Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2022 – 10:10 am BST

PDB ID	:	7QZA
Title	:	Crystal structure of a DyP-type peroxidase 29E4 variant from Pseudomonas putida
Authors	:	Borges, P.T.; Silva, D.; Frazao, C.; Martins, L.O.
Deposited on	:	2022-01-30
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

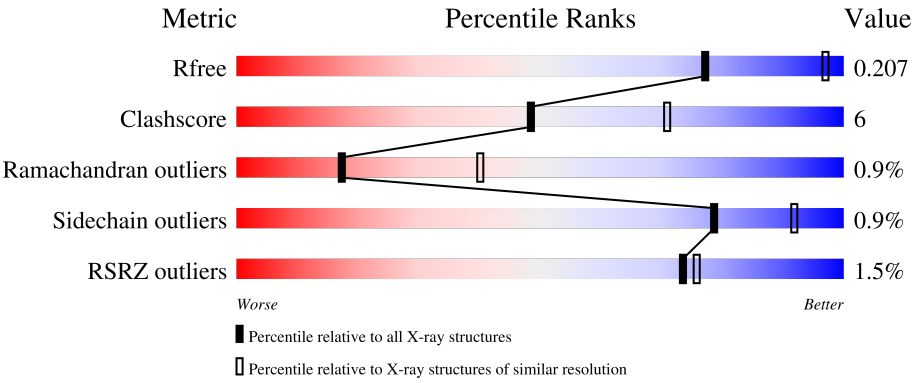
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.70 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.



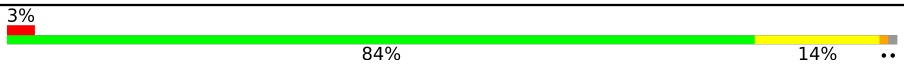
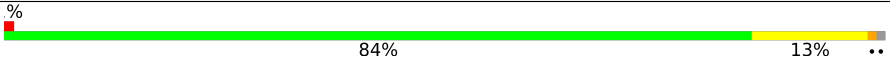
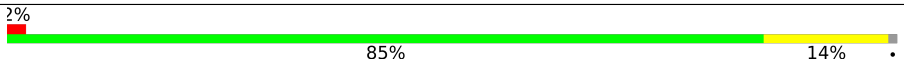
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	287	84% 14% ·
1	B	287	85% 12% ··
1	C	287	87% 10% ··
1	D	287	% 81% 16% ··
1	E	287	3% 84% 13% ··

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	287	
1	G	287	
1	H	287	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17810 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 Dyp-type peroxidase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2182	1388	378	412	4			
1	B	283	Total	C	N	O	S	0	0	0
			2181	1388	378	411	4			
1	C	283	Total	C	N	O	S	0	0	0
			2182	1388	378	412	4			
1	D	283	Total	C	N	O	S	0	0	0
			2182	1388	378	412	4			
1	E	283	Total	C	N	O	S	0	0	0
			2182	1388	378	412	4			
1	F	283	Total	C	N	O	S	0	0	0
			2182	1388	378	412	4			
1	G	283	Total	C	N	O	S	0	0	0
			2182	1388	378	412	4			
1	H	283	Total	C	N	O	S	0	0	0
			2182	1388	378	412	4			

There are 16 discrepancies between the modelled and reference sequences:

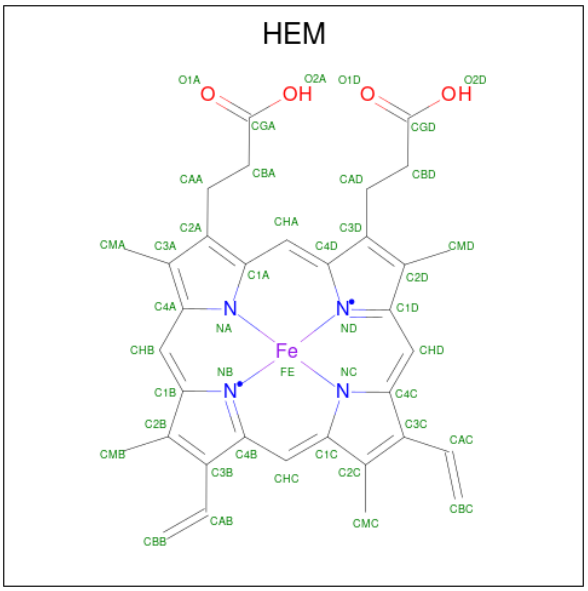
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	TYR	HIS	variant	UNP Q88HV5
A	188	LYS	GLU	variant	UNP Q88HV5
B	125	TYR	HIS	variant	UNP Q88HV5
B	188	LYS	GLU	variant	UNP Q88HV5
C	125	TYR	HIS	variant	UNP Q88HV5
C	188	LYS	GLU	variant	UNP Q88HV5
D	125	TYR	HIS	variant	UNP Q88HV5
D	188	LYS	GLU	variant	UNP Q88HV5
E	125	TYR	HIS	variant	UNP Q88HV5
E	188	LYS	GLU	variant	UNP Q88HV5
F	125	TYR	HIS	variant	UNP Q88HV5
F	188	LYS	GLU	variant	UNP Q88HV5
G	125	TYR	HIS	variant	UNP Q88HV5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	188	LYS	GLU	variant	UNP Q88HV5
H	125	TYR	HIS	variant	UNP Q88HV5
H	188	LYS	GLU	variant	UNP Q88HV5

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is water.

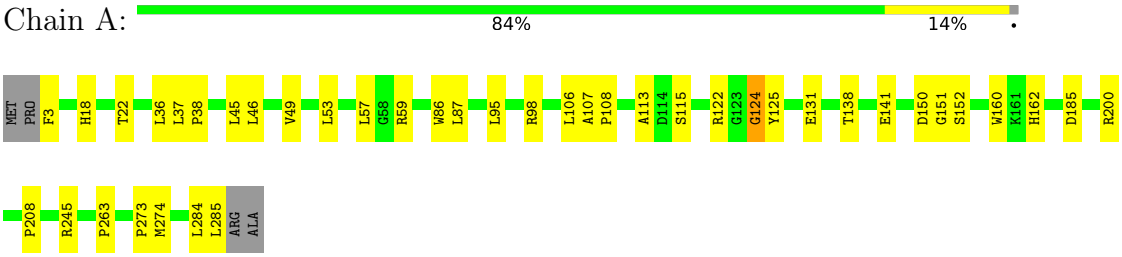
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0
3	B	1	Total O 1 1	0	0
3	C	3	Total O 3 3	0	0
3	D	3	Total O 3 3	0	0
3	H	1	Total O 1 1	0	0

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.

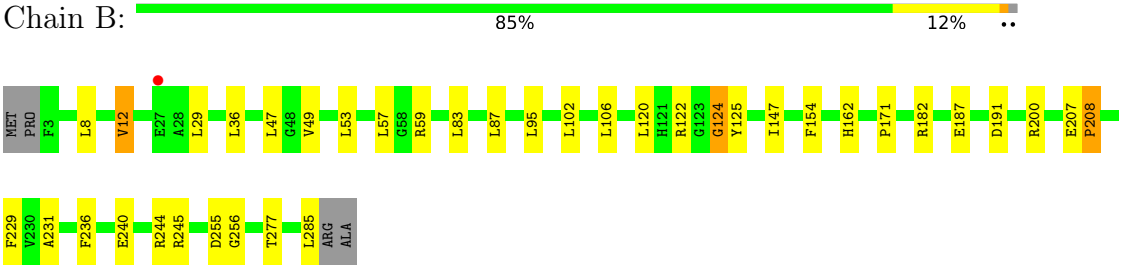
• Molecule 1: Dyp-type peroxidase family protein

Chain A:



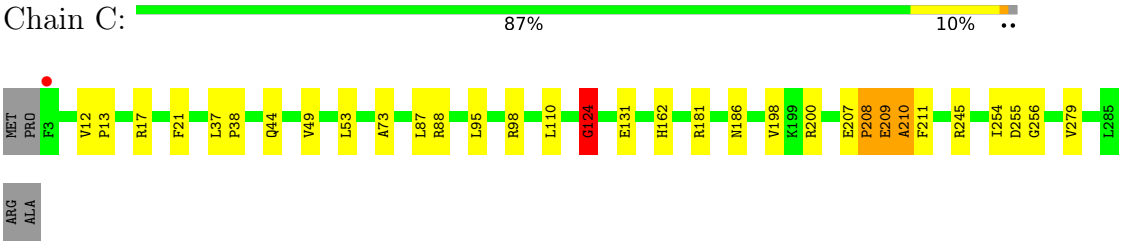
• Molecule 1: Dyp-type peroxidase family protein

Chain B:



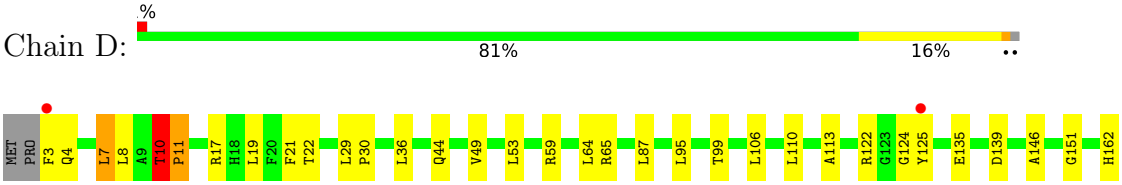
• Molecule 1: Dyp-type peroxidase family protein

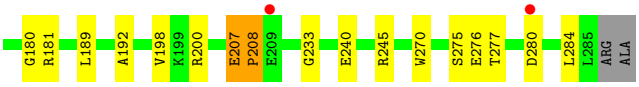
Chain C:



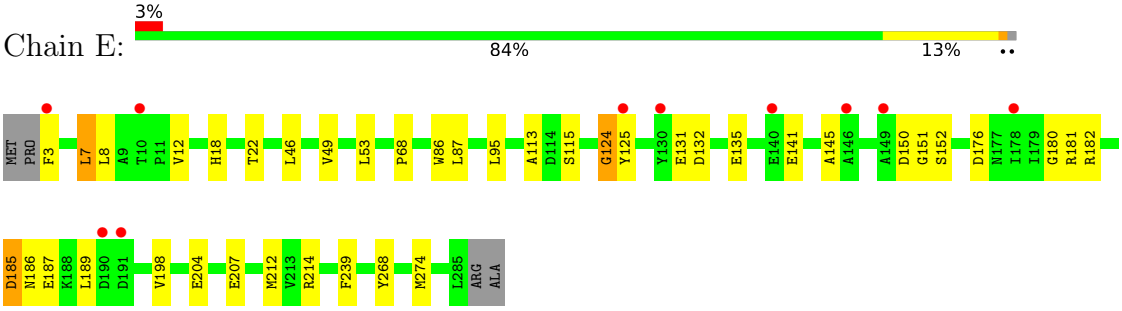
• Molecule 1: Dyp-type peroxidase family protein

Chain D:

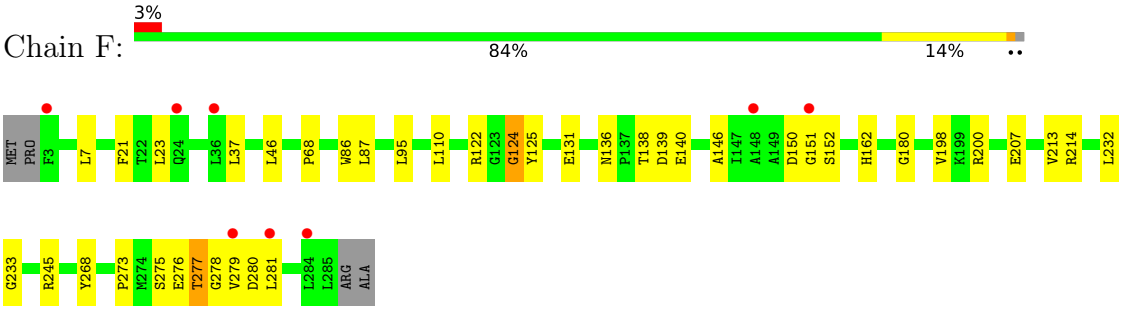




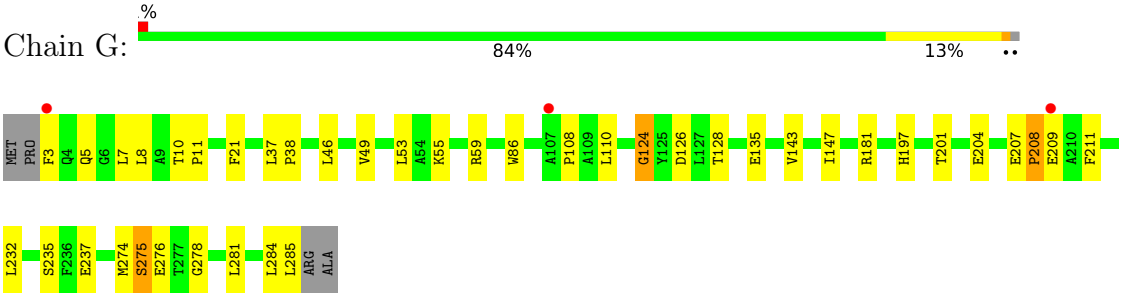
• Molecule 1: Dyp-type peroxidase family protein



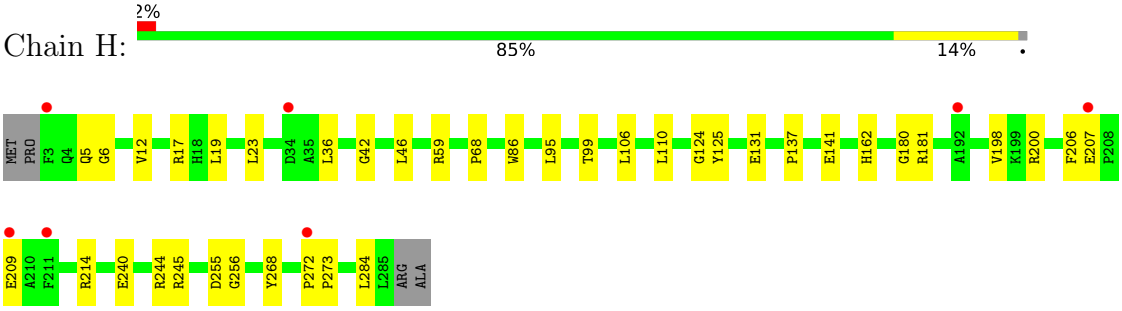
• Molecule 1: Dyp-type peroxidase family protein



• Molecule 1: Dyp-type peroxidase family protein



• Molecule 1: Dyp-type peroxidase family protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.96Å 78.81Å 98.93Å 91.02° 92.93° 94.00°	Depositor
Resolution (Å)	78.60 – 2.70 98.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.8 (78.60-2.70) 90.9 (98.78-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.189 , 0.189 0.197 , 0.207	Depositor DCC
R_{free} test set	1999 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17810	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0/2236	0.66	3/3042 (0.1%)
1	B	0.30	0/2235	0.61	3/3040 (0.1%)
1	C	0.30	0/2236	0.60	3/3042 (0.1%)
1	D	0.30	0/2236	0.49	1/3042 (0.0%)
1	E	0.30	0/2236	0.60	3/3042 (0.1%)
1	F	0.32	0/2236	0.56	3/3042 (0.1%)
1	G	0.31	0/2236	0.62	3/3042 (0.1%)
1	H	0.29	0/2236	0.55	3/3042 (0.1%)
All	All	0.31	0/17887	0.59	22/24334 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
1	H	0	1
All	All	0	7

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	GLY	O-C-N	-16.82	95.79	122.70
1	A	124	GLY	C-N-CA	15.34	160.04	121.70
1	G	124	GLY	O-C-N	-14.92	98.83	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	124	GLY	O-C-N	-14.31	99.80	122.70
1	B	124	GLY	O-C-N	-13.75	100.69	122.70
1	E	124	GLY	O-C-N	-13.45	101.18	122.70
1	E	124	GLY	C-N-CA	12.98	154.15	121.70
1	B	124	GLY	C-N-CA	12.90	153.96	121.70
1	C	124	GLY	C-N-CA	12.68	153.40	121.70
1	G	124	GLY	C-N-CA	12.09	151.92	121.70
1	A	124	GLY	CA-C-N	11.67	142.88	117.20
1	H	124	GLY	O-C-N	-11.04	105.03	122.70
1	F	124	GLY	O-C-N	-10.76	105.49	122.70
1	G	124	GLY	CA-C-N	9.93	139.04	117.20
1	F	124	GLY	C-N-CA	9.86	146.36	121.70
1	B	124	GLY	CA-C-N	9.63	138.40	117.20
1	E	124	GLY	CA-C-N	9.48	138.05	117.20
1	C	124	GLY	CA-C-N	8.77	136.49	117.20
1	H	124	GLY	C-N-CA	7.97	141.63	121.70
1	H	124	GLY	CA-C-N	6.84	132.25	117.20
1	F	124	GLY	CA-C-N	6.61	131.74	117.20
1	D	124	GLY	C-N-CA	5.15	134.58	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	124	GLY	Mainchain
1	D	10	THR	Peptide
1	D	207	GLU	Peptide
1	E	207	GLU	Peptide
1	F	124	GLY	Mainchain
1	F	207	GLU	Peptide
1	H	207	GLU	Peptide

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	2182	0	2128	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2181	0	2128	24	0
1	C	2182	0	2128	20	0
1	D	2182	0	2129	29	0
1	E	2182	0	2127	28	0
1	F	2182	0	2128	20	0
1	G	2182	0	2129	28	0
1	H	2182	0	2129	21	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
2	C	43	0	30	4	0
2	D	43	0	30	4	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
2	G	43	0	30	1	0
2	H	43	0	30	3	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	H	1	0	0	0	0
All	All	17810	0	17266	211	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (211) 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:A:125:TYR:CE1	1:A:131:GLU:HG2	1.72	1.25
1:G:8:LEU:HD11	1:G:147:ILE:HD11	1.49	0.95
1:A:125:TYR:CE1	1:A:131:GLU:CG	2.56	0.89
1:A:125:TYR:CD1	1:A:131:GLU:HG2	2.17	0.79
1:G:143:VAL:HA	1:G:147:ILE:HD13	1.68	0.75
1:G:135:GLU:OE2	1:G:181:ARG:NH1	2.19	0.75
1:A:125:TYR:OH	1:A:131:GLU:OE2	2.03	0.74
1:D:122:ARG:HB2	1:D:125:TYR:HD2	1.51	0.73
1:G:7:LEU:HD12	1:G:8:LEU:HG	1.70	0.73
1:D:19:LEU:HD11	1:D:99:THR:HG22	1.72	0.72
1:D:122:ARG:HB2	1:D:125:TYR:CD2	2.25	0.71
1:G:207:GLU:HG3	1:G:208:PRO:HD3	1.71	0.71
1:E:150:ASP:O	1:E:152:SER:N	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLU:HG3	1:B:208:PRO:HD3	1.74	0.69
1:A:150:ASP:O	1:A:152:SER:N	2.26	0.68
1:A:162:HIS:HE1	2:A:301:HEM:HBB2	1.60	0.67
1:B:122:ARG:HB2	1:B:125:TYR:HD2	1.60	0.66
2:B:301:HEM:HHA	2:B:301:HEM:HBD1	1.78	0.65
1:E:181:ARG:NH1	1:E:186:ASN:OD1	2.30	0.64
1:E:22:THR:HG23	1:E:113:ALA:HB2	1.78	0.64
1:B:36:LEU:HD22	1:B:106:LEU:HD21	1.80	0.64
1:D:10:THR:HG23	1:D:11:PRO:HD2	1.79	0.63
1:C:87:LEU:HB3	1:C:95:LEU:HD22	1.80	0.63
1:H:46:LEU:HB2	1:H:86:TRP:HB3	1.81	0.63
1:C:181:ARG:NH1	1:C:186:ASN:OD1	2.32	0.62
1:A:22:THR:HG23	1:A:113:ALA:HB2	1.82	0.62
1:E:135:GLU:OE2	1:E:181:ARG:NH2	2.32	0.62
1:D:275:SER:O	1:D:277:THR:N	2.33	0.62
1:G:7:LEU:HD13	1:G:232:LEU:HD13	1.82	0.62
2:G:301:HEM:HMC1	2:G:301:HEM:HBC2	1.83	0.61
1:G:3:PHE:O	1:G:274:MET:N	2.29	0.61
1:B:162:HIS:HE1	2:B:301:HEM:HBB2	1.66	0.61
1:B:47:LEU:HD11	1:B:83:LEU:HD11	1.82	0.61
1:F:46:LEU:HB2	1:F:86:TRP:HB3	1.83	0.60
1:D:65:ARG:NH2	1:D:240:GLU:OE1	2.27	0.59
1:F:150:ASP:O	1:F:152:SER:N	2.35	0.59
1:B:122:ARG:HB2	1:B:125:TYR:CD2	2.38	0.59
1:F:180:GLY:HA3	1:F:198:VAL:HG22	1.85	0.59
2:H:301:HEM:HMC1	2:H:301:HEM:HBC2	1.85	0.59
2:B:301:HEM:HBC2	2:B:301:HEM:HMC2	1.85	0.58
1:D:7:LEU:HD12	1:D:8:LEU:HG	1.86	0.58
1:A:138:THR:OG1	1:A:141:GLU:OE1	2.21	0.58
1:F:138:THR:O	1:F:140:GLU:N	2.38	0.57
1:G:46:LEU:HB2	1:G:86:TRP:HB3	1.86	0.57
1:A:49:VAL:HG13	1:A:53:LEU:HD23	1.87	0.56
1:B:191:ASP:O	1:F:122:ARG:NH1	2.36	0.56
1:C:49:VAL:HG13	1:C:53:LEU:HD23	1.87	0.56
1:E:212:MET:HE1	1:E:239:PHE:HA	1.87	0.56
2:F:301:HEM:HMC1	2:F:301:HEM:HBC2	1.88	0.56
2:A:301:HEM:HBB2	2:A:301:HEM:HMB1	1.88	0.56
1:D:17:ARG:HD3	1:D:99:THR:HG21	1.88	0.56
1:E:125:TYR:CD1	1:E:131:GLU:HA	2.41	0.55
1:E:132:ASP:OD1	1:E:214:ARG:NH1	2.37	0.55
1:D:180:GLY:HA3	1:D:198:VAL:HG22	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:GLU:HG3	1:C:208:PRO:HD3	1.88	0.55
1:D:36:LEU:HB2	1:D:106:LEU:HD21	1.89	0.55
1:H:180:GLY:HA3	1:H:198:VAL:HG22	1.89	0.54
2:A:301:HEM:HBC2	2:A:301:HEM:HMC2	1.89	0.54
1:G:281:LEU:HD22	1:G:284:LEU:HD12	1.89	0.54
1:B:207:GLU:CG	1:B:208:PRO:HD3	2.37	0.54
1:E:87:LEU:HB3	1:E:95:LEU:HD22	1.89	0.54
1:B:49:VAL:HG13	1:B:53:LEU:HD23	1.88	0.54
1:E:141:GLU:O	1:E:145:ALA:N	2.33	0.54
1:F:23:LEU:HA	1:F:110:LEU:HD23	1.90	0.54
1:E:131:GLU:OE1	1:E:186:ASN:ND2	2.39	0.53
1:H:19:LEU:HD11	1:H:99:THR:HG22	1.90	0.53
1:A:125:TYR:CZ	1:A:131:GLU:OE2	2.62	0.53
1:D:3:PHE:HB3	1:D:151:GLY:HA3	1.91	0.53
1:D:162:HIS:HE1	2:D:301:HEM:HBB2	1.72	0.53
1:G:59:ARG:NH2	1:G:285:LEU:HD12	2.23	0.53
1:B:12:VAL:HG22	1:B:120:LEU:HD22	1.91	0.53
1:D:22:THR:HG23	1:D:113:ALA:HB2	1.90	0.53
1:F:146:ALA:HA	1:F:233:GLY:HA2	1.90	0.52
1:C:181:ARG:HG3	1:C:198:VAL:HG21	1.91	0.52
1:A:125:TYR:HE1	1:A:131:GLU:CG	2.17	0.52
1:D:87:LEU:HB3	1:D:95:LEU:HD22	1.92	0.51
1:G:49:VAL:HG13	1:G:53:LEU:HD23	1.91	0.51
1:E:181:ARG:HD3	1:E:186:ASN:OD1	2.11	0.51
1:G:275:SER:OG	1:G:276:GLU:N	2.43	0.51
2:C:301:HEM:HMB1	2:C:301:HEM:HBB2	1.91	0.51
1:G:37:LEU:HD21	1:G:281:LEU:HD12	1.93	0.51
1:C:208:PRO:O	1:C:210:ALA:N	2.44	0.51
1:G:207:GLU:CG	1:G:208:PRO:HD3	2.39	0.50
2:E:301:HEM:HBC2	2:E:301:HEM:HMC1	1.93	0.50
1:B:182:ARG:NH2	1:B:187:GLU:OE1	2.43	0.50
2:D:301:HEM:HMC1	2:D:301:HEM:HBC2	1.93	0.50
2:E:301:HEM:HMB1	2:E:301:HEM:HBB2	1.94	0.50
1:B:102:LEU:O	1:B:106:LEU:HD12	2.12	0.49
2:D:301:HEM:HBB2	2:D:301:HEM:HMB1	1.93	0.49
1:F:37:LEU:HD21	1:F:281:LEU:HD12	1.94	0.49
1:G:5:GLN:HG2	1:G:274:MET:HG2	1.95	0.49
1:D:122:ARG:CB	1:D:125:TYR:CD2	2.94	0.49
1:B:59:ARG:NH2	1:B:285:LEU:HD12	2.27	0.49
1:E:176:ASP:HB3	1:E:189:LEU:HD11	1.95	0.49
1:F:7:LEU:HD23	1:F:46:LEU:HD23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:TYR:CE1	1:E:131:GLU:HB2	2.48	0.49
1:F:276:GLU:O	1:F:278:GLY:N	2.45	0.49
1:C:17:ARG:HB3	1:C:87:LEU:HB2	1.95	0.49
1:F:152:SER:HB3	1:F:273:PRO:HG3	1.94	0.49
1:F:68:PRO:HD3	1:F:268:TYR:CZ	2.48	0.48
1:B:162:HIS:HE1	2:B:301:HEM:CBB	2.27	0.48
2:B:301:HEM:HBB2	2:B:301:HEM:HMB1	1.95	0.48
1:C:207:GLU:CG	1:C:208:PRO:HD3	2.43	0.48
2:C:301:HEM:HMC1	2:C:301:HEM:HBC2	1.96	0.48
1:F:213:VAL:HG12	1:F:232:LEU:HB2	1.95	0.48
1:G:59:ARG:HG3	1:G:284:LEU:HA	1.96	0.48
1:E:182:ARG:NE	1:E:185:ASP:OD2	2.43	0.48
1:D:275:SER:HB3	1:D:280:ASP:HB2	1.96	0.48
1:C:73:ALA:HB3	1:C:254:ILE:HD11	1.95	0.47
1:D:49:VAL:HG13	1:D:53:LEU:HD23	1.95	0.47
1:H:162:HIS:HE1	2:H:301:HEM:CBB	2.27	0.47
1:H:137:PRO:HB3	1:H:141:GLU:HG2	1.96	0.47
1:H:68:PRO:HD3	1:H:268:TYR:CZ	2.50	0.47
1:E:182:ARG:NH2	1:E:187:GLU:HB3	2.29	0.47
1:B:29:LEU:HD23	1:B:57:LEU:HD21	1.97	0.47
1:C:13:PRO:HG2	1:C:88:ARG:HB3	1.96	0.47
1:E:182:ARG:NH1	1:E:187:GLU:HB3	2.30	0.47
1:H:6:GLY:N	1:H:42:GLY:O	2.47	0.47
1:C:21:PHE:HB3	1:C:110:LEU:HB3	1.96	0.47
1:A:36:LEU:HB2	1:A:106:LEU:HD21	1.96	0.46
1:A:46:LEU:HB2	1:A:86:TRP:HB3	1.97	0.46
1:D:135:GLU:OE2	1:D:181:ARG:NH1	2.43	0.46
1:D:189:LEU:HB2	1:D:192:ALA:HB2	1.97	0.46
1:E:3:PHE:O	1:E:274:MET:N	2.33	0.46
1:A:45:LEU:HB2	1:A:98:ARG:HH12	1.80	0.46
1:A:150:ASP:C	1:A:152:SER:H	2.17	0.46
1:C:44:GLN:HG3	1:C:98:ARG:HH12	1.81	0.46
1:E:49:VAL:HG13	1:E:53:LEU:HD23	1.97	0.46
1:A:150:ASP:O	1:A:273:PRO:HG3	2.16	0.46
1:D:200:ARG:O	1:D:245:ARG:HD2	2.15	0.46
1:H:59:ARG:HG3	1:H:284:LEU:HA	1.97	0.46
1:F:162:HIS:HE1	2:F:301:HEM:CBB	2.29	0.46
1:C:131:GLU:HB3	1:C:186:ASN:ND2	2.30	0.45
1:H:5:GLN:HB3	1:H:42:GLY:CA	2.46	0.45
1:H:240:GLU:O	1:H:244:ARG:HG3	2.15	0.45
1:A:3:PHE:O	1:A:274:MET:N	2.36	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:HB3	1:B:95:LEU:HD22	1.99	0.45
1:C:207:GLU:CD	1:C:208:PRO:HD3	2.37	0.45
1:A:122:ARG:HB2	1:A:125:TYR:CD2	2.52	0.45
1:H:206:PHE:O	1:H:209:GLU:HG2	2.17	0.44
1:A:59:ARG:NH2	1:A:285:LEU:HD12	2.31	0.44
1:H:36:LEU:HB2	1:H:106:LEU:HD21	1.99	0.44
1:E:150:ASP:C	1:E:152:SER:H	2.21	0.44
1:E:204:GLU:OE1	1:E:204:GLU:N	2.49	0.44
1:H:200:ARG:O	1:H:245:ARG:HD2	2.18	0.44
1:A:57:LEU:HD12	1:A:284:LEU:HG	1.99	0.44
1:A:18:HIS:O	1:A:115:SER:HA	2.18	0.44
1:E:180:GLY:HA3	1:E:198:VAL:HG22	1.99	0.44
1:C:209:GLU:O	1:C:211:PHE:N	2.49	0.44
1:G:21:PHE:HB3	1:G:110:LEU:HB3	1.99	0.43
1:B:8:LEU:HD11	1:B:147:ILE:CD1	2.47	0.43
1:F:136:ASN:HD21	1:F:214:ARG:H	1.66	0.43
1:D:181:ARG:HG3	1:D:198:VAL:HG11	1.99	0.43
1:G:10:THR:N	1:G:11:PRO:HD2	2.34	0.43
1:A:107:ALA:HB3	1:A:108:PRO:HD3	2.00	0.43
1:A:162:HIS:HE1	2:A:301:HEM:CBB	2.30	0.43
1:A:200:ARG:O	1:A:245:ARG:HD2	2.18	0.43
1:E:18:HIS:O	1:E:115:SER:HA	2.18	0.43
1:E:46:LEU:HB2	1:E:86:TRP:HB3	2.01	0.43
1:F:87:LEU:HB3	1:F:95:LEU:HD22	2.00	0.43
1:A:160:TRP:CB	2:A:301:HEM:HBB1	2.49	0.43
1:C:255:ASP:OD1	1:C:256:GLY:N	2.52	0.43
1:D:59:ARG:HB2	1:D:284:LEU:HD23	2.01	0.42
1:D:162:HIS:HE1	2:D:301:HEM:CBB	2.32	0.42
1:E:182:ARG:NH2	1:E:185:ASP:OD2	2.51	0.42
1:G:126:ASP:O	1:G:128:THR:N	2.52	0.42
1:E:182:ARG:CZ	1:E:187:GLU:HB3	2.49	0.42
1:F:125:TYR:CD1	1:F:131:GLU:HA	2.54	0.42
1:H:125:TYR:CD1	1:H:131:GLU:HA	2.55	0.42
1:C:162:HIS:HE1	2:C:301:HEM:HBB2	1.84	0.42
1:H:5:GLN:HB3	1:H:42:GLY:HA2	2.02	0.42
1:B:8:LEU:HD11	1:B:147:ILE:HD11	2.01	0.42
1:G:275:SER:N	1:G:278:GLY:O	2.53	0.42
1:G:209:GLU:HB3	1:G:211:PHE:CE2	2.54	0.42
1:H:23:LEU:HA	1:H:110:LEU:HD23	2.02	0.42
1:H:181:ARG:HD2	2:H:301:HEM:HAA2	2.02	0.42
1:B:229:PHE:CE2	1:B:231:ALA:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:HIS:HE1	2:C:301:HEM:CBB	2.32	0.42
1:D:64:LEU:HD13	1:D:270:TRP:HB2	2.01	0.42
1:D:146:ALA:HA	1:D:233:GLY:HA2	2.01	0.42
1:F:21:PHE:HB3	1:F:110:LEU:HB3	2.02	0.42
1:G:147:ILE:HD12	1:G:147:ILE:N	2.35	0.42
1:F:275:SER:HB3	1:F:280:ASP:HB2	2.02	0.41
1:G:197:HIS:CE1	1:G:201:THR:HG21	2.56	0.41
1:D:29:LEU:HB3	1:D:30:PRO:HD3	2.02	0.41
1:E:7:LEU:HD12	1:E:8:LEU:HG	2.02	0.41
1:E:68:PRO:HD3	1:E:268:TYR:CE2	2.55	0.41
1:G:55:LYS:HE2	1:G:55:LYS:HB2	1.92	0.41
1:G:204:GLU:OE1	1:G:204:GLU:N	2.52	0.41
1:H:95:LEU:O	1:H:99:THR:HG23	2.20	0.41
1:A:37:LEU:N	1:A:38:PRO:HD2	2.35	0.41
1:B:154:PHE:HB3	1:B:236:PHE:CZ	2.56	0.41
1:C:37:LEU:N	1:C:38:PRO:HD2	2.36	0.41
1:G:235:SER:OG	1:G:237:GLU:OE1	2.18	0.41
1:A:160:TRP:CZ3	1:A:263:PRO:HD3	2.56	0.41
1:D:207:GLU:HB2	1:D:208:PRO:HD3	2.03	0.41
1:G:37:LEU:N	1:G:38:PRO:HD2	2.36	0.41
1:B:200:ARG:O	1:B:245:ARG:HD2	2.21	0.41
1:D:21:PHE:HB3	1:D:110:LEU:HB3	2.03	0.41
1:F:200:ARG:O	1:F:245:ARG:HD2	2.20	0.41
1:A:87:LEU:HB3	1:A:95:LEU:HD22	2.02	0.40
1:C:200:ARG:O	1:C:245:ARG:HD2	2.21	0.40
1:E:7:LEU:HB3	1:E:46:LEU:CD2	2.51	0.40
1:H:255:ASP:OD1	1:H:256:GLY:N	2.54	0.40
1:H:272:PRO:HA	1:H:273:PRO:HD3	1.95	0.40
1:B:255:ASP:OD1	1:B:256:GLY:N	2.55	0.40
1:G:59:ARG:HB2	1:G:284:LEU:HD23	2.02	0.40
1:B:171:PRO:HB3	1:D:44:GLN:HB3	2.02	0.40
1:B:240:GLU:O	1:B:244:ARG:HG3	2.21	0.40
2:F:301:HEM:HBB2	2:F:301:HEM:HMB1	2.04	0.40
1:H:17:ARG:HG2	1:H:99:THR:HG21	2.04	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	281/287 (98%)	264 (94%)	15 (5%)	2 (1%)	22	46
1	B	281/287 (98%)	264 (94%)	15 (5%)	2 (1%)	22	46
1	C	281/287 (98%)	261 (93%)	16 (6%)	4 (1%)	11	28
1	D	281/287 (98%)	262 (93%)	14 (5%)	5 (2%)	8	21
1	E	281/287 (98%)	259 (92%)	20 (7%)	2 (1%)	22	46
1	F	281/287 (98%)	265 (94%)	13 (5%)	3 (1%)	14	34
1	G	281/287 (98%)	260 (92%)	18 (6%)	3 (1%)	14	34
1	H	281/287 (98%)	262 (93%)	19 (7%)	0	100	100
All	All	2248/2296 (98%)	2097 (93%)	130 (6%)	21 (1%)	17	40

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	11	PRO
1	D	276	GLU
1	F	139	ASP
1	A	151	GLY
1	D	139	ASP
1	E	151	GLY
1	F	151	GLY
1	C	210	ALA
1	D	10	THR
1	F	277	THR
1	G	275	SER
1	C	209	GLU
1	D	4	GLN
1	A	124	GLY
1	E	124	GLY
1	G	124	GLY
1	C	208	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	208	PRO
1	B	124	GLY
1	B	208	PRO
1	C	124	GLY

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	223/226 (99%)	221 (99%)	2 (1%)	78	92
1	B	223/226 (99%)	221 (99%)	2 (1%)	78	92
1	C	223/226 (99%)	221 (99%)	2 (1%)	78	92
1	D	223/226 (99%)	221 (99%)	2 (1%)	78	92
1	E	223/226 (99%)	220 (99%)	3 (1%)	69	87
1	F	223/226 (99%)	221 (99%)	2 (1%)	78	92
1	G	223/226 (99%)	222 (100%)	1 (0%)	91	97
1	H	223/226 (99%)	221 (99%)	2 (1%)	78	92
All	All	1784/1808 (99%)	1768 (99%)	16 (1%)	78	92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ASP
1	A	208	PRO
1	B	12	VAL
1	B	277	THR
1	C	12	VAL
1	C	279	VAL
1	D	7	LEU
1	D	208	PRO
1	E	7	LEU
1	E	12	VAL
1	E	185	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	277	THR
1	F	279	VAL
1	G	108	PRO
1	H	12	VAL
1	H	214	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	177	ASN
1	F	136	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	E	301	1	41,50,50	1.51	5 (12%)	45,82,82	1.56	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	A	301	1	41,50,50	1.48	5 (12%)	45,82,82	1.52	8 (17%)
2	HEM	F	301	1	41,50,50	1.51	6 (14%)	45,82,82	1.59	8 (17%)
2	HEM	H	301	1	41,50,50	1.49	4 (9%)	45,82,82	1.53	8 (17%)
2	HEM	B	301	1	41,50,50	1.51	6 (14%)	45,82,82	1.68	13 (28%)
2	HEM	D	301	1	41,50,50	1.48	6 (14%)	45,82,82	1.35	5 (11%)
2	HEM	C	301	1	41,50,50	1.50	5 (12%)	45,82,82	1.50	7 (15%)
2	HEM	G	301	1	41,50,50	1.52	6 (14%)	45,82,82	1.42	8 (17%)

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	E	301	1	-	6/12/54/54	-
2	HEM	A	301	1	-	4/12/54/54	-
2	HEM	F	301	1	-	4/12/54/54	-
2	HEM	H	301	1	-	6/12/54/54	-
2	HEM	B	301	1	-	6/12/54/54	-
2	HEM	D	301	1	-	7/12/54/54	-
2	HEM	C	301	1	-	5/12/54/54	-
2	HEM	G	301	1	-	5/12/54/54	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	HEM	C3C-C2C	-3.95	1.34	1.40
2	E	301	HEM	C3C-C2C	-3.92	1.34	1.40
2	H	301	HEM	C3C-C2C	-3.87	1.35	1.40
2	F	301	HEM	C3C-CAC	3.86	1.55	1.47
2	C	301	HEM	C3C-CAC	3.86	1.55	1.47
2	E	301	HEM	C3C-CAC	3.81	1.55	1.47
2	F	301	HEM	C3C-C2C	-3.81	1.35	1.40
2	D	301	HEM	C3C-C2C	-3.80	1.35	1.40
2	D	301	HEM	C3C-CAC	3.79	1.55	1.47
2	A	301	HEM	C3C-C2C	-3.77	1.35	1.40
2	H	301	HEM	C3C-CAC	3.76	1.55	1.47
2	G	301	HEM	C3C-CAC	3.75	1.55	1.47
2	A	301	HEM	C3C-CAC	3.72	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	HEM	C3C-CAC	3.72	1.55	1.47
2	C	301	HEM	C3C-C2C	-3.70	1.35	1.40
2	B	301	HEM	C3C-C2C	-3.69	1.35	1.40
2	G	301	HEM	CAB-C3B	3.05	1.55	1.47
2	E	301	HEM	CAB-C3B	3.02	1.55	1.47
2	A	301	HEM	CAB-C3B	2.94	1.55	1.47
2	H	301	HEM	CAB-C3B	2.93	1.55	1.47
2	C	301	HEM	CAB-C3B	2.91	1.55	1.47
2	B	301	HEM	CAB-C3B	2.90	1.55	1.47
2	F	301	HEM	CAB-C3B	2.86	1.55	1.47
2	D	301	HEM	CAB-C3B	2.85	1.55	1.47
2	B	301	HEM	FE-ND	2.74	2.10	1.96
2	F	301	HEM	FE-NB	2.60	2.09	1.96
2	E	301	HEM	FE-ND	2.45	2.09	1.96
2	G	301	HEM	FE-NB	2.28	2.08	1.96
2	C	301	HEM	FE-NB	2.25	2.08	1.96
2	B	301	HEM	CAA-C2A	2.21	1.55	1.52
2	D	301	HEM	FE-ND	2.19	2.07	1.96
2	B	301	HEM	O1D-CGD	2.17	1.29	1.22
2	D	301	HEM	CAA-C2A	2.10	1.55	1.52
2	E	301	HEM	CMB-C2B	2.08	1.55	1.50
2	F	301	HEM	CAA-C2A	2.07	1.55	1.52
2	G	301	HEM	CAA-C2A	2.07	1.55	1.52
2	A	301	HEM	FE-ND	2.06	2.07	1.96
2	A	301	HEM	CMB-C2B	2.04	1.55	1.50
2	G	301	HEM	CMB-C2B	2.04	1.55	1.50
2	C	301	HEM	CMB-C2B	2.04	1.55	1.50
2	H	301	HEM	CAA-C2A	2.03	1.55	1.52
2	F	301	HEM	CMB-C2B	2.00	1.55	1.50
2	D	301	HEM	CMB-C2B	2.00	1.55	1.50

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	HEM	CAD-C3D-C4D	3.42	130.64	124.66
2	H	301	HEM	CAD-C3D-C4D	3.35	130.51	124.66
2	F	301	HEM	C4D-ND-C1D	3.35	108.53	105.07
2	E	301	HEM	CAD-C3D-C4D	3.28	130.39	124.66
2	C	301	HEM	C4C-CHD-C1D	3.23	126.83	122.56
2	B	301	HEM	CAD-C3D-C4D	3.23	130.31	124.66
2	G	301	HEM	CAD-C3D-C4D	3.23	130.30	124.66
2	H	301	HEM	CAD-C3D-C2D	-3.23	121.86	127.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	HEM	CAD-C3D-C4D	3.19	130.23	124.66
2	B	301	HEM	C4D-ND-C1D	3.14	108.32	105.07
2	F	301	HEM	C4C-CHD-C1D	3.14	126.70	122.56
2	B	301	HEM	C1B-NB-C4B	3.11	108.29	105.07
2	G	301	HEM	C4D-ND-C1D	3.08	108.25	105.07
2	D	301	HEM	C4B-CHC-C1C	3.07	126.62	122.56
2	H	301	HEM	C4D-ND-C1D	3.07	108.25	105.07
2	E	301	HEM	CAD-C3D-C2D	-3.05	122.19	127.88
2	A	301	HEM	CAD-C3D-C2D	-3.04	122.22	127.88
2	C	301	HEM	C4D-ND-C1D	3.00	108.17	105.07
2	F	301	HEM	CAD-C3D-C2D	-2.99	122.31	127.88
2	G	301	HEM	CAD-C3D-C2D	-2.92	122.44	127.88
2	C	301	HEM	CAD-C3D-C4D	2.85	129.64	124.66
2	A	301	HEM	C4B-CHC-C1C	2.84	126.30	122.56
2	A	301	HEM	C4D-ND-C1D	2.79	107.95	105.07
2	E	301	HEM	C4D-ND-C1D	2.79	107.95	105.07
2	E	301	HEM	C1B-NB-C4B	2.78	107.94	105.07
2	D	301	HEM	CAD-C3D-C4D	2.74	129.45	124.66
2	E	301	HEM	CBA-CAA-C2A	-2.71	107.99	112.62
2	E	301	HEM	C4B-CHC-C1C	2.70	126.13	122.56
2	B	301	HEM	CHA-C4D-C3D	2.68	130.36	125.33
2	B	301	HEM	CAD-C3D-C2D	-2.66	122.93	127.88
2	A	301	HEM	C1B-NB-C4B	2.63	107.79	105.07
2	D	301	HEM	C1B-NB-C4B	2.56	107.72	105.07
2	C	301	HEM	C1B-NB-C4B	2.55	107.71	105.07
2	H	301	HEM	C1B-NB-C4B	2.54	107.70	105.07
2	C	301	HEM	CAD-C3D-C2D	-2.52	123.18	127.88
2	D	301	HEM	C4D-ND-C1D	2.52	107.68	105.07
2	H	301	HEM	C3D-C4D-ND	-2.43	107.46	110.17
2	F	301	HEM	C3D-C4D-ND	-2.42	107.48	110.17
2	B	301	HEM	O1D-CGD-CBD	-2.41	115.33	123.08
2	G	301	HEM	C1B-NB-C4B	2.40	107.55	105.07
2	F	301	HEM	C1B-NB-C4B	2.40	107.55	105.07
2	B	301	HEM	C4A-C3A-C2A	2.38	108.65	107.00
2	D	301	HEM	CAD-C3D-C2D	-2.36	123.48	127.88
2	B	301	HEM	C1D-C2D-C3D	2.34	109.41	106.96
2	E	301	HEM	C4C-CHD-C1D	2.32	125.61	122.56
2	B	301	HEM	C4C-CHD-C1D	2.27	125.55	122.56
2	A	301	HEM	CMA-C3A-C4A	-2.24	125.02	128.46
2	B	301	HEM	CHD-C1D-ND	2.22	126.84	124.43
2	B	301	HEM	CMC-C2C-C3C	2.21	128.81	124.68
2	B	301	HEM	C3D-C4D-ND	-2.19	107.73	110.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	HEM	C3D-C4D-ND	-2.18	107.73	110.17
2	A	301	HEM	CMC-C2C-C3C	2.14	128.68	124.68
2	E	301	HEM	CMA-C3A-C4A	-2.13	125.20	128.46
2	B	301	HEM	C3B-C2B-C1B	2.12	108.06	106.49
2	H	301	HEM	CMC-C2C-C3C	2.11	128.63	124.68
2	H	301	HEM	CHA-C4D-C3D	2.09	129.26	125.33
2	F	301	HEM	CHD-C1D-ND	2.09	126.70	124.43
2	E	301	HEM	C3D-C4D-ND	-2.08	107.85	110.17
2	C	301	HEM	CMC-C2C-C3C	2.07	128.56	124.68
2	E	301	HEM	CHA-C4D-C3D	2.07	129.21	125.33
2	G	301	HEM	C4B-CHC-C1C	2.07	125.28	122.56
2	G	301	HEM	CHA-C4D-C3D	2.07	129.20	125.33
2	A	301	HEM	C3D-C4D-ND	-2.07	107.87	110.17
2	F	301	HEM	CMC-C2C-C3C	2.03	128.48	124.68
2	C	301	HEM	C3D-C4D-ND	-2.03	107.91	110.17
2	G	301	HEM	C3B-C2B-C1B	2.02	107.98	106.49
2	H	301	HEM	CMA-C3A-C4A	-2.00	125.39	128.46

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	HEM	C2D-C3D-CAD-CBD
2	A	301	HEM	C4D-C3D-CAD-CBD
2	B	301	HEM	C2D-C3D-CAD-CBD
2	B	301	HEM	C4D-C3D-CAD-CBD
2	F	301	HEM	C2D-C3D-CAD-CBD
2	F	301	HEM	C4D-C3D-CAD-CBD
2	G	301	HEM	C2D-C3D-CAD-CBD
2	G	301	HEM	C4D-C3D-CAD-CBD
2	H	301	HEM	C2D-C3D-CAD-CBD
2	H	301	HEM	C4D-C3D-CAD-CBD
2	D	301	HEM	C2D-C3D-CAD-CBD
2	E	301	HEM	C2D-C3D-CAD-CBD
2	C	301	HEM	C4D-C3D-CAD-CBD
2	D	301	HEM	C4D-C3D-CAD-CBD
2	E	301	HEM	C4D-C3D-CAD-CBD
2	B	301	HEM	C2A-CAA-CBA-CGA
2	G	301	HEM	C2A-CAA-CBA-CGA
2	C	301	HEM	C2D-C3D-CAD-CBD
2	D	301	HEM	C2A-CAA-CBA-CGA
2	D	301	HEM	C3D-CAD-CBD-CGD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	301	HEM	CAA-CBA-CGA-O1A
2	D	301	HEM	CAA-CBA-CGA-O1A
2	B	301	HEM	CAA-CBA-CGA-O2A
2	D	301	HEM	CAA-CBA-CGA-O2A
2	A	301	HEM	CAA-CBA-CGA-O2A
2	C	301	HEM	CAA-CBA-CGA-O2A
2	C	301	HEM	C3D-CAD-CBD-CGD
2	G	301	HEM	CAA-CBA-CGA-O2A
2	C	301	HEM	CAA-CBA-CGA-O1A
2	F	301	HEM	CAA-CBA-CGA-O2A
2	H	301	HEM	CAA-CBA-CGA-O2A
2	A	301	HEM	CAA-CBA-CGA-O1A
2	E	301	HEM	CAA-CBA-CGA-O2A
2	F	301	HEM	CAA-CBA-CGA-O1A
2	G	301	HEM	CAA-CBA-CGA-O1A
2	H	301	HEM	CAA-CBA-CGA-O1A
2	E	301	HEM	CAA-CBA-CGA-O1A
2	B	301	HEM	CAD-CBD-CGD-O2D
2	E	301	HEM	CAD-CBD-CGD-O2D
2	E	301	HEM	CAD-CBD-CGD-O1D
2	H	301	HEM	CAD-CBD-CGD-O2D
2	D	301	HEM	CAD-CBD-CGD-O2D
2	H	301	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

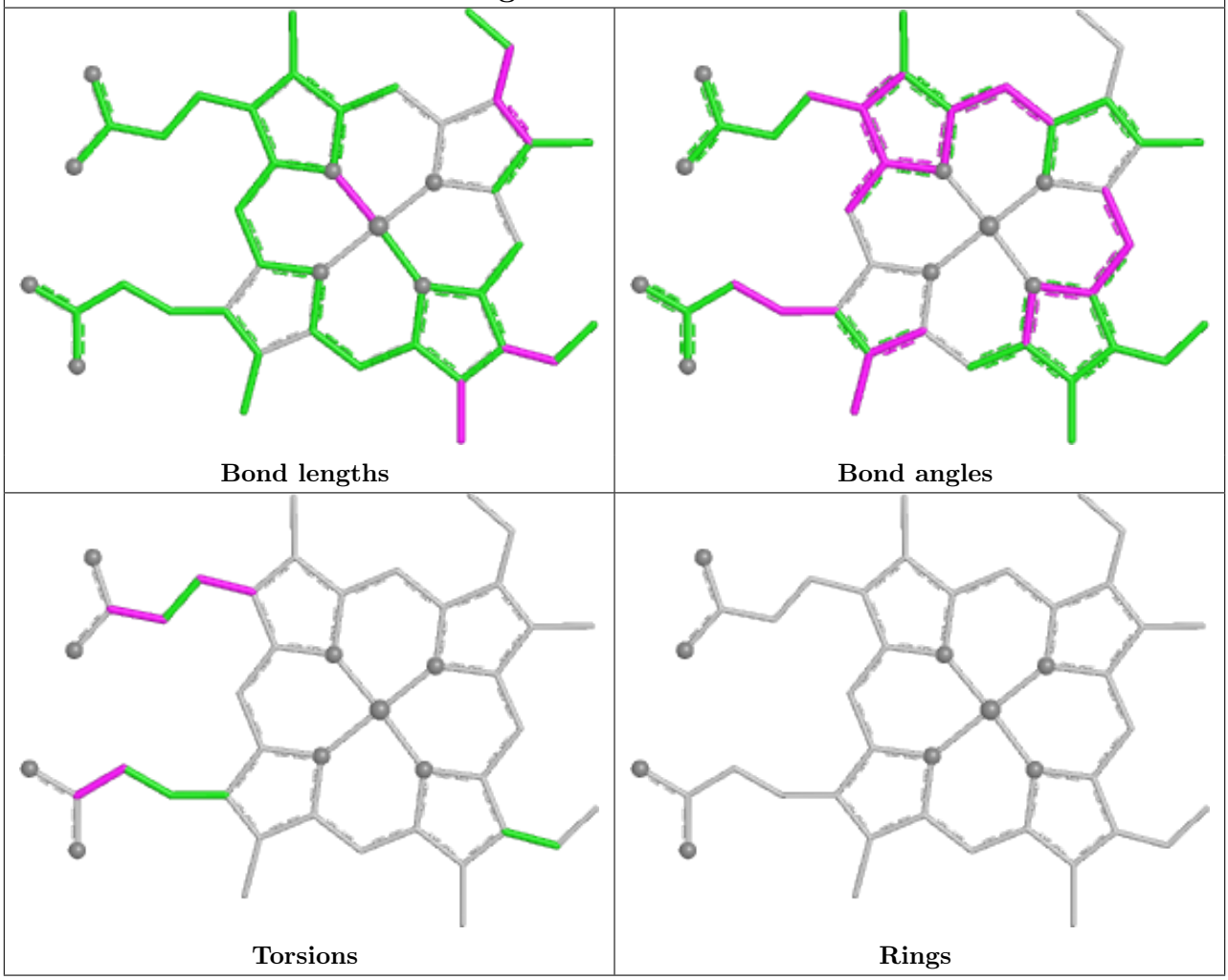
8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	HEM	2	0
2	A	301	HEM	5	0
2	F	301	HEM	3	0
2	H	301	HEM	3	0
2	B	301	HEM	5	0
2	D	301	HEM	4	0
2	C	301	HEM	4	0
2	G	301	HEM	1	0

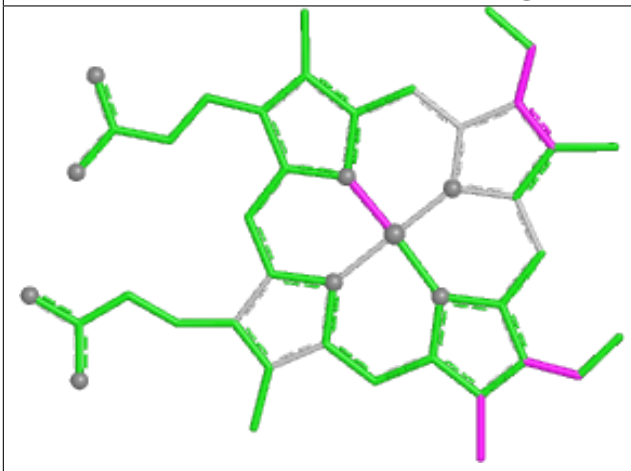
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

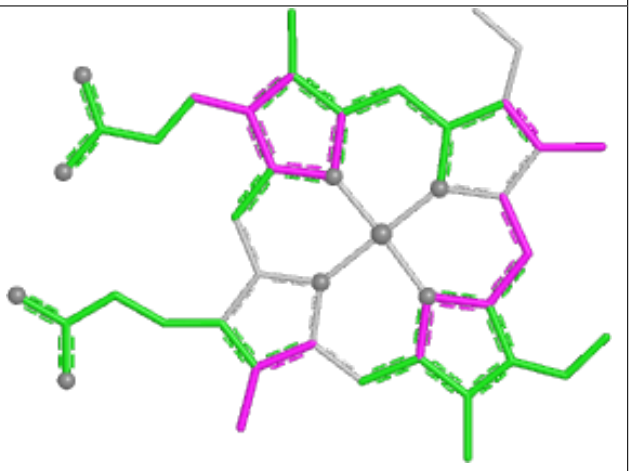
Ligand HEM E 301



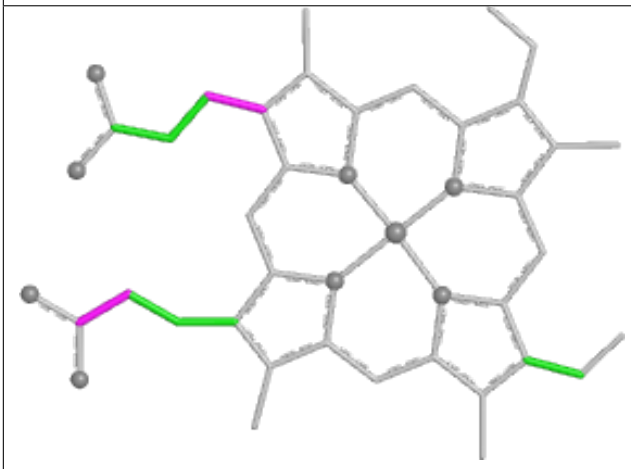
Ligand HEM A 301



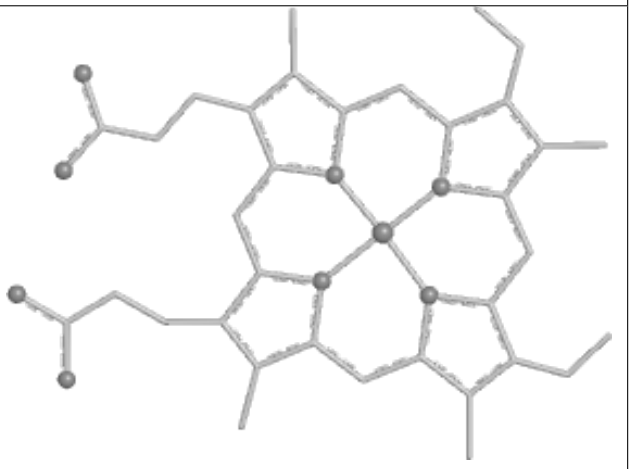
Bond lengths



Bond angles

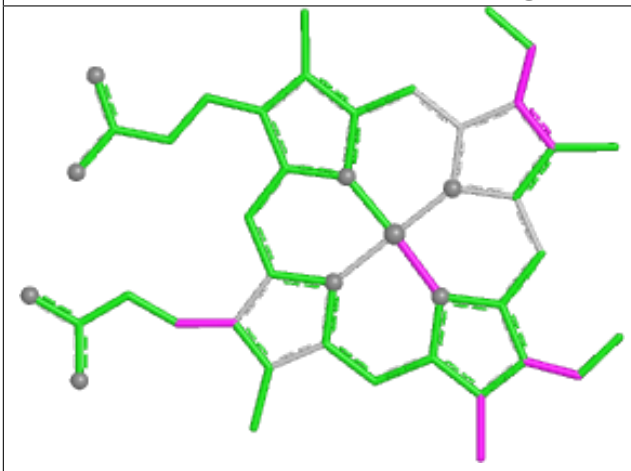


Torsions

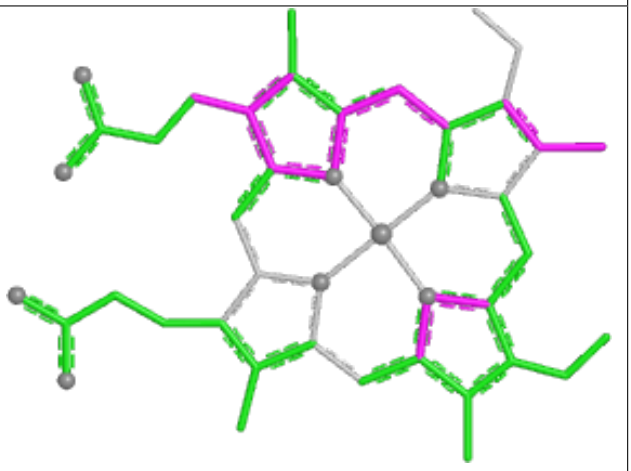


Rings

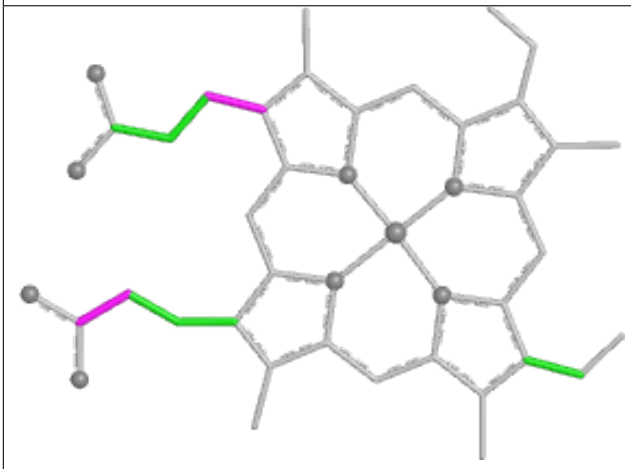
Ligand HEM F 301



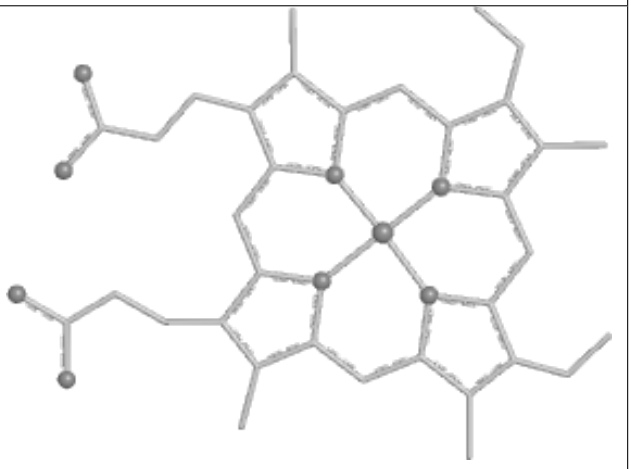
Bond lengths



Bond angles

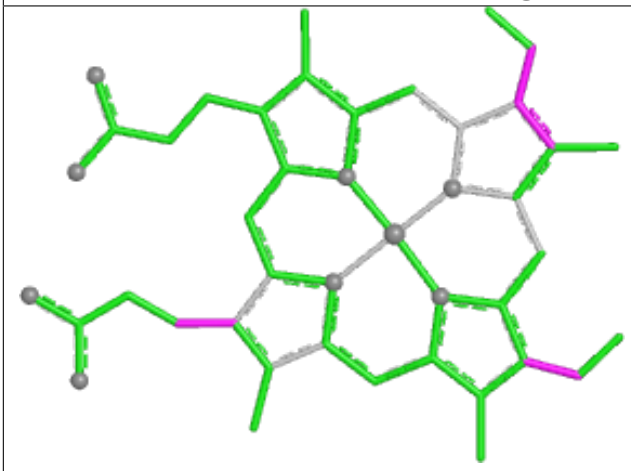


Torsions

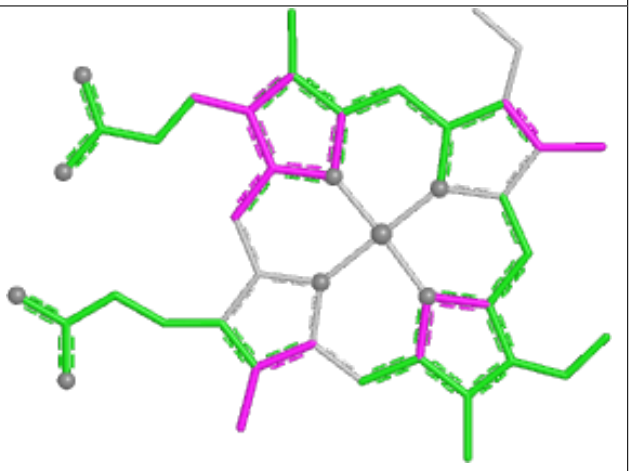


Rings

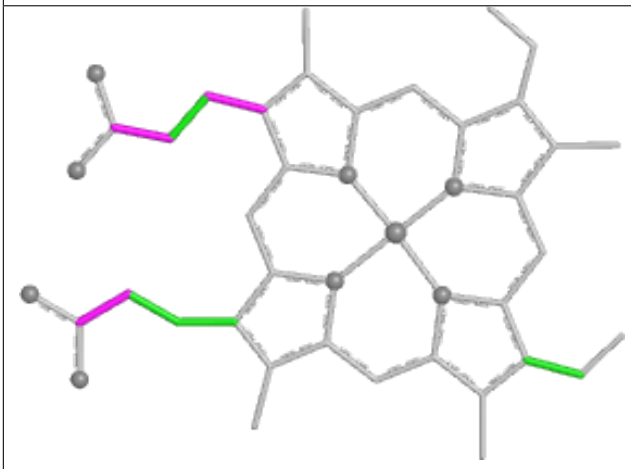
Ligand HEM H 301



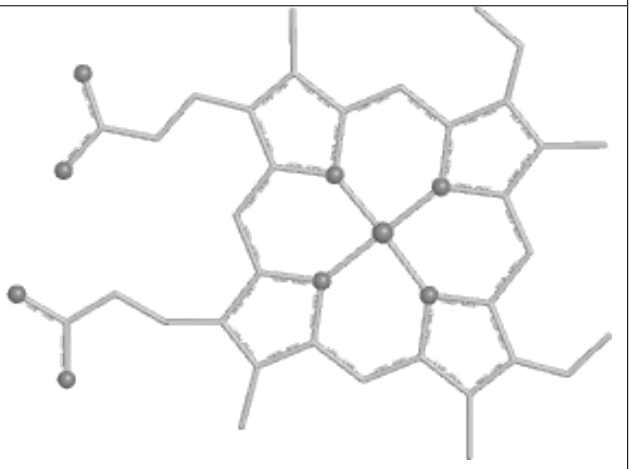
Bond lengths



Bond angles

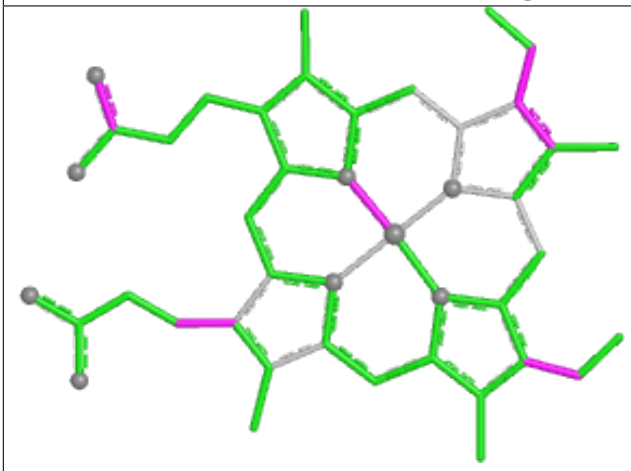


Torsions

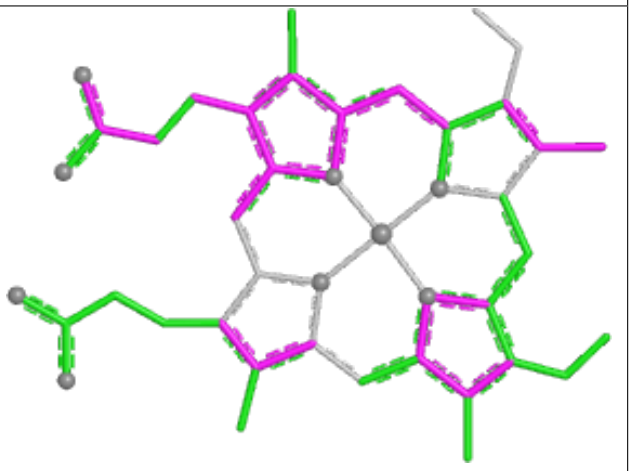


Rings

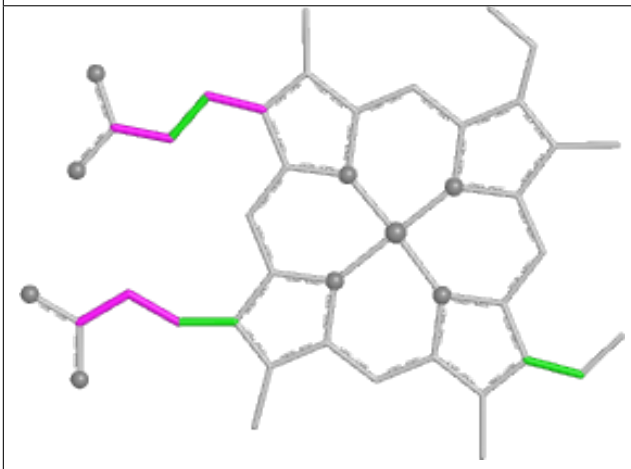
Ligand HEM B 301



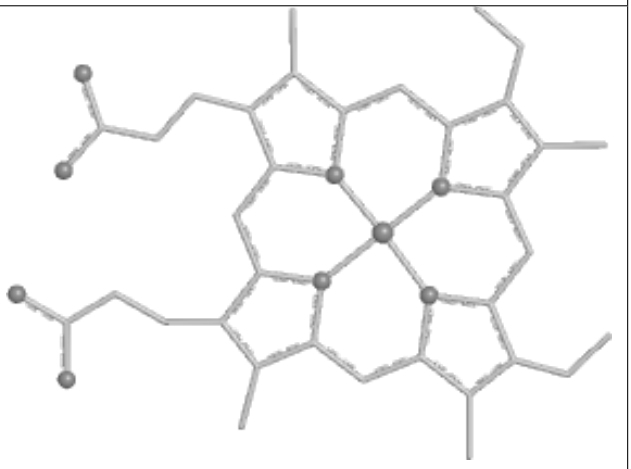
Bond lengths



Bond angles

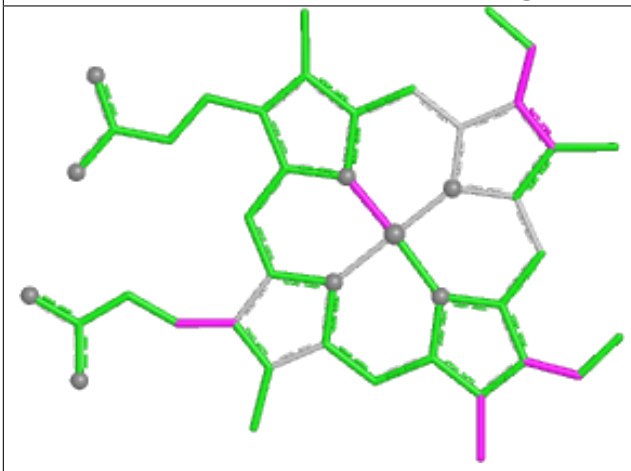


Torsions

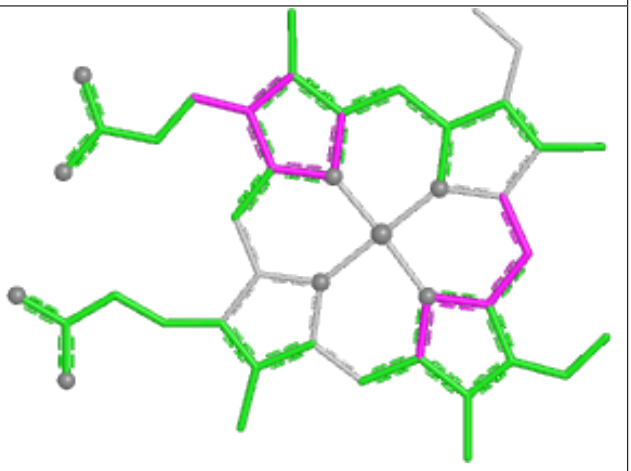


Rings

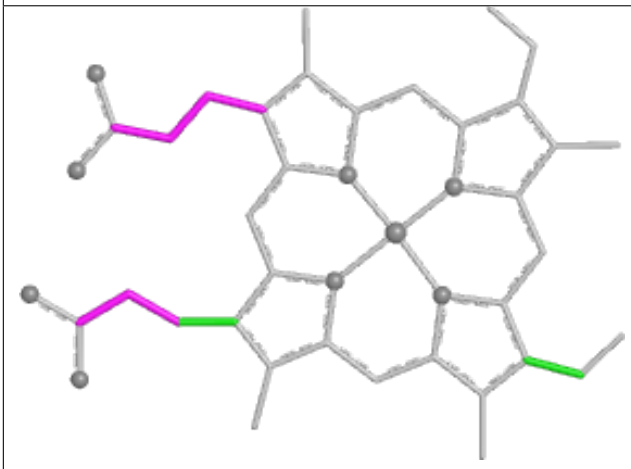
Ligand HEM D 301



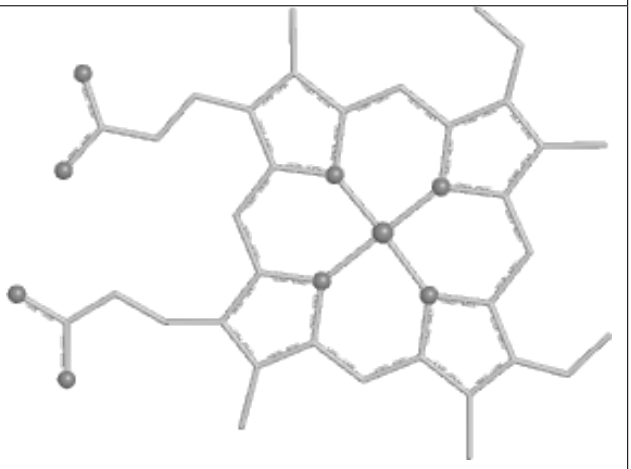
Bond lengths



Bond angles

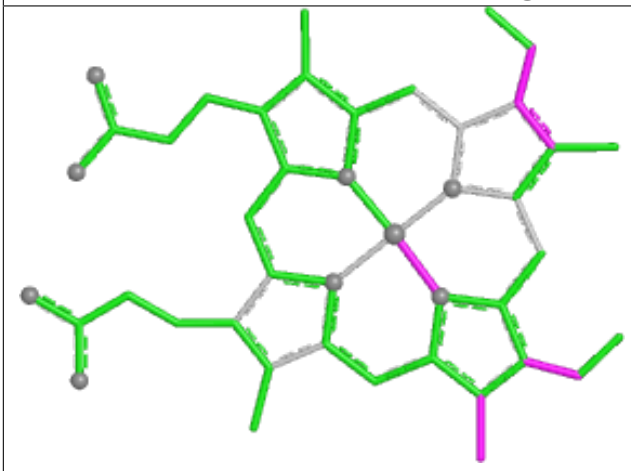


Torsions

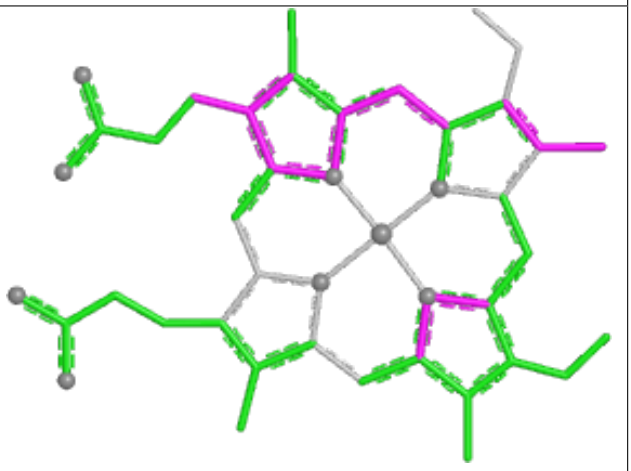


Rings

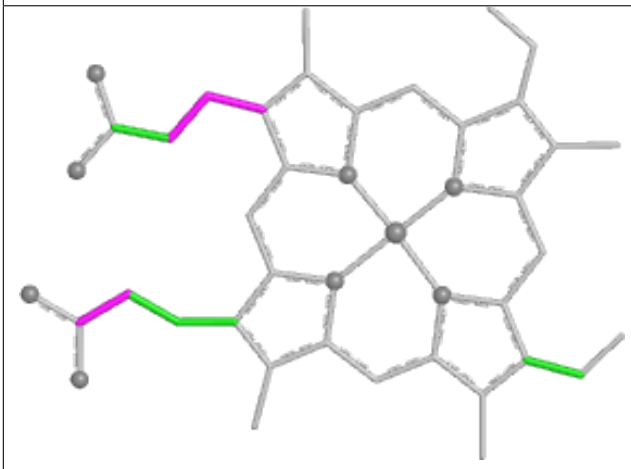
Ligand HEM C 301



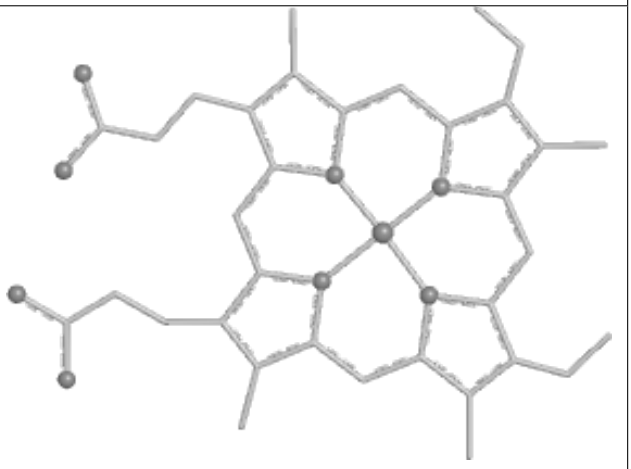
Bond lengths



Bond angles

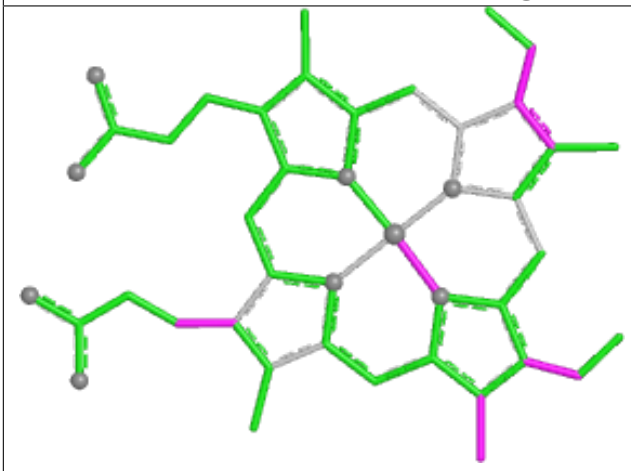


Torsions

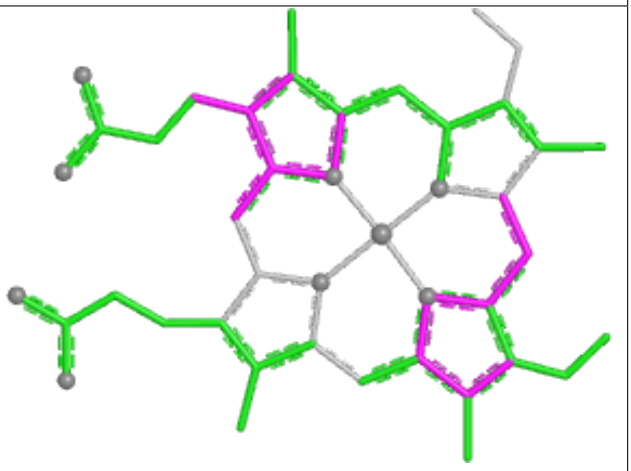


Rings

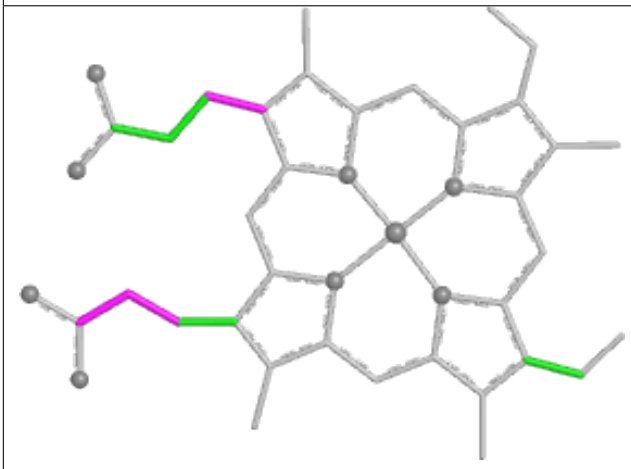
Ligand HEM G 301



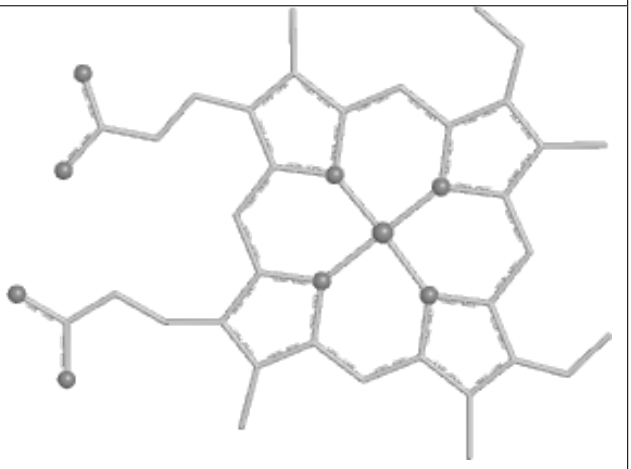
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	283/287 (98%)	-0.04	0 100 100	34, 66, 106, 137	0
1	B	283/287 (98%)	-0.05	1 (0%) 92 93	37, 67, 111, 148	0
1	C	283/287 (98%)	-0.07	1 (0%) 92 93	36, 72, 111, 157	0
1	D	283/287 (98%)	0.05	4 (1%) 75 77	40, 80, 123, 151	0
1	E	283/287 (98%)	0.10	10 (3%) 44 44	42, 81, 136, 198	0
1	F	283/287 (98%)	0.10	8 (2%) 53 54	36, 82, 135, 165	0
1	G	283/287 (98%)	0.12	3 (1%) 80 82	39, 83, 133, 158	0
1	H	283/287 (98%)	0.11	7 (2%) 57 59	36, 86, 136, 184	0
All	All	2264/2296 (98%)	0.04	34 (1%) 73 76	34, 77, 127, 198	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	3	PHE	6.0
1	C	3	PHE	5.6
1	H	3	PHE	5.4
1	D	3	PHE	4.5
1	G	3	PHE	4.3
1	F	3	PHE	3.5
1	B	27	GLU	3.3
1	G	209	GLU	3.3
1	F	279	VAL	3.2
1	F	151	GLY	3.1
1	E	10	THR	3.1
1	H	34	ASP	2.9
1	H	211	PHE	2.8
1	E	140	GLU	2.7
1	E	125	TYR	2.7
1	H	272	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	284	LEU	2.6
1	D	280	ASP	2.5
1	E	191	ASP	2.5
1	F	281	LEU	2.5
1	E	130	TYR	2.4
1	D	125	TYR	2.4
1	H	207	GLU	2.3
1	D	209	GLU	2.3
1	H	192	ALA	2.3
1	E	149	ALA	2.2
1	F	36	LEU	2.2
1	H	209	GLU	2.2
1	E	178	ILE	2.1
1	F	148	ALA	2.1
1	E	146	ALA	2.1
1	F	24	GLN	2.1
1	E	190	ASP	2.1
1	G	107	ALA	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	H	301	43/43	0.95	0.19	86,99,103,106	0
2	HEM	B	301	43/43	0.96	0.19	54,60,80,86	0
2	HEM	E	301	43/43	0.96	0.17	61,70,94,102	0
2	HEM	G	301	43/43	0.96	0.20	78,87,104,114	0
2	HEM	A	301	43/43	0.96	0.19	45,55,69,70	0

Continued on next page...

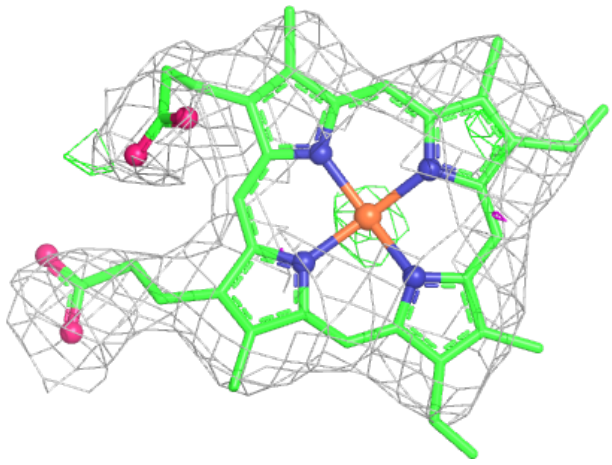
Continued from previous page...

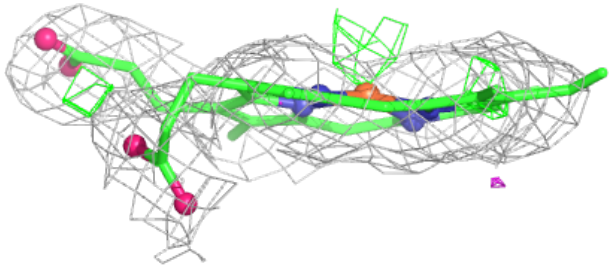
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	F	301	43/43	0.97	0.15	67,74,89,99	0
2	HEM	D	301	43/43	0.97	0.18	57,68,83,91	0
2	HEM	C	301	43/43	0.97	0.17	43,56,81,89	0

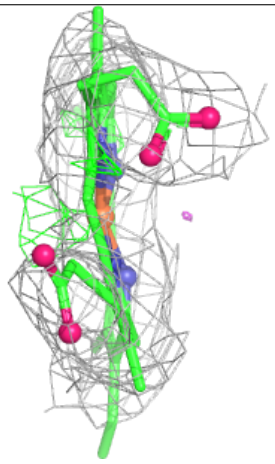
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM H 301:

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

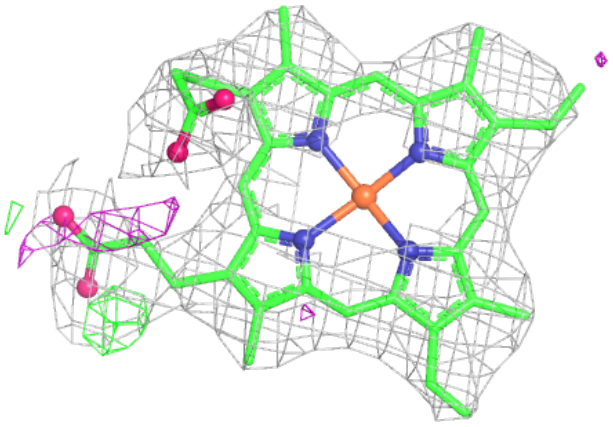


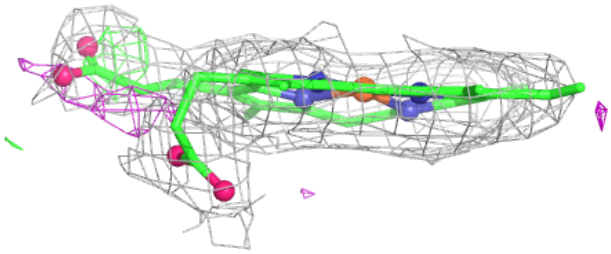


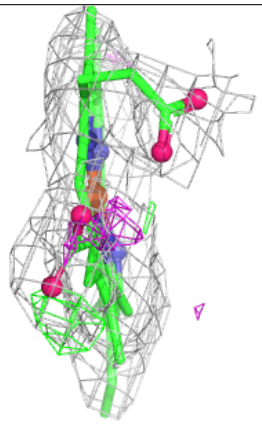


Electron density around HEM B 301:

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

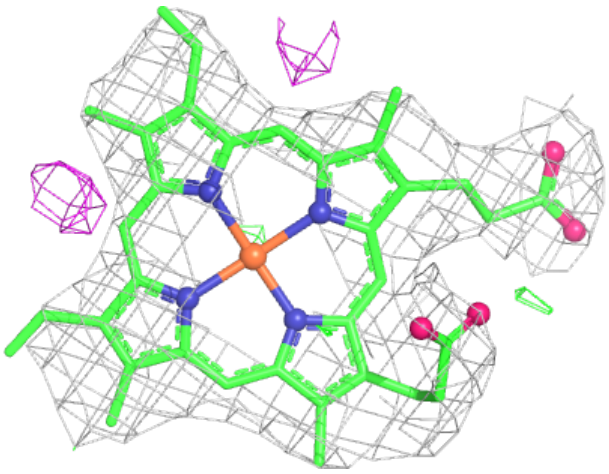


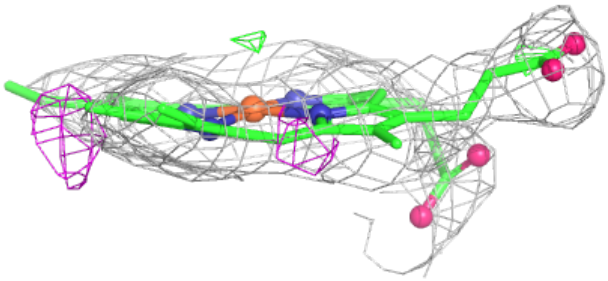




Electron density around HEM E 301:

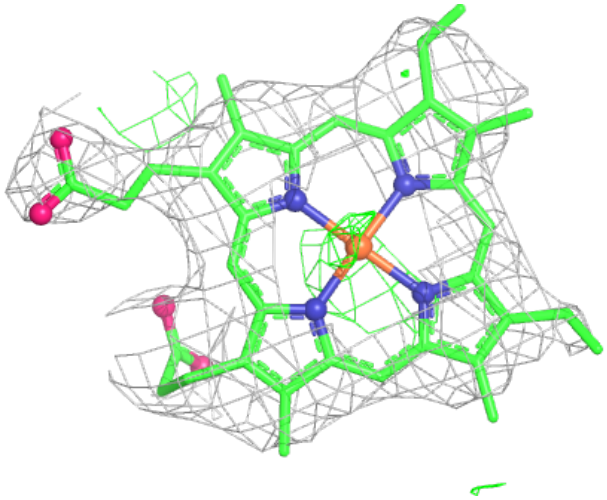
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

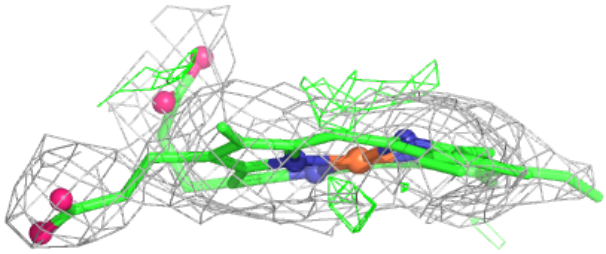


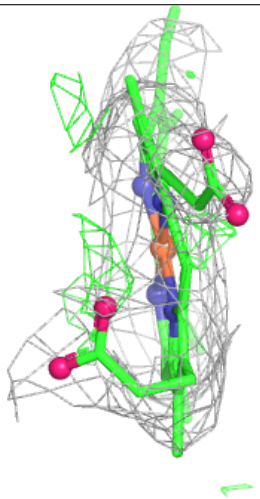


Electron density around HEM G 301:

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

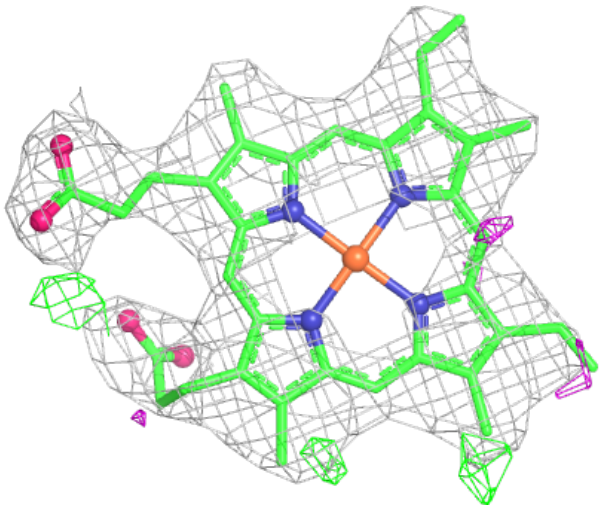


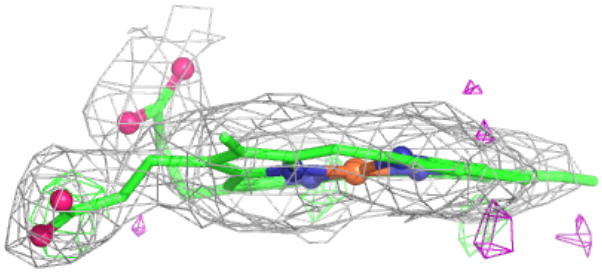


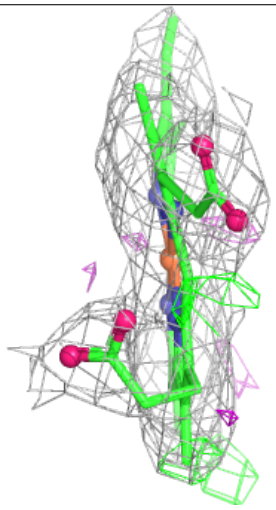


Electron density around HEM A 301:

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

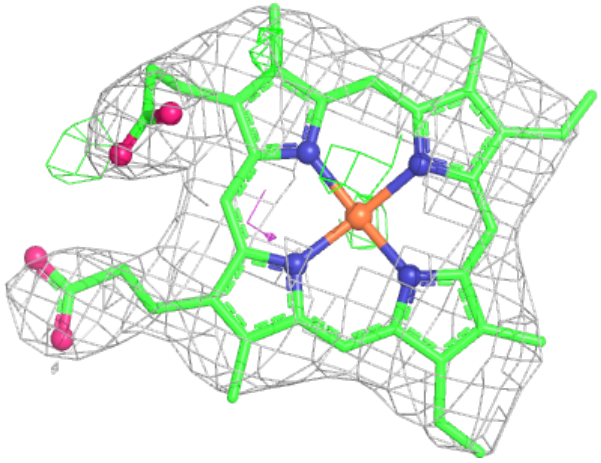


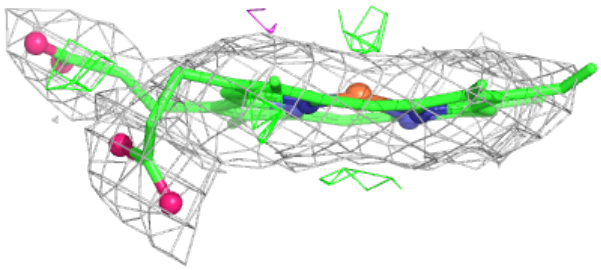


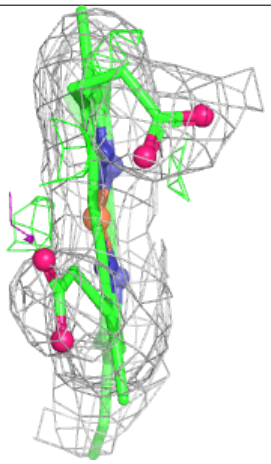


Electron density around HEM F 301:

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

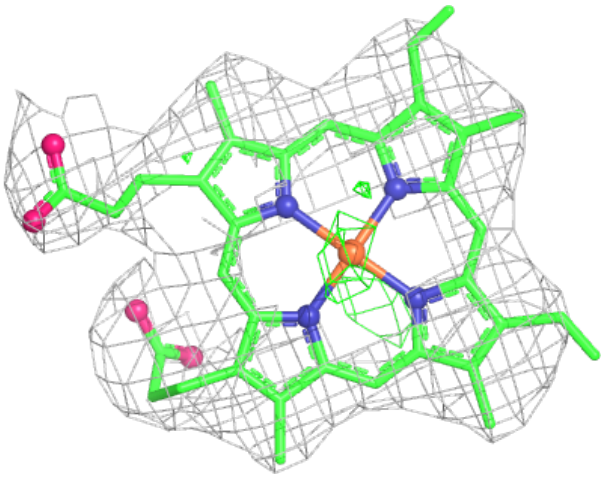


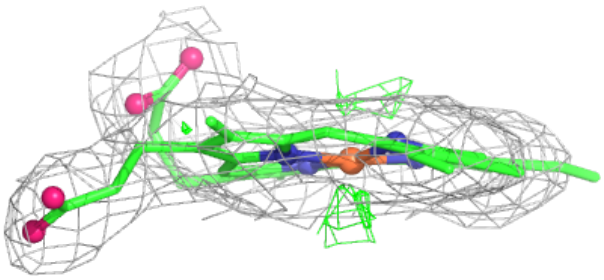


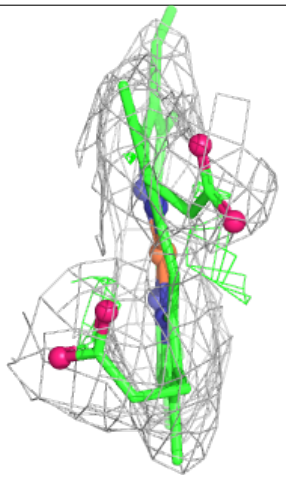


Electron density around HEM D 301:

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

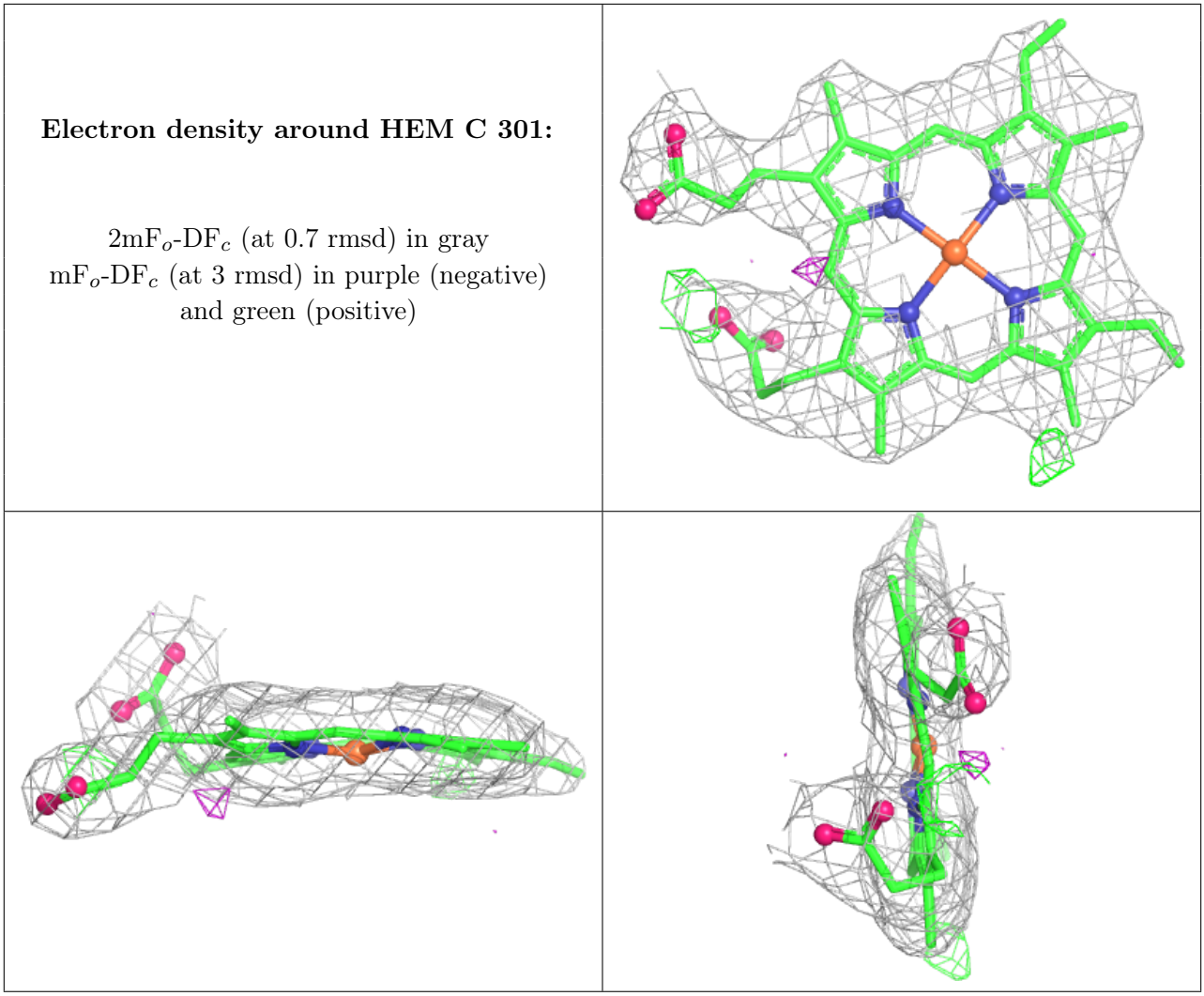






Electron density around HEM C 301:

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



6.5 Other polymers

There are no such residues in this entry.