	9	0
			1402	875	232	293	2			
1	C	184	Total	C	N	O	S	0	7	0
			1389	868	230	289	2			
1	D	184	Total	C	N	O	S	0	8	0
			1395	871	231	291	2			

- Molecule 2 is 5,10,15-Triphenylporphyrin cpntaining FE (three-letter code: WXP) (formula: $C_{38}H_{24}FeN_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	0	1
			49	44	1	4		
2	B	1	Total	C	Fe	N	0	1
			49	44	1	4		

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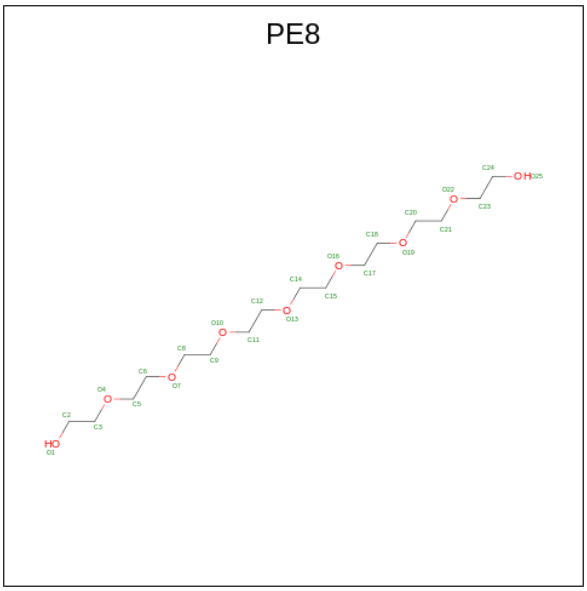
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C Fe N 49 44 1 4	0	1
2	D	1	Total C Fe N 49 44 1 4	0	1

- Molecule 3 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: $C_{16}H_{34}O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 25 16 9	0	0
3	A	1	Total C O 25 16 9	0	0
3	B	1	Total C O 25 16 9	0	0
3	D	1	Total C O 25 16 9	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	127	Total O 127 127	0	0
4	B	117	Total O 117 117	0	0
4	C	115	Total O 115 115	0	0

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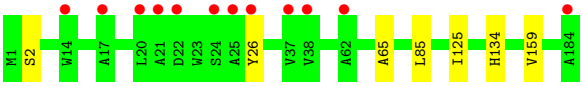
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	117	Total	O	0	0
			117	117		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

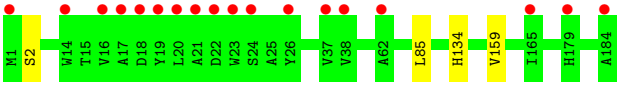
• Molecule 1: Heme acquisition protein HasAp

Chain A:



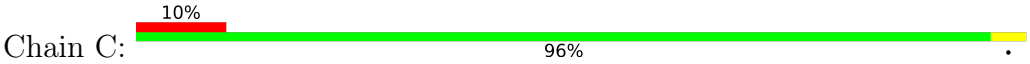
• Molecule 1: Heme acquisition protein HasAp

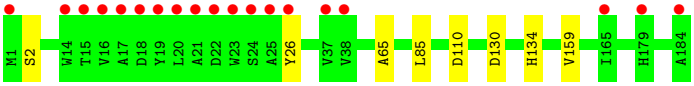
Chain B:



• Molecule 1: Heme acquisition protein HasAp

Chain C:





• Molecule 1: Heme acquisition protein HasAp

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.65Å 83.46Å 83.49Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	19.48 – 1.45 19.48 – 1.45	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.48-1.45) 96.3 (19.48-1.45)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.193 , 0.218 0.202 , 0.225	Depositor DCC
R_{free} test set	5347 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	12.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.466 for -h,l,k 0.467 for -h,-l,-k 0.469 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6343	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PE8, WXP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/1418	0.59	0/1933
1	B	0.35	0/1435	0.62	0/1956
1	C	0.35	0/1422	0.60	0/1939
1	D	0.35	0/1428	0.61	0/1947
All	All	0.35	0/5703	0.61	0/7775

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1385	0	1281	4	0
1	B	1402	0	1305	2	0
1	C	1389	0	1295	5	0
1	D	1395	0	1299	5	0
2	A	49	0	0	1	0
2	B	49	0	0	0	0
2	C	49	0	0	0	0
2	D	49	0	0	0	0
3	A	50	0	68	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	34	0	0
3	D	25	0	34	0	0
4	A	127	0	0	1	1
4	B	117	0	0	0	1
4	C	115	0	0	0	0
4	D	117	0	0	0	0
All	All	6343	0	5316	17	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:H	1:A:134:HIS:HD2	1.42	0.68
1:D:38[B]:VAL:O	1:D:38[B]:VAL:HG22	1.93	0.68
1:C:85:LEU:H	1:C:134:HIS:HD2	1.43	0.67
1:D:85:LEU:H	1:D:134:HIS:HD2	1.42	0.67
1:B:85:LEU:H	1:B:134:HIS:HD2	1.44	0.65
1:D:38[B]:VAL:O	1:D:38[B]:VAL:CG2	2.50	0.60
1:D:2:SER:HB2	1:D:159:VAL:HG11	1.87	0.55
1:B:2[A]:SER:HB2	1:B:159:VAL:HG21	1.88	0.55
1:A:125:ILE:HG22	4:A:416:HOH:O	2.09	0.51
1:D:2:SER:CB	1:D:159:VAL:HG11	2.41	0.51
1:A:2[A]:SER:HB2	1:A:159:VAL:HG21	1.91	0.51
1:C:2:SER:CB	1:C:159[B]:VAL:HG11	2.45	0.47
1:C:2:SER:HB2	1:C:159[A]:VAL:HG21	2.00	0.44
1:A:26[B]:TYR:CD2	1:A:65:ALA:HB2	2.54	0.43
1:C:2:SER:HB2	1:C:159[B]:VAL:HG11	2.01	0.42
1:C:26[B]:TYR:CD2	1:C:65:ALA:HB2	2.55	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:416:HOH:O	4:B:343:HOH:O[2_555]	1.55	0.65

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	189/184 (103%)	182 (96%)	7 (4%)	0	100	100
1	B	191/184 (104%)	189 (99%)	2 (1%)	0	100	100
1	C	189/184 (103%)	183 (97%)	6 (3%)	0	100	100
1	D	190/184 (103%)	183 (96%)	7 (4%)	0	100	100
All	All	759/736 (103%)	737 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	146/139 (105%)	146 (100%)	0	100	100
1	B	148/139 (106%)	148 (100%)	0	100	100
1	C	146/139 (105%)	144 (99%)	2 (1%)	67	37
1	D	147/139 (106%)	147 (100%)	0	100	100
All	All	587/556 (106%)	585 (100%)	2 (0%)	91	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	110	ASP
1	C	130	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	A	149	GLN
1	B	134	HIS
1	C	127	GLN
1	C	134	HIS
1	C	149	GLN
1	D	134	HIS
1	D	149	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	WXP	C	201[A]	-	52,53,53	2.58	20 (38%)	60,84,84	3.75	25 (41%)
3	PE8	B	202	-	24,24,24	0.43	0	23,23,23	0.34	0
2	WXP	A	201[A]	-	52,53,53	2.55	22 (42%)	60,84,84	3.72	26 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	WXP	B	201[B]	-	52,53,53	2.51	20 (38%)	60,84,84	3.75	28 (46%)
3	PE8	D	202	-	24,24,24	0.54	0	23,23,23	0.22	0
2	WXP	C	201[B]	-	52,53,53	2.57	20 (38%)	60,84,84	3.74	26 (43%)
2	WXP	A	201[B]	-	52,53,53	2.54	22 (42%)	60,84,84	3.72	27 (45%)
2	WXP	D	201[A]	-	52,53,53	2.56	20 (38%)	60,84,84	3.75	25 (41%)
2	WXP	B	201[A]	-	52,53,53	2.51	20 (38%)	60,84,84	3.74	26 (43%)
3	PE8	A	202	-	24,24,24	0.43	0	23,23,23	0.33	0
2	WXP	D	201[B]	-	52,53,53	2.54	20 (38%)	60,84,84	3.75	26 (43%)
3	PE8	A	203	-	24,24,24	0.52	0	23,23,23	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WXP	C	201[A]	-	-	0/12/64/64	0/3/11/11
3	PE8	B	202	-	-	2/22/22/22	-
2	WXP	A	201[A]	-	-	0/12/64/64	0/3/11/11
2	WXP	B	201[B]	-	-	0/12/64/64	0/3/11/11
3	PE8	D	202	-	-	10/22/22/22	-
2	WXP	C	201[B]	-	-	0/12/64/64	0/3/11/11
2	WXP	A	201[B]	-	-	0/12/64/64	0/3/11/11
2	WXP	D	201[A]	-	-	0/12/64/64	0/3/11/11
2	WXP	B	201[A]	-	-	0/12/64/64	0/3/11/11
3	PE8	A	202	-	-	0/22/22/22	-
2	WXP	D	201[B]	-	-	0/12/64/64	0/3/11/11
3	PE8	A	203	-	-	11/22/22/22	-

All (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201[A]	WXP	CAV-CAW	-5.95	1.32	1.44
2	C	201[B]	WXP	CAV-CAW	-5.95	1.32	1.44
2	D	201[A]	WXP	CAV-CAW	-5.93	1.32	1.44
2	D	201[B]	WXP	CAV-CAW	-5.93	1.32	1.44
2	B	201[A]	WXP	CAP-CAO	-5.72	1.32	1.44
2	B	201[B]	WXP	CAP-CAO	-5.72	1.32	1.44
2	A	201[A]	WXP	CAP-CAO	-5.62	1.33	1.44
2	A	201[B]	WXP	CAP-CAO	-5.62	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201[A]	WXP	CAV-CAW	-5.35	1.33	1.44
2	A	201[B]	WXP	CAV-CAW	-5.35	1.33	1.44
2	C	201[A]	WXP	FE-NAX	5.28	2.16	1.95
2	C	201[B]	WXP	FE-NAX	5.28	2.16	1.95
2	B	201[A]	WXP	CAV-CAW	-5.27	1.34	1.44
2	B	201[B]	WXP	CAV-CAW	-5.27	1.34	1.44
2	C	201[A]	WXP	CAP-CAO	-5.14	1.34	1.44
2	C	201[B]	WXP	CAP-CAO	-5.14	1.34	1.44
2	D	201[A]	WXP	CAP-CAO	-5.12	1.34	1.44
2	D	201[B]	WXP	CAP-CAO	-5.12	1.34	1.44
2	A	201[A]	WXP	FE-NAX	5.10	2.15	1.95
2	A	201[B]	WXP	FE-NAX	5.10	2.15	1.95
2	B	201[A]	WXP	FE-NAX	4.97	2.15	1.95
2	B	201[B]	WXP	FE-NAX	4.97	2.15	1.95
2	D	201[A]	WXP	FE-NAX	4.83	2.14	1.95
2	D	201[B]	WXP	FE-NAX	4.83	2.14	1.95
2	A	201[A]	WXP	CAU-CAT	-4.75	1.35	1.44
2	A	201[B]	WXP	CAU-CAT	-4.75	1.35	1.44
2	B	201[A]	WXP	CAU-CAT	-4.75	1.35	1.44
2	B	201[B]	WXP	CAU-CAT	-4.75	1.35	1.44
2	B	201[A]	WXP	CAF-CAE	-4.66	1.35	1.44
2	B	201[B]	WXP	CAF-CAE	-4.66	1.35	1.44
2	C	201[A]	WXP	CAF-CAE	-4.65	1.35	1.44
2	C	201[B]	WXP	CAF-CAE	-4.65	1.35	1.44
2	A	201[A]	WXP	CAF-CAE	-4.63	1.35	1.44
2	A	201[B]	WXP	CAF-CAE	-4.63	1.35	1.44
2	D	201[A]	WXP	CAF-CAE	-4.57	1.35	1.44
2	D	201[B]	WXP	CAF-CAE	-4.57	1.35	1.44
2	D	201[A]	WXP	CAQ-CAR	-4.54	1.35	1.44
2	D	201[B]	WXP	CAQ-CAR	-4.54	1.35	1.44
2	C	201[A]	WXP	CAQ-CAR	-4.51	1.35	1.44
2	C	201[B]	WXP	CAQ-CAR	-4.51	1.35	1.44
2	C	201[A]	WXP	FE-NAI	4.49	2.21	1.97
2	C	201[B]	WXP	FE-NAI	4.49	2.21	1.97
2	D	201[A]	WXP	FE-NAI	4.48	2.21	1.97
2	D	201[B]	WXP	FE-NAI	4.48	2.21	1.97
2	C	201[A]	WXP	CAG-CAH	-4.33	1.33	1.43
2	C	201[B]	WXP	CAG-CAH	-4.33	1.33	1.43
2	A	201[A]	WXP	CAG-CAH	-4.32	1.33	1.43
2	A	201[B]	WXP	CAG-CAH	-4.32	1.33	1.43
2	B	201[A]	WXP	CAG-CAH	-4.23	1.33	1.43
2	B	201[B]	WXP	CAG-CAH	-4.23	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201[A]	WXP	CAQ-CAR	-4.17	1.36	1.44
2	B	201[B]	WXP	CAQ-CAR	-4.17	1.36	1.44
2	D	201[A]	WXP	CAG-CAH	-4.17	1.33	1.43
2	D	201[B]	WXP	CAG-CAH	-4.17	1.33	1.43
2	A	201[A]	WXP	CAQ-CAR	-4.15	1.36	1.44
2	A	201[B]	WXP	CAQ-CAR	-4.15	1.36	1.44
2	C	201[A]	WXP	CAU-CAT	-4.09	1.36	1.44
2	C	201[B]	WXP	CAU-CAT	-4.09	1.36	1.44
2	C	201[A]	WXP	CAJ-CAA	-4.07	1.35	1.43
2	C	201[B]	WXP	CAJ-CAA	-4.07	1.35	1.43
2	D	201[A]	WXP	CAU-CAT	-4.03	1.36	1.44
2	D	201[B]	WXP	CAU-CAT	-4.03	1.36	1.44
2	B	201[A]	WXP	CAJ-CAA	-3.97	1.35	1.43
2	B	201[B]	WXP	CAJ-CAA	-3.97	1.35	1.43
2	A	201[A]	WXP	CAZ-CAB	-3.92	1.42	1.49
2	A	201[B]	WXP	CAZ-CAB	-3.92	1.42	1.49
2	D	201[A]	WXP	FE-NAS	3.90	2.18	1.97
2	D	201[B]	WXP	FE-NAS	3.90	2.18	1.97
2	A	201[A]	WXP	CAJ-CAA	-3.89	1.36	1.43
2	A	201[B]	WXP	CAJ-CAA	-3.89	1.36	1.43
2	D	201[A]	WXP	CBK-CAC	-3.86	1.42	1.49
2	C	201[A]	WXP	CAK-CAJ	-3.81	1.33	1.39
2	C	201[B]	WXP	CAK-CAJ	-3.81	1.33	1.39
2	C	201[A]	WXP	CBK-CAC	-3.79	1.42	1.49
2	C	201[A]	WXP	CAZ-CAB	-3.77	1.43	1.49
2	C	201[B]	WXP	CAZ-CAB	-3.77	1.43	1.49
2	B	201[A]	WXP	CAZ-CAB	-3.74	1.43	1.49
2	B	201[B]	WXP	CAZ-CAB	-3.74	1.43	1.49
2	B	201[A]	WXP	CAK-CAJ	-3.72	1.33	1.39
2	B	201[B]	WXP	CAK-CAJ	-3.72	1.33	1.39
2	A	201[A]	WXP	CAK-CAJ	-3.72	1.33	1.39
2	A	201[B]	WXP	CAK-CAJ	-3.72	1.33	1.39
2	D	201[A]	WXP	CAZ-CAB	-3.70	1.43	1.49
2	D	201[B]	WXP	CAZ-CAB	-3.70	1.43	1.49
2	D	201[A]	WXP	CAJ-CAA	-3.70	1.36	1.43
2	D	201[B]	WXP	CAJ-CAA	-3.70	1.36	1.43
2	D	201[A]	WXP	CAY-CAD	-3.70	1.42	1.49
2	D	201[B]	WXP	CAY-CAD	-3.70	1.42	1.49
2	A	201[A]	WXP	CBK-CAC	-3.68	1.42	1.49
2	D	201[A]	WXP	CAK-CAJ	-3.67	1.33	1.39
2	D	201[B]	WXP	CAK-CAJ	-3.67	1.33	1.39
2	A	201[A]	WXP	CAY-CAD	-3.60	1.42	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201[B]	WXP	CAY-CAD	-3.60	1.42	1.49
2	D	201[A]	WXP	CAH-NAI	-3.55	1.32	1.40
2	D	201[B]	WXP	CAH-NAI	-3.55	1.32	1.40
2	C	201[A]	WXP	CAH-NAI	-3.54	1.32	1.40
2	C	201[B]	WXP	CAH-NAI	-3.54	1.32	1.40
2	B	201[A]	WXP	CBK-CAC	-3.53	1.43	1.49
2	C	201[A]	WXP	CAY-CAD	-3.52	1.43	1.49
2	C	201[B]	WXP	CAY-CAD	-3.52	1.43	1.49
2	B	201[A]	WXP	CAY-CAD	-3.50	1.43	1.49
2	B	201[B]	WXP	CAY-CAD	-3.50	1.43	1.49
2	C	201[A]	WXP	FE-NAS	3.47	2.16	1.97
2	C	201[B]	WXP	FE-NAS	3.47	2.16	1.97
2	B	201[A]	WXP	FE-NAI	3.44	2.16	1.97
2	B	201[B]	WXP	FE-NAI	3.44	2.16	1.97
2	A	201[A]	WXP	CAM-CAB	-3.34	1.37	1.47
2	A	201[B]	WXP	CAM-CAB	-3.34	1.37	1.47
2	A	201[A]	WXP	FE-NAS	3.30	2.15	1.97
2	A	201[B]	WXP	FE-NAS	3.30	2.15	1.97
2	A	201[A]	WXP	FE-NAI	3.28	2.15	1.97
2	A	201[B]	WXP	FE-NAI	3.28	2.15	1.97
2	A	201[A]	WXP	CAH-NAI	-3.27	1.33	1.40
2	A	201[B]	WXP	CAH-NAI	-3.27	1.33	1.40
2	B	201[A]	WXP	CAM-CAB	-3.22	1.37	1.47
2	B	201[B]	WXP	CAM-CAB	-3.22	1.37	1.47
2	A	201[A]	WXP	FE-NAN	3.20	2.22	1.96
2	A	201[B]	WXP	FE-NAN	3.20	2.22	1.96
2	B	201[A]	WXP	FE-NAN	3.17	2.22	1.96
2	B	201[B]	WXP	FE-NAN	3.17	2.22	1.96
2	D	201[B]	WXP	CBK-CAC	-3.16	1.43	1.49
2	A	201[B]	WXP	CBK-CAC	-3.15	1.43	1.49
2	B	201[A]	WXP	FE-NAS	3.07	2.14	1.97
2	B	201[B]	WXP	FE-NAS	3.07	2.14	1.97
2	A	201[A]	WXP	CAL-CAM	-3.05	1.34	1.40
2	A	201[B]	WXP	CAL-CAM	-3.05	1.34	1.40
2	C	201[B]	WXP	CBK-CAC	-3.03	1.44	1.49
2	B	201[A]	WXP	CAH-NAI	-3.02	1.34	1.40
2	B	201[B]	WXP	CAH-NAI	-3.02	1.34	1.40
2	B	201[B]	WXP	CBK-CAC	-3.00	1.44	1.49
2	C	201[A]	WXP	CAL-CAM	-2.96	1.35	1.40
2	C	201[B]	WXP	CAL-CAM	-2.96	1.35	1.40
2	D	201[A]	WXP	CAL-CAM	-2.95	1.35	1.40
2	D	201[B]	WXP	CAL-CAM	-2.95	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201[A]	WXP	CAM-CAB	-2.89	1.38	1.47
2	D	201[B]	WXP	CAM-CAB	-2.89	1.38	1.47
2	B	201[A]	WXP	CAL-CAM	-2.88	1.35	1.40
2	B	201[B]	WXP	CAL-CAM	-2.88	1.35	1.40
2	C	201[A]	WXP	CAM-CAB	-2.84	1.39	1.47
2	C	201[B]	WXP	CAM-CAB	-2.84	1.39	1.47
2	D	201[A]	WXP	CAO-NAS	-2.76	1.35	1.40
2	D	201[B]	WXP	CAO-NAS	-2.76	1.35	1.40
2	C	201[A]	WXP	CAO-NAS	-2.58	1.35	1.40
2	C	201[B]	WXP	CAO-NAS	-2.58	1.35	1.40
2	D	201[A]	WXP	FE-NAN	2.46	2.16	1.96
2	D	201[B]	WXP	FE-NAN	2.46	2.16	1.96
2	D	201[A]	WXP	CAE-NAI	-2.36	1.33	1.38
2	D	201[B]	WXP	CAE-NAI	-2.36	1.33	1.38
2	C	201[A]	WXP	FE-NAN	2.27	2.15	1.96
2	C	201[B]	WXP	FE-NAN	2.27	2.15	1.96
2	C	201[A]	WXP	CAE-NAI	-2.23	1.34	1.38
2	C	201[B]	WXP	CAE-NAI	-2.23	1.34	1.38
2	A	201[A]	WXP	CAE-NAI	-2.19	1.34	1.38
2	A	201[B]	WXP	CAE-NAI	-2.19	1.34	1.38
2	B	201[A]	WXP	CAE-NAI	-2.15	1.34	1.38
2	B	201[B]	WXP	CAE-NAI	-2.15	1.34	1.38
2	B	201[A]	WXP	CAW-NAX	-2.14	1.35	1.39
2	B	201[B]	WXP	CAW-NAX	-2.14	1.35	1.39
2	A	201[A]	WXP	CAW-NAX	-2.12	1.35	1.39
2	A	201[B]	WXP	CAW-NAX	-2.12	1.35	1.39
2	A	201[A]	WXP	CAT-NAX	-2.07	1.35	1.39
2	A	201[B]	WXP	CAT-NAX	-2.07	1.35	1.39
2	A	201[A]	WXP	CAO-NAS	-2.03	1.36	1.40
2	A	201[B]	WXP	CAO-NAS	-2.03	1.36	1.40

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201[A]	WXP	CAQ-CAR-NAS	-12.41	99.43	110.42
2	B	201[B]	WXP	CAQ-CAR-NAS	-12.41	99.43	110.42
2	A	201[A]	WXP	CAQ-CAR-NAS	-12.14	99.67	110.42
2	A	201[B]	WXP	CAQ-CAR-NAS	-12.14	99.67	110.42
2	D	201[A]	WXP	CAQ-CAR-NAS	-11.50	100.24	110.42
2	D	201[B]	WXP	CAQ-CAR-NAS	-11.50	100.24	110.42
2	C	201[A]	WXP	CAQ-CAR-NAS	-11.37	100.36	110.42
2	C	201[B]	WXP	CAQ-CAR-NAS	-11.37	100.36	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	201[A]	WXP	CAW-NAX-CAT	10.65	115.78	105.35
2	C	201[B]	WXP	CAW-NAX-CAT	10.65	115.78	105.35
2	D	201[A]	WXP	CAO-NAS-CAR	10.35	115.76	105.07
2	D	201[B]	WXP	CAO-NAS-CAR	10.35	115.76	105.07
2	B	201[A]	WXP	CAW-NAX-CAT	10.32	115.46	105.35
2	B	201[B]	WXP	CAW-NAX-CAT	10.32	115.46	105.35
2	D	201[A]	WXP	CAW-NAX-CAT	10.28	115.42	105.35
2	D	201[B]	WXP	CAW-NAX-CAT	10.28	115.42	105.35
2	C	201[A]	WXP	CAO-NAS-CAR	10.20	115.61	105.07
2	C	201[B]	WXP	CAO-NAS-CAR	10.20	115.61	105.07
2	B	201[A]	WXP	CAO-NAS-CAR	10.13	115.53	105.07
2	B	201[B]	WXP	CAO-NAS-CAR	10.13	115.53	105.07
2	A	201[A]	WXP	CAW-NAX-CAT	10.11	115.24	105.35
2	A	201[B]	WXP	CAW-NAX-CAT	10.11	115.24	105.35
2	A	201[A]	WXP	CAO-NAS-CAR	9.89	115.29	105.07
2	A	201[B]	WXP	CAO-NAS-CAR	9.89	115.29	105.07
2	C	201[A]	WXP	CAU-CAT-NAX	-9.51	98.94	109.93
2	C	201[B]	WXP	CAU-CAT-NAX	-9.51	98.94	109.93
2	D	201[A]	WXP	CAU-CAT-NAX	-9.26	99.24	109.93
2	D	201[B]	WXP	CAU-CAT-NAX	-9.26	99.24	109.93
2	A	201[A]	WXP	CAF-CAE-NAI	-8.91	102.53	110.42
2	A	201[B]	WXP	CAF-CAE-NAI	-8.91	102.53	110.42
2	B	201[A]	WXP	CAU-CAT-NAX	-8.41	100.22	109.93
2	B	201[B]	WXP	CAU-CAT-NAX	-8.41	100.22	109.93
2	B	201[A]	WXP	CAF-CAE-NAI	-8.20	103.16	110.42
2	B	201[B]	WXP	CAF-CAE-NAI	-8.20	103.16	110.42
2	A	201[A]	WXP	CAU-CAT-NAX	-8.20	100.47	109.93
2	A	201[B]	WXP	CAU-CAT-NAX	-8.20	100.47	109.93
2	D	201[A]	WXP	CAF-CAE-NAI	-8.06	103.28	110.42
2	D	201[B]	WXP	CAF-CAE-NAI	-8.06	103.28	110.42
2	C	201[A]	WXP	CAF-CAE-NAI	-8.01	103.32	110.42
2	C	201[B]	WXP	CAF-CAE-NAI	-8.01	103.32	110.42
2	B	201[A]	WXP	CAV-CAW-NAX	-6.81	102.07	109.93
2	B	201[B]	WXP	CAV-CAW-NAX	-6.81	102.07	109.93
2	A	201[A]	WXP	CAV-CAW-NAX	-6.64	102.27	109.93
2	A	201[B]	WXP	CAV-CAW-NAX	-6.64	102.27	109.93
2	C	201[A]	WXP	CAV-CAW-NAX	-6.53	102.39	109.93
2	C	201[B]	WXP	CAV-CAW-NAX	-6.53	102.39	109.93
2	D	201[A]	WXP	CAK-CAJ-NAN	-6.39	104.36	110.09
2	D	201[B]	WXP	CAK-CAJ-NAN	-6.39	104.36	110.09
2	D	201[A]	WXP	CAV-CAW-NAX	-6.35	102.60	109.93
2	D	201[B]	WXP	CAV-CAW-NAX	-6.35	102.60	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201[A]	WXP	CAK-CAJ-NAN	-6.17	104.56	110.09
2	A	201[B]	WXP	CAK-CAJ-NAN	-6.17	104.56	110.09
2	B	201[A]	WXP	CAK-CAJ-NAN	-6.13	104.59	110.09
2	B	201[B]	WXP	CAK-CAJ-NAN	-6.13	104.59	110.09
2	C	201[A]	WXP	CAK-CAJ-NAN	-6.06	104.65	110.09
2	C	201[B]	WXP	CAK-CAJ-NAN	-6.06	104.65	110.09
2	C	201[A]	WXP	CAP-CAO-NAS	-5.95	101.94	108.87
2	C	201[B]	WXP	CAP-CAO-NAS	-5.95	101.94	108.87
2	D	201[A]	WXP	CAP-CAO-NAS	-5.89	102.01	108.87
2	D	201[B]	WXP	CAP-CAO-NAS	-5.89	102.01	108.87
2	B	201[A]	WXP	CAP-CAO-NAS	-5.80	102.11	108.87
2	B	201[B]	WXP	CAP-CAO-NAS	-5.80	102.11	108.87
2	B	201[A]	WXP	CAG-CAH-NAI	-5.76	104.62	109.48
2	B	201[B]	WXP	CAG-CAH-NAI	-5.76	104.62	109.48
2	A	201[A]	WXP	CAP-CAO-NAS	-5.64	102.30	108.87
2	A	201[B]	WXP	CAP-CAO-NAS	-5.64	102.30	108.87
2	D	201[A]	WXP	CAG-CAH-NAI	-5.64	104.71	109.48
2	D	201[B]	WXP	CAG-CAH-NAI	-5.64	104.71	109.48
2	A	201[A]	WXP	CAG-CAH-NAI	-5.63	104.72	109.48
2	A	201[B]	WXP	CAG-CAH-NAI	-5.63	104.72	109.48
2	A	201[A]	WXP	CAE-NAI-CAH	5.30	113.40	106.71
2	A	201[B]	WXP	CAE-NAI-CAH	5.30	113.40	106.71
2	D	201[A]	WXP	CAE-NAI-CAH	5.14	113.19	106.71
2	D	201[B]	WXP	CAE-NAI-CAH	5.14	113.19	106.71
2	C	201[A]	WXP	CAG-CAH-NAI	-5.09	105.18	109.48
2	C	201[B]	WXP	CAG-CAH-NAI	-5.09	105.18	109.48
2	B	201[A]	WXP	CAE-NAI-CAH	4.89	112.88	106.71
2	B	201[B]	WXP	CAE-NAI-CAH	4.89	112.88	106.71
2	C	201[A]	WXP	CAE-NAI-CAH	4.73	112.68	106.71
2	C	201[B]	WXP	CAE-NAI-CAH	4.73	112.68	106.71
2	C	201[A]	WXP	CAV-CAU-CAT	4.71	113.08	107.53
2	C	201[B]	WXP	CAV-CAU-CAT	4.71	113.08	107.53
2	D	201[A]	WXP	CAV-CAU-CAT	4.53	112.86	107.53
2	D	201[B]	WXP	CAV-CAU-CAT	4.53	112.86	107.53
2	B	201[A]	WXP	CAP-CAQ-CAR	4.45	112.83	107.41
2	B	201[B]	WXP	CAP-CAQ-CAR	4.45	112.83	107.41
2	A	201[A]	WXP	CAP-CAQ-CAR	4.36	112.72	107.41
2	A	201[B]	WXP	CAP-CAQ-CAR	4.36	112.72	107.41
2	B	201[A]	WXP	CAV-CAU-CAT	3.98	112.22	107.53
2	B	201[B]	WXP	CAV-CAU-CAT	3.98	112.22	107.53
2	A	201[A]	WXP	CAV-CAU-CAT	3.86	112.08	107.53
2	A	201[B]	WXP	CAV-CAU-CAT	3.86	112.08	107.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	201[A]	WXP	CAP-CAQ-CAR	3.84	112.08	107.41
2	D	201[B]	WXP	CAP-CAQ-CAR	3.84	112.08	107.41
2	C	201[A]	WXP	CAP-CAQ-CAR	3.72	111.94	107.41
2	C	201[B]	WXP	CAP-CAQ-CAR	3.72	111.94	107.41
2	C	201[A]	WXP	CAC-CAT-NAX	3.56	129.77	125.79
2	C	201[B]	WXP	CAC-CAT-NAX	3.56	129.77	125.79
2	B	201[A]	WXP	CAL-CAK-CAJ	3.44	109.23	106.29
2	B	201[B]	WXP	CAL-CAK-CAJ	3.44	109.23	106.29
2	A	201[A]	WXP	CAL-CAK-CAJ	3.41	109.20	106.29
2	A	201[B]	WXP	CAL-CAK-CAJ	3.41	109.20	106.29
2	D	201[A]	WXP	CAC-CAT-NAX	3.39	129.58	125.79
2	D	201[B]	WXP	CAC-CAT-NAX	3.39	129.58	125.79
2	A	201[A]	WXP	CAB-CAO-NAS	3.38	129.76	125.79
2	A	201[B]	WXP	CAB-CAO-NAS	3.38	129.76	125.79
2	D	201[A]	WXP	CAL-CAK-CAJ	3.37	109.17	106.29
2	D	201[B]	WXP	CAL-CAK-CAJ	3.37	109.17	106.29
2	C	201[A]	WXP	CAZ-CAB-CAM	-3.34	113.35	117.56
2	C	201[B]	WXP	CAZ-CAB-CAM	-3.34	113.35	117.56
2	C	201[A]	WXP	CAL-CAK-CAJ	3.33	109.14	106.29
2	C	201[B]	WXP	CAL-CAK-CAJ	3.33	109.14	106.29
2	B	201[A]	WXP	CAB-CAO-NAS	3.26	129.62	125.79
2	B	201[B]	WXP	CAB-CAO-NAS	3.26	129.62	125.79
2	C	201[A]	WXP	CAQ-CAR-CAC	3.23	132.01	125.18
2	C	201[B]	WXP	CAQ-CAR-CAC	3.23	132.01	125.18
2	D	201[A]	WXP	CAZ-CAB-CAM	-3.18	113.56	117.56
2	D	201[B]	WXP	CAZ-CAB-CAM	-3.18	113.56	117.56
2	D	201[A]	WXP	CAQ-CAR-CAC	3.18	131.91	125.18
2	D	201[B]	WXP	CAQ-CAR-CAC	3.18	131.91	125.18
2	B	201[A]	WXP	CAC-CAR-NAS	3.00	129.41	125.46
2	B	201[B]	WXP	CAC-CAR-NAS	3.00	129.41	125.46
2	A	201[A]	WXP	CAF-CAE-CAD	2.97	131.48	125.18
2	A	201[B]	WXP	CAF-CAE-CAD	2.97	131.48	125.18
2	C	201[A]	WXP	CAD-CAW-NAX	2.94	129.07	125.79
2	C	201[B]	WXP	CAD-CAW-NAX	2.94	129.07	125.79
2	A	201[A]	WXP	CAC-CAR-NAS	2.91	129.29	125.46
2	A	201[B]	WXP	CAC-CAR-NAS	2.91	129.29	125.46
2	D	201[A]	WXP	CAD-CAW-NAX	2.83	128.96	125.79
2	D	201[B]	WXP	CAD-CAW-NAX	2.83	128.96	125.79
2	B	201[A]	WXP	CAQ-CAR-CAC	2.82	131.16	125.18
2	B	201[B]	WXP	CAQ-CAR-CAC	2.82	131.16	125.18
2	A	201[A]	WXP	CAQ-CAR-CAC	2.76	131.03	125.18
2	A	201[B]	WXP	CAQ-CAR-CAC	2.76	131.03	125.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	201[A]	WXP	CBL-CBK-CAC	2.76	125.18	120.79
2	D	201[A]	WXP	CAF-CAE-CAD	2.75	131.01	125.18
2	D	201[B]	WXP	CAF-CAE-CAD	2.75	131.01	125.18
2	A	201[A]	WXP	CAZ-CAB-CAM	-2.74	114.11	117.56
2	A	201[B]	WXP	CAZ-CAB-CAM	-2.74	114.11	117.56
2	C	201[A]	WXP	CAF-CAE-CAD	2.62	130.73	125.18
2	C	201[B]	WXP	CAF-CAE-CAD	2.62	130.73	125.18
2	C	201[A]	WXP	CBI-CBJ-CAY	2.59	123.41	120.34
2	C	201[B]	WXP	CBI-CBJ-CAY	2.59	123.41	120.34
2	D	201[A]	WXP	CBL-CBK-CAC	2.57	124.87	120.79
2	B	201[B]	WXP	CBO-CBP-CBK	2.53	123.34	120.34
2	A	201[A]	WXP	CAG-CAF-CAE	2.53	110.49	107.41
2	A	201[B]	WXP	CAG-CAF-CAE	2.53	110.49	107.41
2	B	201[A]	WXP	CAF-CAE-CAD	2.52	130.52	125.18
2	B	201[B]	WXP	CAF-CAE-CAD	2.52	130.52	125.18
2	B	201[A]	WXP	CAZ-CAB-CAM	-2.52	114.39	117.56
2	B	201[B]	WXP	CAZ-CAB-CAM	-2.52	114.39	117.56
2	B	201[A]	WXP	CBB-CBA-CAZ	2.45	123.25	120.34
2	B	201[B]	WXP	CBB-CBA-CAZ	2.45	123.25	120.34
2	A	201[A]	WXP	CBB-CBA-CAZ	2.43	123.22	120.34
2	A	201[B]	WXP	CBB-CBA-CAZ	2.43	123.22	120.34
2	C	201[B]	WXP	CBP-CBK-CBL	-2.36	115.23	118.59
2	A	201[A]	WXP	CAW-CAD-CAE	2.35	129.36	124.29
2	A	201[B]	WXP	CAW-CAD-CAE	2.35	129.36	124.29
2	D	201[A]	WXP	CBI-CBJ-CAY	2.32	123.09	120.34
2	D	201[B]	WXP	CBI-CBJ-CAY	2.32	123.09	120.34
2	B	201[A]	WXP	CAD-CAW-NAX	2.30	128.36	125.79
2	B	201[B]	WXP	CAD-CAW-NAX	2.30	128.36	125.79
2	D	201[B]	WXP	CBO-CBP-CBK	2.29	123.05	120.34
2	B	201[B]	WXP	CBP-CBK-CBL	-2.28	115.34	118.59
2	C	201[B]	WXP	CBO-CBP-CBK	2.27	123.03	120.34
2	A	201[A]	WXP	CAU-CAT-CAC	2.27	131.74	125.73
2	A	201[B]	WXP	CAU-CAT-CAC	2.27	131.74	125.73
2	C	201[A]	WXP	CAQ-CAP-CAO	2.25	110.15	107.41
2	C	201[B]	WXP	CAQ-CAP-CAO	2.25	110.15	107.41
2	D	201[A]	WXP	CAP-CAO-CAB	2.25	129.93	125.97
2	D	201[B]	WXP	CAP-CAO-CAB	2.25	129.93	125.97
2	C	201[A]	WXP	CAB-CAO-NAS	2.23	128.41	125.79
2	C	201[B]	WXP	CAB-CAO-NAS	2.23	128.41	125.79
2	A	201[A]	WXP	CAY-CAD-CAE	-2.22	113.83	117.77
2	A	201[B]	WXP	CAY-CAD-CAE	-2.22	113.83	117.77
2	B	201[A]	WXP	CAU-CAT-CAC	2.21	131.58	125.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201[B]	WXP	CAU-CAT-CAC	2.21	131.58	125.73
2	B	201[A]	WXP	CAQ-CAP-CAO	2.20	110.09	107.41
2	B	201[B]	WXP	CAQ-CAP-CAO	2.20	110.09	107.41
2	B	201[A]	WXP	CAG-CAF-CAE	2.20	110.09	107.41
2	B	201[B]	WXP	CAG-CAF-CAE	2.20	110.09	107.41
2	A	201[A]	WXP	CAQ-CAP-CAO	2.15	110.03	107.41
2	A	201[B]	WXP	CAQ-CAP-CAO	2.15	110.03	107.41
2	D	201[A]	WXP	CAW-CAD-CAE	2.13	128.88	124.29
2	D	201[B]	WXP	CAW-CAD-CAE	2.13	128.88	124.29
2	B	201[A]	WXP	CAU-CAV-CAW	2.11	110.02	107.53
2	B	201[B]	WXP	CAU-CAV-CAW	2.11	110.02	107.53
2	B	201[A]	WXP	CAC-CAT-NAX	2.11	128.15	125.79
2	B	201[B]	WXP	CAC-CAT-NAX	2.11	128.15	125.79
2	D	201[B]	WXP	CBP-CBK-CBL	-2.10	115.59	118.59
2	C	201[A]	WXP	CAP-CAO-CAB	2.08	129.65	125.97
2	C	201[B]	WXP	CAP-CAO-CAB	2.08	129.65	125.97
2	A	201[B]	WXP	CBM-CBL-CBK	2.07	122.79	120.34
2	C	201[A]	WXP	CAU-CAT-CAC	2.05	131.16	125.73
2	C	201[B]	WXP	CAU-CAT-CAC	2.05	131.16	125.73
2	D	201[A]	WXP	CAQ-CAP-CAO	2.05	109.91	107.41
2	D	201[B]	WXP	CAQ-CAP-CAO	2.05	109.91	107.41
2	B	201[A]	WXP	CAW-CAD-CAE	2.05	128.71	124.29
2	B	201[B]	WXP	CAW-CAD-CAE	2.05	128.71	124.29
2	D	201[A]	WXP	CAU-CAT-CAC	2.04	131.13	125.73
2	D	201[B]	WXP	CAU-CAT-CAC	2.04	131.13	125.73
2	A	201[A]	WXP	CAU-CAV-CAW	2.03	109.92	107.53
2	A	201[B]	WXP	CAU-CAV-CAW	2.03	109.92	107.53
2	A	201[A]	WXP	CAD-CAW-NAX	2.02	128.05	125.79
2	A	201[B]	WXP	CAD-CAW-NAX	2.02	128.05	125.79
2	C	201[A]	WXP	CAW-CAD-CAE	2.02	128.64	124.29
2	C	201[B]	WXP	CAW-CAD-CAE	2.02	128.64	124.29
2	D	201[A]	WXP	CBE-CAZ-CAB	2.01	124.10	120.91
2	D	201[B]	WXP	CBE-CAZ-CAB	2.01	124.10	120.91

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	202	PE8	O13-C14-C15-O16
3	D	202	PE8	O19-C20-C21-O22
3	D	202	PE8	O4-C5-C6-O7
3	A	203	PE8	O13-C14-C15-O16

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Mol	Chain	Res	Type	Atoms
3	D	202	PE8	O7-C8-C9-O10
3	D	202	PE8	O16-C17-C18-O19
3	D	202	PE8	O10-C11-C12-O13
3	D	202	PE8	O22-C23-C24-O25
3	A	203	PE8	O19-C20-C21-O22
3	A	203	PE8	O1-C2-C3-O4
3	A	203	PE8	O10-C11-C12-O13
3	D	202	PE8	C2-C3-O4-C5
3	A	203	PE8	C12-C11-O10-C9
3	A	203	PE8	C18-C17-O16-C15
3	D	202	PE8	C15-C14-O13-C12
3	A	203	PE8	O7-C8-C9-O10
3	A	203	PE8	C2-C3-O4-C5
3	D	202	PE8	O1-C2-C3-O4
3	B	202	PE8	O19-C20-C21-O22
3	B	202	PE8	O4-C5-C6-O7
3	A	203	PE8	C15-C14-O13-C12
3	A	203	PE8	O16-C17-C18-O19
3	A	203	PE8	O4-C5-C6-O7

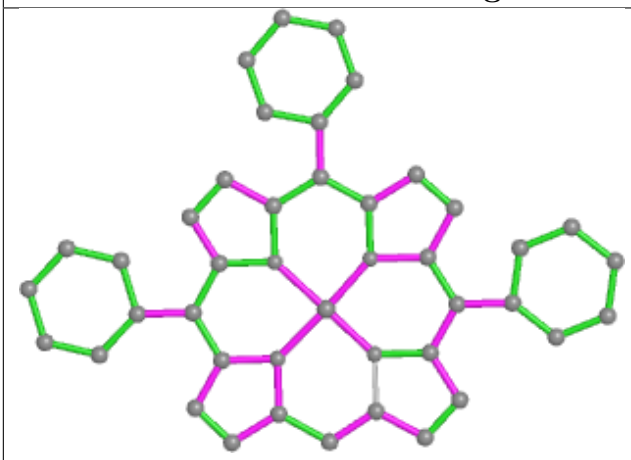
There are no ring outliers.

1 monomer is involved in 1 short contact:

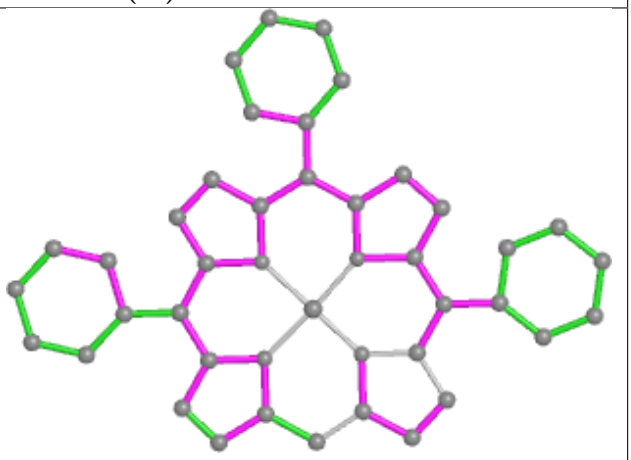
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201[A]	WXP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

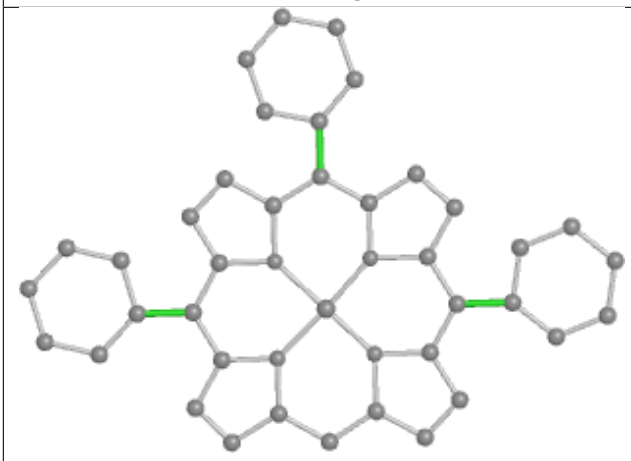
Ligand WXP C 201 (A)



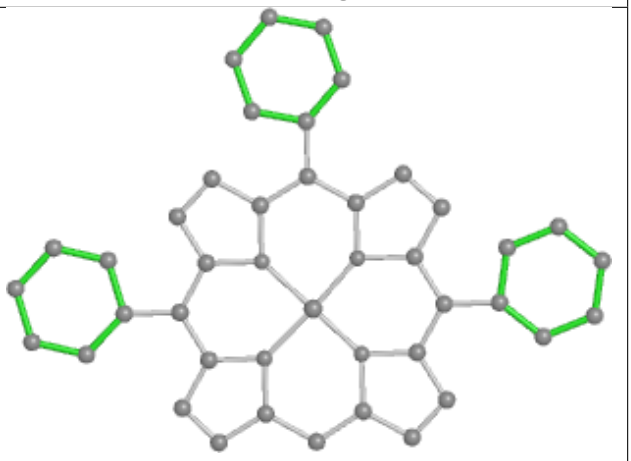
Bond lengths



Bond angles



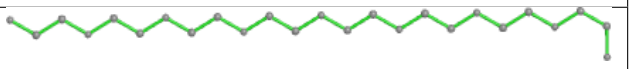
Torsions



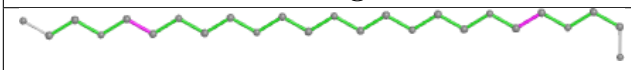
Rings

Ligand PE8 B 202

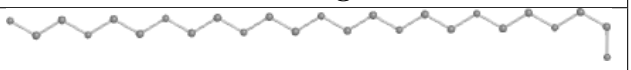
Bond lengths



Bond angles

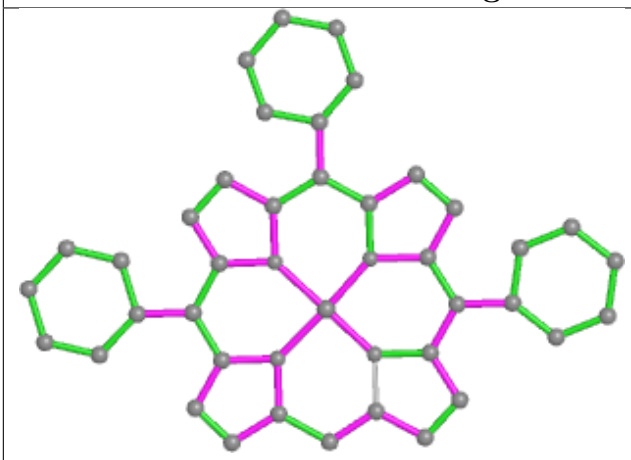


Torsions

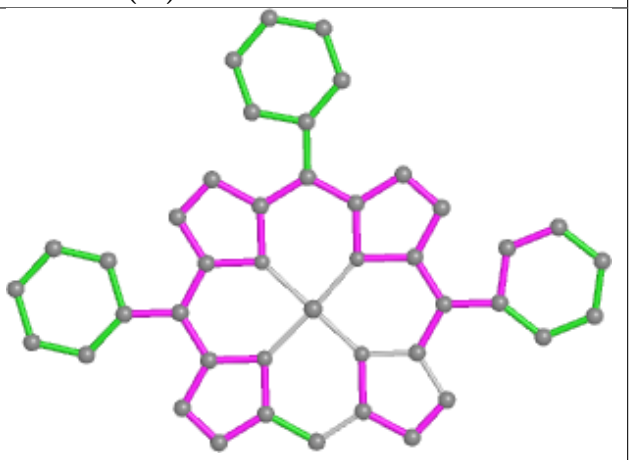


Rings

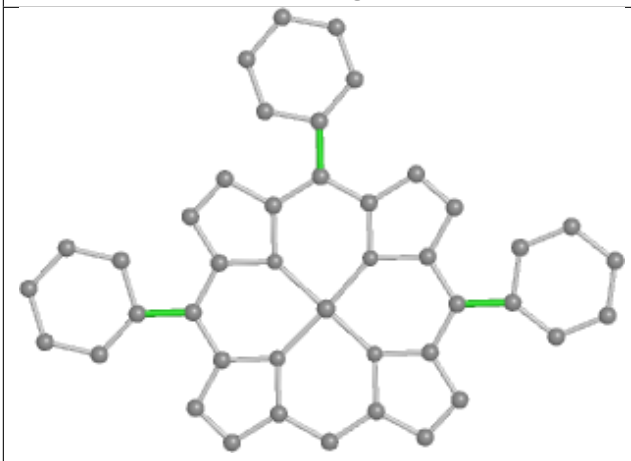
Ligand WXP A 201 (A)



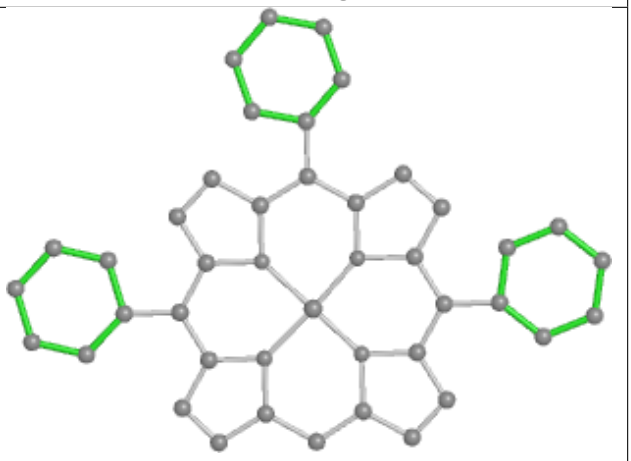
Bond lengths



Bond angles

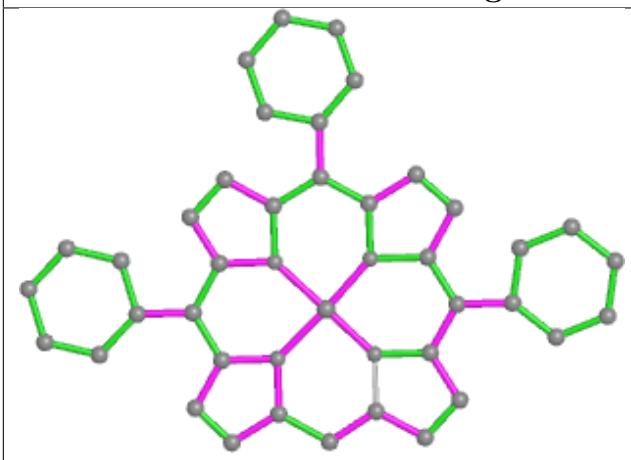


Torsions

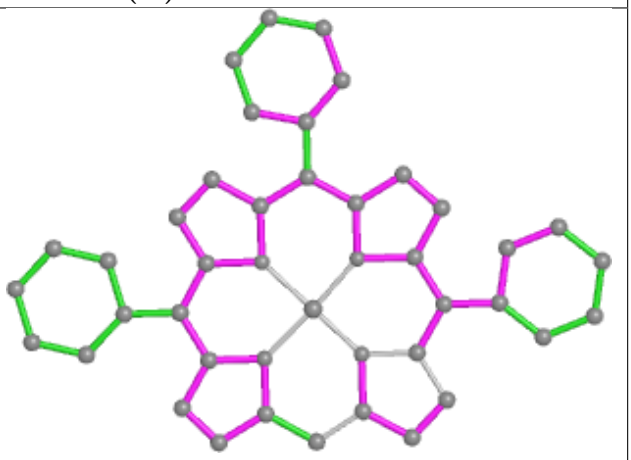


Rings

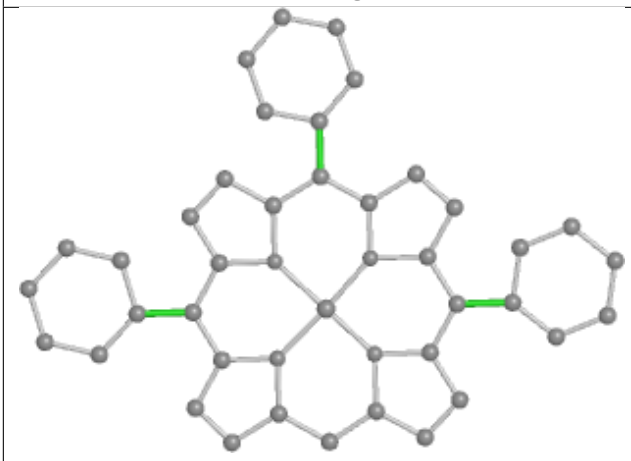
Ligand WXP B 201 (B)



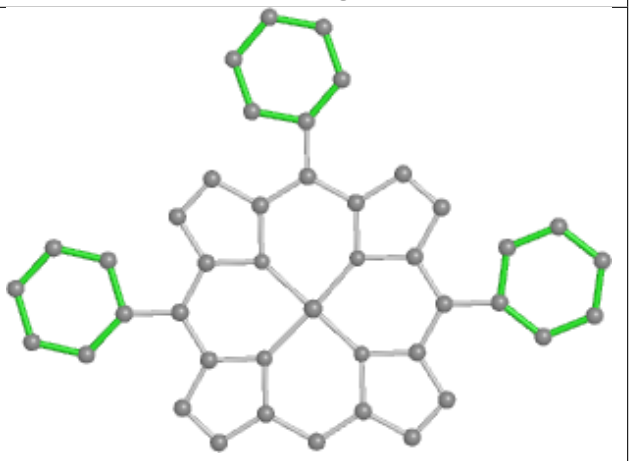
Bond lengths



Bond angles



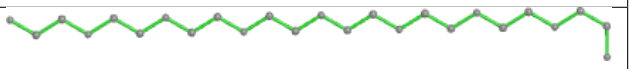
Torsions



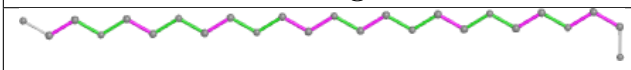
Rings

Ligand PE8 D 202

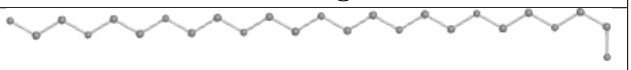
Bond lengths



Bond angles

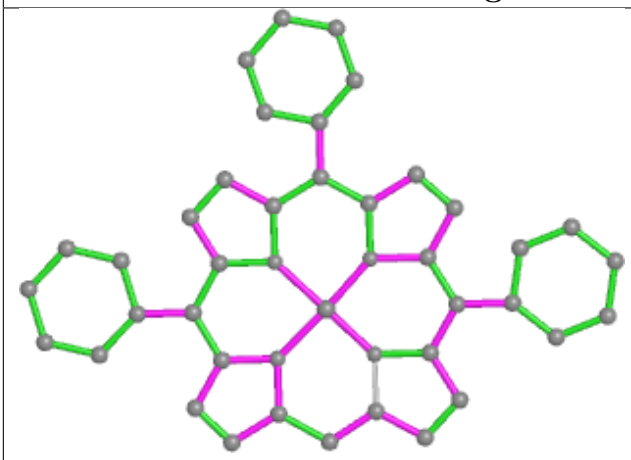


Torsions

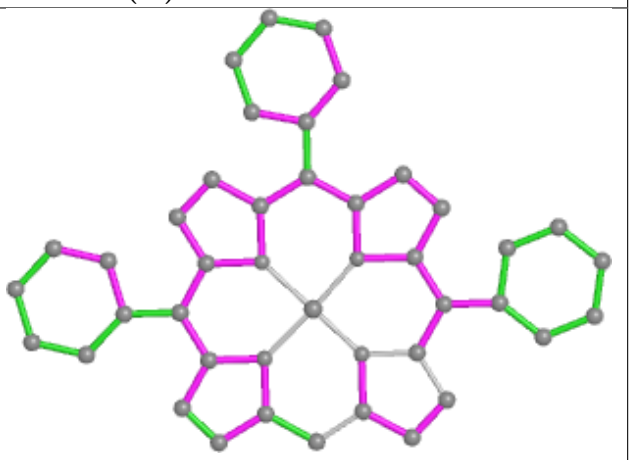


Rings

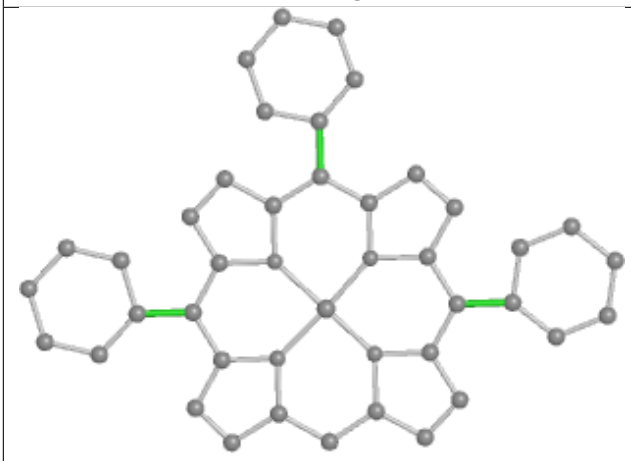
Ligand WXP C 201 (B)



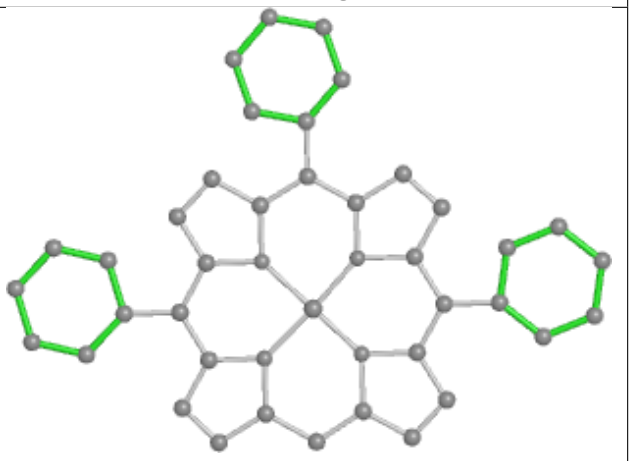
Bond lengths



Bond angles

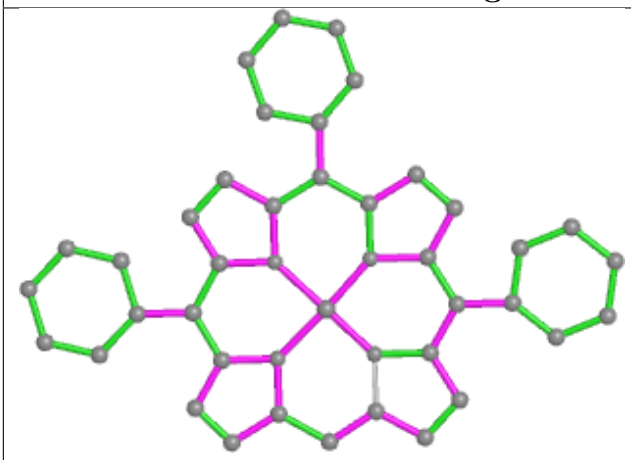


Torsions

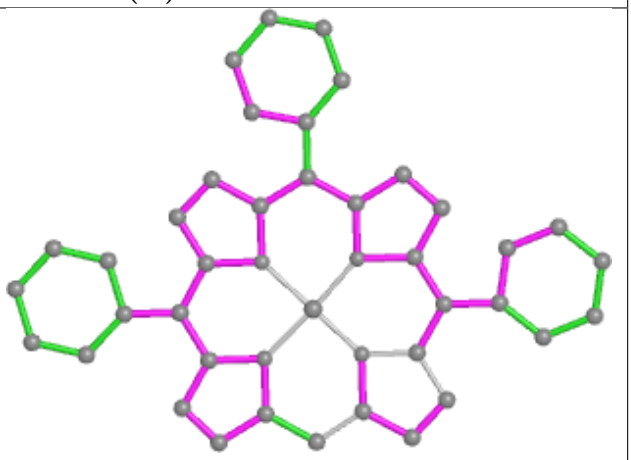


Rings

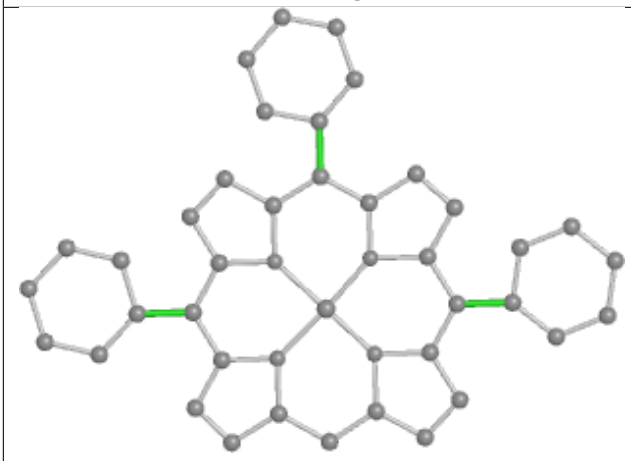
Ligand WXP A 201 (B)



Bond lengths



Bond angles



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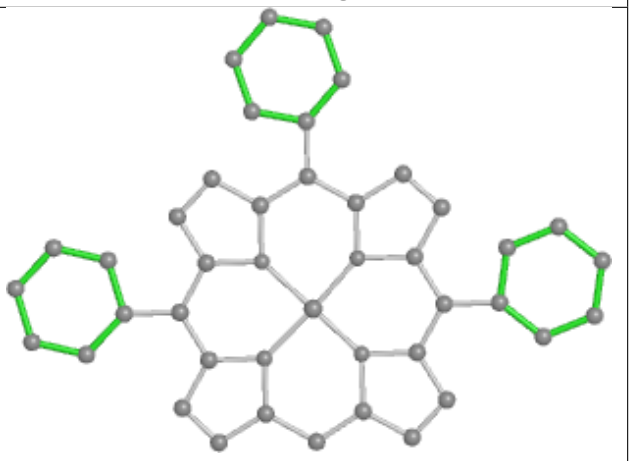
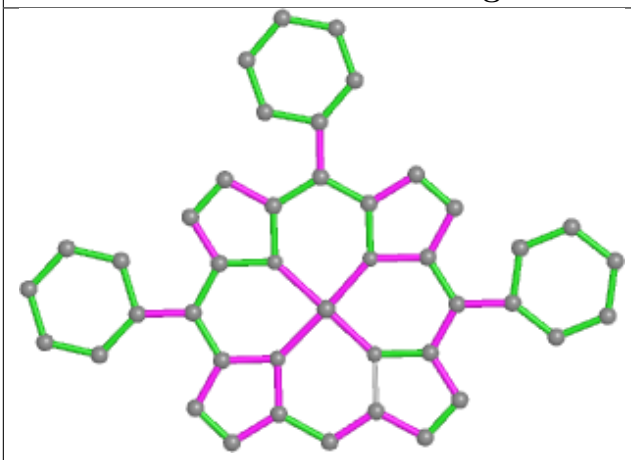
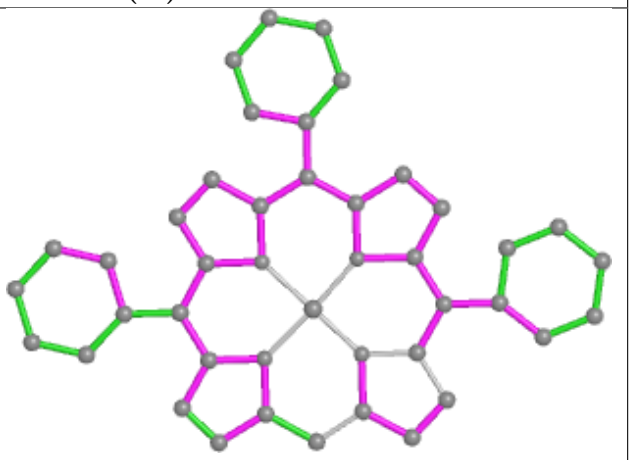


Rings

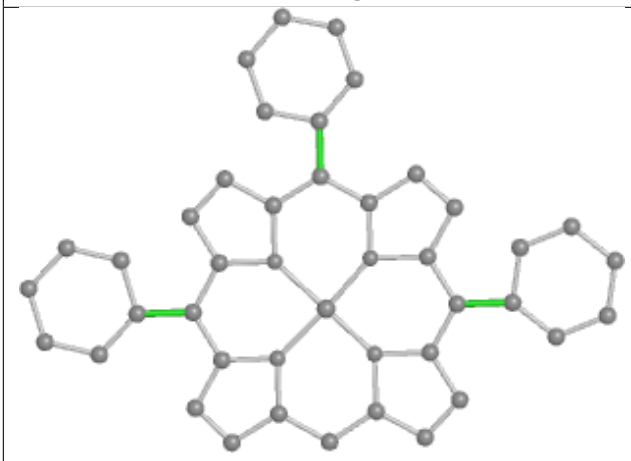
Ligand WXP D 201 (A)



Bond lengths



Bond angles



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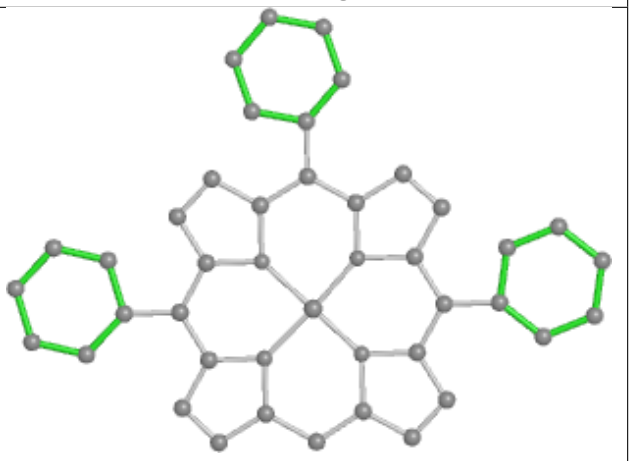
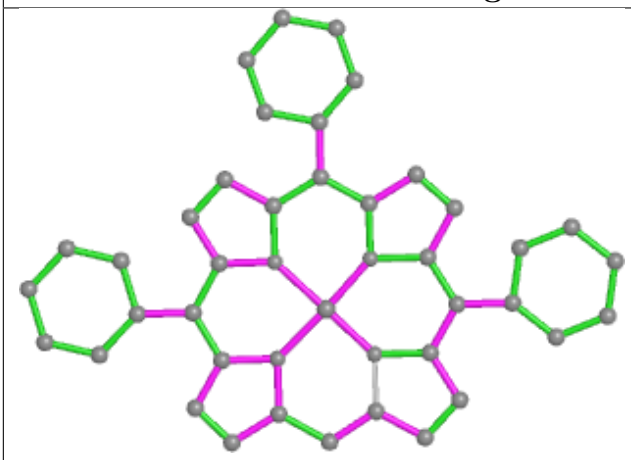
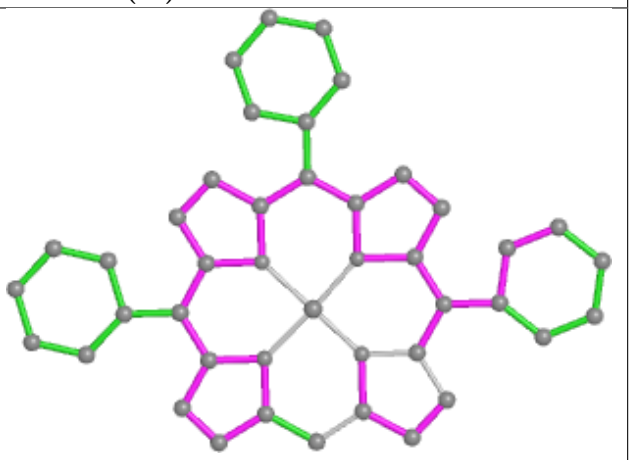


Rings

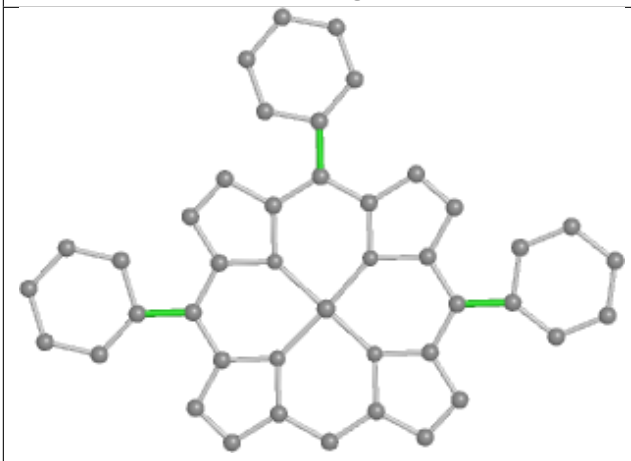
Ligand WXP B 201 (A)



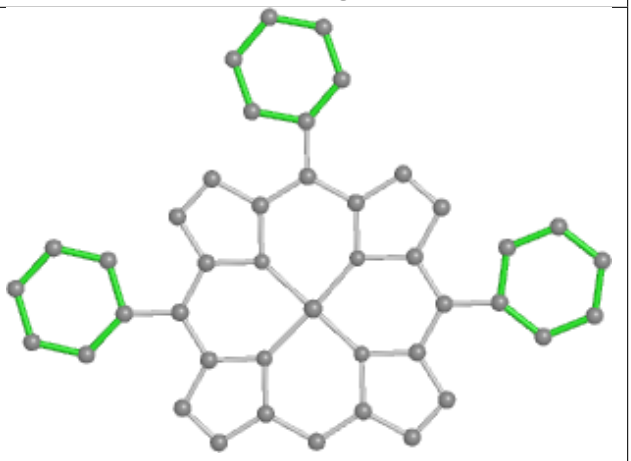
Bond lengths



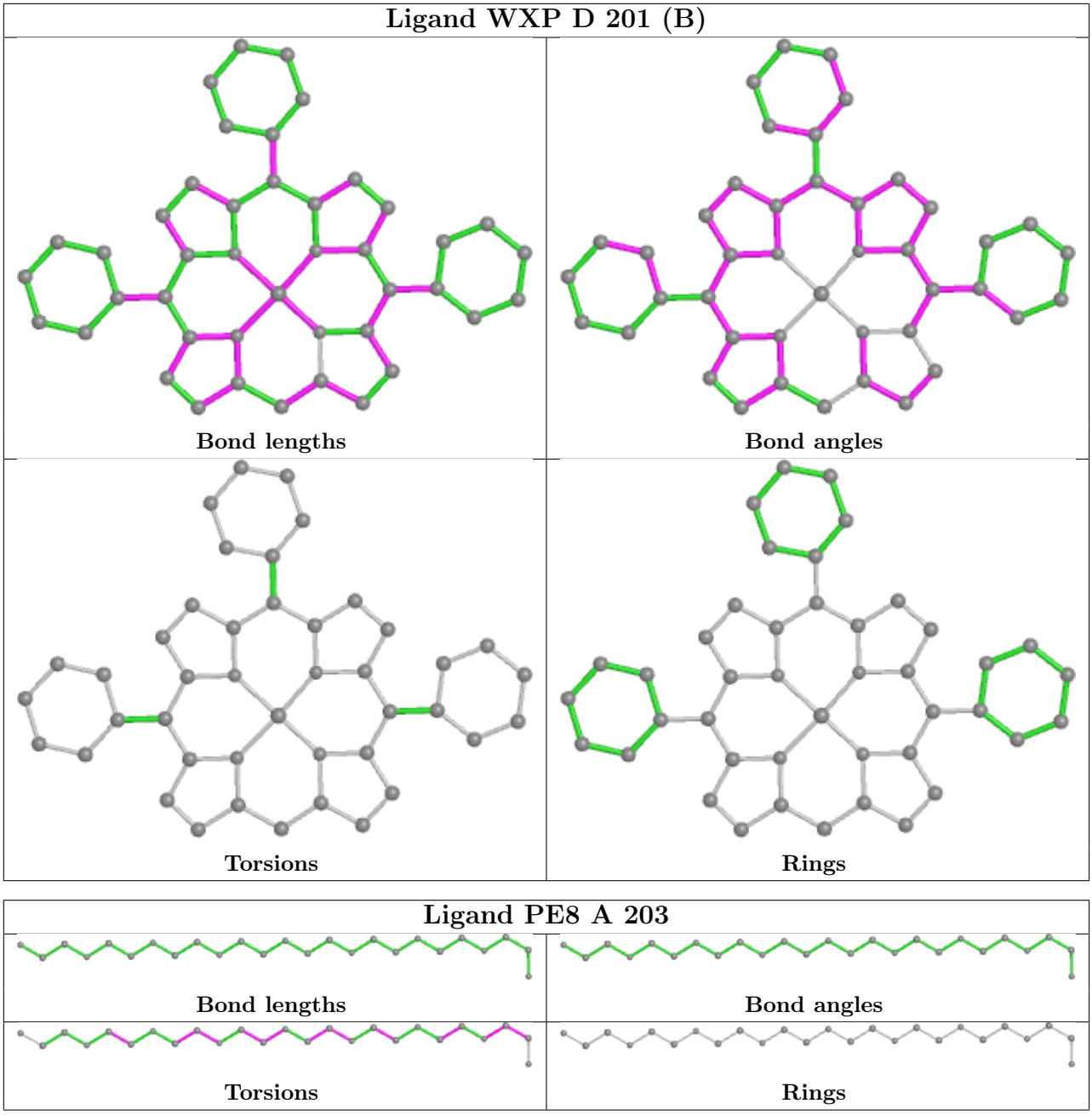
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	184/184 (100%)	0.63	12 (6%) 18 21	7, 13, 20, 32	0
1	B	184/184 (100%)	0.69	18 (9%) 7 9	7, 13, 20, 33	0
1	C	184/184 (100%)	0.70	19 (10%) 6 7	7, 12, 19, 33	0
1	D	184/184 (100%)	0.75	18 (9%) 7 9	7, 13, 20, 36	0
All	All	736/736 (100%)	0.69	67 (9%) 9 11	7, 13, 20, 36	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	184	ALA	7.2
1	D	21	ALA	5.7
1	D	26[A]	TYR	5.7
1	C	184	ALA	5.4
1	B	26[A]	TYR	4.9
1	C	26[A]	TYR	4.8
1	C	14	TRP	4.8
1	A	21	ALA	4.6
1	A	26[A]	TYR	4.6
1	A	14	TRP	4.4
1	B	38	VAL	4.3
1	D	14	TRP	4.3
1	D	38[A]	VAL	4.2
1	B	14	TRP	4.1
1	B	184	ALA	4.0
1	C	20	LEU	3.9
1	D	24	SER	3.9
1	B	20	LEU	3.9
1	C	16	VAL	3.7
1	B	1	MET	3.6
1	C	17	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	3.5
1	D	20	LEU	3.3
1	B	179	HIS	3.2
1	A	20	LEU	3.2
1	C	25	ALA	3.2
1	B	17	ALA	3.1
1	C	38	VAL	3.0
1	D	35	GLY	3.0
1	B	23	TRP	3.0
1	C	23	TRP	3.0
1	A	37	VAL	2.9
1	D	85	LEU	2.9
1	B	62	ALA	2.9
1	B	16	VAL	2.9
1	C	21	ALA	2.8
1	D	165	ILE	2.8
1	C	165	ILE	2.8
1	B	21	ALA	2.8
1	C	22	ASP	2.7
1	B	37	VAL	2.7
1	A	24	SER	2.6
1	B	18	ASP	2.6
1	D	19	TYR	2.5
1	B	22	ASP	2.5
1	D	17	ALA	2.5
1	A	17	ALA	2.5
1	C	179	HIS	2.4
1	C	18	ASP	2.4
1	A	22	ASP	2.4
1	D	183	ALA	2.3
1	A	25	ALA	2.3
1	A	184	ALA	2.3
1	D	16	VAL	2.3
1	C	37	VAL	2.2
1	D	182	PRO	2.2
1	B	19	TYR	2.2
1	A	38	VAL	2.2
1	D	143	GLY	2.2
1	D	163	LEU	2.2
1	B	24	SER	2.1
1	D	1	MET	2.0
1	C	15	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	165	ILE	2.0
1	C	19	TYR	2.0
1	C	24	SER	2.0
1	A	62	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

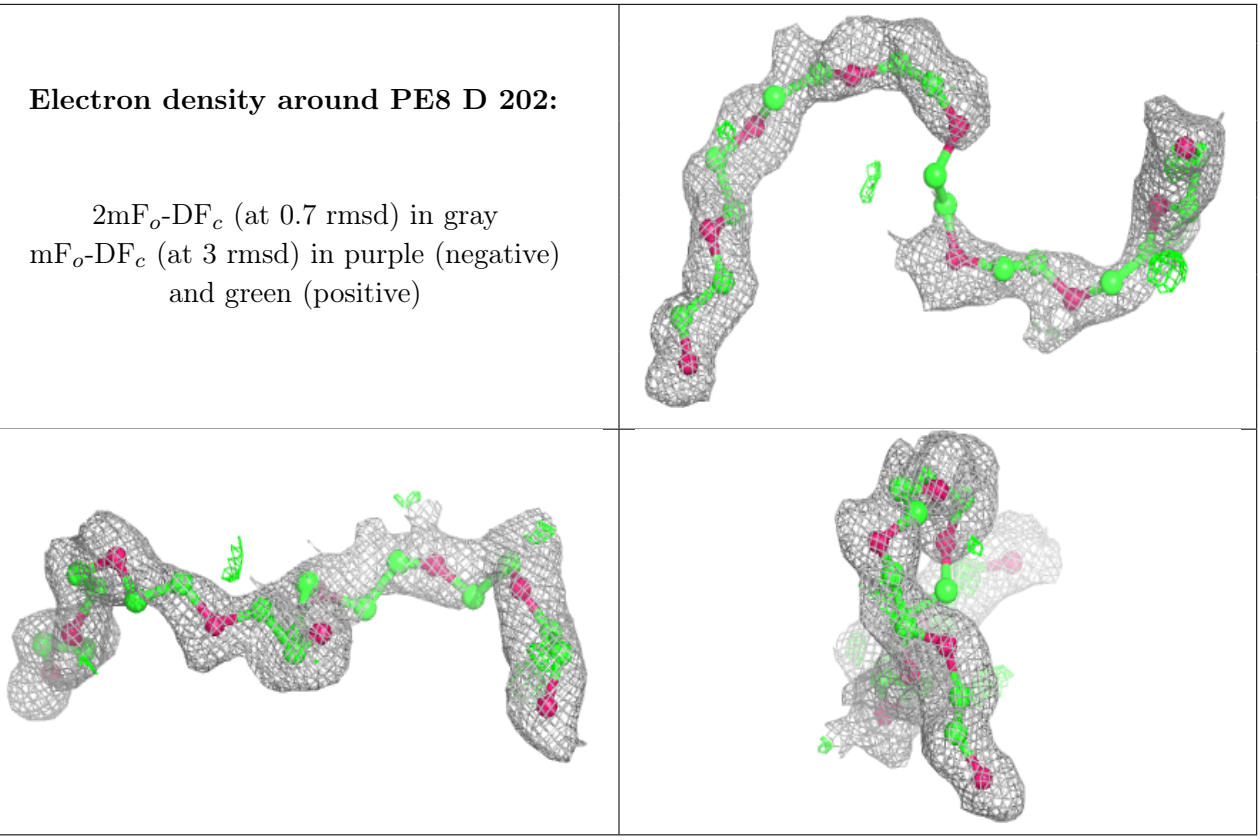
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PE8	D	202	25/25	0.61	0.22	40,42,46,46	0
3	PE8	A	203	25/25	0.65	0.21	39,41,44,45	0
3	PE8	B	202	25/25	0.79	0.16	16,18,21,22	0
3	PE8	A	202	25/25	0.86	0.12	15,16,20,21	0
2	WXP	A	201[A]	43/43	0.95	0.12	9,11,12,13	6
2	WXP	A	201[B]	43/43	0.95	0.12	9,11,12,13	6
2	WXP	C	201[A]	43/43	0.95	0.13	9,11,12,12	6
2	WXP	C	201[B]	43/43	0.95	0.13	9,11,12,12	6
2	WXP	B	201[A]	43/43	0.96	0.14	9,12,13,13	6
2	WXP	B	201[B]	43/43	0.96	0.14	9,12,12,12	6
2	WXP	D	201[A]	43/43	0.97	0.11	9,11,12,12	6
2	WXP	D	201[B]	43/43	0.97	0.11	9,11,12,13	6

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

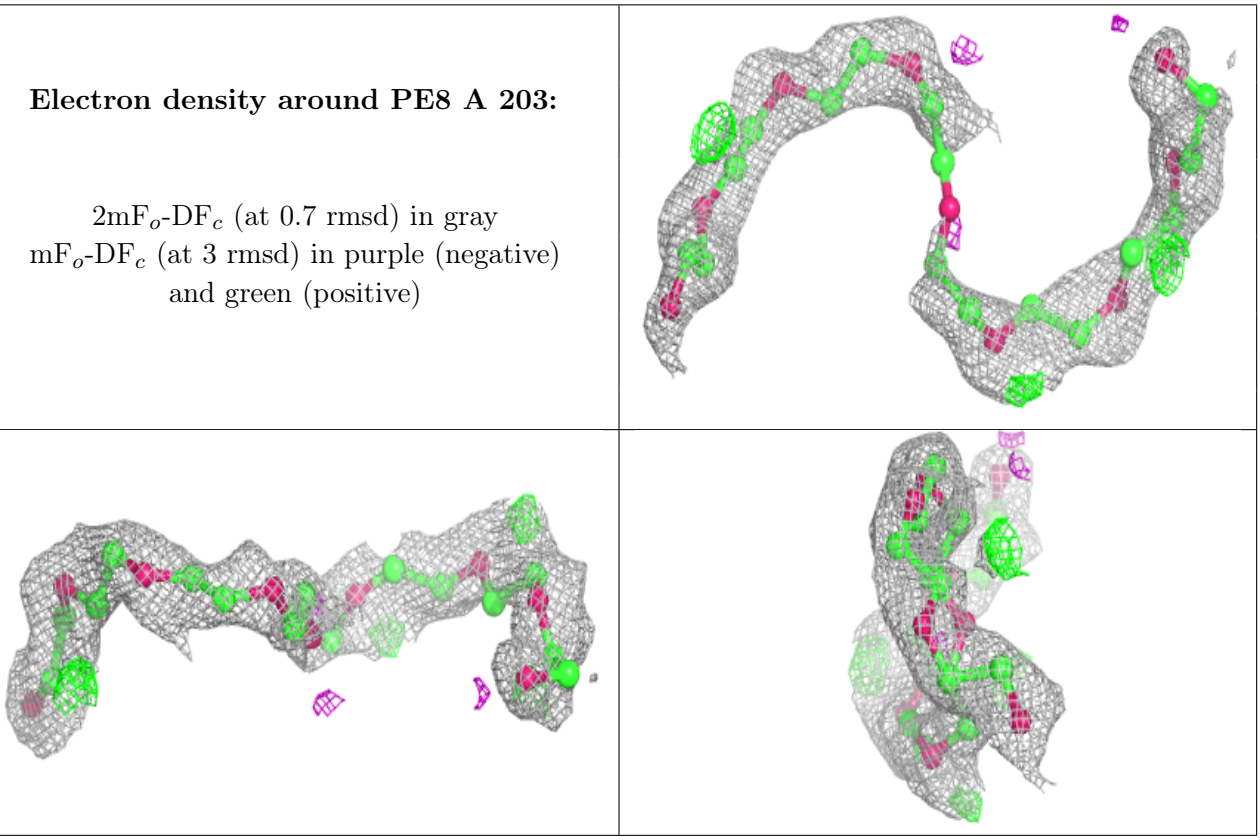
Electron density around PE8 D 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



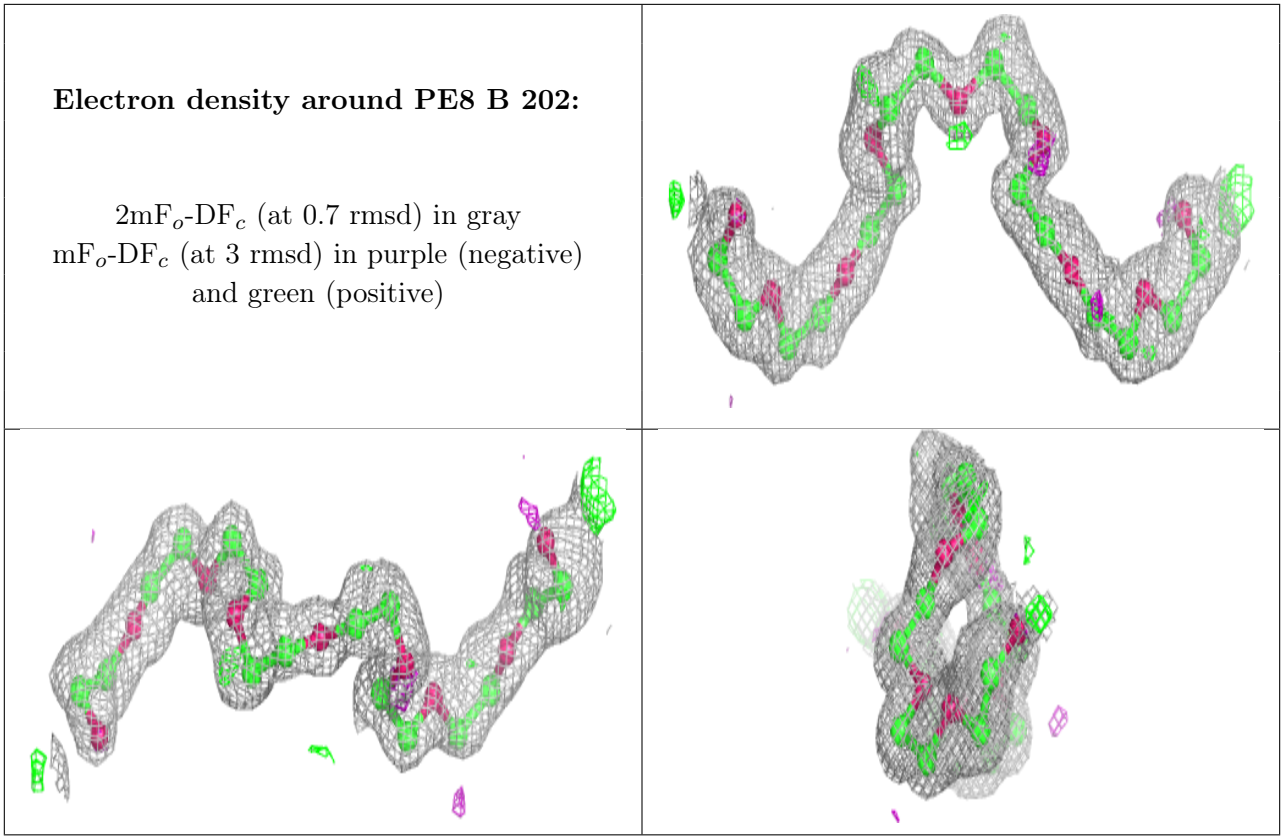
Electron density around PE8 A 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



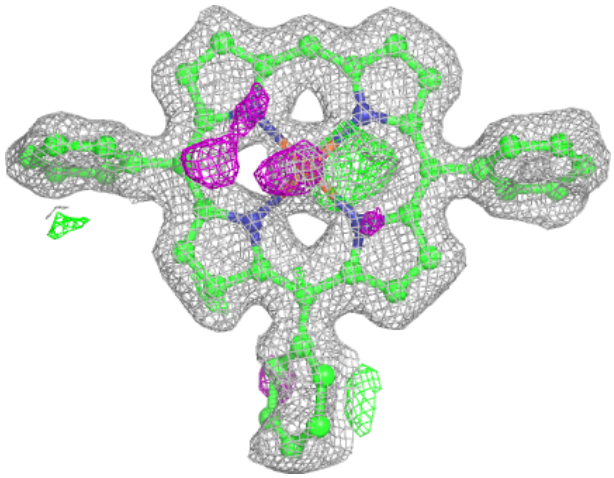
Electron density around PE8 B 202:

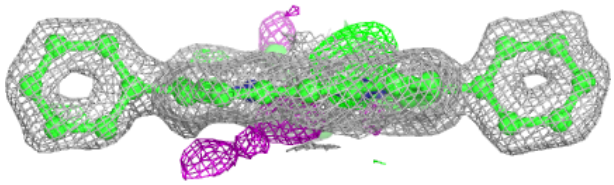
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

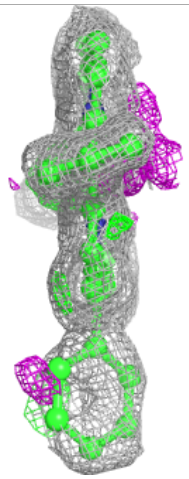


Electron density around WXP A 201 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

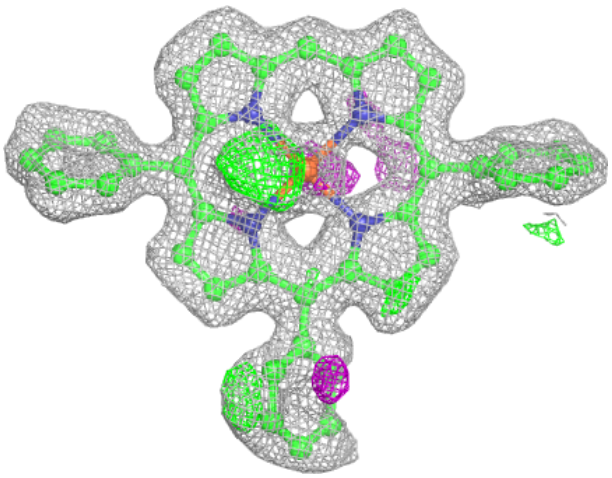


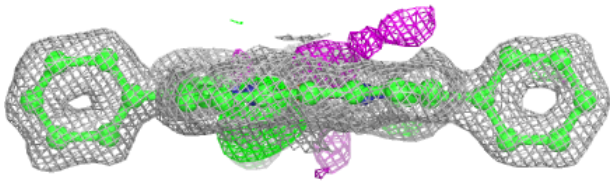


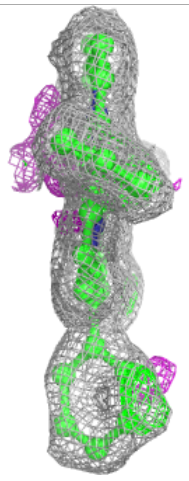


Electron density around WXP A 201 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

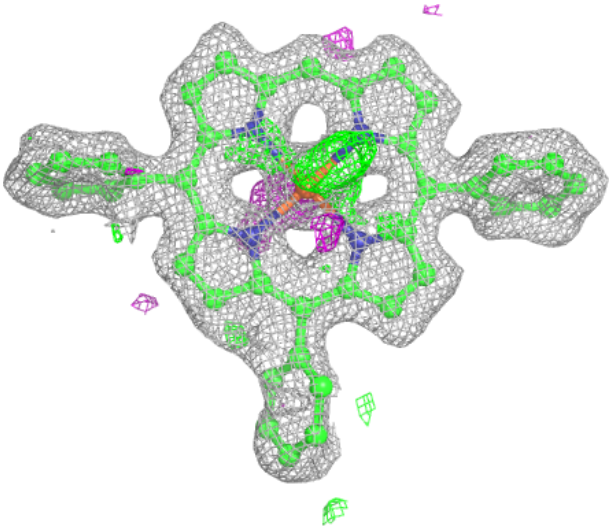


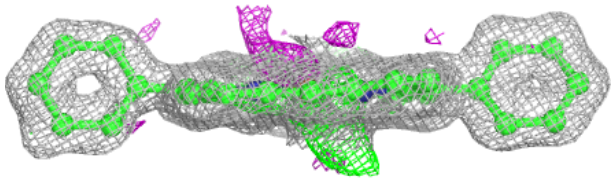


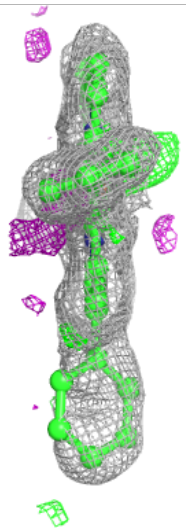


Electron density around WXP C 201 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

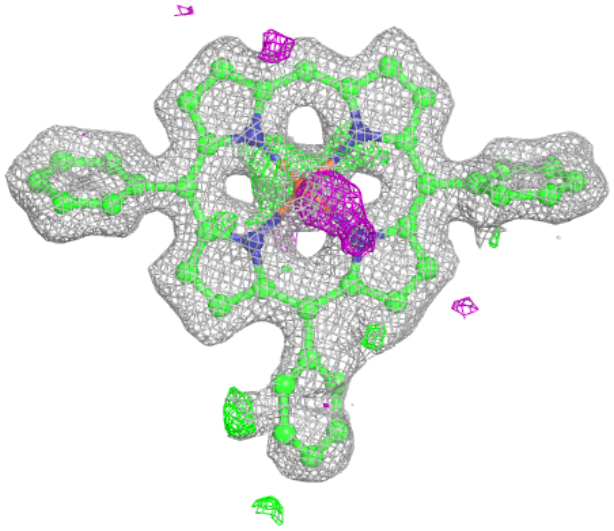


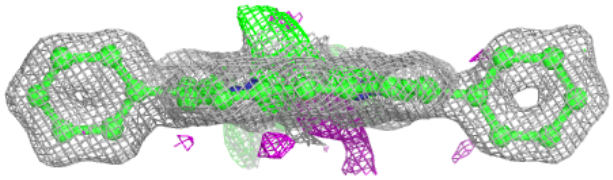


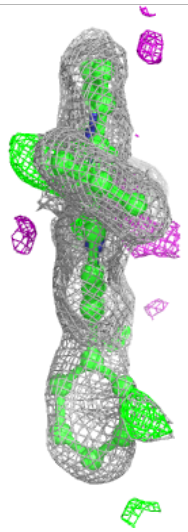


Electron density around WXP C 201 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

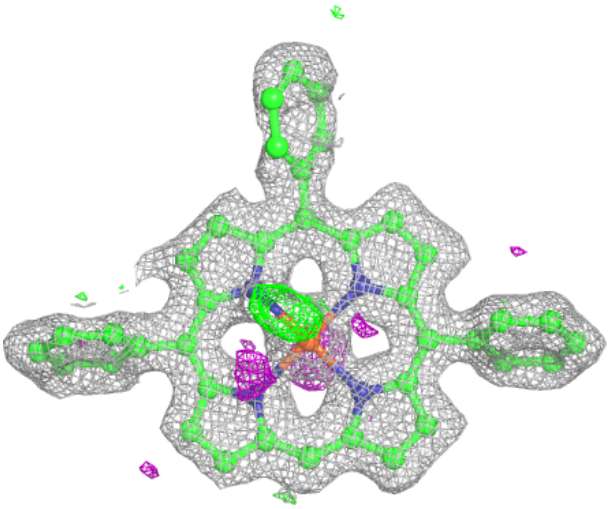


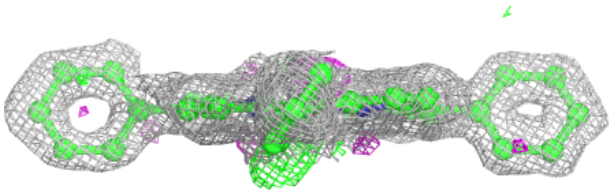


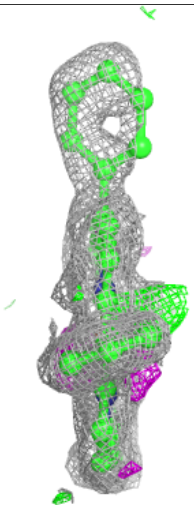


Electron density around WXP B 201 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

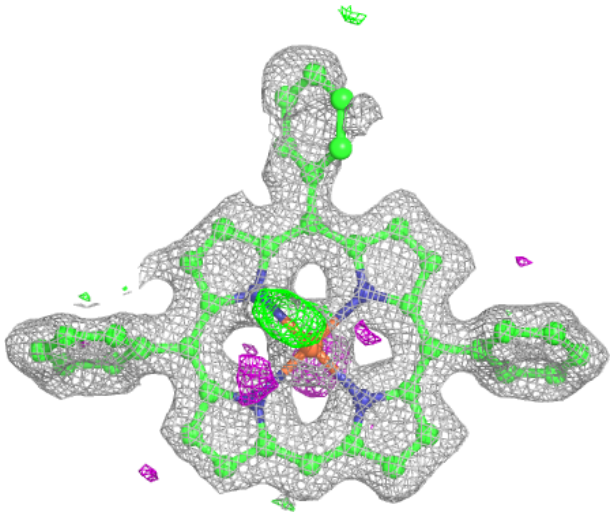


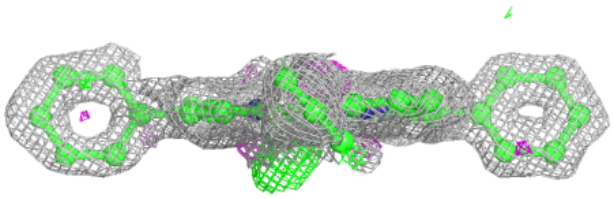


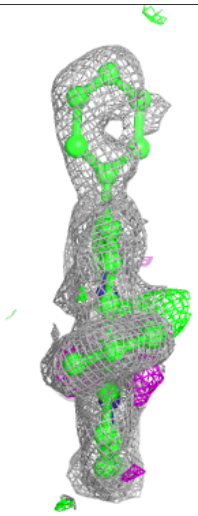


Electron density around WXP B 201 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

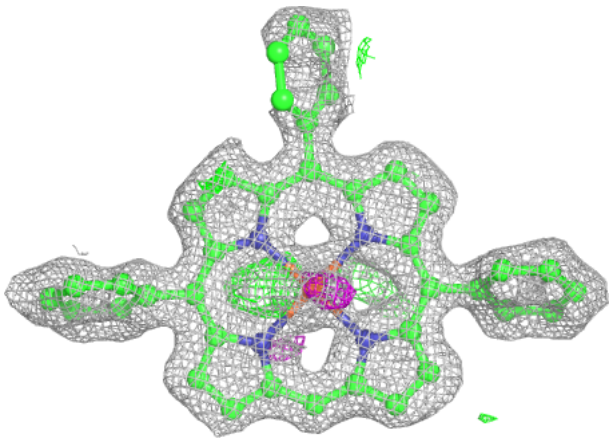


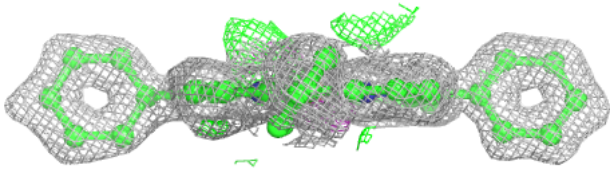


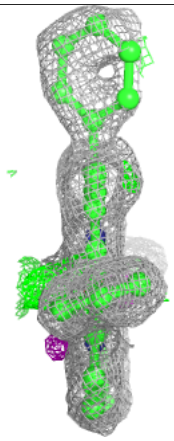


Electron density around WXP D 201 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

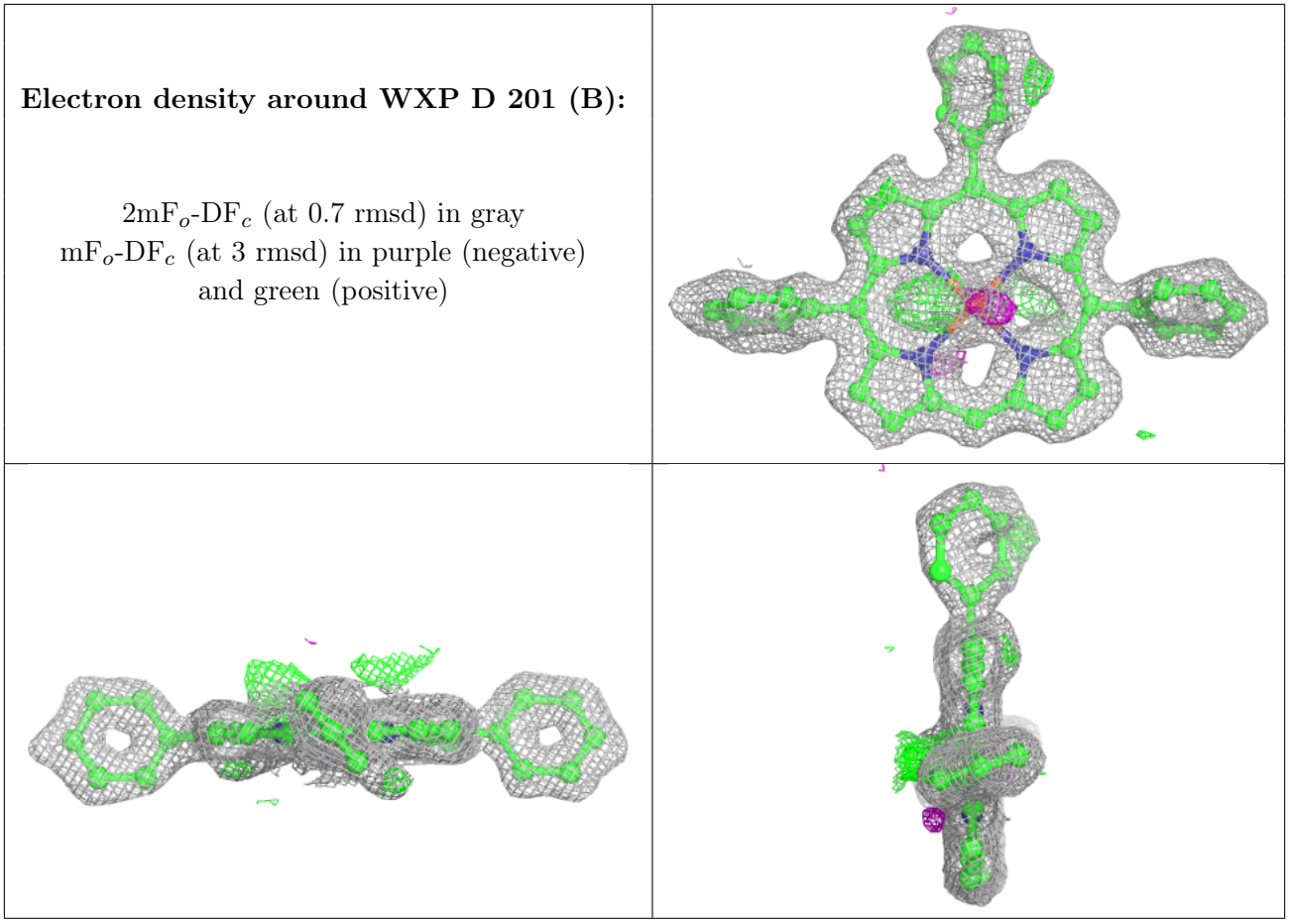






Electron density around WXP D 201 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.