



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:11 PM BST

PDB ID : 4HGG
Title : Crystal structure of P450 BM3 5F5R heme domain variant complexed with styrene
Authors : Shehzad, A.; Panneerselvam, S.; Bocola, M.; Mueller-Dieckmann, J.; Wilmanns, M.; Schwaneberg, U.
Deposited on : 2012-10-08
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

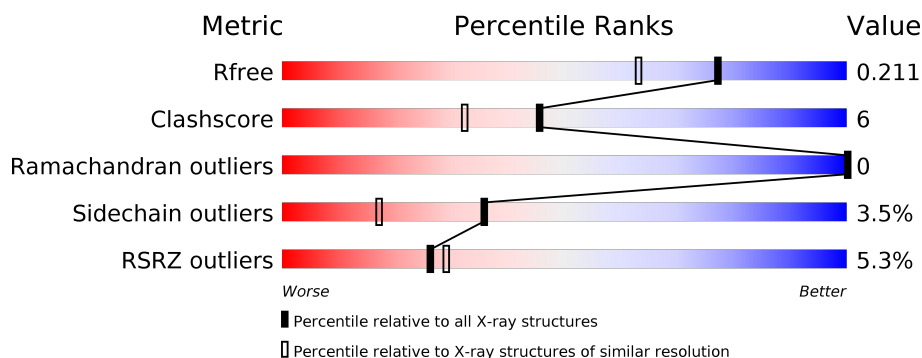
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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 $\leq 5\%$. 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	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• •</div> </div> </div>
1	B	455	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>

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	SYN	A	502	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8111 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.

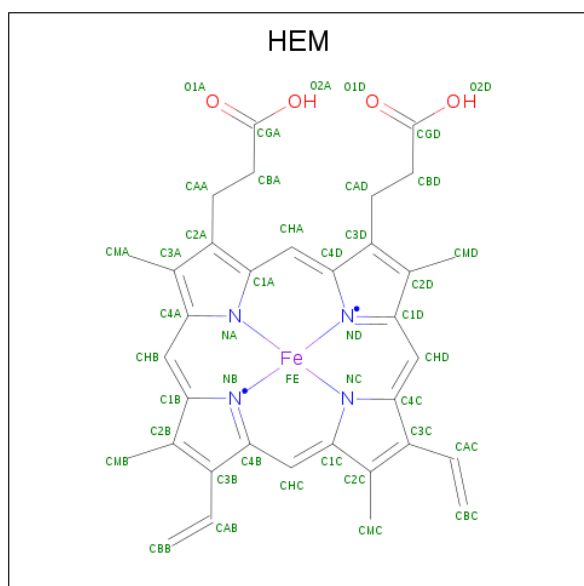
- Molecule 1 is a protein called Bifunctional P-450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	22	0
			3624	2332	607	667	18			
1	B	441	Total	C	N	O	S	0	15	0
			3641	2332	616	675	18			

There are 6 discrepancies between the modelled and reference sequences:

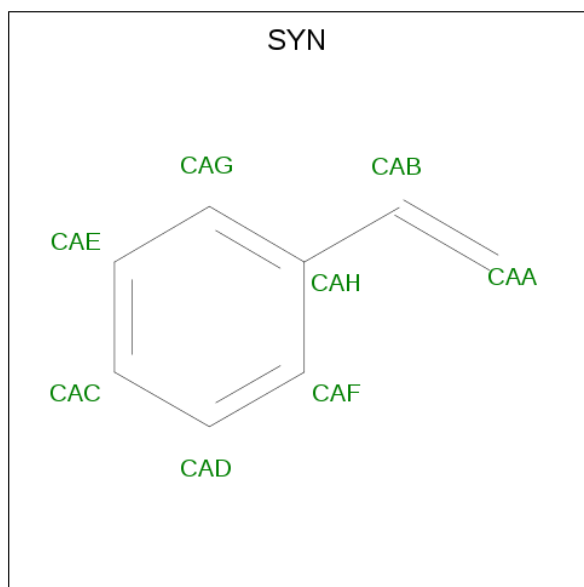
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ALA	PHE	ENGINEERED MUTATION	UNP P14779
A	184	ARG	ALA	ENGINEERED MUTATION	UNP P14779
A	235	ALA	THR	ENGINEERED MUTATION	UNP P14779
B	87	ALA	PHE	ENGINEERED MUTATION	UNP P14779
B	184	ARG	ALA	ENGINEERED MUTATION	UNP P14779
B	235	ALA	THR	ENGINEERED MUTATION	UNP P14779

- 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 ethenylbenzene (three-letter code: SYN) (formula: C_8H_8).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			8	8		
3	B	1	Total	C	0	0
			8	8		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

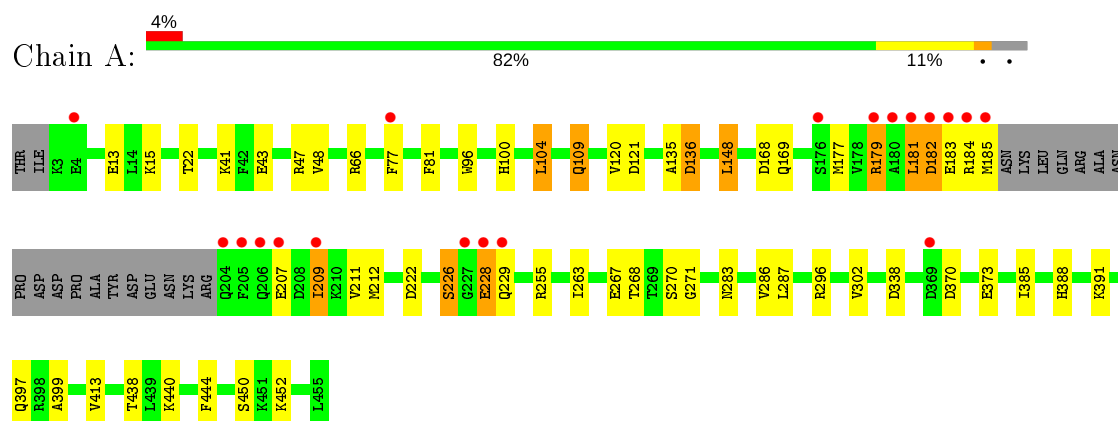
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	357	Total	O	0	0
			357	357		
6	B	339	Total	O	0	0
			339	339		

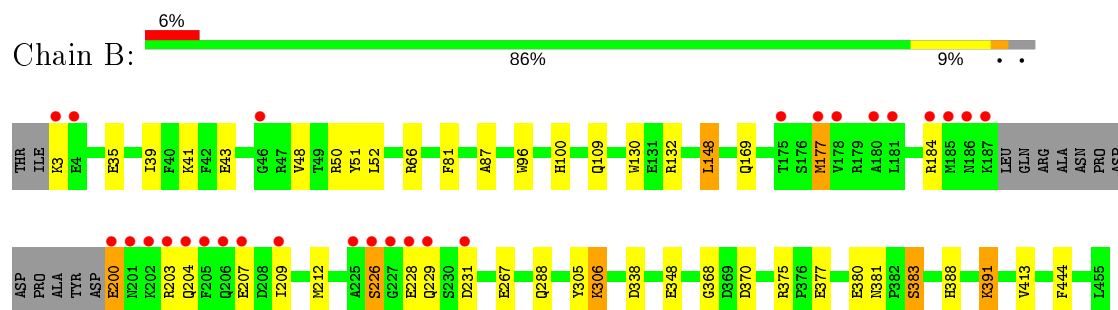
3 Residue-property plots

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 P-450/NADPH-P450 reductase



- Molecule 1: Bifunctional P-450/NADPH-P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.90 Å 147.98 Å 64.01 Å 90.00° 98.37° 90.00°	Depositor
Resolution (Å)	48.11 – 1.70 48.11 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.11-1.70) 100.0 (48.11-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.179 , 0.211 0.178 , 0.211	Depositor DCC
R_{free} test set	5933 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8111	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GOL, SYN, MES, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.08	2/3768 (0.1%)	0.96	7/5087 (0.1%)
1	B	1.08	4/3763 (0.1%)	0.94	7/5078 (0.1%)
All	All	1.08	6/7531 (0.1%)	0.95	14/10165 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	TRP	CD2-CE2	5.84	1.48	1.41
1	B	444	PHE	CE2-CZ	5.59	1.48	1.37
1	B	96	TRP	CD2-CE2	5.29	1.47	1.41
1	A	96	TRP	CD2-CE2	5.25	1.47	1.41
1	B	348	GLU	CD-OE2	-5.10	1.20	1.25
1	A	444	PHE	CG-CD1	5.06	1.46	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	168	ASP	CB-CA-C	-5.96	98.48	110.40
1	B	338	ASP	CB-CG-OD1	5.91	123.61	118.30
1	B	50	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	96	TRP	CA-CB-CG	-5.48	103.28	113.70
1	A	181	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	391	LYS	CD-CE-NZ	-5.45	99.17	111.70
1	B	338	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	182	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	A	255	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	B	66	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	338	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	50	ARG	NE-CZ-NH1	5.13	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	LEU	CB-CG-CD2	-5.08	102.37	111.00

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	3624	0	3671	52	0
1	B	3641	0	3663	37	1
2	A	43	0	30	4	0
2	B	43	0	30	0	0
3	A	8	0	8	5	0
3	B	8	0	7	1	0
4	A	12	0	12	3	0
5	A	24	0	32	4	1
5	B	12	0	16	1	0
6	A	357	0	0	13	0
6	B	339	0	0	8	0
All	All	8111	0	7469	95	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 6.

All (95) 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:226:SER:OG	1:A:228:GLU:HB2	1.43	1.17
1:B:267[A]:GLU:HG3	6:B:833:HOH:O	1.51	1.08
1:A:228:GLU:HA	1:A:228:GLU:OE1	1.50	1.04
1:A:121:ASP:OD2	5:A:507:GOL:H11	1.58	1.02
1:A:267[A]:GLU:HG2	6:A:900:HOH:O	1.72	0.86
1:A:77[B]:PHE:CZ	1:A:184:ARG:HB3	2.14	0.82
1:B:370:ASP:OD2	1:B:375[A]:ARG:NH1	2.11	0.82
1:A:228:GLU:CA	1:A:228:GLU:OE1	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440[A]:LYS:HE2	6:A:771:HOH:O	1.82	0.79
1:B:377:GLU:O	1:B:380[B]:GLU:HG2	1.84	0.78
1:A:43:GLU:HG2	1:A:48[B]:VAL:HG12	1.67	0.76
1:B:177:MET:HB3	1:B:212:MET:HE3	1.68	0.75
1:A:440[A]:LYS:CE	6:A:771:HOH:O	2.35	0.74
1:A:109[B]:GLN:HE22	1:B:368:GLY:HA2	1.52	0.74
1:A:77[B]:PHE:HZ	1:A:184:ARG:HB3	1.51	0.74
1:A:283:ASN:HB3	1:A:286[B]:VAL:HG12	1.67	0.74
1:B:200:GLU:HA	1:B:203:ARG:HG2	1.72	0.72
1:A:440[B]:LYS:HE2	6:A:949:HOH:O	1.88	0.72
1:A:109[A]:GLN:HA	1:A:109[A]:GLN:HE21	1.54	0.70
1:A:397:GLN:O	5:A:506:GOL:H11	1.92	0.70
1:A:179:ARG:O	1:A:182:ASP:HB3	1.92	0.69
1:B:267[B]:GLU:OE1	6:B:939:HOH:O	2.11	0.69
1:A:283:ASN:HB3	1:A:286[B]:VAL:CG1	2.22	0.68
1:B:177:MET:CE	1:B:267[B]:GLU:OE2	2.42	0.67
1:A:222:ASP:OD2	6:A:858:HOH:O	2.13	0.67
1:B:35:GLU:HG3	6:B:887:HOH:O	1.97	0.64
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.80	0.62
1:B:177:MET:HE2	1:B:267[B]:GLU:OE2	2.00	0.62
1:A:296[A]:ARG:NH2	6:A:826:HOH:O	2.32	0.61
1:A:43:GLU:HG2	1:A:48[B]:VAL:CG1	2.31	0.61
1:A:283:ASN:CB	1:A:286[B]:VAL:CG1	2.79	0.61
1:B:226:SER:HB2	1:B:228:GLU:HB3	1.83	0.60
1:B:177:MET:CB	1:B:212:MET:CE	2.80	0.60
1:A:177:MET:HB2	1:A:212:MET:HE3	1.84	0.59
1:A:77[B]:PHE:HZ	1:A:181:LEU:O	1.85	0.59
1:B:177:MET:HB3	1:B:212:MET:CE	2.32	0.58
1:B:177:MET:HB2	1:B:212:MET:HE1	1.86	0.58
1:A:267[A]:GLU:CG	6:A:900:HOH:O	2.41	0.58
1:B:288[A]:GLN:OE1	6:B:880:HOH:O	2.16	0.58
1:B:203:ARG:NH2	1:B:207:GLU:OE1	2.37	0.56
1:B:306:LYS:HG3	6:B:756:HOH:O	2.04	0.56
1:B:177:MET:CB	1:B:212:MET:HE1	2.36	0.56
1:A:77[B]:PHE:CZ	1:A:181:LEU:O	2.60	0.55
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.37	0.55
1:B:288[A]:GLN:CD	6:B:880:HOH:O	2.45	0.55
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.90	0.54
6:A:899:HOH:O	1:B:383:SER:HB3	2.07	0.54
1:A:120:VAL:HG11	1:A:302[A]:VAL:HG13	1.88	0.53
1:B:177:MET:CB	1:B:212:MET:HE3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:503:MES:H71	6:A:663:HOH:O	2.07	0.53
1:A:271:GLY:HA2	1:A:440[B]:LYS:HD3	1.91	0.53
1:B:109:GLN:OE1	1:B:305:TYR:OH	2.26	0.53
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.92	0.52
1:A:385:ILE:HG12	4:A:503:MES:H51	1.92	0.51
1:B:288[A]:GLN:NE2	6:B:880:HOH:O	2.44	0.51
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.93	0.50
1:A:183:GLU:O	1:A:183:GLU:OE1	2.30	0.50
1:A:268:THR:OG1	3:A:502:SYN:H9	2.12	0.50
1:B:200:GLU:CD	1:B:200:GLU:O	2.52	0.48
1:A:399:ALA:O	5:A:506:GOL:H12	2.14	0.48
1:B:41:LYS:HB3	1:B:41:LYS:NZ	2.29	0.47
1:B:177:MET:HE1	1:B:267[B]:GLU:OE2	2.11	0.47
1:A:181:LEU:O	1:A:182:ASP:C	2.53	0.47
2:A:501:HEM:NC	3:A:502:SYN:H6	2.30	0.47
1:A:267[B]:GLU:HG2	1:A:438[B]:THR:OG1	2.14	0.46
1:A:270[B]:SER:OG	1:A:440[B]:LYS:HE3	2.16	0.46
4:A:503:MES:H82	4:A:503:MES:H32	1.57	0.46
1:B:381:ASN:ND2	6:B:909:HOH:O	2.42	0.45
1:A:450:SER:HB3	1:A:452:LYS:HE2	1.97	0.45
1:A:109[B]:GLN:HE22	1:B:368:GLY:CA	2.26	0.45
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.99	0.44
1:A:287:LEU:HD23	1:A:287:LEU:O	2.17	0.44
1:B:100:HIS:HE1	5:B:504:GOL:O2	2.00	0.44
1:A:283:ASN:HB2	1:A:286[B]:VAL:CG1	2.48	0.44
1:B:43:GLU:HG2	1:B:48:VAL:HG22	2.01	0.43
1:A:267[B]:GLU:CD	6:A:867:HOH:O	2.56	0.43
1:A:81:PHE:HE1	1:A:209:ILE:HD11	1.84	0.43
1:A:135:ALA:O	1:A:136[B]:ASP:HB2	2.18	0.42
1:A:283:ASN:O	1:A:286[B]:VAL:CG1	2.68	0.42
1:B:184:ARG:HA	1:B:184:ARG:HD2	1.77	0.42
1:B:226:SER:C	1:B:228:GLU:H	2.23	0.42
1:A:283:ASN:O	1:A:286[B]:VAL:HG13	2.19	0.42
1:B:39:ILE:HA	1:B:51:TYR:O	2.19	0.42
1:A:177:MET:CE	1:A:263[B]:ILE:HD12	2.50	0.42
1:A:268:THR:OG1	3:A:502:SYN:CAA	2.68	0.41
1:A:226:SER:HG	1:A:228:GLU:HB2	1.73	0.41
1:A:207:GLU:O	1:A:211:VAL:HG23	2.21	0.41
1:A:100:HIS:HE1	5:A:506:GOL:O2	2.04	0.41
1:B:81:PHE:HE1	1:B:209:ILE:HD11	1.86	0.41
1:A:370:ASP:HB2	1:A:373:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:502:SYN:CAA	6:A:900:HOH:O	2.67	0.41
3:A:502:SYN:H8	6:A:900:HOH:O	2.20	0.41
1:B:87:ALA:HB1	3:B:502:SYN:H4	2.02	0.41
1:A:15:LYS:HE2	6:A:706:HOH:O	2.21	0.40
2:A:501:HEM:CBC	2:A:501:HEM:HMC2	2.51	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:132:ARG:NE	5:A:507:GOL:O1[2_646]	2.15	0.05

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	453/455 (100%)	438 (97%)	15 (3%)	0	100	100
1	B	452/455 (99%)	438 (97%)	14 (3%)	0	100	100
All	All	905/910 (100%)	876 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	402/398 (101%)	385 (96%)	17 (4%)	30	12
1	B	401/398 (101%)	389 (97%)	12 (3%)	41	22
All	All	803/796 (101%)	774 (96%)	29 (4%)	36	16

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	22	THR
1	A	41	LYS
1	A	47	ARG
1	A	104	LEU
1	A	109[A]	GLN
1	A	109[B]	GLN
1	A	136[A]	ASP
1	A	136[B]	ASP
1	A	148	LEU
1	A	169	GLN
1	A	179	ARG
1	A	185	MET
1	A	209	ILE
1	A	226	SER
1	A	228	GLU
1	A	229	GLN
1	B	3	LYS
1	B	52	LEU
1	B	148	LEU
1	B	169	GLN
1	B	177	MET
1	B	200	GLU
1	B	204	GLN
1	B	226	SER
1	B	229	GLN
1	B	231	ASP
1	B	306	LYS
1	B	383	SER

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

Mol	Chain	Res	Type
1	A	403	GLN

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Mol	Chain	Res	Type
1	B	359	GLN
1	B	403	GLN

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 ⓘ

11 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	$\# Z > 2$
5	GOL	A	504	-	5,5,5	0.49	0	5,5,5	0.46	0
2	HEM	A	501	1	27,50,50	2.19	6 (22%)	17,82,82	1.38	2 (11%)
3	SYN	A	502	-	8,8,8	2.43	2 (25%)	9,9,9	1.62	1 (11%)
3	SYN	B	502	-	8,8,8	2.61	2 (25%)	9,9,9	1.13	1 (11%)
2	HEM	B	501	1	27,50,50	2.14	7 (25%)	17,82,82	2.04	9 (52%)
5	GOL	A	507	-	5,5,5	0.53	0	5,5,5	0.74	0
5	GOL	B	503	-	5,5,5	0.38	0	5,5,5	1.26	0
4	MES	A	503	-	12,12,12	2.47	1 (8%)	14,16,16	2.76	7 (50%)
5	GOL	B	504	-	5,5,5	0.76	0	5,5,5	0.51	0
5	GOL	A	506	-	5,5,5	0.62	0	5,5,5	1.52	1 (20%)
5	GOL	A	505	-	5,5,5	0.46	0	5,5,5	1.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	504	-	-	4/4/4/4	-
2	HEM	A	501	1	-	0/6/54/54	-
3	SYN	A	502	-	-	2/2/2/2	0/1/1/1
3	SYN	B	502	-	-	2/2/2/2	0/1/1/1
2	HEM	B	501	1	-	0/6/54/54	-
5	GOL	A	507	-	-	4/4/4/4	-
5	GOL	B	503	-	-	2/4/4/4	-
4	MES	A	503	-	-	3/6/14/14	0/1/1/1
5	GOL	B	504	-	-	4/4/4/4	-
5	GOL	A	506	-	-	2/4/4/4	-
5	GOL	A	505	-	-	2/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	MES	C8-S	-7.93	1.66	1.77
3	B	502	SYN	CAA-CAB	6.41	1.71	1.29
2	A	501	HEM	C3C-C2C	-5.82	1.32	1.40
3	A	502	SYN	CAA-CAB	5.81	1.67	1.29
2	A	501	HEM	C3B-C2B	-5.70	1.32	1.40
2	B	501	HEM	C3B-C2B	-5.34	1.33	1.40
2	B	501	HEM	C3C-C2C	-5.23	1.33	1.40
2	B	501	HEM	C3D-C2D	4.28	1.50	1.37
2	A	501	HEM	C3D-C2D	3.37	1.47	1.37
2	A	501	HEM	C3C-CAC	3.34	1.54	1.47
2	B	501	HEM	C3C-CAC	3.33	1.54	1.47
2	B	501	HEM	C3B-CAB	2.53	1.53	1.47
2	A	501	HEM	C3B-CAB	2.48	1.53	1.47
2	A	501	HEM	C4B-NB	-2.34	1.31	1.36
3	B	502	SYN	CAH-CAB	-2.30	1.40	1.49
2	B	501	HEM	C4B-CHC	-2.25	1.34	1.41
3	A	502	SYN	CAE-CAG	2.04	1.43	1.38
2	B	501	HEM	C1D-CHD	-2.03	1.35	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	MES	O1S-S-C8	5.20	113.17	106.92
4	A	503	MES	C5-N4-C3	5.10	120.31	108.83
4	A	503	MES	C7-N4-C3	4.39	122.45	111.23
2	B	501	HEM	CBD-CAD-C3D	-3.77	105.54	112.48
3	A	502	SYN	CAH-CAB-CAA	-3.50	106.04	125.66
2	B	501	HEM	C3B-C4B-NB	-3.29	104.96	109.21
4	A	503	MES	O3S-S-C8	2.93	110.50	105.77
4	A	503	MES	O2S-S-O1S	-2.87	104.01	113.95
3	B	502	SYN	CAH-CAB-CAA	-2.71	110.45	125.66
2	A	501	HEM	CMB-C2B-C3B	2.71	129.75	124.68
2	B	501	HEM	CMA-C3A-C4A	-2.56	124.53	128.46
2	B	501	HEM	C4C-C3C-C2C	2.48	108.63	106.90
2	B	501	HEM	C4A-C3A-C2A	2.37	108.64	107.00
2	B	501	HEM	C1D-C2D-C3D	-2.34	105.36	107.00
2	A	501	HEM	C1D-C2D-C3D	-2.33	105.38	107.00
4	A	503	MES	C7-N4-C5	2.32	117.17	111.23
2	B	501	HEM	CBA-CAA-C2A	-2.24	108.35	112.49
2	B	501	HEM	CMB-C2B-C3B	2.23	128.85	124.68
4	A	503	MES	O3S-S-O2S	-2.11	106.12	111.27
2	B	501	HEM	C3C-C4C-NC	-2.07	107.04	110.94
5	A	506	GOL	O3-C3-C2	-2.00	100.60	110.20

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	507	GOL	O1-C1-C2-C3
4	A	503	MES	C8-C7-N4-C3
5	B	504	GOL	C1-C2-C3-O3
5	A	506	GOL	O1-C1-C2-C3
5	A	505	GOL	C1-C2-C3-O3
3	B	502	SYN	CAA-CAB-CAH-CAF
3	B	502	SYN	CAA-CAB-CAH-CAG
5	A	504	GOL	O1-C1-C2-C3
5	A	507	GOL	C1-C2-C3-O3
5	B	503	GOL	C1-C2-C3-O3
5	B	504	GOL	O1-C1-C2-C3
5	A	507	GOL	O1-C1-C2-O2
5	B	504	GOL	O2-C2-C3-O3
5	A	506	GOL	O1-C1-C2-O2
5	A	505	GOL	O2-C2-C3-O3
5	A	504	GOL	O1-C1-C2-O2
5	B	504	GOL	O1-C1-C2-O2

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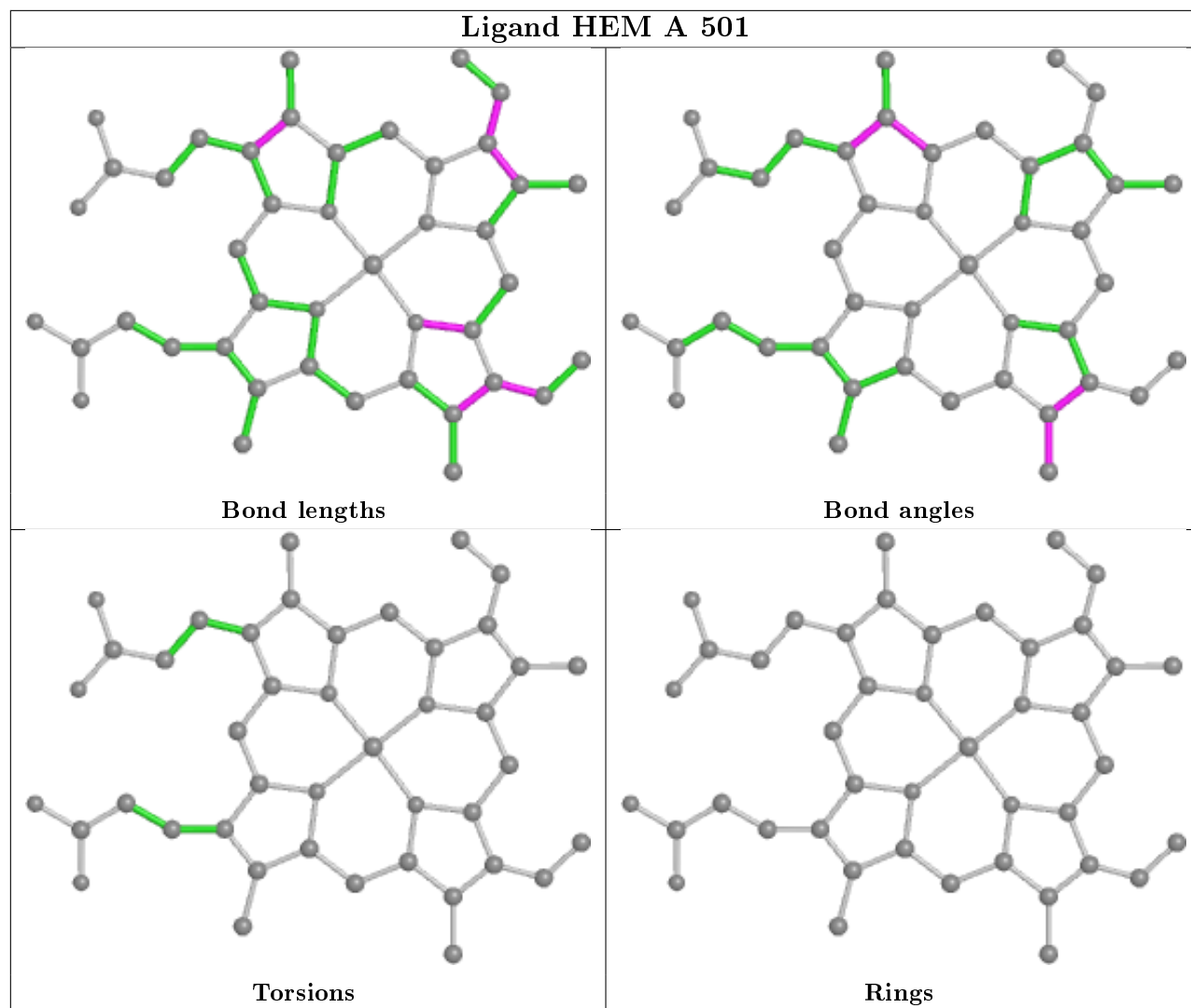
Mol	Chain	Res	Type	Atoms
5	A	507	GOL	O2-C2-C3-O3
5	A	504	GOL	O2-C2-C3-O3
5	B	503	GOL	O2-C2-C3-O3
4	A	503	MES	C7-C8-S-O3S
3	A	502	SYN	CAA-CAB-CAH-CAG
5	A	504	GOL	C1-C2-C3-O3
3	A	502	SYN	CAA-CAB-CAH-CAF
4	A	503	MES	C7-C8-S-O2S

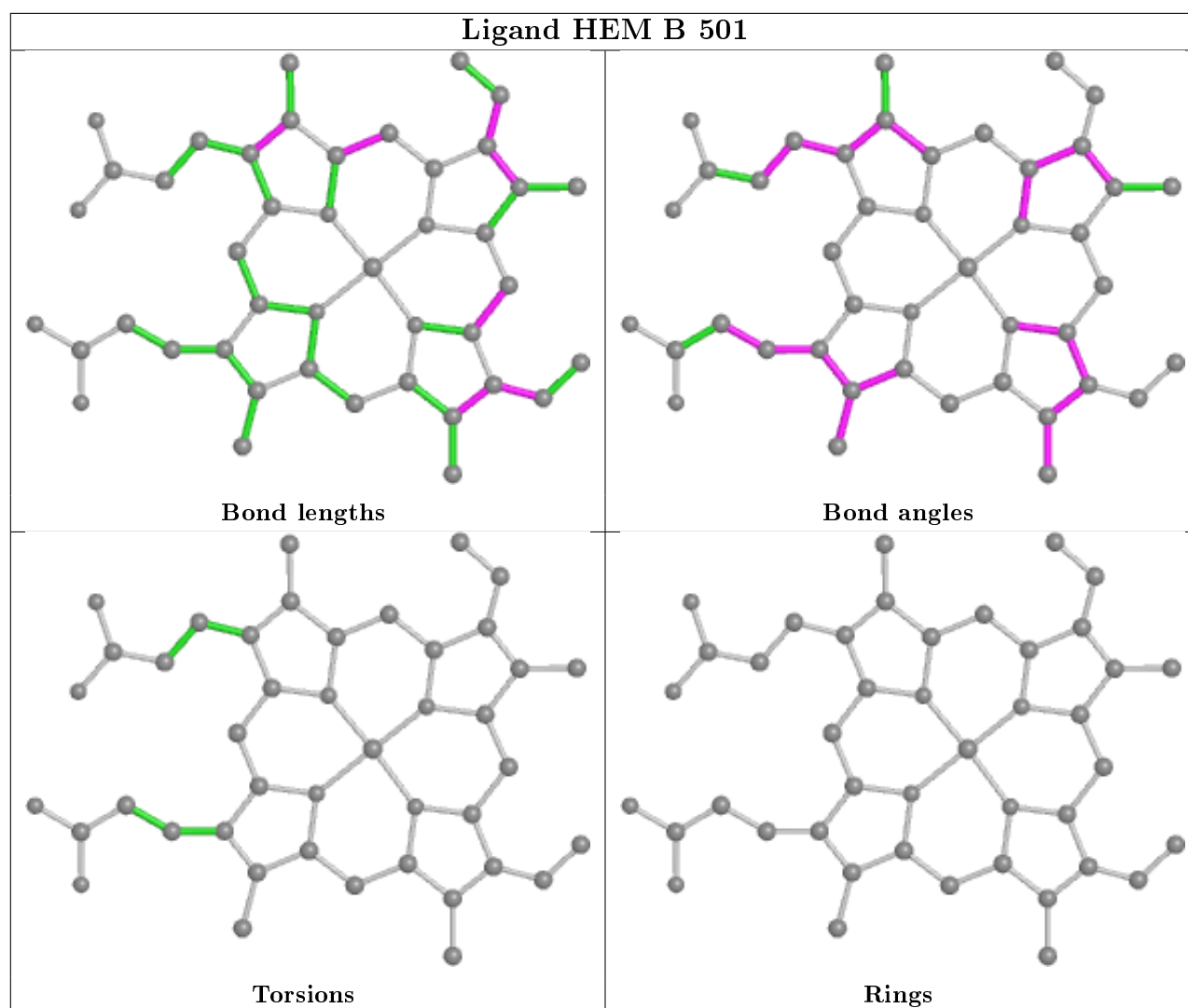
There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	4	0
3	A	502	SYN	5	0
3	B	502	SYN	1	0
5	A	507	GOL	1	1
4	A	503	MES	3	0
5	B	504	GOL	1	0
5	A	506	GOL	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 than 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.





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, 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	435/455 (95%)	-0.18	19 (4%) 34 38	12, 18, 48, 100	0
1	B	441/455 (96%)	-0.02	27 (6%) 21 23	11, 19, 48, 93	0
All	All	876/910 (96%)	-0.10	46 (5%) 26 29	11, 18, 49, 100	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	ALA	7.1
1	A	229	GLN	5.2
1	B	229	GLN	5.0
1	A	206	GLN	4.9
1	B	227	GLY	4.9
1	B	201	ASN	4.8
1	B	228	GLU	4.6
1	B	203	ARG	4.6
1	B	202	LYS	4.5
1	A	182	ASP	4.4
1	A	228	GLU	4.4
1	B	200	GLU	4.4
1	B	186	ASN	4.3
1	A	185	MET	4.3
1	A	227	GLY	4.2
1	A	205	PHE	4.1
1	B	180	ALA	3.9
1	B	184	ARG	3.8
1	B	205	PHE	3.8
1	B	187	LYS	3.5
1	B	177	MET	3.5
1	B	209	ILE	3.4
1	A	183	GLU	3.3
1	B	185	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	3	LYS	3.1
1	A	204	GLN	2.8
1	B	206	GLN	2.8
1	B	178	VAL	2.7
1	A	207	GLU	2.7
1	A	179	ARG	2.7
1	A	209	ILE	2.7
1	A	77[A]	PHE	2.4
1	A	184	ARG	2.4
1	B	207	GLU	2.4
1	B	46	GLY	2.3
1	A	181	LEU	2.3
1	B	226	SER	2.2
1	B	231	ASP	2.2
1	B	4	GLU	2.2
1	B	175	THR	2.2
1	A	369[A]	ASP	2.1
1	B	181	LEU	2.1
1	A	176	SER	2.1
1	B	204	GLN	2.0
1	B	225	ALA	2.0
1	A	4	GLU	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	GOL	A	506	6/6	0.80	0.16	30,37,41,45	0

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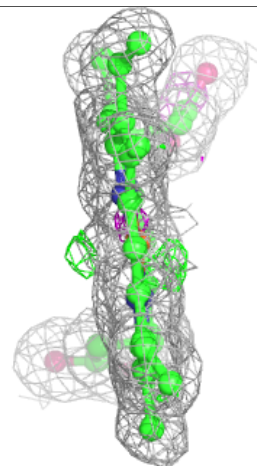
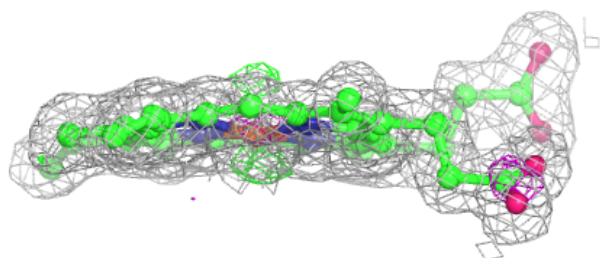
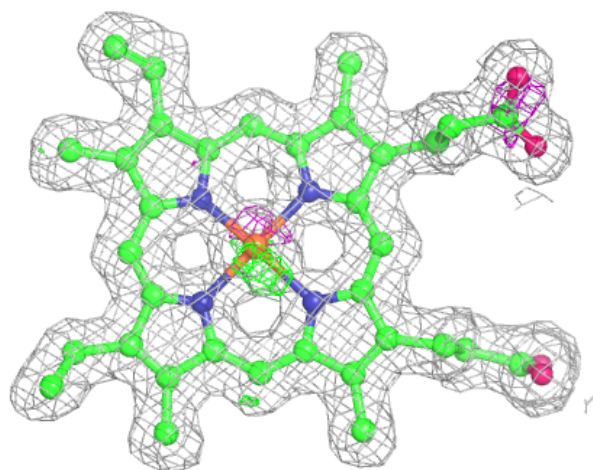
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	B	504	6/6	0.83	0.23	29,43,57,58	0
5	GOL	A	504	6/6	0.85	0.19	35,43,46,48	0
5	GOL	B	503	6/6	0.86	0.27	34,41,52,56	0
4	MES	A	503	12/12	0.86	0.22	34,45,76,98	0
5	GOL	A	505	6/6	0.86	0.20	30,56,60,60	0
3	SYN	B	502	8/8	0.87	0.15	14,36,38,52	0
5	GOL	A	507	6/6	0.89	0.23	35,43,48,53	0
3	SYN	A	502	8/8	0.90	0.14	14,30,39,46	0
2	HEM	A	501	43/43	0.98	0.08	10,13,16,17	0
2	HEM	B	501	43/43	0.98	0.07	9,12,15,16	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.

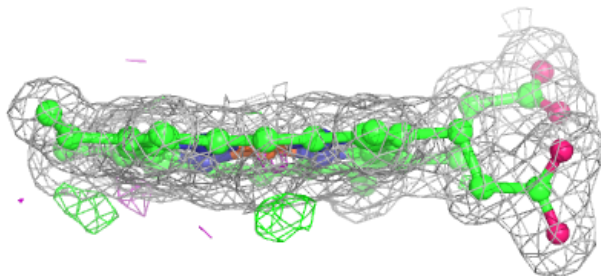
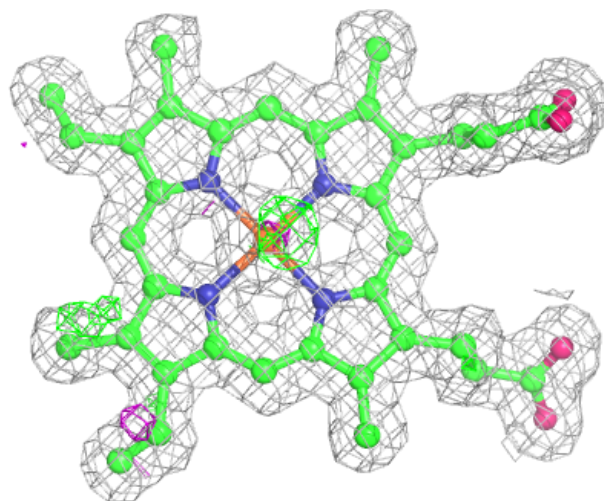
Electron density around HEM A 501:

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 ⓘ

There are no such residues in this entry.