Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 12:42 PM EDT

PDB ID	:	1ZO4
Title	:	Crystal Structure Of A328S Mutant Of The Heme Domain Of P450BM-3
Authors	:	Hegda, A.; Chen, B.; Haines, D.C.; Bondlela, M.; Mullin, D.; Graham, S.E.; Tomchick, D.R.; Machius, M.; Peterson, J.A.
Deposited on	:	2005-05-12
Resolution	:	1.46 Å(reported)

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	:	2.35
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)	:	2.35
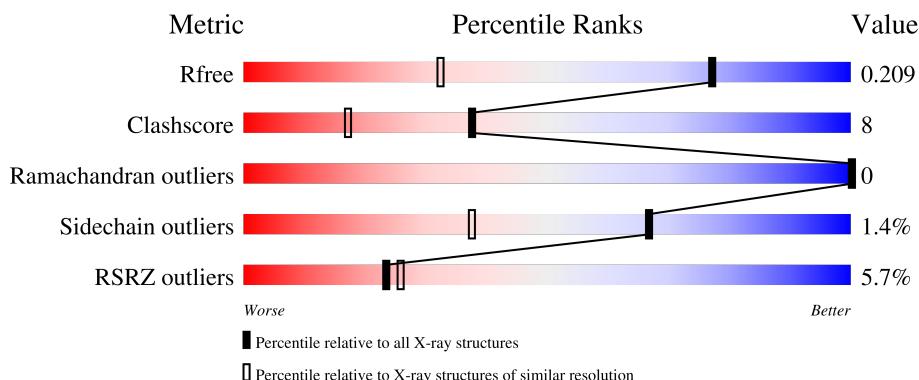
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
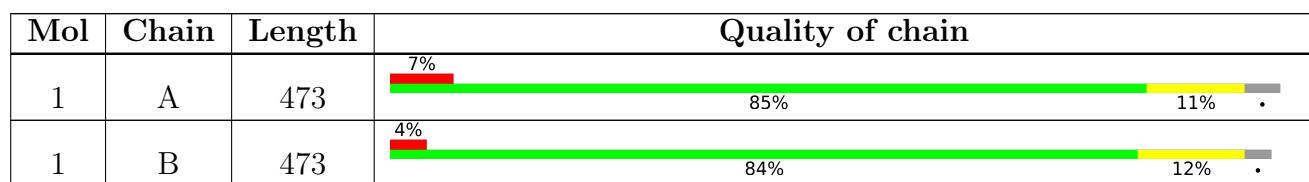
The reported resolution of this entry is 1.46 Å.

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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	473	7% / 85% 11% •
1	B	473	4% / 84% 12% •

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
4	GOL	A	1472	-	-	X	-
4	GOL	B	1474	-	-	X	-
4	GOL	B	1478	-	-	-	X
4	GOL	B	1483	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8734 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.
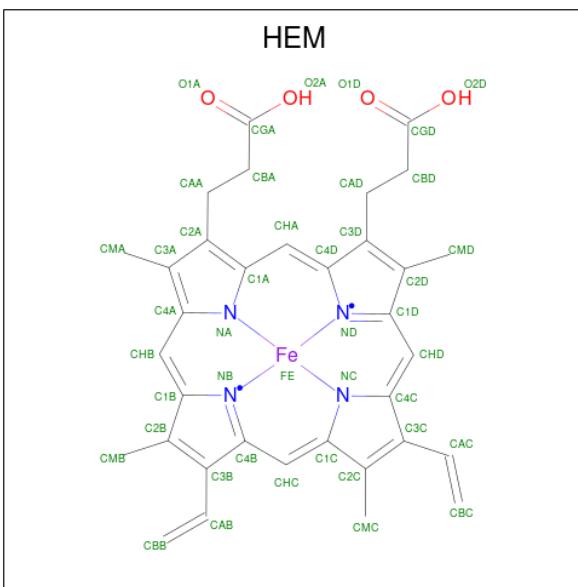
- Molecule 1 is a protein called Bifunctional P-450:NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	18	0
			3829	2440	657	714	18			
1	B	457	Total	C	N	O	S	0	19	0
			3845	2451	659	717	18			

There are 8 discrepancies between the modelled and reference sequences:
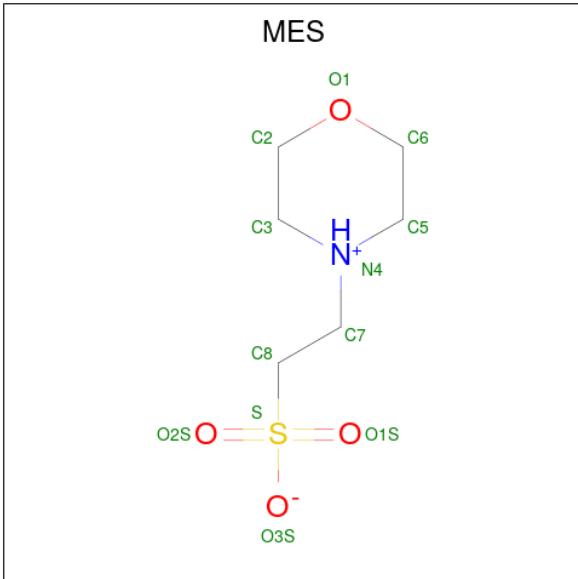
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P14779
A	-1	ALA	-	expression tag	UNP P14779
A	0	MET	-	expression tag	UNP P14779
A	328	SER	ALA	engineered mutation	UNP P14779
B	-2	GLY	-	expression tag	UNP P14779
B	-1	ALA	-	expression tag	UNP P14779
B	0	MET	-	expression tag	UNP P14779
B	328	SER	ALA	engineered mutation	UNP P14779

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

HEM

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

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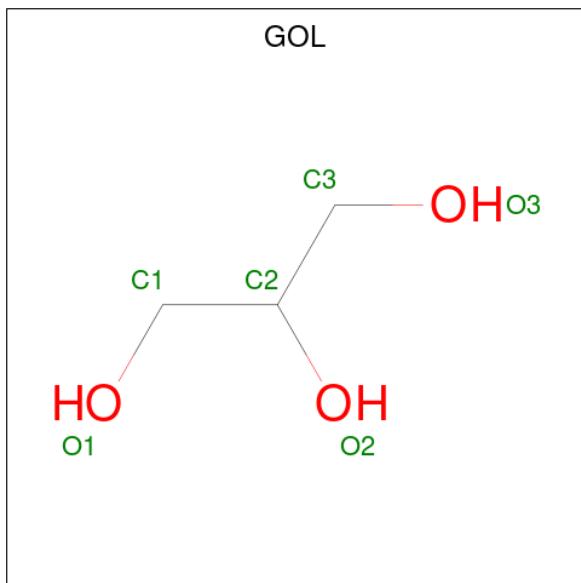
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
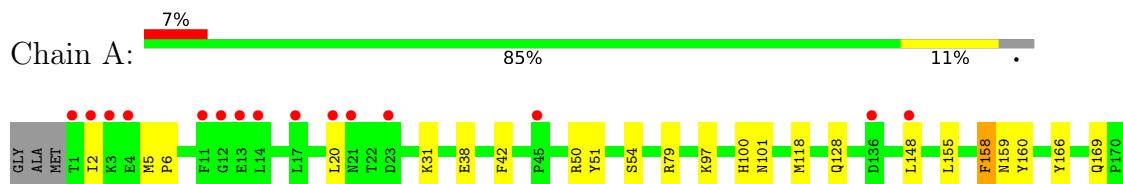
- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	406	Total 406	O 406	0	2
5	B	424	Total 424	O 424	0	2
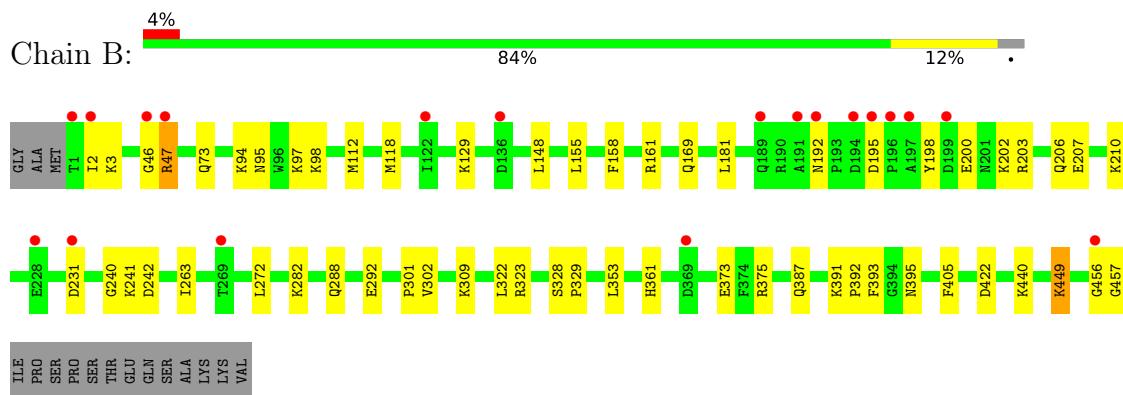
3 Residue-property plots ⓘ

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

Chain A:

• Molecule 1: Bifunctional P-450: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	58.83Å 153.21Å 61.58Å 90.00° 94.33° 90.00°	Depositor
Resolution (Å)	29.30 – 1.46 29.33 – 1.46	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.30-1.46) 94.6 (29.33-1.46)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.46Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.216 0.184 , 0.209	Depositor DCC
R_{free} test set	8896 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8734	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GOL, 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	0.50	0/3914	0.71	2/5283 (0.0%)
1	B	0.51	0/3930	0.72	2/5302 (0.0%)
All	All	0.50	0/7844	0.71	4/10585 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	328	SER	N-CA-C	-6.54	93.33	111.00
1	A	328	SER	N-CA-C	-6.34	93.89	111.00
1	A	329	PRO	N-CA-C	5.86	127.33	112.10
1	B	329	PRO	N-CA-C	5.51	126.42	112.10

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	3829	0	3807	56	0
1	B	3845	0	3825	59	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	12	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	13	0	0
4	A	66	0	88	16	0
4	B	54	0	72	25	0
5	A	406	0	0	13	0
5	B	424	0	0	9	0
All	All	8734	0	7878	122	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 8.

All (122) 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:241:LYS:H	4:B:1483:GOL:H31	1.23	1.01
1:B:392:PRO:HD2	4:B:1474:GOL:H2	1.46	0.96
4:A:1472:GOL:H32	1:B:129:LYS:HE3	1.56	0.87
1:A:2:ILE:HD12	1:A:346:PRO:HD3	1.57	0.87
1:A:171:HIS:HD2	1:A:173:PHE:H	1.20	0.86
1:B:361:HIS:HE1	1:B:391:LYS:H	1.26	0.84
1:A:361:HIS:HE1	1:A:391:LYS:H	1.23	0.84
1:A:169:GLN:HE22	1:B:169:GLN:HE22	1.27	0.83
4:A:1481:GOL:H31	5:A:1690:HOH:O	1.77	0.82
1:B:393:PHE:H	4:B:1474:GOL:H32	1.47	0.80
1:A:388:HIS:HD2	1:A:391:LYS:HZ3	1.30	0.79
1:A:385:ILE:HD13	3:A:1491:MES:H62	1.65	0.78
1:B:393:PHE:HD2	4:B:1474:GOL:H11	1.47	0.78
1:B:393:PHE:HB2	4:B:1474:GOL:C3	2.15	0.76
1:A:171:HIS:CD2	1:A:173:PHE:H	2.07	0.70
1:B:47:ARG:NH2	1:B:73:GLN:HE21	1.90	0.69
1:B:241:LYS:H	4:B:1483:GOL:C3	2.02	0.69
4:B:1474:GOL:H31	4:B:1475:GOL:O3	1.93	0.68
1:A:388:HIS:CD2	1:A:391:LYS:HZ3	2.11	0.67
1:A:50:ARG:HH21	4:A:1484:GOL:H12	1.60	0.67
1:B:94[B]:LYS:HG2	1:B:95:ASN:N	2.10	0.67
4:B:1488:GOL:H32	5:B:1622:HOH:O	1.95	0.67
1:A:198:TYR:HA	1:A:201:ASN:HD22	1.60	0.66
1:A:388:HIS:HD2	1:A:391:LYS:NZ	1.93	0.66
1:B:393:PHE:HB2	4:B:1474:GOL:H32	1.77	0.66
1:B:241:LYS:N	4:B:1483:GOL:H31	2.05	0.65
1:A:158:PHE:CE2	1:A:219:ILE:HD13	2.32	0.65
1:B:393:PHE:H	4:B:1474:GOL:C3	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:PRO:HD2	4:B:1474:GOL:C2	2.26	0.63
1:B:309[B]:LYS:HE2	5:B:1888:HOH:O	1.98	0.63
1:B:301:PRO:CB	1:B:456:GLY:HA3	2.29	0.63
1:B:393:PHE:N	4:B:1474:GOL:H32	2.13	0.62
1:A:100:HIS:HD2	5:A:1504:HOH:O	1.80	0.62
1:B:301:PRO:HB3	1:B:456:GLY:HA3	1.83	0.61
1:A:158:PHE:HE2	1:A:219:ILE:CD1	2.14	0.60
1:B:207:GLU:HA	1:B:210[B]:LYS:HD2	1.84	0.59
1:B:288:GLN:O	1:B:292:GLU:HG3	2.02	0.59
1:B:393:PHE:HB2	4:B:1474:GOL:H31	1.85	0.58
1:B:198:TYR:O	1:B:202[A]:LYS:HG3	2.04	0.57
1:A:210:LYS:HE2	5:A:1838:HOH:O	2.03	0.57
1:B:393:PHE:CD2	4:B:1474:GOL:H11	2.35	0.57
1:A:158:PHE:CE2	1:A:219:ILE:CD1	2.88	0.57
1:B:240:GLY:HA2	4:B:1483:GOL:H32	1.86	0.57
1:B:206:GLN:O	1:B:210[B]:LYS:HG3	2.04	0.57
1:A:166:TYR:HB3	4:A:1472:GOL:H11	1.87	0.56
1:A:223[B]:ARG:NH1	1:A:234:LEU:HD23	2.22	0.55
1:A:449[A]:LYS:HE2	5:A:1806:HOH:O	2.07	0.55
1:A:397:GLN:HB3	4:A:1487:GOL:H11	1.89	0.55
1:B:181:LEU:HD21	1:B:263:ILE:HD12	1.89	0.53
1:B:393:PHE:CB	4:B:1474:GOL:H32	2.38	0.53
1:B:457:GLY:HA2	5:B:1824:HOH:O	2.09	0.53
1:A:370:ASP:OD2	1:A:375[B]:ARG:NH1	2.40	0.53
1:B:395:ASN:HA	4:B:1475:GOL:H11	1.91	0.53
1:A:450:SER:HB3	4:A:1486:GOL:O3	2.09	0.53
1:B:192:ASN:ND2	1:B:195:ASP:HB2	2.24	0.53
4:A:1485:GOL:H11	5:A:1521:HOH:O	2.10	0.52
1:A:118[B]:MET:SD	1:A:155:LEU:HD21	2.51	0.51
1:B:97:LYS:HB2	5:B:1842:HOH:O	2.11	0.51
1:B:47:ARG:HH22	1:B:73:GLN:HE21	1.58	0.51
1:A:158:PHE:CD2	1:A:219:ILE:HD13	2.45	0.51
1:A:437:LEU:HD23	5:A:1781:HOH:O	2.10	0.51
1:A:301:PRO:HD2	5:A:1836:HOH:O	2.11	0.50
1:B:192:ASN:HD21	1:B:195:ASP:HB2	1.76	0.50
1:B:2:ILE:HG12	1:B:3:LYS:N	2.26	0.50
1:A:97:LYS:HB2	5:A:1652:HOH:O	2.12	0.50
1:B:282:LYS:HB3	4:B:1478:GOL:H32	1.93	0.50
1:B:161:ARG:NH2	4:B:1470:GOL:H32	2.27	0.49
1:A:128[B]:GLN:NE2	5:A:1693:HOH:O	2.45	0.49
1:A:160:TYR:OH	1:A:171:HIS:HE1	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LYS:HD3	1:A:440:LYS:HE2	1.95	0.49
1:B:118[A]:MET:SD	1:B:155:LEU:HD21	2.53	0.49
1:B:301:PRO:HB2	1:B:456:GLY:HA3	1.95	0.48
1:B:240:GLY:CA	4:B:1483:GOL:H32	2.43	0.48
1:A:79:ARG:HH21	4:A:1473:GOL:H2	1.79	0.48
1:B:302:VAL:HG23	4:B:1488:GOL:H12	1.97	0.47
1:A:190:ARG:O	1:A:190:ARG:HG3	2.13	0.47
1:A:219:ILE:O	1:A:223[B]:ARG:HG2	2.14	0.47
1:B:46:GLY:O	1:B:47:ARG:HD2	2.14	0.47
1:B:361:HIS:CE1	1:B:391:LYS:H	2.18	0.46
1:A:20:LEU:HG	1:A:42:PHE:CZ	2.50	0.46
1:A:388:HIS:HE1	5:A:1659:HOH:O	1.99	0.46
1:A:323:ARG:HA	1:A:361:HIS:CD2	2.51	0.46
1:A:166:TYR:CB	4:A:1472:GOL:H31	2.46	0.45
1:B:323:ARG:HA	1:B:361:HIS:CD2	2.51	0.45
1:A:20:LEU:HG	1:A:42:PHE:HZ	1.81	0.45
1:A:171:HIS:HD2	1:A:173:PHE:N	2.00	0.45
1:A:50:ARG:NH2	4:A:1484:GOL:H12	2.29	0.45
1:A:198:TYR:HD1	1:A:201:ASN:ND2	2.14	0.45
1:A:51:TYR:OH	4:A:1489:GOL:H31	2.17	0.45
1:B:440:LYS:HD2	5:B:1832:HOH:O	2.18	0.44
1:A:5:MET:HA	1:A:6:PRO:HD3	1.84	0.43
4:B:1488:GOL:H2	5:B:1868:HOH:O	2.17	0.43
1:A:306:LYS:HG2	5:A:1588:HOH:O	2.18	0.43
1:A:361:HIS:CE1	1:A:391:LYS:H	2.15	0.43
1:B:449:LYS:CD	1:B:449:LYS:N	2.81	0.43
1:A:313:TYR:HB2	4:A:1482:GOL:H32	2.01	0.43
1:A:31[A]:LYS:HG3	5:A:1708:HOH:O	2.18	0.42
1:A:97:LYS:HE3	1:A:101:ASN:OD1	2.19	0.42
1:A:166:TYR:HB3	4:A:1472:GOL:H31	2.00	0.42
1:B:301:PRO:HB3	1:B:456:GLY:CA	2.49	0.42
1:B:387[B]:GLN:O	1:B:387[B]:GLN:HG3	2.19	0.42
1:A:2:ILE:HD12	1:A:346:PRO:CD	2.38	0.42
1:B:282:LYS:HD2	4:B:1478:GOL:H11	2.02	0.42
1:A:128[A]:GLN:HA	1:A:128[A]:GLN:OE1	2.19	0.42
1:B:94[B]:LYS:HD3	5:B:1845:HOH:O	2.20	0.42
1:B:200:GLU:OE1	1:B:203:ARG:NE	2.52	0.42
1:A:449[A]:LYS:HA	1:A:449[A]:LYS:HD3	1.85	0.42
1:A:223[B]:ARG:HD3	5:A:1791:HOH:O	2.19	0.41
1:A:38:GLU:HB2	1:A:54:SER:HB3	2.02	0.41
1:B:272:LEU:HD13	1:B:322:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94[A]:LYS:O	1:B:94[A]:LYS:HD3	2.20	0.41
1:B:112:MET:SD	1:B:405:PHE:HA	2.61	0.41
1:B:118[B]:MET:HG3	5:B:1575:HOH:O	2.21	0.41
1:B:200:GLU:OE1	1:B:200:GLU:HA	2.21	0.41
1:B:422:ASP:O	1:B:449:LYS:HD3	2.21	0.41
1:A:338:ASP:OD2	4:A:1471:GOL:H31	2.21	0.41
1:B:98:LYS:HG3	1:B:242:ASP:HB2	2.01	0.40
1:A:158:PHE:HE2	1:A:219:ILE:HD12	1.84	0.40
1:B:373[B]:GLU:OE2	1:B:375:ARG:NH1	2.52	0.40
4:B:1478:GOL:H31	5:B:1879:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	472/473 (100%)	464 (98%)	8 (2%)	0	100	100
1	B	474/473 (100%)	464 (98%)	10 (2%)	0	100	100
All	All	946/946 (100%)	928 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	418/413 (101%)	413 (99%)	5 (1%)	71	43
1	B	419/413 (102%)	413 (99%)	6 (1%)	67	37
All	All	837/826 (101%)	826 (99%)	11 (1%)	67	40

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	158	PHE
1	A	159	ASN
1	A	182	ASP
1	A	344	GLU
1	B	47	ARG
1	B	148	LEU
1	B	158	PHE
1	B	231	ASP
1	B	353	LEU
1	B	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	100	HIS
1	A	110	GLN
1	A	159	ASN
1	A	171	HIS
1	A	201	ASN
1	A	319	ASN
1	A	361	HIS
1	A	388	HIS
1	A	395	ASN
1	A	403	GLN
1	A	426	HIS
1	B	21	ASN
1	B	73	GLN
1	B	95	ASN
1	B	169	GLN
1	B	186	ASN
1	B	213	ASN
1	B	229	GLN

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Mol	Chain	Res	Type
1	B	239	ASN
1	B	359	GLN
1	B	361	HIS
1	B	395	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 ⓘ

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	GOL	A	1489	-	5,5,5	0.52	0	5,5,5	0.21	0
4	GOL	A	1473	-	5,5,5	0.46	0	5,5,5	0.20	0
4	GOL	B	1483	-	5,5,5	0.45	0	5,5,5	0.20	0
4	GOL	B	1478	-	5,5,5	0.45	0	5,5,5	0.16	0
4	GOL	A	1472	-	5,5,5	0.54	0	5,5,5	0.18	0
3	MES	A	1491	-	12,12,12	2.33	6 (50%)	14,16,16	1.12	1 (7%)
4	GOL	A	1487	-	5,5,5	0.72	0	5,5,5	0.10	0
4	GOL	A	1481	-	5,5,5	0.48	0	5,5,5	0.22	0
4	GOL	A	1484	-	5,5,5	0.39	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	HEM	A	471	5,1	41,50,50	1.64	7 (17%)	45,82,82	1.30	8 (17%)
4	GOL	A	1485	-	5,5,5	0.45	0	5,5,5	0.26	0
4	GOL	A	1486	-	5,5,5	0.48	0	5,5,5	0.21	0
4	GOL	B	1474	-	5,5,5	0.58	0	5,5,5	0.30	0
4	GOL	A	1476	-	5,5,5	0.27	0	5,5,5	0.25	0
4	GOL	B	1475	-	5,5,5	0.60	0	5,5,5	0.22	0
4	GOL	B	1470	-	5,5,5	0.62	0	5,5,5	0.18	0
4	GOL	B	1488	-	5,5,5	0.56	0	5,5,5	0.24	0
4	GOL	B	1480	-	5,5,5	0.54	0	5,5,5	0.19	0
4	GOL	B	1477	-	5,5,5	0.48	0	5,5,5	0.24	0
4	GOL	B	1479	-	5,5,5	0.50	0	5,5,5	0.14	0
3	MES	B	1490	-	12,12,12	2.14	5 (41%)	14,16,16	1.07	1 (7%)
2	HEM	B	471	5,1	41,50,50	1.75	11 (26%)	45,82,82	1.32	8 (17%)
4	GOL	A	1482	-	5,5,5	0.48	0	5,5,5	0.20	0
4	GOL	A	1471	-	5,5,5	0.48	0	5,5,5	0.19	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
4	GOL	A	1489	-	-	2/4/4/4	-
4	GOL	A	1473	-	-	2/4/4/4	-
4	GOL	B	1483	-	-	1/4/4/4	-
4	GOL	B	1478	-	-	2/4/4/4	-
4	GOL	A	1472	-	-	2/4/4/4	-
3	MES	A	1491	-	-	2/6/14/14	0/1/1/1
4	GOL	A	1487	-	-	0/4/4/4	-
4	GOL	A	1481	-	-	0/4/4/4	-
4	GOL	A	1484	-	-	0/4/4/4	-
2	HEM	A	471	5,1	-	2/12/54/54	-
4	GOL	A	1485	-	-	1/4/4/4	-
4	GOL	A	1486	-	-	2/4/4/4	-
4	GOL	B	1474	-	-	2/4/4/4	-
4	GOL	A	1476	-	-	2/4/4/4	-
4	GOL	B	1475	-	-	0/4/4/4	-
4	GOL	B	1470	-	-	0/4/4/4	-
4	GOL	B	1488	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	1480	-	-	3/4/4/4	-
4	GOL	B	1477	-	-	2/4/4/4	-
4	GOL	B	1479	-	-	0/4/4/4	-
3	MES	B	1490	-	-	0/6/14/14	0/1/1/1
2	HEM	B	471	5,1	-	2/12/54/54	-
4	GOL	A	1482	-	-	2/4/4/4	-
4	GOL	A	1471	-	-	2/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	471	HEM	CBB-CAB	4.81	1.54	1.30
2	A	471	HEM	CBB-CAB	4.67	1.53	1.30
2	A	471	HEM	CBC-CAC	4.10	1.56	1.29
2	B	471	HEM	CBC-CAC	3.99	1.55	1.29
3	B	1490	MES	C8-S	3.77	1.82	1.77
3	A	1491	MES	C8-S	3.75	1.82	1.77
2	B	471	HEM	C3C-CAC	3.62	1.55	1.47
3	A	1491	MES	O2S-S	-3.59	1.34	1.45
3	B	1490	MES	O2S-S	-3.37	1.35	1.45
3	A	1491	MES	C7-N4	3.31	1.55	1.47
3	A	1491	MES	O1S-S	3.21	1.54	1.45
2	A	471	HEM	C3C-CAC	3.18	1.54	1.47
2	A	471	HEM	CBD-CAD	3.07	1.61	1.52
3	B	1490	MES	O1S-S	3.03	1.54	1.45
2	B	471	HEM	CBD-CAD	3.02	1.61	1.52
2	B	471	HEM	CBD-CGD	-3.00	1.43	1.50
2	A	471	HEM	CBA-CGA	-2.92	1.43	1.50
3	A	1491	MES	C3-N4	2.86	1.54	1.46
3	B	1490	MES	C3-N4	2.64	1.54	1.46
2	B	471	HEM	CBA-CGA	-2.51	1.44	1.50
3	B	1490	MES	C5-N4	2.45	1.53	1.46
2	A	471	HEM	CBD-CGD	-2.43	1.44	1.50
2	B	471	HEM	C4D-C3D	2.39	1.49	1.45
3	A	1491	MES	C5-N4	2.37	1.53	1.46
2	B	471	HEM	CHA-C4D	2.27	1.40	1.35
2	B	471	HEM	C3C-C2C	-2.21	1.37	1.40
2	B	471	HEM	CHB-C1B	2.19	1.40	1.35
2	B	471	HEM	O1A-CGA	2.16	1.29	1.22
2	A	471	HEM	O1A-CGA	2.03	1.28	1.22

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	471	HEM	O2A-CGA-CBA	3.47	125.19	114.03
2	B	471	HEM	CMC-C2C-C3C	2.90	130.11	124.68
2	A	471	HEM	CMC-C2C-C3C	2.89	130.09	124.68
2	A	471	HEM	C4B-CHC-C1C	2.89	126.37	122.56
2	A	471	HEM	C4C-CHD-C1D	2.87	126.35	122.56
3	A	1491	MES	O2S-S-C8	2.76	110.23	106.92
2	B	471	HEM	O1A-CGA-CBA	-2.63	114.62	123.08
3	B	1490	MES	O2S-S-C8	2.62	110.08	106.92
2	B	471	HEM	C4B-CHC-C1C	2.59	125.97	122.56
2	B	471	HEM	CMA-C3A-C4A	-2.53	124.58	128.46
2	B	471	HEM	C4C-CHD-C1D	2.34	125.65	122.56
2	A	471	HEM	O2D-CGD-CBD	2.32	121.49	114.03
2	A	471	HEM	O2A-CGA-CBA	2.22	121.16	114.03
2	B	471	HEM	CMA-C3A-C2A	2.17	129.03	124.94
2	A	471	HEM	CMA-C3A-C4A	-2.12	125.21	128.46
2	A	471	HEM	O2D-CGD-O1D	-2.12	118.03	123.30
2	A	471	HEM	CBB-CAB-C3B	-2.08	117.25	127.62
2	B	471	HEM	O2D-CGD-CBD	2.06	120.65	114.03

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1491	MES	C8-C7-N4-C3
4	A	1473	GOL	O1-C1-C2-C3
4	A	1476	GOL	O1-C1-C2-C3
4	A	1482	GOL	O1-C1-C2-C3
4	A	1489	GOL	O1-C1-C2-C3
4	B	1474	GOL	O1-C1-C2-C3
4	B	1478	GOL	O1-C1-C2-C3
4	B	1480	GOL	O1-C1-C2-C3
4	B	1488	GOL	O1-C1-C2-O2
4	B	1488	GOL	O1-C1-C2-C3
4	B	1474	GOL	O1-C1-C2-O2
4	B	1478	GOL	O1-C1-C2-O2
4	A	1471	GOL	O1-C1-C2-C3
4	A	1486	GOL	O1-C1-C2-C3
4	B	1477	GOL	O1-C1-C2-C3
4	A	1471	GOL	O1-C1-C2-O2
4	A	1473	GOL	O1-C1-C2-O2
4	A	1476	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	1489	GOL	O1-C1-C2-O2
4	B	1480	GOL	O1-C1-C2-O2
4	A	1486	GOL	O1-C1-C2-O2
4	B	1483	GOL	O1-C1-C2-C3
3	A	1491	MES	C8-C7-N4-C5
4	A	1482	GOL	O1-C1-C2-O2
4	A	1472	GOL	O1-C1-C2-O2
4	B	1477	GOL	O1-C1-C2-O2
2	A	471	HEM	CAD-CBD-CGD-O1D
2	A	471	HEM	CAD-CBD-CGD-O2D
4	A	1472	GOL	O1-C1-C2-C3
2	B	471	HEM	CAD-CBD-CGD-O2D
2	B	471	HEM	CAD-CBD-CGD-O1D
4	A	1485	GOL	O2-C2-C3-O3
4	B	1480	GOL	O2-C2-C3-O3
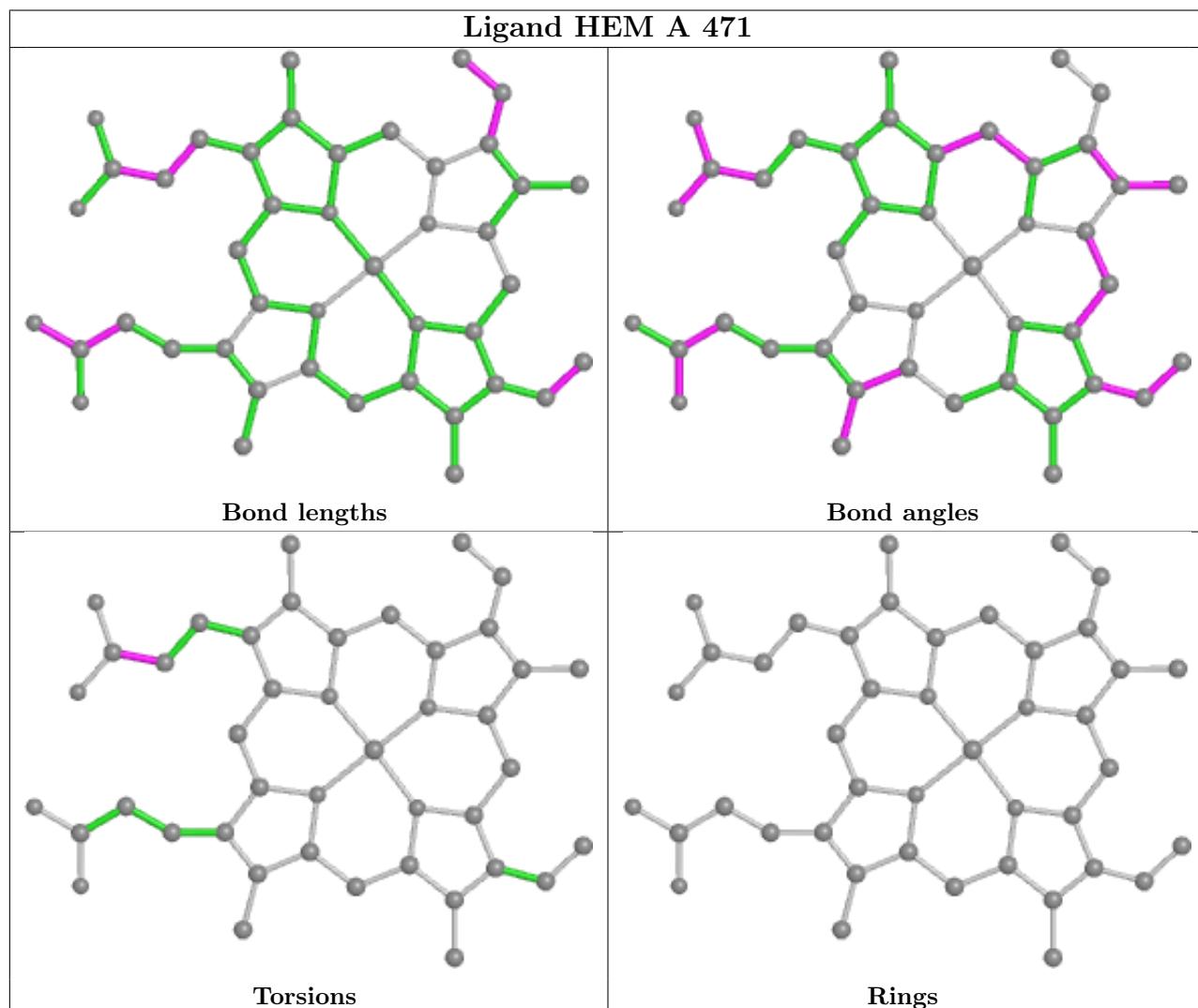
There are no ring outliers.
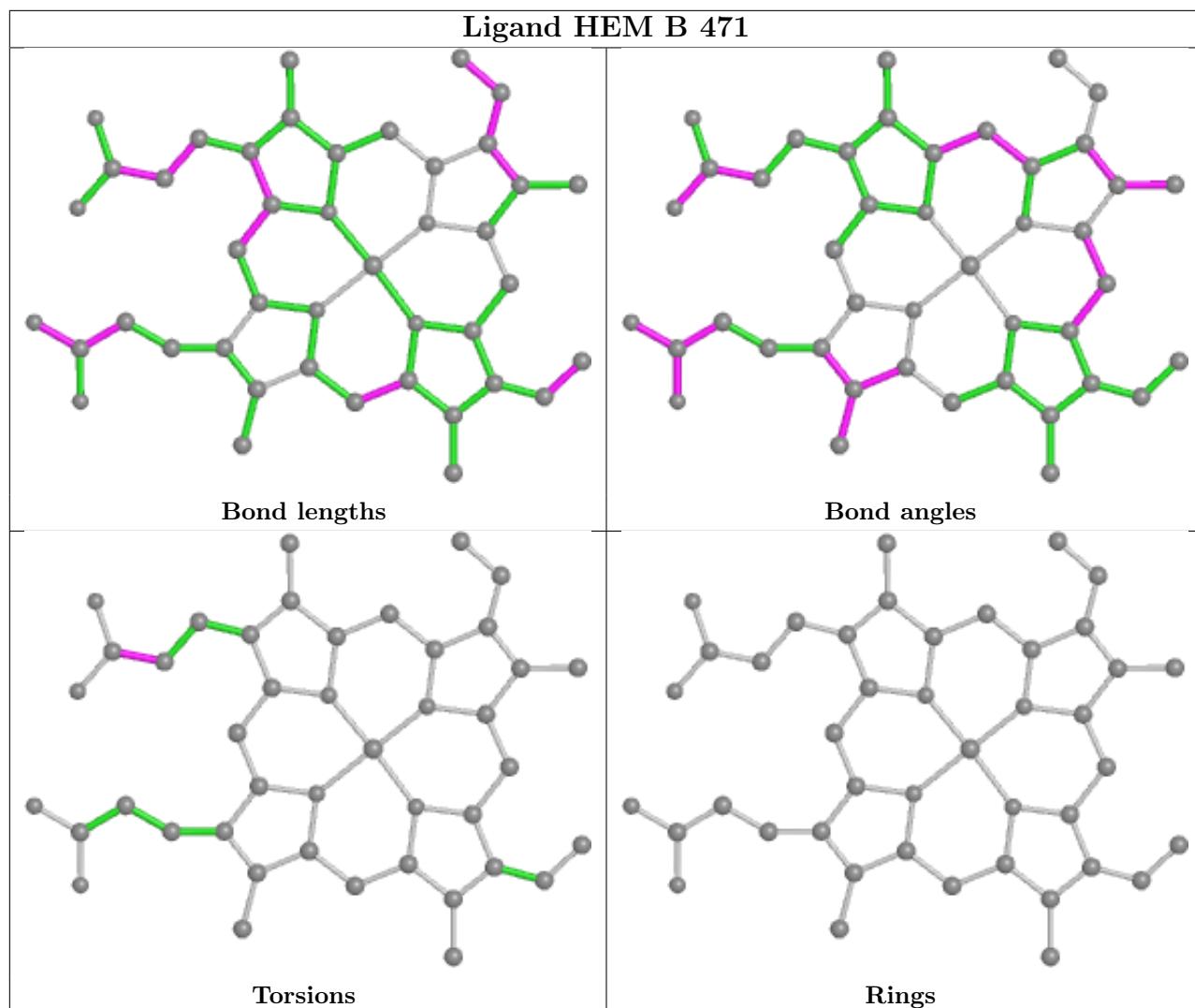
17 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1489	GOL	1	0
4	A	1473	GOL	1	0
4	B	1483	GOL	5	0
4	B	1478	GOL	3	0
4	A	1472	GOL	4	0
3	A	1491	MES	1	0
4	A	1487	GOL	1	0
4	A	1481	GOL	1	0
4	A	1484	GOL	2	0
4	A	1485	GOL	1	0
4	A	1486	GOL	3	0
4	B	1474	GOL	12	0
4	B	1475	GOL	2	0
4	B	1470	GOL	1	0
4	B	1488	GOL	3	0
4	A	1482	GOL	1	0
4	A	1471	GOL	1	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 A 471

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 471

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	456/473 (96%)	0.25	33 (7%)	15	17	14, 23, 45, 57	0
1	B	457/473 (96%)	0.11	19 (4%)	36	39	15, 24, 42, 54	0
All	All	913/946 (96%)	0.18	52 (5%)	23	26	14, 24, 45, 57	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	11.7
1	B	191	ALA	7.9
1	A	1	THR	7.6
1	B	2	ILE	7.4
1	A	191	ALA	6.9
1	A	192	ASN	6.3
1	A	11	PHE	5.9
1	B	196	PRO	5.4
1	A	3	LYS	5.4
1	A	14	LEU	5.3
1	A	196	PRO	5.2
1	B	1	THR	5.2
1	A	198	TYR	4.7
1	B	192	ASN	4.6
1	A	13	GLU	4.4
1	A	21	ASN	4.2
1	A	197	ALA	4.1
1	A	4	GLU	4.0
1	B	47	ARG	3.8
1	B	456	GLY	3.8
1	A	12	GLY	3.8
1	A	194	ASP	3.4
1	B	136	ASP	3.4
1	A	136	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	195	ASP	3.3
1	A	193	PRO	3.3
1	A	384	ALA	3.3
1	B	194	ASP	3.1
1	A	195	ASP	3.1
1	A	369	ASP	3.0
1	A	189	GLN	3.0
1	A	17	LEU	3.0
1	B	231	ASP	2.9
1	B	199	ASP	2.8
1	A	199	ASP	2.7
1	A	20	LEU	2.5
1	A	383	SER	2.5
1	A	45	PRO	2.5
1	A	23	ASP	2.3
1	A	456	GLY	2.3
1	B	197	ALA	2.2
1	B	122	ILE	2.2
1	A	200	GLU	2.2
1	A	227	GLY	2.2
1	B	369	ASP	2.2
1	B	228	GLU	2.2
1	B	269	THR	2.1
1	B	46	GLY	2.1
1	A	263[A]	ILE	2.0
1	B	189	GLN	2.0
1	A	380	GLU	2.0
1	A	148	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.
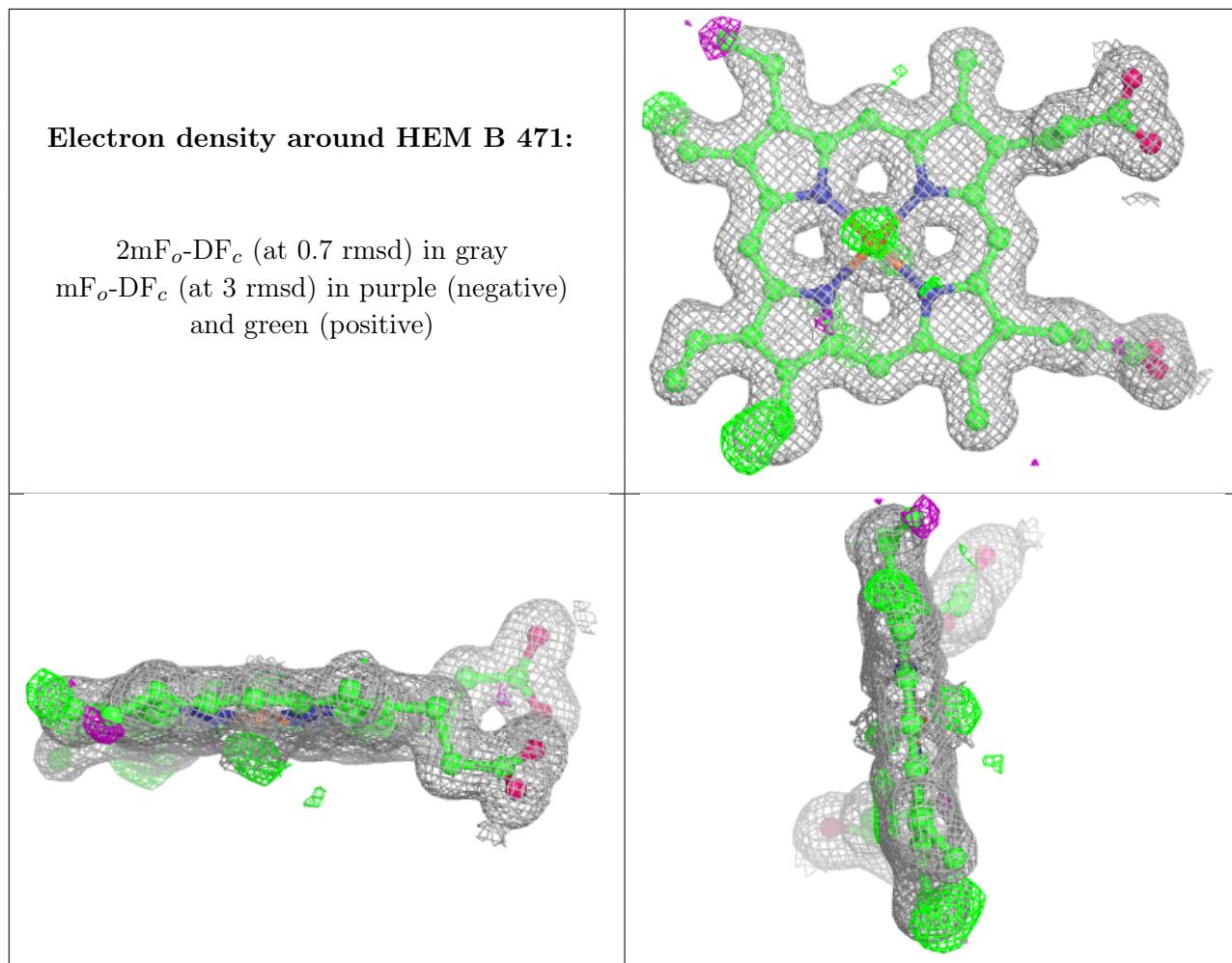
6.4 Ligands ⓘ
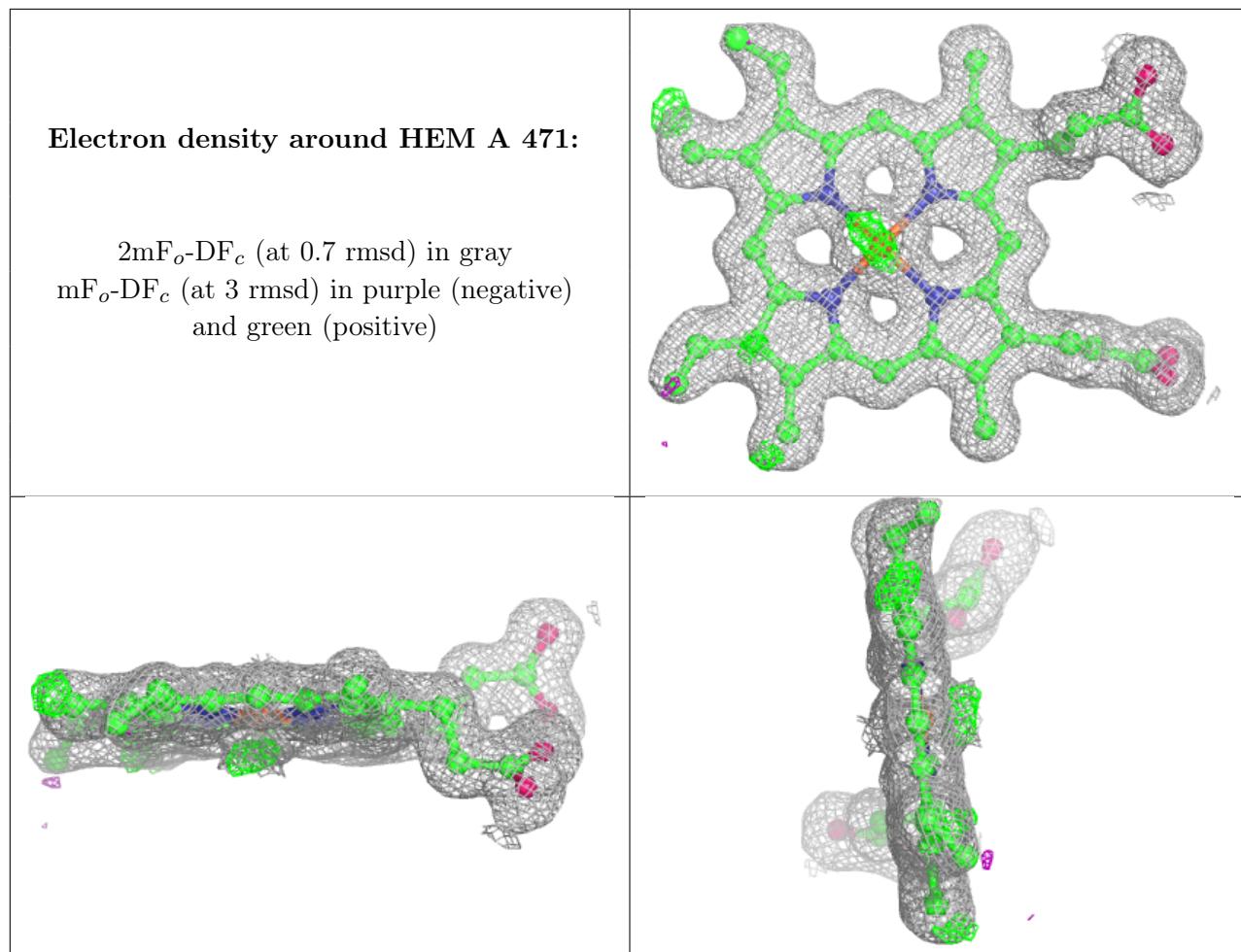
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
4	GOL	A	1481	6/6	0.64	0.25	47,50,52,54	0
4	GOL	A	1489	6/6	0.72	0.22	47,48,48,53	0
4	GOL	B	1480	6/6	0.74	0.37	48,48,50,50	0
4	GOL	B	1478	6/6	0.75	0.46	45,47,50,52	0
3	MES	A	1491	12/12	0.77	0.29	48,52,59,60	0
4	GOL	B	1477	6/6	0.77	0.35	50,52,53,55	0
4	GOL	A	1482	6/6	0.79	0.33	50,51,54,54	0
4	GOL	A	1471	6/6	0.80	0.28	42,47,48,51	0
4	GOL	A	1476	6/6	0.81	0.12	45,47,47,49	0
4	GOL	A	1485	6/6	0.81	0.25	49,50,52,53	0
4	GOL	A	1484	6/6	0.82	0.22	40,46,52,53	0
4	GOL	A	1486	6/6	0.82	0.28	42,46,48,49	0
4	GOL	B	1488	6/6	0.82	0.22	45,47,48,51	0
4	GOL	B	1475	6/6	0.83	0.19	31,43,43,43	0
4	GOL	A	1472	6/6	0.84	0.21	42,45,47,48	0
4	GOL	B	1479	6/6	0.84	0.23	35,46,50,51	0
4	GOL	A	1487	6/6	0.86	0.25	41,41,47,53	0
4	GOL	B	1470	6/6	0.87	0.21	25,44,50,50	0
4	GOL	B	1483	6/6	0.88	0.43	45,47,49,50	0
4	GOL	A	1473	6/6	0.88	0.17	38,43,45,49	0
4	GOL	B	1474	6/6	0.92	0.23	21,41,44,44	0
3	MES	B	1490	12/12	0.93	0.14	36,40,42,42	0
2	HEM	B	471	43/43	0.98	0.11	12,16,18,29	0
2	HEM	A	471	43/43	0.99	0.12	12,14,17,29	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 471:

$2mF_o$-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 471:

$2mF_o$-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.