Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 03:14 PM EDT

PDB ID	:	2R50
Title	:	The crystal structure of nonsymbiotic corn hemoglobin 1
Authors	:	Smagghe, B.J.; Hoy, J.A.; Hargrove, M.S.
Deposited on	:	2007-09-02
Resolution	:	2.20 Å(reported)

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

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

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

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

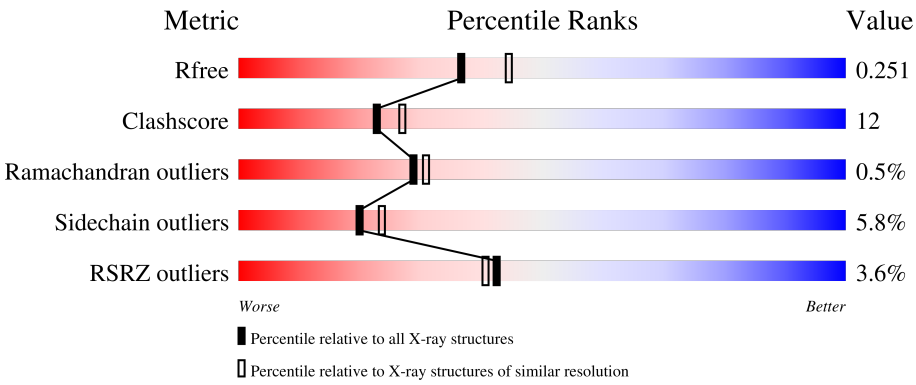
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	165	5% 68% 17% • 12%
1	B	165	% 68% 19% • 12%
1	C	165	4% 65% 21% • • 11%
1	D	165	4% 62% 23% • 12%

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
3	SO4	D	166	-	-	X	-
4	ACY	B	168	-	-	X	-

2 Entry composition (i)

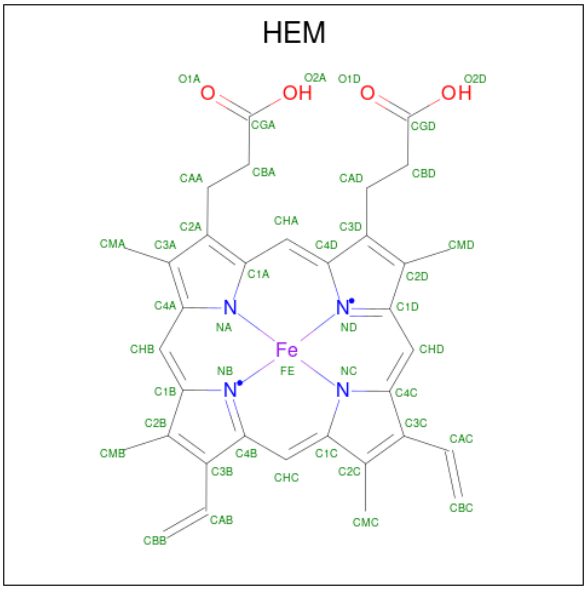
There are 5 unique types of molecules in this entry. The entry contains 5368 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-symbiotic hemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	146	1145	741	195	201	8	0	0	0
1	B	146	1143	738	195	202	8	0	0	0
1	C	147	1155	748	196	203	8	0	0	0
1	D	145	1136	733	194	201	8	0	0	0

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



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

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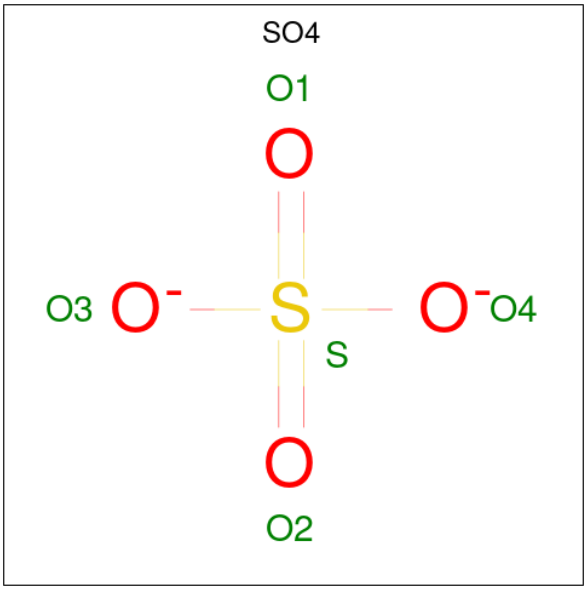
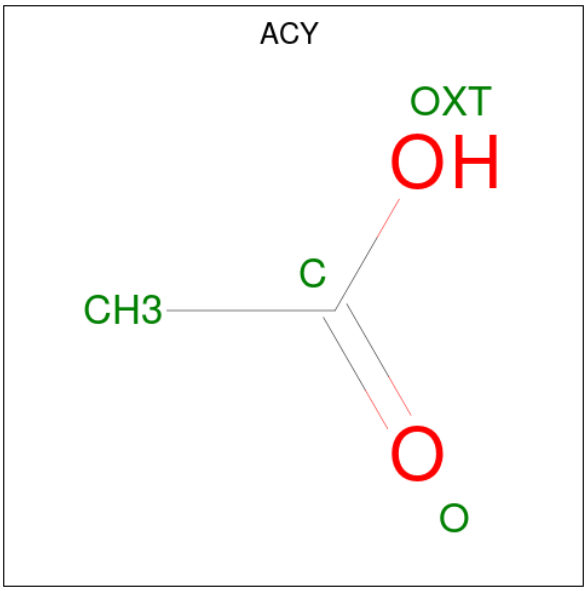
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
2	D	1	43	34	1	4	4	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	B	1	5	4	1	0	0
3	C	1	5	4	1	0	0
3	C	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 5 is water.

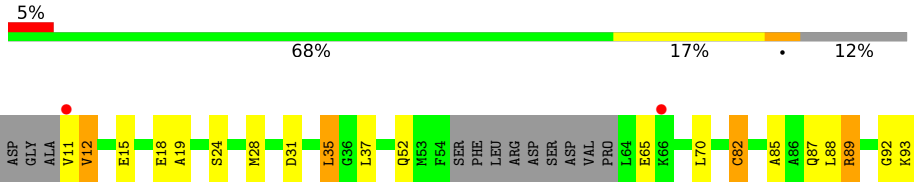
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	161	161	161	0	0
			Total	O		
5	B	172	172	172	0	0
			Total	O		
5	C	142	142	142	0	0
			Total	O		
5	D	109	109	109	0	0

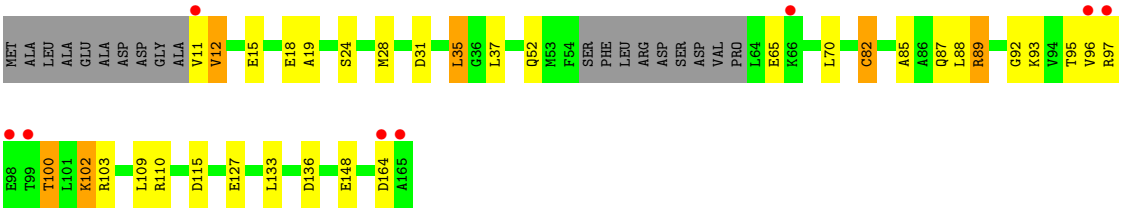
3 Residue-property plots (i)

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-symbiotic hemoglobin

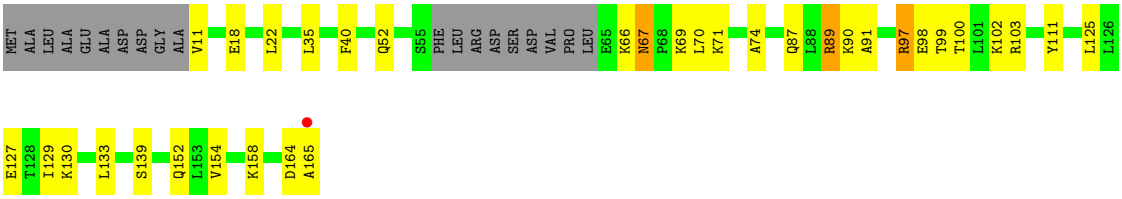
Chain A:





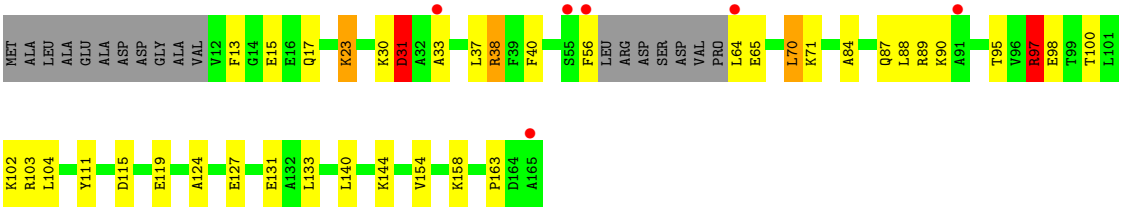
• Molecule 1: Non-symbiotic hemoglobin

Chain B:



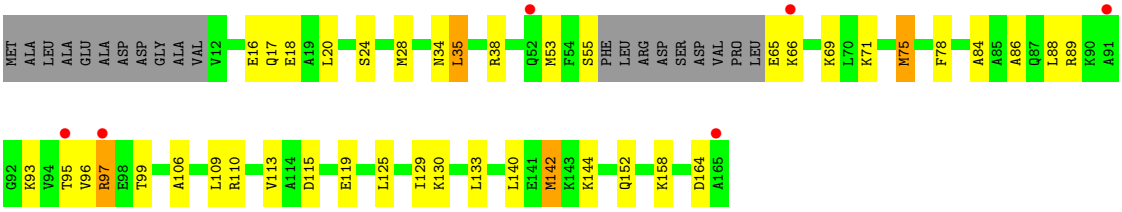
• Molecule 1: Non-symbiotic hemoglobin

Chain C:



• Molecule 1: Non-symbiotic hemoglobin

Chain D:


MET
ALA
LEU
ALA
GLU
ALA
ASP
ASP
GLY
ALA
VAL
V12
E16
Q17
E18
A19
L20
S24
M28
N34
L35
R38
Q52
M53
F54
S55
PHE
LEU
ARG
ASP
SER
ASP
VAL
PRO
LEU
E65
K66
K69
L70
K71
M75
F78
A84
A85
A86
Q87
L88
R89
K90
A91
G92
K93
V94
T95
V96
R97
E98
T99
A106
L109
R110
V113
A114
D115
E119
L125
I129
K130
L133
L140
E141
M142
K143
K144
Q152
K158
D164
A165

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.75Å 89.73Å 157.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.06 – 2.20 26.24 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.6 (79.06-2.20) 80.0 (26.24-1.84)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.201 , 0.253 0.204 , 0.251	Depositor DCC
R_{free} test set	2527 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5368	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1319e-03.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ACY, SO4

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	1.17	1/1166 (0.1%)	0.96	4/1565 (0.3%)
1	B	1.20	2/1164 (0.2%)	0.92	1/1562 (0.1%)
1	C	1.19	2/1177 (0.2%)	0.94	3/1579 (0.2%)
1	D	1.13	1/1157 (0.1%)	0.93	2/1552 (0.1%)
All	All	1.17	6/4664 (0.1%)	0.94	10/6258 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	142	MET	CG-SD	-9.82	1.55	1.81
1	C	131	GLU	CD-OE1	-5.67	1.19	1.25
1	B	130	LYS	CE-NZ	5.23	1.62	1.49
1	A	82	CYS	CB-SG	-5.22	1.73	1.81
1	B	71	LYS	CE-NZ	5.08	1.61	1.49
1	C	124	ALA	CA-CB	-5.01	1.42	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	164	ASP	CB-CG-OD2	7.03	124.63	118.30
1	A	164	ASP	CB-CG-OD2	6.85	124.47	118.30
1	A	115	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	31	ASP	CB-CG-OD2	6.42	124.07	118.30
1	A	136	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	142	MET	CA-CB-CG	-5.46	104.01	113.30
1	C	38	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	31	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	55	SER	CA-C-O	-5.11	109.36	120.10
1	C	97	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1145	0	1188	26	0
1	B	1143	0	1182	21	0
1	C	1155	0	1193	32	0
1	D	1136	0	1173	34	0
2	A	43	0	30	0	0
2	B	43	0	30	2	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
3	B	5	0	0	0	0
3	C	10	0	0	1	0
3	D	10	0	0	2	0
4	B	4	0	3	2	0
4	D	4	0	3	0	0
5	A	161	0	0	6	0
5	B	172	0	0	5	1
5	C	142	0	0	11	1
5	D	109	0	0	6	0
All	All	5368	0	4862	111	1

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 12.

All (111) 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:C:65:GLU:O	5:C:303:HOH:O	1.82	0.97
1:C:23:LYS:HB2	1:C:23:LYS:NZ	1.82	0.94
1:A:15:GLU:HG2	5:A:243:HOH:O	1.72	0.88
1:C:23:LYS:HB2	1:C:23:LYS:HZ3	1.42	0.82
1:C:154:VAL:HG12	1:C:158:LYS:HE2	1.63	0.80
1:A:35:LEU:HG	5:A:251:HOH:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:HG13	5:A:236:HOH:O	1.81	0.79
1:B:97:ARG:HH21	1:B:99:THR:HG23	1.46	0.79
1:D:75:MET:HE1	5:D:257:HOH:O	1.82	0.78
1:D:34:ASN:O	1:D:38:ARG:HG3	1.86	0.74
1:B:139:SER:OG	5:B:300:HOH:O	2.06	0.73
1:C:98:GLU:HG2	1:C:102:LYS:HE2	1.72	0.71
1:C:37:LEU:HB2	5:C:305:HOH:O	1.90	0.71
1:A:87:GLN:HG3	1:A:95:THR:HG22	1.75	0.67
1:D:16:GLU:HG3	1:D:17:GLN:NE2	2.10	0.67
1:C:37:LEU:HG	5:C:258:HOH:O	1.94	0.66
1:A:102:LYS:HD3	1:A:102:LYS:H	1.61	0.66
1:D:125:LEU:O	1:D:129:ILE:HG12	1.95	0.65
1:B:125:LEU:O	1:B:129:ILE:HG13	1.96	0.65
1:B:127:GLU:OE2	5:B:237:HOH:O	2.14	0.65
1:C:64:LEU:HG	1:C:65:GLU:H	1.62	0.64
1:C:38:ARG:NH2	5:C:302:HOH:O	2.25	0.64
1:D:16:GLU:HG3	1:D:17:GLN:HE22	1.65	0.61
1:C:111:TYR:OH	3:C:166:SO4:O2	2.15	0.60
1:D:16:GLU:O	1:D:20:LEU:HG	2.01	0.60
1:A:89:ARG:HH11	1:A:89:ARG:HB3	1.67	0.59
1:A:93:LYS:HB2	5:A:297:HOH:O	2.01	0.59
1:B:52:GLN:HB2	5:B:317:HOH:O	2.03	0.59
1:A:88:LEU:HD23	1:A:93:LYS:HA	1.87	0.57
1:D:66:LYS:HA	1:D:71:LYS:NZ	2.20	0.56
1:C:90:LYS:HG2	5:C:267:HOH:O	2.05	0.56
1:A:37:LEU:HD11	1:A:65:GLU:HG3	1.87	0.56
1:A:100:THR:HG21	1:A:102:LYS:CE	2.36	0.55
1:C:40:PHE:HB3	1:C:70:LEU:HD11	1.89	0.55
1:A:19:ALA:HA	5:A:240:HOH:O	2.08	0.53
1:A:87:GLN:HG3	1:A:95:THR:CG2	2.37	0.53
1:A:100:THR:HG21	1:A:102:LYS:HE2	1.88	0.53
1:A:92:GLY:O	1:A:93:LYS:HB3	2.09	0.53
1:A:18:GLU:OE1	1:A:89:ARG:HD3	2.09	0.52
1:C:127:GLU:CD	5:C:275:HOH:O	2.47	0.52
1:B:40:PHE:HE1	1:B:70:LEU:O	1.91	0.52
1:B:89:ARG:HG3	1:B:90:LYS:N	2.24	0.52
1:C:31:ASP:HB3	5:C:253:HOH:O	2.08	0.52
1:D:129:ILE:O	1:D:133:LEU:HB2	2.09	0.52
1:C:33:ALA:HB2	5:C:300:HOH:O	2.10	0.51
1:D:18:GLU:OE2	1:D:86:ALA:HA	2.10	0.51
1:A:109:LEU:HD21	1:D:110:ARG:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:HD13	1:D:78:PHE:CE2	2.47	0.50
1:D:164:ASP:HB2	3:D:166:SO4:S	2.51	0.50
1:D:164:ASP:HB2	3:D:166:SO4:O2	2.13	0.49
1:D:110:ARG:HH11	1:D:110:ARG:HG3	1.76	0.49
1:C:115:ASP:O	1:C:119:GLU:HG3	2.13	0.49
1:B:69:LYS:HD3	2:B:167:HEM:O2D	2.13	0.48
1:C:64:LEU:HD23	1:C:64:LEU:N	2.28	0.48
1:B:165:ALA:HB2	5:C:240:HOH:O	2.14	0.48
1:D:99:THR:HG22	5:D:275:HOH:O	2.13	0.48
1:D:20:LEU:HB3	1:D:142:MET:HG3	1.94	0.48
1:B:11:VAL:HG21	1:B:152:GLN:NE2	2.29	0.48
1:B:40:PHE:CE1	1:B:74:ALA:HB2	2.49	0.47
1:C:30:LYS:O	1:C:31:ASP:HB2	2.14	0.47
1:D:78:PHE:HE1	1:D:129:ILE:HD11	1.78	0.47
1:B:40:PHE:CG	4:B:168:ACY:H3	2.50	0.47
1:A:24:SER:O	1:A:28:MET:HG3	2.15	0.46
1:B:154:VAL:HG12	1:B:158:LYS:HE2	1.98	0.46
1:A:110:ARG:HA	1:D:109:LEU:HD21	1.97	0.46
1:D:84:ALA:O	1:D:88:LEU:HG	2.16	0.46
1:D:66:LYS:HA	1:D:71:LYS:HZ1	1.80	0.46
1:A:11:VAL:O	1:A:12:VAL:HB	2.16	0.46
1:D:38:ARG:NH1	1:D:38:ARG:HB3	2.31	0.45
1:C:37:LEU:HD13	5:C:257:HOH:O	2.17	0.45
1:A:82:CYS:O	1:A:85:ALA:HB3	2.17	0.45
1:A:96:VAL:HG23	1:A:96:VAL:O	2.17	0.45
1:C:100:THR:HG23	1:C:103:ARG:HH22	1.81	0.44
1:C:100:THR:O	1:C:104:LEU:HG	2.17	0.44
1:D:96:VAL:O	1:D:97:ARG:C	2.55	0.44
1:D:130:LYS:HE3	5:D:239:HOH:O	2.18	0.44
1:B:87:GLN:O	1:B:91:ALA:HB3	2.18	0.44
1:C:140:LEU:HG	1:C:144:LYS:HZ3	1.83	0.44
1:D:152:GLN:NE2	5:D:259:HOH:O	2.49	0.44
1:C:71:LYS:HB2	1:C:71:LYS:NZ	2.33	0.43
1:C:13:PHE:CZ	1:C:17:GLN:HB3	2.53	0.43
1:B:40:PHE:CE1	1:B:70:LEU:O	2.70	0.43
1:C:127:GLU:OE2	5:C:173:HOH:O	2.21	0.43
1:C:23:LYS:CB	1:C:23:LYS:HZ2	2.30	0.43
1:C:84:ALA:O	1:C:88:LEU:HG	2.18	0.43
1:A:96:VAL:HB	1:A:100:THR:HG23	2.01	0.43
1:D:106:ALA:O	1:D:110:ARG:HB2	2.19	0.43
1:D:140:LEU:HG	1:D:144:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HG3	5:A:324:HOH:O	2.19	0.43
1:C:40:PHE:CB	1:C:70:LEU:HD11	2.49	0.42
1:B:97:ARG:NH1	5:B:208:HOH:O	2.50	0.42
2:B:167:HEM:HBC2	5:B:176:HOH:O	2.18	0.42
1:D:115:ASP:OD2	1:D:158:LYS:HE3	2.20	0.42
1:A:89:ARG:HB3	1:A:89:ARG:NH1	2.34	0.42
1:A:103:ARG:HH11	1:A:103:ARG:HG2	1.84	0.42
1:D:53:MET:CE	1:D:113:VAL:HG22	2.50	0.41
1:B:74:ALA:HA	4:B:168:ACY:O	2.20	0.41
1:C:56:PHE:N	1:C:56:PHE:CD2	2.87	0.41
1:C:97:ARG:HA	1:C:97:ARG:HE	1.85	0.41
1:B:98:GLU:O	1:B:102:LYS:HG3	2.20	0.41
1:D:93:LYS:O	1:D:95:THR:HG23	2.21	0.41
1:A:15:GLU:HA	1:A:89:ARG:HD2	2.03	0.41
1:B:100:THR:HG23	1:B:103:ARG:HH21	1.86	0.41
1:D:24:SER:HB2	1:D:28:MET:HE1	2.03	0.41
1:D:34:ASN:CB	5:D:263:HOH:O	2.68	0.41
1:D:78:PHE:HE1	1:D:129:ILE:CD1	2.33	0.41
1:D:115:ASP:O	1:D:119:GLU:HG3	2.21	0.41
1:B:111:TYR:CZ	1:C:163:PRO:HB3	2.56	0.40
1:B:18:GLU:HG2	1:B:22:LEU:HD12	2.03	0.40
1:C:87:GLN:OE1	1:C:95:THR:N	2.51	0.40
1:D:158:LYS:HD3	5:D:176:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:322:HOH:O	5:C:285:HOH:O[3_645]	2.19	0.01

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	142/165 (86%)	135 (95%)	6 (4%)	1 (1%)	22	22
1	B	142/165 (86%)	139 (98%)	2 (1%)	1 (1%)	22	22
1	C	143/165 (87%)	136 (95%)	6 (4%)	1 (1%)	22	22
1	D	141/165 (86%)	137 (97%)	4 (3%)	0	100	100
All	All	568/660 (86%)	547 (96%)	18 (3%)	3 (0%)	29	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	31	ASP
1	B	67	ASN
1	A	12	VAL

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	117/131 (89%)	108 (92%)	9 (8%)	13	13
1	B	117/131 (89%)	111 (95%)	6 (5%)	24	29
1	C	118/131 (90%)	112 (95%)	6 (5%)	24	29
1	D	116/131 (88%)	110 (95%)	6 (5%)	23	28
All	All	468/524 (89%)	441 (94%)	27 (6%)	20	23

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

Mol	Chain	Res	Type
1	A	35	LEU
1	A	52	GLN
1	A	70	LEU
1	A	89	ARG
1	A	100	THR
1	A	102	LYS
1	A	127	GLU
1	A	133	LEU

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Mol	Chain	Res	Type
1	A	148	GLU
1	B	35	LEU
1	B	66	LYS
1	B	67	ASN
1	B	89	ARG
1	B	97	ARG
1	B	133	LEU
1	C	15	GLU
1	C	23	LYS
1	C	70	LEU
1	C	89	ARG
1	C	97	ARG
1	C	133	LEU
1	D	35	LEU
1	D	65	GLU
1	D	69	LYS
1	D	75	MET
1	D	89	ARG
1	D	97	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	C	52	GLN
1	D	52	GLN
1	D	152	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	B	167	1	41,50,50	1.39	7 (17%)	45,82,82	1.40	5 (11%)
3	SO4	D	166	-	4,4,4	0.27	0	6,6,6	0.41	0
4	ACY	D	169	-	3,3,3	0.72	0	3,3,3	1.27	0
2	HEM	A	166	1	41,50,50	1.32	6 (14%)	45,82,82	1.49	10 (22%)
2	HEM	D	168	1	41,50,50	1.25	5 (12%)	45,82,82	1.29	4 (8%)
2	HEM	C	168	1	41,50,50	1.47	6 (14%)	45,82,82	1.42	8 (17%)
3	SO4	C	167	-	4,4,4	0.16	0	6,6,6	0.89	0
3	SO4	C	166	-	4,4,4	0.15	0	6,6,6	0.35	0
3	SO4	D	167	-	4,4,4	0.18	0	6,6,6	0.64	0
4	ACY	B	168	-	3,3,3	0.72	0	3,3,3	0.74	0
3	SO4	B	166	-	4,4,4	0.19	0	6,6,6	0.49	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
2	HEM	C	168	1	-	2/12/54/54	-
2	HEM	A	166	1	-	2/12/54/54	-
2	HEM	B	167	1	-	3/12/54/54	-
2	HEM	D	168	1	-	5/12/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	166	HEM	C3C-C2C	-3.89	1.35	1.40
2	C	168	HEM	C3C-C2C	-3.53	1.35	1.40
2	B	167	HEM	CAB-C3B	-3.39	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	168	HEM	CAB-C3B	-3.29	1.38	1.47
2	A	166	HEM	C1B-NB	-3.13	1.34	1.40
2	B	167	HEM	CBB-CAB	3.07	1.45	1.30
2	D	168	HEM	C3C-CAC	-3.02	1.41	1.47
2	B	167	HEM	C3C-CAC	-2.99	1.41	1.47
2	C	168	HEM	C3B-C4B	2.72	1.50	1.44
2	A	166	HEM	CBB-CAB	2.69	1.43	1.30
2	C	168	HEM	CBB-CAB	2.60	1.43	1.30
2	D	168	HEM	CHB-C1B	2.47	1.41	1.35
2	C	168	HEM	CBD-CGD	2.36	1.56	1.50
2	D	168	HEM	CAB-C3B	-2.32	1.41	1.47
2	D	168	HEM	CBC-CAC	2.28	1.44	1.29
2	B	167	HEM	C3C-C2C	-2.25	1.37	1.40
2	B	167	HEM	CHB-C1B	2.24	1.40	1.35
2	B	167	HEM	C4D-ND	-2.24	1.36	1.40
2	D	168	HEM	CBB-CAB	2.15	1.40	1.30
2	A	166	HEM	CAB-C3B	-2.14	1.41	1.47
2	A	166	HEM	CBC-CAC	2.08	1.43	1.29
2	C	168	HEM	CBC-CAC	2.07	1.43	1.29
2	B	167	HEM	C1A-NA	2.07	1.40	1.36
2	A	166	HEM	C3C-CAC	-2.07	1.43	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	167	HEM	CBA-CAA-C2A	4.77	120.77	112.62
2	D	168	HEM	CBA-CAA-C2A	4.66	120.57	112.62
2	C	168	HEM	O2D-CGD-CBD	3.83	126.33	114.03
2	C	168	HEM	O1A-CGA-CBA	-3.69	111.23	123.08
2	A	166	HEM	CBA-CAA-C2A	3.46	118.52	112.62
2	C	168	HEM	CBA-CAA-C2A	3.32	118.28	112.62
2	B	167	HEM	C4B-CHC-C1C	3.10	126.65	122.56
2	A	166	HEM	CAD-C3D-C4D	2.95	129.82	124.66
2	A	166	HEM	C4B-CHC-C1C	2.78	126.23	122.56
2	C	168	HEM	C4B-CHC-C1C	2.69	126.10	122.56
2	D	168	HEM	C4B-CHC-C1C	2.67	126.08	122.56
2	B	167	HEM	O1A-CGA-CBA	-2.54	114.92	123.08
2	A	166	HEM	C4B-C3B-C2B	-2.50	105.13	107.11
2	C	168	HEM	O2D-CGD-O1D	-2.39	117.33	123.30
2	D	168	HEM	CAD-CBD-CGD	2.37	118.71	113.60
2	A	166	HEM	CMA-C3A-C2A	2.32	129.32	124.94
2	A	166	HEM	C4A-C3A-C2A	-2.29	105.40	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	167	HEM	C2C-C3C-C4C	-2.25	105.32	106.90
2	C	168	HEM	O2A-CGA-CBA	2.23	121.20	114.03
2	A	166	HEM	O2D-CGD-CBD	2.14	120.89	114.03
2	D	168	HEM	C4B-C3B-C2B	-2.12	105.43	107.11
2	C	168	HEM	O1D-CGD-CBD	-2.10	116.34	123.08
2	A	166	HEM	O2A-CGA-O1A	2.08	128.48	123.30
2	A	166	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
2	C	168	HEM	CMD-C2D-C1D	2.06	128.18	125.04
2	A	166	HEM	O1D-CGD-CBD	-2.04	116.53	123.08
2	B	167	HEM	CMA-C3A-C4A	-2.02	125.36	128.46

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	168	HEM	C1A-C2A-CAA-CBA
2	C	168	HEM	C3A-C2A-CAA-CBA
2	D	168	HEM	C2A-CAA-CBA-CGA
2	B	167	HEM	C3D-CAD-CBD-CGD
2	D	168	HEM	C3D-CAD-CBD-CGD
2	D	168	HEM	CAA-CBA-CGA-O2A
2	D	168	HEM	CAA-CBA-CGA-O1A
2	B	167	HEM	CAA-CBA-CGA-O2A
2	B	167	HEM	CAA-CBA-CGA-O1A
2	A	166	HEM	CAA-CBA-CGA-O2A
2	D	168	HEM	C4B-C3B-CAB-CBB
2	A	166	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

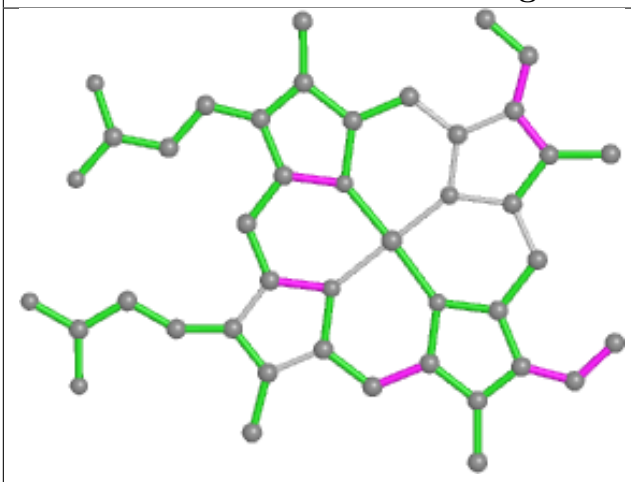
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	167	HEM	2	0
3	D	166	SO4	2	0
3	C	166	SO4	1	0
4	B	168	ACY	2	0

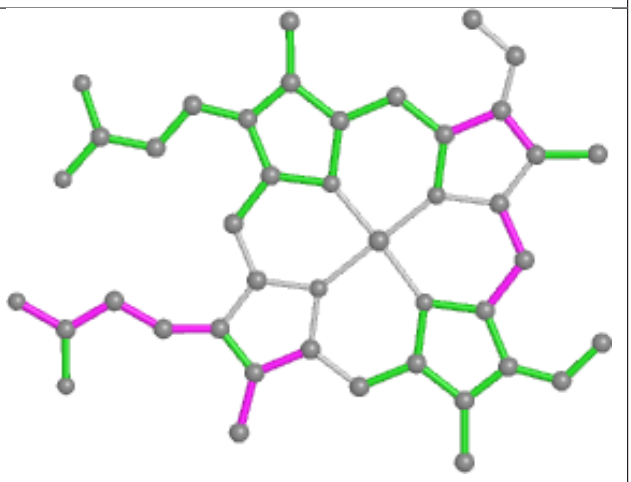
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

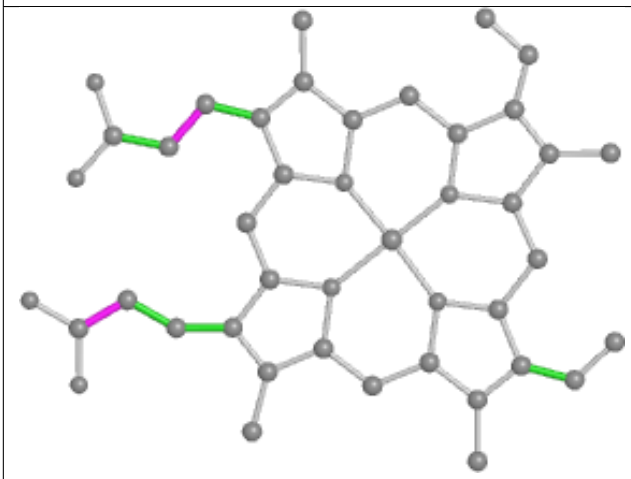
Ligand HEM B 167



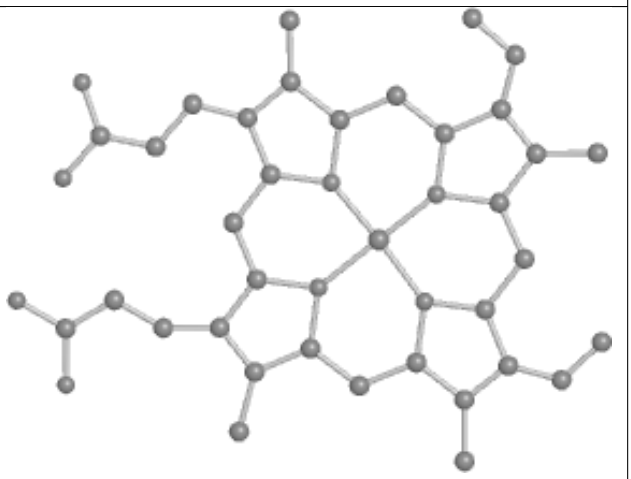
Bond lengths



Bond angles

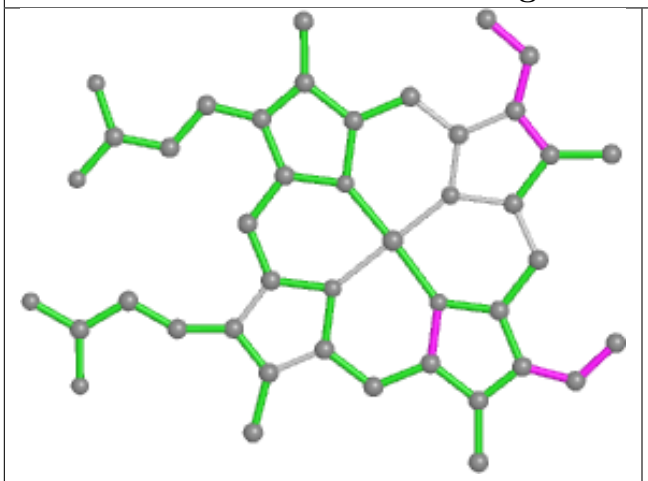


Torsions

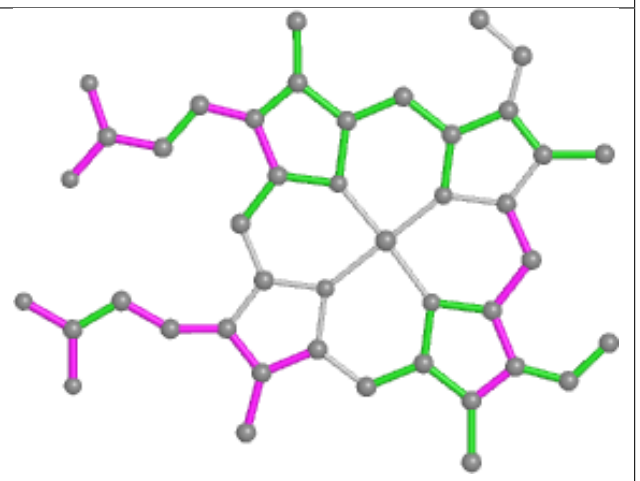


Rings

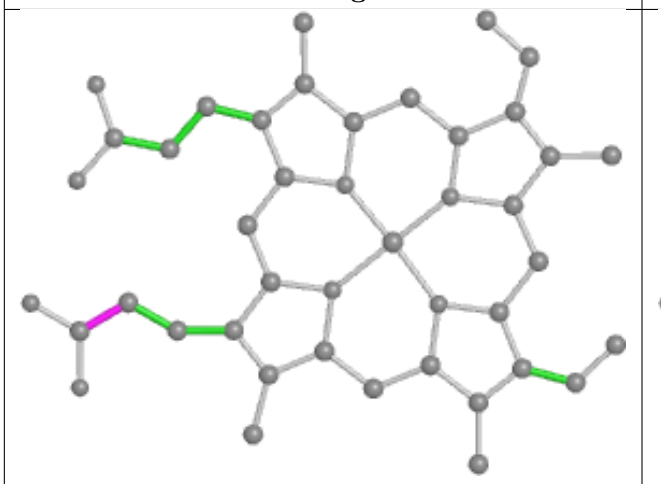
Ligand HEM A 166



Bond lengths



Bond angles



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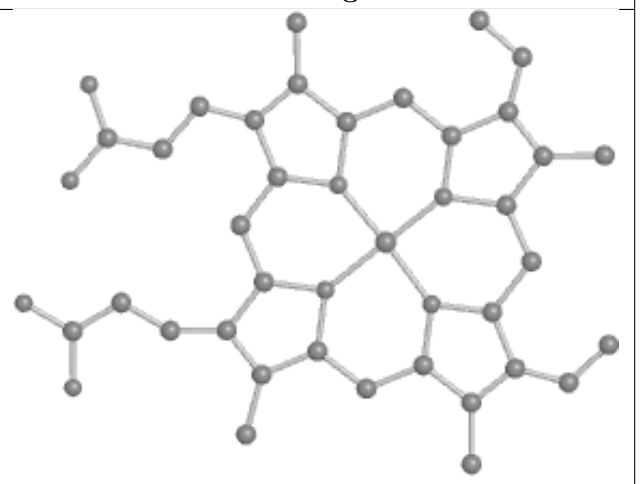
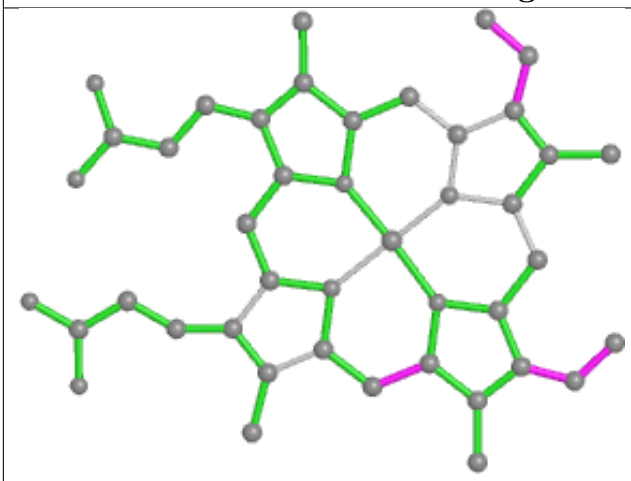
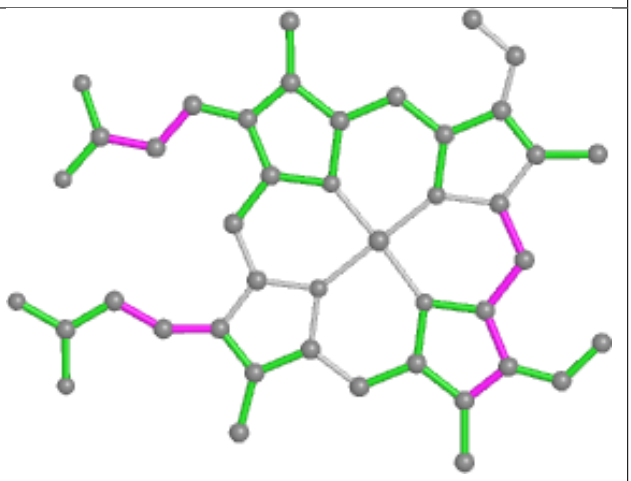


Rings

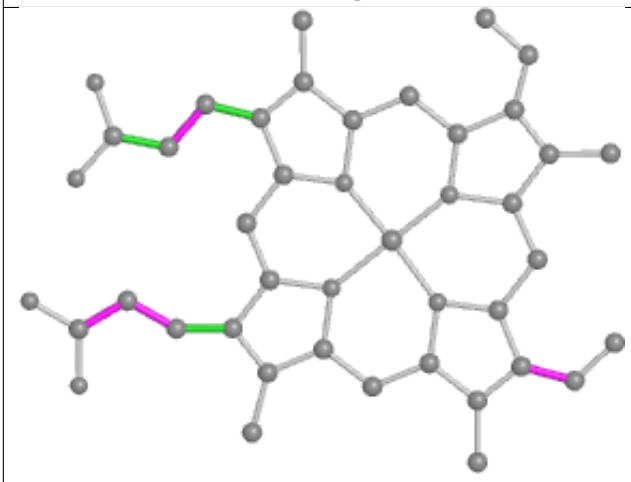
Ligand HEM D 168



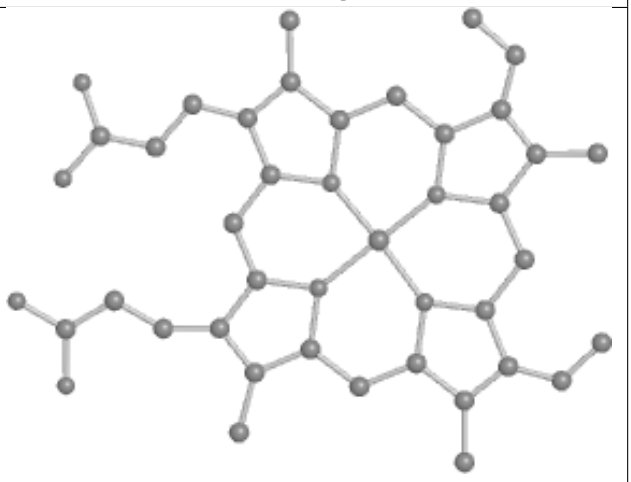
Bond lengths



Bond angles

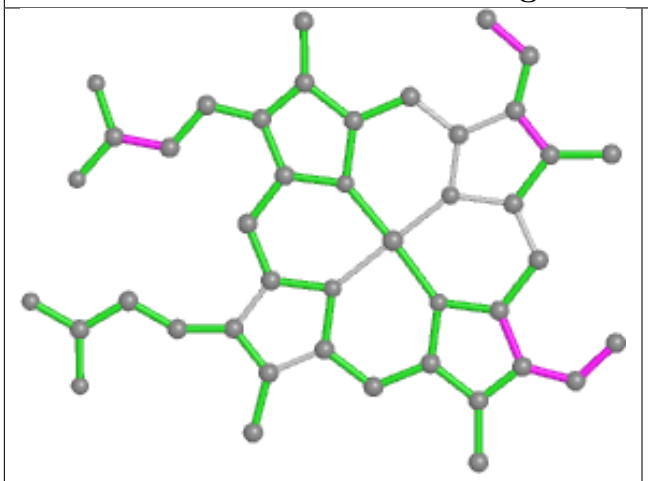


Torsions

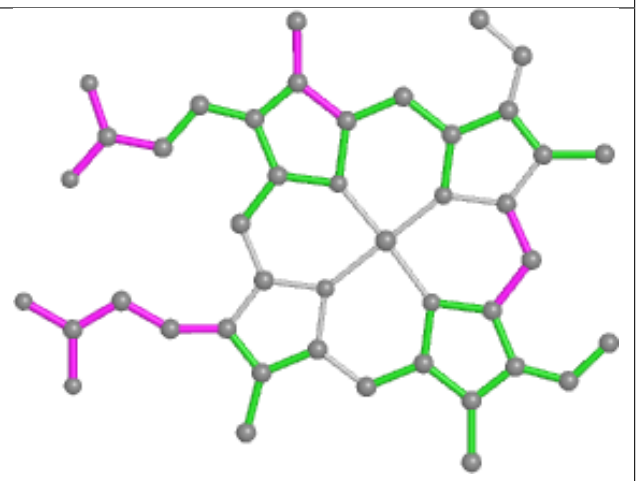


Rings

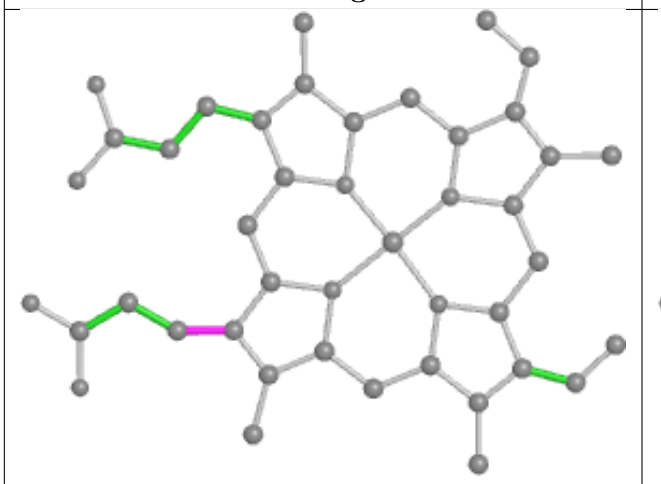
Ligand HEM C 168



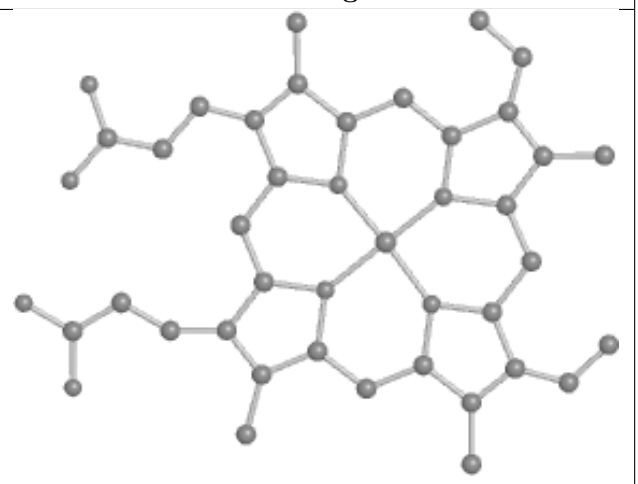
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	146/165 (88%)	-0.12	8 (5%)	25	24	24, 39, 72, 91	0
1	B	146/165 (88%)	-0.34	1 (0%)	87	86	22, 39, 61, 82	1 (0%)
1	C	147/165 (89%)	-0.04	6 (4%)	37	35	26, 40, 69, 93	0
1	D	145/165 (87%)	-0.02	6 (4%)	37	35	26, 42, 73, 93	0
All	All	584/660 (88%)	-0.13	21 (3%)	42	41	22, 40, 72, 93	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	165	ALA	7.6
1	A	165	ALA	7.6
1	C	165	ALA	6.9
1	B	165	ALA	6.8
1	A	97	ARG	5.2
1	C	33	ALA	4.2
1	A	96	VAL	4.1
1	D	66	LYS	3.3
1	D	97	ARG	3.0
1	D	52	GLN	2.9
1	A	99	THR	2.7
1	C	55	SER	2.6
1	C	56	PHE	2.5
1	A	66	LYS	2.5
1	D	91	ALA	2.4
1	C	91	ALA	2.3
1	D	95	THR	2.3
1	A	98	GLU	2.3
1	C	64	LEU	2.2
1	A	11	VAL	2.1
1	A	164	ASP	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

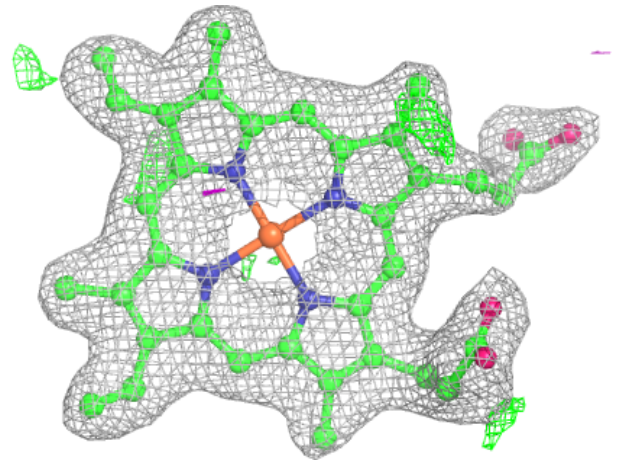
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

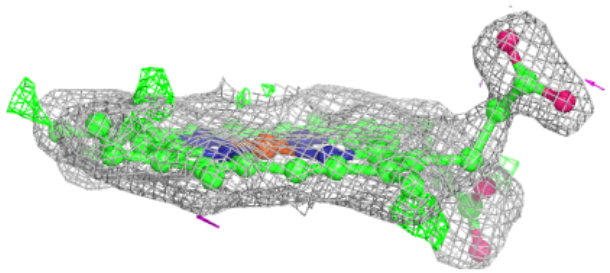
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACY	B	168	4/4	0.89	0.17	40,42,42,42	0
3	SO4	C	167	5/5	0.90	0.19	62,64,65,67	5
3	SO4	D	167	5/5	0.92	0.13	73,73,76,77	0
4	ACY	D	169	4/4	0.92	0.15	37,38,38,38	0
2	HEM	D	168	43/43	0.94	0.15	33,38,61,63	0
2	HEM	C	168	43/43	0.94	0.16	28,35,54,58	0
3	SO4	D	166	5/5	0.94	0.12	80,81,81,82	0
2	HEM	A	166	43/43	0.95	0.16	26,33,57,67	0
2	HEM	B	167	43/43	0.96	0.14	29,34,60,66	0
3	SO4	C	166	5/5	0.97	0.08	68,68,72,75	0
3	SO4	B	166	5/5	0.99	0.07	54,57,59,61	0

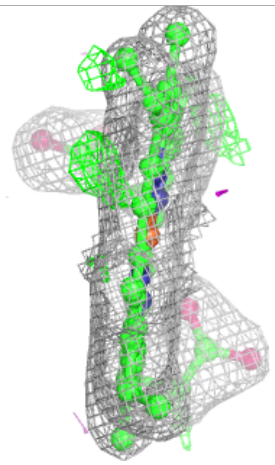
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM D 168:

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

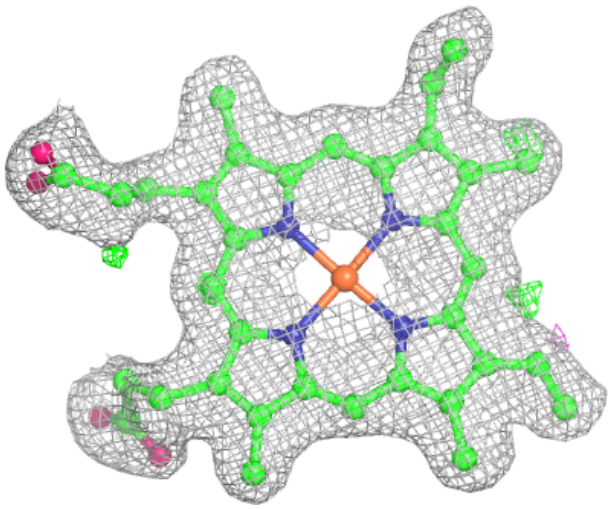


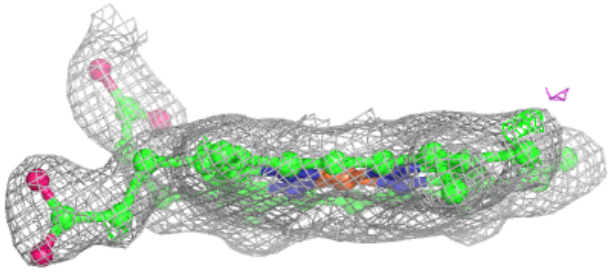


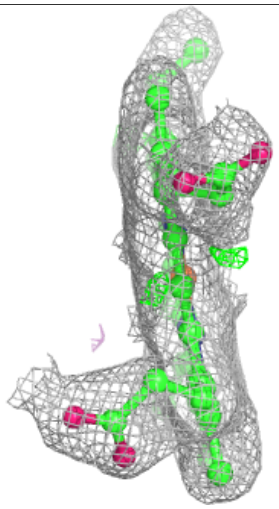


Electron density around HEM C 168:

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

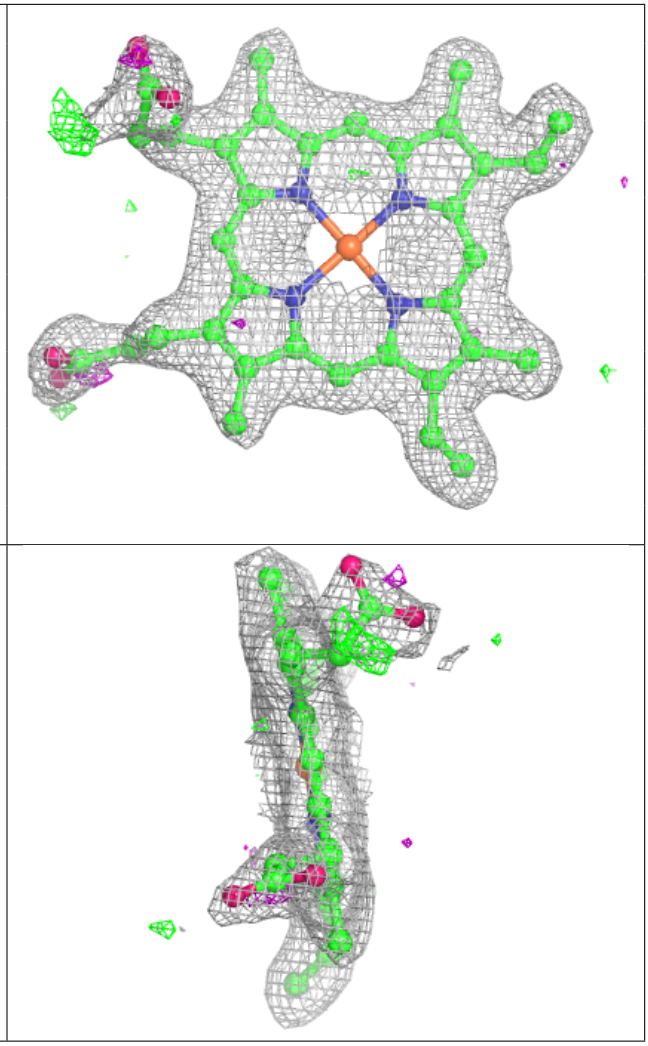






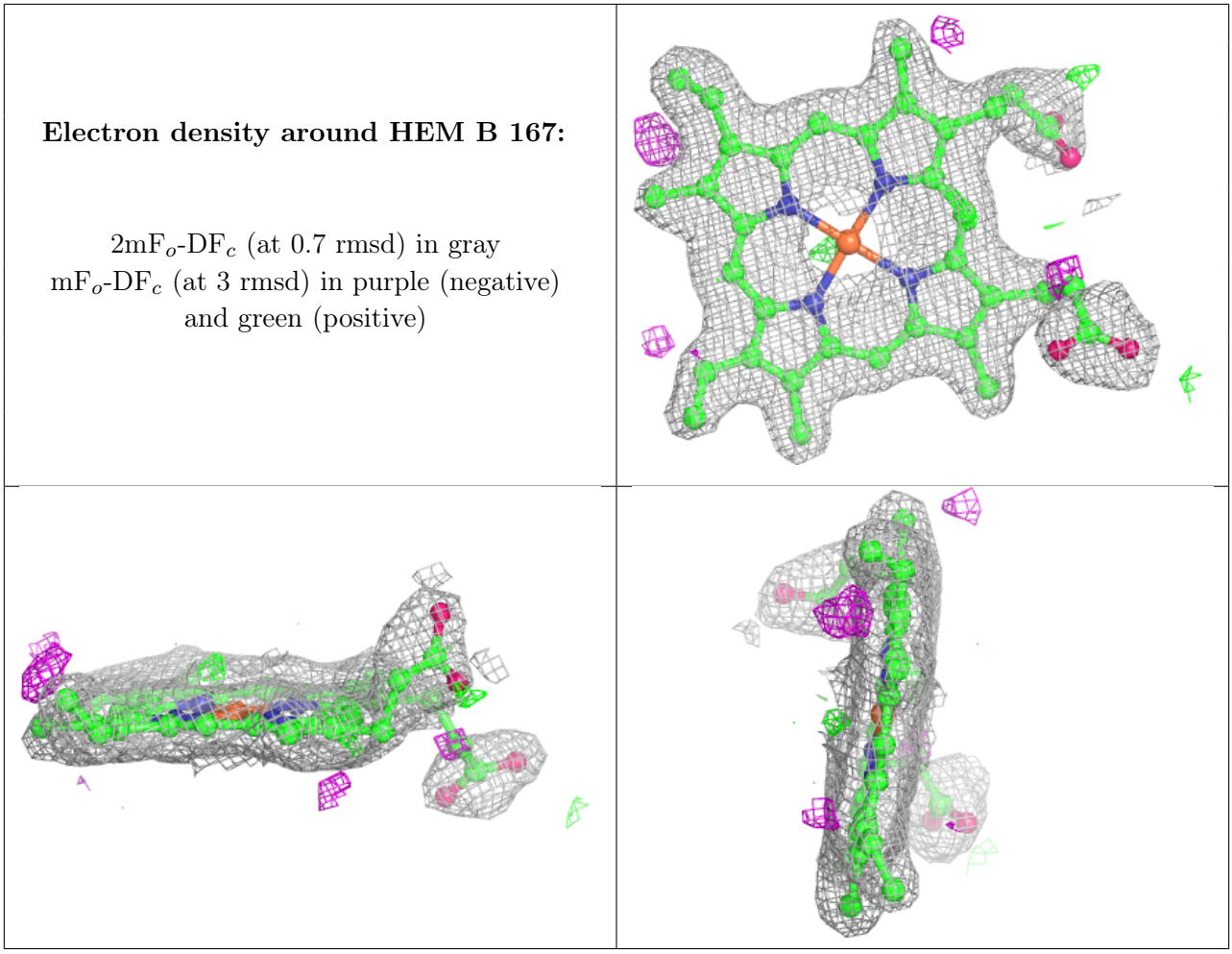
Electron density around HEM A 166:

$2mF_o$-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 167:

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.