



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 09:33 AM EST

PDB ID : 9NSE
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE, ETHYL-
ISOSELENOUREA COMPLEX
Authors : Li, H.; Raman, C.S.; Martasek, P.; Kral, V.; Masters, B.S.S.; Poulos, T.L.
Deposited on : 1999-01-13
Resolution : 2.24 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

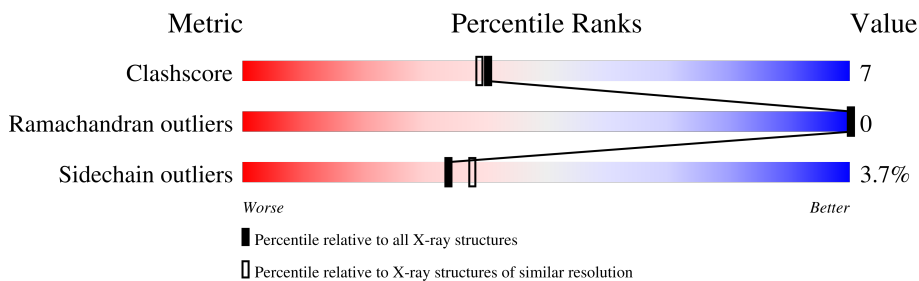
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)

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	 79% 14% • 6%
1	B	444	 75% 17% • 7%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7068 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.

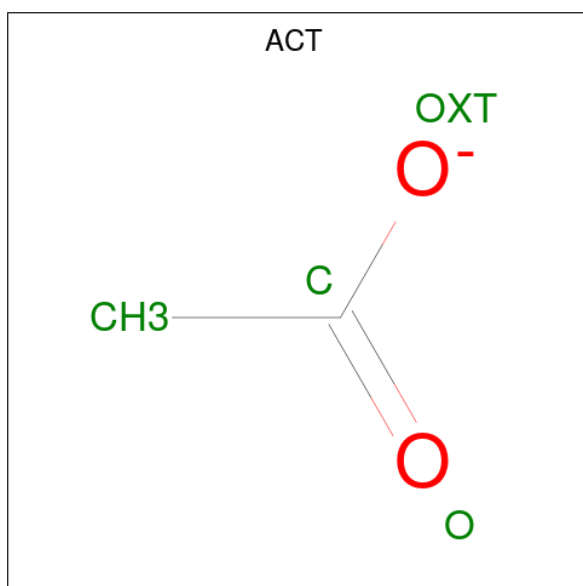
- Molecule 1 is a protein called PROTEIN (NITRIC OXIDE SYNTHASE).

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	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	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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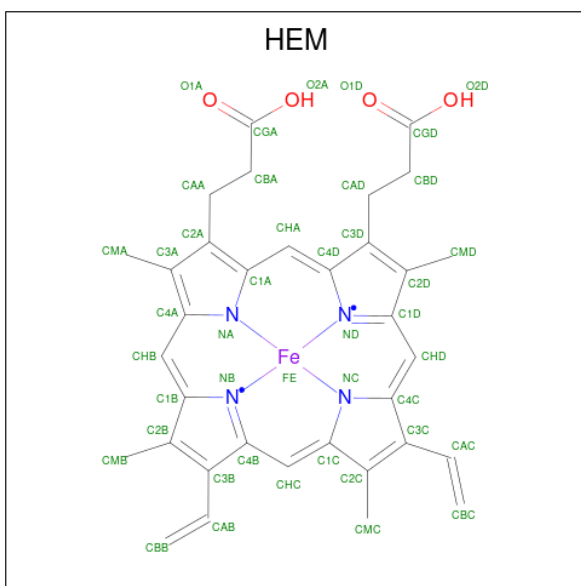
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

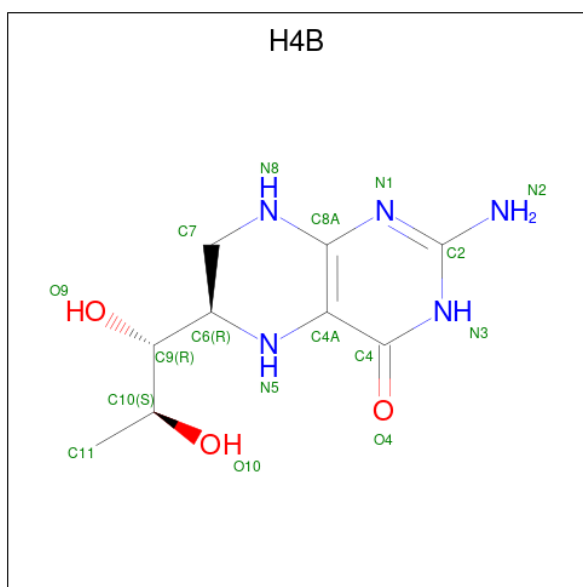
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

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



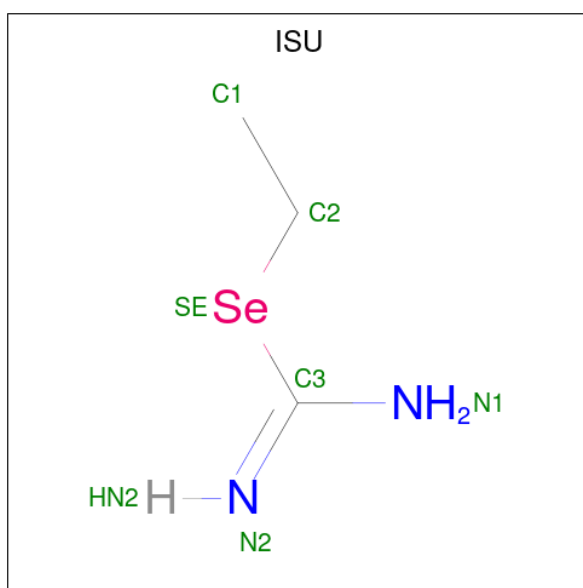
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 6 is SE-ETHYL-ISOSELENOUREA (three-letter code: ISU) (formula: $C_3H_8N_2Se$).



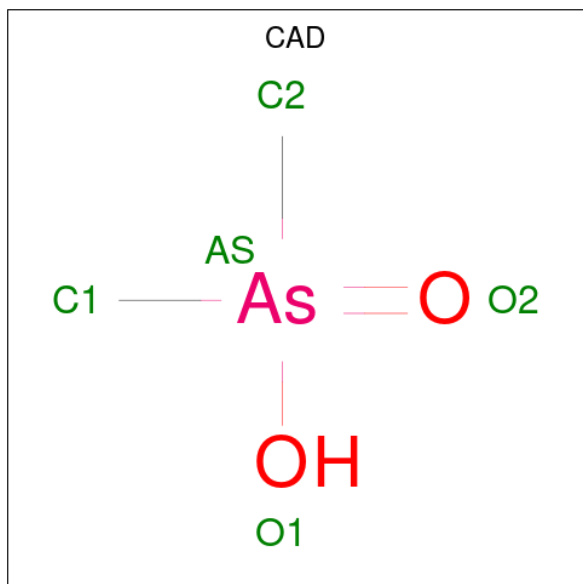
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	Se	0	0
			6	3	2	1		
6	B	1	Total	C	N	Se	0	0
			6	3	2	1		

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

- Molecule 7 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	As	C		
7	A	1	3	1	2	0	0
7	B	1	3	1	2	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	157	Total O 157 157	0	0
9	B	145	Total O 145 145	0	0

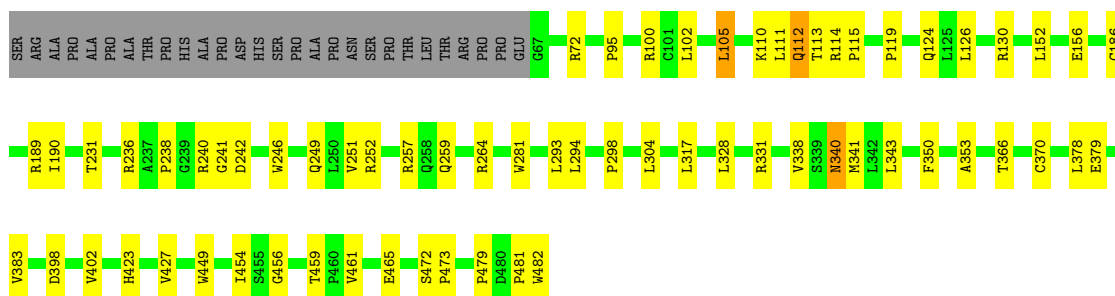
3 Residue-property plots [i](#)

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.

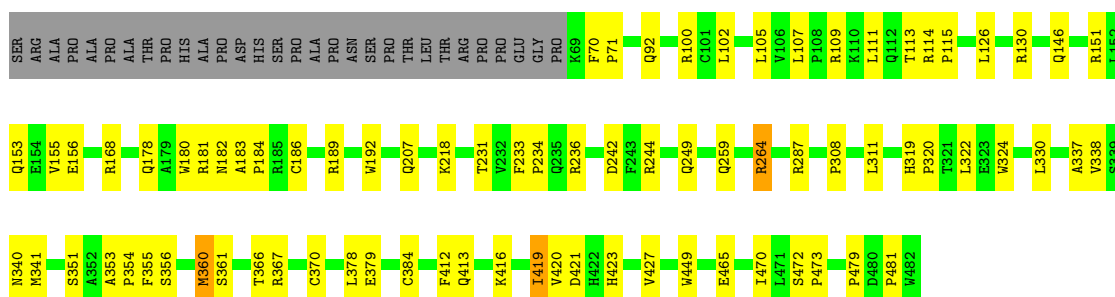
- Molecule 1: PROTEIN (NITRIC OXIDE SYNTHASE)

Chain A: 



- Molecule 1: PROTEIN (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	57.74Å 106.36Å 156.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.24	Depositor
% Data completeness (in resolution range)	84.0 (30.00-2.24)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.197 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7068	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: CAD, GOL, ISU, ZN, H4B, HEM, ACT

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	0.64	0/4631
1	B	0.37	0/3385	0.63	1/4614 (0.0%)
All	All	0.38	0/6782	0.64	1/9245 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	MET	N-CA-C	-5.26	96.81	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	50	0
1	B	3291	0	3205	50	0
2	A	8	0	6	0	0
2	B	8	0	6	0	0
3	A	1	0	0	0	0
4	A	43	0	30	0	0
4	B	43	0	30	1	0
5	A	17	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	17	0	15	2	0
6	A	6	0	0	0	0
6	B	12	0	0	0	0
7	A	3	0	0	0	0
7	B	3	0	0	1	0
8	A	6	0	8	0	0
8	B	6	0	8	0	0
9	A	157	0	0	4	0
9	B	145	0	0	3	0
All	All	7068	0	6538	96	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 7.

All (96) 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:249:GLN:HB2	1:A:252:ARG:HD3	1.43	0.99
1:A:115:PRO:HD3	1:A:479:PRO:HG3	1.44	0.99
1:B:115:PRO:HD3	1:B:479:PRO:HG3	1.46	0.94
1:A:338:VAL:HG11	1:A:341:MET:HE3	1.64	0.78
1:B:338:VAL:HG11	1:B:341:MET:HE3	1.66	0.77
1:A:111:LEU:CD2	9:A:1037:HOH:O	2.35	0.75
1:A:111:LEU:HD21	9:A:1037:HOH:O	1.93	0.69
1:A:459:THR:CG2	1:A:461:VAL:HG22	2.23	0.68
1:A:378:LEU:HB2	9:A:1098:HOH:O	1.94	0.67
1:B:126:LEU:O	1:B:130:ARG:HG3	1.95	0.66
1:B:378:LEU:HB2	9:B:1006:HOH:O	1.97	0.63
1:A:72:ARG:HD2	1:B:109:ARG:NH2	2.14	0.63
1:B:416:LYS:HA	1:B:416:LYS:HE2	1.81	0.62
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.82	0.62
1:B:338:VAL:HG11	1:B:341:MET:CE	2.29	0.62
1:A:111:LEU:HD22	9:A:1037:HOH:O	1.98	0.61
1:A:186:CYS:HB3	1:A:189:ARG:HD2	1.81	0.60
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.82	0.60
1:B:186:CYS:HB3	1:B:189:ARG:HD2	1.84	0.59
1:B:114:ARG:NH1	1:B:479:PRO:HB3	2.17	0.59
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.38	0.59
1:B:264:ARG:HH11	1:B:287:ARG:HG2	1.66	0.59
1:A:119:PRO:HB3	1:A:238:PRO:CG	2.33	0.58
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LEU:HD13	1:B:470:ILE:HD13	1.87	0.57
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.45	0.56
1:A:338:VAL:HG11	1:A:341:MET:CE	2.34	0.55
1:A:340:ASN:H	1:A:340:ASN:HD22	1.55	0.55
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.90	0.54
1:A:481:PRO:HD2	1:A:482:TRP:CE3	2.44	0.53
1:A:111:LEU:O	1:A:111:LEU:HG	2.08	0.53
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.58	0.52
1:B:449:TRP:HA	5:B:601:H4B:N1	2.24	0.52
1:A:115:PRO:HD3	1:A:479:PRO:CG	2.31	0.52
1:B:423:HIS:O	1:B:427:VAL:HG23	2.10	0.52
1:A:481:PRO:HD2	1:A:482:TRP:CZ3	2.45	0.51
1:B:115:PRO:HD3	1:B:479:PRO:CG	2.32	0.51
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.47	0.50
1:A:119:PRO:HB3	1:A:238:PRO:HB3	1.94	0.50
1:A:102:LEU:HD21	1:B:71:PRO:HB3	1.94	0.49
1:A:459:THR:HG22	1:A:461:VAL:HG22	1.95	0.49
1:A:449:TRP:HA	5:A:600:H4B:N1	2.28	0.48
1:B:341:MET:HE1	4:B:500:HEM:HBD2	1.96	0.48
1:A:398:ASP:O	1:A:402:VAL:HG23	2.14	0.48
1:B:151:ARG:O	1:B:155:VAL:HG23	2.14	0.47
1:B:412:PHE:CB	1:B:419:ILE:HG12	2.45	0.47
1:A:343:LEU:HB3	1:A:350:PHE:HB2	1.97	0.47
1:B:366:THR:O	1:B:370:CYS:HB2	2.14	0.47
1:A:95:PRO:CA	1:A:110:LYS:HG3	2.44	0.47
1:A:152:LEU:O	1:A:156:GLU:HG2	2.14	0.47
1:B:341:MET:CE	1:B:355:PHE:HZ	2.28	0.46
1:A:472:SER:HA	1:A:473:PRO:C	2.36	0.46
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.96	0.46
1:B:479:PRO:HG2	9:B:1050:HOH:O	2.16	0.46
1:B:361:SER:OG	1:B:421:ASP:HA	2.15	0.45
1:A:456:GLY:HA3	9:B:965:HOH:O	2.17	0.45
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.16	0.45
1:B:126:LEU:HD11	1:B:156:GLU:HG2	1.98	0.45
1:A:340:ASN:HD22	1:A:340:ASN:N	2.14	0.45
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.51	0.45
1:A:366:THR:HG21	1:A:454:ILE:HG23	2.00	0.44
1:B:231:THR:O	1:B:354:PRO:HD2	2.17	0.44
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.32	0.44
1:B:413:GLN:HG3	1:B:419:ILE:HD11	1.99	0.44
1:B:472:SER:HA	1:B:473:PRO:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:HD2	1:A:241:GLY:O	2.18	0.44
1:A:112:GLN:HE21	1:A:112:GLN:HB2	1.65	0.43
1:B:384:CYS:HA	7:B:950:CAD:C2	2.47	0.43
1:A:119:PRO:HB3	1:A:238:PRO:HG3	2.00	0.43
1:A:119:PRO:HB3	1:A:238:PRO:CB	2.49	0.43
1:B:236:ARG:HD3	1:B:351:SER:HB3	2.00	0.43
1:B:412:PHE:HB3	1:B:419:ILE:CG1	2.49	0.43
1:B:182:ASN:O	1:B:184:PRO:HD3	2.19	0.43
1:B:249:GLN:HA	1:B:337:ALA:O	2.19	0.42
1:B:168:ARG:HA	1:B:168:ARG:HD3	1.93	0.42
1:B:360:MET:HA	1:B:420:VAL:O	2.19	0.42
1:A:126:LEU:O	1:A:130:ARG:HG3	2.20	0.42
1:A:281:TRP:HB2	1:A:304:LEU:HD21	2.00	0.42
1:A:456:GLY:O	1:A:459:THR:HB	2.19	0.42
1:B:186:CYS:O	1:B:189:ARG:HD3	2.19	0.42
1:A:186:CYS:O	1:A:189:ARG:HD3	2.20	0.41
1:B:337:ALA:HB2	1:B:356:SER:HB3	2.02	0.41
1:A:317:LEU:HG	1:A:331:ARG:HA	2.02	0.41
1:A:379:GLU:O	1:A:383:VAL:HG23	2.20	0.41
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.51	0.41
1:A:423:HIS:O	1:A:427:VAL:HG23	2.21	0.41
1:A:251:VAL:O	1:A:252:ARG:HD2	2.21	0.41
1:B:231:THR:O	1:B:353:ALA:HA	2.20	0.41
1:B:367:ARG:HH12	5:B:601:H4B:C4	2.33	0.41
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.61	0.41
1:A:190:ILE:O	1:A:190:ILE:HG12	2.22	0.40
1:B:183:ALA:HA	1:B:184:PRO:HD3	1.88	0.40
1:A:264:ARG:HH11	1:A:264:ARG:HG3	1.87	0.40
1:B:70:PHE:HA	1:B:71:PRO:HD2	1.97	0.40
1:A:231:THR:O	1:A:353:ALA:HA	2.22	0.40
1:A:236:ARG:HG2	1:A:242:ASP:OD1	2.21	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%)	388 (94%)	24 (6%)	0	100	100
All	All	826/888 (93%)	785 (95%)	41 (5%)	0	100	100

There are no Ramachandran outliers to report.

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%)	40	46
1	B	353/377 (94%)	338 (96%)	15 (4%)	30	32
All	All	707/754 (94%)	681 (96%)	26 (4%)	34	38

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	105	LEU
1	A	112	GLN
1	A	113	THR
1	A	114	ARG
1	A	124	GLN
1	A	257	ARG
1	A	259	GLN
1	A	293	LEU
1	A	328	LEU
1	A	340	ASN
1	B	92	GLN
1	B	100	ARG
1	B	102	LEU
1	B	107	LEU

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Mol	Chain	Res	Type
1	B	113	THR
1	B	146	GLN
1	B	153	GLN
1	B	207	GLN
1	B	218	LYS
1	B	259	GLN
1	B	264	ARG
1	B	330	LEU
1	B	340	ASN
1	B	379	GLU
1	B	419	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	146	GLN
1	A	191	GLN
1	A	259	GLN
1	A	278	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	135	GLN
1	B	178	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	340	ASN
1	B	376	ASN
1	B	405	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 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
7	CAD	B	950	1	0,2,4	-	-	0,1,6	-	-
5	H4B	A	600	-	16,18,18	2.05	5 (31%)	11,26,26	4.24	9 (81%)
2	ACT	A	860	-	3,3,3	0.94	0	3,3,3	0.66	0
2	ACT	B	851	-	3,3,3	0.93	0	3,3,3	0.85	0
6	ISU	B	801	-	3,5,5	1.34	1 (33%)	1,5,5	0.37	0
8	GOL	B	881	-	5,5,5	0.15	0	5,5,5	0.22	0
4	HEM	A	500	1	41,50,50	1.29	4 (9%)	45,82,82	1.41	7 (15%)
2	ACT	A	850	-	3,3,3	0.96	0	3,3,3	0.83	0
2	ACT	B	861	-	3,3,3	0.87	0	3,3,3	0.80	0
6	ISU	A	800	-	3,5,5	1.20	0	1,5,5	0.50	0
6	ISU	B	811	-	3,5,5	1.27	0	1,5,5	0.26	0
8	GOL	A	880	-	5,5,5	0.18	0	5,5,5	0.23	0
4	HEM	B	500	1	41,50,50	1.28	3 (7%)	45,82,82	1.39	3 (6%)
7	CAD	A	950	1	0,2,4	-	-	0,1,6	-	-
5	H4B	B	601	-	16,18,18	2.05	4 (25%)	11,26,26	4.20	9 (81%)

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
5	H4B	A	600	-	-	0/8/17/17	0/2/2/2
8	GOL	B	881	-	-	0/4/4/4	-
6	ISU	B	801	-	-	0/1/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	A	500	1	-	2/12/54/54	-
6	ISU	A	800	-	-	0/1/3/3	-
6	ISU	B	811	-	-	0/1/3/3	-
8	GOL	A	880	-	-	0/4/4/4	-
4	HEM	B	500	1	-	2/12/54/54	-
5	H4B	B	601	-	-	0/8/17/17	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	H4B	C4-N3	4.81	1.41	1.33
5	B	601	H4B	C4-N3	4.50	1.40	1.33
5	B	601	H4B	C4A-N5	4.43	1.47	1.38
5	A	600	H4B	C4A-N5	4.16	1.46	1.38
5	B	601	H4B	C6-N5	3.78	1.53	1.45
4	B	500	HEM	C3C-CAC	-3.37	1.40	1.47
4	A	500	HEM	C3C-CAC	-3.31	1.41	1.47
5	A	600	H4B	C6-N5	3.24	1.52	1.45
4	B	500	HEM	C4A-NA	2.80	1.41	1.36
4	B	500	HEM	CAB-C3B	-2.76	1.39	1.47
4	A	500	HEM	C3C-C2C	-2.67	1.36	1.40
4	A	500	HEM	CAB-C3B	-2.39	1.40	1.47
4	A	500	HEM	C1A-NA	2.18	1.40	1.36
6	B	801	ISU	C3-N2	2.16	1.33	1.27
5	A	600	H4B	C4A-C8A	-2.13	1.37	1.41
5	B	601	H4B	C8A-N1	2.11	1.38	1.34
5	A	600	H4B	C8A-N1	2.10	1.38	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	H4B	C8A-C4A-C4	8.45	122.08	114.57
5	B	601	H4B	C8A-C4A-C4	8.31	121.95	114.57
5	B	601	H4B	C2-N3-C4	5.93	125.34	115.93
5	A	600	H4B	C2-N3-C4	5.92	125.33	115.93
5	A	600	H4B	N1-C2-N3	-5.10	117.42	125.42
5	B	601	H4B	N1-C2-N3	-4.91	117.72	125.42
4	B	500	HEM	C4B-CHC-C1C	4.25	128.17	122.56
4	A	500	HEM	C4B-CHC-C1C	4.02	127.86	122.56
5	B	601	H4B	N2-C2-N1	3.99	123.47	117.25
5	A	600	H4B	N2-C2-N1	3.92	123.35	117.25
5	A	600	H4B	C2-N1-C8A	3.69	122.81	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	H4B	C2-N1-C8A	3.68	122.78	114.54
5	A	600	H4B	C4A-C4-N3	-3.58	113.82	124.01
4	B	500	HEM	C2C-C3C-C4C	-3.54	104.42	106.90
5	B	601	H4B	C4A-C4-N3	-3.53	113.97	124.01
5	B	601	H4B	C4A-N5-C6	-3.28	112.22	121.16
5	A	600	H4B	C4A-N5-C6	-3.28	112.23	121.16
4	A	500	HEM	C4B-C3B-C2B	-2.92	104.79	107.11
4	B	500	HEM	CBA-CAA-C2A	-2.90	107.67	112.62
4	A	500	HEM	CAD-C3D-C4D	2.78	129.51	124.66
4	A	500	HEM	C2C-C3C-C4C	-2.48	105.17	106.90
5	B	601	H4B	O9-C9-C6	2.47	114.88	108.98
5	B	601	H4B	C4-C4A-N5	-2.43	117.08	119.12
4	A	500	HEM	CAD-C3D-C2D	-2.32	123.56	127.88
4	A	500	HEM	CMD-C2D-C1D	2.32	128.57	125.04
5	A	600	H4B	O9-C9-C6	2.31	114.50	108.98
5	A	600	H4B	C4-C4A-N5	-2.31	117.19	119.12
4	A	500	HEM	C3B-C2B-C1B	2.15	108.08	106.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	500	HEM	C4D-C3D-CAD-CBD
4	A	500	HEM	C2D-C3D-CAD-CBD
4	B	500	HEM	CAA-CBA-CGA-O2A
4	B	500	HEM	CAA-CBA-CGA-O1A

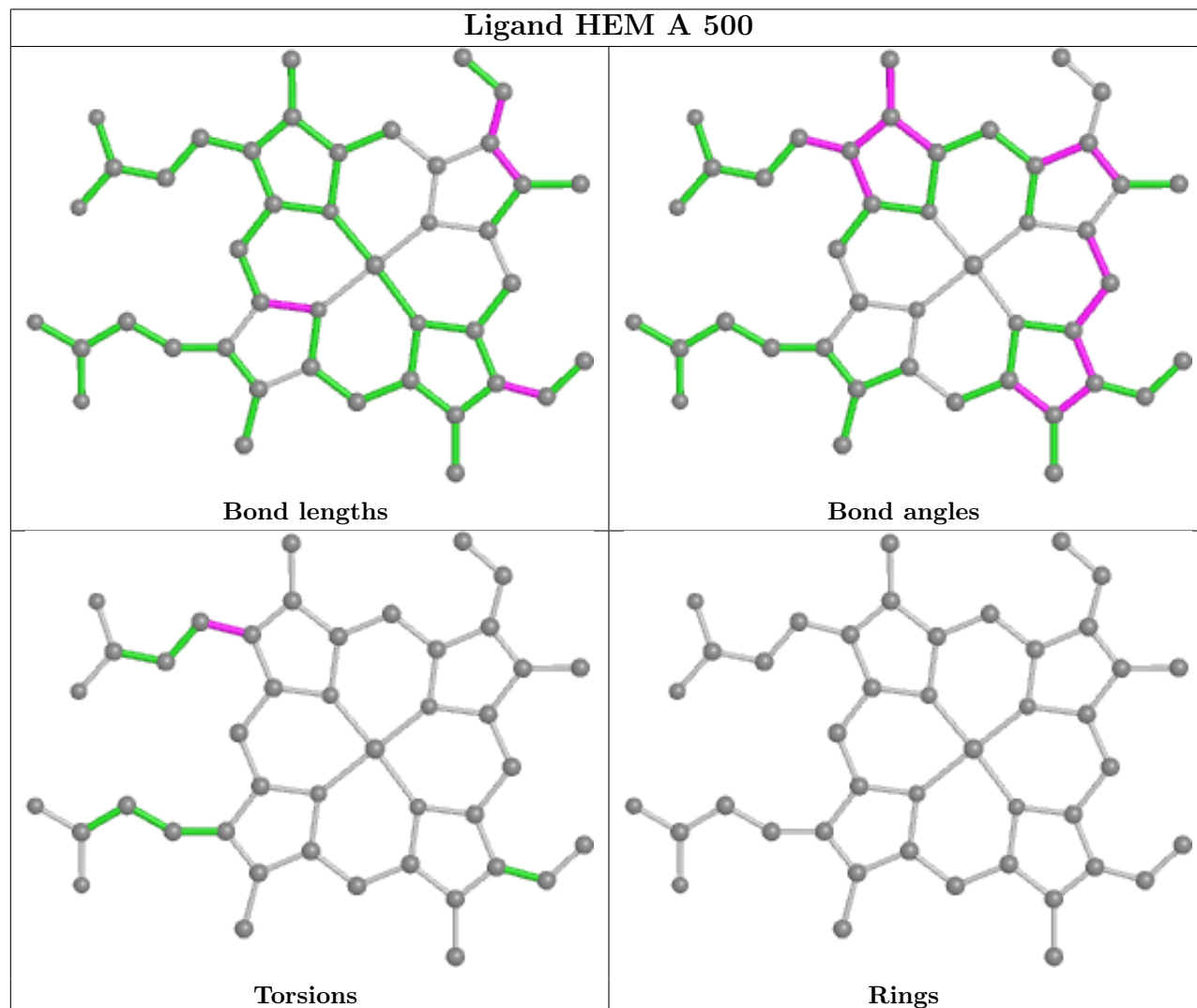
There are no ring outliers.

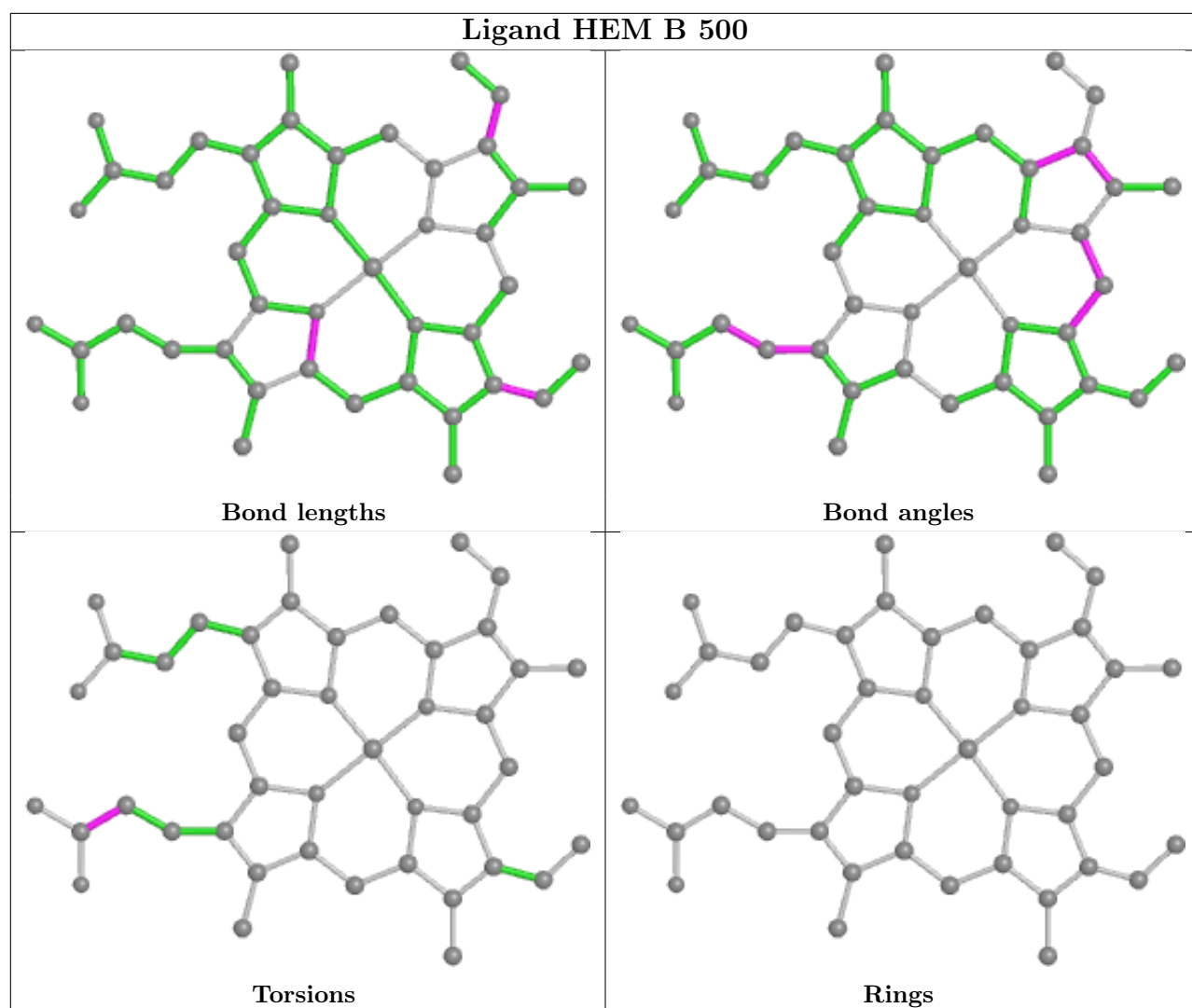
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	950	CAD	1	0
5	A	600	H4B	1	0
4	B	500	HEM	1	0
5	B	601	H4B	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 [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.