Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2023 – 08:28 PM EDT

PDB ID	:	3E08
Title	:	H55S mutant Xanthomonas campestris tryptophan 2,3-dioxygenase
Authors	:	Mowat, C.G.; Campbell, L.P.
Deposited on	:	2008-07-31
Resolution	:	1.90 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:

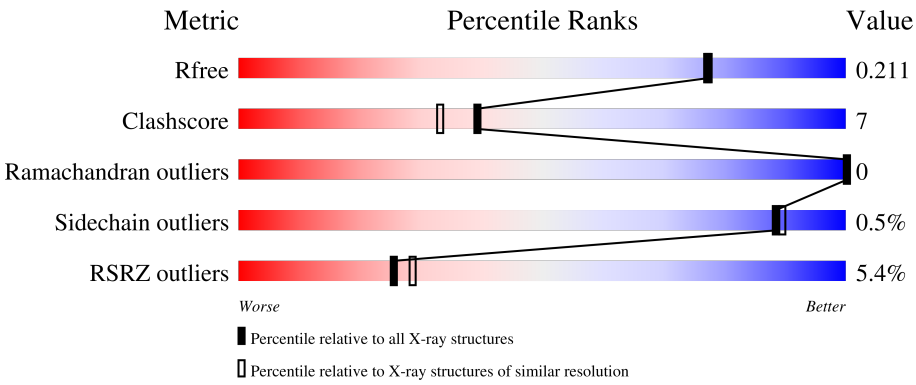
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	298	2%, 78%, 16%, • 6%
1	B	298	%, 82%, 12%, 6%
1	C	298	6%, 83%, 11%, 6%
1	D	298	2%, 82%, 12%, 6%
1	E	298	12%, 77%, 16%, 7%

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Mol	Chain	Length	Quality of chain
1	F	298	7% 79% 13% 7%
1	G	298	7% 79% 14% 7%
1	H	298	3% 81% 11% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20880 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.

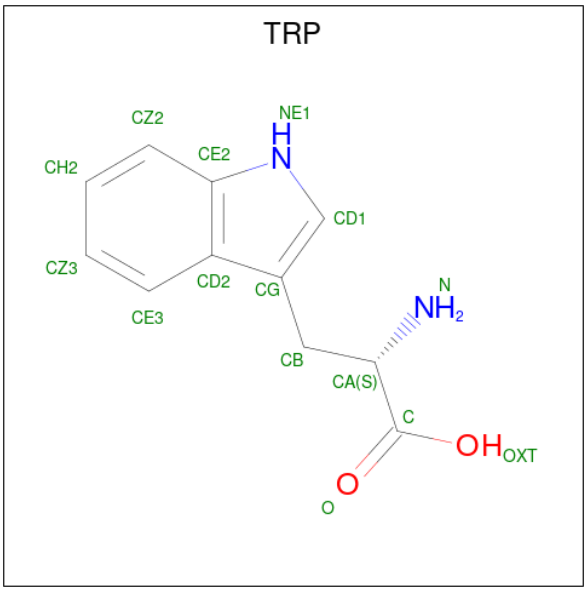
- Molecule 1 is a protein called Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	2300	1467	407	419	7	0	0	0
1	B	280	2305	1473	407	418	7	0	0	0
1	C	280	2309	1475	408	419	7	0	0	0
1	D	280	2303	1469	408	419	7	0	0	0
1	E	278	2284	1459	404	414	7	0	0	0
1	F	276	2278	1458	402	411	7	0	0	0
1	G	277	2286	1462	404	413	7	0	0	0
1	H	276	2276	1454	403	412	7	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	SER	HIS	engineered mutation	UNP Q8PDA8
B	55	SER	HIS	engineered mutation	UNP Q8PDA8
C	55	SER	HIS	engineered mutation	UNP Q8PDA8
D	55	SER	HIS	engineered mutation	UNP Q8PDA8
E	55	SER	HIS	engineered mutation	UNP Q8PDA8
F	55	SER	HIS	engineered mutation	UNP Q8PDA8
G	55	SER	HIS	engineered mutation	UNP Q8PDA8
H	55	SER	HIS	engineered mutation	UNP Q8PDA8

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	11	2	2	0	0
			Total	C	N	O		
2	A	1	15	11	2	2	0	0
			Total	C	N	O		
2	B	1	15	11	2	2	0	0
			Total	C	N	O		
2	B	1	15	11	2	2	0	0
			Total	C	N	O		
2	C	1	15	11	2	2	0	0
			Total	C	N	O		
2	C	1	15	11	2	2	0	0
			Total	C	N	O		
2	D	1	15	11	2	2	0	0
			Total	C	N	O		
2	D	1	15	11	2	2	0	0
			Total	C	N	O		
2	E	1	15	11	2	2	0	0
			Total	C	N	O		
2	E	1	15	11	2	2	0	0
			Total	C	N	O		
2	F	1	15	11	2	2	0	0
			Total	C	N	O		
2	F	1	15	11	2	2	0	0
			Total	C	N	O		
2	G	1	15	11	2	2	0	0
			Total	C	N	O		
2	G	1	15	11	2	2	0	0

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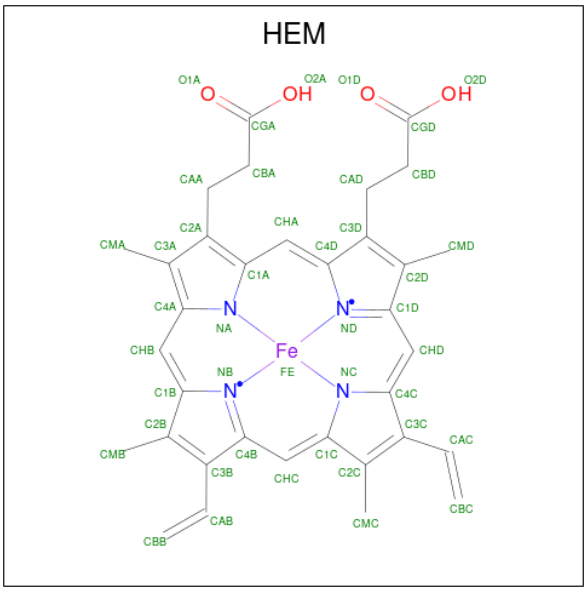
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	H	1	15	11	2	2	0	0
			Total	C	N	O		
2	H	1	15	11	2	2	0	0

- Molecule 3 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		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	E	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	G	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	H	1	43	34	1	4	4	0	0

- Molecule 4 is water.

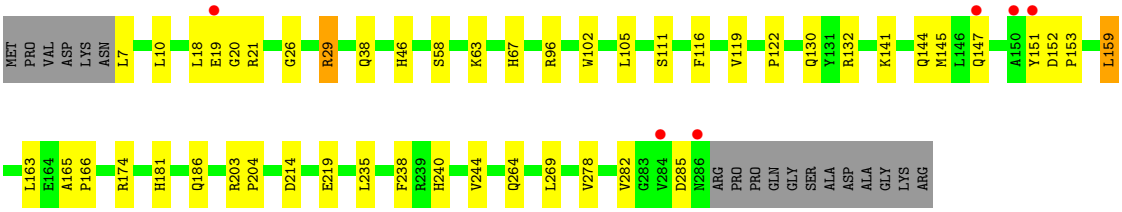
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	306	306	306	0	0
			Total	O		
4	B	325	325	325	0	0
			Total	O		
4	C	245	245	245	0	0
			Total	O		
4	D	268	268	268	0	0
			Total	O		
4	E	147	147	147	0	0
			Total	O		
4	F	217	217	217	0	0
			Total	O		
4	G	195	195	195	0	0
			Total	O		
4	H	252	252	252	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.

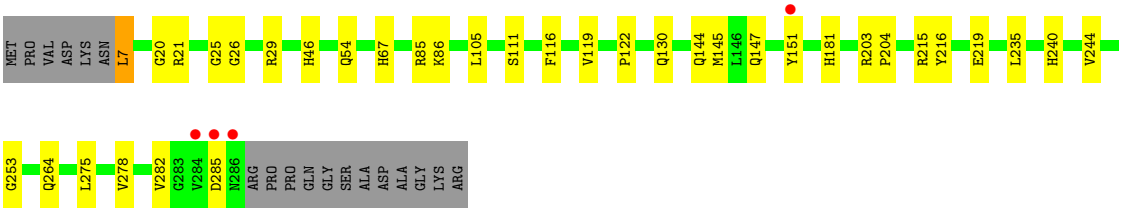
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain A:



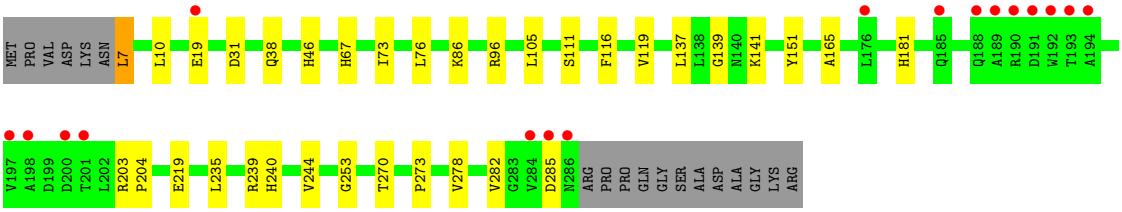
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain B:



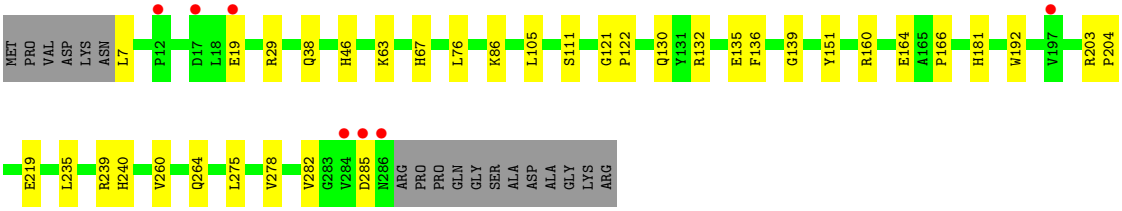
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain C:



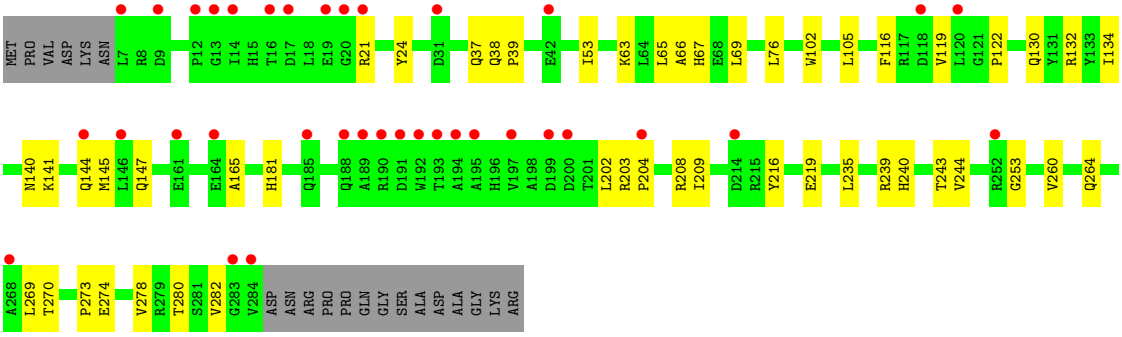
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain D:



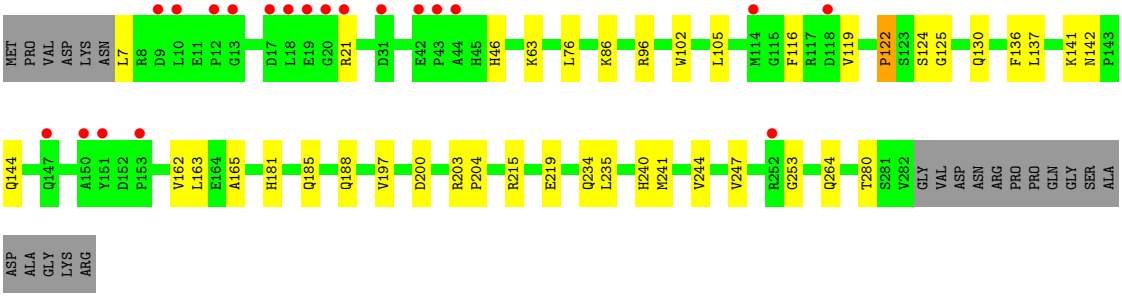
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain E:



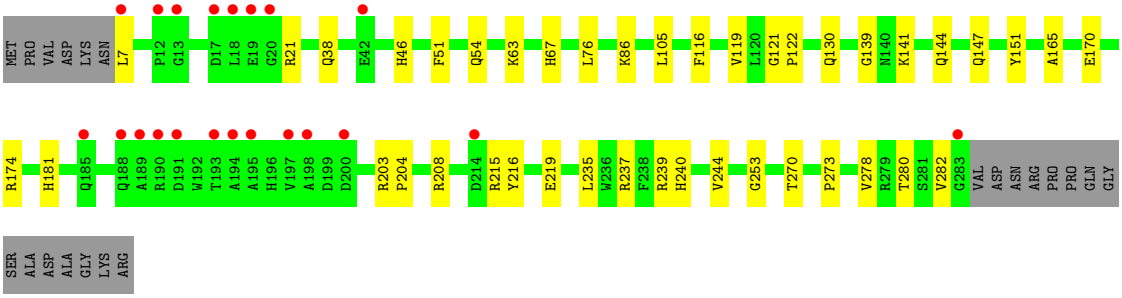
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain F:



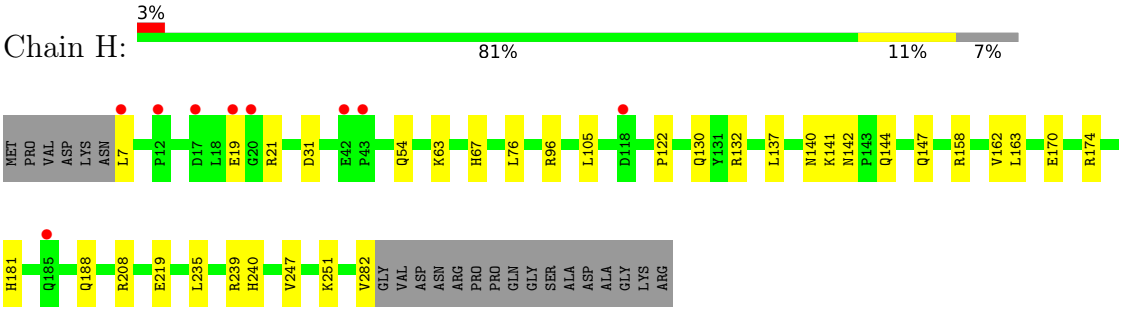
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain G:



• Molecule 1: Tryptophan 2,3-dioxygenase

Chain H:


3%
81%
11%
7%
MET PRO VAL ASP LYS ASN L7 P12 D17 L18 E19 G20 R21 D31 E42 P43 Q54 K63 H67 L76 R96 L105 D118 P122 Q130 Y131 R132 L137 N140 K141 N142 P143 Q144 Q147 R158 V162 L163 E170 R174
H181 Q185 Q188 R208 E219 L235 R239 H240 V247 K251 V282 GLY VAL ASP ASN ARG PRO PRO GLN GLY SER ALA ASP ALA GLY LYS ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.91Å 117.72Å 138.98Å 90.00° 95.64° 90.00°	Depositor
Resolution (Å)	17.56 – 1.90 17.52 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (17.56-1.90) 96.5 (17.52-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 1.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.178 , 0.216 0.173 , 0.211	Depositor DCC
R_{free} test set	9522 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20880	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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	0.35	0/2355	0.51	0/3191
1	B	0.34	0/2362	0.50	0/3202
1	C	0.31	0/2366	0.46	0/3207
1	D	0.32	0/2359	0.47	0/3198
1	E	0.26	0/2339	0.41	0/3169
1	F	0.31	0/2335	0.45	0/3165
1	G	0.29	0/2343	0.42	0/3175
1	H	0.31	0/2332	0.45	0/3161
All	All	0.31	0/18791	0.46	0/25468

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	2300	0	2251	46	0
1	B	2305	0	2253	40	0
1	C	2309	0	2259	31	0
1	D	2303	0	2252	36	0
1	E	2284	0	2241	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2278	0	2231	38	0
1	G	2286	0	2240	36	0
1	H	2276	0	2230	33	0
2	A	30	0	18	1	0
2	B	30	0	18	1	0
2	C	30	0	18	0	0
2	D	30	0	18	1	0
2	E	30	0	18	1	0
2	F	30	0	18	0	0
2	G	30	0	18	2	0
2	H	30	0	18	1	0
3	A	43	0	30	5	0
3	B	43	0	30	4	0
3	C	43	0	30	6	0
3	D	43	0	30	4	0
3	E	43	0	30	6	0
3	F	43	0	30	9	0
3	G	43	0	30	6	0
3	H	43	0	30	4	0
4	A	306	0	0	11	0
4	B	325	0	0	12	0
4	C	245	0	0	10	0
4	D	268	0	0	16	0
4	E	147	0	0	6	0
4	F	217	0	0	7	0
4	G	195	0	0	10	0
4	H	252	0	0	12	0
All	All	20880	0	18341	277	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 7.

All (277) 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)
3:H:401:HEM:HHD	3:H:401:HEM:HBC2	1.44	0.97
3:F:401:HEM:HBC2	3:F:401:HEM:HHD	1.50	0.91
1:H:188:GLN:HG3	4:H:644:HOH:O	1.72	0.89
1:A:20:GLY:O	1:H:188:GLN:NE2	2.08	0.86
3:G:401:HEM:HBC2	3:G:401:HEM:HHD	1.60	0.84
1:C:38:GLN:HG3	4:D:658:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:401:HEM:HBC2	3:D:401:HEM:HHD	1.63	0.81
1:E:105:LEU:HD21	3:E:401:HEM:HAB	1.62	0.81
1:C:7:LEU:HD13	4:D:686:HOH:O	1.81	0.80
1:C:31:ASP:HB2	4:C:626:HOH:O	1.82	0.80
3:C:401:HEM:HBC2	3:C:401:HEM:HHD	1.62	0.80
1:F:280:THR:HG23	4:F:457:HOH:O	1.84	0.78
1:A:58:SER:CB	3:A:401:HEM:HBC1	2.14	0.77
3:E:401:HEM:HBC2	3:E:401:HEM:HHD	1.65	0.77
1:B:151:TYR:HD2	4:B:660:HOH:O	1.69	0.76
1:C:67:HIS:HD2	4:C:678:HOH:O	1.70	0.73
1:H:140:ASN:HB2	4:H:774:HOH:O	1.88	0.72
1:F:188:GLN:HG3	4:F:404:HOH:O	1.90	0.71
3:F:401:HEM:HMB1	3:F:401:HEM:HBB2	1.73	0.70
1:F:96:ARG:HH21	1:H:96:ARG:HH21	1.40	0.70
1:G:38:GLN:HG3	4:H:851:HOH:O	1.92	0.69
1:D:181:HIS:HD2	4:D:625:HOH:O	1.75	0.69
1:D:67:HIS:HD2	4:D:706:HOH:O	1.75	0.69
3:D:401:HEM:HMB1	3:D:401:HEM:HBB2	1.75	0.69
1:B:85:ARG:HB3	4:B:802:HOH:O	1.93	0.68
1:B:29:ARG:NH2	4:B:815:HOH:O	2.27	0.68
1:D:235:LEU:HD13	4:D:837:HOH:O	1.93	0.68
1:B:130:GLN:HG3	4:B:563:HOH:O	1.93	0.68
1:G:7:LEU:HG	4:G:426:HOH:O	1.94	0.68
1:C:240:HIS:HD2	4:C:625:HOH:O	1.76	0.67
1:D:240:HIS:HD2	4:D:622:HOH:O	1.77	0.66
1:D:63:LYS:HB2	1:D:130:GLN:HE22	1.59	0.66
1:B:20:GLY:O	1:F:188:GLN:NE2	2.28	0.65
1:A:181:HIS:HD2	4:A:425:HOH:O	1.80	0.64
4:C:800:HOH:O	1:D:7:LEU:HD13	1.96	0.64
1:F:188:GLN:CG	4:F:404:HOH:O	2.46	0.64
1:H:181:HIS:HD2	4:H:663:HOH:O	1.80	0.63
1:C:181:HIS:HD2	4:C:649:HOH:O	1.81	0.63
1:A:214:ASP:HB2	4:A:630:HOH:O	1.99	0.63
1:F:181:HIS:HD2	4:F:408:HOH:O	1.81	0.63
1:G:280:THR:HG23	4:G:535:HOH:O	1.98	0.62
1:G:235:LEU:HD12	4:G:481:HOH:O	1.98	0.62
1:E:63:LYS:HB2	1:E:130:GLN:HE22	1.63	0.62
1:E:141:LYS:NZ	1:E:165:ALA:O	2.32	0.62
1:A:264:GLN:HG2	4:A:691:HOH:O	1.99	0.62
1:D:239:ARG:HG3	4:D:881:HOH:O	2.00	0.62
1:H:240:HIS:HD2	4:H:653:HOH:O	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HD13	4:B:567:HOH:O	2.00	0.62
1:F:142:ASN:OD1	1:F:144:GLN:HB2	2.00	0.62
1:G:181:HIS:HE1	1:G:219:GLU:OE2	1.82	0.62
1:C:105:LEU:HD21	3:C:401:HEM:HAB	1.81	0.62
1:B:181:HIS:HD2	4:B:565:HOH:O	1.82	0.61
1:F:63:LYS:HB2	1:F:130:GLN:HE22	1.65	0.61
1:B:278:VAL:HG22	1:B:282:VAL:HG13	1.83	0.61
4:A:472:HOH:O	1:B:7:LEU:HD13	2.01	0.61
1:D:105:LEU:HD21	3:D:401:HEM:HAB	1.82	0.60
1:H:67:HIS:HD2	4:H:688:HOH:O	1.84	0.60
1:E:181:HIS:HD2	4:E:425:HOH:O	1.83	0.60
1:B:116:PHE:O	1:B:119:VAL:HG22	2.02	0.60
1:B:240:HIS:HD2	4:B:549:HOH:O	1.85	0.60
1:E:122:PRO:HG3	1:F:21:ARG:NH2	2.16	0.60
1:E:67:HIS:HD2	4:E:484:HOH:O	1.84	0.60
3:F:401:HEM:HBB2	3:F:401:HEM:CMB	2.31	0.59
3:C:401:HEM:HBB2	3:C:401:HEM:HMB1	1.85	0.59
1:E:203:ARG:HB3	1:E:204:PRO:HD3	1.85	0.59
1:F:240:HIS:HD2	4:F:430:HOH:O	1.85	0.58
1:C:19:GLU:HA	1:D:151:TYR:HB2	1.85	0.58
3:E:401:HEM:HBB2	3:E:401:HEM:HMB1	1.84	0.58
1:G:170:GLU:O	1:G:174:ARG:HG3	2.03	0.58
4:G:425:HOH:O	1:H:7:LEU:HG	2.02	0.58
1:H:188:GLN:OE1	1:H:188:GLN:HA	2.03	0.58
1:B:144:GLN:O	1:B:147:GLN:HG2	2.04	0.58
1:F:116:PHE:O	1:F:119:VAL:HG22	2.03	0.58
1:A:67:HIS:HD2	4:A:479:HOH:O	1.86	0.58
1:A:38:GLN:OE1	1:F:215:ARG:NE	2.37	0.57
1:A:20:GLY:O	1:H:188:GLN:CD	2.43	0.57
1:G:244:VAL:HG22	3:G:401:HEM:C1B	2.39	0.57
1:D:235:LEU:HB3	4:D:881:HOH:O	2.04	0.56
1:G:67:HIS:HD2	4:G:493:HOH:O	1.87	0.56
1:H:7:LEU:HD23	4:H:887:HOH:O	2.05	0.56
1:F:105:LEU:HD21	3:F:401:HEM:HAB	1.85	0.56
1:H:208:ARG:NH1	4:H:674:HOH:O	2.37	0.56
1:A:20:GLY:O	1:H:188:GLN:OE1	2.23	0.56
3:E:401:HEM:HBB2	3:E:401:HEM:CMB	2.35	0.56
1:G:63:LYS:HB2	1:G:130:GLN:HE22	1.71	0.56
1:B:85:ARG:CZ	4:B:802:HOH:O	2.53	0.56
1:B:67:HIS:HD2	4:B:579:HOH:O	1.87	0.55
1:D:132:ARG:NH1	4:D:651:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:GLN:HG2	1:H:105:LEU:HD22	1.87	0.55
1:H:144:GLN:O	1:H:147:GLN:HG2	2.05	0.55
1:E:270:THR:HG23	1:E:273:PRO:HG3	1.88	0.54
1:E:132:ARG:HD2	1:E:145:MET:HG3	1.90	0.54
1:A:240:HIS:HD2	4:A:406:HOH:O	1.90	0.54
1:A:181:HIS:HE1	1:A:219:GLU:OE2	1.91	0.54
1:C:139:GLY:HA3	4:C:672:HOH:O	2.07	0.54
1:F:235:LEU:HD21	1:G:239:ARG:HG2	1.90	0.54
1:D:181:HIS:HE1	1:D:219:GLU:OE2	1.90	0.53
1:E:38:GLN:HG3	4:E:508:HOH:O	2.08	0.53
2:E:403:TRP:CE3	1:G:86:LYS:HE2	2.44	0.53
1:A:105:LEU:HD21	3:A:401:HEM:HAB	1.90	0.53
1:A:7:LEU:HD12	4:B:723:HOH:O	2.08	0.53
1:C:7:LEU:N	4:C:818:HOH:O	2.42	0.53
1:G:181:HIS:HD2	4:G:408:HOH:O	1.90	0.53
1:C:181:HIS:HE1	1:C:219:GLU:OE2	1.92	0.52
1:A:141:LYS:HD3	1:A:163:LEU:HD12	1.91	0.52
1:A:235:LEU:HD21	1:D:239:ARG:HG2	1.91	0.52
1:C:203:ARG:HB3	1:C:204:PRO:HD3	1.91	0.52
1:B:105:LEU:HD21	3:B:401:HEM:HAB	1.91	0.52
1:C:151:TYR:HB2	1:D:19:GLU:HA	1.91	0.52
1:G:105:LEU:HD21	3:G:401:HEM:HAB	1.90	0.52
1:A:151:TYR:N	4:A:591:HOH:O	2.43	0.52
1:C:46:HIS:O	1:D:67:HIS:HE1	1.93	0.52
1:B:111:SER:HB2	1:C:285:ASP:HB2	1.90	0.52
1:H:132:ARG:HB2	4:H:751:HOH:O	2.10	0.52
1:H:142:ASN:OD1	1:H:144:GLN:HB2	2.10	0.51
1:F:137:LEU:HD13	1:F:162:VAL:HG23	1.91	0.51
1:A:29:ARG:NH2	4:A:464:HOH:O	2.37	0.51
1:A:151:TYR:CE1	1:A:152:ASP:HB2	2.46	0.51
1:B:26:GLY:O	1:B:29:ARG:HD3	2.11	0.51
1:G:141:LYS:NZ	1:G:165:ALA:O	2.38	0.51
1:A:278:VAL:HG22	1:A:282:VAL:HG13	1.93	0.51
1:B:235:LEU:HD21	1:C:239:ARG:HG2	1.92	0.51
1:G:144:GLN:O	1:G:147:GLN:HG2	2.11	0.50
3:D:401:HEM:HBB2	3:D:401:HEM:CMB	2.40	0.50
1:E:67:HIS:HE1	1:F:46:HIS:O	1.93	0.50
1:G:54:GLN:HG2	1:G:105:LEU:HD22	1.93	0.50
1:C:270:THR:HG23	1:C:273:PRO:HG3	1.94	0.50
4:C:751:HOH:O	1:D:38:GLN:HG3	2.09	0.50
1:B:181:HIS:HE1	1:B:219:GLU:OE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:HIS:HD2	4:E:412:HOH:O	1.94	0.50
1:G:278:VAL:HG22	1:G:282:VAL:HG13	1.94	0.50
1:E:235:LEU:HD21	1:H:239:ARG:HG2	1.94	0.49
1:G:21:ARG:NH2	1:H:122:PRO:HG3	2.27	0.49
1:D:160:ARG:O	1:D:164:GLU:HG3	2.13	0.49
1:F:181:HIS:HE1	1:F:219:GLU:OE2	1.96	0.49
1:B:203:ARG:HB3	1:B:204:PRO:HD3	1.94	0.49
1:F:203:ARG:HB3	1:F:204:PRO:HD3	1.94	0.49
1:C:278:VAL:O	1:C:282:VAL:HG13	2.13	0.49
3:B:401:HEM:HBC2	3:B:401:HEM:HHD	1.94	0.49
1:E:209:ILE:HD13	1:E:219:GLU:HB3	1.94	0.49
1:H:158:ARG:NH2	4:H:755:HOH:O	2.33	0.49
1:C:10:LEU:HD12	4:C:692:HOH:O	2.13	0.48
1:B:21:ARG:HG2	1:F:188:GLN:NE2	2.27	0.48
1:D:63:LYS:CB	1:D:130:GLN:HE22	2.24	0.48
1:G:139:GLY:HA3	4:G:482:HOH:O	2.12	0.48
1:D:29:ARG:CD	4:D:817:HOH:O	2.61	0.48
1:H:208:ARG:NH2	4:H:779:HOH:O	2.45	0.48
1:A:116:PHE:O	1:A:119:VAL:HG22	2.14	0.48
1:A:122:PRO:HG3	1:B:21:ARG:CZ	2.44	0.48
1:A:46:HIS:O	1:B:67:HIS:HE1	1.96	0.48
1:B:264:GLN:NE2	4:B:725:HOH:O	2.46	0.47
1:F:102:TRP:CZ2	1:F:240:HIS:HB2	2.49	0.47
1:G:240:HIS:HD2	4:G:419:HOH:O	1.97	0.47
1:A:63:LYS:HB2	1:A:130:GLN:HE22	1.79	0.47
1:F:86:LYS:HE2	2:H:403:TRP:CE3	2.49	0.47
1:F:200:ASP:HB3	4:F:569:HOH:O	2.15	0.47
1:A:111:SER:HB2	1:D:285:ASP:HB2	1.95	0.47
1:A:285:ASP:HB2	1:D:111:SER:HB2	1.96	0.47
1:C:278:VAL:HG22	1:C:282:VAL:HG13	1.97	0.47
1:A:26:GLY:O	1:A:29:ARG:HD3	2.14	0.47
1:C:116:PHE:O	1:C:119:VAL:HG22	2.15	0.47
1:A:19:GLU:HA	4:A:529:HOH:O	2.13	0.46
1:B:21:ARG:HG2	1:F:188:GLN:CD	2.35	0.46
1:G:181:HIS:CE1	1:G:219:GLU:OE2	2.67	0.46
1:H:31:ASP:HB2	4:H:709:HOH:O	2.15	0.46
1:D:203:ARG:HB3	1:D:204:PRO:HD3	1.97	0.46
1:E:66:ALA:HB2	1:E:134:ILE:HD11	1.97	0.46
1:G:203:ARG:HB3	1:G:204:PRO:HD3	1.97	0.46
1:G:253:GLY:HA3	3:G:401:HEM:O2A	2.14	0.46
1:E:244:VAL:HG22	3:E:401:HEM:C1B	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:GLN:HB3	4:F:588:HOH:O	2.15	0.46
1:E:140:ASN:HB2	4:E:445:HOH:O	2.15	0.46
1:E:253:GLY:HA3	3:E:401:HEM:HMA1	1.98	0.46
1:H:247:VAL:HG11	3:H:401:HEM:CBB	2.47	0.45
1:A:132:ARG:HD2	1:A:145:MET:HG3	1.98	0.45
1:C:73:ILE:CD1	1:C:137:LEU:HD11	2.45	0.45
2:B:403:TRP:CE3	1:D:86:LYS:HE2	2.51	0.45
1:F:141:LYS:NZ	1:F:165:ALA:O	2.45	0.45
1:H:170:GLU:O	1:H:174:ARG:HG3	2.16	0.45
1:B:215:ARG:HD3	1:B:216:TYR:CZ	2.52	0.45
3:G:401:HEM:HHD	3:G:401:HEM:CBC	2.41	0.45
1:F:136:PHE:CE2	1:F:163:LEU:HD13	2.52	0.45
1:A:144:GLN:O	1:A:147:GLN:HG2	2.16	0.45
1:E:102:TRP:CZ2	1:E:240:HIS:HB2	2.52	0.45
1:E:202:LEU:HB2	1:E:274:GLU:HG2	1.99	0.45
1:A:58:SER:HB2	3:A:401:HEM:HBC1	1.96	0.45
1:B:54:GLN:HG2	1:B:105:LEU:HD22	1.97	0.45
1:E:24:TYR:HB2	1:F:124:SER:O	2.16	0.45
1:G:51:PHE:HZ	2:G:402:TRP:CG	2.35	0.45
1:G:141:LYS:HD2	4:G:501:HOH:O	2.17	0.45
1:G:208:ARG:CZ	1:G:216:TYR:OH	2.65	0.45
1:H:63:LYS:HB2	1:H:130:GLN:HE22	1.81	0.45
3:C:401:HEM:HBB2	3:C:401:HEM:CMB	2.46	0.45
1:F:244:VAL:HG22	3:F:401:HEM:C1B	2.52	0.44
1:D:166:PRO:HG3	1:D:192:TRP:CE2	2.53	0.44
1:H:181:HIS:HE1	1:H:219:GLU:OE2	2.00	0.44
1:C:244:VAL:HG22	3:C:401:HEM:C1B	2.52	0.44
1:A:166:PRO:HG2	1:A:174:ARG:NH1	2.33	0.44
1:D:282:VAL:HG12	4:D:772:HOH:O	2.17	0.44
1:E:181:HIS:HE1	1:E:219:GLU:OE2	2.01	0.44
1:E:260:VAL:O	1:E:264:GLN:HG3	2.16	0.44
3:B:401:HEM:HHD	3:B:401:HEM:CBC	2.48	0.44
3:H:401:HEM:CMB	3:H:401:HEM:HBB2	2.47	0.44
1:A:238:PHE:CD2	1:D:235:LEU:HD23	2.53	0.44
2:A:403:TRP:CE3	1:C:86:LYS:HE2	2.53	0.44
1:B:20:GLY:O	1:F:188:GLN:CD	2.57	0.44
1:A:21:ARG:CZ	1:B:122:PRO:HG3	2.48	0.43
1:E:105:LEU:HD23	1:E:243:THR:HG21	2.00	0.43
1:A:151:TYR:O	1:A:153:PRO:HD3	2.18	0.43
1:E:39:PRO:HB2	4:E:495:HOH:O	2.17	0.43
1:G:151:TYR:HB2	1:H:19:GLU:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD12	1:A:159:LEU:HA	1.93	0.43
3:F:401:HEM:HHD	3:F:401:HEM:CBC	2.35	0.43
3:A:401:HEM:HBB2	3:A:401:HEM:CMB	2.48	0.43
1:A:10:LEU:HD11	1:B:145:MET:SD	2.58	0.43
1:B:285:ASP:HB2	1:C:111:SER:HB2	2.00	0.43
1:E:144:GLN:O	1:E:147:GLN:HG2	2.19	0.43
1:F:185:GLN:OE1	1:F:188:GLN:HG3	2.18	0.43
3:G:401:HEM:CMB	3:G:401:HEM:HBB2	2.48	0.43
1:B:85:ARG:NE	4:B:802:HOH:O	2.52	0.43
1:H:141:LYS:HD2	1:H:163:LEU:HD12	2.00	0.43
1:C:253:GLY:HA3	3:C:401:HEM:HMA1	2.01	0.42
1:B:21:ARG:HA	1:F:188:GLN:HE22	1.85	0.42
1:F:125:GLY:HA3	3:F:401:HEM:C1D	2.55	0.42
1:G:215:ARG:HD3	1:G:216:TYR:CE2	2.54	0.42
1:A:67:HIS:HE1	1:B:46:HIS:O	2.02	0.42
1:A:141:LYS:NZ	1:A:165:ALA:O	2.50	0.42
1:D:136:PHE:CB	4:D:627:HOH:O	2.67	0.42
1:D:121:GLY:HA3	1:D:122:PRO:HD3	1.88	0.42
1:D:135:GLU:CG	4:D:651:HOH:O	2.67	0.42
1:G:46:HIS:O	1:H:67:HIS:HE1	2.02	0.42
1:C:76:LEU:HD23	1:C:76:LEU:HA	1.80	0.42
1:D:139:GLY:HA3	4:D:711:HOH:O	2.19	0.42
1:E:280:THR:HA	1:H:251:LYS:HG3	2.01	0.42
1:G:121:GLY:HA3	1:G:122:PRO:HD3	1.86	0.42
1:A:203:ARG:HB3	1:A:204:PRO:HD3	2.01	0.42
1:E:116:PHE:O	1:E:119:VAL:HG22	2.19	0.42
1:E:208:ARG:CZ	1:E:216:TYR:OH	2.68	0.42
1:G:51:PHE:HZ	2:G:402:TRP:CD1	2.38	0.42
1:A:18:LEU:O	1:A:20:GLY:N	2.53	0.41
1:A:102:TRP:CZ2	1:A:240:HIS:HB2	2.55	0.41
1:B:275:LEU:O	1:B:278:VAL:HG12	2.20	0.41
1:C:67:HIS:HE1	1:D:46:HIS:O	2.03	0.41
1:E:239:ARG:HG2	1:H:235:LEU:HD21	2.02	0.41
1:A:244:VAL:HG22	3:A:401:HEM:C1B	2.55	0.41
1:F:241:MET:SD	1:F:264:GLN:HG3	2.60	0.41
1:B:86:LYS:HE2	2:D:403:TRP:CE3	2.55	0.41
3:H:401:HEM:HBB2	3:H:401:HEM:HMB1	2.02	0.41
1:B:203:ARG:N	1:B:204:PRO:HD2	2.36	0.41
1:D:275:LEU:O	1:D:278:VAL:HG12	2.21	0.41
1:E:65:LEU:O	1:E:69:LEU:HG	2.21	0.41
1:G:76:LEU:HD23	1:G:76:LEU:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:PRO:HG3	1:H:21:ARG:CZ	2.50	0.41
1:C:235:LEU:HD12	4:C:773:HOH:O	2.21	0.41
1:A:130:GLN:HG3	4:A:414:HOH:O	2.19	0.41
1:B:240:HIS:O	1:B:244:VAL:HG23	2.21	0.41
1:D:282:VAL:CG1	4:D:772:HOH:O	2.69	0.41
1:F:253:GLY:HA3	3:F:401:HEM:HMA1	2.02	0.41
1:G:116:PHE:O	1:G:119:VAL:HG22	2.20	0.41
1:F:247:VAL:HG11	3:F:401:HEM:CBB	2.51	0.41
1:E:278:VAL:HG22	1:E:282:VAL:HG13	2.03	0.40
1:A:96:ARG:HH21	1:C:96:ARG:HH21	1.67	0.40
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.94	0.40
1:H:137:LEU:HD13	1:H:162:VAL:HG23	2.03	0.40
1:A:269:LEU:HD22	1:B:7:LEU:HB2	2.02	0.40
1:D:29:ARG:NE	4:D:817:HOH:O	2.54	0.40
1:E:21:ARG:NH2	1:F:122:PRO:HG3	2.36	0.40
1:E:37:GLN:HG2	1:E:53:ILE:HD11	2.03	0.40
1:E:76:LEU:HD23	1:E:76:LEU:HA	1.91	0.40
1:E:269:LEU:HD22	1:F:7:LEU:HB2	2.02	0.40
1:G:237:ARG:HG2	4:G:503:HOH:O	2.22	0.40
1:G:270:THR:HG23	1:G:273:PRO:HG3	2.02	0.40
4:A:657:HOH:O	1:B:25:GLY:HA3	2.21	0.40
1:B:253:GLY:HA3	3:B:401:HEM:HMA1	2.03	0.40
1:C:141:LYS:NZ	1:C:165:ALA:O	2.48	0.40
1:D:260:VAL:O	1:D:264:GLN:HG3	2.21	0.40
1:F:76:LEU:HD23	1:F:76:LEU:HA	1.94	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	278/298 (93%)	271 (98%)	7 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	278/298 (93%)	274 (99%)	4 (1%)	0	100	100
1	C	278/298 (93%)	272 (98%)	6 (2%)	0	100	100
1	D	278/298 (93%)	272 (98%)	6 (2%)	0	100	100
1	E	276/298 (93%)	271 (98%)	5 (2%)	0	100	100
1	F	274/298 (92%)	270 (98%)	4 (2%)	0	100	100
1	G	275/298 (92%)	268 (98%)	7 (2%)	0	100	100
1	H	274/298 (92%)	271 (99%)	3 (1%)	0	100	100
All	All	2211/2384 (93%)	2169 (98%)	42 (2%)	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	244/259 (94%)	241 (99%)	3 (1%)	71	70
1	B	244/259 (94%)	243 (100%)	1 (0%)	91	91
1	C	245/259 (95%)	244 (100%)	1 (0%)	91	91
1	D	244/259 (94%)	244 (100%)	0	100	100
1	E	242/259 (93%)	242 (100%)	0	100	100
1	F	241/259 (93%)	239 (99%)	2 (1%)	81	82
1	G	242/259 (93%)	242 (100%)	0	100	100
1	H	241/259 (93%)	239 (99%)	2 (1%)	81	82
All	All	1943/2072 (94%)	1934 (100%)	9 (0%)	88	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	159	LEU

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Mol	Chain	Res	Type
1	A	186	GLN
1	B	7	LEU
1	C	7	LEU
1	F	122	PRO
1	F	197	VAL
1	H	76	LEU
1	H	282	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	130	GLN
1	A	181	HIS
1	A	186	GLN
1	A	240	HIS
1	A	264	GLN
1	B	67	HIS
1	B	130	GLN
1	B	181	HIS
1	B	186	GLN
1	B	240	HIS
1	C	67	HIS
1	C	101	GLN
1	C	130	GLN
1	C	181	HIS
1	C	232	GLN
1	C	240	HIS
1	D	67	HIS
1	D	101	GLN
1	D	130	GLN
1	D	181	HIS
1	D	240	HIS
1	E	32	GLN
1	E	67	HIS
1	E	101	GLN
1	E	130	GLN
1	E	181	HIS
1	E	186	GLN
1	E	240	HIS
1	F	32	GLN
1	F	67	HIS

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Mol	Chain	Res	Type
1	F	130	GLN
1	F	181	HIS
1	F	240	HIS
1	G	67	HIS
1	G	101	GLN
1	G	130	GLN
1	G	181	HIS
1	G	232	GLN
1	G	240	HIS
1	H	32	GLN
1	H	67	HIS
1	H	93	GLN
1	H	101	GLN
1	H	130	GLN
1	H	181	HIS
1	H	240	HIS

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)

24 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	TRP	C	403	-	14,16,16	0.86	0	16,22,22	1.15	2 (12%)
3	HEM	A	401	-	41,50,50	1.85	6 (14%)	45,82,82	1.70	8 (17%)
2	TRP	E	403	-	14,16,16	0.87	1 (7%)	16,22,22	1.13	2 (12%)
3	HEM	B	401	-	41,50,50	1.96	7 (17%)	45,82,82	1.72	9 (20%)
2	TRP	F	403	-	14,16,16	0.86	1 (7%)	16,22,22	1.07	2 (12%)
3	HEM	F	401	-	41,50,50	1.97	8 (19%)	45,82,82	1.76	8 (17%)
3	HEM	C	401	-	41,50,50	1.89	6 (14%)	45,82,82	1.71	9 (20%)
2	TRP	D	403	-	14,16,16	0.86	1 (7%)	16,22,22	1.13	2 (12%)
3	HEM	D	401	-	41,50,50	1.90	4 (9%)	45,82,82	1.63	6 (13%)
2	TRP	B	403	-	14,16,16	0.87	1 (7%)	16,22,22	1.21	2 (12%)
3	HEM	H	401	-	41,50,50	1.98	6 (14%)	45,82,82	1.73	7 (15%)
2	TRP	H	402	-	14,16,16	0.87	1 (7%)	16,22,22	1.19	2 (12%)
2	TRP	D	402	-	14,16,16	0.86	0	16,22,22	1.16	2 (12%)
2	TRP	H	403	-	14,16,16	0.84	1 (7%)	16,22,22	1.13	2 (12%)
2	TRP	G	402	-	14,16,16	0.83	1 (7%)	16,22,22	1.12	3 (18%)
2	TRP	G	403	-	14,16,16	0.87	1 (7%)	16,22,22	1.18	2 (12%)
2	TRP	E	402	-	14,16,16	0.89	1 (7%)	16,22,22	1.15	2 (12%)
2	TRP	B	402	-	14,16,16	0.90	1 (7%)	16,22,22	1.13	2 (12%)
2	TRP	A	402	-	14,16,16	0.94	1 (7%)	16,22,22	0.99	0
3	HEM	E	401	-	41,50,50	1.98	7 (17%)	45,82,82	1.75	6 (13%)
2	TRP	A	403	-	14,16,16	0.87	1 (7%)	16,22,22	1.08	1 (6%)
2	TRP	F	402	-	14,16,16	0.84	0	16,22,22	1.19	2 (12%)
2	TRP	C	402	-	14,16,16	0.90	1 (7%)	16,22,22	1.06	1 (6%)
3	HEM	G	401	-	41,50,50	1.99	8 (19%)	45,82,82	1.82	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	TRP	C	403	-	-	0/7/8/8	0/2/2/2
3	HEM	A	401	-	-	4/12/54/54	-
2	TRP	E	403	-	-	0/7/8/8	0/2/2/2
3	HEM	B	401	-	-	2/12/54/54	-
2	TRP	F	403	-	-	0/7/8/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	F	401	-	-	2/12/54/54	-
3	HEM	C	401	-	-	2/12/54/54	-
2	TRP	D	403	-	-	0/7/8/8	0/2/2/2
3	HEM	D	401	-	-	4/12/54/54	-
2	TRP	B	403	-	-	0/7/8/8	0/2/2/2
3	HEM	H	401	-	-	2/12/54/54	-
2	TRP	H	402	-	-	1/7/8/8	0/2/2/2
2	TRP	D	402	-	-	5/7/8/8	0/2/2/2
2	TRP	H	403	-	-	0/7/8/8	0/2/2/2
2	TRP	G	402	-	-	2/7/8/8	0/2/2/2
2	TRP	G	403	-	-	0/7/8/8	0/2/2/2
2	TRP	E	402	-	-	3/7/8/8	0/2/2/2
2	TRP	B	402	-	-	4/7/8/8	0/2/2/2
2	TRP	A	402	-	-	5/7/8/8	0/2/2/2
3	HEM	E	401	-	-	4/12/54/54	-
2	TRP	A	403	-	-	0/7/8/8	0/2/2/2
2	TRP	F	402	-	-	3/7/8/8	0/2/2/2
2	TRP	C	402	-	-	5/7/8/8	0/2/2/2
3	HEM	G	401	-	-	4/12/54/54	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	HEM	C3D-C2D	8.15	1.54	1.36
3	G	401	HEM	C3D-C2D	7.93	1.53	1.36
3	H	401	HEM	C3D-C2D	7.89	1.53	1.36
3	F	401	HEM	C3D-C2D	7.88	1.53	1.36
3	B	401	HEM	C3D-C2D	7.85	1.53	1.36
3	C	401	HEM	C3D-C2D	7.68	1.53	1.36
3	D	401	HEM	C3D-C2D	7.61	1.52	1.36
3	A	401	HEM	C3D-C2D	7.41	1.52	1.36
3	D	401	HEM	C3C-C2C	-5.04	1.33	1.40
3	B	401	HEM	C3C-C2C	-4.74	1.33	1.40
3	E	401	HEM	C3C-C2C	-4.69	1.33	1.40
3	C	401	HEM	C3C-C2C	-4.67	1.33	1.40
3	F	401	HEM	C3C-C2C	-4.61	1.34	1.40
3	H	401	HEM	C3C-C2C	-4.57	1.34	1.40
3	G	401	HEM	C3C-C2C	-4.52	1.34	1.40
3	A	401	HEM	C3C-C2C	-4.20	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	HEM	C3C-CAC	3.75	1.55	1.47
3	H	401	HEM	C3C-CAC	3.64	1.55	1.47
3	C	401	HEM	C3C-CAC	3.60	1.55	1.47
3	F	401	HEM	C3C-CAC	3.56	1.55	1.47
3	G	401	HEM	C3C-CAC	3.47	1.54	1.47
3	E	401	HEM	C3C-CAC	3.46	1.54	1.47
3	B	401	HEM	C3C-CAC	3.34	1.54	1.47
3	G	401	HEM	FE-ND	3.04	2.11	1.96
3	A	401	HEM	FE-ND	3.00	2.11	1.96
3	H	401	HEM	CAB-C3B	2.98	1.55	1.47
3	B	401	HEM	CAB-C3B	2.97	1.55	1.47
3	C	401	HEM	CAB-C3B	2.91	1.55	1.47
3	A	401	HEM	C3C-CAC	2.80	1.53	1.47
3	G	401	HEM	CAB-C3B	2.79	1.55	1.47
3	D	401	HEM	CAB-C3B	2.77	1.55	1.47
3	F	401	HEM	CAB-C3B	2.77	1.55	1.47
3	A	401	HEM	CAB-C3B	2.76	1.54	1.47
3	E	401	HEM	FE-ND	2.73	2.10	1.96
3	E	401	HEM	CAB-C3B	2.67	1.54	1.47
3	H	401	HEM	FE-ND	2.64	2.09	1.96
3	B	401	HEM	FE-ND	2.48	2.09	1.96
3	F	401	HEM	FE-ND	2.37	2.08	1.96
3	F	401	HEM	FE-NB	2.27	2.08	1.96
3	G	401	HEM	FE-NB	2.23	2.07	1.96
3	B	401	HEM	CAA-C2A	2.22	1.55	1.52
3	F	401	HEM	CAA-C2A	2.18	1.55	1.52
3	A	401	HEM	CAA-C2A	2.14	1.55	1.52
3	G	401	HEM	CMB-C2B	2.14	1.55	1.50
2	C	402	TRP	OXT-C	-2.13	1.23	1.30
3	E	401	HEM	CMB-C2B	2.12	1.55	1.50
3	H	401	HEM	FE-NB	2.11	2.07	1.96
2	H	402	TRP	OXT-C	-2.11	1.23	1.30
2	G	403	TRP	OXT-C	-2.11	1.23	1.30
2	A	403	TRP	OXT-C	-2.10	1.23	1.30
3	F	401	HEM	CMB-C2B	2.10	1.55	1.50
2	D	403	TRP	OXT-C	-2.10	1.23	1.30
3	C	401	HEM	CAA-C2A	2.09	1.55	1.52
2	F	403	TRP	OXT-C	-2.07	1.23	1.30
2	A	402	TRP	OXT-C	-2.07	1.23	1.30
2	E	403	TRP	OXT-C	-2.07	1.23	1.30
2	B	402	TRP	OXT-C	-2.06	1.23	1.30
3	C	401	HEM	CMB-C2B	2.03	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	401	HEM	CAA-C2A	2.02	1.55	1.52
2	E	402	TRP	OXT-C	-2.02	1.23	1.30
2	H	403	TRP	OXT-C	-2.02	1.23	1.30
3	E	401	HEM	CAA-C2A	2.02	1.55	1.52
3	B	401	HEM	CMD-C2D	2.02	1.55	1.50
2	B	403	TRP	OXT-C	-2.01	1.24	1.30
2	G	402	TRP	OXT-C	-2.01	1.24	1.30

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	401	HEM	C4D-ND-C1D	7.27	112.58	105.07
3	F	401	HEM	C4D-ND-C1D	6.66	111.95	105.07
3	E	401	HEM	C4D-ND-C1D	6.65	111.94	105.07
3	H	401	HEM	C4D-ND-C1D	6.30	111.58	105.07
3	B	401	HEM	C4D-ND-C1D	6.18	111.46	105.07
3	C	401	HEM	C4D-ND-C1D	5.85	111.11	105.07
3	A	401	HEM	C4D-ND-C1D	5.78	111.05	105.07
3	D	401	HEM	C4D-ND-C1D	5.71	110.97	105.07
3	H	401	HEM	C4C-CHD-C1D	4.11	127.98	122.56
3	F	401	HEM	C4C-CHD-C1D	3.92	127.74	122.56
3	E	401	HEM	C4B-CHC-C1C	3.52	127.20	122.56
3	D	401	HEM	C4C-CHD-C1D	3.36	126.99	122.56
3	C	401	HEM	CMA-C3A-C4A	-3.34	123.33	128.46
3	D	401	HEM	CBA-CAA-C2A	-3.14	107.25	112.62
3	F	401	HEM	C1B-NB-C4B	3.09	108.27	105.07
3	G	401	HEM	C4B-CHC-C1C	3.08	126.62	122.56
3	A	401	HEM	CMA-C3A-C4A	-2.98	123.89	128.46
3	B	401	HEM	C4B-CHC-C1C	2.98	126.49	122.56
3	C	401	HEM	C4C-CHD-C1D	2.95	126.45	122.56
3	A	401	HEM	C4B-CHC-C1C	2.95	126.45	122.56
2	H	402	TRP	OXT-C-O	-2.92	117.47	124.09
3	E	401	HEM	CBA-CAA-C2A	-2.86	107.73	112.62
3	B	401	HEM	C4C-CHD-C1D	2.86	126.34	122.56
3	A	401	HEM	C1B-NB-C4B	2.85	108.01	105.07
3	G	401	HEM	C1B-NB-C4B	2.83	108.00	105.07
3	C	401	HEM	CHD-C1D-ND	2.82	127.50	124.43
3	H	401	HEM	C1B-NB-C4B	2.79	107.95	105.07
2	G	403	TRP	OXT-C-O	-2.78	117.78	124.09
3	E	401	HEM	C1B-NB-C4B	2.74	107.90	105.07
3	H	401	HEM	CBA-CAA-C2A	-2.73	107.96	112.62
2	B	402	TRP	OXT-C-O	-2.70	117.95	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	401	HEM	C4C-CHD-C1D	2.69	126.10	122.56
3	A	401	HEM	CBD-CAD-C3D	-2.67	105.21	112.63
2	D	402	TRP	OXT-C-O	-2.66	118.05	124.09
3	D	401	HEM	CMA-C3A-C4A	-2.66	124.38	128.46
3	F	401	HEM	C4B-CHC-C1C	2.64	126.04	122.56
3	H	401	HEM	C3B-C2B-C1B	2.63	108.44	106.49
3	B	401	HEM	CMA-C3A-C4A	-2.62	124.43	128.46
3	B	401	HEM	CBD-CAD-C3D	-2.62	105.34	112.63
2	B	403	TRP	OXT-C-O	-2.61	118.16	124.09
3	G	401	HEM	CBA-CAA-C2A	-2.61	108.16	112.62
2	F	402	TRP	OXT-C-CA	2.61	122.27	113.38
2	E	402	TRP	OXT-C-O	-2.55	118.29	124.09
2	E	403	TRP	OXT-C-O	-2.52	118.37	124.09
3	E	401	HEM	C4C-CHD-C1D	2.50	125.86	122.56
3	B	401	HEM	C1B-NB-C4B	2.49	107.64	105.07
3	A	401	HEM	CHC-C4B-NB	2.45	127.09	124.43
2	C	403	TRP	OXT-C-O	-2.44	118.54	124.09
3	D	401	HEM	CHD-C1D-ND	2.44	127.08	124.43
2	H	403	TRP	OXT-C-CA	2.42	121.62	113.38
2	B	403	TRP	OXT-C-CA	2.41	121.60	113.38
2	D	403	TRP	OXT-C-O	-2.41	118.61	124.09
2	D	403	TRP	OXT-C-CA	2.40	121.58	113.38
2	C	402	TRP	OXT-C-O	-2.40	118.64	124.09
2	E	402	TRP	OXT-C-CA	2.37	121.47	113.38
2	A	403	TRP	OXT-C-O	-2.36	118.72	124.09
3	C	401	HEM	CBA-CAA-C2A	-2.36	108.59	112.62
2	C	403	TRP	OXT-C-CA	2.35	121.40	113.38
2	F	402	TRP	OXT-C-O	-2.33	118.80	124.09
3	C	401	HEM	CAD-C3D-C4D	2.32	128.71	124.66
2	H	403	TRP	OXT-C-O	-2.30	118.86	124.09
3	B	401	HEM	CBA-CAA-C2A	-2.29	108.71	112.62
2	G	402	TRP	OXT-C-O	-2.29	118.90	124.09
2	G	403	TRP	OXT-C-CA	2.29	121.17	113.38
2	D	402	TRP	OXT-C-CA	2.27	121.13	113.38
3	G	401	HEM	CHC-C4B-NB	2.23	126.86	124.43
2	H	402	TRP	OXT-C-CA	2.22	120.96	113.38
3	F	401	HEM	C4A-C3A-C2A	2.20	108.53	107.00
3	H	401	HEM	C4B-CHC-C1C	2.20	125.46	122.56
2	E	403	TRP	OXT-C-CA	2.19	120.84	113.38
3	F	401	HEM	CBA-CAA-C2A	-2.18	108.89	112.62
3	H	401	HEM	CBD-CAD-C3D	-2.18	106.58	112.63
3	D	401	HEM	C4B-CHC-C1C	2.17	125.43	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	HEM	C2C-C3C-C4C	2.17	108.42	106.90
3	C	401	HEM	C4B-CHC-C1C	2.17	125.42	122.56
3	C	401	HEM	CHC-C4B-NB	2.16	126.78	124.43
2	B	402	TRP	OXT-C-CA	2.16	120.72	113.38
2	F	403	TRP	OXT-C-O	-2.11	119.30	124.09
3	E	401	HEM	CHC-C4B-NB	2.11	126.72	124.43
3	B	401	HEM	C3B-C2B-C1B	2.09	108.04	106.49
3	F	401	HEM	CHD-C1D-ND	2.08	126.69	124.43
2	G	402	TRP	OXT-C-CA	2.05	120.37	113.38
2	F	403	TRP	OXT-C-CA	2.04	120.34	113.38
3	F	401	HEM	CAD-C3D-C4D	2.03	128.21	124.66
3	C	401	HEM	CAA-CBA-CGA	-2.01	108.11	113.76
3	B	401	HEM	C4A-C3A-C2A	2.01	108.39	107.00
3	A	401	HEM	C4C-CHD-C1D	2.01	125.21	122.56
2	G	402	TRP	CH2-CZ2-CE2	-2.00	117.20	120.08

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	TRP	N-CA-CB-CG
2	A	402	TRP	CA-CB-CG-CD1
2	B	402	TRP	CA-CB-CG-CD1
2	C	402	TRP	CA-CB-CG-CD1
2	D	402	TRP	CA-CB-CG-CD1
2	E	402	TRP	CA-CB-CG-CD1
2	F	402	TRP	CA-CB-CG-CD1
2	G	402	TRP	CA-CB-CG-CD1
2	H	402	TRP	CA-CB-CG-CD1
2	A	402	TRP	O-C-CA-CB
2	B	402	TRP	O-C-CA-CB
2	D	402	TRP	O-C-CA-CB
2	F	402	TRP	O-C-CA-CB
2	A	402	TRP	C-CA-CB-CG
2	C	402	TRP	N-CA-CB-CG
2	D	402	TRP	N-CA-CB-CG
2	D	402	TRP	C-CA-CB-CG
2	B	402	TRP	OXT-C-CA-CB
2	C	402	TRP	O-C-CA-CB
2	D	402	TRP	OXT-C-CA-CB
2	A	402	TRP	OXT-C-CA-CB
2	C	402	TRP	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	F	402	TRP	OXT-C-CA-CB
3	H	401	HEM	CAA-CBA-CGA-O2A
3	F	401	HEM	CAA-CBA-CGA-O2A
3	B	401	HEM	CAA-CBA-CGA-O1A
3	A	401	HEM	CAA-CBA-CGA-O1A
3	C	401	HEM	CAA-CBA-CGA-O2A
3	D	401	HEM	CAA-CBA-CGA-O1A
3	A	401	HEM	CAA-CBA-CGA-O2A
3	G	401	HEM	CAA-CBA-CGA-O1A
3	B	401	HEM	CAA-CBA-CGA-O2A
3	D	401	HEM	CAA-CBA-CGA-O2A
3	H	401	HEM	CAA-CBA-CGA-O1A
3	F	401	HEM	CAA-CBA-CGA-O1A
3	C	401	HEM	CAA-CBA-CGA-O1A
2	E	402	TRP	OXT-C-CA-CB
3	E	401	HEM	CAA-CBA-CGA-O1A
3	E	401	HEM	CAA-CBA-CGA-O2A
3	A	401	HEM	CAD-CBD-CGD-O2D
3	G	401	HEM	CAD-CBD-CGD-O2D
3	D	401	HEM	CAD-CBD-CGD-O2D
3	G	401	HEM	CAA-CBA-CGA-O2A
3	A	401	HEM	CAD-CBD-CGD-O1D
2	E	402	TRP	O-C-CA-CB
2	B	402	TRP	C-CA-CB-CG
2	C	402	TRP	C-CA-CB-CG
3	G	401	HEM	CAD-CBD-CGD-O1D
3	D	401	HEM	CAD-CBD-CGD-O1D
3	E	401	HEM	CAD-CBD-CGD-O2D
2	G	402	TRP	OXT-C-CA-CB
3	E	401	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

14 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	HEM	5	0
2	E	403	TRP	1	0
3	B	401	HEM	4	0
3	F	401	HEM	9	0
3	C	401	HEM	6	0
2	D	403	TRP	1	0
3	D	401	HEM	4	0

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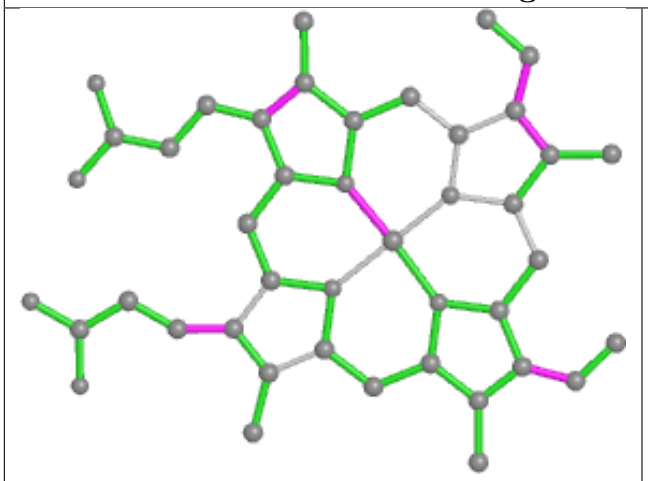
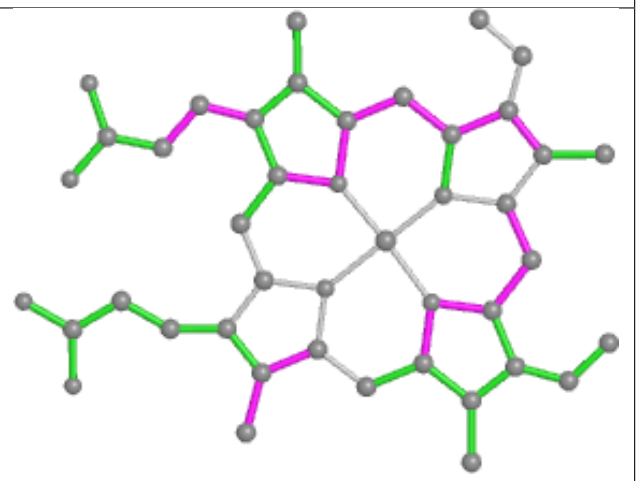
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	403	TRP	1	0
3	H	401	HEM	4	0
2	H	403	TRP	1	0
2	G	402	TRP	2	0
3	E	401	HEM	6	0
2	A	403	TRP	1	0
3	G	401	HEM	6	0

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.

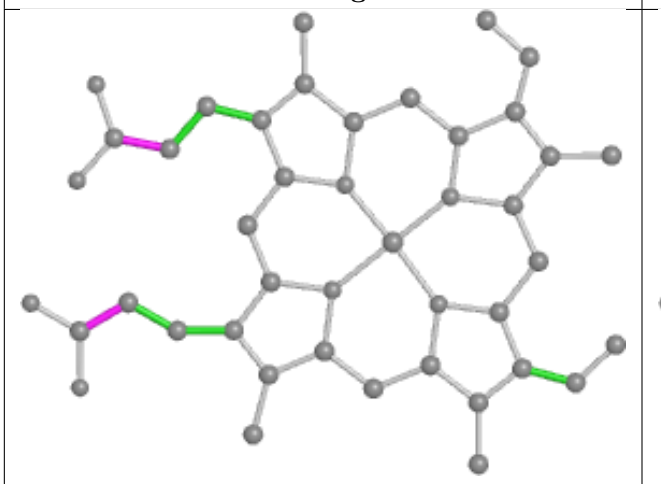
Ligand HEM A 401



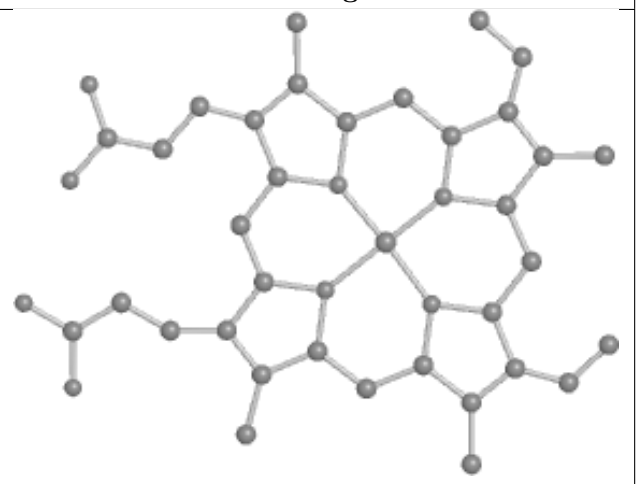
Bond lengths



Bond angles

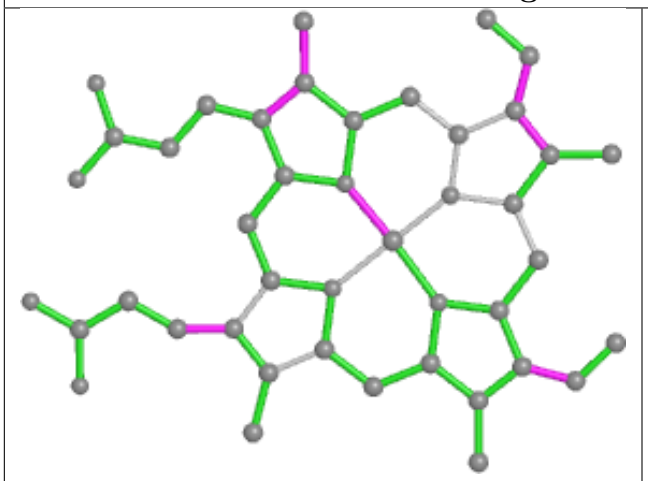


Torsions

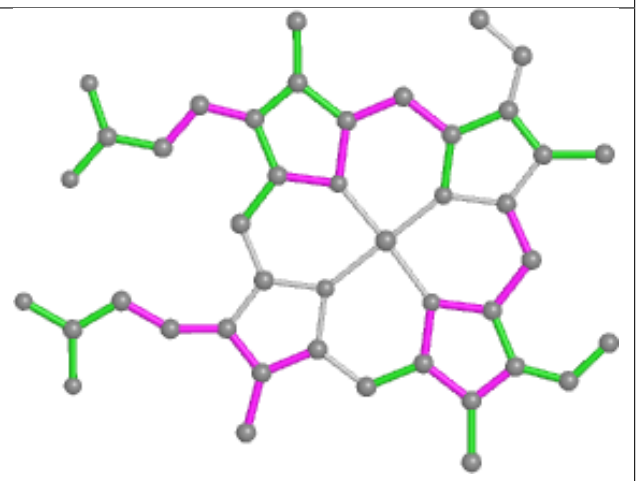


Rings

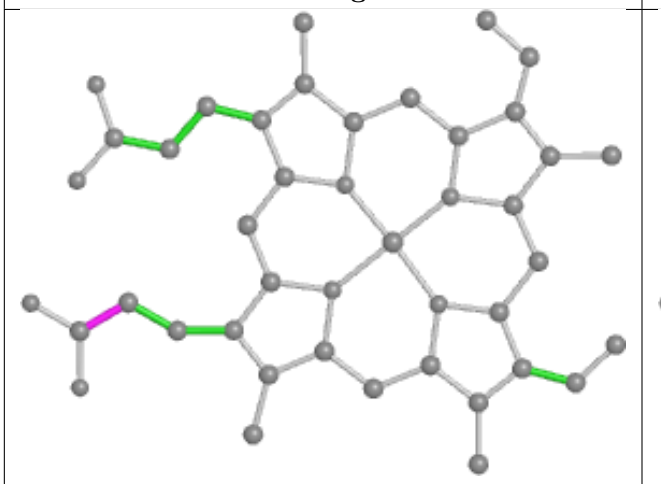
Ligand HEM B 401



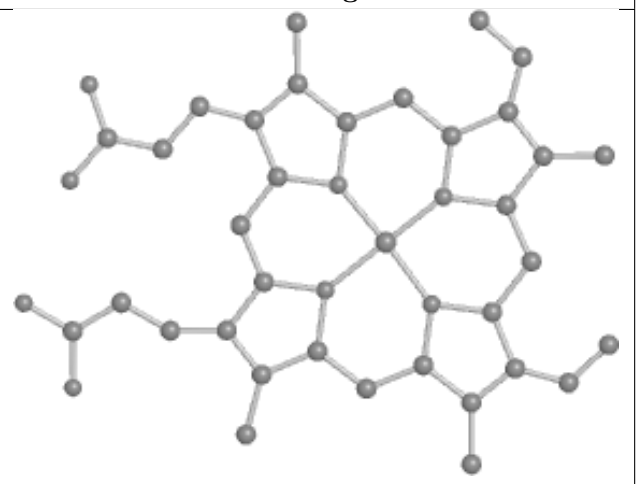
Bond lengths



Bond angles

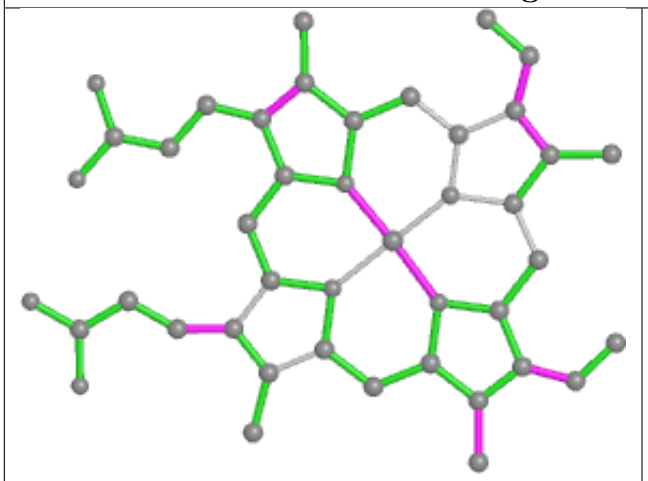


Torsions

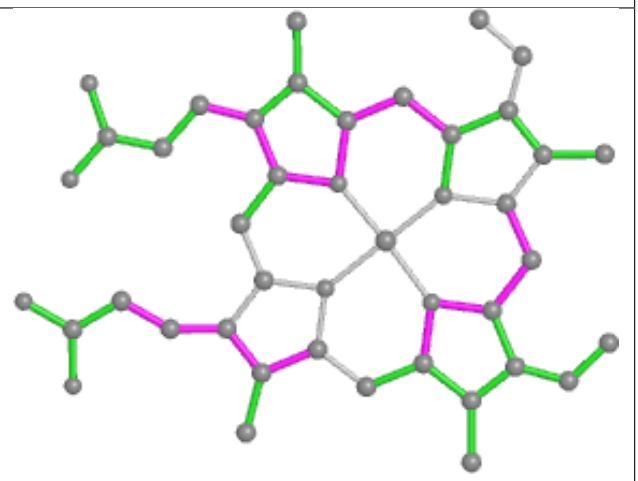


Rings

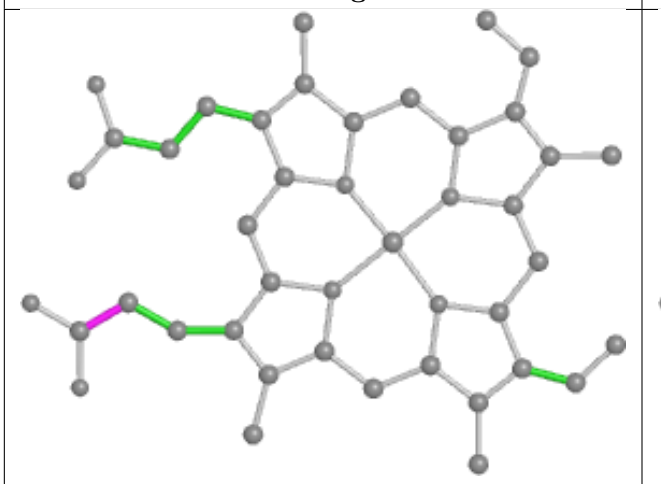
Ligand HEM F 401



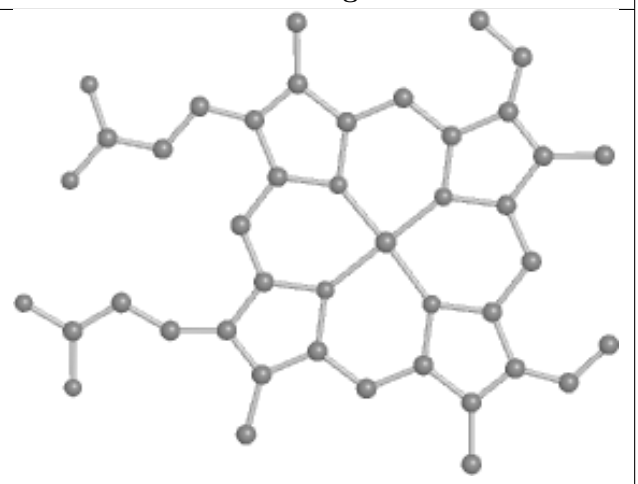
Bond lengths



Bond angles

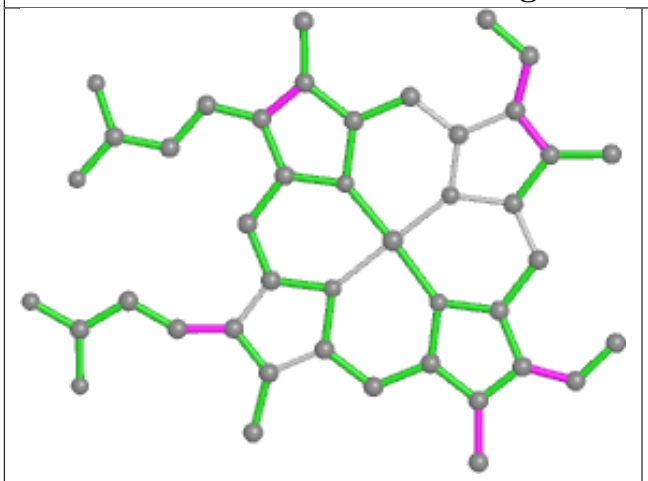


Torsions

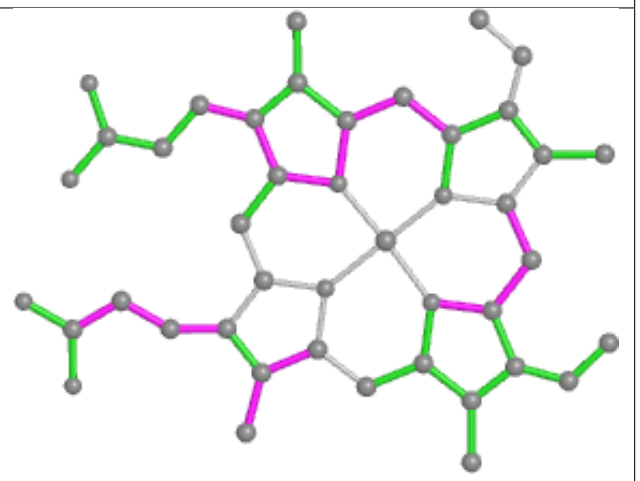


Rings

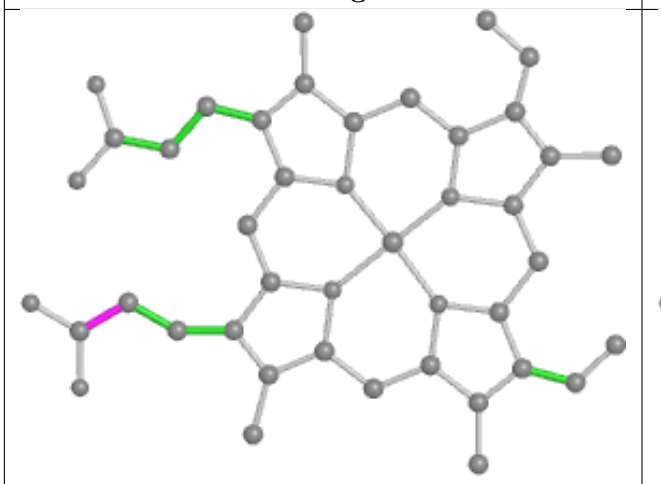
Ligand HEM C 401



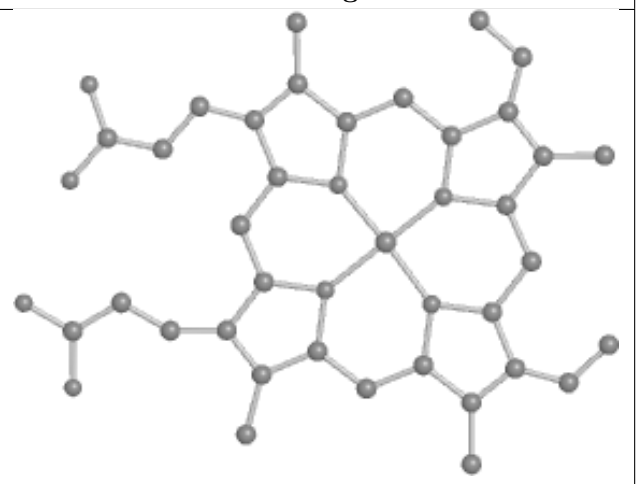
Bond lengths



Bond angles

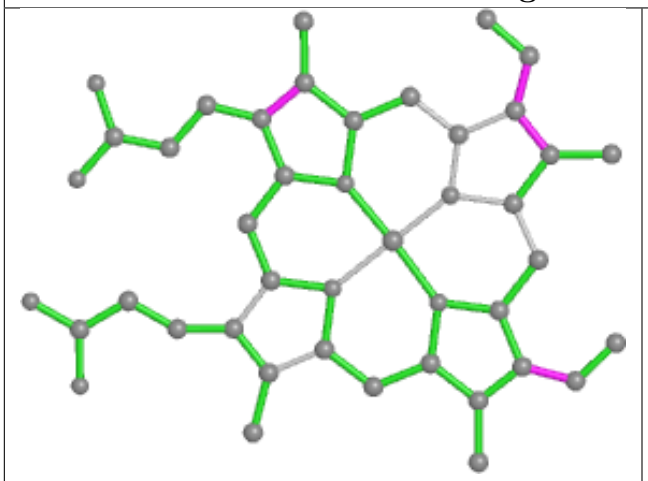


Torsions

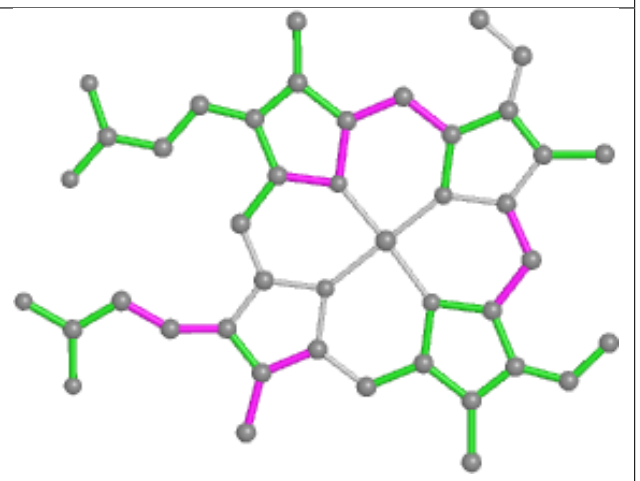


Rings

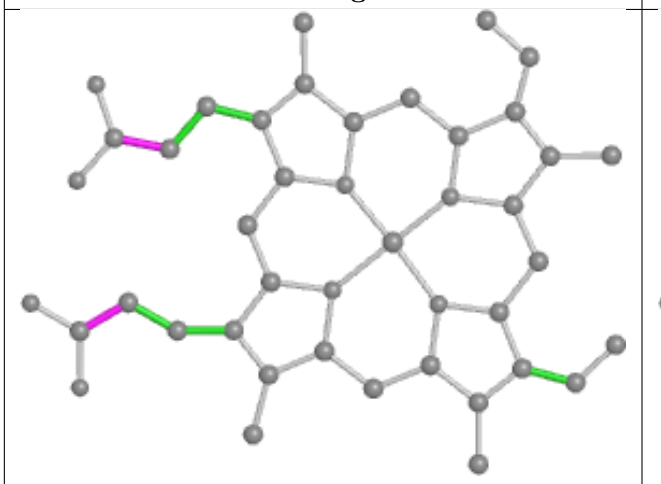
Ligand HEM D 401



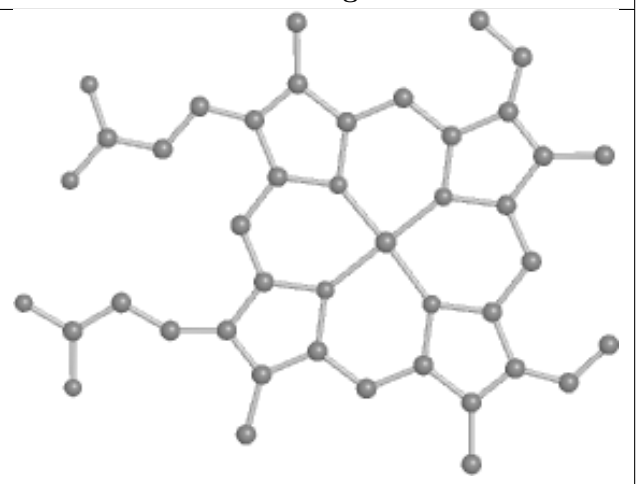
Bond lengths



Bond angles

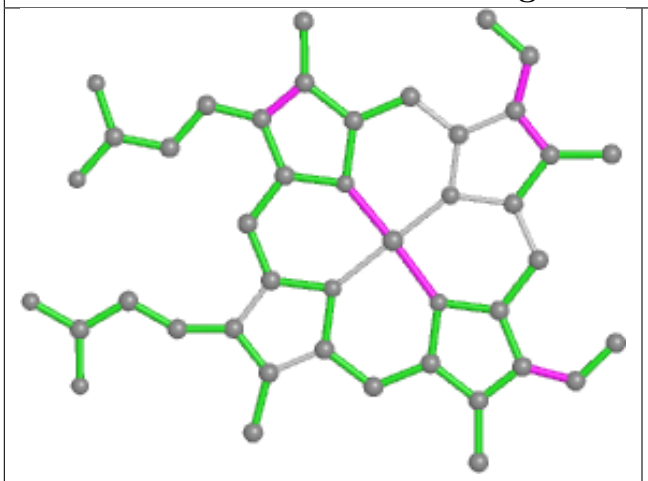


Torsions

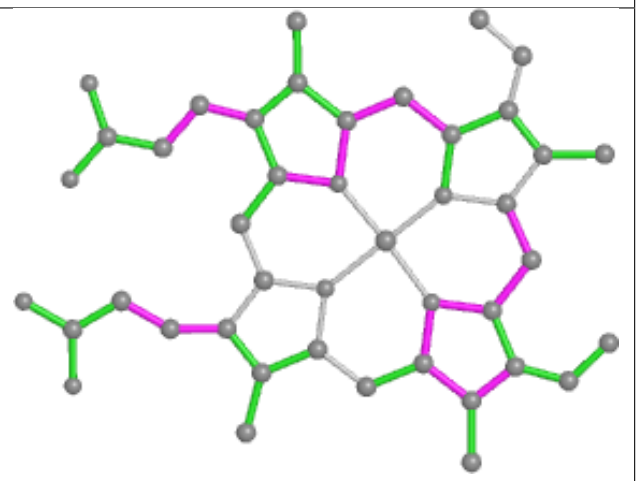


Rings

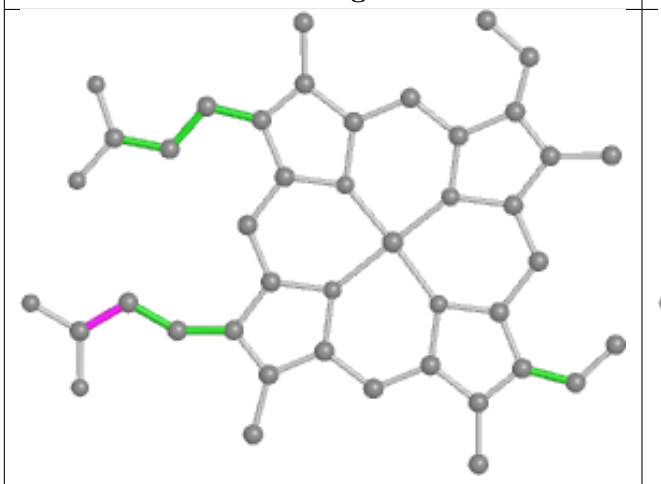
Ligand HEM H 401



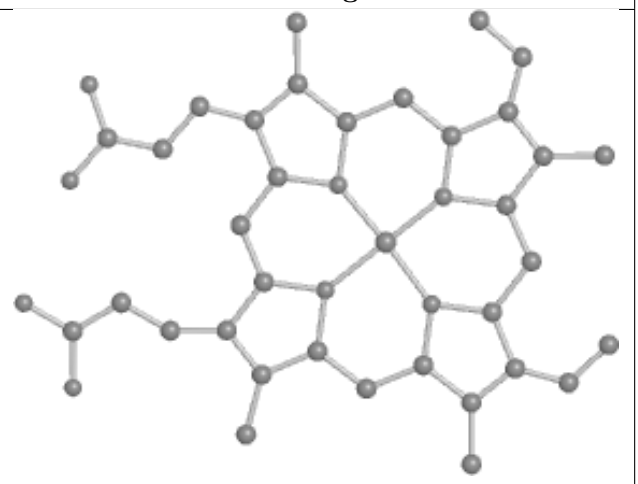
Bond lengths



Bond angles

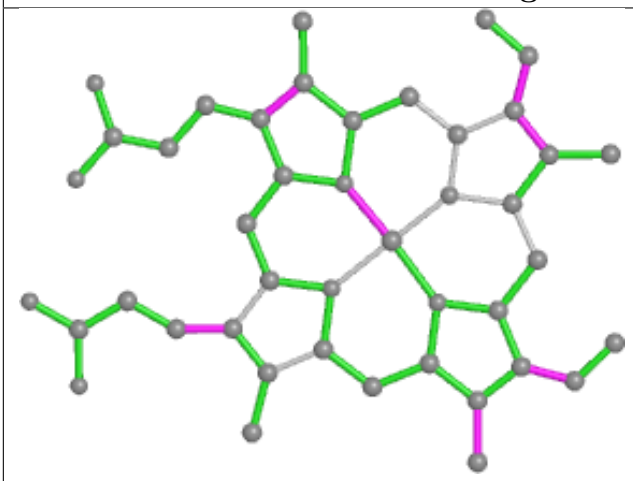


Torsions

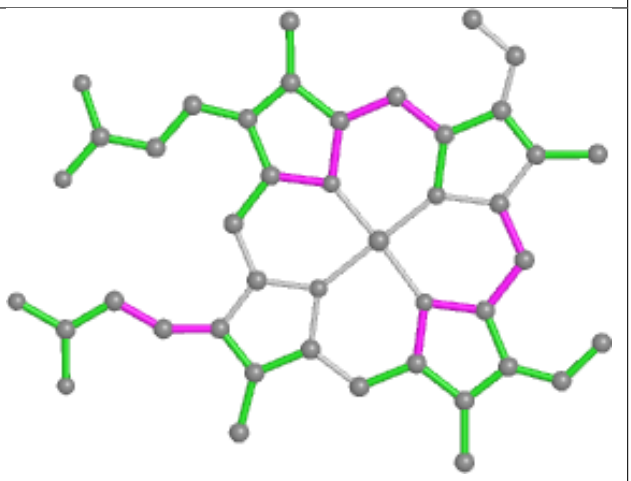


Rings

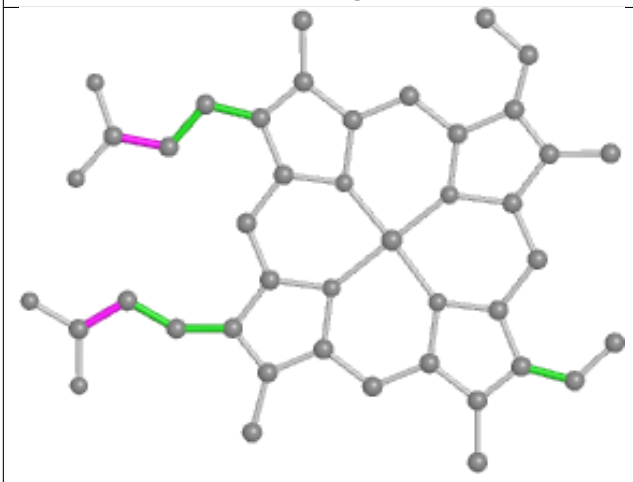
Ligand HEM E 401



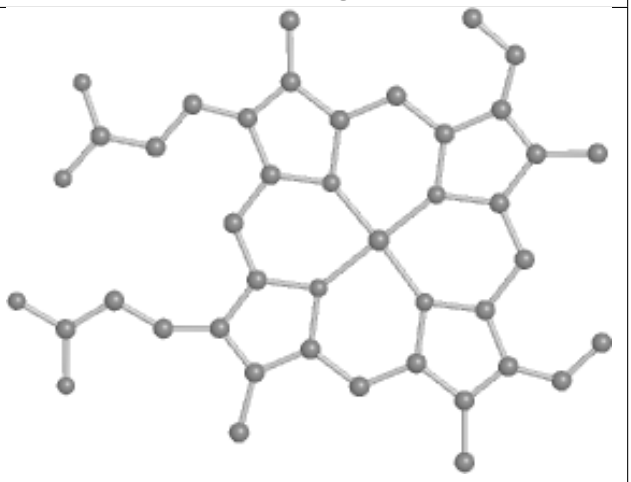
Bond lengths



Bond angles

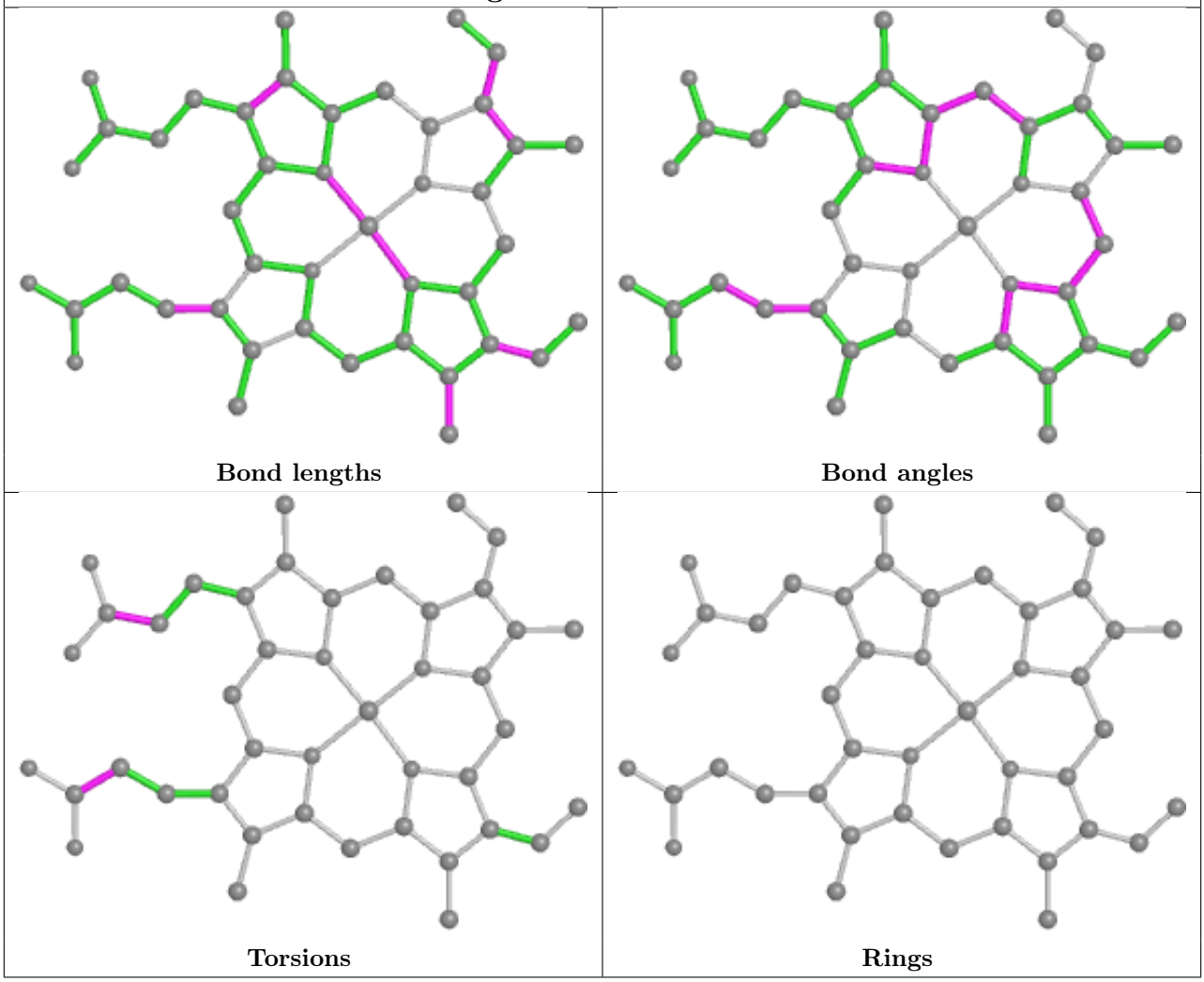


Torsions



Rings

Ligand HEM G 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	280/298 (93%)	-0.19	6 (2%)	63	66	9, 18, 35, 51	0
1	B	280/298 (93%)	-0.24	4 (1%)	75	77	10, 18, 34, 55	0
1	C	280/298 (93%)	0.13	17 (6%)	21	24	13, 25, 46, 61	0
1	D	280/298 (93%)	-0.04	7 (2%)	57	60	13, 23, 40, 60	0
1	E	278/298 (93%)	0.55	36 (12%)	3	3	20, 35, 55, 71	0
1	F	276/298 (92%)	0.06	20 (7%)	15	17	12, 27, 50, 66	0
1	G	277/298 (92%)	0.21	21 (7%)	13	15	17, 28, 49, 63	0
1	H	276/298 (92%)	-0.10	9 (3%)	46	49	14, 25, 41, 61	0
All	All	2227/2384 (93%)	0.05	120 (5%)	25	29	9, 24, 47, 71	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	284	VAL	10.8
1	D	286	ASN	7.2
1	C	286	ASN	7.1
1	G	197	VAL	6.0
1	E	197	VAL	5.9
1	G	283	GLY	5.8
1	E	17	ASP	5.5
1	D	284	VAL	5.4
1	C	284	VAL	5.4
1	E	19	GLU	5.2
1	G	12	PRO	5.1
1	C	197	VAL	4.9
1	E	7	LEU	4.6
1	G	19	GLU	4.6
1	E	185	GLN	4.4
1	G	20	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	189	ALA	4.3
1	H	19	GLU	4.2
1	B	284	VAL	4.2
1	C	198	ALA	4.2
1	F	19	GLU	4.1
1	G	189	ALA	4.1
1	H	17	ASP	4.1
1	C	191	ASP	4.1
1	F	12	PRO	4.1
1	C	190	ARG	4.0
1	F	20	GLY	4.0
1	C	193	THR	3.9
1	A	286	ASN	3.9
1	B	286	ASN	3.8
1	E	20	GLY	3.8
1	E	9	ASP	3.7
1	A	151	TYR	3.7
1	D	197	VAL	3.7
1	E	200	ASP	3.7
1	F	150	ALA	3.6
1	D	19	GLU	3.5
1	A	19	GLU	3.5
1	E	189	ALA	3.5
1	B	151	TYR	3.5
1	E	12	PRO	3.5
1	G	195	ALA	3.3
1	E	188	GLN	3.3
1	H	42	GLU	3.3
1	G	191	ASP	3.2
1	E	192	TRP	3.2
1	E	268	ALA	3.2
1	F	118	ASP	3.2
1	G	13	GLY	3.1
1	G	193	THR	3.1
1	E	283	GLY	3.1
1	E	191	ASP	3.0
1	H	43	PRO	3.0
1	E	190	ARG	3.0
1	G	185	GLN	3.0
1	D	17	ASP	3.0
1	C	285	ASP	3.0
1	E	42	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	20	GLY	3.0
1	G	42	GLU	2.9
1	E	21	ARG	2.9
1	F	43	PRO	2.9
1	F	42	GLU	2.8
1	E	214	ASP	2.8
1	G	190	ARG	2.8
1	E	194	ALA	2.8
1	C	185	GLN	2.8
1	E	146	LEU	2.7
1	C	19	GLU	2.7
1	E	161	GLU	2.7
1	F	9	ASP	2.7
1	F	21	ARG	2.7
1	C	188	GLN	2.7
1	H	12	PRO	2.7
1	C	194	ALA	2.6
1	E	193	THR	2.6
1	A	284	VAL	2.6
1	F	18	LEU	2.6
1	D	285	ASP	2.6
1	E	31	ASP	2.6
1	H	7	LEU	2.6
1	D	12	PRO	2.6
1	G	17	ASP	2.6
1	E	204	PRO	2.5
1	A	147	GLN	2.5
1	F	147	GLN	2.5
1	B	285	ASP	2.5
1	E	144	GLN	2.5
1	F	10	LEU	2.5
1	H	118	ASP	2.4
1	G	7	LEU	2.4
1	G	200	ASP	2.4
1	F	114	MET	2.4
1	G	188	GLN	2.4
1	E	13	GLY	2.4
1	E	199	ASP	2.3
1	F	151	TYR	2.3
1	G	198	ALA	2.3
1	E	16	THR	2.3
1	F	44	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	17	ASP	2.3
1	E	252	ARG	2.3
1	F	31	ASP	2.2
1	G	214	ASP	2.2
1	G	18	LEU	2.2
1	F	153	PRO	2.2
1	C	201	THR	2.2
1	E	118	ASP	2.2
1	A	150	ALA	2.1
1	E	195	ALA	2.1
1	E	14	ILE	2.1
1	E	164	GLU	2.1
1	F	252	ARG	2.1
1	C	176	LEU	2.1
1	F	13	GLY	2.1
1	G	194	ALA	2.0
1	E	120	LEU	2.0
1	C	192	TRP	2.0
1	C	200	ASP	2.0
1	H	185	GLN	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	TRP	E	402	15/15	0.86	0.13	30,32,34,36	0
2	TRP	H	403	15/15	0.90	0.11	16,20,30,34	0
2	TRP	G	403	15/15	0.91	0.11	23,26,31,35	0

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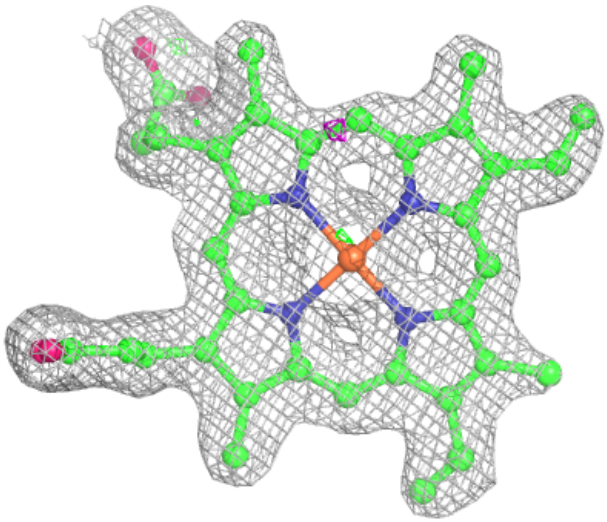
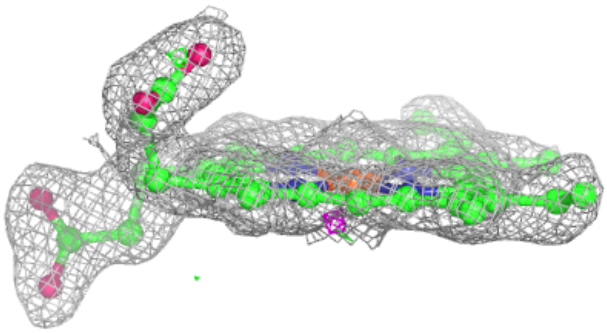
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TRP	F	402	15/15	0.92	0.12	31,32,36,36	0
2	TRP	E	403	15/15	0.93	0.12	27,29,35,35	0
2	TRP	C	402	15/15	0.93	0.10	16,18,23,24	0
2	TRP	C	403	15/15	0.94	0.09	15,18,27,27	0
2	TRP	H	402	15/15	0.94	0.09	27,29,32,33	0
2	TRP	D	402	15/15	0.95	0.09	16,20,22,25	0
2	TRP	G	402	15/15	0.95	0.09	23,28,29,31	0
2	TRP	D	403	15/15	0.95	0.09	13,16,26,26	0
2	TRP	F	403	15/15	0.95	0.08	15,19,28,30	0
3	HEM	E	401	43/43	0.95	0.12	25,29,33,38	0
2	TRP	A	403	15/15	0.96	0.08	15,16,22,23	0
2	TRP	B	402	15/15	0.96	0.09	12,15,18,19	0
2	TRP	B	403	15/15	0.96	0.07	13,17,24,30	0
2	TRP	A	402	15/15	0.96	0.10	9,12,14,21	0
3	HEM	F	401	43/43	0.96	0.10	26,29,34,36	0
3	HEM	G	401	43/43	0.96	0.09	20,25,30,33	0
3	HEM	H	401	43/43	0.96	0.10	20,27,31,34	0
3	HEM	C	401	43/43	0.98	0.09	14,17,22,28	0
3	HEM	D	401	43/43	0.98	0.09	11,16,21,25	0
3	HEM	A	401	43/43	0.99	0.09	7,10,13,17	0
3	HEM	B	401	43/43	0.99	0.09	9,13,15,21	0

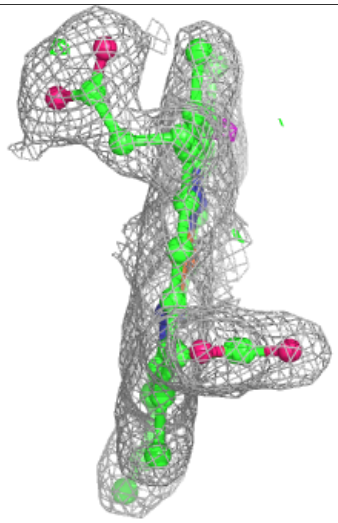
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM E 401:

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

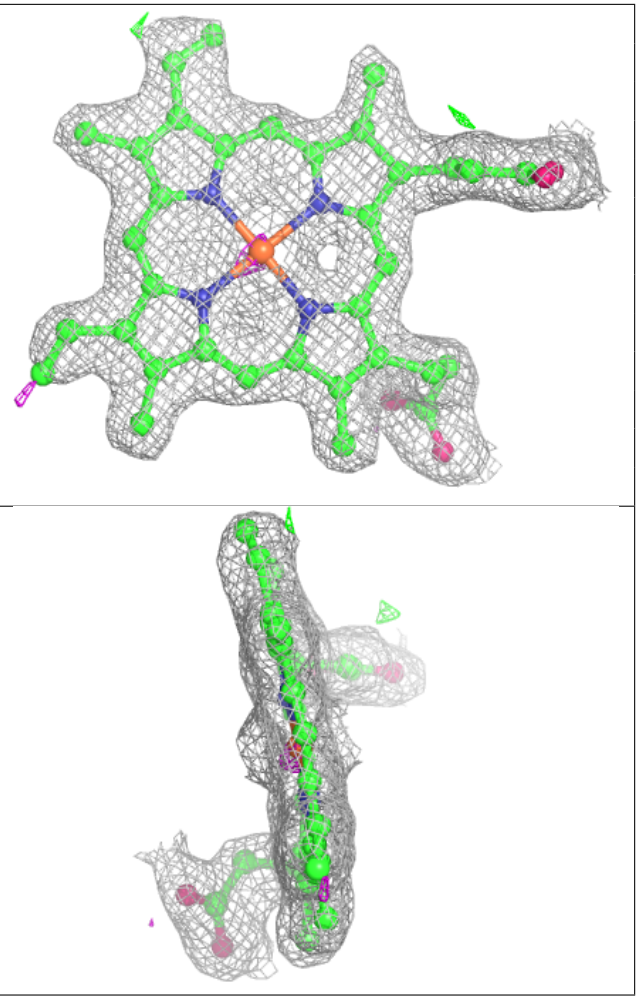






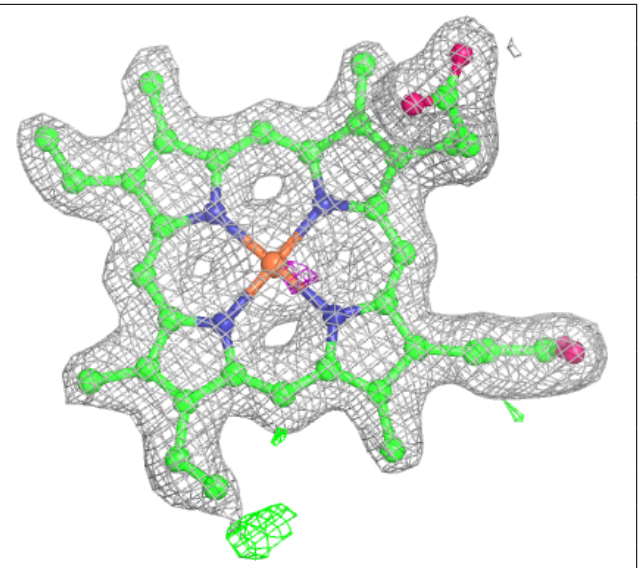
Electron density around HEM F 401:

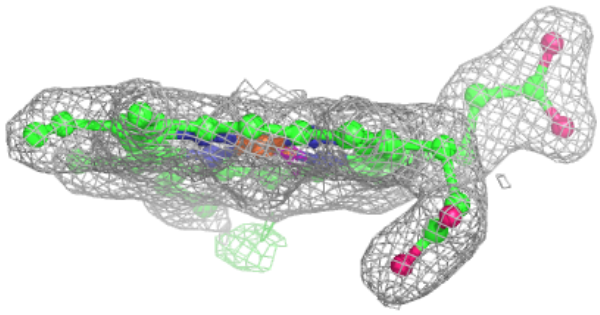
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

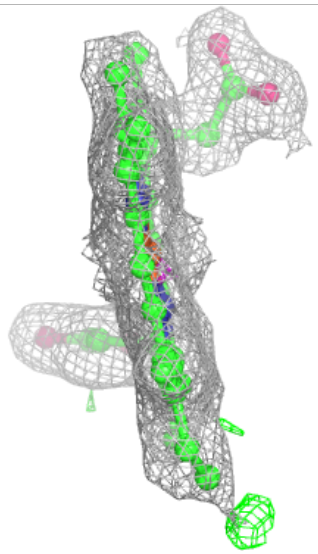


Electron density around HEM G 401:

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

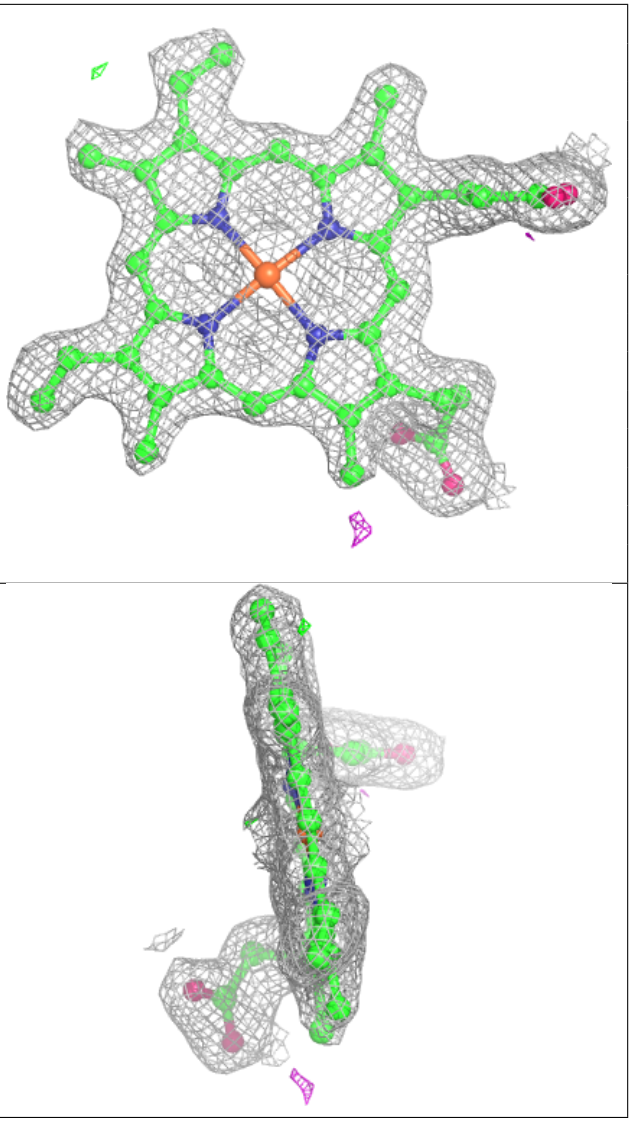






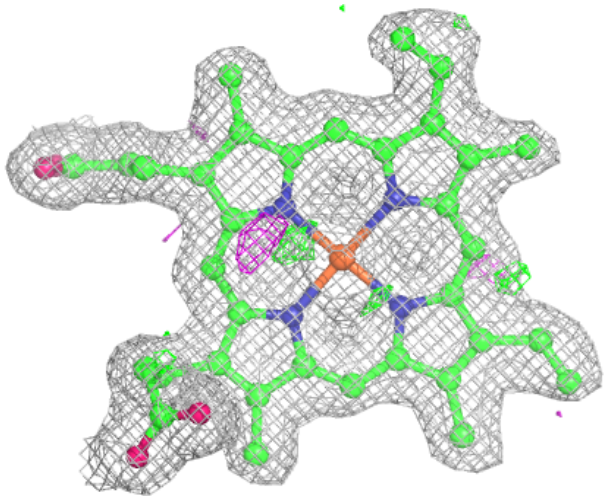
Electron density around HEM H 401:

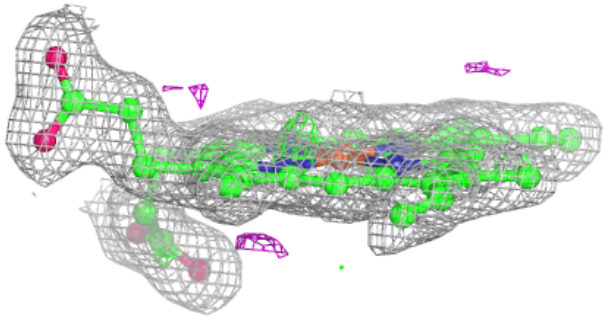
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 401:

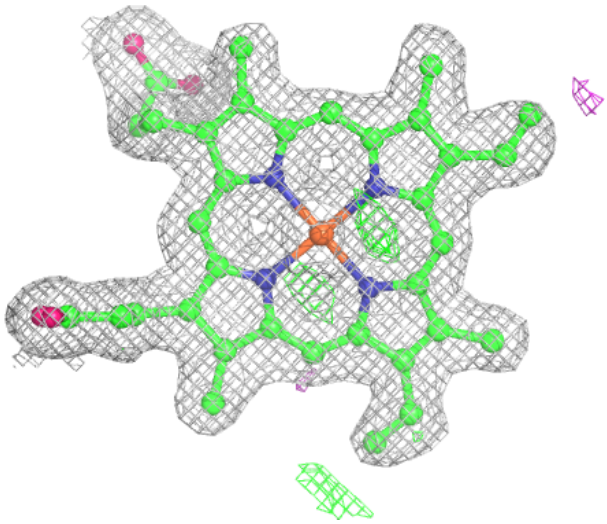
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

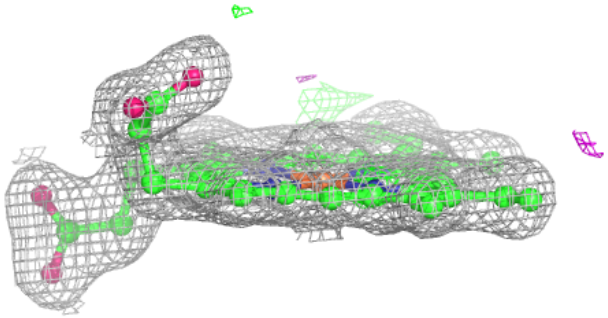




Electron density around HEM D 401:

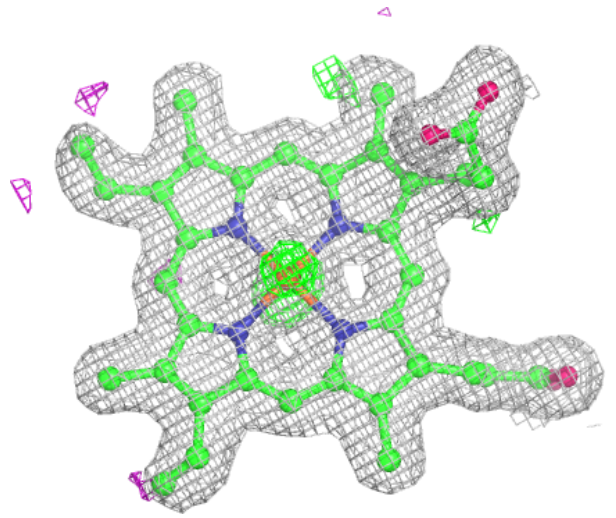
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

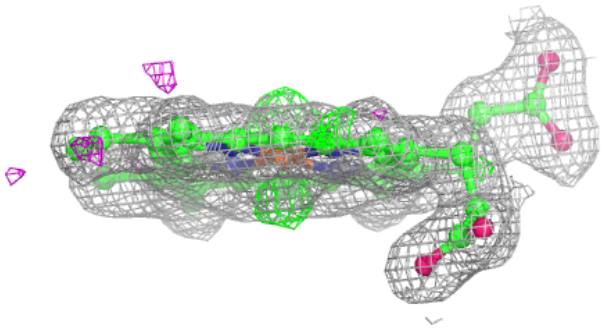


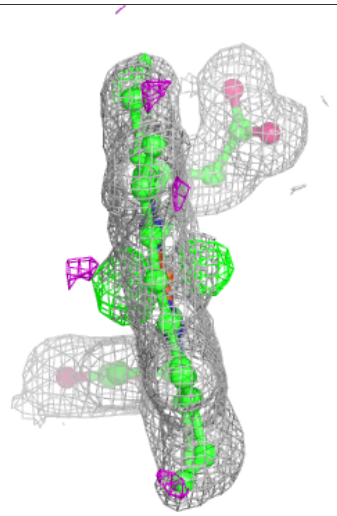


Electron density around HEM A 401:

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

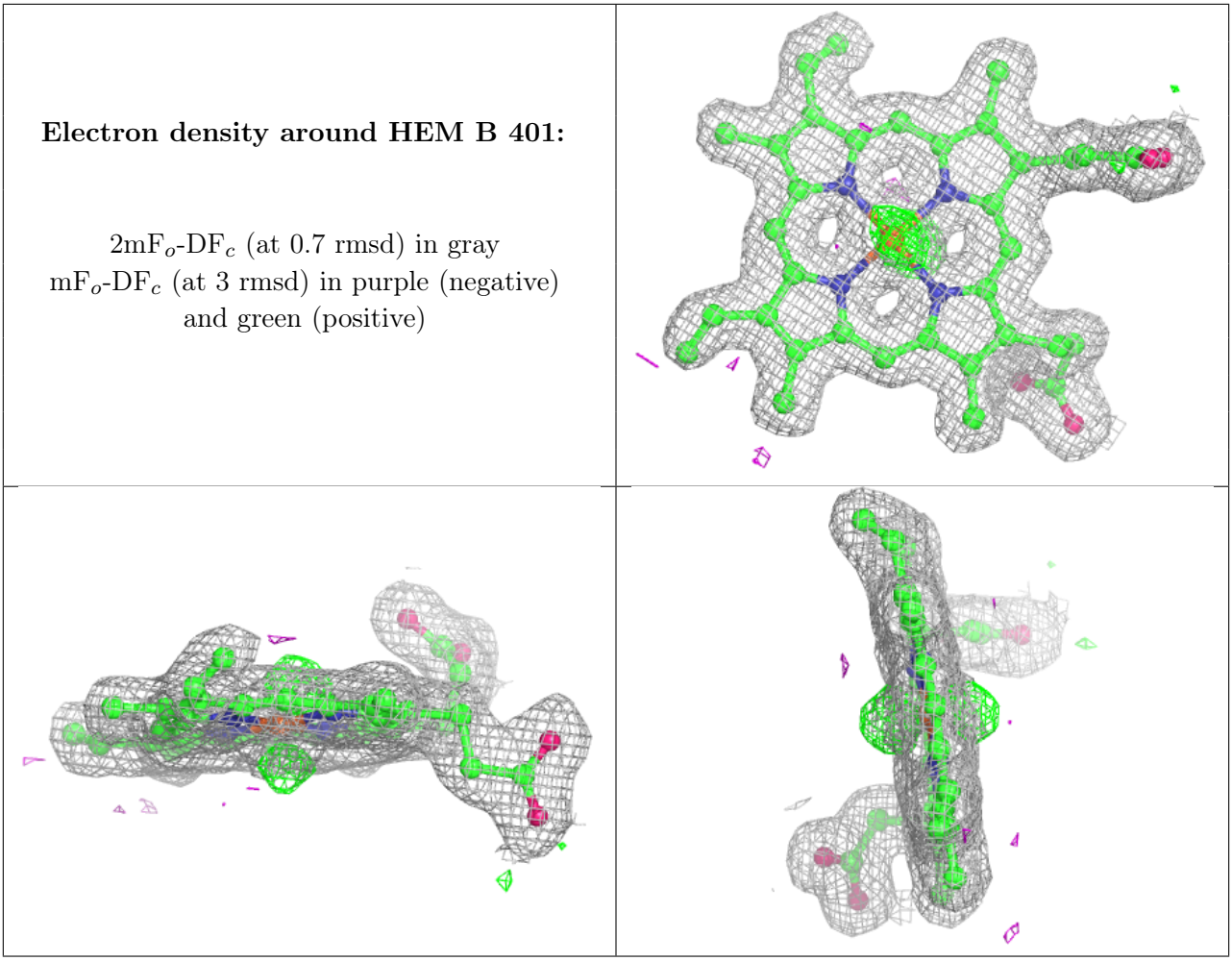






Electron density around HEM B 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.