



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:40 AM GMT

PDB ID : 2NSE  
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE SUBSTRATE COMPLEX  
Authors : Raman, C.S.; Li, H.; Martasek, P.; Kral, V.; Masters, B.S.S.; Poulos, T.L.  
Deposited on : 1998-08-13  
Resolution : 2.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

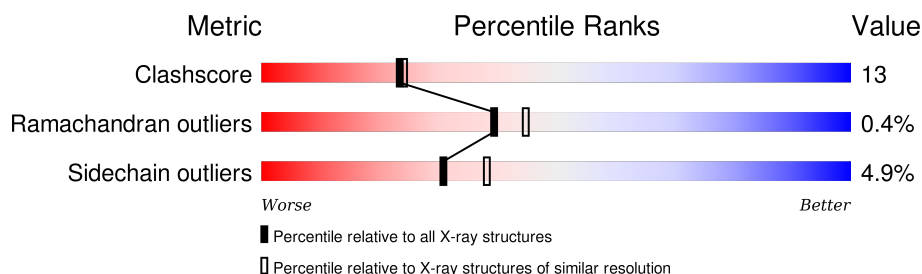
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	444	 65% 26% • 6%
1	B	444	 70% 21% • 7%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7007 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.

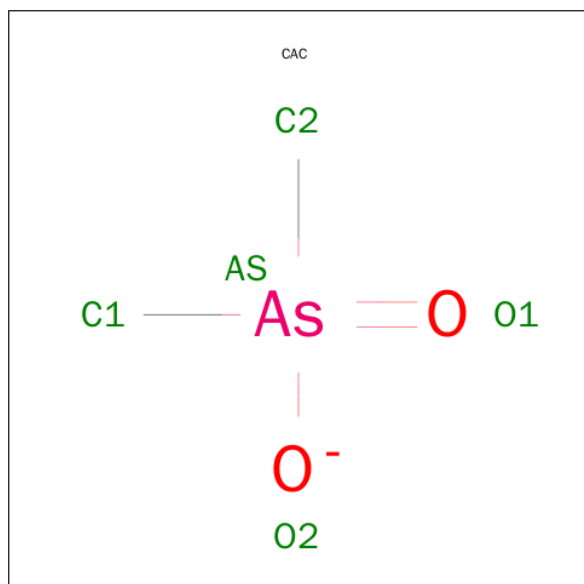
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE.

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	0	0
			1	1		

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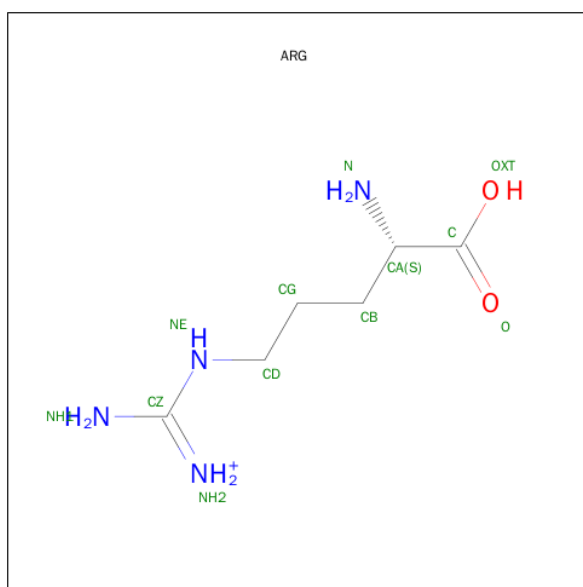
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	As	0	0
			1	1		

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

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

- Molecule 4 is ARGININE (three-letter code: ARG) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>4</sub>O<sub>2</sub>).



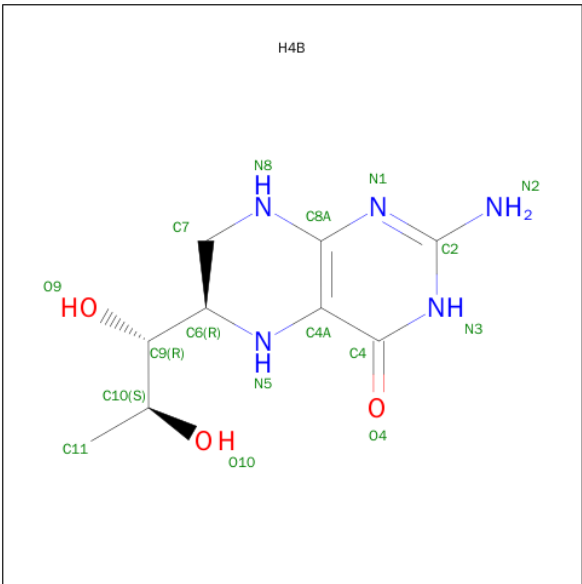
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	6	4	2		
4	B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- 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
6	A	1	Total	C	N	O	0	0
			17	9	5	3		

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

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



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

- Molecule 8 is water.

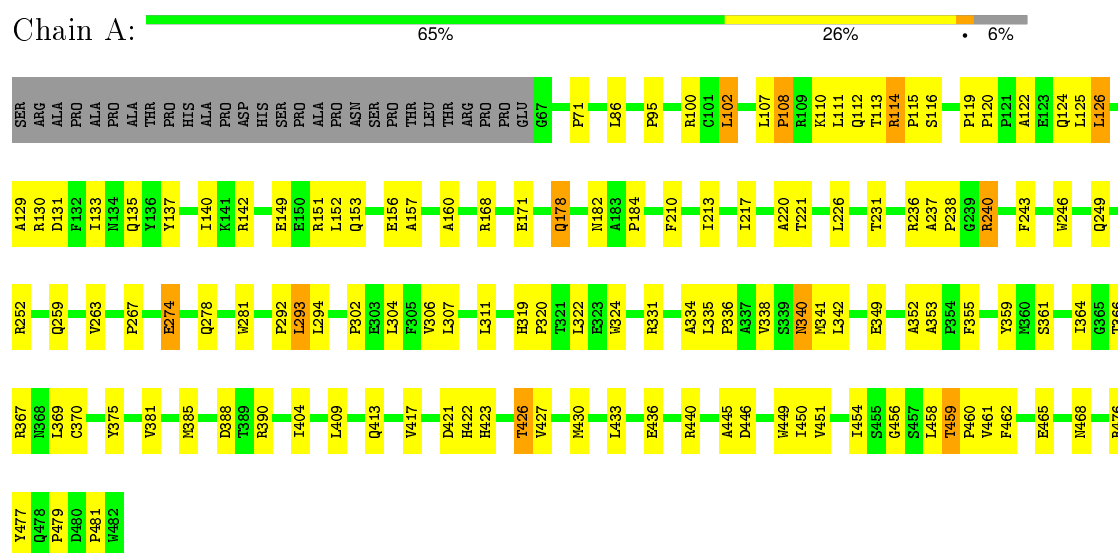
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	149	Total	O	0	0
			149	149		
8	B	112	Total	O	0	0
			112	112		

### 3 Residue-property plots

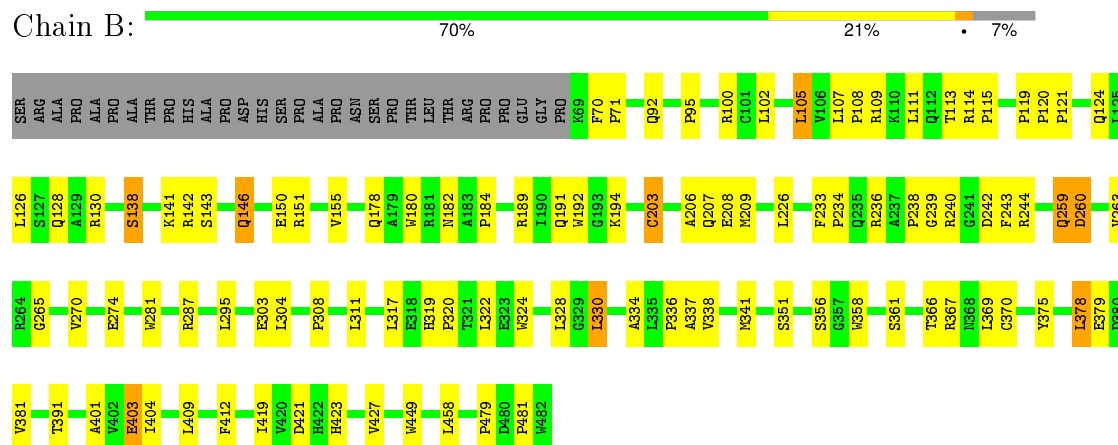
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: NITRIC OXIDE SYNTHASE



#### • Molecule 1: NITRIC OXIDE SYNTHASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.06 Å   106.38 Å   156.38 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.34	Depositor
% Data completeness (in resolution range)	96.2 (30.00-2.34)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.216 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7007	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	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: CAC, GOL, ZN, H4B, 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	0.42	0/3397	0.67	1/4631 (0.0%)
1	B	0.39	0/3385	0.64	0/4614
All	All	0.41	0/6782	0.65	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	A	108	PRO	N-CA-C	-5.20	98.59	112.10

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	107	0
1	B	3291	0	3205	74	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	12	1	0
4	B	12	0	12	0	0
5	A	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	43	0	30	1	0
6	A	17	0	15	2	0
6	B	17	0	15	2	0
7	B	6	0	8	0	0
8	A	149	0	0	0	0
8	B	112	0	0	3	0
All	All	7007	0	6542	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (177) 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:114:ARG:HG3	1:A:115:PRO:HD2	1.43	0.97
1:A:120:PRO:HG2	1:A:125:LEU:HD12	1.42	0.97
1:B:114:ARG:HD3	1:B:479:PRO:HG3	1.47	0.93
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.49	0.92
1:A:113:THR:HG21	1:A:476:ARG:HH11	1.35	0.89
1:B:114:ARG:HD3	1:B:479:PRO:CG	2.05	0.85
1:A:113:THR:CG2	1:A:476:ARG:HH11	1.91	0.83
1:B:409:LEU:HD23	1:B:419:ILE:HD12	1.61	0.82
1:B:111:LEU:HD23	8:B:1051:HOH:O	1.82	0.79
1:A:116:SER:H	1:A:236:ARG:HH22	1.31	0.78
1:B:115:PRO:HD3	1:B:479:PRO:HG2	1.69	0.74
1:A:422:HIS:O	1:A:426:THR:HB	1.88	0.73
1:A:237:ALA:HB3	1:A:240:ARG:HD3	1.71	0.72
1:A:459:THR:CG2	1:A:461:VAL:HG22	2.22	0.70
1:A:95:PRO:HA	1:A:110:LYS:HG3	1.74	0.69
1:A:430:MET:HE1	1:A:433:LEU:HD12	1.73	0.69
1:A:116:SER:H	1:A:236:ARG:NH2	1.91	0.68
1:A:114:ARG:HG3	1:A:115:PRO:CD	2.22	0.67
1:A:426:THR:HG21	1:A:459:THR:HG23	1.77	0.67
1:B:265:GLY:H	1:B:287:ARG:HG2	1.61	0.66
1:A:111:LEU:HG	1:A:111:LEU:O	1.96	0.66
1:B:361:SER:OG	1:B:421:ASP:HA	1.97	0.65
1:A:178:GLN:HA	1:A:178:GLN:HE21	1.62	0.65
1:A:340:ASN:H	1:A:340:ASN:HD22	1.45	0.64
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.79	0.63
1:A:116:SER:N	1:A:236:ARG:HH22	1.98	0.62
1:A:126:LEU:HB3	1:A:130:ARG:HH21	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:THR:OG1	1:A:476:ARG:HD3	2.00	0.61
1:B:95:PRO:HB3	1:B:108:PRO:HG2	1.83	0.61
1:B:111:LEU:HD21	8:B:1006:HOH:O	2.01	0.60
1:B:366:THR:O	1:B:370:CYS:HB2	2.02	0.60
1:A:342:LEU:HD11	1:A:349:GLU:HB3	1.83	0.59
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.84	0.59
4:A:700:ARG:HG3	5:A:500:HEM:HBA1	1.84	0.58
1:A:102:LEU:HD21	1:B:71:PRO:HB3	1.85	0.58
1:A:409:LEU:O	1:A:413:GLN:HG3	2.04	0.57
1:A:178:GLN:NE2	1:A:178:GLN:HA	2.19	0.57
1:B:124:GLN:HG2	1:B:128:GLN:HE21	1.69	0.57
1:B:114:ARG:HD3	1:B:479:PRO:HG2	1.88	0.56
1:B:209:MET:HE3	1:B:295:LEU:HB3	1.87	0.56
1:B:119:PRO:HG3	1:B:238:PRO:HB2	1.88	0.56
1:B:191:GLN:HE22	1:B:194:LYS:HD3	1.71	0.56
1:A:231:THR:O	1:A:353:ALA:HA	2.05	0.56
1:A:338:VAL:HG11	1:A:341:MET:HE3	1.88	0.56
1:B:412:PHE:HB2	1:B:419:ILE:HD13	1.87	0.55
1:B:124:GLN:HG2	1:B:128:GLN:NE2	2.22	0.55
1:B:367:ARG:HH12	6:B:600:H4B:C4	2.19	0.55
1:A:430:MET:HE3	1:A:461:VAL:HG12	1.89	0.55
1:B:209:MET:CE	1:B:295:LEU:HB3	2.37	0.55
1:A:274:GLU:HG2	1:A:278:GLN:HE21	1.72	0.55
1:B:338:VAL:HG11	1:B:341:MET:HE3	1.88	0.55
1:B:449:TRP:HA	6:B:600:H4B:N1	2.22	0.54
1:A:111:LEU:HD23	1:A:477:TYR:CE2	2.43	0.54
1:B:378:LEU:HB2	8:B:1047:HOH:O	2.08	0.54
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.43	0.54
1:A:126:LEU:HB3	1:A:130:ARG:NH2	2.23	0.54
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.90	0.54
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.22	0.54
1:A:426:THR:CG2	1:A:459:THR:HG23	2.39	0.53
1:B:182:ASN:O	1:B:184:PRO:HD3	2.10	0.52
1:A:126:LEU:O	1:A:130:ARG:HG3	2.09	0.52
1:A:86:LEU:HD22	1:A:440:ARG:HB2	1.91	0.52
1:A:249:GLN:HB2	1:A:252:ARG:HD3	1.92	0.51
1:A:178:GLN:CA	1:A:178:GLN:HE21	2.24	0.51
1:A:100:ARG:HH11	1:A:100:ARG:HG3	1.74	0.51
1:A:113:THR:CG2	1:A:476:ARG:HD3	2.41	0.51
1:A:436:GLU:OE1	1:A:440:ARG:HD2	2.11	0.51
1:B:423:HIS:O	1:B:427:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.52	0.50
1:B:259:GLN:HG3	1:B:260:ASP:H	1.75	0.50
1:A:221:THR:HA	1:A:226:LEU:HD13	1.93	0.50
1:B:206:ALA:HB3	1:B:303:GLU:OE2	2.11	0.49
1:A:220:ALA:O	1:A:226:LEU:HA	2.13	0.49
1:A:423:HIS:O	1:A:427:VAL:HG23	2.12	0.49
1:A:71:PRO:HB3	1:B:102:LEU:HD21	1.94	0.49
1:B:126:LEU:O	1:B:130:ARG:HG3	2.13	0.49
1:A:445:ALA:O	1:A:468:ASN:HB2	2.11	0.49
1:A:129:ALA:O	1:A:133:ILE:HG12	2.12	0.49
1:A:292:PRO:HB3	1:A:306:VAL:HG22	1.95	0.48
1:A:459:THR:HG22	1:A:461:VAL:HG22	1.95	0.48
1:A:182:ASN:O	1:A:184:PRO:HD3	2.13	0.48
1:A:359:TYR:CD2	1:A:364:ILE:HD11	2.48	0.48
1:A:151:ARG:HD3	1:A:168:ARG:NH2	2.28	0.48
1:A:113:THR:OG1	1:A:476:ARG:CD	2.62	0.48
1:A:168:ARG:HB2	1:A:171:GLU:HG3	1.94	0.48
1:A:149:GLU:O	1:A:153:GLN:HG3	2.14	0.48
1:A:446:ASP:O	1:A:450:ILE:HG12	2.13	0.48
1:A:381:VAL:O	1:A:385:MET:HG3	2.13	0.48
1:A:213:ILE:O	1:A:217:ILE:HG13	2.13	0.48
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.14	0.47
1:B:234:PRO:HB2	1:B:243:PHE:CE2	2.49	0.47
1:A:334:ALA:HB1	1:A:417:VAL:HG11	1.96	0.47
1:B:412:PHE:CD2	1:B:419:ILE:HG23	2.49	0.47
1:A:112:GLN:OE1	1:A:114:ARG:NH2	2.47	0.47
1:A:114:ARG:CG	1:A:115:PRO:HD2	2.31	0.47
1:A:131:ASP:O	1:A:135:GLN:HG3	2.15	0.47
1:A:451:VAL:HG22	1:A:461:VAL:HG23	1.97	0.47
1:B:281:TRP:HB2	1:B:304:LEU:HD11	1.96	0.47
1:B:287:ARG:HH12	1:B:375:TYR:HA	1.80	0.47
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.96	0.47
1:A:237:ALA:H	1:A:240:ARG:NH1	2.12	0.46
1:B:379:GLU:CD	1:B:379:GLU:H	2.17	0.46
1:A:430:MET:HE1	1:A:433:LEU:CD1	2.43	0.46
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.50	0.46
1:B:226:LEU:HD21	1:B:334:ALA:O	2.15	0.46
1:B:191:GLN:NE2	1:B:194:LYS:HD3	2.31	0.46
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.45	0.46
1:B:236:ARG:HD2	1:B:242:ASP:CG	2.36	0.46
1:A:369:LEU:HA	1:A:375:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:SER:HA	1:B:143:SER:HB2	1.98	0.46
1:B:412:PHE:HB2	1:B:419:ILE:CD1	2.45	0.45
1:A:334:ALA:CB	1:A:417:VAL:HG11	2.46	0.45
1:B:319:HIS:NE2	1:B:403:GLU:HG3	2.31	0.45
1:A:120:PRO:CG	1:A:125:LEU:HD12	2.31	0.45
1:A:281:TRP:HB2	1:A:304:LEU:HD11	1.99	0.45
1:B:180:TRP:O	1:B:189:ARG:HD3	2.17	0.45
1:A:449:TRP:HA	6:A:600:H4B:N1	2.32	0.45
1:A:113:THR:CG2	1:A:476:ARG:NH1	2.72	0.45
1:A:430:MET:CE	1:A:461:VAL:HG12	2.47	0.45
1:B:234:PRO:HB2	1:B:243:PHE:CD2	2.51	0.45
1:A:388:ASP:OD1	1:A:390:ARG:HB2	2.17	0.45
1:A:137:TYR:HA	1:A:140:ILE:HG12	1.98	0.45
1:B:203:CYS:SG	1:B:208:GLU:HB3	2.57	0.45
1:A:122:ALA:O	1:A:126:LEU:HB2	2.17	0.44
1:B:265:GLY:HA2	1:B:287:ARG:HA	1.98	0.44
1:B:369:LEU:HA	1:B:375:TYR:HB2	2.00	0.44
1:A:361:SER:OG	1:A:421:ASP:HA	2.16	0.44
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.53	0.44
1:B:146:GLN:O	1:B:150:GLU:HB2	2.17	0.44
1:A:456:GLY:O	1:A:462:PHE:HB2	2.17	0.44
1:A:246:TRP:CE2	1:A:481:PRO:HB2	2.53	0.44
1:A:210:PHE:HE1	1:A:307:LEU:HD23	1.83	0.43
1:A:226:LEU:H	1:A:226:LEU:CD2	2.31	0.43
1:A:366:THR:HG21	1:A:454:ILE:HG23	2.00	0.43
1:B:239:GLY:O	1:B:240:ARG:HB3	2.17	0.43
1:A:458:LEU:HG	1:B:378:LEU:HD21	2.00	0.43
1:A:100:ARG:NH1	1:A:100:ARG:HG3	2.34	0.43
1:A:249:GLN:HB2	1:A:252:ARG:CG	2.49	0.43
1:B:95:PRO:CB	1:B:108:PRO:HG2	2.47	0.43
1:B:328:LEU:HB3	1:B:330:LEU:HD13	2.01	0.43
1:A:367:ARG:HH12	6:A:600:H4B:C4	2.31	0.43
1:B:308:PRO:O	1:B:311:LEU:HB2	2.19	0.42
1:A:152:LEU:O	1:A:156:GLU:HG2	2.19	0.42
1:A:226:LEU:HD12	1:A:335:LEU:HD12	2.00	0.42
1:B:120:PRO:HA	1:B:121:PRO:HD3	1.93	0.42
1:A:108:PRO:C	1:A:110:LYS:H	2.22	0.42
1:B:70:PHE:HA	1:B:71:PRO:HD2	1.81	0.42
1:A:458:LEU:HD21	1:B:401:ALA:HB2	2.01	0.42
1:A:423:HIS:O	1:A:426:THR:HG22	2.19	0.42
1:A:430:MET:CE	1:A:433:LEU:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD11	1:A:156:GLU:HA	2.02	0.42
1:A:246:TRP:HB2	1:A:294:LEU:HB3	2.00	0.42
1:A:125:LEU:O	1:A:125:LEU:HD23	2.20	0.41
1:B:265:GLY:N	1:B:287:ARG:HG2	2.31	0.41
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.80	0.41
1:A:263:VAL:HG11	1:A:267:PRO:HA	2.02	0.41
1:A:426:THR:CG2	1:A:460:PRO:HD2	2.50	0.41
1:B:259:GLN:HG3	1:B:260:ASP:OD1	2.19	0.41
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.55	0.41
1:B:358:TRP:H	5:B:500:HEM:HAB	1.85	0.41
1:B:194:LYS:O	1:B:194:LYS:HG2	2.20	0.41
1:A:137:TYR:HD1	1:A:142:ARG:HB2	1.86	0.41
1:A:465:GLU:OE1	1:B:105:LEU:HD13	2.20	0.41
1:A:293:LEU:CD2	1:A:307:LEU:HD21	2.51	0.41
1:A:119:PRO:HB3	1:A:238:PRO:HG3	2.03	0.41
1:A:341:MET:HE3	1:A:355:PHE:HZ	1.86	0.41
1:A:335:LEU:HA	1:A:336:PRO:HD2	1.93	0.41
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.55	0.41
1:B:151:ARG:O	1:B:155:VAL:HG23	2.21	0.41
1:B:270:VAL:O	1:B:274:GLU:HG3	2.21	0.41
1:B:191:GLN:HE21	1:B:358:TRP:HH2	1.67	0.41
1:A:243:PHE:O	1:A:352:ALA:HB2	2.20	0.41
1:A:294:LEU:HG	1:A:302:PRO:HB2	2.03	0.40
1:A:157:ALA:O	1:A:160:ALA:HB3	2.21	0.40
1:A:95:PRO:CA	1:A:110:LYS:HG3	2.48	0.40
1:A:370:CYS:SG	1:A:404:ILE:HD12	2.61	0.40
1:B:337:ALA:HA	1:B:356:SER:HB3	2.03	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%)	382 (92%)	32 (8%)	0	100	100
1	B	412/444 (93%)	377 (92%)	32 (8%)	3 (1%)	26	28
All	All	826/888 (93%)	759 (92%)	64 (8%)	3 (0%)	39	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	B	260	ASP
1	B	336	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	354/377 (94%)	339 (96%)	15 (4%)	36	46
1	B	353/377 (94%)	333 (94%)	20 (6%)	25	30
All	All	707/754 (94%)	672 (95%)	35 (5%)	31	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	107	LEU
1	A	114	ARG
1	A	124	GLN
1	A	126	LEU
1	A	178	GLN
1	A	240	ARG
1	A	259	GLN
1	A	274	GLU
1	A	293	LEU
1	A	311	LEU
1	A	331	ARG
1	A	340	ASN

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Mol	Chain	Res	Type
1	A	426	THR
1	A	459	THR
1	B	92	GLN
1	B	100	ARG
1	B	105	LEU
1	B	107	LEU
1	B	109	ARG
1	B	113	THR
1	B	138	SER
1	B	141	LYS
1	B	142	ARG
1	B	146	GLN
1	B	178	GLN
1	B	203	CYS
1	B	207	GLN
1	B	263	VAL
1	B	317	LEU
1	B	330	LEU
1	B	378	LEU
1	B	391	THR
1	B	403	GLU
1	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	178	GLN
1	A	191	GLN
1	A	258	GLN
1	A	278	GLN
1	A	296	GLN
1	A	340	ASN
1	A	468	ASN
1	B	124	GLN
1	B	128	GLN
1	B	146	GLN
1	B	178	GLN
1	B	191	GLN
1	B	222	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 10 ligands modelled in this entry, 1 is monoatomic and 2 are modelled with single atom - leaving 7 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	HEM	A	500	1	30,50,50	2.81	11 (36%)	24,82,82	2.33	8 (33%)
6	H4B	A	600	-	13,18,18	1.66	3 (23%)	11,26,26	3.98	7 (63%)
4	ARG	A	700	-	5,11,11	0.31	0	3,13,13	0.23	0
5	HEM	B	500	1	30,50,50	2.77	7 (23%)	24,82,82	2.28	8 (33%)
6	H4B	B	600	-	13,18,18	1.64	3 (23%)	11,26,26	3.88	6 (54%)
4	ARG	B	700	-	5,11,11	0.29	0	3,13,13	0.27	0
7	GOL	B	880	-	5,5,5	0.11	0	5,5,5	0.12	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
5	HEM	A	500	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	H4B	A	600	-	-	0/8/17/17	0/2/2/2
4	ARG	A	700	-	-	0/5/11/11	0/0/0/0
5	HEM	B	500	1	-	0/10/54/54	0/0/8/8
6	H4B	B	600	-	-	0/8/17/17	0/2/2/2
4	ARG	B	700	-	-	0/5/11/11	0/0/0/0
7	GOL	B	880	-	-	0/4/4/4	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	HEM	C2D-C3D	-7.05	1.33	1.54
5	B	500	HEM	C3B-C4B	-7.01	1.45	1.51
5	A	500	HEM	C3B-C4B	-6.54	1.46	1.51
5	A	500	HEM	C2D-C3D	-6.48	1.35	1.54
5	A	500	HEM	C3C-CAC	-6.43	1.39	1.51
5	B	500	HEM	C3B-CAB	-6.21	1.39	1.51
5	B	500	HEM	C3C-CAC	-5.71	1.40	1.51
5	A	500	HEM	C3D-C4D	-5.49	1.44	1.51
5	A	500	HEM	C3B-CAB	-5.29	1.41	1.51
5	B	500	HEM	C3D-C4D	-4.95	1.45	1.51
5	B	500	HEM	C2C-C1C	-3.63	1.45	1.52
5	A	500	HEM	C2C-C1C	-3.26	1.46	1.52
5	A	500	HEM	C2B-C1B	-2.39	1.44	1.51
5	A	500	HEM	C4A-CHB	-2.29	1.33	1.39
6	A	600	H4B	C4A-C8A	-2.14	1.37	1.41
5	A	500	HEM	C2D-C1D	-2.02	1.45	1.51
5	B	500	HEM	C2D-C1D	-2.00	1.45	1.51
5	A	500	HEM	C1C-NC	2.02	1.38	1.36
6	B	600	H4B	C4A-N5	2.36	1.43	1.38
6	B	600	H4B	C6-N5	2.67	1.51	1.45
6	A	600	H4B	C6-N5	2.90	1.51	1.45
5	A	500	HEM	C4C-NC	3.34	1.40	1.36
6	B	600	H4B	C4-N3	3.47	1.39	1.33
6	A	600	H4B	C4-N3	3.59	1.39	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	H4B	N3-C2-N1	-4.55	118.08	125.53
6	B	600	H4B	N3-C2-N1	-4.13	118.76	125.53
5	B	500	HEM	CBA-CAA-C2A	-2.71	107.67	112.53
6	A	600	H4B	C8A-C4A-N5	2.01	121.39	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	500	HEM	C3B-CAB-CBB	2.11	127.70	124.46
5	A	500	HEM	CMD-C2D-C3D	2.45	125.17	114.35
5	B	500	HEM	CMD-C2D-C3D	2.68	126.18	114.35
6	A	600	H4B	N2-C2-N1	2.87	121.96	117.20
6	A	600	H4B	C4A-C8A-N8	2.88	121.82	118.43
6	B	600	H4B	N2-C2-N1	3.08	122.30	117.20
6	B	600	H4B	C2-N1-C8A	3.09	121.47	114.54
5	B	500	HEM	CMB-C2B-C3B	3.15	124.39	116.53
5	A	500	HEM	C2D-C3D-C4D	3.16	106.86	101.50
5	A	500	HEM	CAD-C3D-C2D	3.22	122.48	113.22
6	A	600	H4B	C2-N1-C8A	3.27	121.88	114.54
6	B	600	H4B	C4A-C8A-N8	3.29	122.31	118.43
5	A	500	HEM	C3C-CAC-CBC	3.49	129.81	124.46
5	B	500	HEM	CAD-C3D-C2D	3.66	123.72	113.22
5	B	500	HEM	C2D-C3D-C4D	3.81	107.96	101.50
5	B	500	HEM	CMC-C2C-C3C	4.05	126.65	116.53
5	B	500	HEM	CAD-C3D-C4D	4.42	128.06	112.47
5	A	500	HEM	CMC-C2C-C3C	4.43	127.60	116.53
5	A	500	HEM	CAD-C3D-C4D	5.08	130.37	112.47
5	B	500	HEM	C3C-CAC-CBC	5.15	132.35	124.46
5	A	500	HEM	CMB-C2B-C3B	5.36	129.91	116.53
6	A	600	H4B	C4-N3-C2	6.21	124.56	115.94
6	B	600	H4B	C4-N3-C2	6.31	124.70	115.94
6	B	600	H4B	C4-C4A-C8A	8.63	122.38	114.56
6	A	600	H4B	C4-C4A-C8A	8.97	122.68	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	HEM	1	0
6	A	600	H4B	2	0
4	A	700	ARG	1	0
5	B	500	HEM	1	0
6	B	600	H4B	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.