Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 09:53 PM EDT

PDB ID	:	5LIV
Title	:	Crystal structure of myxobacterial CYP260A1
Authors	:	Carius, Y.; Khatri, Y.; Bernhardt, R.; Lancaster, C.R.D.
Deposited on	:	2016-07-15
Resolution	:	2.67 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:

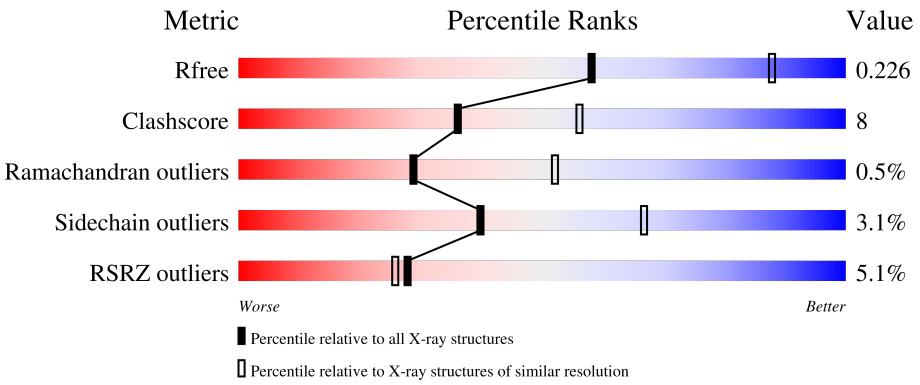
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	450	5%, 76%, 10%, •, 12%
1	B	450	9%, 72%, 13%, •, 14%
1	C	450	%, 73%, 13%, •, 12%
1	D	450	3%, 72%, 13%, •, 14%

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
3	GOL	A	502	-	X	-	-
3	GOL	C	505	-	-	X	-
3	GOL	C	506	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12879 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 CYP260A1,Cytochrome P450 CYP260A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	397	3092	1955	565	555	17	0	2	0
1	B	389	3003	1908	536	543	16	0	1	0
1	C	395	3091	1952	562	561	16	0	2	0
1	D	389	2997	1896	542	543	16	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	HIS	-	expression tag	UNP A9FDB7
A	446	HIS	-	expression tag	UNP A9FDB7
A	447	HIS	-	expression tag	UNP A9FDB7
A	448	HIS	-	expression tag	UNP A9FDB7
A	449	HIS	-	expression tag	UNP A9FDB7
A	450	HIS	-	expression tag	UNP A9FDB7
B	445	HIS	-	expression tag	UNP A9FDB7
B	446	HIS	-	expression tag	UNP A9FDB7
B	447	HIS	-	expression tag	UNP A9FDB7
B	448	HIS	-	expression tag	UNP A9FDB7
B	449	HIS	-	expression tag	UNP A9FDB7
B	450	HIS	-	expression tag	UNP A9FDB7
C	445	HIS	-	expression tag	UNP A9FDB7
C	446	HIS	-	expression tag	UNP A9FDB7
C	447	HIS	-	expression tag	UNP A9FDB7
C	448	HIS	-	expression tag	UNP A9FDB7
C	449	HIS	-	expression tag	UNP A9FDB7
C	450	HIS	-	expression tag	UNP A9FDB7
D	445	HIS	-	expression tag	UNP A9FDB7
D	446	HIS	-	expression tag	UNP A9FDB7
D	447	HIS	-	expression tag	UNP A9FDB7

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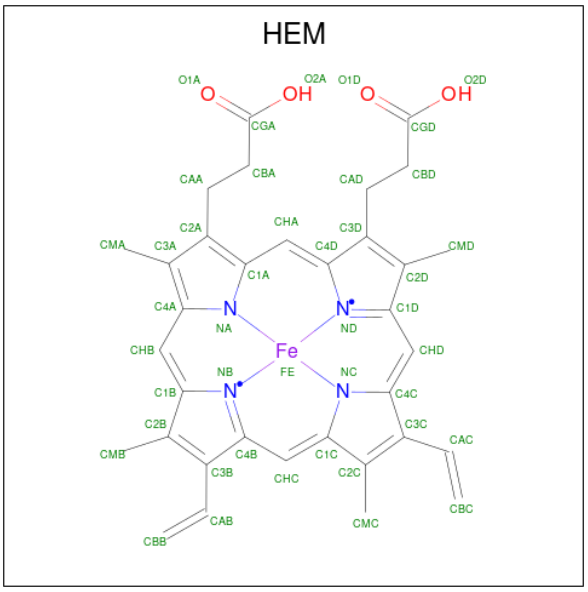
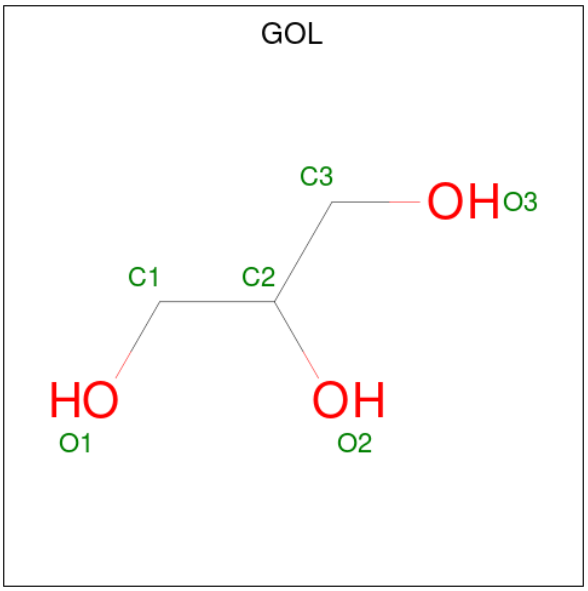
Chain	Residue	Modelled	Actual	Comment	Reference
D	448	HIS	-	expression tag	UNP A9FDB7
D	449	HIS	-	expression tag	UNP A9FDB7
D	450	HIS	-	expression tag	UNP A9FDB7

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



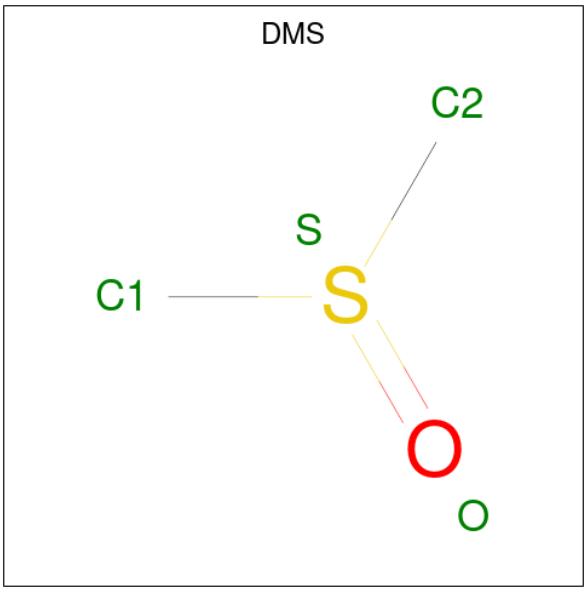
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



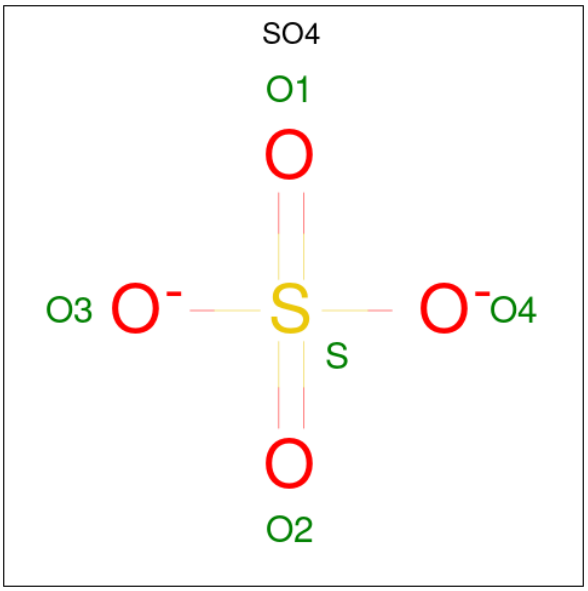
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	A	1	4	2	1	1	0	0
4	B	1	4	2	1	1	0	0
4	C	1	4	2	1	1	0	0
4	D	1	4	2	1	1	0	0
4	D	1	4	2	1	1	0	0
4	D	1	4	2	1	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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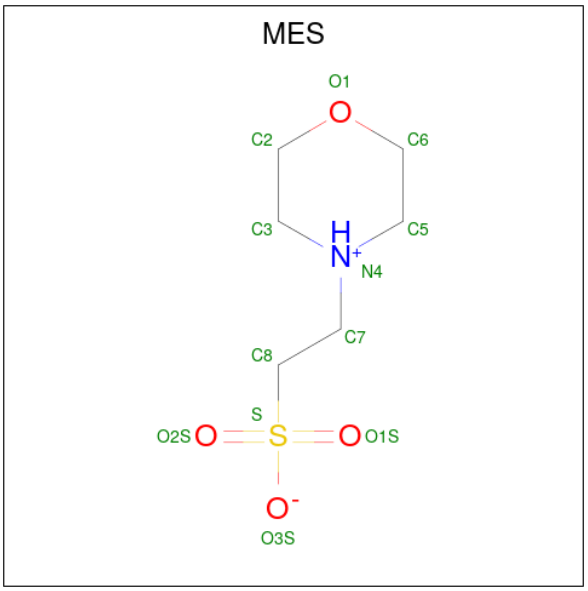
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
5	D	1	5	4	1		0	0
			Total	O	S			
5	D	1	5	4	1		0	0
			Total	O	S			
5	D	1	5	4	1		0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	12	6	1	4	1	0	0

- Molecule 7 is water.

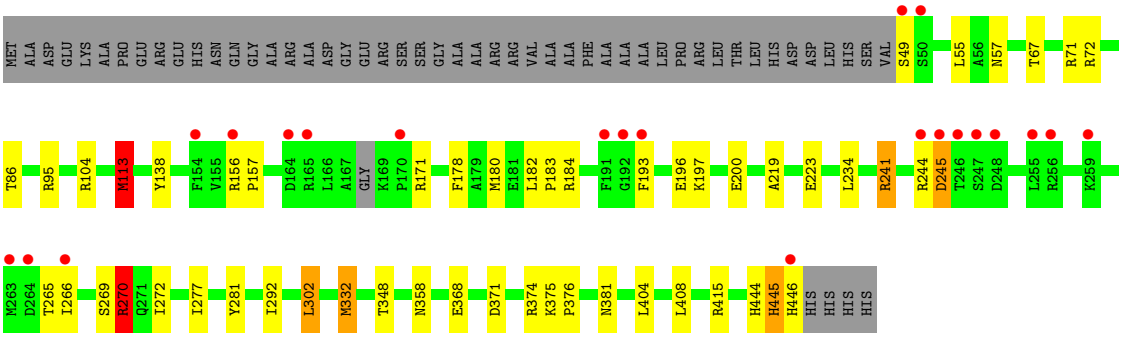
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	78	78	78	0	0
			Total	O		
7	B	66	66	66	0	0
			Total	O		
7	C	117	117	117	0	0
			Total	O		
7	D	76	76	76	0	0

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.

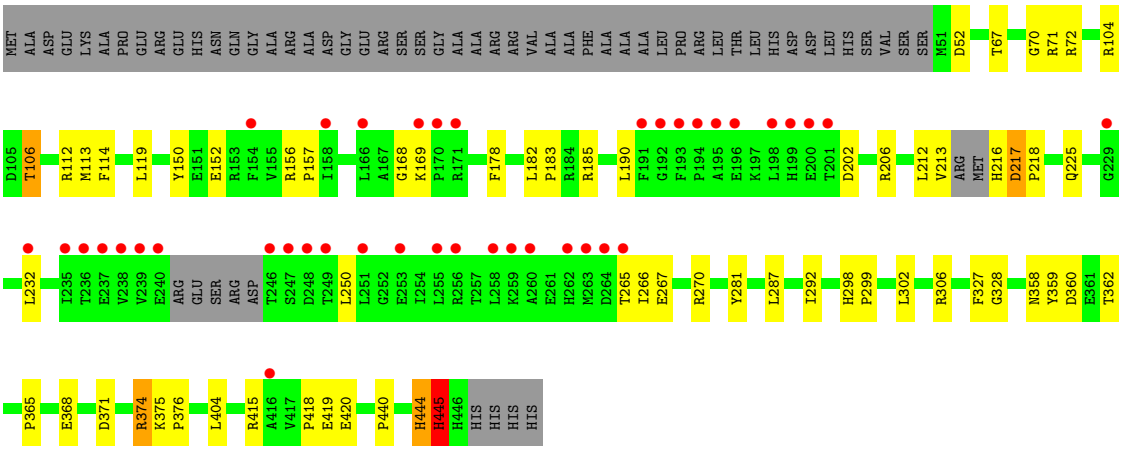
• Molecule 1: Cytochrome P450 CYP260A1,Cytochrome P450 CYP260A1

Chain A:



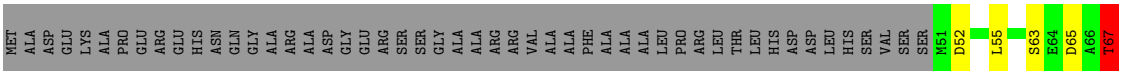
• Molecule 1: Cytochrome P450 CYP260A1,Cytochrome P450 CYP260A1

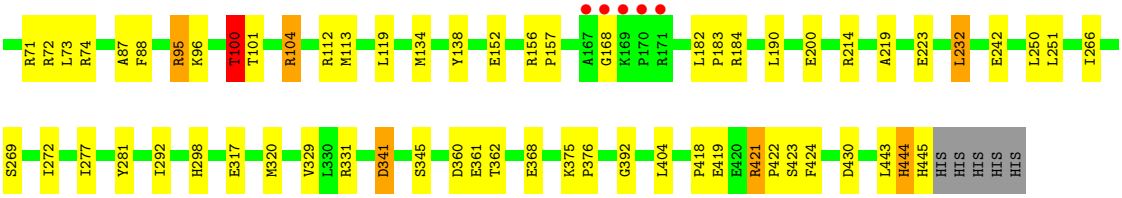
Chain B:



• Molecule 1: Cytochrome P450 CYP260A1,Cytochrome P450 CYP260A1

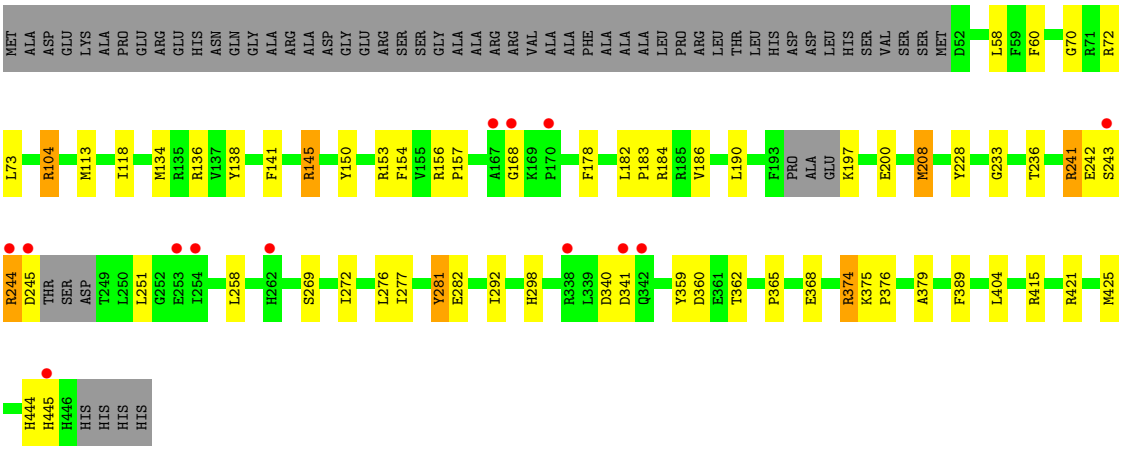
Chain C:





• Molecule 1: Cytochrome P450 CYP260A1,Cytochrome P450 CYP260A1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	234.56Å 234.56Å 96.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.93 – 2.67 69.93 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.7 (69.93-2.67) 99.7 (69.93-2.67)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.187 , 0.223 0.193 , 0.226	Depositor DCC
R_{free} test set	4262 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12879	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: MES, HEM, DMS, SO4, GOL

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	0.83	1/3161 (0.0%)	0.95	6/4284 (0.1%)
1	B	0.79	1/3068 (0.0%)	0.97	9/4164 (0.2%)
1	C	0.94	2/3157 (0.1%)	0.98	10/4281 (0.2%)
1	D	0.85	0/3058	0.99	8/4146 (0.2%)
All	All	0.85	4/12444 (0.0%)	0.97	33/16875 (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	B	0	1
1	C	0	1
1	D	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	GLY	N-CA	-7.92	1.34	1.46
1	C	361	GLU	CG-CD	6.98	1.62	1.51
1	A	113	MET	CG-SD	-5.87	1.65	1.81
1	C	345	SER	CB-OG	-5.80	1.34	1.42

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	104	ARG	NE-CZ-NH1	-9.16	115.72	120.30
1	D	208	MET	CG-SD-CE	-8.16	87.14	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	104	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	C	72	ARG	CG-CD-NE	7.17	126.86	111.80
1	A	113	MET	CB-CG-SD	6.90	133.09	112.40
1	C	341	ASP	CB-CG-OD1	6.87	124.48	118.30
1	B	327	PHE	CA-C-N	6.44	129.08	116.20
1	A	113	MET	CG-SD-CE	6.42	110.47	100.20
1	B	419	GLU	N-CA-C	-6.28	94.03	111.00
1	C	104	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	72	ARG	N-CA-CB	6.07	121.53	110.60
1	A	113	MET	CA-CB-CG	-6.06	103.00	113.30
1	C	67	THR	N-CA-CB	-6.03	98.84	110.30
1	B	106	THR	N-CA-CB	-5.87	99.14	110.30
1	C	88	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	B	374	ARG	CG-CD-NE	-5.73	99.77	111.80
1	C	73	LEU	CB-CG-CD2	5.71	120.71	111.00
1	D	72	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	327	PHE	O-C-N	-5.57	113.73	123.20
1	D	374	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	72	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	332	MET	CG-SD-CE	-5.39	91.58	100.20
1	C	100	THR	N-CA-CB	-5.38	100.09	110.30
1	D	421	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	270	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	112	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	88	PHE	CB-CG-CD1	5.24	124.47	120.80
1	C	152	GLU	CA-CB-CG	5.19	124.81	113.40
1	D	269	SER	N-CA-CB	-5.13	102.80	110.50
1	C	95	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	D	374	ARG	CG-CD-NE	-5.10	101.09	111.80
1	B	306	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	185	ARG	CG-CD-NE	-5.04	101.21	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	418	PRO	Peptide
1	C	168	GLY	Peptide
1	D	168	GLY	Peptide
1	D	242	GLU	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	3092	0	3071	41	0
1	B	3003	0	2977	41	1
1	C	3091	0	3085	48	1
1	D	2997	0	2971	50	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
2	C	43	0	30	5	0
2	D	43	0	30	6	0
3	A	24	0	32	0	0
3	B	6	0	8	0	0
3	C	18	0	24	9	0
3	D	18	0	24	6	0
4	A	4	0	6	0	0
4	B	4	0	6	1	0
4	C	4	0	6	0	0
4	D	12	0	18	0	0
5	A	20	0	0	0	0
5	B	20	0	0	1	0
5	C	20	0	0	1	0
5	D	25	0	0	0	0
6	A	12	0	13	0	0
7	A	78	0	0	1	0
7	B	66	0	0	2	0
7	C	117	0	0	2	0
7	D	76	0	0	4	0
All	All	12879	0	12361	199	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 8.

All (199) 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:C:65:ASP:OD2	1:C:67:THR:HB	1.43	1.17
1:D:60:PHE:HA	1:D:425:MET:HE2	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:HD2	3:D:507:GOL:H2	1.49	0.92
1:D:145:ARG:HD2	1:D:145:ARG:H	1.35	0.92
1:A:445:HIS:O	1:A:446:HIS:CG	2.28	0.87
1:C:444:HIS:O	1:C:444:HIS:ND1	2.08	0.85
1:B:70:GLY:HA3	1:B:359[B]:TYR:CE2	2.12	0.84
1:C:67:THR:CG2	1:C:71:ARG:HE	1.91	0.84
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.60	0.82
1:C:444:HIS:HA	1:C:445:HIS:HB2	1.61	0.82
1:D:70:GLY:HA3	1:D:359:TYR:CE1	2.18	0.78
1:D:60:PHE:CA	1:D:425:MET:HE2	2.14	0.77
2:C:501:HEM:HBC2	2:C:501:HEM:HHD	1.67	0.77
1:C:67:THR:HG22	1:C:71:ARG:HE	1.49	0.77
1:A:193:PHE:CZ	1:A:234:LEU:HD11	2.22	0.74
1:A:371:ASP:OD2	1:D:104:ARG:NH1	2.20	0.74
1:D:365:PRO:O	1:D:374:ARG:NH2	2.21	0.73
1:B:267:GLU:OE1	1:B:270:ARG:NH2	2.23	0.72
1:B:298:HIS:NE2	7:B:601:HOH:O	2.24	0.70
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.72	0.70
1:A:445:HIS:O	1:A:446:HIS:ND1	2.24	0.70
1:D:145:ARG:H	1:D:145:ARG:CD	2.03	0.70
1:D:60:PHE:HA	1:D:425:MET:CE	2.20	0.70
1:D:276:LEU:HD23	2:D:501:HEM:HBC1	1.73	0.69
1:C:298:HIS:NE2	7:C:601:HOH:O	2.26	0.69
1:C:443:LEU:HB2	1:C:445:HIS:HA	1.74	0.69
1:D:415:ARG:NH1	1:D:444:HIS:O	2.25	0.69
1:B:365:PRO:O	1:B:374:ARG:NH1	2.26	0.69
1:D:340:ASP:O	7:D:601:HOH:O	2.09	0.69
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.74	0.68
1:C:63:SER:HB2	1:C:424:PHE:O	1.94	0.68
1:C:138:TYR:CE1	1:C:272:ILE:HD12	2.29	0.67
1:C:87:ALA:O	1:C:214:ARG:NH1	2.27	0.67
1:D:138:TYR:HA	1:D:141:PHE:CE2	2.30	0.67
1:B:216:HIS:HA	1:B:217:ASP:OD2	1.94	0.66
1:C:444:HIS:CA	1:C:445:HIS:HB2	2.24	0.66
1:D:150:TYR:OH	1:D:186:VAL:HG12	1.95	0.66
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.25	0.66
1:B:212:LEU:O	1:B:213:VAL:HB	1.94	0.66
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.76	0.66
3:C:505:GOL:H12	3:C:506:GOL:C3	2.27	0.65
1:D:241:ARG:O	1:D:241:ARG:HG2	1.97	0.64
1:A:193:PHE:CZ	1:A:234:LEU:CD1	2.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:CD	3:D:507:GOL:H2	2.25	0.63
1:B:104:ARG:NH2	4:B:505:DMS:O	2.33	0.62
1:B:70:GLY:HA3	1:B:359[B]:TYR:CZ	2.34	0.62
1:D:60:PHE:CA	1:D:425:MET:CE	2.77	0.62
3:C:505:GOL:H2	3:C:506:GOL:H2	1.80	0.61
1:D:340:ASP:O	1:D:341:ASP:HB2	2.00	0.61
1:A:241:ARG:O	1:A:244:ARG:HB2	2.00	0.61
1:A:57:ASN:ND2	7:A:601:HOH:O	2.26	0.61
1:A:138:TYR:CE1	1:A:272:ILE:HD12	2.36	0.61
2:C:501:HEM:CMB	2:C:501:HEM:HBB2	2.30	0.61
1:A:375:LYS:HA	1:A:376:PRO:C	2.21	0.61
1:A:358:ASN:ND2	1:A:381:ASN:HD22	2.00	0.60
3:D:502:GOL:O3	3:D:505:GOL:O2	2.17	0.60
1:D:118:ILE:HD12	1:D:208:MET:HE2	1.83	0.59
1:C:96:LYS:HB3	3:C:504:GOL:H12	1.83	0.59
3:C:505:GOL:O3	3:C:506:GOL:O1	2.11	0.59
1:C:112[A]:ARG:NH1	5:C:502:SO4:O1	2.35	0.58
1:C:360:ASP:OD2	1:C:362:THR:HB	2.03	0.58
1:B:178:PHE:CE2	1:B:292:ILE:HD11	2.39	0.58
1:D:375:LYS:HA	1:D:376:PRO:C	2.24	0.57
1:A:415:ARG:HH22	1:A:444:HIS:C	2.07	0.57
1:C:292:ILE:HG12	1:C:404:LEU:HD21	1.86	0.57
1:D:190:LEU:HD11	1:D:251:LEU:H	1.68	0.57
1:D:178:PHE:CE2	1:D:292:ILE:HD11	2.40	0.57
1:B:375:LYS:HA	1:B:376:PRO:C	2.24	0.57
1:D:104:ARG:NH2	7:D:602:HOH:O	2.14	0.57
1:A:269:SER:O	1:A:272:ILE:HG22	2.05	0.56
1:B:150:TYR:OH	1:B:250:LEU:HD13	2.04	0.56
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.86	0.56
1:A:178:PHE:CE2	1:A:292:ILE:HD11	2.40	0.56
1:B:212:LEU:O	1:B:213:VAL:CB	2.52	0.56
1:A:292:ILE:HG13	1:A:404:LEU:HD21	1.88	0.56
1:A:302:LEU:HD11	1:A:408:LEU:HD22	1.86	0.56
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.33	0.56
1:B:168:GLY:O	1:B:169:LYS:C	2.43	0.56
3:C:505:GOL:H12	3:C:506:GOL:O3	2.04	0.56
1:C:96:LYS:O	1:C:100:THR:HB	2.06	0.56
1:D:277:ILE:O	1:D:281:TYR:HB3	2.06	0.55
1:B:292:ILE:HG13	1:B:404:LEU:HD21	1.89	0.55
3:C:505:GOL:H12	3:C:506:GOL:H32	1.87	0.55
1:A:49:SER:O	1:A:348:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ARG:HD3	3:C:504:GOL:H32	1.88	0.55
3:D:502:GOL:C3	3:D:505:GOL:O2	2.55	0.55
1:C:375:LYS:HA	1:C:376:PRO:C	2.27	0.54
1:D:444:HIS:HB3	1:D:445:HIS:HA	1.90	0.54
1:A:358:ASN:HD21	1:A:381:ASN:HD22	1.54	0.54
1:C:156:ARG:HB3	1:C:157:PRO:HD3	1.90	0.54
1:B:182:LEU:HB3	1:B:183:PRO:HD3	1.90	0.54
1:C:266:ILE:HG12	1:C:266:ILE:O	2.08	0.54
1:C:269:SER:O	1:C:272:ILE:HG22	2.08	0.53
1:B:265:THR:HG22	1:B:266:ILE:N	2.24	0.53
1:A:95[A]:ARG:HG3	1:A:95[A]:ARG:HH11	1.73	0.53
1:D:444:HIS:CB	1:D:445:HIS:HA	2.39	0.53
1:D:292:ILE:HG13	1:D:404:LEU:HD21	1.90	0.53
1:D:276:LEU:HD23	2:D:501:HEM:CBC	2.39	0.52
1:B:156:ARG:HB3	1:B:157:PRO:HD3	1.91	0.52
1:D:298:HIS:NE2	7:D:603:HOH:O	2.34	0.52
1:B:365:PRO:CG	1:C:100:THR:HG23	2.40	0.52
1:D:156:ARG:HB3	1:D:157:PRO:HD3	1.92	0.52
1:B:70:GLY:CA	1:B:359[B]:TYR:CE2	2.91	0.52
1:D:150:TYR:CD1	1:D:154:PHE:CD2	2.99	0.51
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.41	0.51
1:B:232:LEU:HD22	1:B:270:ARG:HD3	1.93	0.51
1:A:193:PHE:CE1	1:A:197:LYS:HB2	2.45	0.51
1:B:360:ASP:OD1	1:B:362:THR:HB	2.10	0.51
1:C:444:HIS:O	1:C:444:HIS:CG	2.63	0.51
1:C:112[A]:ARG:NH2	7:C:605:HOH:O	2.44	0.51
1:D:360:ASP:OD1	1:D:362:THR:HB	2.11	0.51
1:C:138:TYR:CZ	1:C:272:ILE:HD12	2.46	0.51
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.93	0.50
1:D:182:LEU:HB3	1:D:183:PRO:HD3	1.94	0.49
1:A:184:ARG:HB2	1:A:281:TYR:CE2	2.47	0.49
1:C:67:THR:HG22	1:C:71:ARG:NE	2.25	0.49
3:D:502:GOL:O3	3:D:505:GOL:O1	2.28	0.49
1:A:219:ALA:O	1:A:223:GLU:HG3	2.13	0.49
1:C:182:LEU:HB3	1:C:183:PRO:HD3	1.95	0.49
1:C:329:VAL:CG1	1:C:331:ARG:NH2	2.75	0.49
1:B:202:ASP:HA	1:B:281:TYR:OH	2.13	0.49
1:A:375:LYS:HD2	1:D:389:PHE:CD1	2.47	0.48
1:D:150:TYR:OH	1:D:186:VAL:CG1	2.61	0.48
1:C:190:LEU:HG	1:C:250:LEU:HD23	1.95	0.48
2:D:501:HEM:HBB2	2:D:501:HEM:CMB	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:THR:OG1	1:B:71:ARG:NH1	2.46	0.48
1:D:208:MET:HE1	1:D:228:TYR:CD1	2.49	0.48
1:B:150:TYR:CZ	1:B:250:LEU:HD13	2.49	0.48
1:C:184:ARG:HB2	1:C:281:TYR:CE2	2.49	0.47
1:D:208:MET:HE1	1:D:228:TYR:HD1	1.80	0.47
1:A:178:PHE:CD2	1:A:292:ILE:HD11	2.48	0.47
1:D:374:ARG:HG2	3:D:507:GOL:H32	1.97	0.47
1:A:182:LEU:HB3	1:A:183:PRO:HD3	1.96	0.47
2:A:501:HEM:HBB2	2:A:501:HEM:CHC	2.33	0.47
1:C:219:ALA:O	1:C:223:GLU:HG3	2.15	0.47
1:B:114:PHE:CD1	1:B:119:LEU:HD12	2.50	0.47
1:B:216:HIS:HA	1:B:217:ASP:CG	2.34	0.47
1:B:365:PRO:HG3	1:C:100:THR:CG2	2.45	0.47
1:A:277:ILE:O	1:A:281:TYR:HB3	2.15	0.47
1:C:67:THR:CG2	1:C:71:ARG:NE	2.69	0.47
1:B:168:GLY:O	1:B:169:LYS:O	2.32	0.46
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.46	0.46
1:B:178:PHE:CD2	1:B:292:ILE:HD11	2.51	0.46
1:D:197:LYS:O	1:D:200:GLU:CB	2.63	0.46
1:D:379:ALA:HA	7:D:628:HOH:O	2.15	0.46
1:D:178:PHE:CD2	1:D:292:ILE:HD11	2.50	0.46
1:A:55:LEU:HD22	1:A:86:THR:HG22	1.98	0.46
1:C:421[B]:ARG:HD3	1:C:422:PRO:HD2	1.97	0.46
1:B:420:GLU:HG2	1:B:440:PRO:HG3	1.96	0.46
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	1.97	0.46
1:A:113:MET:HG2	1:A:332:MET:HB2	1.97	0.45
1:B:365:PRO:CG	1:C:100:THR:CG2	2.94	0.45
1:C:292:ILE:HG23	1:C:292:ILE:HD12	1.51	0.45
1:A:193:PHE:CE1	1:A:234:LEU:HD11	2.50	0.45
3:C:505:GOL:C1	3:C:506:GOL:O3	2.64	0.45
1:A:156:ARG:HB3	1:A:157:PRO:HD3	1.98	0.45
1:B:445:HIS:ND1	1:B:445:HIS:N	2.64	0.45
1:D:58:LEU:HD13	1:D:73:LEU:HD23	1.98	0.45
1:A:241:ARG:O	1:A:244:ARG:CB	2.64	0.45
1:D:60:PHE:HB3	1:D:425:MET:CE	2.46	0.45
1:D:190:LEU:HD12	1:D:190:LEU:O	2.16	0.45
1:B:371:ASP:OD2	1:C:104:ARG:NH1	2.49	0.44
1:B:287:LEU:HB2	2:B:501:HEM:HBB1	1.97	0.44
1:B:358:ASN:HB2	1:B:359[B]:TYR:CE2	2.52	0.44
1:D:233:GLY:O	1:D:236:THR:OG1	2.32	0.44
1:A:138:TYR:CZ	1:A:272:ILE:HD12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:O	1:A:270:ARG:HG3	2.17	0.44
1:C:119:LEU:HD11	3:C:505:GOL:H11	1.99	0.44
1:D:150:TYR:HD1	1:D:154:PHE:CD2	2.35	0.43
1:D:258:LEU:HD22	1:D:272:ILE:HD12	1.99	0.43
1:C:392:GLY:HA3	2:C:501:HEM:C3C	2.54	0.43
1:C:277:ILE:O	1:C:281:TYR:HB3	2.18	0.43
1:C:317:GLU:CD	1:C:320:MET:CE	2.87	0.43
1:A:374:ARG:O	1:A:375:LYS:HG2	2.18	0.42
1:D:281:TYR:HD2	1:D:282:GLU:N	2.18	0.42
1:C:292:ILE:HD13	1:C:292:ILE:HA	1.86	0.42
1:C:232:LEU:HD12	1:C:232:LEU:HA	1.79	0.42
1:D:138:TYR:HA	1:D:141:PHE:CD2	2.55	0.42
1:A:445:HIS:O	1:A:446:HIS:CE1	2.73	0.42
1:B:156:ARG:HD3	7:B:627:HOH:O	2.20	0.42
1:A:196:GLU:O	1:A:200:GLU:HG3	2.20	0.42
1:D:60:PHE:C	1:D:425:MET:HE2	2.40	0.42
1:A:265:THR:HG22	1:A:266:ILE:N	2.34	0.41
1:C:100:THR:HG22	1:C:101:THR:N	2.35	0.41
1:B:299:PRO:HD2	5:B:506:SO4:O3	2.20	0.41
1:B:302:LEU:HD23	1:B:302:LEU:O	2.21	0.41
1:C:242:GLU:HG3	1:C:251:LEU:HD23	2.02	0.41
1:A:302:LEU:O	1:A:302:LEU:HD12	2.20	0.41
1:B:299:PRO:HG3	1:B:415:ARG:HH22	1.85	0.41
1:C:292:ILE:HD11	1:C:404:LEU:CD2	2.51	0.41
1:A:55:LEU:HD22	1:A:86:THR:CG2	2.50	0.41
1:A:67:THR:OG1	1:A:71:ARG:NH1	2.54	0.41
1:C:418:PRO:O	1:C:419:GLU:CB	2.68	0.41
2:C:501:HEM:HBC2	2:C:501:HEM:CHD	2.40	0.41
1:D:243:SER:O	1:D:244:ARG:CB	2.68	0.41
1:B:190:LEU:HD22	1:B:250:LEU:HB2	2.02	0.40
1:C:74:ARG:HA	1:C:74:ARG:HD2	1.92	0.40
1:D:178:PHE:HE2	1:D:292:ILE:HD11	1.87	0.40
1:B:232:LEU:HD23	1:B:232:LEU:HA	1.95	0.40

All (1) 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:B:225:GLN:NE2	1:C:423:SER:OG[3_455]	2.19	0.01

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	395/450 (88%)	375 (95%)	18 (5%)	2 (0%)	29	52
1	B	384/450 (85%)	365 (95%)	15 (4%)	4 (1%)	15	34
1	C	395/450 (88%)	379 (96%)	15 (4%)	1 (0%)	41	64
1	D	383/450 (85%)	370 (97%)	12 (3%)	1 (0%)	41	64
All	All	1557/1800 (86%)	1489 (96%)	60 (4%)	8 (0%)	29	52

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	ASP
1	B	218	PRO
1	C	52	ASP
1	D	244	ARG
1	A	445	HIS
1	B	52	ASP
1	B	445	HIS
1	B	444	HIS

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	316/361 (88%)	308 (98%)	8 (2%)	47	74
1	B	307/361 (85%)	299 (97%)	8 (3%)	46	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	320/361 (89%)	307 (96%)	13 (4%)	30	56
1	D	305/361 (84%)	295 (97%)	10 (3%)	38	64
All	All	1248/1444 (86%)	1209 (97%)	39 (3%)	40	67

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	MET
1	A	171	ARG
1	A	180	MET
1	A	241	ARG
1	A	245	ASP
1	A	270	ARG
1	A	302	LEU
1	A	368	GLU
1	B	106	THR
1	B	113	MET
1	B	152	GLU
1	B	206	ARG
1	B	217	ASP
1	B	368	GLU
1	B	444	HIS
1	B	445	HIS
1	C	55	LEU
1	C	67	THR
1	C	100	THR
1	C	113	MET
1	C	134	MET
1	C	200	GLU
1	C	232	LEU
1	C	341	ASP
1	C	368	GLU
1	C	421[A]	ARG
1	C	421[B]	ARG
1	C	430	ASP
1	C	444	HIS
1	D	113	MET
1	D	134	MET
1	D	136	ARG
1	D	145	ARG
1	D	153	ARG

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Mol	Chain	Res	Type
1	D	184	ARG
1	D	241	ARG
1	D	245	ASP
1	D	281	TYR
1	D	368	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	199	HIS
1	A	307	GLN
1	A	358	ASN
1	B	149	GLN
1	B	307	GLN
1	C	78	GLN
1	C	149	GLN
1	C	307	GLN
1	C	445	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)

39 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	$\#\|Z\| > 2$
4	DMS	B	505	-	3,3,3	0.49	0	3,3,3	1.73	1 (33%)
5	SO4	D	511	-	4,4,4	0.44	0	6,6,6	0.36	0
3	GOL	A	506	-	5,5,5	1.09	0	5,5,5	1.21	0
3	GOL	C	506	-	5,5,5	0.59	0	5,5,5	1.93	2 (40%)
5	SO4	A	510	-	4,4,4	0.32	0	6,6,6	0.40	0
5	SO4	B	506	-	4,4,4	0.39	0	6,6,6	0.46	0
3	GOL	D	502	-	5,5,5	0.72	0	5,5,5	1.43	0
2	HEM	C	501	1	41,50,50	1.85	8 (19%)	45,82,82	2.47	17 (37%)
5	SO4	B	507	-	4,4,4	0.43	0	6,6,6	0.09	0
6	MES	A	509	-	12,12,12	2.72	2 (16%)	14,16,16	1.65	4 (28%)
5	SO4	B	503	-	4,4,4	0.56	0	6,6,6	0.60	0
3	GOL	A	504	-	5,5,5	0.98	0	5,5,5	0.78	0
3	GOL	A	503	-	5,5,5	0.75	0	5,5,5	0.39	0
3	GOL	C	505	-	5,5,5	0.56	0	5,5,5	0.94	0
5	SO4	A	511	-	4,4,4	0.50	0	6,6,6	0.92	0
5	SO4	C	509	-	4,4,4	0.39	0	6,6,6	0.25	0
2	HEM	B	501	1	41,50,50	1.57	3 (7%)	45,82,82	2.35	17 (37%)
3	GOL	D	505	-	5,5,5	0.63	0	5,5,5	0.64	0
4	DMS	A	505	-	3,3,3	0.24	0	3,3,3	1.22	0
4	DMS	D	503	-	3,3,3	0.36	0	3,3,3	0.63	0
4	DMS	D	506	-	3,3,3	0.47	0	3,3,3	0.71	0
5	SO4	A	507	-	4,4,4	0.73	0	6,6,6	0.64	0
5	SO4	D	509	-	4,4,4	0.53	0	6,6,6	0.53	0
5	SO4	C	508	-	4,4,4	0.58	0	6,6,6	1.04	0
3	GOL	D	507	-	5,5,5	1.17	0	5,5,5	1.53	1 (20%)
5	SO4	C	502	-	4,4,4	0.46	0	6,6,6	0.30	0
5	SO4	D	510	-	4,4,4	0.70	0	6,6,6	0.56	0
4	DMS	C	507	-	3,3,3	0.43	0	3,3,3	1.41	1 (33%)
5	SO4	D	512	-	4,4,4	0.40	0	6,6,6	0.79	0
4	DMS	D	504	-	3,3,3	0.26	0	3,3,3	1.43	1 (33%)
3	GOL	B	504	-	5,5,5	0.43	0	5,5,5	1.49	1 (20%)
2	HEM	D	501	1	41,50,50	1.78	10 (24%)	45,82,82	2.40	16 (35%)
5	SO4	B	502	-	4,4,4	0.56	0	6,6,6	0.45	0
3	GOL	C	504	-	5,5,5	0.68	0	5,5,5	1.68	1 (20%)
5	SO4	D	508	-	4,4,4	0.50	0	6,6,6	0.52	0
5	SO4	A	508	-	4,4,4	0.36	0	6,6,6	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	502	-	5,5,5	0.72	0	5,5,5	1.40	2 (40%)
5	SO4	C	503	-	4,4,4	0.64	0	6,6,6	0.70	0
2	HEM	A	501	1	41,50,50	1.46	6 (14%)	45,82,82	2.43	20 (44%)

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	GOL	A	504	-	-	0/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	C	505	-	-	2/4/4/4	-
3	GOL	A	506	-	-	4/4/4/4	-
2	HEM	A	501	1	-	1/12/54/54	-
3	GOL	C	506	-	-	2/4/4/4	-
3	GOL	B	504	-	-	2/4/4/4	-
2	HEM	B	501	1	-	0/12/54/54	-
3	GOL	D	507	-	-	4/4/4/4	-
2	HEM	D	501	1	-	0/12/54/54	-
6	MES	A	509	-	-	2/6/14/14	0/1/1/1
3	GOL	C	504	-	-	4/4/4/4	-
3	GOL	D	505	-	-	2/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
2	HEM	C	501	1	-	1/12/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	509	MES	C8-S	-8.79	1.65	1.77
2	D	501	HEM	C4B-NB	-5.12	1.28	1.38
2	C	501	HEM	C1B-NB	-5.10	1.31	1.40
2	C	501	HEM	C4B-NB	-4.90	1.28	1.38
2	B	501	HEM	C1B-NB	-4.44	1.32	1.40
2	A	501	HEM	C1B-NB	-3.96	1.33	1.40
2	B	501	HEM	C4B-NB	-3.93	1.30	1.38
2	C	501	HEM	C4D-ND	-3.81	1.33	1.40
2	C	501	HEM	C3C-C2C	-3.68	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C4D-ND	-3.61	1.34	1.40
2	D	501	HEM	C1B-NB	-3.49	1.34	1.40
2	A	501	HEM	C4D-ND	-3.37	1.34	1.40
2	B	501	HEM	C1D-ND	-3.11	1.32	1.38
2	A	501	HEM	C4B-NB	-2.91	1.32	1.38
2	D	501	HEM	C3C-CAC	-2.76	1.42	1.47
2	A	501	HEM	C1D-ND	-2.74	1.33	1.38
2	C	501	HEM	C3C-CAC	-2.70	1.42	1.47
2	C	501	HEM	CAB-C3B	-2.68	1.40	1.47
2	C	501	HEM	C1A-CHA	-2.63	1.33	1.41
2	D	501	HEM	C3C-C2C	-2.57	1.36	1.40
2	C	501	HEM	O1A-CGA	2.55	1.30	1.22
2	D	501	HEM	O1A-CGA	2.50	1.30	1.22
2	D	501	HEM	CAA-C2A	-2.41	1.48	1.52
2	A	501	HEM	FE-NB	2.29	2.08	1.96
2	D	501	HEM	C1D-ND	-2.27	1.34	1.38
2	D	501	HEM	C1A-CHA	-2.23	1.34	1.41
2	D	501	HEM	C1B-C2B	-2.07	1.40	1.44
6	A	509	MES	C5-N4	2.05	1.52	1.46
2	A	501	HEM	CAA-C2A	-2.01	1.49	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	CHC-C4B-NB	7.48	132.56	124.43
2	A	501	HEM	C1B-NB-C4B	7.18	112.48	105.07
2	D	501	HEM	CHC-C4B-NB	6.93	131.96	124.43
2	B	501	HEM	C1B-NB-C4B	6.80	112.10	105.07
2	C	501	HEM	C1B-NB-C4B	6.71	112.00	105.07
2	B	501	HEM	CHC-C4B-NB	6.54	131.54	124.43
2	D	501	HEM	C1B-NB-C4B	6.25	111.53	105.07
2	D	501	HEM	C2C-C3C-C4C	5.76	110.92	106.90
2	C	501	HEM	C2C-C3C-C4C	4.49	110.04	106.90
2	A	501	HEM	CHC-C4B-NB	4.34	129.15	124.43
2	B	501	HEM	CHB-C1B-NB	4.24	129.62	124.38
2	A	501	HEM	CHD-C1D-C2D	-4.13	118.53	124.98
2	A	501	HEM	C4B-C3B-C2B	4.05	110.33	107.11
2	A	501	HEM	CBA-CAA-C2A	-4.01	105.77	112.62
2	C	501	HEM	CBA-CAA-C2A	-3.96	105.86	112.62
2	A	501	HEM	C3B-C2B-C1B	-3.96	103.55	106.49
2	D	501	HEM	C3B-C2B-C1B	-3.93	103.57	106.49
2	B	501	HEM	CHA-C4D-C3D	-3.87	118.07	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	C3B-C2B-C1B	-3.82	103.65	106.49
2	B	501	HEM	CHA-C4D-ND	3.59	128.81	124.38
2	D	501	HEM	CMC-C2C-C3C	3.54	131.30	124.68
2	B	501	HEM	CHD-C1D-ND	3.43	128.16	124.43
3	D	507	GOL	O3-C3-C2	3.27	125.89	110.20
2	A	501	HEM	CMB-C2B-C1B	3.23	129.96	125.04
2	B	501	HEM	C4B-C3B-C2B	3.23	109.68	107.11
2	C	501	HEM	CHD-C1D-ND	3.20	127.91	124.43
3	C	506	GOL	O2-C2-C3	-3.16	95.21	109.12
2	C	501	HEM	CHA-C4D-C3D	-3.13	119.44	125.33
2	D	501	HEM	C3D-C4D-ND	3.11	113.63	110.17
2	A	501	HEM	C2D-C1D-ND	3.10	113.60	109.88
2	A	501	HEM	CHD-C1D-ND	3.08	127.78	124.43
2	B	501	HEM	C4D-C3D-C2D	-3.06	102.44	106.90
2	C	501	HEM	C3B-C2B-C1B	-3.05	104.23	106.49
6	A	509	MES	C6-C5-N4	2.86	114.43	110.10
2	A	501	HEM	CHB-C1B-NB	2.82	127.86	124.38
2	A	501	HEM	CAD-CBD-CGD	-2.80	107.58	113.60
6	A	509	MES	O3S-S-O2S	2.78	118.07	111.27
2	C	501	HEM	C3D-C4D-ND	2.76	113.24	110.17
2	D	501	HEM	CHB-C1B-NB	2.76	127.79	124.38
2	C	501	HEM	CHD-C1D-C2D	-2.76	120.67	124.98
2	D	501	HEM	CHD-C1D-ND	2.74	127.41	124.43
2	D	501	HEM	C4B-C3B-C2B	2.74	109.29	107.11
2	D	501	HEM	CAD-C3D-C4D	2.73	129.43	124.66
6	A	509	MES	C5-N4-C3	2.73	114.97	108.83
2	B	501	HEM	C1D-C2D-C3D	2.73	109.82	106.96
2	A	501	HEM	CHA-C4D-ND	2.69	127.70	124.38
2	C	501	HEM	CMB-C2B-C1B	2.69	129.13	125.04
2	A	501	HEM	O1D-CGD-CBD	-2.67	114.49	123.08
2	D	501	HEM	CAA-CBA-CGA	-2.67	106.26	113.76
2	A	501	HEM	C2C-C3C-C4C	2.65	108.75	106.90
2	B	501	HEM	C3D-C4D-ND	2.64	113.10	110.17
2	D	501	HEM	CHA-C4D-C3D	-2.53	120.57	125.33
2	D	501	HEM	C4D-C3D-C2D	-2.53	103.21	106.90
2	A	501	HEM	CAB-C3B-C2B	-2.49	120.41	128.60
2	D	501	HEM	CHD-C1D-C2D	-2.44	121.17	124.98
2	A	501	HEM	CMD-C2D-C1D	2.43	128.73	125.04
2	C	501	HEM	CHC-C4B-C3B	-2.42	120.87	124.57
6	A	509	MES	O2S-S-O1S	-2.41	105.61	113.95
2	D	501	HEM	O2D-CGD-O1D	-2.39	117.33	123.30
2	C	501	HEM	C4B-CHC-C1C	2.39	125.72	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	504	GOL	O3-C3-C2	-2.39	98.73	110.20
4	C	507	DMS	C2-S-C1	2.39	110.74	98.44
2	A	501	HEM	CHA-C4D-C3D	-2.38	120.86	125.33
2	B	501	HEM	O2D-CGD-CBD	2.38	121.67	114.03
2	C	501	HEM	CHA-C4D-ND	2.36	127.30	124.38
2	B	501	HEM	CHB-C1B-C2B	-2.36	120.20	126.72
2	B	501	HEM	O2D-CGD-O1D	-2.34	117.47	123.30
4	B	505	DMS	O-S-C1	2.34	118.46	106.54
2	C	501	HEM	CAD-C3D-C4D	2.27	128.63	124.66
2	A	501	HEM	CBD-CAD-C3D	2.27	118.94	112.63
2	B	501	HEM	CAD-C3D-C4D	2.27	128.62	124.66
2	A	501	HEM	C1D-C2D-C3D	-2.24	104.60	106.96
2	C	501	HEM	C3C-C4C-NC	-2.22	106.76	110.94
2	D	501	HEM	C4A-C3A-C2A	2.22	108.54	107.00
2	B	501	HEM	C3C-C4C-NC	-2.20	106.79	110.94
2	A	501	HEM	O2D-CGD-CBD	2.15	120.93	114.03
3	C	506	GOL	O2-C2-C1	2.12	118.48	109.12
3	A	502	GOL	O2-C2-C1	-2.12	99.77	109.12
4	D	504	DMS	C2-S-C1	2.12	109.36	98.44
2	C	501	HEM	CMA-C3A-C4A	-2.09	125.25	128.46
3	C	504	GOL	O3-C3-C2	-2.09	100.19	110.20
2	C	501	HEM	CHB-C1B-NB	2.06	126.93	124.38
2	B	501	HEM	CHD-C1D-C2D	-2.04	121.80	124.98
3	A	502	GOL	O3-C3-C2	2.02	119.90	110.20

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-C3
3	A	503	GOL	C1-C2-C3-O3
3	A	503	GOL	O2-C2-C3-O3
3	A	506	GOL	C1-C2-C3-O3
3	C	504	GOL	O1-C1-C2-C3
3	C	505	GOL	C1-C2-C3-O3
3	C	505	GOL	O2-C2-C3-O3
3	D	502	GOL	C1-C2-C3-O3
6	A	509	MES	C8-C7-N4-C5
3	D	502	GOL	O2-C2-C3-O3
3	A	502	GOL	C1-C2-C3-O3
3	A	506	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	504	GOL	C1-C2-C3-O3
3	C	504	GOL	C1-C2-C3-O3
3	C	506	GOL	O1-C1-C2-C3
3	D	505	GOL	C1-C2-C3-O3
3	D	507	GOL	O1-C1-C2-C3
3	A	506	GOL	O2-C2-C3-O3
3	B	504	GOL	O2-C2-C3-O3
3	C	504	GOL	O1-C1-C2-O2
3	A	506	GOL	O1-C1-C2-O2
3	C	504	GOL	O2-C2-C3-O3
3	D	505	GOL	O2-C2-C3-O3
6	A	509	MES	C8-C7-N4-C3
3	D	507	GOL	O1-C1-C2-O2
3	A	502	GOL	O2-C2-C3-O3
3	C	506	GOL	O1-C1-C2-O2
3	D	507	GOL	C1-C2-C3-O3
3	D	507	GOL	O2-C2-C3-O3
2	A	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

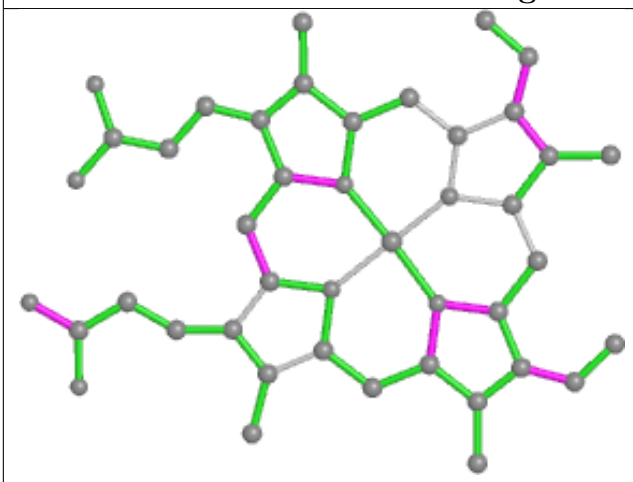
13 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	505	DMS	1	0
3	C	506	GOL	6	0
5	B	506	SO4	1	0
3	D	502	GOL	3	0
2	C	501	HEM	5	0
3	C	505	GOL	7	0
2	B	501	HEM	5	0
3	D	505	GOL	3	0
3	D	507	GOL	3	0
5	C	502	SO4	1	0
2	D	501	HEM	6	0
3	C	504	GOL	2	0
2	A	501	HEM	4	0

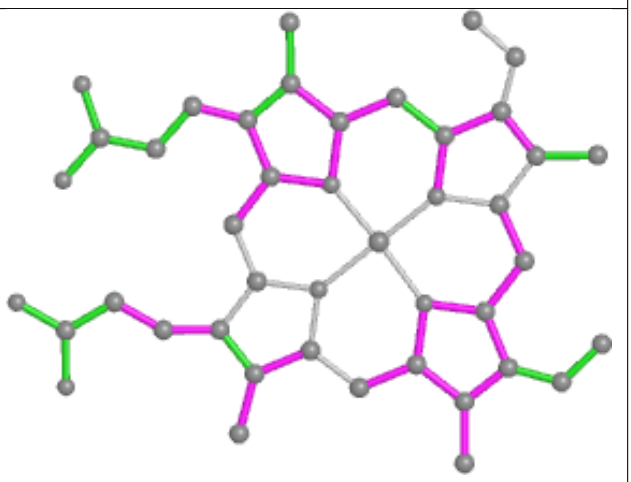
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

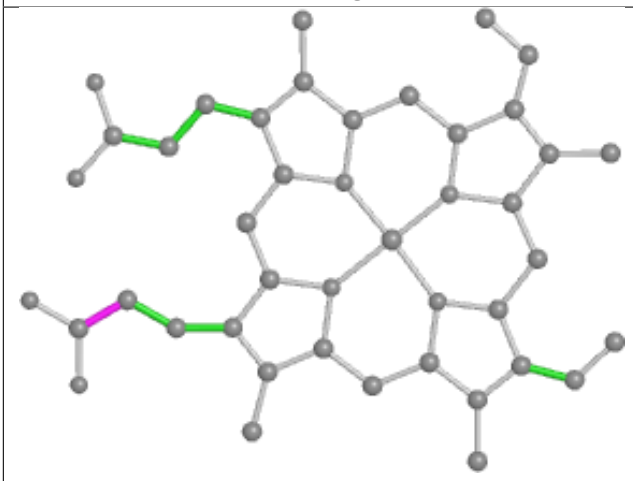
Ligand HEM C 501



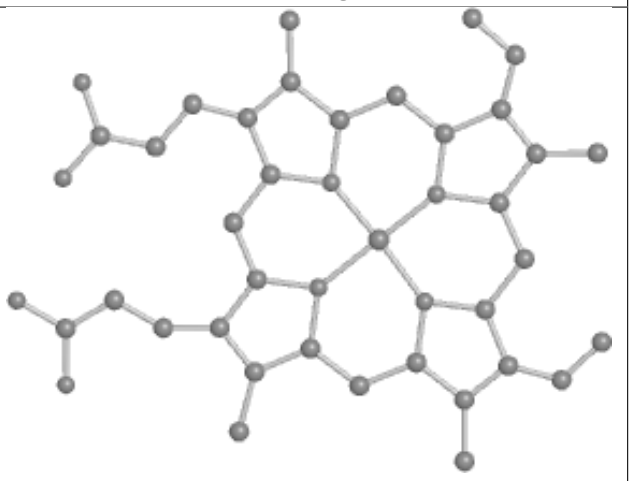
Bond lengths



Bond angles

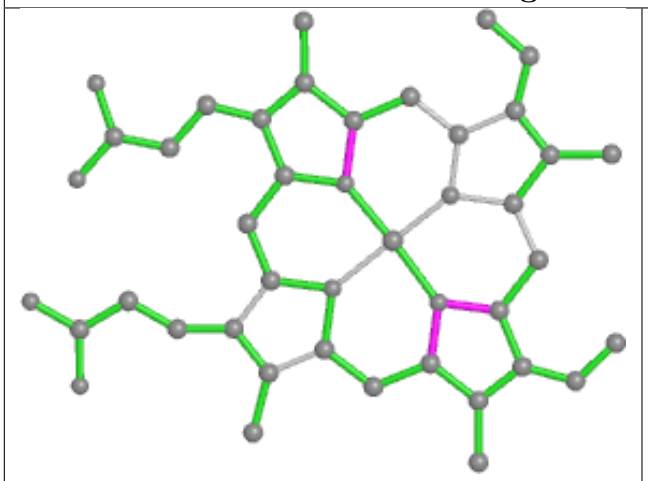


Torsions

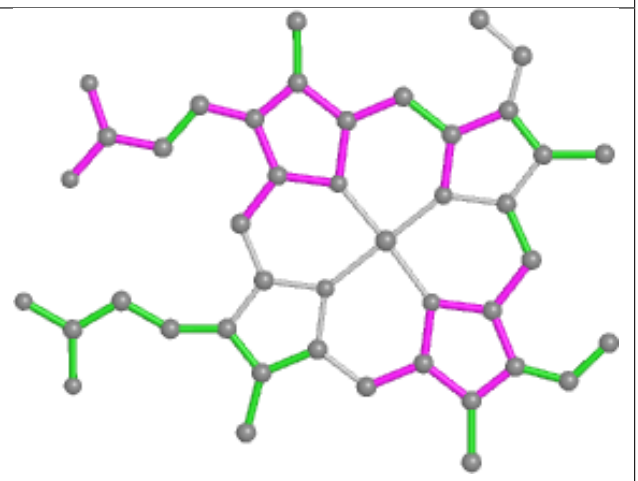


Rings

Ligand HEM B 501



Bond lengths



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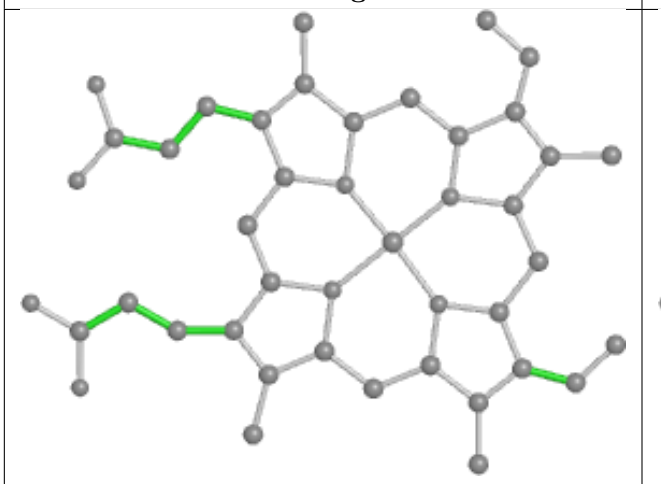
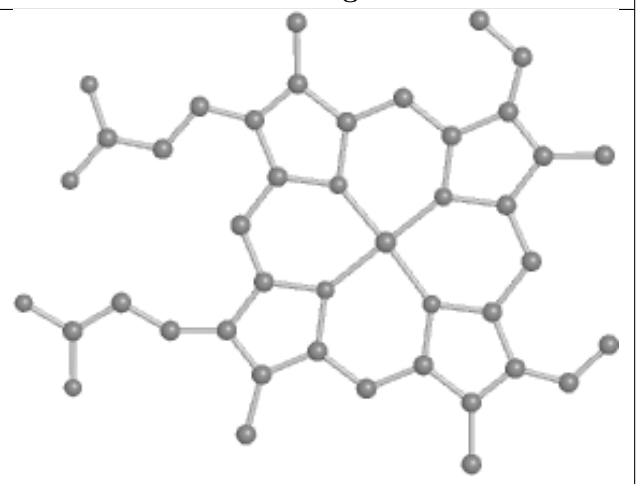
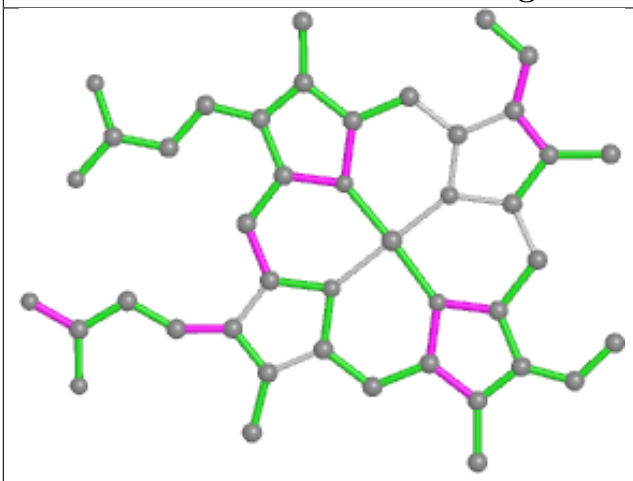


Torsions

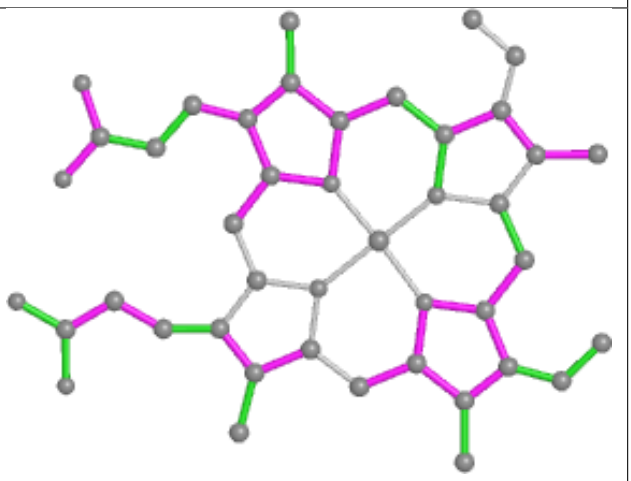


Rings

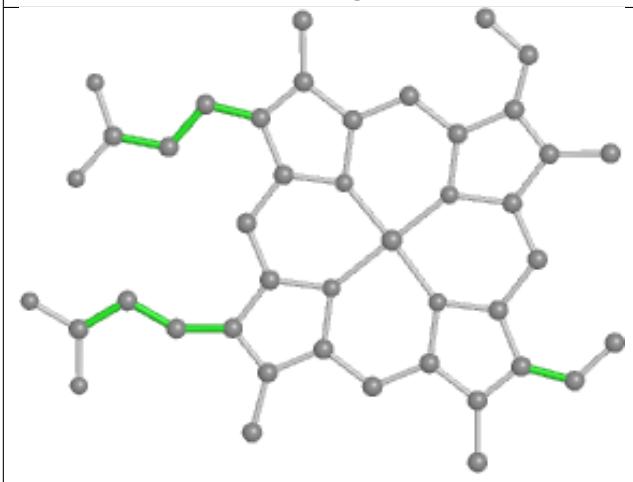
Ligand HEM D 501



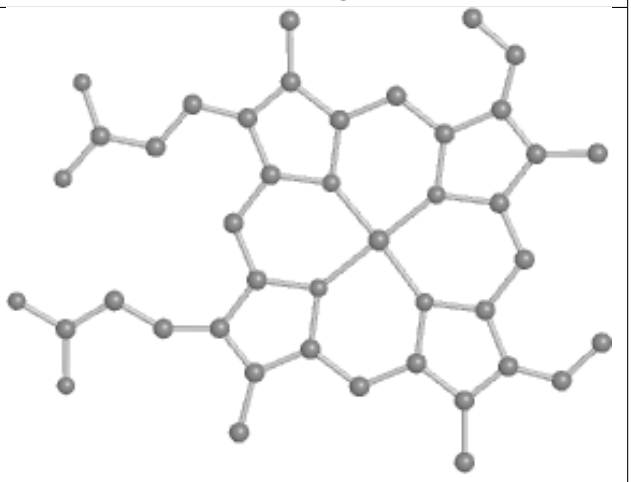
Bond lengths



Bond angles

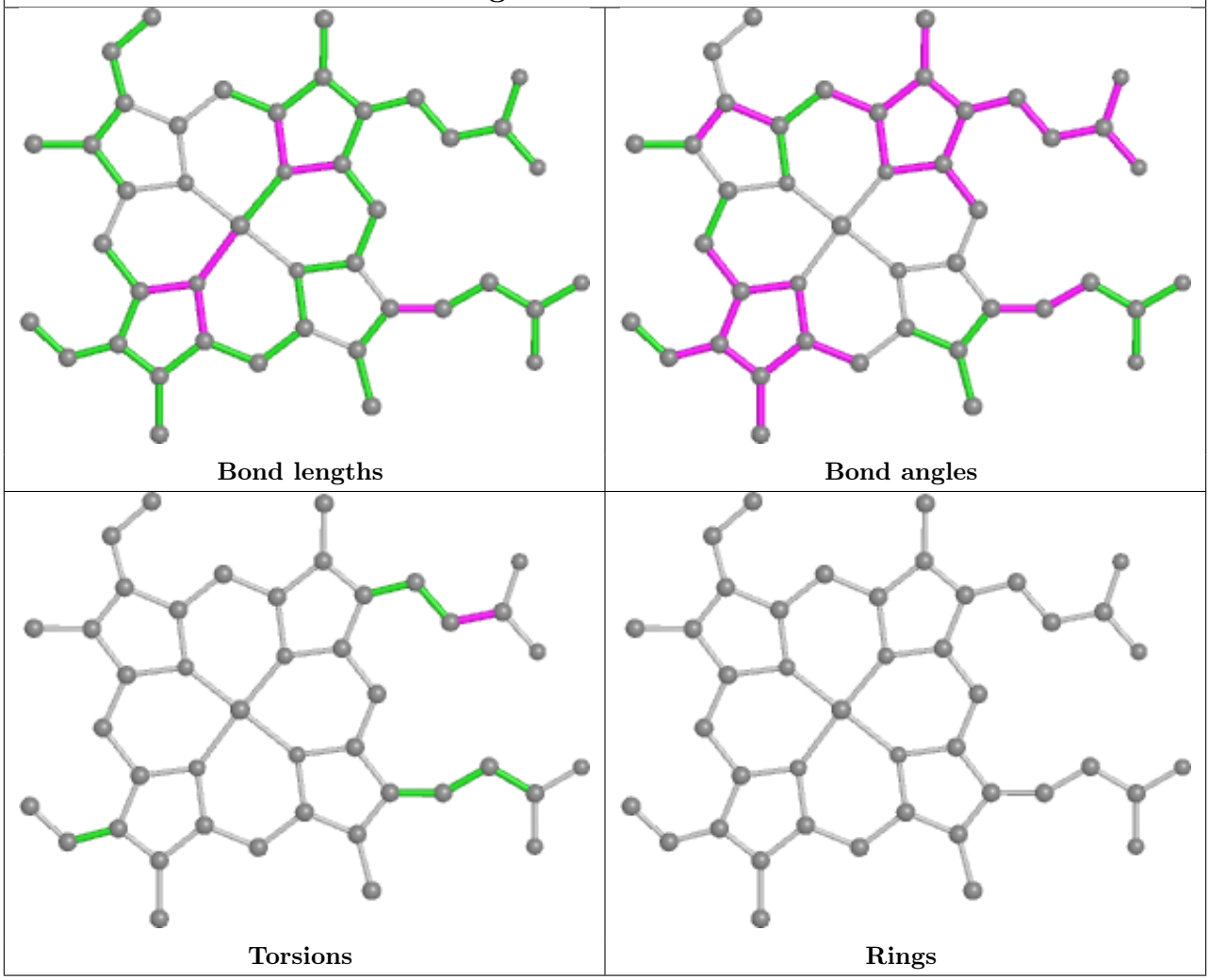


Torsions



Rings

Ligand HEM A 501



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	397/450 (88%)	0.05	22 (5%) 25 23	17, 42, 87, 111	0
1	B	389/450 (86%)	0.24	40 (10%) 6 5	23, 46, 93, 126	0
1	C	395/450 (87%)	-0.23	5 (1%) 77 78	17, 30, 59, 97	0
1	D	389/450 (86%)	-0.05	13 (3%) 46 45	18, 38, 83, 107	0
All	All	1570/1800 (87%)	0.00	80 (5%) 28 26	17, 38, 86, 126	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	VAL	5.3
1	B	194	PRO	5.2
1	B	264	ASP	4.6
1	A	244	ARG	4.5
1	B	238	VAL	4.2
1	A	245	ASP	4.0
1	B	263	MET	3.9
1	A	256	ARG	3.7
1	A	193	PHE	3.6
1	A	255	LEU	3.5
1	B	193	PHE	3.5
1	A	446	HIS	3.3
1	C	171	ARG	3.3
1	D	244	ARG	3.3
1	A	50	SER	3.2
1	B	262	HIS	3.2
1	D	168	GLY	3.1
1	B	195	ALA	3.1
1	C	168	GLY	3.1
1	A	49	SER	3.1
1	A	192	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	198	LEU	3.0
1	B	255	LEU	3.0
1	C	170	PRO	2.9
1	A	248	ASP	2.9
1	A	156	ARG	2.8
1	B	247	SER	2.8
1	D	341	ASP	2.7
1	D	262	HIS	2.7
1	B	192	GLY	2.7
1	B	166	LEU	2.7
1	A	247	SER	2.7
1	A	264	ASP	2.7
1	A	246	THR	2.7
1	B	248	ASP	2.7
1	A	191	PHE	2.7
1	B	240	GLU	2.7
1	A	170	PRO	2.6
1	D	445	HIS	2.6
1	B	246	THR	2.6
1	B	258	LEU	2.5
1	D	338	ARG	2.5
1	A	266	ILE	2.5
1	B	249	THR	2.5
1	A	263	MET	2.5
1	B	235	ILE	2.5
1	D	167	ALA	2.5
1	B	169	LYS	2.5
1	B	170	PRO	2.4
1	B	200	GLU	2.4
1	C	167	ALA	2.4
1	B	201	THR	2.4
1	B	260	ALA	2.4
1	B	191	PHE	2.4
1	B	251	LEU	2.4
1	D	245	ASP	2.4
1	B	171	ARG	2.4
1	B	265	THR	2.3
1	B	154	PHE	2.3
1	A	259	LYS	2.3
1	B	259	LYS	2.3
1	D	170	PRO	2.3
1	A	164	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	253	GLU	2.2
1	B	256	ARG	2.2
1	D	243	SER	2.1
1	B	196	GLU	2.1
1	A	154	PHE	2.1
1	B	237	GLU	2.1
1	A	165	ARG	2.1
1	B	229	GLY	2.1
1	B	232	LEU	2.1
1	B	253	GLU	2.1
1	B	236	THR	2.1
1	D	254	ILE	2.1
1	D	342	GLN	2.0
1	B	158	ILE	2.0
1	B	416	ALA	2.0
1	C	169	LYS	2.0
1	B	199	HIS	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
5	SO4	C	503	5/5	0.81	0.27	65,93,107,111	0
3	GOL	D	507	6/6	0.83	0.28	19,32,38,43	0
3	GOL	A	506	6/6	0.86	0.18	43,48,56,60	0
4	DMS	D	504	4/4	0.87	0.16	51,54,56,61	0
3	GOL	A	502	6/6	0.87	0.24	53,60,64,66	0
5	SO4	D	510	5/5	0.87	0.23	75,75,91,100	0

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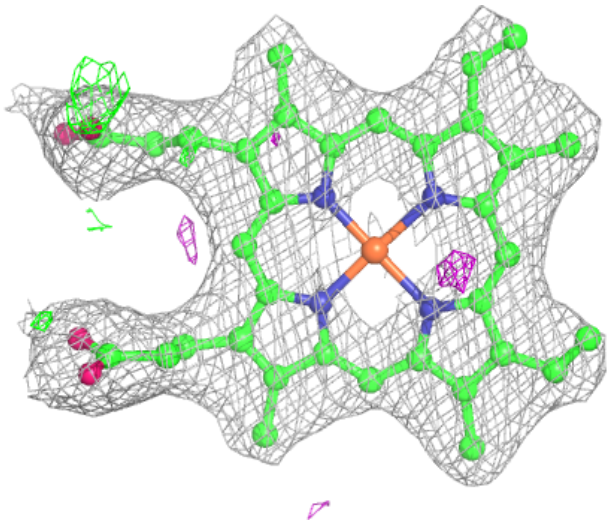
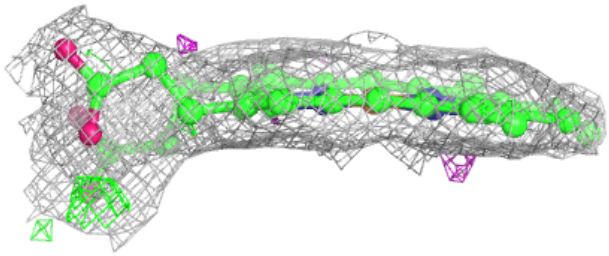
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	A	511	5/5	0.89	0.28	66,68,85,95	0
3	GOL	A	503	6/6	0.89	0.17	33,45,53,56	0
3	GOL	C	504	6/6	0.89	0.22	34,42,46,47	0
3	GOL	D	502	6/6	0.90	0.21	29,49,56,66	0
3	GOL	A	504	6/6	0.90	0.20	35,51,59,60	0
5	SO4	D	511	5/5	0.90	0.32	71,97,101,105	0
3	GOL	D	505	6/6	0.91	0.27	57,62,67,74	0
5	SO4	D	509	5/5	0.91	0.17	62,70,84,87	0
5	SO4	D	508	5/5	0.92	0.28	71,76,81,85	0
5	SO4	C	502	5/5	0.93	0.23	61,79,86,94	0
3	GOL	B	504	6/6	0.93	0.20	40,42,45,50	0
5	SO4	C	508	5/5	0.93	0.20	67,69,76,76	0
5	SO4	C	509	5/5	0.93	0.34	85,87,95,96	0
4	DMS	D	506	4/4	0.94	0.14	90,92,102,107	0
4	DMS	C	507	4/4	0.94	0.18	48,57,58,62	0
5	SO4	B	502	5/5	0.94	0.19	56,73,81,82	0
5	SO4	B	507	5/5	0.94	0.15	68,74,82,87	0
5	SO4	B	506	5/5	0.95	0.23	60,65,75,75	0
4	DMS	B	505	4/4	0.95	0.16	50,53,58,60	0
5	SO4	A	508	5/5	0.95	0.34	69,82,86,87	0
3	GOL	C	506	6/6	0.95	0.19	36,37,41,48	0
4	DMS	A	505	4/4	0.95	0.12	48,54,55,60	0
5	SO4	D	512	5/5	0.95	0.22	83,84,85,92	0
3	GOL	C	505	6/6	0.96	0.15	31,32,34,36	0
5	SO4	A	510	5/5	0.96	0.16	59,61,64,65	5
4	DMS	D	503	4/4	0.96	0.14	52,66,69,79	0
5	SO4	A	507	5/5	0.97	0.13	47,48,58,61	0
6	MES	A	509	12/12	0.97	0.17	39,49,54,55	0
2	HEM	A	501	43/43	0.98	0.14	22,25,35,38	0
2	HEM	B	501	43/43	0.98	0.14	19,22,29,34	0
5	SO4	B	503	5/5	0.98	0.08	50,51,58,63	0
2	HEM	C	501	43/43	0.98	0.14	15,19,21,25	0
2	HEM	D	501	43/43	0.98	0.15	18,23,30,40	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 HEM A 501:

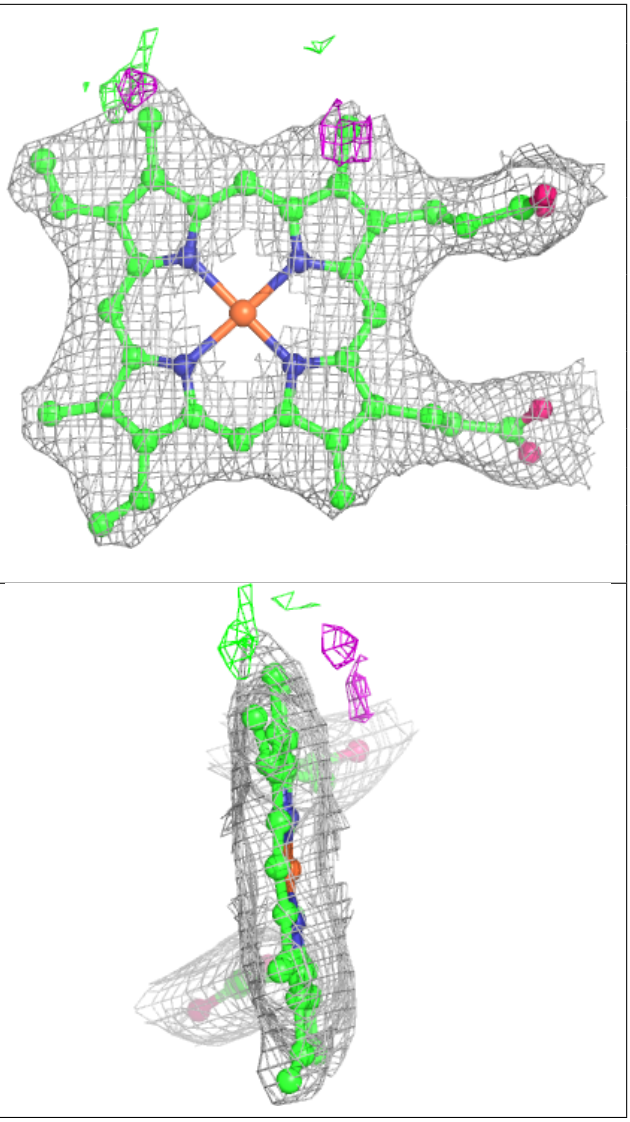
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





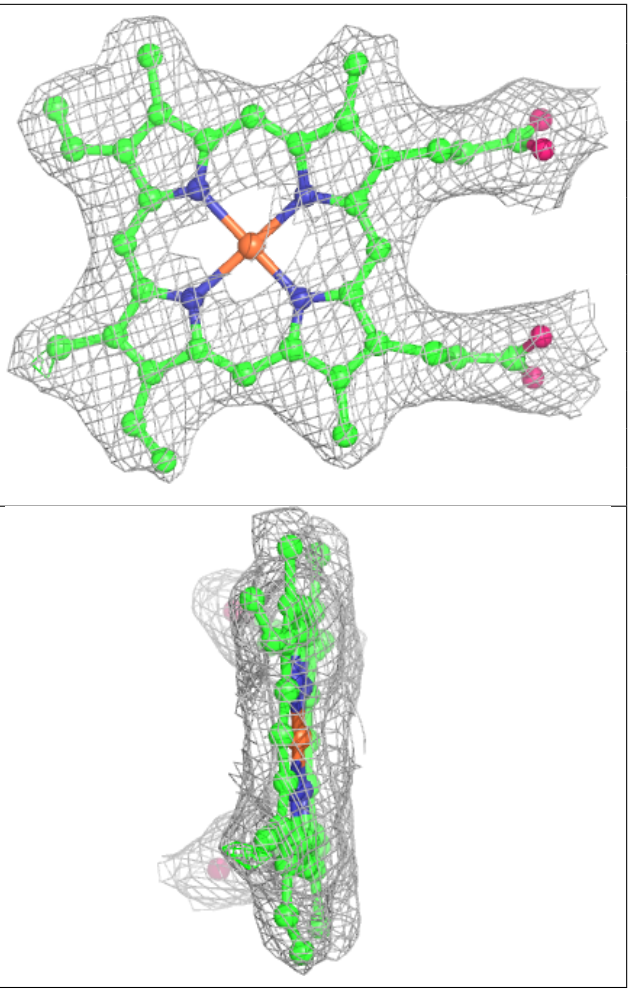
Electron density around HEM B 501:

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



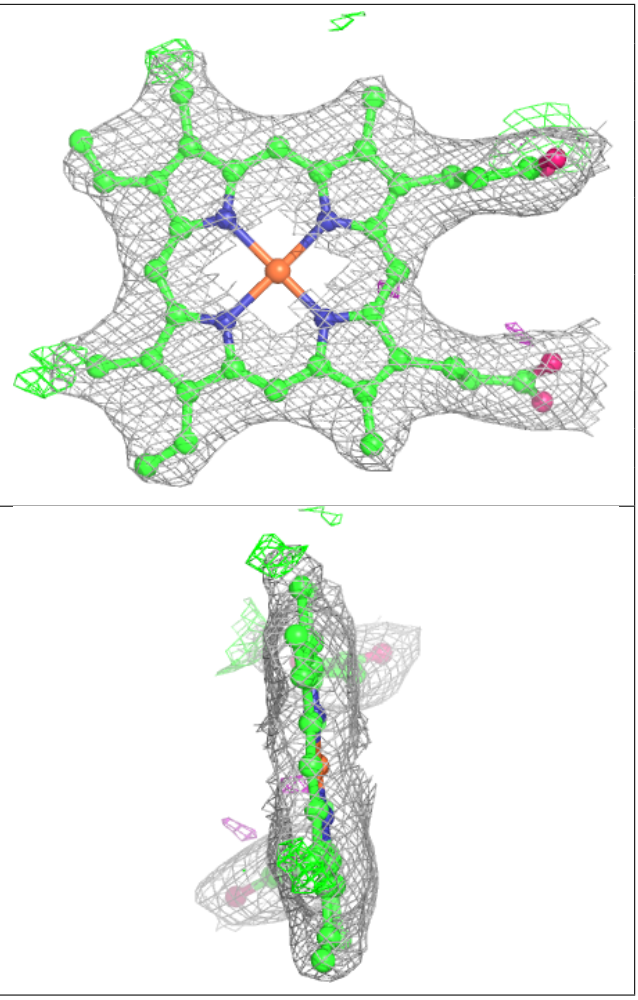
Electron density around HEM C 501:

$2mF_o$-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 D 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.