wwPDB X-ray Structure Validation Summary Report (i)

Dec 19, 2023 – 12:16 PM EST

PDB ID	:	3MM5
Title	:	Dissimilatory sulfite reductase in complex with the substrate sulfite
Authors	:	Parey, K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.
Deposited on	:	2010-04-19
Resolution	:	1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

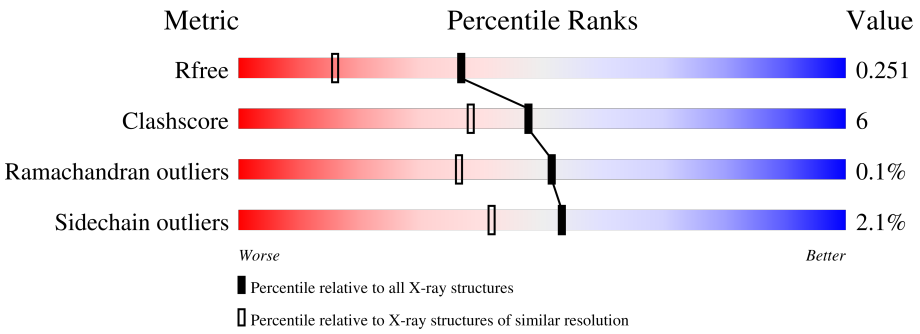
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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%

Mol	Chain	Length	Quality of chain
1	A	418	88% 11%
1	D	418	87% 12% •
2	B	366	90% 8% ••
2	E	366	84% 13% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SRM	A	580	X	-	-	-
3	SRM	B	570	X	-	-	-
3	SRM	D	580	X	-	-	-
3	SRM	E	570	X	-	-	-
4	SF4	E	585	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13810 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.

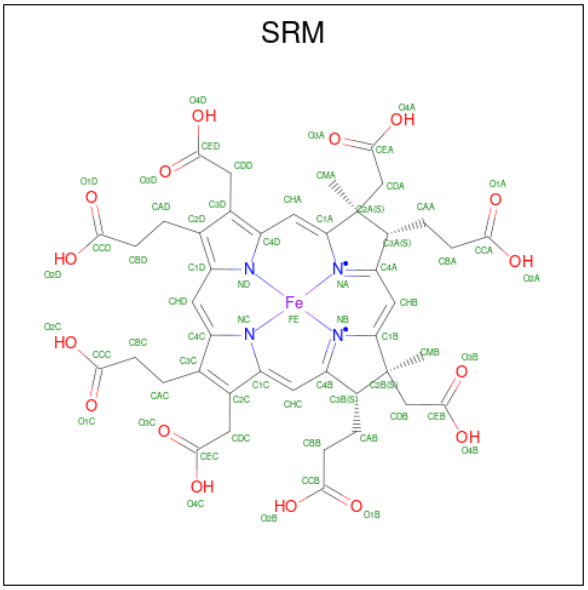
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	3348	2146	557	619	26	0	3	0
1	D	417	3336	2139	558	613	26	0	1	0

- Molecule 2 is a protein called Sulfite reductase, dissimilatory-type subunit beta.

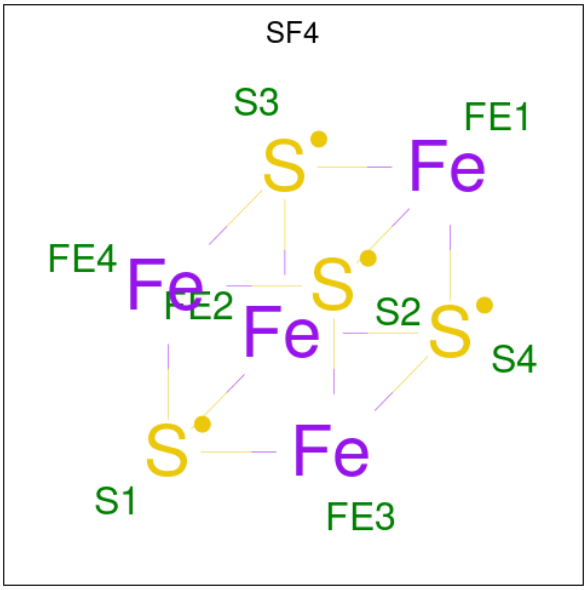
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	363	2930	1883	492	533	22	5	5	0
2	E	363	2901	1862	491	526	22	0	0	0

- Molecule 3 is SIROHEME (three-letter code: SRM) (formula: $C_{42}H_{44}FeN_4O_{16}$).



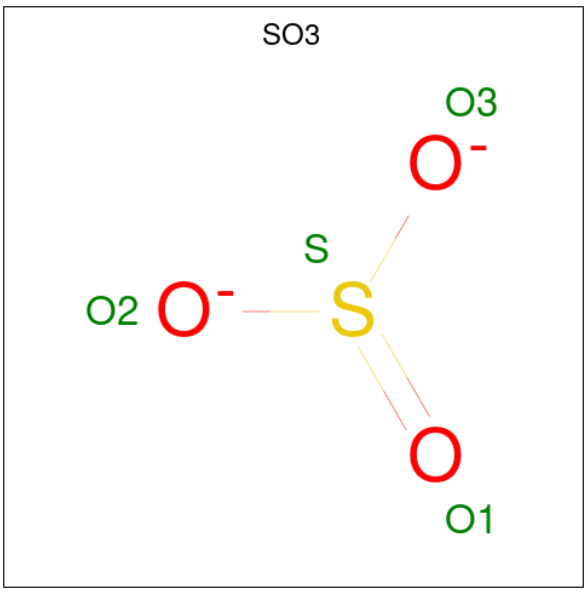
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	63	42	1	4	16	0	0
3	B	1	63	42	1	4	16	0	0
3	D	1	63	42	1	4	16	0	0
3	E	1	63	42	1	4	16	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	8	4	4	0	0
4	A	1	8	4	4	0	0
4	B	1	8	4	4	0	0
4	B	1	8	4	4	0	0
4	D	1	8	4	4	0	0
4	D	1	8	4	4	0	0
4	E	1	8	4	4	0	0
4	E	1	8	4	4	0	0

- Molecule 5 is SULFITE ION (three-letter code: SO3) (formula: O_3S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 4 3 1	0	0
5	D	1	Total O S 4 3 1	0	0

- Molecule 6 is water.

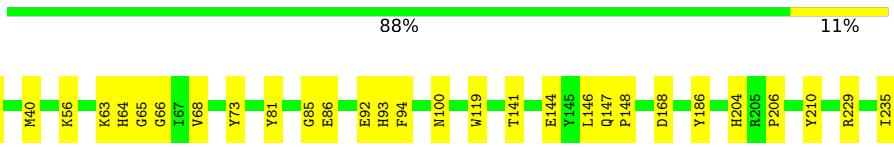
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	229	Total O 229 229	0	0
6	B	565	Total O 565 565	0	0
6	D	92	Total O 92 92	0	0
6	E	85	Total O 85 85	0	0

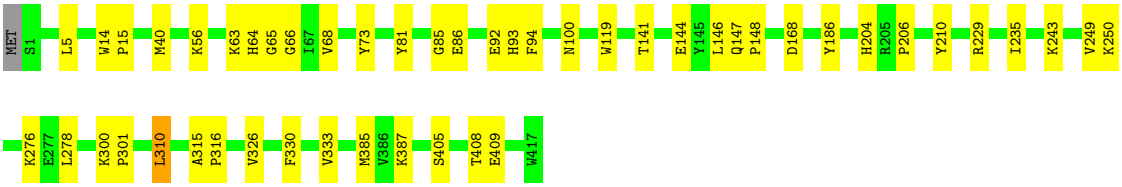
3 Residue-property plots (i)

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. 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. 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: Sulfite reductase, dissimilatory-type subunit alpha

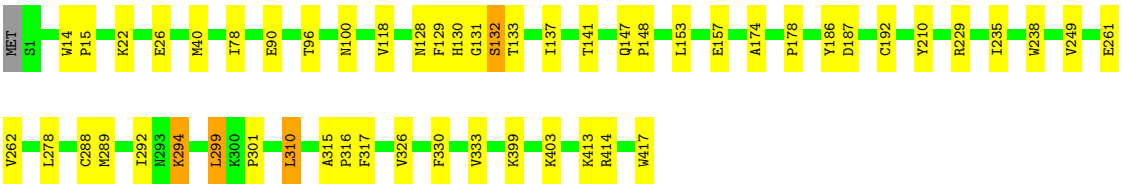
Chain A:





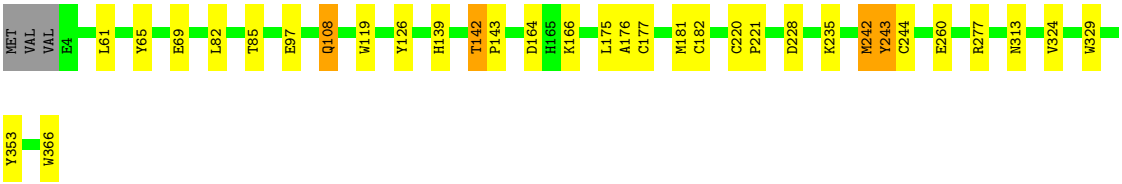
• Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

Chain D:



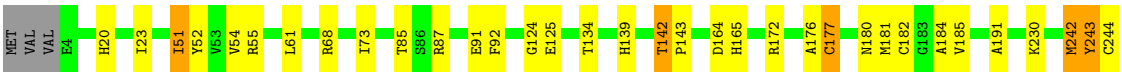
• Molecule 2: Sulfite reductase, dissimilatory-type subunit beta

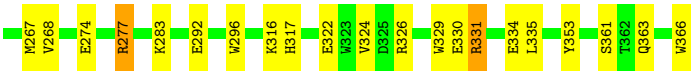
Chain B:



• Molecule 2: Sulfite reductase, dissimilatory-type subunit beta

Chain E:




M267
V268
E274
R277
K283
E292
W296
K316
H317
E322
W323
V324
D325
R326
W329
E330
R331
E334
L335
Y353
S361
T362
Q363
W366

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.60Å 68.90Å 145.10Å 90.00° 107.50° 90.00°	Depositor
Resolution (Å)	15.00 – 1.80 15.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-1.80) 99.3 (15.00-1.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.158 , 0.188 0.230 , 0.251	Depositor DCC
R_{free} test set	8181 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.4	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13810	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, SO3, SRM

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	0.79	0/3444	0.75	0/4646
1	D	0.47	0/3426	0.56	0/4622
2	B	0.81	1/3025 (0.0%)	0.79	1/4114 (0.0%)
2	E	0.47	1/2984 (0.0%)	0.60	3/4058 (0.1%)
All	All	0.66	2/12879 (0.0%)	0.68	4/17440 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	68	ARG	CZ-NH1	5.59	1.40	1.33
2	B	108	GLN	CB-CG	5.20	1.66	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	108	GLN	CA-CB-CG	6.42	127.52	113.40
2	E	277	ARG	NE-CZ-NH1	6.40	123.50	120.30
2	E	331	ARG	NE-CZ-NH1	5.65	123.13	120.30
2	E	277	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3348	0	3294	42	0
1	D	3336	0	3289	39	0
2	B	2930	0	2872	31	0
2	E	2901	0	2837	40	0
3	A	63	0	34	8	0
3	B	63	0	34	1	0
3	D	63	0	34	12	0
3	E	63	0	34	8	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	D	16	0	0	0	0
4	E	16	0	0	3	0
5	A	4	0	0	0	0
5	D	4	0	0	0	0
6	A	229	0	0	5	0
6	B	565	0	0	5	0
6	D	92	0	0	1	0
6	E	85	0	0	1	0
All	All	13810	0	12428	153	0

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 6.

The worst 5 of 153 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)
6:B:588:HOH:O	1:D:403[B]:LYS:HE3	1.20	1.30
3:D:580:SRM:HMB1	3:D:580:SRM:HBB2	1.39	1.04
1:A:85:GLY:HA3	1:A:92[A]:GLU:OE2	1.65	0.96
3:D:580:SRM:HBB2	3:D:580:SRM:CMB	1.95	0.95
3:A:580:SRM:O1A	2:B:139:HIS:HD2	1.55	0.88

There are no symmetry-related clashes.

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	418/418 (100%)	408 (98%)	10 (2%)	0	100	100
1	D	416/418 (100%)	404 (97%)	12 (3%)	0	100	100
2	B	366/366 (100%)	353 (96%)	12 (3%)	1 (0%)	41	27
2	E	361/366 (99%)	347 (96%)	13 (4%)	1 (0%)	41	27
All	All	1561/1568 (100%)	1512 (97%)	47 (3%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	142	THR
2	E	142	THR

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	356/354 (101%)	350 (98%)	6 (2%)	60	51
1	D	354/354 (100%)	346 (98%)	8 (2%)	50	37
2	B	319/317 (101%)	312 (98%)	7 (2%)	52	39
2	E	314/317 (99%)	306 (98%)	8 (2%)	47	34
All	All	1343/1342 (100%)	1314 (98%)	29 (2%)	53	39

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	132	SER
2	E	283	LYS
1	D	294	LYS
2	E	242	MET
1	D	210	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	363	GLN
2	E	180	ASN
1	D	61	HIS
1	D	50	GLN
1	D	100	ASN

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)

14 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	$\#\|Z\| > 2$
4	SF4	B	586	2	0,12,12	-	-	-		
3	SRM	D	580	5,2	68,70,70	2.01	13 (19%)	81,112,112	2.96	29 (35%)
3	SRM	A	580	5,2	68,70,70	1.59	7 (10%)	81,112,112	2.59	28 (34%)
4	SF4	A	575	1	0,12,12	-	-	-		
4	SF4	A	576	1	0,12,12	-	-	-		
3	SRM	E	570	1	68,70,70	2.30	10 (14%)	81,112,112	2.80	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO3	A	590	3	1,3,3	0.26	0	0,3,3	-	-
3	SRM	B	570	1	68,70,70	1.95	14 (20%)	81,112,112	2.75	32 (39%)
4	SF4	D	575	1	0,12,12	-	-	-		
4	SF4	D	576	1	0,12,12	-	-	-		
5	SO3	D	590	3	1,3,3	0.48	0	0,3,3	-	-
4	SF4	B	585	2	0,12,12	-	-	-		
4	SF4	E	585	2	0,12,12	-	-	-		
4	SF4	E	586	2	0,12,12	-	-	-		

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
4	SF4	B	586	2	-	-	0/6/5/5
3	SRM	D	580	5,2	2/2/19/23	12/38/126/126	-
3	SRM	A	580	5,2	1/1/19/23	10/38/126/126	-
4	SF4	A	575	1	-	-	0/6/5/5
4	SF4	A	576	1	-	-	0/6/5/5
3	SRM	E	570	1	1/1/19/23	16/38/126/126	-
3	SRM	B	570	1	1/1/19/23	13/38/126/126	-
4	SF4	D	575	1	-	-	0/6/5/5
4	SF4	D	576	1	-	-	0/6/5/5
4	SF4	B	585	2	-	-	0/6/5/5
4	SF4	E	585	2	-	-	0/6/5/5
4	SF4	E	586	2	-	-	0/6/5/5

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	570	SRM	C4A-NA	-10.53	1.27	1.35
3	E	570	SRM	C3C-C2C	7.05	1.51	1.36
3	D	580	SRM	C3D-C2D	6.45	1.54	1.39
3	E	570	SRM	C3D-C2D	6.17	1.53	1.39
3	B	570	SRM	C4A-NA	-5.91	1.31	1.35

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	580	SRM	CDD-C3D-C4D	-12.11	108.99	127.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	580	SRM	C2A-C3A-C4A	9.78	113.41	100.90
3	D	580	SRM	CAA-C3A-C4A	9.41	127.78	111.19
3	A	580	SRM	C2A-C3A-C4A	8.61	111.92	100.90
3	E	570	SRM	CAB-C3B-C4B	8.47	126.12	111.19

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	580	SRM	NC
3	B	570	SRM	NC
3	D	580	SRM	C3A
3	D	580	SRM	NC
3	E	570	SRM	NC

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	580	SRM	C1B-C2B-CDB-CEB
3	D	580	SRM	CMB-C2B-CDB-CEB
3	D	580	SRM	C3B-C2B-CDB-CEB
3	D	580	SRM	C2B-C3B-CAB-CBB
3	E	570	SRM	C4A-C3A-CAA-CBA

There are no ring outliers.

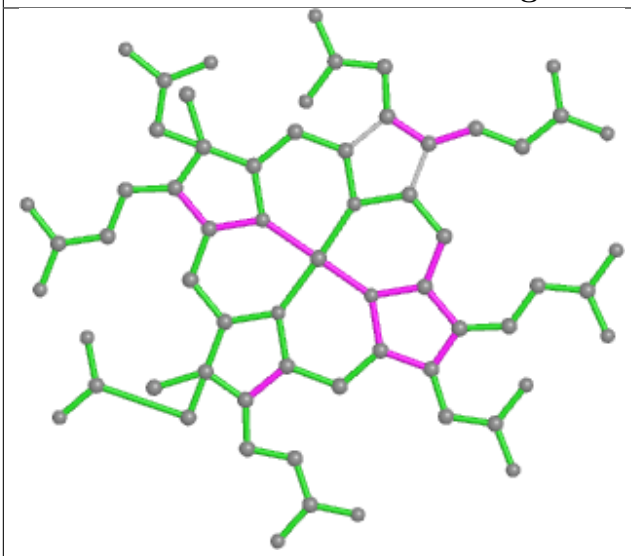
5 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	580	SRM	12	0
3	A	580	SRM	8	0
3	E	570	SRM	8	0
3	B	570	SRM	1	0
4	E	585	SF4	3	0

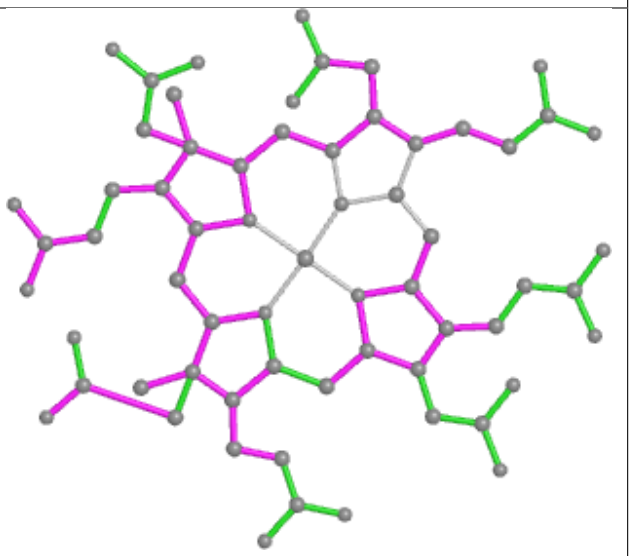
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

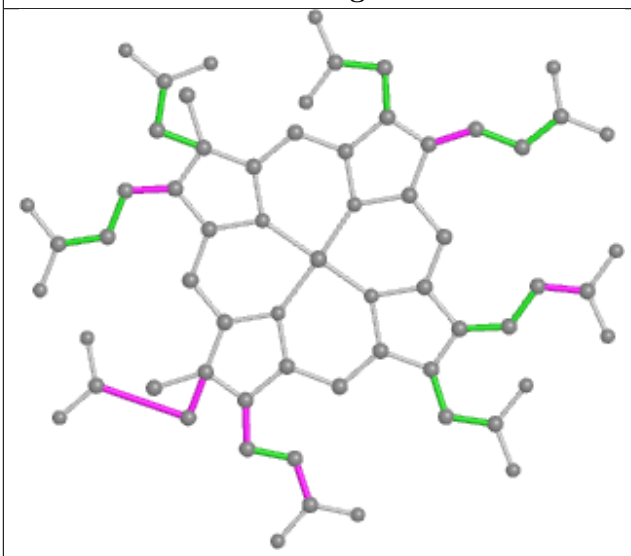
Ligand SRM D 580



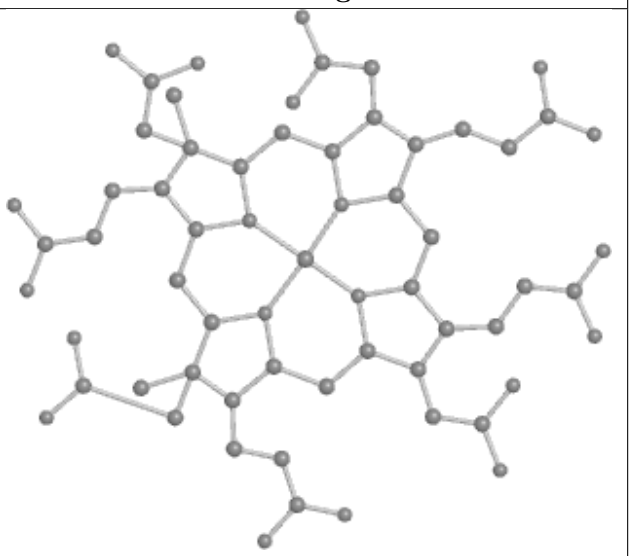
Bond lengths



Bond angles

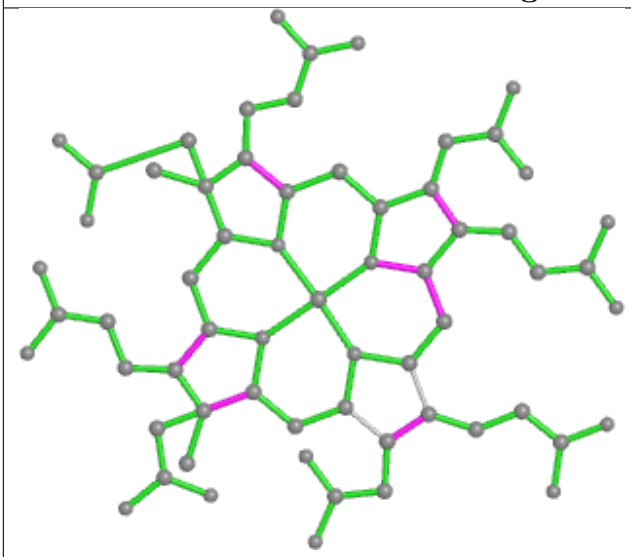


Torsions

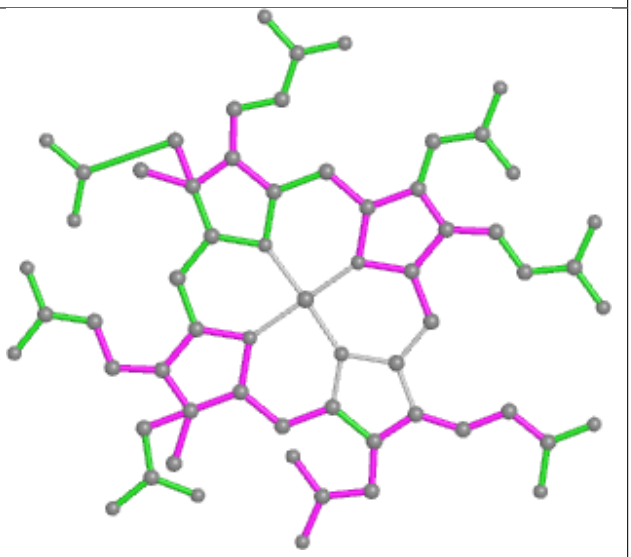


Rings

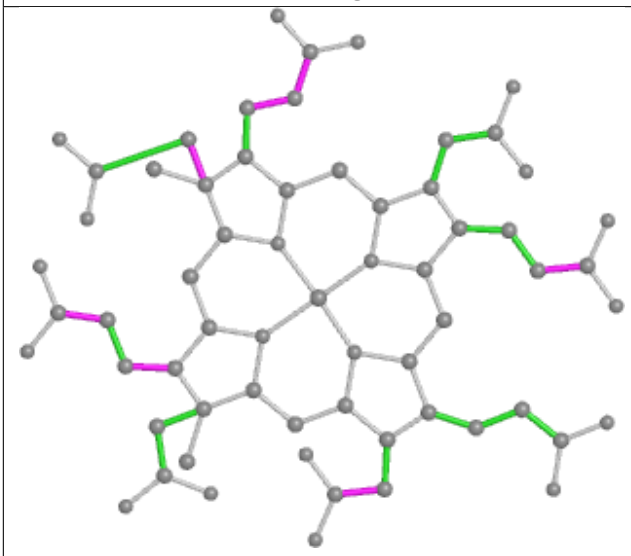
Ligand SRM A 580



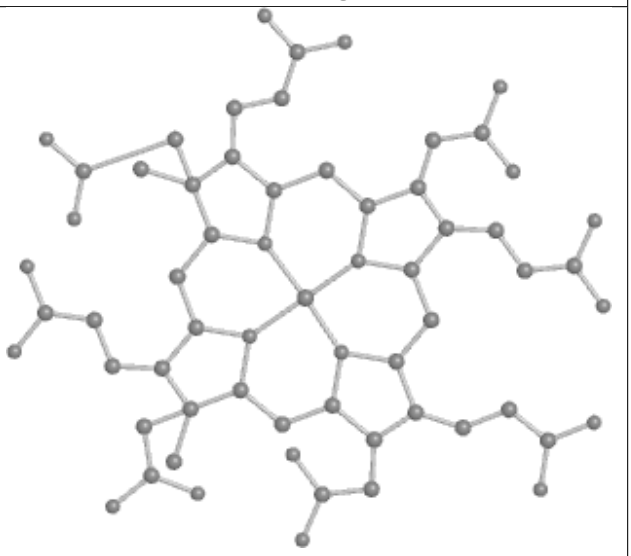
Bond lengths



Bond angles

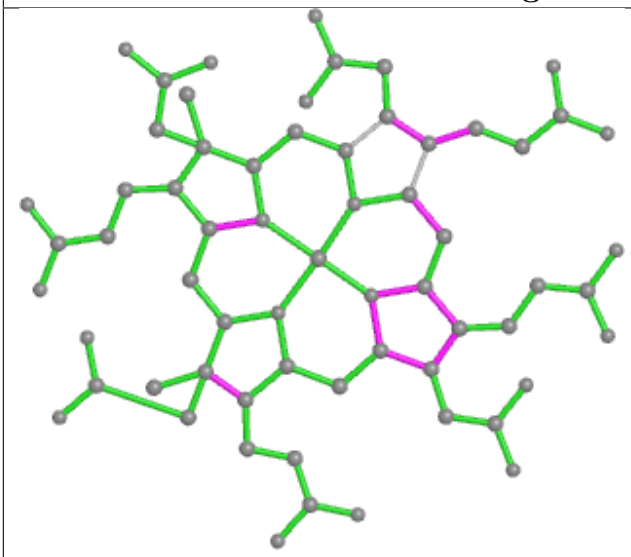


Torsions

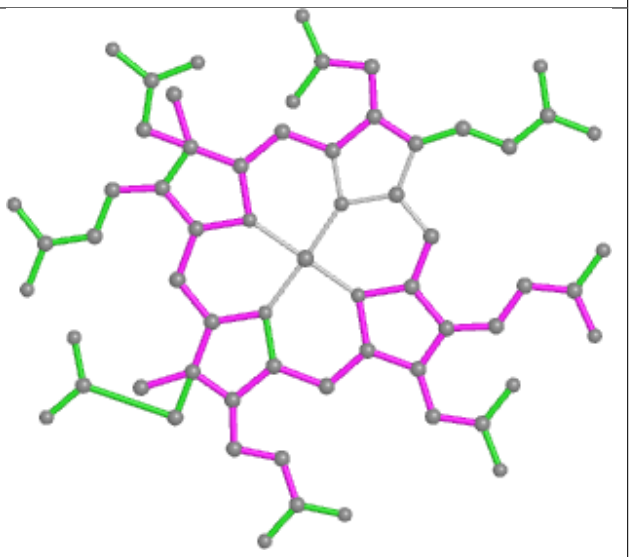


Rings

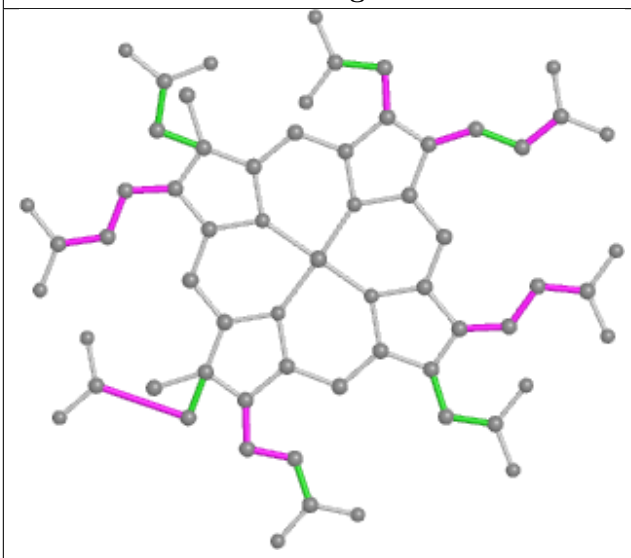
Ligand SRM E 570



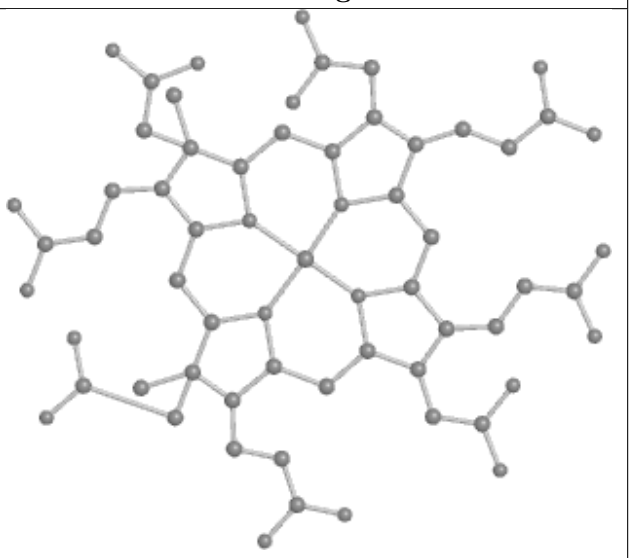
Bond lengths



Bond angles

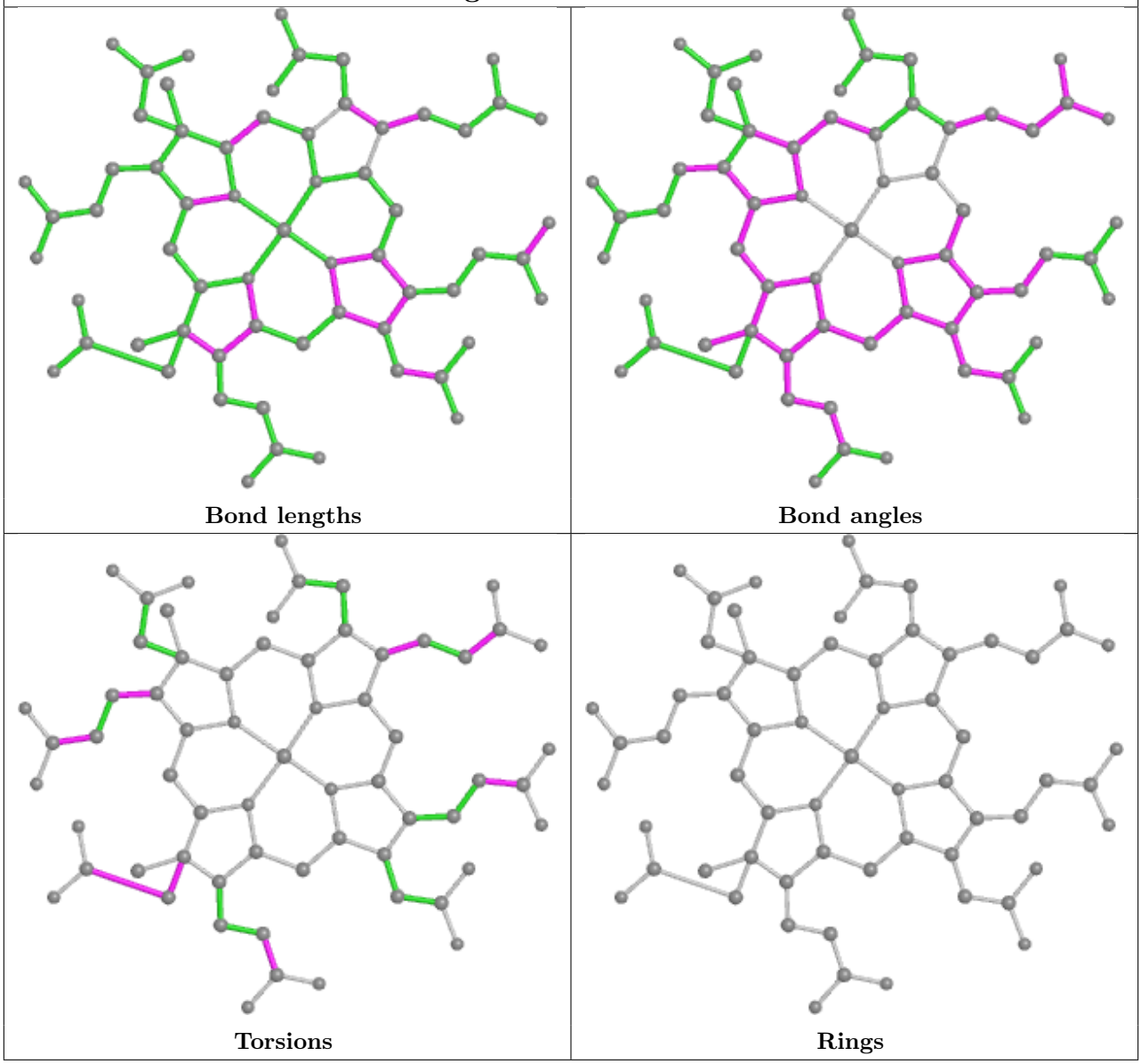


Torsions



Rings

Ligand SRM B 570



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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

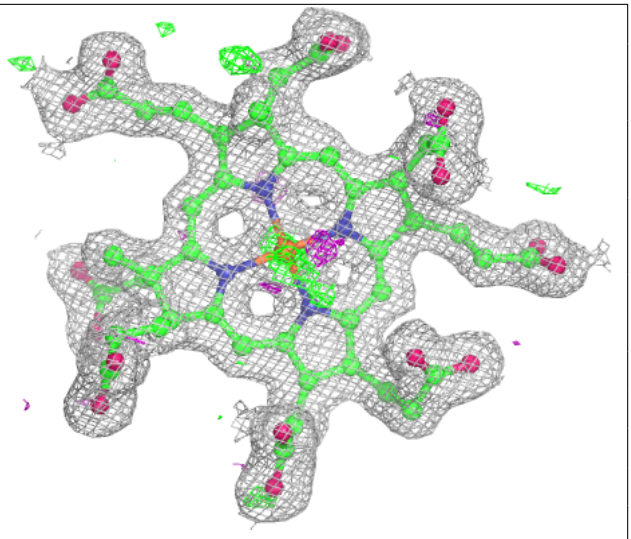
6.4 Ligands (i)

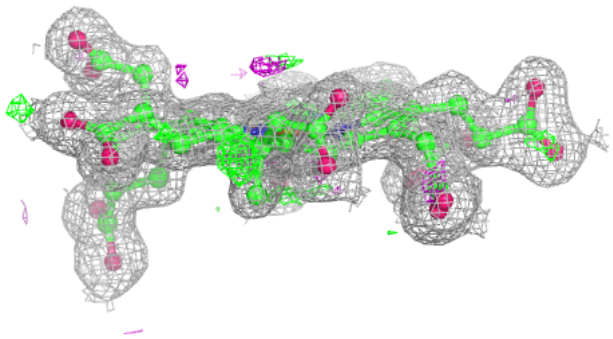
Unable to reproduce the depositors R factor - this section is therefore empty.

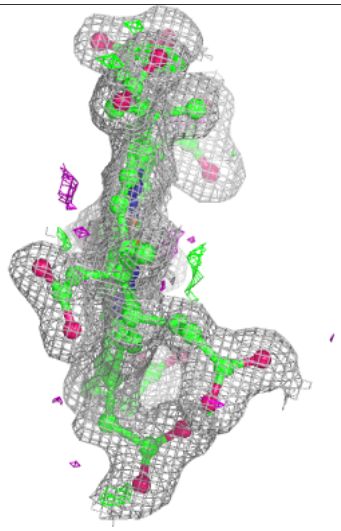
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SRM A 580:

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

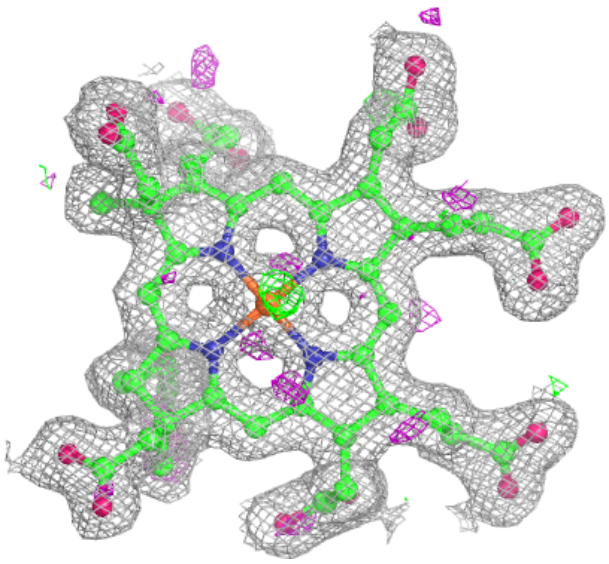


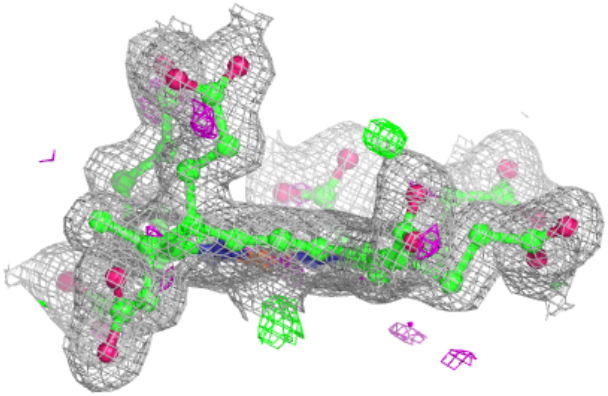


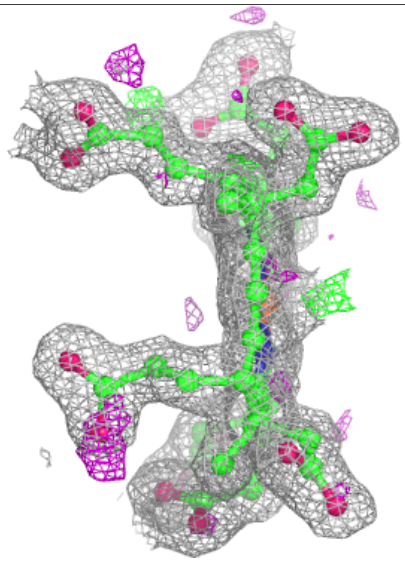


Electron density around SRM B 570:

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

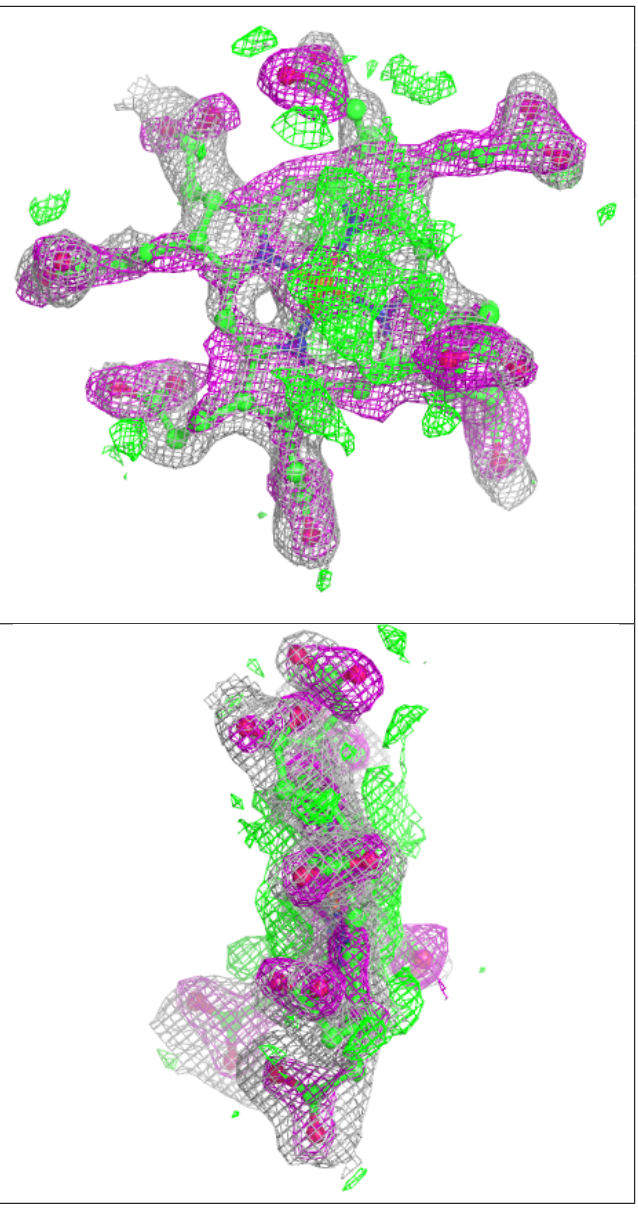






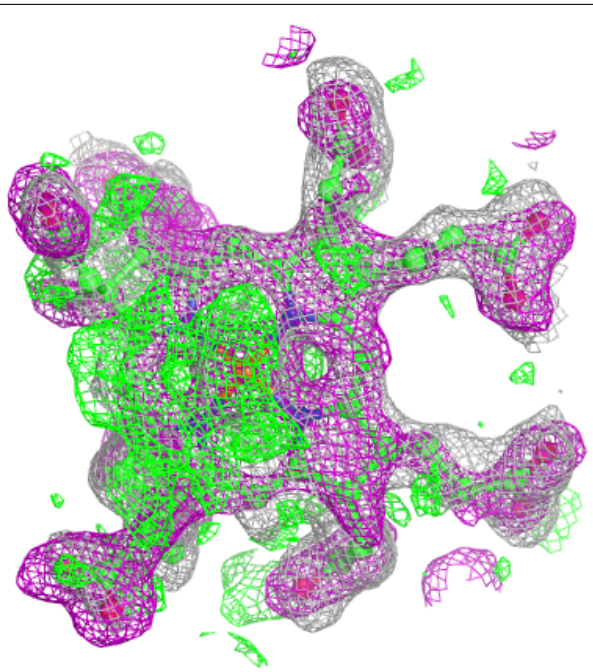
Electron density around SRM D 580:

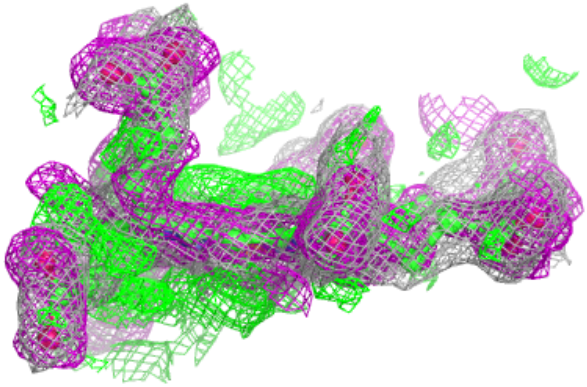
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

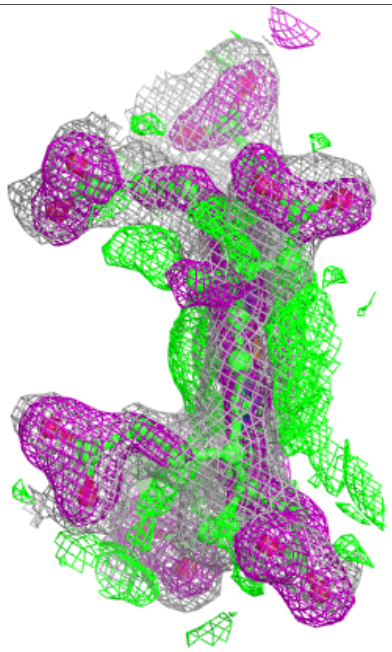


Electron density around SRM E 570:

$2mF_o$-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 (i)

Unable to reproduce the depositors R factor - this section is therefore empty.