Full wwPDB X-ray Structure Validation Report (i)

Apr 5, 2024 – 12:10 PM EDT

PDB ID	:	9BAT
Title	:	Crystal structure of sterol 14 alpha-demethylase (CYP51) from deep-sea fish Coryphaenoides armatus (abyssal grenadier) in the ligand-free state
Deposited on	:	2024-04-04
Resolution	:	2.90 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

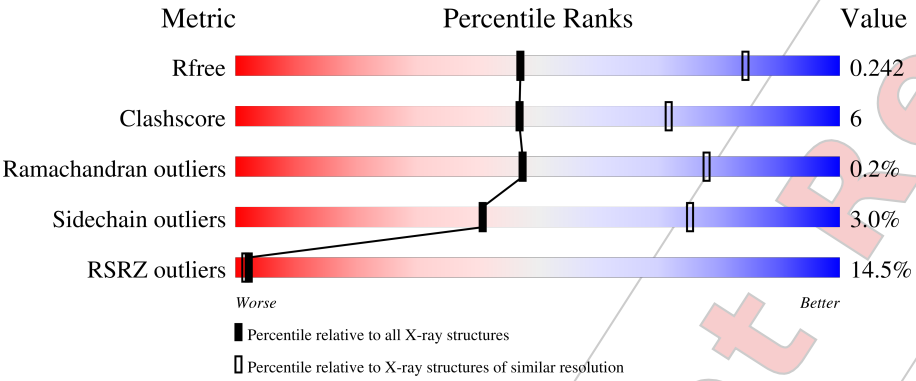
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	449	11% 79% 19%
1	B	449	17% 82% 15%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

2 Entry composition (i)

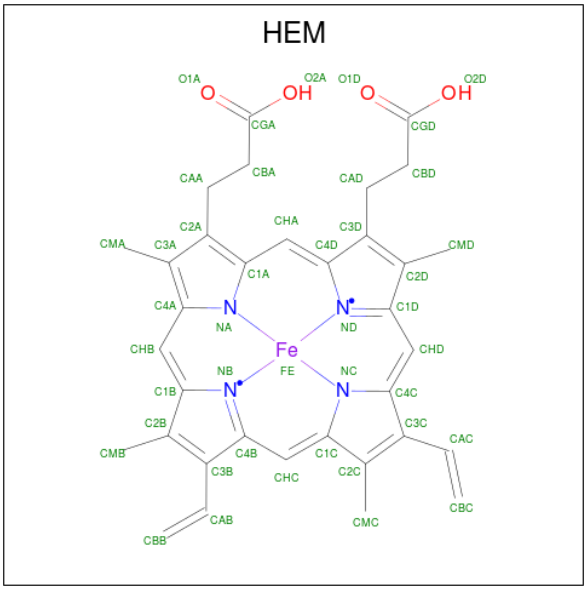
There are 3 unique types of molecules in this entry. The entry contains 7127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lanosterol 14-alpha demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3538	2263	603	652	20			
1	B	435	Total	C	N	O	S	0	0	0
			3481	2228	592	641	20			

- 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		

- Molecule 3 is water.

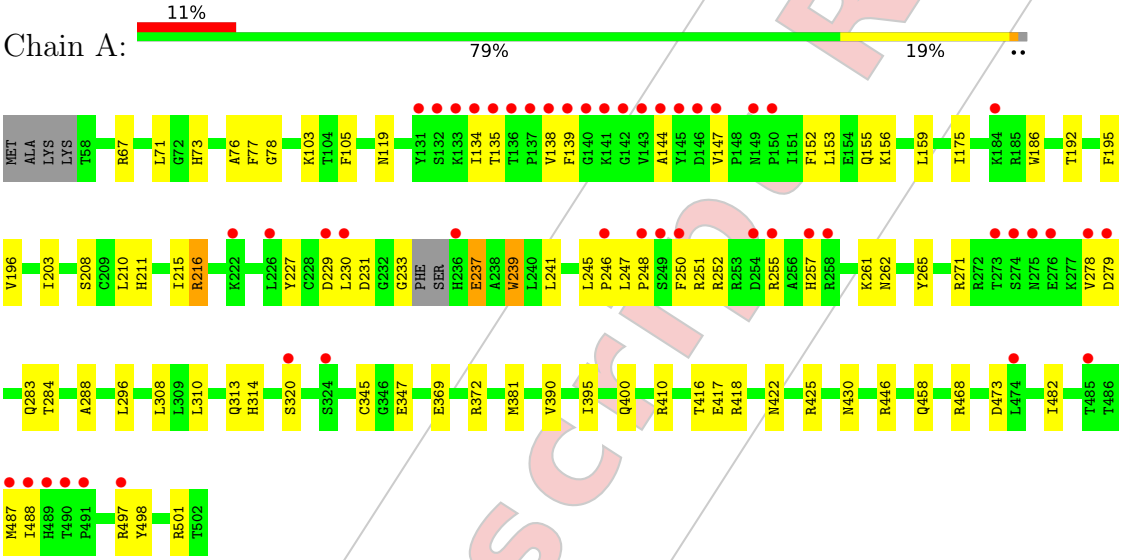
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	14	Total O 14 14	0	0
3	B	8	Total O 8 8	0	0

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.

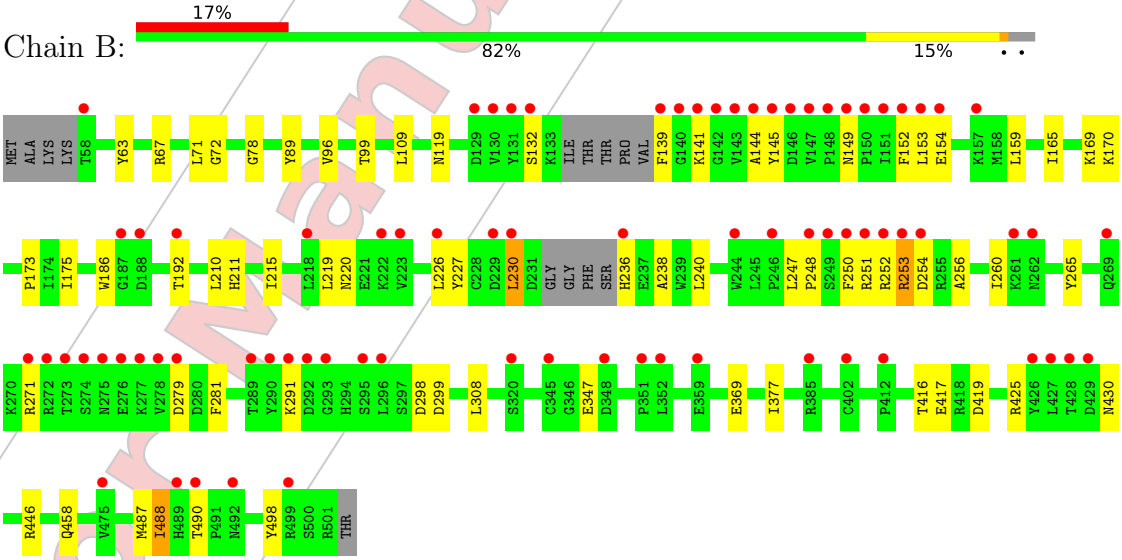
• Molecule 1: Lanosterol 14-alpha demethylase

Chain A:



• Molecule 1: Lanosterol 14-alpha demethylase

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	69.60Å 63.13Å 104.86Å 90.00° 97.59° 90.00°	Depositor
Resolution (Å)	29.09 – 2.90 29.07 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.09-2.90) 97.1 (29.07-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.232 , 0.248 0.232 , 0.242	Depositor DCC
R_{free} test set	1015 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	78.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 68.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7127	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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	0.32	0/3622	0.48	0/4904
1	B	0.31	0/3563	0.51	2/4821 (0.0%)
All	All	0.32	0/7185	0.49	2/9725 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	254	ASP	N-CA-CB	7.25	123.66	110.60
1	B	253	ARG	CB-CA-C	-5.23	99.94	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3538	0	3530	51	0
1	B	3481	0	3464	40	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
3	A	14	0	0	0	0
3	B	8	0	0	0	0
All	All	7127	0	7054	88	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 6.

All (88) 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:229:ASP:HB3	1:A:251:ARG:HB3	1.55	0.87
1:A:138:VAL:HG22	1:A:233:GLY:HA2	1.64	0.79
1:A:134:ILE:HG23	1:A:237:GLU:HA	1.66	0.77
1:A:416:THR:O	1:A:425:ARG:NH2	2.24	0.71
1:B:72:GLY:HA3	1:B:99:THR:HG22	1.78	0.65
1:B:211:HIS:HB3	1:B:215:ILE:HD12	1.79	0.64
1:A:372:ARG:NH2	1:A:418:ARG:O	2.27	0.61
1:A:186:TRP:HB3	1:A:498:TYR:CE1	2.36	0.61
1:B:250:PHE:O	1:B:252:ARG:N	2.34	0.60
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.83	0.60
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.83	0.59
1:A:76:ALA:H	1:B:487:MET:HE2	1.67	0.58
1:A:208:SER:HB3	1:A:216:ARG:HG3	1.84	0.57
1:A:73:HIS:HA	1:B:487:MET:HE3	1.87	0.56
1:B:252:ARG:O	1:B:253:ARG:HB2	2.05	0.56
1:A:345:CYS:SG	1:A:468:ARG:NH2	2.79	0.55
1:B:149:ASN:O	1:B:153:LEU:HG	2.06	0.55
1:B:226:LEU:HD13	1:B:256:ALA:HA	1.88	0.55
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.89	0.55
1:B:227:TYR:HA	1:B:230:LEU:HB2	1.90	0.54
1:B:416:THR:HG22	1:B:417:GLU:HG3	1.89	0.54
1:A:77:PHE:HE2	1:A:239:TRP:HZ2	1.55	0.54
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.90	0.54
1:A:488:ILE:HD12	1:B:67:ARG:HG3	1.90	0.54
1:A:192:THR:HG23	1:A:498:TYR:HE2	1.72	0.53
1:A:245:LEU:HD12	1:A:314:HIS:CD2	2.44	0.53
2:B:601:HEM:HHA	2:B:601:HEM:HBD2	1.91	0.52
1:B:248:PRO:O	1:B:250:PHE:N	2.36	0.52
1:A:67:ARG:NH2	1:B:488:ILE:O	2.43	0.51
1:A:252:ARG:HB3	1:A:255:ARG:HD2	1.92	0.51
1:B:369:GLU:OE2	1:B:425:ARG:NH1	2.43	0.51
1:A:119:ASN:O	1:A:446:ARG:NH1	2.44	0.51
1:A:390:VAL:HG12	1:A:395:ILE:HD13	1.92	0.51
1:A:196:VAL:HG22	1:A:246:PRO:HD3	1.93	0.50
1:A:416:THR:HG22	1:A:417:GLU:HG2	1.93	0.50
1:B:144:ALA:HA	1:B:152:PHE:CZ	2.47	0.50
1:A:369:GLU:OE2	1:A:425:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ALA:HA	1:B:152:PHE:CE1	2.48	0.49
1:B:119:ASN:O	1:B:446:ARG:NH1	2.45	0.48
1:A:195:PHE:HB3	1:A:245:LEU:HD23	1.96	0.47
1:A:278:VAL:H	1:A:283:GLN:HG3	1.79	0.47
1:A:210:LEU:HD13	1:A:308:LEU:HD23	1.97	0.47
1:A:473:ASP:HB3	1:A:497:ARG:HH11	1.80	0.47
1:B:186:TRP:HB3	1:B:498:TYR:CE1	2.50	0.46
1:B:210:LEU:O	1:B:281:PHE:HB3	2.14	0.46
1:A:230:LEU:HG	1:A:310:LEU:HD11	1.98	0.46
1:B:265:TYR:OH	1:B:299:ASP:OD1	2.30	0.46
1:A:241:LEU:HD11	1:A:482:ILE:HD13	1.97	0.46
1:A:71:LEU:HD13	1:B:78:GLY:HA2	1.97	0.46
1:A:248:PRO:O	1:A:250:PHE:N	2.37	0.46
1:A:103:LYS:HB2	1:A:105:PHE:CE1	2.51	0.46
1:A:78:GLY:HA2	1:B:71:LEU:HD13	1.97	0.46
1:B:175:ILE:HD13	1:B:458:GLN:HA	1.98	0.46
1:A:203:ILE:HG13	1:A:313:GLN:OE1	2.17	0.45
1:A:67:ARG:NH1	1:B:490:THR:OG1	2.48	0.45
1:B:236:HIS:C	1:B:238:ALA:H	2.20	0.45
1:A:488:ILE:HA	1:B:67:ARG:HG3	1.99	0.45
1:A:381:MET:SD	1:A:400:GLN:NE2	2.87	0.45
1:A:410:ARG:HG2	1:A:418:ARG:HH11	1.82	0.45
1:B:226:LEU:HB2	1:B:260:ILE:HD11	1.99	0.45
1:B:240:LEU:HD23	1:B:377:ILE:HD13	1.99	0.44
1:B:165:ILE:HG22	1:B:169:LYS:HE3	1.99	0.44
1:A:227:TYR:O	1:A:231:ASP:N	2.51	0.44
1:A:262:ASN:HA	1:A:265:TYR:CD2	2.52	0.44
1:B:226:LEU:HB3	1:B:256:ALA:HB1	2.00	0.44
1:B:139:PHE:HD2	1:B:144:ALA:HB2	1.83	0.43
1:B:230:LEU:HD22	1:B:230:LEU:HA	1.72	0.43
2:A:601:HEM:HHA	2:A:601:HEM:HBD2	2.00	0.43
1:A:468:ARG:O	1:A:501:ARG:HG3	2.18	0.43
1:A:175:ILE:HD13	1:A:458:GLN:HA	2.00	0.43
1:A:390:VAL:HG12	1:A:395:ILE:CD1	2.48	0.43
1:B:159:LEU:HD13	1:B:308:LEU:HD13	2.01	0.43
1:A:257:HIS:O	1:A:261:LYS:HB2	2.19	0.42
1:A:284:THR:O	1:A:288:ALA:HB2	2.20	0.42
1:B:170:LYS:O	1:B:173:PRO:HD2	2.19	0.42
1:A:211:HIS:HB3	1:A:215:ILE:HD12	2.01	0.42
1:B:192:THR:HG23	1:B:498:TYR:HE2	1.85	0.42
1:A:153:LEU:HD23	1:A:156:LYS:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:SER:HB2	1:B:145:TYR:O	2.19	0.42
1:A:139:PHE:HD2	1:A:144:ALA:HB2	1.85	0.41
1:B:89:TYR:HB2	1:B:109:LEU:HD13	2.02	0.41
1:A:422:ASN:O	1:A:425:ARG:HG2	2.20	0.41
1:B:141:LYS:HB3	1:B:141:LYS:HE2	1.90	0.41
1:A:192:THR:HG23	1:A:498:TYR:CE2	2.55	0.41
1:A:250:PHE:HZ	1:B:63:TYR:HD1	1.69	0.40
1:B:154:GLU:OE2	1:B:291:LYS:HG2	2.22	0.40
1:A:147:VAL:HG23	1:A:152:PHE:HB2	2.04	0.40
1:A:155:GLN:O	1:A:159:LEU:HG	2.21	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	439/449 (98%)	408 (93%)	31 (7%)	0	100 100
1	B	429/449 (96%)	396 (92%)	31 (7%)	2 (0%)	29 61
All	All	868/898 (97%)	804 (93%)	62 (7%)	2 (0%)	47 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	ARG
1	B	220	ASN

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	389/394 (99%)	377 (97%)	12 (3%)	40	74
1	B	382/394 (97%)	371 (97%)	11 (3%)	42	76
All	All	771/788 (98%)	748 (97%)	23 (3%)	41	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	THR
1	A	216	ARG
1	A	237	GLU
1	A	239	TRP
1	A	247	LEU
1	A	271	ARG
1	A	279	ASP
1	A	296	LEU
1	A	320	SER
1	A	347	GLU
1	A	430	ASN
1	A	487	MET
1	B	96	VAL
1	B	219	LEU
1	B	230	LEU
1	B	247	LEU
1	B	271	ARG
1	B	279	ASP
1	B	298	ASP
1	B	347	GLU
1	B	419	ASP
1	B	430	ASN
1	B	488	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	430	ASN
1	A	489	HIS
1	B	430	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	601	1	41,50,50	1.47	9 (21%)	45,82,82	1.72	14 (31%)
2	HEM	A	601	1	41,50,50	1.34	6 (14%)	45,82,82	1.92	10 (22%)

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	601	1	-	5/12/54/54	-
2	HEM	A	601	1	-	6/12/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C1B-NB	-3.59	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C4B-NB	-3.21	1.32	1.38
2	B	601	HEM	C3B-C4B	3.06	1.51	1.44
2	B	601	HEM	C4D-C3D	2.83	1.49	1.45
2	A	601	HEM	C4D-C3D	2.76	1.49	1.45
2	B	601	HEM	C4D-ND	-2.74	1.35	1.40
2	B	601	HEM	FE-NB	2.72	2.10	1.96
2	A	601	HEM	FE-NB	2.41	2.08	1.96
2	A	601	HEM	C3B-C4B	2.38	1.49	1.44
2	B	601	HEM	CHB-C1B	2.35	1.41	1.35
2	A	601	HEM	CHA-C4D	2.27	1.40	1.35
2	B	601	HEM	C1D-C2D	2.20	1.48	1.44
2	B	601	HEM	CHA-C4D	2.19	1.40	1.35
2	B	601	HEM	C1B-NB	-2.09	1.36	1.40
2	A	601	HEM	C1A-NA	2.03	1.40	1.36

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	HEM	CHC-C4B-NB	4.79	129.64	124.43
2	A	601	HEM	CAD-C3D-C4D	4.59	132.67	124.66
2	A	601	HEM	C1B-NB-C4B	4.37	109.59	105.07
2	B	601	HEM	CAD-C3D-C4D	3.72	131.16	124.66
2	B	601	HEM	C1B-NB-C4B	3.66	108.86	105.07
2	A	601	HEM	CAD-CBD-CGD	-3.32	106.47	113.60
2	B	601	HEM	CHC-C4B-NB	3.25	127.97	124.43
2	A	601	HEM	CAD-C3D-C2D	-3.23	121.86	127.88
2	A	601	HEM	C4B-C3B-C2B	-2.90	104.81	107.11
2	A	601	HEM	CHD-C1D-ND	2.86	127.54	124.43
2	B	601	HEM	C4B-C3B-C2B	-2.69	104.98	107.11
2	A	601	HEM	CHD-C1D-C2D	-2.69	120.78	124.98
2	B	601	HEM	CAD-CBD-CGD	-2.65	107.89	113.60
2	B	601	HEM	C4B-CHC-C1C	2.63	126.03	122.56
2	A	601	HEM	O2D-CGD-CBD	2.62	122.44	114.03
2	B	601	HEM	CHD-C1D-C2D	-2.57	120.96	124.98
2	B	601	HEM	CHD-C1D-ND	2.51	127.16	124.43
2	B	601	HEM	CAD-C3D-C2D	-2.44	123.33	127.88
2	B	601	HEM	CMD-C2D-C1D	2.42	128.72	125.04
2	B	601	HEM	CHB-C1B-NB	2.28	127.20	124.38
2	B	601	HEM	O2D-CGD-CBD	2.17	120.99	114.03
2	A	601	HEM	O2D-CGD-O1D	-2.12	118.01	123.30
2	B	601	HEM	C2C-C3C-C4C	-2.11	105.42	106.90
2	B	601	HEM	O2D-CGD-O1D	-2.02	118.27	123.30

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEM	C4D-C3D-CAD-CBD
2	B	601	HEM	C4D-C3D-CAD-CBD
2	A	601	HEM	C2D-C3D-CAD-CBD
2	B	601	HEM	C2D-C3D-CAD-CBD
2	B	601	HEM	C3D-CAD-CBD-CGD
2	A	601	HEM	C3D-CAD-CBD-CGD
2	B	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAA-CBA-CGA-O2A

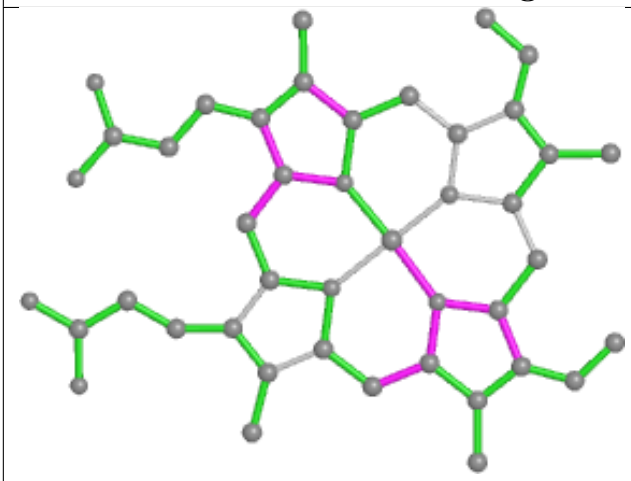
There are no ring outliers.

2 monomers are involved in 6 short contacts:

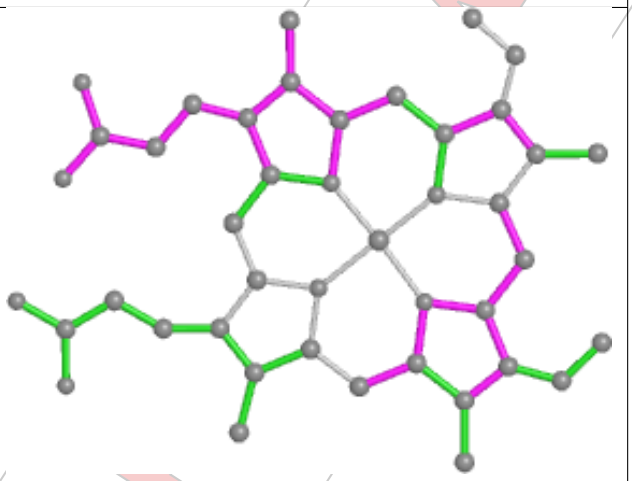
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEM	3	0
2	A	601	HEM	3	0

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.

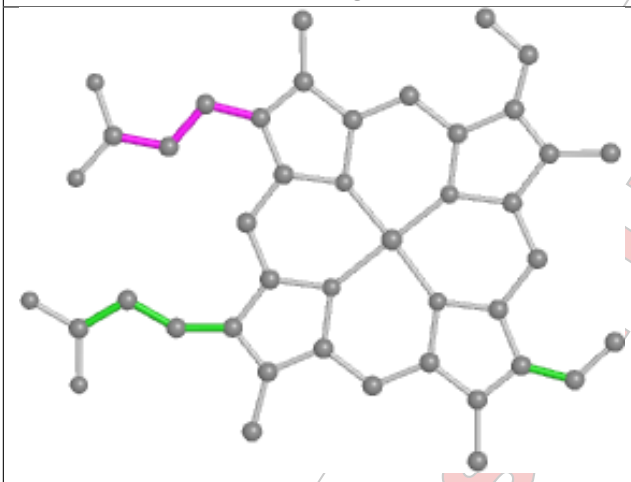
Ligand HEM B 601



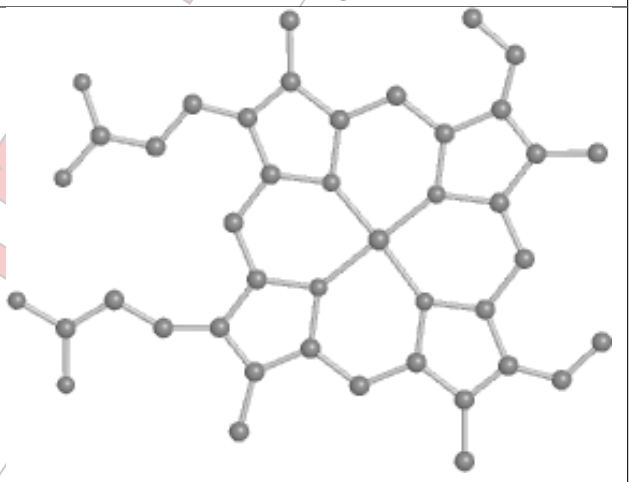
Bond lengths



Bond angles

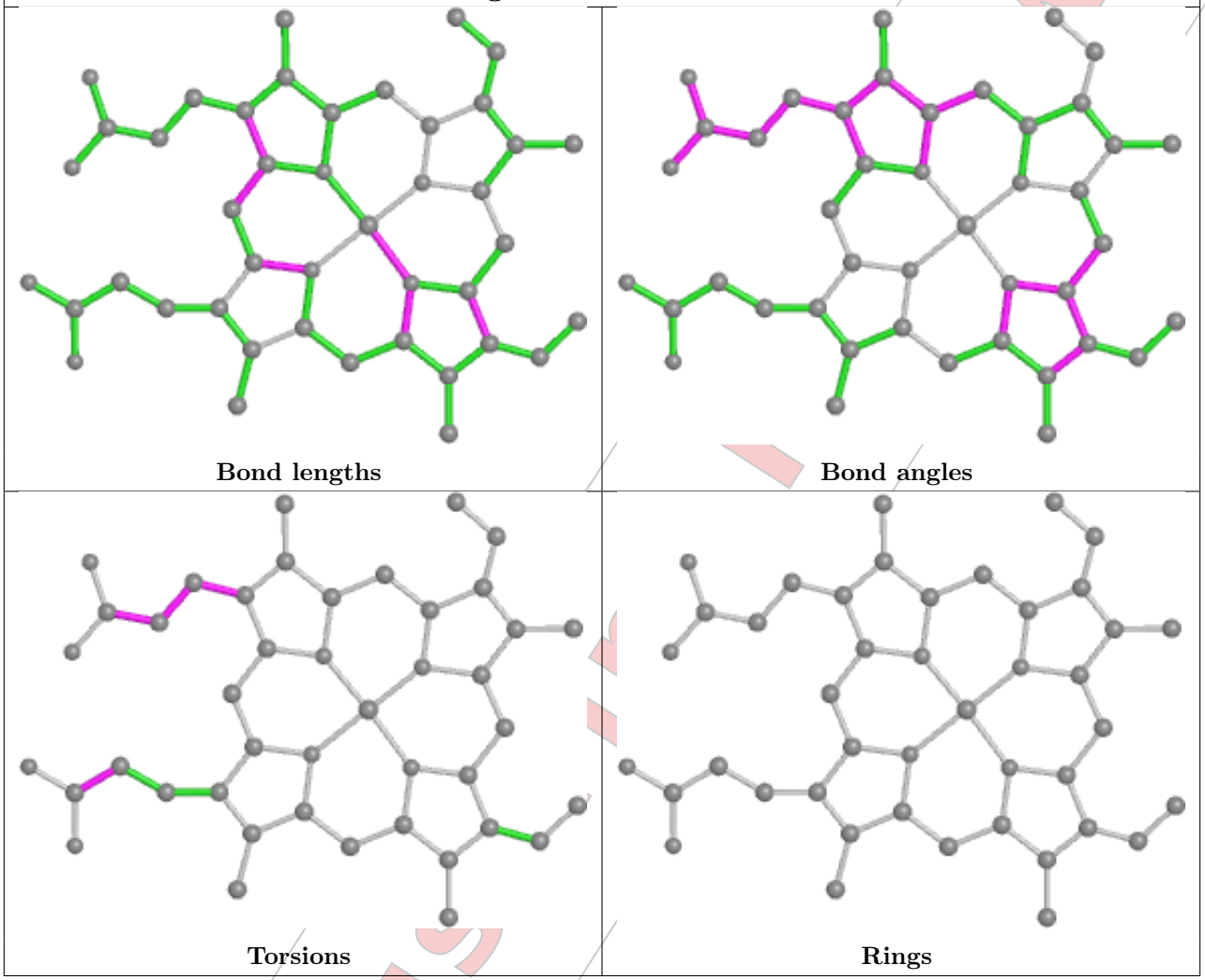


Torsions



Rings

Ligand HEM A 601



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	443/449 (98%)	0.64	49 (11%) 5 4	39, 81, 164, 246	0
1	B	435/449 (96%)	1.14	78 (17%) 1 1	45, 94, 188, 252	0
All	All	878/898 (97%)	0.89	127 (14%) 2 1	39, 89, 182, 252	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	PRO	17.9
1	B	142	GLY	14.1
1	A	136	THR	13.8
1	B	145	TYR	11.1
1	B	275	ASN	10.8
1	B	290	TYR	10.5
1	B	148	PRO	10.2
1	B	272	ARG	10.1
1	B	149	ASN	9.3
1	B	251	ARG	9.1
1	B	246	PRO	8.8
1	B	147	VAL	8.5
1	B	150	PRO	8.5
1	B	141	LYS	8.0
1	A	135	THR	8.0
1	B	132	SER	7.8
1	B	140	GLY	7.7
1	B	146	ASP	7.4
1	B	153	LEU	7.2
1	A	489	HIS	7.2
1	A	279	ASP	7.2
1	A	132	SER	6.8
1	A	144	ALA	6.8
1	A	488	ILE	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	250	PHE	6.4
1	A	145	TYR	6.4
1	B	139	PHE	6.3
1	A	143	VAL	6.2
1	A	255	ARG	6.0
1	B	292	ASP	6.0
1	A	133	LYS	5.3
1	B	277	LYS	5.3
1	A	146	ASP	5.3
1	B	143	VAL	5.2
1	B	273	THR	5.1
1	B	271	ARG	5.0
1	A	222	LYS	5.0
1	B	296	LEU	4.9
1	B	489	HIS	4.8
1	B	223	VAL	4.7
1	A	278	VAL	4.7
1	B	295	SER	4.6
1	A	134	ILE	4.6
1	B	144	ALA	4.5
1	B	248	PRO	4.5
1	A	139	PHE	4.4
1	B	236	HIS	4.4
1	A	138	VAL	4.4
1	B	222	LYS	4.3
1	B	291	LYS	4.3
1	B	278	VAL	4.3
1	A	229	ASP	4.3
1	B	58	THR	4.2
1	B	289	THR	4.2
1	B	188	ASP	4.1
1	A	487	MET	4.1
1	B	250	PHE	4.0
1	A	490	THR	3.9
1	A	141	LYS	3.9
1	A	150	PRO	3.8
1	A	248	PRO	3.8
1	B	352	LEU	3.8
1	B	152	PHE	3.8
1	A	184	LYS	3.7
1	A	257	HIS	3.7
1	A	142	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	276	GLU	3.6
1	B	218	LEU	3.6
1	B	274	SER	3.6
1	A	246	PRO	3.5
1	A	274	SER	3.5
1	A	254	ASP	3.4
1	A	149	ASN	3.4
1	B	131	TYR	3.4
1	B	154	GLU	3.4
1	B	412	PRO	3.4
1	B	151	ILE	3.3
1	B	293	GLY	3.3
1	A	147	VAL	3.3
1	A	140	GLY	3.2
1	B	252	ARG	3.1
1	B	244	TRP	3.1
1	A	485	THR	3.1
1	B	192	THR	3.1
1	A	131	TYR	3.0
1	B	429	ASP	3.0
1	B	269	GLN	3.0
1	B	348	ASP	2.9
1	A	491	PRO	2.9
1	B	229	ASP	2.9
1	B	402	CYS	2.8
1	B	428	THR	2.8
1	B	253	ARG	2.8
1	B	279	ASP	2.8
1	A	249	SER	2.7
1	A	226	LEU	2.7
1	B	226	LEU	2.7
1	B	492	ASN	2.7
1	A	236	HIS	2.6
1	B	249	SER	2.6
1	A	258	ARG	2.6
1	B	427	LEU	2.6
1	A	320	SER	2.6
1	A	276	GLU	2.4
1	A	497	ARG	2.4
1	B	490	THR	2.4
1	A	474	LEU	2.4
1	B	345	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	320	SER	2.4
1	B	426	TYR	2.3
1	B	499	ARG	2.3
1	B	262	ASN	2.3
1	A	230	LEU	2.3
1	B	157	LYS	2.3
1	B	359	GLU	2.2
1	A	273	THR	2.2
1	B	254	ASP	2.2
1	B	385	ARG	2.2
1	B	130	VAL	2.2
1	B	351	PRO	2.1
1	A	324	SER	2.1
1	B	475	VAL	2.1
1	B	129	ASP	2.0
1	B	261	LYS	2.0
1	A	275	ASN	2.0
1	B	187	GLY	2.0
1	B	230	LEU	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.

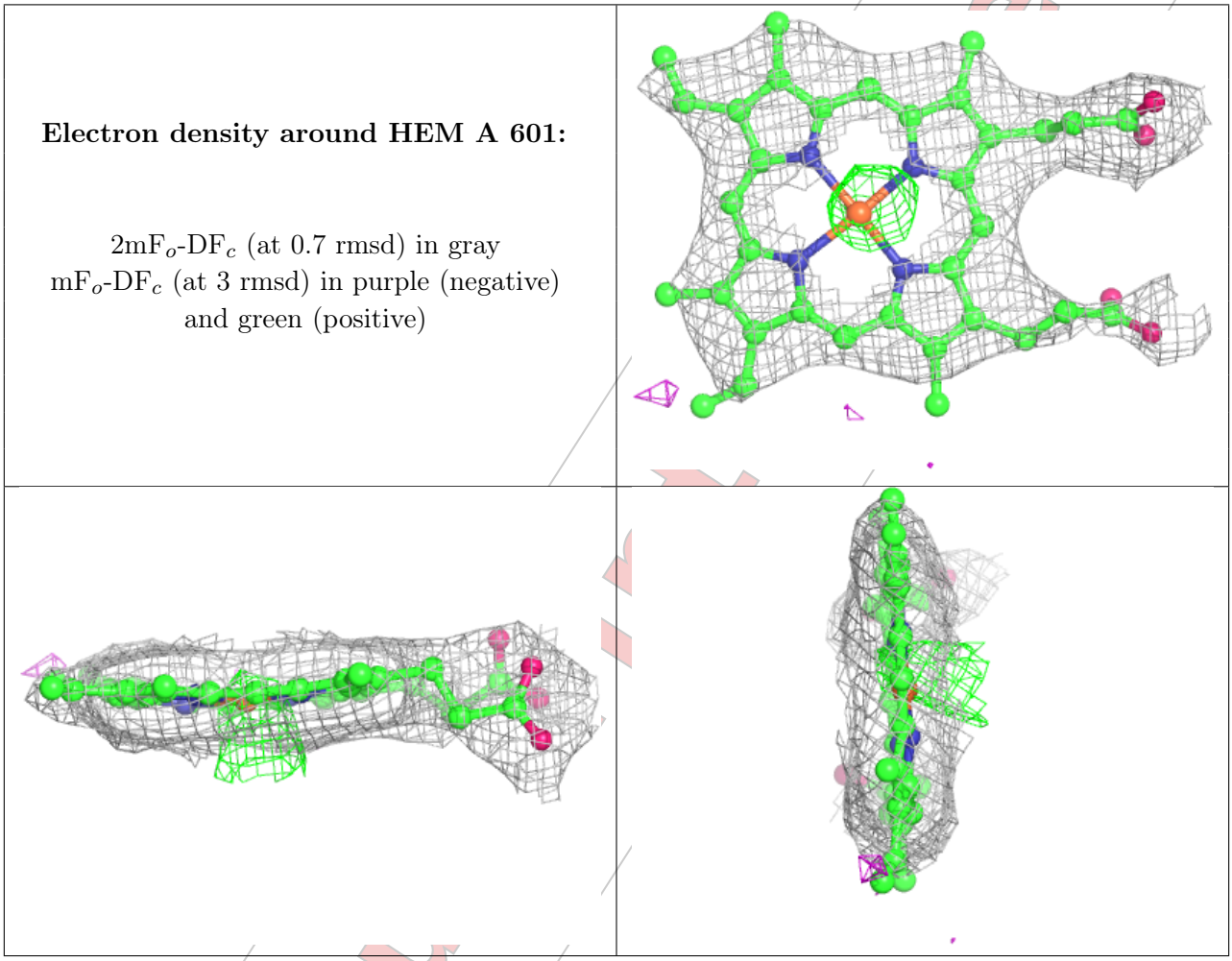
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	A	601	43/43	0.97	0.20	50,60,97,143	0
2	HEM	B	601	43/43	0.98	0.20	36,57,110,147	0

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.

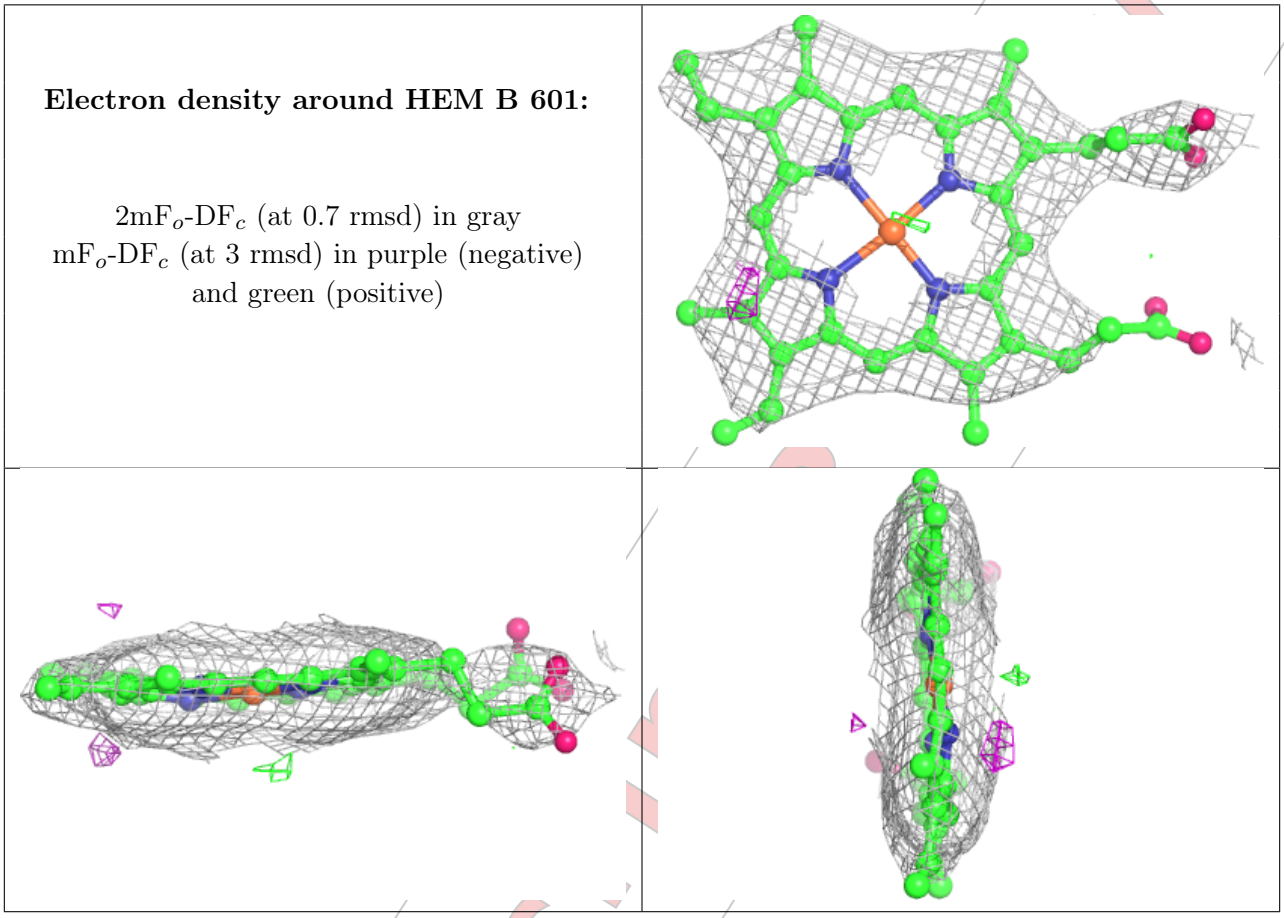
Electron density around HEM A 601:

$2mF_o$-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 601:

$2mF_o$-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.