Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 04:46 PM EDT

PDB ID	:	4XE3
Title	:	OleP, the cytochrome P450 epoxidase from Streptomyces antibioticus involved in Oleandomycin biosynthesis: functional analysis and crystallographic structure in complex with clotrimazole.
Authors	:	Montemiglio, L.C.; Parisi, G.; Scaglione, A.; Savino, C.; Vallone, B.
Deposited on	:	2014-12-22
Resolution	:	2.65 Å(reported)

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

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

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

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

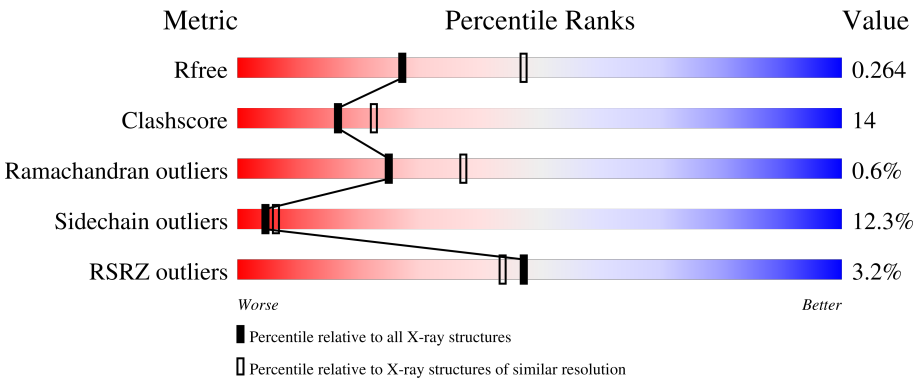
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	407	5% 68% 25%
1	B	407	% 69% 23%

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
4	SO4	A	503	-	-	X	-
4	SO4	A	504	-	-	X	-
4	SO4	A	508	-	-	X	-
4	SO4	B	504	-	-	X	-
4	SO4	B	506	-	-	X	-

2 Entry composition (i)

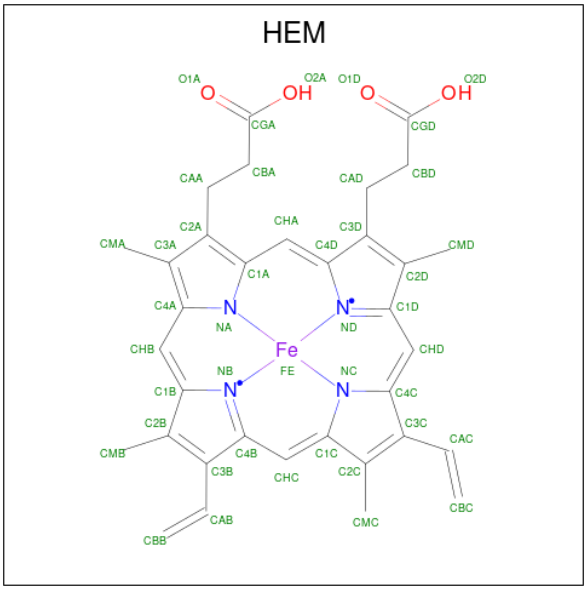
There are 5 unique types of molecules in this entry. The entry contains 6398 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P-450.

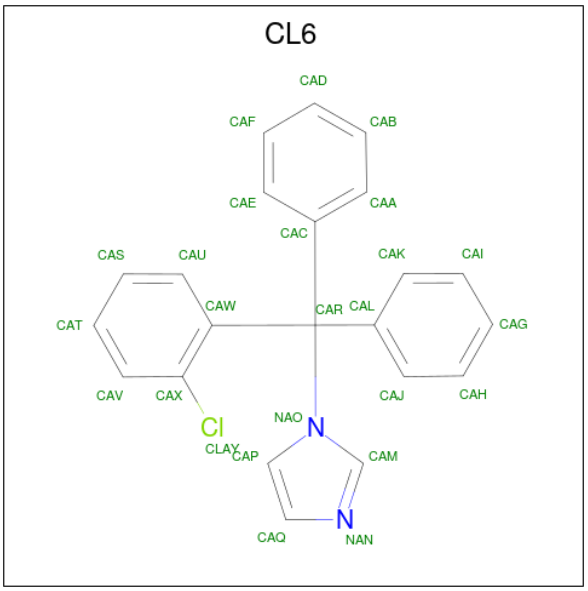
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	394	3085	1942	554	576	13	0	2	0
1	B	394	3070	1932	551	574	13	0	0	0

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



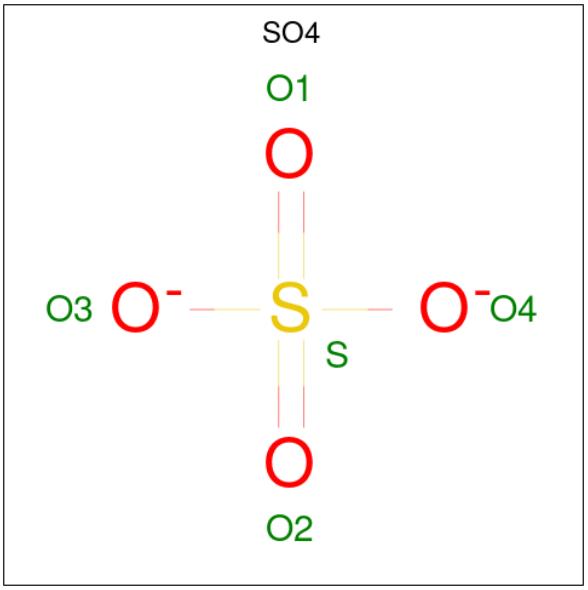
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is 1-[(2-CHLOROPHENYL)(DIPHENYL)METHYL]-1H-IMIDAZOLE (three-letter code: CL6) (formula: $C_{22}H_{17}ClN_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	N		
3	A	1	25	22	1	2	0	0
			Total	C	Cl	N		
3	B	1	25	22	1	2	0	0

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



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

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

- Molecule 5 is water.

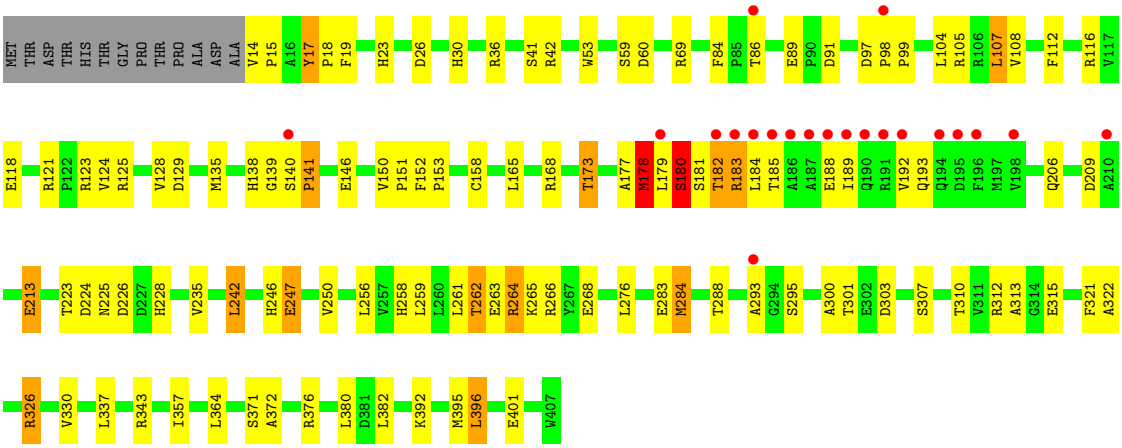
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	28	28	28	0	0
			Total	O		
5	B	29	29	29	0	0

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.

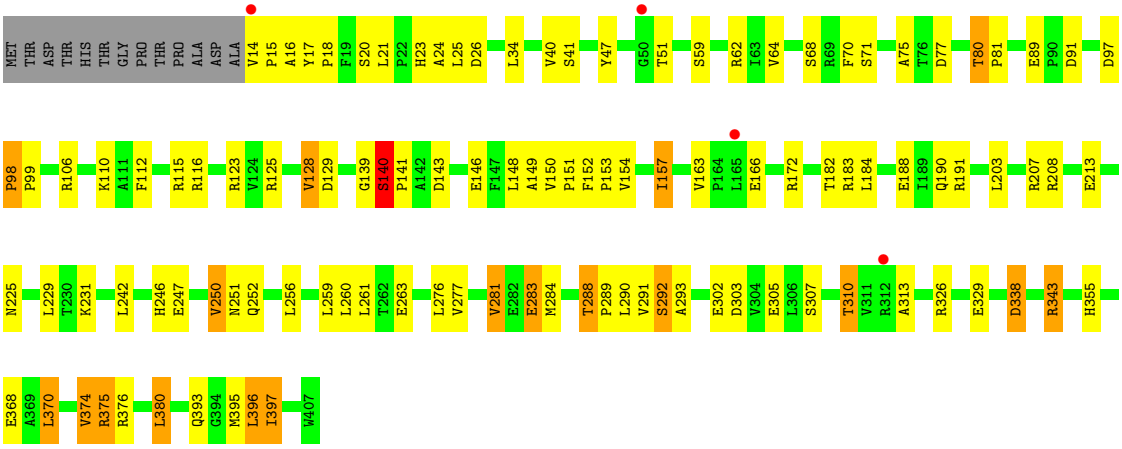
- Molecule 1: Cytochrome P-450

Chain A:



- Molecule 1: Cytochrome P-450

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	115.94Å 117.38Å 174.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.65 48.71 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.76-2.65) 99.4 (48.71-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.207 , 0.260 0.214 , 0.264	Depositor DCC
R_{free} test set	1744 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.034 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6398	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: HEM, SO4, CL6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.59	0/3158	0.93	13/4302 (0.3%)
1	B	0.56	0/3137	0.85	6/4274 (0.1%)
All	All	0.58	0/6295	0.89	19/8576 (0.2%)

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	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	293	ALA	CB-CA-C	13.99	131.08	110.10
1	A	293	ALA	N-CA-C	-10.16	83.56	111.00
1	B	393	GLN	CB-CA-C	-8.32	93.75	110.40
1	A	326	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	B	375	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	375	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	178	MET	CB-CA-C	6.16	122.72	110.40
1	A	121	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	292	SER	N-CA-C	-6.05	94.65	111.00
1	A	326	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	17	TYR	C-N-CD	5.69	140.35	128.40
1	B	128	VAL	CB-CA-C	-5.52	100.91	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	343	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	284	MET	CG-SD-CE	-5.41	91.55	100.20
1	A	264	ARG	CG-CD-NE	5.25	122.83	111.80
1	A	343	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	182	THR	CB-CA-C	-5.07	97.91	111.60
1	A	262	THR	N-CA-CB	5.04	119.88	110.30
1	B	307	SER	CB-CA-C	-5.02	100.56	110.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	GLY	Peptide
1	A	178	MET	Mainchain
1	A	188	GLU	Peptide
1	B	139	GLY	Peptide
1	B	140	SER	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	3085	0	3068	96	3
1	B	3070	0	3044	65	3
2	A	43	0	30	4	0
2	B	43	0	30	3	0
3	A	25	0	17	6	0
3	B	25	0	17	7	0
4	A	30	0	0	10	1
4	B	20	0	0	6	0
5	A	28	0	0	3	0
5	B	29	0	0	4	0
All	All	6398	0	6206	178	4

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 14.

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)
1:A:295:SER:HB3	1:A:321:PHE:CZ	1.58	1.39
1:A:178:MET:HE1	1:A:193:GLN:NE2	1.43	1.31
1:A:178:MET:CE	1:A:193:GLN:NE2	1.94	1.30
1:A:140:SER:OG	1:A:141:PRO:HD3	1.45	1.14
1:A:30:HIS:NE2	4:A:504:SO4:S	2.24	1.10
1:A:178:MET:HE1	1:A:193:GLN:HE21	0.84	0.99
1:A:178:MET:CE	1:A:193:GLN:HE22	1.73	0.99
1:A:178:MET:CE	1:A:193:GLN:HE21	1.67	0.97
1:A:295:SER:CB	1:A:321:PHE:CZ	2.51	0.92
1:A:30:HIS:NE2	4:A:504:SO4:O2	2.03	0.92
1:A:295:SER:HB3	1:A:321:PHE:HZ	1.33	0.91
4:A:508:SO4:O2	1:B:343:ARG:HG3	1.76	0.86
1:A:183:ARG:HB3	1:A:185:THR:HG23	1.60	0.83
1:A:179:LEU:HD13	1:A:247:GLU:HG2	1.61	0.82
1:A:179:LEU:CD1	1:A:247:GLU:HG2	2.10	0.82
1:A:17:TYR:O	1:A:19:PHE:N	2.14	0.81
3:A:502:CL6:HAU	3:A:502:CL6:CAJ	2.09	0.81
1:B:355:HIS:NE2	4:B:503:SO4:O3	2.13	0.80
1:A:183:ARG:HA	1:A:183:ARG:NE	1.95	0.80
1:A:179:LEU:HD12	1:A:247:GLU:CG	2.13	0.79
1:A:140:SER:OG	1:A:141:PRO:CD	2.31	0.79
1:A:179:LEU:CD1	1:A:247:GLU:CG	2.63	0.77
1:A:140:SER:HG	1:A:141:PRO:HD3	1.45	0.76
1:A:178:MET:O	1:A:179:LEU:O	2.03	0.76
1:A:256:LEU:HD22	1:A:284:MET:HB3	1.70	0.74
1:A:322:ALA:O	1:A:326:ARG:HG2	1.88	0.73
1:B:261:LEU:HD11	1:B:380:LEU:HD13	1.69	0.73
1:B:71:SER:OG	1:B:97:ASP:OD2	2.07	0.72
1:A:225:ASN:O	1:A:226:ASP:HB2	1.89	0.72
1:A:312:ARG:N	1:A:315:GLU:OE2	2.22	0.71
1:A:30:HIS:NE2	4:A:504:SO4:O4	2.24	0.69
3:B:502:CL6:CAE	3:B:502:CL6:CLAY	2.77	0.69
1:B:292:SER:O	1:B:293:ALA:HB3	1.92	0.68
1:B:152:PHE:HB3	1:B:153:PRO:HD3	1.75	0.68
1:A:182:THR:OG1	1:A:183:ARG:N	2.26	0.68
1:A:125[B]:ARG:NH2	5:A:605:HOH:O	2.21	0.67
1:A:295:SER:HB3	1:A:321:PHE:CE2	2.25	0.67
1:A:178:MET:HE2	1:A:193:GLN:NE2	2.06	0.67
1:B:284:MET:O	1:B:288:THR:HG23	1.96	0.66
1:A:128:VAL:HG22	1:A:152:PHE:CE1	2.31	0.66
3:B:502:CL6:HAK	3:B:502:CL6:CAA	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:502:CL6:CAM	3:A:502:CL6:HAK	2.25	0.66
1:B:284:MET:O	1:B:288:THR:CG2	2.44	0.65
1:A:259:LEU:HD11	1:A:288:THR:HG22	1.78	0.65
1:A:173:THR:O	1:A:177:ALA:CB	2.45	0.65
1:A:173:THR:O	1:A:177:ALA:HB2	1.97	0.65
1:A:178:MET:HE2	1:A:193:GLN:HE22	1.61	0.64
1:A:295:SER:CB	1:A:321:PHE:HZ	2.04	0.64
1:B:213:GLU:HG2	4:B:506:SO4:O2	1.99	0.63
1:A:295:SER:HB2	2:A:501:HEM:O2A	2.00	0.61
1:B:143:ASP:HB3	1:B:146:GLU:HG2	1.80	0.61
1:B:77:ASP:O	1:B:80:THR:HG22	2.01	0.61
1:A:225:ASN:ND2	1:B:68:SER:OG	2.32	0.60
1:B:251:ASN:HD22	1:B:397:ILE:CG2	2.13	0.60
1:A:258:HIS:HD2	5:A:612:HOH:O	1.83	0.60
1:B:115:ARG:NH1	4:B:504:SO4:S	2.75	0.59
1:B:51:THR:O	1:B:81:PRO:HG2	2.01	0.59
1:A:17:TYR:O	1:A:18:PRO:C	2.37	0.58
4:A:503:SO4:O4	1:B:62:ARG:NH2	2.36	0.58
1:A:303:ASP:OD1	1:A:312:ARG:HD2	2.04	0.58
1:A:30:HIS:CE1	4:A:504:SO4:O4	2.57	0.57
1:A:179:LEU:HD12	1:A:247:GLU:HG3	1.86	0.57
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.86	0.57
3:A:502:CL6:CAJ	3:A:502:CL6:CAU	2.76	0.57
1:A:179:LEU:HD11	1:A:392:LYS:NZ	2.20	0.56
1:A:152:PHE:HB3	1:A:153:PRO:HD3	1.86	0.56
3:B:502:CL6:CLAY	3:B:502:CL6:HAE	2.43	0.56
1:B:302:GLU:HA	1:B:313:ALA:HB2	1.89	0.55
1:B:98:PRO:O	1:B:99:PRO:C	2.43	0.55
1:A:259:LEU:HD11	1:A:288:THR:CG2	2.37	0.55
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.89	0.55
1:B:208:ARG:NH1	1:B:229:LEU:O	2.39	0.55
1:A:14:VAL:HB	1:A:15:PRO:HD3	1.88	0.55
1:B:256:LEU:HD22	1:B:284:MET:HB3	1.89	0.54
1:A:84:PHE:CZ	1:A:396:LEU:CD2	2.91	0.54
1:A:259:LEU:HB2	1:A:284:MET:HE1	1.90	0.54
1:B:115:ARG:NH2	4:B:506:SO4:O4	2.41	0.54
1:A:178:MET:HE3	1:A:193:GLN:NE2	2.11	0.53
1:B:397:ILE:HD13	3:B:502:CL6:HAI	1.90	0.53
1:B:182:THR:HG22	1:B:184:LEU:H	1.74	0.53
1:A:84:PHE:CZ	1:A:396:LEU:HD21	2.44	0.53
1:B:75:ALA:HA	1:B:80:THR:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:502:CL6:HAE	3:B:502:CL6:CAX	2.38	0.53
1:A:84:PHE:HZ	1:A:396:LEU:HG	1.72	0.53
1:B:242:LEU:HD23	1:B:242:LEU:O	2.09	0.53
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.91	0.52
1:A:129:ASP:OD1	1:A:376:ARG:NH1	2.40	0.52
1:A:258:HIS:O	1:A:261:LEU:O	2.28	0.52
3:A:502:CL6:CLAY	3:A:502:CL6:NAO	2.80	0.52
1:A:118:GLU:HG2	4:B:505:SO4:O1	2.10	0.51
4:A:503:SO4:S	1:B:62:ARG:NH2	2.83	0.51
1:B:157:ILE:HG21	1:B:242:LEU:HG	1.93	0.51
1:A:135:MET:O	1:A:138:HIS:O	2.28	0.51
1:A:189:ILE:O	1:A:192:VAL:HB	2.11	0.51
1:B:172:ARG:HG3	5:B:620:HOH:O	2.11	0.50
1:A:105:ARG:CZ	1:A:357:ILE:HG13	2.43	0.49
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.93	0.49
1:B:251:ASN:HD22	1:B:397:ILE:HG22	1.77	0.49
1:A:23:HIS:O	1:A:26:ASP:HB2	2.12	0.48
1:A:246:HIS:O	1:A:250:VAL:HG23	2.13	0.48
1:B:260:LEU:HG	1:B:284:MET:HE3	1.95	0.48
1:B:292:SER:O	1:B:293:ALA:CB	2.56	0.48
1:A:60:ASP:OD2	1:A:307:SER:HB3	2.12	0.48
1:A:300:ALA:O	1:A:313:ALA:O	2.31	0.48
1:B:17:TYR:CD1	1:B:18:PRO:HA	2.49	0.48
3:B:502:CL6:CLAY	3:B:502:CL6:CAL	2.97	0.48
1:B:292:SER:HB2	1:B:395:MET:O	2.13	0.48
1:A:173:THR:O	1:A:177:ALA:HB3	2.14	0.47
1:B:172:ARG:CG	5:B:620:HOH:O	2.62	0.47
1:A:284:MET:O	1:A:288:THR:HG23	2.14	0.47
1:B:17:TYR:HA	1:B:18:PRO:C	2.34	0.47
1:A:17:TYR:C	1:A:17:TYR:CD1	2.88	0.47
1:B:284:MET:O	1:B:288:THR:HG22	2.15	0.47
1:A:261:LEU:O	1:A:262:THR:OG1	2.25	0.46
1:B:106:ARG:NE	5:B:618:HOH:O	2.49	0.46
1:B:129:ASP:OD1	1:B:375:ARG:NH2	2.48	0.46
1:A:179:LEU:HG	1:A:180:SER:N	2.31	0.46
4:A:508:SO4:O1	1:B:343:ARG:NH1	2.48	0.46
1:B:246:HIS:O	1:B:250:VAL:HG12	2.16	0.46
1:B:252:GLN:HG2	1:B:290:LEU:HD13	1.97	0.46
1:B:291:VAL:HG12	1:B:292:SER:N	2.31	0.46
1:B:396:LEU:O	1:B:397:ILE:HD12	2.15	0.46
1:A:179:LEU:HD11	1:A:392:LYS:HZ1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HG3	1:A:53:TRP:CZ3	2.51	0.45
3:B:502:CL6:CAA	3:B:502:CL6:CAK	2.93	0.45
1:A:179:LEU:CD1	1:A:247:GLU:OE2	2.64	0.45
1:A:213:GLU:HB3	4:A:508:SO4:O1	2.15	0.45
1:B:256:LEU:O	1:B:284:MET:HE1	2.17	0.45
1:B:288:THR:HA	1:B:289:PRO:HD3	1.89	0.45
3:A:502:CL6:CAM	3:A:502:CL6:CAK	2.91	0.45
1:B:370:LEU:O	1:B:374:VAL:HG13	2.17	0.45
1:B:24:ALA:O	1:B:25:LEU:HB2	2.17	0.45
1:A:14:VAL:HB	1:A:15:PRO:CD	2.46	0.45
1:A:69:ARG:C	1:A:301:THR:HG22	2.38	0.45
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.48	0.44
1:B:283:GLU:HG3	1:B:338:ASP:O	2.16	0.44
1:A:179:LEU:HD12	1:A:247:GLU:OE2	2.18	0.44
1:A:84:PHE:HZ	1:A:396:LEU:CD2	2.29	0.44
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.47	0.44
1:B:149:ALA:O	1:B:250:VAL:HB	2.17	0.44
1:A:125[B]:ARG:HH22	1:A:372:ALA:HA	1.82	0.43
1:B:23:HIS:ND1	1:B:26:ASP:OD2	2.50	0.43
1:B:116:ARG:HA	5:B:619:HOH:O	2.16	0.43
1:B:115:ARG:NH1	4:B:504:SO4:O2	2.51	0.43
1:A:116:ARG:HG3	5:A:624:HOH:O	2.18	0.43
1:B:260:LEU:HG	1:B:284:MET:CE	2.47	0.43
1:B:277:VAL:O	1:B:281:VAL:HG13	2.19	0.43
1:B:246:HIS:O	1:B:250:VAL:CG1	2.67	0.43
1:A:107:LEU:CD1	1:A:224:ASP:HB2	2.48	0.43
1:A:242:LEU:O	1:A:242:LEU:HG	2.18	0.43
1:A:223:THR:HG22	1:A:224:ASP:N	2.34	0.43
1:B:184:LEU:HB3	1:B:188:GLU:HB2	2.01	0.43
1:A:69:ARG:O	1:A:301:THR:HG22	2.18	0.42
1:A:259:LEU:HB2	1:A:284:MET:CE	2.49	0.42
1:A:264:ARG:NH1	1:A:268:GLU:HG3	2.34	0.42
1:A:128:VAL:HG22	1:A:152:PHE:CZ	2.54	0.42
1:A:30:HIS:CD2	4:A:504:SO4:O2	2.69	0.42
1:A:177:ALA:C	1:A:182:THR:HG21	2.39	0.42
1:B:305:GLU:HA	1:B:310:THR:HB	2.00	0.42
1:A:124:VAL:O	1:A:128:VAL:HG23	2.20	0.42
1:A:158:CYS:HB3	1:A:168:ARG:HD3	2.01	0.41
1:B:64:VAL:HA	1:B:70:PHE:CE2	2.56	0.41
1:B:291:VAL:CG1	1:B:292:SER:N	2.84	0.41
1:A:150:VAL:HB	1:A:151:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:VAL:HB	1:B:151:PRO:HD3	2.01	0.41
1:A:98:PRO:O	1:A:99:PRO:C	2.56	0.41
1:B:21:LEU:HD12	1:B:21:LEU:O	2.21	0.41
1:A:179:LEU:HD12	1:A:247:GLU:CD	2.40	0.41
1:A:264:ARG:HG3	1:A:264:ARG:O	2.20	0.41
1:A:178:MET:O	1:A:179:LEU:C	2.59	0.41
1:B:47:TYR:O	1:B:81:PRO:HA	2.20	0.41
3:A:502:CL6:CAJ	3:A:502:CL6:CAE	2.96	0.41
1:B:259:LEU:HB2	1:B:284:MET:CE	2.51	0.40
1:A:283:GLU:HG3	1:A:337:LEU:HD22	2.03	0.40
1:A:263:GLU:O	1:A:265:LYS:N	2.54	0.40
1:A:178:MET:N	1:A:182:THR:HG21	2.37	0.40
1:B:14:VAL:O	1:B:16:ALA:N	2.52	0.40
1:B:203:LEU:O	1:B:207:ARG:HG2	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:OE2	1:B:140:SER:OG[8_555]	1.58	0.62
1:A:23:HIS:CE1	4:A:504:SO4:O2[4_555]	1.86	0.34
1:B:190:GLN:OE1	1:B:190:GLN:OE1[3_555]	2.07	0.13
1:A:146:GLU:CD	1:B:140:SER:OG[8_555]	2.11	0.09

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	394/407 (97%)	356 (90%)	36 (9%)	2 (0%)	29	43
1	B	392/407 (96%)	365 (93%)	24 (6%)	3 (1%)	19	29
All	All	786/814 (97%)	721 (92%)	60 (8%)	5 (1%)	25	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	SER
1	B	15	PRO
1	B	140	SER
1	B	141	PRO
1	A	141	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	333/341 (98%)	296 (89%)	37 (11%)	6 8
1	B	330/341 (97%)	286 (87%)	44 (13%)	4 5
All	All	663/682 (97%)	582 (88%)	81 (12%)	4 6

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	41	SER
1	A	59	SER
1	A	86	THR
1	A	89	GLU
1	A	91	ASP
1	A	97	ASP
1	A	104	LEU
1	A	107	LEU
1	A	108	VAL
1	A	112	PHE
1	A	123	ARG
1	A	165	LEU
1	A	173	THR
1	A	178	MET
1	A	180	SER
1	A	181	SER
1	A	183	ARG

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Mol	Chain	Res	Type
1	A	184	LEU
1	A	206	GLN
1	A	209	ASP
1	A	213	GLU
1	A	228	HIS
1	A	235	VAL
1	A	242	LEU
1	A	247	GLU
1	A	266	ARG
1	A	276	LEU
1	A	310	THR
1	A	330	VAL
1	A	364	LEU
1	A	371	SER
1	A	380	LEU
1	A	382	LEU
1	A	395	MET
1	A	396	LEU
1	A	401	GLU
1	B	20	SER
1	B	34	LEU
1	B	40	VAL
1	B	41	SER
1	B	59	SER
1	B	80	THR
1	B	89	GLU
1	B	91	ASP
1	B	98	PRO
1	B	110	LYS
1	B	112	PHE
1	B	123	ARG
1	B	125	ARG
1	B	128	VAL
1	B	140	SER
1	B	148	LEU
1	B	154	VAL
1	B	157	ILE
1	B	163	VAL
1	B	166	GLU
1	B	183	ARG
1	B	191	ARG
1	B	225	ASN

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Mol	Chain	Res	Type
1	B	231	LYS
1	B	247	GLU
1	B	250	VAL
1	B	263	GLU
1	B	276	LEU
1	B	281	VAL
1	B	283	GLU
1	B	288	THR
1	B	303	ASP
1	B	310	THR
1	B	326	ARG
1	B	329	GLU
1	B	338	ASP
1	B	343	ARG
1	B	368	GLU
1	B	370	LEU
1	B	374	VAL
1	B	376	ARG
1	B	380	LEU
1	B	396	LEU
1	B	397	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	96	GLN
1	A	193	GLN
1	A	194	GLN
1	A	225	ASN
1	A	258	HIS
1	B	251	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
2	HEM	B	501	1,3	41,50,50	1.50	6 (14%)	45,82,82	1.91	16 (35%)
2	HEM	A	501	1,3	41,50,50	1.46	5 (12%)	45,82,82	1.97	15 (33%)
4	SO4	B	506	-	4,4,4	0.43	0	6,6,6	0.37	0
4	SO4	A	505	-	4,4,4	0.31	0	6,6,6	0.22	0
4	SO4	A	508	-	4,4,4	0.68	0	6,6,6	0.53	0
4	SO4	A	504	-	4,4,4	0.65	0	6,6,6	0.54	0
4	SO4	A	507	-	4,4,4	0.40	0	6,6,6	0.43	0
4	SO4	B	505	-	4,4,4	0.32	0	6,6,6	0.63	0
4	SO4	B	504	-	4,4,4	0.43	0	6,6,6	0.64	0
4	SO4	B	503	-	4,4,4	0.16	0	6,6,6	0.18	0
3	CL6	B	502	2	26,28,28	2.42	6 (23%)	35,39,39	4.37	12 (34%)
3	CL6	A	502	2	26,28,28	1.99	6 (23%)	35,39,39	4.91	12 (34%)
4	SO4	A	503	-	4,4,4	0.46	0	6,6,6	0.47	0
4	SO4	A	506	-	4,4,4	0.19	0	6,6,6	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CL6	B	502	2	-	4/18/24/24	0/4/4/4
2	HEM	B	501	1,3	-	3/12/54/54	-
3	CL6	A	502	2	-	3/18/24/24	0/4/4/4
2	HEM	A	501	1,3	-	0/12/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	CL6	CAP-NAO	-7.07	1.33	1.38
3	B	502	CL6	CAX-CAW	5.95	1.49	1.39
3	A	502	CL6	CAX-CAW	5.55	1.48	1.39
3	A	502	CL6	CAP-NAO	-5.24	1.34	1.38
2	B	501	HEM	C1B-NB	-5.23	1.31	1.40
3	B	502	CL6	CAR-NAO	-4.78	1.45	1.51
2	A	501	HEM	C1B-NB	-4.36	1.32	1.40
3	B	502	CL6	CAR-CAC	-4.31	1.48	1.53
2	A	501	HEM	C4B-NB	-4.18	1.30	1.38
2	A	501	HEM	C4D-ND	-3.44	1.34	1.40
3	A	502	CL6	CAR-CAC	-3.29	1.49	1.53
3	A	502	CL6	CAX-CLAY	3.27	1.81	1.73
2	B	501	HEM	C4D-ND	-3.21	1.34	1.40
3	B	502	CL6	CAX-CLAY	3.08	1.80	1.73
3	A	502	CL6	CAR-CAL	2.45	1.56	1.53
2	B	501	HEM	FE-NB	2.40	2.08	1.96
2	B	501	HEM	C4B-NB	-2.37	1.33	1.38
2	B	501	HEM	C1D-ND	-2.35	1.34	1.38
3	B	502	CL6	CAR-CAL	2.25	1.56	1.53
2	B	501	HEM	C3B-C4B	2.23	1.49	1.44
2	A	501	HEM	FE-NB	2.19	2.07	1.96
3	A	502	CL6	CAR-NAO	-2.16	1.48	1.51
2	A	501	HEM	CHB-C1B	2.07	1.40	1.35

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	CL6	CAR-CAW-CAX	-17.76	111.40	122.65
3	B	502	CL6	CAM-NAO-CAR	-15.28	114.03	126.71
3	A	502	CL6	CAU-CAW-CAR	14.43	131.47	121.05
3	A	502	CL6	CAL-CAR-CAW	-11.78	96.31	112.00
3	B	502	CL6	CAW-CAR-NAO	11.26	123.29	106.11
3	B	502	CL6	CAL-CAR-CAW	-10.80	97.61	112.00
3	B	502	CL6	CAP-NAO-CAM	8.67	113.75	108.25
3	A	502	CL6	CAC-CAR-CAW	6.56	120.74	112.00
3	A	502	CL6	CAP-NAO-CAM	6.39	112.31	108.25
3	B	502	CL6	CAP-NAO-CAR	6.10	132.15	124.95
3	A	502	CL6	CAW-CAR-NAO	5.83	115.00	106.11
3	B	502	CL6	CAC-CAR-CAW	5.58	119.44	112.00
2	A	501	HEM	CHC-C4B-NB	5.39	130.28	124.43
2	A	501	HEM	C1B-NB-C4B	5.21	110.45	105.07
2	A	501	HEM	CHD-C1D-ND	4.28	129.08	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	C1B-NB-C4B	4.23	109.44	105.07
2	B	501	HEM	CHD-C1D-ND	3.94	128.71	124.43
3	A	502	CL6	CAL-CAR-CAC	-3.82	99.33	110.14
2	A	501	HEM	CHD-C1D-C2D	-3.54	119.44	124.98
2	B	501	HEM	C4B-CHC-C1C	3.43	127.09	122.56
2	B	501	HEM	CMC-C2C-C3C	3.15	130.57	124.68
2	B	501	HEM	CMB-C2B-C1B	3.08	129.73	125.04
2	B	501	HEM	C4B-C3B-C2B	-2.85	104.85	107.11
2	B	501	HEM	CHA-C4D-ND	2.81	127.86	124.38
2	A	501	HEM	O2D-CGD-O1D	-2.75	116.45	123.30
2	B	501	HEM	CHA-C4D-C3D	-2.74	120.19	125.33
2	B	501	HEM	O2D-CGD-O1D	-2.72	116.52	123.30
2	B	501	HEM	CHD-C1D-C2D	-2.71	120.75	124.98
3	A	502	CL6	CAP-NAO-CAR	-2.65	121.83	124.95
3	A	502	CL6	CAW-CAX-CLAY	-2.58	118.71	121.68
3	B	502	CL6	CAJ-CAL-CAK	-2.55	114.19	117.97
3	A	502	CL6	CAE-CAC-CAR	2.52	126.04	120.94
3	B	502	CL6	CAV-CAX-CAW	-2.46	118.82	121.79
2	A	501	HEM	CMC-C2C-C3C	2.45	129.26	124.68
2	B	501	HEM	O2A-CGA-CBA	2.44	121.88	114.03
2	A	501	HEM	C4B-CHC-C1C	2.38	125.70	122.56
2	A	501	HEM	CHA-C4D-ND	2.34	127.28	124.38
2	B	501	HEM	C2C-C3C-C4C	2.34	108.53	106.90
2	A	501	HEM	O2A-CGA-O1A	-2.28	117.63	123.30
3	B	502	CL6	CAL-CAR-CAC	-2.27	103.71	110.14
3	A	502	CL6	CAI-CAK-CAL	2.25	123.12	120.76
3	A	502	CL6	CAJ-CAL-CAK	-2.25	114.63	117.97
2	A	501	HEM	CMA-C3A-C4A	-2.24	125.02	128.46
2	B	501	HEM	CAB-C3B-C2B	-2.21	121.32	128.60
3	B	502	CL6	CAK-CAL-CAR	2.20	125.39	120.94
2	A	501	HEM	O2A-CGA-CBA	2.17	121.01	114.03
2	B	501	HEM	CMB-C2B-C3B	-2.11	123.13	128.30
2	A	501	HEM	O2D-CGD-CBD	2.10	120.79	114.03
2	A	501	HEM	CAD-C3D-C4D	2.10	128.32	124.66
3	B	502	CL6	CAH-CAJ-CAL	2.09	122.95	120.76
3	B	502	CL6	CAI-CAK-CAL	2.04	122.90	120.76
2	B	501	HEM	C3C-C4C-NC	-2.03	107.11	110.94
2	A	501	HEM	CHC-C4B-C3B	-2.01	121.49	124.57
2	A	501	HEM	C4A-C3A-C2A	2.01	108.39	107.00
2	B	501	HEM	CAB-C3B-C4B	2.00	133.81	124.47

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	CL6	CAC-CAR-CAW-CAX
3	A	502	CL6	CAC-CAR-CAW-CAU
3	B	502	CL6	CAK-CAL-CAR-NAO
3	B	502	CL6	CAJ-CAL-CAR-NAO
2	B	501	HEM	C4D-C3D-CAD-CBD
2	B	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C2D-C3D-CAD-CBD
3	B	502	CL6	CAA-CAC-CAR-NAO
3	A	502	CL6	CAA-CAC-CAR-CAL
3	B	502	CL6	CAE-CAC-CAR-NAO

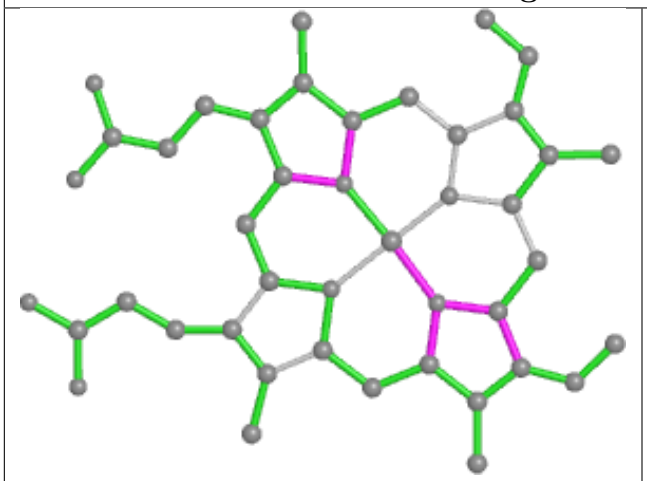
There are no ring outliers.

11 monomers are involved in 37 short contacts:

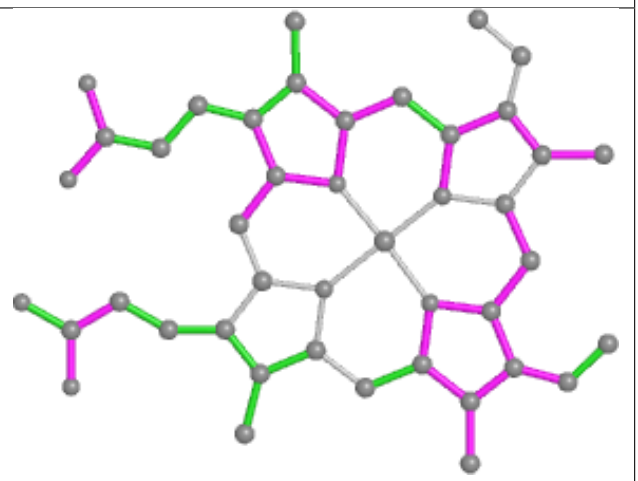
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	3	0
2	A	501	HEM	4	0
4	B	506	SO4	2	0
4	A	508	SO4	3	0
4	A	504	SO4	5	1
4	B	505	SO4	1	0
4	B	504	SO4	2	0
4	B	503	SO4	1	0
3	B	502	CL6	7	0
3	A	502	CL6	6	0
4	A	503	SO4	2	0

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.

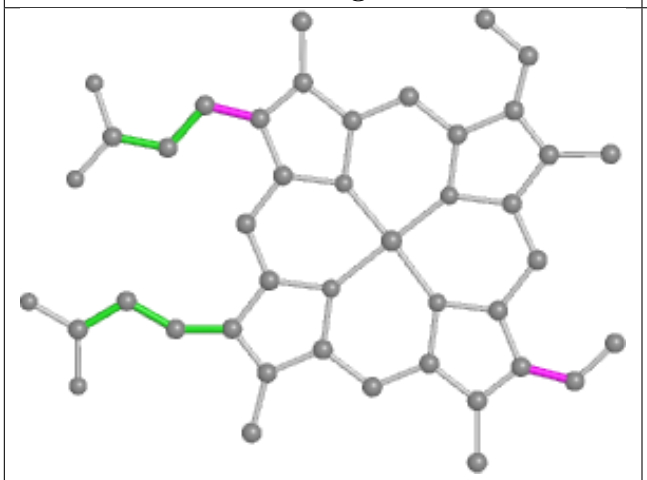
Ligand HEM B 501



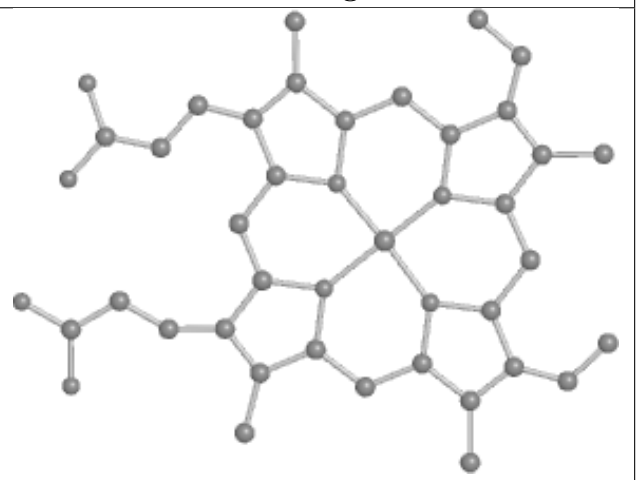
Bond lengths



Bond angles

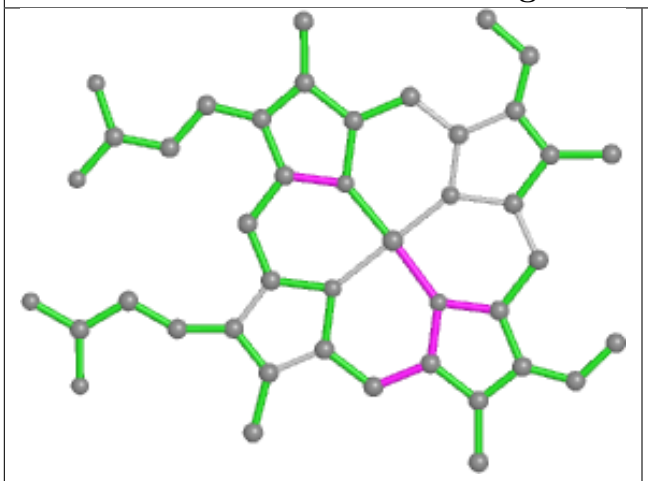


Torsions

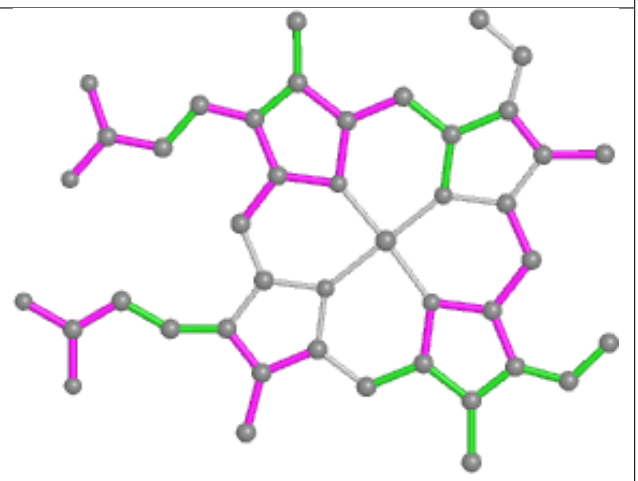


Rings

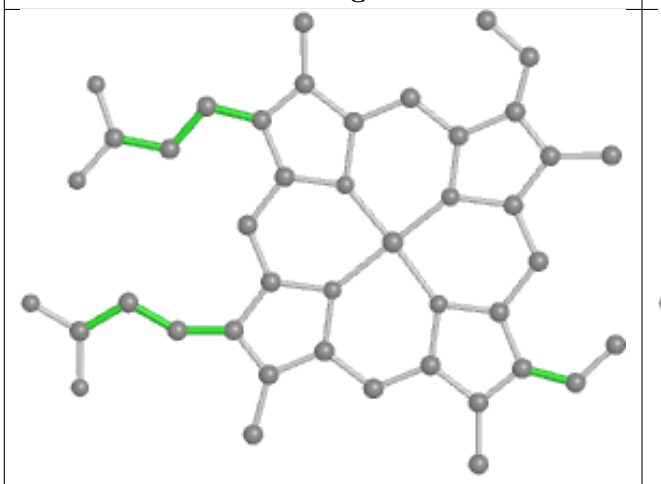
Ligand HEM A 501



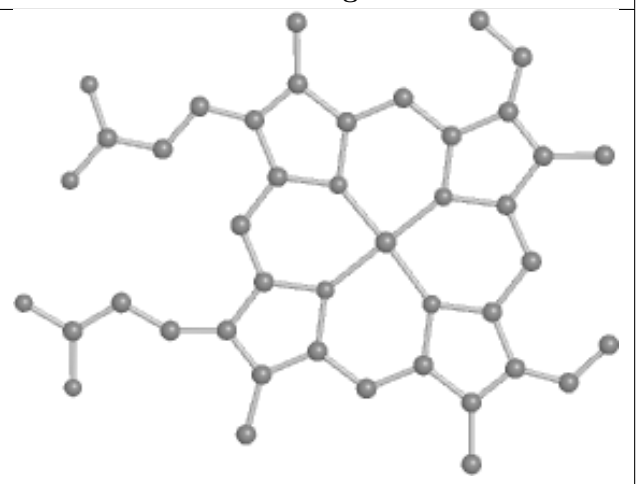
Bond lengths



Bond angles

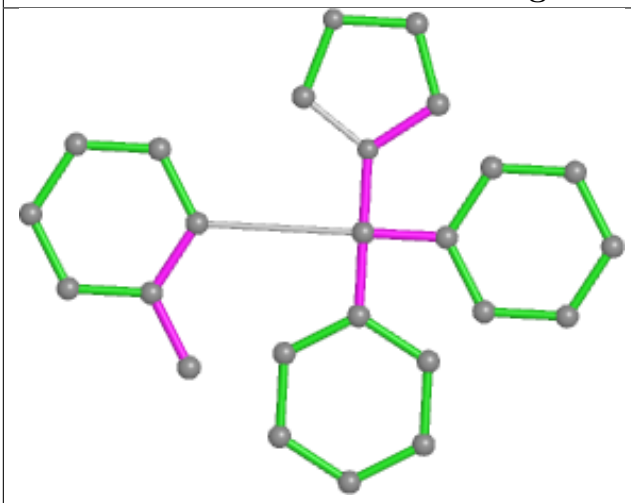


Torsions

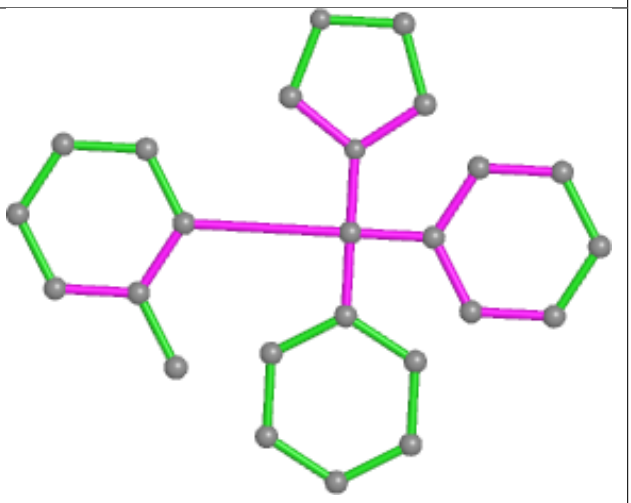


Rings

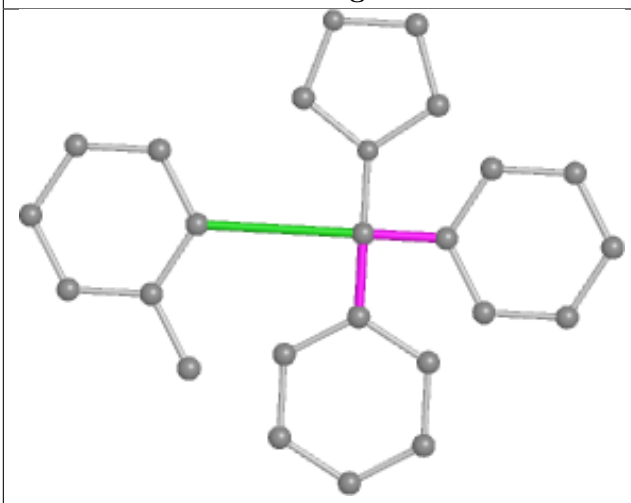
Ligand CL6 B 502



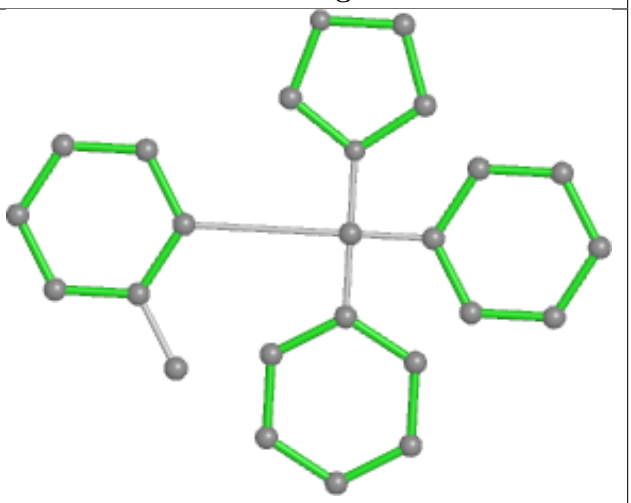
Bond lengths



Bond angles

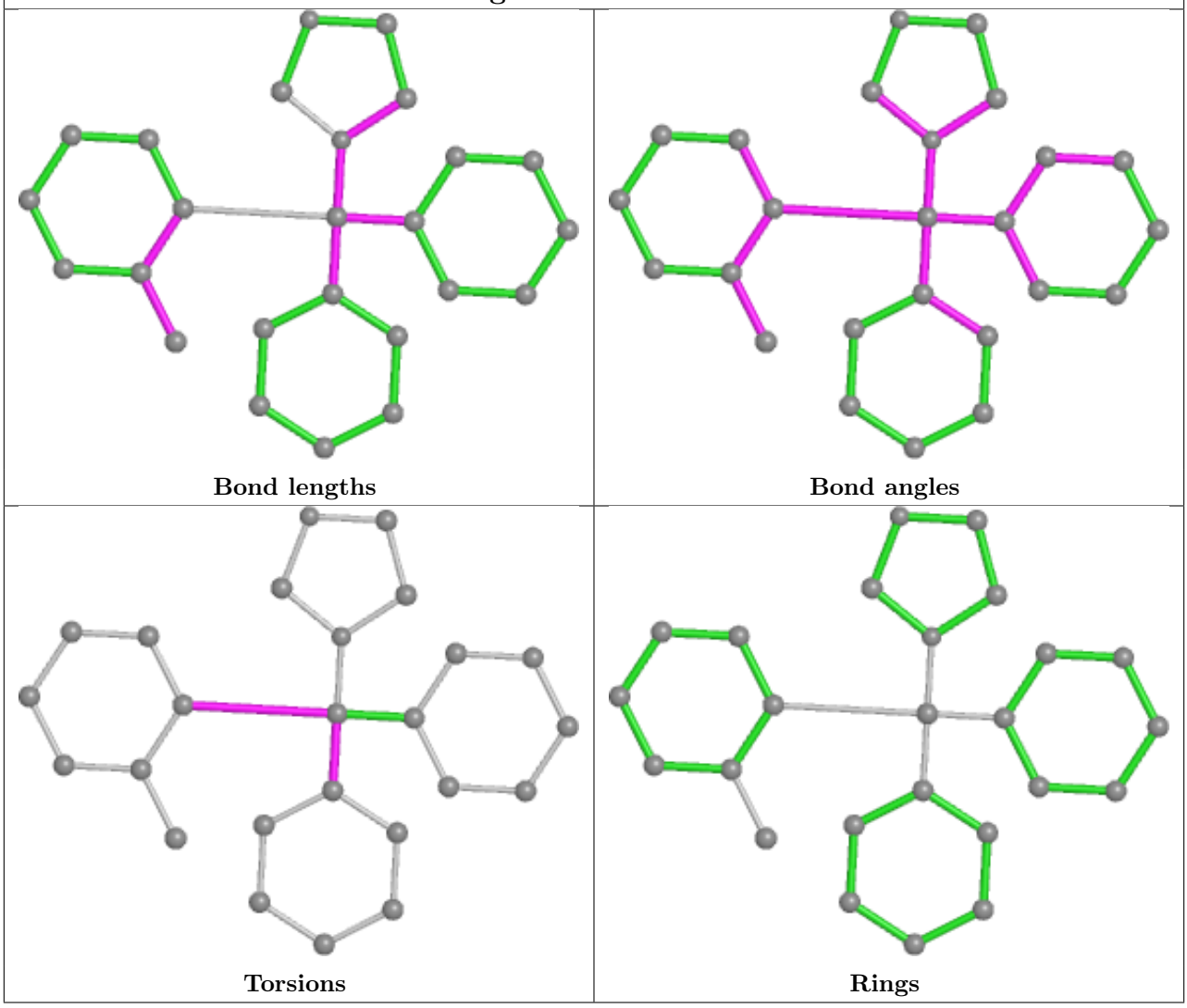


Torsions



Rings

Ligand CL6 A 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	394/407 (96%)	0.16	21 (5%)	26	23	30, 52, 111, 168	0
1	B	394/407 (96%)	-0.00	4 (1%)	82	81	32, 56, 88, 112	0
All	All	788/814 (96%)	0.08	25 (3%)	47	44	30, 54, 97, 168	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ARG	7.3
1	A	184	LEU	6.9
1	A	186	ALA	6.1
1	A	185	THR	6.0
1	A	187	ALA	5.9
1	A	194	GLN	5.2
1	A	189	ILE	4.7
1	A	195	ASP	4.5
1	A	192	VAL	4.4
1	B	14	VAL	4.3
1	B	50	GLY	4.2
1	A	198	VAL	3.3
1	A	182	THR	3.3
1	A	190	GLN	3.2
1	A	191	ARG	3.0
1	A	196	PHE	2.6
1	B	165	LEU	2.6
1	A	98	PRO	2.6
1	B	312	ARG	2.5
1	A	86	THR	2.5
1	A	188	GLU	2.3
1	A	293	ALA	2.3
1	A	210	ALA	2.2
1	A	140	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	179	LEU	2.2

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)

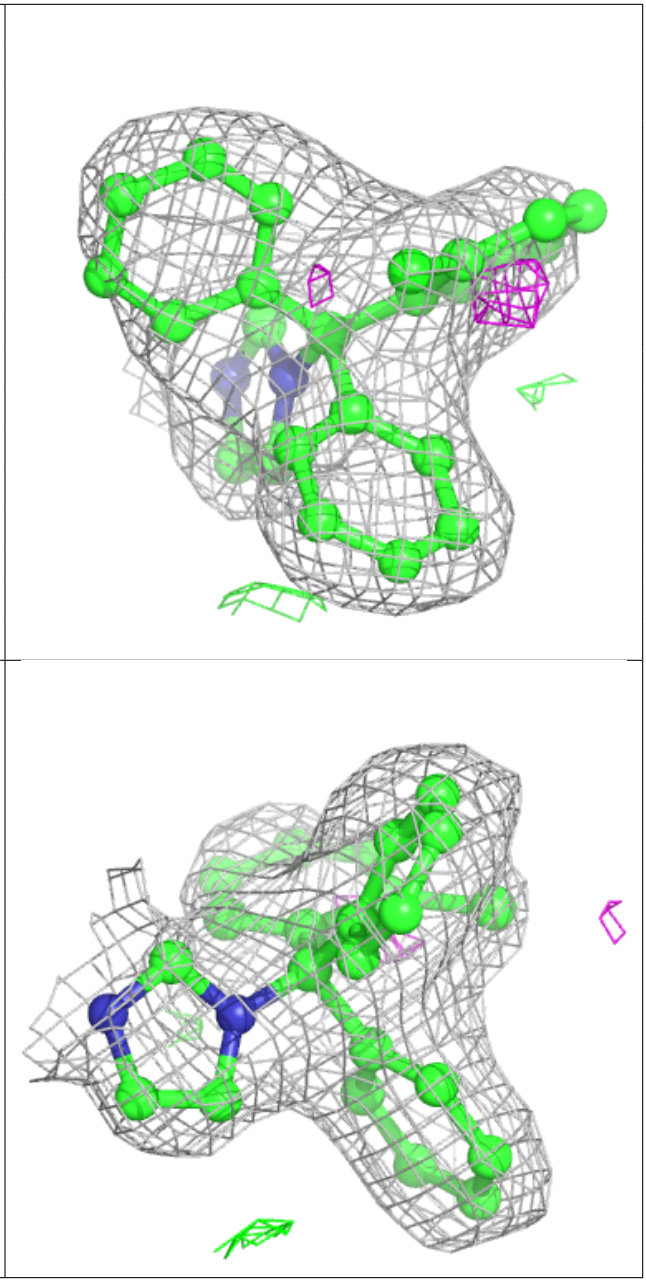
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	507	5/5	0.80	0.24	104,108,114,125	0
4	SO4	B	505	5/5	0.87	0.28	85,90,92,107	0
3	CL6	B	502	25/25	0.95	0.20	52,62,79,96	0
4	SO4	A	508	5/5	0.96	0.14	46,50,57,57	0
3	CL6	A	502	25/25	0.96	0.17	48,59,69,87	0
4	SO4	B	503	5/5	0.97	0.25	47,49,59,61	0
4	SO4	A	505	5/5	0.97	0.13	54,59,63,67	0
4	SO4	B	506	5/5	0.97	0.18	54,56,65,67	0
4	SO4	A	503	5/5	0.98	0.14	55,58,62,63	0
4	SO4	A	504	5/5	0.98	0.19	27,33,37,40	0
4	SO4	B	504	5/5	0.98	0.12	55,56,62,67	0
2	HEM	A	501	43/43	0.98	0.19	38,42,47,59	0
2	HEM	B	501	43/43	0.98	0.18	35,44,55,58	0
4	SO4	A	506	5/5	0.99	0.20	45,45,51,52	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.

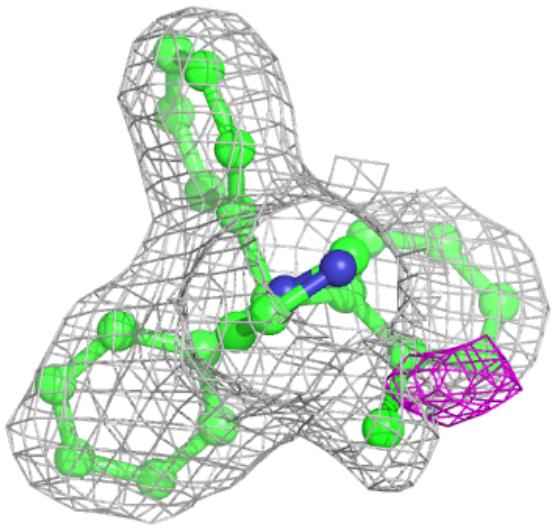
Electron density around CL6 B 502:

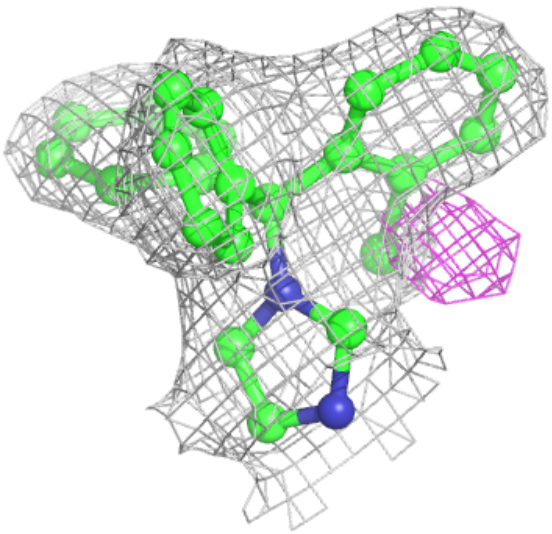
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

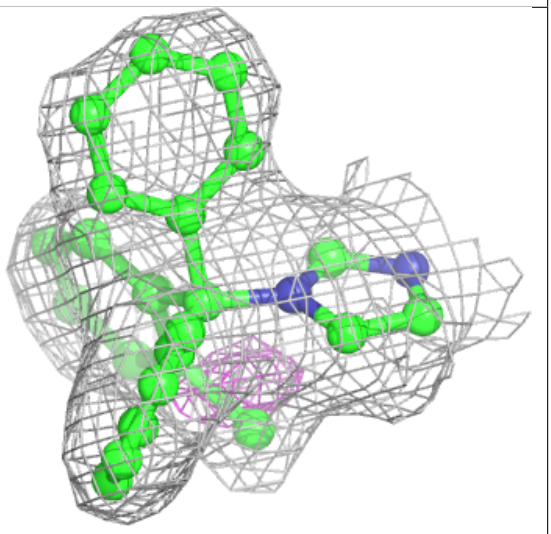


Electron density around CL6 A 502:

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

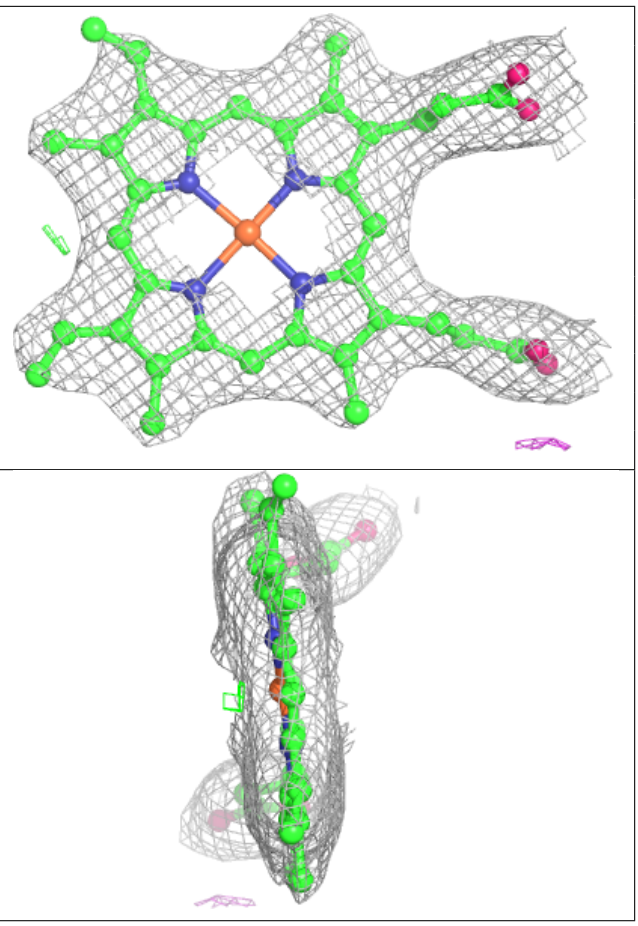


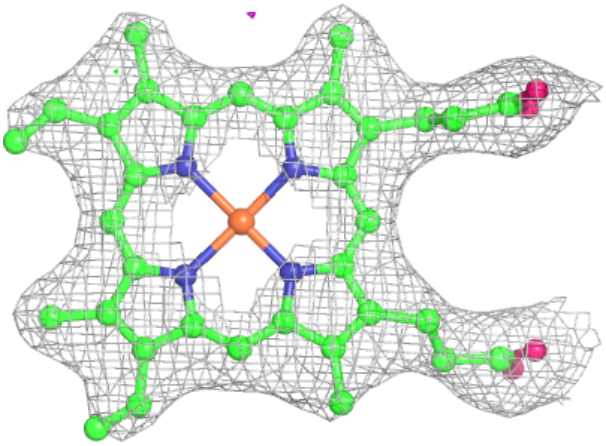
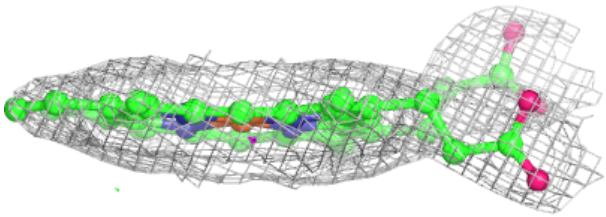
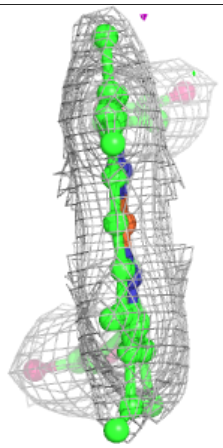




Electron density around HEM A 501:

$2mF_o$-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 501: 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.