Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2025 – 02:10 PM JST

PDB ID	:	9KGP / pdb_00009kgp
Title	:	The structure of natural P450BM3-H derived from Bacillus megaterium for catalyzing the steroid DHEA
Authors	:	Deng, Q.B.; Zhang, L.J.; Li, H.
Deposited on	:	2024-11-08
Resolution	:	1.52 Å(reported)

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

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

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

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

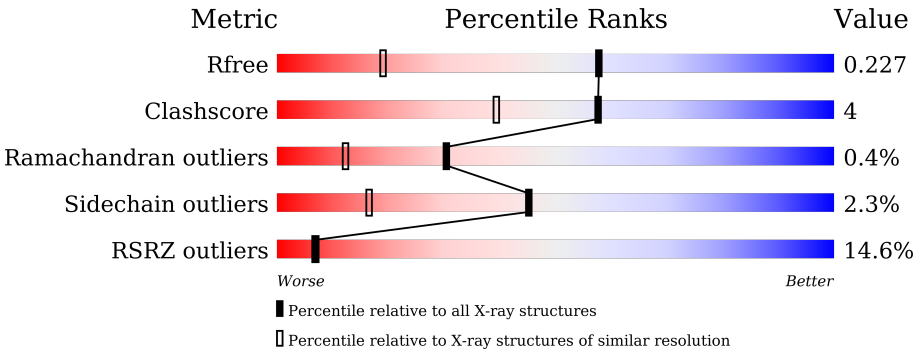
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 1.52 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}	164625	5293 (1.54-1.50)
Clashscore	180529	5759 (1.54-1.50)
Ramachandran outliers	177936	5653 (1.54-1.50)
Sidechain outliers	177891	5650 (1.54-1.50)
RSRZ outliers	164620	5293 (1.54-1.50)

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

Mol	Chain	Length	Quality of chain
1	A	455	16% 88% 11%
1	B	455	13% 87% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7928 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.

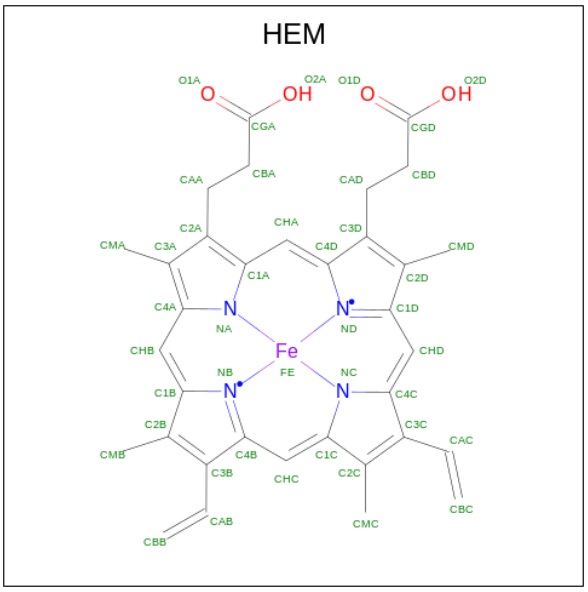
- Molecule 1 is a protein called Bifunctional cytochrome P450/NADPH–P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3642	2324	618	683	17			
1	B	453	Total	C	N	O	S	0	0	0
			3648	2327	621	683	17			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLY	ALA	conflict	UNP P14779
A	87	VAL	PHE	conflict	UNP P14779
A	127	ILE	VAL	conflict	UNP P14779
A	184	ILE	ALA	conflict	UNP P14779
A	207	ASP	GLU	conflict	UNP P14779
A	263	GLY	ILE	conflict	UNP P14779
A	264	GLY	ALA	conflict	UNP P14779
A	297	ILE	VAL	conflict	UNP P14779
A	328	GLY	ALA	conflict	UNP P14779
A	452	GLN	LYS	conflict	UNP P14779
B	74	GLY	ALA	conflict	UNP P14779
B	87	VAL	PHE	conflict	UNP P14779
B	127	ILE	VAL	conflict	UNP P14779
B	184	ILE	ALA	conflict	UNP P14779
B	207	ASP	GLU	conflict	UNP P14779
B	263	GLY	ILE	conflict	UNP P14779
B	264	GLY	ALA	conflict	UNP P14779
B	297	ILE	VAL	conflict	UNP P14779
B	328	GLY	ALA	conflict	UNP P14779
B	452	GLN	LYS	conflict	UNP P14779

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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		

- Molecule 3 is water.

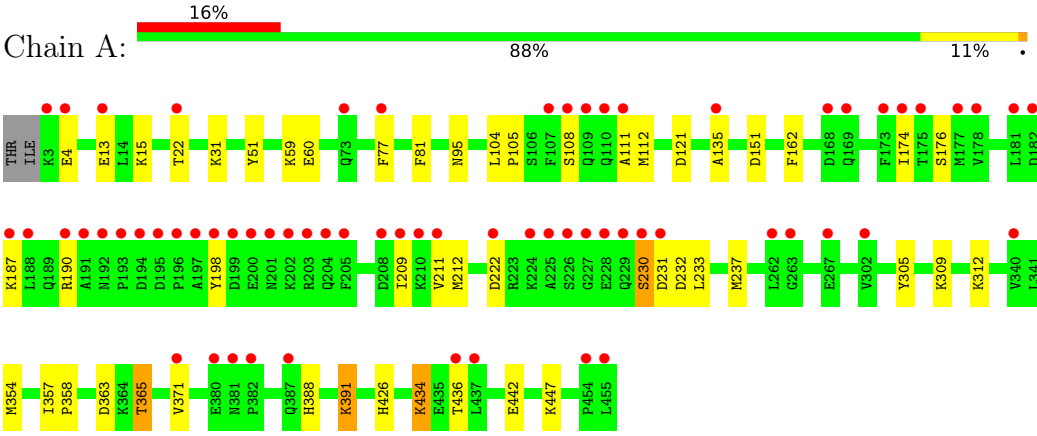
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	266	Total	O	0	0
			266	266		
3	B	286	Total	O	0	0
			286	286		

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.

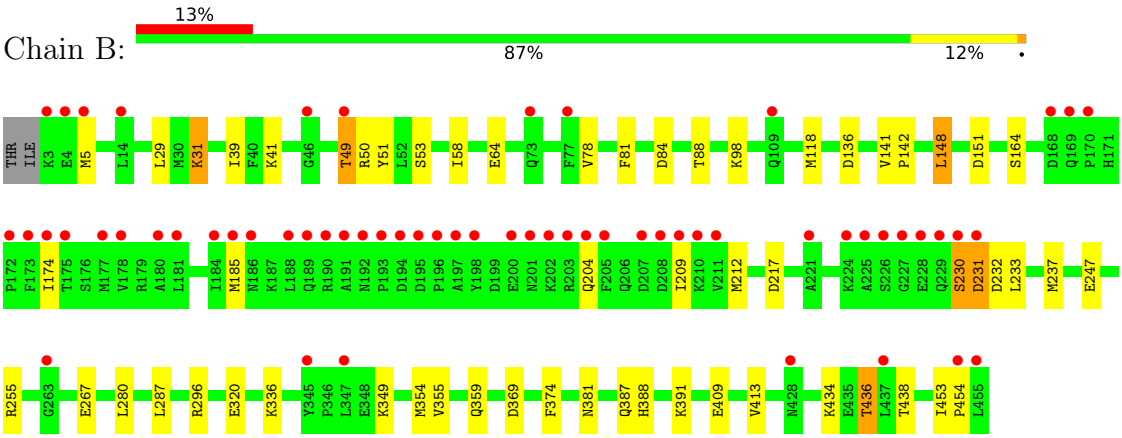
• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain A:



• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.91Å 145.71Å 63.23Å 90.00° 97.51° 90.00°	Depositor
Resolution (Å)	72.82 – 1.52 72.82 – 1.52	Depositor EDS
% Data completeness (in resolution range)	96.9 (72.82-1.52) 96.5 (72.82-1.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.221 , 0.227 0.221 , 0.227	Depositor DCC
R_{free} test set	8020 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 32.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7928	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.63	0/3726	1.05	6/5037 (0.1%)
1	B	0.63	0/3732	1.03	3/5044 (0.1%)
All	All	0.63	0/7458	1.04	9/10081 (0.1%)

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	436	THR	N-CA-C	-7.85	101.22	108.75
1	B	436	THR	CB-CA-C	6.35	125.87	116.53
1	A	391	LYS	CB-CA-C	-5.87	103.60	111.11
1	B	84	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	121	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	222	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	135	ALA	CA-C-N	-5.06	115.04	122.83
1	A	135	ALA	C-N-CA	-5.06	115.04	122.83
1	A	436	THR	CB-CA-C	5.01	120.38	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	296	ARG	Sidechain

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	3642	0	3602	25	0
1	B	3648	0	3613	37	0
2	A	43	0	30	0	0
2	B	43	0	30	4	0
3	A	266	0	0	2	0
3	B	286	0	0	3	0
All	All	7928	0	7275	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (65) 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:230:SER:O	1:A:232:ASP:N	2.25	0.70
1:B:5:MET:HE1	1:B:50:ARG:HG2	1.74	0.69
1:A:15:LYS:NZ	3:A:602:HOH:O	2.25	0.68
1:B:81:PHE:CD1	1:B:212:MET:HE1	2.30	0.67
1:B:5:MET:HE3	1:B:41:LYS:CA	2.25	0.67
1:B:217:ASP:OD1	1:B:255:ARG:NH1	2.27	0.66
1:B:31:LYS:HA	1:B:31:LYS:HE2	1.78	0.66
1:B:5:MET:HE3	1:B:41:LYS:N	2.11	0.65
1:A:190:ARG:HD2	1:A:198:TYR:CE1	2.34	0.62
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.81	0.62
1:A:81:PHE:CD1	1:A:212:MET:HE1	2.35	0.62
1:A:4:GLU:OE2	1:A:4:GLU:HA	2.01	0.61
1:B:369:ASP:HA	3:B:821:HOH:O	2.01	0.60
1:B:49:THR:HG21	1:B:354:MET:HG2	1.84	0.59
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.84	0.59
1:B:5:MET:CE	1:B:41:LYS:HB2	2.35	0.57
1:A:51:TYR:CE1	1:A:354:MET:HG2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LYS:HE3	1:B:247:GLU:HB2	1.87	0.56
1:B:233:LEU:HG	1:B:237:MET:HE3	1.88	0.56
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.88	0.55
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.89	0.55
1:A:187:LYS:HA	1:A:190:ARG:HG3	1.89	0.54
1:B:49:THR:HG22	1:B:50:ARG:H	1.73	0.53
1:B:118:MET:HE2	3:B:613:HOH:O	2.08	0.53
1:B:81:PHE:CG	1:B:212:MET:HE1	2.45	0.52
1:B:5:MET:HE2	1:B:41:LYS:HB2	1.92	0.51
1:B:58:ILE:HD13	1:B:355:VAL:HG13	1.92	0.51
1:A:176:SER:OG	1:A:211:VAL:HG21	2.11	0.50
1:A:108:SER:O	1:A:111:ALA:N	2.45	0.50
1:B:78:VAL:HG12	1:B:88:THR:HG21	1.94	0.50
1:A:81:PHE:CG	1:A:212:MET:HE1	2.49	0.48
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.44	0.48
1:B:185:MET:SD	1:B:436:THR:HA	2.54	0.47
1:A:81:PHE:HB3	1:A:209:ILE:HD12	1.97	0.47
1:B:53:SER:HB3	1:B:359:GLN:HB3	1.96	0.46
1:B:151:ASP:OD1	1:B:164:SER:OG	2.31	0.45
1:B:81:PHE:HB3	1:B:209:ILE:HG12	1.99	0.45
1:A:357:ILE:N	1:A:358:PRO:CD	2.80	0.44
1:B:381:ASN:C	1:B:381:ASN:HD22	2.25	0.44
1:B:230:SER:O	1:B:232:ASP:N	2.51	0.44
1:A:190:ARG:HD2	1:A:198:TYR:CZ	2.53	0.44
1:A:151:ASP:OD1	1:A:162:PHE:HB2	2.17	0.44
1:A:95:ASN:CG	3:A:620:HOH:O	2.60	0.43
1:A:104:LEU:N	1:A:105:PRO:CD	2.81	0.43
1:B:409:GLU:O	1:B:413:VAL:HG23	2.18	0.43
1:B:336:LYS:O	1:B:349:LYS:HE2	2.18	0.43
1:B:29:LEU:HD13	1:B:51:TYR:CE2	2.54	0.43
1:A:305:TYR:CZ	1:A:309:LYS:HE2	2.54	0.42
1:B:141:VAL:HB	1:B:142:PRO:HD3	2.01	0.42
1:A:363:ASP:OD1	1:A:365:THR:HB	2.20	0.42
1:B:39:ILE:HA	1:B:51:TYR:O	2.19	0.42
1:B:280:LEU:HD22	1:B:287:LEU:HA	2.00	0.42
1:B:434:LYS:NZ	3:B:627:HOH:O	2.53	0.41
1:A:77:PHE:CD2	1:A:187:LYS:HE3	2.55	0.41
1:A:312:LYS:HE3	1:B:64:GLU:OE1	2.20	0.41
1:A:426:HIS:CG	1:A:447:LYS:HD2	2.56	0.41
1:A:60:GLU:OE2	1:A:342:GLY:HA2	2.20	0.41
1:A:434:LYS:HB2	1:A:442:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:GLU:OE1	1:B:438:THR:OG1	2.36	0.41
1:B:320:GLU:HG3	1:B:374:PHE:CD1	2.55	0.41
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.51	0.41
1:B:453:ILE:HA	1:B:454:PRO:HD3	1.95	0.41
1:B:31:LYS:HD3	1:B:31:LYS:C	2.46	0.40
1:A:233:LEU:HG	1:A:237:MET:HE3	2.02	0.40
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	451/455 (99%)	434 (96%)	15 (3%)	2 (0%)	30 12
1	B	451/455 (99%)	438 (97%)	11 (2%)	2 (0%)	30 12
All	All	902/910 (99%)	872 (97%)	26 (3%)	4 (0%)	30 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ASP
1	A	230	SER
1	B	230	SER
1	B	231	ASP

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	396/399 (99%)	386 (98%)	10 (2%)	42 14
1	B	397/399 (100%)	389 (98%)	8 (2%)	50 21
All	All	793/798 (99%)	775 (98%)	18 (2%)	45 16

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	22	THR
1	A	31	LYS
1	A	59	LYS
1	A	112	MET
1	A	174	ILE
1	A	185	MET
1	A	365	THR
1	A	371	VAL
1	A	434	LYS
1	B	31	LYS
1	B	49	THR
1	B	136	ASP
1	B	148	LEU
1	B	174	ILE
1	B	204	GLN
1	B	231	ASP
1	B	387	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	70	ASN
1	A	73	GLN
1	A	204	GLN
1	A	213	ASN
1	A	229	GLN
1	A	403	GLN
1	B	70	ASN
1	B	189	GLN

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Mol	Chain	Res	Type
1	B	239	ASN
1	B	381	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	41,50,50	1.62	8 (19%)	45,82,82	1.89	14 (31%)
2	HEM	A	501	1	41,50,50	1.68	9 (21%)	45,82,82	1.95	12 (26%)

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	501	1	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	501	1	-	2/12/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C4D-ND	-5.60	1.30	1.40
2	B	501	HEM	C1B-NB	-4.82	1.32	1.40
2	A	501	HEM	C1B-NB	-3.95	1.33	1.40
2	B	501	HEM	C4D-ND	-3.35	1.34	1.40
2	A	501	HEM	CHA-C4D	3.22	1.43	1.35
2	B	501	HEM	CHB-C1B	3.20	1.43	1.35
2	B	501	HEM	C4D-C3D	3.16	1.50	1.45
2	B	501	HEM	CHA-C4D	2.74	1.42	1.35
2	A	501	HEM	C4B-NB	-2.67	1.33	1.38
2	B	501	HEM	C4B-NB	-2.67	1.33	1.38
2	A	501	HEM	C1A-NA	2.44	1.41	1.36
2	A	501	HEM	C3B-C4B	2.41	1.49	1.44
2	A	501	HEM	O2D-CGD	-2.32	1.22	1.30
2	B	501	HEM	C1D-C2D	2.30	1.49	1.44
2	A	501	HEM	CHB-C1B	2.19	1.40	1.35
2	A	501	HEM	FE-NB	2.16	2.07	1.96
2	B	501	HEM	FE-NB	2.13	2.07	1.96

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	C1B-NB-C4B	4.48	109.70	105.07
2	B	501	HEM	C1B-NB-C4B	3.87	109.07	105.07
2	B	501	HEM	CHD-C1D-ND	3.71	128.46	124.43
2	A	501	HEM	CHD-C1D-C2D	-3.66	119.26	124.98
2	A	501	HEM	CHD-C1D-ND	3.62	128.36	124.43
2	A	501	HEM	C4B-CHC-C1C	3.57	127.27	122.56
2	A	501	HEM	C1D-C2D-C3D	-3.52	103.26	106.96
2	B	501	HEM	CHD-C1D-C2D	-3.49	119.53	124.98
2	B	501	HEM	CHA-C4D-C3D	-3.21	119.30	125.33
2	B	501	HEM	CHA-C4D-ND	3.18	128.31	124.38
2	B	501	HEM	C4B-C3B-C2B	-3.09	104.66	107.11
2	A	501	HEM	CHB-C1B-NB	2.99	128.07	124.38
2	A	501	HEM	C4B-C3B-C2B	-2.97	104.76	107.11
2	A	501	HEM	CHC-C4B-NB	2.90	127.58	124.43
2	A	501	HEM	CHA-C4D-ND	2.90	127.96	124.38
2	A	501	HEM	CMA-C3A-C4A	-2.85	124.08	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	CHC-C4B-NB	2.80	127.48	124.43
2	B	501	HEM	O2A-CGA-CBA	2.72	122.77	114.03
2	A	501	HEM	CHA-C4D-C3D	-2.68	120.30	125.33
2	B	501	HEM	O2D-CGD-O1D	-2.54	116.97	123.30
2	B	501	HEM	O2D-CGD-CBD	2.47	121.96	114.03
2	B	501	HEM	C2C-C3C-C4C	-2.46	105.18	106.90
2	B	501	HEM	C4B-CHC-C1C	2.38	125.70	122.56
2	B	501	HEM	CMB-C2B-C1B	2.16	128.32	125.04
2	B	501	HEM	CBA-CAA-C2A	-2.07	109.09	112.62
2	A	501	HEM	O2D-CGD-CBD	2.01	120.48	114.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O2D

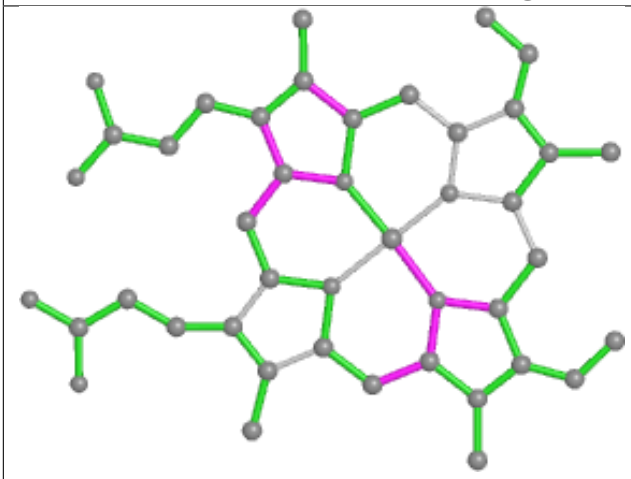
There are no ring outliers.

1 monomer is involved in 4 short contacts:

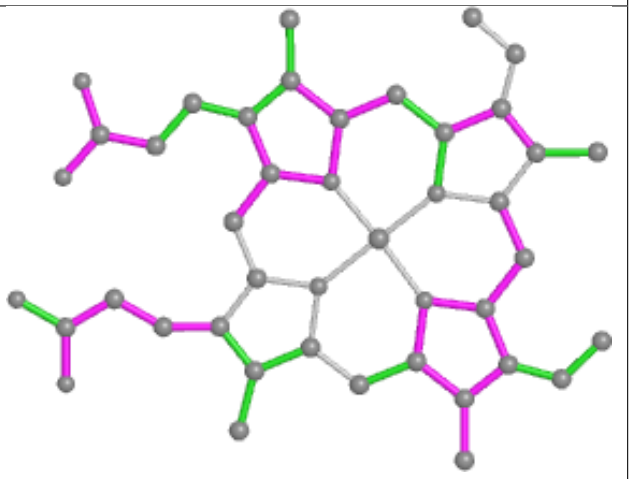
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	4	0

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.

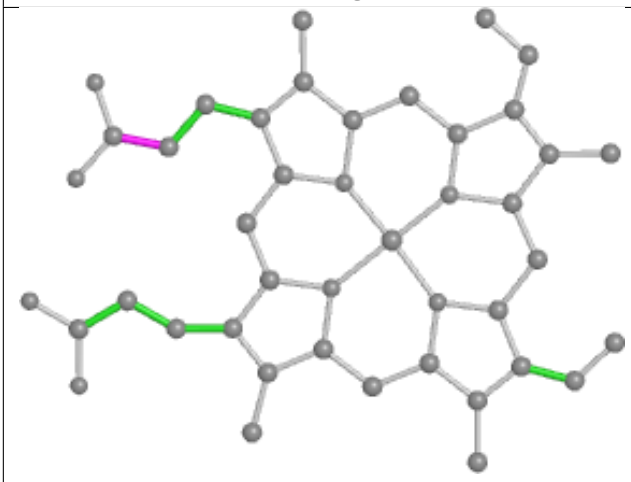
Ligand HEM B 501



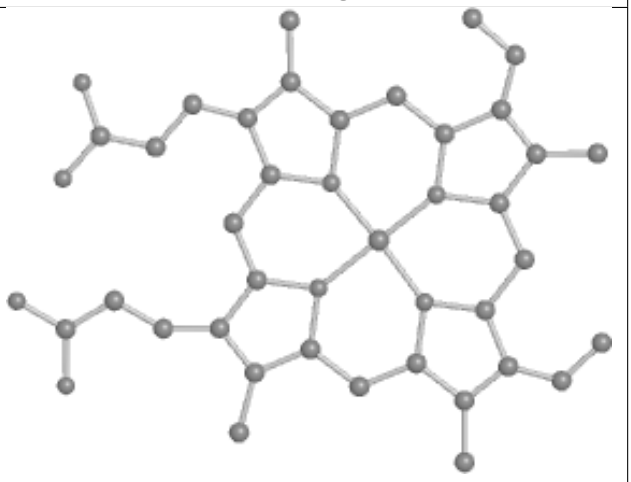
Bond lengths



Bond angles

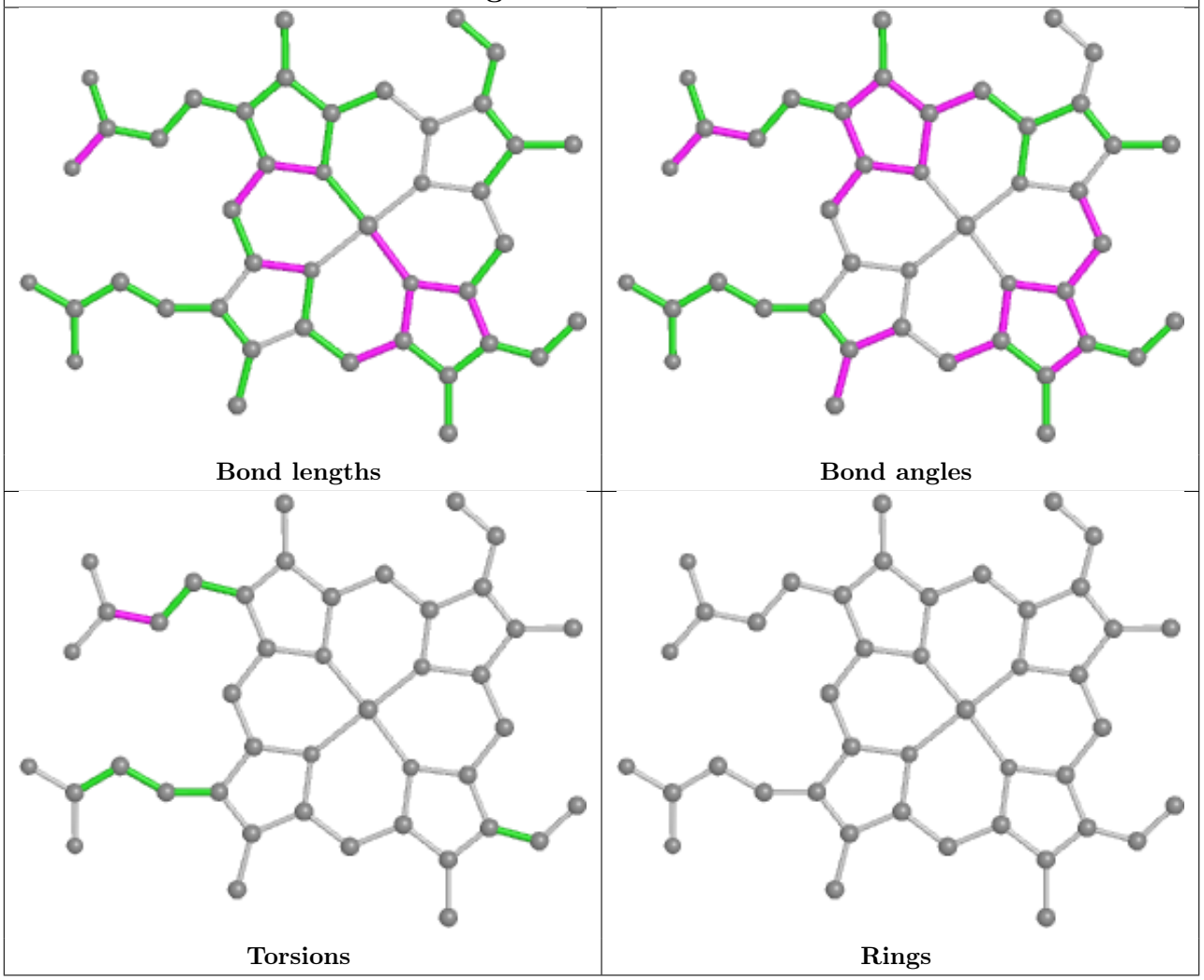


Torsions



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	453/455 (99%)	0.89	71 (15%)	6 5	11, 22, 53, 104	0
1	B	453/455 (99%)	0.81	61 (13%)	8 8	11, 21, 51, 85	0
All	All	906/910 (99%)	0.85	132 (14%)	7 7	11, 22, 52, 104	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	PRO	7.1
1	A	198	TYR	6.4
1	B	229	GLN	6.3
1	B	230	SER	5.6
1	A	230	SER	5.5
1	A	197	ALA	5.3
1	B	227	GLY	5.3
1	A	196	PRO	5.3
1	A	228	GLU	5.0
1	A	191	ALA	4.9
1	B	225	ALA	4.8
1	B	202	LYS	4.7
1	A	229	GLN	4.7
1	A	135	ALA	4.7
1	A	174	ILE	4.7
1	B	205	PHE	4.6
1	B	197	ALA	4.5
1	B	228	GLU	4.5
1	A	202	LYS	4.5
1	A	203	ARG	4.5
1	B	198	TYR	4.4
1	B	193	PRO	4.3
1	B	191	ALA	4.3
1	B	3	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	225	ALA	4.2
1	A	192	ASN	4.1
1	B	204	GLN	4.0
1	A	13	GLU	4.0
1	B	189	GLN	3.8
1	B	226	SER	3.8
1	A	211	VAL	3.8
1	B	192	ASN	3.7
1	B	168	ASP	3.7
1	B	203	ARG	3.7
1	B	437	LEU	3.6
1	A	227	GLY	3.6
1	B	46	GLY	3.6
1	B	455	LEU	3.6
1	A	205	PHE	3.4
1	B	196	PRO	3.4
1	A	188	LEU	3.4
1	A	455	LEU	3.4
1	A	381	ASN	3.4
1	B	169	GLN	3.3
1	A	231	ASP	3.3
1	A	226	SER	3.3
1	A	109	GLN	3.3
1	A	110	GLN	3.3
1	A	201	ASN	3.3
1	B	201	ASN	3.3
1	B	221	ALA	3.2
1	B	194	ASP	3.2
1	A	195	ASP	3.2
1	B	188	LEU	3.1
1	A	204	GLN	3.1
1	A	194	ASP	3.1
1	A	185	MET	3.1
1	A	302	VAL	3.1
1	A	454	PRO	3.0
1	A	177	MET	3.0
1	A	199	ASP	3.0
1	B	178	VAL	3.0
1	A	190	ARG	3.0
1	B	195	ASP	3.0
1	A	436	THR	2.9
1	B	185	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	111	ALA	2.9
1	A	77	PHE	2.9
1	A	200	GLU	2.8
1	B	174	ILE	2.8
1	A	169	GLN	2.8
1	B	207	ASP	2.8
1	A	437	LEU	2.8
1	A	263	GLY	2.8
1	B	224	LYS	2.8
1	B	181	LEU	2.8
1	B	454	PRO	2.8
1	B	200	GLU	2.7
1	A	209	ILE	2.7
1	A	168	ASP	2.7
1	A	208	ASP	2.6
1	A	380	GLU	2.6
1	A	182	ASP	2.6
1	A	181	LEU	2.5
1	B	190	ARG	2.5
1	A	382	PRO	2.5
1	A	262	LEU	2.5
1	B	177	MET	2.4
1	A	3	LYS	2.4
1	B	109	GLN	2.4
1	A	184	ILE	2.4
1	A	178	VAL	2.4
1	B	211	VAL	2.4
1	A	175	THR	2.4
1	B	77	PHE	2.3
1	A	4	GLU	2.3
1	A	222	ASP	2.3
1	B	172	PRO	2.3
1	A	73	GLN	2.3
1	A	345	TYR	2.3
1	B	170	PRO	2.3
1	A	186	ASN	2.2
1	A	224	LYS	2.2
1	B	4	GLU	2.2
1	B	14	LEU	2.2
1	B	263	GLY	2.2
1	B	5	MET	2.2
1	B	175	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	208	ASP	2.2
1	A	371	VAL	2.1
1	B	73	GLN	2.1
1	B	186	ASN	2.1
1	B	173	PHE	2.1
1	B	347	LEU	2.1
1	B	184	ILE	2.1
1	B	345	TYR	2.1
1	A	387	GLN	2.1
1	A	187	LYS	2.1
1	B	49	THR	2.1
1	A	210	LYS	2.1
1	A	267	GLU	2.1
1	A	173	PHE	2.1
1	A	108	SER	2.1
1	A	183	GLU	2.1
1	B	210	LYS	2.0
1	B	231	ASP	2.0
1	B	180	ALA	2.0
1	B	428	ASN	2.0
1	A	22	THR	2.0
1	A	107	PHE	2.0
1	B	209	ILE	2.0
1	A	340	VAL	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)

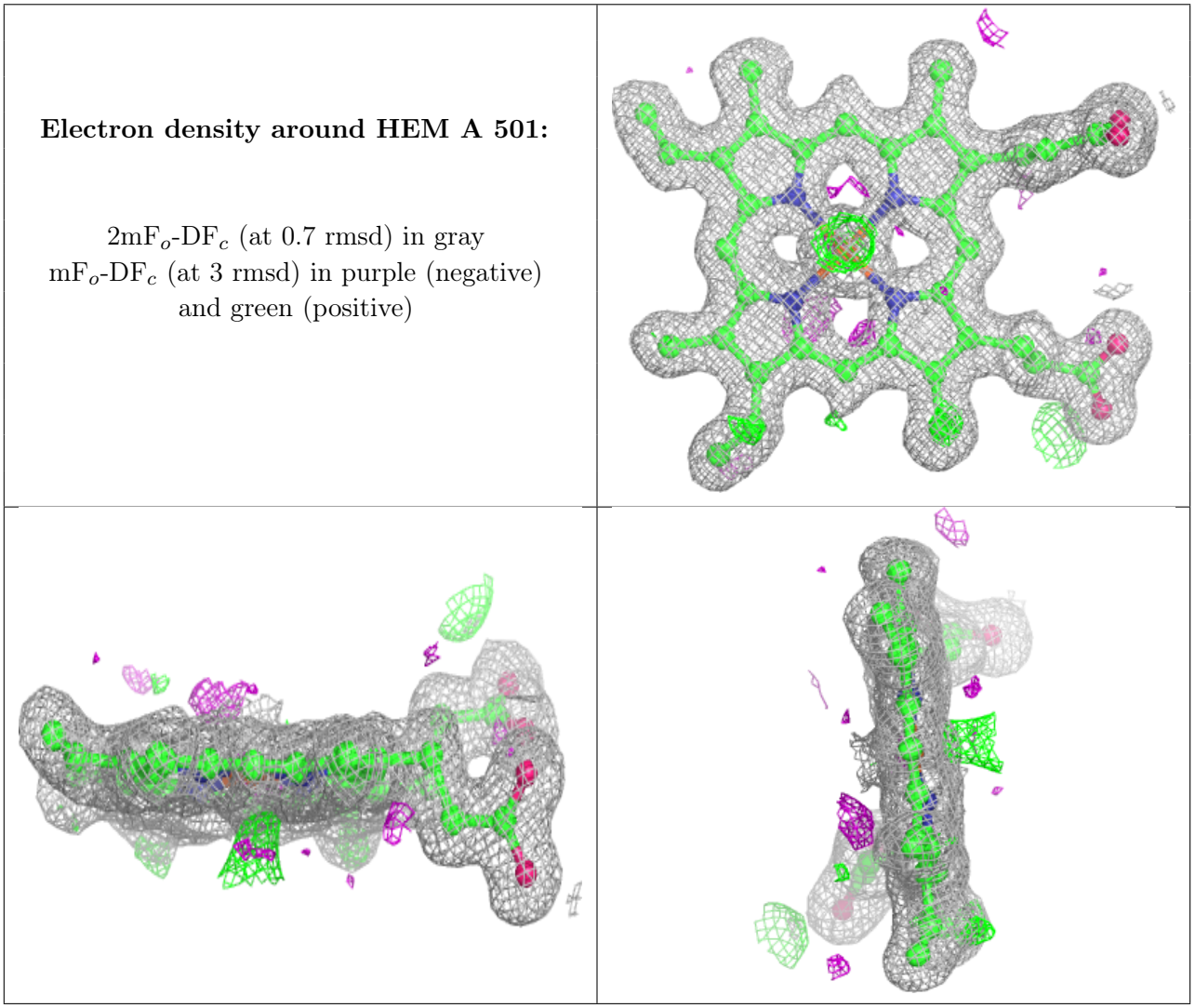
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	A	501	43/43	0.99	0.06	11,13,15,16	0
2	HEM	B	501	43/43	0.99	0.06	11,13,18,20	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.

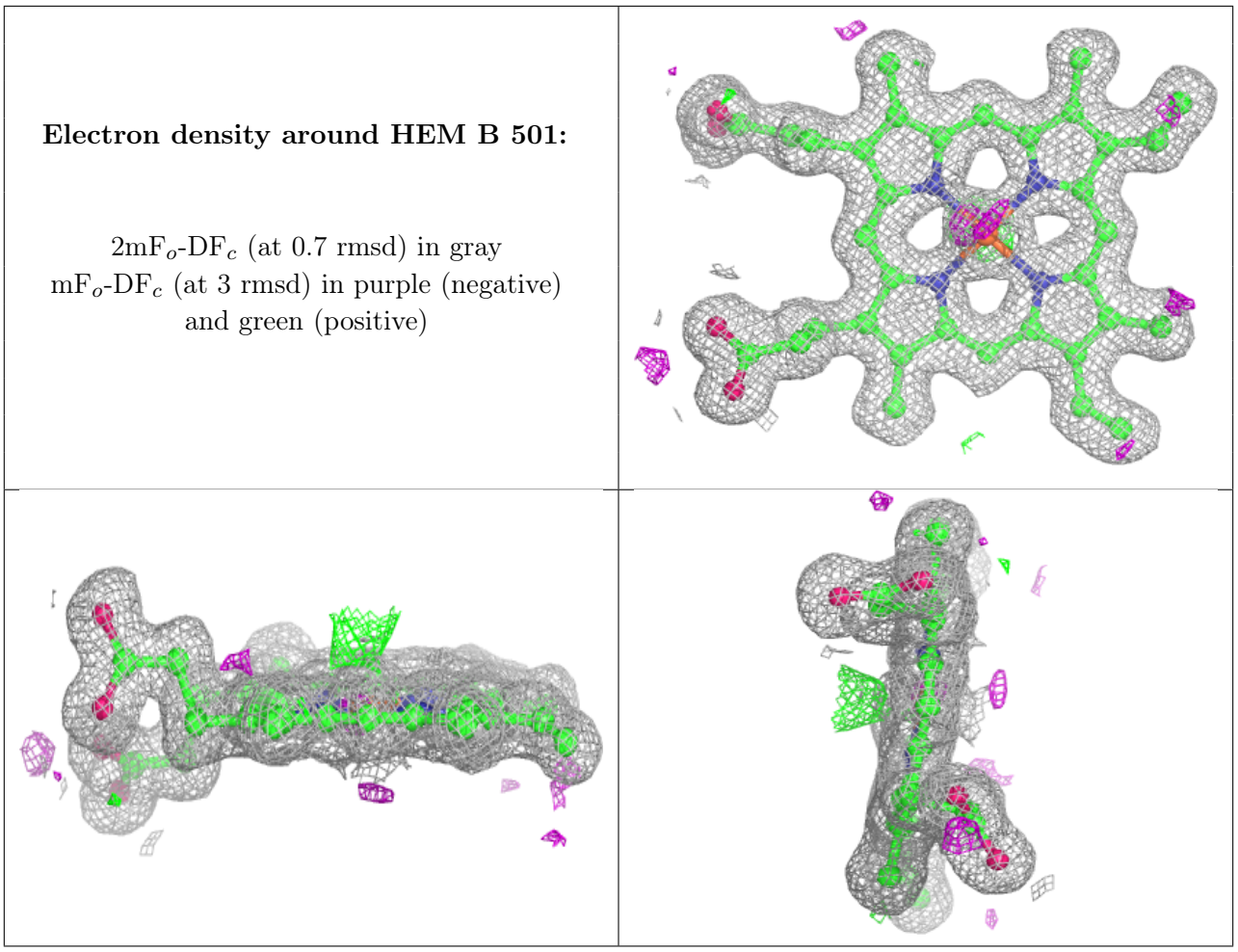
Electron density around HEM A 501:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.