Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 06:40 am GMT

PDB ID	:	2WHW
Title	:	Selective oxidation of carbolide C-H bonds by engineered macrolide P450 monooxygenase
Authors	:	Li, S.; Chaulagain, M.R.; Knauff, A.R.; Podust, L.M.; Montgomery, J.; Sherman, D.H.
Deposited on	:	2009-05-07
Resolution	:	2.20 Å(reported)

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

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

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

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

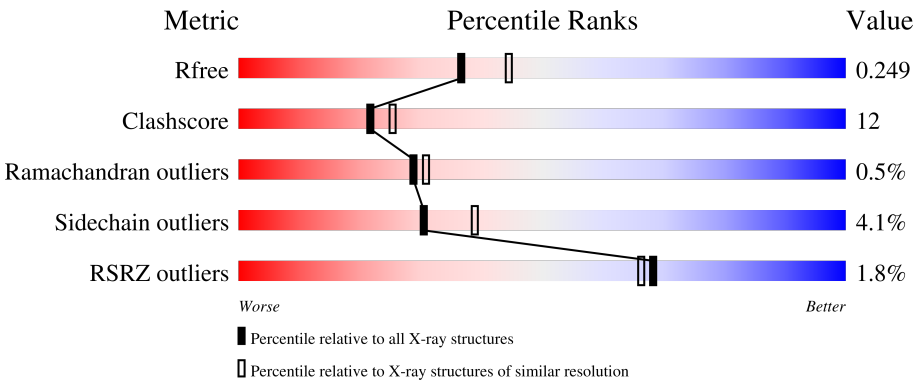
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	436	.% 75% 12% • • 9%
1	B	436	2% 72% 16% • 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7098 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.

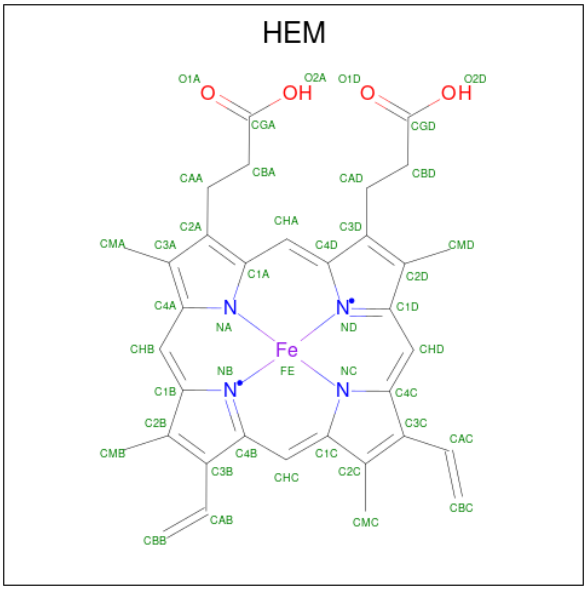
- Molecule 1 is a protein called CYTOCHROME P450 MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3125	1975	564	573	13	0	7	0
1	B	393	3116	1974	557	571	14	0	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	ASN	ASP	engineered mutation	UNP O87605
B	50	ASN	ASP	engineered mutation	UNP O87605

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



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

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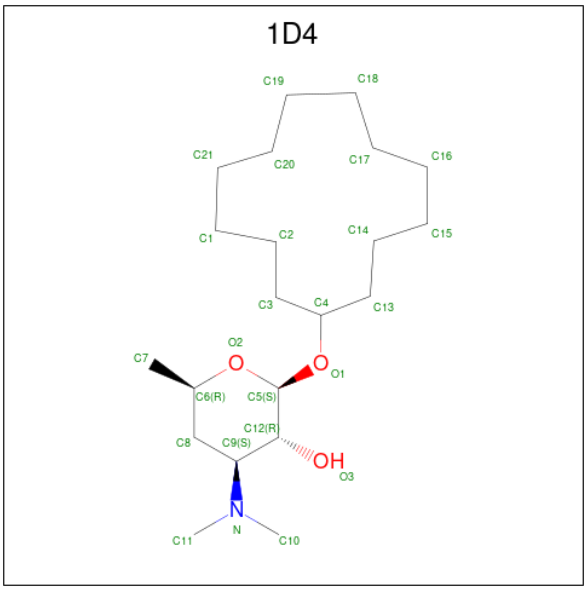
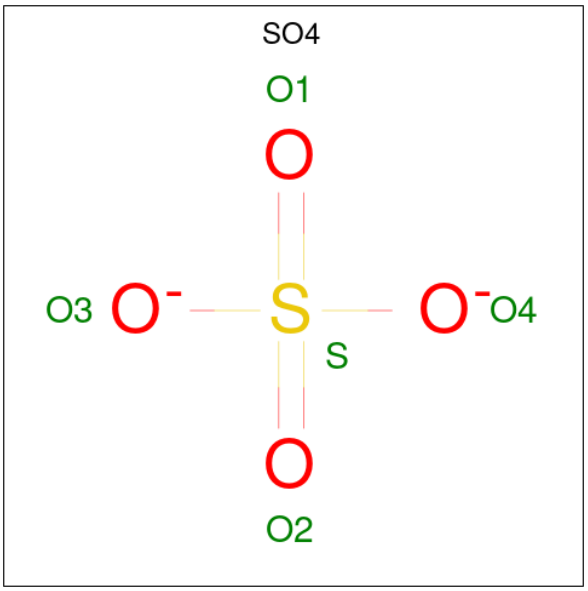
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is CYCLOTRIDECYL 3,4,6-TRIDEOXY-3-(DIMETHYLAMINO)-BETA-D-XYLO-HEXOPYRANOSIDE (three-letter code: 1D4) (formula: $C_{21}H_{41}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O			
3	A	1	25	21	1	3		0	0
			Total	C	N	O			
3	B	1	25	21	1	3		0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

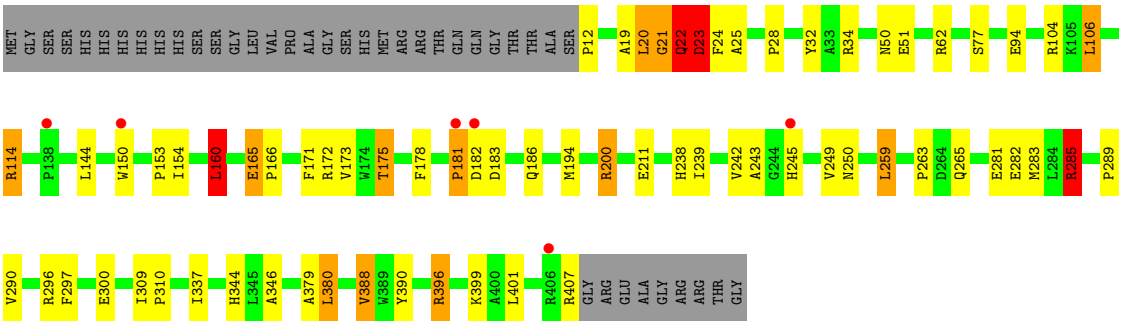
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	355	Total O 355 355	0	0
5	B	356	Total O 356 356	0	0

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.

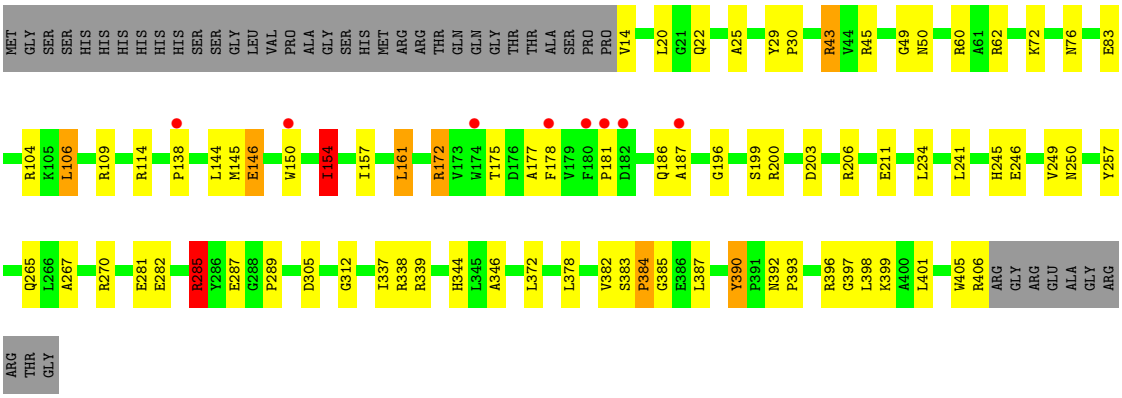
• Molecule 1: CYTOCHROME P450 MONOOXYGENASE

Chain A:



• Molecule 1: CYTOCHROME P450 MONOOXYGENASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.18Å 109.54Å 153.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.09 – 2.20 47.33 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (89.09-2.20) 99.8 (47.33-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.14 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.177 , 0.256 0.171 , 0.249	Depositor DCC
R_{free} test set	2666 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7098	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1D4, SO4, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.06	4/3214 (0.1%)	1.01	14/4386 (0.3%)
1	B	1.09	7/3213 (0.2%)	1.00	10/4382 (0.2%)
All	All	1.07	11/6427 (0.2%)	1.00	24/8768 (0.3%)

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	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405	TRP	C-O	-12.74	0.99	1.23
1	A	50	ASN	C-N	-7.02	1.18	1.34
1	B	146	GLU	CG-CD	6.55	1.61	1.51
1	B	83	GLU	CG-CD	6.00	1.60	1.51
1	A	211	GLU	CG-CD	5.99	1.60	1.51
1	B	405	TRP	C-N	-5.64	1.21	1.34
1	B	49	GLY	C-N	-5.47	1.21	1.34
1	B	109	ARG	CG-CD	5.43	1.65	1.51
1	B	285	ARG	CD-NE	-5.36	1.37	1.46
1	A	285	ARG	CD-NE	-5.34	1.37	1.46
1	A	379	ALA	CA-CB	5.06	1.63	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	285	ARG	NE-CZ-NH2	-14.97	112.81	120.30
1	B	405	TRP	O-C-N	-10.09	106.55	122.70
1	A	285	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	B	285	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	A	160	LEU	CB-CG-CD2	-7.41	98.41	111.00
1	B	62	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	106	LEU	CB-CG-CD1	6.28	121.68	111.00
1	A	285	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	12	PRO	N-CA-CB	5.59	110.00	103.30
1	A	200[A]	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	200[B]	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	396	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	296	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	34	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	62	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	104	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	206	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	154[A]	ILE	CG1-CB-CG2	-5.14	100.08	111.40
1	B	154[B]	ILE	CG1-CB-CG2	-5.14	100.08	111.40
1	B	285	ARG	CG-CD-NE	-5.13	101.02	111.80
1	B	104	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	380	LEU	CA-CB-CG	5.07	126.95	115.30
1	B	106	LEU	CB-CG-CD1	5.06	119.60	111.00
1	A	20	LEU	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	GLY	Peptide
1	A	22	GLN	Peptide

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	3125	0	3103	70	0
1	B	3116	0	3114	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	25	0	41	6	0
3	B	25	0	41	6	0
4	B	10	0	0	0	0
5	A	355	0	0	11	1
5	B	356	0	0	21	0
All	All	7098	0	6359	152	1

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

All (152) 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:150[B]:TRP:CE2	1:A:154:ILE:HD11	1.40	1.56
1:A:178:PHE:CE2	1:A:194:MET:HE1	1.56	1.38
1:A:178:PHE:HE2	1:A:194:MET:CE	1.40	1.34
1:A:150[B]:TRP:NE1	1:A:154:ILE:CD1	1.99	1.26
1:A:150[B]:TRP:CE2	1:A:154:ILE:CD1	2.24	1.21
1:A:178:PHE:CE2	1:A:194:MET:CE	2.20	1.15
1:B:150[A]:TRP:HD1	5:B:2162:HOH:O	1.32	1.12
1:A:150[B]:TRP:CZ2	1:A:154:ILE:HD11	1.85	1.12
1:A:150[B]:TRP:CZ2	1:A:172:ARG:HG3	1.97	1.00
1:B:392:ASN:OD1	1:B:393:PRO:HD2	1.61	0.98
1:A:150[B]:TRP:NE1	1:A:154:ILE:HD12	1.76	0.98
1:A:21:GLY:HA3	1:A:22:GLN:HB2	1.42	0.98
1:B:161[B]:LEU:HD23	1:B:241:LEU:HG	1.47	0.97
1:B:211[B]:GLU:OE2	5:B:2219:HOH:O	1.87	0.92
1:A:150[B]:TRP:NE1	1:A:154:ILE:HD11	1.73	0.91
1:B:390:TYR:HD2	1:B:399:LYS:HE2	1.35	0.91
1:B:150[A]:TRP:CD1	5:B:2162:HOH:O	2.12	0.89
3:B:1410:1D4:H113	5:B:2090:HOH:O	1.73	0.87
1:B:287[B]:GLU:HB2	5:B:2269:HOH:O	1.74	0.87
3:B:1410:1D4:O3	3:B:1410:1D4:H142	1.78	0.83
1:B:344:HIS:HD2	1:B:346:ALA:H	1.27	0.83
1:A:178:PHE:CE2	1:A:194:MET:HE3	2.10	0.82
1:A:22:GLN:H	1:A:24:PHE:H	1.24	0.82
1:A:200[B]:ARG:NH1	5:A:2217:HOH:O	2.12	0.80
1:B:154[A]:ILE:HD12	1:B:245:HIS:CE1	2.16	0.80
1:A:22:GLN:H	1:A:24:PHE:N	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:PHE:HE2	1:A:194:MET:HE1	0.63	0.79
3:B:1410:1D4:H12C	3:B:1410:1D4:H151	1.63	0.79
1:A:150[B]:TRP:CD1	1:A:154:ILE:HD12	2.16	0.78
1:B:145[B]:MET:CE	1:B:398:LEU:HB2	2.15	0.77
1:B:200:ARG:NE	5:B:2201:HOH:O	1.94	0.77
1:B:200:ARG:NH2	5:B:2201:HOH:O	2.15	0.77
1:B:22:GLN:OE1	1:B:25:ALA:HB3	1.88	0.74
1:B:145[B]:MET:HE2	1:B:401:LEU:HB2	1.67	0.74
1:A:282:GLU:OE1	1:A:285:ARG:HD3	1.89	0.73
1:A:344:HIS:HD2	1:A:346:ALA:H	1.37	0.73
1:A:150[B]:TRP:HE1	1:A:154:ILE:CD1	2.00	0.72
1:B:181:PRO:HB3	1:B:187:ALA:HB2	1.73	0.71
1:B:145[B]:MET:HE1	1:B:398:LEU:HB2	1.72	0.70
1:B:154[A]:ILE:HD11	5:B:2179:HOH:O	1.92	0.70
1:B:196:GLY:O	5:B:2197:HOH:O	2.11	0.68
1:B:282:GLU:OE1	1:B:285:ARG:HD3	1.93	0.68
1:B:390:TYR:HD2	1:B:399:LYS:CE	2.05	0.68
1:B:285:ARG:HD2	1:B:339:ARG:HD2	1.77	0.67
1:B:154[B]:ILE:HG13	5:B:2163:HOH:O	1.94	0.66
1:A:388:VAL:HG22	1:A:399:LYS:HD2	1.78	0.66
1:B:406:ARG:C	5:B:2352:HOH:O	2.34	0.66
1:B:196:GLY:HA2	5:B:2197:HOH:O	1.95	0.65
1:B:175:THR:HG22	1:B:246:GLU:OE2	1.96	0.65
1:A:23:ASP:HB2	5:A:2007:HOH:O	1.95	0.64
1:B:161[B]:LEU:HD23	1:B:241:LEU:CG	2.24	0.64
1:A:21:GLY:CA	1:A:22:GLN:HB2	2.24	0.63
1:B:150[A]:TRP:CZ2	1:B:172:ARG:HD2	2.34	0.63
1:B:265:GLN:NE2	1:B:337:ILE:H	1.97	0.63
1:B:154[A]:ILE:CD1	5:B:2179:HOH:O	2.47	0.62
1:A:150[B]:TRP:HZ2	1:A:172:ARG:HG3	1.57	0.62
1:B:199:SER:HB2	5:B:2197:HOH:O	2.00	0.62
1:A:186:GLN:HB2	5:A:2202:HOH:O	2.00	0.61
1:A:249:VAL:HG23	5:A:2265:HOH:O	2.01	0.61
1:A:150[B]:TRP:CE2	1:A:172:ARG:HG3	2.36	0.61
1:B:249[B]:VAL:HG23	5:B:2252:HOH:O	2.01	0.59
1:A:150[B]:TRP:CD1	1:A:172:ARG:NH1	2.71	0.59
1:A:21:GLY:HA3	1:A:22:GLN:CB	2.27	0.59
1:A:250:ASN:HB2	1:A:289:PRO:HB3	1.84	0.58
3:B:1410:1D4:O3	3:B:1410:1D4:H112	2.03	0.58
1:A:173:VAL:HA	5:A:2198:HOH:O	2.04	0.57
1:B:145[B]:MET:HE3	1:B:398:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150[A]:TRP:CE2	1:B:172:ARG:HD2	2.41	0.56
1:B:203:ASP:OD2	5:B:2203:HOH:O	2.18	0.56
1:B:390:TYR:CD2	1:B:399:LYS:HE2	2.27	0.55
1:A:150[B]:TRP:CZ2	1:A:154:ILE:CD1	2.73	0.55
1:A:22:GLN:N	1:A:24:PHE:H	1.99	0.55
1:A:263:PRO:HB3	1:B:267:ALA:HB2	1.90	0.54
1:A:28:PRO:HB2	1:A:32:TYR:CE1	2.43	0.54
1:A:238:HIS:O	1:A:242[A]:VAL:HG23	2.08	0.54
1:B:161[B]:LEU:CD2	1:B:241:LEU:HG	2.29	0.54
3:A:1410:1D4:H142	3:A:1410:1D4:H22C	1.90	0.53
1:B:14:VAL:HG22	1:B:43:ARG:HG2	1.91	0.53
1:B:392:ASN:O	5:B:2346:HOH:O	2.18	0.53
1:A:388:VAL:CG2	1:A:399:LYS:HD2	2.37	0.53
1:A:150[B]:TRP:CZ2	1:A:172:ARG:CG	2.84	0.52
1:B:282:GLU:OE1	1:B:285:ARG:CD	2.57	0.52
1:B:200:ARG:CZ	5:B:2201:HOH:O	2.36	0.52
1:B:157:ILE:HG13	1:B:161[B]:LEU:HD22	1.91	0.52
1:B:29:TYR:HB2	1:B:30:PRO:HD3	1.91	0.52
1:B:60:ARG:NH2	1:B:305:ASP:OD1	2.44	0.51
1:A:175:THR:HG22	1:A:194:MET:SD	2.51	0.50
1:A:259:LEU:HD22	1:A:283:MET:CE	2.42	0.50
1:B:154[A]:ILE:CD1	1:B:245:HIS:CE1	2.92	0.50
1:B:144:LEU:HD23	1:B:401:LEU:HD23	1.94	0.50
1:A:181:PRO:O	1:A:182:ASP:CB	2.59	0.50
1:B:177:ALA:HB1	1:B:186:GLN:HG2	1.94	0.49
1:B:383:SER:O	1:B:384:PRO:C	2.50	0.49
1:A:171:PHE:O	1:A:175:THR:HG23	2.12	0.49
1:B:145[A]:MET:SD	1:B:249[A]:VAL:CG2	3.01	0.49
1:A:114:ARG:NH1	5:A:2139:HOH:O	2.46	0.48
1:B:392:ASN:OD1	1:B:393:PRO:CD	2.49	0.48
3:A:1410:1D4:H11C	3:A:1410:1D4:O1	2.13	0.48
1:B:390:TYR:CE1	1:B:397:GLY:HA3	2.49	0.48
1:B:211[A]:GLU:OE2	5:B:2215:HOH:O	2.20	0.47
1:B:270[A]:ARG:NH1	1:B:372:LEU:O	2.48	0.47
1:A:144:LEU:HD23	1:A:401:LEU:HD23	1.97	0.47
1:A:77:SER:HB2	1:A:297:PHE:CD2	2.49	0.47
1:A:178:PHE:HE1	5:A:2264:HOH:O	1.98	0.46
3:B:1410:1D4:O3	3:B:1410:1D4:H103	2.13	0.46
1:A:344:HIS:CD2	1:A:346:ALA:H	2.25	0.46
1:B:76:ASN:O	1:B:312:GLY:HA2	2.16	0.46
1:B:145[B]:MET:HE3	1:B:398:LEU:CB	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLU:HG3	1:A:166:PRO:N	2.30	0.46
1:A:150[B]:TRP:CZ3	1:A:245:HIS:O	2.69	0.46
1:B:287[A]:GLU:OE2	1:B:396:ARG:NH2	2.43	0.46
1:A:22:GLN:HB3	5:A:2007:HOH:O	2.15	0.46
1:B:250:ASN:HB2	1:B:289:PRO:HB3	1.98	0.45
1:A:21:GLY:CA	1:A:22:GLN:CB	2.92	0.45
1:A:281:GLU:OE1	1:A:344:HIS:HE1	2.00	0.45
1:B:154[A]:ILE:CD1	1:B:245:HIS:NE2	2.80	0.44
1:B:196:GLY:CA	5:B:2197:HOH:O	2.62	0.44
1:B:138:PRO:HD2	5:B:2157:HOH:O	2.16	0.44
1:B:281:GLU:OE1	1:B:344:HIS:HE1	1.99	0.44
3:B:1410:1D4:H172	3:B:1410:1D4:H202	1.48	0.44
1:B:383:SER:O	1:B:385:GLY:N	2.50	0.44
1:A:265:GLN:NE2	1:A:337:ILE:H	2.14	0.44
1:A:194:MET:HB2	1:A:194:MET:HE2	1.27	0.43
1:A:160:LEU:HD12	1:A:160:LEU:HA	1.76	0.43
1:B:344:HIS:CD2	1:B:346:ALA:H	2.20	0.43
1:A:25:ALA:O	1:A:396:ARG:NH1	2.51	0.43
1:A:407:ARG:CB	5:A:2172:HOH:O	2.66	0.43
1:A:150[B]:TRP:CD1	1:A:154:ILE:CD1	2.82	0.43
1:A:172:ARG:NH1	5:A:2199:HOH:O	2.52	0.43
1:A:289:PRO:HG2	2:A:1407:HEM:HMB2	2.00	0.43
1:B:45:ARG:HA	1:B:50:ASN:O	2.19	0.43
1:A:243:ALA:HB2	3:A:1410:1D4:H202	2.00	0.43
1:B:257:TYR:CE1	1:B:387:LEU:CD1	3.02	0.42
1:B:150[A]:TRP:CZ3	1:B:245:HIS:O	2.72	0.42
1:A:265:GLN:NE2	1:A:337:ILE:HG12	2.34	0.42
1:A:282:GLU:OE1	1:A:285:ARG:CD	2.64	0.42
1:B:22:GLN:OE1	1:B:25:ALA:CB	2.64	0.42
1:B:382:VAL:HG11	1:B:387:LEU:HD21	2.02	0.42
1:A:390:TYR:CZ	1:A:399:LYS:HG2	2.54	0.41
1:A:309:ILE:HA	1:A:310:PRO:HD3	1.92	0.41
3:A:1410:1D4:H142	3:A:1410:1D4:C2	2.45	0.41
1:A:19:ALA:HB3	5:A:2004:HOH:O	2.19	0.41
1:B:270[A]:ARG:HH22	1:B:378:LEU:HB3	1.86	0.41
1:B:338:ARG:HH11	1:B:338:ARG:HD3	1.73	0.41
1:B:390:TYR:HE1	1:B:397:GLY:HA3	1.85	0.41
1:A:290:VAL:CG2	3:A:1410:1D4:H161	2.51	0.41
1:B:72:LYS:HB3	1:B:72:LYS:NZ	2.36	0.41
1:A:94:GLU:OE2	3:A:1410:1D4:H71C	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2248:HOH:O	5:A:2317:HOH:O[4_556]	2.05	0.15

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	401/436 (92%)	385 (96%)	13 (3%)	3 (1%)	22	22
1	B	400/436 (92%)	388 (97%)	11 (3%)	1 (0%)	41	46
All	All	801/872 (92%)	773 (96%)	24 (3%)	4 (0%)	29	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	22	GLN
1	A	181	PRO
1	B	384	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	327/354 (92%)	313 (96%)	14 (4%)	29	36
1	B	329/354 (93%)	315 (96%)	14 (4%)	29	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	656/708 (93%)	628 (96%)	28 (4%)	30 36

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	23	ASP
1	A	51	GLU
1	A	106	LEU
1	A	114	ARG
1	A	160	LEU
1	A	165	GLU
1	A	175	THR
1	A	239	ILE
1	A	259	LEU
1	A	285	ARG
1	A	300	GLU
1	A	380	LEU
1	A	388	VAL
1	B	20	LEU
1	B	43	ARG
1	B	106	LEU
1	B	114	ARG
1	B	146	GLU
1	B	154[A]	ILE
1	B	154[B]	ILE
1	B	161[A]	LEU
1	B	161[B]	LEU
1	B	172	ARG
1	B	178	PHE
1	B	234	LEU
1	B	285	ARG
1	B	390	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	208	GLN
1	A	265	GLN
1	A	344	HIS

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Mol	Chain	Res	Type
1	B	188	GLN
1	B	208	GLN
1	B	265	GLN
1	B	344	HIS
1	B	349	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	1D4	A	1410	-	26,26,26	0.71	0	33,33,33	1.90	6 (18%)
4	SO4	B	1408	-	4,4,4	0.05	0	6,6,6	0.36	0
3	1D4	B	1410	-	26,26,26	0.65	0	33,33,33	1.63	7 (21%)
2	HEM	B	1407	1	41,50,50	2.07	11 (26%)	45,82,82	1.97	11 (24%)
4	SO4	B	1409	-	4,4,4	0.29	0	6,6,6	0.47	0
2	HEM	A	1407	1	41,50,50	1.96	13 (31%)	45,82,82	2.04	13 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	1407	1	-	0/12/54/54	-
3	1D4	A	1410	-	-	12/23/39/39	0/1/2/2
2	HEM	A	1407	1	-	0/12/54/54	-
3	1D4	B	1410	-	-	20/23/39/39	0/1/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1407	HEM	C3D-C2D	6.34	1.50	1.36
2	A	1407	HEM	C3D-C2D	5.78	1.49	1.36
2	A	1407	HEM	C3C-C2C	-5.24	1.33	1.40
2	B	1407	HEM	C3C-C2C	-4.65	1.33	1.40
2	B	1407	HEM	C3C-CAC	4.33	1.56	1.47
2	B	1407	HEM	FE-ND	3.40	2.13	1.96
2	B	1407	HEM	CAB-C3B	3.02	1.55	1.47
2	A	1407	HEM	C3C-CAC	2.96	1.53	1.47
2	A	1407	HEM	FE-ND	2.74	2.10	1.96
2	B	1407	HEM	CMD-C2D	2.66	1.56	1.50
2	A	1407	HEM	CMB-C2B	2.64	1.56	1.50
2	A	1407	HEM	C2C-C1C	2.58	1.48	1.42
2	B	1407	HEM	CMB-C2B	2.55	1.56	1.50
2	A	1407	HEM	FE-NB	2.44	2.08	1.96
2	B	1407	HEM	CMA-C3A	2.41	1.56	1.51
2	B	1407	HEM	C4D-ND	-2.32	1.36	1.40
2	A	1407	HEM	CMA-C3A	2.26	1.56	1.51
2	B	1407	HEM	C1B-NB	-2.19	1.36	1.40
2	A	1407	HEM	CBA-CGA	2.18	1.55	1.50
2	B	1407	HEM	C4D-C3D	-2.17	1.41	1.45
2	A	1407	HEM	CAA-C2A	2.16	1.55	1.52
2	A	1407	HEM	CAB-C3B	2.13	1.53	1.47
2	A	1407	HEM	C2A-C3A	-2.01	1.31	1.37
2	A	1407	HEM	CMD-C2D	2.00	1.55	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1407	HEM	C4D-ND-C1D	7.27	112.58	105.07
3	A	1410	1D4	C5-O1-C4	6.08	127.31	114.88
2	A	1407	HEM	C4D-ND-C1D	5.01	110.24	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1410	1D4	O1-C5-C12	4.89	120.77	108.10
3	B	1410	1D4	O1-C4-C13	4.74	116.64	108.34
3	B	1410	1D4	C5-O1-C4	4.13	123.33	114.88
2	A	1407	HEM	C4C-CHD-C1D	4.12	128.00	122.56
2	A	1407	HEM	O2A-CGA-CBA	3.87	126.48	114.03
2	A	1407	HEM	CMD-C2D-C1D	3.84	130.88	125.04
2	B	1407	HEM	C4C-CHD-C1D	3.81	127.58	122.56
3	A	1410	1D4	O1-C4-C13	3.73	114.89	108.34
2	A	1407	HEM	C4B-CHC-C1C	3.41	127.05	122.56
2	A	1407	HEM	O2D-CGD-CBD	3.35	124.80	114.03
2	A	1407	HEM	C4B-C3B-C2B	3.30	109.73	107.11
2	A	1407	HEM	CBD-CAD-C3D	-3.17	103.83	112.63
2	B	1407	HEM	C1B-NB-C4B	3.15	108.33	105.07
2	B	1407	HEM	CHC-C4B-NB	3.15	127.85	124.43
2	B	1407	HEM	CMD-C2D-C1D	3.10	129.75	125.04
2	A	1407	HEM	C1B-NB-C4B	3.09	108.26	105.07
2	A	1407	HEM	CAD-CBD-CGD	-3.01	107.13	113.60
3	A	1410	1D4	O1-C5-O2	-2.96	102.41	110.67
2	B	1407	HEM	CMA-C3A-C4A	-2.86	124.06	128.46
2	A	1407	HEM	O1D-CGD-CBD	-2.79	114.11	123.08
3	A	1410	1D4	O1-C4-C3	-2.68	103.64	108.34
2	B	1407	HEM	CMA-C3A-C2A	2.57	129.78	124.94
3	A	1410	1D4	C5-C12-C9	-2.41	105.25	109.19
3	B	1410	1D4	C11-N-C10	-2.34	103.46	110.38
2	A	1407	HEM	O2A-CGA-O1A	-2.34	117.47	123.30
3	B	1410	1D4	O3-C12-C9	-2.33	105.61	109.77
3	B	1410	1D4	C11-N-C9	-2.24	106.38	113.11
2	A	1407	HEM	O1A-CGA-CBA	-2.21	115.98	123.08
2	B	1407	HEM	CBD-CAD-C3D	-2.19	106.54	112.63
2	B	1407	HEM	C4B-CHC-C1C	2.17	125.43	122.56
3	B	1410	1D4	C3-C4-C13	-2.11	104.68	113.80
2	B	1407	HEM	CHA-C4D-ND	2.08	126.95	124.38
2	B	1407	HEM	CMB-C2B-C1B	-2.05	121.92	125.04
3	B	1410	1D4	C5-O2-C6	2.01	116.09	112.91

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1410	1D4	C14-C13-C4-O1
3	A	1410	1D4	C14-C13-C4-C3
3	B	1410	1D4	C12-C5-O1-C4

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Mol	Chain	Res	Type	Atoms
3	B	1410	1D4	C12-C9-N-C10
3	B	1410	1D4	C14-C13-C4-O1
3	B	1410	1D4	O2-C5-O1-C4
3	A	1410	1D4	O2-C5-O1-C4
3	A	1410	1D4	C12-C5-O1-C4
3	B	1410	1D4	C17-C18-C19-C20
3	B	1410	1D4	C1-C2-C3-C4
3	B	1410	1D4	C8-C9-N-C10
3	B	1410	1D4	C14-C13-C4-C3
3	B	1410	1D4	C2-C3-C4-C13
3	B	1410	1D4	C16-C17-C18-C19
3	A	1410	1D4	C17-C18-C19-C20
3	A	1410	1D4	C15-C16-C17-C18
3	B	1410	1D4	C15-C16-C17-C18
3	B	1410	1D4	C18-C19-C20-C21
3	A	1410	1D4	C19-C20-C21-C1
3	A	1410	1D4	C14-C15-C16-C17
3	B	1410	1D4	C2-C3-C4-O1
3	A	1410	1D4	C21-C1-C2-C3
3	B	1410	1D4	C13-C4-O1-C5
3	B	1410	1D4	C8-C9-N-C11
3	A	1410	1D4	C16-C17-C18-C19
3	B	1410	1D4	C21-C1-C2-C3
3	A	1410	1D4	C4-C13-C14-C15
3	B	1410	1D4	C19-C20-C21-C1
3	B	1410	1D4	C14-C15-C16-C17
3	A	1410	1D4	C13-C14-C15-C16
3	B	1410	1D4	C13-C14-C15-C16
3	B	1410	1D4	C2-C1-C21-C20

There are no ring outliers.

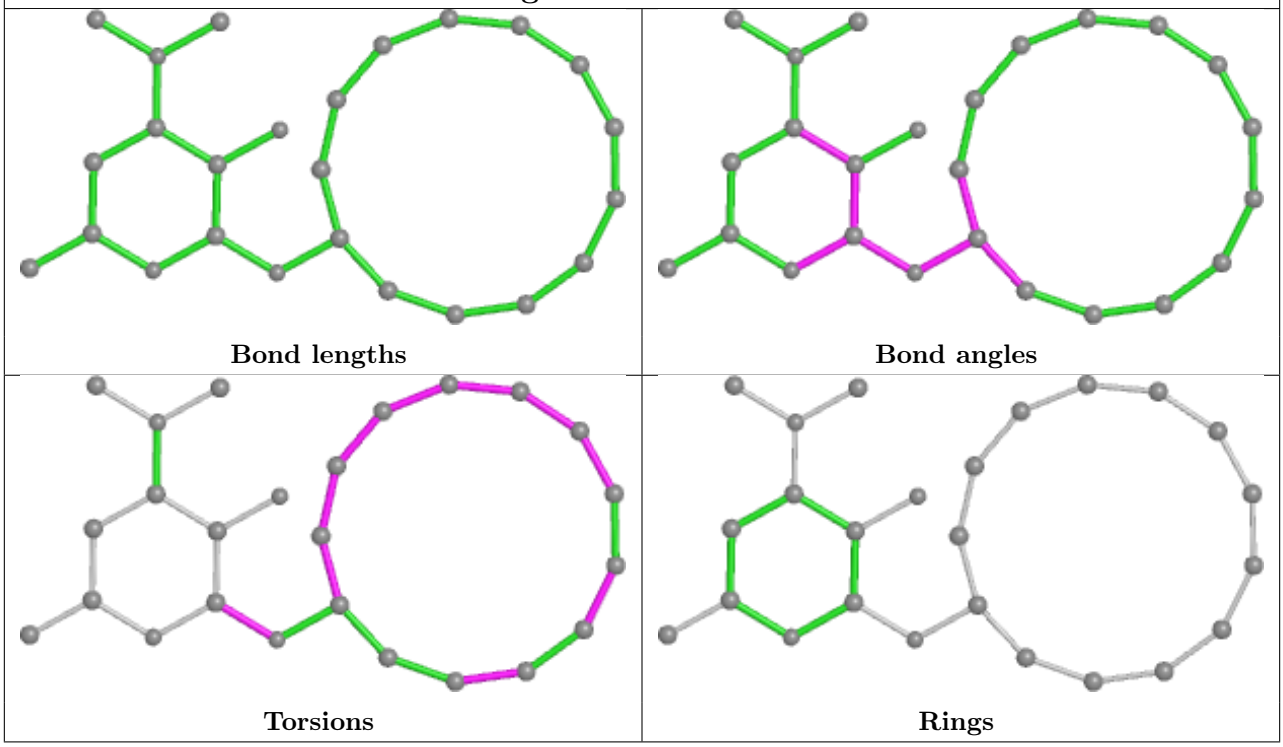
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1410	1D4	6	0
3	B	1410	1D4	6	0
2	A	1407	HEM	1	0

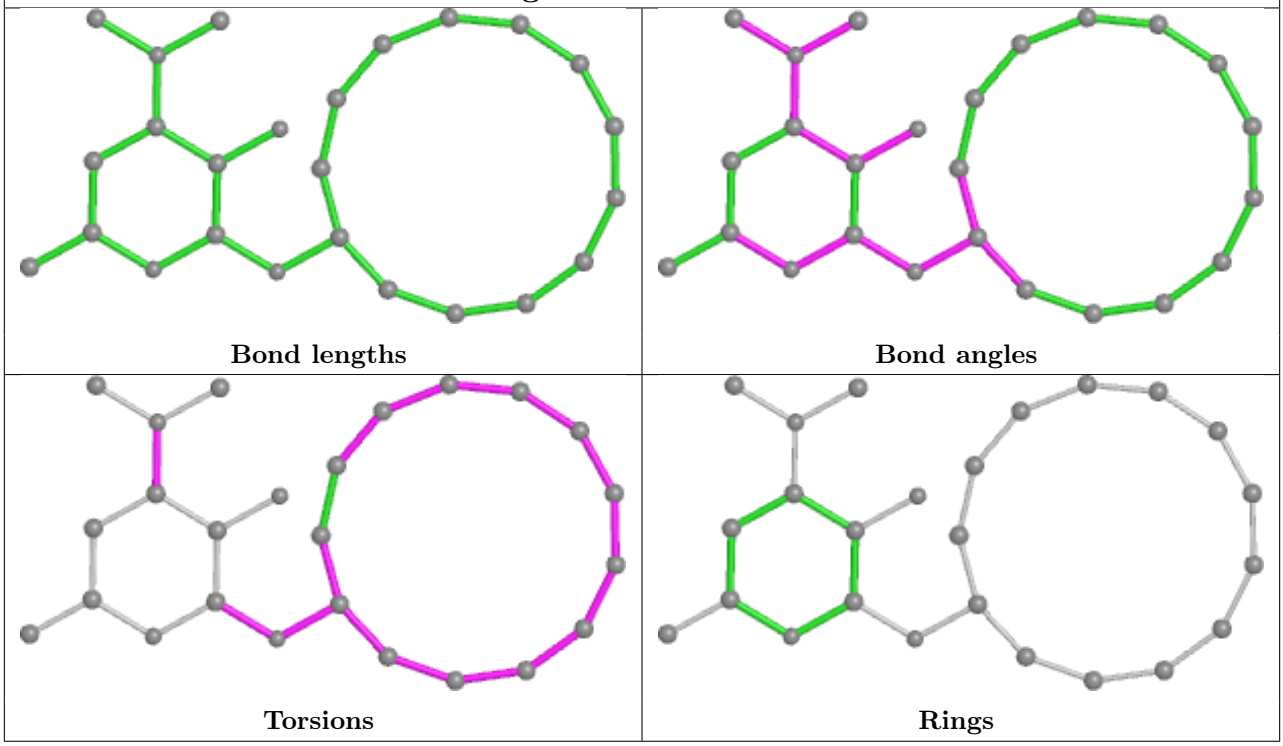
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

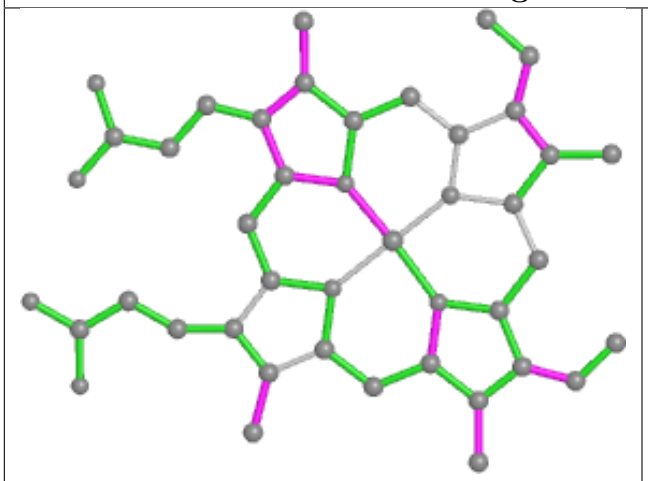
Ligand 1D4 A 1410



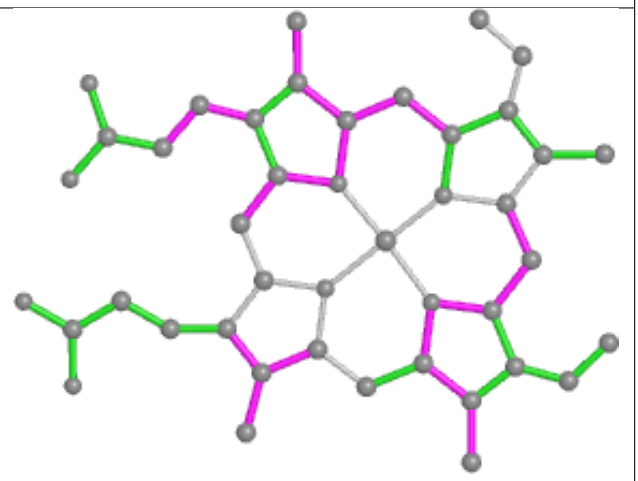
Ligand 1D4 B 1410



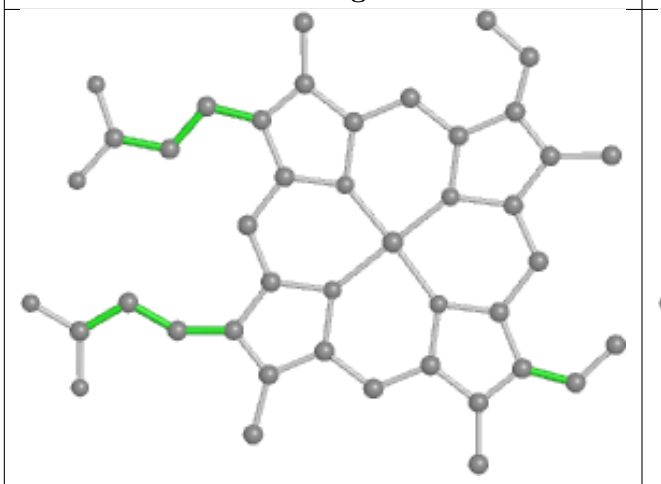
Ligand HEM B 1407



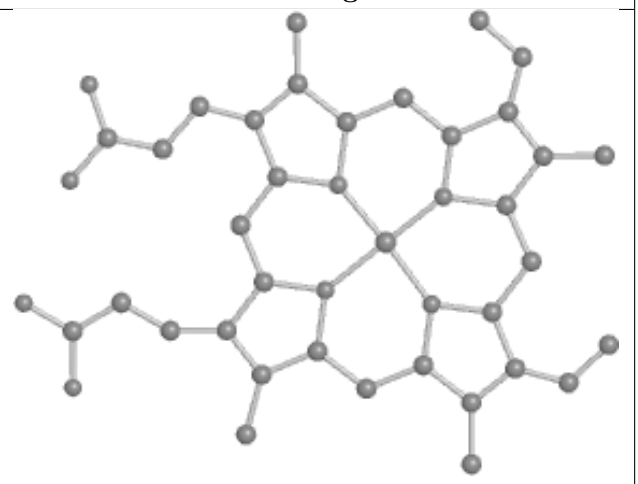
Bond lengths



Bond angles

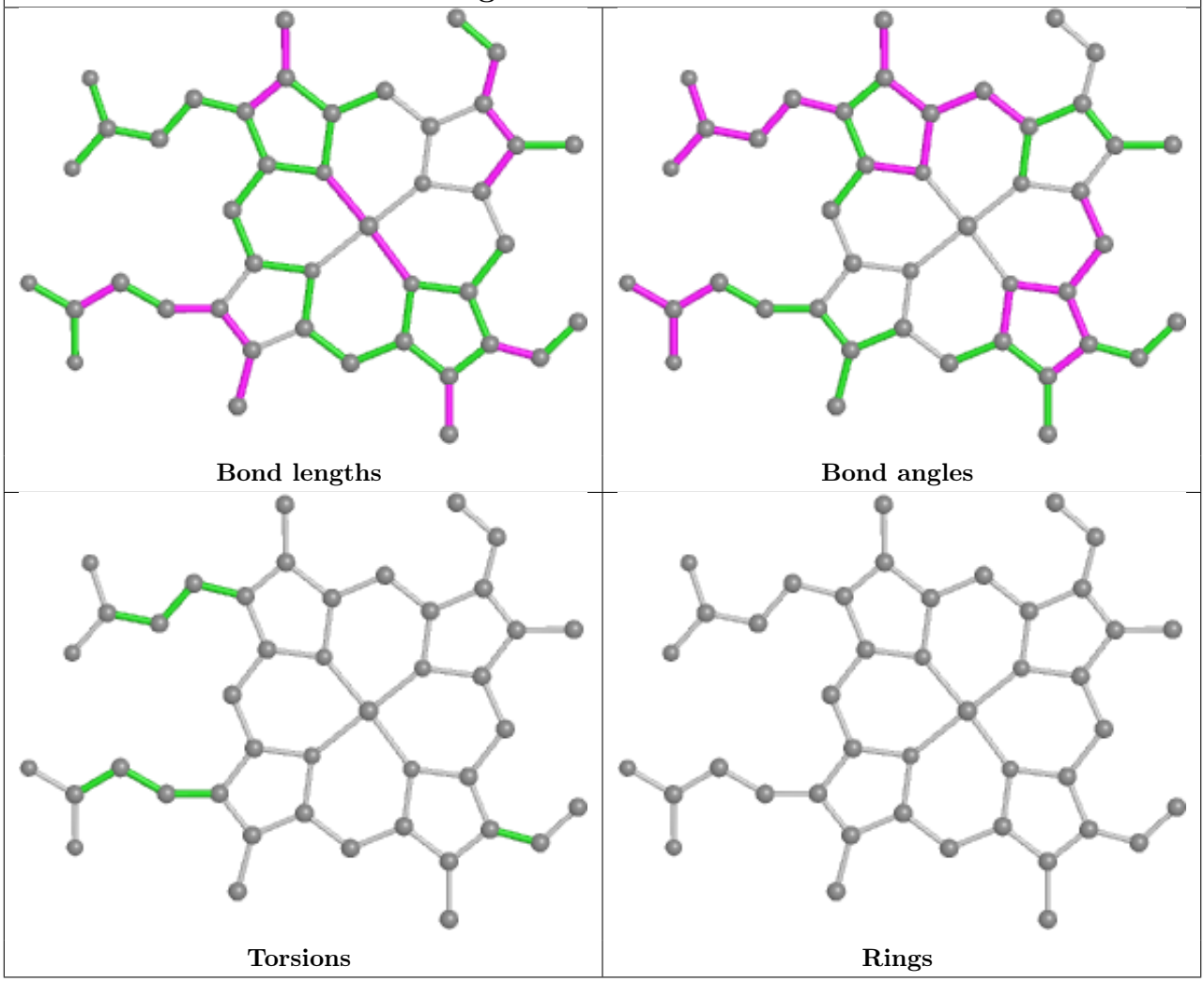


Torsions



Rings

Ligand HEM A 1407



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	50:ASN	C	51:GLU	N	1.17

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	396/436 (90%)	-0.47	6 (1%)	73	72	11, 24, 50, 65	0
1	B	393/436 (90%)	-0.43	8 (2%)	65	63	10, 24, 53, 71	0
All	All	789/872 (90%)	-0.45	14 (1%)	68	66	10, 24, 52, 71	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	PHE	4.1
1	B	181	PRO	3.9
1	B	182	ASP	3.2
1	A	182	ASP	2.9
1	B	180	PHE	2.8
1	B	138	PRO	2.8
1	B	174	TRP	2.5
1	A	406	ARG	2.4
1	A	150[A]	TRP	2.3
1	A	138	PRO	2.3
1	A	181	PRO	2.3
1	B	187	ALA	2.1
1	A	245	HIS	2.1
1	B	150[A]	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

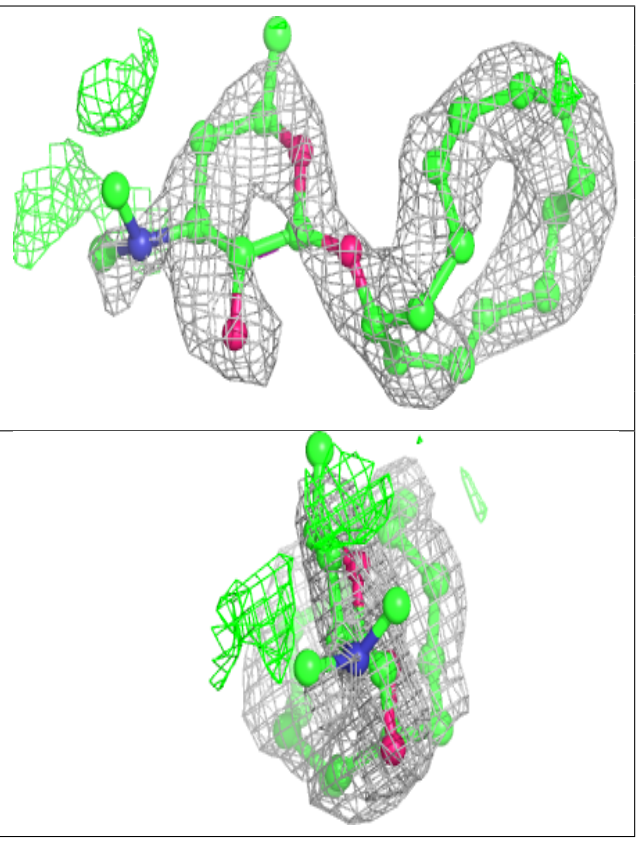
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	1D4	A	1410	25/25	0.69	0.24	45,62,79,80	0
3	1D4	B	1410	25/25	0.80	0.22	39,55,69,70	0
4	SO4	B	1408	5/5	0.85	0.22	90,92,93,93	0
4	SO4	B	1409	5/5	0.89	0.14	74,74,76,77	0
2	HEM	A	1407	43/43	0.99	0.11	7,12,14,23	0
2	HEM	B	1407	43/43	0.99	0.09	8,11,16,24	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.

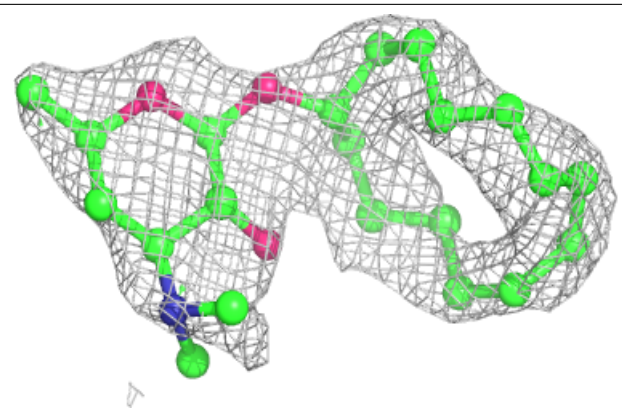
Electron density around 1D4 A 1410:

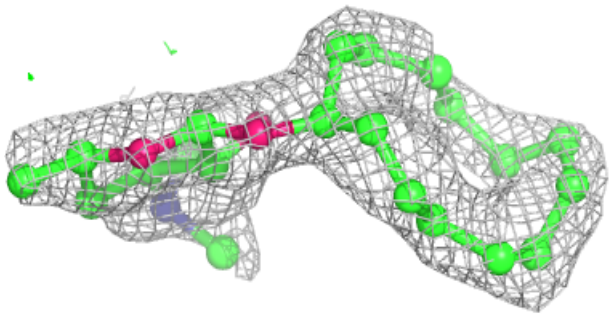
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

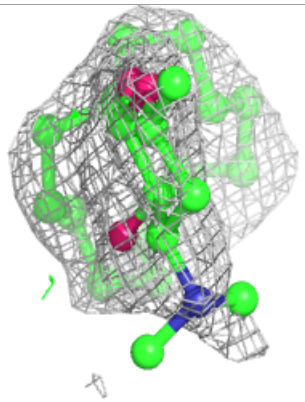


Electron density around 1D4 B 1410:

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

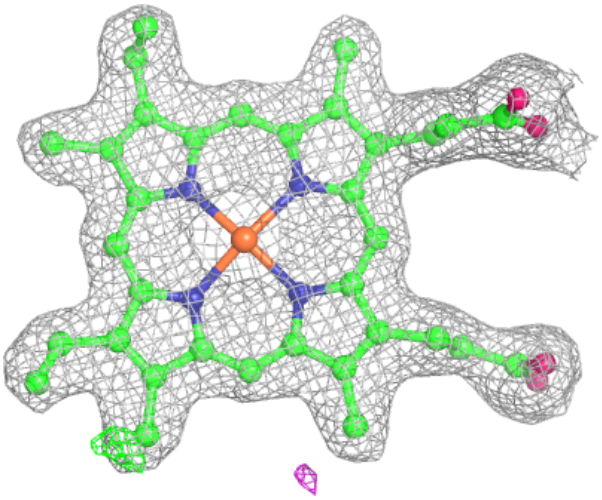


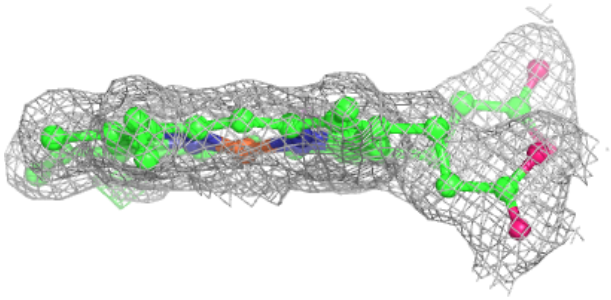


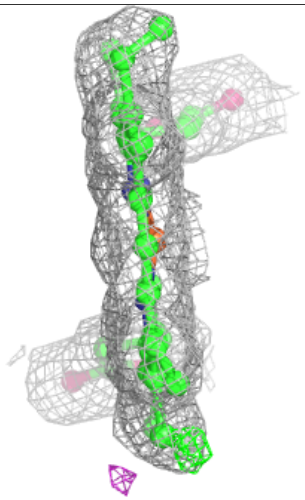


Electron density around HEM A 1407:

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

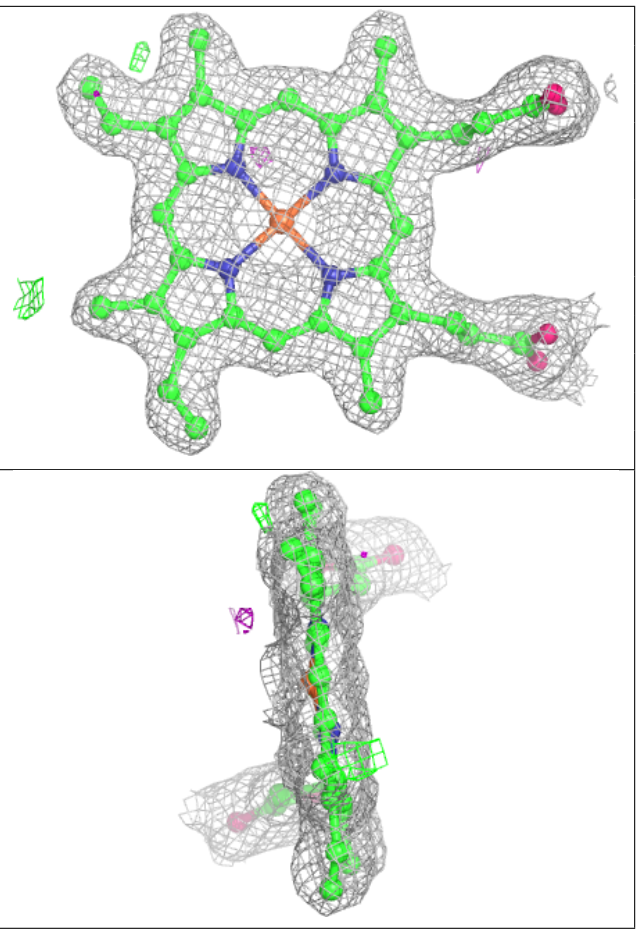






Electron density around HEM B 1407:

$2mF_o$-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.