Full wwPDB X-ray Structure Validation Report

May 26, 2020 – 05:44 pm BST

PDB ID	:	3GAS
Title	:	Crystal Structure of Helicobacter pylori Heme Oxygenase Hugz in Complex with Heme
Authors	:	Jiang, F.; Hu, Y.L.; Guo, Y.; Guo, G.; Zou, Q.M.; Wang, D.C.
Deposited on	:	2009-02-18
Resolution	:	1.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

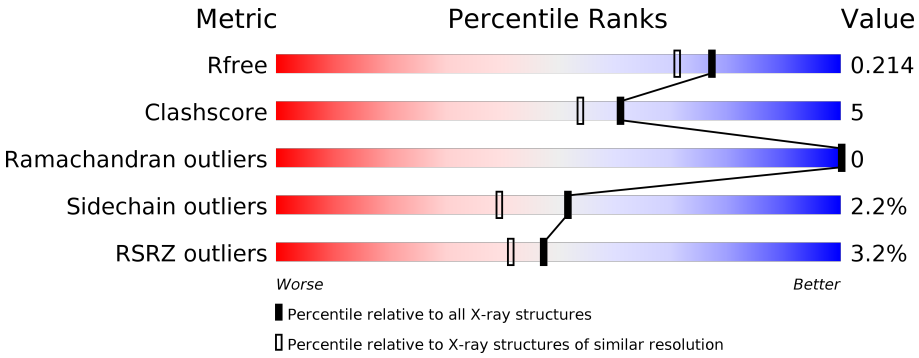
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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)
RSRZ outliers	127900	5850 (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 on 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	259	2% 88% 7% •
1	B	259	3% 85% 10% 5%
1	C	259	5% 85% 11% •
1	D	259	4% 84% 10% • 5%
1	E	259	88% 7% 5%
1	F	259	3% 86% 10% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13497 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 oxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	Se	0	0	0
			1980	1256	349	367	3	5			
1	B	247	Total	C	N	O	S	Se	0	0	0
			1970	1250	346	366	3	5			
1	C	248	Total	C	N	O	S	Se	0	0	0
			1980	1256	349	367	3	5			
1	D	247	Total	C	N	O	S	Se	0	0	0
			1972	1250	348	366	3	5			
1	E	246	Total	C	N	O	S	Se	0	0	0
			1962	1244	345	365	3	5			
1	F	248	Total	C	N	O	S	Se	0	0	0
			1980	1256	349	367	3	5			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	LEU	-	EXPRESSION TAG	UNP C0LU01
A	253	GLU	-	EXPRESSION TAG	UNP C0LU01
A	254	HIS	-	EXPRESSION TAG	UNP C0LU01
A	255	HIS	-	EXPRESSION TAG	UNP C0LU01
A	256	HIS	-	EXPRESSION TAG	UNP C0LU01
A	257	HIS	-	EXPRESSION TAG	UNP C0LU01
A	258	HIS	-	EXPRESSION TAG	UNP C0LU01
A	259	HIS	-	EXPRESSION TAG	UNP C0LU01
B	252	LEU	-	EXPRESSION TAG	UNP C0LU01
B	253	GLU	-	EXPRESSION TAG	UNP C0LU01
B	254	HIS	-	EXPRESSION TAG	UNP C0LU01
B	255	HIS	-	EXPRESSION TAG	UNP C0LU01
B	256	HIS	-	EXPRESSION TAG	UNP C0LU01
B	257	HIS	-	EXPRESSION TAG	UNP C0LU01
B	258	HIS	-	EXPRESSION TAG	UNP C0LU01
B	259	HIS	-	EXPRESSION TAG	UNP C0LU01
C	252	LEU	-	EXPRESSION TAG	UNP C0LU01

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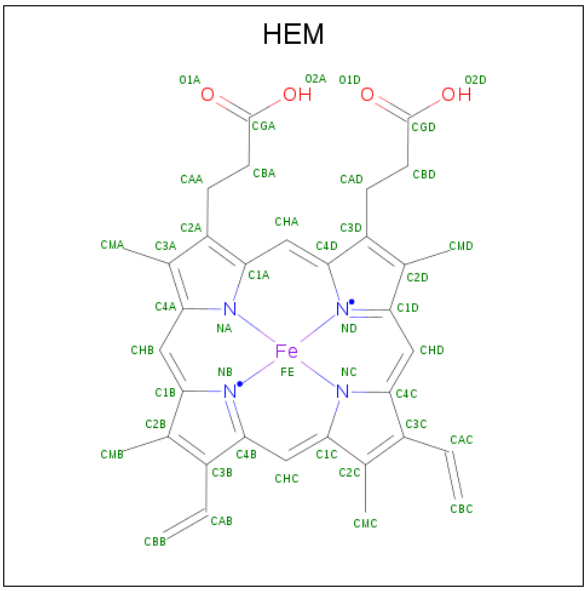
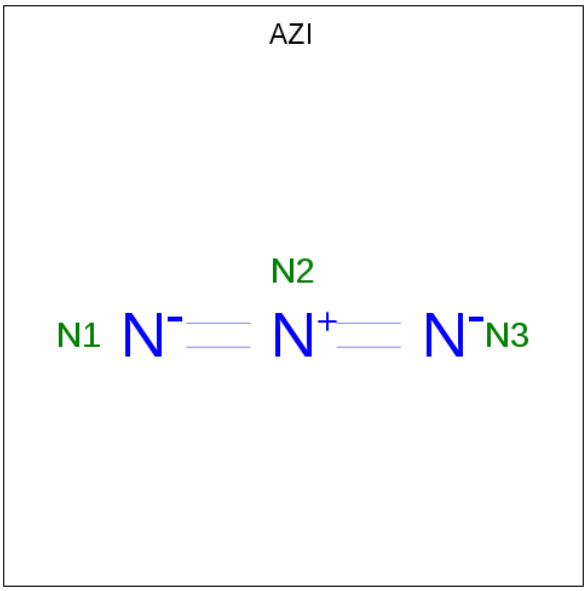
Chain	Residue	Modelled	Actual	Comment	Reference
C	253	GLU	-	EXPRESSION TAG	UNP C0LU01
C	254	HIS	-	EXPRESSION TAG	UNP C0LU01
C	255	HIS	-	EXPRESSION TAG	UNP C0LU01
C	256	HIS	-	EXPRESSION TAG	UNP C0LU01
C	257	HIS	-	EXPRESSION TAG	UNP C0LU01
C	258	HIS	-	EXPRESSION TAG	UNP C0LU01
C	259	HIS	-	EXPRESSION TAG	UNP C0LU01
D	252	LEU	-	EXPRESSION TAG	UNP C0LU01
D	253	GLU	-	EXPRESSION TAG	UNP C0LU01
D	254	HIS	-	EXPRESSION TAG	UNP C0LU01
D	255	HIS	-	EXPRESSION TAG	UNP C0LU01
D	256	HIS	-	EXPRESSION TAG	UNP C0LU01
D	257	HIS	-	EXPRESSION TAG	UNP C0LU01
D	258	HIS	-	EXPRESSION TAG	UNP C0LU01
D	259	HIS	-	EXPRESSION TAG	UNP C0LU01
E	252	LEU	-	EXPRESSION TAG	UNP C0LU01
E	253	GLU	-	EXPRESSION TAG	UNP C0LU01
E	254	HIS	-	EXPRESSION TAG	UNP C0LU01
E	255	HIS	-	EXPRESSION TAG	UNP C0LU01
E	256	HIS	-	EXPRESSION TAG	UNP C0LU01
E	257	HIS	-	EXPRESSION TAG	UNP C0LU01
E	258	HIS	-	EXPRESSION TAG	UNP C0LU01
E	259	HIS	-	EXPRESSION TAG	UNP C0LU01
F	252	LEU	-	EXPRESSION TAG	UNP C0LU01
F	253	GLU	-	EXPRESSION TAG	UNP C0LU01
F	254	HIS	-	EXPRESSION TAG	UNP C0LU01
F	255	HIS	-	EXPRESSION TAG	UNP C0LU01
F	256	HIS	-	EXPRESSION TAG	UNP C0LU01
F	257	HIS	-	EXPRESSION TAG	UNP C0LU01
F	258	HIS	-	EXPRESSION TAG	UNP C0LU01
F	259	HIS	-	EXPRESSION TAG	UNP C0LU01

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



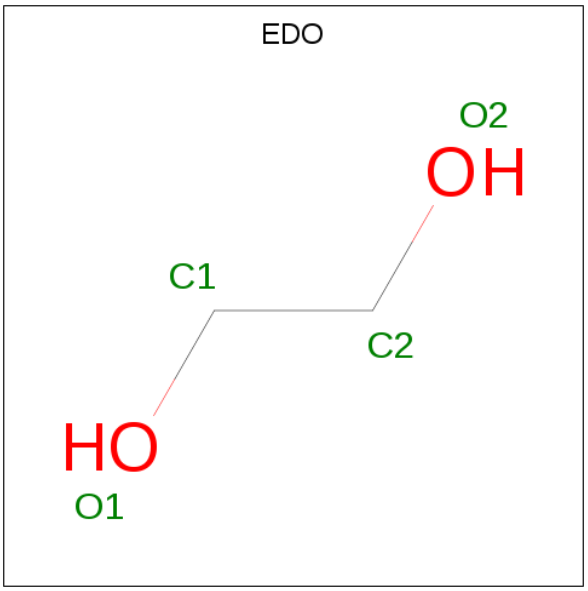
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is AZIDE ION (three-letter code: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 3 3	0	0
3	B	1	Total N 3 3	0	0
3	C	1	Total N 3 3	0	0
3	D	1	Total N 3 3	0	0
3	E	1	Total N 3 3	0	0
3	F	1	Total N 3 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

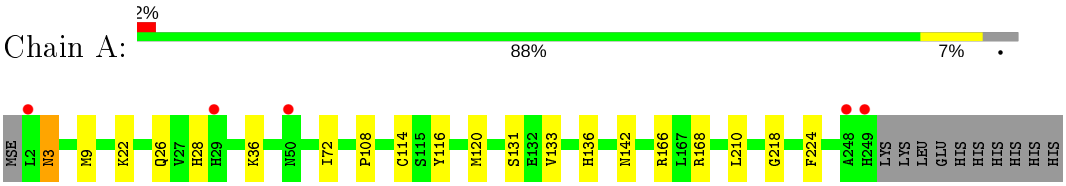
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	251	Total O 251 251	0	0
5	B	197	Total O 197 197	0	0
5	C	184	Total O 184 184	0	0
5	D	181	Total O 181 181	0	0
5	E	243	Total O 243 243	0	0
5	F	233	Total O 233 233	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

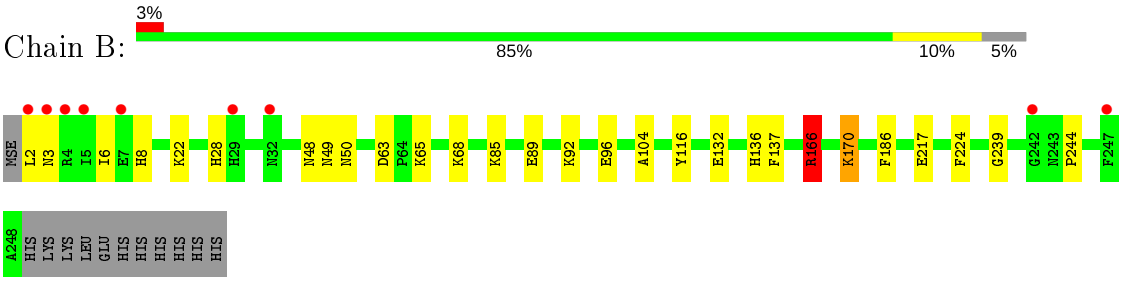
- Molecule 1: heme oxygenase

Chain A:



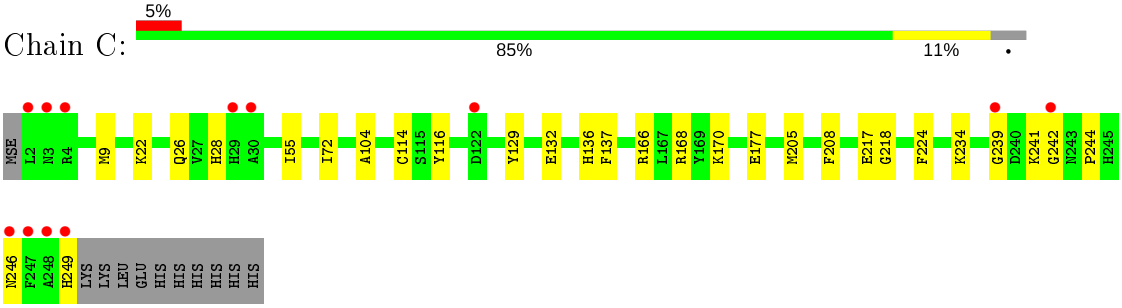
- Molecule 1: heme oxygenase

Chain B:



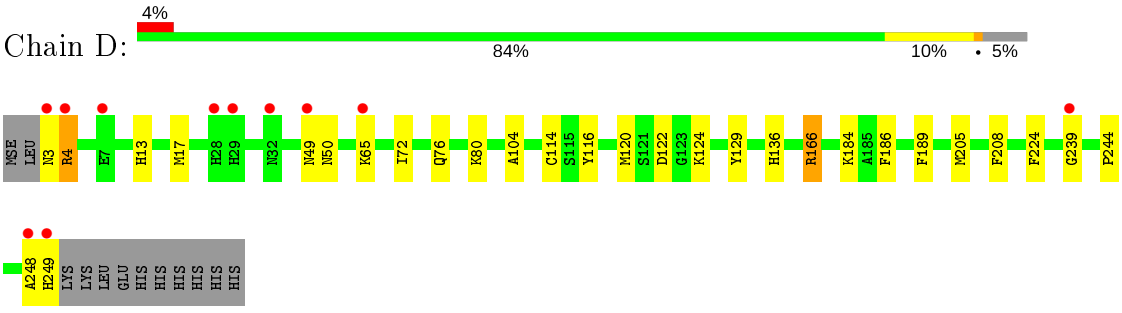
- Molecule 1: heme oxygenase

Chain C:



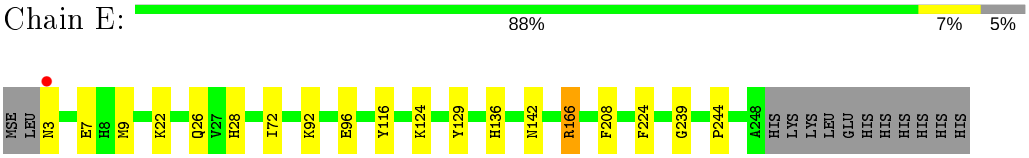
- Molecule 1: heme oxygenase

Chain D:



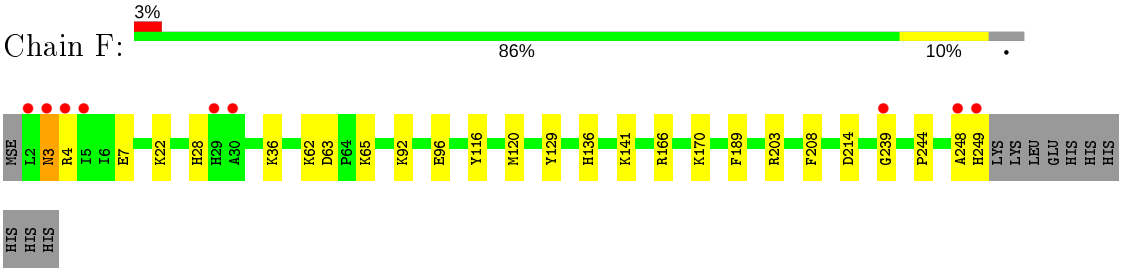
• Molecule 1: heme oxygenase

Chain E:



• Molecule 1: heme oxygenase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.33Å 139.34Å 152.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.87 – 1.80 47.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.6 (47.87-1.80) 94.7 (47.87-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.29 (at 1.79Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.192 , 0.222 0.184 , 0.214	Depositor DCC
R_{free} test set	8304 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13497	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.23% 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: AZI, EDO, HEM

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	0.52	0/2018	0.76	2/2702 (0.1%)
1	B	0.48	0/2007	0.74	3/2687 (0.1%)
1	C	0.45	0/2018	0.71	1/2702 (0.0%)
1	D	0.47	0/2010	0.74	2/2691 (0.1%)
1	E	0.52	0/1999	0.77	2/2676 (0.1%)
1	F	0.51	0/2018	0.71	1/2702 (0.0%)
All	All	0.49	0/12070	0.74	11/16160 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	166	ARG	NE-CZ-NH1	10.91	125.75	120.30
1	B	166	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	D	166	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	D	166	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	E	166	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	A	166	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	B	166	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	166	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	B	170	LYS	N-CA-C	-5.44	96.32	111.00
1	F	170	LYS	N-CA-C	-5.11	97.21	111.00
1	C	170	LYS	N-CA-C	-5.05	97.35	111.00

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	1980	0	1936	19	0
1	B	1970	0	1929	16	0
1	C	1980	0	1936	20	0
1	D	1972	0	1925	24	0
1	E	1962	0	1918	13	0
1	F	1980	0	1936	19	0
2	A	43	0	30	0	0
2	B	43	0	30	4	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
2	E	43	0	30	2	0
2	F	43	0	30	2	0
3	A	3	0	0	0	0
3	B	3	0	0	1	0
3	C	3	0	0	1	0
3	D	3	0	0	1	0
3	E	3	0	0	1	0
3	F	3	0	0	0	0
4	A	12	0	18	1	0
4	B	20	0	30	4	0
4	C	12	0	18	2	0
4	D	12	0	18	0	0
4	E	8	0	12	0	0
4	F	24	0	36	3	0
5	A	251	0	0	2	0
5	B	197	0	0	1	0
5	C	184	0	0	0	0
5	D	181	0	0	1	0
5	E	243	0	0	1	0
5	F	233	0	0	2	0
All	All	13497	0	11892	109	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.

All (109) 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:D:65:LYS:HE2	1:F:62:LYS:HD2	1.42	0.99
1:A:22:LYS:HB2	1:A:22:LYS:NZ	1.99	0.76
1:D:4:ARG:HD2	1:D:4:ARG:H	1.53	0.73
1:E:3:ASN:O	1:E:7:GLU:HG3	1.91	0.71
1:E:22:LYS:HD3	1:E:28:HIS:HD1	1.58	0.69
1:E:166:ARG:HD2	5:E:297:HOH:O	1.94	0.68
1:B:166:ARG:HD2	5:B:279:HOH:O	1.94	0.66
1:B:2:LEU:O	1:B:6:ILE:HG13	1.99	0.63
1:A:120:MSE:HE2	1:A:210:LEU:HD11	1.81	0.63
1:B:63:ASP:CG	1:B:65:LYS:HG2	2.19	0.62
1:A:22:LYS:HG3	1:A:28:HIS:CE1	2.36	0.60
1:C:22:LYS:HG2	1:C:28:HIS:ND1	2.17	0.60
1:F:203:ARG:HG2	4:F:1314:EDO:H21	1.84	0.58
1:D:49:ASN:N	1:D:49:ASN:HD22	1.99	0.58
1:F:3:ASN:O	1:F:7:GLU:HG2	2.02	0.58
1:E:92:LYS:O	1:E:96:GLU:HG3	2.04	0.58
1:F:248:ALA:O	1:F:249:HIS:HB2	2.05	0.57
1:C:217:GLU:CD	1:C:217:GLU:H	2.09	0.56
1:F:92:LYS:O	1:F:96:GLU:HG3	2.06	0.56
1:A:22:LYS:HB2	1:A:22:LYS:HZ3	1.68	0.55
1:B:239:GLY:HA3	2:B:1293:HEM:HBC1	1.89	0.55
1:D:3:ASN:HB3	1:D:4:ARG:NH1	2.22	0.54
1:A:120:MSE:HE2	1:A:210:LEU:CD1	2.38	0.54
1:B:85:LYS:O	1:B:89:GLU:HG3	2.08	0.53
1:F:4:ARG:HG2	1:F:4:ARG:HH11	1.73	0.53
1:F:63:ASP:OD2	1:F:65:LYS:HE3	2.09	0.53
1:E:26:GLN:HA	1:E:26:GLN:HE21	1.74	0.52
1:A:22:LYS:HB2	1:A:22:LYS:HZ2	1.74	0.51
1:D:49:ASN:ND2	1:D:49:ASN:N	2.58	0.51
1:C:9:MSE:HE1	1:C:72:ILE:HG13	1.92	0.51
1:D:129:TYR:CZ	1:D:208:PHE:HB3	2.46	0.51
1:E:244:PRO:HD3	2:E:1291:HEM:HAC	1.92	0.50
1:D:224:PHE:HA	3:D:1300:AZI:N1	2.27	0.50
1:C:217:GLU:CD	1:C:217:GLU:N	2.65	0.50
1:C:205:MSE:HE1	2:D:1294:HEM:HBB2	1.93	0.50
1:F:239:GLY:HA3	2:F:1292:HEM:HBC1	1.94	0.50
1:B:217:GLU:HB3	4:B:1310:EDO:H11	1.93	0.50
1:D:166:ARG:HD2	5:D:333:HOH:O	2.11	0.49
1:C:244:PRO:HD3	2:C:1295:HEM:HAC	1.95	0.49
2:F:1292:HEM:HAB	4:F:1318:EDO:C2	2.43	0.49
1:F:63:ASP:CG	1:F:65:LYS:HG2	2.33	0.49
1:D:4:ARG:H	1:D:4:ARG:CD	2.17	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:ALA:O	1:F:249:HIS:CB	2.60	0.49
1:A:131:SER:OG	1:A:133:VAL:HG22	2.13	0.49
1:C:114:CYS:HB2	1:D:104:ALA:HB2	1.96	0.48
1:F:22:LYS:HG3	1:F:28:HIS:CE1	2.49	0.48
1:C:104:ALA:HB2	1:D:114:CYS:HB2	1.96	0.48
1:D:4:ARG:HH11	1:D:4:ARG:HG3	1.79	0.47
1:A:3:ASN:HD22	1:A:3:ASN:C	2.15	0.47
1:F:22:LYS:HG3	1:F:28:HIS:ND1	2.29	0.47
1:A:114:CYS:HB2	1:B:104:ALA:HB2	1.96	0.47
1:D:120:MSE:HE2	1:D:189:PHE:CD2	2.49	0.47
1:D:244:PRO:HD3	2:D:1294:HEM:HAC	1.97	0.47
2:B:1293:HEM:HAB	4:B:1319:EDO:C2	2.45	0.47
1:E:22:LYS:HD3	1:E:28:HIS:ND1	2.29	0.47
1:F:120:MSE:HG2	1:F:189:PHE:CD1	2.49	0.46
1:C:241:LYS:HB2	1:C:249:HIS:CE1	2.51	0.46
1:E:129:TYR:CZ	1:E:208:PHE:HB3	2.51	0.45
1:D:4:ARG:HG3	1:D:4:ARG:NH1	2.31	0.45
1:A:22:LYS:NZ	1:A:22:LYS:CB	2.75	0.45
1:A:108:PRO:HG3	1:A:142:ASN:HB2	1.98	0.45
1:E:224:PHE:HA	3:E:1297:AZI:N1	2.31	0.45
1:F:36:LYS:NZ	5:F:1095:HOH:O	2.50	0.44
1:A:168:ARG:O	1:A:218:GLY:HA2	2.18	0.44
1:B:8:HIS:CG	1:B:68:LYS:NZ	2.85	0.44
1:D:72:ILE:O	1:D:76:GLN:HG3	2.17	0.44
1:F:4:ARG:HG2	1:F:4:ARG:NH1	2.33	0.44
2:B:1293:HEM:HAB	4:B:1319:EDO:H22	1.99	0.44
1:B:244:PRO:HD3	2:B:1293:HEM:HAC	2.00	0.44
1:C:26:GLN:HE22	1:C:242:GLY:HA3	1.82	0.44
1:E:9:MSE:HE1	1:E:72:ILE:HG13	1.99	0.43
1:D:239:GLY:HA3	2:D:1294:HEM:HBC1	2.00	0.43
1:A:9:MSE:HE1	1:A:72:ILE:HG13	2.01	0.43
1:C:55:ILE:HG23	4:C:1321:EDO:H11	2.00	0.43
1:C:224:PHE:HA	3:C:1301:AZI:N1	2.33	0.43
1:D:248:ALA:O	1:D:249:HIS:HB2	2.18	0.43
1:F:214:ASP:HB2	5:F:1134:HOH:O	2.19	0.43
1:B:132:GLU:HA	1:B:137:PHE:CG	2.54	0.43
1:C:129:TYR:CZ	1:C:208:PHE:HB3	2.53	0.43
1:C:239:GLY:HA3	2:C:1295:HEM:HBC1	2.01	0.43
1:C:55:ILE:CG2	4:C:1321:EDO:H11	2.49	0.43
1:B:224:PHE:HA	3:B:1299:AZI:N1	2.34	0.43
1:B:170:LYS:HG2	4:B:1310:EDO:H12	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:MSE:HE1	1:D:186:PHE:CE1	2.54	0.42
1:F:120:MSE:HE2	1:F:189:PHE:CD2	2.54	0.42
1:A:36:LYS:NZ	5:A:324:HOH:O	2.51	0.42
1:D:3:ASN:HB3	1:D:4:ARG:HH12	1.84	0.42
1:E:239:GLY:HA3	2:E:1291:HEM:HBC1	2.00	0.42
1:C:234:LYS:HA	1:C:234:LYS:HD2	1.81	0.42
1:A:26:GLN:NE2	1:A:28:HIS:NE2	2.68	0.42
1:B:22:LYS:HG3	1:B:28:HIS:ND1	2.35	0.42
1:F:141:LYS:NZ	4:F:1317:EDO:O1	2.52	0.41
1:D:13:HIS:O	1:D:17:MSE:HG3	2.20	0.41
1:A:22:LYS:HE3	1:A:28:HIS:HD1	1.85	0.41
1:B:48:ASN:HB3	1:B:49:ASN:H	1.54	0.41
1:B:92:LYS:O	1:B:96:GLU:HG3	2.19	0.41
1:F:129:TYR:CZ	1:F:208:PHE:HB3	2.55	0.41
1:B:8:HIS:CG	1:B:68:LYS:HZ1	2.39	0.41
1:C:177:GLU:HA	1:C:177:GLU:OE1	2.21	0.41
1:C:168:ARG:O	1:C:218:GLY:HA2	2.21	0.41
1:C:246:ASN:ND2	1:D:205:MSE:HA	2.36	0.41
1:D:122:ASP:OD1	1:D:184:LYS:HE2	2.21	0.41
1:A:224:PHE:HD2	4:A:1312:EDO:H21	1.85	0.41
1:A:22:LYS:HG2	5:A:820:HOH:O	2.21	0.41
1:E:26:GLN:NE2	1:E:26:GLN:HA	2.35	0.41
1:A:22:LYS:HZ3	1:A:22:LYS:CB	2.33	0.41
1:D:4:ARG:HH11	1:D:4:ARG:H	1.68	0.40
1:C:132:GLU:HA	1:C:137:PHE:CG	2.56	0.40
1:E:26:GLN:NE2	1:E:28:HIS:NE2	2.70	0.40

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	246/259 (95%)	238 (97%)	8 (3%)	0	100	100
1	B	245/259 (95%)	236 (96%)	9 (4%)	0	100	100
1	C	246/259 (95%)	237 (96%)	9 (4%)	0	100	100
1	D	245/259 (95%)	235 (96%)	10 (4%)	0	100	100
1	E	244/259 (94%)	237 (97%)	7 (3%)	0	100	100
1	F	246/259 (95%)	236 (96%)	10 (4%)	0	100	100
All	All	1472/1554 (95%)	1419 (96%)	53 (4%)	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	209/214 (98%)	206 (99%)	3 (1%)	67	59
1	B	208/214 (97%)	202 (97%)	6 (3%)	42	29
1	C	209/214 (98%)	206 (99%)	3 (1%)	67	59
1	D	208/214 (97%)	202 (97%)	6 (3%)	42	29
1	E	207/214 (97%)	203 (98%)	4 (2%)	57	46
1	F	209/214 (98%)	204 (98%)	5 (2%)	49	36
All	All	1250/1284 (97%)	1223 (98%)	27 (2%)	52	39

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	116	TYR
1	A	136	HIS
1	B	3	ASN
1	B	50	ASN
1	B	116	TYR
1	B	136	HIS

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Mol	Chain	Res	Type
1	B	166	ARG
1	B	186	PHE
1	C	116	TYR
1	C	136	HIS
1	C	166	ARG
1	D	4	ARG
1	D	50	ASN
1	D	80	LYS
1	D	116	TYR
1	D	124	LYS
1	D	136	HIS
1	E	116	TYR
1	E	124	LYS
1	E	136	HIS
1	E	142	ASN
1	F	3	ASN
1	F	116	TYR
1	F	136	HIS
1	F	166	ARG
1	F	244	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	26	GLN
1	A	59	HIS
1	A	109	ASN
1	B	3	ASN
1	B	246	ASN
1	C	49	ASN
1	D	49	ASN
1	D	143	ASN
1	E	26	GLN
1	E	142	ASN
1	E	143	ASN
1	F	3	ASN
1	F	109	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

34 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	B	1293	1,3	27,50,50	1.70	4 (14%)	17,82,82	2.52	10 (58%)
4	EDO	F	1314	-	3,3,3	0.39	0	2,2,2	0.36	0
4	EDO	B	1319	-	3,3,3	0.49	0	2,2,2	0.23	0
2	HEM	A	1290	1,3	27,50,50	1.77	3 (11%)	17,82,82	2.53	10 (58%)
4	EDO	C	1311	-	3,3,3	0.54	0	2,2,2	0.31	0
4	EDO	F	1304	-	3,3,3	0.65	0	2,2,2	0.39	0
3	AZI	A	1296	2	0,2,2	0.00	-	0,1,1	0.00	-
2	HEM	F	1292	1,3	27,50,50	1.78	5 (18%)	17,82,82	2.54	8 (47%)
2	HEM	C	1295	1,3	27,50,50	1.76	4 (14%)	17,82,82	2.41	8 (47%)
4	EDO	F	1309	-	3,3,3	0.75	0	2,2,2	0.19	0
4	EDO	F	1318	-	3,3,3	0.48	0	2,2,2	0.17	0
4	EDO	C	1321	-	3,3,3	0.50	0	2,2,2	0.24	0
4	EDO	B	1305	-	3,3,3	0.59	0	2,2,2	0.22	0
4	EDO	A	1312	-	3,3,3	0.73	0	2,2,2	0.14	0
4	EDO	B	1315	-	3,3,3	0.53	0	2,2,2	0.35	0
4	EDO	D	1306	-	3,3,3	0.62	0	2,2,2	0.27	0
4	EDO	E	1303	-	3,3,3	0.56	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	AZI	B	1299	2	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	C	1307	-	3,3,3	0.53	0	2,2,2	0.25	0
2	HEM	D	1294	1,3	27,50,50	1.69	4 (14%)	17,82,82	2.59	11 (64%)
4	EDO	F	1317	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	A	1302	-	3,3,3	0.61	0	2,2,2	0.24	0
4	EDO	A	1308	-	3,3,3	0.70	0	2,2,2	0.12	0
3	AZI	F	1298	2	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	E	1313	-	3,3,3	0.54	0	2,2,2	0.35	0
2	HEM	E	1291	1,3	27,50,50	1.72	4 (14%)	17,82,82	2.49	11 (64%)
4	EDO	B	1310	-	3,3,3	0.53	0	2,2,2	0.23	0
3	AZI	E	1297	2	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	F	1322	-	3,3,3	0.50	0	2,2,2	0.36	0
3	AZI	C	1301	2	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	D	1320	-	3,3,3	0.56	0	2,2,2	0.25	0
4	EDO	D	1323	-	3,3,3	0.43	0	2,2,2	0.40	0
4	EDO	B	1316	-	3,3,3	0.50	0	2,2,2	0.34	0
3	AZI	D	1300	2	0,2,2	0.00	-	0,1,1	0.00	-

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	B	1293	1,3	-	0/6/54/54	-
4	EDO	F	1314	-	-	1/1/1/1	-
4	EDO	B	1319	-	-	0/1/1/1	-
2	HEM	A	1290	1,3	-	0/6/54/54	-
4	EDO	C	1311	-	-	0/1/1/1	-
4	EDO	F	1304	-	-	0/1/1/1	-
2	HEM	F	1292	1,3	-	0/6/54/54	-
2	HEM	C	1295	1,3	-	0/6/54/54	-
4	EDO	F	1309	-	-	0/1/1/1	-
4	EDO	F	1318	-	-	0/1/1/1	-
4	EDO	C	1321	-	-	0/1/1/1	-
4	EDO	B	1305	-	-	0/1/1/1	-
4	EDO	A	1312	-	-	1/1/1/1	-
4	EDO	B	1315	-	-	1/1/1/1	-
4	EDO	D	1306	-	-	0/1/1/1	-
4	EDO	E	1303	-	-	0/1/1/1	-
4	EDO	C	1307	-	-	0/1/1/1	-
2	HEM	D	1294	1,3	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	F	1317	-	-	0/1/1/1	-
4	EDO	A	1302	-	-	0/1/1/1	-
4	EDO	A	1308	-	-	0/1/1/1	-
4	EDO	E	1313	-	-	0/1/1/1	-
2	HEM	E	1291	1,3	-	0/6/54/54	-
4	EDO	B	1310	-	-	1/1/1/1	-
4	EDO	F	1322	-	-	1/1/1/1	-
4	EDO	D	1320	-	-	0/1/1/1	-
4	EDO	D	1323	-	-	0/1/1/1	-
4	EDO	B	1316	-	-	0/1/1/1	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1292	HEM	C3C-CAC	-6.20	1.35	1.47
2	B	1293	HEM	C3C-CAC	-6.06	1.35	1.47
2	A	1290	HEM	C3C-CAC	-5.99	1.35	1.47
2	E	1291	HEM	C3C-CAC	-5.77	1.36	1.47
2	C	1295	HEM	C3C-CAC	-5.71	1.36	1.47
2	D	1294	HEM	C3C-CAC	-5.58	1.36	1.47
2	F	1292	HEM	C4B-NB	3.72	1.43	1.36
2	C	1295	HEM	C4B-NB	3.31	1.43	1.36
2	C	1295	HEM	C3B-C2B	3.24	1.44	1.40
2	B	1293	HEM	C4B-NB	3.10	1.42	1.36
2	A	1290	HEM	C4B-NB	3.09	1.42	1.36
2	A	1290	HEM	C4A-CHB	-3.07	1.32	1.41
2	E	1291	HEM	C4B-NB	3.03	1.42	1.36
2	E	1291	HEM	C4A-CHB	-2.74	1.33	1.41
2	C	1295	HEM	C4A-CHB	-2.70	1.33	1.41
2	D	1294	HEM	C4A-CHB	-2.64	1.33	1.41
2	F	1292	HEM	C4A-CHB	-2.58	1.33	1.41
2	D	1294	HEM	C3B-C2B	2.46	1.43	1.40
2	B	1293	HEM	C4A-CHB	-2.45	1.34	1.41
2	B	1293	HEM	C3B-C2B	2.42	1.43	1.40
2	D	1294	HEM	C4B-NB	2.41	1.41	1.36
2	F	1292	HEM	C1C-C2C	2.15	1.47	1.42
2	E	1291	HEM	C3B-C2B	2.10	1.43	1.40
2	F	1292	HEM	C4D-C3D	2.01	1.47	1.42

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1294	HEM	C4C-C3C-C2C	-5.24	103.24	106.90
2	B	1293	HEM	C4C-C3C-C2C	-5.09	103.35	106.90
2	E	1291	HEM	C4C-C3C-C2C	-5.02	103.39	106.90
2	A	1290	HEM	C4C-C3C-C2C	-5.01	103.40	106.90
2	C	1295	HEM	C4C-C3C-C2C	-4.79	103.55	106.90
2	F	1292	HEM	C4C-C3C-C2C	-4.55	103.72	106.90
2	E	1291	HEM	CMA-C3A-C4A	-4.18	122.04	128.46
2	F	1292	HEM	CMA-C3A-C4A	-3.91	122.45	128.46
2	D	1294	HEM	CBD-CAD-C3D	-3.83	105.42	112.48
2	C	1295	HEM	C1D-C2D-C3D	-3.69	104.43	107.00
2	B	1293	HEM	CMA-C3A-C4A	-3.65	122.86	128.46
2	B	1293	HEM	C1D-C2D-C3D	-3.64	104.46	107.00
2	A	1290	HEM	CMA-C3A-C4A	-3.61	122.91	128.46
2	F	1292	HEM	C1D-C2D-C3D	-3.59	104.50	107.00
2	F	1292	HEM	CBD-CAD-C3D	-3.59	105.86	112.48
2	A	1290	HEM	C1D-C2D-C3D	-3.52	104.55	107.00
2	D	1294	HEM	C1D-C2D-C3D	-3.52	104.55	107.00
2	D	1294	HEM	CAD-CBD-CGD	3.46	118.48	112.67
2	C	1295	HEM	CMA-C3A-C4A	-3.41	123.22	128.46
2	E	1291	HEM	C1D-C2D-C3D	-3.22	104.76	107.00
2	A	1290	HEM	CBD-CAD-C3D	-3.17	106.64	112.48
2	B	1293	HEM	CBD-CAD-C3D	-3.01	106.93	112.48
2	E	1291	HEM	C3B-C4B-NB	2.96	113.04	109.21
2	C	1295	HEM	CBD-CAD-C3D	-2.96	107.02	112.48
2	C	1295	HEM	CMD-C2D-C3D	2.94	130.48	124.94
2	D	1294	HEM	C3B-C4B-NB	2.92	112.99	109.21
2	B	1293	HEM	CAD-CBD-CGD	2.89	117.52	112.67
2	A	1290	HEM	C4A-C3A-C2A	2.88	109.00	107.00
2	E	1291	HEM	CBD-CAD-C3D	-2.83	107.25	112.48
2	A	1290	HEM	CMD-C2D-C3D	2.80	130.23	124.94
2	D	1294	HEM	CMD-C2D-C3D	2.77	130.16	124.94
2	F	1292	HEM	CAD-CBD-CGD	2.75	117.29	112.67
2	B	1293	HEM	CMD-C2D-C3D	2.75	130.12	124.94
2	C	1295	HEM	C3B-C4B-NB	2.73	112.74	109.21
2	F	1292	HEM	C4A-C3A-C2A	2.66	108.85	107.00
2	B	1293	HEM	C3B-C4B-NB	2.66	112.65	109.21
2	D	1294	HEM	CMA-C3A-C4A	-2.65	124.40	128.46
2	F	1292	HEM	C3B-C4B-NB	2.65	112.63	109.21
2	F	1292	HEM	CMD-C2D-C3D	2.64	129.92	124.94
2	E	1291	HEM	C4A-C3A-C2A	2.61	108.81	107.00
2	A	1290	HEM	C3B-C4B-NB	2.49	112.43	109.21
2	D	1294	HEM	C4A-C3A-C2A	2.37	108.65	107.00
2	C	1295	HEM	C4A-C3A-C2A	2.37	108.64	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1291	HEM	CAD-CBD-CGD	2.33	116.58	112.67
2	A	1290	HEM	CMB-C2B-C3B	2.24	128.88	124.68
2	E	1291	HEM	CMA-C3A-C2A	2.23	129.15	124.94
2	C	1295	HEM	CMD-C2D-C1D	-2.20	125.08	128.46
2	A	1290	HEM	CAD-CBD-CGD	2.19	116.35	112.67
2	D	1294	HEM	CMB-C2B-C3B	2.17	128.73	124.68
2	E	1291	HEM	CMB-C2B-C3B	2.14	128.69	124.68
2	E	1291	HEM	CMC-C2C-C3C	2.14	128.69	124.68
2	E	1291	HEM	CMD-C2D-C3D	2.12	128.94	124.94
2	A	1290	HEM	CMD-C2D-C1D	-2.12	125.21	128.46
2	B	1293	HEM	CMB-C2B-C3B	2.09	128.59	124.68
2	D	1294	HEM	CMD-C2D-C1D	-2.08	125.27	128.46
2	B	1293	HEM	C4A-C3A-C2A	2.05	108.42	107.00
2	D	1294	HEM	CMC-C2C-C3C	2.00	128.43	124.68
2	B	1293	HEM	CMA-C3A-C2A	2.00	128.72	124.94

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1310	EDO	O1-C1-C2-O2
4	F	1314	EDO	O1-C1-C2-O2
4	B	1315	EDO	O1-C1-C2-O2
4	A	1312	EDO	O1-C1-C2-O2
4	F	1322	EDO	O1-C1-C2-O2

There are no ring outliers.

16 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1293	HEM	4	0
4	F	1314	EDO	1	0
4	B	1319	EDO	2	0
2	F	1292	HEM	2	0
2	C	1295	HEM	2	0
4	F	1318	EDO	1	0
4	C	1321	EDO	2	0
4	A	1312	EDO	1	0
3	B	1299	AZI	1	0
2	D	1294	HEM	3	0
4	F	1317	EDO	1	0

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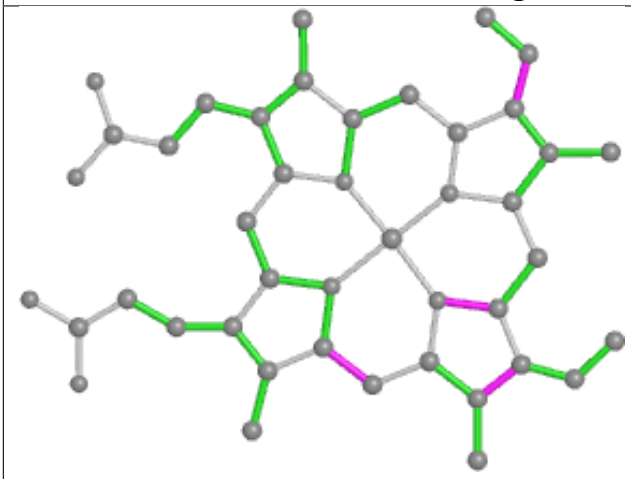
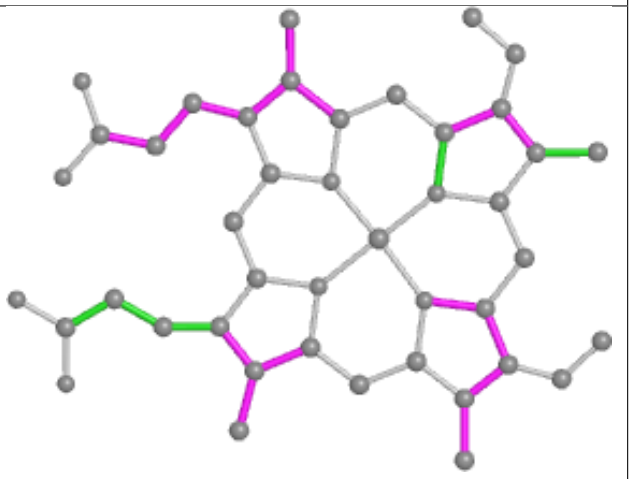
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1291	HEM	2	0
4	B	1310	EDO	2	0
3	E	1297	AZI	1	0
3	C	1301	AZI	1	0
3	D	1300	AZI	1	0

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.

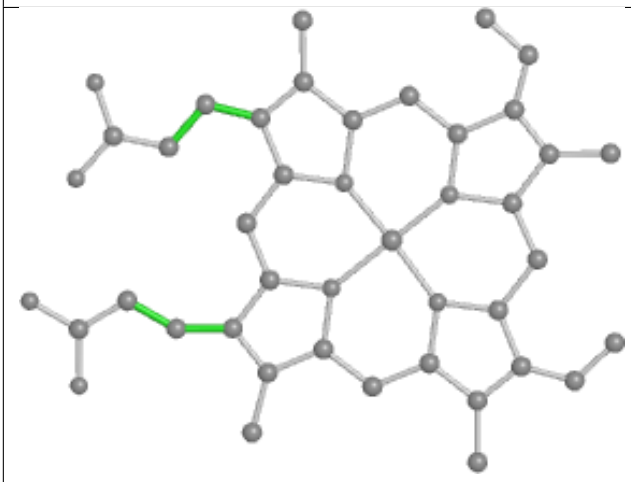
Ligand HEM B 1293



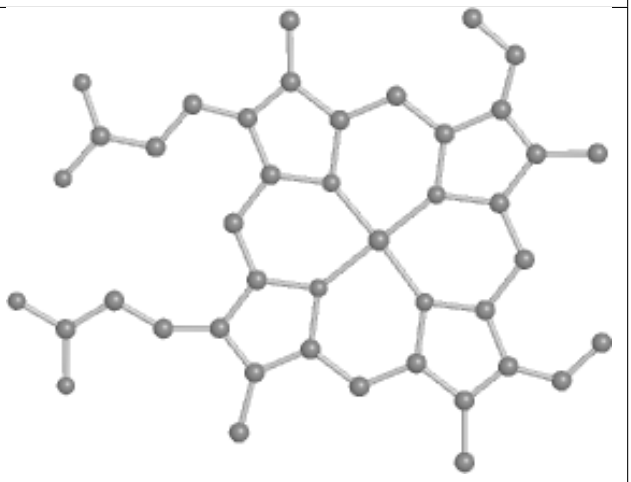
Bond lengths



Bond angles

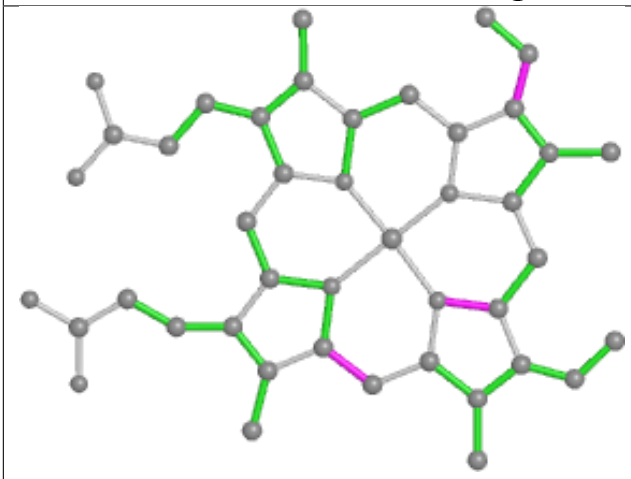


Torsions

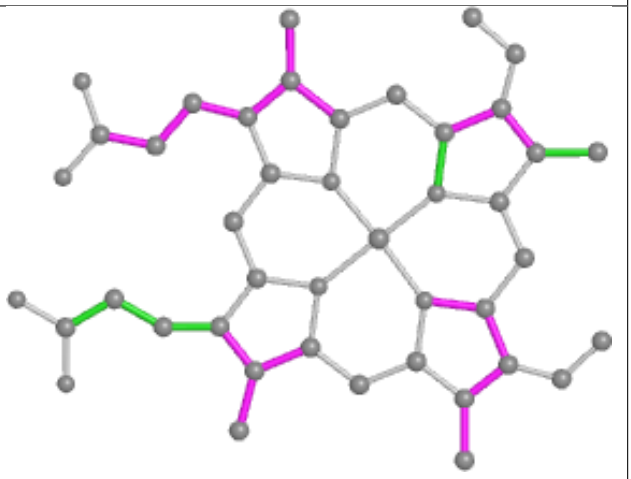


Rings

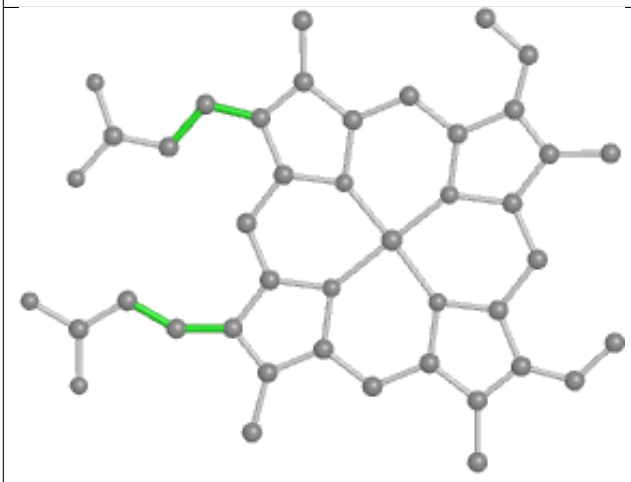
Ligand HEM A 1290



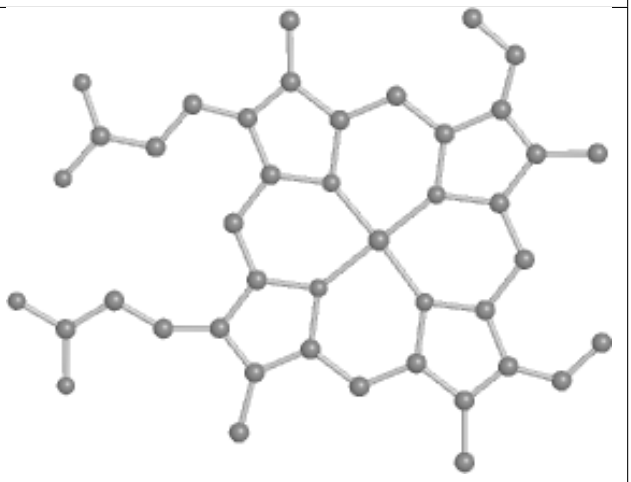
Bond lengths



Bond angles

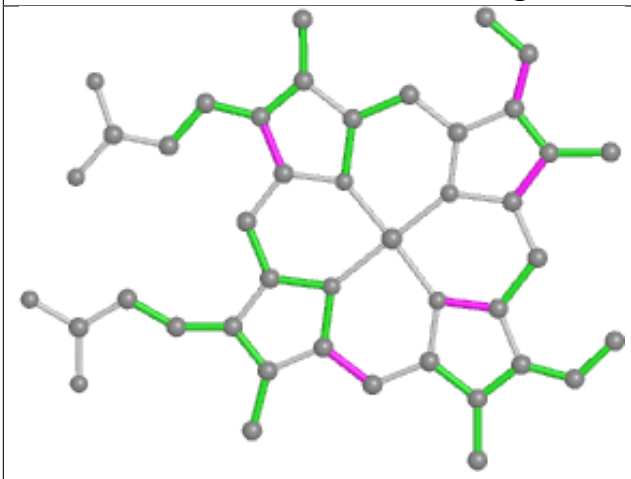


Torsions

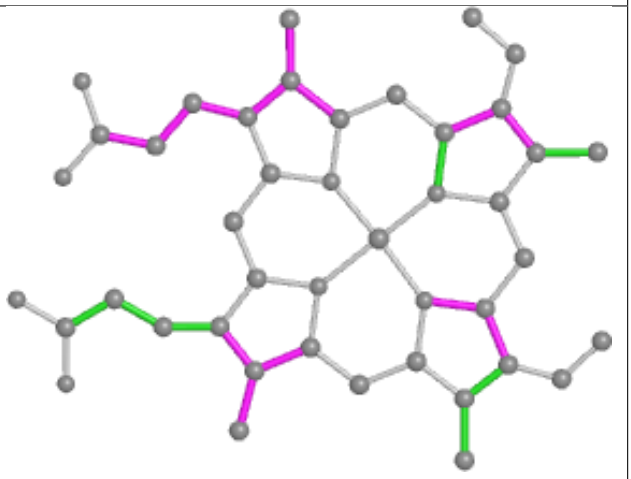


Rings

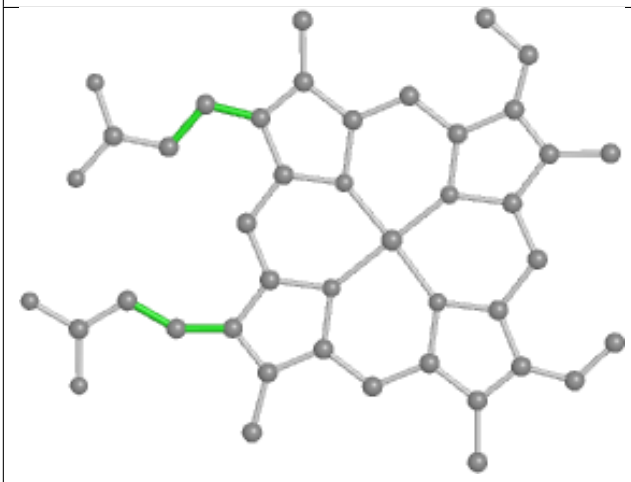
Ligand HEM F 1292



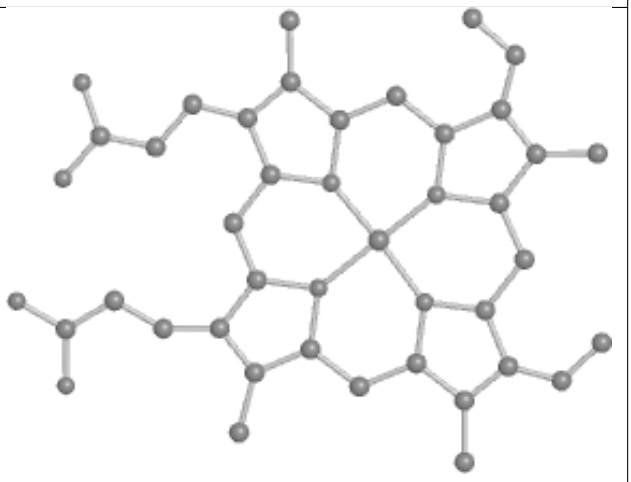
Bond lengths



Bond angles

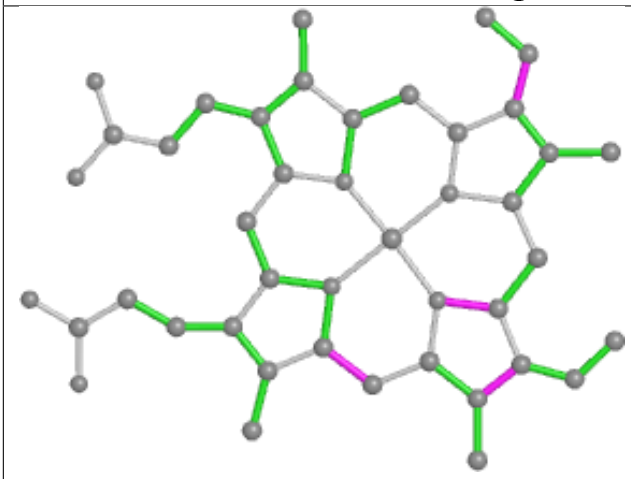


Torsions

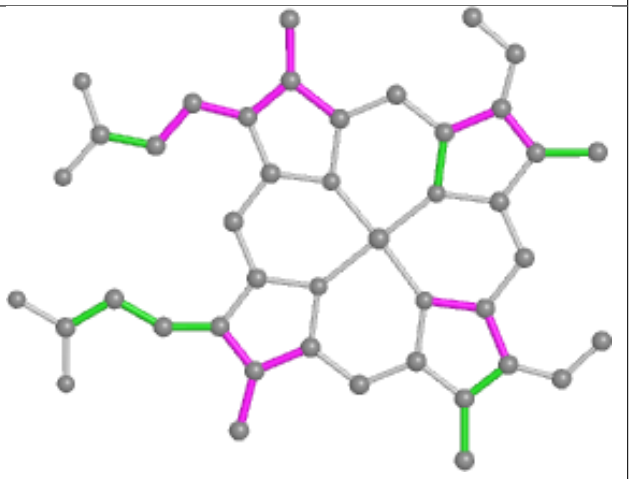


Rings

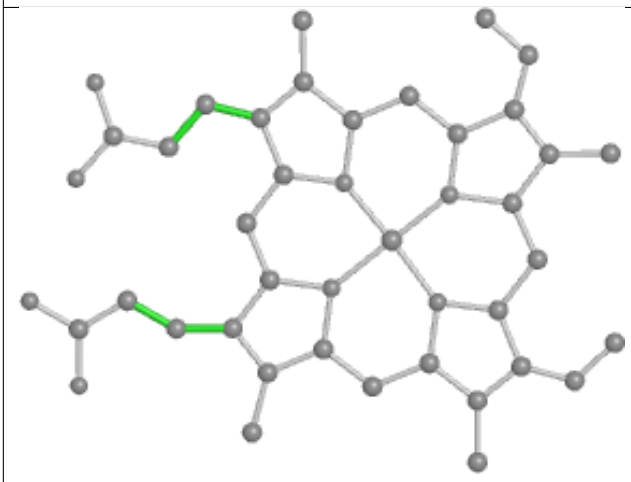
Ligand HEM C 1295



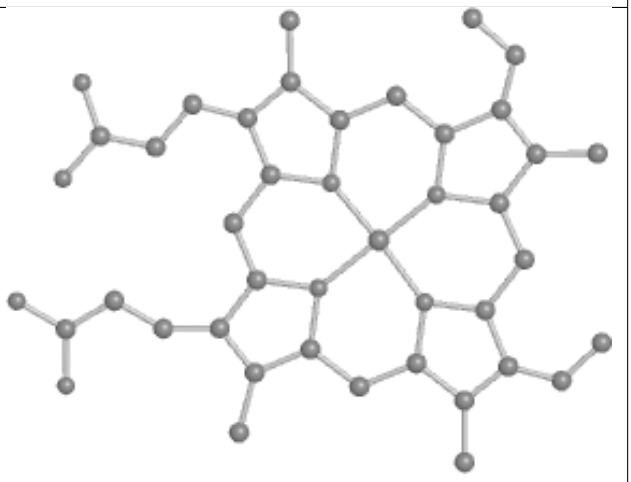
Bond lengths



Bond angles

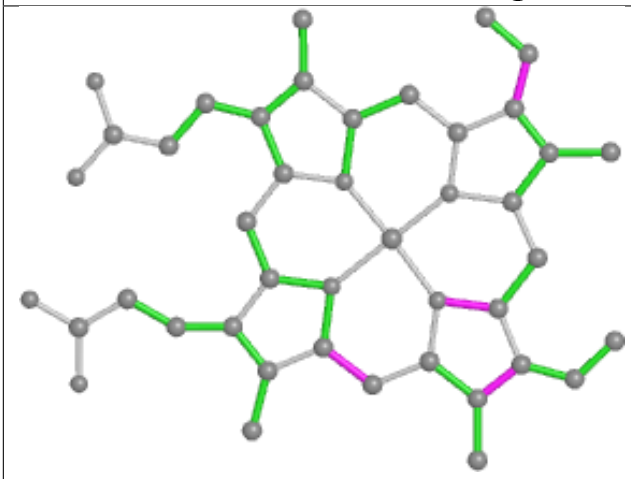


Torsions

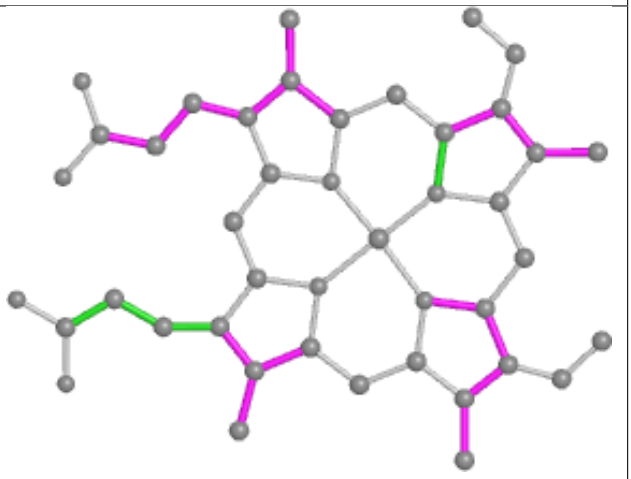


Rings

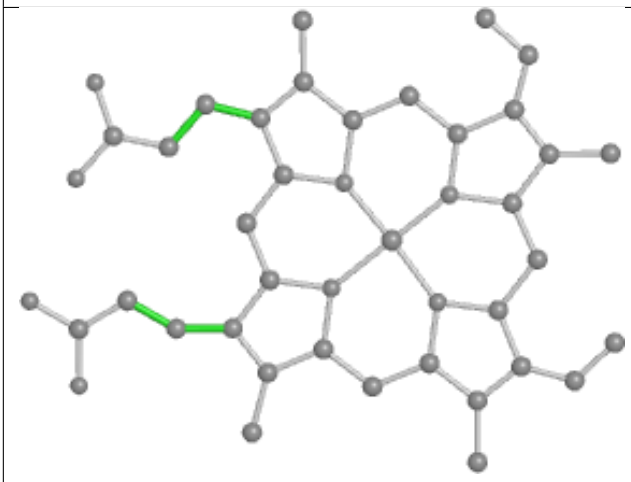
Ligand HEM D 1294



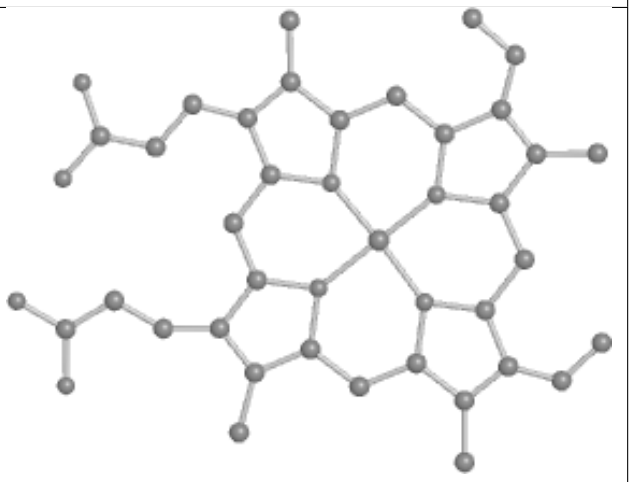
Bond lengths



Bond angles

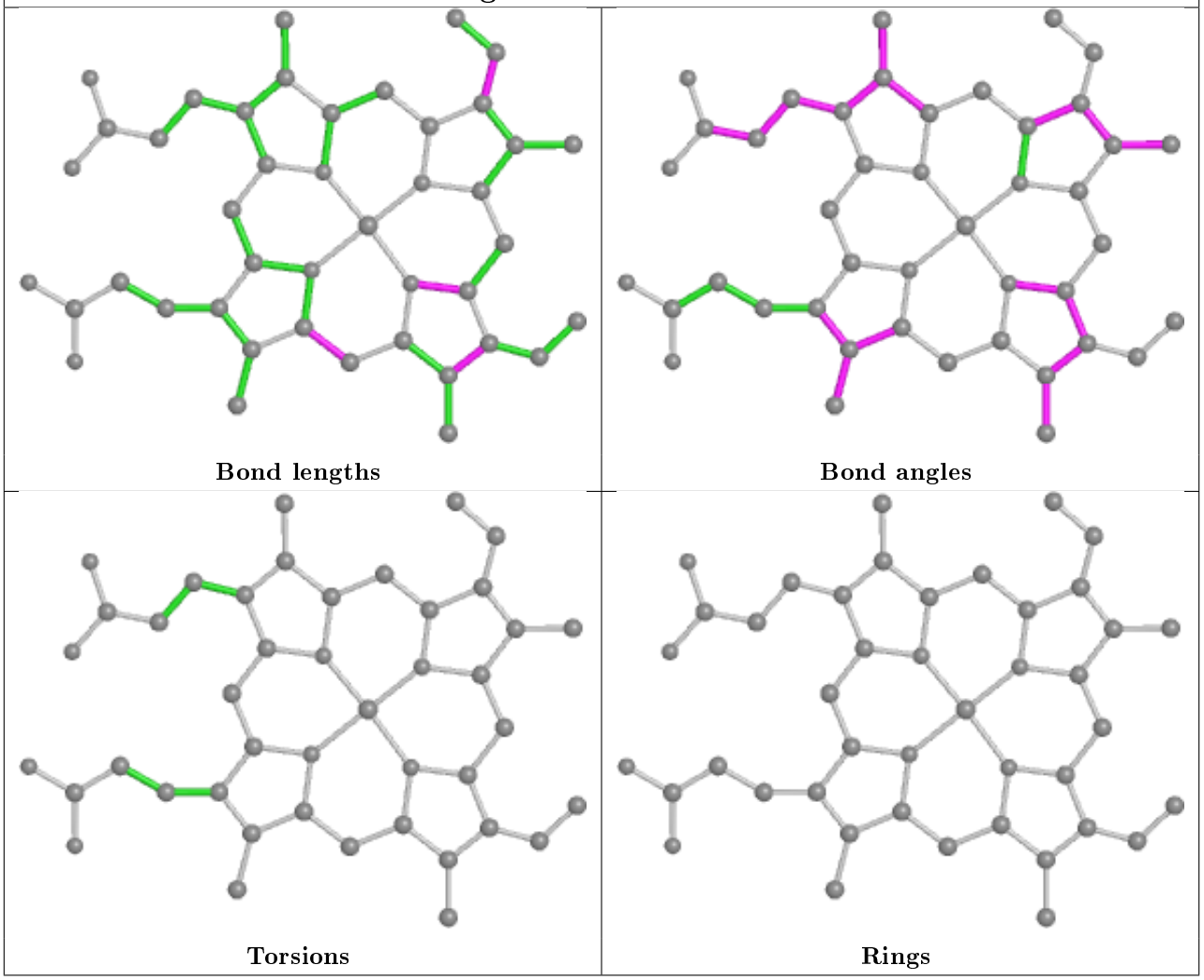


Torsions



Rings

Ligand HEM E 1291



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	243/259 (93%)	-0.07	5 (2%)	63	59	10, 21, 36, 61	1 (0%)
1	B	242/259 (93%)	0.10	9 (3%)	41	36	13, 26, 49, 71	0
1	C	243/259 (93%)	0.08	12 (4%)	29	24	15, 26, 47, 66	0
1	D	242/259 (93%)	0.09	11 (4%)	33	27	14, 26, 52, 71	0
1	E	241/259 (93%)	-0.06	1 (0%)	92	90	12, 22, 39, 48	0
1	F	243/259 (93%)	0.05	9 (3%)	41	36	12, 22, 42, 60	0
All	All	1454/1554 (93%)	0.03	47 (3%)	47	41	10, 24, 44, 71	1 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	LEU	10.4
1	D	3	ASN	8.3
1	C	249	HIS	7.5
1	D	249	HIS	5.5
1	F	249	HIS	5.4
1	F	2	LEU	5.0
1	C	2	LEU	4.9
1	A	249	HIS	4.9
1	B	3	ASN	4.9
1	F	3	ASN	4.6
1	B	4	ARG	4.4
1	A	2	LEU	4.3
1	C	3	ASN	4.3
1	D	248	ALA	3.8
1	B	29	HIS	3.5
1	D	29	HIS	3.4
1	D	4	ARG	3.3
1	C	248	ALA	3.1
1	C	247	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	239	GLY	3.0
1	B	247	PHE	2.9
1	A	29	HIS	2.9
1	C	29	HIS	2.8
1	C	30	ALA	2.8
1	F	29	HIS	2.8
1	F	5	ILE	2.8
1	D	65	LYS	2.6
1	A	50	ASN	2.6
1	D	28	HIS	2.6
1	F	4	ARG	2.6
1	B	5	ILE	2.6
1	B	242	GLY	2.5
1	F	248	ALA	2.5
1	D	49	ASN	2.5
1	F	30	ALA	2.4
1	B	7	GLU	2.4
1	C	239	GLY	2.4
1	E	3	ASN	2.4
1	B	32	ASN	2.3
1	C	4	ARG	2.3
1	F	239	GLY	2.2
1	C	246	ASN	2.2
1	D	32	ASN	2.2
1	A	248	ALA	2.2
1	C	242	GLY	2.2
1	D	7	GLU	2.1
1	C	122	ASP	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 carbohydrates 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,

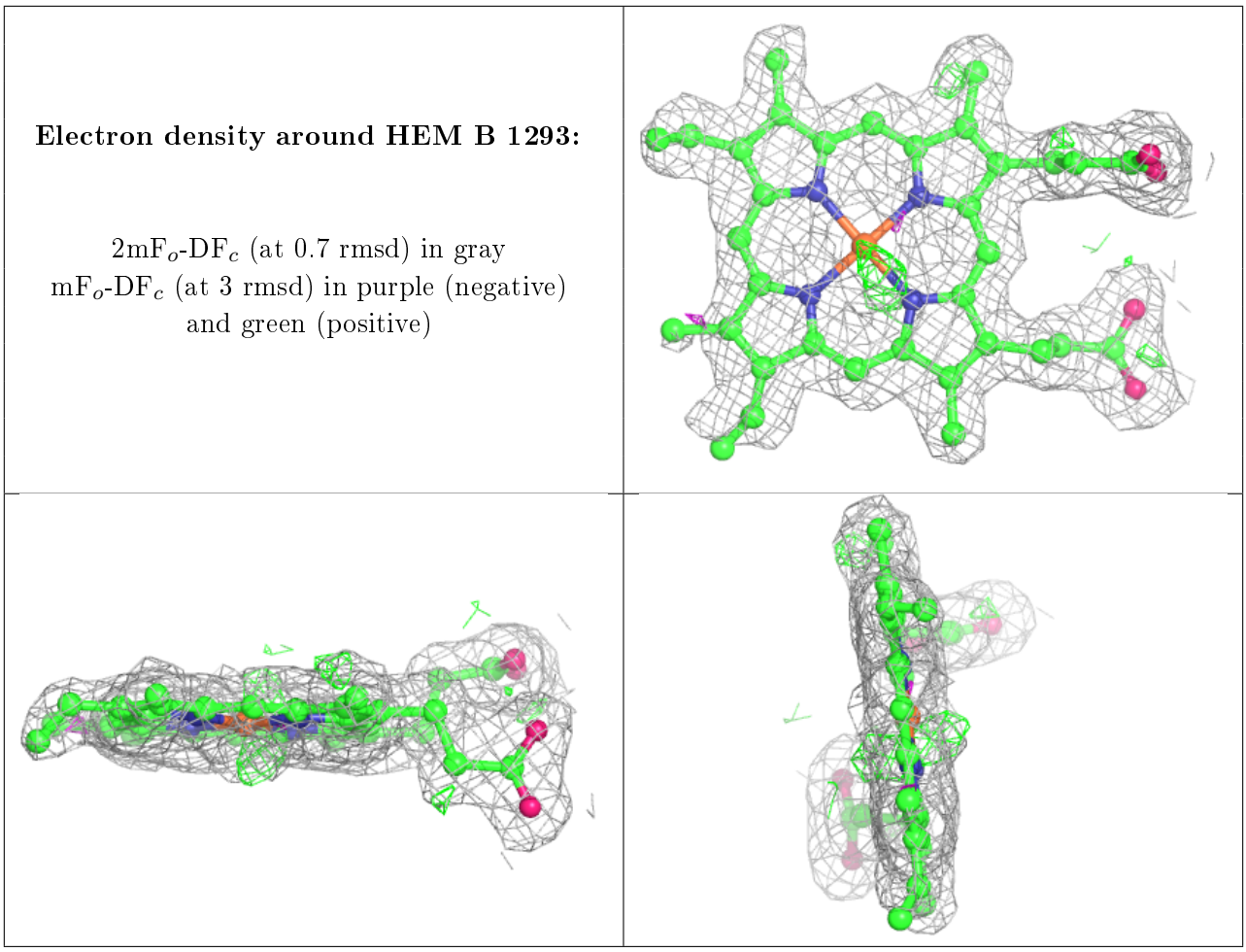
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	F	1317	4/4	0.74	0.13	45,46,46,50	0
4	EDO	B	1310	4/4	0.76	0.22	41,42,43,43	0
4	EDO	F	1314	4/4	0.80	0.33	47,48,48,50	0
4	EDO	A	1312	4/4	0.81	0.16	34,35,36,38	0
4	EDO	D	1323	4/4	0.82	0.14	37,38,39,40	0
4	EDO	F	1322	4/4	0.83	0.14	37,38,40,43	0
4	EDO	B	1316	4/4	0.84	0.12	50,51,51,52	0
4	EDO	B	1315	4/4	0.88	0.20	37,37,37,40	0
4	EDO	C	1321	4/4	0.89	0.16	34,36,39,40	0
4	EDO	D	1320	4/4	0.89	0.21	32,35,35,39	0
3	AZI	D	1300	3/3	0.89	0.13	19,19,24,31	0
4	EDO	C	1311	4/4	0.90	0.15	30,31,32,37	0
3	AZI	C	1301	3/3	0.91	0.14	26,26,33,34	0
3	AZI	A	1296	3/3	0.92	0.13	18,18,26,29	0
4	EDO	F	1318	4/4	0.93	0.15	31,33,34,35	0
3	AZI	F	1298	3/3	0.94	0.10	23,23,28,31	0
4	EDO	F	1309	4/4	0.94	0.12	23,24,24,31	0
4	EDO	B	1319	4/4	0.95	0.15	31,32,33,33	0
3	AZI	E	1297	3/3	0.95	0.12	18,18,25,28	0
4	EDO	B	1305	4/4	0.95	0.10	26,27,28,29	0
4	EDO	E	1313	4/4	0.95	0.12	33,36,38,40	0
2	HEM	B	1293	43/43	0.96	0.12	14,22,31,41	0
2	HEM	C	1295	43/43	0.96	0.11	16,24,30,32	0
3	AZI	B	1299	3/3	0.96	0.08	23,23,30,32	0
4	EDO	F	1304	4/4	0.96	0.13	16,18,18,21	0
4	EDO	A	1308	4/4	0.96	0.15	19,23,25,27	0
2	HEM	F	1292	43/43	0.97	0.12	12,20,28,34	0
2	HEM	D	1294	43/43	0.97	0.10	14,23,28,32	0
2	HEM	A	1290	43/43	0.97	0.12	11,19,24,31	0
2	HEM	E	1291	43/43	0.97	0.11	12,18,25,30	0
4	EDO	C	1307	4/4	0.98	0.10	28,29,30,32	0
4	EDO	E	1303	4/4	0.98	0.11	21,23,23,25	0
4	EDO	D	1306	4/4	0.98	0.08	24,24,25,26	0
4	EDO	A	1302	4/4	0.98	0.10	18,20,21,22	0

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.

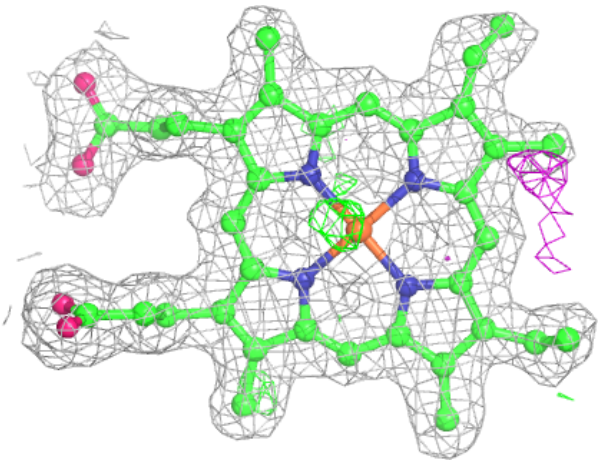
Electron density around HEM B 1293:

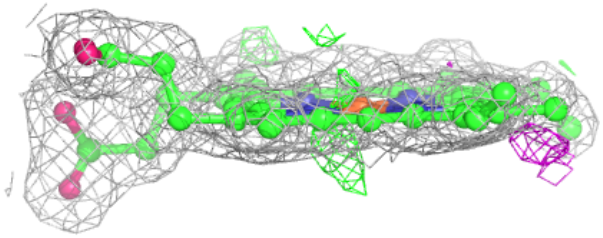
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

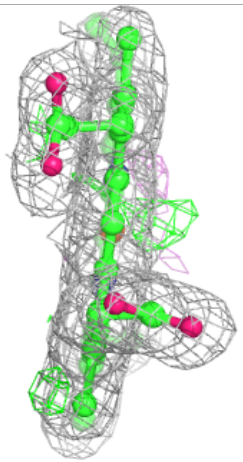


Electron density around HEM C 1295:

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

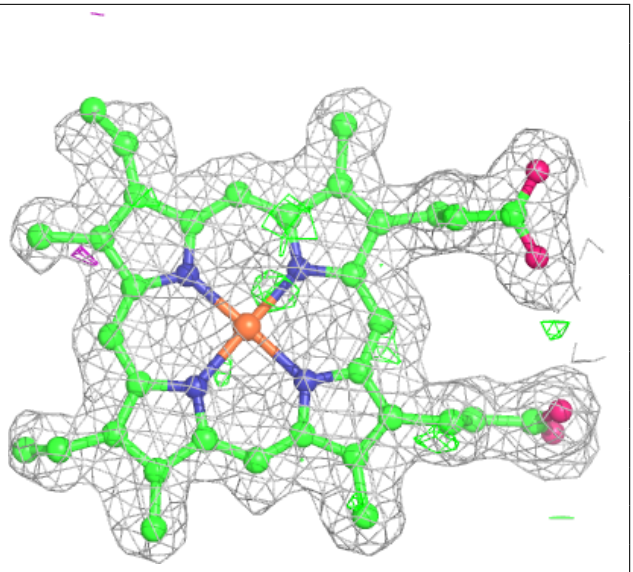


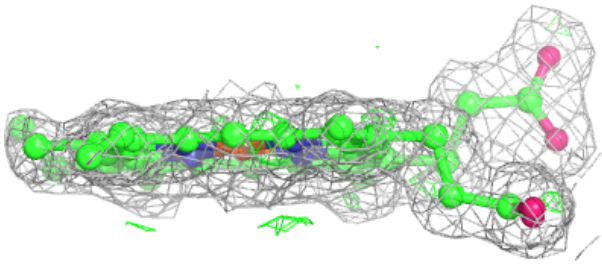


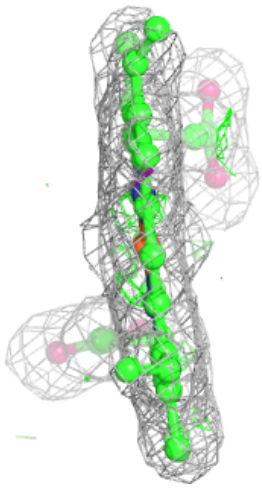


Electron density around HEM F 1292:

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

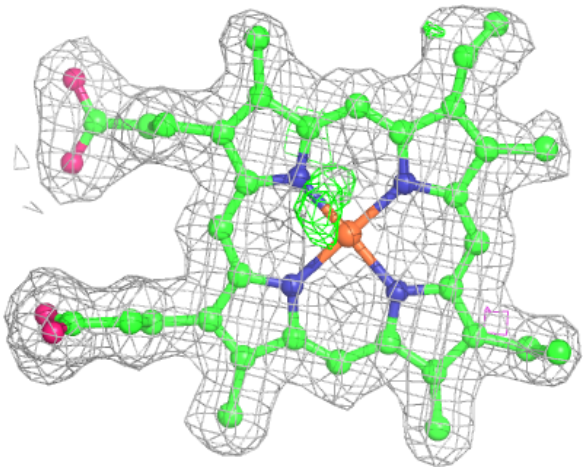


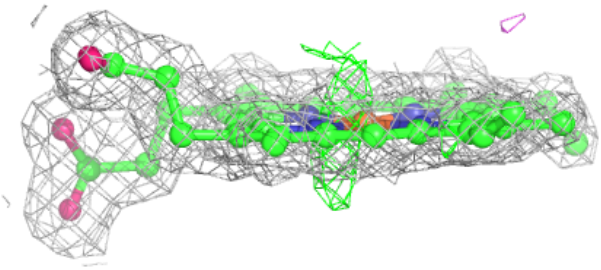


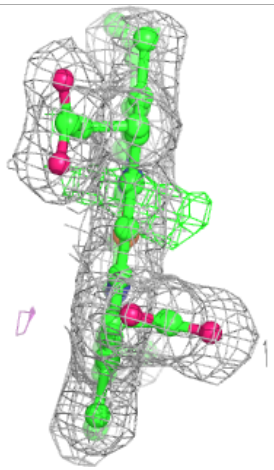


Electron density around HEM D 1294:

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

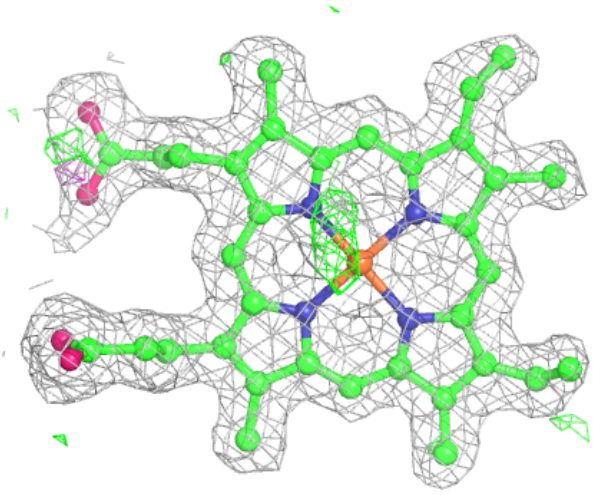


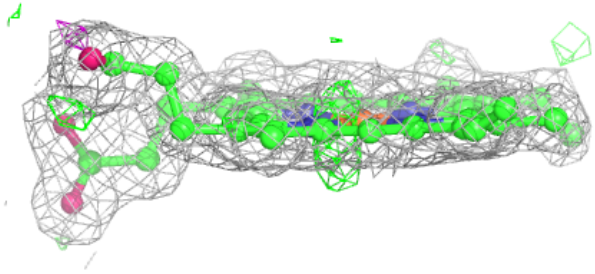


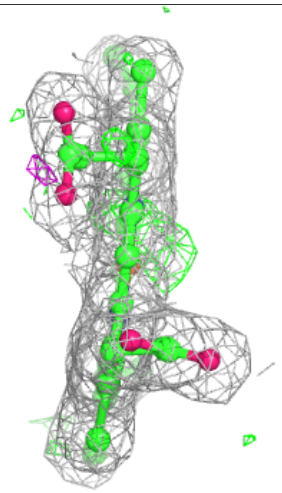


Electron density around HEM A 1290:

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

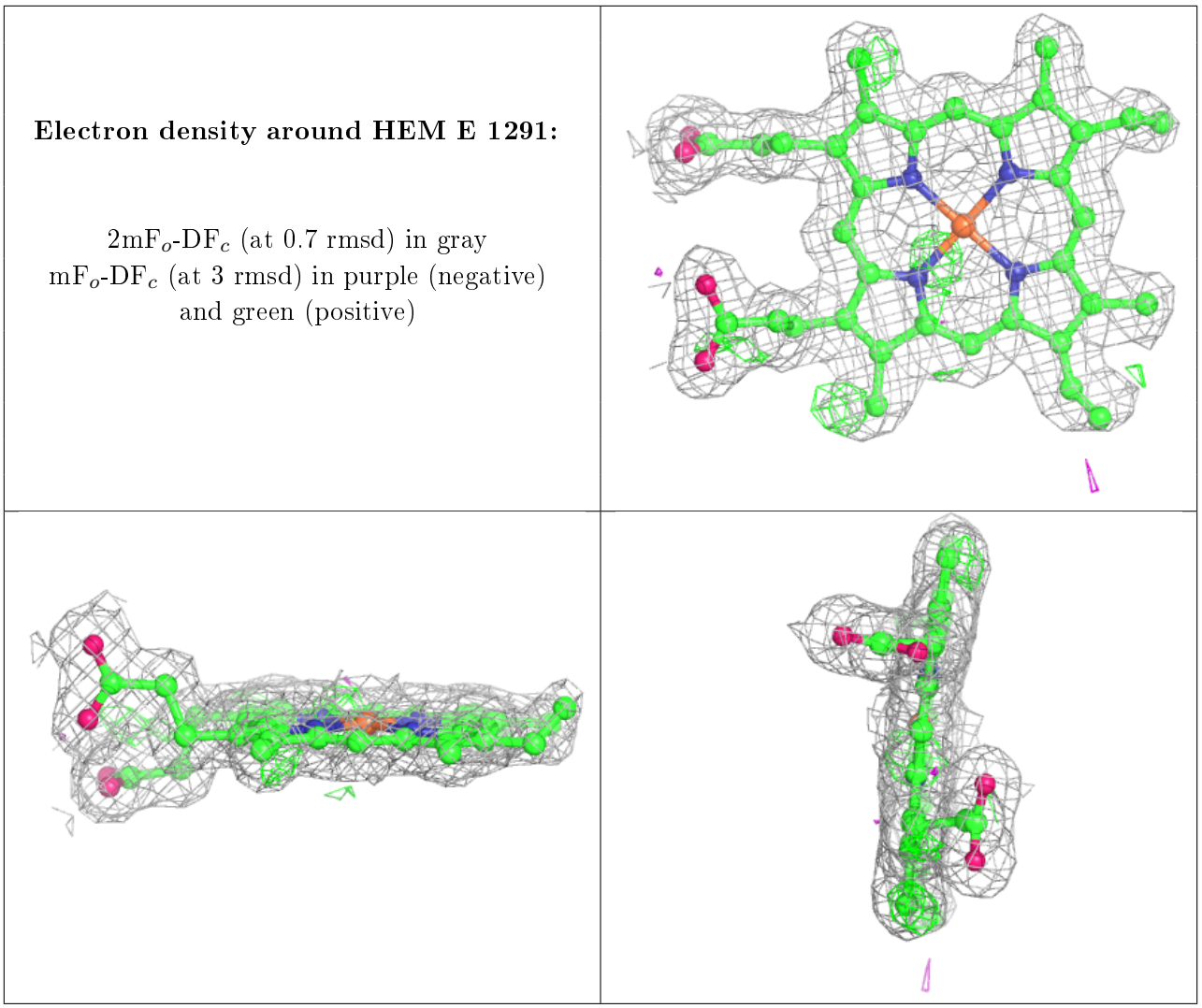






Electron density around HEM E 1291:

$2mF_o$-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.