



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:46 PM GMT

PDB ID : 1D1X  
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN  
COMPLEXED WITH 1,4-PBITU (H4B BOUND)  
Authors : Raman, C.S.; Li, H.; Martasek, P.; Southan, G.J.; Masters, B.S.S.; Poulos,  
T.L.  
Deposited on : 1999-09-21  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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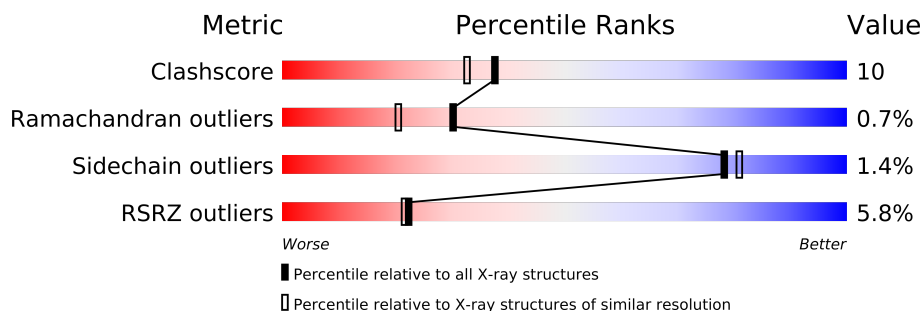
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 7156 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

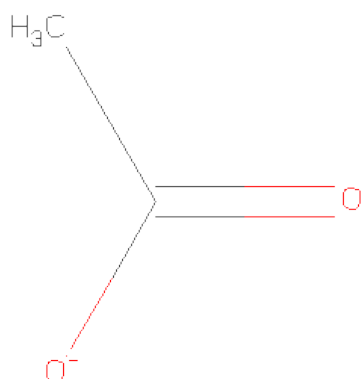
- Molecule 1 is a protein called BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN.

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 (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

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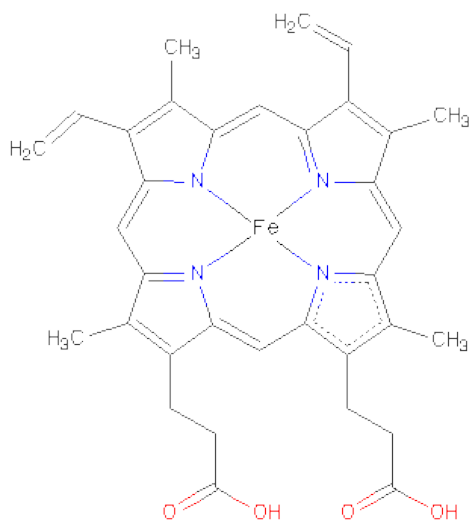
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

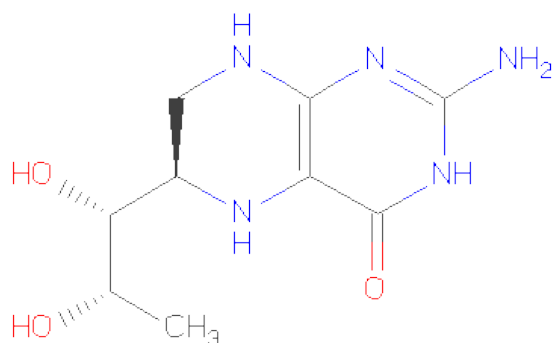
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

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



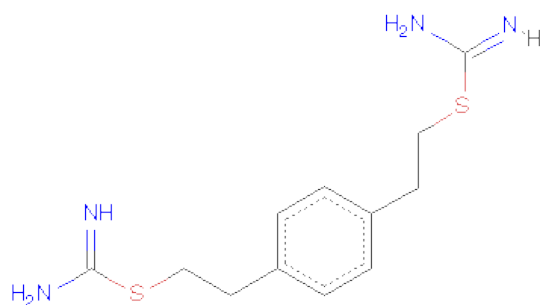
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 2-{2-[4-(2-CARBAMIMIDOYLSULFANYL-ETHYL)-PHENYL]-ETHYL}-IS OTHIOUREA (three-letter code: 4BT) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>S<sub>2</sub>).



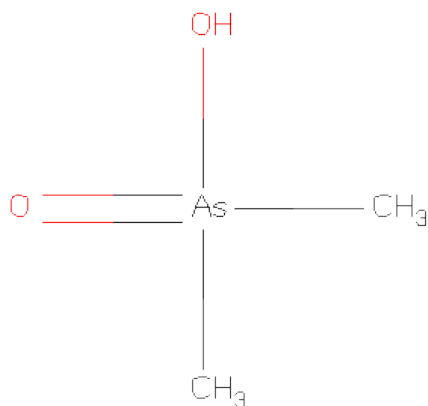
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	S	0	0
			18	12	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	S	0	0
			18	12	4	2		

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



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

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



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

- Molecule 9 is water.

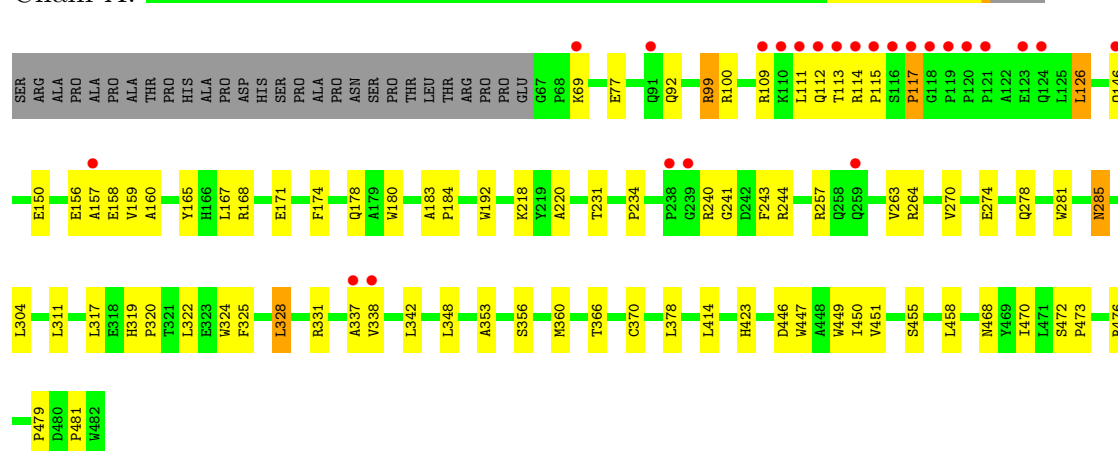
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	193	Total	O	0	0
			193	193		
9	B	179	Total	O	0	0
			179	179		

### 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.

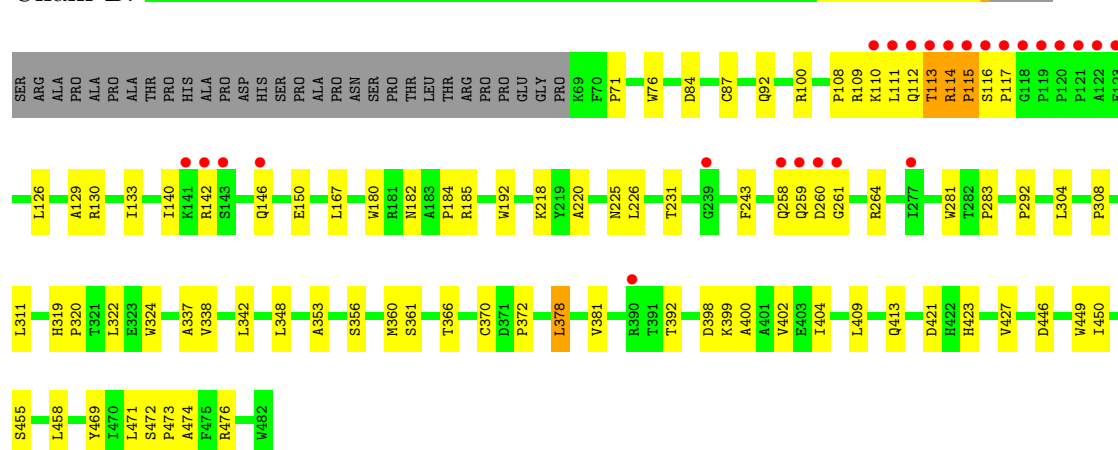
#### • Molecule 1: BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN

Chain A:



#### • Molecule 1: BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.53Å 106.73Å 156.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.61 – 2.00 36.61 – 2.00	Depositor EDS
% Data completeness (in resolution range)	79.7 (36.61-2.00) 82.8 (36.61-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.00Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.220 , 0.254 0.214 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 62691 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, 4BT, ACT, HEM, CAD

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	0.36	0/3397	0.63	1/4631 (0.0%)
1	B	0.35	0/3385	0.62	2/4614 (0.0%)
All	All	0.36	0/6782	0.63	3/9245 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	MET	N-CA-C	-5.06	97.34	111.00
1	A	360	MET	N-CA-C	-5.05	97.37	111.00
1	B	243	PHE	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3302	0	3215	62	0
1	B	3291	0	3205	71	0
2	A	8	0	6	0	0
2	B	8	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	43	0	30	2	0
4	B	43	0	30	1	0
5	A	17	0	15	1	0
5	B	17	0	15	1	0
6	A	18	0	16	2	0
6	B	18	0	16	2	0
7	A	3	0	0	0	0
7	B	3	0	0	0	0
8	A	6	0	8	1	0
8	B	6	0	8	0	0
9	A	193	0	0	3	0
9	B	179	0	0	6	0
All	All	7156	0	6570	133	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (133) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.47	0.95
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.54	0.87
1:B:140:ILE:HD12	1:B:142:ARG:HH11	1.41	0.85
1:A:146:GLN:O	1:A:150:GLU:HG3	1.87	0.74
1:B:114:ARG:HH11	1:B:115:PRO:HD3	1.52	0.74
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.72	0.71
1:B:114:ARG:HH11	1:B:114:ARG:HA	1.59	0.68
1:A:274:GLU:O	1:A:278:GLN:HG3	1.95	0.65
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.78	0.65
1:B:259:GLN:HG3	1:B:260:ASP:OD1	1.97	0.65
1:A:270:VAL:O	1:A:274:GLU:HG3	1.97	0.64
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.79	0.64
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.33	0.64
1:A:126:LEU:CD1	1:A:156:GLU:HG2	2.23	0.64
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.81	0.63
1:B:114:ARG:NH1	1:B:115:PRO:HD3	2.13	0.63
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.35	0.62
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.30	0.62
1:B:366:THR:O	1:B:370:CYS:HB2	2.00	0.61
1:A:99:ARG:HG3	1:A:99:ARG:HH11	1.65	0.61
1:A:111:LEU:HD22	1:A:476:ARG:NH1	2.17	0.60
1:B:399:LYS:NZ	9:B:1096:HOH:O	2.33	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:449:TRP:HA	5:B:601:H4B:N1	2.17	0.60
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.41	0.59
1:A:115:PRO:O	1:A:117:PRO:HD3	2.03	0.58
1:A:113:THR:HG21	1:A:342:LEU:HD22	1.84	0.58
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.84	0.58
1:A:99:ARG:HH11	1:A:99:ARG:CG	2.17	0.58
1:B:258:GLN:C	1:B:259:GLN:HG2	2.23	0.58
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.86	0.57
1:A:115:PRO:C	1:A:117:PRO:HD3	2.25	0.57
1:B:113:THR:HG21	1:B:342:LEU:HD13	1.87	0.56
1:A:167:LEU:HG	1:A:348:LEU:HD12	1.87	0.56
1:B:114:ARG:HD3	1:B:115:PRO:CD	2.34	0.56
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.88	0.55
1:A:168:ARG:HB2	1:A:171:GLU:HG3	1.87	0.55
1:A:92:GLN:NE2	1:A:111:LEU:HD23	2.22	0.55
1:B:423:HIS:O	1:B:427:VAL:HG23	2.07	0.55
1:B:146:GLN:HG3	9:B:1043:HOH:O	2.07	0.55
1:A:240:ARG:HG2	1:A:241:GLY:N	2.22	0.54
1:A:257:ARG:HH21	1:A:263:VAL:HG23	1.73	0.54
1:A:325:PHE:O	1:A:328:LEU:HB2	2.08	0.53
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.90	0.53
1:B:126:LEU:O	1:B:130:ARG:HG3	2.08	0.53
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.89	0.53
1:A:126:LEU:HD23	1:A:159:VAL:HG11	1.89	0.53
1:B:113:THR:HG21	1:B:342:LEU:CD1	2.38	0.53
1:B:378:LEU:HB2	9:B:1021:HOH:O	2.08	0.52
1:B:409:LEU:O	1:B:413:GLN:HG3	2.10	0.52
1:A:115:PRO:HD3	1:A:479:PRO:CG	2.35	0.52
1:B:399:LYS:HE2	9:B:1096:HOH:O	2.09	0.52
1:B:109:ARG:O	1:B:110:LYS:HG3	2.10	0.52
1:B:361:SER:OG	1:B:421:ASP:HA	2.09	0.51
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.92	0.51
1:A:414:LEU:HD23	9:A:1091:HOH:O	2.11	0.51
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.45	0.51
1:B:146:GLN:O	1:B:150:GLU:HG3	2.12	0.50
1:B:281:TRP:O	1:B:283:PRO:HD3	2.11	0.50
1:A:472:SER:HA	1:A:473:PRO:C	2.32	0.50
1:A:257:ARG:HH21	1:A:263:VAL:CG2	2.24	0.50
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.93	0.50
1:A:285:ASN:C	1:A:285:ASN:HD22	2.15	0.50
1:B:259:GLN:HG3	1:B:260:ASP:H	1.77	0.49
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:500:HEM:HMC1	4:A:500:HEM:HBC2	1.94	0.49
1:A:111:LEU:HD21	1:A:470:ILE:HD13	1.95	0.49
1:A:449:TRP:HA	5:A:600:H4B:N1	2.28	0.49
1:B:108:PRO:HB3	1:B:111:LEU:HD13	1.95	0.48
1:B:319:HIS:CE1	1:B:322:LEU:HG	2.48	0.48
1:B:472:SER:HA	1:B:473:PRO:C	2.34	0.48
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.53	0.48
1:B:399:LYS:CE	9:B:1096:HOH:O	2.62	0.47
1:B:292:PRO:CG	1:B:304:LEU:HD11	2.45	0.47
1:A:378:LEU:HB2	9:A:1134:HOH:O	2.13	0.47
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.50	0.47
1:B:218:LYS:HE3	1:B:311:LEU:HD11	1.95	0.47
1:B:182:ASN:O	1:B:184:PRO:HD3	2.14	0.47
1:B:114:ARG:NH1	1:B:114:ARG:HA	2.28	0.47
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.49	0.47
1:B:129:ALA:O	1:B:133:ILE:HG12	2.15	0.47
8:A:880:GOL:O3	1:B:76:TRP:HB3	2.15	0.46
1:A:285:ASN:C	1:A:285:ASN:ND2	2.68	0.46
1:B:92:GLN:NE2	1:B:476:ARG:HH21	2.13	0.46
1:A:111:LEU:CD2	1:A:470:ILE:HD13	2.46	0.46
1:A:111:LEU:CD2	1:A:476:ARG:NH1	2.79	0.46
1:A:337:ALA:HB2	1:A:356:SER:HB3	1.97	0.46
1:B:231:THR:O	1:B:353:ALA:HA	2.16	0.45
1:B:471:LEU:O	1:B:474:ALA:HB2	2.16	0.45
1:A:77:GLU:HG3	1:B:372:PRO:CG	2.45	0.45
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.51	0.45
1:A:126:LEU:HA	1:A:126:LEU:HD22	1.80	0.45
2:B:861:ACT:H1	4:B:500:HEM:HMB3	1.97	0.45
1:B:140:ILE:O	1:B:142:ARG:HG3	2.17	0.45
1:A:114:ARG:HD2	1:A:479:PRO:CG	2.46	0.45
1:A:174:PHE:CZ	1:A:178:GLN:HG3	2.52	0.44
1:A:264:ARG:HG3	1:A:264:ARG:HH11	1.83	0.43
1:B:87:CYS:HA	1:B:469:TYR:CE1	2.53	0.43
1:B:338:VAL:HG23	6:B:831:4BT:C1	2.49	0.43
1:A:366:THR:O	1:A:370:CYS:HB2	2.19	0.43
1:A:446:ASP:O	1:A:450:ILE:HG12	2.19	0.43
4:A:500:HEM:O2D	6:A:830:4BT:S'	2.76	0.43
1:B:71:PRO:HG2	1:B:84:ASP:HB3	2.00	0.43
1:A:109:ARG:HD3	1:A:109:ARG:HA	1.87	0.43
1:B:226:LEU:HD12	1:B:226:LEU:N	2.33	0.43
1:A:157:ALA:O	1:A:160:ALA:HB3	2.19	0.43
1:B:220:ALA:O	1:B:226:LEU:HA	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:116:SER:N	1:B:117:PRO:CD	2.81	0.42
1:A:338:VAL:HG23	6:A:830:4BT:C1	2.48	0.42
1:A:69:LYS:HG2	1:A:69:LYS:O	2.18	0.42
1:B:140:ILE:HD12	1:B:142:ARG:HD2	2.02	0.42
1:B:381:VAL:HG21	1:B:404:ILE:CD1	2.50	0.42
1:A:114:ARG:HD2	1:A:479:PRO:HG2	2.01	0.42
1:B:130:ARG:HD3	9:B:1087:HOH:O	2.19	0.42
1:A:257:ARG:NH2	1:A:263:VAL:CG2	2.83	0.42
1:B:337:ALA:CB	1:B:356:SER:HB3	2.48	0.42
1:B:308:PRO:O	1:B:311:LEU:HB2	2.19	0.42
1:A:111:LEU:HD22	1:A:476:ARG:HH11	1.84	0.42
1:A:231:THR:O	1:A:353:ALA:HA	2.19	0.42
1:B:398:ASP:O	1:B:402:VAL:HG23	2.20	0.41
1:A:158:GLU:HG2	1:A:165:TYR:HA	2.02	0.41
1:B:400:ALA:O	1:B:404:ILE:HG13	2.20	0.41
1:B:446:ASP:O	1:B:450:ILE:HG12	2.21	0.41
1:B:338:VAL:HG23	6:B:831:4BT:C6	2.51	0.41
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.56	0.41
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.90	0.41
1:B:264:ARG:HH11	1:B:264:ARG:HG3	1.85	0.41
1:A:220:ALA:HB1	9:A:1122:HOH:O	2.21	0.41
1:B:258:GLN:HG3	1:B:259:GLN:HG2	2.03	0.40
1:A:447:TRP:CZ2	1:A:451:VAL:HG21	2.57	0.40
1:B:185:ARG:HD3	1:B:449:TRP:CD2	2.56	0.40
1:A:423:HIS:HB2	1:B:392:THR:HB	2.03	0.40
1:B:258:GLN:O	1:B:259:GLN:HG2	2.22	0.40
1:A:317:LEU:HG	1:A:331:ARG:HA	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	414/444 (93%)	388 (94%)	24 (6%)	2 (0%)	38 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	412/444 (93%)	380 (92%)	28 (7%)	4 (1%)	22	12
All	All	826/888 (93%)	768 (93%)	52 (6%)	6 (1%)	30	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	112	GLN
1	A	112	GLN
1	A	117	PRO
1	B	261	GLY
1	B	113	THR
1	B	115	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%)	348 (98%)	6 (2%)	73	75
1	B	353/377 (94%)	349 (99%)	4 (1%)	84	86
All	All	707/754 (94%)	697 (99%)	10 (1%)	78	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	100	ARG
1	A	126	LEU
1	A	285	ASN
1	A	328	LEU
1	A	468	ASN
1	B	100	ARG
1	B	114	ARG
1	B	225	ASN
1	B	378	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	124	GLN
1	A	153	GLN
1	A	191	GLN
1	A	196	GLN
1	A	278	GLN
1	A	285	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	89	GLN
1	B	92	GLN
1	B	112	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	278	GLN
1	B	405	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected



value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	HEM	A	500	1	49,50,50	2.28	15 (30%)	46,82,82	1.63	9 (19%)
5	H4B	A	600	-	18,18,18	1.65	4 (22%)	24,26,26	2.51	10 (41%)
6	4BT	A	830	-	18,18,18	1.94	2 (11%)	22,22,22	1.28	3 (13%)
2	ACT	A	850	-	1,3,3	1.64	0	0,3,3	0.00	-
2	ACT	A	860	-	1,3,3	4.47	1 (100%)	0,3,3	0.00	-
8	GOL	A	880	-	5,5,5	0.13	0	5,5,5	0.29	0
7	CAD	A	950	1	2,2,4	0.45	0	0,1,6	0.00	-
4	HEM	B	500	1	49,50,50	1.88	13 (26%)	46,82,82	1.41	6 (13%)
5	H4B	B	601	-	18,18,18	1.52	4 (22%)	24,26,26	2.57	10 (41%)
6	4BT	B	831	-	18,18,18	1.85	2 (11%)	22,22,22	1.10	2 (9%)
2	ACT	B	851	-	1,3,3	3.09	1 (100%)	0,3,3	0.00	-
2	ACT	B	861	-	1,3,3	1.17	0	0,3,3	0.00	-
8	GOL	B	881	-	5,5,5	0.37	0	5,5,5	0.59	0
7	CAD	B	951	1	2,2,4	0.47	0	0,1,6	0.00	-

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
4	HEM	A	500	1	-	0/14/114/114	0/0/8/8
5	H4B	A	600	-	-	0/8/17/17	0/0/2/2
6	4BT	A	830	-	-	0/12/12/12	0/1/1/1
2	ACT	A	850	-	-	0/0/0/0	0/0/0/0
2	ACT	A	860	-	-	0/0/0/0	0/0/0/0
8	GOL	A	880	-	-	0/4/4/4	0/0/0/0
7	CAD	A	950	1	-	0/0/0/0	0/0/0/0
4	HEM	B	500	1	-	0/14/114/114	0/0/8/8
5	H4B	B	601	-	-	0/8/17/17	0/0/2/2
6	4BT	B	831	-	-	0/12/12/12	0/1/1/1
2	ACT	B	851	-	-	0/0/0/0	0/0/0/0
2	ACT	B	861	-	-	0/0/0/0	0/0/0/0
8	GOL	B	881	-	-	0/4/4/4	0/0/0/0
7	CAD	B	951	1	-	0/0/0/0	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	HEM	C2D-C1D	8.11	1.46	1.44
6	A	830	4BT	CC-CD	-6.15	1.35	1.52
6	B	831	4BT	CC-CD	-5.54	1.37	1.52
4	A	500	HEM	C3D-C2D	-5.26	1.34	1.43
4	B	500	HEM	C3C-C2C	-4.69	1.35	1.43
2	A	860	ACT	CH3-C	4.47	1.55	1.48
4	B	500	HEM	C3B-C2B	-4.47	1.35	1.43
4	A	500	HEM	C4A-C3A	4.46	1.45	1.40
4	B	500	HEM	CHB-C1B	4.22	1.41	1.35
4	A	500	HEM	C3B-C4B	4.12	1.49	1.44
5	A	600	H4B	C6-N5	3.98	1.54	1.46
4	A	500	HEM	C3C-C2C	-3.76	1.37	1.43
4	B	500	HEM	C3D-C2D	-3.70	1.37	1.43
4	A	500	HEM	C3B-C2B	-3.64	1.37	1.43
5	B	601	H4B	C6-N5	3.45	1.53	1.46
4	B	500	HEM	CHA-C4D	3.38	1.40	1.35
4	B	500	HEM	C2D-C1D	3.34	1.45	1.44
4	B	500	HEM	C2B-C1B	3.26	1.45	1.44
4	A	500	HEM	C4A-NA	3.21	1.42	1.36
2	B	851	ACT	CH3-C	3.09	1.53	1.48
4	B	500	HEM	C4A-C3A	3.05	1.44	1.40
4	A	500	HEM	CHD-C4C	2.99	1.41	1.36
4	A	500	HEM	CHA-C4D	2.92	1.40	1.35
5	B	601	H4B	C4-N3	2.82	1.41	1.37
5	A	600	H4B	C4A-N5	2.70	1.47	1.38
5	B	601	H4B	C8A-N1	2.62	1.39	1.34
4	A	500	HEM	CHC-C1C	2.60	1.41	1.36
4	A	500	HEM	C2B-C1B	2.59	1.45	1.44
4	A	500	HEM	C1C-NC	2.52	1.41	1.38
5	B	601	H4B	C4A-N5	2.45	1.46	1.38
5	A	600	H4B	C4-N3	2.35	1.41	1.37
4	A	500	HEM	C4C-NC	2.33	1.41	1.38
4	B	500	HEM	C4A-NA	2.29	1.41	1.36
4	B	500	HEM	FE-NA	2.27	2.02	1.92
4	B	500	HEM	C1C-NC	2.26	1.41	1.38
5	A	600	H4B	C2-N1	2.21	1.36	1.33
4	B	500	HEM	C3D-C4D	-2.19	1.44	1.44
4	A	500	HEM	C1A-NA	2.17	1.40	1.36
4	B	500	HEM	CMD-C2D	2.15	1.54	1.47
6	B	831	4BT	C2-C1	2.15	1.43	1.38
6	A	830	4BT	C5-C4	2.15	1.43	1.38
4	A	500	HEM	CHB-C1B	2.06	1.38	1.35

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	H4B	C4-C4A-C8A	8.84	122.75	114.56
5	A	600	H4B	C4-C4A-C8A	8.40	122.34	114.56
4	A	500	HEM	C4A-CHB-C1B	-4.16	121.99	127.47
4	A	500	HEM	C3A-C4A-NA	3.90	112.35	109.41
4	B	500	HEM	CBA-CAA-C2A	-3.82	105.97	112.69
6	A	830	4BT	CA-CB-C1	-3.81	107.44	114.06
4	B	500	HEM	C1A-CHA-C4D	-3.69	122.61	127.47
4	A	500	HEM	C3B-C4B-NB	-3.62	111.41	114.00
5	A	600	H4B	C2-N1-C8A	3.57	122.68	117.61
4	A	500	HEM	C4A-C3A-C2A	-3.48	104.58	107.00
5	A	600	H4B	C4-N3-C2	3.28	125.24	119.51
5	B	601	H4B	C4-N3-C2	3.23	125.16	119.51
5	B	601	H4B	C2-N1-C8A	3.18	122.13	117.61
4	B	500	HEM	C4C-NC-C1C	-3.05	102.36	105.53
4	A	500	HEM	C1A-C2A-C3A	2.86	109.88	106.92
4	B	500	HEM	CBD-CAD-C3D	-2.80	108.25	114.37
4	B	500	HEM	C4A-CHB-C1B	-2.80	123.78	127.47
5	B	601	H4B	C4A-N5-C6	-2.80	113.55	121.16
4	A	500	HEM	C4A-NA-C1A	-2.79	103.09	106.76
5	A	600	H4B	N3-C2-N1	-2.78	117.89	121.78
6	A	830	4BT	CC-S'-C'	2.73	111.03	103.31
5	B	601	H4B	N3-C2-N1	-2.73	117.96	121.78
6	B	831	4BT	CA-S-C	2.71	110.97	103.31
5	A	600	H4B	C4A-N5-C6	-2.67	113.88	121.16
5	A	600	H4B	C4A-C8A-N8	2.66	122.88	119.23
6	B	831	4BT	CC-S'-C'	2.64	110.77	103.31
4	B	500	HEM	C3B-C4B-NB	-2.55	112.17	114.00
6	A	830	4BT	CA-S-C	2.41	110.12	103.31
4	A	500	HEM	C1A-CHA-C4D	-2.40	124.31	127.47
5	B	601	H4B	N8-C8A-N1	2.38	119.31	115.82
5	B	601	H4B	C4A-C8A-N8	2.34	122.44	119.23
5	A	600	H4B	O9-C9-C6	2.28	114.59	109.07
5	A	600	H4B	N8-C8A-N1	2.20	119.04	115.82
5	A	600	H4B	C4A-C8A-N1	-2.16	118.04	121.50
5	B	601	H4B	C9-C6-N5	-2.10	105.77	109.69
5	B	601	H4B	O9-C9-C6	2.09	114.14	109.07
4	A	500	HEM	CHC-C1C-NC	-2.09	122.92	124.73
5	A	600	H4B	N2-C2-N1	2.04	123.06	120.31
5	B	601	H4B	C4A-C8A-N1	-2.04	118.24	121.50
4	A	500	HEM	C4C-NC-C1C	-2.01	103.45	105.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	416/444 (93%)	0.25	24 (5%) 22 22	26, 38, 66, 100	0
1	B	414/444 (93%)	0.33	25 (6%) 21 20	28, 42, 72, 100	0
All	All	830/888 (93%)	0.29	49 (5%) 22 21	26, 40, 69, 100	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	LEU	12.0
1	A	113	THR	11.6
1	B	117	PRO	10.2
1	B	113	THR	9.3
1	A	117	PRO	9.2
1	B	115	PRO	8.5
1	A	115	PRO	8.4
1	A	111	LEU	8.1
1	A	119	PRO	7.7
1	A	112	GLN	7.6
1	B	116	SER	7.5
1	A	114	ARG	7.4
1	B	119	PRO	6.9
1	A	116	SER	6.3
1	B	110	LYS	6.1
1	B	114	ARG	6.1
1	B	120	PRO	6.1
1	B	118	GLY	6.0
1	B	112	GLN	5.9
1	A	110	LYS	5.7
1	B	121	PRO	5.6
1	A	239	GLY	5.4
1	A	118	GLY	5.1
1	A	259	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	120	PRO	4.5
1	B	258	GLN	3.8
1	A	121	PRO	3.6
1	B	146	GLN	3.4
1	B	261	GLY	3.4
1	B	239	GLY	3.4
1	A	91	GLN	3.4
1	B	260	ASP	3.3
1	A	123	GLU	3.3
1	B	123	GLU	3.3
1	A	109	ARG	3.0
1	A	69	LYS	2.9
1	B	122	ALA	2.9
1	B	142	ARG	2.9
1	B	259	GLN	2.8
1	B	390	ARG	2.6
1	B	141	LYS	2.5
1	A	124	GLN	2.5
1	A	238	PRO	2.4
1	A	146	GLN	2.3
1	A	338	VAL	2.3
1	A	157	ALA	2.3
1	B	143	SER	2.3
1	A	337	ALA	2.2
1	B	277	ILE	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	GOL	A	880	6/6	0.19	1.69	54,54,56,58	0
2	ACT	A	850	4/4	0.15	1.57	41,42,42,42	0
8	GOL	B	881	6/6	0.14	1.26	43,47,48,49	0
2	ACT	B	861	4/4	0.10	1.16	45,46,46,47	0
5	H4B	B	601	17/17	0.13	0.90	30,31,33,34	0
5	H4B	A	600	17/17	0.14	0.48	31,32,33,36	0
4	HEM	A	500	43/43	0.16	0.46	27,29,32,33	0
2	ACT	A	860	4/4	0.10	0.38	41,42,43,44	0
7	CAD	A	950	3/5	0.10	0.32	54,54,54,61	0
4	HEM	B	500	43/43	0.14	0.28	26,28,31,33	0
6	4BT	A	830	18/18	0.16	0.14	34,40,47,47	0
6	4BT	B	831	18/18	0.15	-0.03	32,41,44,44	0
7	CAD	B	951	3/5	0.11	-0.87	69,69,69,72	0
2	ACT	B	851	4/4	0.11	-0.98	39,39,40,40	0
3	ZN	A	901	1/1	0.03	-4.12	38,38,38,38	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.