



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:31 am BST

PDB ID : 1ED6  
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN  
COMPLEXED WITH L-NIO (H4B FREE)  
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T.L.  
Deposited on : 2000-01-26  
Resolution : 2.05 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

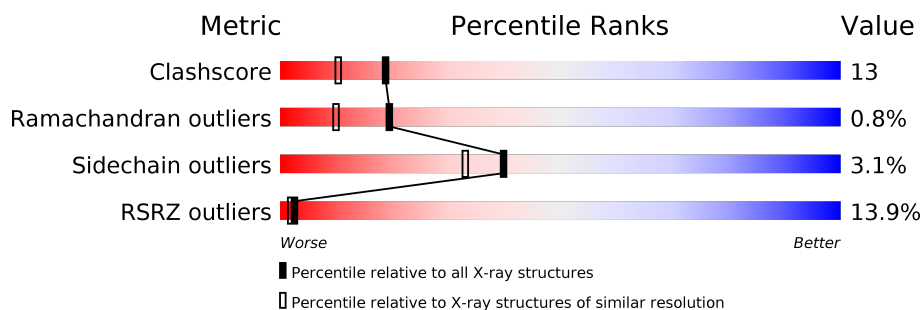
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	444	<div> <div>14%</div> <div>70%</div> <div>21%</div> <div>6%</div> </div>
1	B	444	<div> <div>12%</div> <div>70%</div> <div>21%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7105 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.

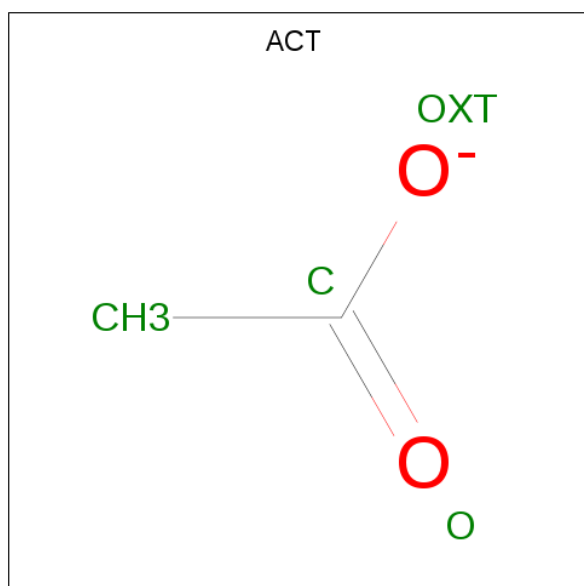
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE.

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

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<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

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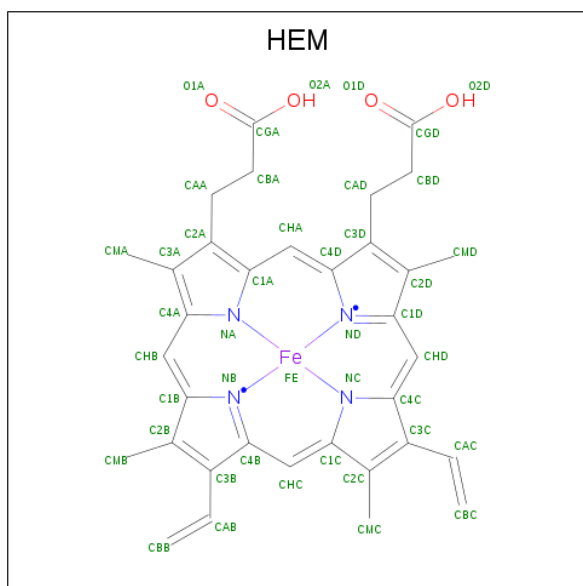
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

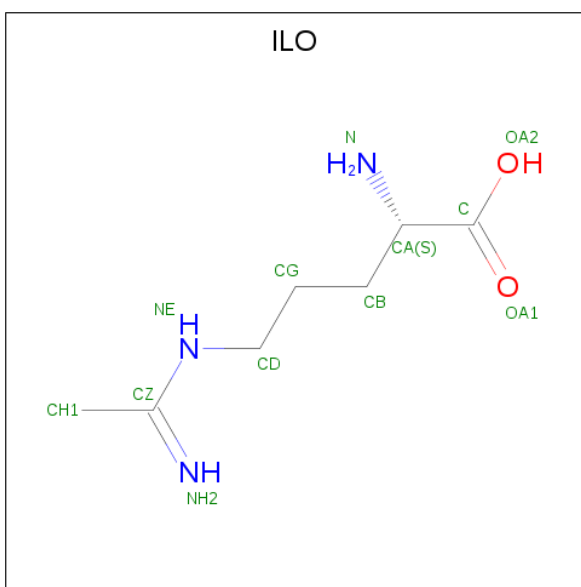
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



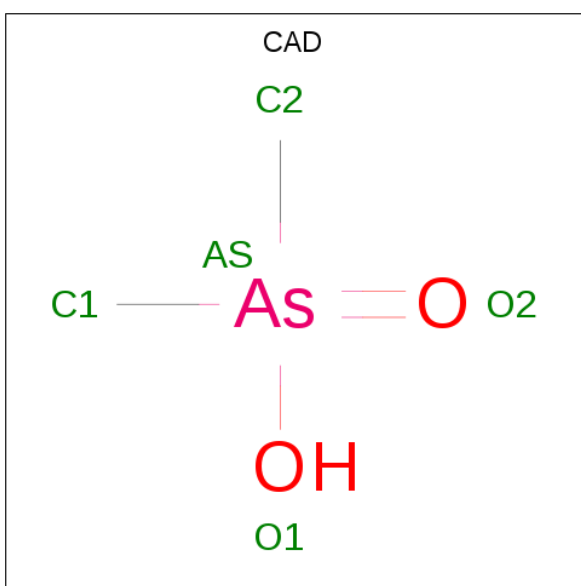
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is N5-IMINOETHYL-L-ORNITHINE (three-letter code: ILO) (formula:  $C_7H_{15}N_3O_2$ ).



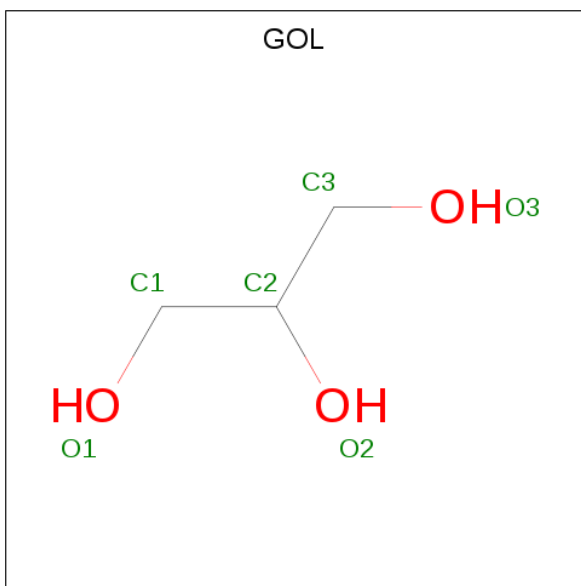
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	7	3	2		
5	B	1	Total	C	N	O	0	0
			12	7	3	2		

- Molecule 6 is CACODYLIC ACID (three-letter code: CAD) (formula: C<sub>2</sub>H<sub>7</sub>AsO<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	As	C	0	0
			3	1	2		
6	B	1	Total	As	C	0	0
			3	1	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

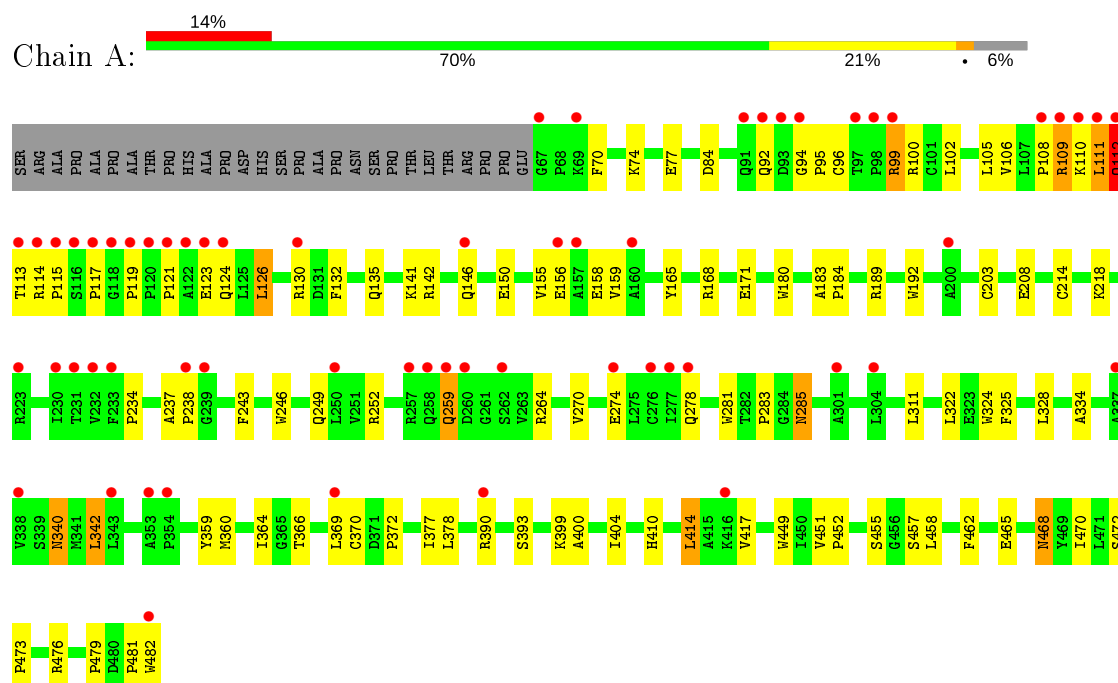
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	197	Total	O	0	0
			197	197		
8	B	178	Total	O	0	0
			178	178		

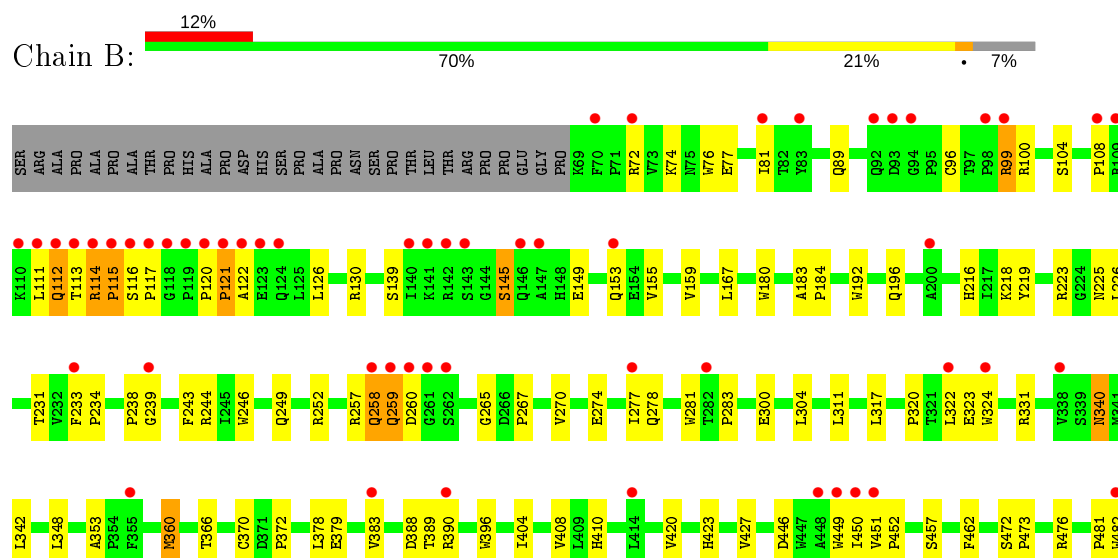
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



#### • Molecule 1: NITRIC OXIDE SYNTHASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.12Å 106.16Å 156.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.66 – 2.05 32.66 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.1 (32.66-2.05) 78.0 (32.66-2.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.74 (at 2.05Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.241 , 0.275 0.233 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 55.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7105	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, ZN, ILO, ACT, HEM, CAD

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	0.36	0/3397	0.61	1/4631 (0.0%)
1	B	0.36	0/3385	0.62	2/4614 (0.0%)
All	All	0.36	0/6782	0.62	3/9245 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	MET	N-CA-C	-5.68	95.66	111.00
1	A	360	MET	N-CA-C	-5.16	97.07	111.00
1	B	243	PHE	N-CA-C	-5.09	97.26	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	87	0
1	B	3291	0	3205	87	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
4	A	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	43	0	30	2	0
5	A	12	0	13	1	0
5	B	12	0	13	1	0
6	A	3	0	0	0	0
6	B	3	0	0	1	0
7	A	6	0	8	1	0
7	B	6	0	8	2	0
8	A	197	0	0	3	0
8	B	178	0	0	5	0
All	All	7105	0	6528	173	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 13.

All (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:HH11	1:A:99:ARG:HB2	1.17	1.09
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.36	1.06
1:B:258:GLN:HA	1:B:258:GLN:HE21	1.30	0.92
1:B:112:GLN:HG3	1:B:113:THR:H	1.32	0.92
1:A:249:GLN:HB2	1:A:252:ARG:HD3	1.54	0.88
1:A:119:PRO:HG3	1:A:238:PRO:HB3	1.54	0.88
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.54	0.87
1:B:259:GLN:HG3	1:B:260:ASP:H	1.42	0.84
1:B:249:GLN:HB2	1:B:252:ARG:HD3	1.59	0.84
1:B:114:ARG:HH11	1:B:114:ARG:HA	1.44	0.83
1:A:109:ARG:O	1:A:110:LYS:HD2	1.80	0.81
1:B:378:LEU:HB2	8:B:2955:HOH:O	1.78	0.81
1:A:115:PRO:O	1:A:117:PRO:HD3	1.85	0.77
1:A:126:LEU:HD12	1:A:130:ARG:HE	1.51	0.75
1:A:111:LEU:HG	1:A:470:ILE:HD13	1.67	0.75
1:B:259:GLN:HG3	1:B:260:ASP:OD1	1.86	0.75
1:B:89:GLN:HA	1:B:89:GLN:HE21	1.51	0.74
1:A:111:LEU:H	1:A:111:LEU:HD12	1.52	0.73
1:A:99:ARG:NH1	1:A:99:ARG:HB2	1.99	0.73
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.72	0.72
4:B:2500:HEM:HBC2	4:B:2500:HEM:HMC2	1.71	0.71
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.73	0.70
1:B:218:LYS:HE3	1:B:311:LEU:HD11	1.73	0.70
1:B:72:ARG:NE	1:B:81:ILE:HG21	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:HD22	1:A:340:ASN:H	1.41	0.69
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.58	0.68
1:B:258:GLN:HA	1:B:258:GLN:NE2	2.08	0.67
1:A:259:GLN:H	1:A:259:GLN:CD	1.99	0.66
1:A:113:THR:HG21	1:A:342:LEU:HD22	1.76	0.66
1:A:146:GLN:O	1:A:150:GLU:HG3	1.97	0.63
1:A:378:LEU:HB2	8:A:1951:HOH:O	1.98	0.63
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.27	0.63
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.33	0.62
1:A:119:PRO:CG	1:A:238:PRO:HB3	2.29	0.62
1:B:116:SER:O	1:B:238:PRO:HA	2.00	0.61
1:B:113:THR:HG21	1:B:342:LEU:HD13	1.82	0.60
1:A:77:GLU:HG3	1:B:372:PRO:CG	2.32	0.60
1:B:379:GLU:O	1:B:383:VAL:HG23	2.02	0.59
1:A:114:ARG:HG3	1:A:115:PRO:HD2	1.82	0.59
1:B:126:LEU:O	1:B:130:ARG:HG3	2.03	0.58
1:A:94:GLY:O	1:A:110:LYS:HE2	2.04	0.58
1:A:99:ARG:CB	1:A:99:ARG:HH11	2.05	0.57
1:B:89:GLN:HA	1:B:89:GLN:NE2	2.19	0.57
1:A:95:PRO:HB3	1:A:108:PRO:HB2	1.86	0.57
1:B:149:GLU:O	1:B:153:GLN:HG3	2.05	0.57
1:B:258:GLN:HE21	1:B:258:GLN:CA	1.97	0.57
1:B:113:THR:HG23	1:B:476:ARG:NH2	2.19	0.56
1:A:113:THR:CG2	1:A:476:ARG:HD2	2.35	0.56
1:B:155:VAL:O	1:B:159:VAL:HG23	2.06	0.56
1:B:258:GLN:CA	1:B:258:GLN:NE2	2.68	0.55
1:A:115:PRO:C	1:A:117:PRO:HD3	2.25	0.55
1:B:249:GLN:HB2	1:B:252:ARG:CD	2.34	0.55
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.89	0.55
1:A:249:GLN:HB2	1:A:252:ARG:CD	2.32	0.55
1:B:112:GLN:HG3	1:B:113:THR:N	2.13	0.55
1:A:158:GLU:HG2	1:A:165:TYR:HA	1.89	0.54
1:A:472:SER:HA	1:A:473:PRO:C	2.28	0.54
1:B:72:ARG:CZ	1:B:81:ILE:HG21	2.38	0.54
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.89	0.53
1:A:214:CYS:O	1:A:218:LYS:HG3	2.08	0.53
1:B:122:ALA:O	1:B:126:LEU:HB2	2.08	0.53
1:A:274:GLU:O	1:A:278:GLN:HG3	2.08	0.53
1:A:110:LYS:HB2	1:A:111:LEU:HD12	1.89	0.53
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.91	0.53
1:B:117:PRO:HA	1:B:239:GLY:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.23	0.53
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.45	0.52
1:A:340:ASN:HD22	1:A:340:ASN:N	2.03	0.52
1:B:340:ASN:HD22	1:B:340:ASN:H	1.55	0.52
1:A:340:ASN:ND2	1:A:340:ASN:H	2.06	0.52
1:A:281:TRP:O	1:A:283:PRO:HD3	2.10	0.52
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.91	0.51
7:B:2890:GOL:H12	8:B:3099:HOH:O	2.10	0.51
1:B:324:TRP:HB2	6:B:2950:CAD:C1	2.40	0.51
1:A:372:PRO:HB2	1:B:77:GLU:HG3	1.93	0.50
1:B:265:GLY:O	1:B:267:PRO:HD3	2.12	0.50
1:A:112:GLN:HA	1:A:112:GLN:HE21	1.77	0.50
1:B:320:PRO:HG3	1:B:410:HIS:CG	2.46	0.50
1:B:277:ILE:HD11	1:B:283:PRO:HB3	1.94	0.49
1:B:389:THR:HA	1:B:396:TRP:CD1	2.47	0.49
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.94	0.49
1:B:472:SER:HA	1:B:473:PRO:C	2.32	0.49
1:A:111:LEU:CD1	1:A:111:LEU:H	2.24	0.49
1:A:400:ALA:O	1:A:404:ILE:HG13	2.12	0.49
1:A:74:LYS:O	1:A:465:GLU:HG3	2.13	0.49
1:B:476:ARG:HD2	8:B:3123:HOH:O	2.13	0.49
1:A:399:LYS:NZ	8:A:2147:HOH:O	2.42	0.49
4:A:1500:HEM:HBA2	5:A:1765:ILO:HCG1	1.95	0.49
1:A:246:TRP:CD1	1:A:481:PRO:HG3	2.48	0.49
4:B:2500:HEM:HBA2	5:B:2765:ILO:HCG1	1.94	0.49
1:B:360:MET:HA	1:B:420:VAL:O	2.12	0.49
1:A:111:LEU:N	1:A:111:LEU:HD12	2.26	0.48
1:A:113:THR:HG23	1:A:476:ARG:HD2	1.94	0.48
1:A:334:ALA:HB1	1:A:417:VAL:HG11	1.95	0.48
1:B:145:SER:O	1:B:149:GLU:HG2	2.13	0.48
1:A:285:ASN:C	1:A:285:ASN:HD22	2.16	0.48
1:A:259:GLN:N	1:A:259:GLN:CD	2.64	0.48
1:B:423:HIS:O	1:B:427:VAL:HG23	2.14	0.48
1:A:102:LEU:HB3	1:A:105:LEU:HD22	1.95	0.48
1:A:92:GLN:HE22	1:A:111:LEU:HA	1.79	0.47
1:B:317:LEU:HG	1:B:331:ARG:HA	1.96	0.47
1:B:72:ARG:HG3	1:B:81:ILE:CG2	2.44	0.47
1:B:116:SER:N	1:B:117:PRO:CD	2.78	0.47
1:B:74:LYS:HE2	1:B:76:TRP:CE3	2.50	0.47
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.50	0.47
1:A:325:PHE:O	1:A:328:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ASN:ND2	1:B:340:ASN:H	2.13	0.46
1:A:124:GLN:HE21	1:A:124:GLN:HA	1.81	0.46
1:A:124:GLN:NE2	1:A:124:GLN:HA	2.30	0.45
1:B:366:THR:O	1:B:370:CYS:HB2	2.17	0.45
1:B:249:GLN:CB	1:B:252:ARG:HD3	2.40	0.45
1:B:340:ASN:HD22	1:B:340:ASN:N	2.12	0.45
1:A:449:TRP:CE2	7:A:1890:GOL:H2	2.52	0.45
1:B:259:GLN:CG	1:B:260:ASP:N	2.80	0.45
1:B:476:ARG:CD	8:B:3123:HOH:O	2.65	0.45
1:B:246:TRP:CH2	1:B:482:TRP:HB3	2.51	0.45
1:A:203:CYS:SG	1:A:208:GLU:HB3	2.57	0.45
1:B:446:ASP:O	1:B:450:ILE:HG12	2.17	0.45
1:A:141:LYS:O	1:A:142:ARG:NH1	2.45	0.44
1:B:120:PRO:O	1:B:121:PRO:C	2.56	0.44
1:A:246:TRP:CE3	1:A:482:TRP:HE3	2.35	0.44
1:B:259:GLN:HG3	1:B:260:ASP:N	2.22	0.44
1:B:449:TRP:CD2	7:B:2890:GOL:H32	2.52	0.44
1:A:285:ASN:C	1:A:285:ASN:ND2	2.71	0.44
1:A:334:ALA:CB	1:A:417:VAL:HG11	2.47	0.44
1:B:231:THR:O	1:B:353:ALA:HA	2.18	0.44
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.85	0.43
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.49	0.43
1:A:96:CYS:HB3	1:B:96:CYS:HB3	1.99	0.43
1:B:257:ARG:HH11	1:B:270:VAL:HG11	1.83	0.43
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.54	0.43
1:B:216:HIS:C	1:B:216:HIS:CD2	2.92	0.43
1:A:259:GLN:NE2	1:A:259:GLN:H	2.15	0.43
1:A:111:LEU:HG	1:A:470:ILE:CD1	2.43	0.43
1:A:457:SER:HA	1:A:462:PHE:CG	2.54	0.43
1:B:233:PHE:HB3	1:B:234:PRO:HD2	2.00	0.42
1:A:111:LEU:HD22	8:A:1966:HOH:O	2.18	0.42
1:A:184:PRO:HB3	1:A:468:ASN:ND2	2.35	0.42
1:A:264:ARG:HG3	1:A:264:ARG:HH11	1.85	0.42
1:A:270:VAL:O	1:A:274:GLU:HG3	2.19	0.42
1:B:300:GLU:HG3	8:B:3121:HOH:O	2.18	0.42
1:A:155:VAL:O	1:A:159:VAL:HG23	2.20	0.42
1:A:237:ALA:HA	1:A:238:PRO:HD3	1.89	0.41
1:B:183:ALA:HA	1:B:184:PRO:HD3	1.84	0.41
1:B:196:GLN:HG2	1:B:219:TYR:CZ	2.55	0.41
1:B:226:LEU:HD12	1:B:226:LEU:N	2.34	0.41
1:B:388:ASP:OD1	1:B:390:ARG:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PRO:O	1:A:110:LYS:N	2.53	0.41
1:B:257:ARG:HG3	1:B:257:ARG:HH11	1.84	0.41
1:A:132:PHE:O	1:A:135:GLN:HB2	2.21	0.41
1:B:278:GLN:HG2	1:B:278:GLN:O	2.20	0.41
1:B:342:LEU:C	1:B:342:LEU:HD23	2.41	0.41
1:A:249:GLN:CB	1:A:252:ARG:HD3	2.39	0.41
1:B:74:LYS:HE2	1:B:76:TRP:CD2	2.55	0.41
1:A:366:THR:O	1:A:370:CYS:HB2	2.21	0.41
1:A:390:ARG:HE	1:A:390:ARG:HB2	1.54	0.41
1:B:257:ARG:NH1	1:B:274:GLU:OE1	2.54	0.41
1:A:168:ARG:HB2	1:A:171:GLU:HG3	2.01	0.41
1:A:234:PRO:HB2	1:A:243:PHE:CD1	2.56	0.41
1:A:369:LEU:O	1:A:377:ILE:HG12	2.21	0.41
1:A:121:PRO:C	1:A:123:GLU:N	2.75	0.41
1:B:99:ARG:HH11	1:B:99:ARG:CB	2.29	0.40
1:A:183:ALA:O	1:A:189:ARG:CZ	2.69	0.40
1:A:359:TYR:CD2	1:A:364:ILE:HD11	2.56	0.40
1:B:451:VAL:HA	1:B:452:PRO:HD3	1.87	0.40
1:B:457:SER:HA	1:B:462:PHE:CG	2.56	0.40
1:A:70:PHE:HB3	1:A:84:ASP:O	2.22	0.40
1:A:410:HIS:NE2	1:A:414:LEU:HD12	2.36	0.40
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.57	0.40
1:B:404:ILE:O	1:B:408:VAL:HG23	2.21	0.40
1:A:106:VAL:HB	1:B:76:TRP:CZ2	2.55	0.40
1:B:72:ARG:NH1	1:B:81:ILE:HD13	2.36	0.40
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.61	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	414/444 (93%)	389 (94%)	23 (6%)	2 (0%)	29	18
1	B	412/444 (93%)	380 (92%)	27 (7%)	5 (1%)	13	5
All	All	826/888 (93%)	769 (93%)	50 (6%)	7 (1%)	19	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	A	109	ARG
1	A	112	GLN
1	B	112	GLN
1	B	115	PRO
1	B	145	SER
1	B	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%)	342 (97%)	12 (3%)	37	30
1	B	353/377 (94%)	343 (97%)	10 (3%)	43	37
All	All	707/754 (94%)	685 (97%)	22 (3%)	40	33

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	100	ARG
1	A	111	LEU
1	A	112	GLN
1	A	126	LEU
1	A	259	GLN
1	A	285	ASN
1	A	340	ASN
1	A	342	LEU

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Mol	Chain	Res	Type
1	A	393	SER
1	A	414	LEU
1	A	468	ASN
1	B	99	ARG
1	B	100	ARG
1	B	104	SER
1	B	114	ARG
1	B	139	SER
1	B	223	ARG
1	B	225	ASN
1	B	258	GLN
1	B	323	GLU
1	B	340	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	124	GLN
1	A	153	GLN
1	A	191	GLN
1	A	278	GLN
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	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	258	GLN
1	B	278	GLN
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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	CAD	A	1950	1	0,2,4	0.00	-	0,1,6	0.00	-
2	ACT	B	2860	-	1,3,3	3.01	1 (100%)	0,3,3	0.00	-
4	HEM	A	1500	1	27,50,50	1.69	4 (14%)	17,82,82	1.34	2 (11%)
2	ACT	A	1860	-	1,3,3	3.45	1 (100%)	0,3,3	0.00	-
7	GOL	A	1890	-	5,5,5	0.25	0	5,5,5	0.29	0
6	CAD	B	2950	1	0,2,4	0.00	-	0,1,6	0.00	-
5	ILO	B	2765	-	7,11,11	1.37	0	4,13,13	4.36	1 (25%)
7	GOL	B	2890	-	5,5,5	0.28	0	5,5,5	0.21	0
5	ILO	A	1765	-	7,11,11	1.53	2 (28%)	4,13,13	4.23	1 (25%)
4	HEM	B	2500	1	27,50,50	1.56	5 (18%)	17,82,82	1.20	2 (11%)

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	HEM	A	1500	1	-	0/6/54/54	-
7	GOL	A	1890	-	-	0/4/4/4	-
5	ILO	B	2765	-	-	0/6/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	2890	-	-	2/4/4/4	-
5	ILO	A	1765	-	-	0/6/11/11	-
4	HEM	B	2500	1	-	0/6/54/54	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1500	HEM	C3B-C2B	-4.99	1.33	1.40
4	B	2500	HEM	C3B-C2B	-4.17	1.34	1.40
4	A	1500	HEM	C3C-CAC	-3.67	1.40	1.47
4	A	1500	HEM	C3B-CAB	-3.56	1.40	1.47
2	A	1860	ACT	CH3-C	3.45	1.53	1.48
4	B	2500	HEM	C3C-CAC	-3.02	1.41	1.47
2	B	2860	ACT	CH3-C	3.01	1.52	1.48
4	A	1500	HEM	C3C-C2C	-2.96	1.36	1.40
4	B	2500	HEM	C3B-CAB	-2.74	1.42	1.47
5	A	1765	ILO	CG-CD	-2.39	1.41	1.51
5	A	1765	ILO	CH1-CZ	-2.35	1.42	1.49
4	B	2500	HEM	C1A-NA	2.04	1.40	1.36
4	B	2500	HEM	C3C-C2C	-2.00	1.37	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2765	ILO	CH1-CZ-NE	8.65	125.32	114.24
5	A	1765	ILO	CH1-CZ-NE	8.31	124.89	114.24
4	A	1500	HEM	C4C-C3C-C2C	-3.26	104.62	106.90
4	A	1500	HEM	C4A-C3A-C2A	-3.24	104.74	107.00
4	B	2500	HEM	C3B-C4B-NB	2.40	112.31	109.21
4	B	2500	HEM	CBA-CAA-C2A	-2.02	108.77	112.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

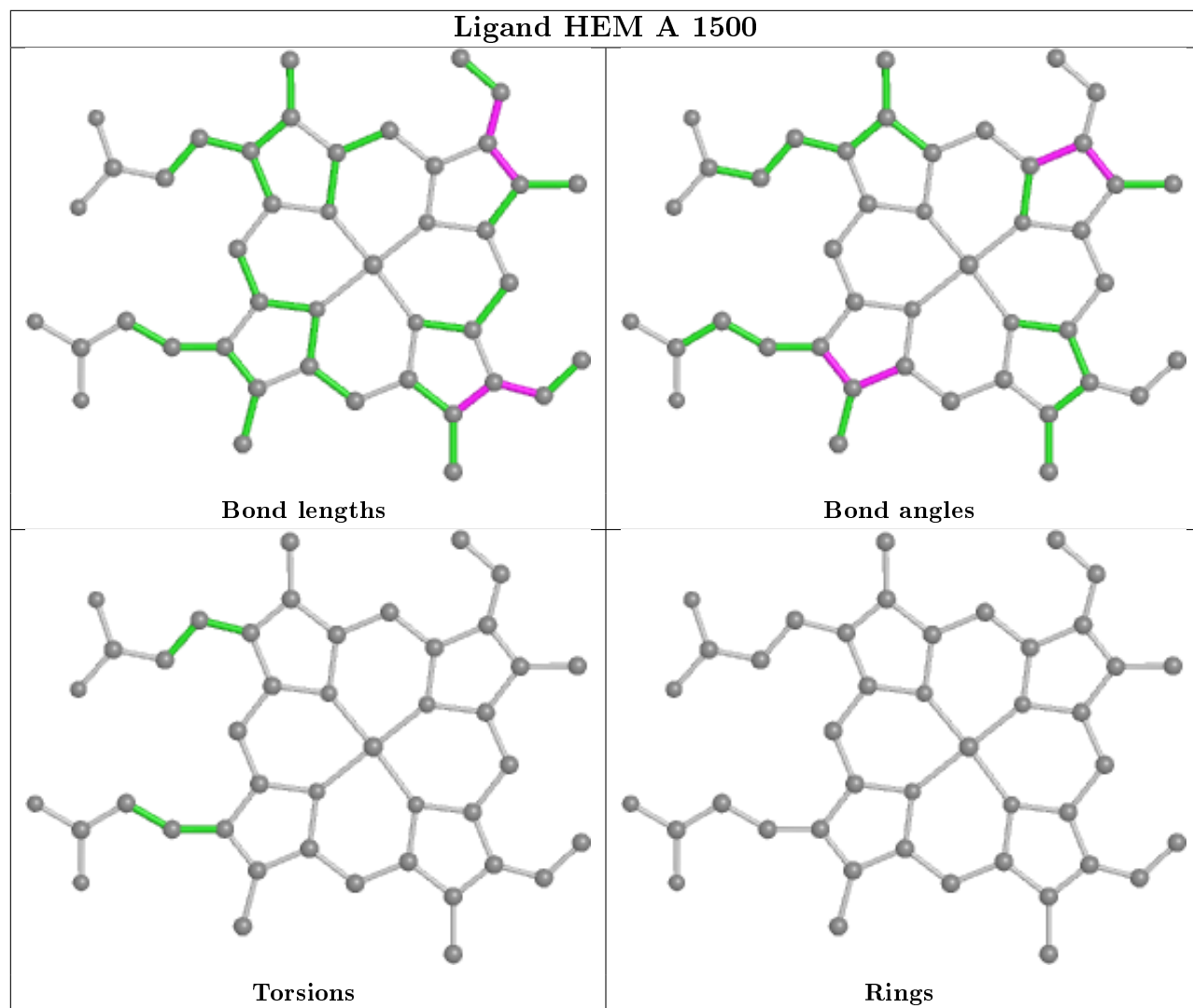
Mol	Chain	Res	Type	Atoms
7	B	2890	GOL	O1-C1-C2-C3
7	B	2890	GOL	O1-C1-C2-O2

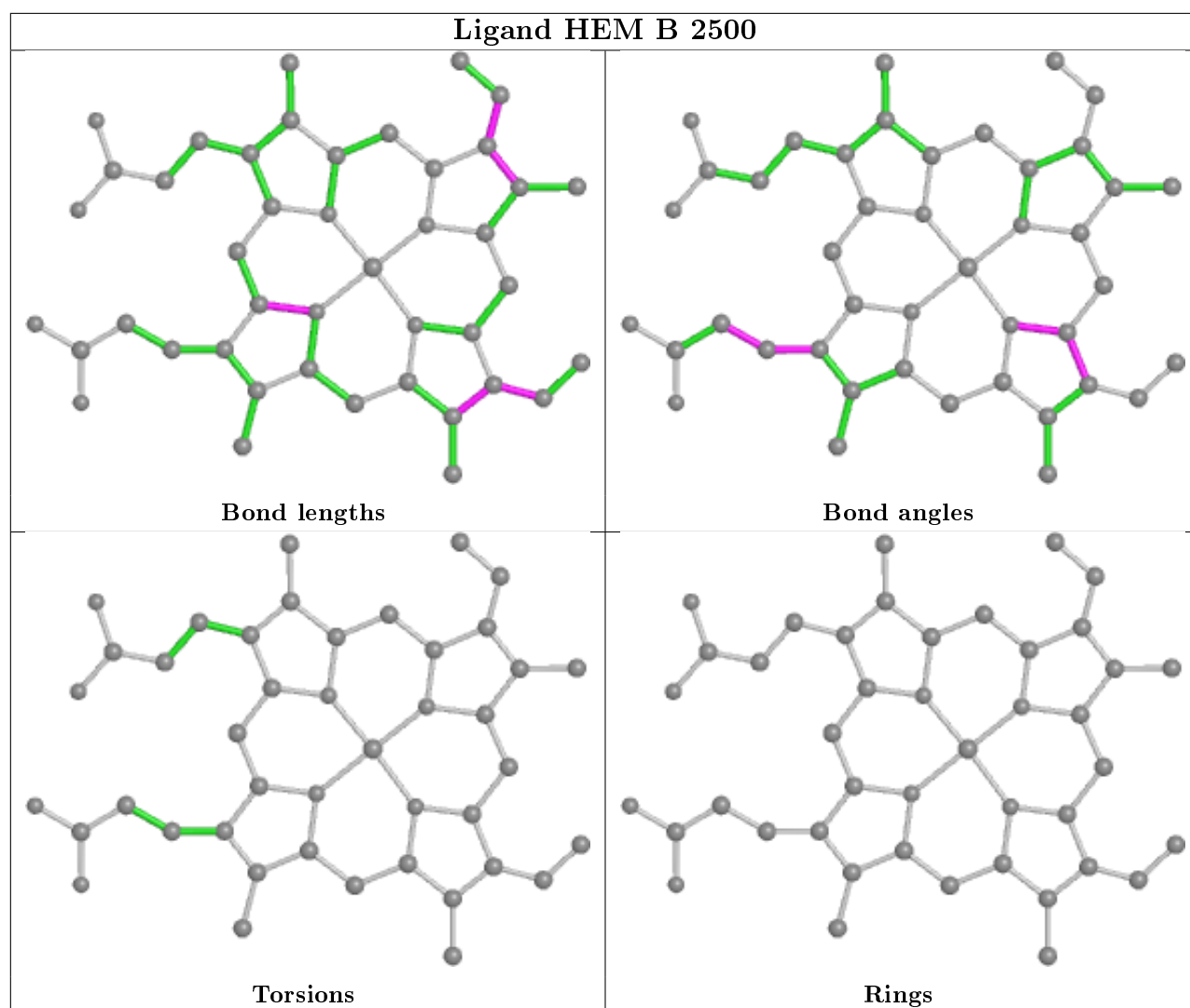
There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1500	HEM	1	0
7	A	1890	GOL	1	0
6	B	2950	CAD	1	0
5	B	2765	ILO	1	0
7	B	2890	GOL	2	0
5	A	1765	ILO	1	0
4	B	2500	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	416/444 (93%)	0.91	60 (14%) 2 2	32, 45, 69, 83	0
1	B	414/444 (93%)	0.88	55 (13%) 3 2	34, 49, 69, 84	0
All	All	830/888 (93%)	0.89	115 (13%) 2 2	32, 47, 69, 84	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	LEU	12.0
1	A	113	THR	12.0
1	A	117	PRO	11.1
1	B	115	PRO	11.0
1	A	119	PRO	10.7
1	B	113	THR	10.1
1	B	117	PRO	9.5
1	A	115	PRO	9.3
1	A	111	LEU	9.2
1	B	119	PRO	9.2
1	B	116	SER	8.2
1	A	118	GLY	7.8
1	B	120	PRO	7.3
1	B	112	GLN	7.3
1	A	122	ALA	7.2
1	B	110	LYS	7.1
1	B	114	ARG	6.7
1	A	114	ARG	6.5
1	A	120	PRO	6.3
1	B	118	GLY	6.3
1	B	121	PRO	5.5
1	A	116	SER	5.4
1	A	112	GLN	5.3
1	A	239	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	5.0
1	B	108	PRO	4.6
1	A	109	ARG	4.6
1	A	121	PRO	4.5
1	A	67	GLY	4.4
1	B	260	ASP	4.4
1	A	110	LYS	4.2
1	A	123	GLU	4.1
1	B	72	ARG	4.1
1	B	142	ARG	4.0
1	B	259	GLN	3.9
1	A	99	ARG	3.8
1	A	259	GLN	3.8
1	A	97	THR	3.7
1	B	146	GLN	3.7
1	B	258	GLN	3.6
1	A	124	GLN	3.6
1	A	238	PRO	3.5
1	B	123	GLU	3.5
1	A	92	GLN	3.5
1	A	258	GLN	3.4
1	B	98	PRO	3.3
1	B	122	ALA	3.3
1	A	160	ALA	3.3
1	A	69	LYS	3.2
1	A	231	THR	3.2
1	A	277	ILE	3.1
1	B	277	ILE	3.1
1	B	261	GLY	3.0
1	A	343	LEU	3.0
1	B	70	PHE	3.0
1	B	83	TYR	3.0
1	A	146	GLN	3.0
1	B	451	VAL	3.0
1	B	141	LYS	2.9
1	A	260	ASP	2.9
1	A	301	ALA	2.9
1	A	262	SER	2.8
1	A	338	VAL	2.8
1	B	282	THR	2.8
1	A	93	ASP	2.8
1	B	390	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	98	PRO	2.6
1	A	304	LEU	2.6
1	B	482	TRP	2.6
1	B	147	ALA	2.6
1	A	130	ARG	2.6
1	B	140	ILE	2.6
1	B	94	GLY	2.6
1	A	223	ARG	2.5
1	A	250	LEU	2.5
1	A	94	GLY	2.5
1	B	200	ALA	2.5
1	A	257	ARG	2.5
1	B	81	ILE	2.5
1	A	390	ARG	2.5
1	A	482	TRP	2.5
1	A	200	ALA	2.5
1	B	109	ARG	2.4
1	B	262	SER	2.4
1	B	449	TRP	2.4
1	B	239	GLY	2.4
1	B	124	GLN	2.4
1	B	143	SER	2.3
1	B	383	VAL	2.3
1	B	92	GLN	2.3
1	A	232	VAL	2.3
1	B	93	ASP	2.3
1	B	448	ALA	2.2
1	A	233	PHE	2.2
1	B	153	GLN	2.2
1	A	230	ILE	2.2
1	A	337	ALA	2.2
1	B	414	LEU	2.2
1	B	338	VAL	2.2
1	A	91	GLN	2.2
1	A	157	ALA	2.2
1	A	353	ALA	2.2
1	B	355	PHE	2.2
1	A	369	LEU	2.2
1	A	156	GLU	2.2
1	B	99	ARG	2.1
1	A	278	GLN	2.1
1	A	276	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	233	PHE	2.1
1	A	416	LYS	2.1
1	B	322	LEU	2.1
1	B	324	TRP	2.0
1	A	354	PRO	2.0
1	B	450	ILE	2.0
1	A	274	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

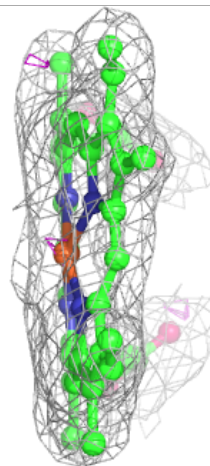
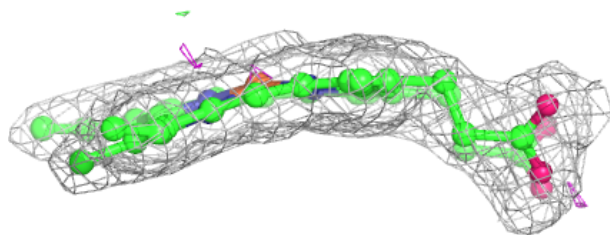
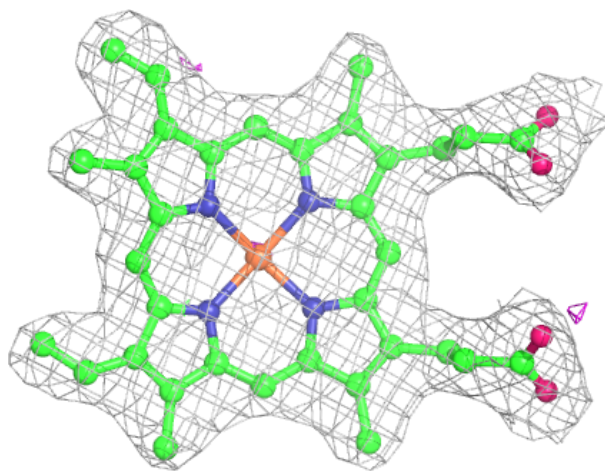
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	A	1890	6/6	0.86	0.39	74,74,74,74	0
2	ACT	A	1860	4/4	0.87	0.16	51,52,53,54	0
7	GOL	B	2890	6/6	0.87	0.33	61,62,62,62	0
6	CAD	B	2950	3/5	0.94	0.29	61,61,61,63	3
5	ILO	A	1765	12/12	0.95	0.23	32,36,39,39	0
5	ILO	B	2765	12/12	0.96	0.20	30,34,35,36	0
2	ACT	B	2860	4/4	0.96	0.10	52,52,52,52	0
6	CAD	A	1950	3/5	0.96	0.26	43,43,44,45	3
4	HEM	A	1500	43/43	0.98	0.17	30,33,39,41	0
4	HEM	B	2500	43/43	0.98	0.18	32,34,38,39	0
3	ZN	A	900	1/1	0.99	0.04	62,62,62,62	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.

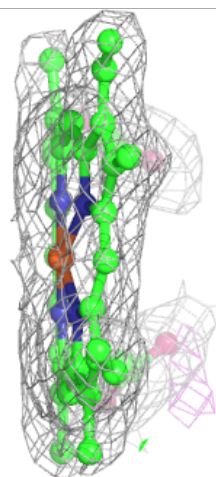
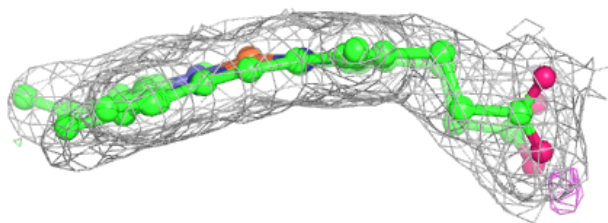
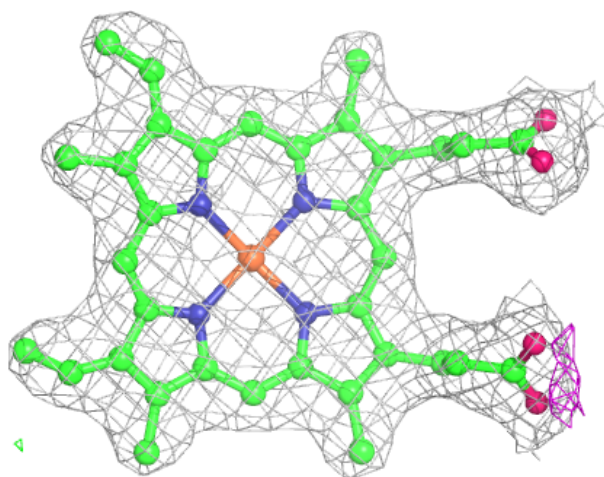
**Electron density around HEM A 1500:**

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



**Electron density around HEM B 2500:**

$2mF_o-DF_c$  (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.