Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 08:00 AM EDT

PDB ID	:	3WFC / pdb_00003wfc
Title	:	Reduced and carbonmonoxide-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	:	2.50 Å(reported)

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

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

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

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

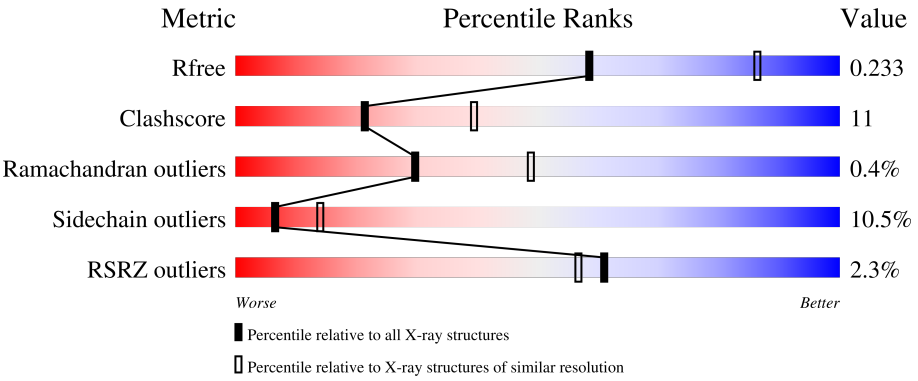
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	78% 17%
2	H	225	2% 75% 22%
3	B	465	3% 72% 20% 5%
4	C	146	3% 82% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HEC	C	201	X	-	-	-
7	CMO	B	804	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 8541 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.

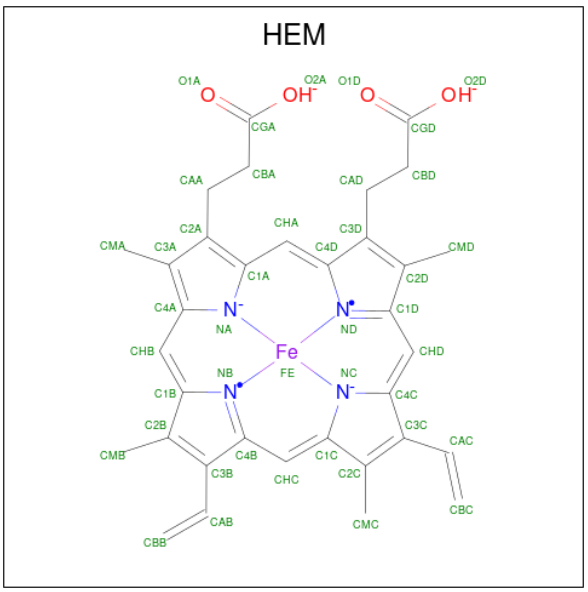
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	142	Total	C	N	O	S	0	0	0
			1123	720	195	202	6			

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 (CCD ID: HEM) (formula:

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

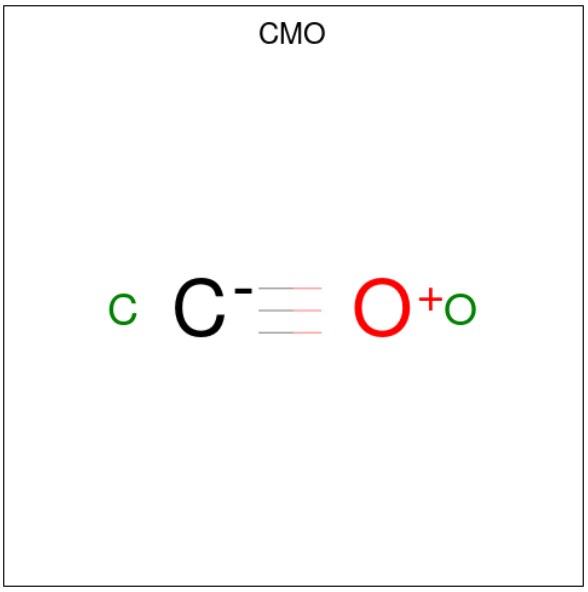


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

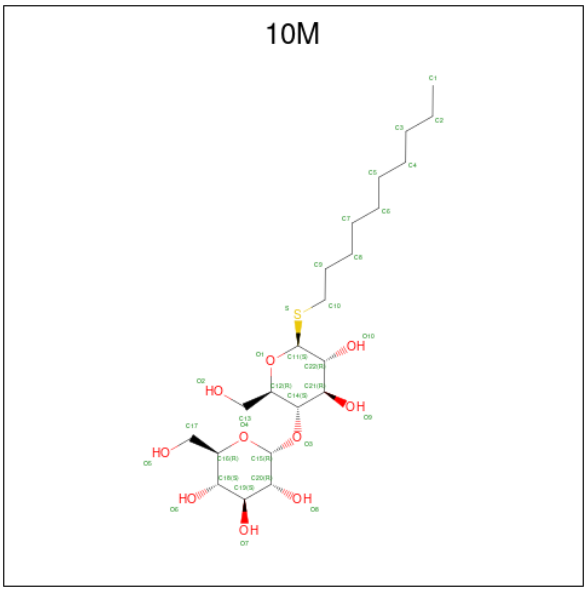
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe	0	0
			1	1		

- Molecule 7 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

- Molecule 8 is decyl 4-O-alpha-D-glucopyranosyl-1-thio-beta-D-glucopyranoside (CCD ID: 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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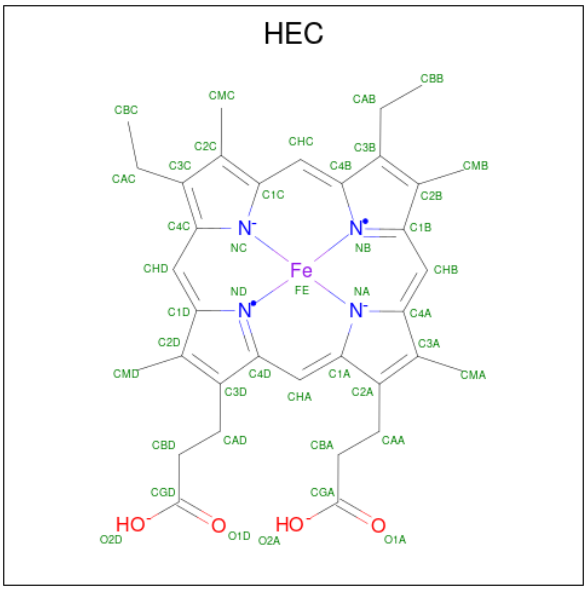
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O S 33 22 10 1	0	0

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 10 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 11 is water.

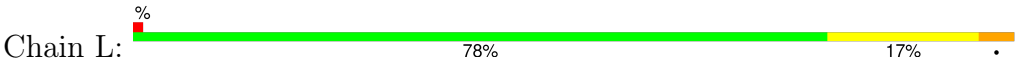
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	90	Total O 90 90	0	0
11	H	86	Total O 86 86	0	0
11	B	52	Total O 52 52	0	0
11	C	52	Total O 52 52	0	0

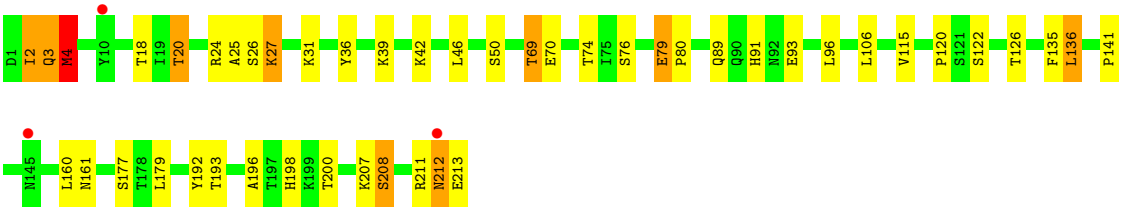
3 Residue-property plots (i)

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: antibody fab fragment light chain

Chain L:

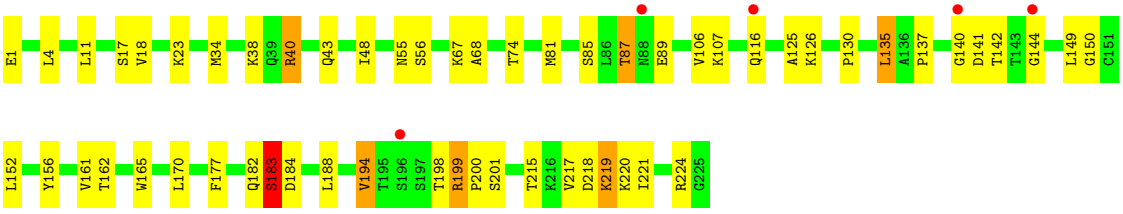




• Molecule 2: antibody fab fragment heavy chain

Chain H:

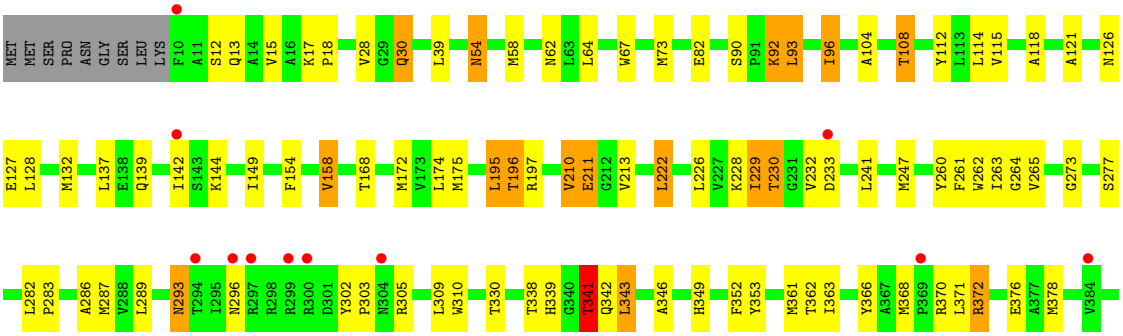


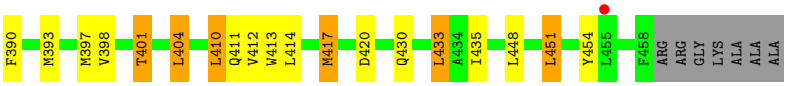


• Molecule 3: Nitric oxide reductase subunit B

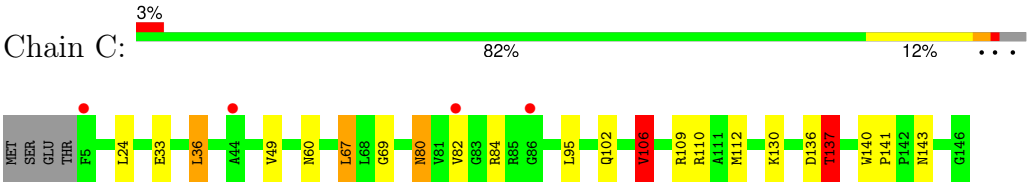
Chain B:







• 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	90.67Å 107.07Å 196.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.37 – 2.50 33.37 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (33.37-2.50) 98.6 (33.37-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.34 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.191 , 0.232 0.191 , 0.233	Depositor DCC
R_{free} test set	3348 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.0	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	8541	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: CMO, 10M, HEM, FE, CA, HEC

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	0.93	0/1709	1.05	3/2317 (0.1%)
2	H	0.93	0/1735	1.10	2/2367 (0.1%)
3	B	0.77	0/3693	1.02	3/5039 (0.1%)
4	C	0.74	0/1153	1.06	5/1559 (0.3%)
All	All	0.84	0/8290	1.05	13/11282 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	106	VAL	CB-CA-C	7.59	118.00	110.94
4	C	137	THR	N-CA-C	-6.34	103.68	112.30
3	B	417	MET	CA-C-N	-6.09	114.37	120.21
3	B	417	MET	C-N-CA	-6.09	114.37	120.21
1	L	4	MET	CB-CG-SD	-5.80	95.30	112.70
1	L	208	SER	N-CA-C	5.51	115.82	108.38
1	L	93	GLU	CB-CA-C	-5.42	100.23	110.16
2	H	177	PHE	CA-C-N	-5.36	114.26	119.78
2	H	177	PHE	C-N-CA	-5.36	114.26	119.78
4	C	141	PRO	CA-C-N	5.31	125.38	119.32
4	C	141	PRO	C-N-CA	5.31	125.38	119.32
4	C	106	VAL	N-CA-CB	5.29	115.89	110.23
3	B	341	THR	N-CA-CB	-5.25	103.08	111.43

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	36	0
2	H	1692	0	1647	32	0
3	B	3576	0	3619	93	0
4	C	1123	0	1092	27	0
5	B	86	0	60	10	0
6	B	1	0	0	0	0
7	B	4	0	0	3	0
8	B	66	0	84	4	0
9	B	1	0	0	0	0
10	C	43	0	30	2	0
11	B	52	0	0	1	0
11	C	52	0	0	1	0
11	H	86	0	0	2	0
11	L	90	0	0	3	0
All	All	8541	0	8138	178	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 11.

All (178) 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	1.35	1.05
2:H:107:LYS:HB2	11:H:319:HOH:O	1.63	0.99
3:B:211:GLU:OE2	7:B:805:CMO:C	2.13	0.95
8:B:806:10M:H17	8:B:807:10M:O8	1.69	0.93
2:H:48:ILE:HG21	2:H:81:MET:HE1	1.49	0.92
2:H:48:ILE:HG21	2:H:81:MET:CE	2.02	0.89
1:L:79:GLU:HG3	1:L:80:PRO:HD2	1.52	0.88
3:B:230:THR:HG23	3:B:232:VAL:H	1.39	0.86
3:B:104:ALA:O	3:B:108:THR:HG23	1.76	0.84
3:B:126:ASN:HB2	3:B:132:MET:HE2	1.59	0.83
3:B:126:ASN:HB2	3:B:132:MET:CE	2.08	0.82
1:L:79:GLU:HG3	1:L:80:PRO:CD	2.10	0.80
3:B:338:THR:O	3:B:341:THR:HB	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:137:LEU:HA	3:B:139:GLN:HE22	1.46	0.80
2:H:48:ILE:HD13	2:H:81:MET:HE1	1.62	0.80
2:H:87:THR:HG22	2:H:89:GLU:H	1.49	0.77
2:H:183:SER:OG	2:H:184:ASP:N	2.10	0.75
2:H:40:ARG:O	2:H:43:GLN:HB2	1.90	0.70
3:B:352:PHE:HB3	5:B:801:HEM:HBC1	1.73	0.70
3:B:302:TYR:OH	3:B:370:ARG:NH1	2.26	0.69
3:B:195:LEU:HD11	4:C:67:LEU:HD13	1.74	0.68
3:B:104:ALA:O	3:B:108:THR:CG2	2.41	0.68
3:B:197:ARG:HD3	4:C:36:LEU:HD23	1.75	0.68
3:B:126:ASN:CB	3:B:132:MET:HE2	2.24	0.68
3:B:229:ILE:HD11	3:B:366:TYR:HD2	1.58	0.67
3:B:430:GLN:HE21	4:C:110:ARG:HH22	1.40	0.67
2:H:55:ASN:O	2:H:56:SER:HB2	1.95	0.67
8:B:806:10M:C17	8:B:807:10M:O8	2.42	0.66
3:B:126:ASN:CB	3:B:132:MET:CE	2.73	0.66
3:B:121:ALA:CA	3:B:132:MET:HE1	2.22	0.64
3:B:137:LEU:HA	3:B:139:GLN:NE2	2.13	0.64
1:L:50:SER:H	1:L:91:HIS:HE1	1.46	0.63
2:H:194:VAL:HG13	2:H:198:THR:HB	1.80	0.63
1:L:136:LEU:HD23	1:L:136:LEU:N	2.14	0.62
3:B:126:ASN:ND2	3:B:132:MET:HE2	2.14	0.62
3:B:197:ARG:CD	4:C:36:LEU:HD23	2.30	0.62
3:B:196:THR:HB	3:B:263:ILE:O	2.00	0.62
3:B:341:THR:CG2	3:B:343:LEU:H	2.14	0.61
3:B:139:GLN:HE21	3:B:144:LYS:HE3	1.65	0.60
4:C:80:ASN:HD22	4:C:80:ASN:H	1.48	0.60
3:B:430:GLN:HE21	4:C:110:ARG:NH2	2.00	0.60
3:B:126:ASN:CG	3:B:132:MET:HE2	2.26	0.60
4:C:137:THR:HG21	4:C:140:TRP:O	2.02	0.59
1:L:161:ASN:HD22	1:L:177:SER:HA	1.66	0.59
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.86	0.59
3:B:420:ASP:OD1	4:C:143:ASN:HB2	2.02	0.59
1:L:3:GLN:HG2	1:L:26:SER:HB3	1.83	0.59
3:B:168:THR:O	3:B:172:MET:HG2	2.03	0.59
3:B:222:LEU:HD12	3:B:287:MET:HE2	1.84	0.59
3:B:229:ILE:HD11	3:B:366:TYR:CD2	2.37	0.59
1:L:2:ILE:CD1	1:L:25:ALA:HB1	2.33	0.58
2:H:4:LEU:HD22	2:H:34:MET:HE1	1.85	0.58
2:H:87:THR:HG22	2:H:89:GLU:N	2.16	0.58
1:L:135:PHE:C	1:L:136:LEU:HD23	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:218:ASP:O	2:H:219:LYS:HD2	2.03	0.57
3:B:341:THR:HG22	3:B:343:LEU:H	1.69	0.57
1:L:160:LEU:HD11	2:H:182:GLN:HG3	1.85	0.57
3:B:411:GLN:HB2	3:B:433:LEU:HD21	1.86	0.56
3:B:126:ASN:CG	3:B:132:MET:CE	2.78	0.56
3:B:393:MET:HE3	3:B:451:LEU:HB2	1.87	0.56
2:H:87:THR:CG2	2:H:89:GLU:H	2.17	0.56
1:L:50:SER:H	1:L:91:HIS:CE1	2.24	0.55
3:B:352:PHE:HB3	5:B:801:HEM:CBC	2.37	0.55
1:L:136:LEU:HD13	1:L:196:ALA:HB2	1.89	0.55
1:L:24:ARG:HG3	1:L:25:ALA:N	2.22	0.55
3:B:393:MET:HE1	3:B:451:LEU:HD23	1.88	0.54
2:H:125:ALA:HB2	2:H:184:ASP:HB3	1.90	0.53
3:B:210:VAL:CG1	5:B:802:HEM:C2B	2.91	0.53
3:B:341:THR:HG22	3:B:343:LEU:N	2.24	0.53
4:C:80:ASN:HD21	4:C:84:ARG:HH22	1.55	0.53
1:L:115:VAL:HG13	1:L:136:LEU:HD22	1.90	0.52
3:B:142:ILE:HG12	11:B:922:HOH:O	2.09	0.52
3:B:413:TRP:HA	3:B:417:MET:HG3	1.92	0.52
3:B:264:GLY:HA2	4:C:136:ASP:O	2.09	0.52
3:B:261:PHE:HB3	3:B:262:TRP:CE2	2.46	0.51
3:B:397:MET:O	3:B:401:THR:HG23	2.11	0.51
1:L:141:PRO:O	1:L:198:HIS:HE1	1.94	0.51
3:B:197:ARG:CZ	4:C:33:GLU:OE2	2.59	0.51
3:B:226:LEU:O	3:B:230:THR:HG22	2.11	0.50
3:B:397:MET:O	3:B:401:THR:CG2	2.60	0.50
1:L:27:LYS:HD3	11:L:342:HOH:O	2.11	0.50
3:B:158:VAL:HG13	3:B:175:MET:SD	2.52	0.49
2:H:199:ARG:HA	2:H:201:SER:N	2.27	0.49
1:L:161:ASN:ND2	1:L:177:SER:OG	2.45	0.49
3:B:349:HIS:CD2	5:B:801:HEM:NC	2.80	0.49
1:L:193:THR:OG1	1:L:208:SER:HB3	2.12	0.49
5:B:802:HEM:C4A	7:B:804:CMO:C	2.86	0.49
4:C:80:ASN:ND2	4:C:84:ARG:HH22	2.11	0.49
2:H:137:PRO:HD3	2:H:149:LEU:CD2	2.43	0.48
3:B:341:THR:HG22	3:B:343:LEU:HB2	1.95	0.48
3:B:13:GLN:NE2	3:B:82:GLU:HB2	2.28	0.48
3:B:229:ILE:CD1	3:B:366:TYR:CD2	2.96	0.48
4:C:137:THR:CG2	4:C:140:TRP:O	2.61	0.48
2:H:38:LYS:HE2	2:H:40:ARG:HD3	1.96	0.48
2:H:4:LEU:CD2	2:H:34:MET:HE1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:ALA:HB1	2:H:81:MET:HE2	1.96	0.48
1:L:2:ILE:HD11	1:L:25:ALA:HB1	1.96	0.47
1:L:160:LEU:CD1	2:H:182:GLN:HG3	2.44	0.47
2:H:165:TRP:HZ3	2:H:221:ILE:CD1	2.27	0.47
3:B:273:GLY:O	3:B:277:SER:HB2	2.14	0.47
1:L:122:SER:O	1:L:126:THR:HG23	2.15	0.47
1:L:193:THR:HA	1:L:208:SER:HB3	1.97	0.47
2:H:135:LEU:HB2	2:H:150:GLY:C	2.40	0.47
3:B:58:MET:HE2	4:C:60:ASN:ND2	2.30	0.47
3:B:139:GLN:O	3:B:144:LYS:NZ	2.45	0.47
2:H:199:ARG:HD2	2:H:200:PRO:HA	1.96	0.47
3:B:54:ASN:H	3:B:54:ASN:HD22	1.62	0.47
1:L:39:LYS:NZ	11:L:376:HOH:O	2.48	0.46
3:B:260:TYR:HB3	3:B:265:VAL:HG21	1.96	0.46
3:B:310:TRP:HB3	3:B:362:THR:OG1	2.16	0.46
8:B:807:10M:H15	8:B:807:10M:O9	2.15	0.46
1:L:4:MET:HE3	1:L:4:MET:HB2	1.52	0.46
1:L:69:THR:HG22	1:L:70:GLU:HG2	1.96	0.46
1:L:212:ASN:HB2	1:L:213:GLU:H	1.54	0.46
3:B:118:ALA:O	3:B:121:ALA:HB3	2.16	0.46
4:C:80:ASN:ND2	4:C:84:ARG:NH2	2.63	0.46
4:C:82:VAL:HG21	4:C:130:LYS:HA	1.97	0.46
3:B:82:GLU:OE1	3:B:228:LYS:HE3	2.15	0.46
4:C:106:VAL:HG22	4:C:109:ARG:HB2	1.98	0.46
3:B:430:GLN:NE2	4:C:110:ARG:HH22	2.10	0.46
3:B:282:LEU:N	3:B:283:PRO:HD2	2.31	0.46
1:L:42:LYS:NZ	11:L:334:HOH:O	2.47	0.46
3:B:289:LEU:O	3:B:293:ASN:HB2	2.16	0.46
4:C:80:ASN:HD22	4:C:80:ASN:N	2.09	0.46
3:B:353:TYR:N	5:B:801:HEM:HBC1	2.31	0.45
3:B:342:GLN:H	3:B:411:GLN:HE22	1.64	0.45
2:H:130:PRO:HB3	2:H:156:TYR:HB3	1.98	0.45
1:L:4:MET:HE3	1:L:4:MET:N	2.32	0.45
5:B:802:HEM:C1B	7:B:804:CMO:C	2.97	0.45
3:B:12:SER:O	3:B:15:VAL:HG22	2.17	0.45
3:B:62:ASN:ND2	3:B:112:TYR:OH	2.49	0.45
1:L:120:PRO:O	2:H:224:ARG:NH2	2.50	0.45
3:B:352:PHE:CB	5:B:801:HEM:HBC1	2.45	0.45
3:B:372:ARG:HH21	3:B:378:MET:HE1	1.82	0.45
4:C:80:ASN:HD21	4:C:84:ARG:NH2	2.14	0.45
3:B:92:LYS:O	3:B:96:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:73:MET:HG2	3:B:154:PHE:CE1	2.52	0.44
3:B:390:PHE:C	3:B:390:PHE:CD1	2.94	0.44
3:B:393:MET:HE3	3:B:451:LEU:CB	2.47	0.44
2:H:140:GLY:O	2:H:142:THR:HG22	2.17	0.44
2:H:183:SER:HG	2:H:184:ASP:N	2.12	0.44
3:B:412:VAL:HG11	8:B:807:10M:H5	2.00	0.44
1:L:192:TYR:O	1:L:208:SER:CB	2.65	0.44
3:B:30:GLN:NE2	3:B:67:TRP:HE1	2.15	0.44
3:B:28:VAL:HG22	3:B:451:LEU:CD1	2.47	0.44
3:B:342:GLN:H	3:B:411:GLN:NE2	2.16	0.44
3:B:410:LEU:HD22	3:B:414:LEU:CD1	2.48	0.43
4:C:112:MET:CE	10:C:201:HEC:NB	2.82	0.43
1:L:2:ILE:HD13	1:L:25:ALA:HB1	2.00	0.43
1:L:36:TYR:HE2	1:L:89:GLN:HE21	1.65	0.43
3:B:210:VAL:HG11	5:B:802:HEM:C2B	2.54	0.43
1:L:136:LEU:N	1:L:136:LEU:CD2	2.82	0.42
3:B:230:THR:HG23	3:B:232:VAL:N	2.21	0.42
1:L:115:VAL:HA	1:L:135:PHE:O	2.20	0.42
1:L:18:THR:OG1	1:L:76:SER:O	2.26	0.42
3:B:361:MET:HE3	3:B:454:TYR:CD2	2.55	0.42
4:C:112:MET:HE1	10:C:201:HEC:C1B	2.49	0.42
4:C:137:THR:HG23	4:C:140:TRP:H	1.85	0.42
3:B:210:VAL:HG13	5:B:802:HEM:C2B	2.54	0.41
3:B:341:THR:CG2	3:B:343:LEU:HB2	2.49	0.41
4:C:33:GLU:HA	4:C:36:LEU:HD22	2.02	0.41
3:B:139:GLN:H	3:B:139:GLN:CD	2.28	0.41
3:B:339:HIS:CD2	4:C:69:GLY:HA3	2.55	0.41
3:B:17:LYS:N	3:B:18:PRO:HD2	2.34	0.41
3:B:127:GLU:H	3:B:127:GLU:CD	2.28	0.41
3:B:247:MET:HE1	3:B:286:ALA:HB2	2.03	0.41
3:B:346:ALA:HB2	3:B:404:LEU:HB3	2.02	0.41
3:B:13:GLN:O	3:B:371:LEU:HD21	2.20	0.41
3:B:412:VAL:O	3:B:417:MET:HG2	2.21	0.41
3:B:303:PRO:HG3	3:B:376:GLU:OE1	2.21	0.41
4:C:102:GLN:NE2	11:C:313:HOH:O	2.53	0.41
1:L:20:THR:HB	1:L:74:THR:OG1	2.21	0.41
2:H:140:GLY:O	2:H:142:THR:N	2.52	0.41
2:H:194:VAL:HG13	2:H:198:THR:CB	2.49	0.40
3:B:197:ARG:NE	4:C:33:GLU:OE2	2.54	0.40
3:B:90:SER:OG	3:B:93:LEU:HB2	2.21	0.40
2:H:137:PRO:HD3	2:H:149:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:SER:HB3	11:H:376:HOH:O	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%)	200 (95%)	10 (5%)	1 (0%)	24 43
2	H	223/225 (99%)	211 (95%)	9 (4%)	3 (1%)	9 18
3	B	447/465 (96%)	426 (95%)	21 (5%)	0	100 100
4	C	140/146 (96%)	136 (97%)	4 (3%)	0	100 100
All	All	1021/1049 (97%)	973 (95%)	44 (4%)	4 (0%)	30 49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	141	ASP
1	L	211	ARG
2	H	183	SER
2	H	144	GLY

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%)	11 24
2	H	192/192 (100%)	167 (87%)	25 (13%)	4 8
3	B	360/371 (97%)	318 (88%)	42 (12%)	5 11
4	C	116/120 (97%)	108 (93%)	8 (7%)	14 30
All	All	857/872 (98%)	767 (90%)	90 (10%)	6 14

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

Mol	Chain	Res	Type
1	L	2	ILE
1	L	3	GLN
1	L	4	MET
1	L	20	THR
1	L	27	LYS
1	L	31	LYS
1	L	46	LEU
1	L	69	THR
1	L	79	GLU
1	L	96	LEU
1	L	106	LEU
1	L	136	LEU
1	L	179	LEU
1	L	207	LYS
1	L	212	ASN
2	H	1	GLU
2	H	11	LEU
2	H	18	VAL
2	H	23	LYS
2	H	40	ARG
2	H	67	LYS
2	H	74	THR
2	H	85	SER
2	H	87	THR
2	H	106	VAL
2	H	116	GLN
2	H	126	LYS
2	H	135	LEU
2	H	152	LEU
2	H	161	VAL
2	H	162	THR
2	H	170	LEU
2	H	183	SER

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Mol	Chain	Res	Type
2	H	188	LEU
2	H	194	VAL
2	H	199	ARG
2	H	215	THR
2	H	217	VAL
2	H	219	LYS
2	H	220	LYS
3	B	30	GLN
3	B	39	LEU
3	B	54	ASN
3	B	64	LEU
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	128	LEU
3	B	149	ILE
3	B	158	VAL
3	B	174	LEU
3	B	195	LEU
3	B	196	THR
3	B	210	VAL
3	B	211	GLU
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	293	ASN
3	B	296	ASN
3	B	305	ARG
3	B	309	LEU
3	B	330	THR
3	B	341	THR
3	B	343	LEU
3	B	363	ILE
3	B	368	MET
3	B	372	ARG
3	B	398	VAL

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Mol	Chain	Res	Type
3	B	401	THR
3	B	404	LEU
3	B	410	LEU
3	B	433	LEU
3	B	435	ILE
3	B	448	LEU
3	B	451	LEU
4	C	24	LEU
4	C	36	LEU
4	C	49	VAL
4	C	67	LEU
4	C	80	ASN
4	C	95	LEU
4	C	106	VAL
4	C	137	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	3	GLN
1	L	89	GLN
1	L	91	HIS
1	L	137	ASN
1	L	156	GLN
1	L	161	ASN
1	L	198	HIS
2	H	43	GLN
2	H	116	GLN
2	H	182	GLN
3	B	13	GLN
3	B	30	GLN
3	B	54	ASN
3	B	62	ASN
3	B	139	GLN
3	B	296	ASN
3	B	304	ASN
3	B	342	GLN
3	B	383	GLN
3	B	411	GLN
3	B	415	GLN
3	B	430	GLN
4	C	31	HIS

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Mol	Chain	Res	Type
4	C	60	ASN
4	C	80	ASN
4	C	96	GLN
4	C	102	GLN
4	C	105	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 oligosaccharides 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	9,3	50,50,50	1.81	7 (14%)	67,82,82	2.45	26 (38%)
7	CMO	B	804	-	0,1,1	-	-	-		
7	CMO	B	805	5,6	0,1,1	-	-	-		
8	10M	B	807	-	34,34,34	1.60	7 (20%)	44,45,45	1.21	5 (11%)
5	HEM	B	802	9,7,3	50,50,50	1.87	9 (18%)	67,82,82	2.29	28 (41%)
8	10M	B	806	-	34,34,34	1.15	2 (5%)	44,45,45	1.37	6 (13%)
10	HEC	C	201	4	50,50,50	1.60	7 (14%)	68,82,82	1.24	8 (11%)

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	9,3	-	4/14/54/54	-
8	10M	B	807	-	-	8/19/59/59	0/2/2/2
5	HEM	B	802	9,7,3	-	7/14/54/54	-
8	10M	B	806	-	-	8/19/59/59	0/2/2/2
10	HEC	C	201	4	1/1/3/7	6/14/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	HEM	C3D-C2D	7.90	1.53	1.36
5	B	801	HEM	C3D-C2D	7.48	1.52	1.36
10	C	201	HEC	C3D-C2D	6.92	1.51	1.36
5	B	802	HEM	FE-NA	5.15	2.12	1.95
5	B	801	HEM	FE-ND	4.57	2.09	1.94
8	B	806	10M	O1-C11	3.85	1.48	1.42
8	B	807	10M	C10-S	3.78	1.86	1.81
5	B	802	HEM	FE-NB	3.47	2.05	1.94
5	B	801	HEM	FE-NC	3.22	2.05	1.95
10	C	201	HEC	FE-ND	3.08	2.04	1.94
5	B	802	HEM	CAC-C3C	3.01	1.55	1.47
8	B	806	10M	C11-S	2.98	1.85	1.80
8	B	807	10M	O3-C15	2.97	1.50	1.41
8	B	807	10M	O4-C16	2.86	1.51	1.44
5	B	802	HEM	CAB-C3B	2.84	1.55	1.47
5	B	802	HEM	CMC-C2C	2.84	1.56	1.50
8	B	807	10M	O1-C11	2.83	1.46	1.42
5	B	801	HEM	CMB-C2B	2.80	1.56	1.50
5	B	801	HEM	CAC-C3C	2.80	1.54	1.47
5	B	801	HEM	CAB-C3B	2.77	1.54	1.47
5	B	801	HEM	CMC-C2C	2.74	1.56	1.50
8	B	807	10M	C14-C12	2.40	1.59	1.52
10	C	201	HEC	C3C-C2C	-2.25	1.33	1.38
10	C	201	HEC	CAC-C3C	2.22	1.56	1.51
10	C	201	HEC	CMC-C2C	2.17	1.55	1.50
5	B	802	HEM	CMA-C3A	2.13	1.55	1.50
10	C	201	HEC	O2A-CGA	-2.11	1.23	1.30
8	B	807	10M	C18-C16	2.08	1.57	1.53
10	C	201	HEC	CMA-C3A	2.08	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	HEM	O1A-CGA	2.06	1.28	1.22
8	B	807	10M	O4-C15	2.03	1.47	1.41
5	B	802	HEM	C2A-C3A	-2.01	1.33	1.38

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	801	HEM	C4C-C3C-C2C	6.72	112.64	106.81
5	B	801	HEM	CHC-C4B-NB	6.69	131.62	124.42
5	B	801	HEM	C4D-ND-C1D	6.57	112.99	105.21
5	B	802	HEM	CMD-C2D-C1D	6.33	134.93	125.03
5	B	801	HEM	C3C-C2C-C1C	-5.58	101.76	107.05
5	B	802	HEM	CHB-C1B-NB	-4.95	118.25	124.37
5	B	801	HEM	CMC-C2C-C1C	4.81	133.21	124.73
5	B	802	HEM	CHA-C1A-NA	-4.81	115.13	123.86
5	B	802	HEM	C4A-CHB-C1B	4.65	137.18	126.25
8	B	806	10M	O4-C16-C18	4.34	117.51	109.70
5	B	802	HEM	C1D-C2D-C3D	-4.23	102.53	106.98
5	B	802	HEM	O2A-CGA-O1A	4.04	133.72	123.33
5	B	801	HEM	CHC-C1C-NC	-3.92	120.19	124.45
5	B	801	HEM	CMA-C3A-C2A	3.72	133.51	125.62
5	B	802	HEM	CBB-CAB-C3B	-3.64	109.35	127.53
8	B	807	10M	C21-C14-C12	3.52	118.74	110.93
5	B	802	HEM	CMB-C2B-C1B	-3.51	119.54	125.03
8	B	806	10M	C11-O1-C12	3.47	118.79	112.56
5	B	802	HEM	O2A-CGA-CBA	-3.40	103.27	114.00
5	B	801	HEM	CBC-CAC-C3C	-3.35	110.78	127.53
5	B	801	HEM	CHA-C4D-ND	3.31	128.46	124.37
10	C	201	HEC	CBC-CAC-C3C	3.22	121.15	112.42
5	B	802	HEM	CAB-C3B-C2B	3.09	138.47	128.43
10	C	201	HEC	C1D-ND-C4D	3.07	108.84	105.21
8	B	806	10M	C15-O3-C14	-3.07	110.71	117.98
5	B	801	HEM	CMB-C2B-C1B	3.05	129.80	125.03
5	B	802	HEM	CBA-CAA-C2A	-2.99	104.27	112.53
5	B	802	HEM	C3B-C4B-NB	2.97	111.60	109.47
5	B	802	HEM	CHB-C4A-NA	-2.96	118.49	123.86
8	B	807	10M	C18-C19-C20	2.94	116.00	110.83
5	B	802	HEM	CHA-C1A-C2A	2.93	131.70	125.30
5	B	802	HEM	O1D-CGD-CBD	-2.85	114.06	123.09
5	B	801	HEM	CMA-C3A-C4A	-2.83	121.10	125.42
5	B	802	HEM	C4D-ND-C1D	2.79	108.51	105.21
8	B	807	10M	O3-C15-C20	2.77	114.90	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	802	HEM	CAA-CBA-CGA	-2.75	106.38	113.67
5	B	802	HEM	CHC-C1C-NC	2.66	127.35	124.45
10	C	201	HEC	CAC-C3C-C2C	2.65	131.08	126.89
5	B	801	HEM	O2D-CGD-CBD	2.63	122.31	114.00
5	B	802	HEM	C2A-C1A-NA	2.63	113.06	110.15
8	B	806	10M	O3-C14-C21	-2.62	100.56	107.23
5	B	801	HEM	CHC-C4B-C3B	-2.58	119.92	125.07
5	B	801	HEM	O1A-CGA-CBA	-2.54	115.03	123.09
5	B	802	HEM	CMC-C2C-C1C	-2.53	120.28	124.73
5	B	801	HEM	CHA-C1A-NA	-2.46	119.41	123.86
10	C	201	HEC	C1D-C2D-C3D	-2.43	104.42	106.98
5	B	802	HEM	C1A-CHA-C4D	2.43	131.95	126.25
5	B	802	HEM	CMA-C3A-C2A	2.42	130.75	125.62
10	C	201	HEC	CMC-C2C-C1C	-2.39	121.78	125.42
5	B	802	HEM	CHA-C4D-ND	2.38	127.32	124.37
8	B	807	10M	C15-O3-C14	-2.37	112.36	117.98
8	B	806	10M	O1-C12-C14	2.31	114.50	109.72
5	B	801	HEM	C4D-C3D-C2D	-2.31	103.53	106.89
5	B	801	HEM	CAD-CBD-CGD	2.31	119.79	113.67
5	B	802	HEM	CMA-C3A-C4A	-2.29	121.93	125.42
5	B	802	HEM	CHD-C1D-ND	-2.26	121.99	124.42
10	C	201	HEC	CBD-CAD-C3D	-2.23	106.36	112.53
5	B	801	HEM	CHB-C4A-C3A	-2.23	120.95	127.43
5	B	801	HEM	O2D-CGD-O1D	-2.22	117.61	123.33
5	B	801	HEM	CAA-CBA-CGA	-2.21	107.79	113.67
5	B	801	HEM	CMD-C2D-C1D	2.20	128.47	125.03
5	B	801	HEM	C4B-C3B-C2B	2.17	109.27	107.28
8	B	806	10M	O1-C11-C22	2.15	113.28	110.32
5	B	801	HEM	CAC-C3C-C2C	-2.14	121.46	128.43
5	B	801	HEM	C1C-CHC-C4B	-2.12	121.52	126.02
5	B	802	HEM	C2D-C1D-ND	2.11	112.34	109.90
5	B	802	HEM	CAB-C3B-C4B	-2.10	115.09	124.39
5	B	801	HEM	C1B-NB-C4B	2.09	107.68	105.21
10	C	201	HEC	CBB-CAB-C3B	-2.06	106.82	112.42
5	B	802	HEM	CMB-C2B-C3B	2.05	133.40	128.43
10	C	201	HEC	C1C-C2C-C3C	2.04	109.15	106.82
5	B	801	HEM	C4C-CHD-C1D	2.03	130.34	126.02
8	B	807	10M	O4-C16-C18	2.00	113.31	109.70

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
10	C	201	HEC	NA

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	806	10M	C22-C11-S-C10
8	B	806	10M	O4-C16-C17-O5
10	C	201	HEC	C2C-C3C-CAC-CBC
8	B	806	10M	C18-C16-C17-O5
10	C	201	HEC	C4C-C3C-CAC-CBC
10	C	201	HEC	C2B-C3B-CAB-CBB
8	B	806	10M	C7-C8-C9-C10
8	B	806	10M	C4-C5-C6-C7
8	B	807	10M	C3-C4-C5-C6
8	B	807	10M	C4-C5-C6-C7
8	B	806	10M	C6-C7-C8-C9
8	B	807	10M	C6-C7-C8-C9
8	B	807	10M	C5-C6-C7-C8
5	B	801	HEM	C2C-C3C-CAC-CBC
8	B	807	10M	C21-C14-O3-C15
10	C	201	HEC	C4B-C3B-CAB-CBB
5	B	801	HEM	C4C-C3C-CAC-CBC
8	B	806	10M	C1-C2-C3-C4
8	B	806	10M	C2-C3-C4-C5
8	B	807	10M	C7-C8-C9-C10
5	B	801	HEM	CAA-CBA-CGA-O1A
5	B	801	HEM	CAA-CBA-CGA-O2A
5	B	802	HEM	CAA-CBA-CGA-O2A
5	B	802	HEM	CAA-CBA-CGA-O1A
10	C	201	HEC	CAD-CBD-CGD-O1D
10	C	201	HEC	CAD-CBD-CGD-O2D
8	B	807	10M	C12-C14-O3-C15
5	B	802	HEM	C4B-C3B-CAB-CBB
5	B	802	HEM	C4C-C3C-CAC-CBC
5	B	802	HEM	CAD-CBD-CGD-O1D
5	B	802	HEM	CAD-CBD-CGD-O2D
8	B	807	10M	C2-C3-C4-C5
5	B	802	HEM	C2C-C3C-CAC-CBC

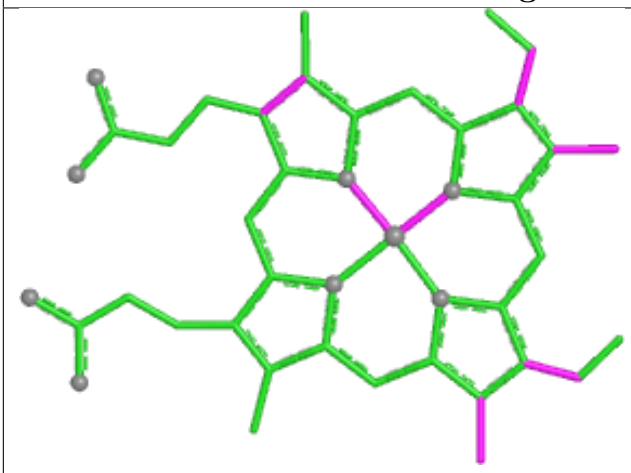
There are no ring outliers.

7 monomers are involved in 17 short contacts:

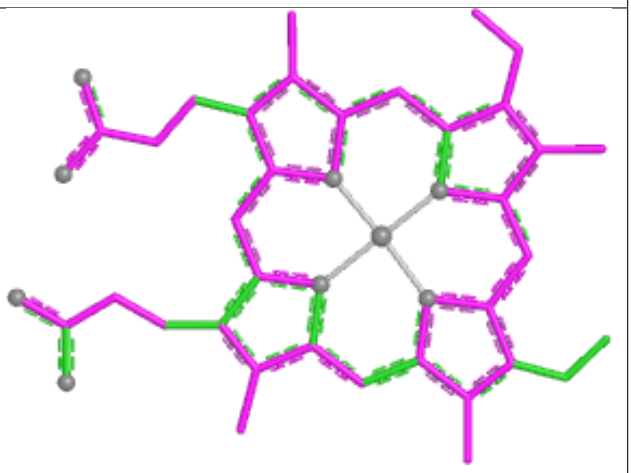
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	801	HEM	5	0
7	B	804	CMO	2	0
7	B	805	CMO	1	0
8	B	807	10M	4	0
5	B	802	HEM	5	0
8	B	806	10M	2	0
10	C	201	HEC	2	0

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.

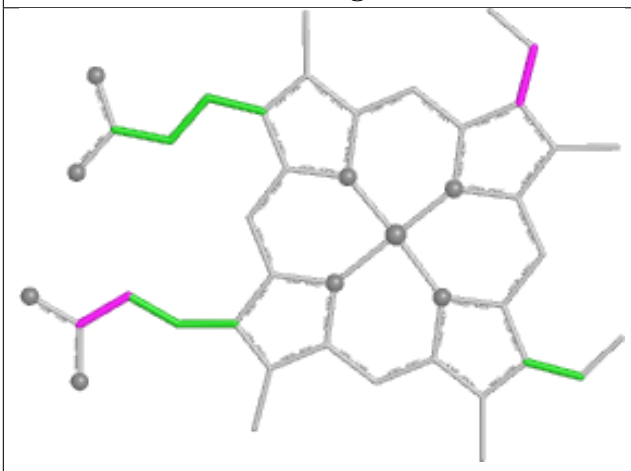
Ligand HEM B 801



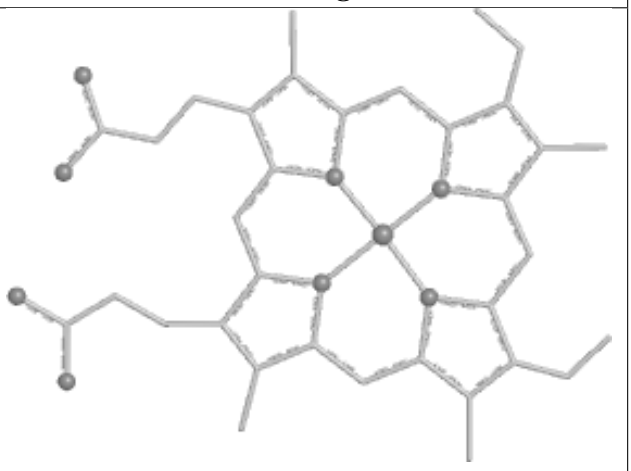
Bond lengths



Bond angles

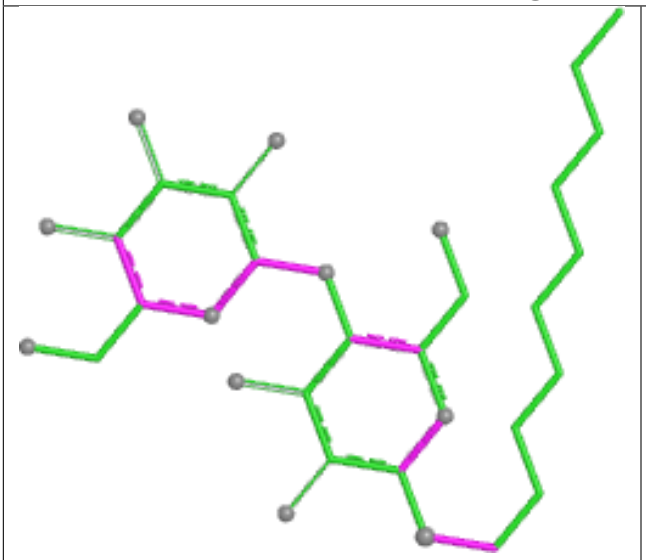


Torsions

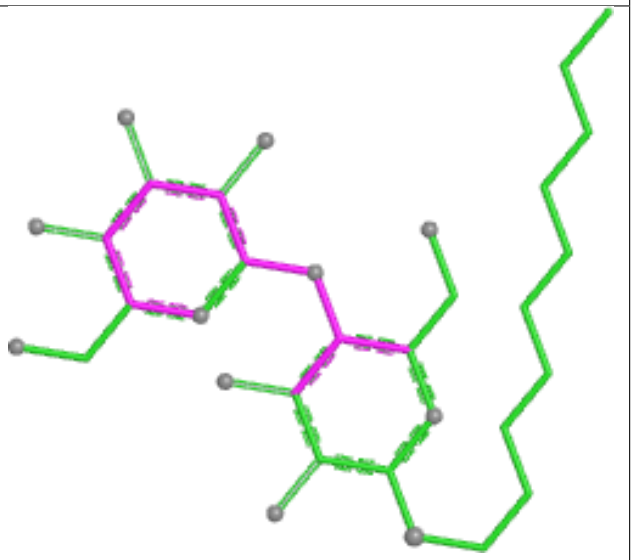


Rings

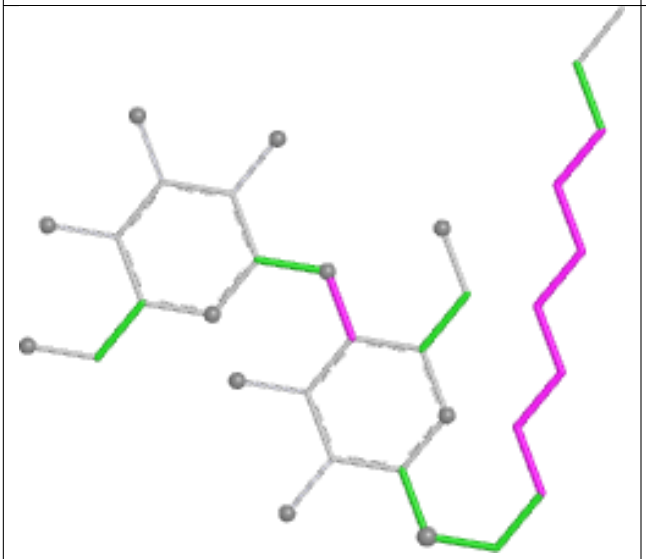
Ligand 10M B 807



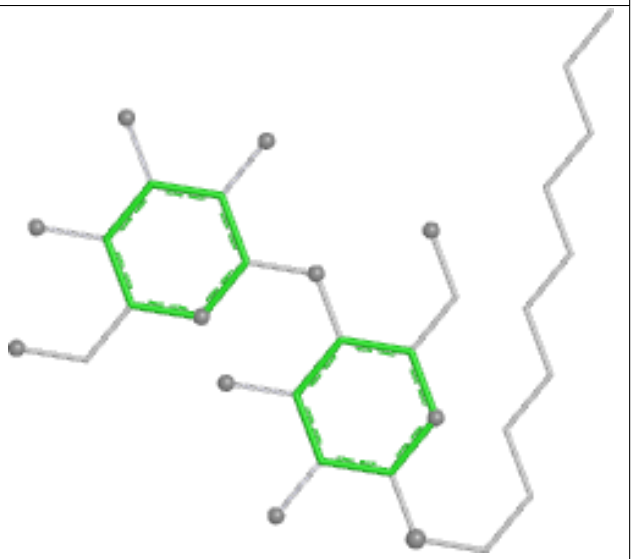
Bond lengths



Bond angles

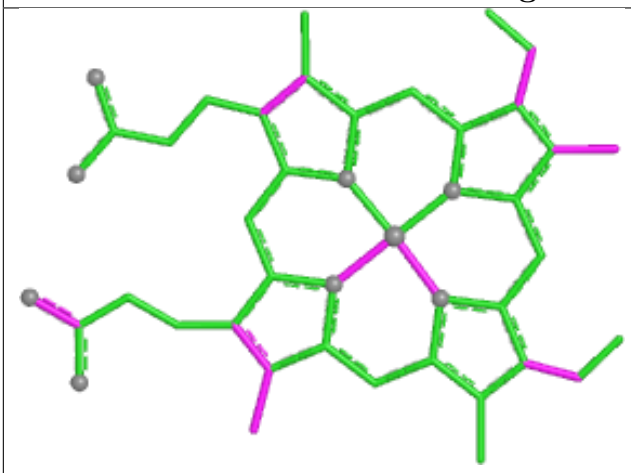


Torsions

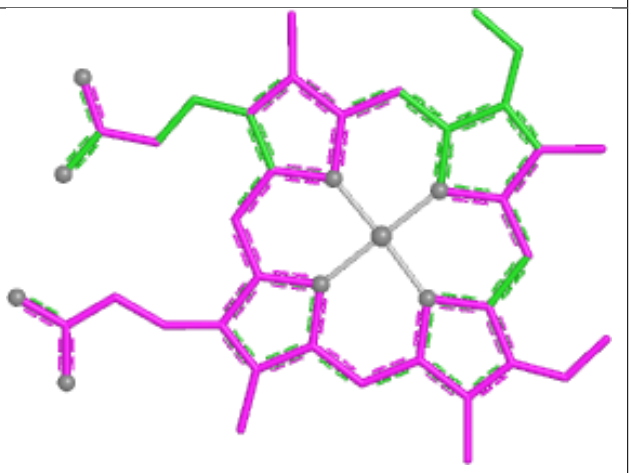


Rings

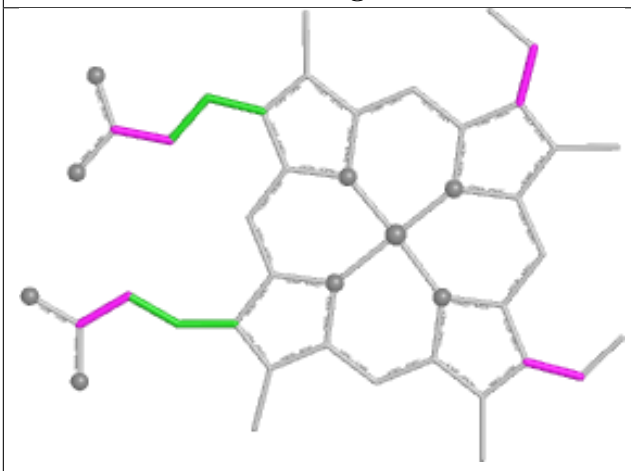
Ligand HEM B 802



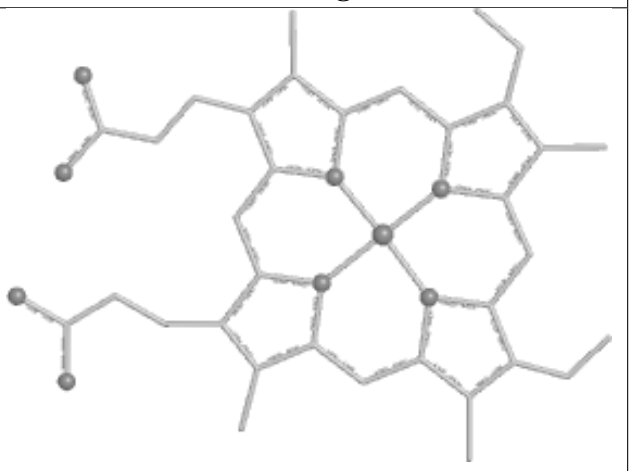
Bond lengths



Bond angles

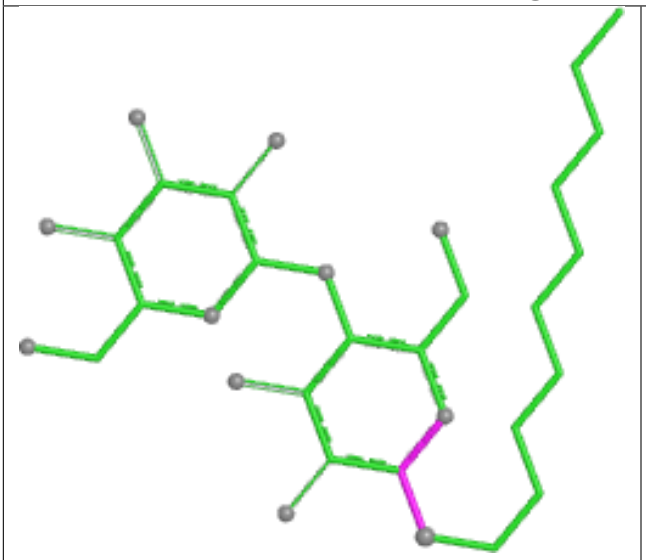


Torsions

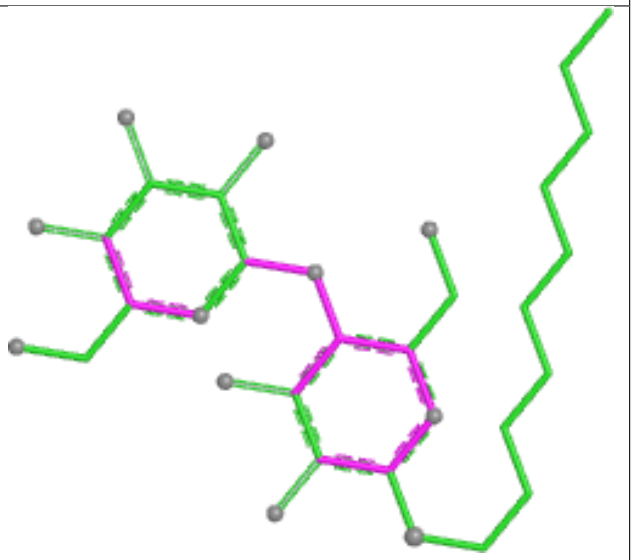


Rings

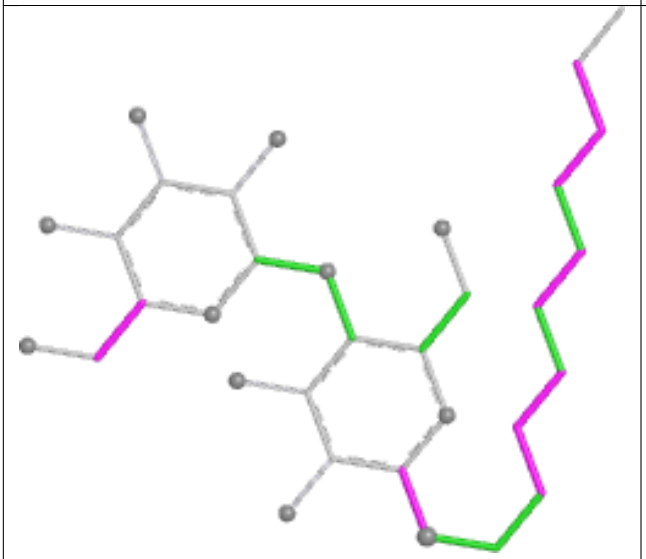
Ligand 10M B 806



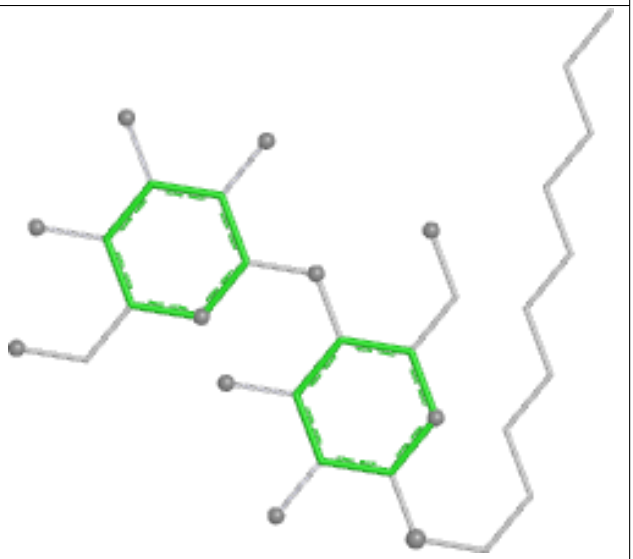
Bond lengths



Bond angles

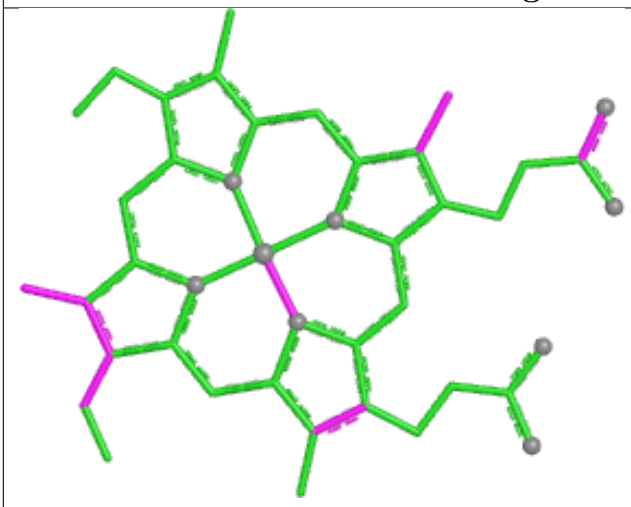


Torsions

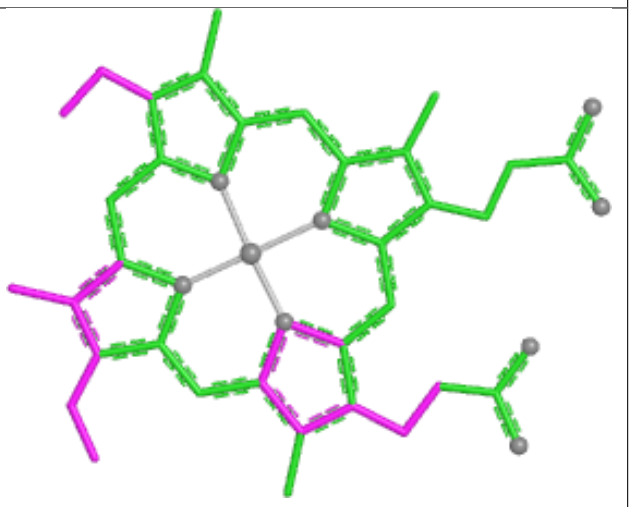


Rings

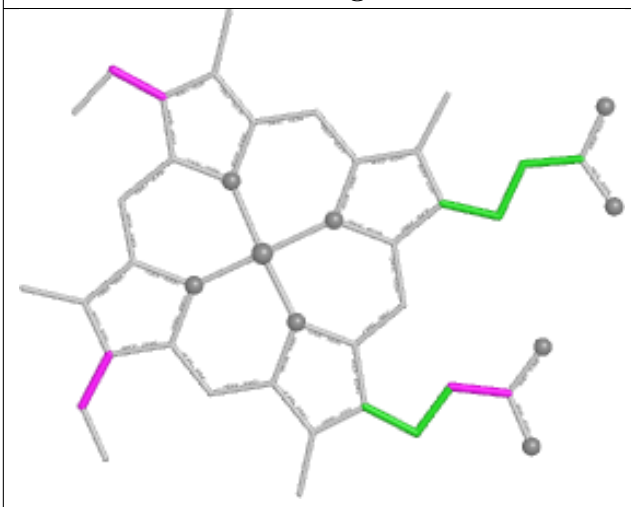
Ligand HEC C 201



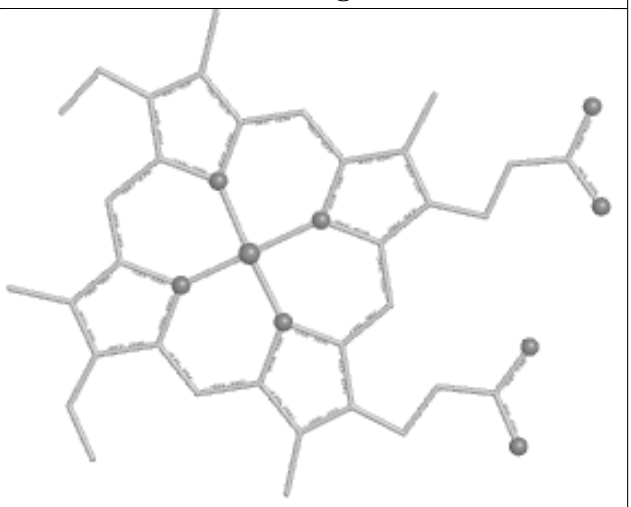
Bond lengths



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%)	-0.22	3 (1%)	73	70	33, 44, 62, 108	0
2	H	225/225 (100%)	-0.20	5 (2%)	62	58	33, 43, 72, 134	0
3	B	449/465 (96%)	0.23	12 (2%)	56	51	37, 58, 96, 124	0
4	C	142/146 (97%)	0.01	4 (2%)	55	50	35, 56, 80, 99	0
All	All	1029/1049 (98%)	0.01	24 (2%)	61	57	33, 52, 87, 134	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	212	ASN	3.6
3	B	384	VAL	2.9
3	B	296	ASN	2.9
3	B	10	PHE	2.8
3	B	369	PRO	2.6
4	C	86	GLY	2.5
3	B	233	ASP	2.5
3	B	294	THR	2.5
3	B	299	ARG	2.4
1	L	10	TYR	2.4
2	H	116	GLN	2.3
3	B	300	ARG	2.2
2	H	88	ASN	2.2
2	H	140	GLY	2.2
3	B	304	ASN	2.1
1	L	145	ASN	2.1
3	B	142	ILE	2.1
3	B	297	ARG	2.1
3	B	455	LEU	2.1
4	C	44	ALA	2.0
2	H	196	SER	2.0

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Mol	Chain	Res	Type	RSRZ
4	C	5	PHE	2.0
4	C	82	VAL	2.0
2	H	144	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

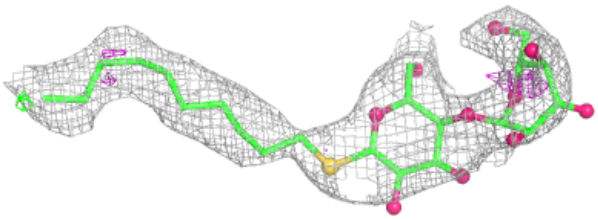
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

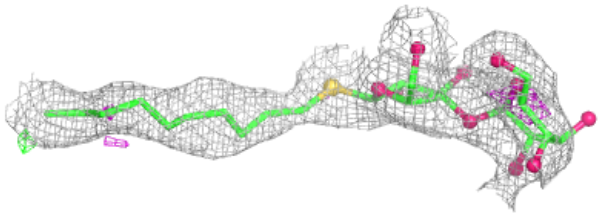
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	10M	B	807	33/33	0.74	0.17	73,91,107,108	0
8	10M	B	806	33/33	0.91	0.13	65,74,87,89	0
7	CMO	B	805	2/2	0.97	0.06	39,39,39,40	0
5	HEM	B	801	43/43	0.98	0.08	37,40,45,49	0
5	HEM	B	802	43/43	0.98	0.07	36,40,43,44	0
7	CMO	B	804	2/2	0.98	0.06	40,40,40,41	0
6	FE	B	803	1/1	0.99	0.03	42,42,42,42	0
9	CA	B	808	1/1	0.99	0.02	46,46,46,46	0
10	HEC	C	201	43/43	0.99	0.06	35,37,39,41	0

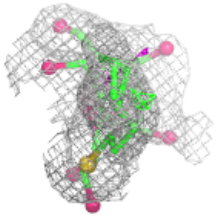
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 10M B 807:

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

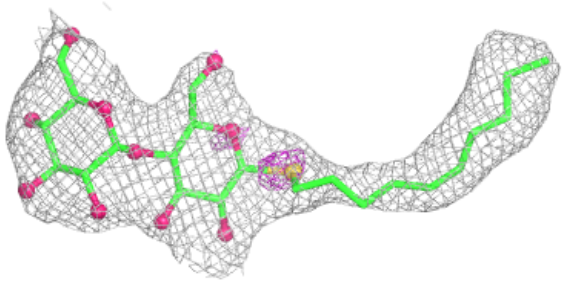


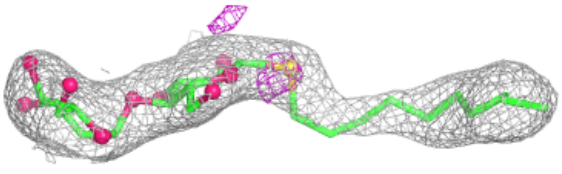


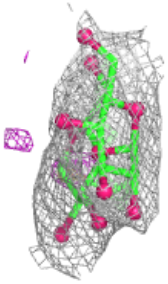


Electron density around 10M B 806:

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

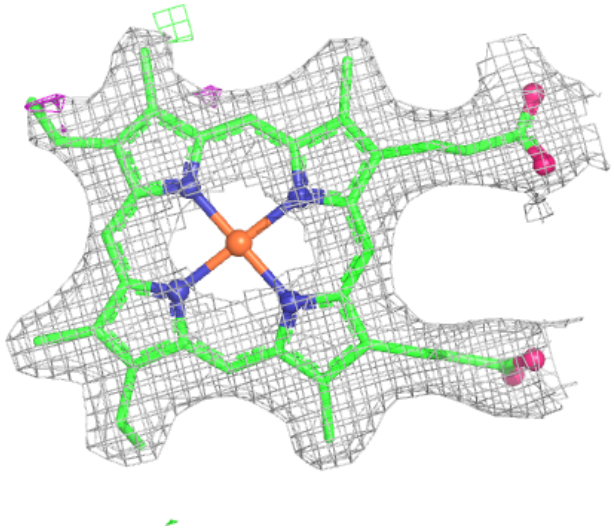


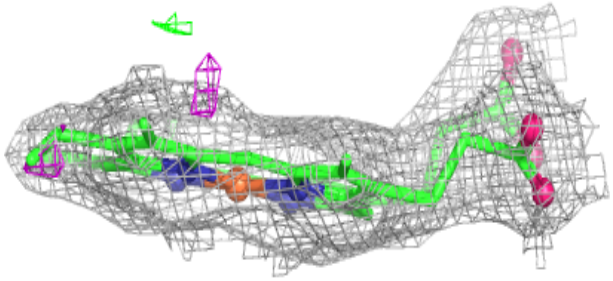


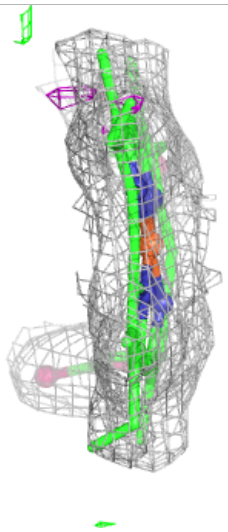


Electron density around HEM B 801:

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

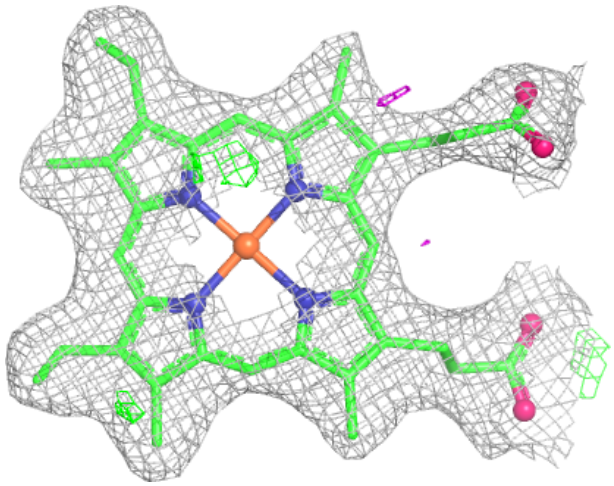


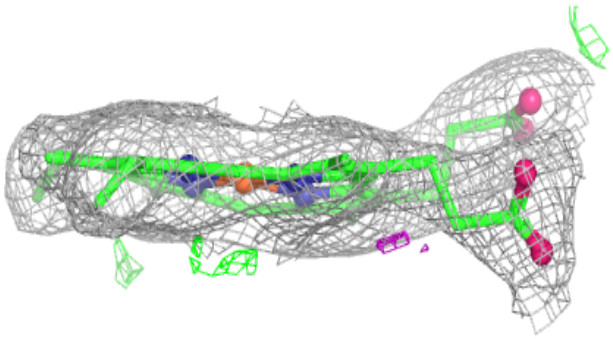


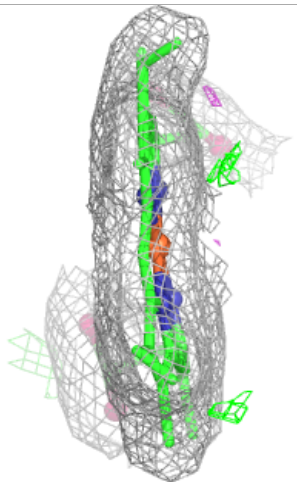


Electron density around HEM B 802:

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

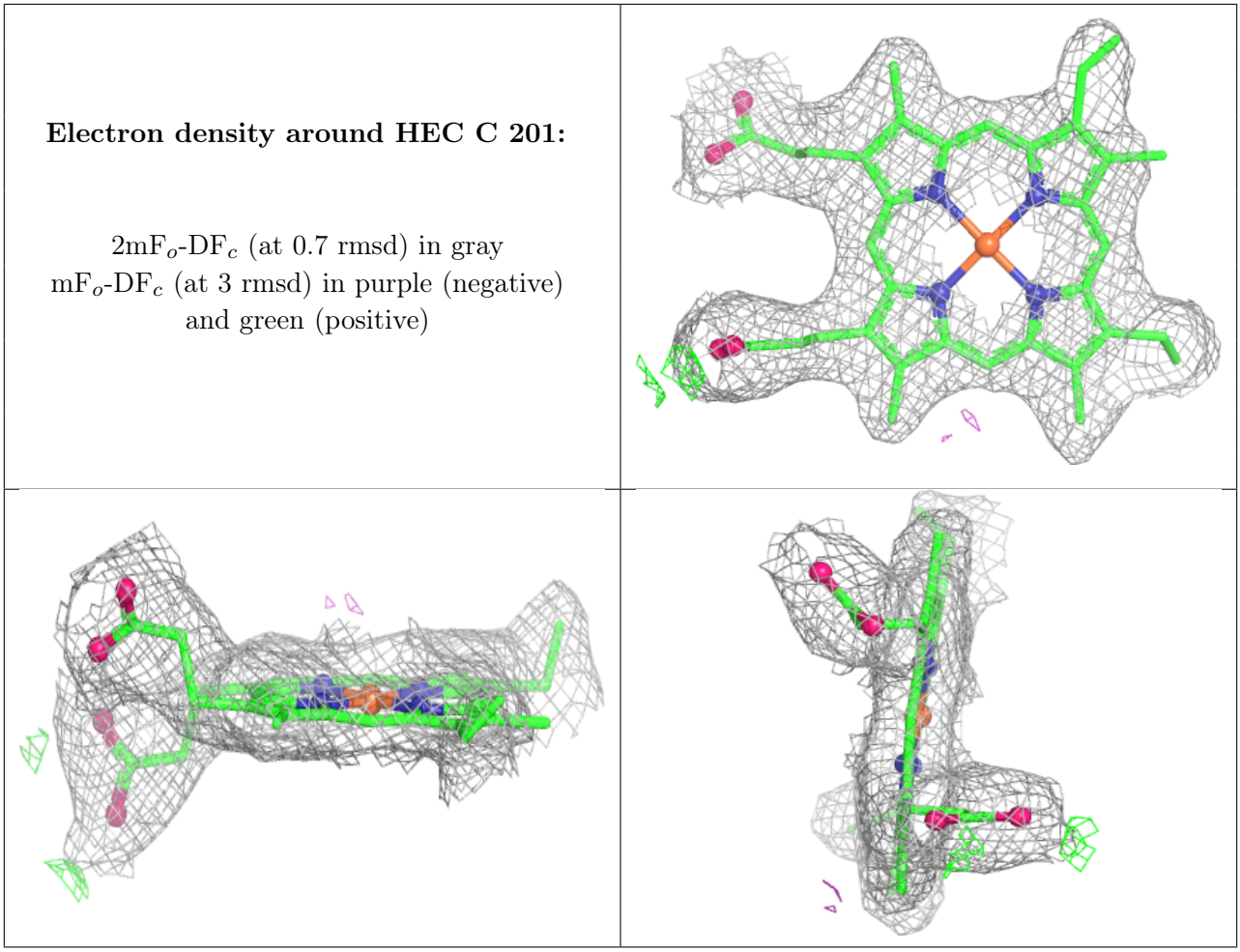






Electron density around HEC C 201:

$2mF_o$-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.