Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 04:52 PM EDT

PDB ID	:	1P2H
Title	:	H61M mutant of flavocytochrome c3
Authors	:	Rothery, E.L.; Mowat, C.G.; Miles, C.S.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on	:	2003-04-15
Resolution	:	2.10 Å(reported)

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

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

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

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

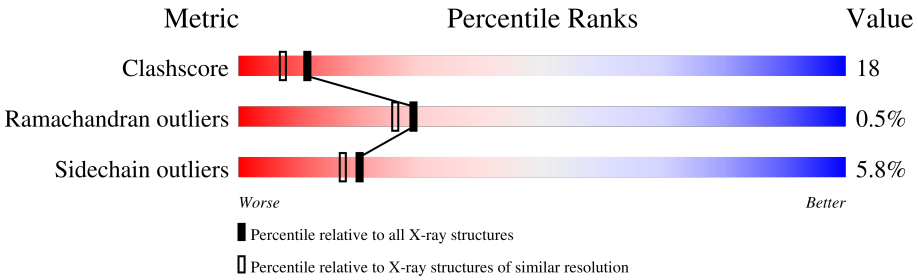
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	571	61% 31% 7% ••

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
5	TEO	A	806	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4994 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 flavocytochrome c3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	568	4178	2592	733	827	26	0	0	0

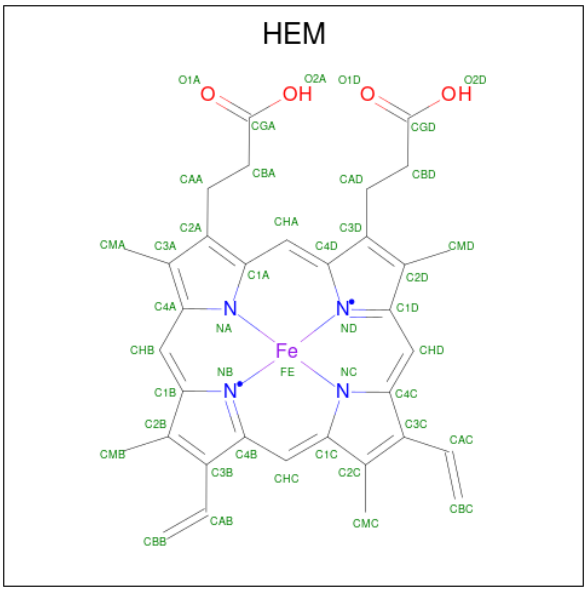
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MET	HIS	engineered mutation	UNP Q02469

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

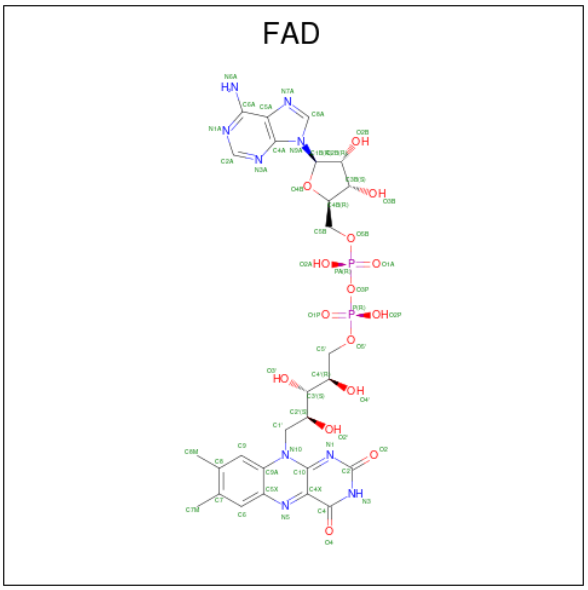
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



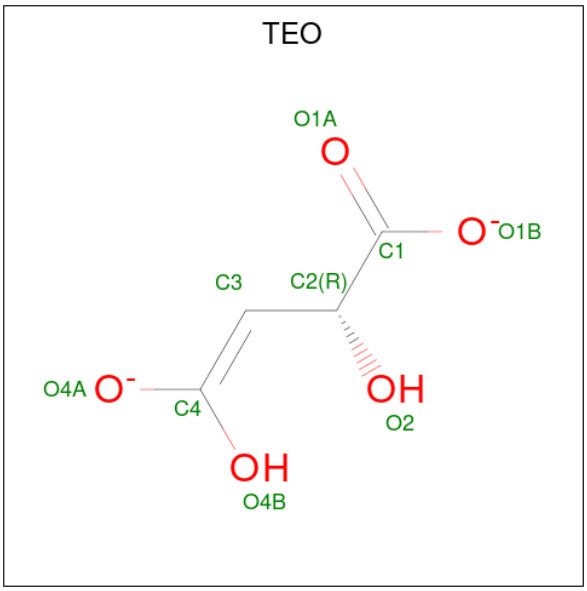
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is MALATE LIKE INTERMEDIATE (three-letter code: TEO) (formula: $C_4H_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 4 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	581	Total O 581 581	0	0

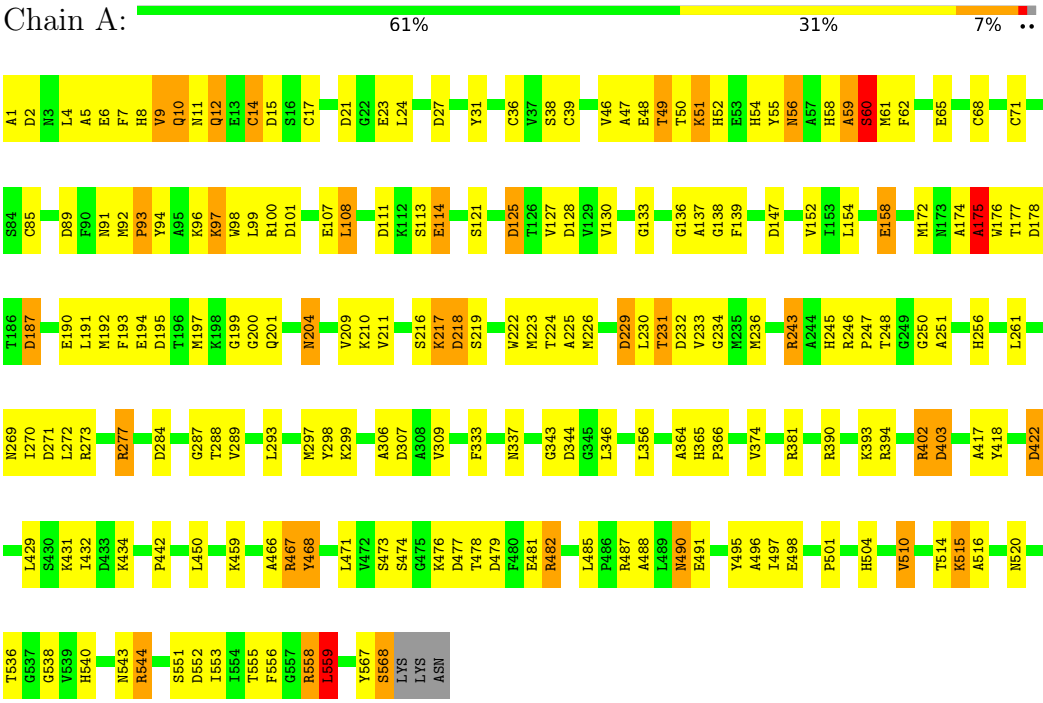
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

- Molecule 1: flavocytochrome c3

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.69Å 87.29Å 76.99Å 90.00° 104.35° 90.00°	Depositor
Resolution (Å)	17.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (17.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4994	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, TEO, FAD, NA

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	0.91	1/4247 (0.0%)	2.00	117/5750 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	TRP	N-CA	-5.02	1.36	1.46

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	390	ARG	NE-CZ-NH1	21.44	131.02	120.30
1	A	175	ALA	C-N-CA	20.05	171.81	121.70
1	A	390	ARG	NE-CZ-NH2	-19.66	110.47	120.30
1	A	467	ARG	CD-NE-CZ	14.84	144.38	123.60
1	A	403	ASP	CB-CG-OD1	14.49	131.34	118.30
1	A	277	ARG	NE-CZ-NH1	-12.89	113.86	120.30
1	A	175	ALA	N-CA-CB	11.55	126.27	110.10
1	A	147	ASP	CB-CG-OD1	11.14	128.32	118.30
1	A	12	GLN	CA-CB-CG	10.00	135.40	113.40
1	A	273	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	A	125	ASP	CB-CG-OD2	9.83	127.15	118.30
1	A	31	TYR	CB-CG-CD2	-9.83	115.10	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	307	ASP	CB-CG-OD1	-9.76	109.52	118.30
1	A	100	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	A	176	TRP	N-CA-CB	9.05	126.90	110.60
1	A	552	ASP	CB-CG-OD2	8.94	126.35	118.30
1	A	482	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	495	TYR	CB-CG-CD2	8.70	126.22	121.00
1	A	487	ARG	NE-CZ-NH2	8.65	124.62	120.30
1	A	510	VAL	CB-CA-C	-8.56	95.14	111.40
1	A	96	LYS	N-CA-CB	8.42	125.76	110.60
1	A	381	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	A	394	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	A	544	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	A	243	ARG	NE-CZ-NH2	8.01	124.31	120.30
1	A	284	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	A	31	TYR	CB-CG-CD1	7.83	125.70	121.00
1	A	298	TYR	CB-CG-CD2	-7.80	116.32	121.00
1	A	394	ARG	CD-NE-CZ	7.79	134.50	123.60
1	A	94	TYR	CB-CG-CD2	-7.71	116.37	121.00
1	A	487	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	A	423	ASP	CB-CG-OD2	7.57	125.11	118.30
1	A	187	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	426	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	125	ASP	CB-CG-OD1	-7.40	111.64	118.30
1	A	15	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	A	510	VAL	CG1-CB-CG2	7.31	122.60	110.90
1	A	2	ASP	CB-CG-OD1	-7.23	111.79	118.30
1	A	100	ARG	CD-NE-CZ	7.18	133.65	123.60
1	A	284	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	559	LEU	CA-CB-CG	7.09	131.61	115.30
1	A	187	ASP	CB-CG-OD2	-6.97	112.02	118.30
1	A	180	GLN	CG-CD-OE1	-6.86	107.87	121.60
1	A	422	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	93	PRO	C-N-CA	6.81	138.74	121.70
1	A	510	VAL	N-CA-CB	6.80	126.47	111.50
1	A	38	SER	O-C-N	-6.65	112.06	122.70
1	A	243	ARG	CD-NE-CZ	6.56	132.79	123.60
1	A	229	ASP	CB-CG-OD1	6.54	124.18	118.30
1	A	403	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	60	SER	N-CA-C	6.32	128.07	111.00
1	A	14	CYS	CA-CB-SG	-6.25	102.75	114.00
1	A	94	TYR	CB-CG-CD1	6.06	124.64	121.00
1	A	231	THR	CA-CB-OG1	6.06	121.73	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	12	GLN	CB-CA-C	5.97	122.34	110.40
1	A	558	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	51	LYS	CA-C-O	5.85	132.38	120.10
1	A	467	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	A	293	LEU	CB-CG-CD1	-5.82	101.10	111.00
1	A	552	ASP	OD1-CG-OD2	-5.80	112.28	123.30
1	A	147	ASP	OD1-CG-OD2	-5.78	112.32	123.30
1	A	14	CYS	CB-CA-C	-5.77	98.85	110.40
1	A	277	ARG	NE-CZ-NH2	5.77	123.18	120.30
1	A	402	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	A	466	ALA	CA-C-N	5.75	129.84	117.20
1	A	498	GLU	OE1-CD-OE2	5.75	130.19	123.30
1	A	271	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	534	GLU	O-C-N	-5.69	113.59	122.70
1	A	211	VAL	CG1-CB-CG2	-5.66	101.84	110.90
1	A	364	ALA	N-CA-CB	5.66	118.02	110.10
1	A	231	THR	CA-CB-CG2	-5.62	104.53	112.40
1	A	130	VAL	O-C-N	5.61	131.68	122.70
1	A	59	ALA	C-N-CA	5.61	135.72	121.70
1	A	467	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	211	VAL	CA-CB-CG1	5.53	119.19	110.90
1	A	333	PHE	N-CA-CB	-5.52	100.66	110.60
1	A	536	THR	CA-CB-CG2	-5.50	104.70	112.40
1	A	495	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	A	298	TYR	CB-CG-CD1	5.42	124.25	121.00
1	A	111	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	51	LYS	C-N-CA	5.38	135.15	121.70
1	A	271	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	218	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	556	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	A	468	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	A	178	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	434	LYS	CA-C-O	-5.32	108.93	120.10
1	A	426	ARG	CD-NE-CZ	5.32	131.04	123.60
1	A	114	GLU	CA-CB-CG	5.31	125.08	113.40
1	A	195	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	488	ALA	O-C-N	-5.30	114.22	122.70
1	A	175	ALA	CA-C-O	5.29	131.21	120.10
1	A	309	VAL	CA-CB-CG1	-5.28	102.98	110.90
1	A	79	MET	N-CA-CB	-5.27	101.12	110.60
1	A	236	MET	CG-SD-CE	5.27	108.62	100.20
1	A	158	GLU	OE1-CD-OE2	-5.26	116.98	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	482	ARG	NH1-CZ-NH2	5.26	125.18	119.40
1	A	97	LYS	N-CA-CB	-5.24	101.16	110.60
1	A	424	SER	CB-CA-C	5.23	120.04	110.10
1	A	536	THR	CA-CB-OG1	5.23	119.99	109.00
1	A	567	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	A	467	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	A	60	SER	CA-C-O	5.17	130.97	120.10
1	A	551	SER	CB-CA-C	5.17	119.93	110.10
1	A	287	GLY	O-C-N	-5.17	114.42	122.70
1	A	51	LYS	O-C-N	-5.15	114.45	122.70
1	A	434	LYS	CA-C-N	5.14	128.50	117.20
1	A	172	MET	CG-SD-CE	-5.10	92.04	100.20
1	A	176	TRP	CB-CA-C	5.10	120.60	110.40
1	A	559	LEU	N-CA-CB	5.08	120.56	110.40
1	A	108	LEU	CB-CG-CD1	-5.07	102.39	111.00
1	A	152	VAL	CA-CB-CG2	-5.07	103.30	110.90
1	A	488	ALA	CA-C-N	5.06	128.33	117.20
1	A	223	MET	CG-SD-CE	5.03	108.25	100.20
1	A	175	ALA	O-C-N	-5.01	114.68	122.70
1	A	568	SER	CA-C-O	-5.01	109.58	120.10
1	A	27	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ASP	Mainchain
1	A	158	GLU	Mainchain
1	A	175	ALA	Peptide
1	A	192	MET	Mainchain
1	A	266	VAL	Mainchain
1	A	417	ALA	Mainchain
1	A	9	VAL	Mainchain

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	4178	0	4072	148	0
2	A	1	0	0	0	0
3	A	172	0	120	36	0
4	A	53	0	31	1	0
5	A	9	0	2	1	0
6	A	581	0	0	28	0
All	All	4994	0	4225	154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASN:HD22	1:A:204:ASN:H	1.01	0.98
1:A:71:CYS:SG	3:A:803:HEM:CAC	2.53	0.96
1:A:85:CYS:SG	3:A:804:HEM:CAC	2.59	0.91
1:A:229:ASP:H	1:A:256:HIS:HE1	1.13	0.87
1:A:82:CYS:SG	3:A:804:HEM:CAB	2.64	0.85
3:A:804:HEM:HMB1	3:A:804:HEM:HBB2	1.57	0.85
1:A:68:CYS:SG	3:A:803:HEM:CAB	2.65	0.85
1:A:14:CYS:SG	3:A:801:HEM:CAB	2.66	0.83
1:A:48:GLU:HG3	6:A:967:HOH:O	1.78	0.82
1:A:229:ASP:H	1:A:256:HIS:CE1	2.00	0.80
1:A:17:CYS:SG	3:A:801:HEM:CAC	2.71	0.79
1:A:418:TYR:HB3	6:A:1368:HOH:O	1.81	0.79
1:A:204:ASN:H	1:A:204:ASN:ND2	1.82	0.77
1:A:14:CYS:HG	3:A:801:HEM:CAB	1.98	0.75
1:A:36:CYS:SG	3:A:802:HEM:CAB	2.75	0.75
1:A:204:ASN:HD22	1:A:204:ASN:N	1.80	0.73
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.53	0.72
1:A:39:CYS:HG	3:A:802:HEM:CAC	2.04	0.70
1:A:55:TYR:OH	1:A:89:ASP:HB3	1.91	0.70
1:A:422:ASP:OD2	1:A:424:SER:HB3	1.92	0.69
1:A:71:CYS:SG	3:A:803:HEM:HAC	2.32	0.69
1:A:39:CYS:SG	3:A:802:HEM:CAC	2.83	0.67
1:A:218:ASP:HB3	6:A:1338:HOH:O	1.95	0.66
1:A:516:ALA:HB2	1:A:559:LEU:HD21	1.78	0.65
3:A:802:HEM:HMB1	3:A:802:HEM:HBB2	1.77	0.65
1:A:180:GLN:HB3	1:A:185:ILE:HB	1.76	0.65
1:A:108:LEU:HD23	6:A:1378:HOH:O	1.98	0.64
1:A:114:GLU:HB2	6:A:1074:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:CYS:HG	3:A:804:HEM:CAB	2.11	0.63
1:A:101:ASP:HB3	6:A:1097:HOH:O	1.99	0.63
1:A:12:GLN:HB2	6:A:991:HOH:O	1.98	0.62
1:A:61:MET:HG2	6:A:909:HOH:O	2.00	0.62
1:A:230:LEU:O	1:A:245:HIS:HB3	2.00	0.62
1:A:393:LYS:HE3	6:A:993:HOH:O	1.99	0.62
1:A:442:PRO:HD2	1:A:496:ALA:O	2.01	0.61
1:A:246:ARG:HB2	1:A:247:PRO:CD	2.31	0.61
1:A:366:PRO:HD3	1:A:402:ARG:HG2	1.82	0.61
1:A:154:LEU:HD23	1:A:272:LEU:HD13	1.81	0.61
1:A:232:ASP:HB3	1:A:246:ARG:HG2	1.82	0.61
1:A:62:PHE:HZ	3:A:804:HEM:HMC3	1.66	0.61
1:A:190:GLU:O	1:A:194:GLU:HG2	2.01	0.61
1:A:9:VAL:O	1:A:11:ASN:N	2.34	0.60
1:A:200:GLY:O	1:A:201:GLN:HB2	2.00	0.60
1:A:268:ARG:O	1:A:269:ASN:HB2	2.01	0.60
1:A:246:ARG:HB2	1:A:247:PRO:HD2	1.83	0.59
1:A:402:ARG:HH22	5:A:806:TEO:C3	2.15	0.59
1:A:365:HIS:O	1:A:501:PRO:HA	2.02	0.59
1:A:92:MET:HG3	3:A:803:HEM:C3D	2.38	0.58
1:A:265:ALA:HA	1:A:270:ILE:HD12	1.85	0.58
1:A:219:SER:OG	1:A:555:THR:OG1	2.14	0.58
1:A:520:ASN:HD21	1:A:524:GLN:HB2	1.67	0.58
1:A:52:HIS:HB2	1:A:55:TYR:O	2.04	0.58
1:A:476:LYS:HD2	1:A:478:THR:HG22	1.85	0.58
1:A:127:VAL:O	1:A:306:ALA:HA	2.04	0.58
1:A:79:MET:HE3	1:A:98:TRP:CE3	2.39	0.58
1:A:266:VAL:O	1:A:267:LYS:C	2.41	0.57
1:A:174:ALA:HA	1:A:216:SER:HB2	1.86	0.57
1:A:193:PHE:O	1:A:197:MET:HG2	2.06	0.56
1:A:197:MET:SD	1:A:209:VAL:HG21	2.46	0.56
1:A:515:LYS:O	1:A:516:ALA:HB3	2.05	0.56
1:A:14:CYS:SG	3:A:801:HEM:HAB	2.45	0.55
1:A:467:ARG:HD2	1:A:479:ASP:OD2	2.06	0.55
1:A:139:PHE:HB3	1:A:261:LEU:HB3	1.88	0.55
1:A:431:LYS:NZ	3:A:804:HEM:O1D	2.38	0.55
1:A:516:ALA:HB2	1:A:559:LEU:CD2	2.35	0.55
1:A:54:HIS:HB2	6:A:1357:HOH:O	2.06	0.55
1:A:175:ALA:O	1:A:217:LYS:HG2	2.06	0.55
1:A:191:LEU:HA	1:A:194:GLU:HG2	1.88	0.54
3:A:803:HEM:CMB	3:A:803:HEM:HBB2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLN:NE2	1:A:187:ASP:OD2	2.40	0.54
1:A:496:ALA:HB1	6:A:1368:HOH:O	2.07	0.54
1:A:82:CYS:SG	3:A:804:HEM:CBB	2.96	0.54
1:A:217:LYS:HD3	6:A:865:HOH:O	2.07	0.54
1:A:520:ASN:ND2	1:A:524:GLN:HB2	2.22	0.54
1:A:490:ASN:HD22	1:A:490:ASN:C	2.11	0.53
1:A:234:GLY:HA3	1:A:246:ARG:NH2	2.22	0.53
1:A:46:VAL:HG21	3:A:803:HEM:HMB3	1.90	0.53
1:A:56:ASN:HB3	1:A:59:ALA:HB2	1.92	0.52
1:A:468:TYR:O	1:A:471:LEU:HB2	2.09	0.52
1:A:482:ARG:HG2	1:A:485:LEU:HD23	1.91	0.52
1:A:1:ALA:HB3	6:A:1203:HOH:O	2.08	0.52
1:A:24:LEU:HD11	3:A:801:HEM:HBA1	1.91	0.52
1:A:229:ASP:N	1:A:256:HIS:HE1	1.95	0.51
1:A:11:ASN:O	1:A:12:GLN:HB3	2.09	0.51
3:A:804:HEM:HBB2	3:A:804:HEM:CMB	2.35	0.51
1:A:4:LEU:HD21	3:A:802:HEM:HMB2	1.94	0.50
1:A:179:GLN:HA	6:A:1230:HOH:O	2.11	0.50
1:A:4:LEU:O	1:A:8:HIS:ND1	2.32	0.49
1:A:199:GLY:O	1:A:543:ASN:HB3	2.13	0.49
1:A:540:HIS:HB3	1:A:544:ARG:HB2	1.94	0.48
1:A:217:LYS:HE2	6:A:861:HOH:O	2.11	0.48
1:A:299:LYS:HB2	6:A:1058:HOH:O	2.13	0.48
1:A:226:MET:HG3	6:A:1277:HOH:O	2.13	0.48
1:A:366:PRO:CD	1:A:402:ARG:HG2	2.44	0.48
1:A:17:CYS:SG	3:A:801:HEM:C3C	3.07	0.47
1:A:9:VAL:O	1:A:12:GLN:N	2.39	0.47
1:A:85:CYS:SG	3:A:804:HEM:CBC	3.02	0.47
1:A:514:THR:CB	6:A:902:HOH:O	2.62	0.47
1:A:137:ALA:HB2	1:A:553:ILE:HB	1.96	0.47
1:A:222:TRP:CE3	1:A:558:ARG:HD2	2.50	0.47
1:A:224:THR:O	1:A:225:ALA:C	2.50	0.47
1:A:490:ASN:HD22	1:A:491:GLU:N	2.12	0.47
1:A:5:ALA:O	1:A:9:VAL:N	2.46	0.46
1:A:17:CYS:SG	3:A:801:HEM:CBC	3.03	0.46
1:A:46:VAL:O	1:A:49:THR:HG23	2.16	0.46
1:A:107:GLU:HB3	6:A:973:HOH:O	2.17	0.45
1:A:4:LEU:HD21	3:A:802:HEM:CMB	2.46	0.45
1:A:423:ASP:O	1:A:424:SER:C	2.54	0.45
1:A:128:ASP:HB3	1:A:568:SER:O	2.16	0.45
1:A:346:LEU:HD22	1:A:356:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ILE:N	6:A:1368:HOH:O	2.50	0.45
1:A:559:LEU:C	1:A:559:LEU:HD23	2.37	0.45
1:A:9:VAL:O	1:A:10:GLN:C	2.55	0.45
1:A:193:PHE:CE1	1:A:197:MET:HG3	2.52	0.45
1:A:429:LEU:HD23	1:A:432:ILE:HG13	1.98	0.45
1:A:210:LYS:O	1:A:210:LYS:HG2	2.17	0.44
1:A:85:CYS:SG	3:A:804:HEM:C3C	3.10	0.44
1:A:343:GLY:O	1:A:346:LEU:HB2	2.17	0.44
1:A:177:THR:OG1	1:A:245:HIS:HE1	2.00	0.44
1:A:180:GLN:HG2	1:A:233:VAL:HG11	1.99	0.44
1:A:6:GLU:O	1:A:7:PHE:C	2.54	0.44
1:A:83:ASP:HB2	1:A:98:TRP:HB2	1.99	0.44
1:A:114:GLU:HG2	6:A:1066:HOH:O	2.18	0.44
1:A:191:LEU:HA	1:A:194:GLU:CG	2.48	0.44
1:A:97:LYS:O	1:A:98:TRP:C	2.55	0.44
1:A:243:ARG:O	1:A:245:HIS:HD2	2.01	0.43
1:A:231:THR:OG1	1:A:248:THR:OG1	2.34	0.43
1:A:39:CYS:SG	3:A:802:HEM:C3C	3.12	0.43
1:A:47:ALA:HA	1:A:50:THR:OG1	2.18	0.43
1:A:477:ASP:O	1:A:481:GLU:HA	2.18	0.43
1:A:514:THR:HB	6:A:902:HOH:O	2.19	0.43
1:A:12:GLN:HE22	3:A:802:HEM:CBC	2.32	0.43
1:A:82:CYS:HG	3:A:804:HEM:CBB	2.30	0.42
3:A:801:HEM:CMC	6:A:1124:HOH:O	2.67	0.42
1:A:6:GLU:HA	1:A:9:VAL:HG22	2.00	0.42
4:A:805:FAD:H1'1	6:A:854:HOH:O	2.19	0.42
1:A:231:THR:O	1:A:233:VAL:HG23	2.20	0.42
1:A:232:ASP:OD2	1:A:250:GLY:N	2.52	0.42
1:A:297:MET:HE1	6:A:1065:HOH:O	2.19	0.42
1:A:365:HIS:HB2	1:A:504:HIS:CG	2.55	0.42
1:A:490:ASN:C	1:A:490:ASN:ND2	2.73	0.42
1:A:277:ARG:HH21	1:A:344:ASP:CB	2.32	0.41
1:A:393:LYS:HE2	6:A:1286:HOH:O	2.20	0.41
1:A:92:MET:HG3	3:A:803:HEM:C2D	2.54	0.41
1:A:92:MET:HG2	1:A:93:PRO:HD2	2.03	0.41
1:A:133:GLY:O	1:A:138:GLY:HA3	2.21	0.41
1:A:218:ASP:HA	6:A:1112:HOH:O	2.21	0.41
1:A:538:GLY:HA2	6:A:1157:HOH:O	2.20	0.41
1:A:71:CYS:SG	3:A:803:HEM:C3C	3.14	0.41
1:A:247:PRO:HD2	1:A:251:ALA:O	2.21	0.41
1:A:374:VAL:HB	3:A:804:HEM:CMD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD11	1:A:8:HIS:HE1	1.86	0.40
1:A:136:GLY:HA3	1:A:553:ILE:HD12	2.02	0.40
1:A:47:ALA:HB2	1:A:58:HIS:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	566/571 (99%)	532 (94%)	31 (6%)	3 (0%)	29 26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	60	SER
1	A	51	LYS

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	430/445 (97%)	405 (94%)	25 (6%)	20 17

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	23	GLU
1	A	49	THR
1	A	56	ASN
1	A	60	SER
1	A	65	GLU
1	A	91	ASN
1	A	99	LEU
1	A	113	SER
1	A	121	SER
1	A	204	ASN
1	A	217	LYS
1	A	288	THR
1	A	289	VAL
1	A	337	ASN
1	A	403	ASP
1	A	424	SER
1	A	450	LEU
1	A	459	LYS
1	A	473	SER
1	A	474	SER
1	A	490	ASN
1	A	510	VAL
1	A	515	LYS
1	A	559	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	56	ASN
1	A	91	ASN
1	A	201	GLN
1	A	204	ASN
1	A	245	HIS
1	A	256	HIS
1	A	490	ASN

5.3.3 RNA

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)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
4	FAD	A	805	-	53,58,58	1.83	13 (24%)	68,89,89	2.01	19 (27%)
3	HEM	A	804	1,6	41,50,50	1.53	4 (9%)	45,82,82	1.99	13 (28%)
3	HEM	A	803	1	41,50,50	1.49	5 (12%)	45,82,82	1.66	8 (17%)
5	TEO	A	806	-	6,8,8	4.68	4 (66%)	4,10,10	1.73	1 (25%)
3	HEM	A	802	1	41,50,50	1.40	4 (9%)	45,82,82	1.46	5 (11%)
3	HEM	A	801	1	41,50,50	1.77	9 (21%)	45,82,82	1.68	12 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	A	805	-	-	7/30/50/50	0/6/6/6
3	HEM	A	804	1,6	-	2/12/54/54	-
3	HEM	A	803	1	-	2/12/54/54	-
3	HEM	A	801	1	-	3/12/54/54	-
3	HEM	A	802	1	-	3/12/54/54	-
5	TEO	A	806	-	1/1/3/4	5/6/8/8	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	806	TEO	O2-C2	-9.97	1.31	1.43
4	A	805	FAD	C2A-N3A	4.73	1.39	1.32
3	A	801	HEM	C3C-C2C	-4.71	1.33	1.40
3	A	803	HEM	C3C-C2C	-4.63	1.33	1.40
3	A	802	HEM	C3C-C2C	-4.27	1.34	1.40
4	A	805	FAD	C6-C5X	4.25	1.46	1.40
4	A	805	FAD	C2'-C3'	4.24	1.61	1.53
3	A	804	HEM	C3C-C2C	-4.11	1.34	1.40
5	A	806	TEO	O4B-C4	4.11	1.50	1.30
3	A	801	HEM	CAA-C2A	3.88	1.57	1.52
3	A	804	HEM	CAA-C2A	3.76	1.57	1.52
3	A	804	HEM	C3C-CAC	3.58	1.55	1.47
4	A	805	FAD	O4-C4	-3.55	1.16	1.23
3	A	801	HEM	CAB-C3B	3.41	1.56	1.47
4	A	805	FAD	C2B-C1B	3.35	1.58	1.53
4	A	805	FAD	C4'-C3'	3.30	1.59	1.53
3	A	801	HEM	C3C-CAC	3.28	1.54	1.47
3	A	803	HEM	C3C-CAC	3.11	1.54	1.47
4	A	805	FAD	C8A-N7A	-3.11	1.29	1.34
3	A	802	HEM	C3C-CAC	3.10	1.54	1.47
5	A	806	TEO	C2-C1	2.82	1.59	1.54
3	A	803	HEM	CMD-C2D	2.81	1.56	1.50
4	A	805	FAD	P-O1P	-2.81	1.40	1.50
4	A	805	FAD	C10-N1	-2.79	1.27	1.33
3	A	803	HEM	CAB-C3B	2.73	1.54	1.47
3	A	804	HEM	CAB-C3B	2.72	1.54	1.47
5	A	806	TEO	O1B-C1	-2.56	1.22	1.30
4	A	805	FAD	C8-C7	2.45	1.47	1.40
3	A	802	HEM	CAB-C3B	2.37	1.53	1.47
3	A	801	HEM	C3B-C2B	-2.36	1.32	1.37
3	A	801	HEM	CMD-C2D	2.32	1.55	1.50
3	A	801	HEM	C1A-NA	2.29	1.40	1.36
4	A	805	FAD	C9-C8	2.28	1.42	1.39
4	A	805	FAD	O2'-C2'	2.24	1.48	1.43
4	A	805	FAD	O2-C2	-2.23	1.20	1.24
3	A	802	HEM	CMD-C2D	2.16	1.55	1.50
3	A	803	HEM	CMC-C2C	2.11	1.56	1.51
3	A	801	HEM	CMB-C2B	2.10	1.55	1.50
3	A	801	HEM	O1D-CGD	2.08	1.29	1.22

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	HEM	CAD-CBD-CGD	6.94	128.54	113.60
4	A	805	FAD	O4B-C1B-C2B	-6.42	97.54	106.93
4	A	805	FAD	O4'-C4'-C3'	-5.10	96.69	109.10
3	A	804	HEM	CMA-C3A-C4A	-4.96	120.83	128.46
4	A	805	FAD	O5'-C5'-C4'	-4.92	96.22	109.36
3	A	802	HEM	CAD-CBD-CGD	4.48	123.24	113.60
3	A	804	HEM	C4C-CHD-C1D	4.26	128.17	122.56
3	A	804	HEM	C4B-CHC-C1C	4.10	127.97	122.56
3	A	804	HEM	CMA-C3A-C2A	4.03	132.54	124.94
4	A	805	FAD	C4-N3-C2	-3.84	118.55	125.64
3	A	804	HEM	CAA-CBA-CGA	3.84	124.51	113.76
3	A	802	HEM	CMA-C3A-C4A	-3.76	122.69	128.46
3	A	803	HEM	CMA-C3A-C4A	-3.70	122.78	128.46
4	A	805	FAD	O3'-C3'-C2'	-3.57	100.18	108.81
4	A	805	FAD	C4X-C10-N10	3.54	121.66	116.48
3	A	804	HEM	CBA-CAA-C2A	-3.49	106.67	112.62
4	A	805	FAD	O4'-C4'-C5'	3.33	117.40	109.92
4	A	805	FAD	C5A-C6A-N6A	3.31	125.39	120.35
3	A	801	HEM	CAD-CBD-CGD	3.22	120.53	113.60
3	A	801	HEM	CMC-C2C-C3C	3.17	130.60	124.68
3	A	801	HEM	C4B-CHC-C1C	3.14	126.70	122.56
3	A	804	HEM	CHC-C4B-C3B	3.08	129.29	124.57
4	A	805	FAD	C7M-C7-C6	2.78	124.63	119.49
4	A	805	FAD	N3-C2-N1	2.75	124.78	119.38
3	A	803	HEM	CBA-CAA-C2A	2.68	117.19	112.62
3	A	804	HEM	CMC-C2C-C3C	2.66	129.65	124.68
3	A	803	HEM	CHC-C4B-NB	2.64	127.30	124.43
4	A	805	FAD	C9A-N10-C10	-2.64	116.66	120.77
4	A	805	FAD	O2'-C2'-C1'	2.62	116.14	109.80
3	A	801	HEM	C3D-C4D-ND	-2.62	107.25	110.17
3	A	801	HEM	C4D-ND-C1D	2.60	107.76	105.07
3	A	801	HEM	CMA-C3A-C4A	-2.60	124.47	128.46
3	A	803	HEM	CMA-C3A-C2A	2.57	129.79	124.94
4	A	805	FAD	C5'-C4'-C3'	2.57	117.17	112.20
3	A	801	HEM	O2D-CGD-CBD	2.53	122.15	114.03
3	A	803	HEM	C3B-C2B-C1B	2.51	108.35	106.49
5	A	806	TEO	O2-C2-C1	2.50	116.08	109.61
3	A	804	HEM	CHC-C4B-NB	-2.45	121.76	124.43
3	A	804	HEM	CMB-C2B-C1B	-2.41	121.37	125.04
3	A	804	HEM	O2A-CGA-CBA	2.41	121.77	114.03
3	A	801	HEM	O1D-CGD-CBD	-2.40	115.38	123.08
3	A	801	HEM	CMD-C2D-C1D	-2.39	121.40	125.04
3	A	801	HEM	CHA-C4D-C3D	2.39	129.81	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	805	FAD	O2B-C2B-C1B	-2.32	102.29	110.85
3	A	802	HEM	CMA-C3A-C2A	2.32	129.31	124.94
3	A	802	HEM	CMC-C2C-C3C	2.31	129.01	124.68
4	A	805	FAD	C2A-N1A-C6A	2.24	122.58	118.75
3	A	801	HEM	C3B-C2B-C1B	2.23	108.14	106.49
4	A	805	FAD	C9-C8-C7	2.20	122.81	119.67
3	A	803	HEM	CBB-CAB-C3B	-2.17	116.81	127.62
3	A	802	HEM	C4D-ND-C1D	2.16	107.30	105.07
3	A	801	HEM	CAA-CBA-CGA	2.15	119.78	113.76
4	A	805	FAD	N10-C10-N1	-2.10	112.31	118.35
3	A	803	HEM	O1A-CGA-CBA	-2.09	116.38	123.08
3	A	804	HEM	CHA-C4D-ND	2.06	126.92	124.38
4	A	805	FAD	O4-C4-N3	-2.03	116.23	120.12
3	A	804	HEM	CHB-C1B-NB	2.02	126.88	124.38
4	A	805	FAD	C7M-C7-C8	-2.01	116.63	120.74

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	806	TEO	C2

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	HEM	C2A-CAA-CBA-CGA
4	A	805	FAD	N10-C1'-C2'-O2'
5	A	806	TEO	C1-C2-C3-C4
5	A	806	TEO	O2-C2-C3-C4
3	A	802	HEM	C3D-CAD-CBD-CGD
3	A	803	HEM	C3D-CAD-CBD-CGD
5	A	806	TEO	O1A-C1-C2-O2
5	A	806	TEO	O1B-C1-C2-O2
4	A	805	FAD	C2'-C3'-C4'-C5'
3	A	801	HEM	C3D-CAD-CBD-CGD
4	A	805	FAD	P-O3P-PA-O1A
4	A	805	FAD	C2'-C3'-C4'-O4'
4	A	805	FAD	P-O3P-PA-O2A
3	A	804	HEM	CAA-CBA-CGA-O2A
3	A	802	HEM	CAD-CBD-CGD-O1D
3	A	801	HEM	CAD-CBD-CGD-O1D
3	A	804	HEM	CAA-CBA-CGA-O1A
3	A	802	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	A	801	HEM	CAD-CBD-CGD-O2D
4	A	805	FAD	O4B-C4B-C5B-O5B
5	A	806	TEO	O1B-C1-C2-C3
4	A	805	FAD	N10-C1'-C2'-C3'

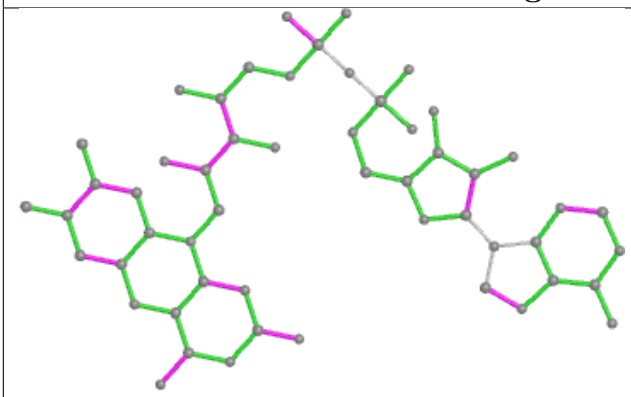
There are no ring outliers.

6 monomers are involved in 38 short contacts:

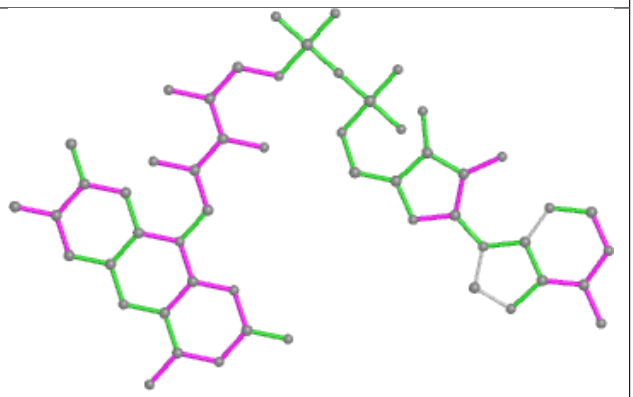
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	805	FAD	1	0
3	A	804	HEM	12	0
3	A	803	HEM	8	0
5	A	806	TEO	1	0
3	A	802	HEM	8	0
3	A	801	HEM	8	0

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.

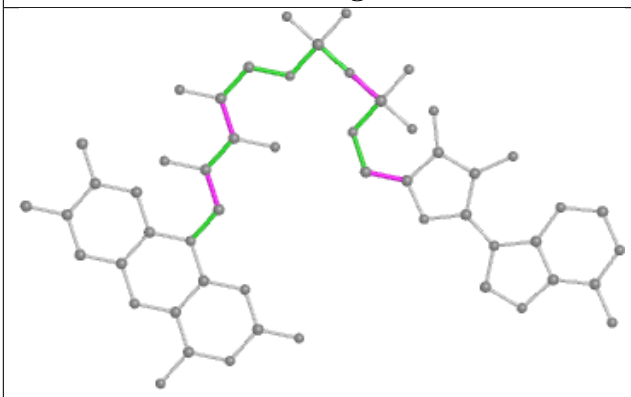
Ligand FAD A 805



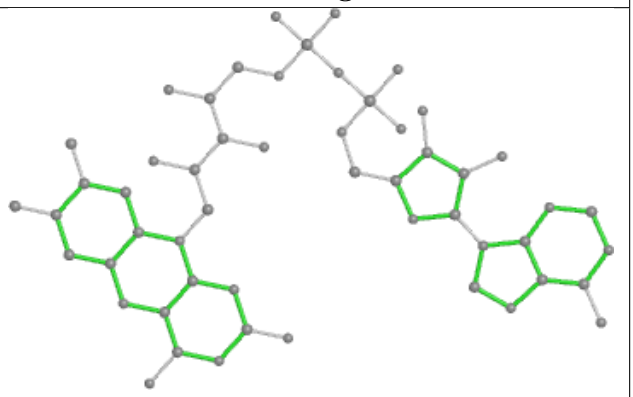
Bond lengths



Bond angles

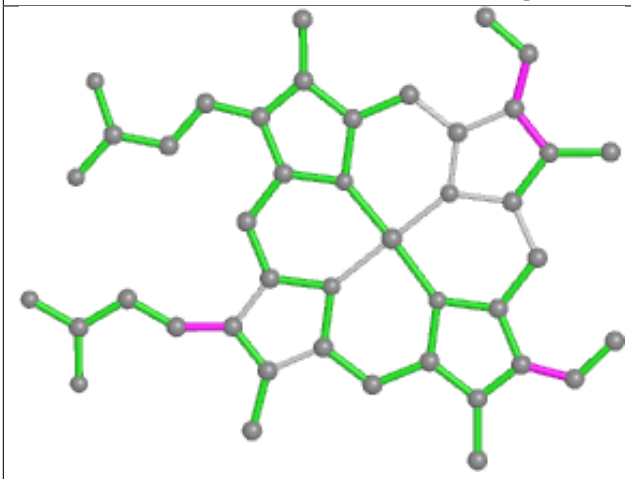


Torsions

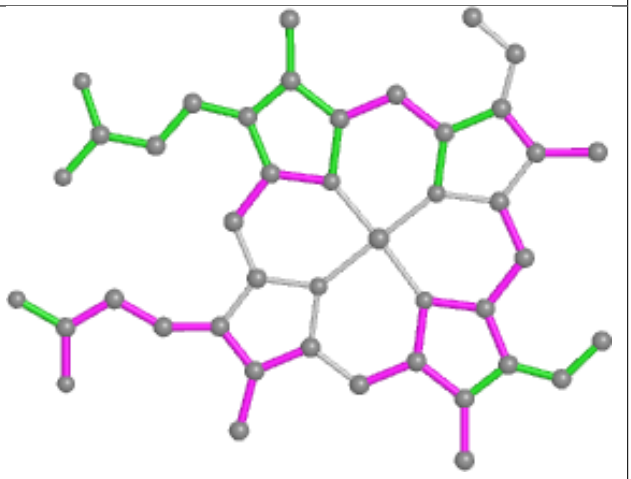


Rings

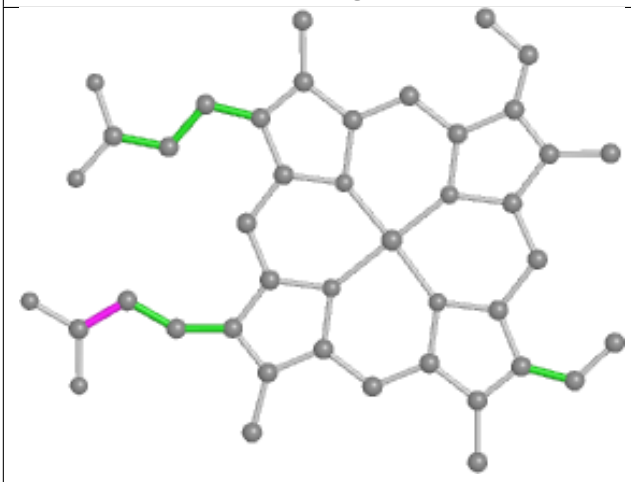
Ligand HEM A 804



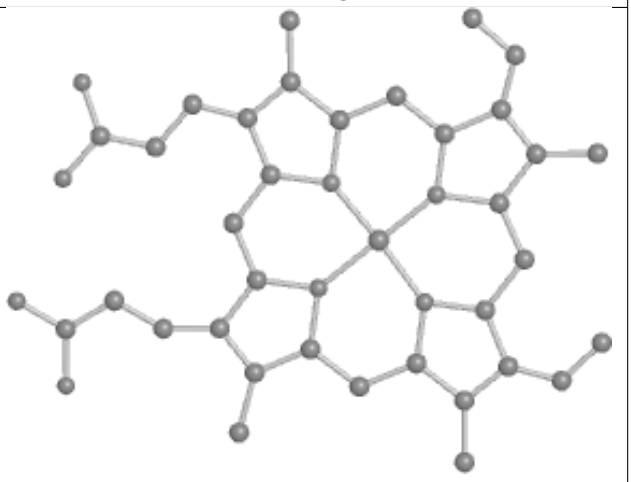
Bond lengths



Bond angles

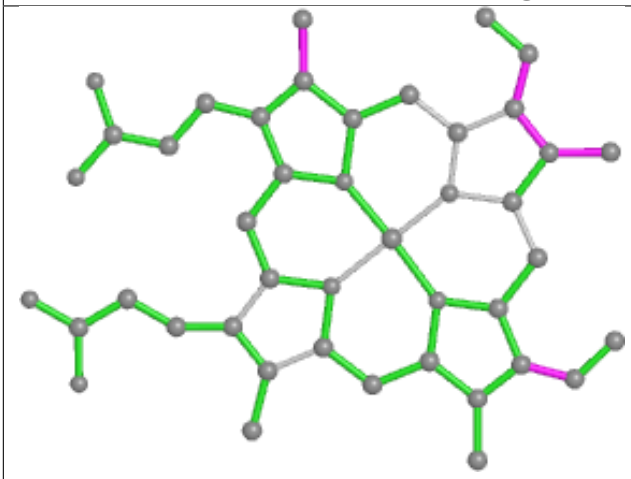


Torsions

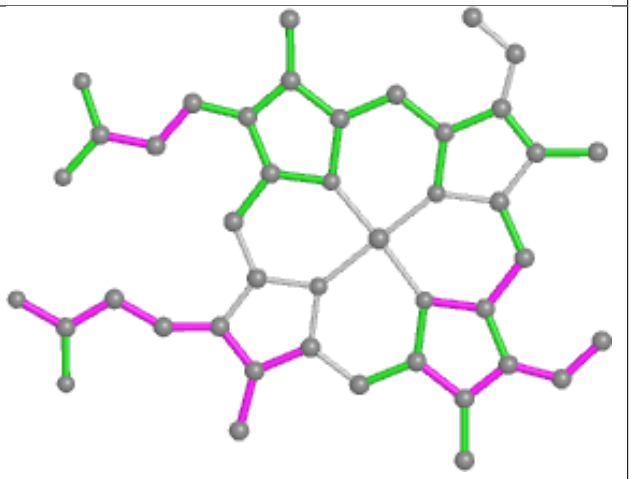


Rings

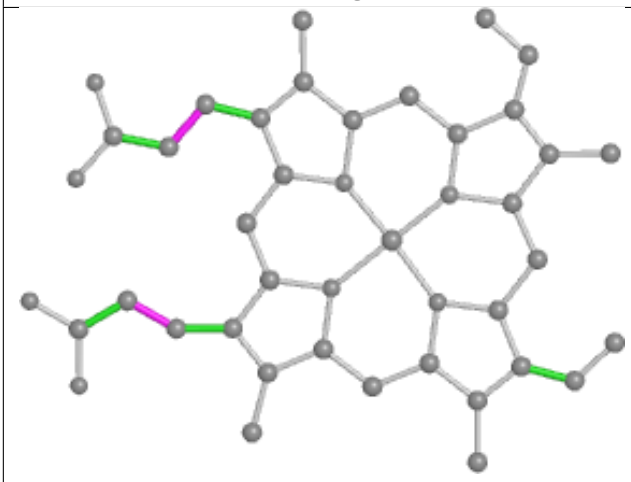
Ligand HEM A 803



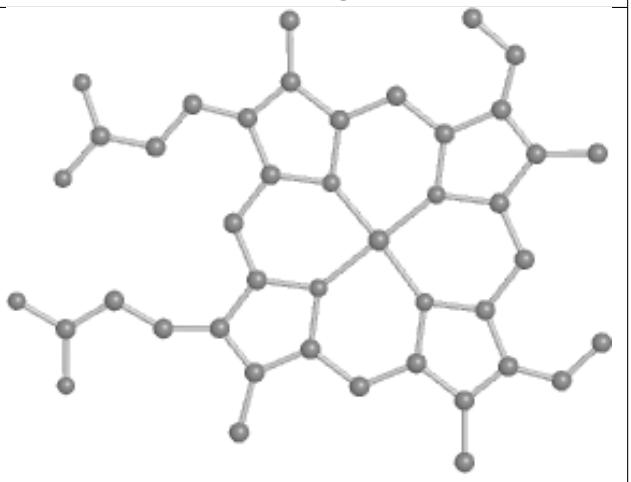
Bond lengths



Bond angles

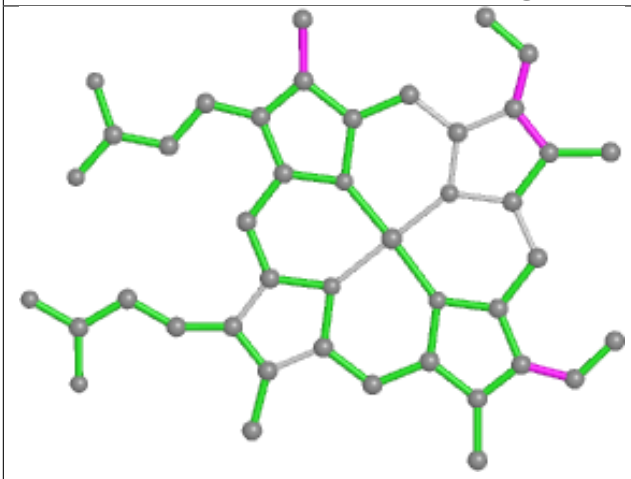


Torsions

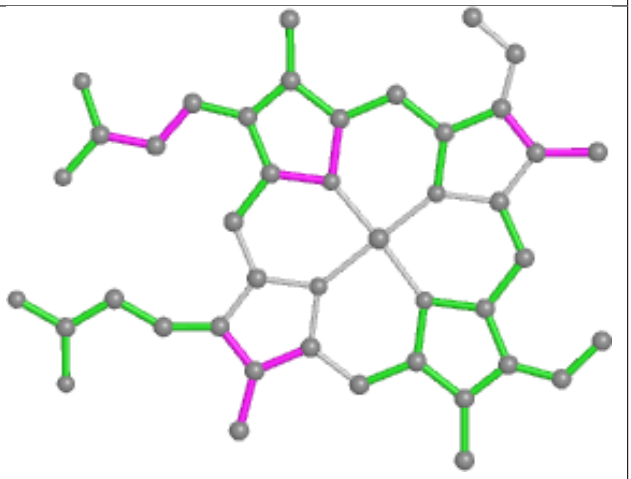


Rings

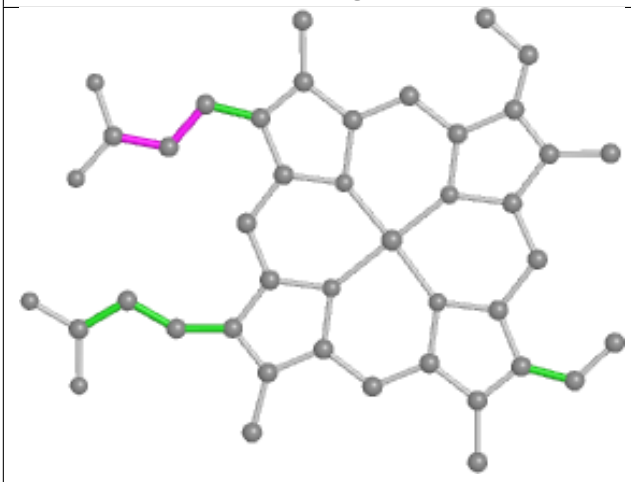
Ligand HEM A 802



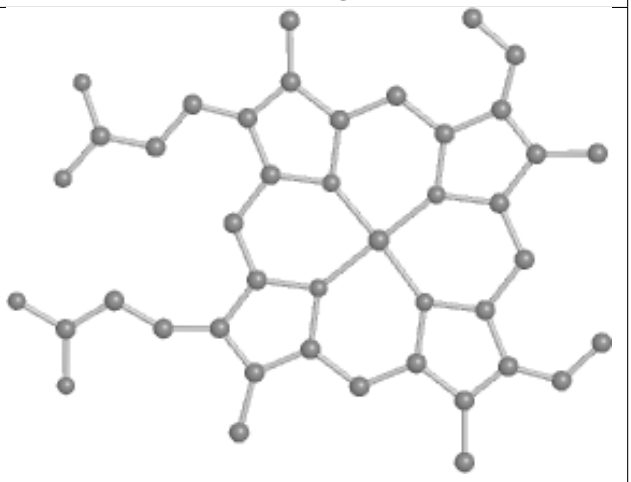
Bond lengths



Bond angles

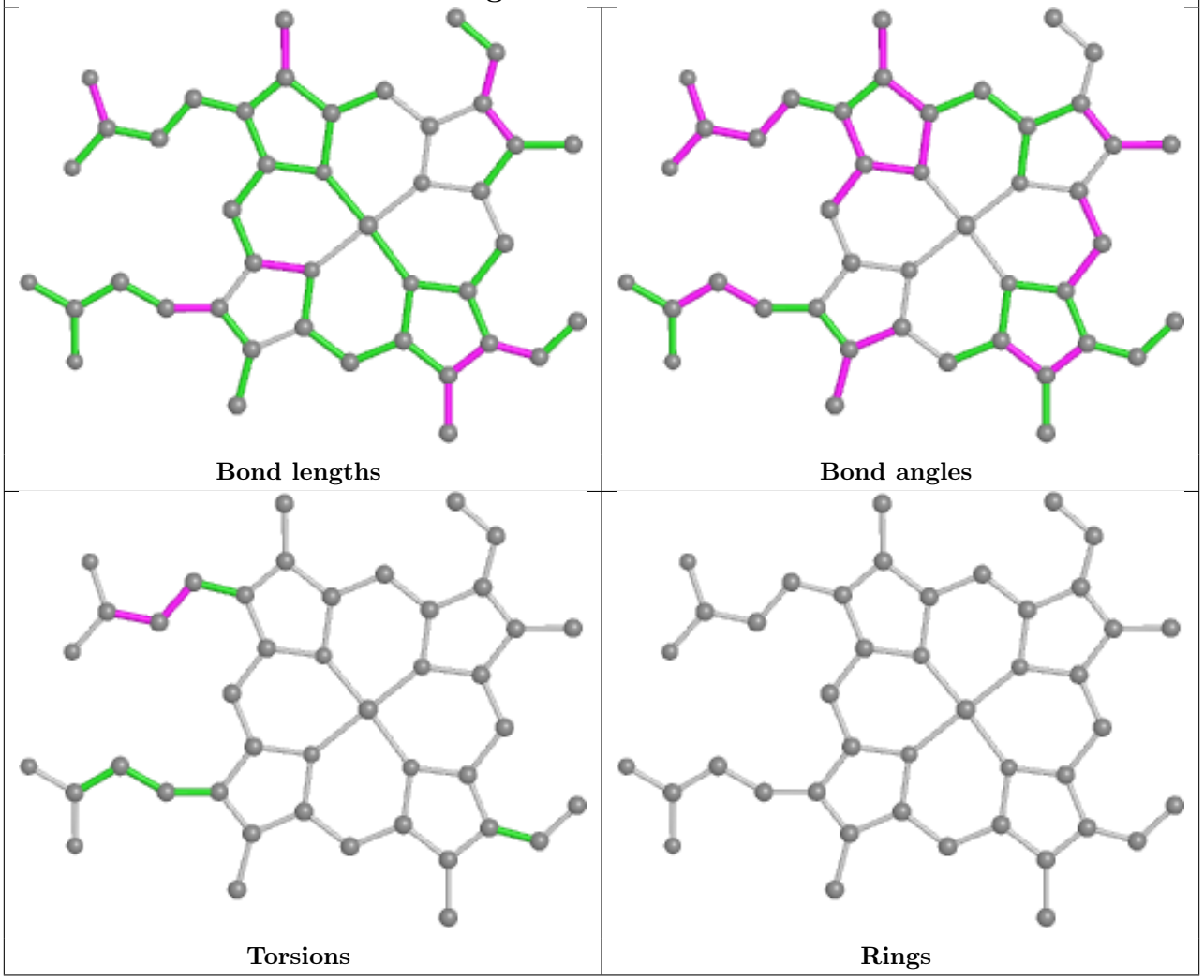


Torsions



Rings

Ligand HEM A 801



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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.