



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 07:37 AM EST

PDB ID : 1NSE
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE
Authors : Raman, C.S.; Li, H.; Martasek, P.; Kral, V.; Masters, B.S.S.; Poulos, T.L.
Deposited on : 1998-05-14
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

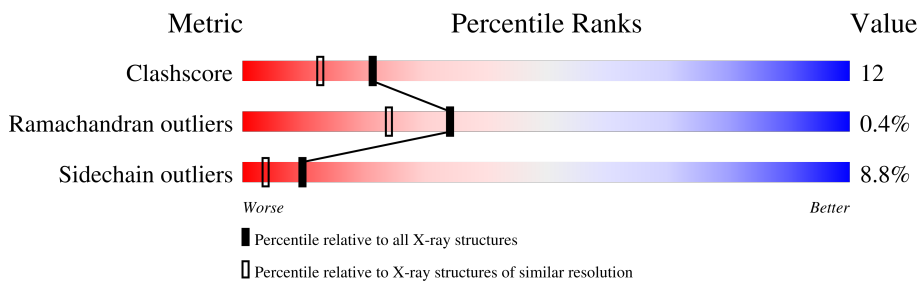
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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

Note EDS was not executed.

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

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7355 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
			Total	C	N	O	S			
1	A	416	3302	2099	584	603	16	0	0	0
1	B	414	3291	2092	582	601	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: C₂H₃O₂).



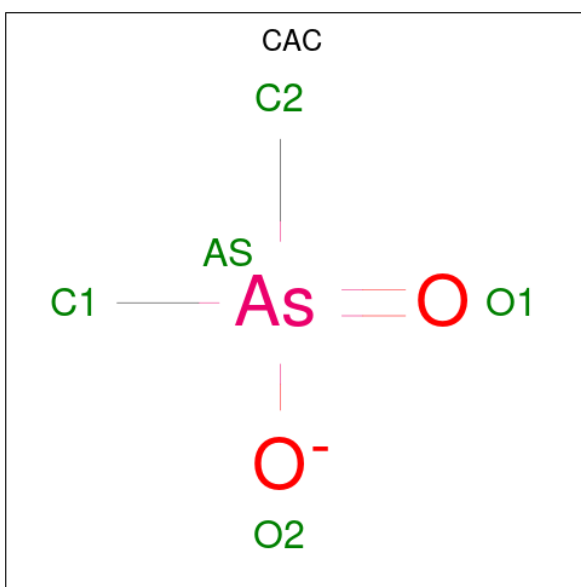
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0

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

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



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

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

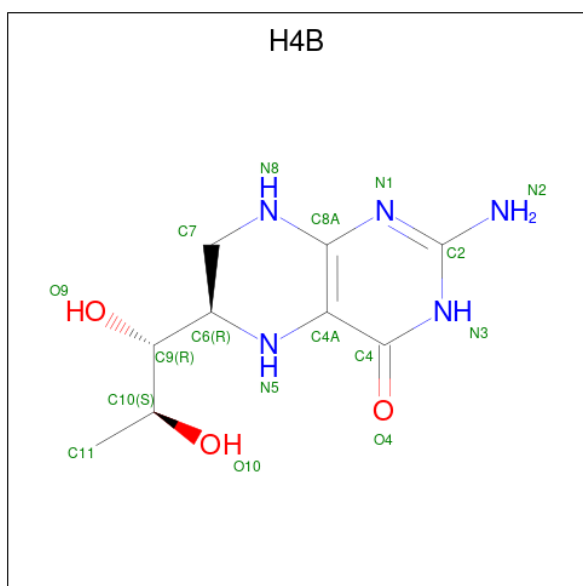
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 6 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



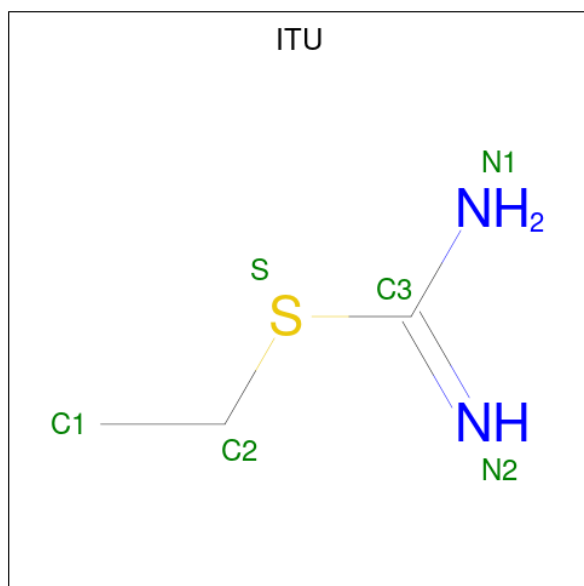
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
			Total	C	N			O	
6	A	1	Total	17	9	5	3	0	0

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

- Molecule 7 is ETHYLISOTHIOUREA (three-letter code: ITU) (formula: $C_3H_8N_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
7	A	1	6	3	2	1	0	0
7	B	1	6	3	2	1	0	0

- 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 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	299	Total O 299 299	0	0
9	B	292	Total O 292 292	0	0

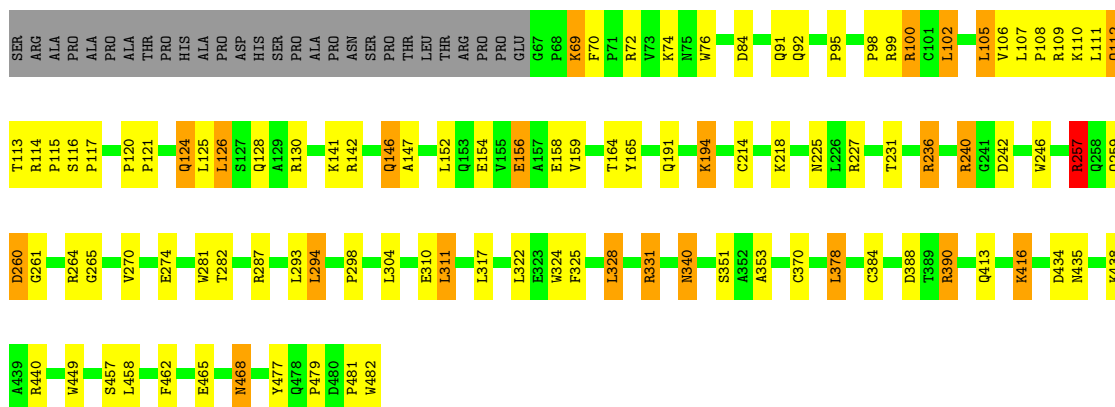
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

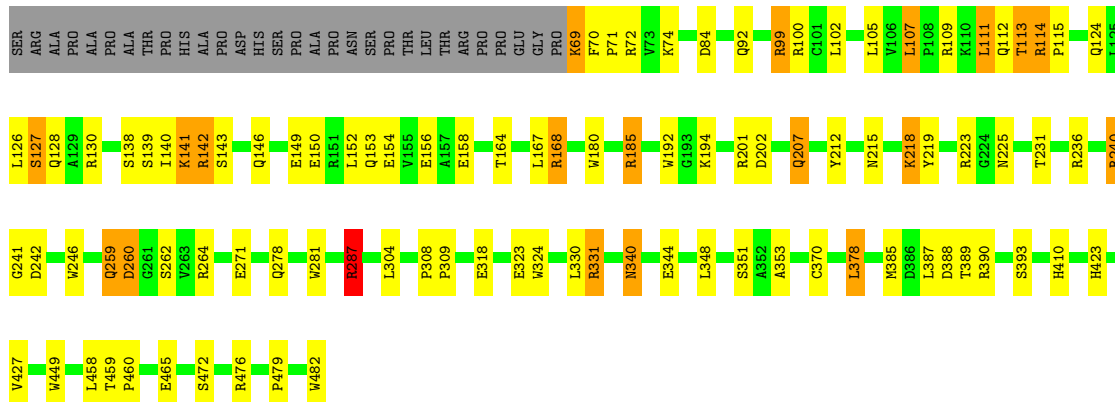
- Molecule 1: NITRIC OXIDE SYNTHASE

Chain A: 



- Molecule 1: NITRIC OXIDE SYNTHASE

Chain B: 



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.00Å 106.55Å 156.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	98.0 (10.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.206 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7355	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

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: ZN, HEM, GOL, ACT, H4B, CAC, ITU

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	0.46	4/3397 (0.1%)	0.98	7/4631 (0.2%)
1	B	0.43	3/3385 (0.1%)	0.94	6/4614 (0.1%)
All	All	0.44	7/6782 (0.1%)	0.96	13/9245 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	ARG	CZ-NH1	10.43	1.46	1.33
1	B	114	ARG	CG-CD	7.47	1.70	1.51
1	A	109	ARG	CB-CG	6.65	1.70	1.52
1	A	109	ARG	NE-CZ	6.40	1.41	1.33
1	B	114	ARG	NE-CZ	5.85	1.40	1.33
1	B	114	ARG	CD-NE	5.25	1.55	1.46
1	A	109	ARG	CD-NE	5.08	1.55	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	A	331	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	A	109	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	B	331	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	440	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	287	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	257	ARG	CD-NE-CZ	6.40	132.55	123.60
1	A	227	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	331	ARG	CD-NE-CZ	6.14	132.19	123.60
1	B	287	ARG	CD-NE-CZ	5.74	131.64	123.60
1	B	185	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	114	ARG	CG-CD-NE	-5.04	101.23	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	88	0
1	B	3291	0	3205	73	0
2	A	8	0	6	0	0
2	B	12	0	9	0	0
3	A	3	0	0	1	0
3	B	3	0	0	1	0
4	A	1	0	0	0	0
5	A	43	0	30	2	0
5	B	43	0	30	1	0
6	A	17	0	15	1	0
6	B	17	0	15	0	0
7	A	6	0	7	0	0
7	B	6	0	7	0	0
8	A	6	0	8	2	0
8	B	6	0	8	0	0
9	A	299	0	0	10	0
9	B	292	0	0	17	0
All	All	7355	0	6555	159	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 12.

All (159) 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:146:GLN:HE21	1:A:147:ALA:H	0.94	0.90
1:B:115:PRO:HD3	1:B:479:PRO:HG2	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLN:HE21	1:A:147:ALA:N	1.77	0.82
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.69	0.74
1:A:413:GLN:O	1:A:416:LYS:HE3	1.88	0.74
1:A:270:VAL:O	1:A:274:GLU:HG3	1.87	0.74
1:A:146:GLN:NE2	1:A:147:ALA:H	1.79	0.74
1:B:287:ARG:HD2	9:B:1028:HOH:O	1.89	0.72
1:A:236:ARG:NH1	1:A:351:SER:HB3	2.07	0.70
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.74	0.69
1:A:294:LEU:HD13	1:A:304:LEU:HD13	1.74	0.68
1:B:240:ARG:HD2	1:B:241:GLY:O	1.93	0.68
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.77	0.67
1:A:152:LEU:O	1:A:156:GLU:HG2	1.94	0.67
1:B:236:ARG:HD2	1:B:242:ASP:OD1	1.94	0.67
1:B:126:LEU:O	1:B:130:ARG:HG3	1.96	0.66
1:A:98:PRO:HD2	9:A:1215:HOH:O	1.95	0.66
1:A:126:LEU:HB3	1:A:130:ARG:HH21	1.61	0.65
1:A:236:ARG:HG2	1:A:242:ASP:OD1	1.96	0.65
1:B:324:TRP:HB2	3:B:950:CAC:C1	2.27	0.65
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.62	0.64
1:A:434:ASP:O	1:A:438:LYS:HE2	1.99	0.63
1:A:340:ASN:H	1:A:340:ASN:HD22	1.47	0.61
1:A:191:GLN:HE22	1:A:194:LYS:NZ	2.00	0.60
1:A:115:PRO:O	1:A:117:PRO:HD3	2.01	0.59
1:B:423:HIS:O	1:B:427:VAL:HG23	2.03	0.59
1:A:310:GLU:HG2	1:A:311:LEU:HD13	1.85	0.58
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.85	0.58
1:A:378:LEU:HB2	9:A:1097:HOH:O	2.04	0.57
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.68	0.57
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.44	0.57
1:B:323:GLU:CG	9:B:1115:HOH:O	2.52	0.56
1:B:152:LEU:O	1:B:156:GLU:HG3	2.05	0.56
1:B:69:LYS:HG2	1:B:70:PHE:CE2	2.40	0.56
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.87	0.56
1:B:378:LEU:HB2	9:B:1136:HOH:O	2.06	0.56
1:B:185:ARG:HG2	1:B:449:TRP:CG	2.41	0.56
1:A:236:ARG:HH12	1:A:351:SER:HB3	1.70	0.56
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.34	0.56
1:A:317:LEU:HG	1:A:331:ARG:HA	1.88	0.56
1:B:393:SER:HB3	9:B:1146:HOH:O	2.04	0.55
1:A:111:LEU:O	1:A:111:LEU:HG	2.05	0.55
1:A:264:ARG:NH1	1:A:287:ARG:HG3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:SER:O	1:B:141:LYS:HD2	2.07	0.54
1:B:323:GLU:HG2	9:B:1115:HOH:O	2.08	0.54
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.90	0.53
1:B:140:ILE:HG13	1:B:142:ARG:HG2	1.90	0.53
1:B:318:GLU:HG3	1:B:410:HIS:CD2	2.44	0.53
1:B:112:GLN:OE1	1:B:114:ARG:NH2	2.41	0.53
1:B:388:ASP:OD1	1:B:390:ARG:HG3	2.10	0.52
1:B:271:GLU:OE1	1:B:482:TRP:HZ2	1.92	0.52
1:A:69:LYS:O	1:A:69:LYS:HG2	2.10	0.52
1:A:70:PHE:HB3	1:A:84:ASP:O	2.11	0.51
1:B:128:GLN:HB3	9:B:1015:HOH:O	2.10	0.51
1:B:71:PRO:HG2	1:B:84:ASP:HB3	1.92	0.51
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.91	0.51
1:A:72:ARG:HD2	1:B:109:ARG:NH2	2.25	0.51
1:B:99:ARG:HB2	1:B:99:ARG:NH1	2.25	0.51
1:A:384:CYS:HA	3:A:950:CAC:C1	2.41	0.51
1:A:257:ARG:HG3	1:A:257:ARG:NH1	2.27	0.50
1:A:111:LEU:HB3	9:A:1209:HOH:O	2.11	0.50
1:A:264:ARG:HH11	1:A:264:ARG:HG3	1.77	0.49
1:A:106:VAL:HG21	8:A:880:GOL:H12	1.93	0.49
1:A:435:ASN:HA	1:A:438:LYS:CE	2.43	0.49
1:A:99:ARG:HG3	9:A:1215:HOH:O	2.13	0.49
1:A:154:GLU:O	1:A:158:GLU:HG3	2.12	0.49
1:A:214:CYS:O	1:A:218:LYS:HG3	2.13	0.49
1:A:100:ARG:NH1	1:A:102:LEU:HD22	2.27	0.48
1:A:111:LEU:HD22	9:A:1190:HOH:O	2.13	0.48
1:B:69:LYS:O	1:B:69:LYS:HG3	2.13	0.48
1:A:115:PRO:HD3	1:A:479:PRO:CG	2.42	0.48
1:A:99:ARG:HD3	9:B:1157:HOH:O	2.14	0.47
1:B:111:LEU:HD12	1:B:111:LEU:O	2.14	0.47
1:A:481:PRO:HD2	1:A:482:TRP:CZ3	2.48	0.47
1:A:111:LEU:HD23	1:A:477:TYR:CE2	2.49	0.47
1:A:92:GLN:HA	1:A:92:GLN:OE1	2.14	0.47
1:A:340:ASN:HD22	1:A:340:ASN:N	2.08	0.47
1:A:481:PRO:HD2	1:A:482:TRP:CE3	2.50	0.46
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.96	0.46
1:A:121:PRO:O	1:A:124:GLN:N	2.48	0.46
1:B:150:GLU:O	1:B:154:GLU:HG3	2.15	0.46
1:B:388:ASP:OD2	1:B:390:ARG:NH2	2.48	0.46
1:B:130:ARG:HB3	1:B:130:ARG:NH1	2.31	0.46
1:B:218:LYS:HD3	1:B:219:TYR:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLU:HG2	1:A:156:GLU:H	1.62	0.46
1:B:240:ARG:NH2	9:B:1008:HOH:O	2.49	0.46
1:A:191:GLN:HE22	1:A:194:LYS:HZ3	1.63	0.46
1:B:111:LEU:HG	9:B:1234:HOH:O	2.14	0.46
1:A:325:PHE:O	1:A:328:LEU:HB2	2.15	0.46
1:A:477:TYR:OH	5:A:500:HEM:O1D	2.29	0.46
1:B:113:THR:HG21	1:B:476:ARG:HD2	1.98	0.45
1:B:218:LYS:NZ	9:B:1217:HOH:O	2.50	0.45
1:B:340:ASN:HD22	1:B:340:ASN:H	1.65	0.45
1:A:74:LYS:HE2	1:A:76:TRP:CE3	2.52	0.45
1:A:141:LYS:NZ	9:A:1234:HOH:O	2.50	0.45
1:A:388:ASP:OD1	1:A:390:ARG:NE	2.49	0.45
1:B:107:LEU:HB3	9:B:1199:HOH:O	2.17	0.45
1:A:449:TRP:HA	6:A:600:H4B:N1	2.31	0.45
1:A:231:THR:O	1:A:353:ALA:HA	2.17	0.45
1:A:260:ASP:OD1	1:A:260:ASP:N	2.49	0.45
1:B:72:ARG:NH1	9:B:1088:HOH:O	2.50	0.45
1:A:124:GLN:NE2	1:A:128:GLN:OE1	2.50	0.45
1:A:257:ARG:NH1	1:A:261:GLY:O	2.50	0.45
1:B:215:ASN:ND2	9:B:1173:HOH:O	2.41	0.45
1:A:240:ARG:NH2	9:A:1240:HOH:O	2.50	0.44
1:B:246:TRP:CZ3	1:B:482:TRP:HB3	2.52	0.44
1:A:126:LEU:HD22	1:A:159:VAL:HG11	1.99	0.44
1:B:115:PRO:CD	1:B:479:PRO:HG2	2.38	0.44
1:A:130:ARG:NH1	9:A:1179:HOH:O	2.49	0.44
1:B:194:LYS:NZ	9:B:1203:HOH:O	2.50	0.44
5:A:500:HEM:HMC2	5:A:500:HEM:HBC2	2.00	0.44
1:A:106:VAL:HG12	1:A:107:LEU:HG	1.99	0.43
1:A:120:PRO:HA	1:A:121:PRO:HD2	1.87	0.43
1:A:225:ASN:ND2	9:A:1134:HOH:O	2.50	0.43
1:B:344:GLU:OE1	1:B:472:SER:OG	2.29	0.43
1:B:459:THR:HB	1:B:460:PRO:HD2	2.00	0.43
1:B:69:LYS:HG2	1:B:70:PHE:CZ	2.53	0.43
1:B:74:LYS:NZ	9:B:1120:HOH:O	2.50	0.43
1:A:72:ARG:HD2	1:B:109:ARG:HH21	1.83	0.43
1:B:158:GLU:HG2	1:B:164:THR:O	2.18	0.43
1:B:389:THR:HG22	1:B:389:THR:O	2.19	0.43
1:B:113:THR:CG2	1:B:476:ARG:HD2	2.49	0.43
1:B:246:TRP:CH2	1:B:482:TRP:HB3	2.54	0.43
1:B:138:SER:HA	1:B:143:SER:HB2	2.00	0.42
1:A:164:THR:HG23	1:A:165:TYR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HH12	1:A:287:ARG:HG3	1.83	0.42
1:B:168:ARG:HD3	1:B:168:ARG:HA	1.48	0.42
1:B:231:THR:O	1:B:353:ALA:HA	2.19	0.42
1:A:294:LEU:HD13	1:A:304:LEU:CD1	2.43	0.42
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.59	0.42
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.54	0.42
1:B:308:PRO:HA	1:B:309:PRO:HD3	1.92	0.42
1:A:126:LEU:O	1:A:130:ARG:HG3	2.19	0.42
1:B:167:LEU:HG	1:B:348:LEU:HD12	2.02	0.42
1:A:74:LYS:HE2	1:A:76:TRP:CD2	2.55	0.42
1:A:236:ARG:HH11	1:A:236:ARG:HG3	1.84	0.42
1:B:318:GLU:HG3	1:B:410:HIS:HD2	1.82	0.42
1:A:265:GLY:HA2	1:A:287:ARG:O	2.20	0.42
1:B:99:ARG:HH11	1:B:99:ARG:CB	2.32	0.42
1:B:202:ASP:OD1	1:B:212:TYR:OH	2.29	0.42
1:A:112:GLN:HE21	1:A:112:GLN:HB2	1.40	0.41
1:B:388:ASP:OD1	1:B:390:ARG:CG	2.68	0.41
1:A:236:ARG:NH1	1:A:236:ARG:HG3	2.35	0.41
1:A:106:VAL:CG2	8:A:880:GOL:H12	2.50	0.41
1:A:468:ASN:ND2	9:A:1135:HOH:O	2.52	0.41
1:B:105:LEU:HD23	1:B:105:LEU:N	2.34	0.41
1:B:207:GLN:HB2	9:B:1112:HOH:O	2.19	0.41
1:B:259:GLN:H	1:B:259:GLN:HG3	1.59	0.41
1:A:457:SER:HA	1:A:462:PHE:CG	2.56	0.41
1:A:95:PRO:CA	1:A:110:LYS:HG3	2.50	0.41
1:B:141:LYS:HD2	1:B:141:LYS:HA	1.65	0.41
1:B:124:GLN:O	1:B:127:SER:OG	2.30	0.41
1:B:385:MET:HB2	1:B:387:LEU:HG	2.02	0.41
5:B:500:HEM:HMC2	5:B:500:HEM:HBC2	2.03	0.41
1:A:105:LEU:HD23	1:A:105:LEU:N	2.35	0.41
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.55	0.41
1:A:95:PRO:HB3	1:A:108:PRO:HB2	2.03	0.40
1:B:115:PRO:HG3	9:B:1161:HOH:O	2.21	0.40
1:A:126:LEU:HB3	1:A:130:ARG:NH2	2.32	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%)	397 (96%)	17 (4%)	0	100	100
1	B	412/444 (93%)	393 (95%)	16 (4%)	3 (1%)	22	12
All	All	826/888 (93%)	790 (96%)	33 (4%)	3 (0%)	34	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	262	SER
1	B	259	GLN
1	B	260	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	354/377 (94%)	322 (91%)	32 (9%)	9	3
1	B	353/377 (94%)	323 (92%)	30 (8%)	10	4
All	All	707/754 (94%)	645 (91%)	62 (9%)	10	4

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	91	GLN
1	A	100	ARG

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Mol	Chain	Res	Type
1	A	102	LEU
1	A	105	LEU
1	A	112	GLN
1	A	113	THR
1	A	114	ARG
1	A	116	SER
1	A	124	GLN
1	A	125	LEU
1	A	126	LEU
1	A	142	ARG
1	A	146	GLN
1	A	156	GLU
1	A	194	LYS
1	A	236	ARG
1	A	240	ARG
1	A	257	ARG
1	A	259	GLN
1	A	260	ASP
1	A	282	THR
1	A	293	LEU
1	A	294	LEU
1	A	311	LEU
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	390	ARG
1	A	416	LYS
1	A	458	LEU
1	A	468	ASN
1	B	69	LYS
1	B	92	GLN
1	B	99	ARG
1	B	100	ARG
1	B	102	LEU
1	B	107	LEU
1	B	111	LEU
1	B	113	THR
1	B	127	SER
1	B	139	SER
1	B	141	LYS
1	B	142	ARG
1	B	146	GLN

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Mol	Chain	Res	Type
1	B	149	GLU
1	B	153	GLN
1	B	168	ARG
1	B	207	GLN
1	B	218	LYS
1	B	223	ARG
1	B	225	ASN
1	B	240	ARG
1	B	260	ASP
1	B	264	ARG
1	B	278	GLN
1	B	287	ARG
1	B	330	LEU
1	B	331	ARG
1	B	340	ASN
1	B	378	LEU
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	146	GLN
1	A	191	GLN
1	A	258	GLN
1	A	278	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	278	GLN
1	B	340	ASN
1	B	376	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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
3	CAC	B	950	1	0,2,4	-	-	0,1,6	-	-
2	ACT	B	850	-	3,3,3	0.92	0	3,3,3	0.64	0
3	CAC	A	950	1	0,2,4	-	-	0,1,6	-	-
6	H4B	A	600	-	16,18,18	1.77	4 (25%)	11,26,26	4.30	8 (72%)
2	ACT	A	860	-	3,3,3	0.89	0	3,3,3	0.55	0
8	GOL	A	880	-	5,5,5	0.25	0	5,5,5	0.23	0
2	ACT	A	850	-	3,3,3	0.91	0	3,3,3	1.01	0
7	ITU	A	800	-	4,5,5	0.83	0	4,5,5	2.64	1 (25%)
8	GOL	B	880	-	5,5,5	0.30	0	5,5,5	0.51	0
7	ITU	B	800	-	4,5,5	0.78	0	4,5,5	1.70	1 (25%)
2	ACT	B	870	-	3,3,3	0.84	0	3,3,3	0.56	0
5	HEM	A	500	1	41,50,50	1.26	3 (7%)	45,82,82	1.31	4 (8%)
5	HEM	B	500	1	41,50,50	1.26	3 (7%)	45,82,82	1.13	3 (6%)
6	H4B	B	600	-	16,18,18	1.82	3 (18%)	11,26,26	3.95	8 (72%)
2	ACT	B	860	-	3,3,3	0.94	0	3,3,3	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	H4B	A	600	-	-	0/8/17/17	0/2/2/2
8	GOL	A	880	-	-	2/4/4/4	-
7	ITU	A	800	-	-	1/3/3/3	-
8	GOL	B	880	-	-	2/4/4/4	-
7	ITU	B	800	-	-	0/3/3/3	-
5	HEM	A	500	1	-	0/12/54/54	-
5	HEM	B	500	1	-	0/12/54/54	-
6	H4B	B	600	-	-	0/8/17/17	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	H4B	C4-N3	4.89	1.41	1.33
6	A	600	H4B	C4-N3	4.23	1.40	1.33
5	A	500	HEM	C3C-CAC	-4.09	1.39	1.47
5	B	500	HEM	C3C-CAC	-4.08	1.39	1.47
6	B	600	H4B	C4A-N5	3.68	1.45	1.38
6	A	600	H4B	C4A-N5	3.56	1.45	1.38
5	A	500	HEM	C3C-C2C	-3.44	1.35	1.40
5	B	500	HEM	C3C-C2C	-3.18	1.36	1.40
6	A	600	H4B	C6-N5	2.92	1.51	1.45
5	A	500	HEM	CAB-C3B	-2.82	1.39	1.47
5	B	500	HEM	CAB-C3B	-2.82	1.39	1.47
6	B	600	H4B	C6-N5	2.44	1.50	1.45
6	A	600	H4B	C4A-C8A	-2.20	1.37	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	H4B	C8A-C4A-C4	9.54	123.04	114.57
6	A	600	H4B	C8A-C4A-C4	9.11	122.67	114.57
6	A	600	H4B	C2-N3-C4	5.80	125.14	115.93
7	A	800	ITU	C2-S-C3	4.99	108.43	103.20
6	A	600	H4B	N1-C2-N3	-4.84	117.83	125.42
6	B	600	H4B	C2-N3-C4	3.96	122.21	115.93
6	A	600	H4B	C4A-C4-N3	-3.63	113.69	124.01
6	B	600	H4B	N1-C2-N3	-3.57	119.81	125.42
6	A	600	H4B	C2-N1-C8A	3.50	122.39	114.54
6	B	600	H4B	C2-N1-C8A	3.46	122.29	114.54
6	A	600	H4B	N2-C2-N1	3.41	122.56	117.25
7	B	800	ITU	C2-S-C3	3.34	106.71	103.20
6	A	600	H4B	C4A-N5-C6	-3.27	112.27	121.16
6	B	600	H4B	C4-C4A-N5	-3.25	116.39	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	H4B	C4-C4A-N5	-3.16	116.47	119.12
6	B	600	H4B	C4A-N5-C6	-3.16	112.56	121.16
6	B	600	H4B	C4A-C4-N3	-3.14	115.10	124.01
5	A	500	HEM	C1B-NB-C4B	-2.80	102.18	105.07
5	A	500	HEM	C4D-ND-C1D	-2.45	102.54	105.07
5	B	500	HEM	C4B-CHC-C1C	2.43	125.76	122.56
5	A	500	HEM	CBD-CAD-C3D	2.32	119.07	112.63
5	A	500	HEM	CAD-C3D-C4D	2.19	128.48	124.66
5	B	500	HEM	CHB-C1B-C2B	-2.13	120.83	126.72
6	B	600	H4B	N2-C2-N1	2.07	120.47	117.25
5	B	500	HEM	CMA-C3A-C4A	-2.02	125.36	128.46

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	880	GOL	O1-C1-C2-C3
7	A	800	ITU	C1-C2-S-C3
8	A	880	GOL	O1-C1-C2-O2
8	B	880	GOL	O1-C1-C2-O2
8	B	880	GOL	O1-C1-C2-C3

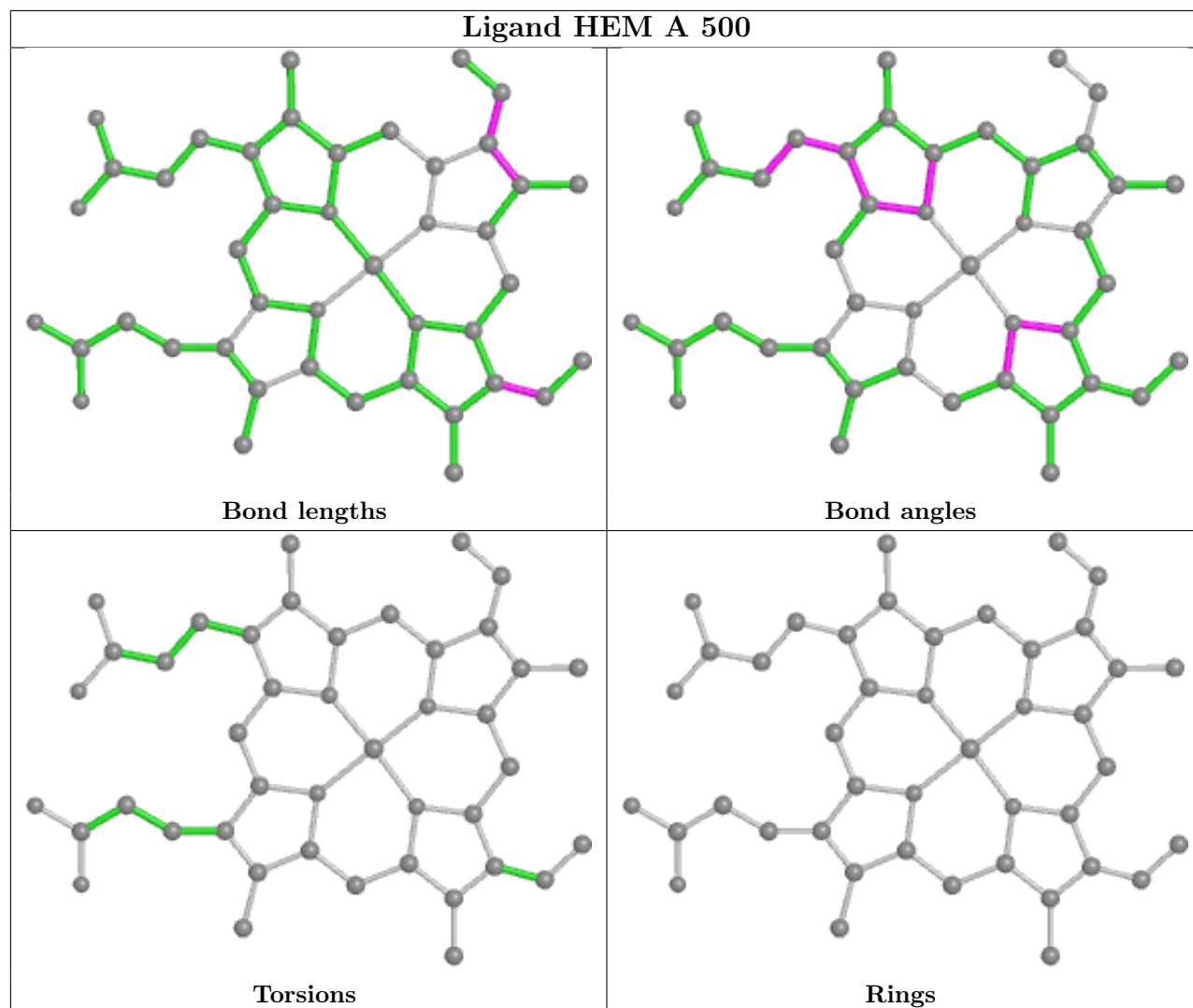
There are no ring outliers.

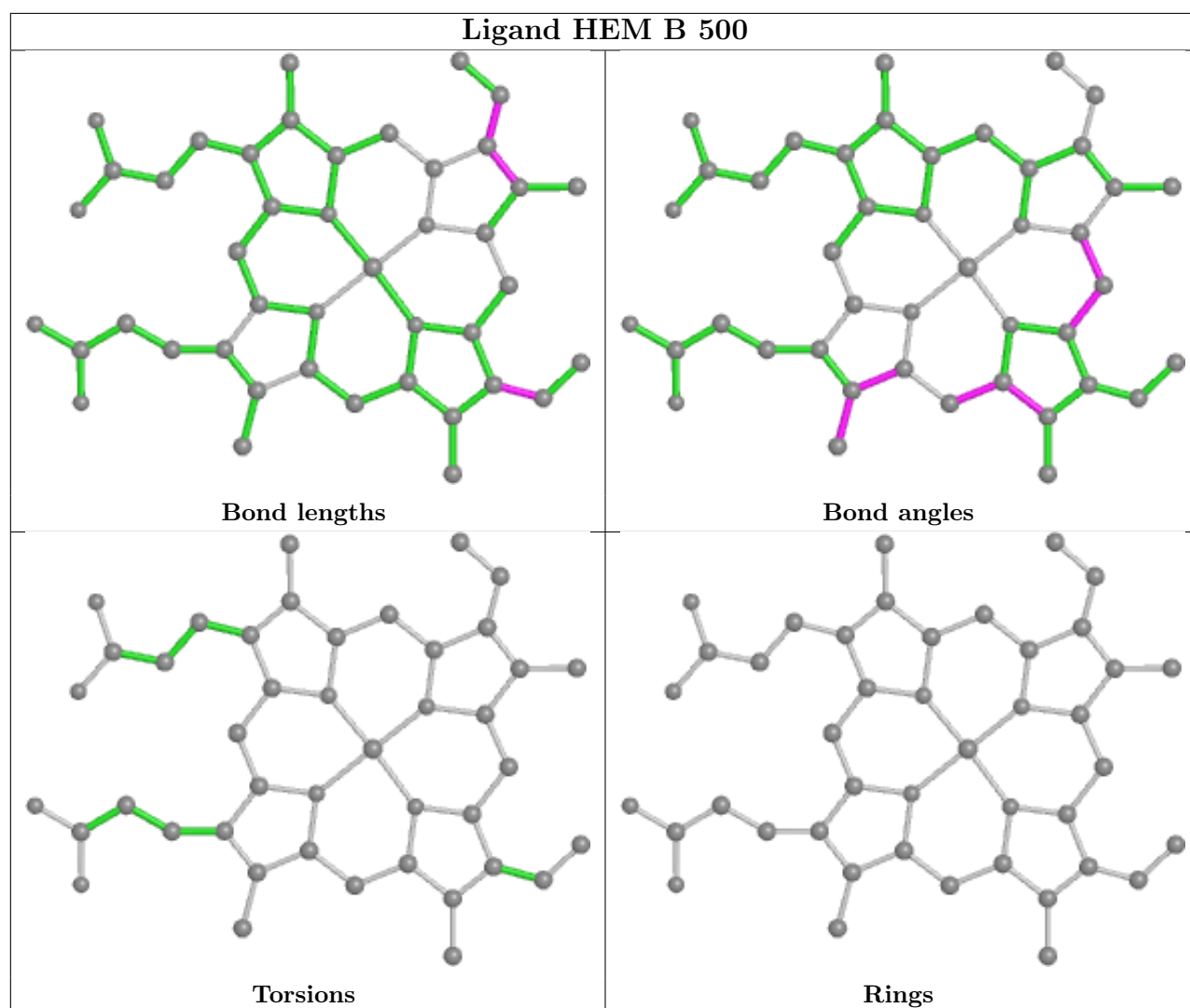
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	950	CAC	1	0
3	A	950	CAC	1	0
6	A	600	H4B	1	0
8	A	880	GOL	2	0
5	A	500	HEM	2	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.