WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2024 – 09:08 AM EST

PDB ID	:	1FOI
Title	:	BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN COMPLEXED WITH 1400W(H4B-FREE)
Authors	:	Raman, C.S.; Li, H.; Martasek, P.; Masters, B.S.S.; Poulos, T.L.
Deposited on	:	2000-08-28
Resolution	:	1.93 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	:	2.36
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)	:	2.36

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 1.93 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.

| | Percentile relative to all X-ray structures |
| | Percentile relative to X-ray structures of similar resolution |
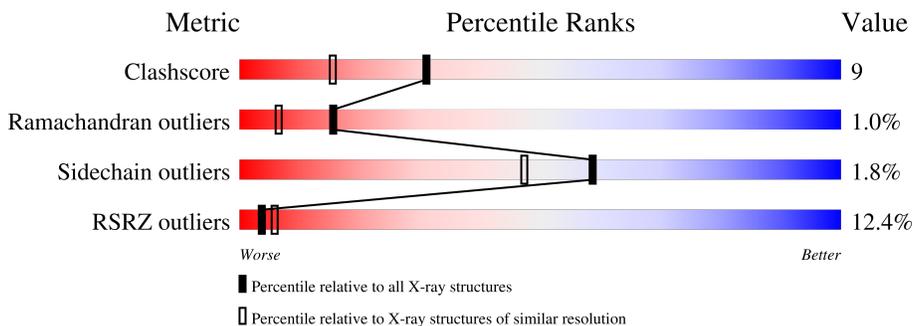
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	444	
1	B	444	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7382 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 NITRIC-OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total 3302	C 2099	N 584	O 603	S 16	0	0	0
1	B	414	Total 3291	C 2092	N 582	O 601	S 16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	conflict	UNP P29473
B	100	ARG	CYS	conflict	UNP P29473

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
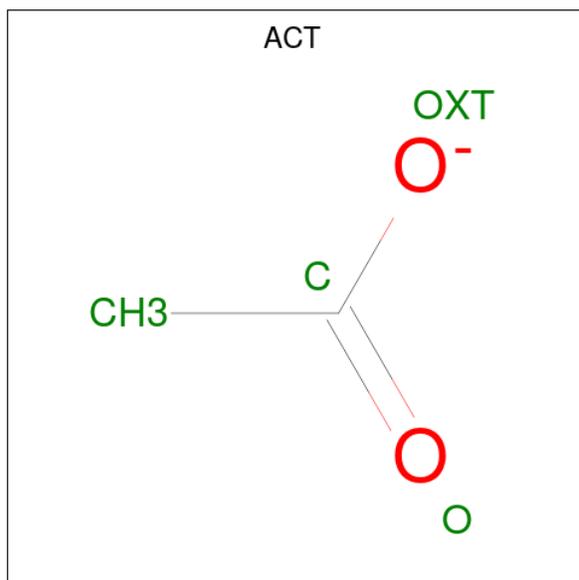
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total C O			0	0
			4	2	2		

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).
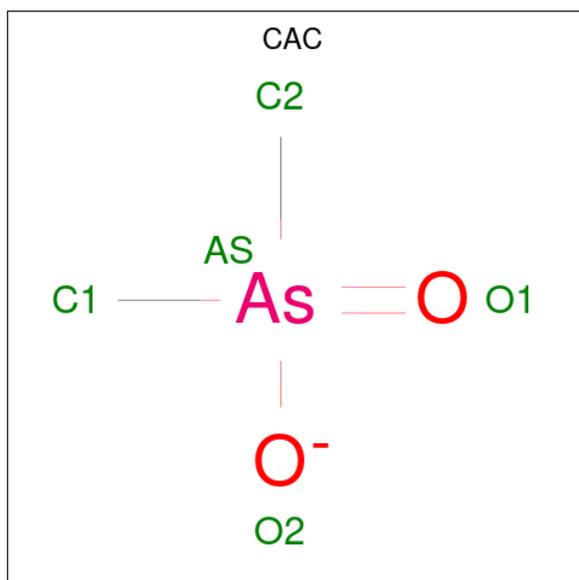
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total As C			0	0
			3	1	2		
3	B	1	Total As C			0	0
			3	1	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total Zn		0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

HEM

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N O 4 4	0	0
5	B	1	Total 43	C 34	Fe 1	N O 4 4	0	0

- Molecule 6 is N-(3-(AMINOMETHYL)BENZYL)ACETAMIDINE (three-letter code: 14W) (formula: $C_{10}H_{15}N_3$).

14W

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 11	C 9	N 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 11	C 9	N 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
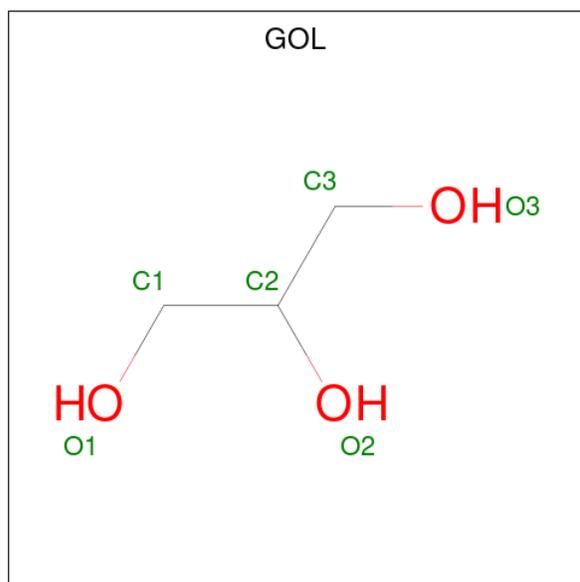
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 5	C 2	O 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	340	Total 340	O 340	0	0
8	B	315	Total 315	O 315	0	0

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: NITRIC-OXIDE SYNTHASE

Chain A:

- Molecule 1: NITRIC-OXIDE SYNTHASE

Chain B:
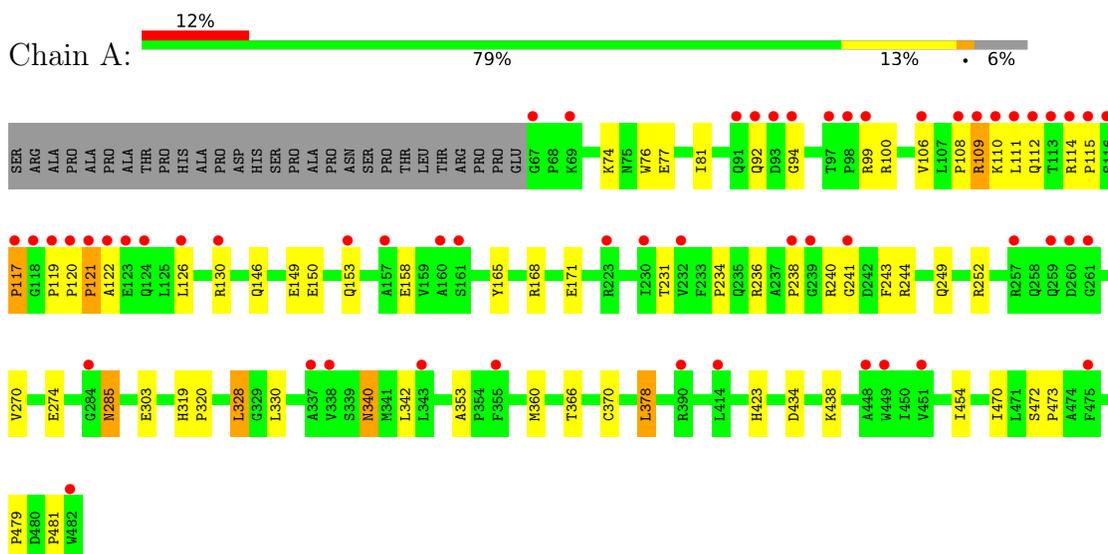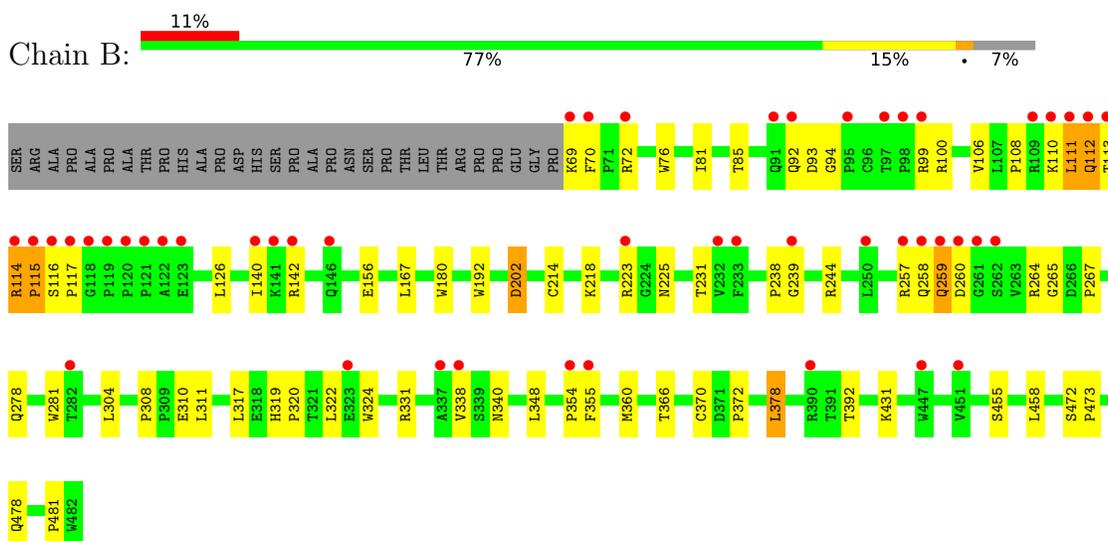
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.19Å 106.64Å 156.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.08 – 1.93 39.08 – 1.92	Depositor EDS
% Data completeness (in resolution range)	85.3 (39.08-1.93) 82.0 (39.08-1.92)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.92Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.251 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å²)	27.5	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.37 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7382	wwPDB-VP
Average B, all atoms (Å²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: 14W, ZN, HEM, ACT, CAC, GOL

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	0.34	0/3397	0.59	1/4631 (0.0%)
1	B	0.33	0/3385	0.59	1/4614 (0.0%)
All	All	0.34	0/6782	0.59	2/9245 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	360	MET	N-CA-C	-5.81	95.30	111.00
1	A	360	MET	N-CA-C	-5.60	95.89	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	3302	0	3215	59	0
1	B	3291	0	3205	66	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	43	0	30	0	0
5	B	43	0	30	1	0
6	A	11	0	10	0	0
6	B	11	0	10	0	0
7	A	6	0	8	0	0
7	B	5	0	3	1	0
8	A	340	0	0	3	0
8	B	315	0	0	2	0
All	All	7382	0	6517	120	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 9.

All (120) 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:114:ARG:HA	1:B:114:ARG:HH11	1.24	1.00
1:B:259:GLN:HG2	1:B:260:ASP:H	1.34	0.92
1:B:308:PRO:HB2	1:B:311:LEU:HD13	1.54	0.90
1:B:112:GLN:HG3	1:B:113:THR:H	1.38	0.89
1:A:249:GLN:HB2	1:A:252:ARG:HD3	1.53	0.88
1:B:259:GLN:HG2	1:B:260:ASP:N	1.93	0.84
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.61	0.82
1:A:115:PRO:O	1:A:117:PRO:HD3	1.80	0.81
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.64	0.79
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.50	0.76
1:B:142:ARG:HG2	1:B:142:ARG:HH11	1.54	0.71
1:A:168:ARG:HD3	8:A:2157:HOH:O	1.90	0.71
1:A:119:PRO:HG3	1:A:238:PRO:HB3	1.72	0.70
1:B:114:ARG:HA	1:B:114:ARG:NH1	2.04	0.70
1:B:99:ARG:HB2	1:B:99:ARG:NH1	2.07	0.70
1:B:116:SER:O	1:B:238:PRO:HA	1.92	0.70
1:A:149:GLU:O	1:A:153:GLN:HG2	1.90	0.70
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.74	0.69
1:A:111:LEU:HD12	1:A:111:LEU:H	1.56	0.69
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.75	0.68
7:B:2880:GOL:C2	7:B:2880:GOL:O1	2.42	0.67
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.78	0.66
1:B:258:GLN:NE2	1:B:264:ARG:HB2	2.13	0.64
1:B:214:CYS:O	1:B:218:LYS:HG3	1.98	0.63
1:A:378:LEU:HB2	8:A:1954:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:O	1:A:130:ARG:HG3	1.99	0.62
1:A:270:VAL:O	1:A:274:GLU:HG3	2.00	0.62
1:B:310:GLU:HG2	1:B:311:LEU:HD12	1.82	0.61
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.41	0.61
1:B:70:PHE:HD2	1:B:85:THR:HA	1.66	0.60
1:B:378:LEU:HB2	8:B:2961:HOH:O	2.01	0.59
1:B:142:ARG:HG2	1:B:142:ARG:NH1	2.14	0.59
1:A:303:GLU:HB3	8:A:2261:HOH:O	2.03	0.59
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.32	0.58
1:B:117:PRO:HA	1:B:239:GLY:H	1.68	0.58
1:A:94:GLY:O	1:A:110:LYS:HE2	2.03	0.58
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.44	0.58
1:B:431:LYS:HG3	8:B:3035:HOH:O	2.05	0.57
1:B:72:ARG:CZ	1:B:81:ILE:HD13	2.34	0.56
1:B:126:LEU:HD21	1:B:156:GLU:OE2	2.06	0.55
1:B:117:PRO:HA	1:B:239:GLY:HA2	1.87	0.55
5:B:500:HEM:HBB2	5:B:500:HEM:HHC	1.88	0.55
1:A:130:ARG:HB3	1:A:130:ARG:HH11	1.72	0.54
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.90	0.54
1:A:111:LEU:HD12	1:A:111:LEU:N	2.23	0.53
1:B:114:ARG:HH11	1:B:115:PRO:HD3	1.73	0.53
1:A:77:GLU:HG3	1:B:372:PRO:CG	2.38	0.53
1:B:112:GLN:HE21	1:B:478:GLN:HA	1.74	0.53
1:A:366:THR:HG21	1:A:454:ILE:HG23	1.91	0.52
1:B:114:ARG:HD3	1:B:115:PRO:CD	2.39	0.52
1:B:110:LYS:C	1:B:112:GLN:H	2.13	0.52
1:A:285:ASN:HD22	1:A:285:ASN:C	2.13	0.51
1:A:249:GLN:HB2	1:A:252:ARG:CD	2.33	0.51
1:B:112:GLN:NE2	1:B:478:GLN:HA	2.26	0.51
1:A:342:LEU:C	1:A:342:LEU:HD23	2.32	0.49
1:B:472:SER:HA	1:B:473:PRO:C	2.32	0.49
1:B:265:GLY:O	1:B:267:PRO:HD3	2.13	0.49
1:A:130:ARG:HB3	1:A:130:ARG:NH1	2.28	0.49
1:B:72:ARG:NH2	1:B:81:ILE:HD13	2.27	0.49
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.48	0.49
1:A:285:ASN:C	1:A:285:ASN:ND2	2.65	0.49
1:A:434:ASP:OD1	1:A:438:LYS:NZ	2.45	0.49
1:B:114:ARG:NH1	1:B:115:PRO:HD3	2.27	0.49
1:B:112:GLN:CG	1:B:113:THR:H	2.18	0.48
1:A:92:GLN:NE2	1:A:470:ILE:HG22	2.28	0.48
1:A:99:ARG:HH22	1:B:92:GLN:C	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLN:HG3	1:B:113:THR:N	2.17	0.48
1:A:340:ASN:H	1:A:340:ASN:HD22	1.62	0.48
1:B:366:THR:O	1:B:370:CYS:HB2	2.14	0.47
1:B:70:PHE:CD2	1:B:85:THR:HA	2.48	0.47
1:A:158:GLU:HG2	1:A:165:TYR:HA	1.97	0.47
1:B:117:PRO:HA	1:B:239:GLY:N	2.30	0.47
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.49	0.47
1:B:338:VAL:HB	1:B:355:PHE:CZ	2.49	0.47
1:B:69:LYS:HE2	1:B:69:LYS:HB2	1.85	0.46
1:B:202:ASP:CG	1:B:202:ASP:O	2.53	0.46
1:A:110:LYS:HB2	1:A:111:LEU:HD12	1.98	0.46
1:A:249:GLN:CB	1:A:252:ARG:HD3	2.37	0.46
1:A:146:GLN:O	1:A:150:GLU:HG3	2.16	0.46
1:A:472:SER:HA	1:A:473:PRO:C	2.35	0.45
1:B:116:SER:N	1:B:117:PRO:CD	2.79	0.45
1:B:117:PRO:HA	1:B:239:GLY:CA	2.46	0.45
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.99	0.45
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.82	0.45
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.52	0.45
1:A:153:GLN:HA	1:A:153:GLN:OE1	2.17	0.45
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.31	0.44
1:B:317:LEU:HG	1:B:331:ARG:HA	1.99	0.44
1:A:328:LEU:HB3	1:A:330:LEU:HG	1.99	0.44
1:A:106:VAL:HB	1:B:76:TRP:CZ2	2.53	0.44
1:A:236:ARG:HB3	1:A:236:ARG:NH1	2.33	0.43
1:A:76:TRP:CZ2	1:B:106:VAL:HB	2.53	0.43
1:A:423:HIS:HB2	1:B:392:THR:HB	2.01	0.43
1:A:108:PRO:O	1:A:110:LYS:N	2.48	0.43
1:A:122:ALA:O	1:A:126:LEU:HG	2.19	0.43
1:B:94:GLY:HA2	1:B:111:LEU:HD21	2.01	0.43
1:A:378:LEU:HD12	1:A:378:LEU:HA	1.89	0.43
1:B:264:ARG:HH11	1:B:264:ARG:HG3	1.85	0.42
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.54	0.42
1:A:92:GLN:HE21	1:A:92:GLN:HB2	1.61	0.42
1:B:140:ILE:O	1:B:142:ARG:HG3	2.19	0.42
1:A:120:PRO:HA	1:A:121:PRO:HD3	1.98	0.42
1:B:117:PRO:CA	1:B:239:GLY:H	2.32	0.42
1:A:111:LEU:HG	1:A:470:ILE:HD13	2.02	0.42
1:A:109:ARG:HA	1:A:109:ARG:HD3	1.91	0.41
1:A:244:ARG:CZ	1:A:481:PRO:HG3	2.50	0.41
1:A:111:LEU:H	1:A:111:LEU:CD1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.55	0.41
1:A:252:ARG:HA	1:A:252:ARG:HD2	1.93	0.41
1:A:99:ARG:NH1	1:B:93:ASP:OD2	2.54	0.41
1:A:231:THR:O	1:A:353:ALA:HA	2.21	0.41
1:A:168:ARG:HB2	1:A:171:GLU:HG3	2.01	0.41
1:A:366:THR:O	1:A:370:CYS:HB2	2.21	0.41
1:B:111:LEU:N	1:B:111:LEU:HD12	2.35	0.41
1:B:231:THR:O	1:B:354:PRO:HD2	2.21	0.41
1:A:114:ARG:HD2	1:A:479:PRO:CG	2.51	0.41
1:A:114:ARG:HD2	1:A:479:PRO:HG2	2.03	0.41
1:A:340:ASN:HD22	1:A:340:ASN:N	2.18	0.40
1:A:240:ARG:HG2	1:A:241:GLY:N	2.37	0.40
1:A:74:LYS:HB2	1:A:81:ILE:CD1	2.51	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	414/444 (93%)	397 (96%)	13 (3%)	4 (1%)	15	6
1	B	412/444 (93%)	391 (95%)	17 (4%)	4 (1%)	15	6
All	All	826/888 (93%)	788 (95%)	30 (4%)	8 (1%)	15	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	B	111	LEU
1	A	109	ARG
1	B	112	GLN
1	B	259	GLN

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Mol	Chain	Res	Type
1	A	117	PRO
1	B	115	PRO
1	A	121	PRO

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	354/377 (94%)	349 (99%)	5 (1%)	67	58
1	B	353/377 (94%)	345 (98%)	8 (2%)	50	38
All	All	707/754 (94%)	694 (98%)	13 (2%)	59	47

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	285	ASN
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	B	100	ARG
1	B	114	ARG
1	B	202	ASP
1	B	225	ASN
1	B	257	ARG
1	B	278	GLN
1	B	340	ASN
1	B	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	112	GLN

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Mol	Chain	Res	Type
1	A	124	GLN
1	A	191	GLN
1	A	278	GLN
1	A	279	HIS
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	89	GLN
1	B	112	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	258	GLN
1	B	279	HIS
1	B	340	ASN
1	B	405	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 ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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	$\#\|Z\| > 2$
6	14W	A	810	-	11,11,13	1.67	2 (18%)	10,13,16	2.60	1 (10%)
7	GOL	A	1880	-	5,5,5	0.22	0	5,5,5	0.21	0
6	14W	B	810	-	11,11,13	1.67	2 (18%)	10,13,16	2.65	1 (10%)
7	GOL	B	2880	-	3,3,5	0.45	0	2,2,5	0.22	0
2	ACT	B	2860	-	3,3,3	1.00	0	3,3,3	0.79	0
5	HEM	B	500	1	41,50,50	1.28	6 (14%)	45,82,82	1.29	5 (11%)
3	CAC	B	2950	1	0,2,4	-	-	0,1,6	-	-
5	HEM	A	500	1	41,50,50	1.32	6 (14%)	45,82,82	1.10	2 (4%)
2	ACT	A	1860	-	3,3,3	0.90	0	3,3,3	0.70	0
3	CAC	A	1950	1	0,2,4	-	-	0,1,6	-	-

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
6	14W	A	810	-	-	1/4/5/7	0/1/1/1
7	GOL	A	1880	-	-	0/4/4/4	-
7	GOL	B	2880	-	-	0/1/1/4	-
5	HEM	B	500	1	-	3/12/54/54	-
6	14W	B	810	-	-	1/4/5/7	0/1/1/1
5	HEM	A	500	1	-	4/12/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	HEM	C3C-CAC	-3.50	1.40	1.47
5	A	500	HEM	C3C-C2C	-2.97	1.36	1.40
5	B	500	HEM	C3C-CAC	-2.77	1.42	1.47
5	B	500	HEM	CHB-C1B	2.68	1.41	1.35
5	A	500	HEM	CAB-C3B	-2.58	1.40	1.47
5	B	500	HEM	C3C-C2C	-2.38	1.37	1.40
5	B	500	HEM	CHA-C4D	2.38	1.41	1.35
5	B	500	HEM	CAB-C3B	-2.32	1.41	1.47
5	A	500	HEM	CHB-C1B	2.31	1.40	1.35
5	A	500	HEM	C1A-NA	2.20	1.40	1.36
5	A	500	HEM	C4A-NA	2.12	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	HEM	C1A-NA	2.08	1.40	1.36
6	A	810	14W	C9-N11	2.08	1.33	1.27
6	B	810	14W	C6-C1	2.04	1.43	1.38
6	A	810	14W	C7-N8	2.03	1.50	1.46
6	B	810	14W	C9-N11	2.02	1.33	1.27

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	810	14W	C10-C9-N8	8.28	124.86	114.24
6	A	810	14W	C10-C9-N8	8.13	124.66	114.24
5	B	500	HEM	CBA-CAA-C2A	-3.34	106.92	112.62
5	A	500	HEM	CBA-CAA-C2A	-3.30	107.00	112.62
5	B	500	HEM	C4B-CHC-C1C	2.96	126.47	122.56
5	B	500	HEM	C3B-C2B-C1B	2.39	108.26	106.49
5	B	500	HEM	C4B-C3B-C2B	-2.19	105.37	107.11
5	B	500	HEM	CAB-C3B-C2B	-2.08	121.76	128.60
5	A	500	HEM	C4D-ND-C1D	-2.01	103.00	105.07

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	500	HEM	C4B-C3B-CAB-CBB
6	A	810	14W	C1-C7-N8-C9
6	B	810	14W	C1-C7-N8-C9
5	A	500	HEM	CAD-CBD-CGD-O2D
5	A	500	HEM	CAA-CBA-CGA-O2A
5	B	500	HEM	CAA-CBA-CGA-O2A
5	A	500	HEM	CAA-CBA-CGA-O1A
5	A	500	HEM	CAD-CBD-CGD-O1D
5	B	500	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	2880	GOL	1	0
5	B	500	HEM	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 B 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 500
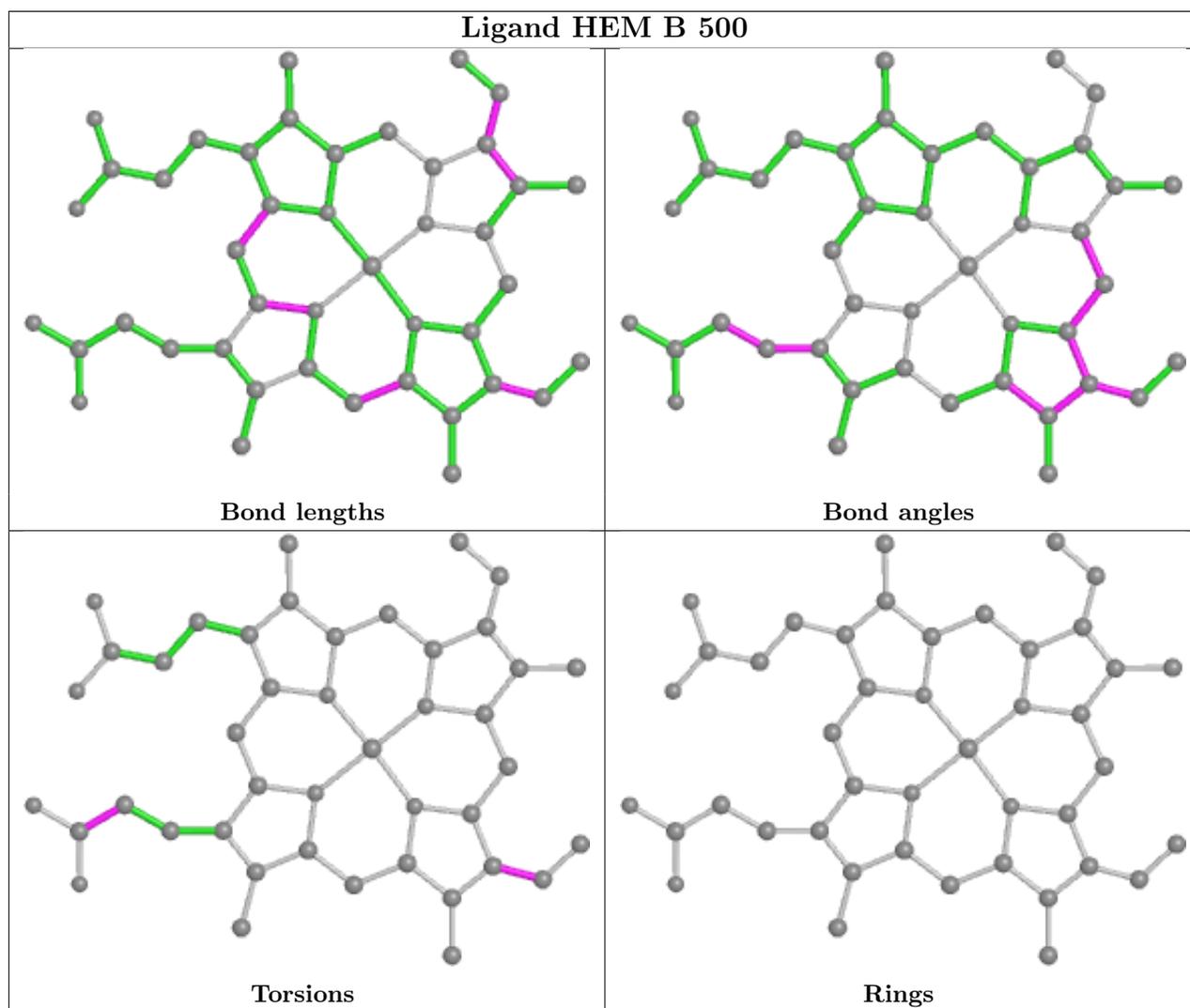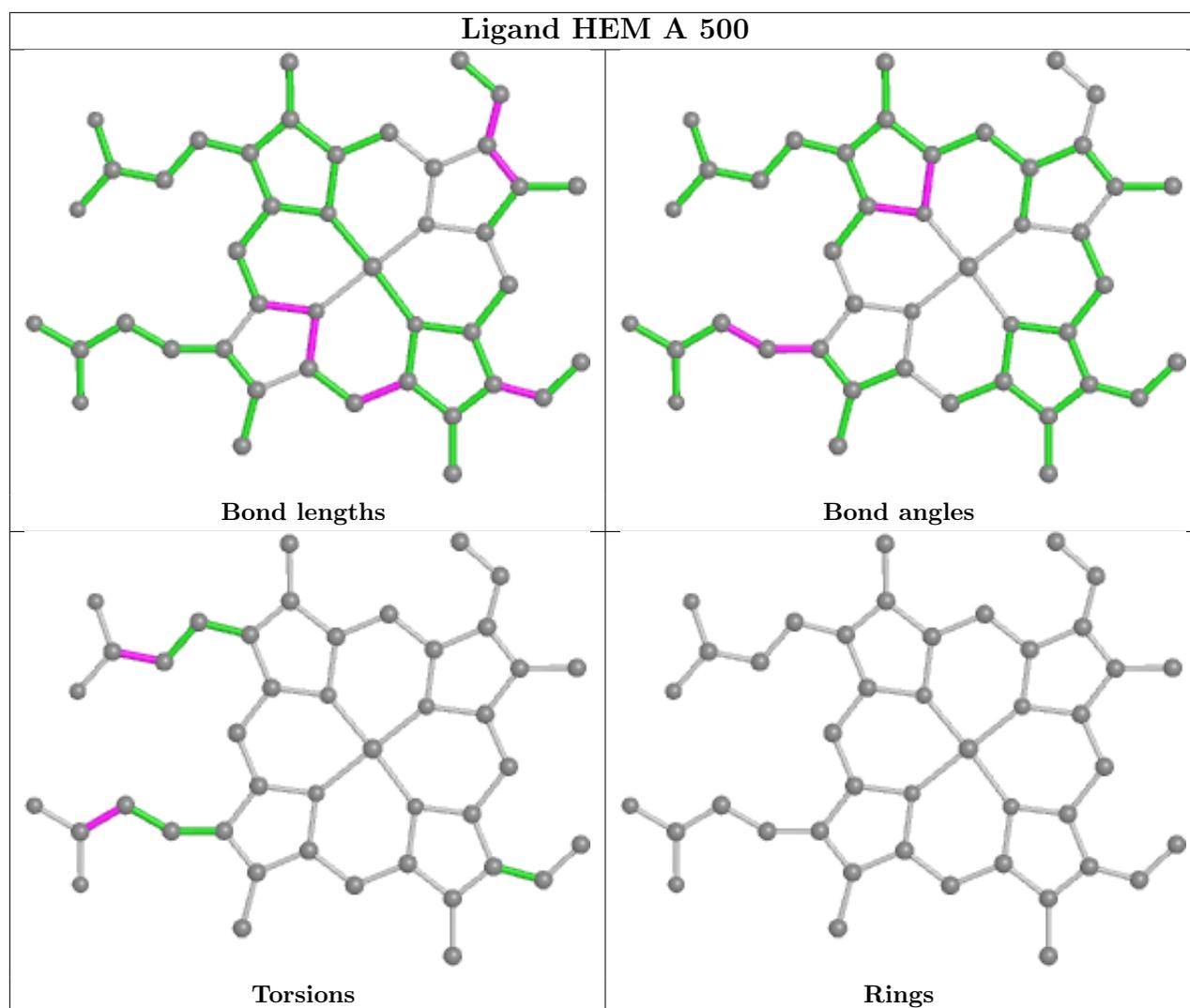
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	416/444 (93%)	0.89	55 (13%)	3	4	24, 34, 56, 85	0
1	B	414/444 (93%)	0.85	48 (11%)	4	7	25, 38, 58, 82	0
All	All	830/888 (93%)	0.87	103 (12%)	4	6	24, 36, 58, 85	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	PRO	13.3
1	A	118	GLY	12.8
1	A	113	THR	12.4
1	A	117	PRO	12.4
1	B	117	PRO	11.6
1	B	113	THR	11.5
1	A	111	LEU	10.1
1	B	119	PRO	9.2
1	B	110	LYS	8.6
1	B	118	GLY	8.5
1	B	115	PRO	8.2
1	A	116	SER	8.0
1	A	115	PRO	7.7
1	A	121	PRO	7.4
1	A	114	ARG	7.3
1	B	116	SER	7.0
1	A	122	ALA	6.9
1	B	111	LEU	6.8
1	A	120	PRO	6.8
1	B	114	ARG	6.5
1	A	123	GLU	6.3
1	B	120	PRO	6.2
1	A	259	GLN	6.0
1	A	239	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	110	LYS	5.9
1	B	259	GLN	5.2
1	A	67	GLY	5.1
1	A	112	GLN	4.9
1	B	261	GLY	4.8
1	B	112	GLN	4.3
1	A	109	ARG	4.2
1	A	160	ALA	4.2
1	B	99	ARG	4.1
1	A	157	ALA	4.1
1	A	238	PRO	4.0
1	A	161	SER	4.0
1	B	98	PRO	3.8
1	A	153	GLN	3.8
1	A	92	GLN	3.8
1	B	121	PRO	3.8
1	A	99	ARG	3.7
1	A	124	GLN	3.6
1	A	126	LEU	3.3
1	B	92	GLN	3.3
1	A	261	GLY	3.2
1	A	69	LYS	3.1
1	B	122	ALA	3.1
1	B	232	VAL	3.0
1	A	91	GLN	3.0
1	B	260	ASP	3.0
1	B	142	ARG	2.9
1	A	449	TRP	2.9
1	A	108	PRO	2.9
1	A	338	VAL	2.9
1	B	323	GLU	2.9
1	B	239	GLY	2.9
1	B	91	GLN	2.9
1	A	390	ARG	2.8
1	B	69	LYS	2.8
1	A	230	ILE	2.7
1	B	70	PHE	2.7
1	B	258	GLN	2.7
1	B	146	GLN	2.6
1	B	338	VAL	2.6
1	A	482	TRP	2.5
1	B	282	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	123	GLU	2.5
1	A	337	ALA	2.5
1	B	250	LEU	2.5
1	A	93	ASP	2.4
1	B	97	THR	2.4
1	B	141	LYS	2.4
1	A	475	PHE	2.4
1	A	260	ASP	2.4
1	B	257	ARG	2.4
1	A	414	LEU	2.3
1	B	390	ARG	2.3
1	B	109	ARG	2.3
1	B	95	PRO	2.3
1	A	97	THR	2.3
1	B	140	ILE	2.3
1	A	284	GLY	2.2
1	B	451	VAL	2.2
1	B	354	PRO	2.2
1	A	448	ALA	2.2
1	A	257	ARG	2.2
1	A	130	ARG	2.2
1	A	223	ARG	2.2
1	A	106	VAL	2.2
1	A	232	VAL	2.1
1	A	94	GLY	2.1
1	B	337	ALA	2.1
1	A	355	PHE	2.1
1	B	233	PHE	2.1
1	A	343	LEU	2.1
1	A	451	VAL	2.1
1	B	72	ARG	2.1
1	B	223	ARG	2.1
1	A	98	PRO	2.1
1	B	447	TRP	2.1
1	B	262	SER	2.1
1	A	241	GLY	2.0
1	B	355	PHE	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 ⓘ

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
2	ACT	A	1860	4/4	0.82	0.18	38,38,38,38	0
7	GOL	B	2880	5/6	0.84	0.35	48,49,49,49	0
7	GOL	A	1880	6/6	0.91	0.23	43,44,44,45	0
2	ACT	B	2860	4/4	0.91	0.13	39,39,39,39	0
6	14W	A	810	11/13	0.93	0.31	36,36,37,38	0
6	14W	B	810	11/13	0.93	0.23	36,37,38,38	0
5	HEM	A	500	43/43	0.97	0.17	24,26,31,32	0
5	HEM	B	500	43/43	0.97	0.15	25,26,30,32	0
3	CAC	A	1950	3/5	0.99	0.13	43,43,43,45	0
3	CAC	B	2950	3/5	0.99	0.11	51,51,51,51	0
4	ZN	A	900	1/1	1.00	0.04	46,46,46,46	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 500:

$2mF_o$-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 500:

$2mF_o$-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.