



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:47 pm BST

PDB ID : 1FOP
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN
COMPLEXED WITH L-ARG AND NO(H4B-BOUND)
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Deposited on : 2000-08-28
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

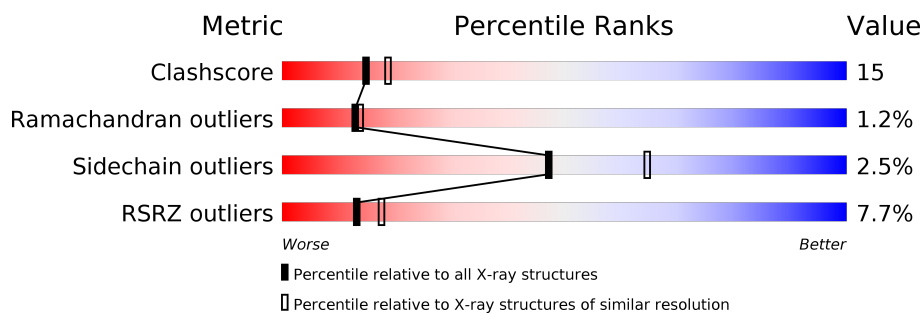
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	444	
1	B	444	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	1860	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7047 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.

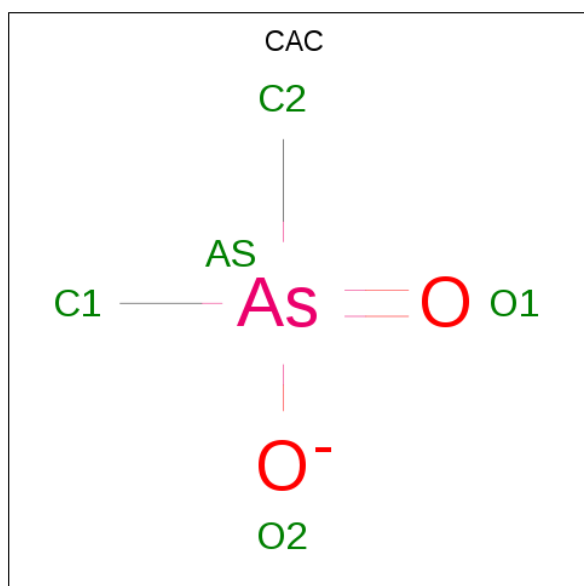
- Molecule 1 is a protein called NITRIC-OXIDE SYNTHASE.

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 CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



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

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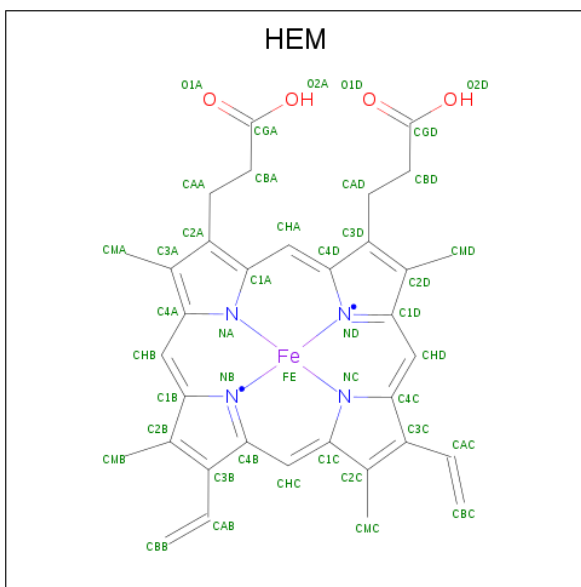
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	As	C	0	0
			3	1	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



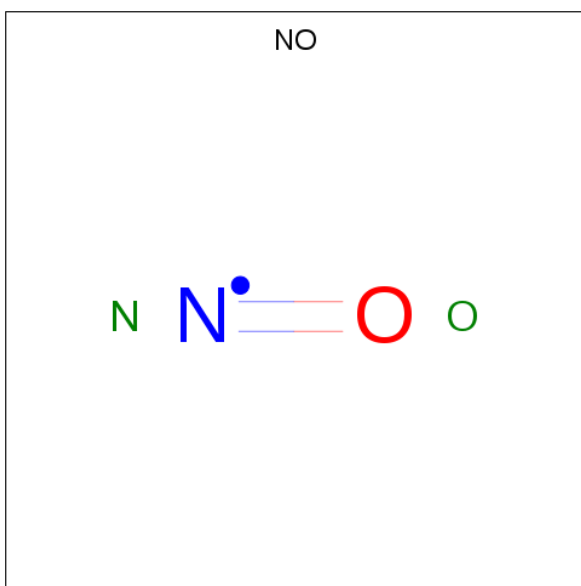
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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



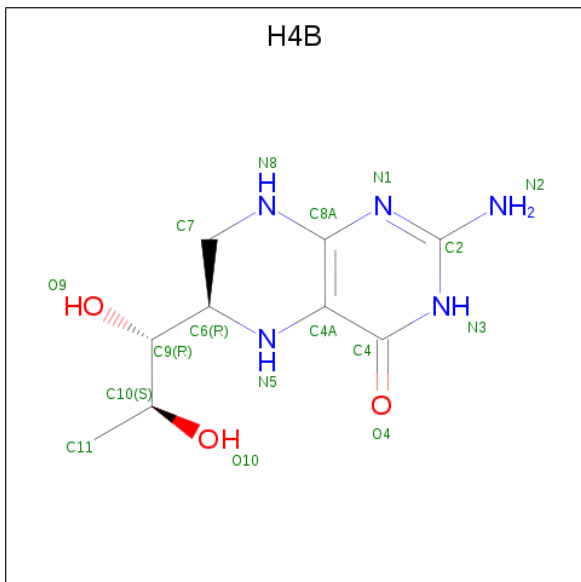
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is NITRIC OXIDE (three-letter code: NO) (formula: NO).



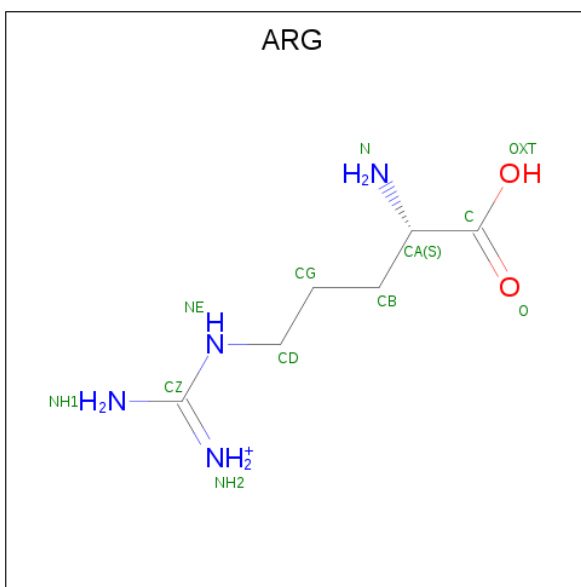
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			2	1	1		
5	B	1	Total	N	O	0	0
			2	1	1		

- Molecule 6 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 17	C 9	N 5	O 3	0	0
6	B	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 7 is ARGinine (three-letter code: ARG) (formula: $\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			12	6	4	2		
7	B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Zn	0	0
			1	1		

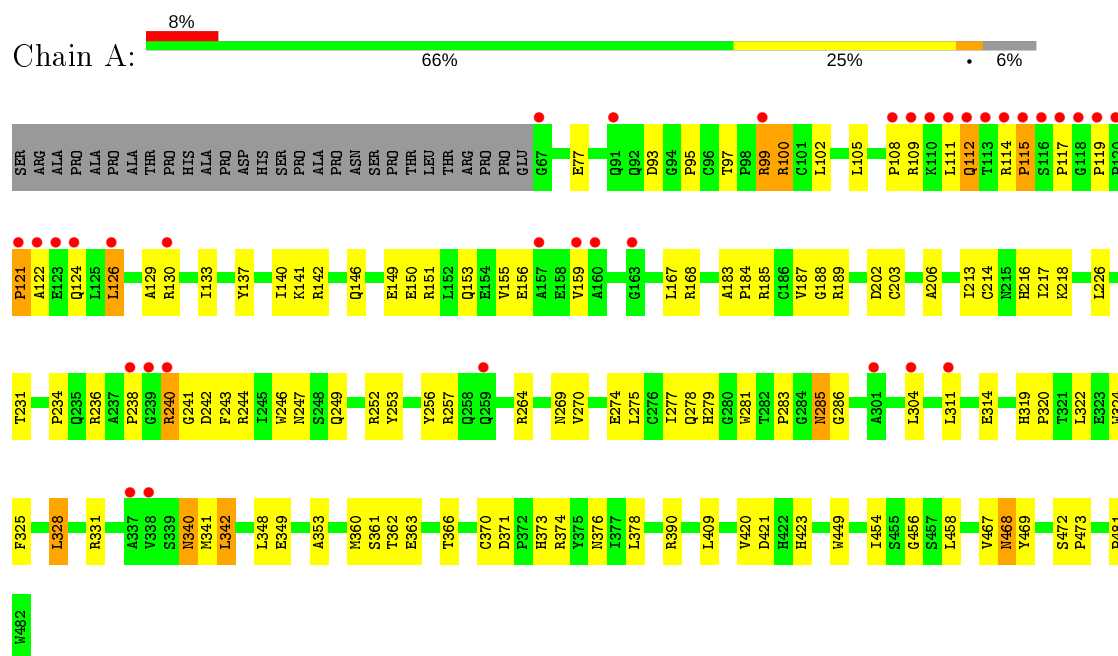
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	144	Total	O	0	0
			144	144		
10	B	135	Total	O	0	0
			135	135		

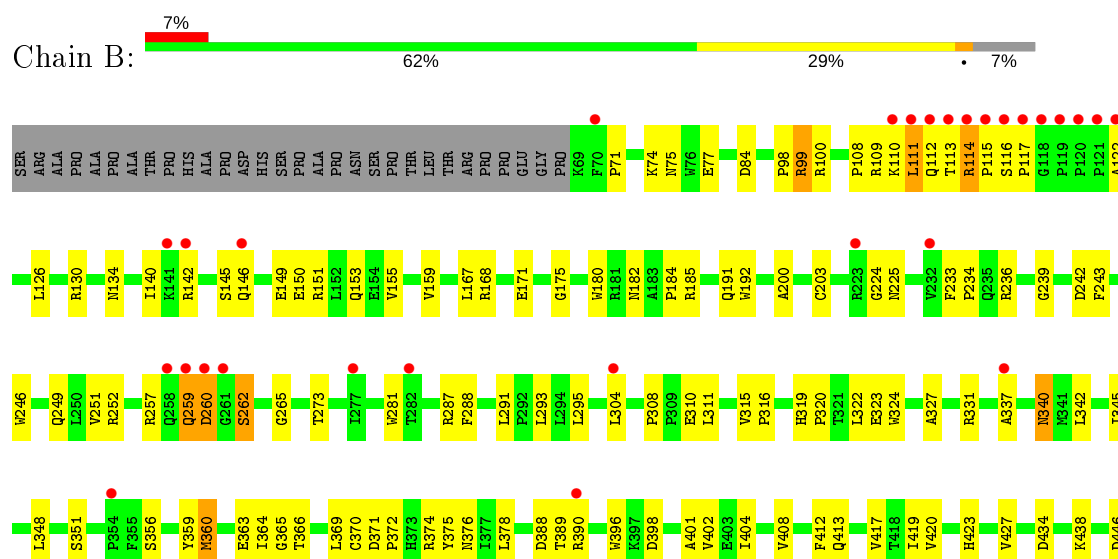
3 Residue-property plots

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



W449	I450	S455	G456	S457	L458	T459	P460	V461	F462	E465	R466	V467	R468	Y469	I470	L471	S472	P473	A474	P481	W482
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.55Å 106.25Å 156.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.19 – 2.30 39.19 – 2.29	Depositor EDS
% Data completeness (in resolution range)	78.5 (39.19-2.30) 83.7 (39.19-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.277 0.235 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7047	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, NO, ACT, CAC, 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	0.38	0/3397	0.62	0/4631
1	B	0.37	0/3385	0.62	2/4614 (0.0%)
All	All	0.37	0/6782	0.62	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(°)	Ideal(°)
1	B	243	PHE	N-CA-C	-5.19	96.98	111.00
1	B	360	MET	N-CA-C	-5.00	97.49	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	102	0
1	B	3291	0	3205	102	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	4	0	3	2	0
3	B	4	0	3	1	0
4	A	43	0	30	2	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	2	0	0	1	0
5	B	2	0	0	0	0
6	A	17	0	15	1	0
6	B	17	0	15	1	0
7	A	12	0	12	2	0
7	B	12	0	12	1	0
8	A	6	0	8	0	0
8	B	6	0	8	0	0
9	B	1	0	0	0	0
10	A	144	0	0	4	0
10	B	135	0	0	4	0
All	All	7047	0	6556	202	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 15.

All (202) 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:119:PRO:HG3	1:A:238:PRO:HB3	1.44	0.97
1:A:99:ARG:HB2	1:A:99:ARG:HH11	1.28	0.97
1:B:259:GLN:HG2	1:B:260:ASP:H	1.30	0.95
1:B:340:ASN:HD22	1:B:340:ASN:H	1.24	0.85
1:B:378:LEU:HB2	10:B:2964:HOH:O	1.76	0.85
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.59	0.84
1:A:285:ASN:C	1:A:285:ASN:HD22	1.82	0.83
1:A:264:ARG:HG3	1:A:264:ARG:HH11	1.48	0.77
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.17	0.74
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.69	0.74
1:B:251:VAL:O	1:B:252:ARG:HG2	1.91	0.70
1:B:259:GLN:HG2	1:B:260:ASP:N	2.04	0.70
1:A:115:PRO:O	1:A:117:PRO:HD3	1.93	0.69
1:B:388:ASP:OD1	1:B:390:ARG:HB3	1.94	0.67
1:A:285:ASN:C	1:A:285:ASN:ND2	2.49	0.66
1:B:293:LEU:HB3	1:B:295:LEU:HD21	1.78	0.65
1:B:423:HIS:O	1:B:427:VAL:HG23	1.97	0.65
1:B:114:ARG:HA	1:B:114:ARG:HH11	1.61	0.64
1:B:182:ASN:O	1:B:184:PRO:HD3	1.98	0.63
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.78	0.63
1:A:111:LEU:HD12	1:A:111:LEU:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLU:O	1:A:153:GLN:HG2	1.99	0.62
1:A:99:ARG:NH1	1:A:99:ARG:HB2	2.09	0.62
1:A:126:LEU:HD12	1:A:130:ARG:HD2	1.81	0.61
1:A:151:ARG:HD3	1:A:168:ARG:CZ	2.30	0.61
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.66	0.61
1:B:110:LYS:C	1:B:112:GLN:H	2.04	0.60
1:B:471:LEU:O	1:B:474:ALA:HB2	2.01	0.60
1:A:184:PRO:HB3	1:A:468:ASN:HD21	1.67	0.60
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.84	0.59
1:B:151:ARG:O	1:B:155:VAL:HG23	2.03	0.59
1:B:110:LYS:O	1:B:112:GLN:N	2.35	0.59
1:B:149:GLU:O	1:B:153:GLN:HG3	2.02	0.59
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.39	0.58
1:B:122:ALA:O	1:B:126:LEU:HB2	2.02	0.58
1:B:449:TRP:HA	6:B:2600:H4B:N1	2.18	0.58
1:B:109:ARG:HB2	10:B:2969:HOH:O	2.04	0.58
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.85	0.57
1:B:389:THR:HA	1:B:396:TRP:CD1	2.39	0.57
1:A:151:ARG:HD3	1:A:168:ARG:NH2	2.20	0.57
1:A:378:LEU:HB2	10:A:2079:HOH:O	2.05	0.57
1:A:126:LEU:HD11	1:A:156:GLU:CG	2.35	0.57
1:B:71:PRO:HG2	1:B:84:ASP:HB3	1.87	0.57
1:B:259:GLN:HG2	1:B:260:ASP:OD1	2.04	0.57
1:B:265:GLY:HA2	1:B:287:ARG:HA	1.88	0.56
1:A:188:GLY:HA2	3:A:1860:ACT:CH3	2.35	0.56
1:B:175:GLY:HA3	1:B:345:ILE:HD13	1.88	0.56
1:A:146:GLN:O	1:A:150:GLU:HG3	2.06	0.56
1:A:270:VAL:O	1:A:274:GLU:HG3	2.07	0.55
1:B:446:ASP:O	1:B:450:ILE:HG12	2.06	0.55
1:A:246:TRP:CD1	1:A:481:PRO:HG3	2.43	0.54
1:B:363:GLU:OE2	7:B:2700:ARG:HB2	2.08	0.54
1:A:264:ARG:NH1	1:A:264:ARG:HG3	2.19	0.54
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.43	0.54
1:B:140:ILE:O	1:B:142:ARG:HG2	2.08	0.54
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.73	0.54
1:A:472:SER:HA	1:A:473:PRO:O	2.09	0.53
1:A:363:GLU:OE2	7:A:1700:ARG:HB2	2.08	0.53
1:B:249:GLN:HB2	1:B:252:ARG:HD2	1.90	0.53
1:A:121:PRO:O	1:A:124:GLN:N	2.41	0.53
1:A:472:SER:HA	1:A:473:PRO:C	2.29	0.53
1:A:340:ASN:HD22	1:A:340:ASN:H	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:HA	1:A:140:ILE:HG12	1.90	0.53
1:A:458:LEU:HD11	1:B:401:ALA:CB	2.40	0.52
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.39	0.52
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.25	0.52
1:A:105:LEU:HA	1:B:465:GLU:HG2	1.92	0.52
1:B:472:SER:HA	1:B:473:PRO:C	2.30	0.52
1:B:108:PRO:HG3	10:B:2983:HOH:O	2.10	0.52
1:B:404:ILE:O	1:B:408:VAL:HG23	2.10	0.52
1:A:111:LEU:HD22	10:A:2050:HOH:O	2.10	0.52
1:B:434:ASP:OD1	1:B:438:LYS:HE3	2.10	0.51
1:A:240:ARG:HD3	1:A:241:GLY:O	2.11	0.51
1:A:366:THR:HG21	1:A:454:ILE:HG23	1.93	0.51
1:A:109:ARG:HG2	1:A:109:ARG:NH1	2.26	0.51
1:A:458:LEU:HD11	1:B:401:ALA:HB2	1.92	0.51
1:B:310:GLU:CD	1:B:310:GLU:H	2.14	0.51
1:A:188:GLY:HA2	3:A:1860:ACT:H3	1.91	0.51
1:B:457:SER:HA	1:B:462:PHE:CG	2.46	0.51
1:A:114:ARG:HG3	1:A:115:PRO:HD2	1.92	0.50
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.92	0.50
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.92	0.50
1:A:146:GLN:HG2	1:A:150:GLU:OE2	2.12	0.49
1:B:340:ASN:N	1:B:340:ASN:HD22	1.95	0.49
1:B:342:LEU:HD23	1:B:342:LEU:C	2.33	0.49
1:A:325:PHE:O	1:A:328:LEU:HB2	2.12	0.49
1:B:340:ASN:H	1:B:340:ASN:ND2	2.03	0.49
1:A:342:LEU:HD11	1:A:349:GLU:HB3	1.95	0.49
1:A:141:LYS:O	1:A:142:ARG:NH1	2.45	0.49
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.94	0.49
1:A:360:MET:CE	1:A:362:THR:OG1	2.61	0.49
1:B:116:SER:N	1:B:236:ARG:NH2	2.59	0.49
1:B:251:VAL:C	1:B:252:ARG:HG2	2.32	0.49
1:A:253:TYR:O	1:A:269:ASN:ND2	2.43	0.49
1:B:308:PRO:HB3	1:B:310:GLU:OE1	2.12	0.48
1:A:275:LEU:O	1:A:279:HIS:HD2	1.96	0.48
1:B:323:GLU:HG2	1:B:324:TRP:N	2.28	0.48
1:B:324:TRP:O	1:B:327:ALA:HB3	2.13	0.48
1:A:93:ASP:HB3	1:B:98:PRO:HB3	1.95	0.48
1:B:108:PRO:HB2	1:B:111:LEU:HB2	1.95	0.48
1:B:116:SER:N	1:B:236:ARG:HH22	2.11	0.48
1:B:246:TRP:CD1	1:B:481:PRO:HG3	2.48	0.48
1:A:360:MET:HA	1:A:420:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:GLY:HA2	1:B:369:LEU:HD12	1.95	0.48
1:A:226:LEU:HD12	1:A:226:LEU:N	2.29	0.47
1:A:373:HIS:ND1	1:B:77:GLU:HA	2.28	0.47
1:B:249:GLN:HB2	1:B:252:ARG:CD	2.43	0.47
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.96	0.47
1:A:102:LEU:HB3	1:A:105:LEU:HD22	1.96	0.47
4:B:500:HEM:HBC2	4:B:500:HEM:HMC1	1.95	0.47
1:B:74:LYS:CG	1:B:75:ASN:N	2.77	0.47
1:A:213:ILE:O	1:A:217:ILE:HG13	2.15	0.47
1:A:360:MET:HE1	1:A:362:THR:OG1	2.15	0.47
1:B:155:VAL:O	1:B:159:VAL:HG23	2.15	0.47
1:A:216:HIS:CD2	1:A:216:HIS:C	2.88	0.46
1:B:116:SER:N	1:B:117:PRO:CD	2.78	0.46
1:B:273:THR:OG1	1:B:291:LEU:HD21	2.15	0.46
1:A:234:PRO:HB2	1:A:243:PHE:CD1	2.51	0.46
1:A:449:TRP:HA	6:A:1600:H4B:N1	2.31	0.46
1:A:155:VAL:O	1:A:159:VAL:HG23	2.16	0.46
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.98	0.46
1:A:249:GLN:HB2	1:A:252:ARG:CG	2.44	0.46
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.50	0.46
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.51	0.46
1:B:366:THR:O	1:B:370:CYS:HB2	2.16	0.46
1:A:214:CYS:O	1:A:218:LYS:HG3	2.16	0.45
1:B:146:GLN:HE21	1:B:150:GLU:CG	2.29	0.45
1:B:412:PHE:CG	1:B:419:ILE:HD12	2.51	0.45
1:A:184:PRO:HB3	1:A:468:ASN:ND2	2.31	0.45
1:B:168:ARG:HB2	1:B:171:GLU:HG3	1.98	0.45
1:B:308:PRO:HB2	1:B:311:LEU:HD13	1.98	0.45
1:A:274:GLU:O	1:A:278:GLN:HG3	2.16	0.45
1:A:285:ASN:HD22	1:A:286:GLY:N	2.15	0.45
1:A:421:ASP:OD2	1:A:423:HIS:HB2	2.17	0.45
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.52	0.44
1:A:121:PRO:O	1:A:122:ALA:C	2.55	0.44
1:A:236:ARG:NE	1:A:242:ASP:OD1	2.49	0.44
1:B:281:TRP:HB2	1:B:304:LEU:HD21	2.00	0.44
1:A:409:LEU:HD21	1:A:421:ASP:HB3	1.99	0.44
1:A:99:ARG:CB	1:A:99:ARG:HH11	2.13	0.44
1:A:390:ARG:HB2	1:A:390:ARG:HE	1.59	0.44
1:B:224:GLY:O	1:B:417:VAL:HA	2.17	0.44
1:B:200:ALA:O	1:B:203:CYS:HB2	2.16	0.44
1:B:457:SER:HA	1:B:462:PHE:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:THR:HB	1:B:460:PRO:HD2	1.99	0.44
1:A:167:LEU:HG	1:A:348:LEU:HD12	1.99	0.44
5:A:1910:NO:O	7:A:1700:ARG:HD3	2.18	0.44
1:B:388:ASP:C	1:B:390:ARG:H	2.21	0.43
1:A:95:PRO:HB3	1:A:108:PRO:HB2	1.99	0.43
1:B:371:ASP:HB2	1:B:374:ARG:CG	2.48	0.43
1:A:340:ASN:N	1:A:340:ASN:HD22	2.13	0.43
1:A:341:MET:SD	4:A:500:HEM:HBD2	2.58	0.43
1:A:371:ASP:HB2	1:A:374:ARG:HG2	2.01	0.43
1:A:97:THR:HG23	1:A:100:ARG:NH1	2.34	0.43
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.54	0.43
1:B:185:ARG:HD3	1:B:449:TRP:CD2	2.53	0.43
1:B:323:GLU:HG2	1:B:324:TRP:H	1.83	0.43
1:B:109:ARG:HG2	1:B:109:ARG:NH1	2.33	0.43
1:B:310:GLU:N	1:B:310:GLU:OE2	2.47	0.43
1:A:231:THR:O	1:A:353:ALA:HA	2.19	0.43
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.59	0.43
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.88	0.43
1:A:226:LEU:CD1	1:A:226:LEU:H	2.32	0.43
1:B:191:GLN:HB3	10:B:2954:HOH:O	2.18	0.43
1:B:242:ASP:HB3	1:B:351:SER:OG	2.18	0.43
1:B:337:ALA:CB	1:B:356:SER:HB3	2.49	0.42
1:A:226:LEU:H	1:A:226:LEU:HD12	1.84	0.42
1:A:206:ALA:HB2	10:A:2063:HOH:O	2.19	0.42
1:A:202:ASP:OD1	1:A:203:CYS:N	2.53	0.42
1:A:361:SER:OG	1:A:421:ASP:HA	2.19	0.42
1:B:467:VAL:HG12	1:B:469:TYR:HD2	1.84	0.42
1:B:113:THR:HG21	1:B:342:LEU:HD13	2.02	0.42
1:B:375:TYR:O	1:B:376:ASN:C	2.57	0.42
1:A:126:LEU:HD23	1:A:159:VAL:HG11	2.01	0.42
1:B:360:MET:HA	1:B:420:VAL:O	2.20	0.42
1:A:257:ARG:HA	1:A:257:ARG:HD2	1.82	0.42
1:A:378:LEU:HA	1:A:378:LEU:HD12	1.93	0.42
1:A:467:VAL:HG12	1:A:469:TYR:HD2	1.85	0.42
1:B:288:PHE:HB2	1:B:331:ARG:HD3	2.01	0.42
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.55	0.42
1:A:183:ALA:O	1:A:189:ARG:CZ	2.68	0.42
1:B:249:GLN:HB2	1:B:252:ARG:CG	2.50	0.42
1:B:191:GLN:HG3	3:B:2860:ACT:H2	2.01	0.41
1:A:187:VAL:O	1:A:187:VAL:HG22	2.20	0.41
1:B:109:ARG:HH11	1:B:109:ARG:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:TYR:HB2	1:A:264:ARG:HB3	2.02	0.41
1:A:340:ASN:ND2	1:A:340:ASN:H	2.18	0.41
1:A:129:ALA:O	1:A:133:ILE:HG12	2.21	0.41
1:A:371:ASP:HB2	1:A:374:ARG:CG	2.51	0.41
1:B:260:ASP:C	1:B:262:SER:H	2.24	0.41
4:A:500:HEM:HAD1	10:A:2070:HOH:O	2.20	0.41
1:A:247:ASN:OD1	1:A:247:ASN:N	2.54	0.41
1:A:314:GLU:CD	1:A:331:ARG:HH21	2.25	0.41
4:B:500:HEM:CMC	4:B:500:HEM:HBC2	2.50	0.41
1:B:117:PRO:O	1:B:239:GLY:N	2.54	0.41
1:B:130:ARG:O	1:B:134:ASN:ND2	2.54	0.41
1:A:277:ILE:HD11	1:A:283:PRO:HB3	2.02	0.40
1:B:398:ASP:O	1:B:402:VAL:HG23	2.20	0.40
1:B:315:VAL:HA	1:B:316:PRO:HD3	1.87	0.40
1:B:359:TYR:CD2	1:B:364:ILE:HD11	2.55	0.40
1:B:467:VAL:HG12	1:B:469:TYR:CD2	2.56	0.40
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.62	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%)	380 (92%)	30 (7%)	4 (1%)	15	17
1	B	412/444 (93%)	373 (90%)	33 (8%)	6 (2%)	10	10
All	All	826/888 (93%)	753 (91%)	63 (8%)	10 (1%)	13	14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLN

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Mol	Chain	Res	Type
1	B	111	LEU
1	B	259	GLN
1	B	260	ASP
1	B	145	SER
1	B	262	SER
1	A	121	PRO
1	A	115	PRO
1	B	115	PRO
1	A	456	GLY

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%)	343 (97%)	11 (3%)	40	55
1	B	353/377 (94%)	346 (98%)	7 (2%)	55	72
All	All	707/754 (94%)	689 (98%)	18 (2%)	47	65

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	100	ARG
1	A	112	GLN
1	A	126	LEU
1	A	240	ARG
1	A	285	ASN
1	A	328	LEU
1	A	340	ASN
1	A	342	LEU
1	A	376	ASN
1	A	468	ASN
1	B	99	ARG
1	B	100	ARG
1	B	114	ARG

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Mol	Chain	Res	Type
1	B	225	ASN
1	B	257	ARG
1	B	340	ASN
1	B	413	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	191	GLN
1	A	278	GLN
1	A	279	HIS
1	A	285	ASN
1	A	296	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	89	GLN
1	B	92	GLN
1	B	134	ASN
1	B	146	GLN
1	B	191	GLN
1	B	215	ASN
1	B	222	ASN
1	B	225	ASN
1	B	278	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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$
5	NO	A	1910	4	0,1,1	0.00	-	-		
8	GOL	A	1880	-	5,5,5	0.21	0	5,5,5	0.27	0
8	GOL	B	2880	-	5,5,5	0.23	0	5,5,5	0.20	0
4	HEM	A	500	1,5	27,50,50	1.47	5 (18%)	17,82,82	1.61	2 (11%)
2	CAC	A	1950	1	0,2,4	0.00	-	0,1,6	0.00	-
3	ACT	B	2860	-	1,3,3	3.51	1 (100%)	0,3,3	0.00	-
6	H4B	A	1600	-	16,18,18	2.17	5 (31%)	11,26,26	4.19	8 (72%)
6	H4B	B	2600	-	16,18,18	2.20	3 (18%)	11,26,26	4.34	8 (72%)
5	NO	B	2910	4	0,1,1	0.00	-	-		
3	ACT	A	1860	-	1,3,3	3.22	1 (100%)	0,3,3	0.00	-
2	CAC	B	2950	1	0,2,4	0.00	-	0,1,6	0.00	-
4	HEM	B	500	1,5	27,50,50	1.57	4 (14%)	17,82,82	1.66	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
8	GOL	A	1880	-	-	0/4/4/4	-
8	GOL	B	2880	-	-	0/4/4/4	-
4	HEM	A	500	1,5	-	0/6/54/54	-
6	H4B	B	2600	-	-	0/8/17/17	0/2/2/2
6	H4B	A	1600	-	-	0/8/17/17	0/2/2/2
4	HEM	B	500	1,5	-	0/6/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2600	H4B	C4-N3	5.80	1.43	1.33
6	A	1600	H4B	C4-N3	5.13	1.42	1.33
6	A	1600	H4B	C6-N5	4.23	1.54	1.45
6	A	1600	H4B	C4A-N5	4.11	1.46	1.38
6	B	2600	H4B	C4A-N5	4.05	1.46	1.38
4	B	500	HEM	C3B-C2B	-3.61	1.35	1.40
4	B	500	HEM	C3B-CAB	-3.52	1.40	1.47
3	B	2860	ACT	CH3-C	3.51	1.53	1.48
6	B	2600	H4B	C6-N5	3.48	1.52	1.45
4	A	500	HEM	C3B-CAB	-3.30	1.41	1.47
3	A	1860	ACT	CH3-C	3.22	1.52	1.48
4	A	500	HEM	C4A-NA	3.19	1.42	1.36
4	B	500	HEM	C3C-C2C	-3.15	1.36	1.40
4	A	500	HEM	C3C-CAC	-3.05	1.41	1.47
4	A	500	HEM	C3B-C2B	-2.44	1.37	1.40
6	A	1600	H4B	C8A-N1	2.27	1.38	1.34
4	B	500	HEM	C3C-CAC	-2.19	1.43	1.47
4	A	500	HEM	C4B-NB	2.15	1.40	1.36
6	A	1600	H4B	C7-N8	2.04	1.48	1.44

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2600	H4B	C4-C4A-C8A	9.38	122.90	114.57
6	A	1600	H4B	C4-C4A-C8A	8.82	122.40	114.57
6	A	1600	H4B	C4-N3-C2	5.70	124.99	115.93
6	B	2600	H4B	C4-N3-C2	5.49	124.65	115.93
6	B	2600	H4B	N3-C2-N1	-5.32	117.07	125.42
4	B	500	HEM	CBA-CAA-C2A	-4.99	103.28	112.49
6	A	1600	H4B	N3-C2-N1	-4.97	117.63	125.42
4	A	500	HEM	C4A-C3A-C2A	-4.93	103.57	107.00
6	A	1600	H4B	N2-C2-N1	3.70	123.01	117.25
6	B	2600	H4B	C2-N1-C8A	3.64	122.69	114.54
6	B	2600	H4B	C4A-C4-N3	-3.61	113.75	124.01
6	A	1600	H4B	C2-N1-C8A	3.60	122.60	114.54
6	A	1600	H4B	C4A-C4-N3	-3.51	114.03	124.01
6	B	2600	H4B	N2-C2-N1	3.42	122.57	117.25
6	B	2600	H4B	C4-C4A-N5	-3.00	116.60	119.12
6	A	1600	H4B	C4A-N5-C6	-2.74	113.71	121.16
6	B	2600	H4B	C4A-N5-C6	-2.58	114.13	121.16
6	A	1600	H4B	C4-C4A-N5	-2.45	117.07	119.12
4	B	500	HEM	C4C-C3C-C2C	-2.38	105.23	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	HEM	C1D-C2D-C3D	-2.02	105.59	107.00

There are no chirality outliers.

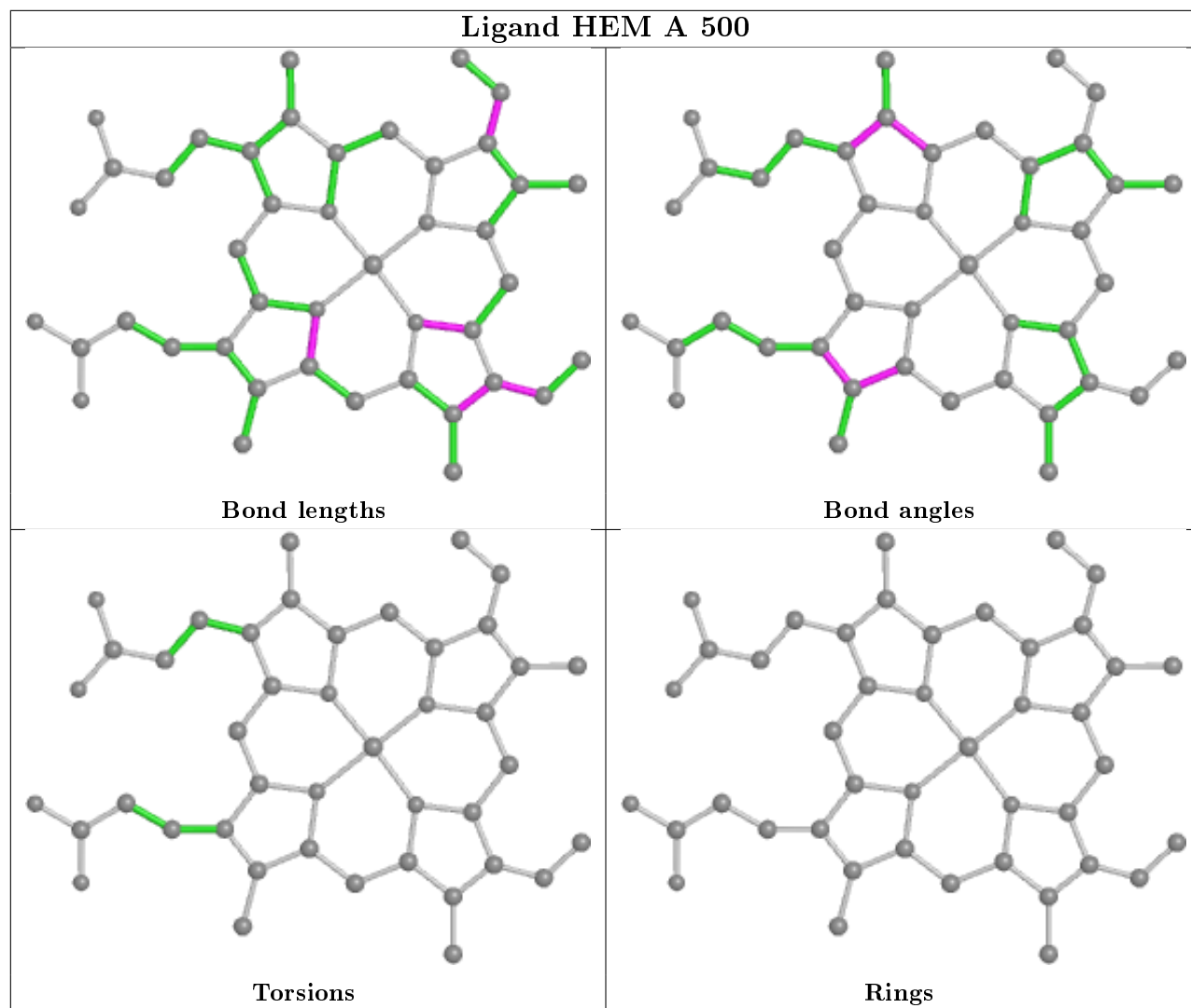
There are no torsion outliers.

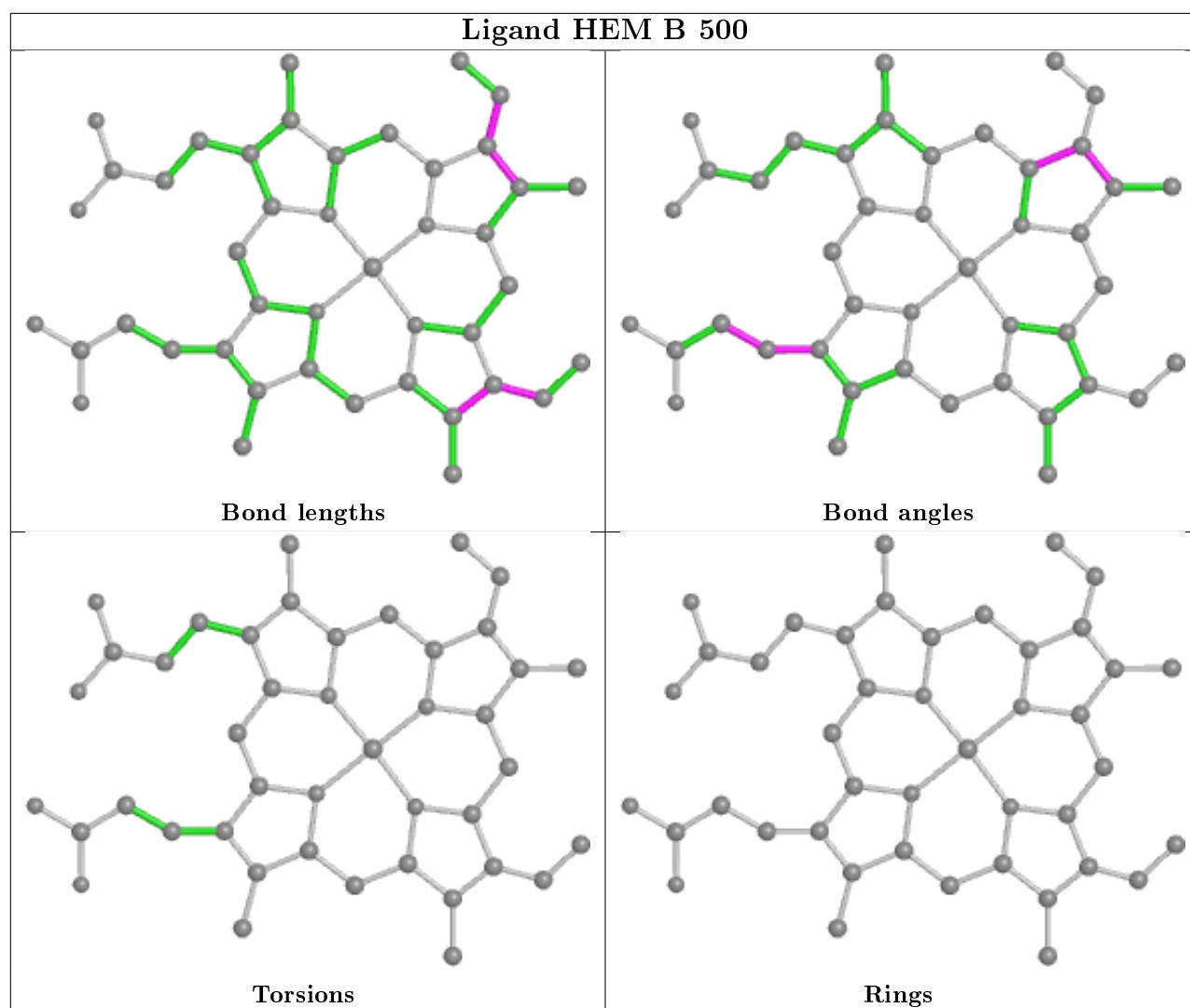
There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1910	NO	1	0
4	A	500	HEM	2	0
3	B	2860	ACT	1	0
6	A	1600	H4B	1	0
6	B	2600	H4B	1	0
3	A	1860	ACT	2	0
4	B	500	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	416/444 (93%)	0.47	35 (8%) 11 15	26, 47, 73, 101	0
1	B	414/444 (93%)	0.50	29 (7%) 16 21	28, 51, 75, 101	0
All	All	830/888 (93%)	0.49	64 (7%) 13 17	26, 49, 74, 101	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	PRO	11.4
1	A	118	GLY	10.7
1	B	119	PRO	9.6
1	A	119	PRO	9.5
1	B	118	GLY	8.7
1	A	117	PRO	8.7
1	B	113	THR	8.4
1	A	113	THR	7.8
1	B	115	PRO	7.2
1	A	111	LEU	7.0
1	B	111	LEU	6.8
1	A	115	PRO	6.7
1	B	116	SER	6.6
1	B	110	LYS	6.5
1	A	116	SER	6.4
1	B	120	PRO	5.8
1	A	120	PRO	5.0
1	B	114	ARG	5.0
1	A	121	PRO	4.9
1	B	121	PRO	4.6
1	A	239	GLY	4.3
1	A	123	GLU	4.0
1	A	114	ARG	4.0
1	B	112	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	122	ALA	3.8
1	A	110	LYS	3.8
1	B	277	ILE	3.7
1	A	159	VAL	3.5
1	A	259	GLN	3.5
1	A	157	ALA	3.4
1	B	259	GLN	3.3
1	B	146	GLN	3.0
1	A	238	PRO	3.0
1	B	142	ARG	2.9
1	A	124	GLN	2.9
1	B	261	GLY	2.8
1	A	160	ALA	2.8
1	B	70	PHE	2.8
1	B	223	ARG	2.6
1	A	99	ARG	2.6
1	B	390	ARG	2.5
1	A	301	ALA	2.5
1	A	109	ARG	2.5
1	B	260	ASP	2.5
1	B	258	GLN	2.5
1	A	338	VAL	2.5
1	A	130	ARG	2.5
1	A	126	LEU	2.4
1	B	122	ALA	2.4
1	A	108	PRO	2.4
1	A	112	GLN	2.4
1	A	91	GLN	2.4
1	A	163	GLY	2.3
1	B	304	LEU	2.3
1	A	304	LEU	2.3
1	B	354	PRO	2.2
1	B	337	ALA	2.2
1	B	141	LYS	2.1
1	B	282	THR	2.1
1	B	232	VAL	2.1
1	A	240	ARG	2.1
1	A	337	ALA	2.1
1	A	67	GLY	2.0
1	A	311	LEU	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](#)

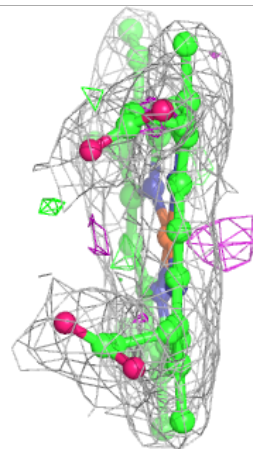
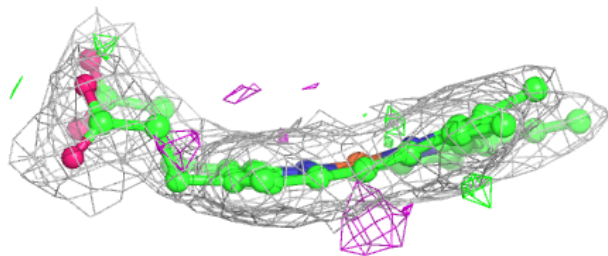
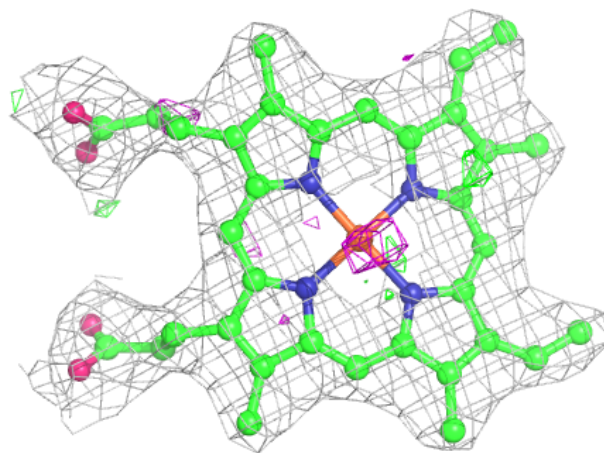
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GOL	B	2880	6/6	0.87	0.29	55,57,59,62	0
7	ARG	A	1700	12/12	0.90	0.29	38,39,42,42	0
8	GOL	A	1880	6/6	0.92	0.26	55,55,56,58	0
3	ACT	B	2860	4/4	0.93	0.14	62,62,63,63	0
3	ACT	A	1860	4/4	0.94	0.24	71,72,72,72	0
6	H4B	B	2600	17/17	0.95	0.21	33,35,36,39	0
6	H4B	A	1600	17/17	0.95	0.24	43,45,47,49	0
7	ARG	B	2700	12/12	0.96	0.25	31,34,37,37	0
4	HEM	A	500	43/43	0.97	0.19	28,33,40,43	0
5	NO	B	2910	2/2	0.97	0.19	34,34,34,36	0
2	CAC	A	1950	3/5	0.97	0.10	65,65,65,70	0
4	HEM	B	500	43/43	0.97	0.16	25,33,35,39	0
2	CAC	B	2950	3/5	0.98	0.17	81,81,82,84	0
5	NO	A	1910	2/2	0.98	0.14	34,34,34,38	0
9	ZN	B	900	1/1	1.00	0.07	43,43,43,43	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.

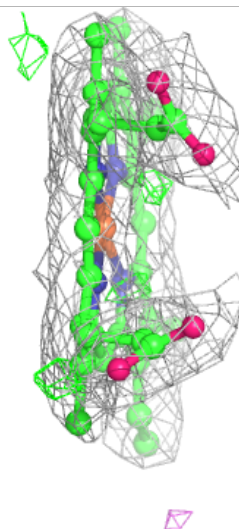
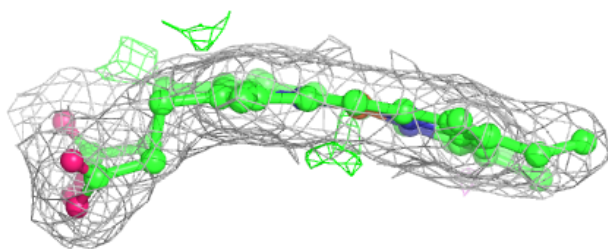
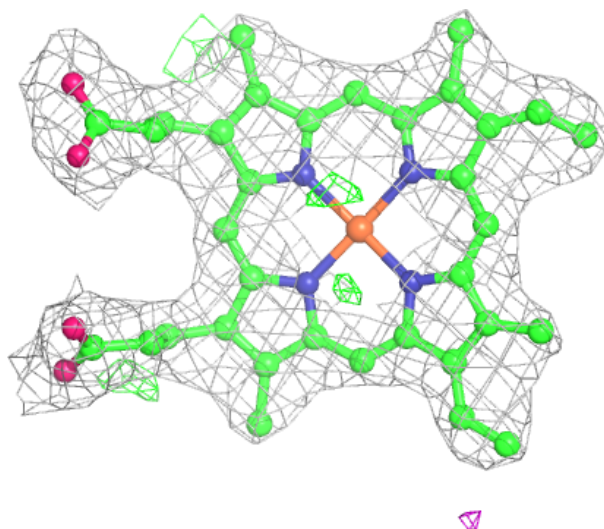
Electron density around HEM A 500:

$2mF_o-DF_c$ (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.