Full wwPDB X-ray Structure Validation Report (i)

Mar 13, 2024 – 05:13 PM JST

PDB ID	:	5GT2
Title	:	Crystal Structure and Biochemical Features of dye-decolorizing peroxidase YfeX from Escherichia coli O157
Authors	:	Ma, Y.L.; Yuan, Z.G.; Liu, S.; Wang, J.X.; Gu, L.C.; Liu, X.H.
Deposited on	:	2016-08-18
Resolution	:	2.09 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 (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:

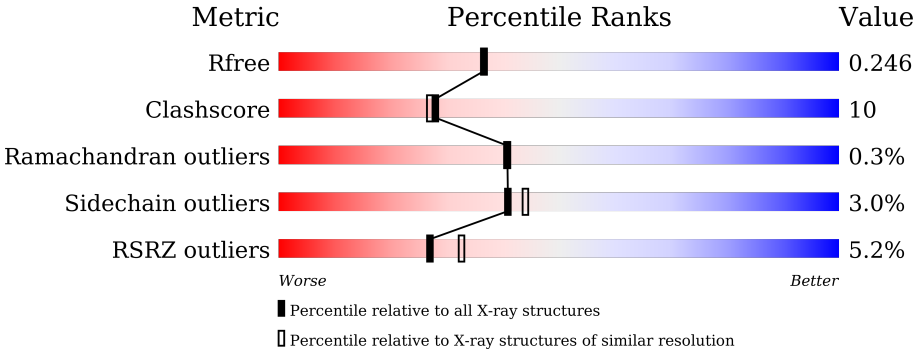
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	307	2%, 79%, 16%, • •
1	B	307	2%, 81%, 14%, • •
1	C	307	5%, 79%, 16%, • •
1	D	307	11%, 72%, 23%, • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10155 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 Probable deferrochelatase/peroxidase YfeX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2305	1448	406	440	11	0	0	0
1	B	296	2305	1448	406	440	11	0	0	0
1	C	296	2305	1448	406	440	11	0	0	0
1	D	296	2305	1448	406	440	11	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	MET	VAL	engineered mutation	UNP P76536
A	302	LEU	-	expression tag	UNP P76536
A	303	GLU	-	expression tag	UNP P76536
A	304	HIS	-	expression tag	UNP P76536
A	305	HIS	-	expression tag	UNP P76536
A	306	HIS	-	expression tag	UNP P76536
A	307	HIS	-	expression tag	UNP P76536
A	308	HIS	-	expression tag	UNP P76536
A	309	HIS	-	expression tag	UNP P76536
B	195	MET	VAL	engineered mutation	UNP P76536
B	302	LEU	-	expression tag	UNP P76536
B	303	GLU	-	expression tag	UNP P76536
B	304	HIS	-	expression tag	UNP P76536
B	305	HIS	-	expression tag	UNP P76536
B	306	HIS	-	expression tag	UNP P76536
B	307	HIS	-	expression tag	UNP P76536
B	308	HIS	-	expression tag	UNP P76536
B	309	HIS	-	expression tag	UNP P76536
C	195	MET	VAL	engineered mutation	UNP P76536
C	302	LEU	-	expression tag	UNP P76536
C	303	GLU	-	expression tag	UNP P76536

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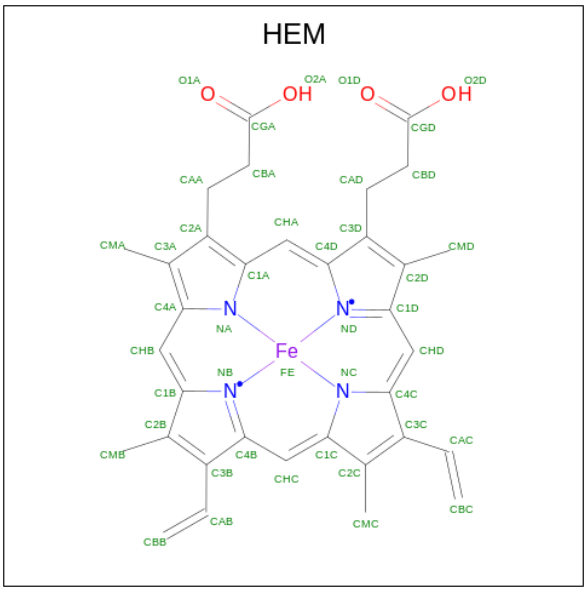
Chain	Residue	Modelled	Actual	Comment	Reference
C	304	HIS	-	expression tag	UNP P76536
C	305	HIS	-	expression tag	UNP P76536
C	306	HIS	-	expression tag	UNP P76536
C	307	HIS	-	expression tag	UNP P76536
C	308	HIS	-	expression tag	UNP P76536
C	309	HIS	-	expression tag	UNP P76536
D	195	MET	VAL	engineered mutation	UNP P76536
D	302	LEU	-	expression tag	UNP P76536
D	303	GLU	-	expression tag	UNP P76536
D	304	HIS	-	expression tag	UNP P76536
D	305	HIS	-	expression tag	UNP P76536
D	306	HIS	-	expression tag	UNP P76536
D	307	HIS	-	expression tag	UNP P76536
D	308	HIS	-	expression tag	UNP P76536
D	309	HIS	-	expression tag	UNP P76536

- 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
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0

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

- Molecule 3 is water.

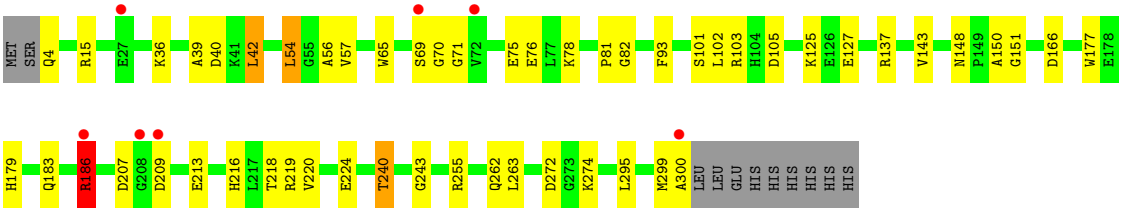
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	218	218	218	0	0
			Total	O		
3	B	198	198	198	0	0
			Total	O		
3	C	200	200	200	0	0
			Total	O		
3	D	147	147	147	0	0

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 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.

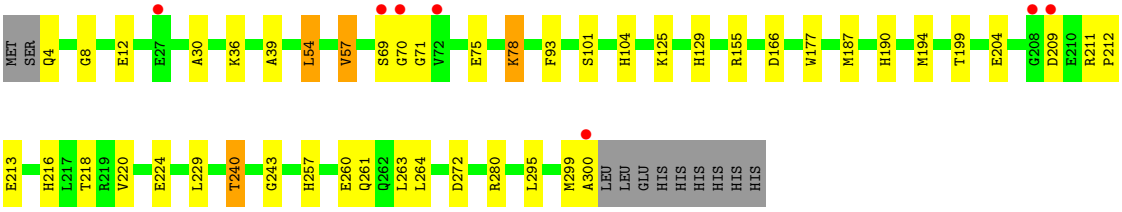
• Molecule 1: Probable deferrochelatase/peroxidase YfeX

Chain A:



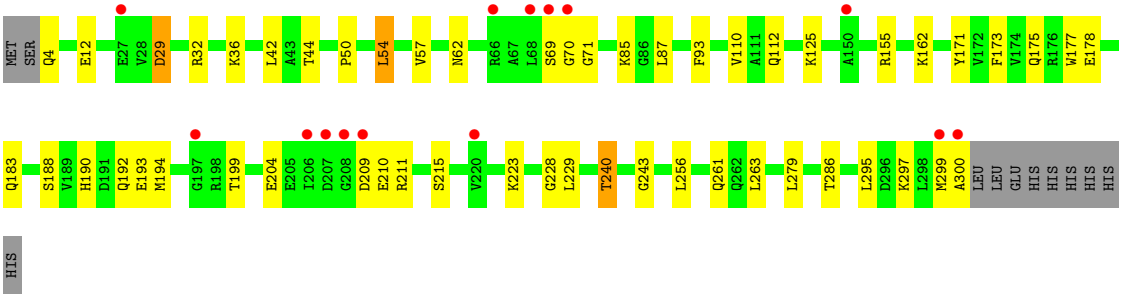
• Molecule 1: Probable deferrochelatase/peroxidase YfeX

Chain B:



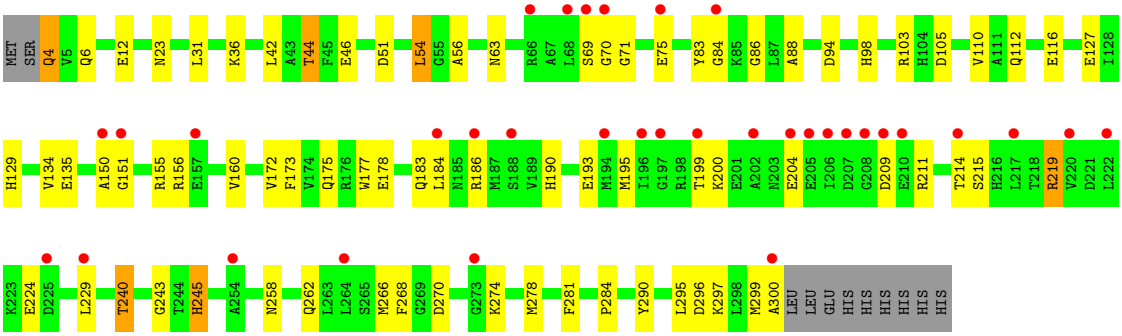
• Molecule 1: Probable deferrochelatase/peroxidase YfeX

Chain C:



• Molecule 1: Probable deferrochelatase/peroxidase YfeX

Chain D:


MET SER Q4 V5 Q6 E12 N23 L31 K36 L42 A43 T44 F45 E46 D51 L54 G55 A56 N63 R66 A67 L68 S69 G70 G71 E75 Y83 G84 K85 G86 L87 A88 D94 H98 R103 H104 D105 V110 A111 Q112 E116 E127 I128
H129 V134 E135 A150 G151 R155 R156 E157 V160 V172 F173 V174 Q175 R176 W177 E178 Q183 L184 N185 R186 M187 S188 V189 H190 E193 M194 M195 I196 G197 R198 T199 K200 E201 A202 N203 E204 E205 I206 D207 G208 D209 E210 R211 T214 S215 H216 L217 T218 R219 V220 D221 L222
K223 E224 D225 L229 T240 G243 T244 H245 A254 N258 Q262 L263 L264 S265 M266 F268 G269 D270 G273 K274 M278 F281 P284 Y290 L295 D296 K297 L298 M299 A300 LEU LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	121.57Å 101.60Å 114.30Å 90.00° 111.51° 90.00°	Depositor
Resolution (Å)	36.69 – 2.09 45.84 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.7 (36.69-2.09) 92.5 (45.84-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.61 (at 2.10Å)	Xtriage
Refinement program	PHENIX (dev_2411: ???)	Depositor
R, R_{free}	0.220 , 0.248 0.217 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.822	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10155	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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

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	0.32	0/2353	0.53	1/3176 (0.0%)
1	B	0.30	0/2353	0.49	0/3176
1	C	0.29	0/2353	0.49	0/3176
1	D	0.33	0/2353	0.51	0/3176
All	All	0.31	0/9412	0.51	1/12704 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	ARG	NE-CZ-NH2	-5.97	117.32	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	2305	0	2233	44	0
1	B	2305	0	2233	37	1
1	C	2305	0	2233	41	0
1	D	2305	0	2233	52	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	3	0
2	D	43	0	30	5	0
3	A	218	0	0	11	1
3	B	198	0	0	14	0
3	C	200	0	0	13	0
3	D	147	0	0	13	2
All	All	10155	0	9052	183	2

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 10.

All (183) 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:B:199:THR:HG22	1:B:204:GLU:H	1.27	0.94
1:A:224:GLU:OE1	3:A:501:HOH:O	1.84	0.94
1:C:112:GLN:OE1	3:C:501:HOH:O	1.85	0.94
1:B:240:THR:HG22	1:B:243:GLY:H	1.32	0.91
1:A:240:THR:HG22	1:A:243:GLY:H	1.36	0.91
1:B:229:LEU:O	3:B:501:HOH:O	1.91	0.88
1:D:86:GLY:O	3:D:501:HOH:O	1.94	0.84
1:C:261:GLN:NE2	3:C:502:HOH:O	2.03	0.83
1:A:186:ARG:HA	1:A:186:ARG:HE	1.42	0.83
1:A:4:GLN:N	3:A:502:HOH:O	2.13	0.82
1:A:69:SER:HB3	1:A:70:GLY:HA2	1.62	0.82
1:C:240:THR:HG22	1:C:243:GLY:H	1.45	0.80
1:A:219:ARG:NH1	3:A:503:HOH:O	2.13	0.79
1:C:36:LYS:NZ	3:C:506:HOH:O	2.15	0.79
1:B:166:ASP:OD1	3:B:503:HOH:O	2.01	0.77
2:D:401:HEM:O1D	3:D:503:HOH:O	2.02	0.77
1:B:69:SER:HB3	1:B:70:GLY:HA2	1.68	0.74
1:D:299:MET:SD	3:D:639:HOH:O	2.46	0.73
1:B:204:GLU:OE1	3:B:504:HOH:O	2.06	0.72
1:D:270:ASP:OD2	3:D:504:HOH:O	2.09	0.71
1:C:178:GLU:OE2	3:C:503:HOH:O	2.08	0.70
1:A:183:GLN:HA	1:A:186:ARG:HG2	1.73	0.70
1:B:224:GLU:OE2	3:B:506:HOH:O	2.10	0.69
1:B:69:SER:HB3	1:B:71:GLY:HA2	1.75	0.69
1:D:178:GLU:OE2	3:D:505:HOH:O	2.13	0.66
1:C:69:SER:OG	1:C:70:GLY:HA2	1.96	0.66
2:B:401:HEM:O2D	3:B:507:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASP:OD2	3:A:504:HOH:O	2.13	0.66
1:B:261:GLN:NE2	3:B:505:HOH:O	2.09	0.65
1:C:193:GLU:OE2	3:C:505:HOH:O	2.14	0.65
1:A:4:GLN:O	1:A:295:LEU:N	2.29	0.65
1:D:56:ALA:O	3:D:506:HOH:O	2.14	0.64
1:C:87:LEU:HD21	1:C:279:LEU:HD13	1.78	0.64
1:D:224:GLU:HB2	1:D:229:LEU:HD11	1.81	0.63
1:B:12:GLU:O	3:B:508:HOH:O	2.15	0.62
1:B:36:LYS:HA	1:B:300:ALA:HB2	1.82	0.61
1:C:229:LEU:O	3:C:507:HOH:O	2.16	0.61
1:D:199:THR:HG22	1:D:204:GLU:H	1.66	0.60
1:A:186:ARG:HE	1:A:186:ARG:CA	2.12	0.59
1:D:229:LEU:HD23	1:D:258:ASN:HA	1.86	0.58
1:A:78:LYS:NZ	3:A:514:HOH:O	2.36	0.57
1:D:44:THR:HG21	3:D:633:HOH:O	2.04	0.57
1:A:240:THR:HG22	1:A:243:GLY:N	2.15	0.57
2:A:401:HEM:HBB2	2:A:401:HEM:HMB2	1.85	0.57
1:A:224:GLU:OE2	3:A:505:HOH:O	2.18	0.57
1:A:186:ARG:HG3	3:A:543:HOH:O	2.06	0.56
1:D:219:ARG:NH1	1:D:274:LYS:HB3	2.21	0.56
1:B:54:LEU:HD23	1:B:101:SER:HB3	1.89	0.55
1:B:30:ALA:O	3:B:509:HOH:O	2.18	0.55
1:C:29:ASP:O	3:C:509:HOH:O	2.18	0.55
1:A:69:SER:HB3	1:A:71:GLY:HA2	1.88	0.54
1:C:4:GLN:NE2	3:C:517:HOH:O	2.39	0.54
1:B:104:HIS:HD2	3:B:578:HOH:O	1.89	0.54
1:A:255:ARG:NE	3:A:516:HOH:O	2.39	0.54
1:C:240:THR:HG22	1:C:243:GLY:N	2.20	0.54
1:A:148:ASN:ND2	3:A:518:HOH:O	2.41	0.54
2:D:401:HEM:HBC2	2:D:401:HEM:HMC1	1.90	0.53
1:D:54:LEU:HD11	1:D:110:VAL:HG21	1.89	0.53
1:D:199:THR:CG2	1:D:204:GLU:H	2.20	0.53
1:D:183:GLN:HA	1:D:186:ARG:HH11	1.72	0.53
1:A:219:ARG:CZ	3:A:503:HOH:O	2.54	0.53
1:C:297:LYS:C	1:C:299:MET:H	2.09	0.53
2:D:401:HEM:HMB1	2:D:401:HEM:HBB2	1.92	0.52
1:B:299:MET:HB2	3:B:533:HOH:O	2.09	0.52
1:D:297:LYS:C	1:D:299:MET:H	2.13	0.52
1:D:6:GLN:O	3:D:507:HOH:O	2.19	0.52
1:A:127:GLU:CD	1:C:240:THR:HG23	2.30	0.51
1:C:193:GLU:HG2	1:C:199:THR:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD23	1:A:101:SER:HB3	1.92	0.51
1:C:36:LYS:HG3	1:C:300:ALA:HB2	1.92	0.51
1:C:54:LEU:HD11	1:C:110:VAL:HG21	1.92	0.51
1:C:85:LYS:NZ	3:C:504:HOH:O	2.14	0.51
1:C:211:ARG:HD3	1:C:215:SER:OG	2.11	0.51
1:D:172:VAL:HG13	1:D:290:TYR:HB2	1.93	0.51
1:A:36:LYS:HE2	1:A:299:MET:O	2.11	0.50
1:A:166:ASP:OD1	3:A:506:HOH:O	2.19	0.50
1:B:190:HIS:O	1:B:194:MET:HG2	2.11	0.50
1:C:223:LYS:HA	1:C:228:GLY:HA2	1.94	0.50
1:D:63:ASN:OD1	3:D:508:HOH:O	2.19	0.50
1:C:183:GLN:HG3	3:C:616:HOH:O	2.11	0.50
1:C:199:THR:CG2	1:C:204:GLU:H	2.25	0.49
1:C:190:HIS:O	1:C:194:MET:HG2	2.11	0.49
1:B:213:GLU:HA	1:B:218:THR:HG21	1.93	0.49
1:A:36:LYS:HA	1:A:300:ALA:HB2	1.94	0.49
1:A:39:ALA:HB3	1:A:300:ALA:HB1	1.93	0.49
1:A:75:GLU:HG3	1:A:76:GLU:N	2.26	0.49
1:D:4:GLN:O	1:D:295:LEU:N	2.42	0.49
1:C:62:ASN:N	3:C:519:HOH:O	2.43	0.49
1:A:183:GLN:HA	1:A:186:ARG:CG	2.42	0.48
1:D:69:SER:HB2	1:D:70:GLY:HA2	1.94	0.48
1:B:78:LYS:NZ	3:B:502:HOH:O	1.95	0.48
1:B:199:THR:HG21	3:B:504:HOH:O	2.14	0.48
1:B:272:ASP:OD2	1:B:272:ASP:N	2.45	0.48
1:A:216:HIS:O	1:A:220:VAL:HG22	2.14	0.47
1:B:129:HIS:HB3	3:B:657:HOH:O	2.14	0.47
1:D:177:TRP:CG	2:D:401:HEM:HBB1	2.49	0.47
1:B:39:ALA:HB3	1:B:300:ALA:HB1	1.96	0.47
2:C:401:HEM:HMB1	2:C:401:HEM:HBB2	1.96	0.47
1:C:93:PHE:CZ	1:C:125:LYS:HD2	2.50	0.47
1:B:240:THR:HG22	1:B:243:GLY:N	2.14	0.47
1:D:262:GLN:O	1:D:266:MET:HG3	2.15	0.47
1:B:224:GLU:OE2	1:B:257:HIS:NE2	2.34	0.47
1:B:194:MET:CE	1:B:212:PRO:HD3	2.45	0.46
1:D:23:ASN:HA	1:D:94:ASP:HB2	1.97	0.46
1:D:112:GLN:OE1	3:D:510:HOH:O	2.21	0.46
1:B:75:GLU:HG2	3:B:545:HOH:O	2.15	0.46
1:D:129:HIS:HB3	3:D:611:HOH:O	2.15	0.46
1:C:4:GLN:O	1:C:295:LEU:N	2.46	0.45
1:C:171:TYR:HB3	1:C:256:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:GLU:HG2	1:D:54:LEU:HB3	1.98	0.45
1:D:69:SER:CB	1:D:70:GLY:HA2	2.47	0.45
1:A:36:LYS:HD2	1:A:40:ASP:OD2	2.17	0.45
1:A:70:GLY:HA2	1:A:71:GLY:HA2	1.59	0.45
1:D:184:LEU:HB2	1:D:281:PHE:CD2	2.52	0.45
1:D:245:HIS:HE1	3:D:524:HOH:O	1.99	0.45
1:A:137:ARG:HA	1:A:143:VAL:HA	1.99	0.45
2:C:401:HEM:HMC2	2:C:401:HEM:HBC2	1.98	0.45
1:A:81:PRO:HB2	1:A:82:GLY:O	2.15	0.45
1:B:70:GLY:HA2	1:B:71:GLY:HA2	1.61	0.45
1:C:70:GLY:HA2	1:C:71:GLY:HA2	1.59	0.45
1:D:214:THR:HG23	1:D:274:LYS:HE3	1.98	0.45
1:A:127:GLU:OE1	1:C:240:THR:HG23	2.15	0.45
2:B:401:HEM:HBC2	2:B:401:HEM:HMC2	1.99	0.45
2:B:401:HEM:HMB1	2:B:401:HEM:HBB2	1.99	0.45
1:D:70:GLY:HA2	1:D:71:GLY:HA2	1.58	0.45
1:C:50:PRO:HG3	3:C:572:HOH:O	2.16	0.45
1:D:150:ALA:HA	1:D:151:GLY:HA2	1.66	0.45
1:D:88:ALA:HB2	1:D:268:PHE:CE1	2.53	0.44
1:B:260:GLU:O	1:B:264:LEU:HD23	2.16	0.44
1:D:173:PHE:CZ	1:D:175:GLN:HB2	2.53	0.44
1:C:32:ARG:NH1	1:C:299:MET:SD	2.90	0.44
1:D:103:ARG:HB3	1:D:105:ASP:OD1	2.18	0.44
1:D:112:GLN:O	1:D:116:GLU:HG2	2.16	0.44
1:D:190:HIS:O	1:D:193:GLU:HB2	2.18	0.44
1:A:213:GLU:HA	1:A:218:THR:HG21	2.00	0.44
1:B:4:GLN:O	1:B:295:LEU:N	2.48	0.44
1:D:240:THR:CG2	1:D:243:GLY:H	2.31	0.44
1:A:103:ARG:HB3	1:A:105:ASP:OD1	2.17	0.44
1:B:194:MET:HE3	1:B:211:ARG:HA	1.98	0.44
1:C:173:PHE:CZ	1:C:175:GLN:HB2	2.53	0.44
1:B:216:HIS:O	1:B:220:VAL:HG22	2.18	0.43
1:D:177:TRP:CD2	2:D:401:HEM:HBB1	2.53	0.43
1:B:187:MET:SD	1:B:280:ARG:HD3	2.57	0.43
1:D:195:MET:SD	1:D:278:MET:HA	2.59	0.43
1:A:42:LEU:HD11	1:A:56:ALA:HB3	2.00	0.43
2:A:401:HEM:HMC2	2:A:401:HEM:HBC2	2.01	0.43
1:D:215:SER:O	1:D:219:ARG:HG2	2.18	0.43
1:D:134:VAL:HG12	1:D:135:GLU:HG3	2.00	0.43
1:B:93:PHE:CE1	1:B:125:LYS:HG3	2.53	0.43
1:D:84:GLY:O	3:D:509:HOH:O	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:TRP:CZ3	1:D:284:PRO:HD3	2.53	0.43
1:A:177:TRP:CD2	2:A:401:HEM:HBB1	2.54	0.43
1:D:12:GLU:HG2	1:D:155:ARG:CZ	2.49	0.43
1:B:12:GLU:HG2	1:B:155:ARG:CZ	2.48	0.43
1:C:69:SER:OG	1:C:71:GLY:HA2	2.18	0.43
1:B:240:THR:HG23	1:D:127:GLU:OE1	2.19	0.43
1:C:175:GLN:HG3	1:C:286:THR:O	2.19	0.43
1:D:83:TYR:HB2	1:D:88:ALA:HB3	2.01	0.43
1:A:150:ALA:HA	1:A:151:GLY:HA2	1.72	0.42
1:D:36:LYS:HG3	1:D:300:ALA:HB2	2.01	0.42
2:A:401:HEM:HBB2	2:A:401:HEM:CMB	2.49	0.42
1:D:156:ARG:O	1:D:160:VAL:HG12	2.19	0.42
1:A:272:ASP:HB3	1:A:274:LYS:HG3	2.02	0.42
1:A:15:ARG:HD2	1:A:102:LEU:O	2.20	0.42
1:C:188:SER:O	1:C:192:GLN:HG3	2.20	0.41
1:A:93:PHE:CE1	1:A:125:LYS:HG3	2.55	0.41
1:C:177:TRP:CD2	2:C:401:HEM:HBB1	2.56	0.41
1:C:12:GLU:HG2	1:C:155:ARG:CZ	2.51	0.41
1:C:297:LYS:C	1:C:299:MET:N	2.73	0.41
1:A:65:TRP:O	1:A:69:SER:HB2	2.21	0.41
1:A:65:TRP:O	1:A:69:SER:N	2.53	0.41
1:D:211:ARG:HD3	1:D:215:SER:OG	2.20	0.41
1:A:262:GLN:OE1	2:A:401:HEM:HAC	2.20	0.41
1:B:177:TRP:CD2	2:B:401:HEM:HBB1	2.56	0.41
1:D:56:ALA:HA	1:D:98:HIS:O	2.21	0.41
1:D:75:GLU:H	1:D:75:GLU:CD	2.24	0.41
1:A:186:ARG:HA	1:A:186:ARG:NE	2.22	0.41
2:B:401:HEM:HBB2	2:B:401:HEM:CMB	2.51	0.41
1:D:4:GLN:HA	1:D:296:ASP:OD2	2.21	0.41
1:C:87:LEU:HD21	1:C:279:LEU:CD1	2.47	0.40
1:B:8:GLY:HA3	1:B:57:VAL:HG12	2.04	0.40
1:C:162:LYS:NZ	3:C:529:HOH:O	2.50	0.40
1:C:209:ASP:OD2	1:C:210:GLU:HG3	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:GLN:NE2	3:D:501:HOH:O[4_555]	2.11	0.09
3:A:605:HOH:O	3:D:642:HOH:O[4_556]	2.17	0.03

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	294/307 (96%)	280 (95%)	13 (4%)	1 (0%)	41	41
1	B	294/307 (96%)	284 (97%)	9 (3%)	1 (0%)	41	41
1	C	294/307 (96%)	280 (95%)	14 (5%)	0	100	100
1	D	294/307 (96%)	276 (94%)	16 (5%)	2 (1%)	22	18
All	All	1176/1228 (96%)	1120 (95%)	52 (4%)	4 (0%)	41	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	209	ASP
1	A	209	ASP
1	B	209	ASP
1	D	200	LYS

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	238/249 (96%)	230 (97%)	8 (3%)	37	39
1	B	238/249 (96%)	233 (98%)	5 (2%)	53	59
1	C	238/249 (96%)	231 (97%)	7 (3%)	42	46
1	D	238/249 (96%)	229 (96%)	9 (4%)	33	34
All	All	952/996 (96%)	923 (97%)	29 (3%)	41	44

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	54	LEU
1	A	57	VAL
1	A	179	HIS
1	A	186	ARG
1	A	207	ASP
1	A	240	THR
1	A	263	LEU
1	B	54	LEU
1	B	57	VAL
1	B	78	LYS
1	B	240	THR
1	B	263	LEU
1	C	29	ASP
1	C	42	LEU
1	C	44	THR
1	C	54	LEU
1	C	57	VAL
1	C	240	THR
1	C	263	LEU
1	D	4	GLN
1	D	31	LEU
1	D	42	LEU
1	D	44	THR
1	D	51	ASP
1	D	54	LEU
1	D	219	ARG
1	D	240	THR
1	D	245	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

4 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	401	1	41,50,50	1.44	4 (9%)	45,82,82	1.40	6 (13%)
2	HEM	C	401	1	41,50,50	1.49	6 (14%)	45,82,82	1.45	6 (13%)
2	HEM	D	401	1	41,50,50	1.46	6 (14%)	45,82,82	1.42	6 (13%)
2	HEM	B	401	1,3	41,50,50	1.48	5 (12%)	45,82,82	1.39	6 (13%)

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	401	1	-	4/12/54/54	-
2	HEM	C	401	1	-	4/12/54/54	-
2	HEM	D	401	1	-	4/12/54/54	-
2	HEM	B	401	1,3	-	4/12/54/54	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	C3C-CAC	3.83	1.55	1.47
2	D	401	HEM	C3C-CAC	3.83	1.55	1.47
2	C	401	HEM	C3C-CAC	3.77	1.55	1.47
2	A	401	HEM	C3C-C2C	-3.76	1.35	1.40
2	B	401	HEM	C3C-C2C	-3.75	1.35	1.40
2	C	401	HEM	C3C-C2C	-3.71	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	C3C-CAC	3.64	1.55	1.47
2	D	401	HEM	C3C-C2C	-3.54	1.35	1.40
2	D	401	HEM	CAB-C3B	2.95	1.55	1.47
2	C	401	HEM	CAB-C3B	2.86	1.55	1.47
2	A	401	HEM	CAB-C3B	2.71	1.54	1.47
2	B	401	HEM	CAB-C3B	2.68	1.54	1.47
2	A	401	HEM	CMB-C2B	2.30	1.55	1.50
2	B	401	HEM	CMB-C2B	2.27	1.55	1.50
2	C	401	HEM	FE-NB	2.23	2.07	1.96
2	B	401	HEM	CAA-C2A	2.13	1.55	1.52
2	C	401	HEM	CMB-C2B	2.11	1.55	1.50
2	D	401	HEM	CMB-C2B	2.11	1.55	1.50
2	D	401	HEM	FE-ND	2.06	2.07	1.96
2	D	401	HEM	CMD-C2D	2.02	1.55	1.50
2	C	401	HEM	CMD-C2D	2.01	1.55	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	HEM	C1B-NB-C4B	3.43	108.61	105.07
2	B	401	HEM	C4B-CHC-C1C	3.28	126.89	122.56
2	C	401	HEM	C4C-CHD-C1D	3.14	126.70	122.56
2	C	401	HEM	C1B-NB-C4B	3.14	108.31	105.07
2	A	401	HEM	C1B-NB-C4B	3.10	108.27	105.07
2	D	401	HEM	C4C-CHD-C1D	2.99	126.50	122.56
2	D	401	HEM	C4D-ND-C1D	2.98	108.15	105.07
2	C	401	HEM	C4D-ND-C1D	2.89	108.06	105.07
2	C	401	HEM	C4B-CHC-C1C	2.88	126.36	122.56
2	A	401	HEM	C4C-CHD-C1D	2.83	126.29	122.56
2	D	401	HEM	C4B-CHC-C1C	2.68	126.10	122.56
2	D	401	HEM	C1B-NB-C4B	2.64	107.80	105.07
2	A	401	HEM	C4B-CHC-C1C	2.64	126.04	122.56
2	B	401	HEM	C4C-CHD-C1D	2.58	125.97	122.56
2	A	401	HEM	C4D-ND-C1D	2.49	107.64	105.07
2	B	401	HEM	C4D-ND-C1D	2.35	107.50	105.07
2	D	401	HEM	CMC-C2C-C3C	2.28	128.95	124.68
2	B	401	HEM	CMA-C3A-C4A	-2.28	124.97	128.46
2	D	401	HEM	CMA-C3A-C4A	-2.27	124.97	128.46
2	A	401	HEM	CHD-C1D-ND	2.20	126.82	124.43
2	A	401	HEM	CMA-C3A-C4A	-2.15	125.16	128.46
2	C	401	HEM	CAD-CBD-CGD	-2.08	109.13	113.60
2	B	401	HEM	CHD-C1D-ND	2.06	126.67	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	HEM	CMA-C3A-C4A	-2.03	125.35	128.46

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAD-CBD-CGD-O2D
2	A	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAD-CBD-CGD-O1D
2	B	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAD-CBD-CGD-O2D
2	A	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAD-CBD-CGD-O1D
2	A	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

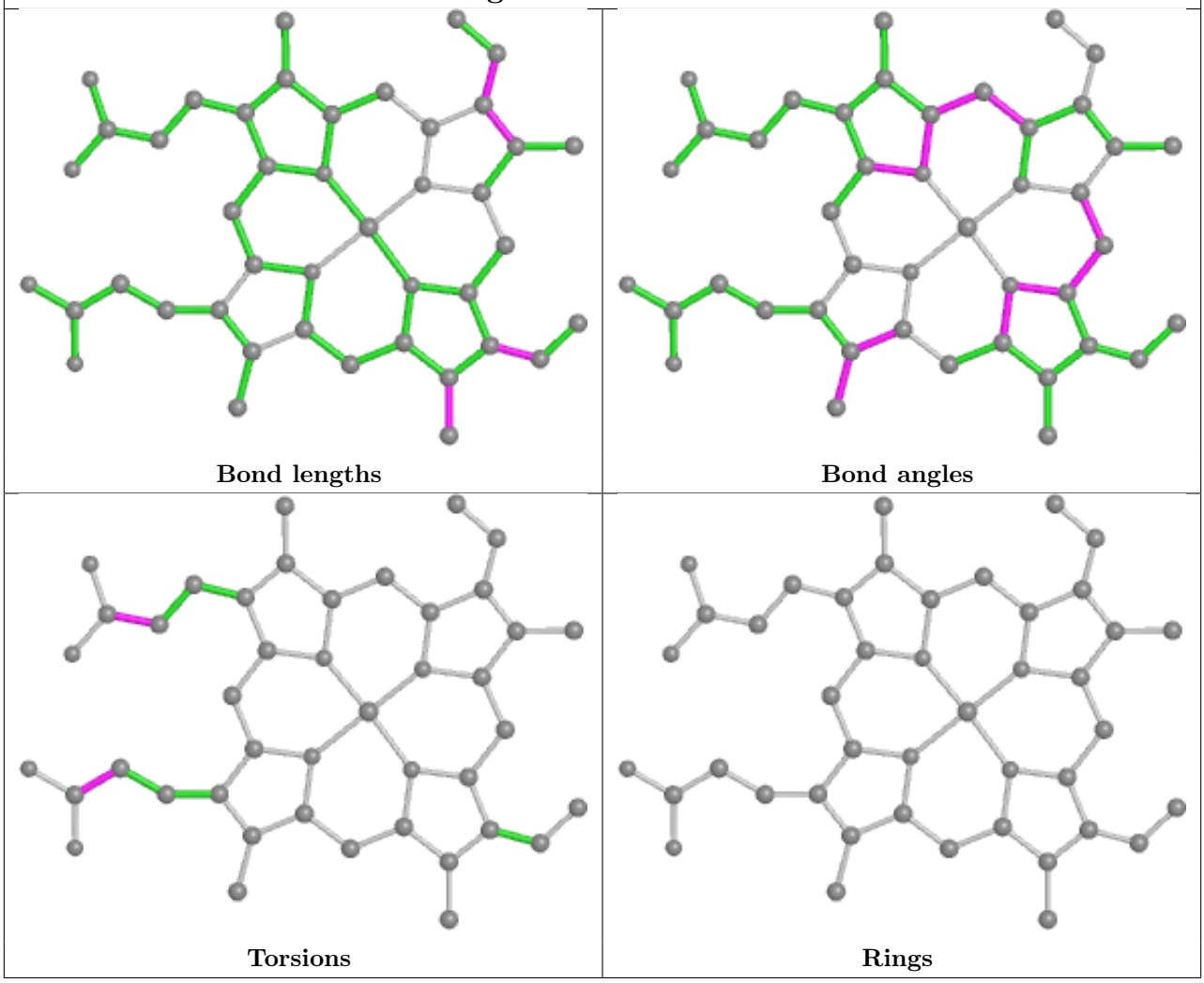
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	5	0
2	C	401	HEM	3	0
2	D	401	HEM	5	0
2	B	401	HEM	5	0

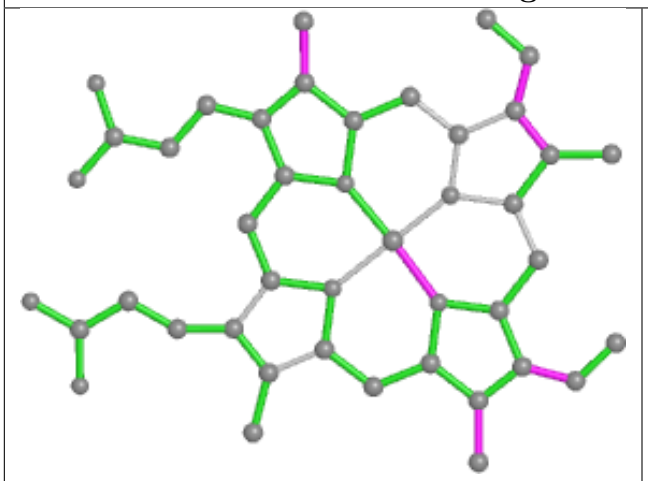
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

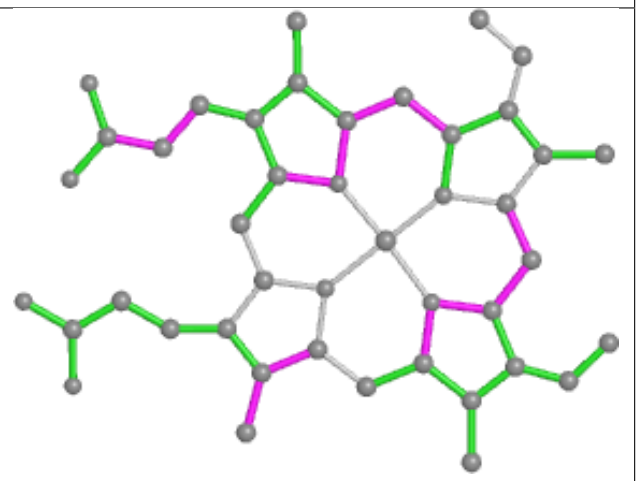
Ligand HEM A 401



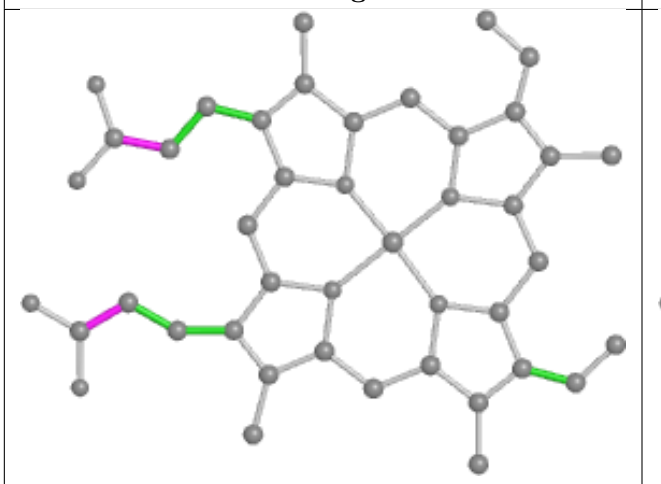
Ligand HEM C 401



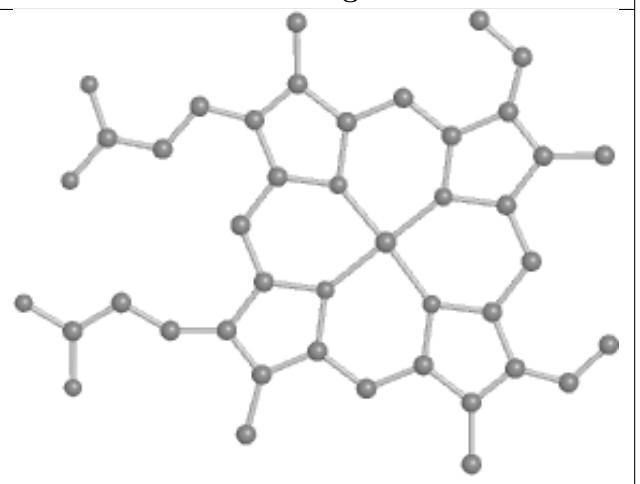
Bond lengths



Bond angles

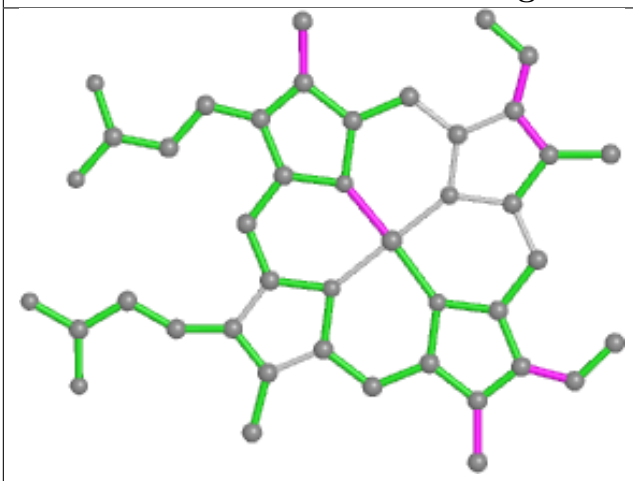


Torsions



Rings

Ligand HEM D 401



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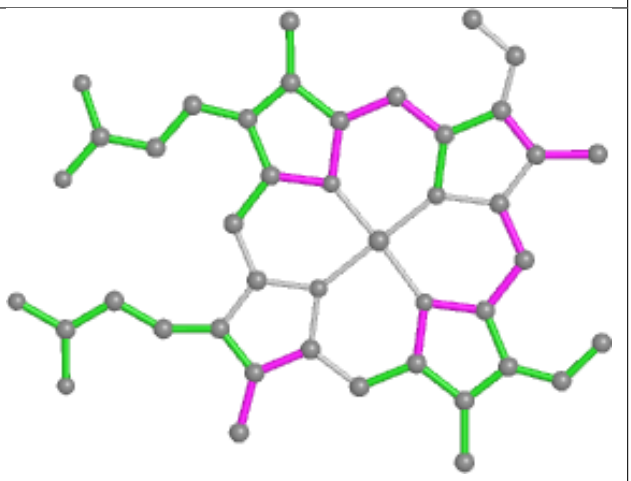

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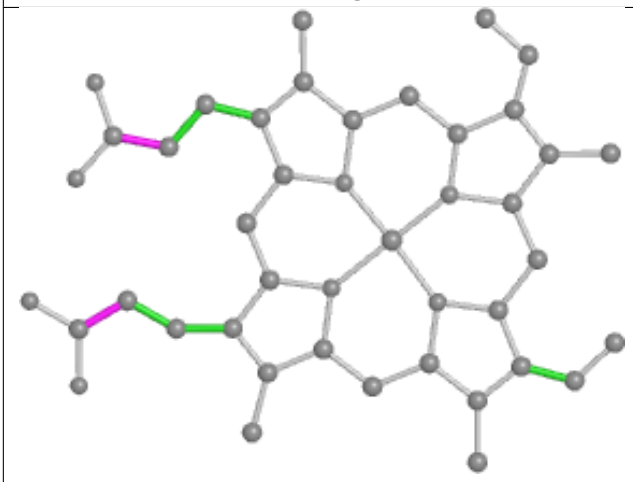
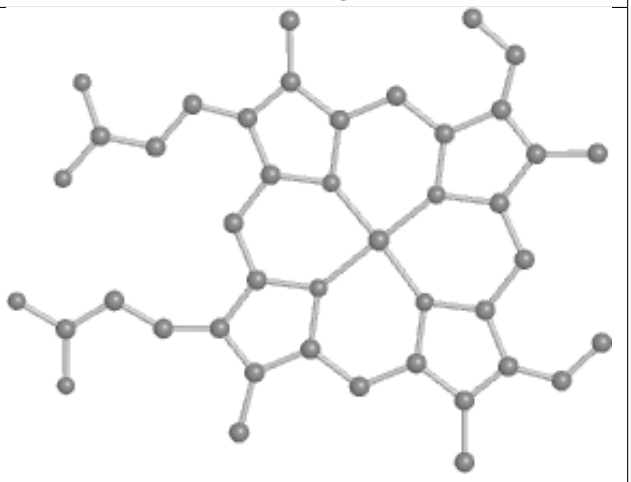
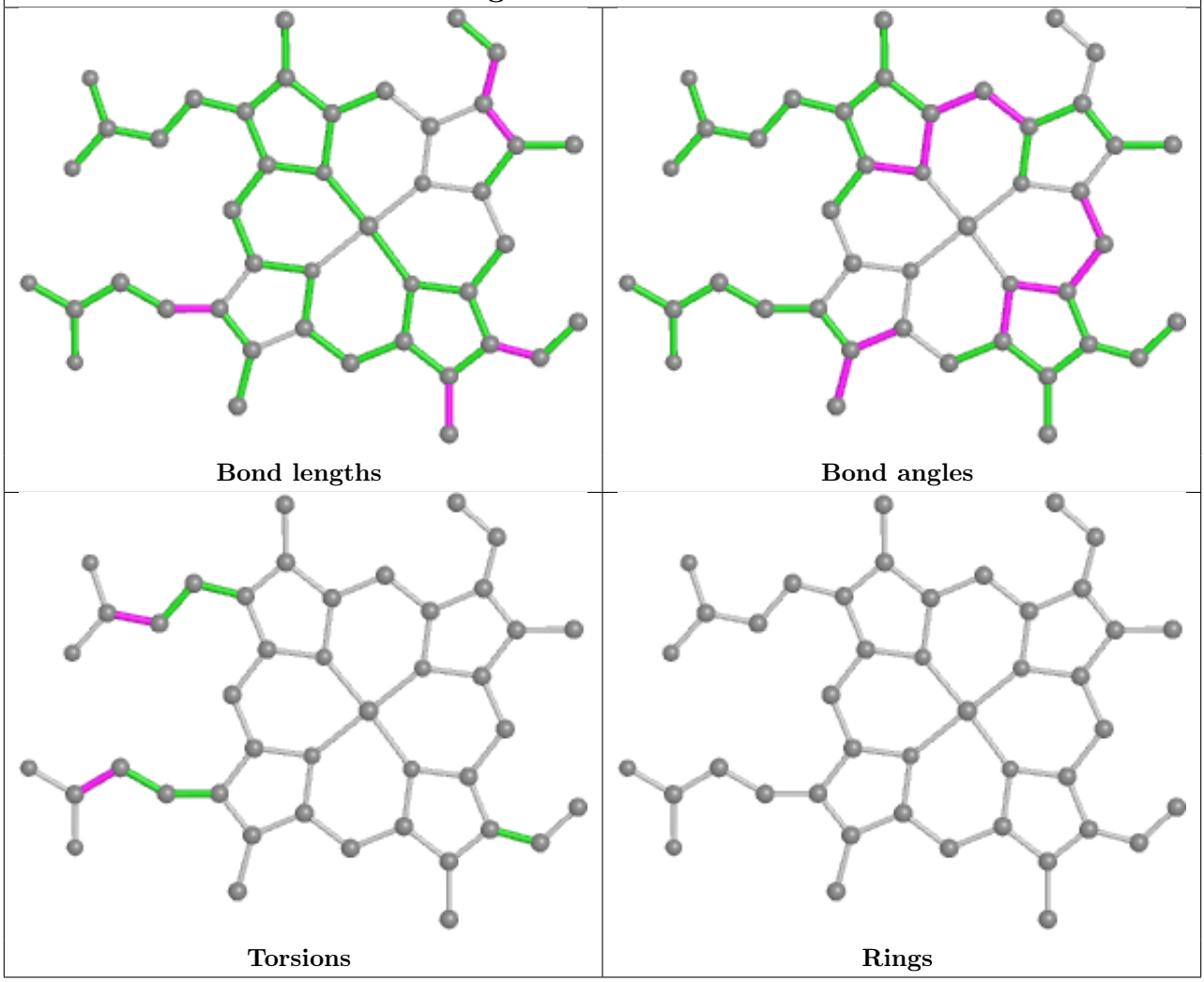


Torsions



Rings

Ligand HEM B 401



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)

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, 95th 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	296/307 (96%)	0.08	7 (2%)	59	64	14, 31, 58, 71	0
1	B	296/307 (96%)	0.15	7 (2%)	59	64	14, 32, 60, 71	0
1	C	296/307 (96%)	0.41	14 (4%)	31	37	15, 35, 69, 107	0
1	D	296/307 (96%)	0.72	34 (11%)	4	6	15, 39, 84, 117	0
All	All	1184/1228 (96%)	0.34	62 (5%)	27	32	14, 34, 70, 117	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	208	GLY	7.2
1	D	207	ASP	6.3
1	B	72	VAL	5.8
1	D	210	GLU	5.1
1	A	186	ARG	4.8
1	D	208	GLY	4.4
1	B	69	SER	4.2
1	C	209	ASP	4.1
1	D	214	THR	4.0
1	D	217	LEU	3.9
1	B	300	ALA	3.8
1	C	207	ASP	3.6
1	D	209	ASP	3.6
1	D	70	GLY	3.6
1	A	72	VAL	3.6
1	C	69	SER	3.5
1	D	220	VAL	3.4
1	D	197	GLY	3.4
1	D	68	LEU	3.3
1	C	197	GLY	3.2
1	C	299	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	69	SER	3.1
1	D	300	ALA	3.0
1	D	206	ILE	3.0
1	D	186	ARG	2.9
1	C	70	GLY	2.9
1	A	27	GLU	2.9
1	D	150	ALA	2.9
1	C	150	ALA	2.8
1	C	300	ALA	2.8
1	D	204	GLU	2.7
1	A	300	ALA	2.7
1	D	66	ARG	2.6
1	D	157	GLU	2.6
1	B	70	GLY	2.5
1	B	208	GLY	2.5
1	C	27	GLU	2.5
1	B	209	ASP	2.5
1	D	273	GLY	2.5
1	C	220	VAL	2.5
1	D	188	SER	2.5
1	A	208	GLY	2.5
1	D	196	ILE	2.5
1	A	209	ASP	2.4
1	D	229	LEU	2.4
1	C	206	ILE	2.4
1	D	225	ASP	2.4
1	D	222	LEU	2.3
1	D	205	GLU	2.3
1	D	194	MET	2.3
1	B	27	GLU	2.3
1	D	75	GLU	2.3
1	C	68	LEU	2.2
1	D	202	ALA	2.2
1	D	264	LEU	2.2
1	D	69	SER	2.2
1	D	151	GLY	2.1
1	D	254	ALA	2.1
1	D	84	GLY	2.1
1	D	184	LEU	2.0
1	D	199	THR	2.0
1	C	66	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

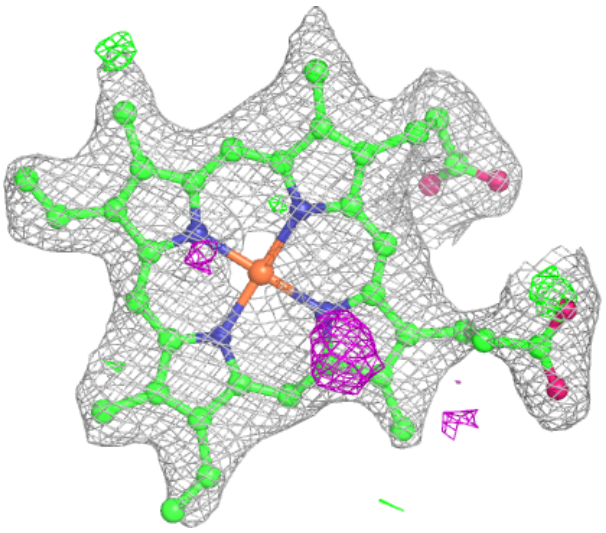
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

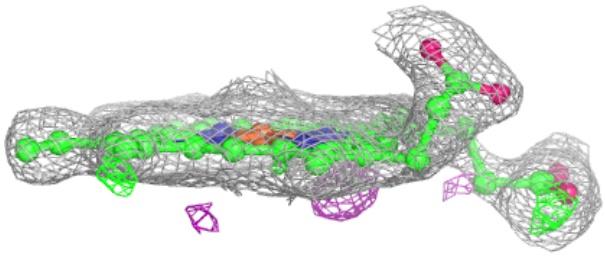
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	D	401	43/43	0.94	0.15	32,38,56,64	0
2	HEM	C	401	43/43	0.96	0.12	27,32,37,39	0
2	HEM	B	401	43/43	0.96	0.12	18,22,28,35	0
2	HEM	A	401	43/43	0.97	0.11	19,21,26,27	0

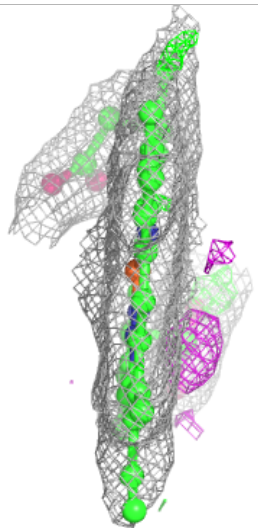
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM D 401:

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

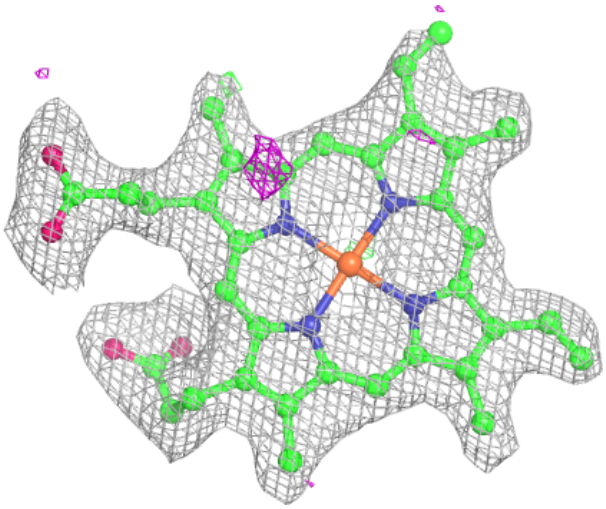


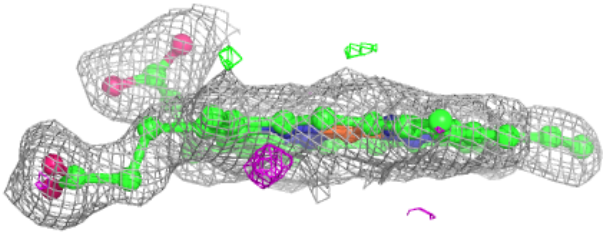


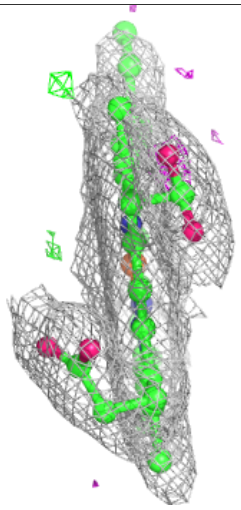


Electron density around HEM C 401:

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

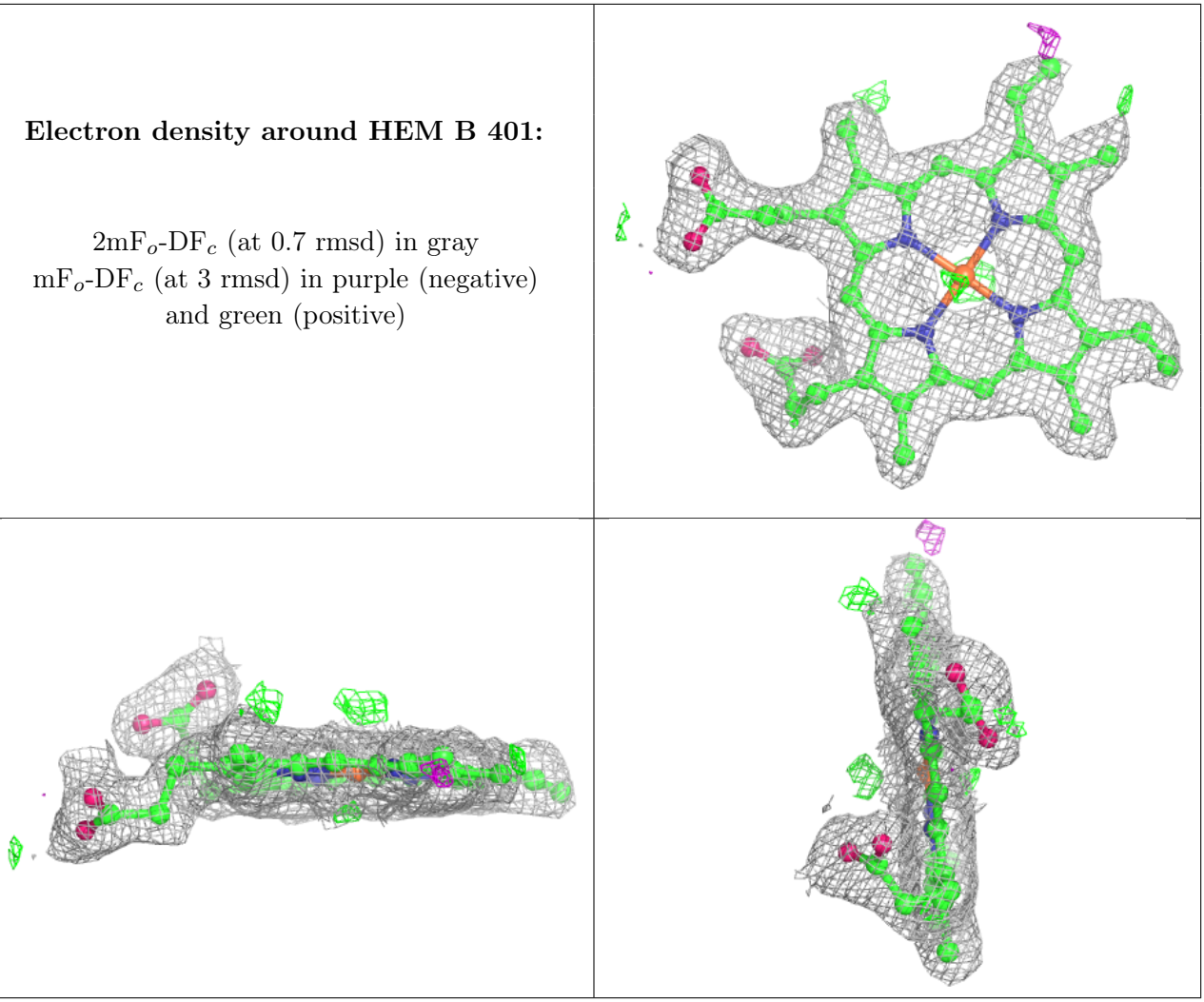






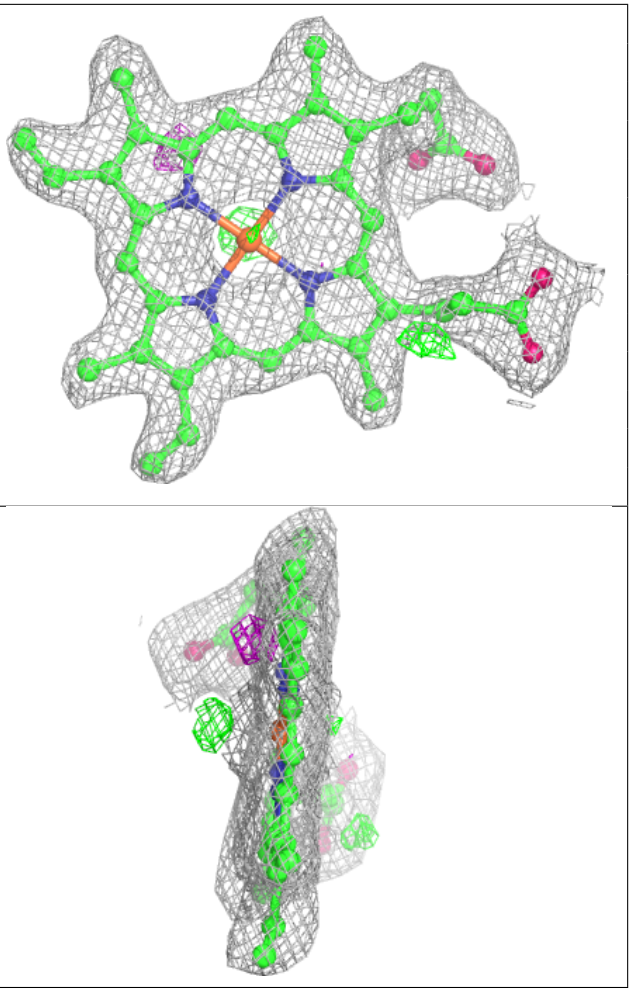
Electron density around HEM B 401:

$2mF_o$-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 401:

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)

There are no such residues in this entry.