Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 10:49 AM EDT

PDB ID	:	2OIF / pdb_00002oif
Title	:	The crystal structure of ferric cyanide bound barley hexacoordinate hemoglobin.
Authors	:	Hoy, J.A.
Deposited on	:	2007-01-10
Resolution	:	1.80 Å(reported)

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

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

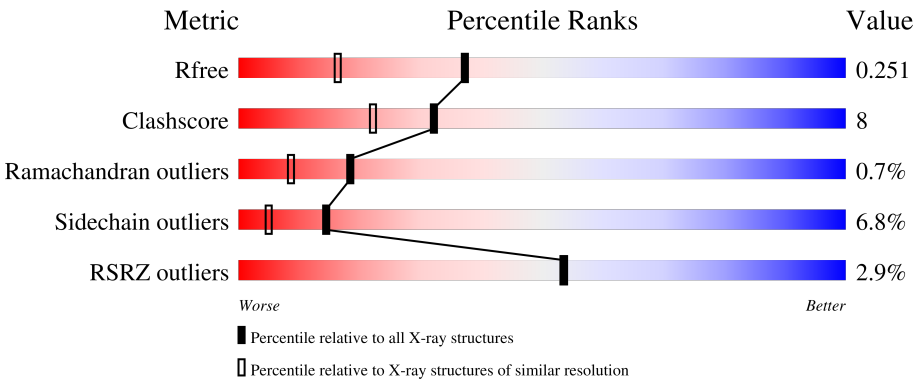
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	162	3% 84% 10% • 6%
1	B	162	2% 77% 15% • 7%
1	C	162	4% 79% 12% •• 6%
1	D	162	% 74% 15% • • 6%
1	E	162	6% 70% 21% •• 6%

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Mol	Chain	Length	Quality of chain
1	F	162	% 78% 12% • • 6%
1	G	162	4% 81% 12% • 5%
1	H	162	% 80% 13% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PGO	A	1210	X	-	-	-
4	PGO	A	1211	X	-	-	-
4	PGO	A	1215	X	-	-	-
4	PGO	B	1217	X	-	-	-
4	PGO	C	1218	X	-	-	-
4	PGO	D	1209	X	-	-	-
4	PGO	D	1219	X	-	X	-
4	PGO	E	1212	X	-	-	-
4	PGO	E	1216	X	-	X	-
4	PGO	F	1220	X	-	-	-
4	PGO	G	1214	X	-	-	-
4	PGO	H	1213	X	-	-	-
4	PGO	H	1221	X	-	-	-

2 Entry composition (i)

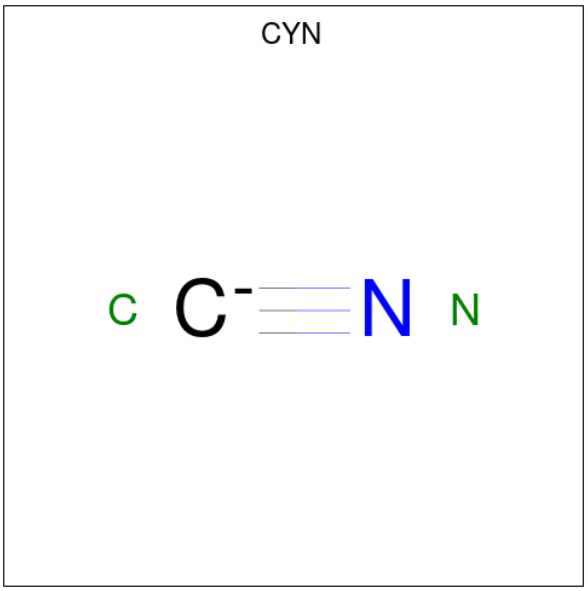
There are 5 unique types of molecules in this entry. The entry contains 10949 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Non-legume hemoglobin.

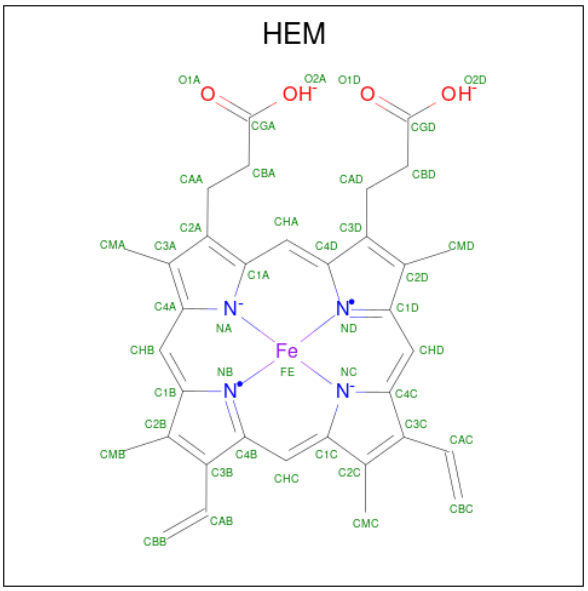
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1208	780	207	214	7	0	0	0
1	B	151	1197	772	205	213	7	0	0	0
1	C	152	1204	777	206	214	7	0	0	0
1	D	152	1204	777	206	214	7	0	0	0
1	E	153	1211	782	207	215	7	0	0	0
1	F	152	1204	777	206	214	7	0	0	0
1	G	154	1216	785	208	216	7	0	0	0
1	H	152	1204	777	206	214	7	0	0	0

- Molecule 2 is CYANIDE ION (CCD ID: CYN) (formula: CN).



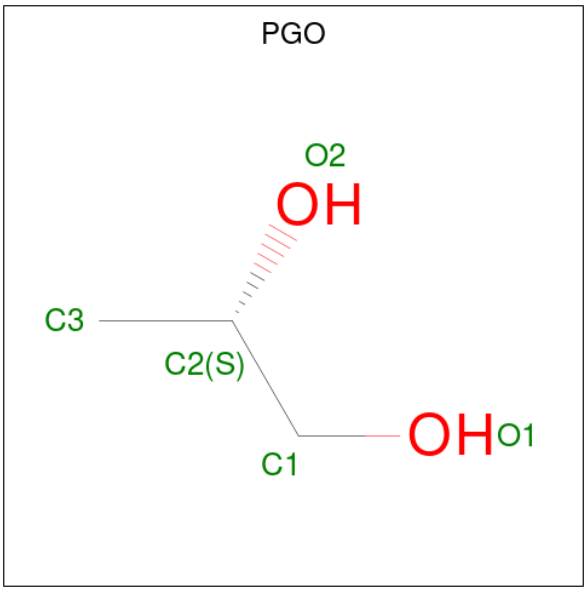
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	2	1	1	0	0
2	B	1	2	1	1	0	0
2	C	1	2	1	1	0	0
2	D	1	2	1	1	0	0
2	E	1	2	1	1	0	0
2	F	1	2	1	1	0	0
2	G	1	2	1	1	0	0
2	H	1	2	1	1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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 S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	5	3	2	0	0
4	A	1	5	3	2	0	0
4	A	1	5	3	2	0	0
4	B	1	5	3	2	0	0
4	C	1	5	3	2	0	0
4	D	1	5	3	2	0	0
4	D	1	5	3	2	0	0
4	E	1	5	3	2	0	0
4	E	1	5	3	2	0	0
4	F	1	5	3	2	0	0
4	G	1	5	3	2	0	0
4	H	1	5	3	2	0	0
4	H	1	5	3	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	116	116	116	0	0
			Total	O		
5	B	106	106	106	0	0
			Total	O		
5	C	97	97	97	0	0
			Total	O		
5	D	107	107	107	0	0
			Total	O		
5	E	109	109	109	0	0
			Total	O		
5	F	108	108	108	0	0
			Total	O		
5	G	99	99	99	0	0
			Total	O		
5	H	134	134	134	0	0

3 Residue-property plots (i)

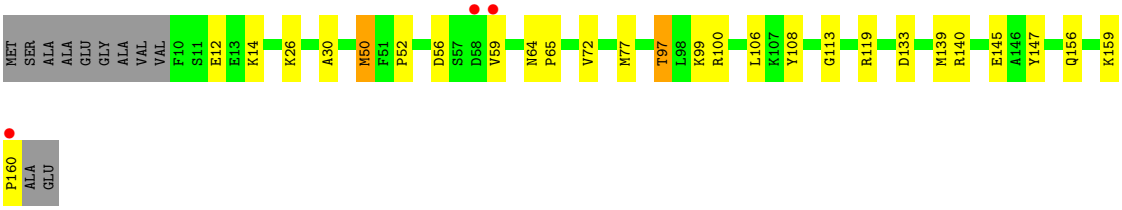
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Non-legume hemoglobin

Chain A:

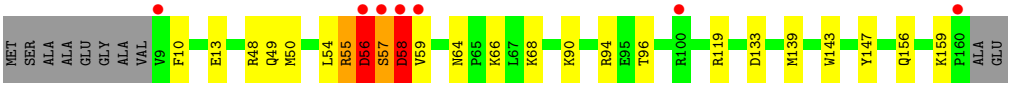
• Molecule 1: Non-legume hemoglobin

Chain B:



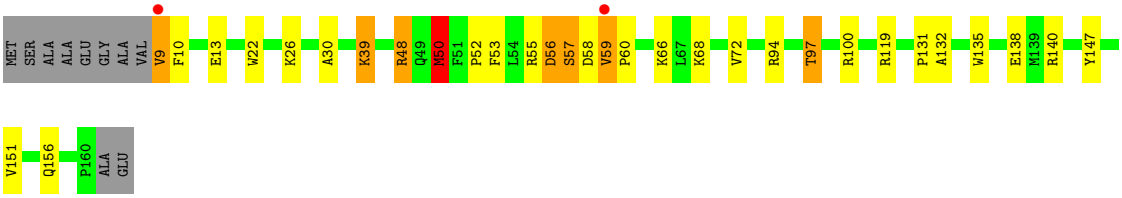
• Molecule 1: Non-legume hemoglobin

Chain C:



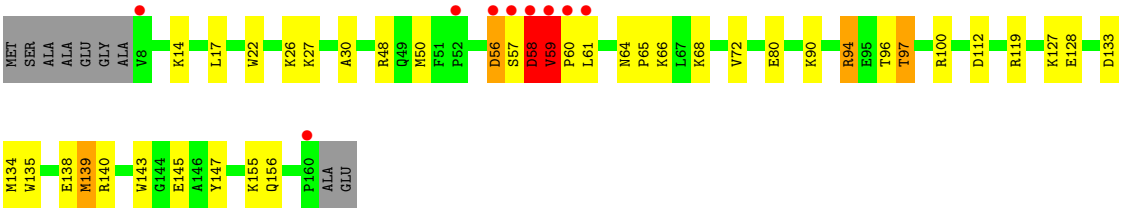
• Molecule 1: Non-legume hemoglobin

Chain D:



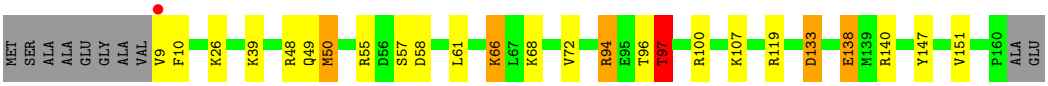
• Molecule 1: Non-legume hemoglobin

Chain E:



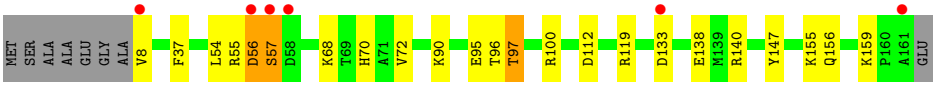
- Molecule 1: Non-legume hemoglobin

Chain F:



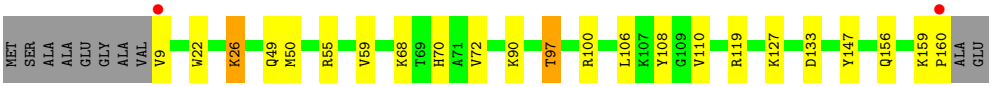
- Molecule 1: Non-legume hemoglobin

Chain G:



- Molecule 1: Non-legume hemoglobin

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.74Å 60.56Å 145.80Å 99.17° 96.97° 92.43°	Depositor
Resolution (Å)	30.00 – 1.80 30.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	87.4 (30.00-1.80) 87.4 (30.00-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.200 , 0.250 0.199 , 0.251	Depositor DCC
R_{free} test set	6195 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 28.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10949	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.53% 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: PGO, CYN, 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	1.05	1/1234 (0.1%)	1.05	3/1663 (0.2%)
1	B	0.94	2/1223 (0.2%)	1.04	2/1648 (0.1%)
1	C	0.96	1/1230 (0.1%)	1.08	2/1658 (0.1%)
1	D	0.94	0/1230	1.06	3/1658 (0.2%)
1	E	0.98	0/1237	1.06	3/1668 (0.2%)
1	F	0.97	0/1230	1.08	3/1658 (0.2%)
1	G	1.01	0/1242	1.03	2/1675 (0.1%)
1	H	0.97	0/1230	1.05	2/1658 (0.1%)
All	All	0.98	4/9856 (0.0%)	1.06	20/13286 (0.2%)

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	E	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	56	ASP	C-N	-13.39	1.15	1.33
1	A	50	MET	SD-CE	-7.86	1.59	1.79
1	B	77	MET	SD-CE	5.63	1.93	1.79
1	B	139	MET	SD-CE	5.15	1.92	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	56	ASP	O-C-N	-15.38	102.14	122.59
1	C	58	ASP	N-CA-C	-8.79	101.50	113.18
1	E	58	ASP	N-CA-C	-7.04	100.49	110.35
1	A	50	MET	CG-SD-CE	-6.88	85.76	100.90
1	B	133	ASP	N-CA-C	6.63	119.36	111.33
1	G	55	ARG	N-CA-C	-6.23	105.39	112.87
1	H	133	ASP	N-CA-C	6.13	119.60	111.75
1	B	133	ASP	CB-CA-C	-5.67	101.04	110.68
1	G	37	PHE	N-CA-C	5.58	117.44	111.36
1	A	133	ASP	N-CA-C	5.54	118.84	111.75
1	D	50	MET	CG-SD-CE	-5.51	88.79	100.90
1	F	133	ASP	N-CA-C	5.50	118.20	111.82
1	F	97	THR	N-CA-CB	-5.39	101.49	111.53
1	H	133	ASP	CB-CA-C	-5.26	100.26	110.46
1	E	133	ASP	CB-CA-C	-5.22	100.34	110.46
1	A	133	ASP	CB-CA-C	-5.14	100.50	110.46
1	E	134	MET	CG-SD-CE	-5.13	89.61	100.90
1	D	132	ALA	CA-C-N	5.13	127.15	120.28
1	D	132	ALA	C-N-CA	5.13	127.15	120.28
1	F	107	LYS	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	56	ASP	Mainchain
1	E	59	VAL	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	1208	0	1239	12	0
1	B	1197	0	1225	16	0
1	C	1204	0	1233	10	0
1	D	1204	0	1234	32	0
1	E	1211	0	1243	43	0
1	F	1204	0	1234	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1216	0	1248	10	0
1	H	1204	0	1234	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	1	0
2	H	2	0	0	1	0
3	A	43	0	30	0	0
3	B	43	0	30	0	0
3	C	43	0	30	1	0
3	D	43	0	30	2	0
3	E	43	0	30	1	0
3	F	43	0	30	1	0
3	G	43	0	30	0	0
3	H	43	0	30	0	0
4	A	15	0	20	0	0
4	B	5	0	8	1	0
4	C	5	0	8	0	0
4	D	10	0	16	5	0
4	E	10	0	16	7	0
4	F	5	0	8	0	0
4	G	5	0	8	0	0
4	H	10	0	16	3	0
5	A	116	0	0	3	0
5	B	106	0	0	5	0
5	C	97	0	0	1	0
5	D	107	0	0	4	0
5	E	109	0	0	11	0
5	F	108	0	0	5	0
5	G	99	0	0	2	0
5	H	134	0	0	0	0
All	All	10949	0	10230	163	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 8.

All (163) 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:9:VAL:HG12	1:A:10:PHE:H	1.15	1.10
1:C:139:MET:HE2	1:C:143:TRP:CD1	1.86	1.09
1:F:9:VAL:HG12	1:F:10:PHE:H	1.12	1.09
1:E:58:ASP:OD1	5:E:855:HOH:O	1.69	1.08
1:E:59:VAL:HB	1:E:60:PRO:HD3	1.36	1.04
1:E:139:MET:HE3	1:E:139:MET:HA	1.40	1.03
1:C:139:MET:HE2	1:C:143:TRP:HD1	1.25	0.99
1:E:14:LYS:HE2	1:E:145:GLU:OE1	1.61	0.99
1:A:9:VAL:CG1	1:A:10:PHE:H	1.78	0.95
1:D:97:THR:HG22	1:D:100:ARG:H	1.30	0.95
1:A:128:GLU:OE1	5:A:337:HOH:O	1.86	0.94
1:F:97:THR:HG22	1:F:100:ARG:H	1.35	0.91
1:D:59:VAL:CG2	1:D:60:PRO:HA	2.04	0.88
1:E:17:LEU:HB3	1:E:139:MET:CE	2.03	0.88
1:F:96:THR:HG22	1:F:97:THR:H	1.38	0.87
1:D:59:VAL:HG23	1:D:60:PRO:HA	1.56	0.86
1:B:97:THR:HG23	5:B:1250:HOH:O	1.75	0.85
1:E:17:LEU:HB3	1:E:139:MET:HE1	1.57	0.84
1:G:97:THR:HG22	1:G:100:ARG:H	1.42	0.83
1:E:58:ASP:CG	5:E:855:HOH:O	2.17	0.81
1:F:9:VAL:HG12	1:F:10:PHE:N	1.94	0.81
1:D:59:VAL:CB	1:D:60:PRO:HA	2.11	0.81
1:D:59:VAL:HB	1:D:60:PRO:HA	1.64	0.78
1:E:96:THR:HG22	1:E:97:THR:H	1.50	0.76
1:A:9:VAL:HG12	1:A:10:PHE:N	1.97	0.75
1:E:59:VAL:HB	1:E:60:PRO:CD	2.16	0.75
1:D:59:VAL:HB	1:D:60:PRO:CA	2.17	0.74
1:F:9:VAL:CG1	1:F:10:PHE:H	1.95	0.74
1:G:68:LYS:O	1:G:72:VAL:HG23	1.88	0.73
1:E:135:TRP:HE1	4:E:1216:PGO:H2	1.52	0.73
4:E:1216:PGO:H11	5:E:827:HOH:O	1.89	0.71
1:G:54:LEU:C	1:G:56:ASP:H	1.98	0.71
1:E:97:THR:HG22	1:E:100:ARG:HB2	1.72	0.70
1:F:68:LYS:O	1:F:72:VAL:HG23	1.91	0.70
1:H:127:LYS:NZ	4:H:1221:PGO:H2	2.06	0.70
1:E:139:MET:HA	1:E:139:MET:CE	2.19	0.69
1:D:48:ARG:HH21	1:D:59:VAL:HG11	1.56	0.69
1:D:22:TRP:CZ2	1:D:26:LYS:HG3	2.30	0.67
1:H:97:THR:HG22	1:H:100:ARG:H	1.60	0.66
1:E:48:ARG:HD3	1:E:61:LEU:HD21	1.78	0.66
1:H:68:LYS:O	1:H:72:VAL:HG23	1.96	0.65
4:D:1219:PGO:H33	5:D:1274:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ASP:O	1:C:58:ASP:N	2.30	0.64
1:D:59:VAL:HG12	5:D:1323:HOH:O	1.97	0.64
1:E:127:LYS:HZ1	4:E:1216:PGO:H33	1.62	0.64
1:E:127:LYS:NZ	4:E:1216:PGO:H33	2.13	0.63
1:D:30:ALA:HA	1:D:72:VAL:HG22	1.80	0.63
1:A:9:VAL:CG1	1:A:10:PHE:N	2.49	0.63
1:F:48:ARG:HD3	1:F:61:LEU:HD21	1.81	0.62
1:E:80:GLU:OE1	1:E:94:ARG:CD	2.48	0.61
1:D:59:VAL:CB	1:D:60:PRO:CA	2.77	0.61
1:D:55:ARG:O	1:D:56:ASP:CG	2.44	0.61
1:E:97:THR:HG22	1:E:100:ARG:H	1.66	0.60
1:E:145:GLU:HG3	5:E:643:HOH:O	2.00	0.60
1:D:9:VAL:HG12	1:D:10:PHE:H	1.67	0.60
1:G:54:LEU:C	1:G:56:ASP:N	2.60	0.60
1:E:140:ARG:NH1	5:E:640:HOH:O	2.35	0.59
1:C:13:GLU:HG3	5:C:787:HOH:O	2.03	0.59
1:D:59:VAL:HB	1:D:60:PRO:C	2.29	0.58
1:E:80:GLU:OE1	1:E:94:ARG:HD3	2.03	0.58
1:F:96:THR:HG22	1:F:97:THR:N	2.14	0.58
1:C:139:MET:CE	1:C:143:TRP:CD1	2.75	0.58
1:F:50:MET:HG3	5:F:416:HOH:O	2.04	0.56
1:F:138:GLU:H	1:F:138:GLU:CD	2.14	0.56
1:B:30:ALA:HA	1:B:72:VAL:CG2	2.37	0.55
1:F:48:ARG:HD2	5:F:373:HOH:O	2.07	0.55
1:C:48:ARG:HG2	1:C:54:LEU:HB3	1.87	0.55
1:E:97:THR:HG21	5:E:851:HOH:O	2.07	0.54
1:H:97:THR:CG2	1:H:100:ARG:H	2.21	0.54
1:D:30:ALA:HA	1:D:72:VAL:CG2	2.38	0.53
1:E:68:LYS:O	1:E:72:VAL:HG23	2.07	0.53
1:B:14:LYS:HE2	1:B:145:GLU:OE1	2.08	0.53
1:B:30:ALA:HA	1:B:72:VAL:HG22	1.89	0.53
1:B:97:THR:HG22	1:B:100:ARG:H	1.73	0.53
1:E:17:LEU:HB3	1:E:139:MET:HE3	1.86	0.53
1:E:127:LYS:NZ	4:E:1216:PGO:C3	2.71	0.53
1:D:140:ARG:NH1	5:D:1319:HOH:O	1.85	0.53
1:E:97:THR:CG2	1:E:100:ARG:H	2.22	0.53
1:H:119:ARG:HB2	1:H:147:TYR:CE1	2.43	0.53
1:A:119:ARG:HB2	1:A:147:TYR:CE1	2.44	0.52
1:D:68:LYS:O	1:D:72:VAL:HG23	2.10	0.52
1:A:62:GLU:O	1:A:68:LYS:NZ	2.43	0.52
1:F:96:THR:HG23	1:F:100:ARG:CZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:TRP:HE1	4:D:1219:PGO:C2	2.23	0.52
1:G:97:THR:HG21	5:G:1262:HOH:O	2.10	0.51
1:H:127:LYS:HZ2	4:H:1221:PGO:H2	1.75	0.51
1:B:160:PRO:HB3	1:H:108:TYR:CZ	2.46	0.51
1:H:127:LYS:HZ3	4:H:1221:PGO:H2	1.76	0.51
1:D:147:TYR:CE1	1:D:151:VAL:HG21	2.46	0.51
1:E:50:MET:HE3	5:E:715:HOH:O	2.11	0.51
1:E:139:MET:HE2	1:E:143:TRP:CD1	2.45	0.51
1:A:68:LYS:O	1:A:72:VAL:HG23	2.11	0.50
1:D:57:SER:O	1:D:59:VAL:HG22	2.11	0.50
1:D:97:THR:HB	1:D:100:ARG:HD3	1.93	0.50
1:H:22:TRP:CZ2	1:H:26:LYS:HG3	2.47	0.50
1:E:22:TRP:CZ2	1:E:26:LYS:HG3	2.47	0.49
1:E:17:LEU:CB	1:E:139:MET:HE1	2.37	0.49
1:C:49:GLN:O	1:C:55:ARG:HD3	2.12	0.48
1:C:139:MET:HE3	1:C:139:MET:HA	1.95	0.48
1:D:59:VAL:HG23	1:D:60:PRO:CA	2.38	0.48
1:F:119:ARG:HB2	1:F:147:TYR:CE1	2.48	0.48
1:E:112:ASP:OD1	1:E:155:LYS:HE2	2.13	0.48
1:F:94:ARG:HB2	1:F:94:ARG:NH1	2.29	0.47
1:F:140:ARG:NH1	5:F:463:HOH:O	2.48	0.47
1:F:147:TYR:CE1	1:F:151:VAL:HG21	2.49	0.47
1:F:50:MET:HE2	1:F:50:MET:HB2	1.62	0.47
1:G:70:HIS:NE2	2:G:207:CYN:N	2.56	0.47
1:B:113:GLY:HA3	4:D:1209:PGO:H12	1.95	0.47
1:D:52:PRO:HD2	3:D:163:HEM:O1D	2.14	0.47
1:D:135:TRP:CD1	4:D:1219:PGO:H31	2.50	0.47
1:H:97:THR:HG22	1:H:100:ARG:HG3	1.97	0.47
1:A:140:ARG:NH1	5:A:386:HOH:O	2.47	0.47
1:E:96:THR:HG22	1:E:97:THR:N	2.25	0.47
3:E:163:HEM:HHA	3:E:163:HEM:HBA1	1.97	0.47
1:G:112:ASP:OD1	1:G:155:LYS:HE2	2.15	0.46
1:H:49:GLN:O	1:H:55:ARG:HD3	2.15	0.46
1:E:119:ARG:HB2	1:E:147:TYR:CE2	2.50	0.46
1:F:49:GLN:NE2	1:F:55:ARG:HG2	2.32	0.45
1:E:127:LYS:HZ1	4:E:1216:PGO:C3	2.29	0.45
1:E:94:ARG:NH1	5:E:753:HOH:O	2.49	0.45
1:B:108:TYR:CZ	1:H:160:PRO:HB3	2.51	0.45
1:F:66:LYS:HB2	5:F:376:HOH:O	2.16	0.45
1:A:37:PHE:HA	1:A:40:ILE:HD12	1.98	0.45
1:A:129:ALA:O	1:D:131:PRO:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:TRP:NE1	4:E:1216:PGO:H2	2.27	0.45
1:E:128:GLU:HG3	5:E:845:HOH:O	2.17	0.44
3:F:163:HEM:HMB1	3:F:163:HEM:HBB2	1.99	0.44
1:G:140:ARG:NH1	5:G:1295:HOH:O	2.48	0.44
1:D:48:ARG:NH2	1:D:59:VAL:HG11	2.27	0.44
3:D:163:HEM:HHA	3:D:163:HEM:HBA1	1.98	0.44
1:B:12:GLU:HG2	5:B:1302:HOH:O	2.16	0.44
4:B:1217:PGO:C3	5:B:1321:HOH:O	2.66	0.43
1:B:50:MET:HE2	1:B:50:MET:HB2	1.46	0.43
1:H:70:HIS:NE2	2:H:208:CYN:N	2.56	0.43
1:B:64:ASN:HA	1:B:65:PRO:HD3	1.89	0.43
3:C:163:HEM:HMB2	3:C:163:HEM:HBB2	1.99	0.43
1:D:56:ASP:O	1:D:56:ASP:OD1	2.36	0.43
4:D:1219:PGO:H12	5:D:1257:HOH:O	2.16	0.43
1:H:97:THR:CG2	1:H:100:ARG:HG3	2.48	0.43
1:B:106:LEU:HG	1:H:106:LEU:HG	2.00	0.43
1:B:119:ARG:HB2	1:B:147:TYR:CE2	2.54	0.43
1:E:30:ALA:HA	1:E:72:VAL:CG2	2.49	0.43
1:B:97:THR:HG22	1:B:99:LYS:N	2.34	0.42
1:B:140:ARG:NH1	5:B:1236:HOH:O	2.49	0.42
1:D:119:ARG:HB2	1:D:147:TYR:CE1	2.54	0.42
1:F:39:LYS:NZ	5:F:384:HOH:O	2.53	0.42
1:C:119:ARG:HB2	1:C:147:TYR:CE2	2.55	0.42
1:D:50:MET:HB2	1:D:50:MET:HE2	1.41	0.42
1:E:64:ASN:HA	1:E:65:PRO:HD3	1.82	0.42
1:E:96:THR:HG23	1:E:100:ARG:CZ	2.50	0.42
1:C:64:ASN:O	1:C:68:LYS:HG3	2.19	0.42
1:B:97:THR:HG21	5:B:1252:HOH:O	2.20	0.41
1:D:53:PHE:HB2	1:D:66:LYS:HD2	2.01	0.41
1:E:145:GLU:CG	5:E:643:HOH:O	2.64	0.41
1:G:96:THR:HG22	1:G:100:ARG:NH2	2.35	0.41
1:D:13:GLU:H	1:D:13:GLU:CD	2.28	0.41
1:G:119:ARG:HB2	1:G:147:TYR:CE2	2.56	0.41
1:A:65:PRO:HD2	5:A:322:HOH:O	2.20	0.41
1:E:27:LYS:NZ	5:E:513:HOH:O	2.50	0.40
1:H:50:MET:HE1	1:H:110:VAL:HA	2.02	0.40
1:E:30:ALA:HA	1:E:72:VAL:HG22	2.02	0.40
1:E:56:ASP:C	1:E:58:ASP:H	2.30	0.40
1:D:39:LYS:HB2	1:D:39:LYS:HE3	1.80	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	151/162 (93%)	150 (99%)	1 (1%)	0	100	100
1	B	149/162 (92%)	147 (99%)	2 (1%)	0	100	100
1	C	150/162 (93%)	144 (96%)	3 (2%)	3 (2%)	6	1
1	D	150/162 (93%)	144 (96%)	4 (3%)	2 (1%)	9	3
1	E	151/162 (93%)	146 (97%)	3 (2%)	2 (1%)	9	3
1	F	150/162 (93%)	146 (97%)	4 (3%)	0	100	100
1	G	152/162 (94%)	146 (96%)	5 (3%)	1 (1%)	18	8
1	H	150/162 (93%)	149 (99%)	1 (1%)	0	100	100
All	All	1203/1296 (93%)	1172 (97%)	23 (2%)	8 (1%)	18	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	10	PHE
1	C	56	ASP
1	C	57	SER
1	D	59	VAL
1	E	59	VAL
1	D	56	ASP
1	E	57	SER
1	G	57	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	126/131 (96%)	123 (98%)	3 (2%)	43	31
1	B	125/131 (95%)	117 (94%)	8 (6%)	16	6
1	C	126/131 (96%)	114 (90%)	12 (10%)	8	2
1	D	126/131 (96%)	116 (92%)	10 (8%)	11	3
1	E	127/131 (97%)	117 (92%)	10 (8%)	11	3
1	F	126/131 (96%)	117 (93%)	9 (7%)	13	4
1	G	127/131 (97%)	117 (92%)	10 (8%)	11	3
1	H	126/131 (96%)	119 (94%)	7 (6%)	19	8
All	All	1009/1048 (96%)	940 (93%)	69 (7%)	14	5

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	26	LYS
1	A	95	GLU
1	B	26	LYS
1	B	50	MET
1	B	52	PRO
1	B	56	ASP
1	B	59	VAL
1	B	97	THR
1	B	156	GLN
1	B	159	LYS
1	C	50	MET
1	C	55	ARG
1	C	57	SER
1	C	58	ASP
1	C	59	VAL
1	C	66	LYS
1	C	90	LYS
1	C	94	ARG
1	C	96	THR
1	C	133	ASP
1	C	156	GLN
1	C	159	LYS
1	D	9	VAL
1	D	39	LYS
1	D	48	ARG
1	D	50	MET

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Mol	Chain	Res	Type
1	D	57	SER
1	D	58	ASP
1	D	94	ARG
1	D	97	THR
1	D	138	GLU
1	D	156	GLN
1	E	56	ASP
1	E	58	ASP
1	E	59	VAL
1	E	66	LYS
1	E	90	LYS
1	E	94	ARG
1	E	97	THR
1	E	138	GLU
1	E	139	MET
1	E	156	GLN
1	F	26	LYS
1	F	50	MET
1	F	57	SER
1	F	58	ASP
1	F	66	LYS
1	F	94	ARG
1	F	97	THR
1	F	133	ASP
1	F	138	GLU
1	G	8	VAL
1	G	56	ASP
1	G	57	SER
1	G	90	LYS
1	G	95	GLU
1	G	97	THR
1	G	133	ASP
1	G	138	GLU
1	G	156	GLN
1	G	159	LYS
1	H	9	VAL
1	H	26	LYS
1	H	59	VAL
1	H	90	LYS
1	H	97	THR
1	H	156	GLN
1	H	159	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	B	149	GLN
1	C	31	ASN
1	D	31	ASN
1	F	49	GLN
1	F	84	GLN
1	G	49	GLN
1	H	149	GLN
1	H	156	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

29 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	CYN	E	205	-	1,1,1	0.10	0	-		
4	PGO	D	1209	-	4,4,4	0.69	0	4,4,4	0.42	0
3	HEM	C	163	1	50,50,50	1.14	4 (8%)	67,82,82	1.10	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PGO	B	1217	-	4,4,4	0.77	0	4,4,4	0.65	0
3	HEM	F	163	1	50,50,50	1.34	6 (12%)	67,82,82	1.06	1 (1%)
3	HEM	H	163	1	50,50,50	1.18	3 (6%)	67,82,82	1.06	5 (7%)
4	PGO	D	1219	-	4,4,4	0.60	0	4,4,4	1.34	0
2	CYN	B	202	-	1,1,1	0.06	0	-		
3	HEM	E	163	1	50,50,50	1.23	4 (8%)	67,82,82	1.20	4 (5%)
2	CYN	H	208	-	1,1,1	0.24	0	-		
2	CYN	A	201	-	1,1,1	0.20	0	-		
4	PGO	A	1211	-	4,4,4	0.62	0	4,4,4	0.66	0
4	PGO	E	1216	-	4,4,4	0.58	0	4,4,4	0.95	0
4	PGO	H	1221	-	4,4,4	0.70	0	4,4,4	0.72	0
4	PGO	C	1218	-	4,4,4	0.72	0	4,4,4	0.66	0
2	CYN	D	204	-	1,1,1	0.08	0	-		
4	PGO	F	1220	-	4,4,4	0.71	0	4,4,4	0.84	0
2	CYN	F	206	-	1,1,1	0.22	0	-		
3	HEM	D	163	1	50,50,50	1.12	3 (6%)	67,82,82	1.08	3 (4%)
3	HEM	A	163	1	50,50,50	1.16	4 (8%)	67,82,82	1.04	3 (4%)
4	PGO	H	1213	-	4,4,4	0.56	0	4,4,4	0.61	0
4	PGO	E	1212	-	4,4,4	0.73	0	4,4,4	0.39	0
4	PGO	A	1210	4	4,4,4	0.57	0	4,4,4	0.87	0
2	CYN	C	203	-	1,1,1	0.05	0	-		
3	HEM	G	163	1	50,50,50	1.19	3 (6%)	67,82,82	1.26	6 (8%)
4	PGO	A	1215	4	4,4,4	0.59	0	4,4,4	0.75	0
4	PGO	G	1214	-	4,4,4	0.67	0	4,4,4	0.53	0
3	HEM	B	163	1	50,50,50	1.22	6 (12%)	67,82,82	1.10	3 (4%)
2	CYN	G	207	-	1,1,1	0.05	0	-		

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
4	PGO	D	1209	-	1/1/1/1	0/2/2/2	-
3	HEM	C	163	1	-	7/14/54/54	-
4	PGO	B	1217	-	1/1/1/1	0/2/2/2	-
3	HEM	F	163	1	-	5/14/54/54	-
3	HEM	H	163	1	-	5/14/54/54	-
4	PGO	D	1219	-	1/1/1/1	0/2/2/2	-
3	HEM	E	163	1	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGO	A	1211	-	1/1/1/1	0/2/2/2	-
4	PGO	E	1216	-	1/1/1/1	0/2/2/2	-
4	PGO	H	1221	-	1/1/1/1	0/2/2/2	-
4	PGO	C	1218	-	1/1/1/1	0/2/2/2	-
4	PGO	F	1220	-	1/1/1/1	0/2/2/2	-
3	HEM	D	163	1	-	7/14/54/54	-
3	HEM	A	163	1	-	7/14/54/54	-
4	PGO	H	1213	-	1/1/1/1	0/2/2/2	-
4	PGO	E	1212	-	1/1/1/1	0/2/2/2	-
4	PGO	A	1210	4	1/1/1/1	0/2/2/2	-
3	HEM	G	163	1	-	6/14/54/54	-
4	PGO	A	1215	4	1/1/1/1	0/2/2/2	-
4	PGO	G	1214	-	1/1/1/1	0/2/2/2	-
3	HEM	B	163	1	-	6/14/54/54	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	163	HEM	CBC-CAC	3.73	1.48	1.30
3	G	163	HEM	CBC-CAC	3.66	1.48	1.30
3	E	163	HEM	CAB-C3B	-3.58	1.37	1.47
3	F	163	HEM	CBC-CAC	3.52	1.47	1.30
3	C	163	HEM	CBC-CAC	3.49	1.47	1.30
3	E	163	HEM	CBC-CAC	3.42	1.46	1.30
3	H	163	HEM	CBC-CAC	3.27	1.46	1.30
3	B	163	HEM	CBC-CAC	3.25	1.46	1.30
3	D	163	HEM	CBC-CAC	3.19	1.45	1.30
3	C	163	HEM	CBB-CAB	2.92	1.44	1.30
3	B	163	HEM	CBB-CAB	2.90	1.44	1.30
3	F	163	HEM	C4D-ND	-2.90	1.35	1.40
3	H	163	HEM	CBB-CAB	2.87	1.44	1.30
3	C	163	HEM	CAB-C3B	-2.80	1.39	1.47
3	F	163	HEM	CAB-C3B	-2.80	1.39	1.47
3	D	163	HEM	CBB-CAB	2.71	1.43	1.30
3	F	163	HEM	CBB-CAB	2.68	1.43	1.30
3	G	163	HEM	CBB-CAB	2.53	1.42	1.30
3	E	163	HEM	CAC-C3C	-2.50	1.40	1.47
3	F	163	HEM	CAC-C3C	-2.45	1.40	1.47
3	A	163	HEM	CBB-CAB	2.44	1.42	1.30
3	G	163	HEM	C4C-NC	-2.43	1.35	1.39
3	D	163	HEM	CAB-C3B	-2.39	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	163	HEM	CAB-C3B	-2.34	1.41	1.47
3	B	163	HEM	C4C-NC	-2.28	1.35	1.39
3	F	163	HEM	C4C-NC	-2.22	1.35	1.39
3	A	163	HEM	CMB-C2B	2.13	1.55	1.50
3	A	163	HEM	CAB-C3B	-2.11	1.41	1.47
3	B	163	HEM	C2A-C3A	-2.05	1.33	1.38
3	B	163	HEM	CMA-C3A	2.04	1.55	1.50
3	B	163	HEM	CAB-C3B	-2.04	1.41	1.47
3	C	163	HEM	CMA-C3A	2.02	1.54	1.50
3	E	163	HEM	CBB-CAB	2.00	1.40	1.30

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	163	HEM	C3B-C4B-NB	4.64	112.80	109.47
3	H	163	HEM	C3B-C4B-NB	3.89	112.26	109.47
3	B	163	HEM	C3B-C4B-NB	3.86	112.24	109.47
3	C	163	HEM	C3B-C4B-NB	3.83	112.22	109.47
3	F	163	HEM	C3B-C4B-NB	3.80	112.19	109.47
3	A	163	HEM	C3B-C4B-NB	3.19	111.76	109.47
3	E	163	HEM	C3B-C2B-C1B	-2.83	104.29	106.41
3	D	163	HEM	C4C-C3C-C2C	-2.53	104.62	106.81
3	E	163	HEM	CAA-C2A-C1A	2.51	129.85	124.94
3	A	163	HEM	CBC-CAC-C3C	-2.50	115.02	127.53
3	E	163	HEM	C4B-C3B-C2B	2.37	109.46	107.28
3	G	163	HEM	CAD-C3D-C4D	2.34	128.78	124.70
3	A	163	HEM	CBD-CAD-C3D	-2.28	106.22	112.53
3	H	163	HEM	CHD-C4C-NC	-2.27	121.98	124.45
3	E	163	HEM	CBD-CAD-C3D	-2.26	106.30	112.53
3	D	163	HEM	C3B-C4B-NB	2.20	111.05	109.47
3	G	163	HEM	CHD-C4C-NC	-2.20	122.06	124.45
3	B	163	HEM	CAD-C3D-C4D	2.17	128.48	124.70
3	G	163	HEM	C4D-ND-C1D	-2.15	102.66	105.21
3	D	163	HEM	CHD-C1D-ND	2.15	126.73	124.42
3	G	163	HEM	C3D-C4D-ND	2.10	112.47	110.17
3	C	163	HEM	C4C-C3C-C2C	-2.09	105.00	106.81
3	B	163	HEM	C2B-C1B-NB	2.09	112.24	109.84
3	H	163	HEM	C1B-NB-C4B	-2.08	102.74	105.21
3	G	163	HEM	C4B-C3B-C2B	-2.04	105.40	107.28
3	H	163	HEM	C2B-C1B-NB	2.03	112.18	109.84
3	H	163	HEM	CAD-CBD-CGD	-2.01	108.33	113.67

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1210	PGO	C2
4	A	1211	PGO	C2
4	A	1215	PGO	C2
4	B	1217	PGO	C2
4	C	1218	PGO	C2
4	D	1209	PGO	C2
4	D	1219	PGO	C2
4	E	1212	PGO	C2
4	E	1216	PGO	C2
4	F	1220	PGO	C2
4	G	1214	PGO	C2
4	H	1213	PGO	C2
4	H	1221	PGO	C2

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	163	HEM	C1A-C2A-CAA-CBA
3	D	163	HEM	C2C-C3C-CAC-CBC
3	C	163	HEM	C3D-CAD-CBD-CGD
3	F	163	HEM	C3D-CAD-CBD-CGD
3	E	163	HEM	C1A-C2A-CAA-CBA
3	E	163	HEM	C2C-C3C-CAC-CBC
3	H	163	HEM	C2C-C3C-CAC-CBC
3	E	163	HEM	C3A-C2A-CAA-CBA
3	D	163	HEM	C4C-C3C-CAC-CBC
3	H	163	HEM	C4C-C3C-CAC-CBC
3	D	163	HEM	C3A-C2A-CAA-CBA
3	A	163	HEM	C3D-CAD-CBD-CGD
3	A	163	HEM	C2C-C3C-CAC-CBC
3	B	163	HEM	C2C-C3C-CAC-CBC
3	C	163	HEM	C2C-C3C-CAC-CBC
3	F	163	HEM	C2C-C3C-CAC-CBC
3	G	163	HEM	C2C-C3C-CAC-CBC
3	E	163	HEM	C4C-C3C-CAC-CBC
3	B	163	HEM	C4C-C3C-CAC-CBC
3	D	163	HEM	CAD-CBD-CGD-O1D
3	D	163	HEM	CAD-CBD-CGD-O2D
3	A	163	HEM	CAA-CBA-CGA-O2A
3	A	163	HEM	CAA-CBA-CGA-O1A
3	A	163	HEM	CAD-CBD-CGD-O2D
3	B	163	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
3	H	163	HEM	CAD-CBD-CGD-O2D
3	F	163	HEM	CAD-CBD-CGD-O1D
3	G	163	HEM	CAA-CBA-CGA-O2A
3	E	163	HEM	CAD-CBD-CGD-O1D
3	G	163	HEM	CAA-CBA-CGA-O1A
3	A	163	HEM	CAD-CBD-CGD-O1D
3	E	163	HEM	CAD-CBD-CGD-O2D
3	B	163	HEM	CAD-CBD-CGD-O2D
3	H	163	HEM	CAD-CBD-CGD-O1D
3	G	163	HEM	CAD-CBD-CGD-O2D
3	F	163	HEM	CAD-CBD-CGD-O2D
3	G	163	HEM	CAD-CBD-CGD-O1D
3	C	163	HEM	CAD-CBD-CGD-O1D
3	A	163	HEM	C4C-C3C-CAC-CBC
3	C	163	HEM	C4C-C3C-CAC-CBC
3	F	163	HEM	C4C-C3C-CAC-CBC
3	G	163	HEM	C4C-C3C-CAC-CBC
3	B	163	HEM	CAA-CBA-CGA-O2A
3	C	163	HEM	CAD-CBD-CGD-O2D
3	C	163	HEM	CAA-CBA-CGA-O1A
3	D	163	HEM	CAA-CBA-CGA-O2A
3	H	163	HEM	CAA-CBA-CGA-O2A
3	B	163	HEM	CAA-CBA-CGA-O1A
3	C	163	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

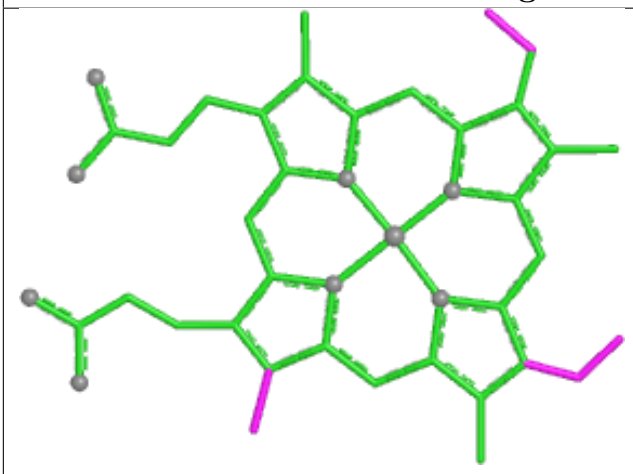
11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1209	PGO	1	0
3	C	163	HEM	1	0
4	B	1217	PGO	1	0
3	F	163	HEM	1	0
4	D	1219	PGO	4	0
3	E	163	HEM	1	0
2	H	208	CYN	1	0
4	E	1216	PGO	7	0
4	H	1221	PGO	3	0
3	D	163	HEM	2	0
2	G	207	CYN	1	0

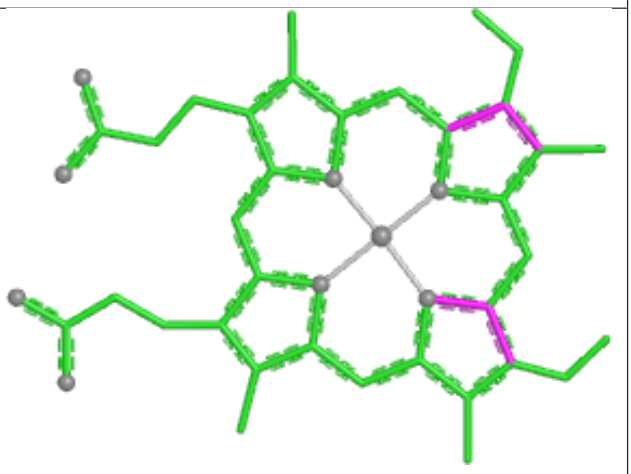
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

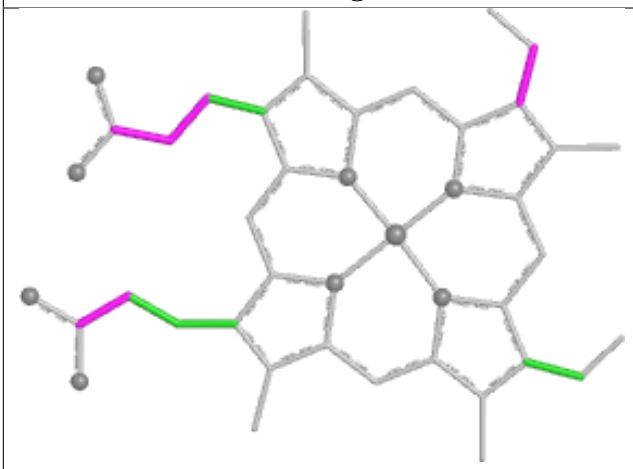
Ligand HEM C 163



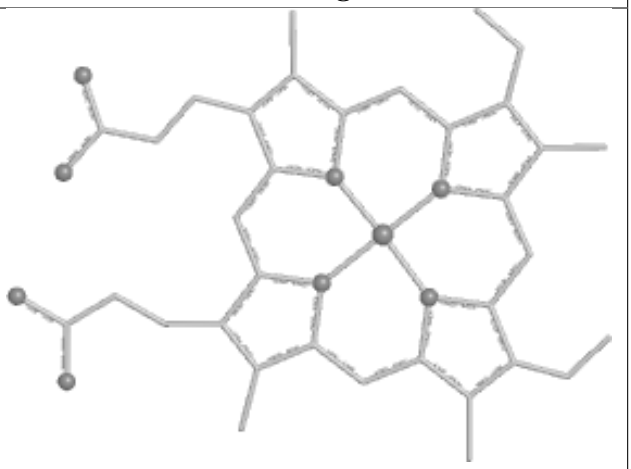
Bond lengths



Bond angles

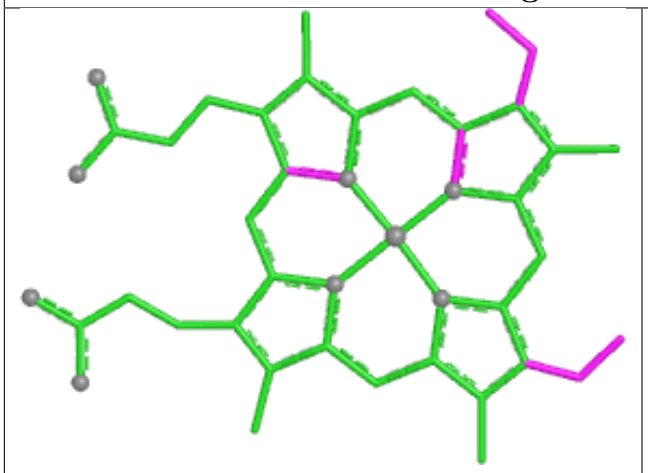


Torsions

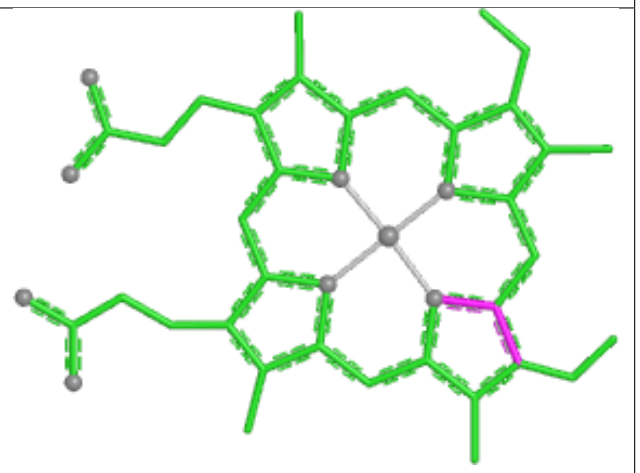


Rings

Ligand HEM F 163



Bond lengths



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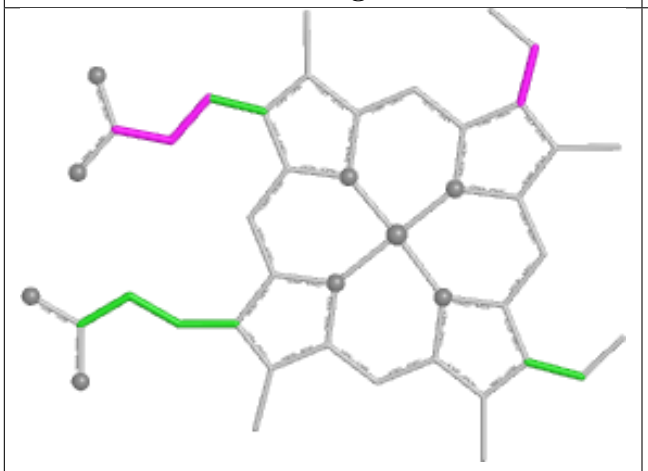

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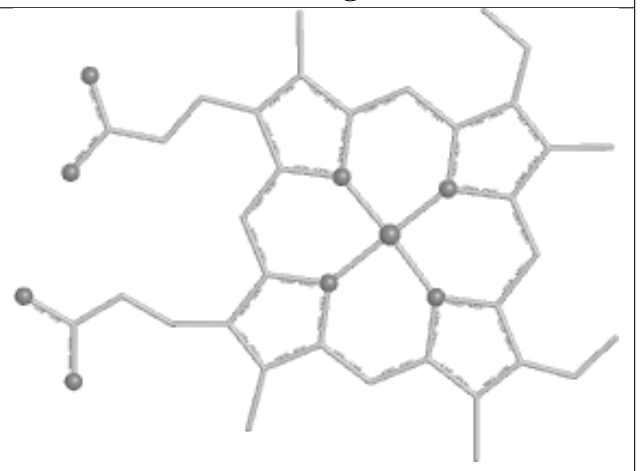
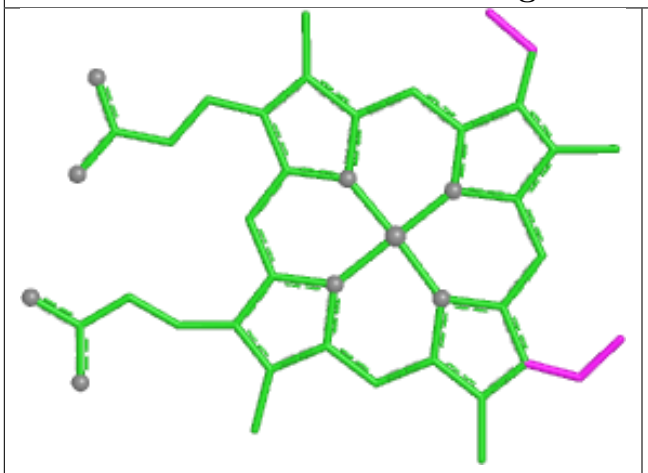
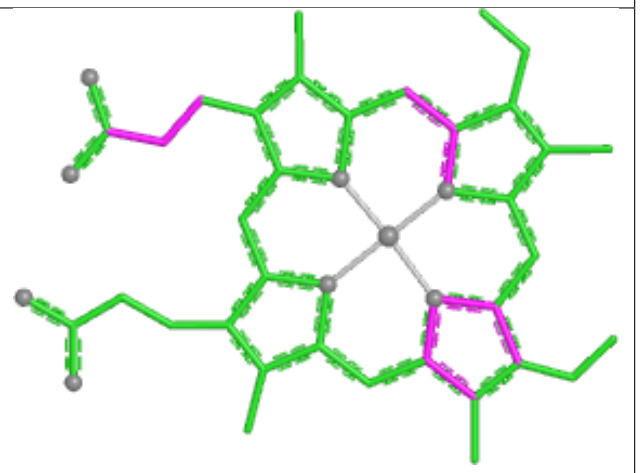


Rings

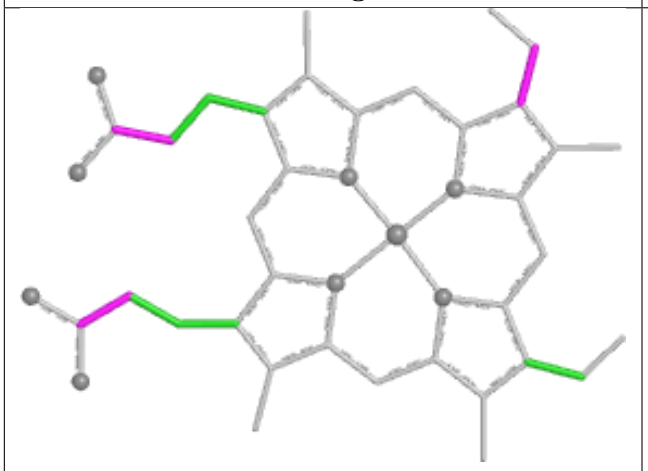
Ligand HEM H 163



Bond lengths



Bond angles



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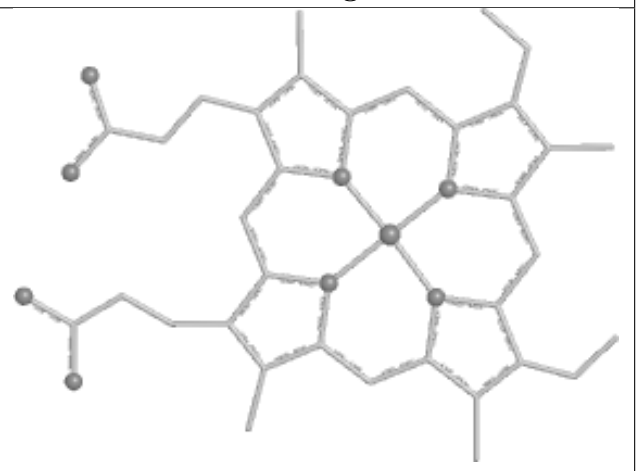
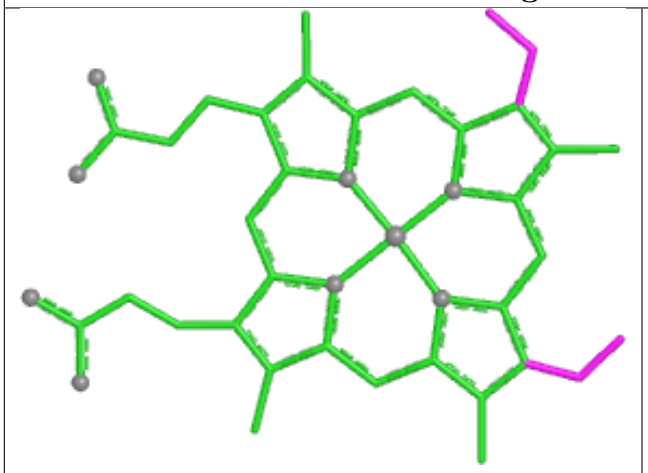


Rings

Ligand HEM E 163



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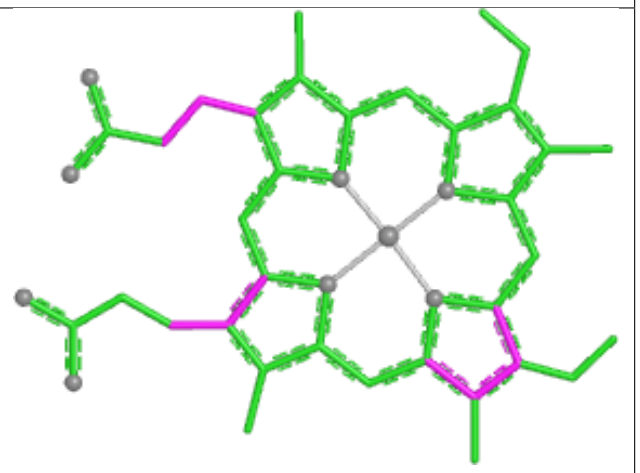
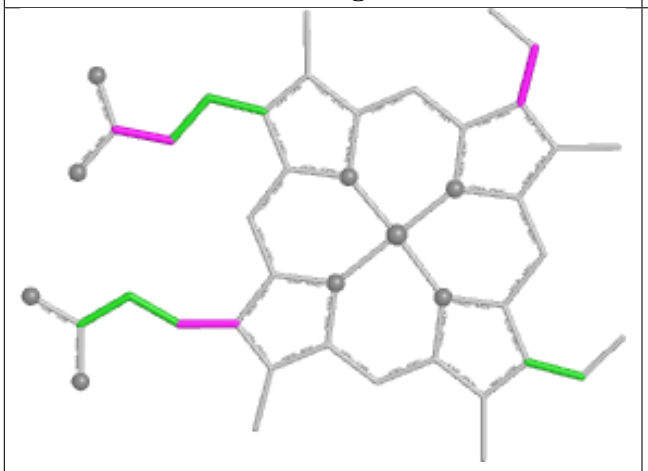
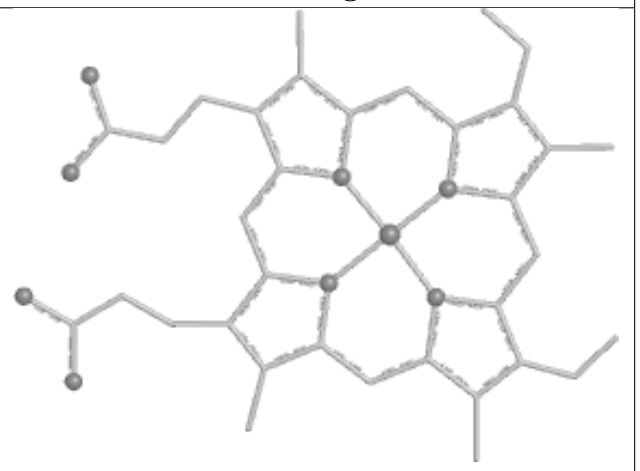


Bond angles

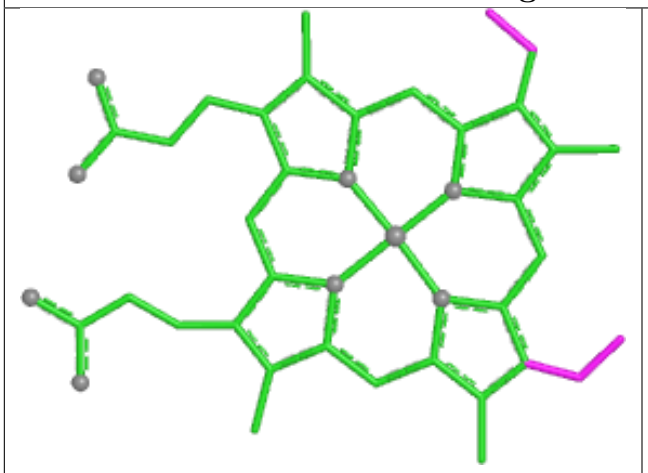


Torsions

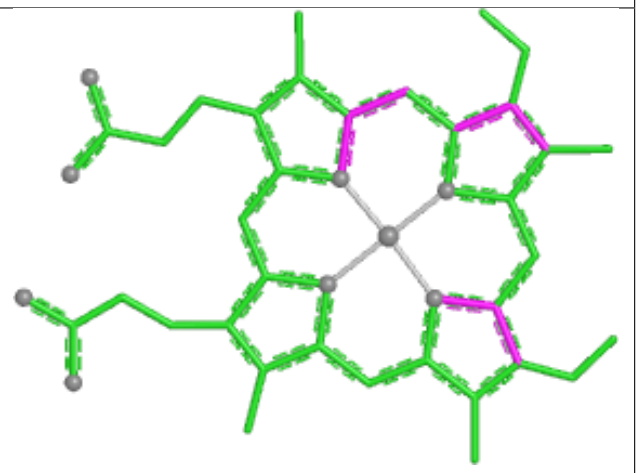


Rings

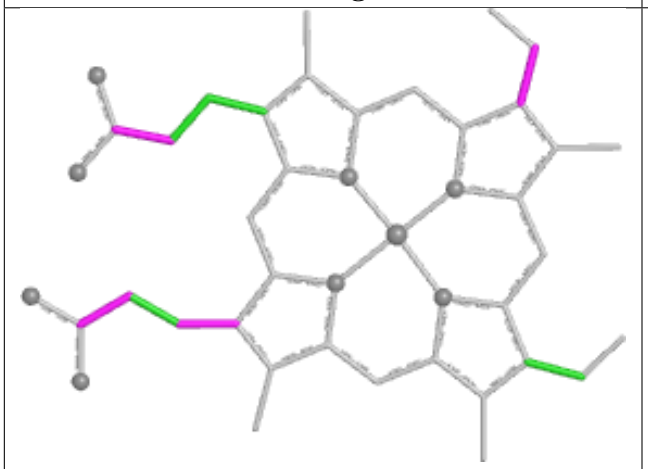
Ligand HEM D 163



Bond lengths



Bond angles



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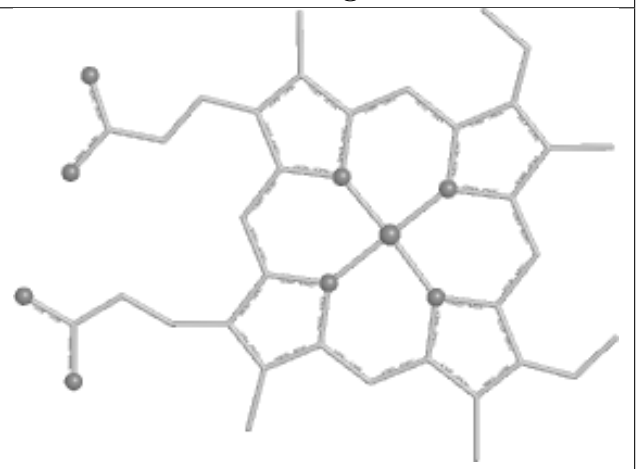
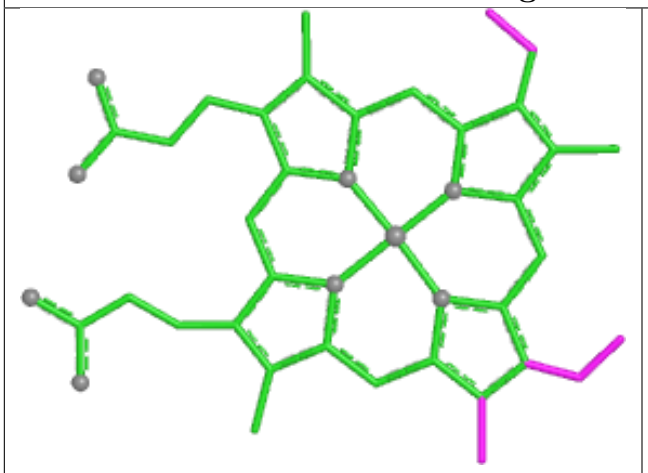


Rings

Ligand HEM A 163



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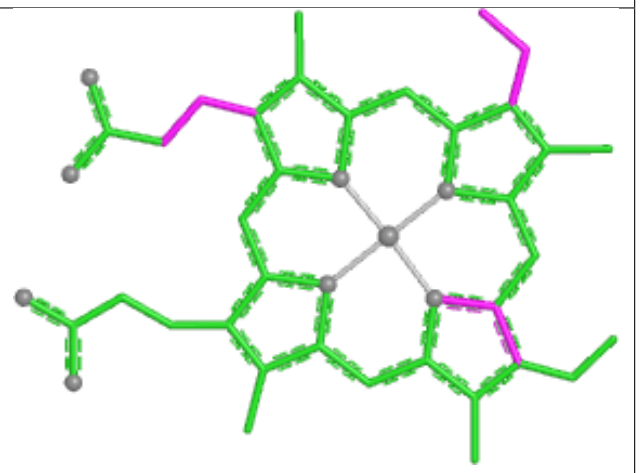
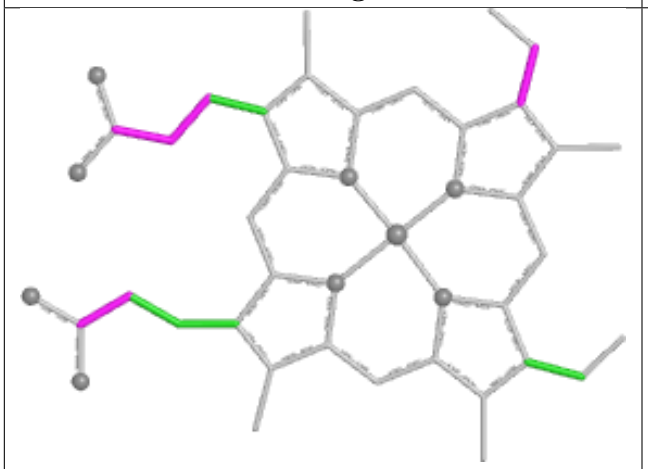


Bond angles



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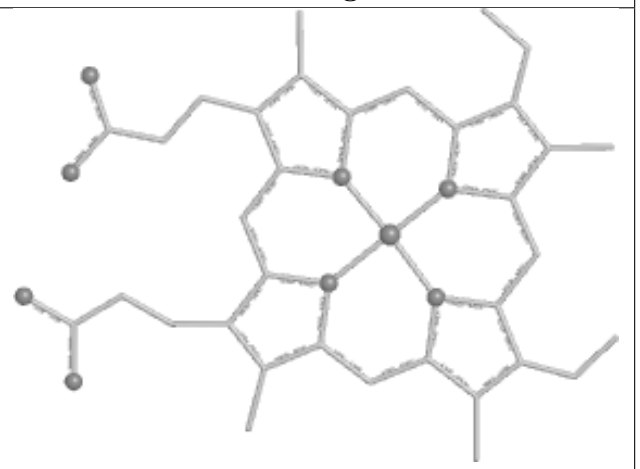
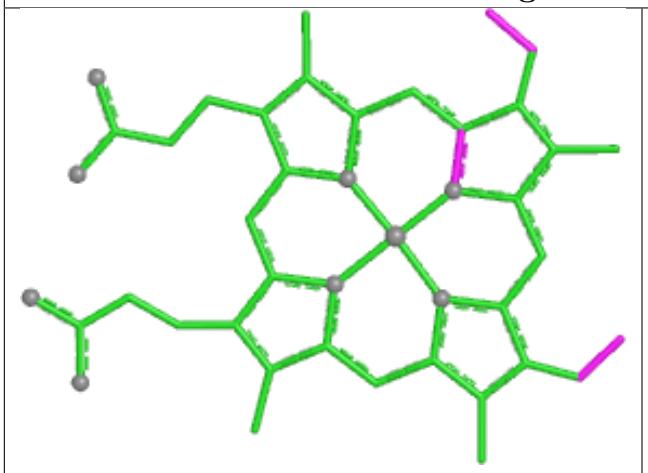
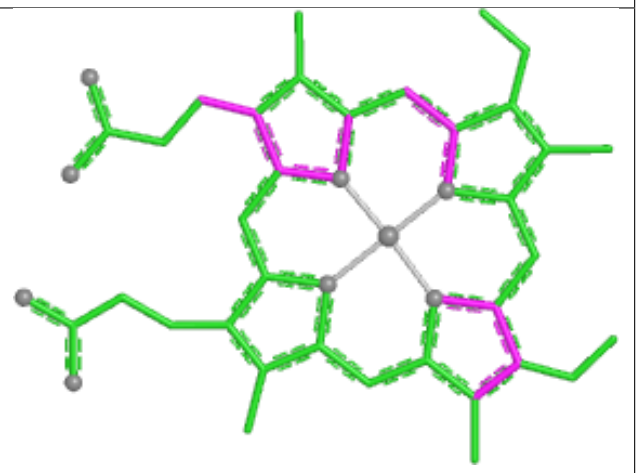


Rings

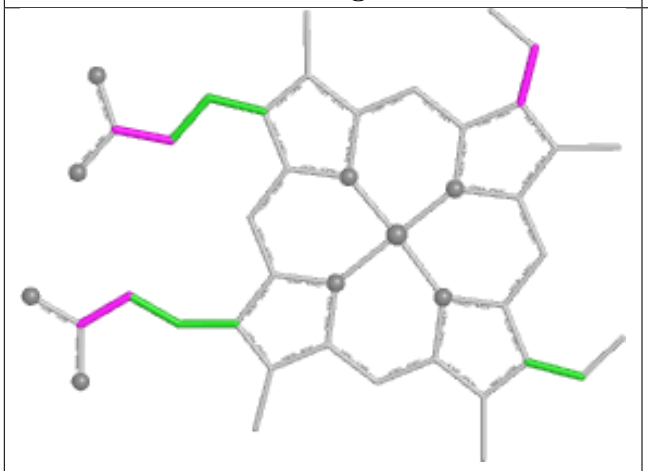
Ligand HEM G 163



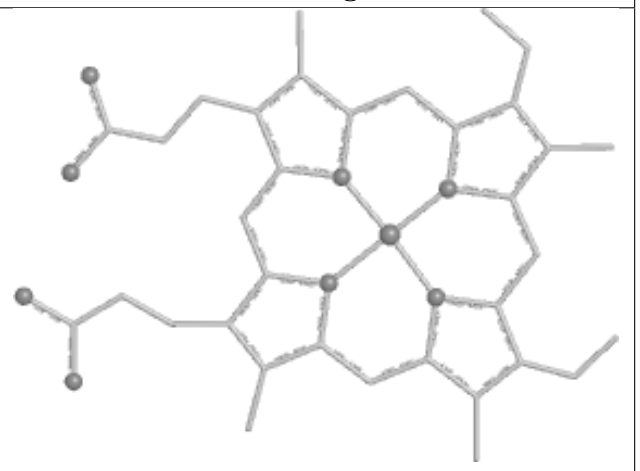
Bond lengths



Bond angles

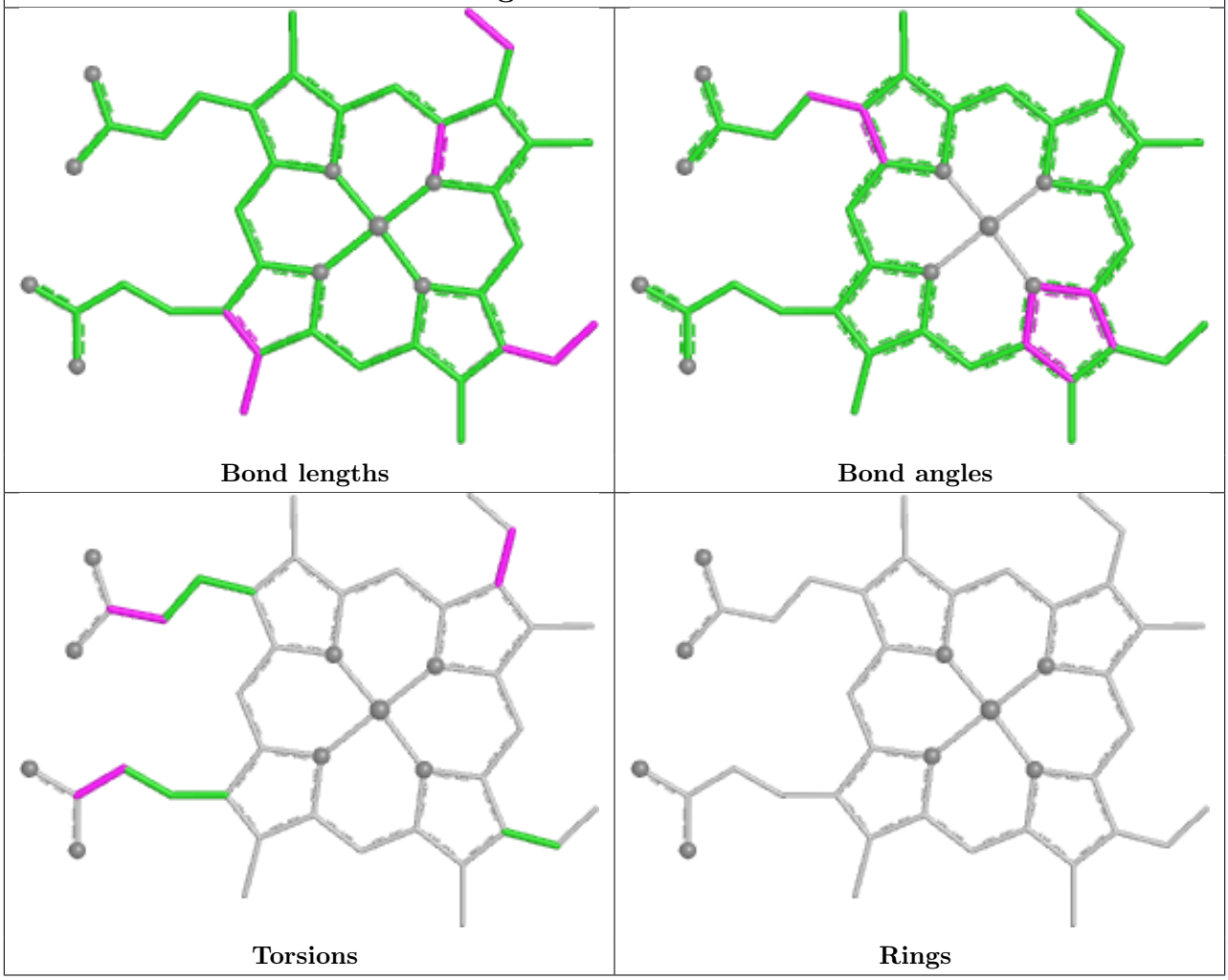


Torsions



Rings

Ligand HEM B 163



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	56:ASP	C	57:SER	N	1.14

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	153/162 (94%)	0.03	5 (3%)	49	49	21, 31, 47, 53	0
1	B	151/162 (93%)	0.16	3 (1%)	65	65	22, 34, 52, 68	0
1	C	152/162 (93%)	0.28	7 (4%)	37	36	22, 36, 54, 66	0
1	D	152/162 (93%)	0.09	2 (1%)	75	75	22, 33, 51, 69	0
1	E	153/162 (94%)	0.17	9 (5%)	28	27	22, 33, 56, 78	0
1	F	152/162 (93%)	0.09	1 (0%)	84	85	21, 33, 46, 55	0
1	G	154/162 (95%)	0.11	6 (3%)	43	43	20, 32, 51, 68	0
1	H	152/162 (93%)	0.01	2 (1%)	75	75	21, 32, 43, 49	0
All	All	1219/1296 (94%)	0.12	35 (2%)	53	53	20, 33, 50, 78	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	9	VAL	5.2
1	D	59	VAL	5.1
1	C	9	VAL	4.9
1	E	59	VAL	4.2
1	F	9	VAL	4.0
1	E	58	ASP	3.9
1	G	57	SER	3.8
1	A	161	ALA	3.8
1	H	9	VAL	3.4
1	B	58	ASP	3.3
1	G	133	ASP	3.1
1	G	58	ASP	3.0
1	E	60	PRO	3.0
1	E	8	VAL	3.0
1	A	9	VAL	2.9
1	G	8	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	58	ASP	2.8
1	C	56	ASP	2.8
1	B	160	PRO	2.7
1	C	59	VAL	2.7
1	A	59	VAL	2.7
1	E	56	ASP	2.5
1	E	57	SER	2.4
1	H	160	PRO	2.3
1	E	61	LEU	2.3
1	G	161	ALA	2.3
1	E	52	PRO	2.3
1	E	160	PRO	2.3
1	B	59	VAL	2.3
1	C	160	PRO	2.2
1	G	56	ASP	2.2
1	C	100	ARG	2.2
1	C	58	ASP	2.1
1	C	57	SER	2.1
1	A	100	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides 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
4	PGO	A	1211	5/5	0.69	0.22	68,68,69,71	0
4	PGO	C	1218	5/5	0.70	0.22	79,79,80,80	0
4	PGO	F	1220	5/5	0.70	0.23	70,70,71,73	0
4	PGO	E	1216	5/5	0.71	0.18	63,63,64,65	0

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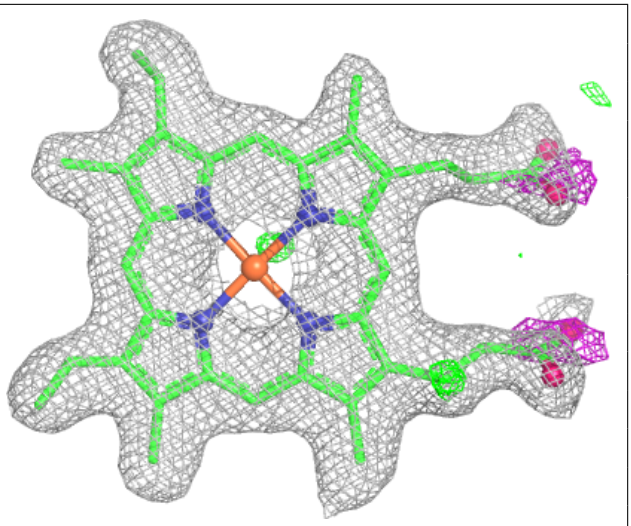
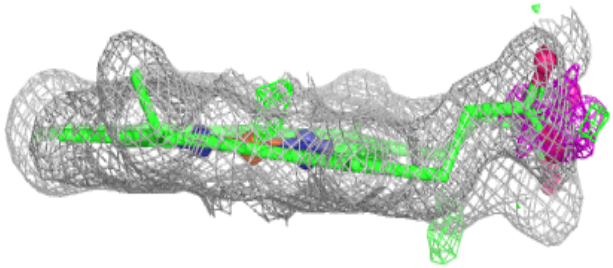
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PGO	H	1221	5/5	0.77	0.15	69,69,69,70	0
4	PGO	B	1217	5/5	0.78	0.16	59,60,62,62	0
4	PGO	G	1214	5/5	0.79	0.16	74,74,75,75	0
4	PGO	A	1210	5/5	0.79	0.25	33,34,35,36	5
4	PGO	A	1215	5/5	0.80	0.28	31,31,34,35	5
4	PGO	D	1219	5/5	0.81	0.13	44,49,50,52	0
4	PGO	H	1213	5/5	0.87	0.15	58,60,62,63	0
4	PGO	D	1209	5/5	0.88	0.16	62,64,64,65	0
4	PGO	E	1212	5/5	0.89	0.15	56,57,58,59	0
2	CYN	E	205	2/2	0.91	0.12	32,32,32,32	0
2	CYN	B	202	2/2	0.94	0.08	28,28,28,28	0
3	HEM	E	163	43/43	0.96	0.09	24,29,44,52	0
2	CYN	G	207	2/2	0.96	0.08	27,27,27,28	0
3	HEM	C	163	43/43	0.97	0.08	26,31,52,55	0
3	HEM	D	163	43/43	0.97	0.09	24,27,46,52	0
3	HEM	A	163	43/43	0.97	0.08	22,27,48,51	0
3	HEM	G	163	43/43	0.97	0.08	22,26,49,54	0
3	HEM	H	163	43/43	0.97	0.08	23,28,50,51	0
3	HEM	B	163	43/43	0.97	0.08	25,30,50,54	0
2	CYN	C	203	2/2	0.98	0.06	29,29,29,31	0
2	CYN	H	208	2/2	0.98	0.04	22,22,22,23	0
3	HEM	F	163	43/43	0.98	0.07	24,27,48,52	0
2	CYN	D	204	2/2	0.98	0.04	30,30,30,30	0
2	CYN	A	201	2/2	0.98	0.06	25,25,25,26	0
2	CYN	F	206	2/2	0.98	0.05	26,26,26,26	0

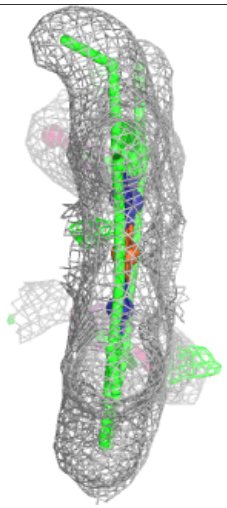
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM E 163:

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

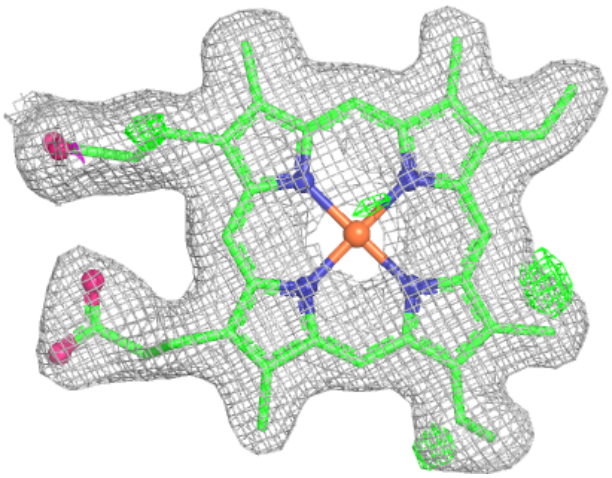


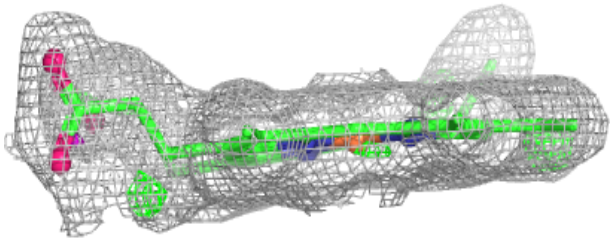


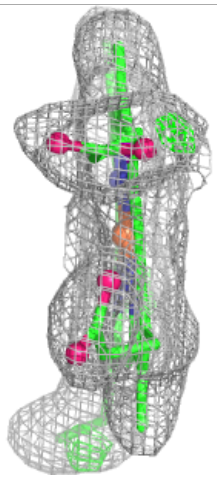


Electron density around HEM C 163:

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

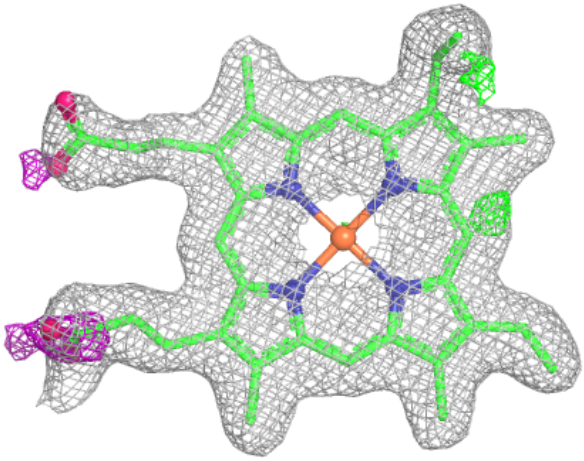


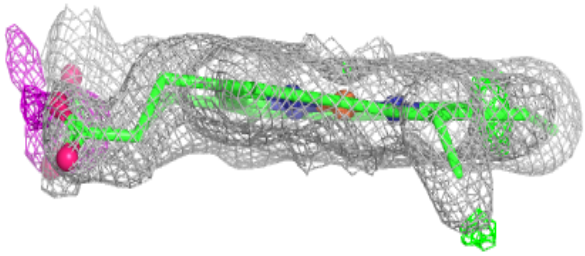


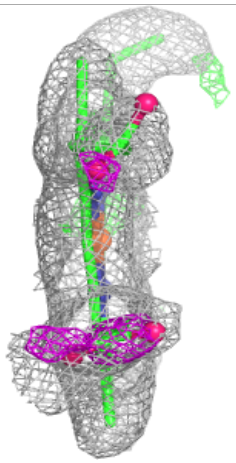


Electron density around HEM D 163:

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

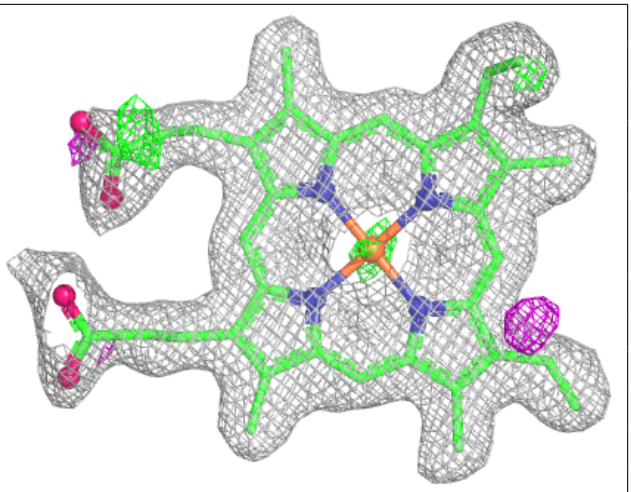


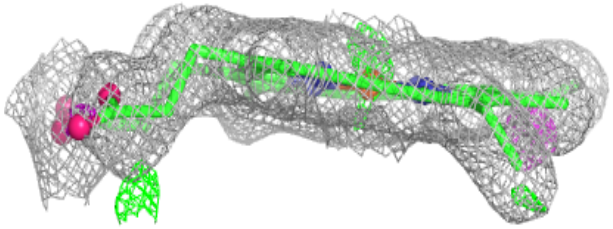


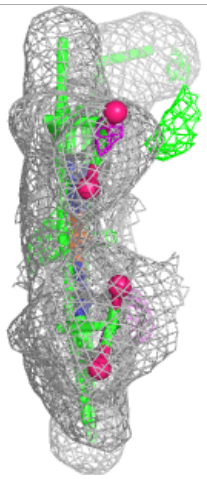


Electron density around HEM A 163:

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

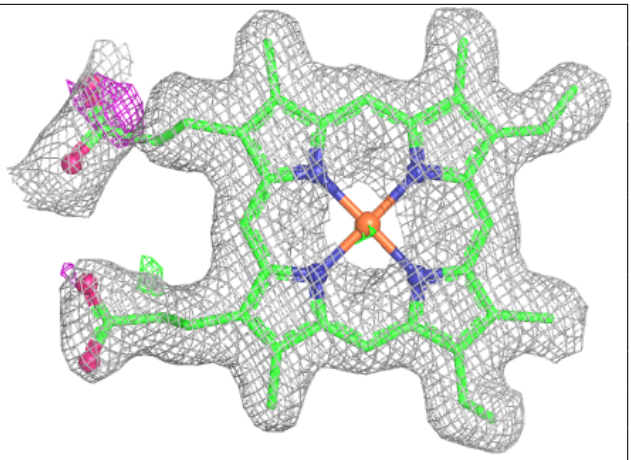


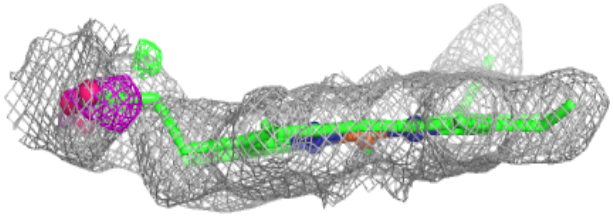


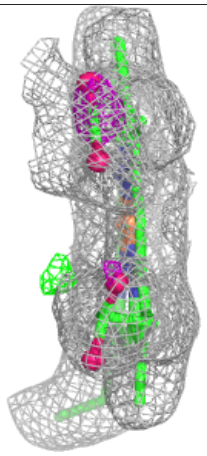


Electron density around HEM G 163:

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

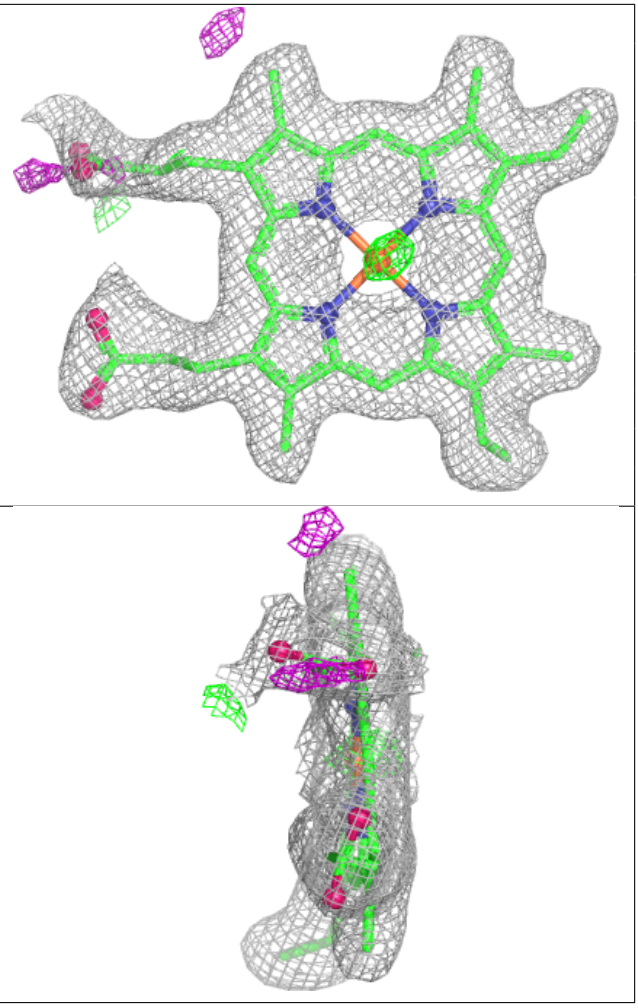






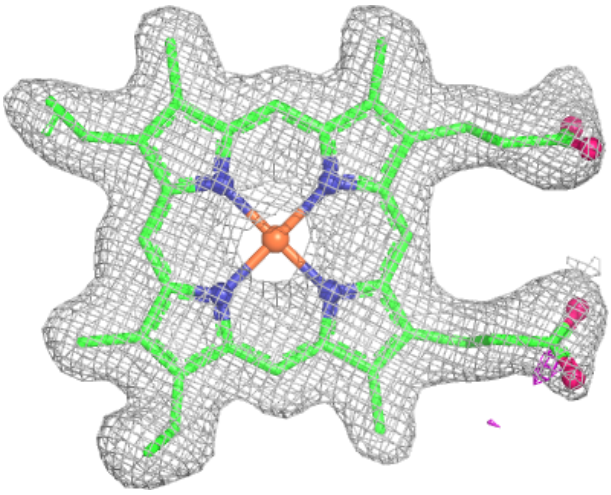
Electron density around HEM H 163:

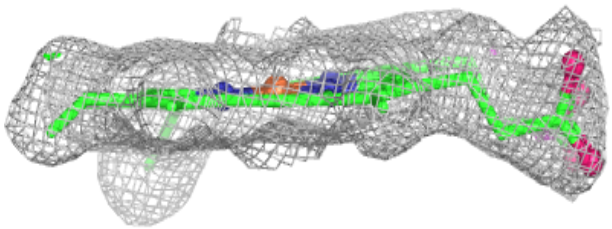
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

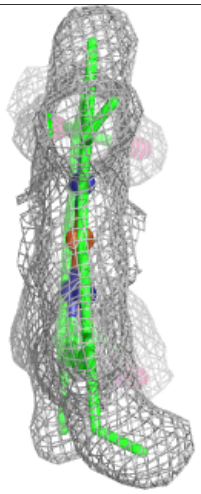


Electron density around HEM B 163:

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

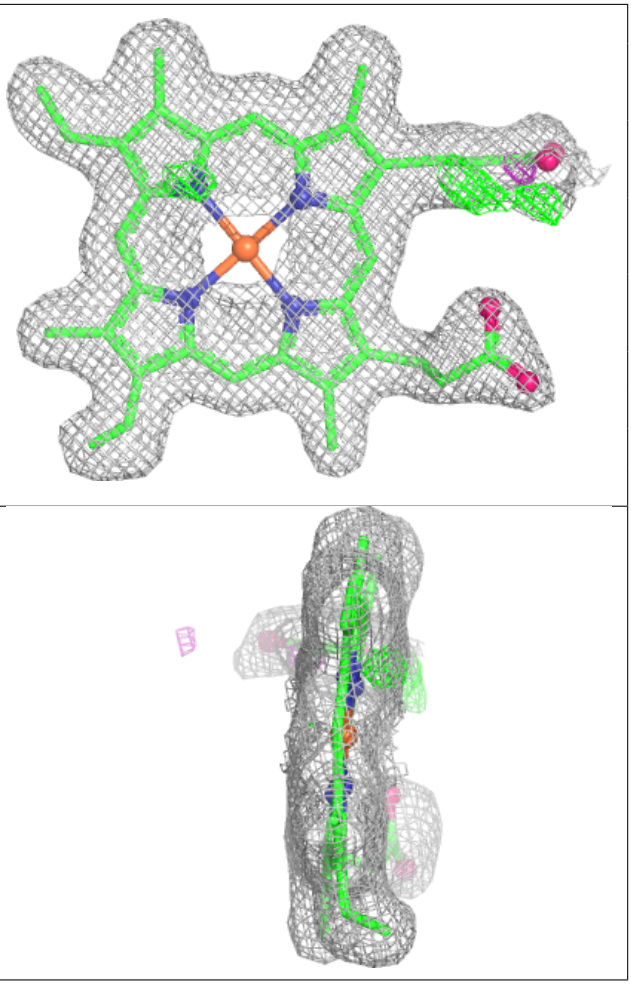






Electron density around HEM F 163:

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.