



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:32 PM UTC

PDB ID : 3NSE / pdb_00003nse
Title : BOVINE ENOS, H4B-FREE, SEITU COMPLEX
Authors : Raman, C.S.; Li, H.; Martasek, P.; Kral, V.; Masters, B.S.S.; Poulos, T.L.
Deposited on : 1998-09-23
Resolution : 2.10 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

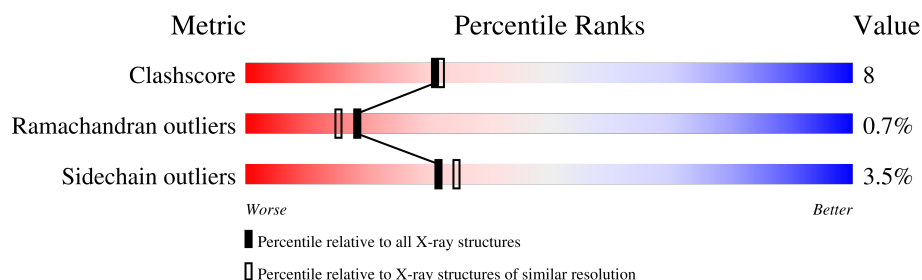
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	 75% 17% • 6%
1	B	444	 70% 19% • 7%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7080 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 (CCD ID: ACT) (formula: C₂H₃O₂).



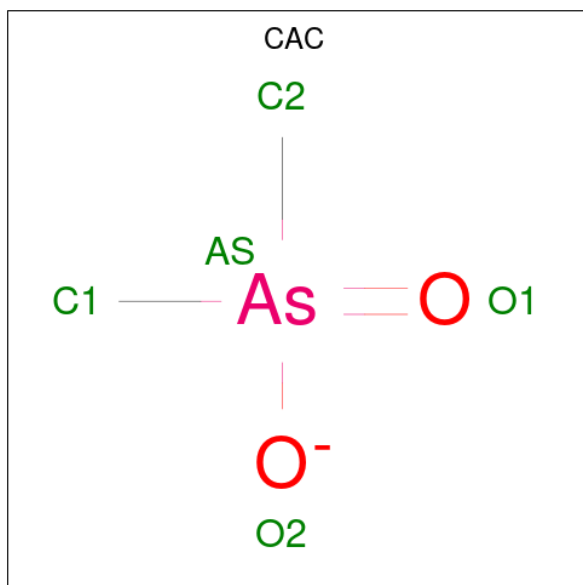
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

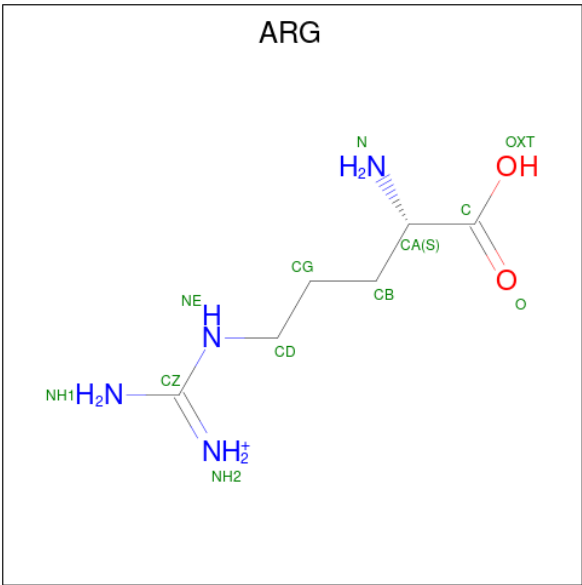
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



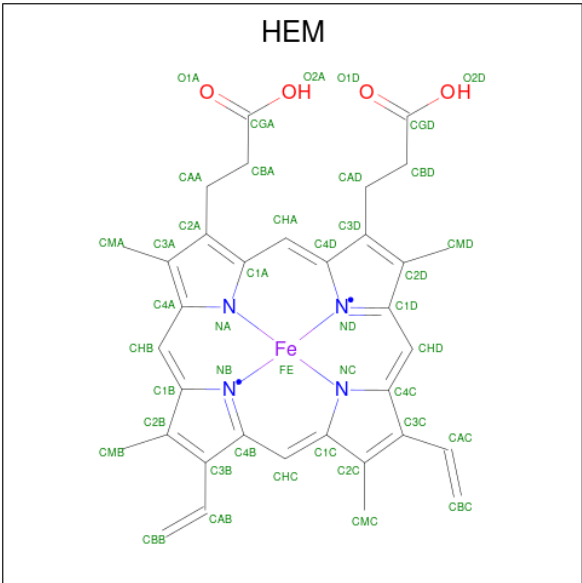
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	As	C	0	0
			3	1	2		
3	B	1	Total	As	C	0	0
			3	1	2		

- Molecule 4 is ARGININE (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



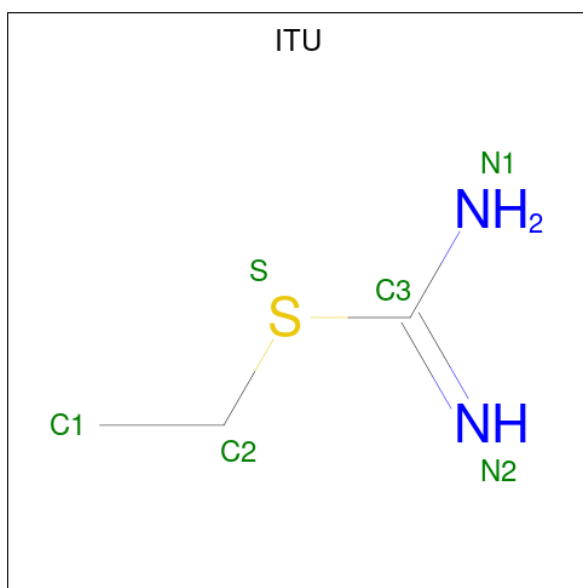
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 6 is ETHYLISOTHIOUREA (CCD ID: ITU) (formula: $C_3H_8N_2S$).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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 ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	178	Total	O	0	0
			178	178		
9	B	158	Total	O	0	0
			158	158		

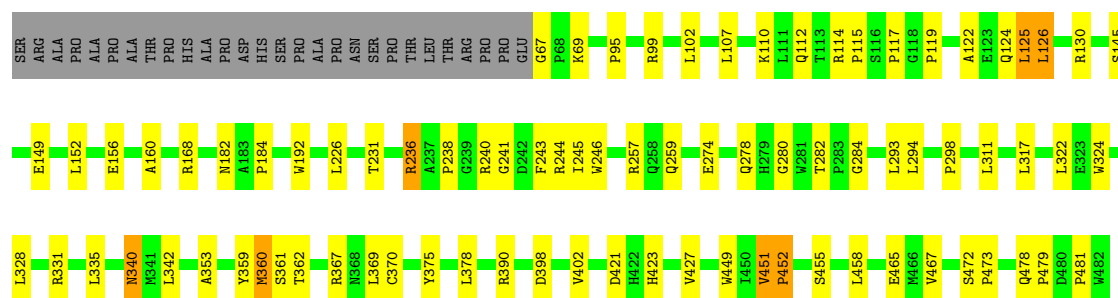
3 Residue-property plots

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.

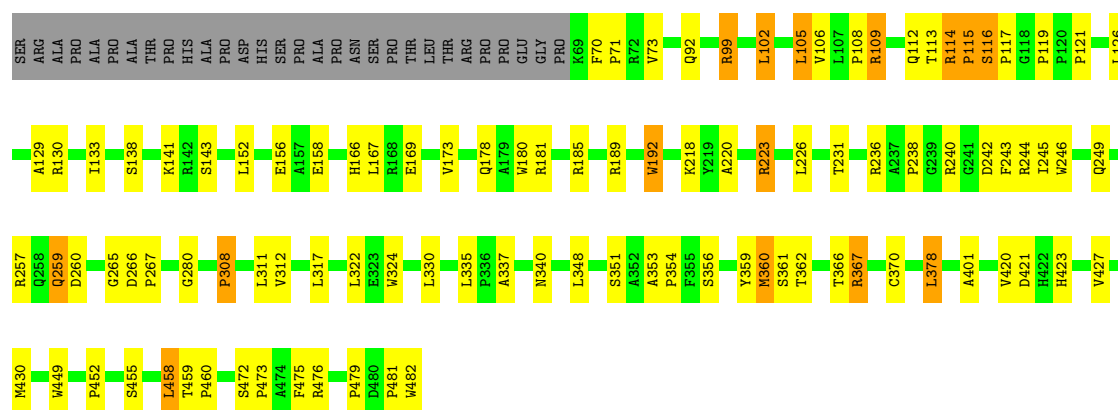
• Molecule 1: NITRIC OXIDE SYNTHASE

Chain A: 



• Molecule 1: NITRIC OXIDE SYNTHASE

Chain B: 



4 Data and refinement statistics

Xtriage (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	58.17Å 107.14Å 156.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	99.6 (30.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.197 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7080	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ITU, GOL, HEM, ACT, CAC

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	0.52	0/3397	1.00	21/4631 (0.5%)
1	B	0.49	0/3385	1.00	21/4614 (0.5%)
All	All	0.50	0/6782	1.00	42/9245 (0.5%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	LEU	CA-C-N	-7.73	111.95	120.14
1	A	107	LEU	C-N-CA	-7.73	111.95	120.14
1	B	360	MET	N-CA-C	-7.57	96.89	109.07
1	A	360	MET	N-CA-C	-7.36	97.22	109.07
1	B	243	PHE	N-CA-C	-7.15	97.59	109.46
1	B	335	LEU	N-CA-C	6.91	121.13	108.69
1	B	245	ILE	N-CA-C	-6.65	98.16	107.80
1	A	451	VAL	CA-C-N	6.45	124.37	119.66
1	A	451	VAL	C-N-CA	6.45	124.37	119.66
1	A	335	LEU	N-CA-C	6.34	120.11	108.69
1	B	240	ARG	N-CA-C	6.31	117.73	108.14
1	A	359	TYR	N-CA-C	6.18	118.69	110.53
1	A	452	PRO	CA-C-N	6.15	125.85	119.82
1	A	452	PRO	C-N-CA	6.15	125.85	119.82
1	A	243	PHE	N-CA-C	-5.99	99.44	108.96
1	B	192	TRP	N-CA-C	5.96	119.38	111.75
1	A	117	PRO	N-CA-C	-5.81	108.01	114.92
1	B	367	ARG	N-CA-C	5.79	117.46	111.03
1	A	282	THR	CA-C-N	5.70	125.67	120.03
1	A	282	THR	C-N-CA	5.70	125.67	120.03
1	B	189	ARG	N-CA-C	5.58	119.56	112.87
1	A	284	GLY	N-CA-C	-5.52	106.16	112.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	LEU	N-CA-C	5.50	117.83	110.35
1	A	245	ILE	N-CA-C	-5.46	99.88	107.80
1	B	266	ASP	CA-C-N	5.45	125.12	119.56
1	B	266	ASP	C-N-CA	5.45	125.12	119.56
1	B	317	LEU	N-CA-C	5.45	117.63	108.96
1	B	459	THR	CA-C-N	5.35	125.17	119.28
1	B	459	THR	C-N-CA	5.35	125.17	119.28
1	A	280	GLY	N-CA-C	5.35	122.70	115.32
1	A	67	GLY	CA-C-N	5.32	125.24	119.76
1	A	67	GLY	C-N-CA	5.32	125.24	119.76
1	B	475	PHE	N-CA-C	-5.30	100.67	109.46
1	B	312	VAL	N-CA-C	5.27	114.19	106.55
1	A	192	TRP	N-CA-C	5.25	117.68	111.33
1	B	308	PRO	CA-C-N	5.20	125.50	119.47
1	B	308	PRO	C-N-CA	5.20	125.50	119.47
1	A	168	ARG	N-CA-C	-5.18	103.55	110.55
1	B	359	TYR	N-CA-C	5.17	117.35	110.53
1	B	452	PRO	CA-C-N	5.14	125.21	119.87
1	B	452	PRO	C-N-CA	5.14	125.21	119.87
1	B	280	GLY	N-CA-C	5.08	122.59	115.43

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	53	0
1	B	3291	0	3205	58	0
2	A	8	0	6	0	0
2	B	8	0	6	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	12	0	12	1	0
5	A	43	0	30	0	0
5	B	43	0	30	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	6	0	7	0	0
6	B	6	0	7	0	0
7	A	12	0	16	4	0
7	B	6	0	8	1	0
8	B	1	0	0	0	0
9	A	178	0	0	3	0
9	B	158	0	0	4	0
All	All	7080	0	6542	109	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ARG:HB3	1:B:115:PRO:HD2	1.64	0.79
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.49	0.77
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.69	0.74
1:B:114:ARG:HD3	1:B:479:PRO:HG3	1.68	0.74
1:B:126:LEU:HD11	1:B:156:GLU:HG2	1.70	0.73
1:A:114:ARG:HG3	1:A:115:PRO:HD2	1.68	0.73
1:A:478:GLN:HB3	9:A:995:HOH:O	1.91	0.70
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.76	0.67
1:B:126:LEU:O	1:B:130:ARG:HG3	1.96	0.66
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.37	0.65
1:A:378:LEU:HB2	9:A:989:HOH:O	1.94	0.65
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.78	0.65
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.81	0.63
1:A:69:LYS:O	1:A:69:LYS:HG2	1.98	0.62
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.82	0.61
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.65	0.61
1:A:95:PRO:HA	1:A:110:LYS:HG3	1.82	0.60
1:B:121:PRO:HB2	9:B:1095:HOH:O	2.02	0.59
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.84	0.59
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.50	0.58
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.85	0.58
1:A:423:HIS:O	1:A:427:VAL:HG23	2.04	0.58
1:B:366:THR:O	1:B:370:CYS:HB2	2.04	0.57
1:A:398:ASP:O	1:A:402:VAL:HG23	2.05	0.55
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.47	0.55
1:B:472:SER:HA	1:B:473:PRO:C	2.32	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ARG:HB3	1:B:115:PRO:CD	2.35	0.55
1:A:340:ASN:H	1:A:340:ASN:HD22	1.55	0.55
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.42	0.55
1:A:360:MET:HE3	1:A:362:THR:OG1	2.07	0.54
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.90	0.54
1:B:223:ARG:HH11	1:B:223:ARG:CG	2.21	0.53
1:A:119:PRO:HB3	1:A:238:PRO:HB3	1.91	0.52
1:A:449:TRP:CE2	7:A:890:GOL:H2	2.45	0.52
1:A:95:PRO:CA	1:A:110:LYS:HG3	2.40	0.52
1:B:152:LEU:O	1:B:156:GLU:HG3	2.08	0.52
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.09	0.52
1:A:236:ARG:HH11	1:A:236:ARG:HG3	1.74	0.52
1:B:236:ARG:HD2	1:B:242:ASP:CG	2.34	0.51
1:A:472:SER:HA	1:A:473:PRO:C	2.36	0.51
1:B:361:SER:OG	1:B:421:ASP:HA	2.11	0.50
1:B:108:PRO:HD2	9:B:1034:HOH:O	2.11	0.50
1:A:114:ARG:HH21	1:A:479:PRO:HG3	1.76	0.49
1:A:361:SER:OG	1:A:421:ASP:HA	2.13	0.49
1:B:337:ALA:CB	1:B:356:SER:HB3	2.43	0.48
1:A:367:ARG:HH22	7:A:880:GOL:H32	1.78	0.48
1:B:259:GLN:HG3	1:B:260:ASP:H	1.79	0.48
1:A:317:LEU:HG	1:A:331:ARG:HA	1.96	0.47
1:A:125:LEU:O	1:A:125:LEU:HD22	2.15	0.47
1:A:236:ARG:HG3	1:A:236:ARG:NH1	2.30	0.47
1:B:185:ARG:HD3	1:B:449:TRP:CD2	2.50	0.47
1:A:156:GLU:O	1:A:160:ALA:HB2	2.15	0.46
1:A:119:PRO:HB3	1:A:238:PRO:CB	2.44	0.46
1:A:126:LEU:HD11	1:A:156:GLU:HB3	1.97	0.46
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.46	0.46
1:B:113:THR:HG21	1:B:476:ARG:HD2	1.97	0.46
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.30	0.46
1:A:112:GLN:OE1	1:A:114:ARG:NH2	2.48	0.46
1:B:265:GLY:O	1:B:267:PRO:HD3	2.16	0.45
1:B:158:GLU:OE2	1:B:166:HIS:HD2	1.99	0.45
1:A:152:LEU:O	1:A:156:GLU:HG2	2.16	0.45
1:A:342:LEU:HD13	9:A:995:HOH:O	2.15	0.45
1:B:178:GLN:HE22	1:B:181:ARG:NH1	2.15	0.45
1:B:169:GLU:O	1:B:173:VAL:HG23	2.16	0.45
4:A:700:ARG:NH2	1:B:367:ARG:HH12	2.15	0.45
1:B:114:ARG:HD3	1:B:479:PRO:CG	2.40	0.44
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASN:O	1:A:184:PRO:HD3	2.17	0.44
1:B:119:PRO:HB3	1:B:238:PRO:HB3	2.00	0.44
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.81	0.44
1:A:367:ARG:NH2	7:A:880:GOL:H32	2.32	0.44
1:A:115:PRO:CD	1:A:479:PRO:HG2	2.45	0.43
1:A:369:LEU:HA	1:A:375:TYR:HB2	2.00	0.43
1:A:126:LEU:HB3	1:A:130:ARG:HH21	1.83	0.43
7:A:880:GOL:H31	9:B:1032:HOH:O	2.18	0.43
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.91	0.42
1:B:423:HIS:O	1:B:427:VAL:HG23	2.19	0.42
1:B:455:SER:HB3	1:B:458:LEU:CD2	2.48	0.42
1:B:115:PRO:O	1:B:116:SER:HB3	2.19	0.42
1:B:129:ALA:O	1:B:133:ILE:HG12	2.19	0.42
1:B:231:THR:O	1:B:354:PRO:HD2	2.19	0.42
1:B:249:GLN:HA	1:B:337:ALA:O	2.19	0.42
1:B:360:MET:HA	1:B:420:VAL:O	2.19	0.42
1:A:112:GLN:OE1	1:A:479:PRO:HG3	2.20	0.42
1:A:145:SER:O	1:A:149:GLU:HG2	2.19	0.42
1:B:109:ARG:NH2	9:B:1104:HOH:O	2.52	0.42
1:A:99:ARG:HA	1:A:99:ARG:HD3	1.91	0.42
1:B:246:TRP:CH2	1:B:482:TRP:HB3	2.55	0.42
1:B:308:PRO:HD2	1:B:311:LEU:HD12	2.02	0.42
1:B:231:THR:O	1:B:353:ALA:HA	2.19	0.42
1:A:340:ASN:H	1:A:340:ASN:ND2	2.18	0.41
1:B:138:SER:HA	1:B:143:SER:HB2	2.01	0.41
1:A:458:LEU:HD21	1:B:401:ALA:HB2	2.02	0.41
1:A:119:PRO:HD3	1:A:238:PRO:HB2	2.02	0.41
1:B:106:VAL:HG11	7:B:880:GOL:O1	2.20	0.41
1:B:430:MET:HG3	1:B:460:PRO:HB2	2.02	0.41
1:A:274:GLU:O	1:A:278:GLN:HG3	2.20	0.41
1:A:455:SER:O	1:A:458:LEU:HB2	2.19	0.41
1:A:126:LEU:HB3	1:A:130:ARG:NH2	2.35	0.41
1:A:240:ARG:HD2	1:A:241:GLY:O	2.21	0.41
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.56	0.41
1:A:467:VAL:HG13	1:B:102:LEU:CD1	2.51	0.41
1:B:70:PHE:HA	1:B:71:PRO:HD2	1.96	0.41
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.36	0.40
1:B:360:MET:HE3	1:B:362:THR:OG1	2.21	0.40
1:A:231:THR:O	1:A:353:ALA:HA	2.22	0.40
1:B:220:ALA:O	1:B:226:LEU:HA	2.22	0.40
1:B:115:PRO:O	1:B:116:SER:CB	2.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLN:HG2	1:B:114:ARG:HG2	2.02	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%)	395 (95%)	18 (4%)	1 (0%)	43	44
1	B	412/444 (93%)	384 (93%)	23 (6%)	5 (1%)	10	7
All	All	826/888 (93%)	779 (94%)	41 (5%)	6 (1%)	18	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	ARG
1	B	116	SER
1	B	259	GLN
1	A	122	ALA
1	B	115	PRO
1	B	117	PRO

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%)	343 (97%)	11 (3%)	35	39
1	B	353/377 (94%)	339 (96%)	14 (4%)	28	29
All	All	707/754 (94%)	682 (96%)	25 (4%)	32	35

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	124	GLN
1	A	125	LEU
1	A	126	LEU
1	A	236	ARG
1	A	259	GLN
1	A	293	LEU
1	A	311	LEU
1	A	328	LEU
1	A	340	ASN
1	A	390	ARG
1	B	73	VAL
1	B	92	GLN
1	B	99	ARG
1	B	102	LEU
1	B	105	LEU
1	B	109	ARG
1	B	141	LYS
1	B	218	LYS
1	B	223	ARG
1	B	257	ARG
1	B	330	LEU
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	91	GLN
1	A	146	GLN
1	A	278	GLN
1	A	340	ASN
1	A	410	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	413	GLN
1	A	437	GLN
1	A	468	ASN
1	B	92	GLN
1	B	166	HIS
1	B	178	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	340	ASN
1	B	376	ASN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	ACT	A	860	-	3,3,3	0.90	0	3,3,3	0.84	0
3	CAC	A	950	1	0,2,4	-	-	0,1,6	-	-
2	ACT	A	850	-	3,3,3	0.97	0	3,3,3	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ITU	A	800	-	4,5,5	2.42	1 (25%)	3,5,5	3.35	1 (33%)
5	HEM	B	500	1	50,50,50	1.10	3 (6%)	67,82,82	1.12	4 (5%)
7	GOL	B	880	-	5,5,5	0.24	0	5,5,5	0.44	0
2	ACT	B	850	-	3,3,3	0.98	0	3,3,3	0.79	0
3	CAC	B	950	1	0,2,4	-	-	0,1,6	-	-
4	ARG	A	700	-	10,11,11	0.79	0	9,13,13	0.65	0
6	ITU	B	800	-	4,5,5	2.49	1 (25%)	3,5,5	2.35	1 (33%)
2	ACT	B	860	-	3,3,3	0.93	0	3,3,3	0.77	0
7	GOL	A	890	-	5,5,5	0.17	0	5,5,5	0.21	0
5	HEM	A	500	1	50,50,50	1.05	2 (4%)	67,82,82	1.27	5 (7%)
7	GOL	A	880	-	5,5,5	0.21	0	5,5,5	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ITU	A	800	-	-	1/3/3/3	-
5	HEM	B	500	1	-	0/14/54/54	-
7	GOL	B	880	-	-	2/4/4/4	-
4	ARG	A	700	-	-	3/11/11/11	-
6	ITU	B	800	-	-	0/3/3/3	-
7	GOL	A	890	-	-	0/4/4/4	-
5	HEM	A	500	1	-	0/14/54/54	-
7	GOL	A	880	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	800	ITU	C3-S	4.89	1.80	1.75
6	A	800	ITU	C3-S	4.71	1.80	1.75
5	B	500	HEM	CAB-C3B	-2.78	1.40	1.47
5	A	500	HEM	FE-NC	2.75	2.04	1.95
5	B	500	HEM	FE-NC	2.53	2.03	1.95
5	B	500	HEM	CAC-C3C	-2.40	1.41	1.47
5	A	500	HEM	CAB-C3B	-2.24	1.41	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	800	ITU	C2-S-C3	5.78	109.15	103.15
6	B	800	ITU	C2-S-C3	4.06	107.37	103.15
5	A	500	HEM	C3B-C4B-NB	3.70	112.12	109.47
5	B	500	HEM	C3B-C4B-NB	3.49	111.97	109.47
5	A	500	HEM	C4B-C3B-C2B	-2.79	104.71	107.28
5	A	500	HEM	CMD-C2D-C1D	2.53	128.98	125.03
5	B	500	HEM	CBD-CAD-C3D	-2.34	106.05	112.53
5	A	500	HEM	CHD-C4C-NC	-2.32	121.93	124.45
5	B	500	HEM	C2D-C1D-ND	2.31	112.58	109.90
5	A	500	HEM	CHB-C1B-C2B	-2.14	120.87	126.95
5	B	500	HEM	C4D-ND-C1D	-2.01	102.82	105.21

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	700	ARG	OXT-C-CA-N
6	A	800	ITU	C1-C2-S-C3
7	B	880	GOL	C1-C2-C3-O3
7	B	880	GOL	O2-C2-C3-O3
4	A	700	ARG	O-C-CA-CB
4	A	700	ARG	OXT-C-CA-CB

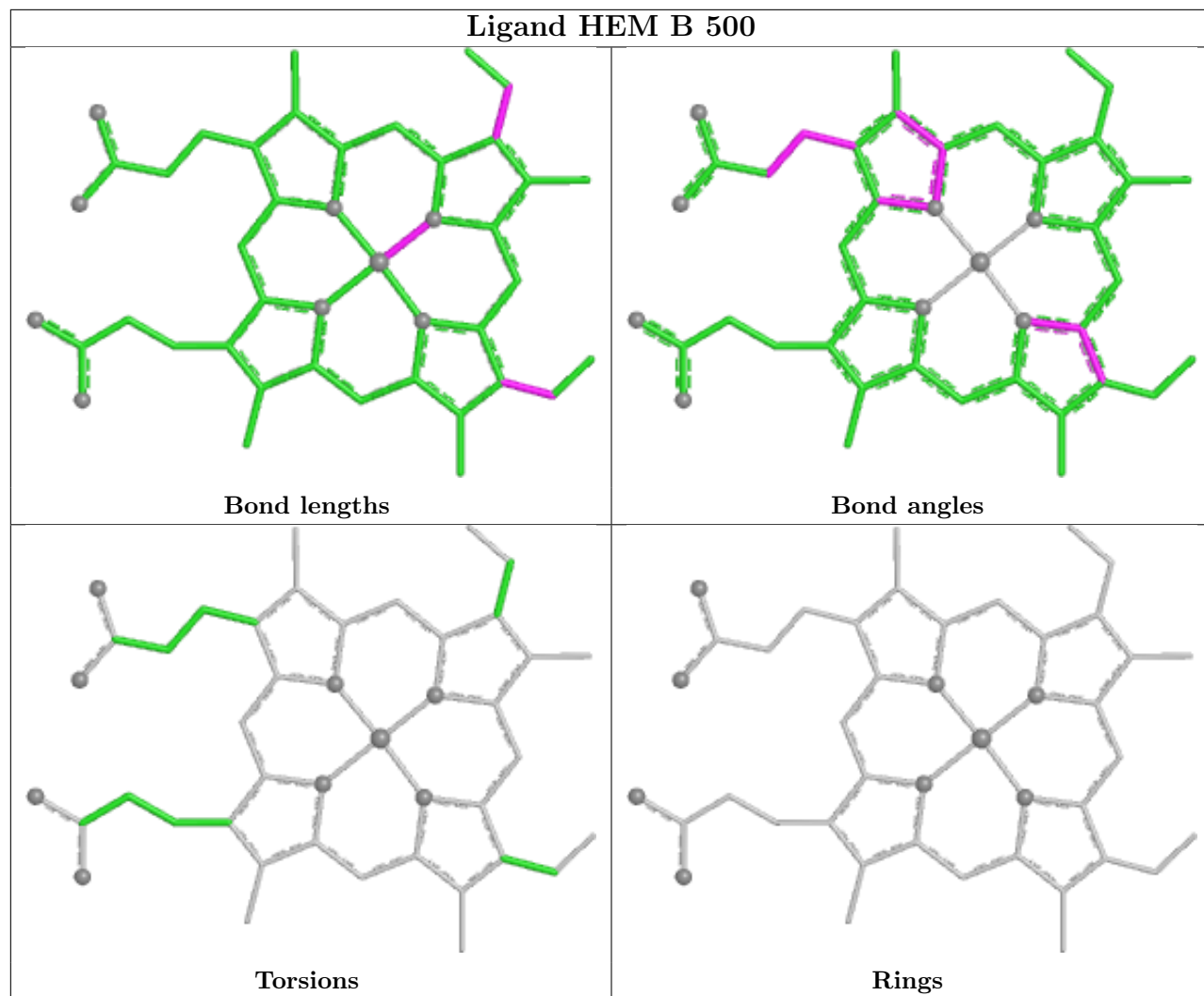
There are no ring outliers.

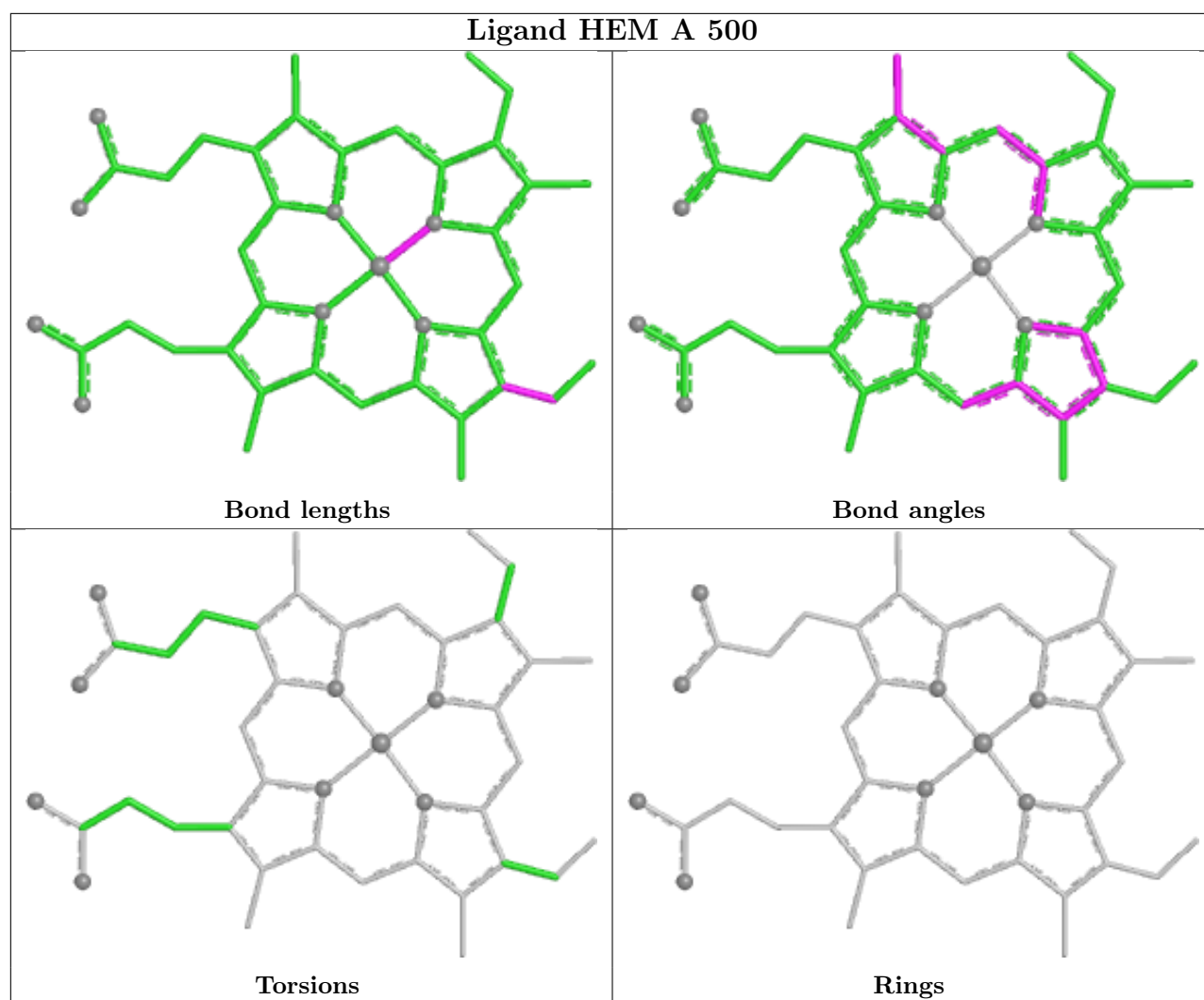
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	880	GOL	1	0
4	A	700	ARG	1	0
7	A	890	GOL	1	0
7	A	880	GOL	3	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.