Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 09:24 PM EDT

PDB ID	:	3B75
Title	:	Crystal Structure of Glycated Human Haemoglobin
Authors	:	Saraswathi, N.T.; Syakhovich, V.E.; Bokut, S.B.; Moras, D.; Ruff, M.
Deposited on	:	2007-10-30
Resolution	:	2.30 Å(reported)

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

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

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

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

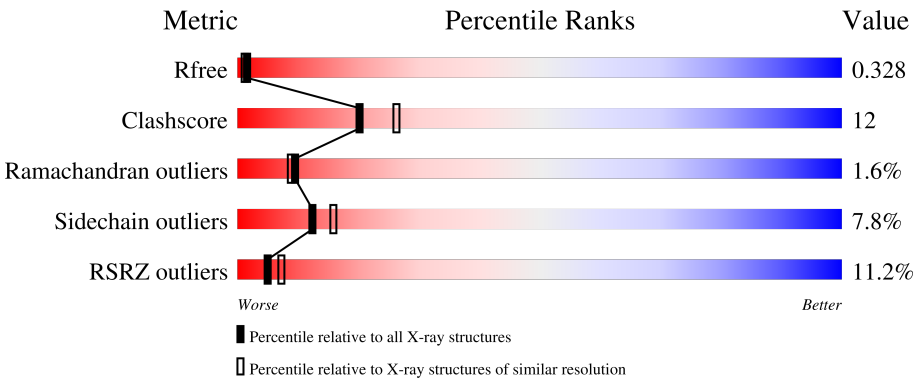
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	141	.%, 79%, 17%, .
1	C	141	85%, 13%, ..
1	E	141	35%, 64%, 30%, 6%
1	G	141	9%, 70%, 26%, .
1	S	141	13%, 67%, 32%, .

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Mol	Chain	Length	Quality of chain
2	B	146	3% 79% 18%
2	D	146	2% 74% 25%
2	F	146	5% 71% 25% 5%
2	H	146	27% 58% 38%
2	T	146	16% 68% 30%

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	FRU	A	142	X	-	-	-
5	OXY	B	151	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11931 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.

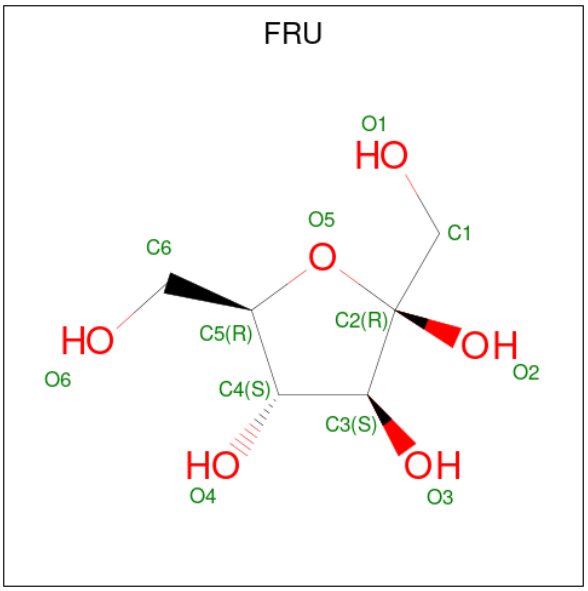
- Molecule 1 is a protein called Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1068	685	187	193	3	0	0	0
1	C	141	1068	685	187	193	3	0	0	0
1	E	141	1068	685	187	193	3	0	0	0
1	G	141	1068	685	187	193	3	0	0	0
1	S	141	1068	685	187	193	3	0	0	0

- Molecule 2 is a protein called Hemoglobin subunit beta.

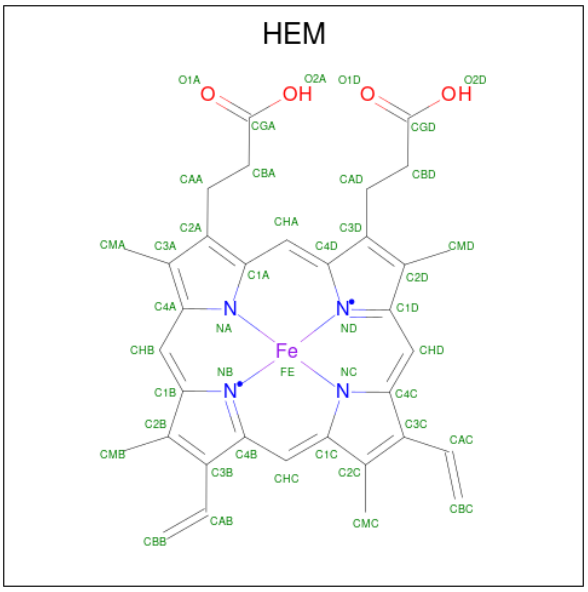
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	146	1122	724	195	200	3	0	0	0
2	D	146	1122	724	195	200	3	0	0	0
2	F	146	1122	724	195	200	3	0	0	0
2	H	146	1122	724	195	200	3	0	0	0
2	T	146	1122	724	195	200	3	0	0	0

- Molecule 3 is beta-D-fructofuranose (three-letter code: FRU) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	11	6	5	0	0
			Total	C	O		
3	E	1	11	6	5	0	0

- Molecule 4 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		
4	A	1	43	34	1	4	4	0	0

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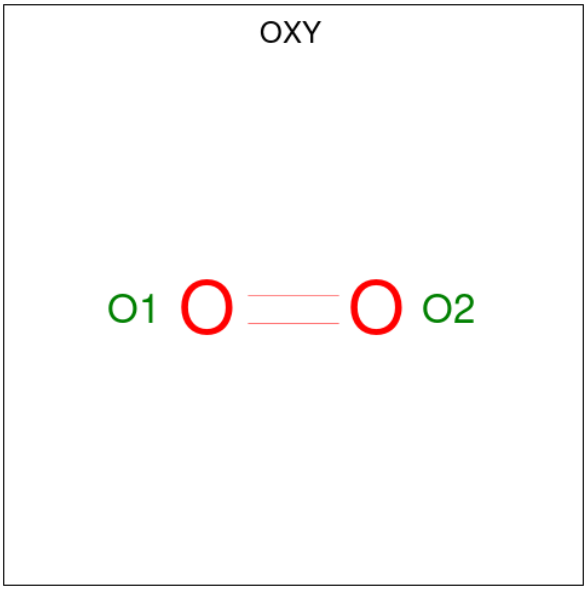
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
4	B	1	43	34	1	4	4	0	0
4	C	1	43	34	1	4	4	0	0
4	D	1	43	34	1	4	4	0	0
4	E	1	43	34	1	4	4	0	0
4	F	1	43	34	1	4	4	0	0
4	G	1	43	34	1	4	4	0	0
4	H	1	43	34	1	4	4	0	0
4	S	1	43	34	1	4	4	0	0
4	T	1	43	34	1	4	4	0	0

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	1	2	2	0	0
5	B	1	2	2	0	0

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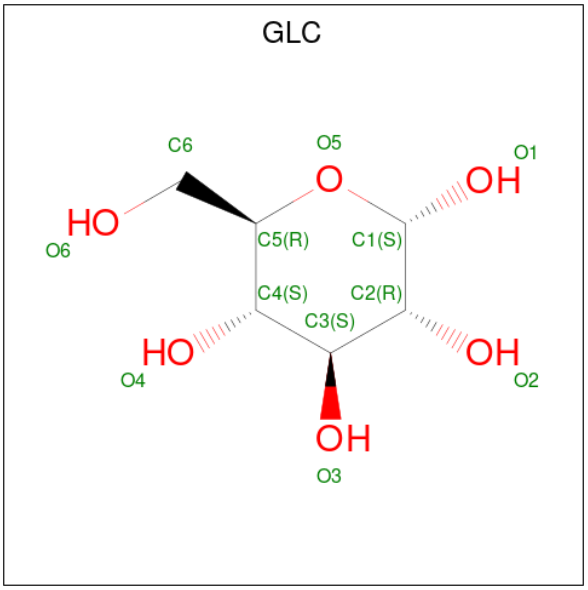
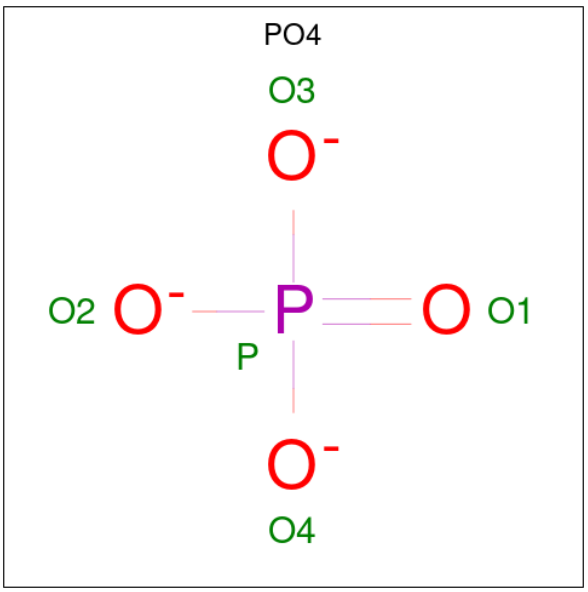
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O 2 2	0	0
5	D	1	Total O 2 2	0	0
5	E	1	Total O 2 2	0	0
5	F	1	Total O 2 2	0	0
5	G	1	Total O 2 2	0	0
5	H	1	Total O 2 2	0	0
5	S	1	Total O 2 2	0	0
5	T	1	Total O 2 2	0	0

- Molecule 6 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 12 6 6	0	0
6	C	1	Total C O 12 6 6	0	0
6	T	1	Total C O 12 6 6	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total O P 5 4 1	0	0

- Molecule 8 is water.

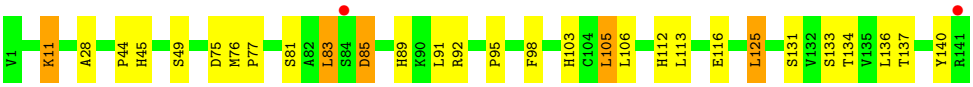
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	46	Total O 46 46	0	0
8	B	66	Total O 66 66	0	0
8	C	51	Total O 51 51	0	0
8	D	52	Total O 52 52	0	0
8	E	29	Total O 29 29	0	0
8	F	61	Total O 61 61	0	0
8	G	31	Total O 31 31	0	0
8	H	35	Total O 35 35	0	0
8	S	46	Total O 46 46	0	0
8	T	51	Total O 51 51	0	0

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: Hemoglobin subunit alpha

Chain A:

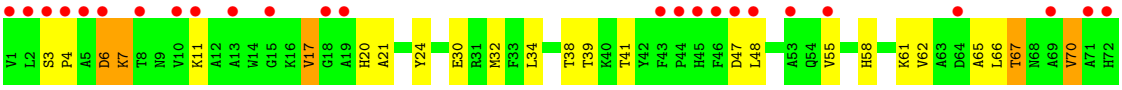


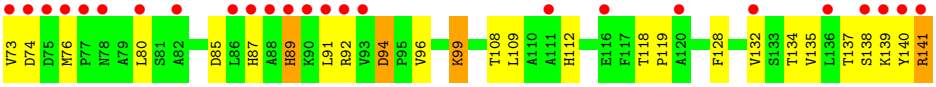
• Molecule 1: Hemoglobin subunit alpha

Chain C:

• Molecule 1: Hemoglobin subunit alpha

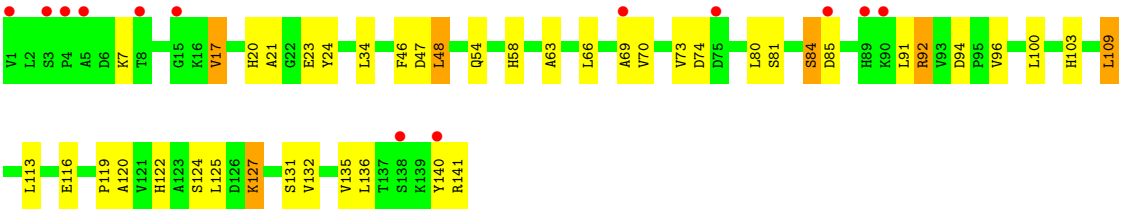
Chain E:





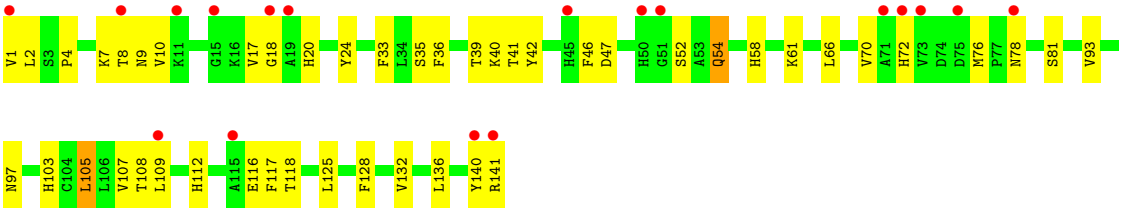
• Molecule 1: Hemoglobin subunit alpha

Chain G:



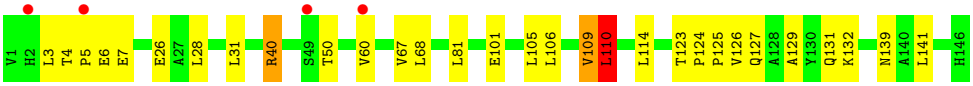
• Molecule 1: Hemoglobin subunit alpha

Chain S:



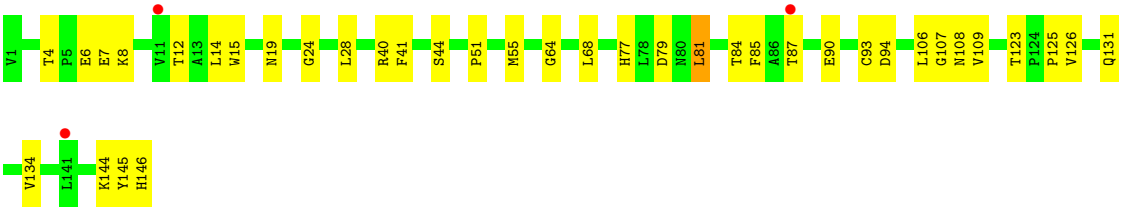
• Molecule 2: Hemoglobin subunit beta

Chain B:



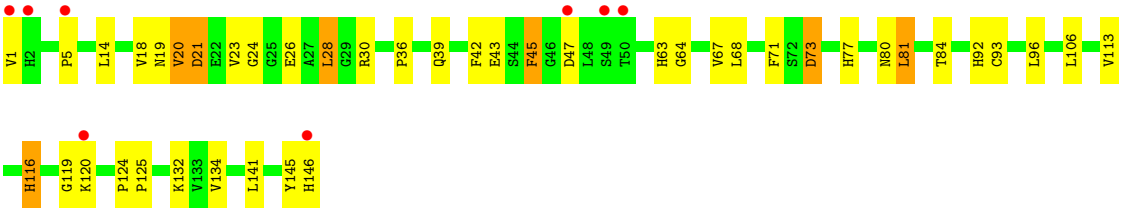
• Molecule 2: Hemoglobin subunit beta

Chain D:



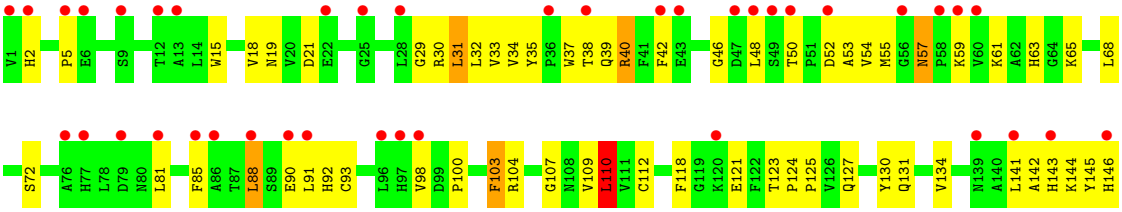
• Molecule 2: Hemoglobin subunit beta

Chain F:



• Molecule 2: Hemoglobin subunit beta

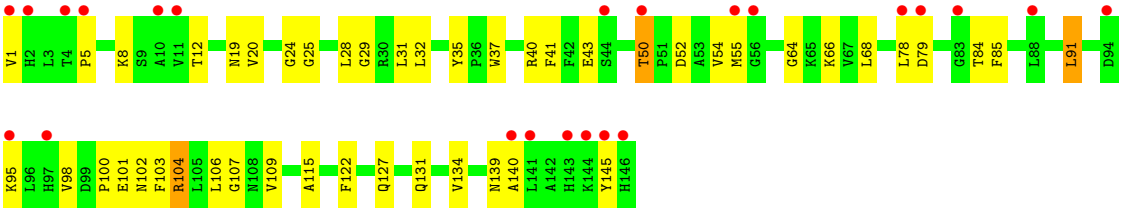
Chain H:



• Molecule 2: Hemoglobin subunit beta

Chain T:

16%
68%
30%


V1 H2 L3 T4 P5 K8 S9 A10 V11 T12 N19 V20 G24 G25 L28 G29 R30 L31 L32 Y35 P36 W37 R40 F41 F42 E43 S44 T50 P51 D52 A53 V54 M55 G56 G64 K65 K66 V67 L68 L78 D79 G83 T84 F85 L88 L91 D94
K95 L96 H97 V98 D99 P100 E101 N102 F103 R104 L105 L106 G107 N108 V109 A115 F122 Q127 Q131 V134 N139 A140 L141 A142 H143 K144 Y145 H146

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	237.99Å 59.27Å 137.02Å 90.00° 125.36° 90.00°	Depositor
Resolution (Å)	14.90 – 2.30 14.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.3 (14.90-2.30) 87.3 (14.89-2.30)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.244 , 0.331 0.242 , 0.328	Depositor DCC
R_{free} test set	3191 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11931	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: GLC, FRU, PO4, OXY, 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	0.66	0/1096	0.74	0/1491
1	C	0.66	0/1096	0.69	1/1491 (0.1%)
1	E	0.49	0/1096	0.60	0/1491
1	G	0.58	0/1096	0.70	0/1491
1	S	0.56	0/1096	0.69	0/1491
2	B	0.70	0/1152	0.81	3/1566 (0.2%)
2	D	0.63	0/1152	0.71	0/1566
2	F	0.60	0/1152	0.71	1/1566 (0.1%)
2	H	0.55	0/1152	0.68	2/1566 (0.1%)
2	T	0.52	0/1152	0.61	0/1566
All	All	0.60	0/11240	0.70	7/15285 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	40	ARG	NE-CZ-NH1	8.35	124.48	120.30
2	B	40	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	C	105	LEU	CA-CB-CG	6.40	130.02	115.30
2	H	31	LEU	CA-CB-CG	5.60	128.18	115.30
2	F	14	LEU	CA-CB-CG	5.43	127.79	115.30
2	B	110	LEU	CA-CB-CG	5.32	127.55	115.30
2	H	110	LEU	CA-CB-CG	5.26	127.39	115.30

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	1068	0	1070	27	0
1	C	1068	0	1073	18	1
1	E	1068	0	1070	48	0
1	G	1068	0	1073	25	0
1	S	1068	0	1073	29	0
2	B	1122	0	1118	18	0
2	D	1122	0	1118	25	0
2	F	1122	0	1118	24	0
2	H	1122	0	1118	48	0
2	T	1122	0	1118	34	0
3	A	11	0	9	1	0
3	E	11	0	9	0	0
4	A	43	0	30	4	0
4	B	43	0	30	1	0
4	C	43	0	30	0	0
4	D	43	0	30	4	0
4	E	43	0	30	7	0
4	F	43	0	30	1	0
4	G	43	0	30	0	0
4	H	43	0	30	2	0
4	S	43	0	30	2	0
4	T	43	0	30	3	0
5	A	2	0	0	0	0
5	B	2	0	0	2	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	1	0
5	H	2	0	0	0	0
5	S	2	0	0	0	0
5	T	2	0	0	0	0
6	B	12	0	12	0	0
6	C	12	0	12	0	0
6	T	12	0	12	0	0
7	G	5	0	0	0	0
8	A	46	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	66	0	0	1	1
8	C	51	0	0	4	1
8	D	52	0	0	2	0
8	E	29	0	0	2	0
8	F	61	0	0	0	0
8	G	31	0	0	0	0
8	H	35	0	0	1	0
8	S	46	0	0	0	1
8	T	51	0	0	0	0
All	All	11931	0	11303	284	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (284) 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:S:140:TYR:O	1:S:141:ARG:HG2	1.60	1.01
1:E:61:LYS:HE2	4:E:150:HEM:HAA1	1.49	0.94
1:E:134:THR:O	1:E:137:THR:HB	1.67	0.93
1:E:11:LYS:HG2	8:E:165:HOH:O	1.69	0.91
1:S:1:VAL:HG12	1:S:2:LEU:H	1.38	0.88
4:H:150:HEM:HMA2	4:H:150:HEM:HBA2	1.60	0.84
2:D:24:GLY:HA3	2:D:64:GLY:O	1.77	0.84
2:F:20:VAL:O	2:F:21:ASP:HB2	1.78	0.84
1:A:45:HIS:H	1:A:45:HIS:CD2	1.98	0.82
1:C:38:THR:CG2	8:C:196:HOH:O	2.29	0.80
1:E:137:THR:HG23	1:E:140:TYR:CB	2.13	0.78
2:F:26:GLU:O	2:F:30:ARG:HG2	1.85	0.77
1:C:29:LEU:HD11	1:C:58:HIS:HD2	1.50	0.77
1:C:38:THR:HG23	8:C:196:HOH:O	1.86	0.76
1:E:65:ALA:HB2	4:E:150:HEM:HMA1	1.68	0.75
2:T:29:GLY:HA3	2:T:55:MET:CE	2.16	0.75
2:H:29:GLY:O	2:H:33:VAL:HG23	1.87	0.74
1:S:66:LEU:O	1:S:70:VAL:HG23	1.88	0.74
1:A:44:PRO:HD2	1:A:45:HIS:HD2	1.52	0.74
1:E:137:THR:HG23	1:E:140:TYR:HB2	1.70	0.73
2:T:29:GLY:HA3	2:T:55:MET:HE1	1.69	0.73
2:H:130:TYR:O	2:H:134:VAL:HG12	1.93	0.69
2:T:101:GLU:OE2	2:T:104:ARG:NH1	2.26	0.69
4:E:150:HEM:HHD	4:E:150:HEM:HBC2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:HIS:NE2	5:G:151:OXY:O2	2.24	0.68
2:F:18:VAL:HG13	2:F:23:VAL:HG21	1.75	0.68
1:A:44:PRO:HD2	1:A:45:HIS:CD2	2.29	0.68
1:G:91:LEU:O	1:G:92:ARG:HB2	1.94	0.66
1:E:11:LYS:HB2	8:E:163:HOH:O	1.97	0.65
1:E:85:ASP:O	1:E:89:HIS:HB2	1.97	0.65
1:E:137:THR:HG23	1:E:140:TYR:HB3	1.77	0.65
4:A:150:HEM:HBA2	8:A:191:HOH:O	1.97	0.65
2:T:28:LEU:O	2:T:32:LEU:HD13	1.97	0.65
1:E:134:THR:O	1:E:137:THR:CB	2.45	0.64
2:F:73:ASP:O	2:F:77:HIS:HD2	1.79	0.64
2:H:88:LEU:HD12	2:H:88:LEU:H	1.63	0.64
2:T:24:GLY:HA3	2:T:68:LEU:HB2	1.79	0.64
2:H:104:ARG:HD3	8:H:225:HOH:O	1.99	0.63
1:G:103:HIS:HE1	2:H:131:GLN:OE1	1.82	0.63
1:S:140:TYR:O	1:S:141:ARG:CG	2.44	0.63
1:S:1:VAL:CG1	1:S:2:LEU:H	2.09	0.62
1:G:7:LYS:HD3	1:G:73:VAL:HG11	1.80	0.62
2:H:15:TRP:HA	2:H:18:VAL:HG23	1.79	0.62
1:G:66:LEU:O	1:G:70:VAL:HG23	1.98	0.62
1:S:46:PHE:HA	1:S:54:GLN:HE22	1.64	0.62
4:S:150:HEM:HMB2	4:S:150:HEM:HBB2	1.80	0.62
1:E:140:TYR:CE2	2:H:37:TRP:HE3	2.18	0.62
4:H:150:HEM:HBA2	4:H:150:HEM:CMA	2.29	0.61
2:B:4:THR:HB	2:B:5:PRO:HD2	1.80	0.61
1:C:24:TYR:HE1	1:C:112:HIS:HD1	1.43	0.61
1:E:32:MET:HE3	1:E:39:THR:HB	1.81	0.61
2:F:113:VAL:O	2:F:116:HIS:HB2	2.01	0.61
2:B:105:LEU:O	2:B:109:VAL:HG13	2.01	0.61
2:T:106:LEU:HD23	4:T:150:HEM:CAB	2.32	0.60
1:E:58:HIS:O	1:E:62:VAL:HG23	2.02	0.60
2:T:29:GLY:CA	2:T:55:MET:HE1	2.32	0.60
2:D:123:THR:OG1	2:D:126:VAL:HG23	2.02	0.60
1:E:128:PHE:O	1:E:132:VAL:HG23	2.03	0.59
1:E:3:SER:HB2	1:E:4:PRO:CD	2.32	0.59
1:E:3:SER:HB2	1:E:4:PRO:HD2	1.85	0.59
1:S:39:THR:HG22	1:S:97:ASN:HD22	1.67	0.59
1:S:10:VAL:HG22	1:S:125:LEU:HD23	1.85	0.59
1:S:76:MET:HE3	1:S:132:VAL:HG22	1.85	0.58
1:S:1:VAL:HG12	1:S:2:LEU:N	2.15	0.58
1:E:66:LEU:HG	4:E:150:HEM:HMB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:HIS:HE1	4:A:150:HEM:O1D	1.86	0.58
2:H:142:ALA:O	2:H:145:TYR:HB2	2.04	0.57
2:B:124:PRO:HB2	2:B:125:PRO:HD3	1.86	0.57
1:E:141:ARG:HD2	1:G:127:LYS:HD2	1.86	0.56
4:D:150:HEM:CMD	4:D:150:HEM:HBD2	2.35	0.56
2:F:26:GLU:HG2	2:F:30:ARG:HE	1.70	0.56
1:S:72:HIS:O	1:S:76:MET:HG2	2.06	0.56
1:E:141:ARG:HA	1:G:127:LYS:HE3	1.88	0.56
2:F:146:HIS:CE1	2:H:2:HIS:HB2	2.41	0.56
1:E:70:VAL:O	1:E:73:VAL:HG23	2.07	0.55
1:S:103:HIS:O	1:S:107:VAL:HG23	2.07	0.55
2:F:42:PHE:O	2:F:45:PHE:HB2	2.06	0.55
2:H:90:GLU:HA	2:H:144:LYS:HD3	1.88	0.55
1:S:35:SER:HB3	2:T:131:GLN:HG3	1.88	0.55
2:T:66:LYS:HD3	4:T:150:HEM:HAA2	1.87	0.55
1:C:29:LEU:HD11	1:C:58:HIS:CD2	2.38	0.55
2:D:41:PHE:HB3	4:D:150:HEM:HMD2	1.90	0.54
2:F:93:CYS:HB2	2:F:145:TYR:CE2	2.43	0.54
2:F:1:VAL:HG11	2:F:132:LYS:HB3	1.89	0.54
2:T:37:TRP:HE1	2:T:102:ASN:HD21	1.55	0.54
1:A:45:HIS:H	1:A:45:HIS:HD2	1.51	0.54
1:A:44:PRO:CD	1:A:45:HIS:HD2	2.18	0.54
2:B:28:LEU:HD22	2:B:60:VAL:HG13	1.88	0.54
2:B:123:THR:OG1	2:B:126:VAL:HG23	2.08	0.54
2:H:50:THR:O	2:H:54:VAL:HG23	2.08	0.54
1:C:51:GLY:O	1:C:52:SER:C	2.47	0.53
1:G:46:PHE:HB2	1:G:48:LEU:HD13	1.90	0.53
1:S:47:ASP:H	1:S:54:GLN:NE2	2.06	0.53
1:A:85:ASP:O	1:A:89:HIS:HB2	2.08	0.53
1:C:103:HIS:HE1	2:D:131:GLN:OE1	1.90	0.53
2:D:51:PRO:O	2:D:55:MET:HG2	2.09	0.53
2:H:53:ALA:O	2:H:57:ASN:HB2	2.09	0.53
1:S:105:LEU:O	1:S:109:LEU:HD13	2.09	0.53
2:T:25:GLY:HA2	2:T:64:GLY:HA3	1.91	0.53
1:E:41:THR:HG22	2:H:40:ARG:HH12	1.74	0.52
1:E:87:HIS:HA	1:E:91:LEU:HD12	1.90	0.52
2:F:124:PRO:HB2	2:F:125:PRO:HD3	1.91	0.52
2:T:107:GLY:HA3	2:T:134:VAL:CG1	2.40	0.52
1:A:103:HIS:HE1	2:B:131:GLN:OE1	1.93	0.52
1:E:112:HIS:CE1	2:F:120:LYS:HG3	2.45	0.52
1:E:65:ALA:HB2	4:E:150:HEM:CMA	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:THR:O	2:D:7:GLU:N	2.43	0.52
1:A:83:LEU:HB3	1:A:136:LEU:HD22	1.90	0.52
1:C:24:TYR:CE1	1:C:112:HIS:ND1	2.72	0.52
2:T:24:GLY:H	2:T:68:LEU:HG	1.74	0.52
1:A:98:PHE:HB3	1:A:133:SER:HB3	1.92	0.51
1:E:92:ARG:CZ	2:H:39:GLN:HB2	2.40	0.51
1:E:17:VAL:HG12	1:E:21:ALA:HB2	1.92	0.51
2:T:50:THR:O	2:T:54:VAL:HG23	2.10	0.51
1:S:4:PRO:HA	1:S:7:LYS:HZ2	1.75	0.51
1:S:4:PRO:HA	1:S:7:LYS:NZ	2.26	0.51
1:E:138:SER:C	1:E:140:TYR:H	2.14	0.51
2:F:145:TYR:O	2:F:146:HIS:HB2	2.11	0.51
1:G:21:ALA:HB1	1:G:63:ALA:HB1	1.93	0.51
2:H:107:GLY:CA	2:H:134:VAL:HG21	2.40	0.51
1:E:96:VAL:O	1:E:99:LYS:HB2	2.11	0.51
2:B:67:VAL:CG2	5:B:151:OXY:O2	2.60	0.50
2:F:19:ASN:O	2:F:21:ASP:N	2.44	0.50
2:F:26:GLU:CD	2:F:30:ARG:HH21	2.15	0.50
1:S:20:HIS:HB3	1:S:24:TYR:CZ	2.47	0.50
1:E:32:MET:CE	1:E:39:THR:HB	2.42	0.50
2:B:31:LEU:HD22	2:B:106:LEU:HD13	1.94	0.50
2:H:30:ARG:O	2:H:34:VAL:HG23	2.11	0.50
2:D:77:HIS:O	2:D:81:LEU:HD13	2.12	0.49
1:E:89:HIS:CD2	1:E:139:LYS:HG3	2.47	0.49
1:S:128:PHE:O	1:S:132:VAL:HG23	2.12	0.49
1:E:76:MET:HB3	1:E:135:VAL:HG11	1.94	0.49
2:T:127:GLN:O	2:T:131:GLN:HG2	2.12	0.49
1:E:61:LYS:CE	4:E:150:HEM:HAA1	2.34	0.49
2:H:88:LEU:HA	2:H:91:LEU:HD12	1.94	0.49
1:G:20:HIS:O	1:G:23:GLU:N	2.46	0.49
1:A:28:ALA:HB1	1:A:105:LEU:CD1	2.43	0.49
2:B:3:LEU:HD22	2:B:7:GLU:HB3	1.95	0.48
4:F:150:HEM:HHC	4:F:150:HEM:HBB2	1.95	0.48
2:T:115:ALA:HB2	2:T:122:PHE:CD2	2.47	0.48
2:D:68:LEU:O	2:D:68:LEU:HD23	2.13	0.48
1:C:83:LEU:HB3	1:C:136:LEU:HD22	1.95	0.48
4:D:150:HEM:HBD2	4:D:150:HEM:HMD1	1.95	0.48
1:C:29:LEU:CD1	1:C:58:HIS:HD2	2.22	0.48
2:H:48:LEU:HD23	2:H:54:VAL:HA	1.96	0.48
1:C:82:ALA:O	1:C:85:ASP:HB2	2.14	0.48
1:E:24:TYR:O	1:E:108:THR:HG21	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:GLU:O	2:F:30:ARG:CG	2.60	0.48
2:H:107:GLY:HA2	2:H:134:VAL:HG21	1.95	0.48
2:T:29:GLY:HA3	2:T:55:MET:HE2	1.95	0.48
1:E:65:ALA:CB	4:E:150:HEM:HMA1	2.39	0.47
2:H:88:LEU:HD12	2:H:88:LEU:N	2.29	0.47
2:F:80:ASN:O	2:F:84:THR:OG1	2.20	0.47
1:A:112:HIS:O	1:A:113:LEU:HD23	2.14	0.47
2:H:143:HIS:C	2:H:145:TYR:H	2.16	0.47
1:E:94:ASP:HB3	1:E:96:VAL:HB	1.97	0.47
1:A:95:PRO:HB3	1:A:137:THR:HG21	1.96	0.47
1:E:96:VAL:O	1:E:99:LYS:N	2.46	0.47
2:H:110:LEU:HD22	2:H:110:LEU:O	2.15	0.47
1:A:98:PHE:HE1	1:A:136:LEU:HD12	1.80	0.47
1:A:28:ALA:HB1	1:A:105:LEU:HD13	1.97	0.47
1:A:45:HIS:CE1	4:A:150:HEM:O1D	2.68	0.47
1:G:47:ASP:H	1:G:54:GLN:NE2	2.13	0.47
1:G:113:LEU:HB3	1:G:116:GLU:HB2	1.97	0.47
2:H:103:PHE:CD1	2:H:103:PHE:N	2.83	0.46
2:H:103:PHE:N	2:H:103:PHE:HD1	2.13	0.46
2:T:40:ARG:O	2:T:43:GLU:HG3	2.15	0.46
1:A:28:ALA:CB	1:A:105:LEU:HD12	2.46	0.46
2:H:85:PHE:HD2	2:H:141:LEU:HD21	1.81	0.46
1:C:114:PRO:HG3	8:D:183:HOH:O	2.15	0.46
1:E:58:HIS:HA	1:E:61:LYS:HD3	1.97	0.46
1:G:119:PRO:HG3	2:H:55:MET:HE3	1.98	0.46
1:G:17:VAL:HG23	1:G:24:TYR:HD1	1.79	0.46
1:S:33:PHE:CD1	1:S:40:LYS:HG2	2.51	0.46
1:A:11:LYS:NZ	8:A:179:HOH:O	2.45	0.46
2:D:87:THR:HG22	8:D:189:HOH:O	2.16	0.45
1:E:112:HIS:HE1	2:F:120:LYS:HG3	1.81	0.45
2:T:55:MET:CE	2:T:55:MET:HA	2.46	0.45
2:B:127:GLN:O	2:B:131:GLN:HG2	2.16	0.45
2:B:67:VAL:HG21	5:B:151:OXY:O2	2.17	0.45
2:H:92:HIS:HD2	2:H:98:VAL:HG21	1.80	0.45
1:A:76:MET:N	1:A:77:PRO:CD	2.80	0.45
2:D:94:ASP:OD2	2:D:144:LYS:HE2	2.16	0.45
1:A:28:ALA:CB	1:A:105:LEU:CD1	2.94	0.45
2:T:5:PRO:HA	2:T:8:LYS:HB2	1.98	0.45
1:E:48:LEU:HD23	1:E:55:VAL:CG2	2.46	0.45
2:D:4:THR:O	2:D:7:GLU:HB2	2.16	0.45
2:D:8:LYS:O	2:D:12:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:THR:OG1	2:D:125:PRO:HD2	2.17	0.45
2:F:28:LEU:HD21	2:F:63:HIS:HD2	1.82	0.45
2:F:92:HIS:HA	2:F:96:LEU:HD12	1.99	0.45
1:S:1:VAL:CG1	1:S:2:LEU:N	2.78	0.45
1:E:4:PRO:HA	1:E:7:LYS:HG2	1.99	0.44
2:B:3:LEU:HD23	2:B:132:LYS:HD3	1.97	0.44
1:C:31:ARG:HG2	1:C:31:ARG:HH11	1.82	0.44
2:T:100:PRO:HD3	2:T:145:TYR:CE2	2.52	0.44
1:A:76:MET:HE1	1:A:131:SER:HB3	1.99	0.44
2:D:79:ASP:OD2	2:H:5:PRO:HB3	2.17	0.44
4:S:150:HEM:HBB2	4:S:150:HEM:CMB	2.46	0.44
2:T:107:GLY:HA3	2:T:134:VAL:HG11	1.99	0.44
1:A:91:LEU:O	2:D:40:ARG:HD2	2.18	0.44
1:S:108:THR:O	1:S:112:HIS:HB2	2.17	0.44
1:E:67:THR:O	1:E:70:VAL:HG23	2.18	0.44
1:E:4:PRO:C	1:E:6:ASP:H	2.21	0.44
8:C:164:HOH:O	2:D:109:VAL:HG12	2.18	0.44
2:T:41:PHE:CE1	2:T:98:VAL:HG22	2.52	0.44
1:A:45:HIS:CD2	1:A:45:HIS:N	2.77	0.43
2:D:108:ASN:ND2	2:D:131:GLN:HE22	2.15	0.43
1:G:34:LEU:HD12	2:H:124:PRO:HB2	2.00	0.43
2:D:106:LEU:HD23	4:D:150:HEM:CAB	2.48	0.43
1:A:45:HIS:HE1	4:A:150:HEM:CGD	2.31	0.43
2:F:1:VAL:H1	2:F:81:LEU:HD22	1.84	0.43
1:G:69:ALA:HB2	1:G:80:LEU:HD21	1.99	0.43
1:S:8:THR:O	1:S:10:VAL:N	2.51	0.43
1:E:48:LEU:HD23	1:E:55:VAL:HG22	2.01	0.43
1:G:120:ALA:O	1:G:124:SER:OG	2.36	0.43
2:D:15:TRP:CZ2	2:D:68:LEU:HD21	2.53	0.43
1:G:122:HIS:ND1	2:H:30:ARG:HD3	2.34	0.43
1:S:132:VAL:O	1:S:136:LEU:HG	2.19	0.43
2:T:107:GLY:HA3	2:T:134:VAL:HG13	2.01	0.43
1:A:106:LEU:CD2	1:A:125:LEU:HB3	2.49	0.42
1:G:46:PHE:N	1:G:46:PHE:CD2	2.87	0.42
2:H:61:LYS:O	2:H:65:LYS:HG3	2.20	0.42
2:H:15:TRP:CE3	2:H:18:VAL:HG21	2.54	0.42
2:T:1:VAL:HG12	2:T:78:LEU:HD22	2.02	0.42
2:T:85:PHE:HB2	2:T:140:ALA:HB1	2.01	0.42
1:G:109:LEU:HD23	1:G:125:LEU:HD13	2.00	0.42
2:H:50:THR:HG22	2:H:52:ASP:H	1.85	0.42
2:H:127:GLN:O	2:H:131:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:31:LEU:HD12	2:T:35:TYR:HD1	1.84	0.42
3:A:142:FRU:H61	2:B:101:GLU:HG2	2.01	0.42
1:S:42:TYR:CE1	1:S:93:VAL:HA	2.55	0.42
2:T:100:PRO:HA	2:T:103:PHE:CD2	2.55	0.42
1:E:137:THR:CG2	1:E:140:TYR:HB2	2.45	0.42
1:G:46:PHE:CB	1:G:48:LEU:HD13	2.49	0.42
1:C:119:PRO:HG2	2:D:55:MET:HG3	2.02	0.42
1:G:94:ASP:CG	1:G:96:VAL:HG12	2.40	0.42
2:H:107:GLY:CA	2:H:134:VAL:CG2	2.97	0.42
2:B:110:LEU:O	2:B:114:LEU:HG	2.20	0.42
2:B:139:ASN:HD21	2:D:146:HIS:HD2	1.67	0.42
2:F:36:PRO:HA	2:F:39:GLN:HE21	1.84	0.42
2:H:32:LEU:HD23	2:H:39:GLN:HG2	2.02	0.42
2:H:118:PHE:O	2:H:121:GLU:HG2	2.19	0.42
2:T:106:LEU:O	2:T:109:VAL:HG22	2.19	0.42
1:S:2:LEU:HD21	1:S:128:PHE:HB2	2.02	0.42
1:G:84:SER:HB3	1:G:135:VAL:O	2.20	0.42
1:S:58:HIS:HA	1:S:61:LYS:HD2	2.02	0.41
2:H:118:PHE:HB3	2:H:121:GLU:HG3	2.01	0.41
2:T:31:LEU:HD12	2:T:35:TYR:CD1	2.54	0.41
1:A:140:TYR:HA	1:C:3:SER:HB3	2.01	0.41
2:B:40:ARG:NH2	8:B:192:HOH:O	2.53	0.41
1:C:27:GLU:OE2	1:C:31:ARG:NH2	2.46	0.41
2:H:100:PRO:HA	2:H:103:PHE:CD1	2.55	0.41
1:S:116:GLU:O	1:S:118:THR:N	2.47	0.41
1:E:3:SER:CB	1:E:4:PRO:CD	2.98	0.41
2:T:29:GLY:C	2:T:55:MET:HE1	2.41	0.41
2:B:7:GLU:HG2	2:B:129:ALA:HB2	2.01	0.41
1:E:140:TYR:CE2	2:H:37:TRP:CE3	3.05	0.41
1:G:132:VAL:O	1:G:136:LEU:HD23	2.21	0.41
2:H:123:THR:HB	2:H:125:PRO:HD2	2.02	0.41
2:T:106:LEU:CD2	4:T:150:HEM:CAB	2.98	0.41
1:E:17:VAL:CG1	1:E:21:ALA:HB2	2.51	0.41
2:D:15:TRP:CZ2	2:D:68:LEU:CD2	3.04	0.41
2:D:81:LEU:O	2:D:85:PHE:HD1	2.03	0.41
1:E:80:LEU:HD21	1:E:132:VAL:HG13	2.02	0.41
2:H:15:TRP:CD2	2:H:18:VAL:HG21	2.55	0.41
2:H:107:GLY:HA2	2:H:134:VAL:CG2	2.51	0.41
1:S:76:MET:CE	1:S:132:VAL:HG22	2.50	0.41
1:C:47:ASP:H	1:C:54:GLN:NE2	2.18	0.41
2:H:42:PHE:HE2	2:H:63:HIS:CD2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:THR:HG21	8:C:196:HOH:O	2.13	0.40
2:T:20:VAL:HG23	2:T:68:LEU:HD12	2.03	0.40
1:A:85:ASP:HA	1:A:89:HIS:CD2	2.55	0.40
2:D:107:GLY:HA3	2:D:134:VAL:HG22	2.03	0.40
2:F:67:VAL:HG11	2:F:106:LEU:HD21	2.03	0.40
1:G:46:PHE:N	1:G:46:PHE:HD2	2.18	0.40
2:T:91:LEU:O	2:T:95:LYS:HB2	2.20	0.40
2:B:106:LEU:HD23	4:B:150:HEM:CAB	2.51	0.40
2:D:93:CYS:SG	2:D:145:TYR:CE2	3.05	0.40
2:H:35:TYR:HB3	2:H:37:TRP:CE2	2.56	0.40
2:H:88:LEU:H	2:H:88:LEU:CD1	2.32	0.40
2:H:109:VAL:O	2:H:112:CYS:HB2	2.21	0.40
2:F:24:GLY:HA3	2:F:64:GLY:O	2.20	0.40
2:H:85:PHE:HB3	2:H:141:LEU:HD23	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:191:HOH:O	8:C:176:HOH:O[1_565]	2.13	0.07
1:C:11:LYS:NZ	8:S:217:HOH:O[2_546]	2.13	0.07

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	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22 26
1	C	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22 26
1	E	139/141 (99%)	115 (83%)	21 (15%)	3 (2%)	6 5
1	G	139/141 (99%)	126 (91%)	12 (9%)	1 (1%)	22 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	139/141 (99%)	121 (87%)	12 (9%)	6 (4%)	2	1
2	B	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	D	144/146 (99%)	136 (94%)	6 (4%)	2 (1%)	11	11
2	F	144/146 (99%)	126 (88%)	13 (9%)	5 (4%)	3	2
2	H	144/146 (99%)	130 (90%)	11 (8%)	3 (2%)	7	5
2	T	144/146 (99%)	129 (90%)	14 (10%)	1 (1%)	22	26
All	All	1415/1435 (99%)	1290 (91%)	102 (7%)	23 (2%)	9	9

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	17	VAL
2	F	20	VAL
2	F	21	ASP
1	S	9	ASN
1	C	52	SER
2	F	43	GLU
1	G	92	ARG
2	H	46	GLY
1	S	18	GLY
2	T	19	ASN
2	F	119	GLY
2	H	93	CYS
1	S	17	VAL
1	S	52	SER
2	D	19	ASN
1	E	7	LYS
2	F	5	PRO
1	S	41	THR
1	S	117	PHE
1	A	75	ASP
2	D	6	GLU
2	H	57	ASN
1	E	119	PRO

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	113/113 (100%)	103 (91%)	10 (9%)	10	12
1	C	113/113 (100%)	110 (97%)	3 (3%)	44	61
1	E	113/113 (100%)	98 (87%)	15 (13%)	4	4
1	G	113/113 (100%)	101 (89%)	12 (11%)	6	7
1	S	113/113 (100%)	108 (96%)	5 (4%)	28	39
2	B	118/118 (100%)	110 (93%)	8 (7%)	16	21
2	D	118/118 (100%)	112 (95%)	6 (5%)	24	33
2	F	118/118 (100%)	108 (92%)	10 (8%)	10	13
2	H	118/118 (100%)	105 (89%)	13 (11%)	6	7
2	T	118/118 (100%)	110 (93%)	8 (7%)	16	21
All	All	1155/1155 (100%)	1065 (92%)	90 (8%)	12	16

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	49	SER
1	A	81	SER
1	A	83	LEU
1	A	85	ASP
1	A	92	ARG
1	A	105	LEU
1	A	116	GLU
1	A	125	LEU
1	A	134	THR
2	B	6	GLU
2	B	26	GLU
2	B	50	THR
2	B	68	LEU
2	B	81	LEU
2	B	109	VAL
2	B	110	LEU
2	B	141	LEU
1	C	38	THR
1	C	52	SER
1	C	105	LEU
2	D	14	LEU

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Mol	Chain	Res	Type
2	D	28	LEU
2	D	44	SER
2	D	81	LEU
2	D	84	THR
2	D	90	GLU
1	E	6	ASP
1	E	20	HIS
1	E	30	GLU
1	E	34	LEU
1	E	38	THR
1	E	47	ASP
1	E	67	THR
1	E	70	VAL
1	E	74	ASP
1	E	89	HIS
1	E	94	ASP
1	E	99	LYS
1	E	109	LEU
1	E	118	THR
1	E	141	ARG
2	F	28	LEU
2	F	45	PHE
2	F	47	ASP
2	F	68	LEU
2	F	71	PHE
2	F	73	ASP
2	F	81	LEU
2	F	116	HIS
2	F	134	VAL
2	F	141	LEU
1	G	17	VAL
1	G	48	LEU
1	G	74	ASP
1	G	81	SER
1	G	84	SER
1	G	85	ASP
1	G	100	LEU
1	G	109	LEU
1	G	127	LYS
1	G	131	SER
1	G	140	TYR
1	G	141	ARG

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Mol	Chain	Res	Type
2	H	19	ASN
2	H	21	ASP
2	H	31	LEU
2	H	38	THR
2	H	40	ARG
2	H	59	LYS
2	H	68	LEU
2	H	72	SER
2	H	81	LEU
2	H	88	LEU
2	H	103	PHE
2	H	110	LEU
2	H	146	HIS
1	S	36	PHE
1	S	54	GLN
1	S	78	ASN
1	S	81	SER
1	S	105	LEU
2	T	12	THR
2	T	50	THR
2	T	52	ASP
2	T	79	ASP
2	T	84	THR
2	T	91	LEU
2	T	104	ARG
2	T	139	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	45	HIS
1	A	54	GLN
1	A	89	HIS
1	A	97	ASN
1	A	103	HIS
2	B	77	HIS
1	C	54	GLN
1	C	58	HIS
1	C	97	ASN
1	C	103	HIS
2	D	63	HIS

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Mol	Chain	Res	Type
2	D	77	HIS
2	D	108	ASN
2	D	146	HIS
1	E	20	HIS
1	E	122	HIS
2	F	39	GLN
2	F	77	HIS
2	F	108	ASN
2	F	143	HIS
1	G	54	GLN
1	G	103	HIS
2	H	19	ASN
2	H	63	HIS
2	H	97	HIS
2	H	108	ASN
1	S	9	ASN
1	S	54	GLN
1	S	78	ASN
1	S	97	ASN
1	S	122	HIS
2	T	77	HIS
2	T	102	ASN
2	T	108	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)

26 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	$\#\|Z\| > 2$
3	FRU	A	142	1	11,11,12	1.00	0	15,17,18	12.84	6 (40%)
5	OXY	D	151	4	1,1,1	0.19	0	-		
5	OXY	T	151	4	1,1,1	0.13	0	-		
4	HEM	B	150	2,5	41,50,50	2.09	11 (26%)	45,82,82	1.91	15 (33%)
6	GLC	B	147	-	12,12,12	0.63	0	17,17,17	1.71	4 (23%)
5	OXY	A	151	4	1,1,1	0.09	0	-		
4	HEM	D	150	2,5	41,50,50	2.03	7 (17%)	45,82,82	1.89	9 (20%)
4	HEM	T	150	2,5	41,50,50	2.02	9 (21%)	45,82,82	1.70	8 (17%)
5	OXY	E	151	4	1,1,1	0.46	0	-		
5	OXY	S	151	4	1,1,1	0.22	0	-		
4	HEM	E	150	1,5	41,50,50	2.02	7 (17%)	45,82,82	1.78	8 (17%)
5	OXY	B	151	4	1,1,1	0.16	0	-		
4	HEM	A	150	1,5	41,50,50	2.08	9 (21%)	45,82,82	1.77	8 (17%)
6	GLC	T	147	-	12,12,12	0.55	0	17,17,17	0.79	0
4	HEM	C	150	1,5	41,50,50	1.99	6 (14%)	45,82,82	1.82	12 (26%)
4	HEM	S	150	1,5	41,50,50	1.97	8 (19%)	45,82,82	2.11	11 (24%)
5	OXY	F	151	4	1,1,1	0.26	0	-		
5	OXY	G	151	4	1,1,1	0.16	0	-		
5	OXY	H	151	4	1,1,1	0.15	0	-		
4	HEM	F	150	2,5	41,50,50	2.00	10 (24%)	45,82,82	1.67	8 (17%)
4	HEM	H	150	2,5	41,50,50	2.01	8 (19%)	45,82,82	1.92	8 (17%)
5	OXY	C	151	4	1,1,1	0.17	0	-		
6	GLC	C	142	-	12,12,12	0.55	0	17,17,17	1.40	2 (11%)
7	PO4	G	142	-	4,4,4	0.75	0	6,6,6	0.48	0
4	HEM	G	150	1,5	41,50,50	1.99	6 (14%)	45,82,82	1.96	10 (22%)
3	FRU	E	142	1	11,11,12	0.77	0	15,17,18	2.63	3 (20%)

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
3	FRU	A	142	1	1/1/4/4	0/2/21/24	0/1/1/1
4	HEM	C	150	1,5	-	5/12/54/54	-
4	HEM	S	150	1,5	-	4/12/54/54	-
4	HEM	D	150	2,5	-	4/12/54/54	-
6	GLC	T	147	-	-	2/2/22/22	0/1/1/1
4	HEM	T	150	2,5	-	5/12/54/54	-
4	HEM	B	150	2,5	-	4/12/54/54	-
4	HEM	E	150	1,5	-	9/12/54/54	-
6	GLC	B	147	-	-	0/2/22/22	0/1/1/1
4	HEM	F	150	2,5	-	4/12/54/54	-
6	GLC	C	142	-	-	0/2/22/22	0/1/1/1
4	HEM	H	150	2,5	-	9/12/54/54	-
4	HEM	G	150	1,5	-	7/12/54/54	-
4	HEM	A	150	1,5	-	6/12/54/54	-
3	FRU	E	142	1	-	0/2/21/24	0/1/1/1

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	150	HEM	C3D-C2D	8.40	1.54	1.36
4	G	150	HEM	C3D-C2D	8.39	1.54	1.36
4	D	150	HEM	C3D-C2D	8.20	1.54	1.36
4	A	150	HEM	C3D-C2D	8.02	1.53	1.36
4	E	150	HEM	C3D-C2D	7.95	1.53	1.36
4	F	150	HEM	C3D-C2D	7.83	1.53	1.36
4	C	150	HEM	C3D-C2D	7.81	1.53	1.36
4	T	150	HEM	C3D-C2D	7.81	1.53	1.36
4	B	150	HEM	C3D-C2D	7.71	1.53	1.36
4	S	150	HEM	C3D-C2D	7.59	1.52	1.36
4	E	150	HEM	C3C-C2C	-4.73	1.33	1.40
4	A	150	HEM	C3C-C2C	-4.43	1.34	1.40
4	B	150	HEM	C3C-C2C	-4.13	1.34	1.40
4	T	150	HEM	C3C-C2C	-4.13	1.34	1.40
4	B	150	HEM	C3C-CAC	4.11	1.56	1.47
4	C	150	HEM	C3C-CAC	3.97	1.56	1.47
4	S	150	HEM	C3C-C2C	-3.90	1.35	1.40
4	G	150	HEM	C3C-CAC	3.89	1.55	1.47
4	S	150	HEM	C3C-CAC	3.85	1.55	1.47
4	A	150	HEM	C3C-CAC	3.80	1.55	1.47
4	T	150	HEM	C3C-CAC	3.76	1.55	1.47
4	E	150	HEM	C3C-CAC	3.75	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	150	HEM	C3C-CAC	3.72	1.55	1.47
4	D	150	HEM	C3C-CAC	3.70	1.55	1.47
4	C	150	HEM	C3C-C2C	-3.64	1.35	1.40
4	H	150	HEM	C3C-C2C	-3.62	1.35	1.40
4	G	150	HEM	C3C-C2C	-3.60	1.35	1.40
4	H	150	HEM	C3C-CAC	3.55	1.55	1.47
4	C	150	HEM	CAA-C2A	3.45	1.57	1.52
4	S	150	HEM	CAB-C3B	3.41	1.56	1.47
4	D	150	HEM	CAB-C3B	3.40	1.56	1.47
4	D	150	HEM	C3C-C2C	-3.38	1.35	1.40
4	H	150	HEM	CAB-C3B	3.33	1.56	1.47
4	F	150	HEM	FE-ND	3.32	2.13	1.96
4	F	150	HEM	CAB-C3B	3.22	1.56	1.47
4	D	150	HEM	FE-NB	3.22	2.12	1.96
4	G	150	HEM	CAB-C3B	3.19	1.56	1.47
4	T	150	HEM	CAB-C3B	3.04	1.55	1.47
4	E	150	HEM	CAB-C3B	3.03	1.55	1.47
4	S	150	HEM	CAA-C2A	2.93	1.56	1.52
4	A	150	HEM	FE-NB	2.93	2.11	1.96
4	F	150	HEM	CMB-C2B	2.90	1.56	1.50
4	A	150	HEM	CAB-C3B	2.90	1.55	1.47
4	T	150	HEM	FE-ND	2.87	2.11	1.96
4	C	150	HEM	CAB-C3B	2.87	1.55	1.47
4	D	150	HEM	FE-ND	2.85	2.11	1.96
4	B	150	HEM	CAA-C2A	2.83	1.56	1.52
4	E	150	HEM	FE-ND	2.78	2.10	1.96
4	F	150	HEM	CAA-C2A	2.75	1.56	1.52
4	T	150	HEM	CAA-C2A	2.73	1.56	1.52
4	H	150	HEM	FE-NB	2.72	2.10	1.96
4	B	150	HEM	CAB-C3B	2.64	1.54	1.47
4	G	150	HEM	CAA-C2A	2.63	1.55	1.52
4	B	150	HEM	CMA-C3A	2.61	1.57	1.51
4	D	150	HEM	CMB-C2B	2.60	1.56	1.50
4	H	150	HEM	CAA-C2A	2.60	1.55	1.52
4	F	150	HEM	C3C-C2C	-2.51	1.36	1.40
4	B	150	HEM	CMD-C2D	2.50	1.56	1.50
4	T	150	HEM	FE-NB	2.47	2.09	1.96
4	B	150	HEM	CMB-C2B	2.46	1.56	1.50
4	S	150	HEM	FE-NB	2.43	2.08	1.96
4	B	150	HEM	C1A-NA	2.41	1.41	1.36
4	S	150	HEM	CMB-C2B	2.37	1.55	1.50
4	A	150	HEM	CAA-C2A	2.36	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	150	HEM	FE-NB	2.35	2.08	1.96
4	E	150	HEM	CAA-C2A	2.34	1.55	1.52
4	C	150	HEM	CMB-C2B	2.34	1.55	1.50
4	F	150	HEM	CMD-C2D	2.29	1.55	1.50
4	S	150	HEM	CMA-C3A	2.29	1.56	1.51
4	H	150	HEM	FE-ND	2.28	2.08	1.96
4	F	150	HEM	CMA-C3A	2.26	1.56	1.51
4	T	150	HEM	CMB-C2B	2.24	1.55	1.50
4	B	150	HEM	FE-ND	2.17	2.07	1.96
4	A	150	HEM	C2C-C1C	2.15	1.47	1.42
4	H	150	HEM	CMB-C2B	2.13	1.55	1.50
4	T	150	HEM	CMD-C2D	2.11	1.55	1.50
4	A	150	HEM	CMD-C2D	2.07	1.55	1.50
4	A	150	HEM	CMB-C2B	2.04	1.55	1.50
4	B	150	HEM	CHB-C1B	2.04	1.40	1.35
4	G	150	HEM	CHB-C1B	2.03	1.40	1.35
4	E	150	HEM	CMD-C2D	2.01	1.55	1.50

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	142	FRU	O5-C2-C1	-35.56	83.66	107.46
3	A	142	FRU	O2-C2-O5	-33.67	87.85	109.99
3	E	142	FRU	O5-C2-C1	8.21	112.95	107.46
4	S	150	HEM	C4D-ND-C1D	7.40	112.71	105.07
4	H	150	HEM	C4D-ND-C1D	7.33	112.64	105.07
4	A	150	HEM	C4D-ND-C1D	6.73	112.02	105.07
4	E	150	HEM	C4D-ND-C1D	5.96	111.22	105.07
4	T	150	HEM	C4D-ND-C1D	5.94	111.21	105.07
4	G	150	HEM	C4D-ND-C1D	5.87	111.14	105.07
4	B	150	HEM	C4D-ND-C1D	5.80	111.07	105.07
4	D	150	HEM	C4D-ND-C1D	5.74	111.01	105.07
4	S	150	HEM	C4B-CHC-C1C	5.40	129.69	122.56
4	C	150	HEM	C4D-ND-C1D	5.18	110.42	105.07
4	F	150	HEM	C4D-ND-C1D	5.15	110.39	105.07
3	A	142	FRU	O5-C2-C3	-5.13	94.22	104.70
4	C	150	HEM	C4B-CHC-C1C	5.11	129.30	122.56
3	E	142	FRU	O2-C2-O5	-5.03	106.68	109.99
4	S	150	HEM	CAD-CBD-CGD	-4.75	103.39	113.60
4	E	150	HEM	C4C-CHD-C1D	4.73	128.81	122.56
4	G	150	HEM	C1B-NB-C4B	4.59	109.82	105.07
4	D	150	HEM	CBA-CAA-C2A	-4.21	105.44	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	150	HEM	C4C-CHD-C1D	4.05	127.91	122.56
3	A	142	FRU	C2-O5-C5	3.98	117.60	109.22
4	H	150	HEM	C4B-CHC-C1C	3.94	127.75	122.56
4	G	150	HEM	C3B-C2B-C1B	3.87	109.36	106.49
3	A	142	FRU	O2-C2-C3	3.77	118.25	109.31
4	C	150	HEM	C1B-NB-C4B	3.65	108.84	105.07
3	A	142	FRU	O2-C2-C1	3.57	118.55	111.87
4	G	150	HEM	C4C-CHD-C1D	3.56	127.26	122.56
4	D	150	HEM	C3B-C2B-C1B	3.51	109.09	106.49
4	H	150	HEM	C4C-CHD-C1D	3.50	127.18	122.56
4	G	150	HEM	CHB-C1B-NB	3.50	128.70	124.38
4	D	150	HEM	C1B-NB-C4B	3.48	108.67	105.07
4	F	150	HEM	C4C-CHD-C1D	3.48	127.16	122.56
4	F	150	HEM	C1B-NB-C4B	3.47	108.66	105.07
6	C	142	GLC	C1-O5-C5	3.47	120.22	113.66
4	A	150	HEM	C4C-CHD-C1D	3.46	127.13	122.56
4	E	150	HEM	C1B-NB-C4B	3.46	108.64	105.07
4	T	150	HEM	C1B-NB-C4B	3.43	108.61	105.07
4	B	150	HEM	C1B-NB-C4B	3.37	108.55	105.07
4	B	150	HEM	C4C-CHD-C1D	3.37	127.00	122.56
4	S	150	HEM	CHA-C4D-ND	3.35	128.52	124.38
4	E	150	HEM	C3B-C2B-C1B	3.31	108.94	106.49
4	T	150	HEM	C4C-CHD-C1D	3.21	126.79	122.56
4	G	150	HEM	C2B-C1B-NB	-3.15	106.11	109.84
4	S	150	HEM	C3D-C4D-ND	-3.14	106.67	110.17
4	A	150	HEM	C4B-CHC-C1C	3.13	126.69	122.56
4	B	150	HEM	CHB-C1B-NB	3.11	128.22	124.38
4	D	150	HEM	C4B-CHC-C1C	3.08	126.62	122.56
6	B	147	GLC	O2-C2-C1	3.02	116.16	109.16
4	H	150	HEM	C1B-NB-C4B	3.00	108.17	105.07
4	H	150	HEM	CMA-C3A-C4A	-2.99	123.86	128.46
4	B	150	HEM	CBD-CAD-C3D	-2.89	104.59	112.63
4	C	150	HEM	CBA-CAA-C2A	2.89	117.55	112.62
6	B	147	GLC	O3-C3-C4	2.88	117.00	110.35
6	B	147	GLC	C4-C3-C2	-2.83	105.89	110.82
4	S	150	HEM	CMA-C3A-C4A	-2.82	124.14	128.46
4	S	150	HEM	CMD-C2D-C1D	2.79	129.29	125.04
4	E	150	HEM	CHD-C1D-ND	2.72	127.38	124.43
4	A	150	HEM	C3B-C2B-C1B	2.71	108.50	106.49
4	B	150	HEM	C4B-C3B-C2B	2.69	109.25	107.11
4	C	150	HEM	C4C-CHD-C1D	2.67	126.09	122.56
6	B	147	GLC	C1-O5-C5	2.66	118.69	113.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	150	HEM	CBD-CAD-C3D	-2.61	105.38	112.63
4	B	150	HEM	CAA-CBA-CGA	-2.57	106.55	113.76
4	T	150	HEM	C4B-CHC-C1C	2.54	125.91	122.56
4	C	150	HEM	CMD-C2D-C1D	2.53	128.90	125.04
4	G	150	HEM	CHD-C1D-ND	2.52	127.17	124.43
4	G	150	HEM	CHC-C4B-NB	2.51	127.16	124.43
4	A	150	HEM	C1B-NB-C4B	2.50	107.66	105.07
4	F	150	HEM	CMC-C2C-C3C	2.48	129.31	124.68
4	A	150	HEM	C1D-C2D-C3D	-2.45	104.38	106.96
4	B	150	HEM	C2C-C3C-C4C	2.44	108.60	106.90
4	T	150	HEM	CMA-C3A-C4A	-2.42	124.75	128.46
4	F	150	HEM	CMA-C3A-C4A	-2.42	124.75	128.46
4	F	150	HEM	CAD-CBD-CGD	-2.39	108.46	113.60
4	B	150	HEM	CHC-C4B-NB	2.31	126.94	124.43
6	C	142	GLC	C4-C3-C2	-2.30	106.81	110.82
4	T	150	HEM	C4A-C3A-C2A	2.29	108.59	107.00
4	B	150	HEM	CHD-C1D-ND	2.28	126.91	124.43
4	D	150	HEM	C2B-C1B-NB	-2.27	107.15	109.84
4	S	150	HEM	O1A-CGA-CBA	-2.26	115.81	123.08
4	G	150	HEM	C4A-C3A-C2A	2.25	108.56	107.00
4	B	150	HEM	CMA-C3A-C4A	-2.23	125.03	128.46
4	E	150	HEM	C2B-C1B-NB	-2.23	107.19	109.84
4	T	150	HEM	CMD-C2D-C1D	2.23	128.43	125.04
4	B	150	HEM	CAD-C3D-C4D	2.22	128.54	124.66
3	E	142	FRU	C6-C5-C4	-2.22	109.73	115.09
4	S	150	HEM	C1D-C2D-C3D	-2.21	104.63	106.96
4	T	150	HEM	C3B-C2B-C1B	2.21	108.12	106.49
4	H	150	HEM	CBA-CAA-C2A	2.19	116.36	112.62
4	A	150	HEM	CHA-C4D-ND	2.18	127.07	124.38
4	C	150	HEM	C4A-C3A-C2A	2.18	108.51	107.00
4	C	150	HEM	CHC-C4B-NB	2.17	126.79	124.43
4	A	150	HEM	CHB-C1B-NB	2.15	127.04	124.38
4	D	150	HEM	O2D-CGD-CBD	2.13	120.87	114.03
4	E	150	HEM	C4B-CHC-C1C	2.13	125.37	122.56
4	B	150	HEM	C3B-C2B-C1B	2.12	108.06	106.49
4	D	150	HEM	O1D-CGD-CBD	-2.12	116.26	123.08
4	E	150	HEM	C4A-C3A-C2A	2.12	108.47	107.00
4	C	150	HEM	CMA-C3A-C4A	-2.11	125.22	128.46
4	S	150	HEM	O2A-CGA-CBA	2.09	120.75	114.03
4	C	150	HEM	CHA-C4D-ND	2.09	126.97	124.38
4	C	150	HEM	C2B-C1B-NB	-2.08	107.37	109.84
4	B	150	HEM	C3D-C4D-ND	-2.07	107.86	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	150	HEM	C3C-C4C-NC	-2.07	107.03	110.94
4	F	150	HEM	CHC-C4B-C3B	2.05	127.71	124.57
4	G	150	HEM	CHA-C4D-ND	2.03	126.89	124.38
4	S	150	HEM	O1D-CGD-CBD	-2.02	116.58	123.08
4	B	150	HEM	CMC-C2C-C3C	2.02	128.46	124.68
4	H	150	HEM	C2D-C1D-ND	-2.02	107.47	109.88
4	F	150	HEM	C2C-C3C-C4C	2.01	108.30	106.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	142	FRU	C2

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	150	HEM	C2B-C3B-CAB-CBB
4	D	150	HEM	C2D-C3D-CAD-CBD
4	E	150	HEM	C2B-C3B-CAB-CBB
4	G	150	HEM	C2A-CAA-CBA-CGA
4	H	150	HEM	C1A-C2A-CAA-CBA
4	H	150	HEM	C3A-C2A-CAA-CBA
4	T	150	HEM	C2B-C3B-CAB-CBB
4	T	150	HEM	C4B-C3B-CAB-CBB
4	D	150	HEM	C4D-C3D-CAD-CBD
6	T	147	GLC	O5-C5-C6-O6
4	T	150	HEM	C2A-CAA-CBA-CGA
4	H	150	HEM	C3D-CAD-CBD-CGD
6	T	147	GLC	C4-C5-C6-O6
4	D	150	HEM	C3D-CAD-CBD-CGD
4	H	150	HEM	C2D-C3D-CAD-CBD
4	H	150	HEM	C4D-C3D-CAD-CBD
4	A	150	HEM	C4B-C3B-CAB-CBB
4	E	150	HEM	C4B-C3B-CAB-CBB
4	G	150	HEM	C2B-C3B-CAB-CBB
4	A	150	HEM	C2A-CAA-CBA-CGA
4	A	150	HEM	C3A-C2A-CAA-CBA
4	E	150	HEM	C1A-C2A-CAA-CBA
4	E	150	HEM	C3A-C2A-CAA-CBA
4	S	150	HEM	C1A-C2A-CAA-CBA
4	S	150	HEM	C3A-C2A-CAA-CBA
4	C	150	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
4	E	150	HEM	C2A-CAA-CBA-CGA
4	C	150	HEM	CAD-CBD-CGD-O2D
4	B	150	HEM	CAD-CBD-CGD-O1D
4	B	150	HEM	CAD-CBD-CGD-O2D
4	C	150	HEM	CAA-CBA-CGA-O2A
4	G	150	HEM	CAD-CBD-CGD-O2D
4	E	150	HEM	CAD-CBD-CGD-O2D
4	G	150	HEM	CAD-CBD-CGD-O1D
4	F	150	HEM	CAD-CBD-CGD-O1D
4	B	150	HEM	CAA-CBA-CGA-O1A
4	E	150	HEM	CAD-CBD-CGD-O1D
4	C	150	HEM	CAA-CBA-CGA-O1A
4	H	150	HEM	CAD-CBD-CGD-O1D
4	B	150	HEM	CAA-CBA-CGA-O2A
4	T	150	HEM	CAD-CBD-CGD-O1D
4	T	150	HEM	CAD-CBD-CGD-O2D
4	C	150	HEM	CAD-CBD-CGD-O1D
4	F	150	HEM	CAD-CBD-CGD-O2D
4	A	150	HEM	CAD-CBD-CGD-O2D
4	G	150	HEM	CAA-CBA-CGA-O2A
4	S	150	HEM	CAD-CBD-CGD-O2D
4	F	150	HEM	CAA-CBA-CGA-O2A
4	E	150	HEM	CAA-CBA-CGA-O2A
4	H	150	HEM	CAD-CBD-CGD-O2D
4	A	150	HEM	CAD-CBD-CGD-O1D
4	E	150	HEM	CAA-CBA-CGA-O1A
4	H	150	HEM	CAA-CBA-CGA-O1A
4	S	150	HEM	CAD-CBD-CGD-O1D
4	G	150	HEM	C4B-C3B-CAB-CBB
4	F	150	HEM	CAA-CBA-CGA-O1A
4	G	150	HEM	CAA-CBA-CGA-O1A
4	H	150	HEM	CAA-CBA-CGA-O2A
4	D	150	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

11 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	142	FRU	1	0
4	B	150	HEM	1	0
4	D	150	HEM	4	0
4	T	150	HEM	3	0

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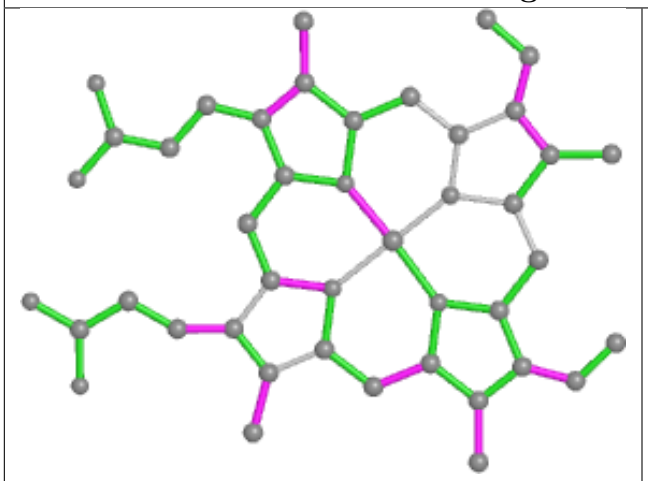
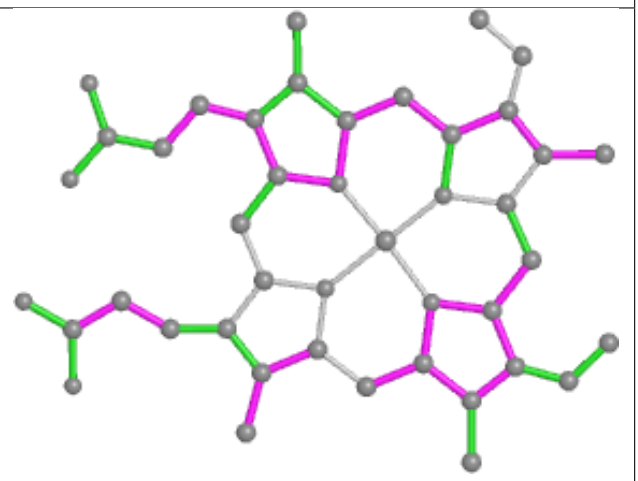
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	150	HEM	7	0
5	B	151	OXY	2	0
4	A	150	HEM	4	0
4	S	150	HEM	2	0
5	G	151	OXY	1	0
4	F	150	HEM	1	0
4	H	150	HEM	2	0

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.

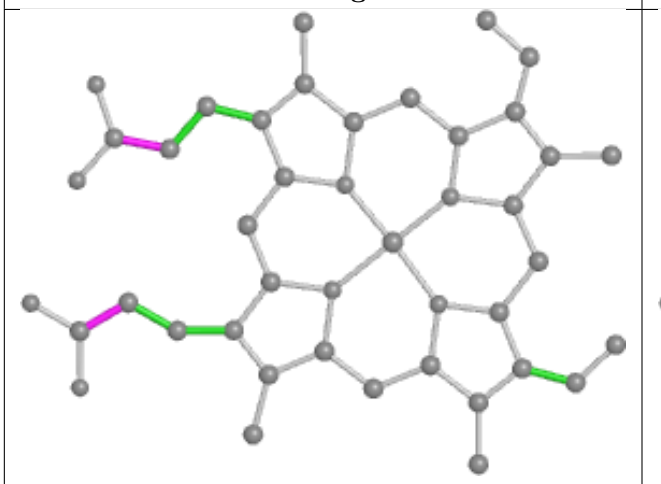
Ligand HEM B 150



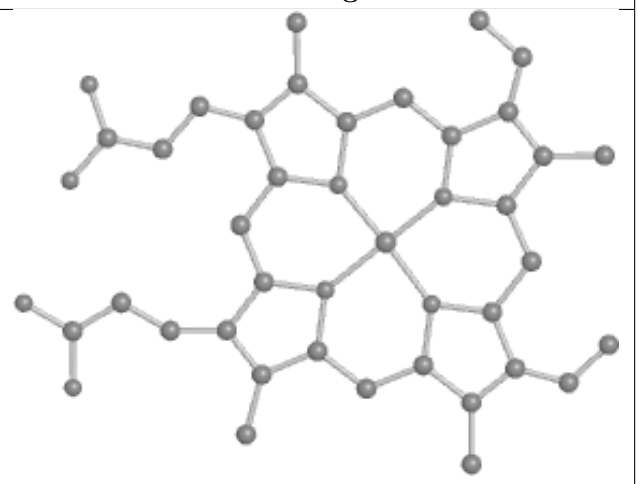
Bond lengths



Bond angles

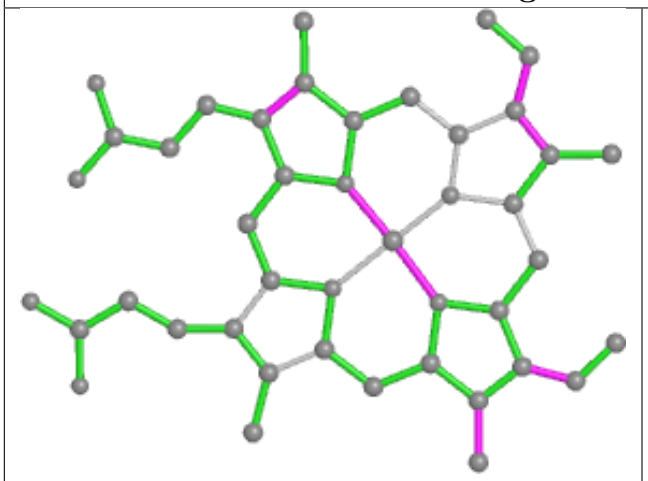


Torsions

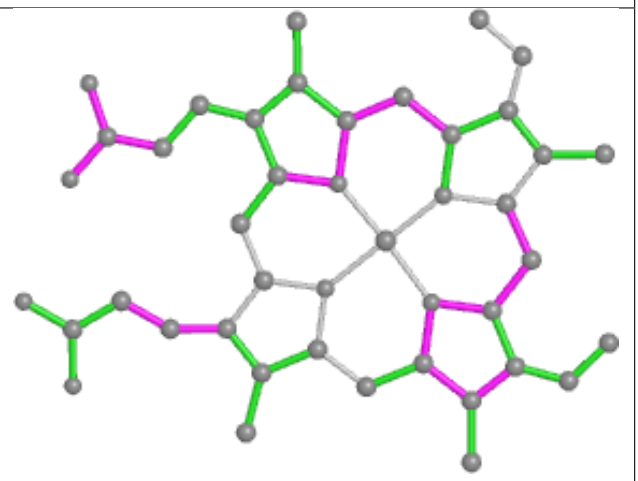


Rings

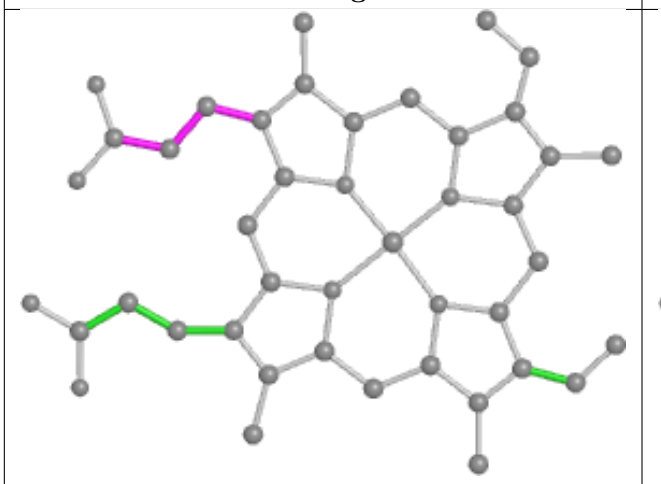
Ligand HEM D 150



Bond lengths



Bond angles



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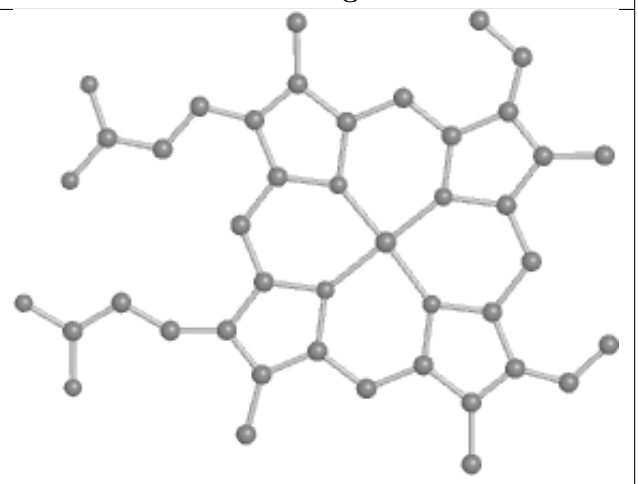
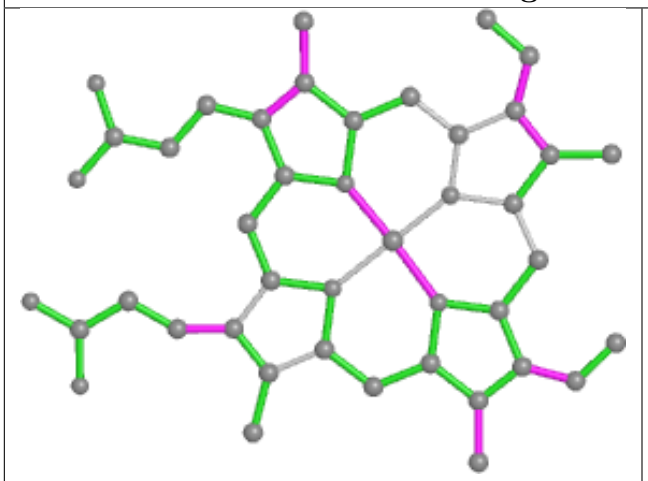
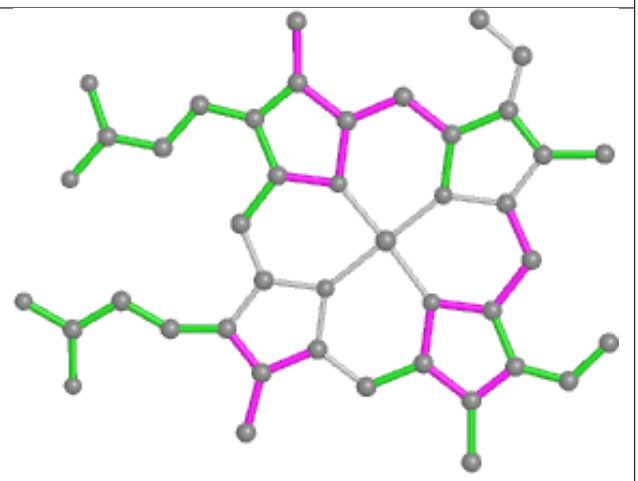


Rings

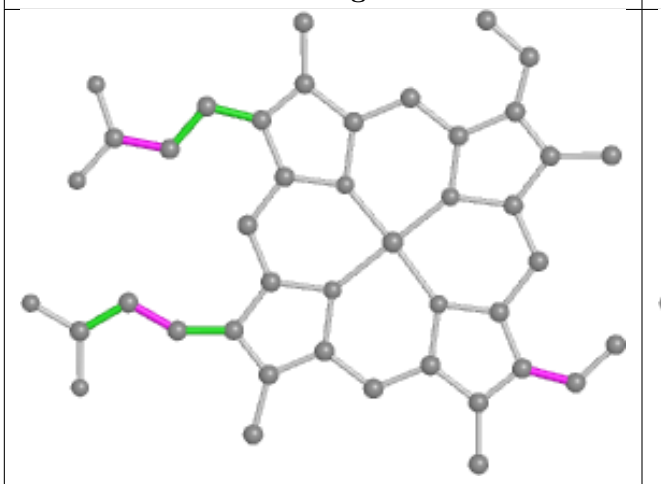
Ligand HEM T 150



Bond lengths



Bond angles



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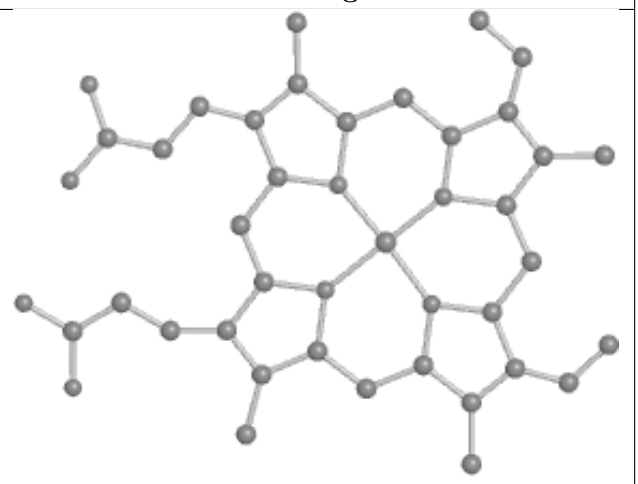
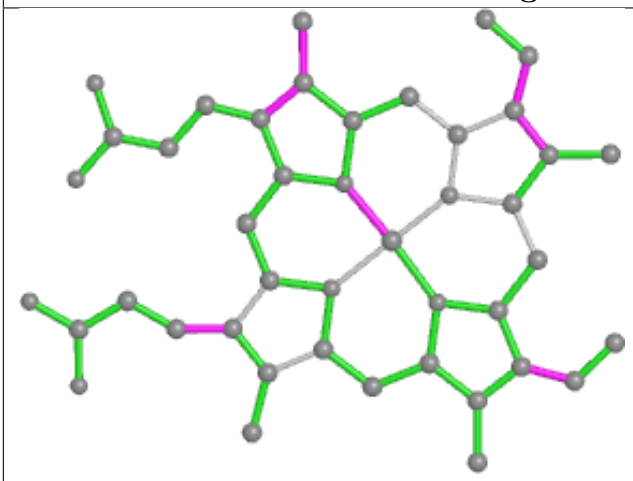
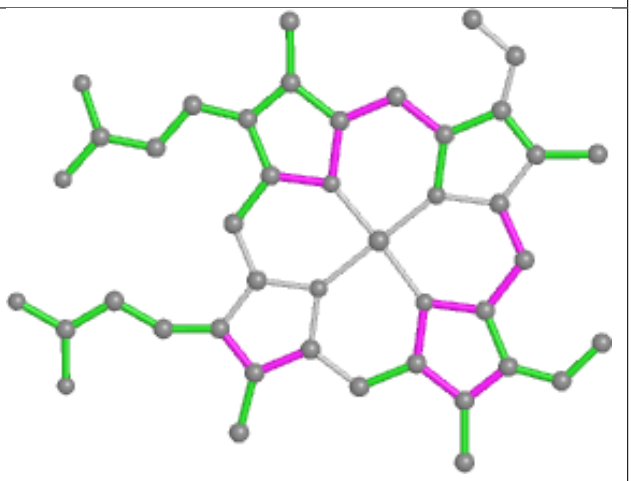


Rings

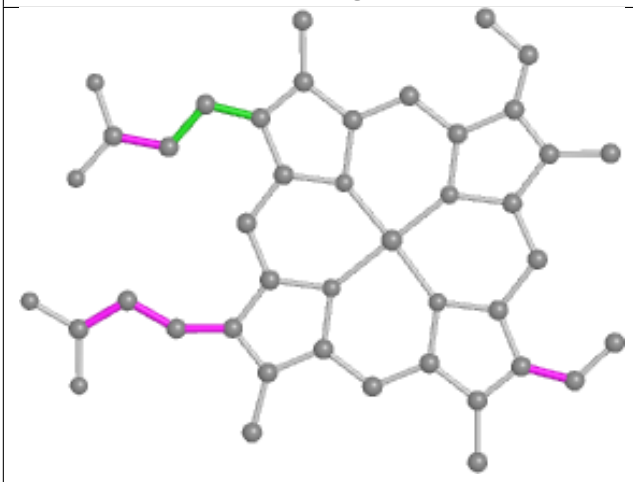
Ligand HEM E 150



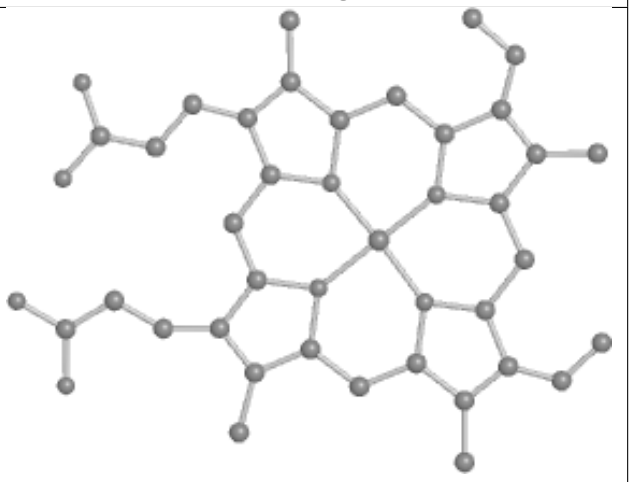
Bond lengths



Bond angles

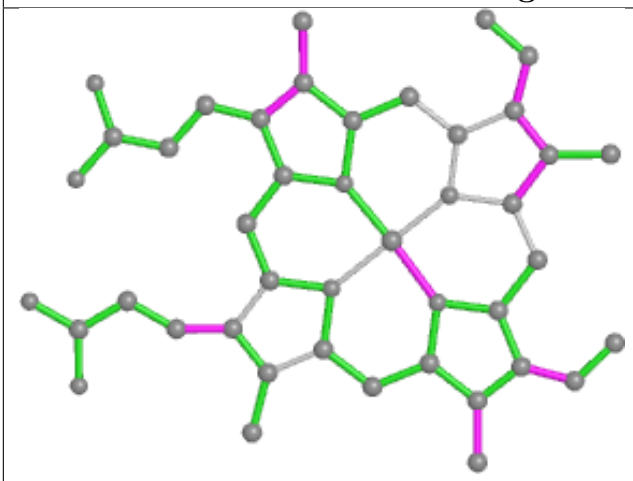


Torsions

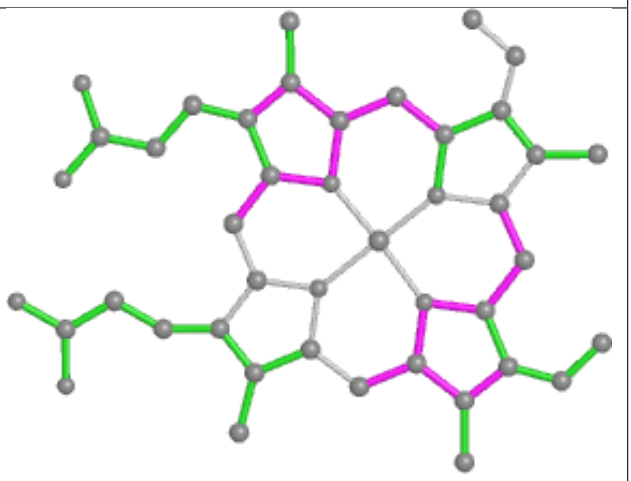


Rings

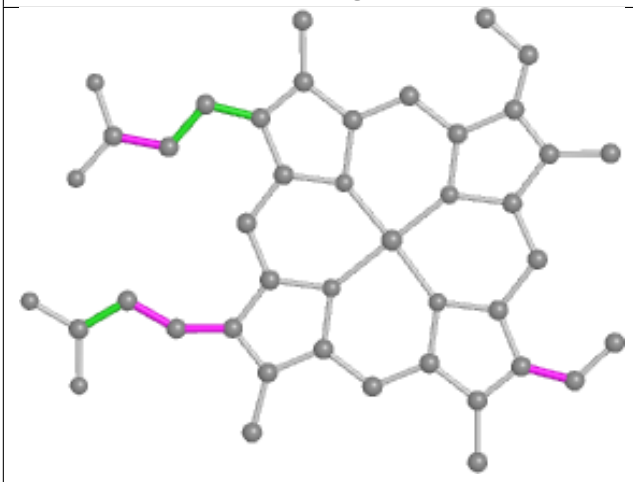
Ligand HEM A 150



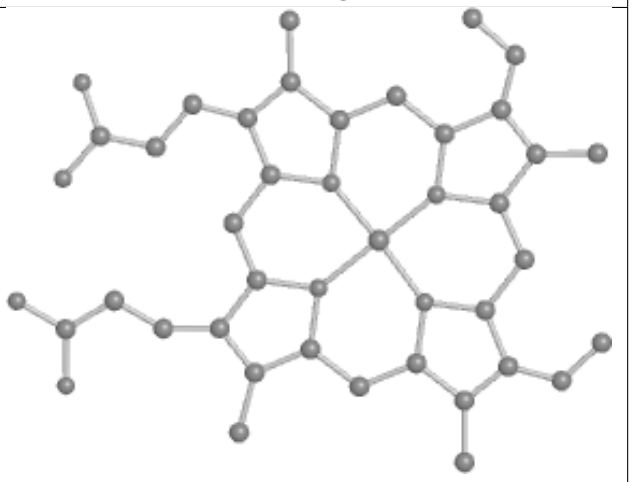
Bond lengths



Bond angles

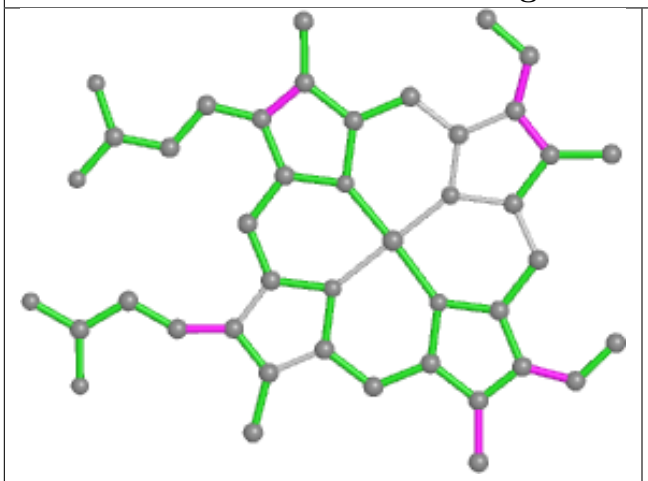


Torsions

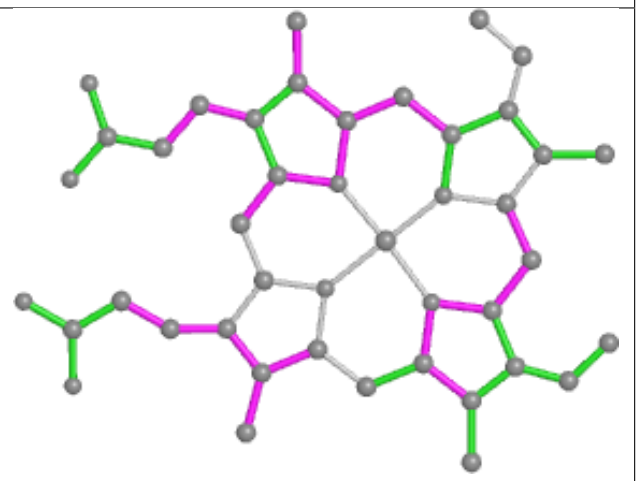


Rings

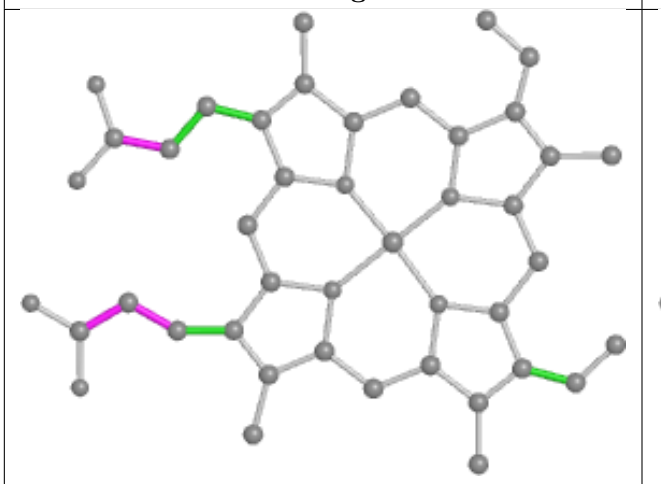
Ligand HEM C 150



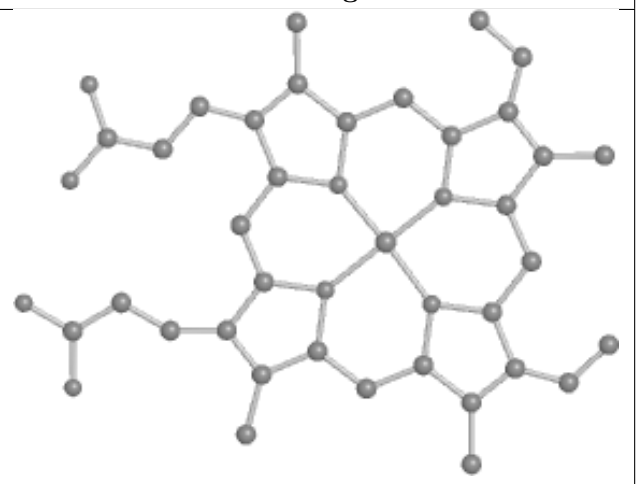
Bond lengths



Bond angles

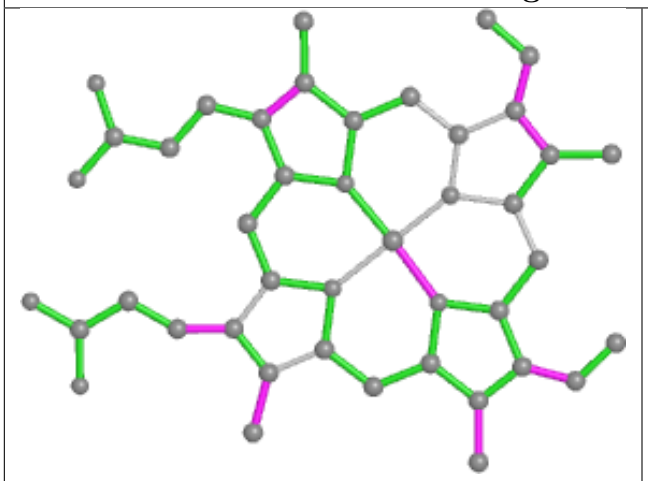


Torsions

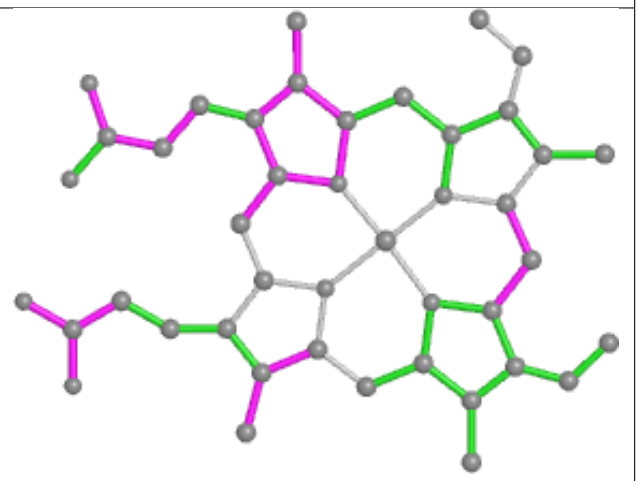


Rings

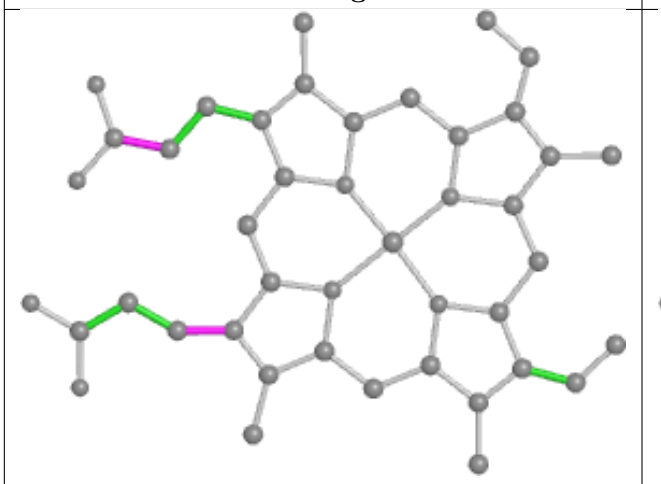
Ligand HEM S 150



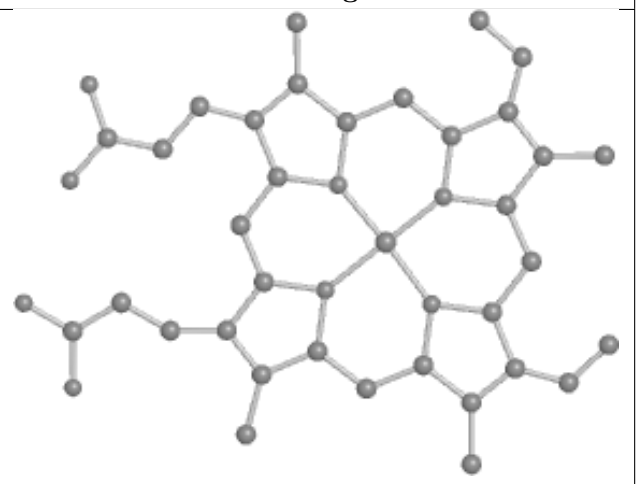
Bond lengths



Bond angles

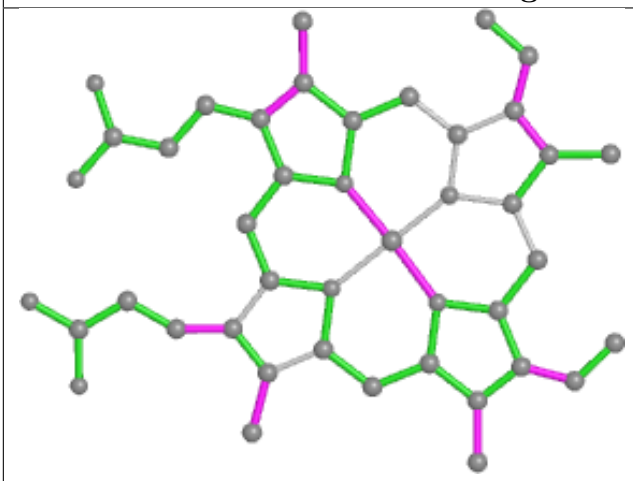


Torsions

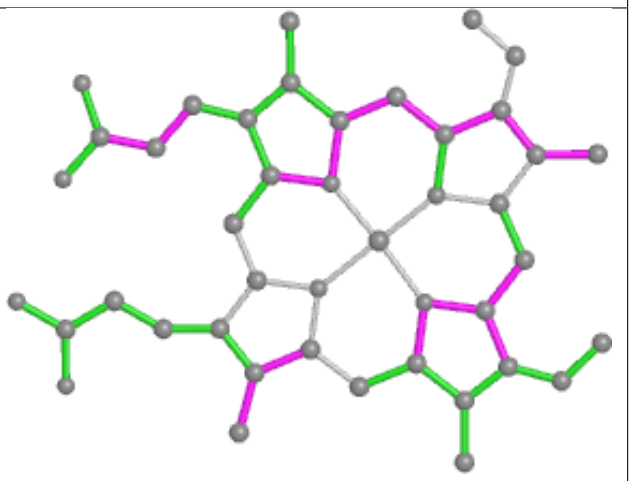


Rings

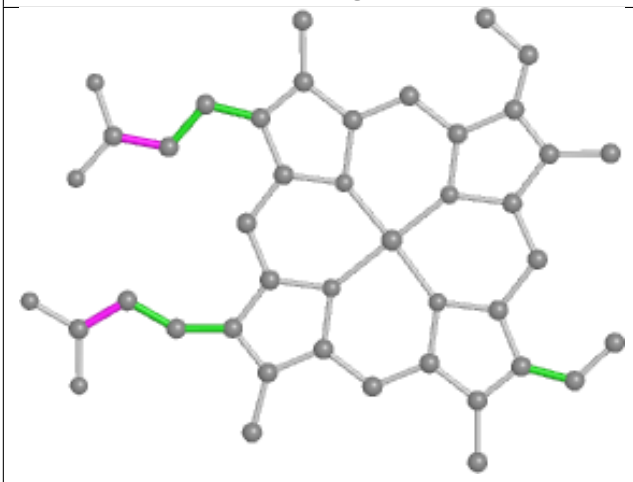
Ligand HEM F 150



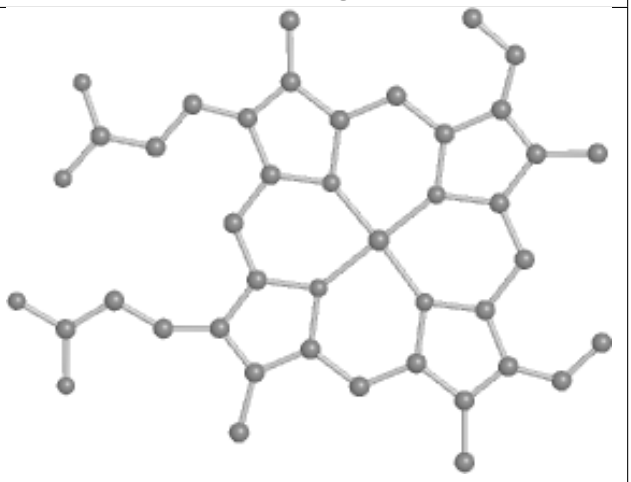
Bond lengths



Bond angles

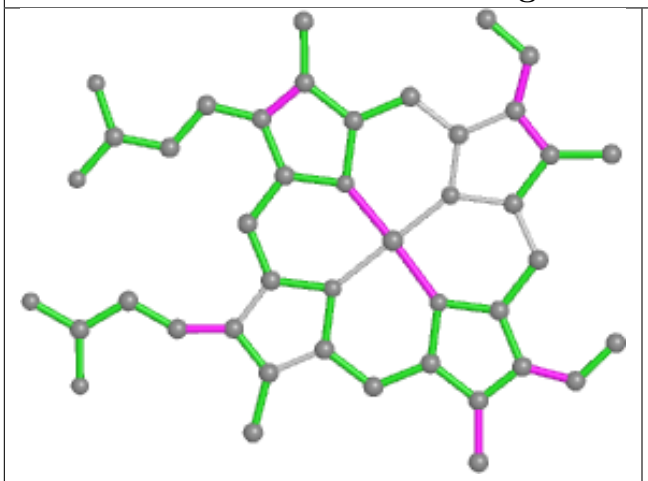


Torsions

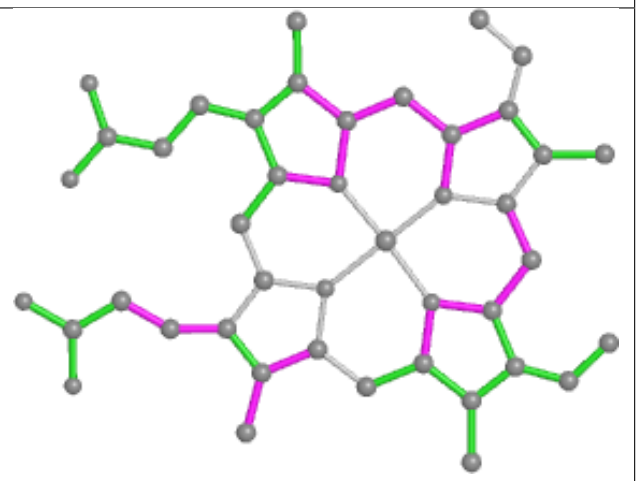


Rings

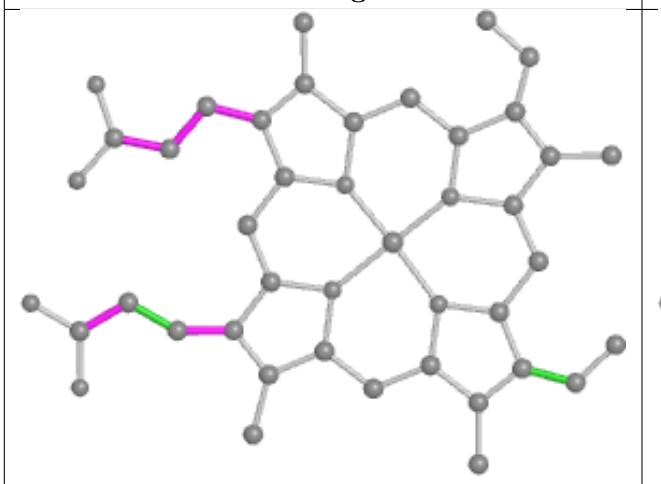
Ligand HEM H 150



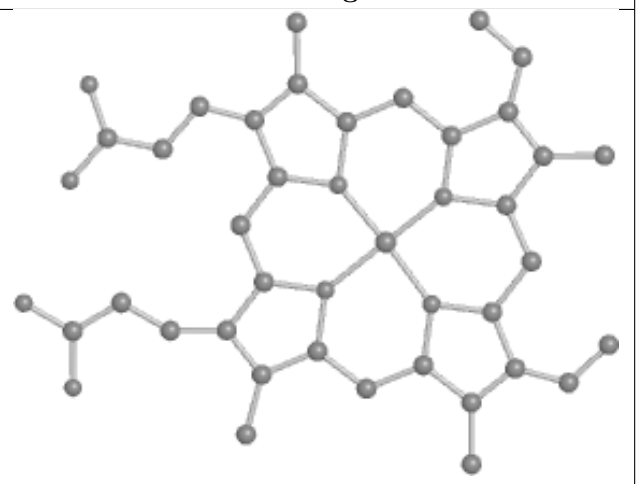
Bond lengths



Bond angles

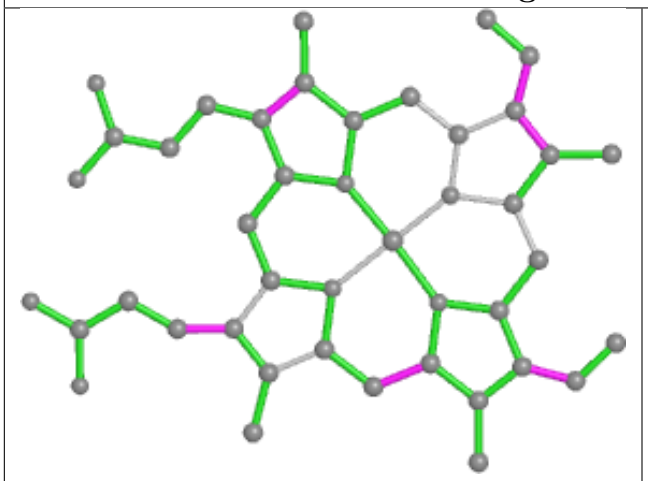


Torsions

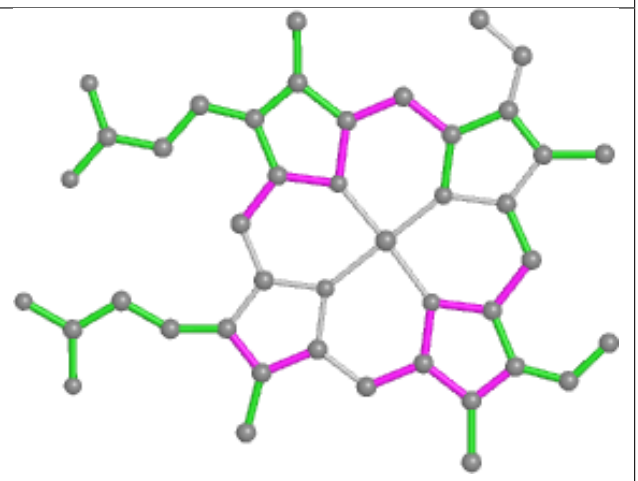


Rings

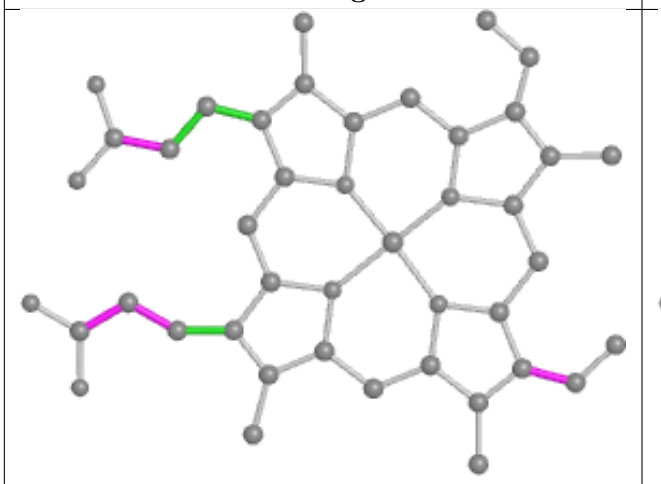
Ligand HEM G 150



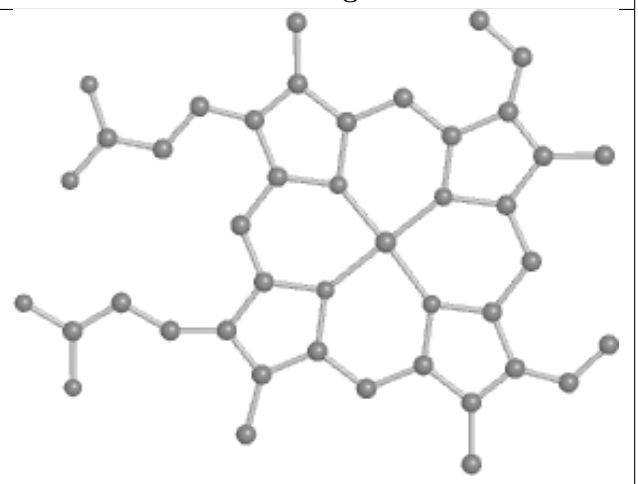
Bond lengths



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	141/141 (100%)	-0.06	2 (1%) 75 80	29, 43, 52, 59	0
1	C	141/141 (100%)	0.07	0 100 100	29, 44, 60, 66	0
1	E	141/141 (100%)	1.71	50 (35%) 0 0	51, 83, 110, 117	0
1	G	141/141 (100%)	0.57	13 (9%) 9 12	36, 60, 86, 94	0
1	S	141/141 (100%)	0.67	18 (12%) 3 5	39, 63, 74, 78	0
2	B	146/146 (100%)	0.05	4 (2%) 54 62	25, 42, 57, 72	0
2	D	146/146 (100%)	0.24	3 (2%) 63 70	30, 49, 59, 62	0
2	F	146/146 (100%)	0.45	8 (5%) 25 31	31, 55, 77, 80	0
2	H	146/146 (100%)	1.29	40 (27%) 0 0	45, 77, 85, 88	0
2	T	146/146 (100%)	1.02	23 (15%) 2 2	46, 77, 94, 105	0
All	All	1435/1435 (100%)	0.60	161 (11%) 5 7	25, 55, 89, 117	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	4	PRO	8.7
1	E	1	VAL	7.2
1	E	5	ALA	6.1
1	E	48	LEU	5.2
1	E	8	THR	4.8
2	T	56	GLY	4.8
2	H	47	ASP	4.7
2	H	77	HIS	4.7
2	T	4	THR	4.7
1	S	141	ARG	4.7
1	E	53	ALA	4.6
1	G	1	VAL	4.6
1	E	15	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	19	ALA	4.5
1	E	86	LEU	4.4
1	E	72	HIS	4.4
1	E	6	ASP	4.3
1	E	77	PRO	4.3
1	E	91	LEU	4.3
2	T	5	PRO	4.3
1	G	75	ASP	4.2
1	E	75	ASP	4.2
2	T	94	ASP	4.1
2	H	141	LEU	4.1
2	H	146	HIS	4.1
2	T	2	HIS	4.1
2	T	141	LEU	4.0
1	S	45	HIS	3.9
1	E	2	LEU	3.9
2	H	88	LEU	3.8
2	H	2	HIS	3.8
1	E	92	ARG	3.7
2	H	50	THR	3.7
1	E	45	HIS	3.7
1	E	71	ALA	3.6
2	D	141	LEU	3.6
1	E	73	VAL	3.6
1	E	89	HIS	3.6
2	B	2	HIS	3.6
2	F	49	SER	3.6
2	T	79	ASP	3.5
1	E	55	VAL	3.5
2	H	120	LYS	3.5
1	E	78	ASN	3.5
1	E	18	GLY	3.5
2	T	50	THR	3.5
2	T	143	HIS	3.5
1	G	4	PRO	3.4
2	H	28	LEU	3.4
2	H	49	SER	3.4
1	E	82	ALA	3.4
1	E	3	SER	3.4
1	G	140	TYR	3.4
1	E	80	LEU	3.4
2	F	50	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	141	ARG	3.3
2	H	97	HIS	3.3
1	S	71	ALA	3.2
1	E	47	ASP	3.2
1	E	13	ALA	3.2
2	T	83	GLY	3.2
1	S	75	ASP	3.1
1	G	8	THR	3.1
2	T	146	HIS	3.1
1	A	84	SER	3.1
1	E	11	LYS	3.1
1	E	140	TYR	3.0
1	E	90	LYS	3.0
2	H	143	HIS	3.0
1	E	44	PRO	3.0
2	H	81	LEU	3.0
2	F	2	HIS	3.0
2	T	78	LEU	3.0
2	F	5	PRO	3.0
2	H	13	ALA	2.9
1	E	116	GLU	2.9
2	T	97	HIS	2.9
1	E	139	LYS	2.9
1	G	85	ASP	2.9
1	E	64	ASP	2.9
1	S	1	VAL	2.9
2	T	55	MET	2.8
1	S	140	TYR	2.8
2	H	85	PHE	2.8
2	F	1	VAL	2.8
1	S	19	ALA	2.8
2	H	79	ASP	2.8
2	H	12	THR	2.7
2	H	48	LEU	2.7
2	H	139	ASN	2.7
1	S	18	GLY	2.7
2	H	98	VAL	2.7
1	G	5	ALA	2.7
2	H	56	GLY	2.7
2	H	9	SER	2.7
2	T	44	SER	2.7
1	E	74	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	T	10	ALA	2.6
1	E	43	PHE	2.6
2	H	42	PHE	2.6
2	H	58	PRO	2.6
1	G	69	ALA	2.6
2	H	90	GLU	2.6
2	H	86	ALA	2.6
1	S	73	VAL	2.5
2	H	36	PRO	2.5
1	E	69	ALA	2.5
1	S	115	ALA	2.5
2	T	144	LYS	2.5
2	H	25	GLY	2.5
2	T	95	LYS	2.5
1	G	90	LYS	2.5
2	H	96	LEU	2.5
1	E	10	VAL	2.4
2	T	11	VAL	2.4
2	H	91	LEU	2.4
1	E	132	VAL	2.4
1	S	72	HIS	2.4
1	E	138	SER	2.4
1	S	50	HIS	2.4
1	E	136	LEU	2.4
2	H	52	ASP	2.4
2	H	76	ALA	2.4
2	T	145	TYR	2.4
1	E	88	ALA	2.4
1	E	120	ALA	2.4
2	H	43	GLU	2.4
1	G	138	SER	2.4
2	H	6	GLU	2.3
2	T	1	VAL	2.3
2	B	5	PRO	2.3
2	F	120	LYS	2.3
1	E	87	HIS	2.3
1	A	141	ARG	2.3
2	H	59	LYS	2.3
2	T	88	LEU	2.3
2	H	38	THR	2.2
1	S	78	ASN	2.2
2	D	11	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	76	MET	2.2
1	S	51	GLY	2.2
2	H	22	GLU	2.2
2	H	5	PRO	2.2
1	E	111	ALA	2.2
1	S	109	LEU	2.2
2	H	60	VAL	2.1
2	T	140	ALA	2.1
2	F	47	ASP	2.1
2	B	60	VAL	2.1
2	F	146	HIS	2.1
1	S	11	LYS	2.1
2	H	1	VAL	2.1
1	E	93	VAL	2.1
1	E	46	PHE	2.1
1	G	3	SER	2.1
1	G	89	HIS	2.1
1	G	15	GLY	2.0
1	S	15	GLY	2.0
1	S	8	THR	2.0
2	B	49	SER	2.0
2	D	87	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FRU	E	142	11/12	0.59	0.29	72,75,75,76	0

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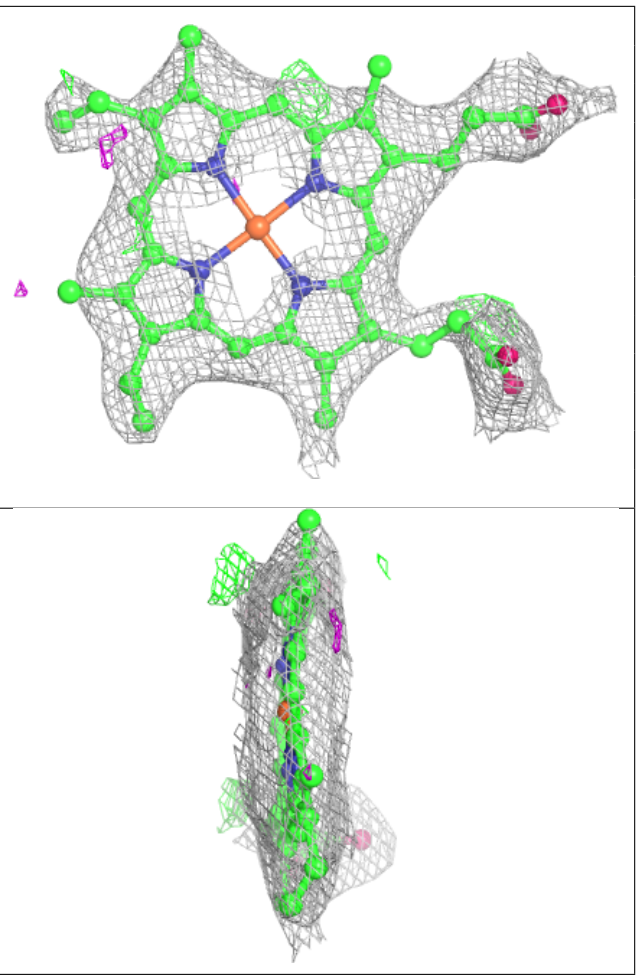
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GLC	B	147	12/12	0.62	0.30	67,70,72,72	0
3	FRU	A	142	11/12	0.65	0.26	64,68,69,69	0
6	GLC	T	147	12/12	0.66	0.37	100,102,102,102	0
6	GLC	C	142	12/12	0.79	0.21	74,76,77,77	0
7	PO4	G	142	5/5	0.79	0.32	96,96,97,97	0
4	HEM	H	150	43/43	0.83	0.20	65,69,72,74	0
4	HEM	E	150	43/43	0.84	0.20	71,73,77,79	0
4	HEM	S	150	43/43	0.88	0.19	37,47,56,57	0
4	HEM	T	150	43/43	0.89	0.19	74,77,80,80	0
4	HEM	G	150	43/43	0.91	0.15	40,50,56,59	0
4	HEM	D	150	43/43	0.92	0.15	38,46,53,57	0
4	HEM	C	150	43/43	0.92	0.18	22,38,52,58	0
4	HEM	F	150	43/43	0.94	0.15	35,40,52,59	0
5	OXY	E	151	2/2	0.94	0.23	76,76,76,76	0
4	HEM	A	150	43/43	0.94	0.14	21,38,42,44	0
4	HEM	B	150	43/43	0.96	0.13	20,31,45,50	0
5	OXY	F	151	2/2	0.97	0.16	46,46,46,49	0
5	OXY	T	151	2/2	0.97	0.14	73,73,73,74	0
5	OXY	C	151	2/2	0.97	0.19	37,37,37,44	0
5	OXY	S	151	2/2	0.98	0.12	52,52,52,56	0
5	OXY	B	151	2/2	0.98	0.20	33,33,33,40	0
5	OXY	D	151	2/2	0.98	0.08	45,45,45,48	0
5	OXY	A	151	2/2	0.99	0.14	40,40,40,47	0
5	OXY	G	151	2/2	0.99	0.18	50,50,50,53	0
5	OXY	H	151	2/2	0.99	0.07	70,70,70,71	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.

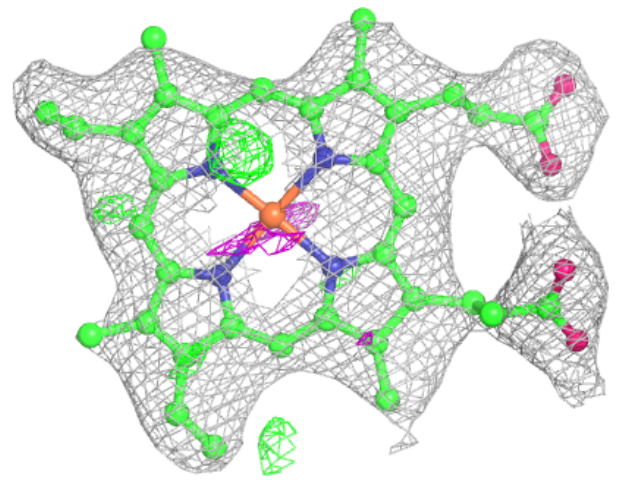
Electron density around HEM H 150:

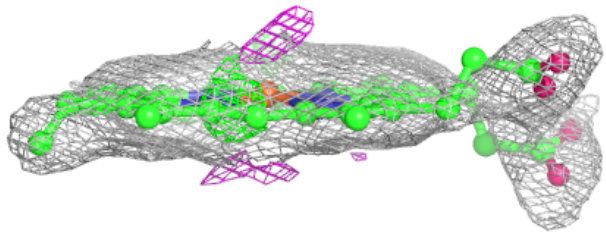
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

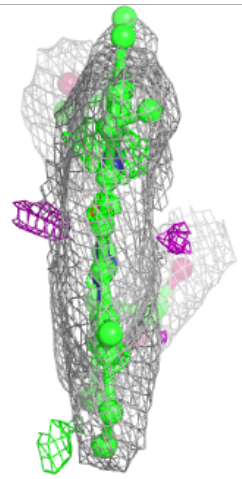


Electron density around HEM E 150:

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

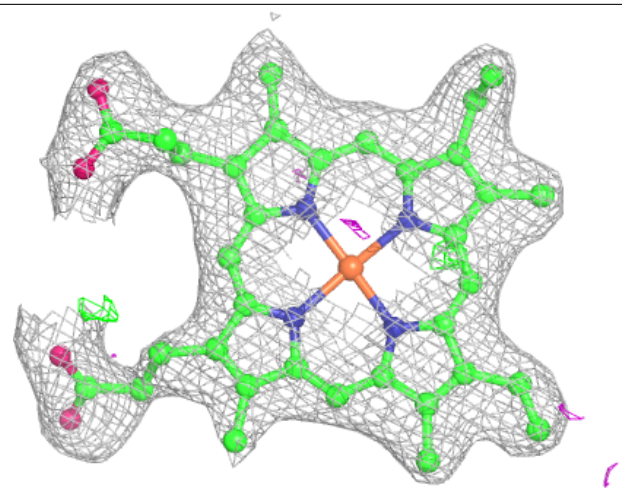


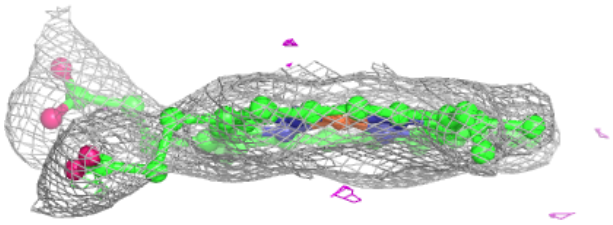


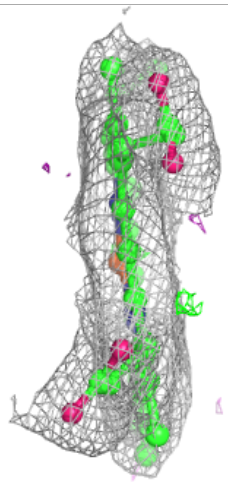


Electron density around HEM S 150:

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

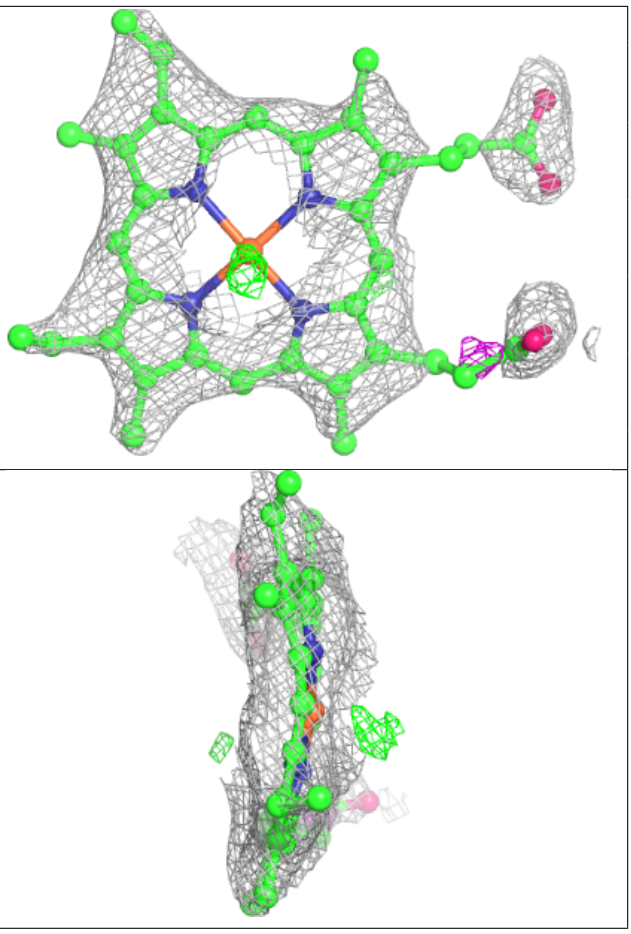


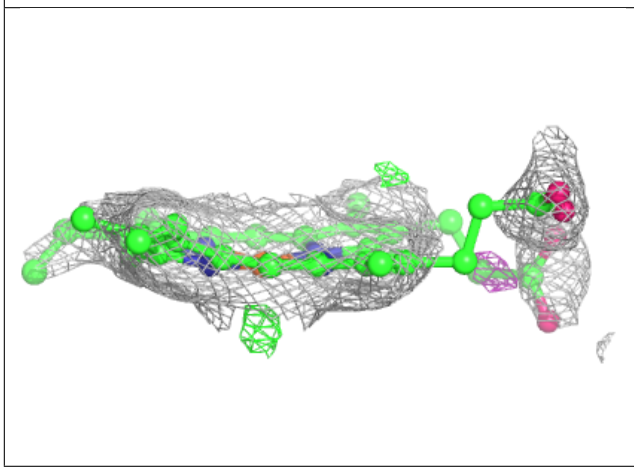




Electron density around HEM T 150:

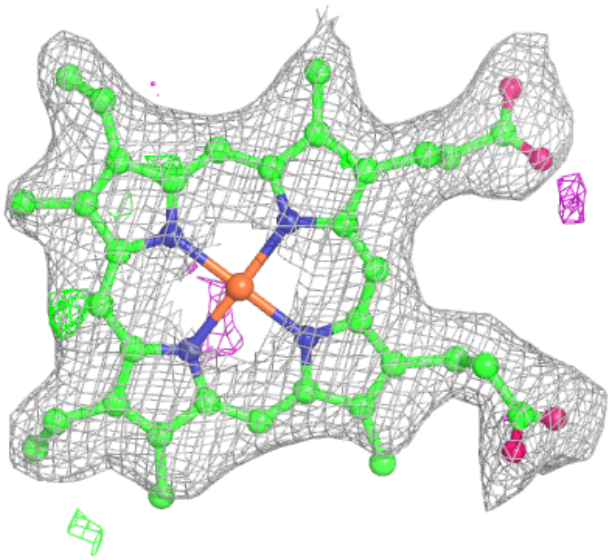
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

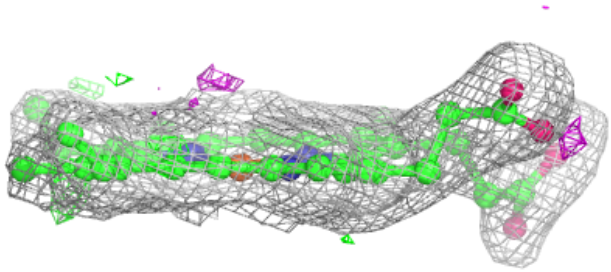


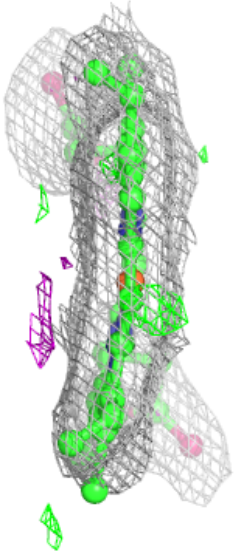


Electron density around HEM G 150:

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

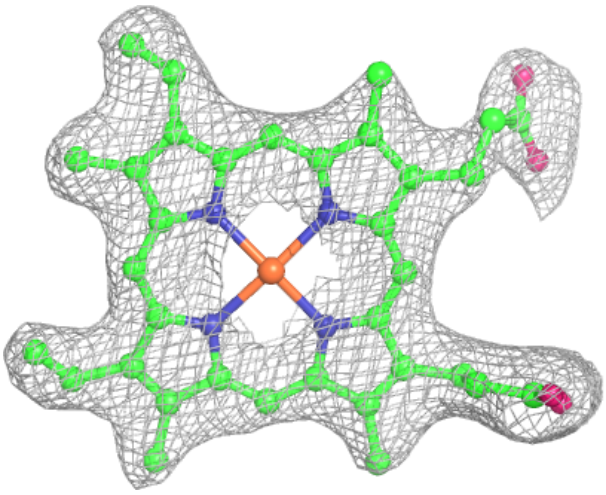


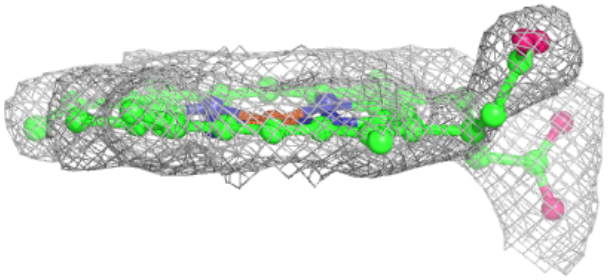


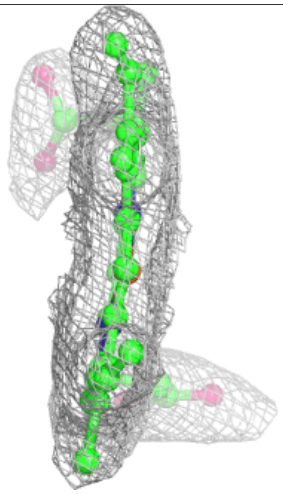


Electron density around HEM D 150:

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

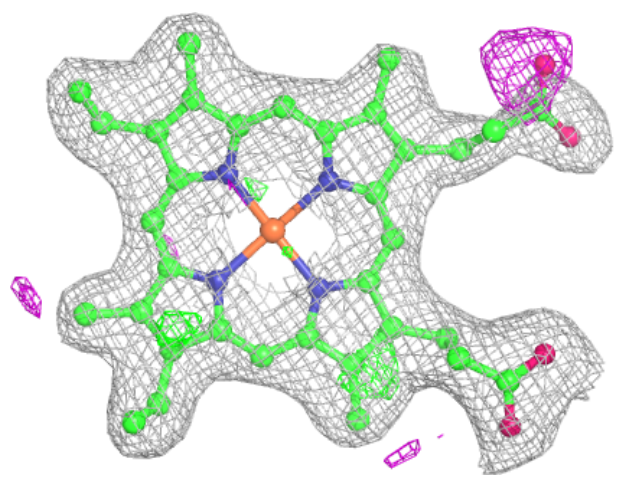


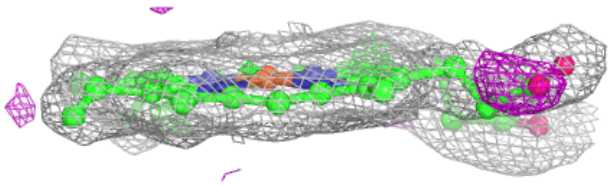


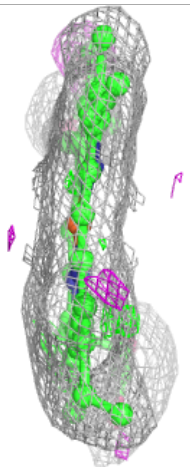


Electron density around HEM C 150:

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

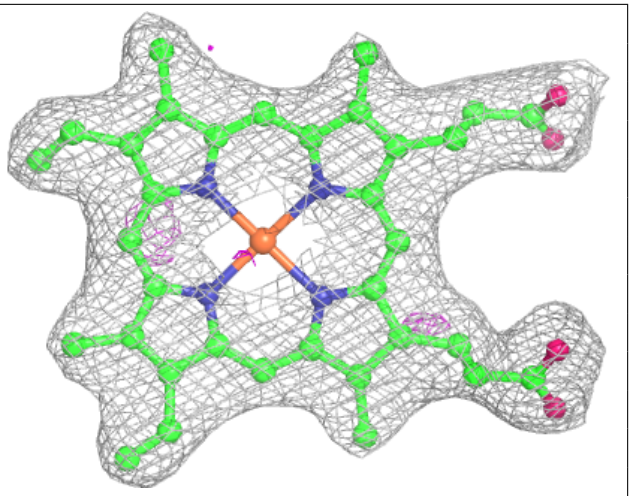


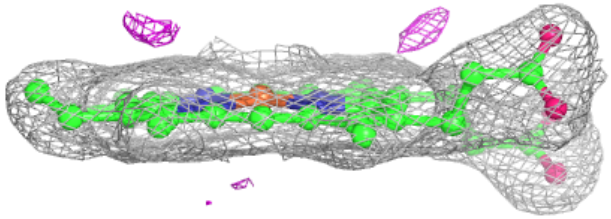


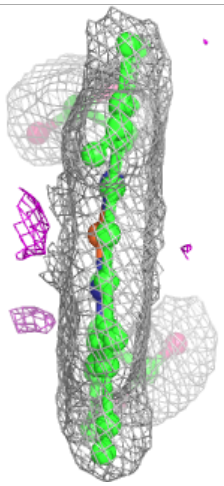


Electron density around HEM F 150:

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

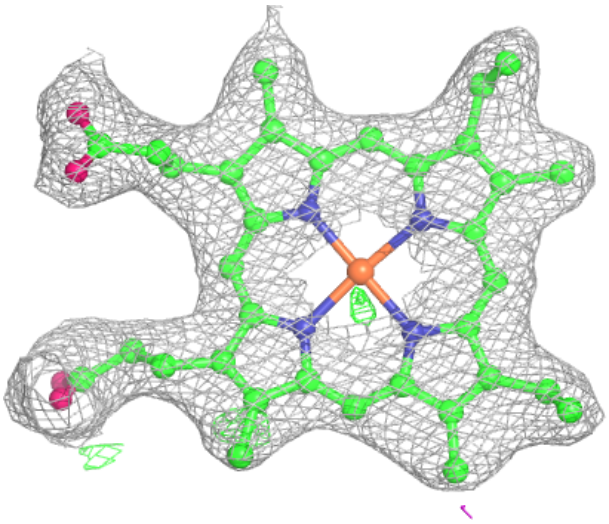


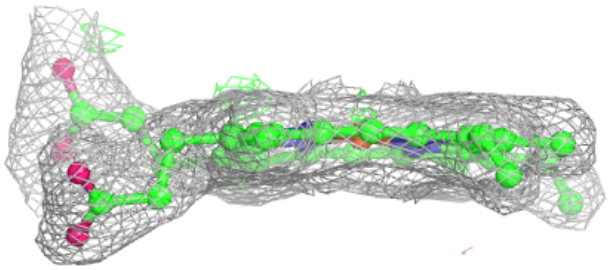


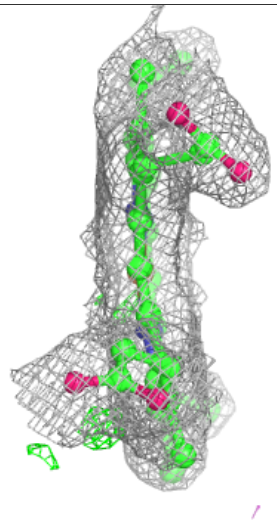


Electron density around HEM A 150:

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

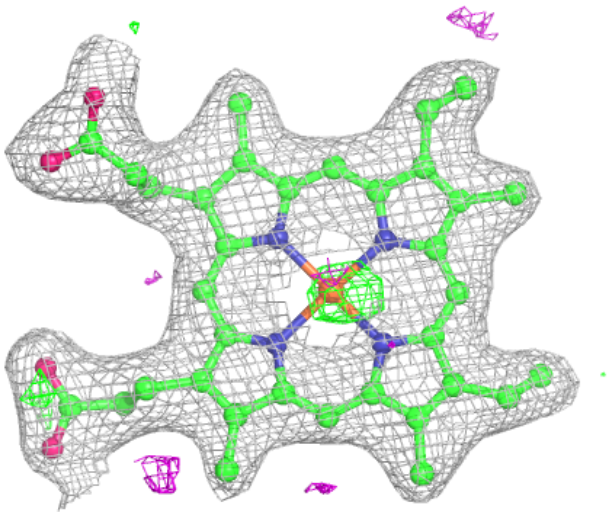


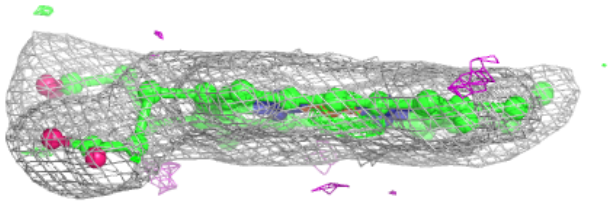


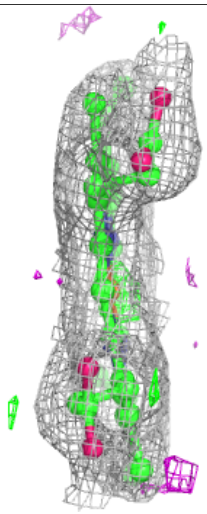


Electron density around HEM B 150:

$2mF_o$-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.