



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:46 AM UTC

PDB ID : 4HGH / pdb_00004hgh
Title : Crystal structure of P450 BM3 5F5 heme domain variant complexed with styrene (dataset I)
Authors : Shehzad, A.; Panneerselvam, S.; Bocola, M.; Mueller-Dieckmann, J.; Wilmanns, M.; Schwaneberg, U.
Deposited on : 2012-10-08
Resolution : 1.40 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

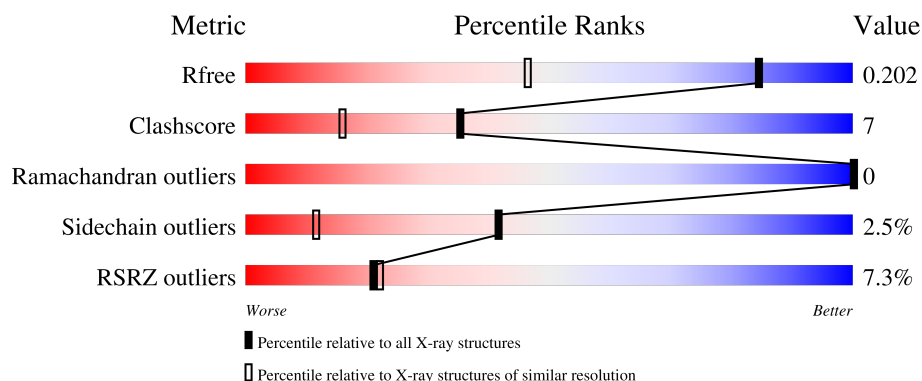
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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 $\leq 5\%$. 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	3% 84% 15% .
1	B	455	12% 82% 16% .

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	B	502	-	X	-	-
6	PEG	A	505	-	-	X	-

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.

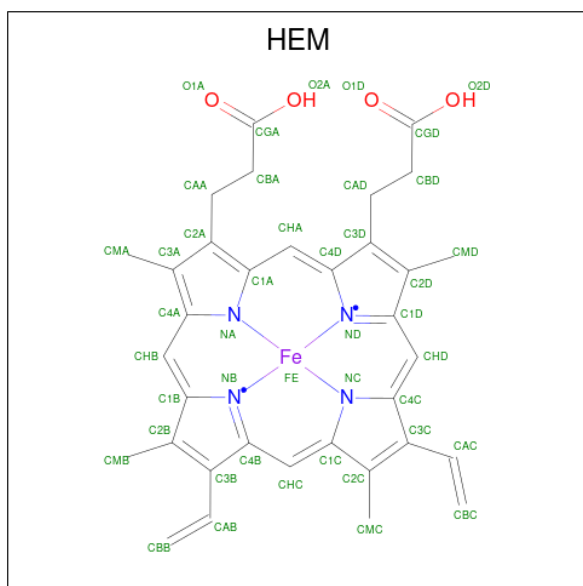
- Molecule 1 is a protein called Bifunctional P-450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	28	0
			3817	2458	636	704	19			
1	B	455	Total	C	N	O	S	0	33	0
			3851	2480	642	710	19			

There are 4 discrepancies between the modelled and reference sequences:

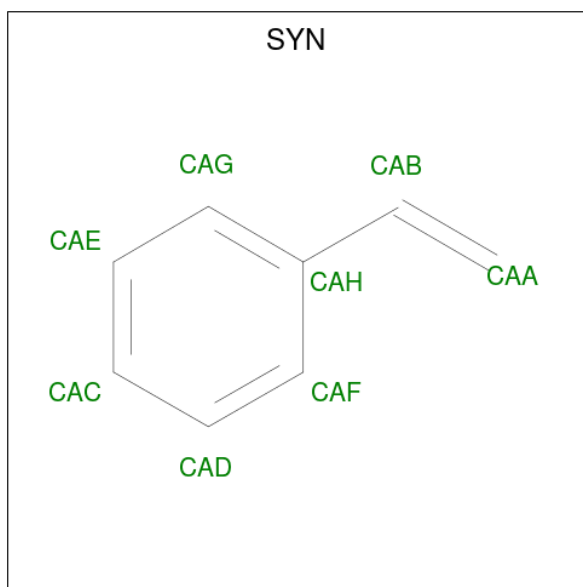
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ALA	PHE	engineered mutation	UNP P14779
A	235	ALA	THR	engineered mutation	UNP P14779
B	87	ALA	PHE	engineered mutation	UNP P14779
B	235	ALA	THR	engineered mutation	UNP P14779

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 3 is ethenylbenzene (CCD ID: SYN) (formula: C₈H₈).



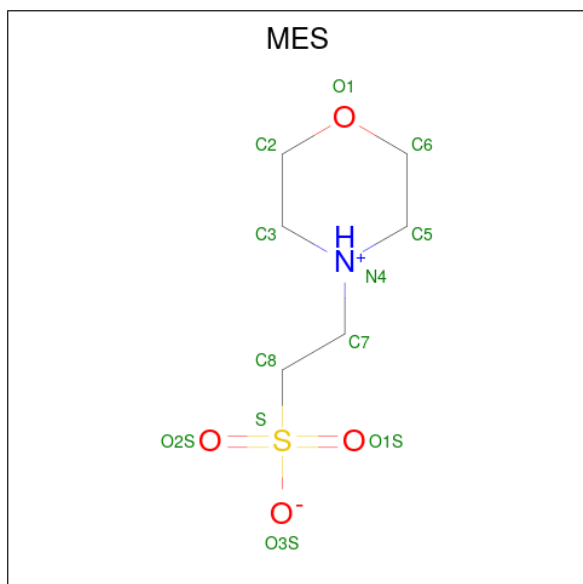
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C		
			8	8	0	0
3	B	1	Total	C		
			8	8	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

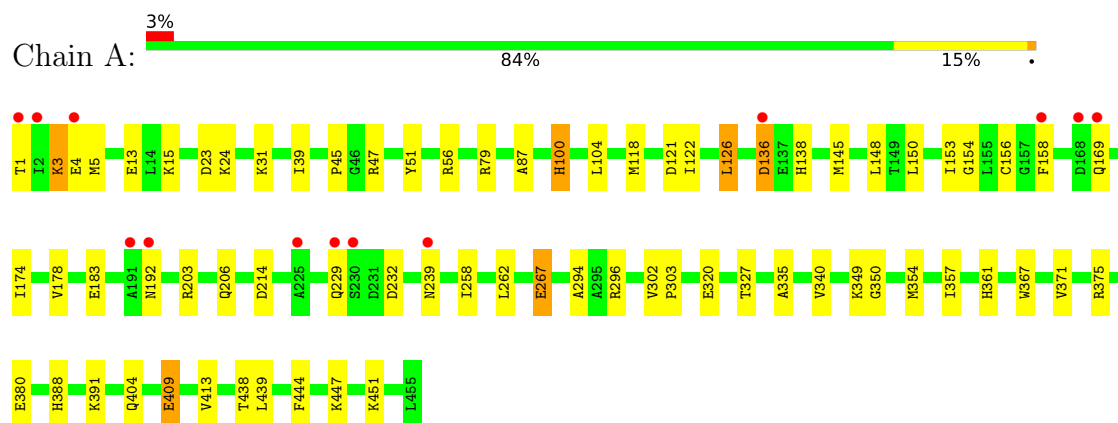
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	536	Total	O	0	0
			536	536		
7	B	475	Total	O	0	0
			475	475		

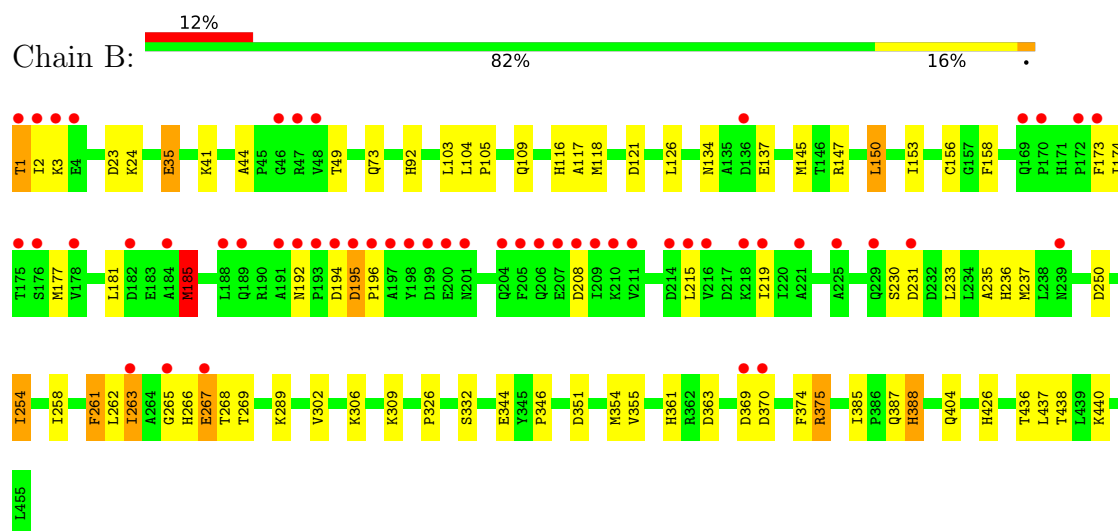
3 Residue-property plots

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	59.09Å 149.27Å 65.16Å 90.00° 98.38° 90.00°	Depositor
Resolution (Å)	19.87 – 1.40 19.87 – 1.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (19.87-1.40) 96.3 (19.87-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.190 , 0.204 0.188 , 0.202	Depositor DCC
R_{free} test set	818 reflections (0.37%)	wwPDB-VP
Wilson B-factor (Å ²)	12.3	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8824	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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, MES, SYN, PEG, 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	1.60	34/3978 (0.9%)	1.26	13/5373 (0.2%)
1	B	1.59	34/4016 (0.8%)	1.25	12/5425 (0.2%)
All	All	1.60	68/7994 (0.9%)	1.26	25/10798 (0.2%)

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	VAL	CA-CB	8.70	1.61	1.54
1	B	426	HIS	CE1-NE2	8.23	1.40	1.32
1	B	156	CYS	C-O	8.21	1.33	1.24
1	B	268[A]	THR	C-O	-7.93	1.14	1.24
1	B	268[B]	THR	C-O	-7.93	1.14	1.24
1	A	361	HIS	ND1-CE1	7.83	1.40	1.32
1	A	451	LYS	N-CA	7.28	1.55	1.46
1	A	39	ILE	C-O	7.20	1.31	1.23
1	A	183	GLU	N-CA	7.11	1.54	1.46
1	B	137	GLU	C-O	-7.05	1.14	1.23
1	B	361	HIS	ND1-CE1	6.97	1.39	1.32
1	B	326	PRO	C-O	6.94	1.32	1.23
1	A	178	VAL	CA-C	6.81	1.61	1.52
1	A	100	HIS	ND1-CE1	6.59	1.39	1.32
1	B	302	VAL	CA-C	6.21	1.58	1.53
1	A	203	ARG	C-O	6.16	1.31	1.24
1	A	206	GLN	CA-C	6.01	1.60	1.52
1	B	117	ALA	C-O	5.98	1.31	1.24
1	A	138	HIS	ND1-CE1	5.96	1.38	1.32
1	B	92	HIS	C-O	-5.95	1.16	1.24
1	B	145	MET	N-CA	5.92	1.53	1.46
1	A	121	ASP	N-CA	5.89	1.53	1.46
1	B	254	ILE	N-CA	5.88	1.53	1.46
1	A	388	HIS	ND1-CE1	5.84	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	ILE	CA-CB	5.82	1.57	1.53
1	A	444	PHE	N-CA	5.74	1.53	1.46
1	B	134	ASN	C-O	-5.62	1.16	1.23
1	A	340	VAL	C-O	5.61	1.30	1.24
1	B	351	ASP	N-CA	5.55	1.52	1.46
1	B	302	VAL	C-O	-5.50	1.18	1.24
1	B	235	ALA	CA-CB	-5.49	1.44	1.53
1	B	261	PHE	C-O	-5.48	1.17	1.24
1	B	355	VAL	CA-C	-5.46	1.46	1.52
1	A	267[A]	GLU	C-O	-5.43	1.17	1.24
1	A	267[B]	GLU	C-O	-5.43	1.17	1.24
1	B	35	GLU	C-O	-5.43	1.17	1.24
1	B	344	GLU	C-O	5.43	1.29	1.24
1	B	363	ASP	CA-CB	5.40	1.59	1.53
1	A	303	PRO	N-CA	5.39	1.53	1.47
1	A	232	ASP	C-O	5.35	1.30	1.23
1	A	47	ARG	N-CA	5.34	1.52	1.46
1	B	236	HIS	CA-C	-5.33	1.45	1.52
1	B	374	PHE	C-O	-5.32	1.17	1.24
1	A	375	ARG	CZ-NH1	5.29	1.40	1.32
1	B	237	MET	C-O	-5.29	1.17	1.24
1	B	44	ALA	C-O	5.25	1.28	1.24
1	A	214	ASP	C-O	5.24	1.30	1.24
1	A	15	LYS	CA-C	5.22	1.57	1.53
1	B	147	ARG	CA-C	5.22	1.59	1.52
1	A	56	ARG	NE-CZ	5.20	1.38	1.33
1	B	375[A]	ARG	C-O	-5.20	1.18	1.24
1	B	375[B]	ARG	C-O	-5.20	1.18	1.24
1	B	24	LYS	N-CA	5.19	1.52	1.46
1	B	388	HIS	CE1-NE2	5.17	1.37	1.32
1	A	320	GLU	C-O	5.15	1.30	1.24
1	A	294	ALA	N-CA	5.13	1.52	1.46
1	A	154	GLY	C-O	5.12	1.29	1.23
1	A	335	ALA	C-O	5.11	1.29	1.24
1	B	121	ASP	C-O	5.10	1.29	1.24
1	A	192	ASN	C-N	5.09	1.39	1.34
1	B	73	GLN	N-CA	5.06	1.52	1.46
1	A	232	ASP	N-CA	5.06	1.52	1.45
1	A	156	CYS	C-O	-5.06	1.18	1.24
1	B	116	HIS	C-O	5.06	1.29	1.24
1	A	409[A]	GLU	CG-CD	-5.03	1.39	1.52
1	A	409[B]	GLU	CG-CD	-5.03	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	ARG	C-O	-5.02	1.17	1.24
1	B	436	THR	C-O	-5.01	1.17	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASP	N-CA-C	7.52	122.17	113.38
1	A	5	MET	CA-C-N	-6.80	113.68	120.21
1	A	5	MET	C-N-CA	-6.80	113.68	120.21
1	A	391	LYS	CA-C-N	-6.22	113.21	119.56
1	A	391	LYS	C-N-CA	-6.22	113.21	119.56
1	B	254	ILE	N-CA-C	-6.11	104.55	110.72
1	B	208	ASP	N-CA-C	6.04	117.86	111.28
1	A	87	ALA	N-CA-C	5.91	118.68	111.82
1	B	137	GLU	N-CA-C	-5.87	103.19	110.41
1	A	302	VAL	N-CA-CB	-5.71	106.31	112.37
1	A	239	ASN	CB-CA-C	-5.66	99.33	109.24
1	B	302	VAL	CA-C-O	-5.59	114.25	119.62
1	B	185	MET	N-CA-C	-5.54	104.87	111.69
1	B	263[A]	ILE	CB-CA-C	-5.54	104.78	112.04
1	B	263[B]	ILE	CB-CA-C	-5.54	104.78	112.04
1	A	380	GLU	CA-C-N	-5.54	116.45	123.15
1	A	380	GLU	C-N-CA	-5.54	116.45	123.15
1	B	269	THR	N-CA-C	-5.37	105.51	111.36
1	B	195	ASP	CA-C-N	5.32	124.99	119.56
1	B	195	ASP	C-N-CA	5.32	124.99	119.56
1	A	451	LYS	N-CA-C	-5.29	106.60	113.16
1	B	369	ASP	N-CA-C	5.27	118.87	112.23
1	A	169	GLN	CA-C-N	-5.17	115.25	120.21
1	A	169	GLN	C-N-CA	-5.17	115.25	120.21
1	B	121	ASP	N-CA-C	-5.10	105.61	111.07

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	3817	0	3879	31	0
1	B	3851	0	3919	81	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	8	0	8	0	0
3	B	8	0	8	0	0
4	A	12	0	16	1	0
5	A	12	0	12	0	0
5	B	12	0	12	1	0
6	A	7	0	10	4	0
7	A	536	0	0	11	0
7	B	475	0	0	12	0
All	All	8824	0	7924	117	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 7.

All (117) 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:B:150[A]:LEU:HD11	1:B:174:ILE:CD1	1.30	1.58
1:B:150[A]:LEU:CD1	1:B:174:ILE:CD1	1.99	1.39
1:B:150[A]:LEU:CD1	1:B:174:ILE:HD13	1.56	1.35
1:B:158[A]:PHE:CE1	1:B:258:ILE:HG12	1.78	1.17
1:B:150[A]:LEU:CD1	1:B:174:ILE:HD11	1.75	1.14
1:B:375[B]:ARG:NH2	5:B:503:MES:O2S	1.84	1.09
1:B:261:PHE:O	1:B:265[B]:GLY:N	1.87	1.07
1:B:150[A]:LEU:HD11	1:B:174:ILE:HD11	1.25	1.06
1:B:158[B]:PHE:CE2	1:B:262[B]:LEU:HD21	1.91	1.04
1:B:158[B]:PHE:HE2	1:B:262[B]:LEU:HD21	1.21	1.03
1:B:150[A]:LEU:HD12	1:B:174:ILE:HD13	1.46	0.98
1:B:150[A]:LEU:HD11	1:B:174:ILE:CG1	1.94	0.98
1:B:150[B]:LEU:HD13	1:B:266[B]:HIS:CE1	1.98	0.98
1:B:267[B]:GLU:CG	1:B:438[B]:THR:HG21	1.95	0.97
1:B:267[B]:GLU:HG2	1:B:438[B]:THR:HG21	1.50	0.93
1:B:150[A]:LEU:HD11	1:B:174:ILE:HD13	1.18	0.93
1:B:177:MET:HE1	1:B:266[B]:HIS:HE1	1.33	0.92
1:B:150[B]:LEU:CD1	1:B:266[B]:HIS:CE1	2.53	0.92
1:B:158[A]:PHE:HE1	1:B:258:ILE:HG12	1.31	0.88
1:B:150[B]:LEU:HD13	1:B:266[B]:HIS:CG	2.08	0.87
1:A:267[B]:GLU:OE2	7:A:1021:HOH:O	1.95	0.85
1:B:370:ASP:OD2	1:B:375[A]:ARG:NH1	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150[B]:LEU:HD13	1:B:266[B]:HIS:ND1	1.91	0.84
1:B:150[A]:LEU:HD13	1:B:174:ILE:HD11	1.62	0.81
1:B:233[B]:LEU:HD21	1:B:261:PHE:CD2	2.15	0.80
1:A:118[B]:MET:SD	7:A:866:HOH:O	2.40	0.79
1:A:3:LYS:HE2	7:A:1004:HOH:O	1.81	0.79
1:A:327:THR:O	1:A:438[B]:THR:HG23	1.87	0.75
1:A:438[B]:THR:HG22	1:A:439:LEU:N	2.01	0.75
1:B:150[B]:LEU:HD13	1:B:266[B]:HIS:CD2	2.22	0.74
1:B:118[A]:MET:SD	7:B:802:HOH:O	2.46	0.73
1:B:375[A]:ARG:NE	7:B:877:HOH:O	2.13	0.73
1:A:136:ASP:O	1:A:447:LYS:NZ	2.24	0.71
1:B:177:MET:HE1	1:B:266[B]:HIS:CE1	2.21	0.70
1:B:261:PHE:O	1:B:265[B]:GLY:CA	2.39	0.69
1:B:267[B]:GLU:HG2	1:B:438[B]:THR:CG2	2.21	0.69
1:B:158[B]:PHE:HE2	1:B:262[B]:LEU:CD2	2.01	0.68
1:B:150[B]:LEU:HD11	1:B:266[B]:HIS:CE1	2.29	0.67
1:B:177:MET:SD	1:B:263[B]:ILE:HG12	2.35	0.67
1:A:3:LYS:CE	7:A:1004:HOH:O	2.41	0.66
1:B:233[B]:LEU:HD21	1:B:261:PHE:CE2	2.32	0.65
1:B:153[A]:ILE:HG13	7:B:812:HOH:O	1.97	0.64
1:B:2:ILE:HD13	1:B:346[A]:PRO:HG3	1.81	0.62
1:B:185:MET:HE2	1:B:437:LEU:HA	1.80	0.62
1:B:150[A]:LEU:HD11	1:B:174:ILE:HG12	1.80	0.62
1:B:267[B]:GLU:HG3	1:B:438[B]:THR:HG21	1.77	0.61
1:A:349:LYS:HE2	6:A:505:PEG:H32	1.83	0.60
1:B:266[A]:HIS:CE1	1:B:267[A]:GLU:OE2	2.54	0.59
1:A:23[A]:ASP:OD2	7:A:1061:HOH:O	2.15	0.59
1:B:150[B]:LEU:HD13	1:B:266[B]:HIS:NE2	2.18	0.59
1:A:153[A]:ILE:HG13	7:A:978:HOH:O	2.03	0.58
1:B:185:MET:HE1	1:B:437:LEU:HD23	1.86	0.58
1:A:350:GLY:HA2	6:A:505:PEG:H41	1.84	0.58
1:A:158[B]:PHE:CE1	1:A:258:ILE:HG12	2.39	0.57
6:A:505:PEG:H11	7:A:768:HOH:O	2.03	0.56
1:B:109:GLN:NE2	1:B:404[B]:GLN:HG3	2.20	0.56
1:A:438[B]:THR:HG22	1:A:439:LEU:H	1.68	0.56
1:B:261:PHE:O	1:B:265[B]:GLY:HA3	2.05	0.56
1:B:375[A]:ARG:CG	7:B:877:HOH:O	2.54	0.55
1:B:49[A]:THR:CG2	1:B:354[A]:MET:HG2	2.36	0.55
1:B:385:ILE:HD12	7:B:957:HOH:O	2.07	0.55
1:A:150[A]:LEU:HD13	1:A:174:ILE:HD13	1.89	0.55
1:B:185:MET:CE	1:B:437:LEU:HD23	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HD22	1:B:233[B]:LEU:CD1	2.37	0.55
1:B:158[B]:PHE:CZ	1:B:262[B]:LEU:HD21	2.39	0.54
1:B:23:ASP:OD2	7:B:1004:HOH:O	2.19	0.52
1:A:350:GLY:CA	6:A:505:PEG:H41	2.39	0.52
1:B:375[A]:ARG:HG2	7:B:877:HOH:O	2.09	0.52
1:A:438[B]:THR:CG2	1:A:439:LEU:H	2.22	0.52
1:B:150[B]:LEU:CD1	1:B:266[B]:HIS:ND1	2.68	0.52
1:B:387:GLN:HG2	1:B:388:HIS:CD2	2.47	0.50
1:B:181:LEU:HD11	1:B:263[B]:ILE:HG23	1.92	0.50
1:B:267[A]:GLU:HG3	7:B:963:HOH:O	2.11	0.49
1:A:148[B]:LEU:HD11	1:A:413:VAL:HG21	1.94	0.49
1:A:296[A]:ARG:NH1	7:A:995:HOH:O	2.40	0.49
1:B:263[A]:ILE:O	1:B:263[A]:ILE:HG22	2.11	0.49
1:B:375[A]:ARG:CD	7:B:877:HOH:O	2.60	0.49
1:B:262[B]:LEU:O	1:B:266[B]:HIS:ND1	2.39	0.48
1:A:100:HIS:HE1	4:A:506:GOL:O2	1.96	0.48
1:A:51:TYR:CE2	1:A:354[B]:MET:HG2	2.49	0.47
1:B:258:ILE:O	1:B:262[B]:LEU:HG	2.14	0.47
1:A:126[B]:LEU:HD21	1:A:145:MET:HE1	1.97	0.47
1:A:31[A]:LYS:HE2	7:A:746:HOH:O	2.15	0.47
1:B:173:PHE:CE2	1:B:262[B]:LEU:HD13	2.50	0.47
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.97	0.46
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.96	0.46
1:A:153[B]:ILE:HG23	1:A:262:LEU:HD23	1.96	0.46
1:B:195:ASP:HA	1:B:196:PRO:HD3	1.83	0.45
1:B:103:LEU:HD22	1:B:233[B]:LEU:HD11	1.98	0.45
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.47	0.45
1:B:173:PHE:HB2	1:B:215:LEU:HD22	1.98	0.44
1:B:250:ASP:O	1:B:254:ILE:HG13	2.17	0.44
1:B:309[B]:LYS:HA	1:B:309[B]:LYS:HD2	1.74	0.44
1:A:150[B]:LEU:HG	1:A:174:ILE:HD13	1.99	0.44
1:B:332:SER:HB2	1:B:354[B]:MET:HE1	1.98	0.44
1:A:23[B]:ASP:HB3	1:A:24:LYS:HG3	1.99	0.44
1:B:1:THR:HG22	1:B:2:ILE:N	2.32	0.44
1:B:233[B]:LEU:HD11	1:B:261:PHE:CE2	2.53	0.44
1:B:35:GLU:HG3	7:B:1030:HOH:O	2.17	0.44
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.48	0.43
1:B:306:LYS:HB2	1:B:306:LYS:HE2	1.76	0.43
1:B:177:MET:SD	1:B:263[B]:ILE:CG1	3.05	0.43
1:B:267[A]:GLU:HG3	7:B:1074:HOH:O	2.18	0.43
1:A:404[B]:GLN:NE2	7:A:981:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289[A]:LYS:HG3	7:B:824:HOH:O	2.18	0.43
1:A:31[A]:LYS:HG3	7:A:746:HOH:O	2.19	0.42
1:B:177:MET:CE	1:B:266[B]:HIS:HE1	2.19	0.42
1:B:266[A]:HIS:CE1	1:B:267[A]:GLU:HG2	2.54	0.42
1:B:2:ILE:HD13	1:B:346[B]:PRO:HG2	2.02	0.42
1:B:103:LEU:CD2	1:B:233[B]:LEU:HD12	2.50	0.42
1:B:266[A]:HIS:HE1	1:B:267[A]:GLU:OE2	2.03	0.41
1:B:104:LEU:HB3	1:B:105:PRO:HD3	2.03	0.41
1:A:150[B]:LEU:HG	1:A:174:ILE:CD1	2.51	0.41
1:A:367:TRP:HB2	1:A:371:VAL:HG12	2.02	0.41
1:A:104[B]:LEU:HA	1:A:104[B]:LEU:HD23	1.78	0.41
1:B:215:LEU:O	1:B:219:ILE:HG12	2.21	0.41
1:A:122:ILE:HG22	1:A:148[B]:LEU:HD23	2.03	0.41

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	481/455 (106%)	466 (97%)	15 (3%)	0	100	100
1	B	486/455 (107%)	468 (96%)	18 (4%)	0	100	100
All	All	967/910 (106%)	934 (97%)	33 (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	424/397 (107%)	414 (98%)	10 (2%)	43	12
1	B	428/397 (108%)	413 (96%)	15 (4%)	32	6
All	All	852/794 (107%)	827 (97%)	25 (3%)	42	9

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	3	LYS
1	A	4	GLU
1	A	13	GLU
1	A	45	PRO
1	A	126[A]	LEU
1	A	126[B]	LEU
1	A	229	GLN
1	A	409[A]	GLU
1	A	409[B]	GLU
1	B	1	THR
1	B	3	LYS
1	B	41	LYS
1	B	126[A]	LEU
1	B	126[B]	LEU
1	B	150[A]	LEU
1	B	150[B]	LEU
1	B	185	MET
1	B	192	ASN
1	B	194	ASP
1	B	230	SER
1	B	231	ASP
1	B	267[A]	GLU
1	B	267[B]	GLU
1	B	440	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	70	ASN

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Mol	Chain	Res	Type
1	A	169	GLN
1	A	189	GLN
1	A	239	ASN
1	B	70	ASN
1	B	169	GLN
1	B	285	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	MES	B	503	-	12,12,12	1.97	1 (8%)	15,16,16	2.65	7 (46%)
4	GOL	A	506	-	5,5,5	0.58	0	5,5,5	1.09	0
3	SYN	A	502	-	8,8,8	1.78	2 (25%)	9,9,9	1.02	1 (11%)
5	MES	A	504	-	12,12,12	1.61	1 (8%)	15,16,16	2.21	6 (40%)
3	SYN	B	502	-	8,8,8	1.84	4 (50%)	9,9,9	2.71	5 (55%)
6	PEG	A	505	-	6,6,6	1.06	0	5,5,5	1.83	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	501	1,7	50,50,50	2.05	12 (24%)	67,82,82	1.65	16 (23%)
2	HEM	B	501	1,7	50,50,50	2.14	11 (22%)	67,82,82	1.88	13 (19%)
4	GOL	A	503	-	5,5,5	0.53	0	5,5,5	1.42	1 (20%)

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	MES	B	503	-	-	3/6/14/14	0/1/1/1
4	GOL	A	506	-	-	0/4/4/4	-
3	SYN	A	502	-	-	0/2/2/2	0/1/1/1
5	MES	A	504	-	-	4/6/14/14	0/1/1/1
3	SYN	B	502	-	-	2/2/2/2	0/1/1/1
6	PEG	A	505	-	-	2/4/4/4	-
2	HEM	A	501	1,7	-	2/14/54/54	-
2	HEM	B	501	1,7	-	2/14/54/54	-
4	GOL	A	503	-	-	3/4/4/4	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	MES	C8-S	-6.20	1.68	1.77
2	B	501	HEM	FE-ND	6.08	2.13	1.94
2	B	501	HEM	FE-NC	6.02	2.15	1.95
2	B	501	HEM	FE-NB	5.75	2.12	1.94
2	A	501	HEM	FE-ND	5.52	2.11	1.94
2	A	501	HEM	FE-NC	5.51	2.13	1.95
2	A	501	HEM	FE-NA	5.49	2.13	1.95
2	B	501	HEM	C3D-C2D	5.37	1.48	1.36
5	A	504	MES	C8-S	-5.03	1.70	1.77
2	A	501	HEM	C3D-C2D	4.85	1.47	1.36
2	B	501	HEM	O2A-CGA	-3.92	1.17	1.30
2	B	501	HEM	FE-NA	3.82	2.07	1.95
3	A	502	SYN	CAA-CAB	3.75	1.52	1.29
2	A	501	HEM	FE-NB	3.56	2.05	1.94
2	A	501	HEM	O2D-CGD	-3.30	1.19	1.30
2	B	501	HEM	C4C-NC	-3.25	1.33	1.39
2	A	501	HEM	O2A-CGA	-3.08	1.20	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	SYN	CAA-CAB	2.92	1.47	1.29
3	B	502	SYN	CAE-CAG	2.67	1.43	1.38
2	A	501	HEM	CAB-C3B	2.62	1.54	1.47
2	A	501	HEM	C3B-C2B	-2.53	1.32	1.37
2	A	501	HEM	CAA-C2A	2.46	1.57	1.51
3	B	502	SYN	CAG-CAH	2.28	1.44	1.39
2	A	501	HEM	C2A-C3A	-2.27	1.33	1.38
2	B	501	HEM	C4D-C3D	-2.17	1.41	1.45
3	A	502	SYN	CAF-CAH	2.17	1.43	1.39
2	B	501	HEM	CAA-C2A	2.07	1.56	1.51
3	B	502	SYN	CAH-CAB	-2.06	1.41	1.49
2	B	501	HEM	CMC-C2C	2.03	1.54	1.50
2	A	501	HEM	CMB-C2B	2.02	1.54	1.50
2	B	501	HEM	CAC-C3C	2.01	1.52	1.47

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	MES	C5-N4-C3	6.37	122.57	108.84
2	B	501	HEM	C3B-C4B-NB	-5.97	105.18	109.47
3	B	502	SYN	CAC-CAD-CAF	5.90	127.52	120.24
2	B	501	HEM	C4D-ND-C1D	5.72	111.97	105.21
2	B	501	HEM	C1B-NB-C4B	5.39	111.59	105.21
5	A	504	MES	C5-N4-C3	4.80	119.19	108.84
2	A	501	HEM	C2A-C1A-NA	-4.77	104.86	110.15
5	B	503	MES	O1S-S-C8	4.67	113.78	106.73
5	A	504	MES	C7-N4-C5	4.66	123.67	111.24
2	B	501	HEM	C2B-C1B-NB	-3.72	105.56	109.84
2	A	501	HEM	C3B-C4B-NB	-3.62	106.87	109.47
5	B	503	MES	C7-N4-C3	3.53	120.64	111.24
3	B	502	SYN	CAD-CAF-CAH	-3.39	116.67	120.64
2	A	501	HEM	C4D-ND-C1D	3.34	109.16	105.21
5	B	503	MES	C8-C7-N4	-3.08	100.72	112.36
5	A	504	MES	C2-C3-N4	3.05	114.75	110.12
2	B	501	HEM	C4B-C3B-C2B	2.82	109.87	107.28
2	A	501	HEM	CMA-C3A-C4A	-2.81	121.13	125.42
6	A	505	PEG	O2-C2-C1	2.76	122.26	110.11
2	A	501	HEM	CHD-C1D-ND	2.73	127.36	124.42
2	A	501	HEM	C4A-NA-C1A	2.71	110.24	105.82
2	A	501	HEM	C3B-C2B-C1B	2.69	108.43	106.41
2	A	501	HEM	CHD-C4C-C3C	2.68	129.72	125.21
2	B	501	HEM	CMB-C2B-C1B	-2.66	120.87	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C3D-C4D-ND	-2.65	107.26	110.17
4	A	503	GOL	C3-C2-C1	-2.64	102.11	111.80
2	B	501	HEM	O1A-CGA-CBA	-2.64	114.72	123.09
2	B	501	HEM	C4C-CHD-C1D	2.61	131.57	126.02
2	A	501	HEM	C3A-C4A-NA	-2.59	106.00	110.14
6	A	505	PEG	O2-C3-C4	2.54	121.32	110.11
5	B	503	MES	O1-C6-C5	-2.51	106.36	111.77
2	B	501	HEM	O1D-CGD-CBD	-2.35	115.63	123.09
2	A	501	HEM	CMD-C2D-C1D	2.35	128.70	125.03
3	B	502	SYN	CAC-CAE-CAG	-2.33	117.37	120.24
5	A	504	MES	C7-N4-C3	2.22	117.14	111.24
2	A	501	HEM	C1C-CHC-C4B	2.21	130.72	126.02
5	A	504	MES	C8-C7-N4	2.20	120.67	112.36
2	A	501	HEM	C4A-C3A-C2A	2.19	109.33	106.82
3	B	502	SYN	CAE-CAG-CAH	2.19	123.20	120.64
2	B	501	HEM	C4A-C3A-C2A	2.19	109.32	106.82
2	A	501	HEM	CHC-C1C-C2C	2.17	129.99	125.49
3	B	502	SYN	CAE-CAC-CAD	-2.16	116.92	119.87
5	A	504	MES	O1-C2-C3	-2.15	107.13	111.77
2	A	501	HEM	C1B-NB-C4B	2.12	107.72	105.21
2	B	501	HEM	C1C-CHC-C4B	2.10	130.49	126.02
2	A	501	HEM	CHC-C4B-C3B	2.10	129.26	125.07
5	B	503	MES	C7-N4-C5	2.08	116.79	111.24
3	A	502	SYN	CAC-CAD-CAF	-2.07	117.68	120.24
2	B	501	HEM	CMC-C2C-C1C	-2.04	121.13	124.73
2	A	501	HEM	C4C-NC-C1C	2.02	109.11	105.82
5	B	503	MES	O3S-S-O2S	-2.02	106.35	111.40

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	MES	C8-C7-N4-C5
5	A	504	MES	C7-C8-S-O2S
5	A	504	MES	C7-C8-S-O3S
3	B	502	SYN	CAA-CAB-CAH-CAF
3	B	502	SYN	CAA-CAB-CAH-CAG
6	A	505	PEG	O2-C3-C4-O4
4	A	503	GOL	C1-C2-C3-O3
6	A	505	PEG	O1-C1-C2-O2
4	A	503	GOL	O2-C2-C3-O3
5	B	503	MES	C8-C7-N4-C5

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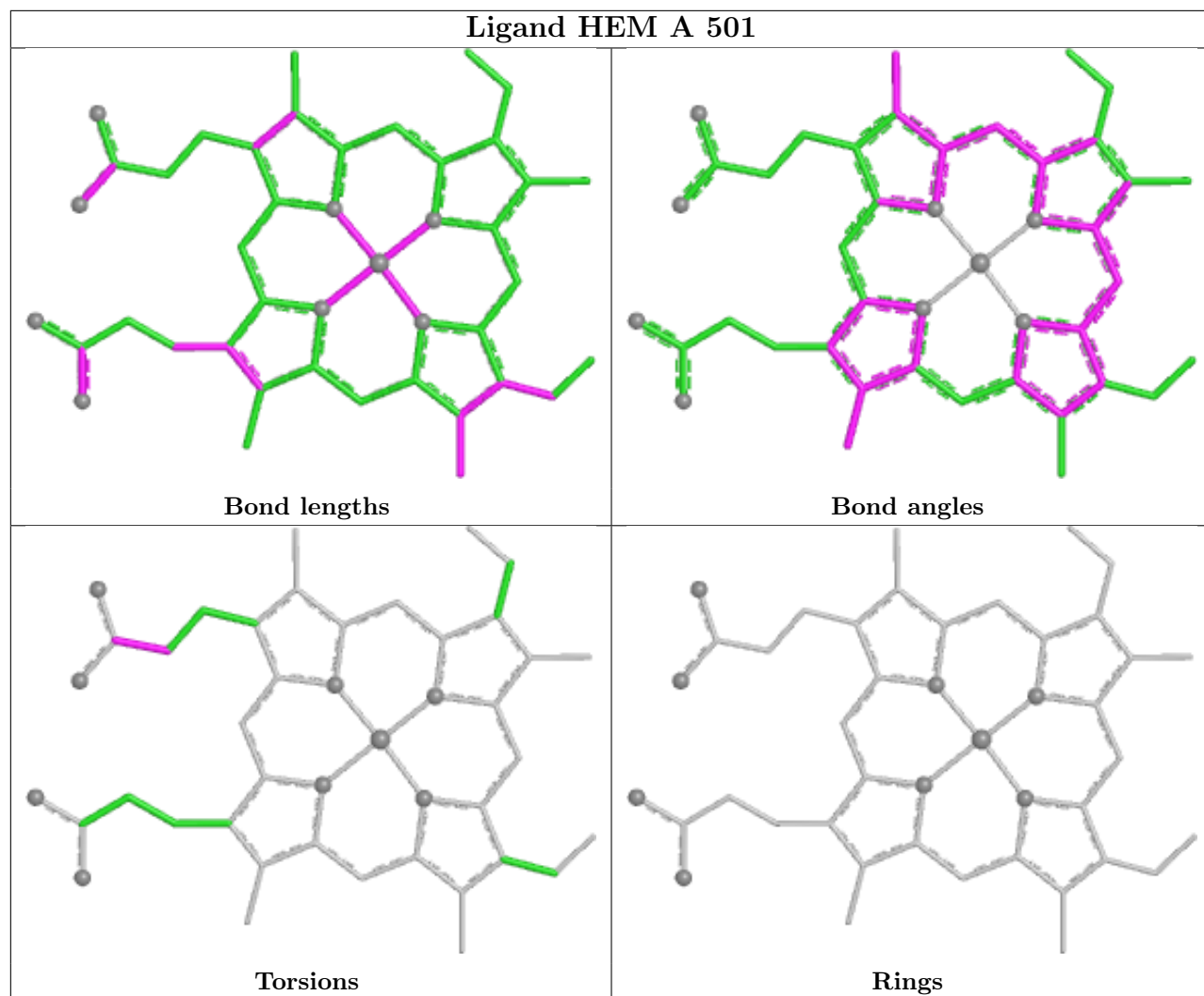
Mol	Chain	Res	Type	Atoms
4	A	503	GOL	O1-C1-C2-O2
5	A	504	MES	C7-C8-S-O1S
5	B	503	MES	C7-C8-S-O2S
5	B	503	MES	N4-C7-C8-S
2	A	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O1D

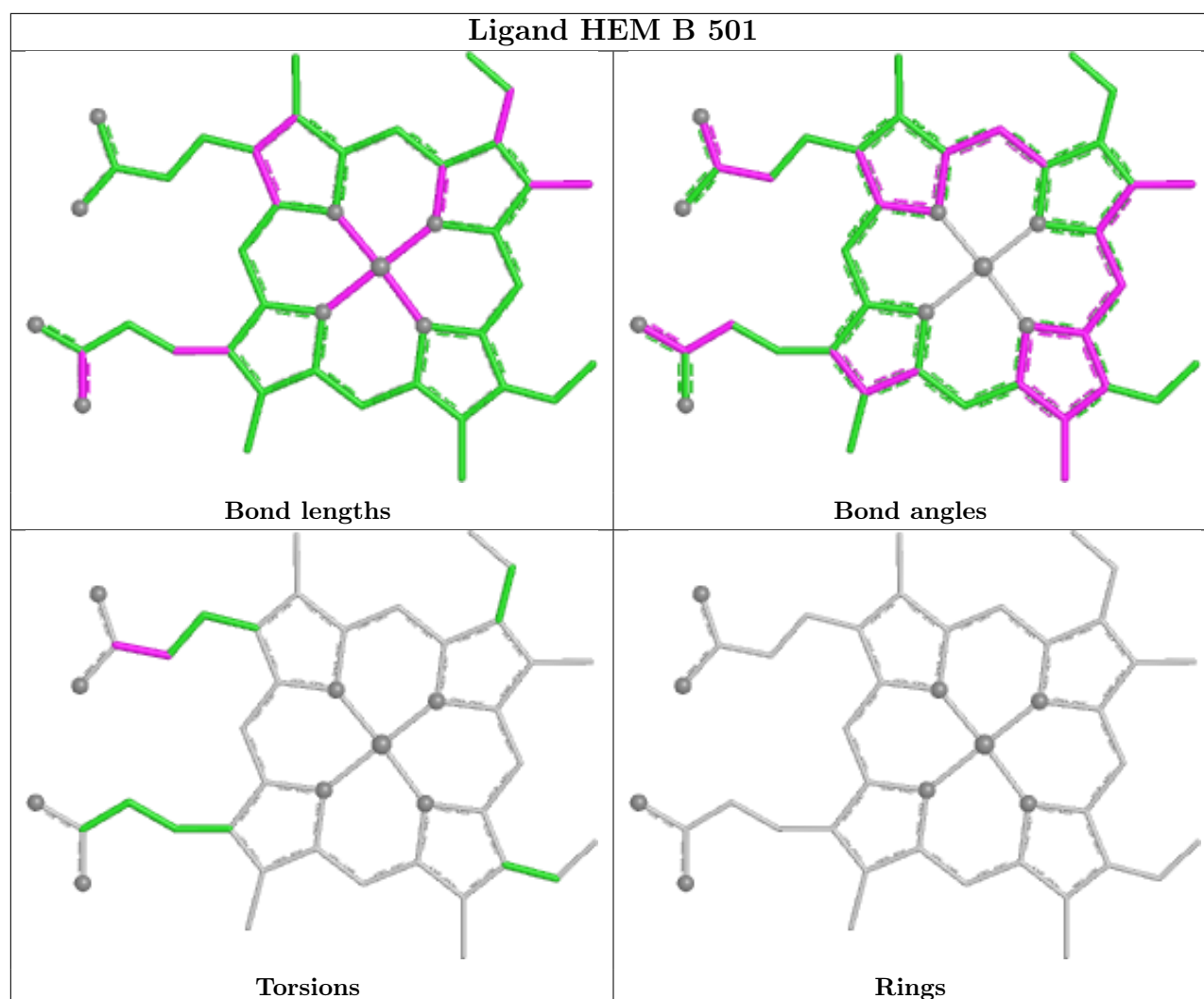
There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	503	MES	1	0
4	A	506	GOL	1	0
6	A	505	PEG	4	0
2	A	501	HEM	2	0
2	B	501	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	455/455 (100%)	-0.04	13 (2%)	53	56	5, 13, 29, 107	28 (6%)
1	B	455/455 (100%)	0.34	53 (11%)	9	9	5, 14, 51, 142	33 (7%)
All	All	910/910 (100%)	0.15	66 (7%)	21	22	5, 13, 41, 142	61 (6%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	ALA	7.9
1	B	136	ASP	7.7
1	B	191	ALA	7.5
1	B	1	THR	6.9
1	A	1	THR	6.8
1	B	2	ILE	5.9
1	A	2	ILE	5.6
1	B	194	ASP	5.5
1	B	196	PRO	5.4
1	B	215	LEU	4.9
1	B	210	LYS	4.8
1	B	195	ASP	4.6
1	B	199	ASP	4.6
1	A	136	ASP	4.5
1	B	193	PRO	4.5
1	B	192	ASN	4.3
1	B	175	THR	4.1
1	B	211	VAL	4.0
1	B	369	ASP	3.9
1	B	182	ASP	3.7
1	B	198	TYR	3.7
1	B	209	ILE	3.6
1	B	189	GLN	3.5
1	A	191	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	47	ARG	3.4
1	B	201	ASN	3.4
1	B	225	ALA	3.4
1	B	221	ALA	3.3
1	A	225	ALA	3.2
1	A	4	GLU	3.2
1	B	3	LYS	3.1
1	A	239	ASN	3.1
1	B	4	GLU	3.0
1	A	158[A]	PHE	2.9
1	B	229	GLN	2.9
1	B	169	GLN	2.9
1	B	214	ASP	2.9
1	B	178	VAL	2.8
1	B	46	GLY	2.8
1	B	219	ILE	2.8
1	B	216	VAL	2.7
1	B	173	PHE	2.7
1	B	239	ASN	2.7
1	A	230	SER	2.7
1	B	207	GLU	2.7
1	B	205	PHE	2.7
1	B	218	LYS	2.6
1	B	231	ASP	2.6
1	B	263[A]	ILE	2.6
1	B	200	GLU	2.4
1	B	265[A]	GLY	2.4
1	B	208	ASP	2.4
1	A	192	ASN	2.3
1	B	188	LEU	2.3
1	B	172	PRO	2.3
1	A	169	GLN	2.2
1	B	206	GLN	2.2
1	B	170	PRO	2.2
1	B	48	VAL	2.2
1	B	184	ALA	2.1
1	B	176	SER	2.1
1	B	204	GLN	2.0
1	B	267[A]	GLU	2.0
1	B	370	ASP	2.0
1	A	229	GLN	2.0
1	A	168	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

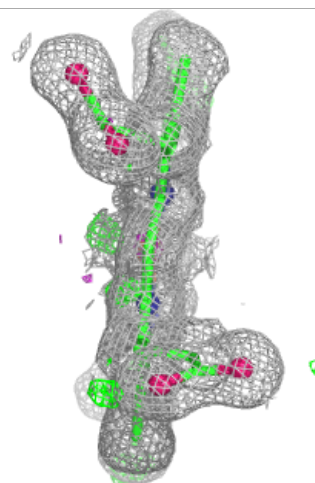
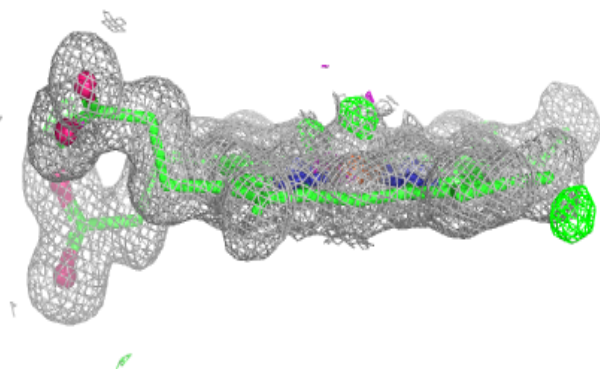
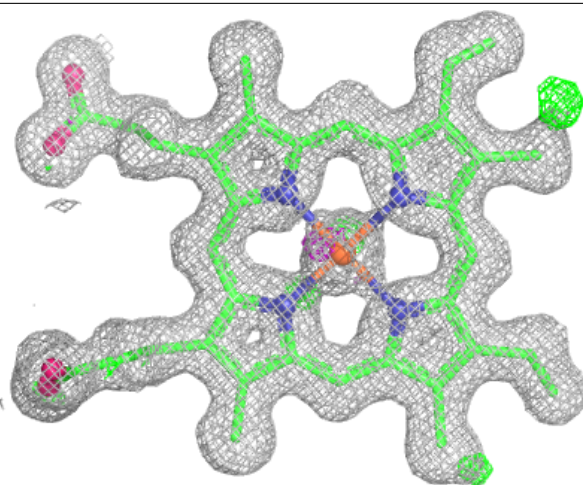
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MES	A	504	12/12	0.63	0.23	30,43,80,123	0
5	MES	B	503	12/12	0.70	0.17	34,45,71,80	0
3	SYN	B	502	8/8	0.84	0.15	26,31,41,43	0
4	GOL	A	506	6/6	0.84	0.14	26,28,30,41	0
3	SYN	A	502	8/8	0.85	0.12	23,26,29,30	0
6	PEG	A	505	7/7	0.85	0.15	29,32,38,41	0
4	GOL	A	503	6/6	0.90	0.14	21,34,45,47	0
2	HEM	B	501	43/43	0.99	0.05	6,8,10,22	0
2	HEM	A	501	43/43	0.99	0.05	5,7,10,17	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.

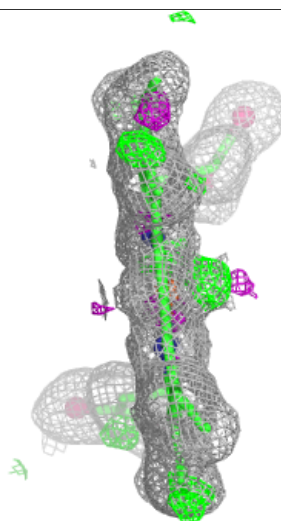
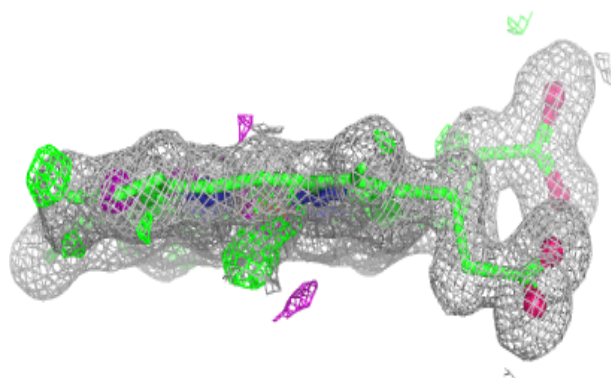
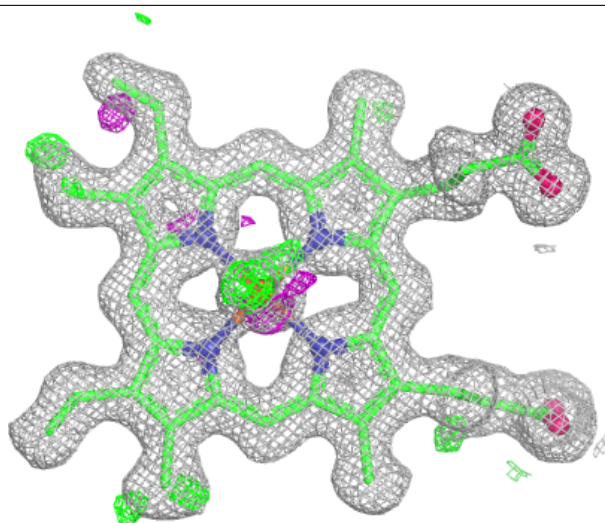
Electron density around HEM B 501:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.