wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2023 – 10:40 AM EDT

PDB ID	:	3A18
Title	:	Crystal Structure of Aldoxime Dehydratase (OxdRE) in Complex with Butyraldoxime (soaked crystal)
Authors	:	Sawai, H.; Sugimoto, H.; Kato, Y.; Asano, Y.; Shiro, Y.; Aono, S.
Deposited on	:	2009-03-26
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:

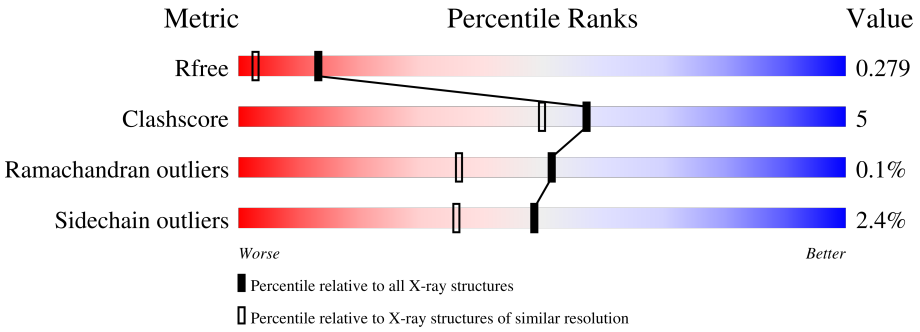
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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	373	83% 10% • 5%
1	B	373	83% 10% • 5%
1	C	373	86% 8% • 5%
1	D	373	82% 12% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12589 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 Aldoxime dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	353	2928	1848	515	553	12	0	15	0
1	B	353	2843	1790	504	537	12	0	4	0
1	C	353	2828	1779	500	537	12	0	2	0
1	D	352	2926	1850	515	549	12	0	16	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q76K71
A	-18	GLY	-	expression tag	UNP Q76K71
A	-17	SER	-	expression tag	UNP Q76K71
A	-16	SER	-	expression tag	UNP Q76K71
A	-15	HIS	-	expression tag	UNP Q76K71
A	-14	HIS	-	expression tag	UNP Q76K71
A	-13	HIS	-	expression tag	UNP Q76K71
A	-12	HIS	-	expression tag	UNP Q76K71
A	-11	HIS	-	expression tag	UNP Q76K71
A	-10	HIS	-	expression tag	UNP Q76K71
A	-9	SER	-	expression tag	UNP Q76K71
A	-8	SER	-	expression tag	UNP Q76K71
A	-7	GLY	-	expression tag	UNP Q76K71
A	-6	LEU	-	expression tag	UNP Q76K71
A	-5	VAL	-	expression tag	UNP Q76K71
A	-4	PRO	-	expression tag	UNP Q76K71
A	-3	ARG	-	expression tag	UNP Q76K71
A	-2	GLY	-	expression tag	UNP Q76K71
A	-1	SER	-	expression tag	UNP Q76K71
A	0	HIS	-	expression tag	UNP Q76K71
B	-19	MET	-	initiating methionine	UNP Q76K71

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q76K71
B	-17	SER	-	expression tag	UNP Q76K71
B	-16	SER	-	expression tag	UNP Q76K71
B	-15	HIS	-	expression tag	UNP Q76K71
B	-14	HIS	-	expression tag	UNP Q76K71
B	-13	HIS	-	expression tag	UNP Q76K71
B	-12	HIS	-	expression tag	UNP Q76K71
B	-11	HIS	-	expression tag	UNP Q76K71
B	-10	HIS	-	expression tag	UNP Q76K71
B	-9	SER	-	expression tag	UNP Q76K71
B	-8	SER	-	expression tag	UNP Q76K71
B	-7	GLY	-	expression tag	UNP Q76K71
B	-6	LEU	-	expression tag	UNP Q76K71
B	-5	VAL	-	expression tag	UNP Q76K71
B	-4	PRO	-	expression tag	UNP Q76K71
B	-3	ARG	-	expression tag	UNP Q76K71
B	-2	GLY	-	expression tag	UNP Q76K71
B	-1	SER	-	expression tag	UNP Q76K71
B	0	HIS	-	expression tag	UNP Q76K71
C	-19	MET	-	initiating methionine	UNP Q76K71
C	-18	GLY	-	expression tag	UNP Q76K71
C	-17	SER	-	expression tag	UNP Q76K71
C	-16	SER	-	expression tag	UNP Q76K71
C	-15	HIS	-	expression tag	UNP Q76K71
C	-14	HIS	-	expression tag	UNP Q76K71
C	-13	HIS	-	expression tag	UNP Q76K71
C	-12	HIS	-	expression tag	UNP Q76K71
C	-11	HIS	-	expression tag	UNP Q76K71
C	-10	HIS	-	expression tag	UNP Q76K71
C	-9	SER	-	expression tag	UNP Q76K71
C	-8	SER	-	expression tag	UNP Q76K71
C	-7	GLY	-	expression tag	UNP Q76K71
C	-6	LEU	-	expression tag	UNP Q76K71
C	-5	VAL	-	expression tag	UNP Q76K71
C	-4	PRO	-	expression tag	UNP Q76K71
C	-3	ARG	-	expression tag	UNP Q76K71
C	-2	GLY	-	expression tag	UNP Q76K71
C	-1	SER	-	expression tag	UNP Q76K71
C	0	HIS	-	expression tag	UNP Q76K71
D	-19	MET	-	initiating methionine	UNP Q76K71
D	-18	GLY	-	expression tag	UNP Q76K71
D	-17	SER	-	expression tag	UNP Q76K71

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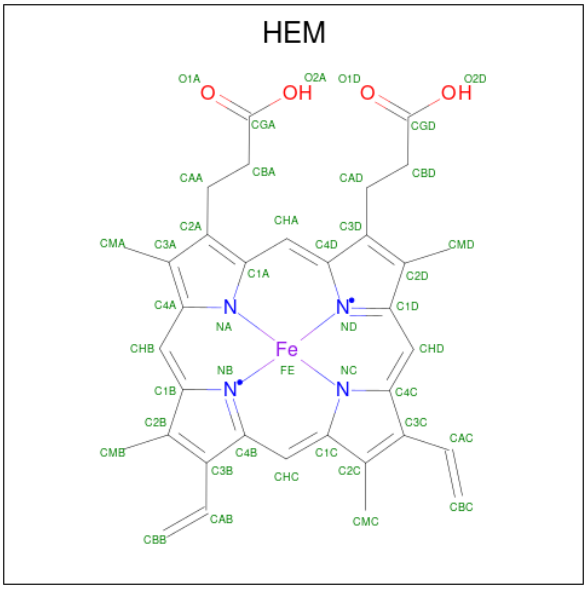
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q76K71
D	-15	HIS	-	expression tag	UNP Q76K71
D	-14	HIS	-	expression tag	UNP Q76K71
D	-13	HIS	-	expression tag	UNP Q76K71
D	-12	HIS	-	expression tag	UNP Q76K71
D	-11	HIS	-	expression tag	UNP Q76K71
D	-10	HIS	-	expression tag	UNP Q76K71
D	-9	SER	-	expression tag	UNP Q76K71
D	-8	SER	-	expression tag	UNP Q76K71
D	-7	GLY	-	expression tag	UNP Q76K71
D	-6	LEU	-	expression tag	UNP Q76K71
D	-5	VAL	-	expression tag	UNP Q76K71
D	-4	PRO	-	expression tag	UNP Q76K71
D	-3	ARG	-	expression tag	UNP Q76K71
D	-2	GLY	-	expression tag	UNP Q76K71
D	-1	SER	-	expression tag	UNP Q76K71
D	0	HIS	-	expression tag	UNP Q76K71

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0

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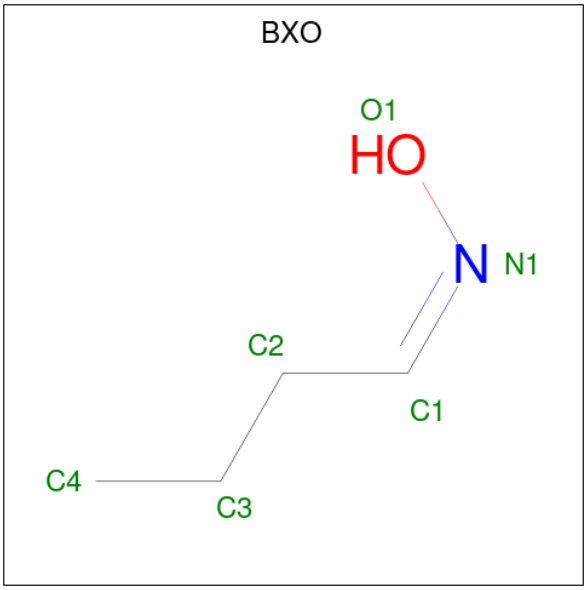
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
2	D	1	43	34	1	4	4	0	0

- Molecule 3 is (1Z)-butanal oxime (three-letter code: BXO) (formula: C_4H_9NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	6	4	1	1	0	0
3	B	1	6	4	1	1	0	0
3	C	1	6	4	1	1	0	0
3	D	1	6	4	1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	238	238	238	0	0
4	B	225	225	225	0	0
4	C	214	214	214	0	0

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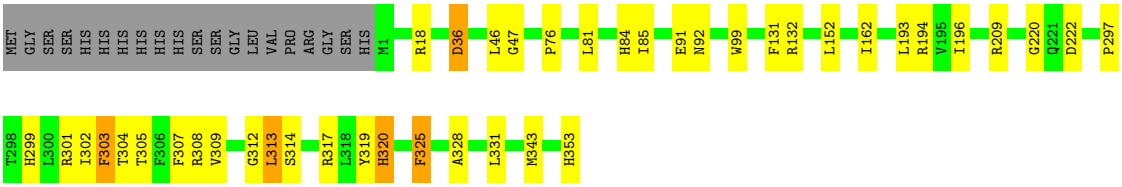
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	191	191	191	0	0

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.

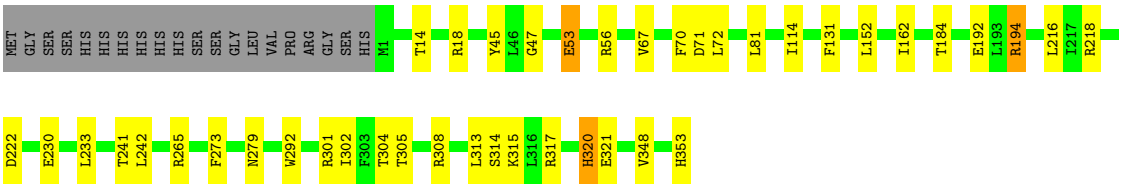
• Molecule 1: Aldoxime dehydratase

Chain A:



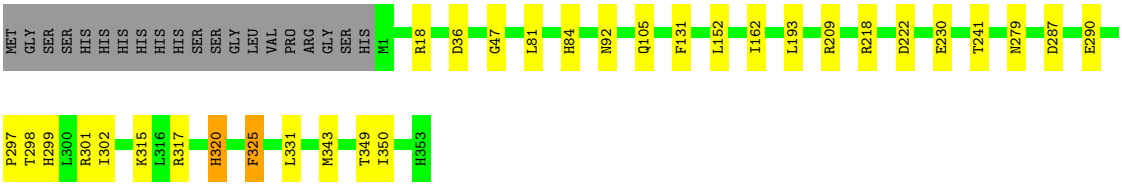
• Molecule 1: Aldoxime dehydratase

Chain B:



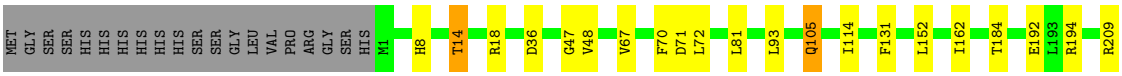
• Molecule 1: Aldoxime dehydratase

Chain C:



• Molecule 1: Aldoxime dehydratase

Chain D:



R218
D222
E230
L233
T241
L242
R265
F273
N279
D287
R291
R301
I302
F303
T304
T305
F306
F307
R308
V309
G312
L313
L316
R317
H320
V348
E352
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.12Å 148.57Å 79.11Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	19.93 – 1.80 19.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.93-1.80) 98.8 (19.93-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.247 , 0.280 0.247 , 0.279	Depositor DCC
R_{free} test set	6625 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	15.4	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 23.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12589	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 5.76% 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: HEM, BXO

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	0.44	2/3017 (0.1%)	0.58	2/4103 (0.0%)
1	B	0.40	0/2932	0.56	0/3985
1	C	0.44	3/2911 (0.1%)	0.57	0/3959
1	D	0.40	0/3017	0.56	0/4103
All	All	0.42	5/11877 (0.0%)	0.57	2/16150 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	325	PHE	CE1-CZ	-5.51	1.26	1.37
1	A	325	PHE	CG-CD1	-5.34	1.30	1.38
1	C	325	PHE	CG-CD2	-5.29	1.30	1.38
1	C	325	PHE	CE2-CZ	-5.13	1.27	1.37
1	A	325	PHE	CE2-CZ	-5.04	1.27	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	313[A]	LEU	C-N-CA	-5.68	107.50	121.70
1	A	313[B]	LEU	C-N-CA	-5.68	107.50	121.70

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	2928	0	2764	36	0
1	B	2843	0	2691	30	0
1	C	2828	0	2663	18	0
1	D	2926	0	2779	41	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	6	0	9	0	0
3	B	6	0	9	0	0
3	C	6	0	9	0	0
3	D	6	0	9	0	0
4	A	238	0	0	0	0
4	B	225	0	0	2	0
4	C	214	0	0	3	0
4	D	191	0	0	0	0
All	All	12589	0	11053	111	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 5.

The worst 5 of 111 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:C:241:THR:HG23	4:C:374:HOH:O	1.81	0.78
1:B:241:THR:HG22	1:B:301:ARG:HH21	1.48	0.77
1:A:36[B]:ASP:CG	1:D:194:ARG:HH21	1.89	0.75
1:D:241:THR:HG22	1:D:301:ARG:HH21	1.50	0.74
1:D:301:ARG:O	1:D:305[A]:THR:N	2.18	0.70

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	366/373 (98%)	360 (98%)	5 (1%)	1 (0%)	41	27
1	B	355/373 (95%)	348 (98%)	7 (2%)	0	100	100
1	C	353/373 (95%)	344 (98%)	9 (2%)	0	100	100
1	D	366/373 (98%)	355 (97%)	11 (3%)	0	100	100
All	All	1440/1492 (96%)	1407 (98%)	32 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	SER

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	307/312 (98%)	296 (96%)	11 (4%)	35	20
1	B	299/312 (96%)	292 (98%)	7 (2%)	50	37
1	C	297/312 (95%)	288 (97%)	9 (3%)	41	27
1	D	307/312 (98%)	302 (98%)	5 (2%)	62	54
All	All	1210/1248 (97%)	1178 (97%)	32 (3%)	49	32

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	71	ASP
1	D	81	LEU
1	B	53	GLU
1	B	14	THR
1	D	105	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	HIS
1	B	353	HIS
1	C	105	GLN
1	D	105	GLN
1	D	288	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)

8 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	HEM	A	354	3,1	41,50,50	1.91	6 (14%)	45,82,82	1.85	8 (17%)
2	HEM	C	354	3,1	41,50,50	1.83	6 (14%)	45,82,82	1.82	6 (13%)
3	BXO	C	355	2	5,5,5	1.22	1 (20%)	2,4,4	9.32	1 (50%)
3	BXO	A	355	2	5,5,5	1.16	1 (20%)	2,4,4	9.52	1 (50%)
3	BXO	D	355	2	5,5,5	1.30	1 (20%)	2,4,4	8.73	1 (50%)
2	HEM	B	354	3,1	41,50,50	1.86	5 (12%)	45,82,82	1.84	7 (15%)
3	BXO	B	355	2	5,5,5	1.26	1 (20%)	2,4,4	8.49	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	D	354	3,1	41,50,50	1.86	7 (17%)	45,82,82	1.78	7 (15%)

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	HEM	A	354	3,1	-	6/12/54/54	-
2	HEM	C	354	3,1	-	6/12/54/54	-
3	BXO	C	355	2	-	0/2/3/3	-
3	BXO	A	355	2	-	0/2/3/3	-
3	BXO	D	355	2	-	0/2/3/3	-
2	HEM	B	354	3,1	-	4/12/54/54	-
3	BXO	B	355	2	-	0/2/3/3	-
2	HEM	D	354	3,1	-	4/12/54/54	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	354	HEM	C3D-C2D	7.62	1.52	1.36
2	C	354	HEM	C3D-C2D	7.62	1.52	1.36
2	B	354	HEM	C3D-C2D	7.61	1.52	1.36
2	D	354	HEM	C3D-C2D	7.50	1.52	1.36
2	A	354	HEM	C3C-C2C	-4.51	1.34	1.40

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	355	BXO	O1-N1-C1	13.46	124.32	111.70
3	C	355	BXO	O1-N1-C1	13.18	124.06	111.70
3	D	355	BXO	O1-N1-C1	12.34	123.27	111.70
3	B	355	BXO	O1-N1-C1	12.01	122.96	111.70
2	A	354	HEM	C4D-ND-C1D	6.97	112.27	105.07

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	354	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	C	354	HEM	C2B-C3B-CAB-CBB
2	A	354	HEM	C4B-C3B-CAB-CBB
2	C	354	HEM	C4B-C3B-CAB-CBB
2	B	354	HEM	CAA-CBA-CGA-O1A

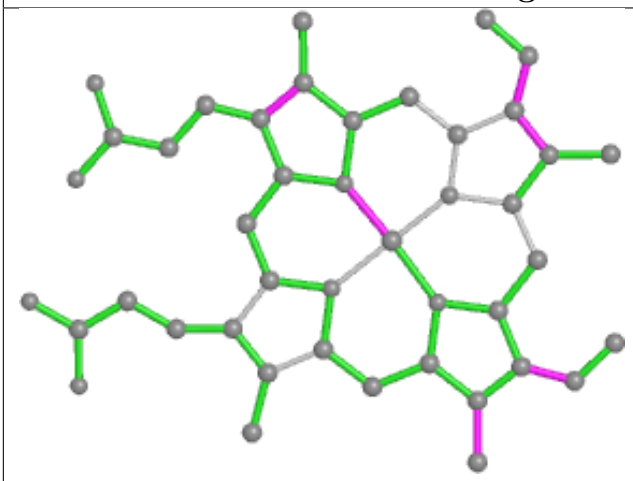
There are no ring outliers.

4 monomers are involved in 11 short contacts:

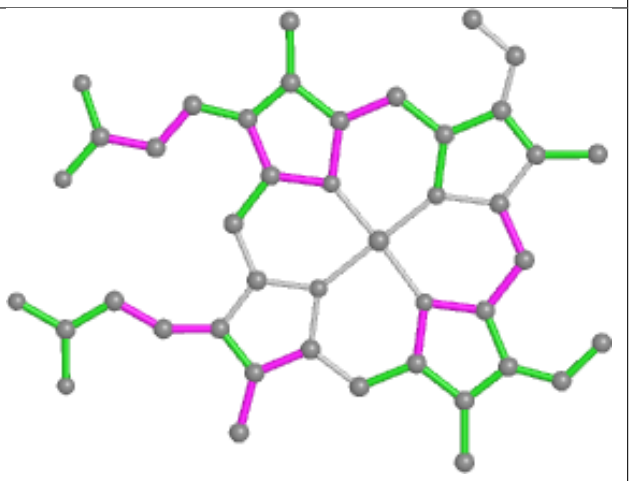
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	354	HEM	2	0
2	C	354	HEM	2	0
2	B	354	HEM	4	0
2	D	354	HEM	3	0

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.

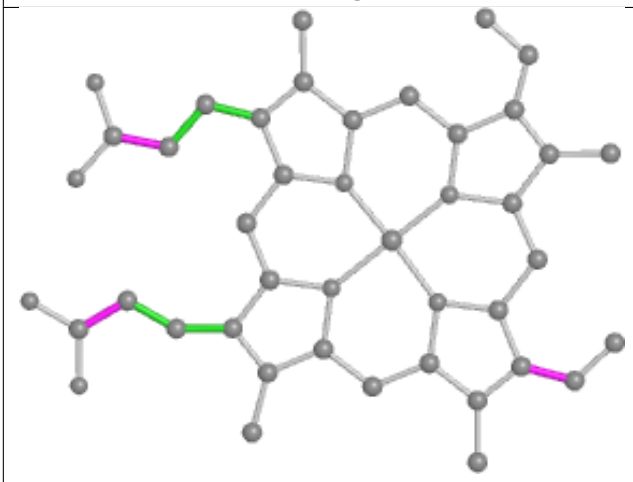
Ligand HEM A 354



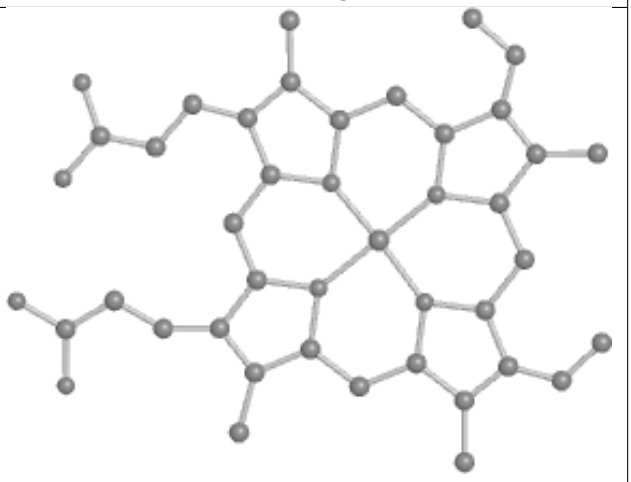
Bond lengths



Bond angles

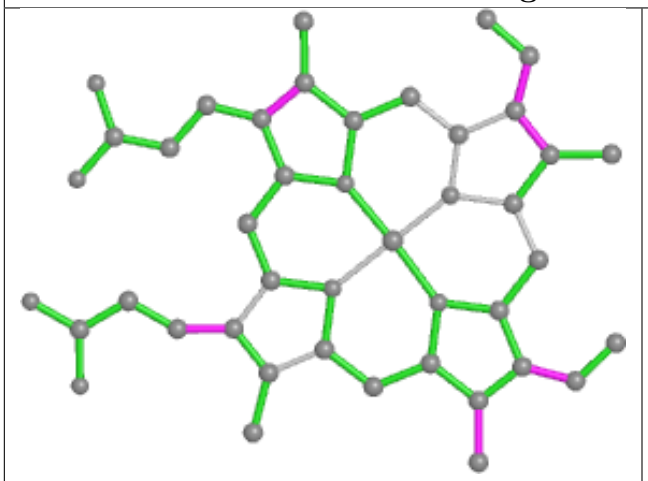


Torsions

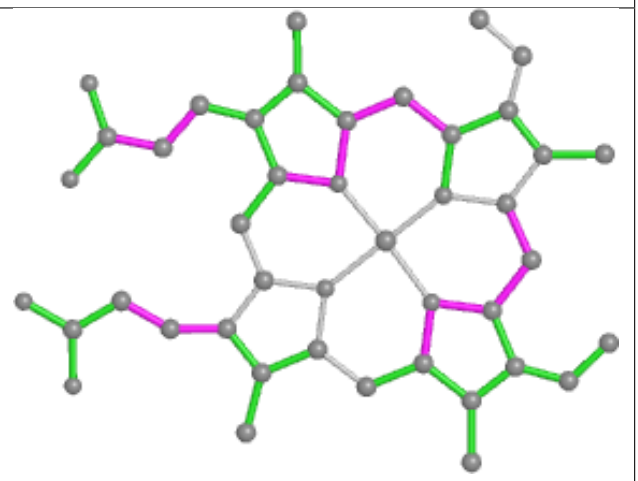


Rings

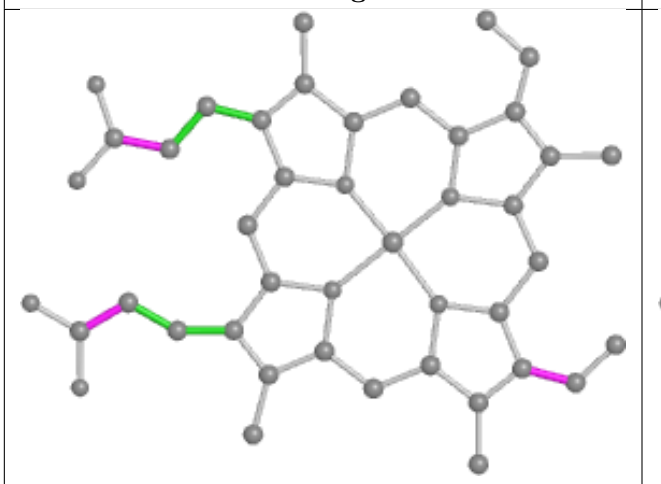
Ligand HEM C 354



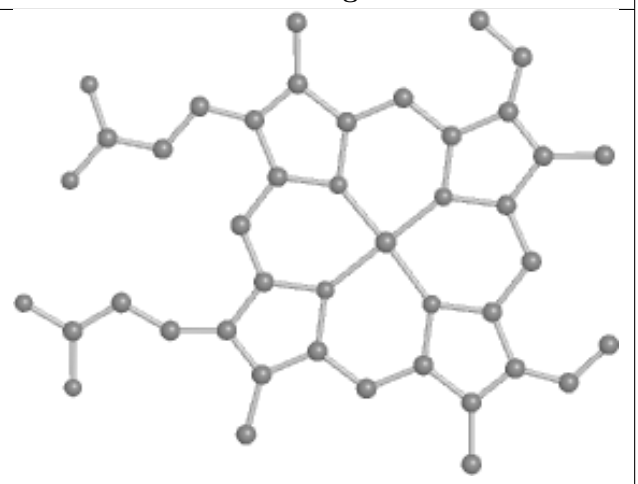
Bond lengths



Bond angles

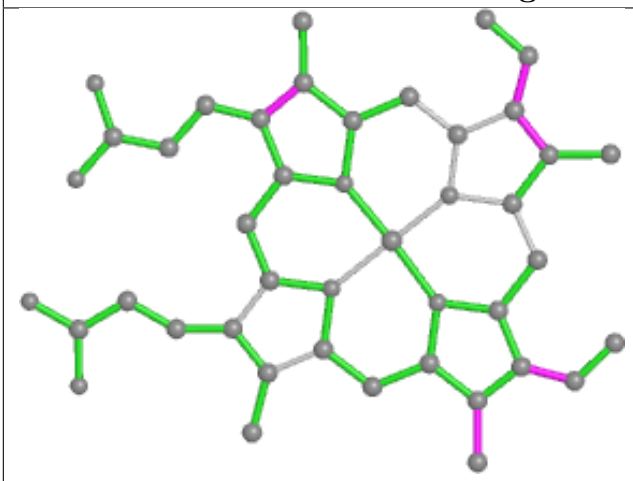


Torsions

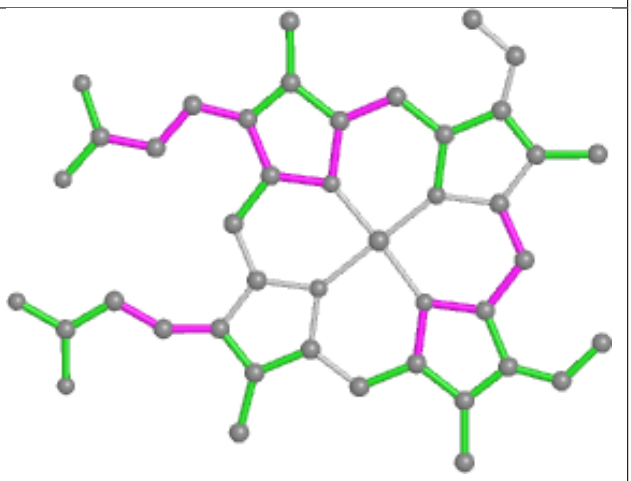


Rings

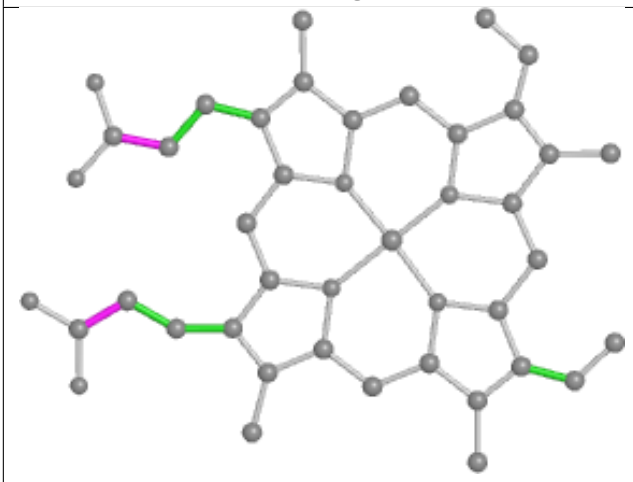
Ligand HEM B 354



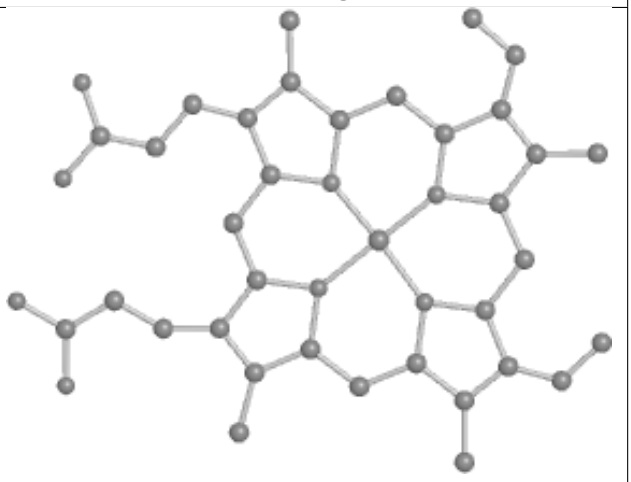
Bond lengths



Bond angles

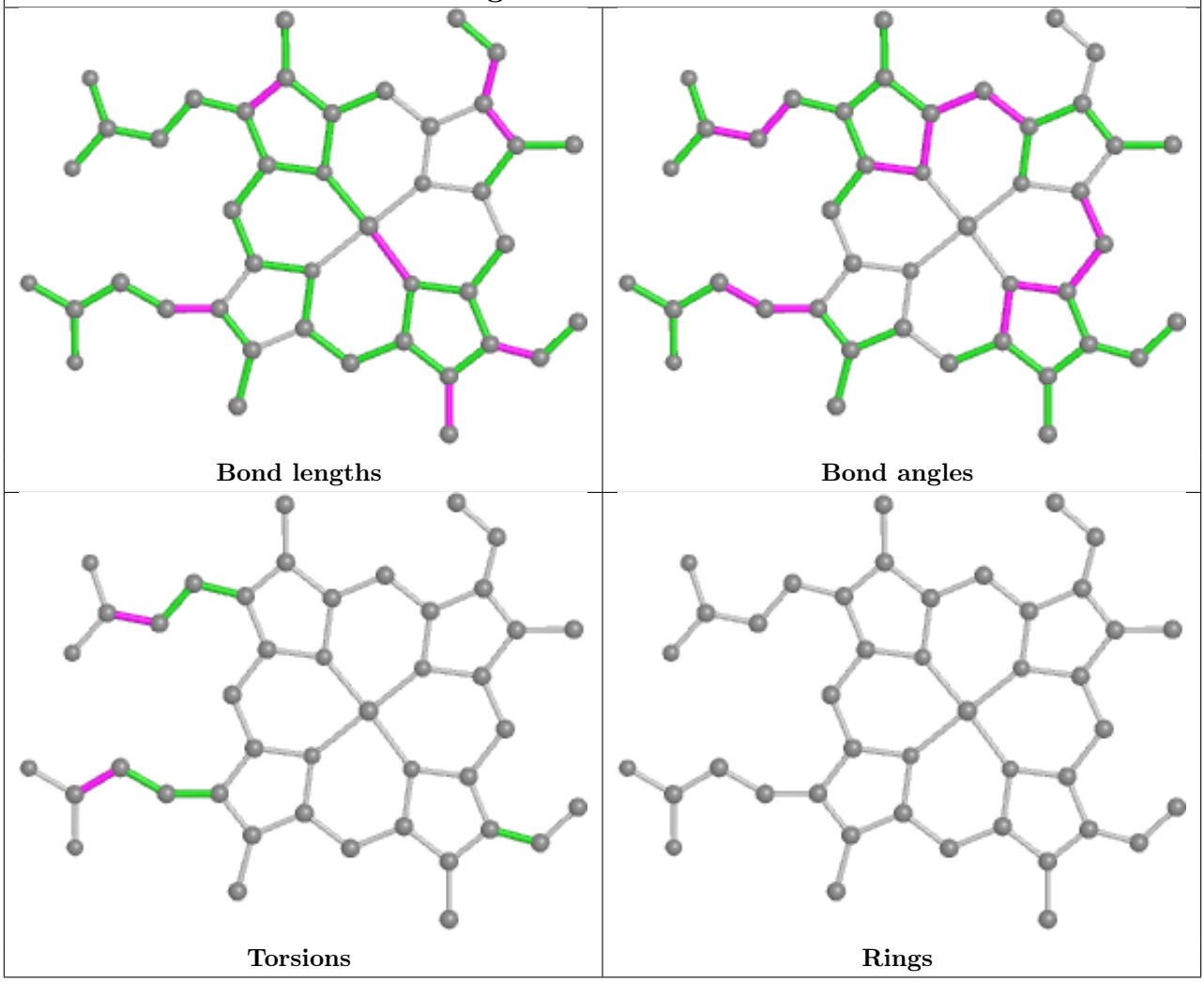


Torsions



Rings

Ligand HEM D 354



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.

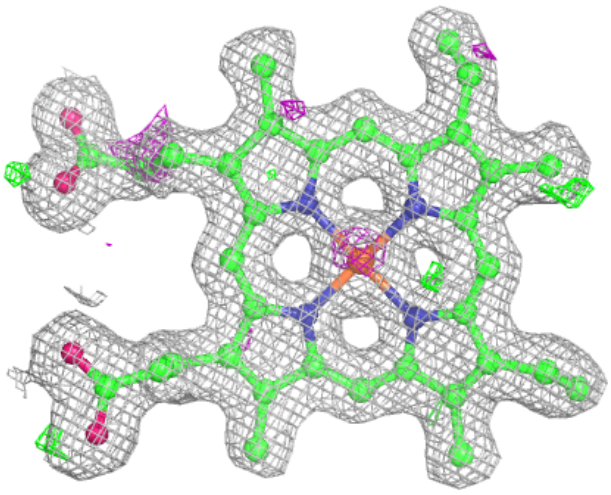
6.4 Ligands (i)

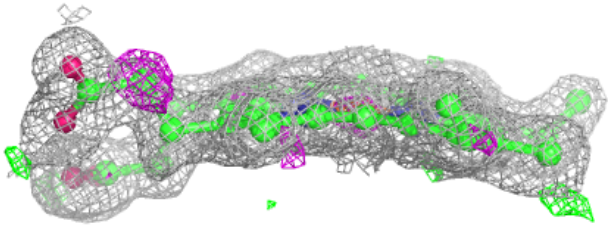
Unable to reproduce the depositors R factor - this section is therefore empty.

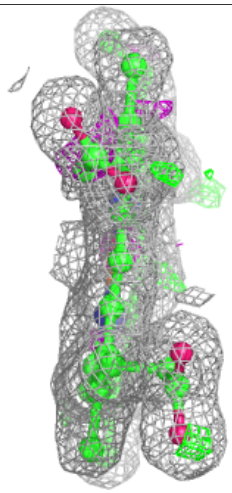
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM A 354:

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

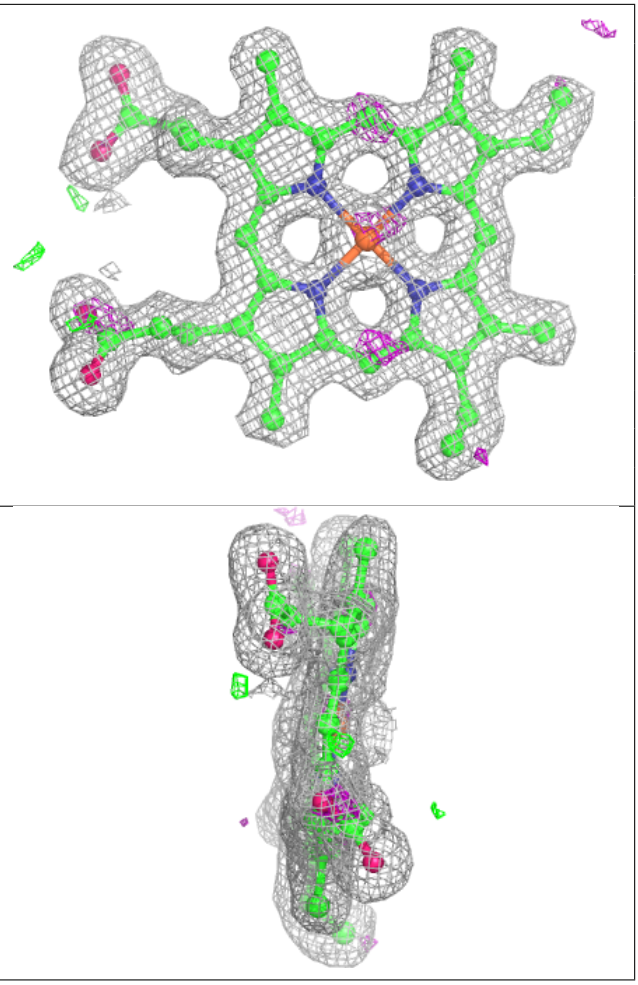






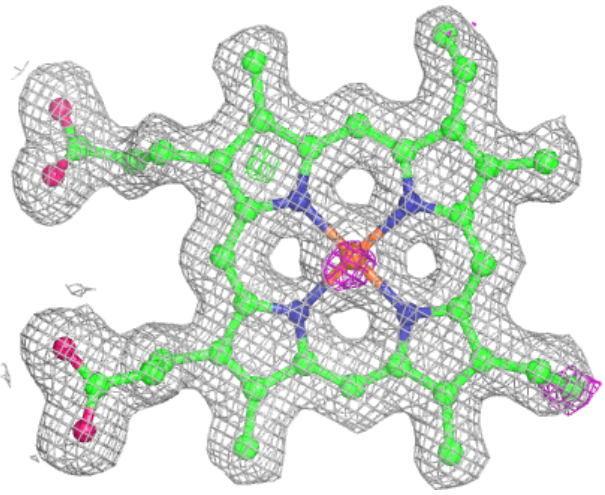
Electron density around HEM B 354:

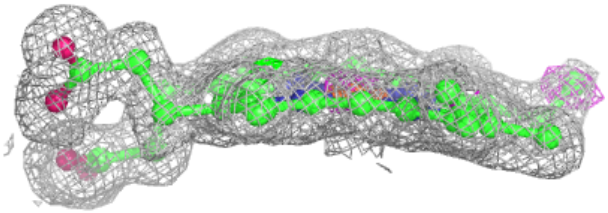
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

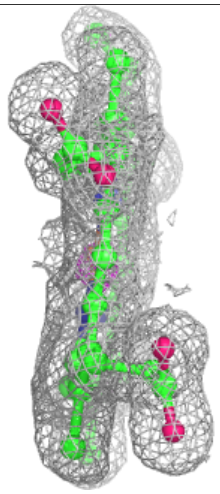


Electron density around HEM C 354:

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

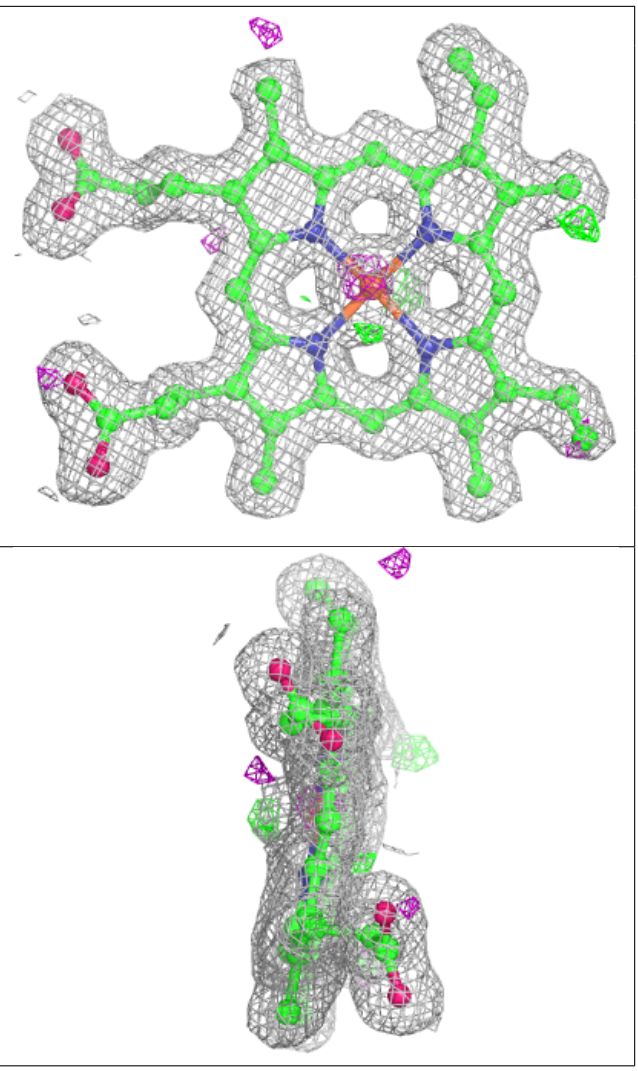






Electron density around HEM D 354:

$2mF_o$-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.