Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 10:05 PM EDT

PDB ID	:	3WFE
Title	:	Reduced and cyanide-bound cytochrome c-dependent nitric oxide reductase (cNOR) from Pseudomonas aeruginosa in complex with antibody fragment
Authors	:	Sato, N.; Ishii, S.; Hino, T.; Sugimoto, H.; Fukumori, Y.; Shiro, Y.; Tosha, T.
Deposited on	:	2013-07-18
Resolution	:	2.49 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:

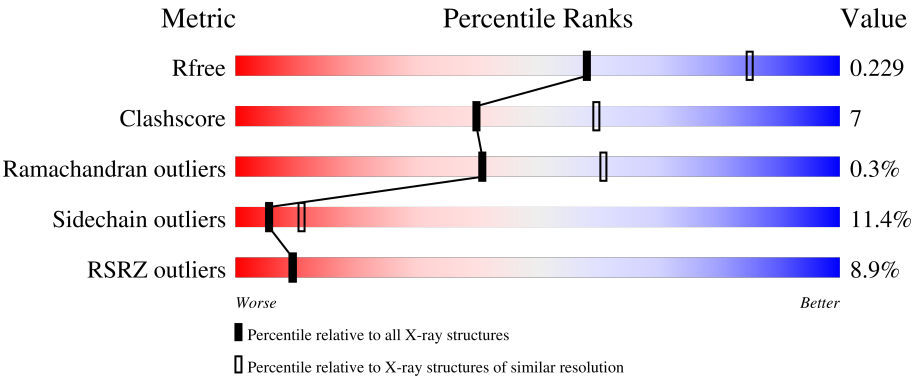
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	L	213	% 81% 17%
2	H	225	6% 83% 14%
3	B	465	15% 74% 19%
4	C	146	5% 79% 14%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 8503 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 antibody fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1669	1047	277	338	7			

- Molecule 2 is a protein called antibody fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	225	Total	C	N	O	S	0	0	0
			1692	1065	280	338	9			

- Molecule 3 is a protein called Nitric oxide reductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	449	Total	C	N	O	S	0	0	0
			3576	2416	563	572	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ARG	deletion	UNP Q59647

- Molecule 4 is a protein called Nitric oxide reductase subunit C.

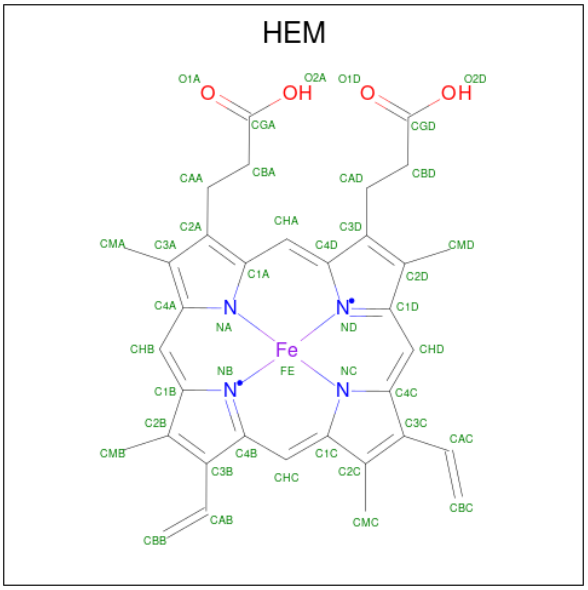
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	142	Total	C	N	O	S	0	0	0
			1123	720	195	202	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	100	LYS	ASN	conflict	UNP Q59646

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: $C_{34}H_{32}FeN_4O_4$).

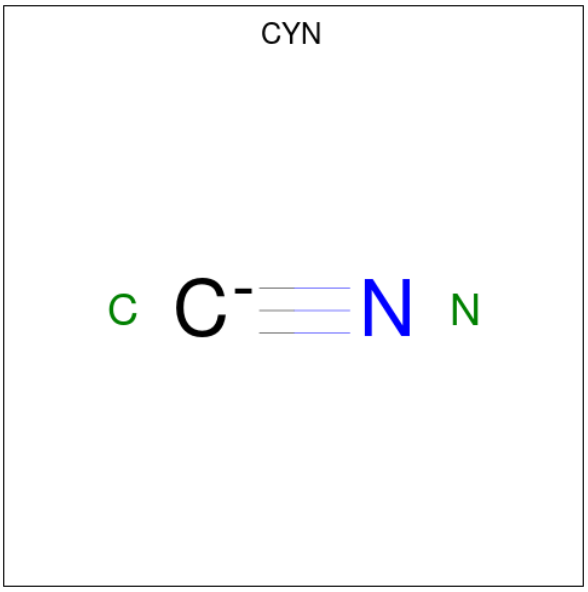


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

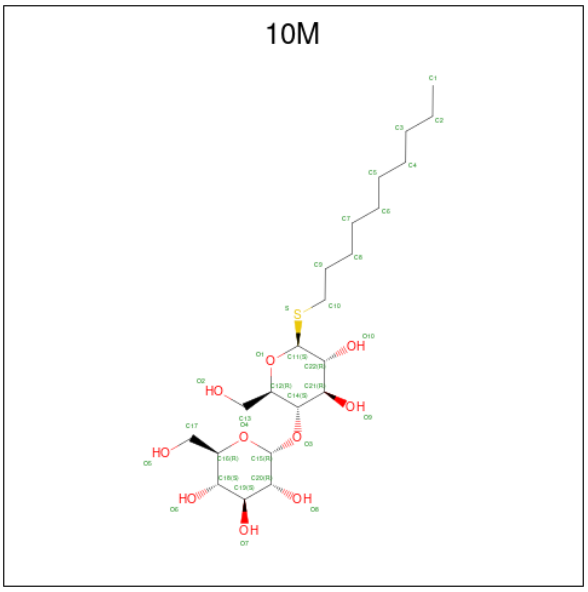
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe	0	0
			1	1		

- Molecule 7 is CYANIDE ION (three-letter code: CYN) (formula: CN).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N 2 1 1	0	0
7	B	1	Total C N 2 1 1	0	0

- Molecule 8 is decyl 4-O-alpha-D-glucopyranosyl-1-thio-beta-D-glucopyranoside (three-letter code: 10M) (formula: $C_{22}H_{42}O_{10}S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O S 33 22 10 1	0	0

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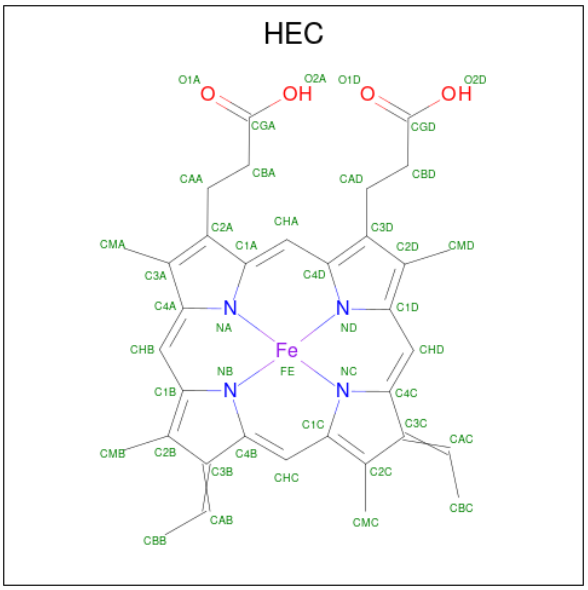
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O	S	0	0
			33	22	10	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Ca	0	0
			1	1		

- Molecule 10 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

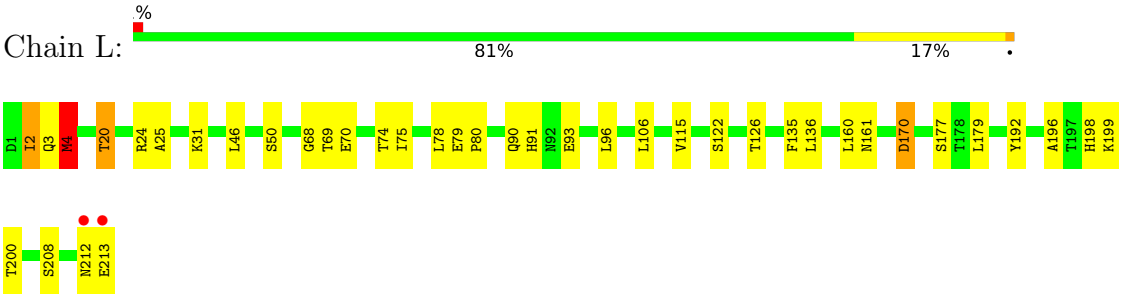
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	80	Total	O	0	0
			80	80		
11	H	77	Total	O	0	0
			77	77		
11	B	47	Total	O	0	0
			47	47		
11	C	38	Total	O	0	0
			38	38		

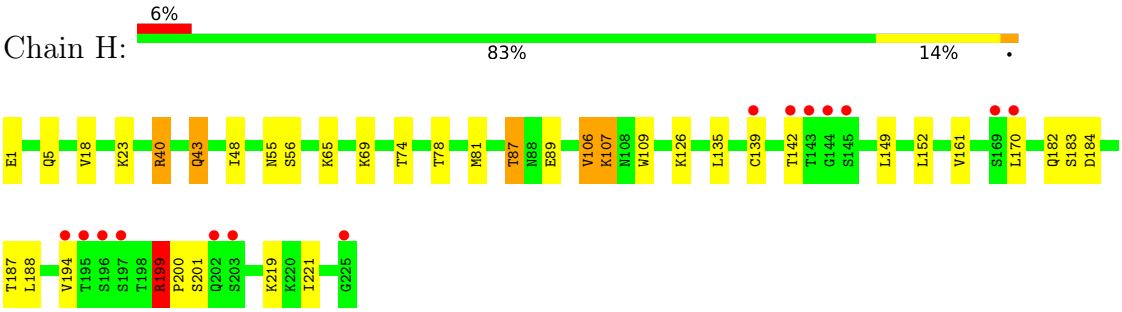
3 Residue-property plots (i)

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.

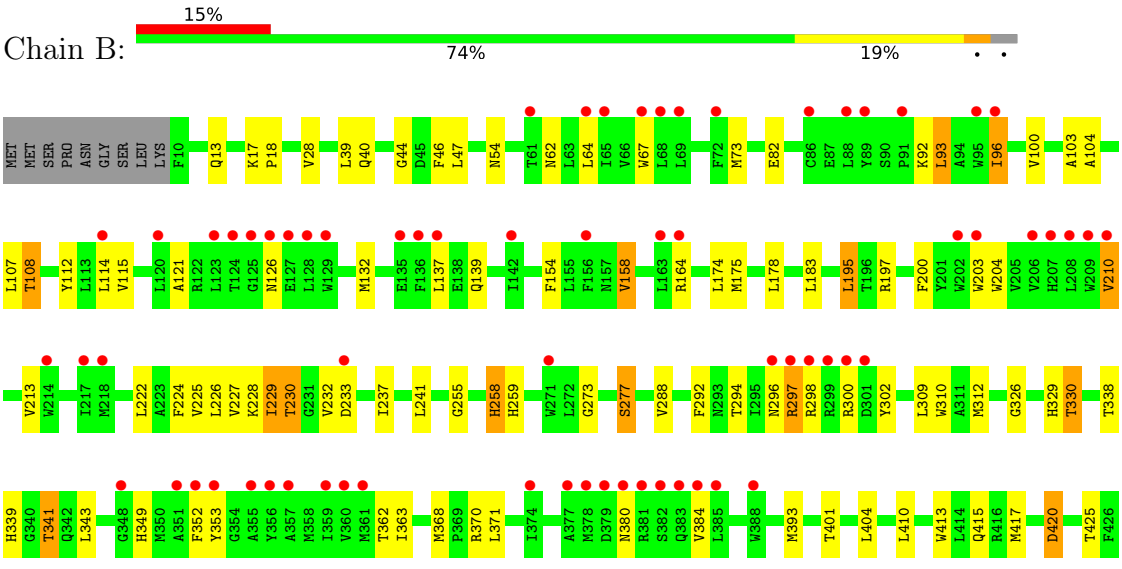
• Molecule 1: antibody fab fragment light chain

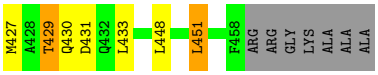


• Molecule 2: antibody fab fragment heavy chain

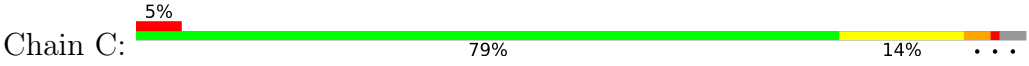


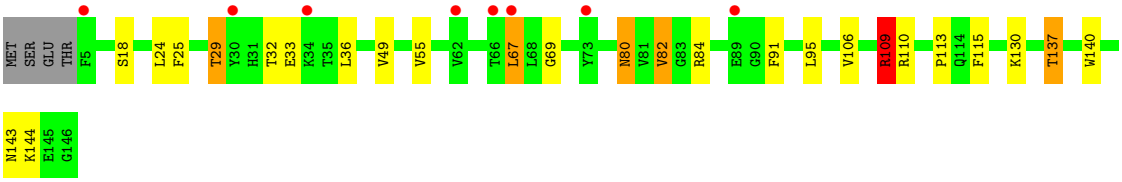
• Molecule 3: Nitric oxide reductase subunit B





• Molecule 4: Nitric oxide reductase subunit C





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.69Å 107.38Å 195.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.16 – 2.49 35.16 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.4 (35.16-2.49) 98.4 (35.16-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.24 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.189 , 0.227 0.194 , 0.229	Depositor DCC
R_{free} test set	3358 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8503	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, 10M, HEM, CYN, FE, CA

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	L	0.87	0/1709	0.93	3/2317 (0.1%)
2	H	0.86	0/1735	0.90	1/2367 (0.0%)
3	B	0.64	0/3693	0.79	3/5039 (0.1%)
4	C	0.68	2/1153 (0.2%)	0.79	0/1559
All	All	0.74	2/8290 (0.0%)	0.84	7/11282 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	109	ARG	CZ-NH1	-5.30	1.26	1.33
4	C	109	ARG	CZ-NH2	-5.03	1.26	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	199	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	L	4	MET	CB-CA-C	-5.65	99.09	110.40
3	B	420	ASP	CB-CG-OD1	5.62	123.36	118.30
3	B	371	LEU	CA-CB-CG	5.57	128.10	115.30
1	L	170	ASP	CB-CG-OD1	5.49	123.24	118.30
3	B	431	ASP	CB-CG-OD1	5.33	123.10	118.30
1	L	93	GLU	CB-CA-C	-5.18	100.04	110.40

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	L	1669	0	1606	26	0
2	H	1692	0	1647	20	0
3	B	3576	0	3619	58	0
4	C	1123	0	1092	22	0
5	B	86	0	60	8	0
6	B	1	0	0	0	0
7	B	4	0	0	1	0
8	B	66	0	84	1	0
9	B	1	0	0	0	0
10	C	43	0	30	6	0
11	B	47	0	0	0	0
11	C	38	0	0	0	0
11	H	77	0	0	3	0
11	L	80	0	0	1	0
All	All	8503	0	8138	120	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 7.

All (120) 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)
3:B:121:ALA:HA	3:B:132:MET:HE1	1.49	0.91
2:H:48:ILE:HG21	2:H:81:MET:CE	2.09	0.82
4:C:25:PHE:O	4:C:29:THR:HG23	1.85	0.77
3:B:121:ALA:HA	3:B:132:MET:CE	2.18	0.74
3:B:137:LEU:HA	3:B:139:GLN:HE22	1.52	0.72
2:H:182:GLN:HE21	2:H:187:THR:HG21	1.55	0.71
2:H:48:ILE:HG21	2:H:81:MET:HE3	1.71	0.71
1:L:3:GLN:C	1:L:4:MET:HE2	2.12	0.71
4:C:109:ARG:NH2	10:C:201:HEC:O1D	2.24	0.70
3:B:425:THR:O	3:B:429:THR:HG23	1.93	0.69
3:B:126:ASN:HB2	3:B:132:MET:CE	2.23	0.69
3:B:338:THR:O	3:B:341:THR:HB	1.91	0.68
3:B:197:ARG:NE	4:C:33:GLU:OE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:161:ASN:HD22	1:L:177:SER:HA	1.64	0.63
2:H:107:LYS:HB2	11:H:323:HOH:O	1.97	0.63
1:L:160:LEU:CD1	2:H:182:GLN:HG2	2.29	0.62
3:B:104:ALA:O	3:B:108:THR:HG22	1.99	0.62
3:B:302:TYR:OH	3:B:370:ARG:NH1	2.33	0.62
3:B:427:MET:HE3	10:C:201:HEC:HAD1	1.82	0.62
2:H:183:SER:OG	2:H:184:ASP:N	2.33	0.61
4:C:82:VAL:HG21	4:C:130:LYS:HG2	1.83	0.60
4:C:137:THR:HG21	4:C:140:TRP:O	2.02	0.60
1:L:79:GLU:HG3	1:L:80:PRO:HD2	1.83	0.60
3:B:427:MET:CE	10:C:201:HEC:HAD1	2.32	0.60
3:B:273:GLY:O	3:B:277:SER:HB2	2.03	0.58
3:B:393:MET:HE1	3:B:451:LEU:HD23	1.85	0.58
3:B:230:THR:OG1	3:B:294:THR:O	2.21	0.58
3:B:226:LEU:O	3:B:230:THR:HG22	2.03	0.57
2:H:69:LYS:HE3	11:H:349:HOH:O	2.04	0.57
3:B:137:LEU:HA	3:B:139:GLN:NE2	2.20	0.57
2:H:48:ILE:HG21	2:H:81:MET:HE1	1.87	0.56
2:H:182:GLN:HE21	2:H:187:THR:CG2	2.19	0.56
1:L:135:PHE:C	1:L:136:LEU:HD23	2.27	0.55
1:L:4:MET:N	1:L:4:MET:CE	2.70	0.55
1:L:4:MET:HE2	1:L:4:MET:N	2.22	0.54
3:B:225:VAL:O	3:B:229:ILE:HB	2.08	0.54
3:B:62:ASN:ND2	3:B:112:TYR:OH	2.41	0.53
3:B:158:VAL:CG1	3:B:175:MET:SD	2.96	0.53
2:H:199:ARG:HA	2:H:201:SER:N	2.24	0.53
3:B:415:GLN:HB2	3:B:429:THR:HG21	1.89	0.53
3:B:82:GLU:OE1	3:B:228:LYS:HE3	2.09	0.52
8:B:806:10M:O8	8:B:807:10M:H17	2.10	0.52
1:L:2:ILE:HD13	1:L:25:ALA:HB1	1.92	0.52
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.94	0.51
3:B:200:PHE:CZ	4:C:29:THR:HB	2.46	0.50
1:L:115:VAL:HG13	1:L:136:LEU:HD22	1.92	0.50
1:L:192:TYR:O	1:L:208:SER:HB2	2.13	0.49
2:H:182:GLN:NE2	2:H:187:THR:HG21	2.27	0.49
2:H:199:ARG:HB2	2:H:200:PRO:HA	1.95	0.49
1:L:2:ILE:CD1	1:L:25:ALA:HB1	2.42	0.49
1:L:161:ASN:ND2	1:L:177:SER:OG	2.45	0.49
3:B:158:VAL:HG12	3:B:175:MET:SD	2.53	0.49
3:B:210:VAL:HG13	5:B:802:HEM:C3B	2.47	0.49
3:B:430:GLN:HE21	4:C:110:ARG:HH22	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:137:THR:CG2	4:C:140:TRP:O	2.60	0.48
2:H:40:ARG:O	2:H:43:GLN:HB2	2.13	0.48
5:B:802:HEM:C4A	7:B:804:CYN:C	2.78	0.48
4:C:109:ARG:NH2	10:C:201:HEC:CGD	2.77	0.48
1:L:50:SER:H	1:L:91:HIS:HE1	1.62	0.48
3:B:349:HIS:CD2	5:B:801:HEM:NC	2.81	0.48
3:B:230:THR:HG23	3:B:232:VAL:H	1.78	0.47
3:B:174:LEU:HD13	3:B:178:LEU:HD12	1.95	0.47
3:B:430:GLN:HE21	4:C:110:ARG:NH2	2.12	0.47
3:B:40:GLN:O	3:B:44:GLY:HA2	2.15	0.47
3:B:326:GLY:O	3:B:330:THR:HB	2.15	0.47
4:C:80:ASN:HD21	4:C:84:ARG:HH22	1.61	0.47
1:L:136:LEU:HD23	1:L:136:LEU:N	2.30	0.47
3:B:352:PHE:HB3	5:B:801:HEM:HBC1	1.96	0.47
2:H:107:LYS:CB	11:H:323:HOH:O	2.59	0.47
4:C:113:PRO:HD3	10:C:201:HEC:HBC2	1.97	0.47
1:L:20:THR:HB	1:L:74:THR:OG1	2.15	0.47
3:B:28:VAL:HG22	3:B:451:LEU:HD13	1.97	0.47
3:B:126:ASN:ND2	3:B:132:MET:HE2	2.30	0.46
3:B:13:GLN:HE22	3:B:82:GLU:HG3	1.80	0.46
1:L:115:VAL:HG13	1:L:136:LEU:CD2	2.45	0.46
2:H:149:LEU:HD11	2:H:199:ARG:HD3	1.97	0.46
3:B:230:THR:HG23	3:B:232:VAL:HG23	1.97	0.46
4:C:80:ASN:HD22	4:C:80:ASN:H	1.63	0.46
1:L:136:LEU:HD13	1:L:196:ALA:HB2	1.98	0.46
3:B:46:PHE:CE2	3:B:47:LEU:HG	2.51	0.46
3:B:93:LEU:HA	3:B:96:ILE:HG22	1.98	0.45
5:B:801:HEM:HMB1	5:B:801:HEM:HBB2	1.98	0.45
3:B:353:TYR:N	5:B:801:HEM:HBC1	2.32	0.45
4:C:115:PHE:HZ	10:C:201:HEC:HMC2	1.82	0.45
4:C:32:THR:O	4:C:36:LEU:HD13	2.17	0.45
4:C:82:VAL:HG23	4:C:91:PHE:CD2	2.52	0.44
5:B:801:HEM:HBB2	5:B:801:HEM:CMB	2.47	0.44
1:L:75:ILE:HG21	1:L:78:LEU:HD23	2.00	0.44
3:B:126:ASN:HB2	3:B:132:MET:HE3	2.00	0.43
3:B:204:TRP:HZ2	4:C:29:THR:HG21	1.83	0.43
3:B:104:ALA:O	3:B:108:THR:CG2	2.65	0.43
3:B:203:TRP:CZ3	3:B:259:HIS:CE1	3.05	0.43
3:B:224:PHE:CE1	3:B:228:LYS:HE2	2.52	0.43
4:C:82:VAL:HG23	4:C:91:PHE:CG	2.53	0.43
3:B:227:VAL:HG23	3:B:237:ILE:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:310:TRP:HB3	3:B:362:THR:OG1	2.19	0.43
3:B:73:MET:HG2	3:B:154:PHE:CE1	2.53	0.43
3:B:339:HIS:CD2	4:C:69:GLY:HA3	2.53	0.43
3:B:292:PHE:CE1	3:B:312:MET:HG2	2.54	0.43
3:B:425:THR:O	3:B:429:THR:CG2	2.65	0.43
3:B:258:HIS:CE1	5:B:802:HEM:CHD	3.01	0.42
3:B:420:ASP:OD1	4:C:143:ASN:HB2	2.19	0.42
1:L:70:GLU:HG3	11:L:322:HOH:O	2.20	0.42
3:B:17:LYS:N	3:B:18:PRO:HD2	2.34	0.42
1:L:4:MET:HE3	1:L:4:MET:HB2	1.71	0.42
2:H:199:ARG:HA	2:H:201:SER:H	1.85	0.42
1:L:122:SER:O	1:L:126:THR:HG23	2.19	0.42
3:B:13:GLN:NE2	3:B:82:GLU:HG3	2.34	0.41
1:L:115:VAL:HA	1:L:135:PHE:O	2.20	0.41
3:B:96:ILE:O	3:B:100:VAL:HG23	2.20	0.41
2:H:87:THR:HG22	2:H:89:GLU:H	1.84	0.41
1:L:4:MET:CE	1:L:4:MET:CA	2.99	0.41
1:L:50:SER:H	1:L:91:HIS:CE1	2.38	0.41
2:H:87:THR:CG2	2:H:89:GLU:H	2.34	0.41
3:B:297:ARG:HH11	3:B:297:ARG:CG	2.34	0.41
4:C:80:ASN:ND2	4:C:84:ARG:HH22	2.19	0.41
1:L:91:HIS:HD2	2:H:109:TRP:CE3	2.39	0.40
2:H:55:ASN:O	2:H:56:SER:HB2	2.21	0.40
3:B:195:LEU:HD11	4:C:67:LEU:HD13	2.03	0.40
3:B:103:ALA:O	3:B:107:LEU:HB2	2.20	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	L	211/213 (99%)	202 (96%)	8 (4%)	1 (0%)	29 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	223/225 (99%)	213 (96%)	9 (4%)	1 (0%)	34 54
3	B	447/465 (96%)	428 (96%)	18 (4%)	1 (0%)	47 68
4	C	140/146 (96%)	135 (96%)	5 (4%)	0	100 100
All	All	1021/1049 (97%)	978 (96%)	40 (4%)	3 (0%)	41 61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	68	GLY
3	B	255	GLY
2	H	106	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	189/189 (100%)	174 (92%)	15 (8%)	12 24
2	H	192/192 (100%)	168 (88%)	24 (12%)	4 8
3	B	360/371 (97%)	314 (87%)	46 (13%)	4 8
4	C	116/120 (97%)	103 (89%)	13 (11%)	6 11
All	All	857/872 (98%)	759 (89%)	98 (11%)	5 11

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	4	MET
1	L	20	THR
1	L	24	ARG
1	L	31	LYS
1	L	46	LEU
1	L	69	THR
1	L	90	GLN

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Mol	Chain	Res	Type
1	L	96	LEU
1	L	106	LEU
1	L	170	ASP
1	L	179	LEU
1	L	199	LYS
1	L	212	ASN
1	L	213	GLU
2	H	1	GLU
2	H	5	GLN
2	H	18	VAL
2	H	23	LYS
2	H	40	ARG
2	H	43	GLN
2	H	65	LYS
2	H	74	THR
2	H	78	THR
2	H	87	THR
2	H	106	VAL
2	H	107	LYS
2	H	126	LYS
2	H	135	LEU
2	H	139	CYS
2	H	142	THR
2	H	152	LEU
2	H	161	VAL
2	H	170	LEU
2	H	188	LEU
2	H	194	VAL
2	H	199	ARG
2	H	219	LYS
2	H	221	ILE
3	B	39	LEU
3	B	54	ASN
3	B	64	LEU
3	B	67	TRP
3	B	92	LYS
3	B	93	LEU
3	B	96	ILE
3	B	108	THR
3	B	114	LEU
3	B	115	VAL
3	B	158	VAL

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Mol	Chain	Res	Type
3	B	164	ARG
3	B	183	LEU
3	B	195	LEU
3	B	210	VAL
3	B	213	VAL
3	B	222	LEU
3	B	229	ILE
3	B	230	THR
3	B	233	ASP
3	B	241	LEU
3	B	258	HIS
3	B	277	SER
3	B	288	VAL
3	B	296	ASN
3	B	297	ARG
3	B	298	ARG
3	B	300	ARG
3	B	309	LEU
3	B	329	HIS
3	B	330	THR
3	B	341	THR
3	B	343	LEU
3	B	363	ILE
3	B	368	MET
3	B	380	ASN
3	B	384	VAL
3	B	401	THR
3	B	404	LEU
3	B	410	LEU
3	B	413	TRP
3	B	417	MET
3	B	429	THR
3	B	433	LEU
3	B	448	LEU
3	B	451	LEU
4	C	18	SER
4	C	24	LEU
4	C	29	THR
4	C	49	VAL
4	C	55	VAL
4	C	67	LEU
4	C	80	ASN

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Mol	Chain	Res	Type
4	C	82	VAL
4	C	95	LEU
4	C	106	VAL
4	C	109	ARG
4	C	137	THR
4	C	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
1	L	91	HIS
1	L	137	ASN
1	L	156	GLN
1	L	161	ASN
1	L	190	ASN
1	L	198	HIS
2	H	182	GLN
3	B	30	GLN
3	B	54	ASN
3	B	62	ASN
3	B	126	ASN
3	B	139	GLN
3	B	296	ASN
3	B	329	HIS
3	B	411	GLN
3	B	430	GLN
4	C	31	HIS
4	C	60	ASN
4	C	80	ASN
4	C	96	GLN
4	C	102	GLN
4	C	105	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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
5	HEM	B	801	3,9	41,50,50	1.86	7 (17%)	45,82,82	2.63	17 (37%)
5	HEM	B	802	3,9,7	41,50,50	1.88	6 (14%)	45,82,82	2.53	19 (42%)
7	CYN	B	805	6	0,1,1	-	-	-		
8	10M	B	807	-	34,34,34	1.17	3 (8%)	44,45,45	1.26	6 (13%)
7	CYN	B	804	5	0,1,1	-	-	-		
8	10M	B	806	-	34,34,34	0.96	2 (5%)	44,45,45	1.17	4 (9%)
10	HEC	C	201	4	32,50,50	2.56	4 (12%)	24,82,82	1.80	8 (33%)

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
5	HEM	B	801	3,9	-	3/12/54/54	-
5	HEM	B	802	3,9,7	-	4/12/54/54	-
8	10M	B	807	-	-	3/19/59/59	0/2/2/2
8	10M	B	806	-	-	9/19/59/59	0/2/2/2
10	HEC	C	201	4	-	2/10/54/54	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	201	HEC	C3C-C2C	-9.01	1.31	1.40
10	C	201	HEC	C2B-C3B	-7.66	1.32	1.40
5	B	802	HEM	C3D-C2D	6.69	1.51	1.36
5	B	801	HEM	C3D-C2D	6.37	1.50	1.36
5	B	802	HEM	C3C-C2C	-5.93	1.32	1.40
10	C	201	HEC	C3D-C2D	4.86	1.52	1.37
5	B	801	HEM	C3C-C2C	-4.25	1.34	1.40
8	B	807	10M	O1-C11	4.10	1.48	1.42
5	B	802	HEM	C3C-CAC	3.09	1.54	1.47
5	B	801	HEM	C3C-CAC	3.03	1.54	1.47
5	B	801	HEM	C1B-NB	-2.93	1.35	1.40
5	B	801	HEM	C3B-C2B	-2.91	1.31	1.37
5	B	801	HEM	CAB-C3B	2.74	1.54	1.47
8	B	807	10M	C11-S	2.72	1.85	1.80
5	B	802	HEM	O1A-CGA	2.64	1.30	1.22
8	B	806	10M	C10-S	2.62	1.84	1.81
8	B	807	10M	C10-S	2.41	1.84	1.81
5	B	801	HEM	C1D-ND	-2.24	1.34	1.38
10	C	201	HEC	C1B-CHB	-2.15	1.35	1.41
5	B	802	HEM	CMD-C2D	2.12	1.55	1.50
5	B	802	HEM	C2A-C3A	-2.03	1.31	1.37
8	B	806	10M	O3-C15	2.02	1.47	1.41

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	801	HEM	C2C-C3C-C4C	10.30	114.09	106.90
5	B	802	HEM	CBA-CAA-C2A	-6.92	100.81	112.62
5	B	802	HEM	C1D-C2D-C3D	-6.54	100.08	106.96
5	B	801	HEM	C4D-ND-C1D	5.69	110.95	105.07
5	B	802	HEM	CMB-C2B-C1B	-5.59	116.53	125.04
5	B	801	HEM	CMA-C3A-C4A	-5.54	119.95	128.46
5	B	802	HEM	O2A-CGA-O1A	5.19	136.24	123.30
10	C	201	HEC	CMB-C2B-C3B	4.49	131.10	125.82
5	B	801	HEM	C4A-C3A-C2A	4.38	110.05	107.00
5	B	802	HEM	CHB-C1B-NB	-4.26	119.11	124.38
5	B	801	HEM	CHA-C4D-ND	3.94	129.24	124.38
10	C	201	HEC	CMB-C2B-C1B	-3.62	122.90	128.46
5	B	802	HEM	O2A-CGA-CBA	-3.55	102.63	114.03
5	B	802	HEM	C2D-C1D-ND	3.41	113.97	109.88
8	B	807	10M	C17-C16-C18	-3.29	105.30	113.00
5	B	801	HEM	C3C-C4C-NC	-3.29	104.74	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	802	HEM	CBB-CAB-C3B	-3.27	111.36	127.62
8	B	806	10M	C18-C19-C20	3.11	116.25	110.82
5	B	802	HEM	CMD-C2D-C1D	3.07	129.71	125.04
5	B	801	HEM	CHC-C4B-NB	3.04	127.73	124.43
8	B	806	10M	C11-O1-C12	-2.98	107.08	112.58
8	B	807	10M	O4-C16-C17	2.93	113.71	106.44
5	B	802	HEM	CHD-C1D-C2D	-2.89	120.46	124.98
8	B	806	10M	C15-C20-C19	2.88	115.99	110.00
5	B	801	HEM	C4D-C3D-C2D	-2.87	102.71	106.90
5	B	802	HEM	CAA-CBA-CGA	-2.74	106.07	113.76
8	B	807	10M	O4-C16-C18	2.72	114.63	109.69
5	B	802	HEM	CHA-C4D-ND	2.70	127.72	124.38
5	B	801	HEM	C4C-CHD-C1D	2.64	126.04	122.56
5	B	801	HEM	CMA-C3A-C2A	2.59	129.83	124.94
5	B	801	HEM	O2D-CGD-O1D	-2.58	116.88	123.30
10	C	201	HEC	C1D-C2D-C3D	-2.57	105.21	107.00
5	B	802	HEM	C2C-C3C-C4C	-2.55	105.12	106.90
5	B	801	HEM	CAD-CBD-CGD	-2.53	108.16	113.60
8	B	806	10M	C22-C21-C14	2.48	115.34	109.68
5	B	801	HEM	O2D-CGD-CBD	2.45	121.90	114.03
8	B	807	10M	C11-O1-C12	2.45	117.09	112.58
10	C	201	HEC	CBD-CAD-C3D	-2.40	108.53	112.62
5	B	802	HEM	CMB-C2B-C3B	2.37	134.10	128.30
5	B	801	HEM	CMD-C2D-C1D	2.34	128.60	125.04
10	C	201	HEC	CBA-CAA-C2A	-2.33	108.68	112.60
8	B	807	10M	O10-C22-C11	2.23	114.37	110.27
5	B	802	HEM	CAB-C3B-C4B	-2.18	114.31	124.47
10	C	201	HEC	O2D-CGD-CBD	2.17	121.00	114.03
5	B	801	HEM	CHA-C4D-C3D	-2.13	121.33	125.33
10	C	201	HEC	O1D-CGD-CBD	-2.09	116.38	123.08
8	B	807	10M	O1-C12-C14	2.08	114.14	109.75
5	B	802	HEM	CAD-C3D-C2D	-2.07	124.03	127.88
5	B	802	HEM	CHA-C4D-C3D	-2.06	121.47	125.33
5	B	801	HEM	CBD-CAD-C3D	-2.02	107.00	112.63
10	C	201	HEC	CMC-C2C-C1C	-2.02	125.36	128.46
5	B	802	HEM	CMC-C2C-C3C	2.02	128.45	124.68
5	B	801	HEM	CAD-C3D-C2D	-2.01	124.13	127.88
5	B	802	HEM	CAB-C3B-C2B	2.01	135.22	128.60

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	807	10M	C7-C8-C9-C10
8	B	806	10M	C7-C8-C9-C10
8	B	806	10M	C2-C3-C4-C5
8	B	806	10M	C4-C5-C6-C7
8	B	806	10M	C6-C7-C8-C9
8	B	806	10M	C3-C4-C5-C6
8	B	807	10M	C6-C7-C8-C9
8	B	806	10M	C5-C6-C7-C8
8	B	806	10M	C1-C2-C3-C4
8	B	806	10M	C21-C14-O3-C15
8	B	807	10M	C18-C16-C17-O5
8	B	806	10M	C12-C14-O3-C15
5	B	801	HEM	CAA-CBA-CGA-O1A
10	C	201	HEC	CAD-CBD-CGD-O2D
5	B	801	HEM	CAA-CBA-CGA-O2A
5	B	802	HEM	CAA-CBA-CGA-O1A
5	B	802	HEM	CAD-CBD-CGD-O2D
10	C	201	HEC	CAD-CBD-CGD-O1D
5	B	802	HEM	CAA-CBA-CGA-O2A
5	B	802	HEM	CAD-CBD-CGD-O1D
5	B	801	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

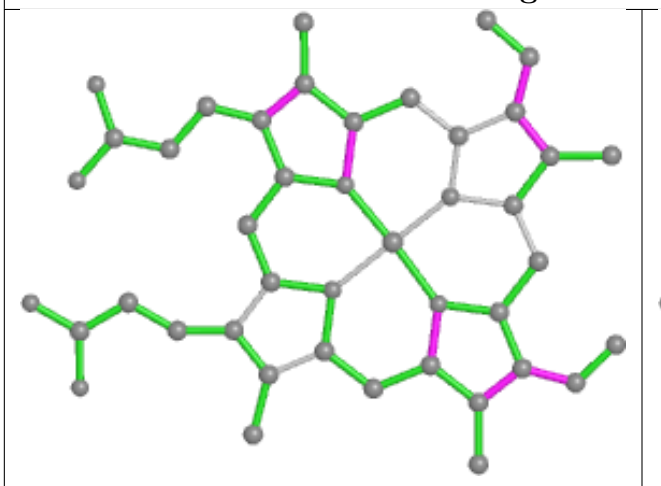
6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	801	HEM	5	0
5	B	802	HEM	3	0
8	B	807	10M	1	0
7	B	804	CYN	1	0
8	B	806	10M	1	0
10	C	201	HEC	6	0

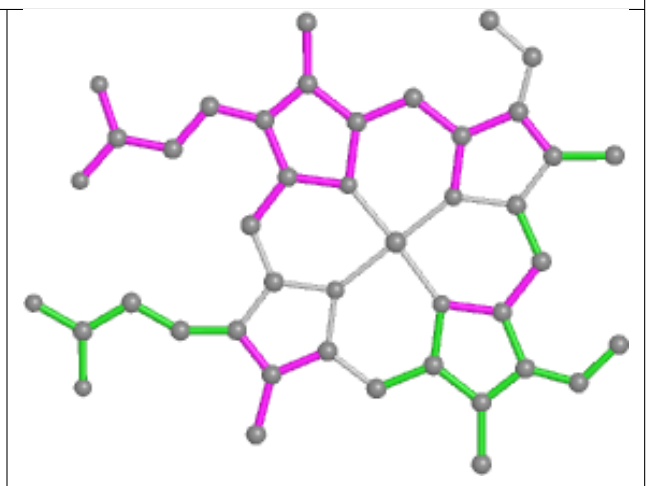
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

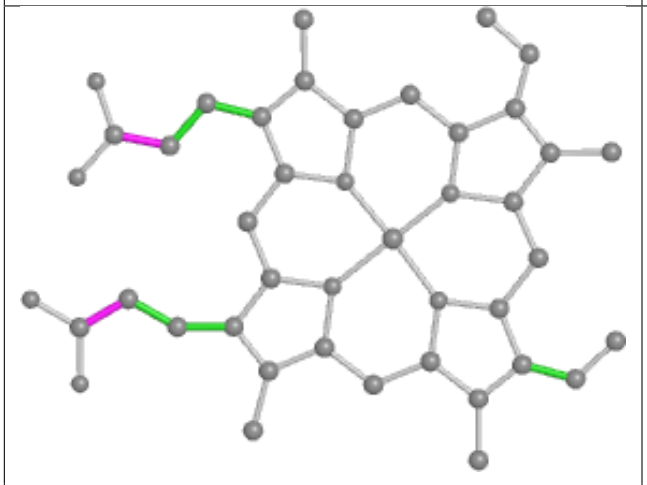
Ligand HEM B 801



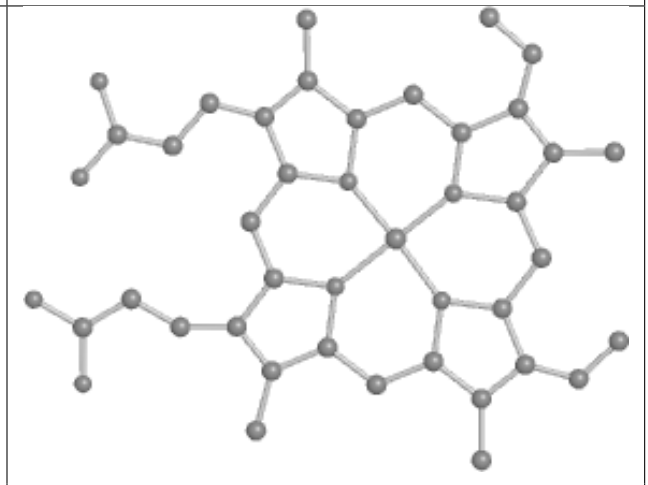
Bond lengths



Bond angles

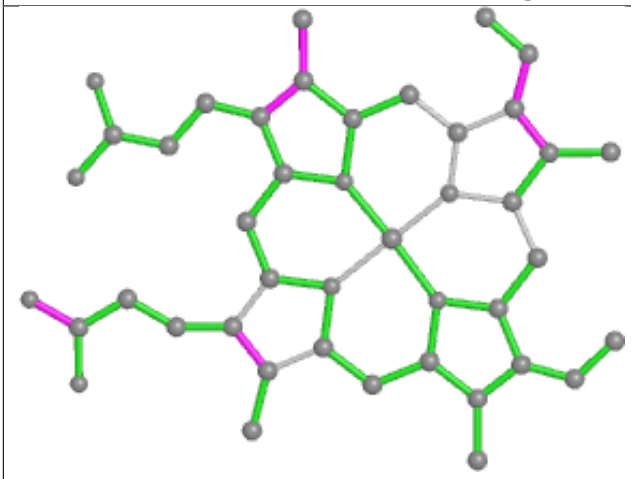


Torsions

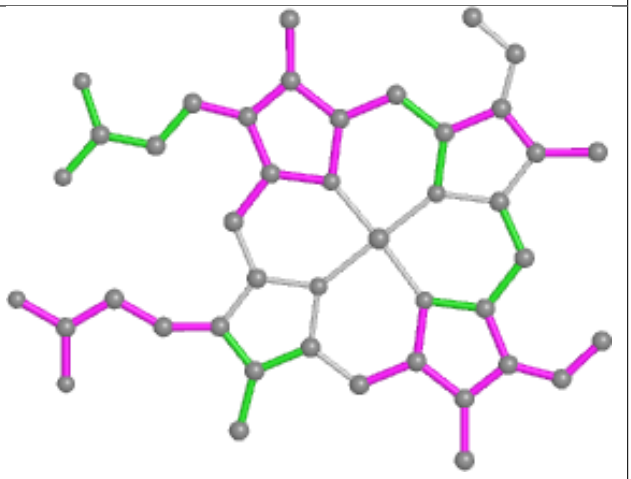


Rings

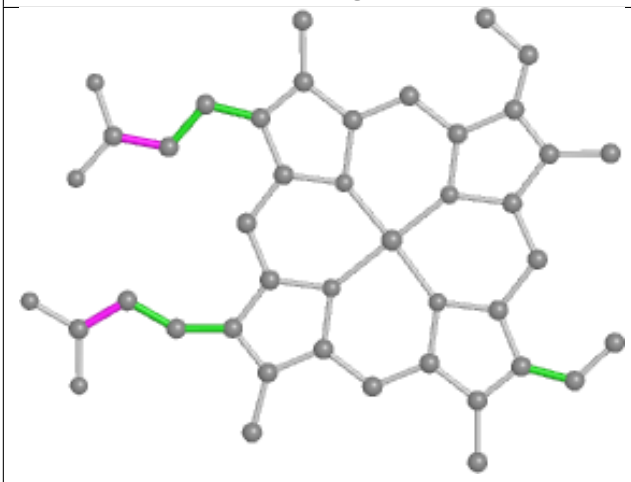
Ligand HEM B 802



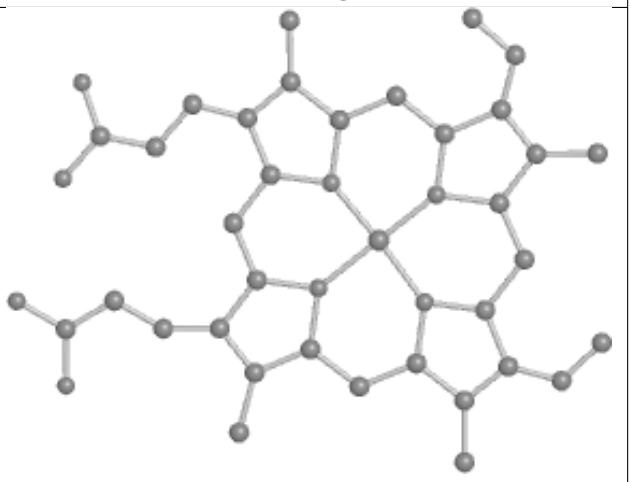
Bond lengths



Bond angles

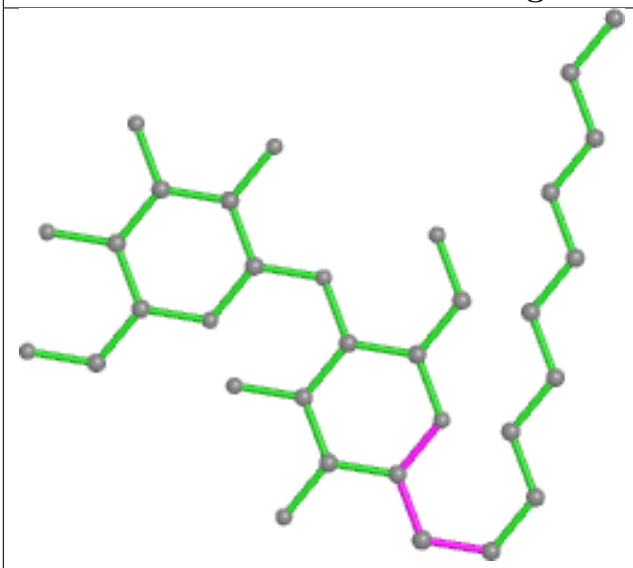


Torsions

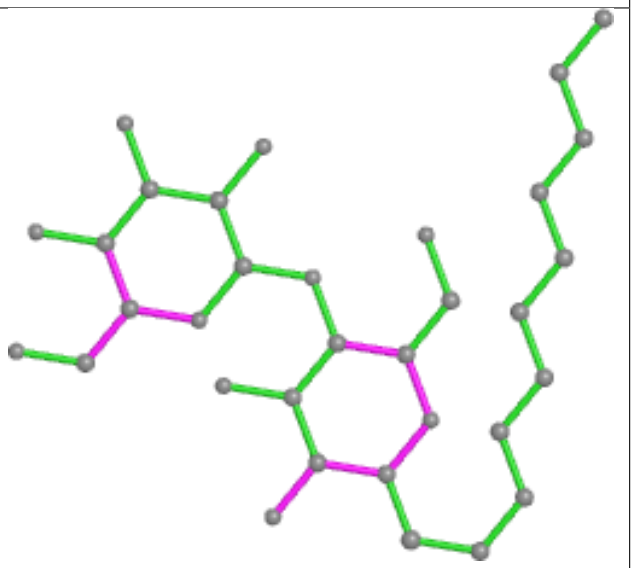


Rings

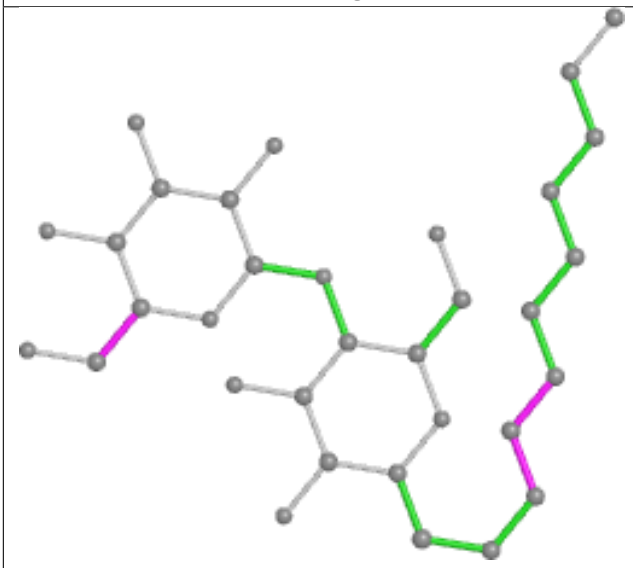
Ligand 10M B 807



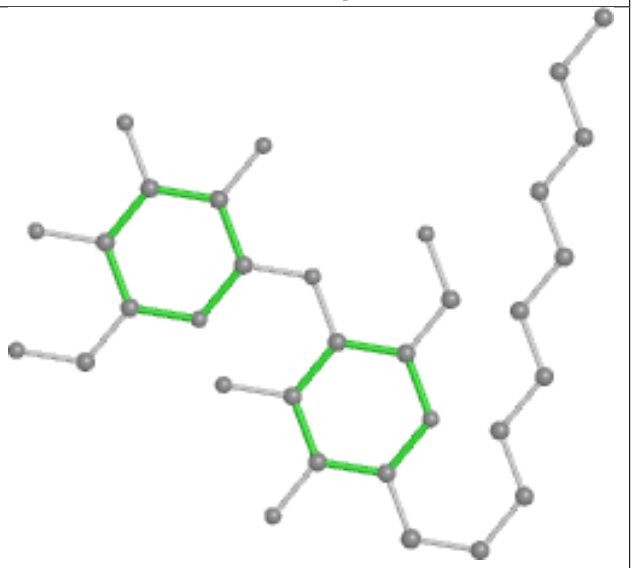
Bond lengths



Bond angles

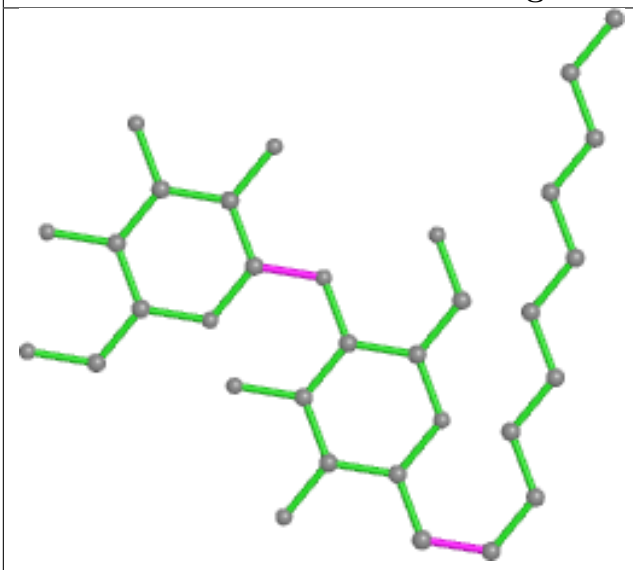


Torsions

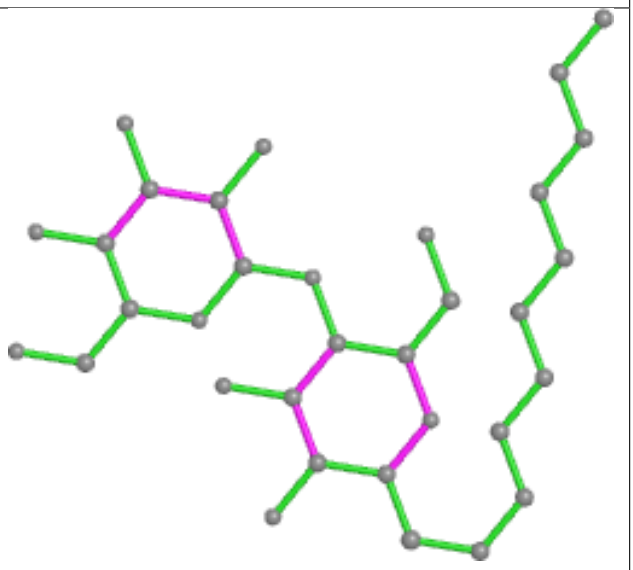


Rings

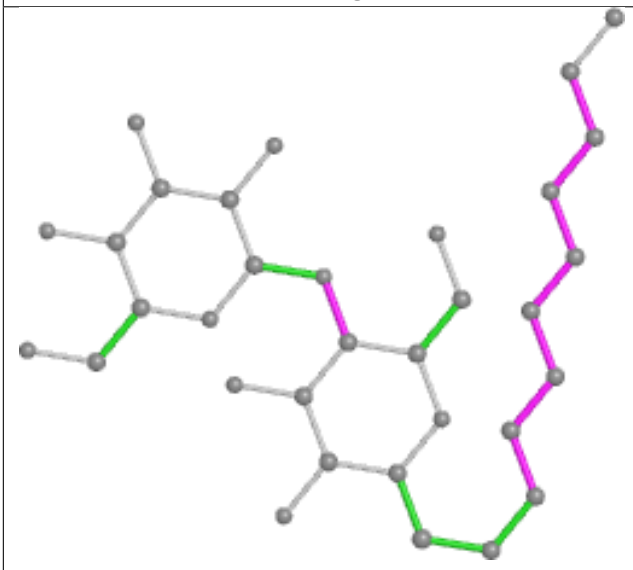
Ligand 10M B 806



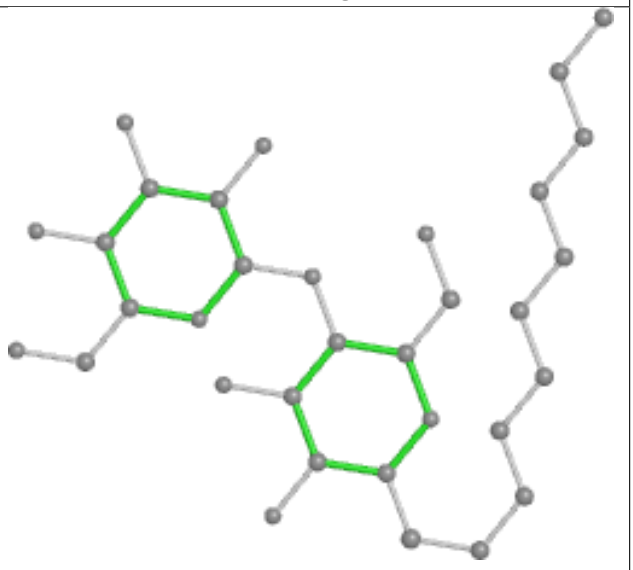
Bond lengths



Bond angles

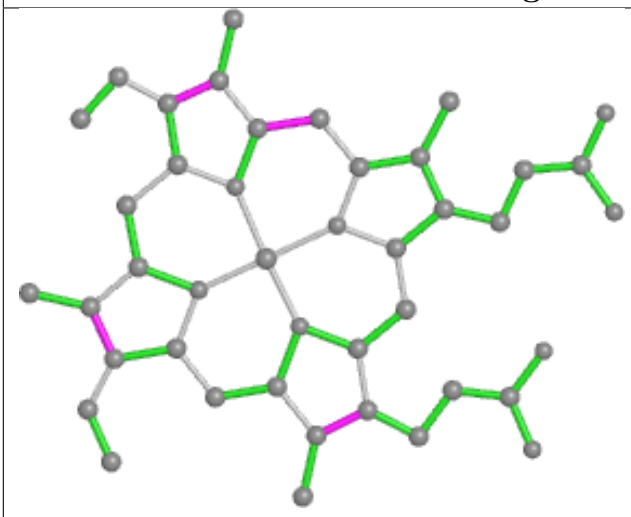


Torsions

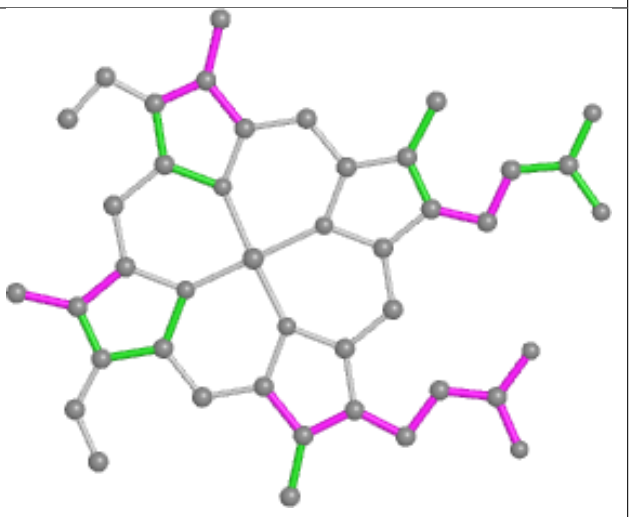


Rings

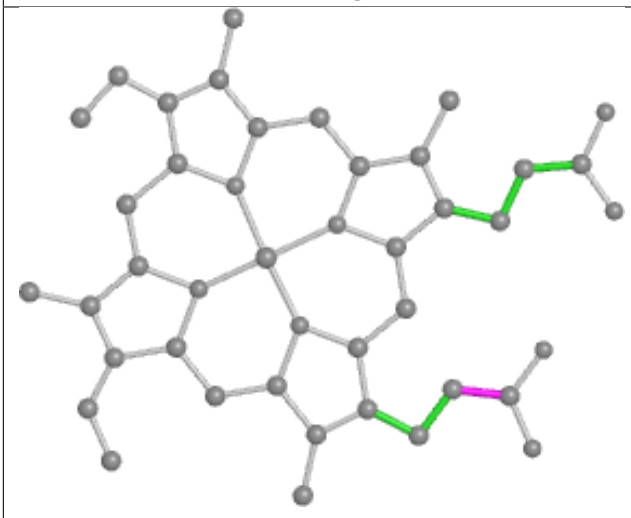
Ligand HEC C 201



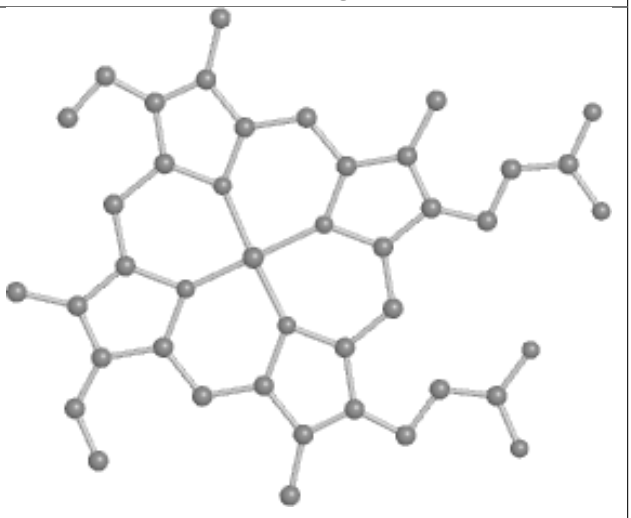
Bond lengths



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	L	213/213 (100%)	-0.32	2 (0%) 84 86	37, 49, 70, 113	0
2	H	225/225 (100%)	-0.01	14 (6%) 20 21	37, 49, 83, 163	0
3	B	449/465 (96%)	0.54	68 (15%) 2 1	42, 65, 100, 137	0
4	C	142/146 (97%)	0.21	8 (5%) 24 25	41, 64, 91, 106	0
All	All	1029/1049 (98%)	0.20	92 (8%) 9 9	37, 58, 95, 163	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	65	ILE	7.1
3	B	352	PHE	6.3
3	B	136	PHE	6.0
2	H	225	GLY	5.9
3	B	206	VAL	5.7
3	B	88	LEU	5.7
3	B	68	LEU	5.6
3	B	297	ARG	5.5
3	B	299	ARG	5.4
3	B	129	TRP	4.9
3	B	388	TRP	4.8
2	H	142	THR	4.8
3	B	381	ARG	4.8
3	B	69	LEU	4.5
3	B	214	TRP	4.4
3	B	356	TYR	4.3
3	B	209	TRP	4.3
3	B	128	LEU	4.2
3	B	384	VAL	4.2
3	B	296	ASN	4.2
3	B	301	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
3	B	64	LEU	4.1
3	B	202	TRP	4.1
3	B	210	VAL	4.1
2	H	145	SER	3.9
3	B	127	GLU	3.9
3	B	89	TYR	3.8
3	B	357	ALA	3.8
3	B	218	MET	3.7
3	B	156	PHE	3.7
3	B	385	LEU	3.6
4	C	30	TYR	3.6
3	B	359	ILE	3.6
2	H	143	THR	3.4
3	B	217	ILE	3.4
3	B	164	ARG	3.4
3	B	72	PHE	3.3
3	B	382	SER	3.3
2	H	144	GLY	3.2
3	B	351	ALA	3.2
4	C	5	PHE	3.2
3	B	377	ALA	3.1
2	H	139	CYS	3.1
4	C	34	LYS	3.1
3	B	360	VAL	3.0
3	B	124	THR	3.0
3	B	203	TRP	3.0
3	B	355	ALA	3.0
1	L	212	ASN	2.9
3	B	67	TRP	2.8
2	H	170	LEU	2.7
3	B	96	ILE	2.7
2	H	195	THR	2.7
3	B	208	LEU	2.7
3	B	114	LEU	2.7
3	B	298	ARG	2.7
3	B	379	ASP	2.6
3	B	95	TRP	2.6
3	B	137	LEU	2.5
3	B	374	ILE	2.5
3	B	125	GLY	2.5
3	B	61	THR	2.5
3	B	380	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
4	C	73	TYR	2.4
4	C	89	GLU	2.4
3	B	233	ASP	2.4
3	B	207	HIS	2.4
2	H	203	SER	2.4
3	B	163	LEU	2.4
4	C	67	LEU	2.4
3	B	142	ILE	2.4
3	B	135	GLU	2.4
2	H	194	VAL	2.3
3	B	300	ARG	2.3
2	H	169	SER	2.3
2	H	202	GLN	2.3
1	L	213	GLU	2.3
3	B	353	TYR	2.3
3	B	361	MET	2.3
4	C	66	THR	2.2
2	H	197	SER	2.2
3	B	123	LEU	2.2
4	C	62	VAL	2.2
3	B	383	GLN	2.1
3	B	120	LEU	2.1
3	B	348	GLY	2.1
3	B	86	CYS	2.1
3	B	91	PRO	2.1
3	B	378	MET	2.1
2	H	196	SER	2.1
3	B	271	TRP	2.0
3	B	126	ASN	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

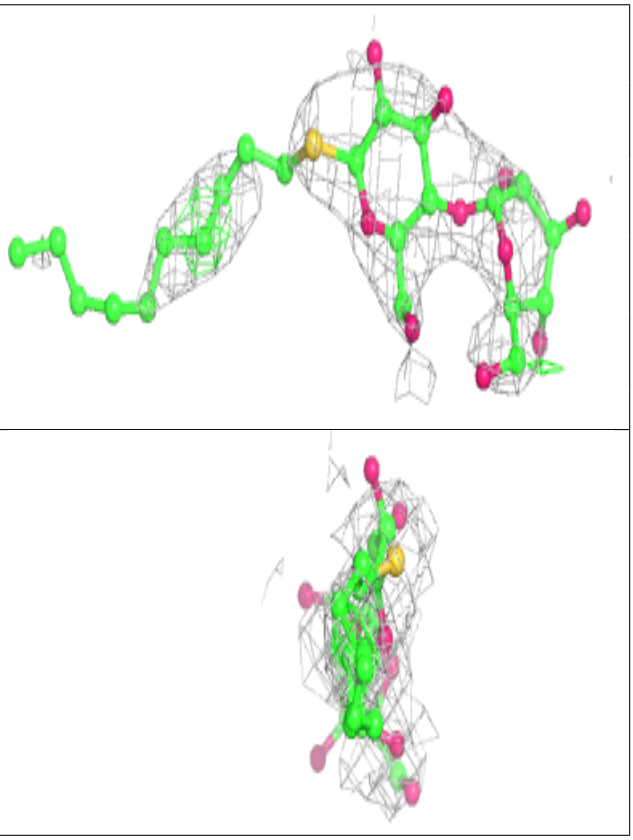
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	10M	B	806	33/33	0.81	0.44	101,131,158,159	0
8	10M	B	807	33/33	0.94	0.34	76,86,108,117	0
5	HEM	B	801	43/43	0.96	0.28	41,48,57,64	0
5	HEM	B	802	43/43	0.97	0.27	40,45,46,48	0
10	HEC	C	201	43/43	0.98	0.17	35,42,49,53	0
6	FE	B	803	1/1	0.99	0.17	47,47,47,47	0
7	CYN	B	804	2/2	0.99	0.24	47,47,47,49	0
9	CA	B	808	1/1	0.99	0.23	53,53,53,53	0
7	CYN	B	805	2/2	0.99	0.23	39,39,39,42	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.

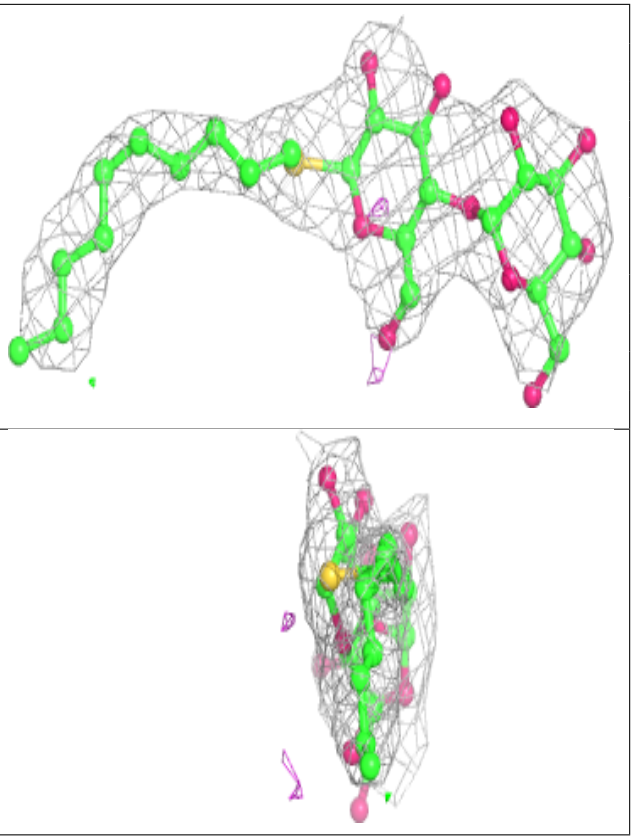
Electron density around 10M B 806:

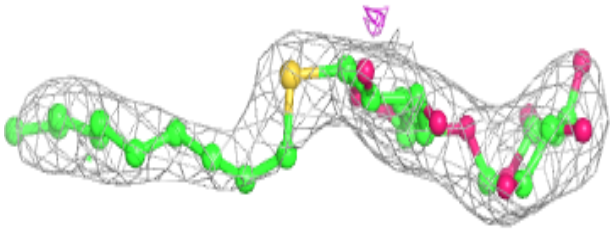
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 10M B 807:

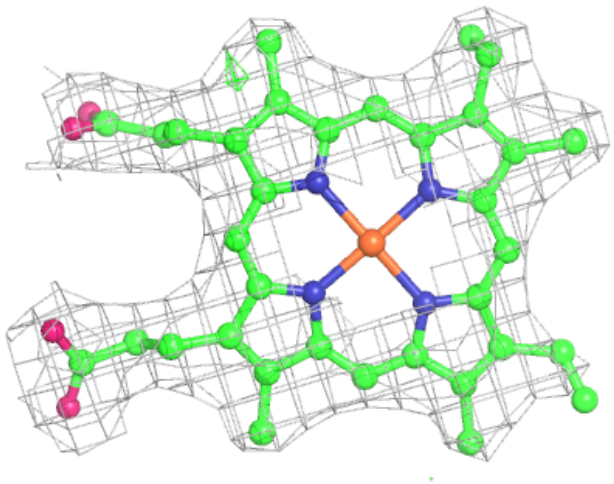
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

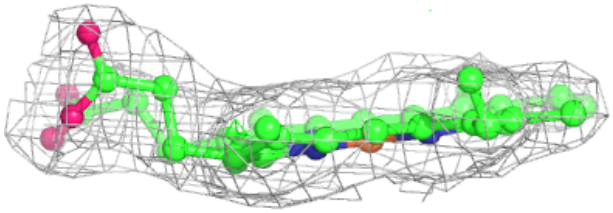


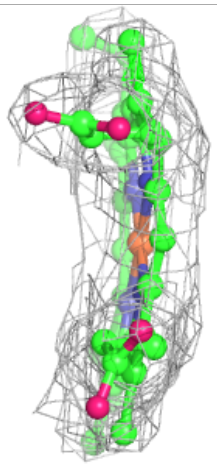


Electron density around HEM B 801:

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

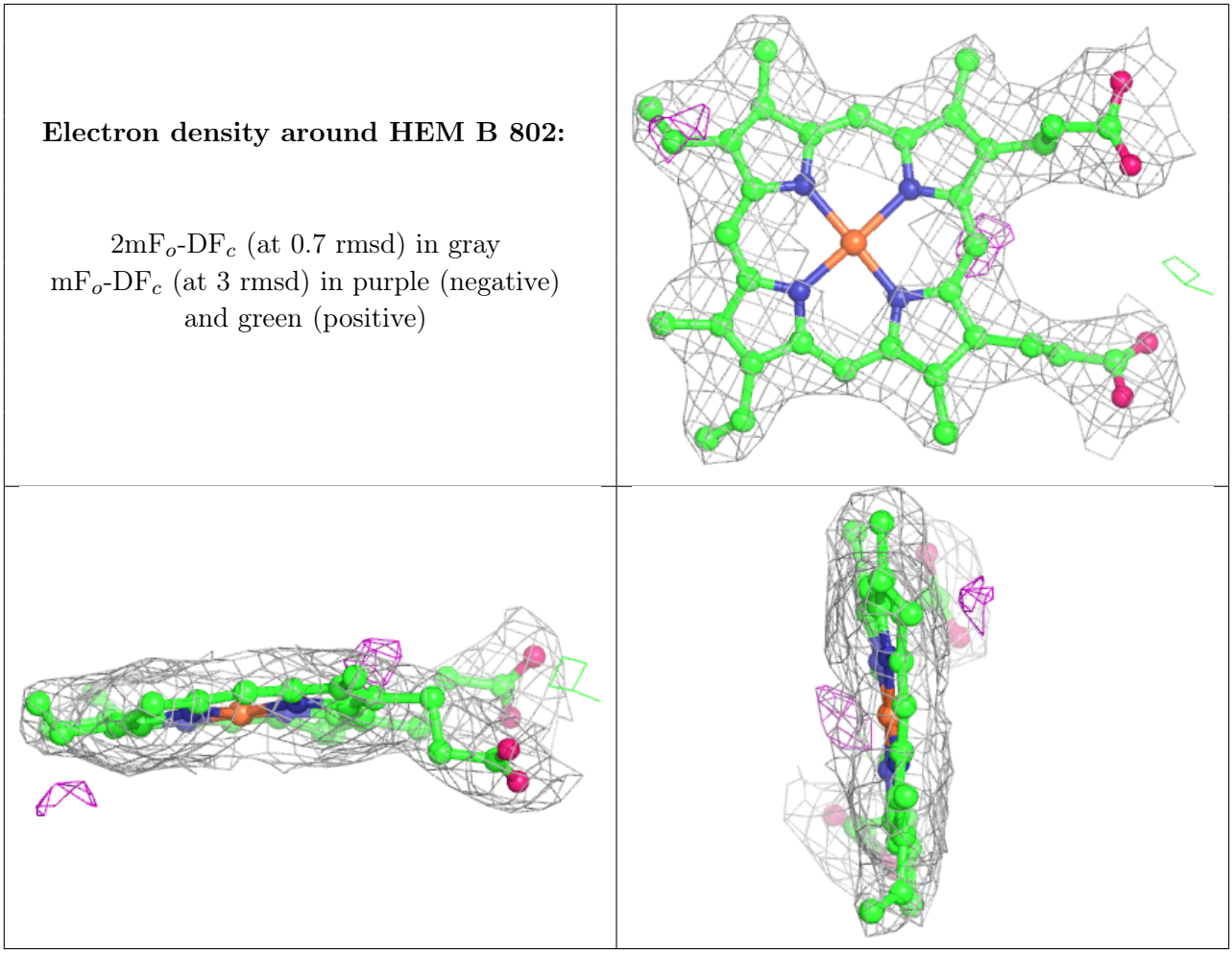






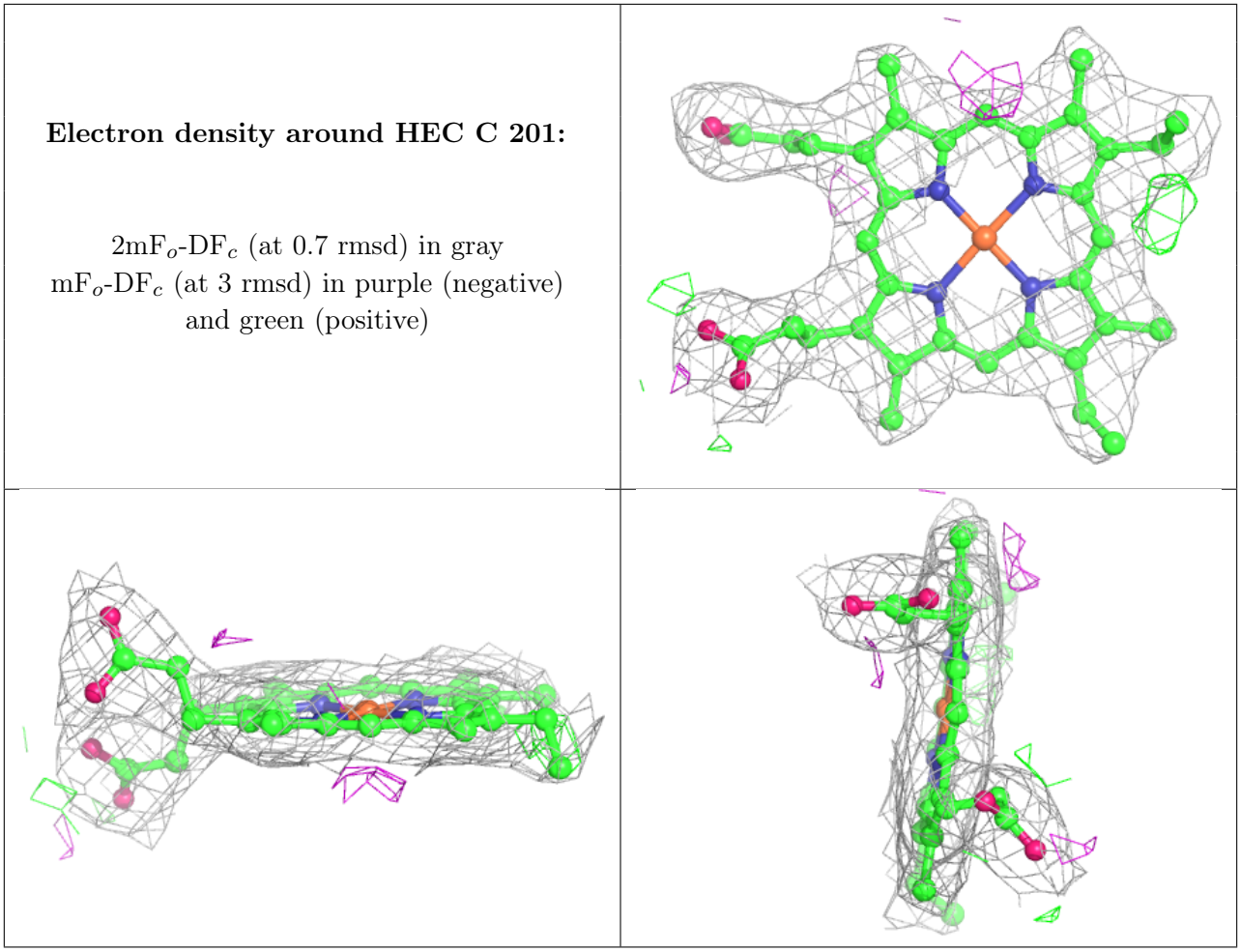
Electron density around HEM B 802:

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



Electron density around HEC C 201:

$2mF_o$-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.