



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:00 PM GMT

PDB ID : 1DMI  
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN  
COMPLEXED WITH 6S-H4B  
Authors : Raman, C.S.; Li, H.; Martasek, P.; Kotsonis, P.; Pfeleiderer, W.; Schmidt,  
H.H.H.W.; Masters, B.S.S.; Poulos, T.L.  
Deposited on : 1999-12-14  
Resolution : 2.00 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

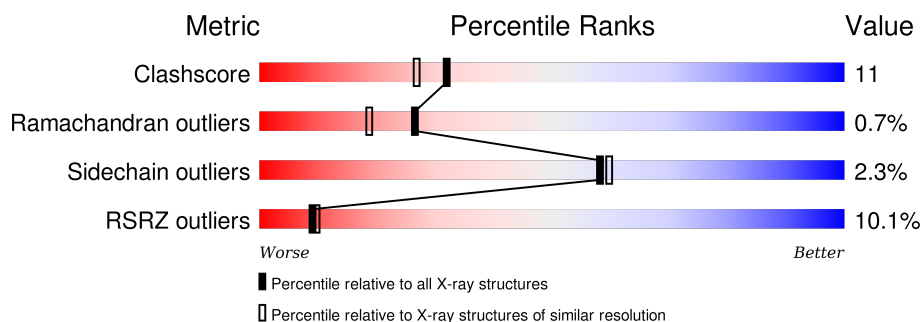
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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.

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 7148 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.

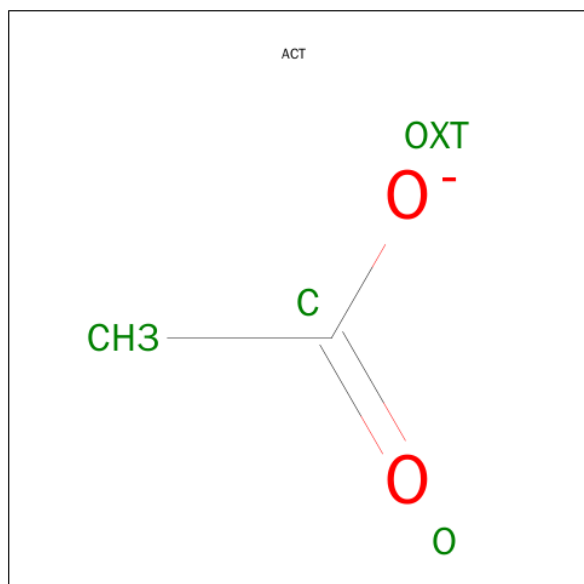
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE.

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



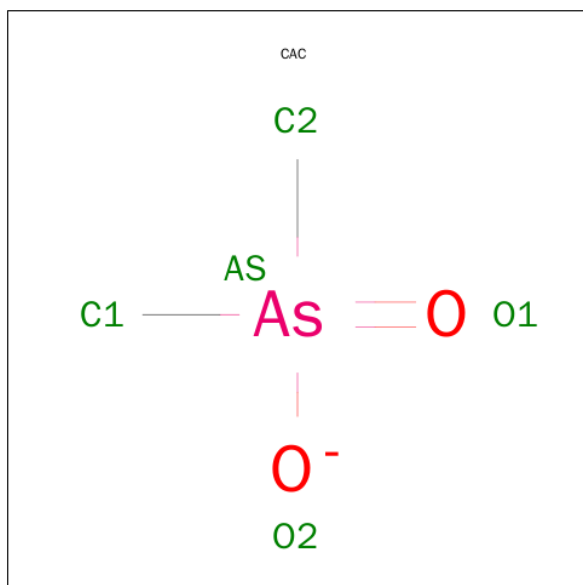
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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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 (three-letter code: 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 ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

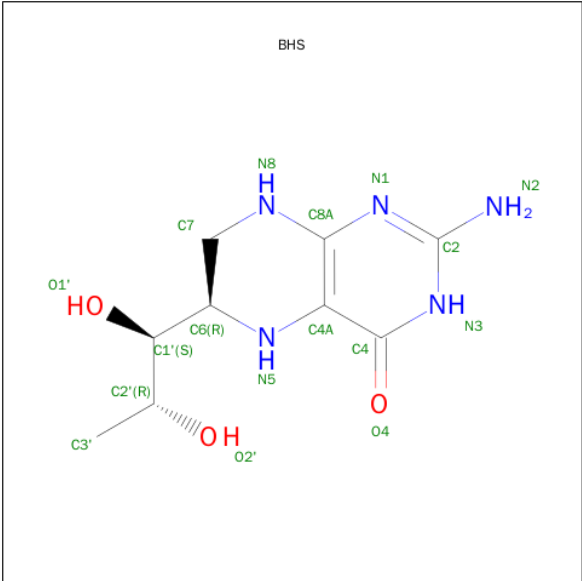
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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



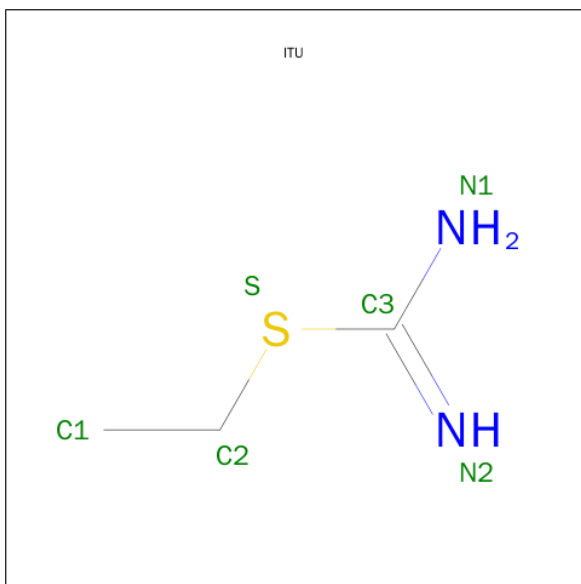
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			17	9	5	3		

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



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

- 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		

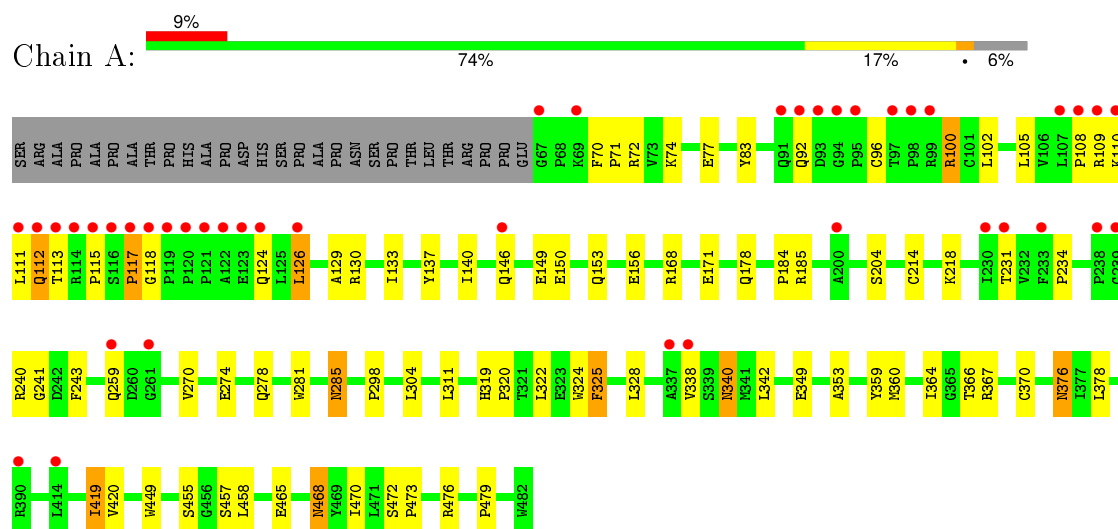
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	199	Total	O	0	0
			199	199		
9	B	189	Total	O	0	0
			189	189		

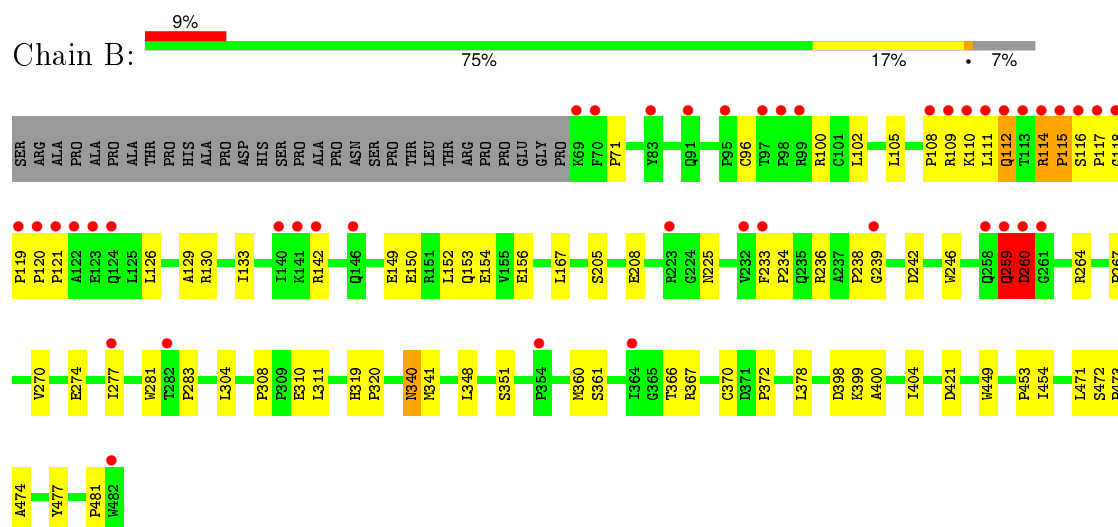
### 3 Residue-property plots

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: NITRIC OXIDE SYNTHASE



#### • Molecule 1: NITRIC OXIDE SYNTHASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.63Å 106.56Å 156.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.59 – 2.00 32.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.2 (32.59-2.00) 80.1 (32.59-2.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.00Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.229 , 0.264 0.219 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 61177 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7148	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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, ACT, CAC, HEM, BHS, ITU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.39	1/3397 (0.0%)	0.64	2/4631 (0.0%)
1	B	0.36	0/3385	0.61	1/4614 (0.0%)
All	All	0.38	1/6782 (0.0%)	0.62	3/9245 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	PHE	CD2-CE2	-5.21	1.28	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	PHE	CB-CG-CD1	-5.83	116.72	120.80
1	A	360	MET	N-CA-C	-5.40	96.42	111.00
1	B	360	MET	N-CA-C	-5.16	97.08	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	75	0
1	B	3291	0	3205	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0	0	0	0
5	A	43	0	30	0	0
5	B	43	0	30	2	0
6	A	17	0	15	1	0
6	B	17	0	15	2	0
7	A	6	0	7	2	0
7	B	6	0	7	0	0
8	A	6	0	8	0	0
8	B	6	0	8	0	0
9	A	199	0	0	4	0
9	B	189	0	0	3	0
All	All	7148	0	6552	141	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 11.

All (141) 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:115:PRO:HD3	1:A:479:PRO:HG2	1.28	1.15
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.37	1.02
1:B:126:LEU:HD11	1:B:156:GLU:HG2	1.53	0.89
1:B:108:PRO:HB3	1:B:111:LEU:HD13	1.57	0.84
1:B:114:ARG:HH11	1:B:114:ARG:HA	1.41	0.84
1:B:116:SER:HB2	1:B:236:ARG:NH2	1.98	0.78
1:B:270:VAL:O	1:B:274:GLU:HG2	1.82	0.77
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.66	0.77
1:A:92:GLN:NE2	1:A:111:LEU:HD23	1.99	0.76
1:A:204:SER:OG	9:A:2062:HOH:O	2.05	0.73
1:B:114:ARG:NH1	1:B:114:ARG:HA	2.07	0.70
1:A:338:VAL:HG23	7:A:1800:ITU:H11	1.73	0.69
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.77	0.66
1:A:111:LEU:HD22	1:A:476:ARG:NH1	2.11	0.66
1:B:378:LEU:HB2	9:B:3033:HOH:O	1.96	0.66
1:A:178:GLN:HG2	9:A:2058:HOH:O	1.95	0.65
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.79	0.65
1:A:146:GLN:O	1:A:150:GLU:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:HD22	1:A:340:ASN:H	1.46	0.64
1:B:114:ARG:HH11	1:B:115:PRO:HD3	1.64	0.63
1:B:259:GLN:HG2	1:B:260:ASP:H	1.64	0.62
1:B:149:GLU:O	1:B:153:GLN:HG3	1.99	0.62
1:A:378:LEU:HB2	9:A:2070:HOH:O	1.98	0.62
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.80	0.62
1:A:96:CYS:HB3	1:B:96:CYS:HB3	1.82	0.61
1:B:126:LEU:O	1:B:130:ARG:HG3	2.00	0.60
1:A:111:LEU:HD21	1:A:470:ILE:HG21	1.82	0.60
1:A:168:ARG:HB2	1:A:171:GLU:HG3	1.83	0.59
1:A:270:VAL:O	1:A:274:GLU:HG3	2.03	0.59
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.41	0.59
1:A:115:PRO:O	1:A:117:PRO:HD3	2.04	0.58
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.39	0.57
1:A:214:CYS:O	1:A:218:LYS:HG3	2.04	0.57
1:B:310:GLU:HG2	1:B:311:LEU:HD12	1.87	0.56
1:B:119:PRO:HA	1:B:238:PRO:CG	2.36	0.55
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.88	0.55
1:A:113:THR:HG21	1:A:342:LEU:HD22	1.88	0.55
1:A:149:GLU:O	1:A:153:GLN:HG3	2.07	0.55
1:A:105:LEU:CB	1:A:108:PRO:HG3	2.37	0.55
1:B:150:GLU:O	1:B:154:GLU:HG3	2.07	0.55
1:B:449:TRP:HA	6:B:2610:BHS:N1	2.22	0.55
1:A:115:PRO:C	1:A:117:PRO:HD3	2.27	0.54
1:B:236:ARG:HD2	1:B:242:ASP:CG	2.27	0.54
1:A:111:LEU:HD11	1:A:470:ILE:CD1	2.38	0.54
1:B:102:LEU:HB3	1:B:105:LEU:HD22	1.90	0.54
1:A:111:LEU:HD11	1:A:470:ILE:HD12	1.90	0.54
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.38	0.54
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.37	0.54
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.91	0.53
1:A:342:LEU:HD11	1:A:349:GLU:HB3	1.90	0.52
1:A:105:LEU:HB2	1:A:108:PRO:HG3	1.90	0.52
1:B:400:ALA:O	1:B:404:ILE:HG13	2.10	0.52
1:A:111:LEU:HD21	1:A:470:ILE:HG13	1.92	0.52
1:A:74:LYS:O	1:A:465:GLU:HG3	2.09	0.52
1:B:152:LEU:O	1:B:156:GLU:HG3	2.09	0.52
1:B:111:LEU:O	1:B:112:GLN:O	2.26	0.52
1:A:285:ASN:C	1:A:285:ASN:HD22	2.13	0.51
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.93	0.51
1:B:119:PRO:N	1:B:238:PRO:HB3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ARG:NH1	1:B:115:PRO:HD3	2.27	0.50
1:A:109:ARG:O	1:A:110:LYS:HD2	2.12	0.50
1:B:119:PRO:HA	1:B:238:PRO:HG3	1.94	0.50
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.12	0.50
1:A:274:GLU:O	1:A:278:GLN:HG3	2.11	0.50
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.47	0.49
1:B:130:ARG:HB3	1:B:130:ARG:NH1	2.27	0.49
1:A:340:ASN:ND2	1:A:340:ASN:H	2.10	0.49
1:A:457:SER:OG	1:B:453:PRO:HB2	2.12	0.49
1:B:471:LEU:O	1:B:474:ALA:HB2	2.12	0.49
1:A:340:ASN:HD22	1:A:340:ASN:N	2.07	0.49
1:B:116:SER:HB2	1:B:236:ARG:HH22	1.76	0.49
1:A:419:ILE:HG13	1:A:420:VAL:N	2.28	0.49
1:A:231:THR:O	1:A:353:ALA:HA	2.13	0.48
1:B:472:SER:HA	1:B:473:PRO:C	2.33	0.48
1:A:100:ARG:H	1:A:100:ARG:HD3	1.79	0.48
1:A:115:PRO:HD3	1:A:479:PRO:CG	2.20	0.47
1:A:102:LEU:HD21	1:B:71:PRO:HB3	1.96	0.47
1:A:338:VAL:HG23	7:A:1800:ITU:C1	2.43	0.47
1:A:126:LEU:O	1:A:130:ARG:HG3	2.15	0.47
1:B:117:PRO:O	1:B:239:GLY:N	2.48	0.47
1:A:240:ARG:HD2	1:A:241:GLY:O	2.14	0.47
1:B:308:PRO:HB2	1:B:311:LEU:HD13	1.97	0.46
1:B:116:SER:HB2	1:B:236:ARG:CZ	2.45	0.46
1:B:281:TRP:CB	1:B:304:LEU:HD21	2.42	0.46
1:B:120:PRO:HA	1:B:121:PRO:HD3	1.88	0.46
1:B:129:ALA:O	1:B:133:ILE:HG12	2.16	0.46
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.51	0.46
1:B:205:SER:OG	1:B:208:GLU:HG3	2.16	0.46
1:B:236:ARG:HD2	1:B:242:ASP:OD2	2.16	0.45
1:A:92:GLN:HE22	1:A:111:LEU:HD23	1.77	0.45
1:A:472:SER:HA	1:A:473:PRO:C	2.36	0.45
1:A:83:TYR:HE2	1:B:109:ARG:HH22	1.65	0.45
1:A:72:ARG:HB2	1:B:109:ARG:NH2	2.32	0.45
1:B:277:ILE:HD13	1:B:283:PRO:HG3	1.99	0.45
1:A:325:PHE:O	1:A:328:LEU:HB2	2.17	0.45
1:A:77:GLU:HG3	1:B:372:PRO:CG	2.46	0.45
1:B:366:THR:HG21	1:B:454:ILE:HG23	1.99	0.45
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.51	0.45
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.99	0.44
1:A:111:LEU:HD22	1:A:476:ARG:HH12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:O	1:A:112:GLN:C	2.56	0.44
1:B:108:PRO:HB3	1:B:111:LEU:HB2	2.00	0.43
1:B:340:ASN:HD22	1:B:341:MET:N	2.16	0.43
1:B:116:SER:N	1:B:117:PRO:CD	2.81	0.43
1:B:366:THR:O	1:B:370:CYS:HB2	2.18	0.43
1:A:285:ASN:C	1:A:285:ASN:ND2	2.72	0.43
1:B:399:LYS:NZ	9:B:3039:HOH:O	2.48	0.43
1:B:246:TRP:CD1	1:B:481:PRO:HG3	2.54	0.43
1:A:113:THR:HG21	1:A:476:ARG:HD2	2.01	0.43
1:A:70:PHE:O	1:B:109:ARG:NH2	2.52	0.42
1:A:109:ARG:HA	1:A:109:ARG:HD3	1.86	0.42
1:B:118:GLY:C	1:B:238:PRO:HB3	2.40	0.42
1:B:109:ARG:HG3	1:B:110:LYS:HG3	2.01	0.42
1:B:267:PRO:O	1:B:270:VAL:HG23	2.19	0.42
1:B:117:PRO:O	1:B:239:GLY:CA	2.67	0.42
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.50	0.42
1:A:359:TYR:CD2	1:A:364:ILE:HD11	2.54	0.42
1:B:112:GLN:NE2	1:B:477:TYR:C	2.73	0.42
1:B:310:GLU:HG2	1:B:311:LEU:CD1	2.48	0.42
1:A:71:PRO:HB3	1:B:102:LEU:HD21	2.02	0.42
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.54	0.42
1:A:129:ALA:O	1:A:133:ILE:HG12	2.21	0.41
1:A:366:THR:O	1:A:370:CYS:HB2	2.20	0.41
1:A:184:PRO:HB3	1:A:468:ASN:ND2	2.36	0.41
5:B:2500:HEM:CMC	5:B:2500:HEM:HBC2	2.50	0.41
1:A:113:THR:CG2	1:A:476:ARG:CD	2.99	0.41
1:B:264:ARG:HG3	1:B:264:ARG:HH11	1.85	0.41
1:B:114:ARG:HD3	1:B:115:PRO:HD3	2.02	0.41
1:A:111:LEU:CD2	1:A:476:ARG:NH1	2.83	0.41
5:B:2500:HEM:HBC2	5:B:2500:HEM:HMC1	2.03	0.40
1:B:259:GLN:HG2	1:B:260:ASP:N	2.34	0.40
1:B:233:PHE:HB3	1:B:234:PRO:HD2	2.02	0.40
1:A:137:TYR:HA	1:A:140:ILE:HG12	2.02	0.40
1:B:361:SER:OG	1:B:421:ASP:HA	2.21	0.40
1:A:376:ASN:ND2	9:A:2070:HOH:O	2.41	0.40
1:A:110:LYS:HA	1:A:110:LYS:HE3	2.04	0.40
1:A:117:PRO:O	1:A:118:GLY:C	2.58	0.40
1:B:367:ARG:HH12	6:B:2610:BHS:C4	2.34	0.40
1:A:367:ARG:HH12	6:A:1610:BHS:C4	2.34	0.40
1:B:142:ARG:HG2	1:B:142:ARG:NH1	2.35	0.40
1:A:96:CYS:HB2	9:B:2987:HOH:O	2.22	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%)	392 (95%)	20 (5%)	2 (0%)	34	26
1	B	412/444 (93%)	387 (94%)	21 (5%)	4 (1%)	19	11
All	All	826/888 (93%)	779 (94%)	41 (5%)	6 (1%)	26	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	PRO
1	B	112	GLN
1	B	259	GLN
1	A	112	GLN
1	B	115	PRO
1	B	260	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	354/377 (94%)	345 (98%)	9 (2%)	55	55
1	B	353/377 (94%)	346 (98%)	7 (2%)	63	65
All	All	707/754 (94%)	691 (98%)	16 (2%)	58	60

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	124	GLN
1	A	126	LEU
1	A	259	GLN
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	419	ILE
1	A	468	ASN
1	B	100	ARG
1	B	114	ARG
1	B	225	ASN
1	B	259	GLN
1	B	260	ASP
1	B	340	ASN
1	B	398	ASP

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	259	GLN
1	A	278	GLN
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	112	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	259	GLN
1	B	340	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 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	$\# Z  > 2$
5	HEM	A	1500	1	30,50,50	2.58	9 (30%)	24,82,82	2.39	9 (37%)
6	BHS	A	1610	-	13,18,18	2.23	3 (23%)	11,26,26	3.70	7 (63%)
7	ITU	A	1800	-	4,5,5	0.75	0	4,5,5	2.19	1 (25%)
2	ACT	A	1850	-	1,3,3	2.74	1 (100%)	0,3,3	0.00	-
2	ACT	A	1860	-	1,3,3	1.67	0	0,3,3	0.00	-
8	GOL	A	1880	-	5,5,5	0.43	0	5,5,5	1.51	1 (20%)
3	CAC	A	950	1	0,2,4	0.00	-	0,1,6	0.00	-
5	HEM	B	2500	1	30,50,50	2.68	8 (26%)	24,82,82	2.13	8 (33%)
6	BHS	B	2610	-	13,18,18	2.36	4 (30%)	11,26,26	3.89	7 (63%)
7	ITU	B	2800	-	4,5,5	0.76	0	4,5,5	2.36	1 (25%)
2	ACT	B	2850	-	1,3,3	3.62	1 (100%)	0,3,3	0.00	-
2	ACT	B	2860	-	1,3,3	1.98	0	0,3,3	0.00	-
8	GOL	B	2880	-	5,5,5	0.19	0	5,5,5	0.26	0
3	CAC	B	950	1	0,2,4	0.00	-	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
5	HEM	A	1500	1	-	0/10/54/54	0/0/8/8
6	BHS	A	1610	-	-	0/8/17/17	0/2/2/2
7	ITU	A	1800	-	-	0/3/3/3	0/0/0/0
2	ACT	A	1850	-	-	0/0/0/0	0/0/0/0
2	ACT	A	1860	-	-	0/0/0/0	0/0/0/0
8	GOL	A	1880	-	-	0/4/4/4	0/0/0/0
3	CAC	A	950	1	-	0/0/0/0	0/0/0/0
5	HEM	B	2500	1	-	0/10/54/54	0/0/8/8
6	BHS	B	2610	-	-	0/8/17/17	0/2/2/2
7	ITU	B	2800	-	-	0/3/3/3	0/0/0/0
2	ACT	B	2850	-	-	0/0/0/0	0/0/0/0
2	ACT	B	2860	-	-	0/0/0/0	0/0/0/0
8	GOL	B	2880	-	-	0/4/4/4	0/0/0/0
3	CAC	B	950	1	-	0/0/0/0	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1500	HEM	C2D-C3D	-6.81	1.34	1.54
5	B	2500	HEM	C3B-C4B	-6.52	1.46	1.51
5	B	2500	HEM	C2D-C3D	-6.14	1.36	1.54
5	A	1500	HEM	C3B-CAB	-5.79	1.40	1.51
5	B	2500	HEM	C3D-C4D	-5.63	1.44	1.51
5	B	2500	HEM	C3B-CAB	-5.34	1.41	1.51
5	B	2500	HEM	C3C-CAC	-5.25	1.41	1.51
5	A	1500	HEM	C3D-C4D	-5.11	1.45	1.51
5	A	1500	HEM	C3C-CAC	-5.09	1.41	1.51
5	B	2500	HEM	C2C-C1C	-4.19	1.44	1.52
5	A	1500	HEM	C2C-C1C	-4.05	1.44	1.52
6	B	2610	BHS	C7-N8	-3.50	1.41	1.46
6	A	1610	BHS	C7-N8	-3.03	1.42	1.46
5	A	1500	HEM	C3B-C4B	-2.30	1.49	1.51
5	B	2500	HEM	C2D-C1D	-2.23	1.44	1.51
5	A	1500	HEM	CMA-C3A	2.06	1.55	1.51
6	B	2610	BHS	C2-N3	2.24	1.39	1.35
5	A	1500	HEM	C4C-NC	2.46	1.39	1.36
2	A	1850	ACT	CH3-C	2.74	1.52	1.48
5	B	2500	HEM	C4C-NC	2.78	1.39	1.36
6	A	1610	BHS	C8A-N1	2.82	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2610	BHS	C8A-N1	2.98	1.40	1.34
2	B	2850	ACT	CH3-C	3.62	1.53	1.48
5	A	1500	HEM	C1C-NC	3.90	1.40	1.36
6	A	1610	BHS	C4-N3	6.31	1.44	1.33
6	B	2610	BHS	C4-N3	6.43	1.45	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1610	BHS	N3-C2-N1	-4.40	118.32	125.53
6	B	2610	BHS	N3-C2-N1	-4.39	118.34	125.53
5	B	2500	HEM	CBA-CAA-C2A	-2.62	107.84	112.53
5	A	1500	HEM	CBD-CAD-C3D	-2.11	107.42	113.55
5	A	1500	HEM	C3B-CAB-CBB	2.02	127.56	124.46
6	A	1610	BHS	N2-C2-N1	2.03	120.56	117.20
8	A	1880	GOL	O3-C3-C2	2.17	120.70	110.18
5	B	2500	HEM	C3B-CAB-CBB	2.36	128.08	124.46
6	A	1610	BHS	N2-C2-N3	2.37	121.12	117.20
6	B	2610	BHS	N2-C2-N3	2.52	121.37	117.20
6	B	2610	BHS	C7-C6-N5	2.59	115.83	110.45
5	B	2500	HEM	C2D-C3D-C4D	2.64	105.97	101.50
5	B	2500	HEM	CMD-C2D-C3D	2.76	126.56	114.35
5	A	1500	HEM	CMD-C2D-C3D	2.78	126.64	114.35
6	B	2610	BHS	C2-N1-C8A	3.60	122.63	114.54
5	B	2500	HEM	CMB-C2B-C3B	3.67	125.69	116.53
5	A	1500	HEM	CAD-C3D-C4D	3.68	125.44	112.47
6	A	1610	BHS	C2-N1-C8A	3.71	122.88	114.54
5	B	2500	HEM	CAD-C3D-C4D	3.90	126.23	112.47
5	A	1500	HEM	C2D-C3D-C4D	3.94	108.18	101.50
6	B	2610	BHS	C4A-C8A-N8	4.09	123.25	118.43
6	A	1610	BHS	C4A-C8A-N8	4.15	123.31	118.43
5	B	2500	HEM	CMC-C2C-C3C	4.15	126.89	116.53
7	A	1800	ITU	C2-S-C3	4.26	107.77	101.53
5	A	1500	HEM	CMC-C2C-C3C	4.51	127.80	116.53
7	B	2800	ITU	C2-S-C3	4.57	108.23	101.53
5	A	1500	HEM	CAD-C3D-C2D	4.57	126.35	113.22
5	A	1500	HEM	CMB-C2B-C3B	4.60	128.02	116.53
5	A	1500	HEM	C3C-CAC-CBC	4.65	131.60	124.46
5	B	2500	HEM	CAD-C3D-C2D	5.03	127.67	113.22
6	B	2610	BHS	C4-N3-C2	5.33	123.33	115.94
6	A	1610	BHS	C4-N3-C2	5.34	123.35	115.94
6	A	1610	BHS	C4-C4A-C8A	7.64	121.47	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	B	2610	BHS	C4-C4A-C8A	8.43	122.19	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1610	BHS	1	0
7	A	1800	ITU	2	0
5	B	2500	HEM	2	0
6	B	2610	BHS	2	0

## 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

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%)	0.56	42 (10%) 9 10	32, 47, 89, 99	0
1	B	414/444 (93%)	0.64	42 (10%) 9 10	35, 52, 88, 99	0
All	All	830/888 (93%)	0.60	84 (10%) 9 10	32, 49, 89, 99	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	PRO	14.0
1	B	118	GLY	13.0
1	A	113	THR	12.8
1	A	115	PRO	12.6
1	A	119	PRO	12.2
1	B	113	THR	12.0
1	B	117	PRO	11.9
1	A	111	LEU	11.3
1	B	120	PRO	10.6
1	B	115	PRO	10.4
1	A	118	GLY	9.9
1	B	119	PRO	9.9
1	B	114	ARG	7.5
1	B	116	SER	7.4
1	A	109	ARG	7.3
1	B	111	LEU	7.3
1	B	110	LYS	7.3
1	A	110	LYS	7.1
1	A	116	SER	6.9
1	B	261	GLY	6.6
1	A	239	GLY	6.4
1	A	114	ARG	6.3
1	B	112	GLN	6.2
1	A	120	PRO	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	259	GLN	5.9
1	A	112	GLN	5.8
1	A	108	PRO	5.4
1	B	121	PRO	5.1
1	A	107	LEU	5.0
1	B	259	GLN	5.0
1	B	98	PRO	4.9
1	A	99	ARG	4.6
1	A	123	GLU	4.6
1	A	121	PRO	4.5
1	A	122	ALA	4.3
1	A	69	LYS	4.2
1	A	67	GLY	4.0
1	B	109	ARG	3.8
1	B	260	ASP	3.6
1	A	92	GLN	3.5
1	A	98	PRO	3.5
1	A	390	ARG	3.5
1	B	91	GLN	3.3
1	B	97	THR	3.3
1	A	124	GLN	3.3
1	B	70	PHE	3.2
1	A	91	GLN	3.2
1	B	258	GLN	3.2
1	B	123	GLU	3.2
1	B	122	ALA	3.1
1	A	95	PRO	3.1
1	B	95	PRO	3.1
1	A	261	GLY	2.9
1	B	140	ILE	2.9
1	B	69	LYS	2.8
1	B	146	GLN	2.8
1	A	93	ASP	2.8
1	B	99	ARG	2.8
1	A	97	THR	2.8
1	A	94	GLY	2.7
1	A	146	GLN	2.6
1	A	233	PHE	2.6
1	B	223	ARG	2.6
1	A	238	PRO	2.6
1	A	126	LEU	2.5
1	B	141	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	142	ARG	2.4
1	A	338	VAL	2.3
1	A	230	ILE	2.3
1	A	200	ALA	2.3
1	B	233	PHE	2.3
1	B	482	TRP	2.2
1	A	337	ALA	2.2
1	A	414	LEU	2.2
1	B	354	PRO	2.2
1	B	364	ILE	2.1
1	B	239	GLY	2.1
1	B	232	VAL	2.1
1	B	277	ILE	2.1
1	A	231	THR	2.1
1	B	124	GLN	2.1
1	B	282	THR	2.1
1	B	83	TYR	2.1
1	B	108	PRO	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACT	B	2850	4/4	0.85	0.20	2.00	49,50,50,50	0
2	ACT	A	1850	4/4	0.93	0.18	1.35	50,50,51,52	0
6	BHS	A	1610	17/17	0.89	0.20	1.15	63,65,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	GOL	B	2880	6/6	0.88	0.17	1.13	61,65,66,68	0
6	BHS	B	2610	17/17	0.93	0.17	0.80	66,66,67,67	0
5	HEM	B	2500	43/43	0.98	0.17	0.75	33,35,46,51	0
5	HEM	A	1500	43/43	0.98	0.15	0.56	29,34,45,48	0
3	CAC	A	950	3/5	0.98	0.11	0.54	69,69,69,75	0
8	GOL	A	1880	6/6	0.86	0.15	0.43	63,64,65,65	0
7	ITU	A	1800	6/6	0.98	0.17	0.11	37,39,40,40	0
2	ACT	A	1860	4/4	0.93	0.10	-0.18	52,52,53,54	0
7	ITU	B	2800	6/6	0.98	0.16	-0.23	44,45,46,47	0
2	ACT	B	2860	4/4	0.98	0.08	-1.30	55,55,55,56	0
4	ZN	A	900	1/1	0.98	0.03	-3.23	69,69,69,69	0
3	CAC	B	950	3/5	0.97	0.16	-	85,85,85,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.