



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:54 PM GMT

PDB ID : 1D1Y  
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN  
COMPLEXED WITH 1,3-PBITU (H4B FREE)  
Authors : Raman, C.S.; Li, H.; Martasek, P.; Southan, G.J.; Masters, B.S.S.; Poulos,  
T.L.  
Deposited on : 1999-09-21  
Resolution : 2.20 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

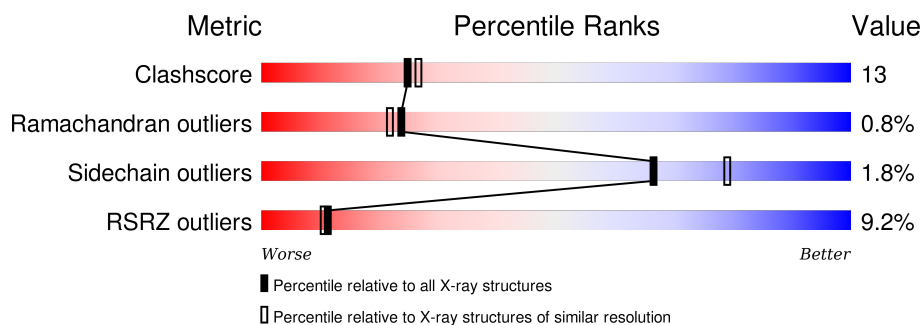
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	<div> <div>9%</div> <div>69%</div> <div>23%</div> <div>6%</div> </div>
1	B	444	<div> <div>9%</div> <div>71%</div> <div>21%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GOL	A	890	-	-	-	X
8	GOL	B	891	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7086 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.

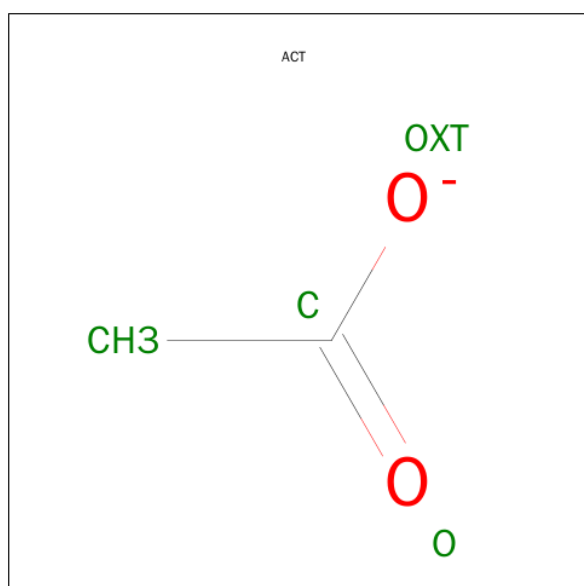
- Molecule 1 is a protein called BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN.

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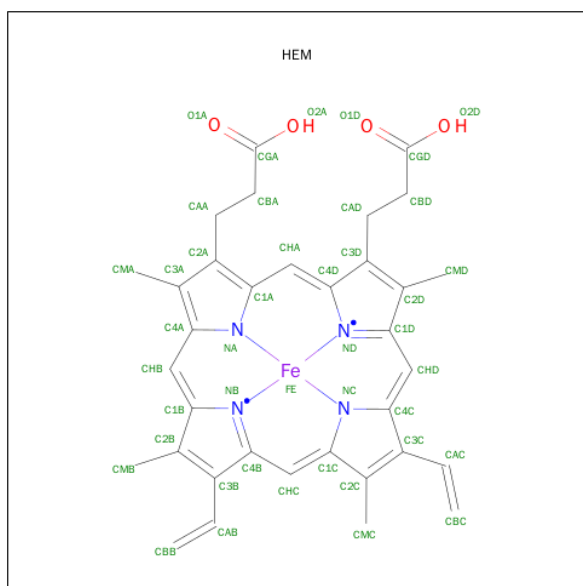
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

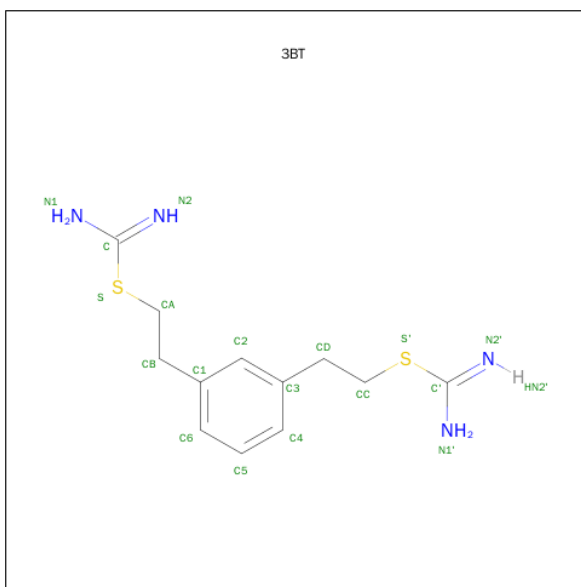
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- 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 2-{2-[3-(2-CARBAMIMIDOYLSULFANYL-ETHYL)-PHENYL]-ETHYL}-ISOTHIUREA (three-letter code: 3BT) (formula:  $C_{12}H_{18}N_4S_2$ ).



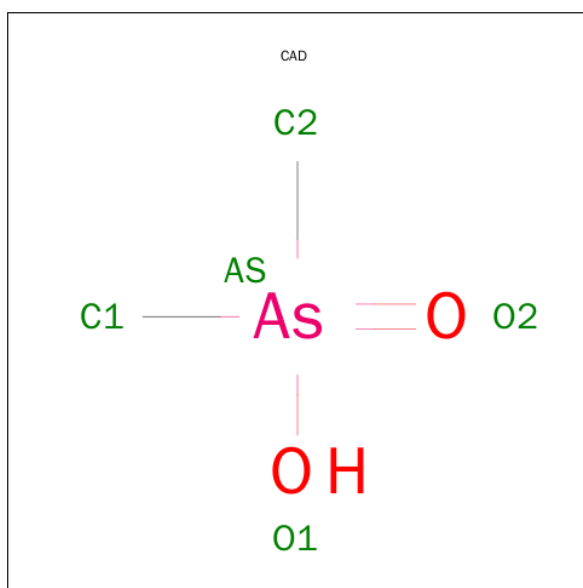
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	S	0	0
			18	12	4	2		
5	B	1	Total	C	N	S	0	0
			18	12	4	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

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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		

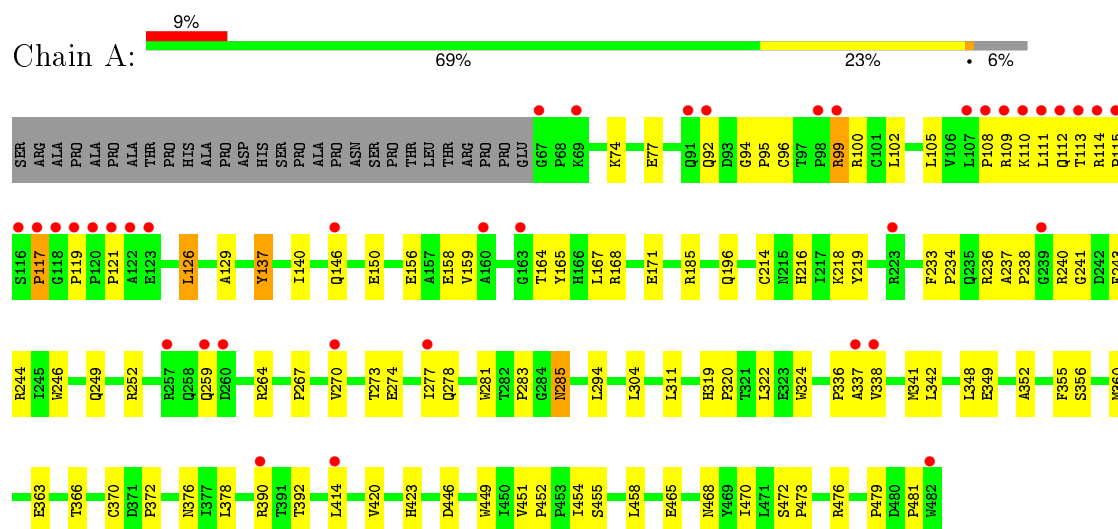
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	170	Total	O	0	0
			170	170		
9	B	152	Total	O	0	0
			152	152		

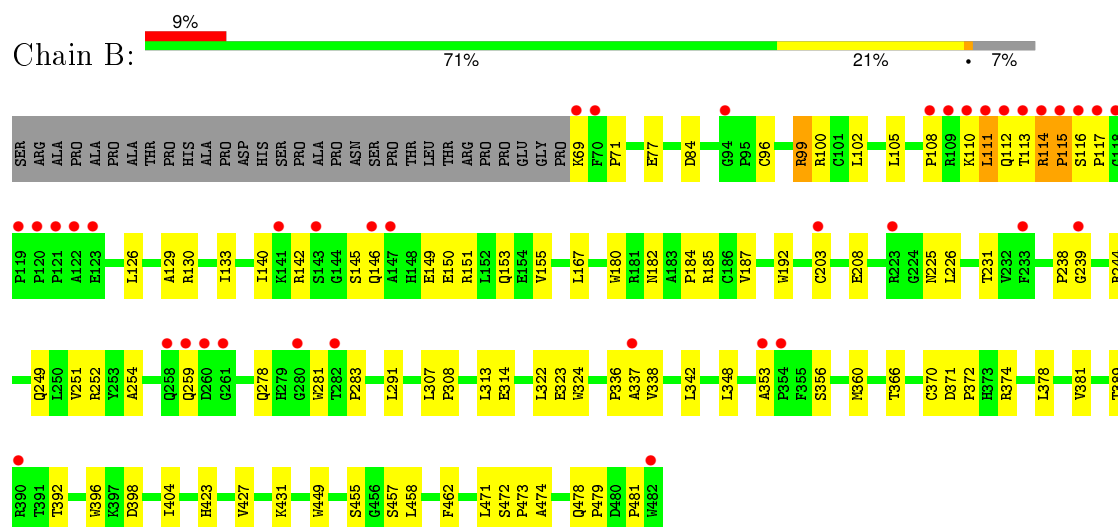
### 3 Residue-property plots

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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.66Å 106.25Å 156.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.32 – 2.20 30.32 – 2.20	Depositor EDS
% Data completeness (in resolution range)	76.4 (30.32-2.20) 82.8 (30.32-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.20Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.223 , 0.268 0.227 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 49052 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 3BT, EDO, 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	0.38	0/3397	0.62	0/4631
1	B	0.39	0/3385	0.63	1/4614 (0.0%)
All	All	0.38	0/6782	0.63	1/9245 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	360	MET	N-CA-C	-5.06	97.35	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	TYR	Sidechain

### 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	88	0
1	B	3291	0	3205	84	0
2	A	8	0	6	0	0
2	B	8	0	6	0	0
3	B	1	0	0	0	0
4	A	43	0	30	0	0
4	B	43	0	30	4	0
5	A	18	0	18	2	0
5	B	18	0	18	3	0
6	A	4	0	6	0	0
6	B	4	0	6	0	0
7	A	3	0	0	0	0
7	B	3	0	0	1	0
8	A	12	0	16	2	0
8	B	6	0	8	1	0
9	A	170	0	0	3	0
9	B	152	0	0	6	0
All	All	7086	0	6564	170	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 (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLN:HB2	1:B:252:ARG:HD3	1.25	1.14
1:B:99:ARG:HH11	1:B:99:ARG:HG3	1.15	1.08
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.42	0.99
1:A:249:GLN:HB2	1:A:252:ARG:HD3	1.49	0.93
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.53	0.91
1:B:114:ARG:HH11	1:B:114:ARG:HA	1.48	0.78
1:A:338:VAL:HG11	1:A:341:MET:HG3	1.65	0.78
1:A:146:GLN:O	1:A:150:GLU:HG3	1.86	0.76
1:B:112:GLN:HG3	1:B:113:THR:H	1.53	0.73
1:A:277:ILE:HD11	1:A:283:PRO:HB3	1.71	0.71
1:B:99:ARG:NH1	1:B:99:ARG:HG3	1.95	0.71
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.26	0.70
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.07	0.70
1:A:168:ARG:HB2	1:A:171:GLU:HG3	1.73	0.69
1:A:99:ARG:HH11	1:A:99:ARG:HG3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:O	1:A:117:PRO:HD3	1.94	0.68
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.76	0.67
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.76	0.67
1:B:378:LEU:HB2	9:B:958:HOH:O	1.95	0.67
1:A:119:PRO:HG3	1:A:238:PRO:HB3	1.76	0.67
1:B:153:GLN:HB2	9:B:1057:HOH:O	1.93	0.67
1:A:102:LEU:HB3	1:A:105:LEU:HD22	1.78	0.66
1:A:378:LEU:HB2	9:A:1088:HOH:O	1.97	0.65
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.81	0.63
1:A:96:CYS:HB3	1:B:96:CYS:HB3	1.81	0.63
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.82	0.61
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.82	0.61
1:A:113:THR:HG21	1:A:342:LEU:HD22	1.82	0.61
1:A:94:GLY:O	1:A:110:LYS:HE2	2.00	0.61
1:A:285:ASN:C	1:A:285:ASN:HD22	2.03	0.61
1:B:116:SER:O	1:B:238:PRO:HA	2.01	0.60
1:A:449:TRP:CD2	8:A:890:GOL:H11	2.36	0.59
1:B:69:LYS:NZ	1:B:69:LYS:HB2	2.18	0.59
1:A:77:GLU:HG3	1:B:372:PRO:CG	2.33	0.59
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.84	0.58
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.84	0.58
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.18	0.58
1:A:277:ILE:HD12	1:A:283:PRO:HD3	1.86	0.57
1:B:313:LEU:HD12	1:B:314:GLU:H	1.68	0.57
1:B:102:LEU:HB3	1:B:105:LEU:HD22	1.86	0.57
1:A:338:VAL:CG1	1:A:341:MET:HG3	2.35	0.56
1:A:277:ILE:CD1	1:A:283:PRO:HB3	2.34	0.56
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.87	0.56
1:B:117:PRO:HA	1:B:239:GLY:H	1.69	0.56
1:A:115:PRO:C	1:A:117:PRO:HD3	2.25	0.56
1:A:249:GLN:HB2	1:A:252:ARG:CD	2.31	0.56
1:B:149:GLU:O	1:B:153:GLN:HG3	2.06	0.55
1:A:472:SER:HA	1:A:473:PRO:C	2.26	0.55
1:A:273:THR:O	1:A:277:ILE:HG12	2.07	0.55
1:A:336:PRO:HB2	5:A:820:3BT:H61	1.88	0.55
1:A:126:LEU:HD11	1:A:156:GLU:CG	2.32	0.54
1:B:113:THR:HG21	1:B:342:LEU:HD13	1.90	0.54
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.43	0.54
1:A:237:ALA:HB3	1:A:240:ARG:HB3	1.89	0.54
1:A:294:LEU:HD21	1:A:304:LEU:HD13	1.90	0.54
1:B:112:GLN:HE21	1:B:478:GLN:HA	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ALA:O	1:B:133:ILE:HG12	2.08	0.53
1:A:99:ARG:CG	1:A:99:ARG:HH11	2.19	0.53
1:B:126:LEU:O	1:B:130:ARG:HG3	2.08	0.53
1:B:249:GLN:CB	1:B:252:ARG:HD3	2.18	0.53
1:B:471:LEU:O	1:B:474:ALA:HB2	2.08	0.53
1:A:372:PRO:HB2	1:B:77:GLU:HG3	1.90	0.53
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.48	0.53
1:B:113:THR:HG21	1:B:342:LEU:CD1	2.39	0.53
1:B:472:SER:HA	1:B:473:PRO:C	2.29	0.53
1:A:264:ARG:HG3	1:A:264:ARG:HH11	1.73	0.53
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.49	0.52
1:B:366:THR:O	1:B:370:CYS:HB2	2.09	0.52
1:A:95:PRO:HB3	1:A:108:PRO:HB2	1.92	0.52
1:B:278:GLN:NE2	9:B:1039:HOH:O	2.41	0.52
1:B:185:ARG:HD3	1:B:449:TRP:CD2	2.45	0.52
1:A:111:LEU:H	1:A:111:LEU:HD12	1.74	0.52
1:B:449:TRP:CE2	8:B:891:GOL:H2	2.45	0.52
1:A:236:ARG:HD3	1:A:349:GLU:HB2	1.90	0.52
1:A:214:CYS:O	1:A:218:LYS:HG3	2.10	0.52
1:B:249:GLN:HB2	1:B:252:ARG:CD	2.18	0.51
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.46	0.51
1:B:342:LEU:HD23	1:B:342:LEU:C	2.31	0.51
1:B:203:CYS:SG	1:B:208:GLU:HB3	2.52	0.50
1:B:108:PRO:HG3	9:B:1064:HOH:O	2.11	0.50
1:A:285:ASN:C	1:A:285:ASN:ND2	2.64	0.50
1:B:99:ARG:HH11	1:B:99:ARG:CG	2.04	0.50
1:B:457:SER:HA	1:B:462:PHE:CG	2.46	0.50
1:A:274:GLU:O	1:A:278:GLN:HG3	2.12	0.50
1:B:110:LYS:C	1:B:112:GLN:H	2.16	0.50
1:A:74:LYS:O	1:A:465:GLU:HG3	2.12	0.50
1:A:240:ARG:HG2	1:A:241:GLY:N	2.28	0.49
1:B:187:VAL:O	1:B:187:VAL:HG22	2.12	0.49
1:B:337:ALA:CB	1:B:356:SER:HB3	2.43	0.49
4:B:500:HEM:HMC1	4:B:500:HEM:HBC2	1.95	0.48
1:A:115:PRO:HD3	1:A:479:PRO:CG	2.29	0.48
1:A:109:ARG:O	1:A:110:LYS:HD2	2.13	0.48
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.42	0.48
1:A:446:ASP:HB2	9:A:1075:HOH:O	2.14	0.47
1:B:478:GLN:HB2	1:B:479:PRO:HD2	1.97	0.47
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.78	0.47
1:A:113:THR:CG2	1:A:476:ARG:HD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:TRP:CE2	8:A:890:GOL:H11	2.49	0.47
1:A:137:TYR:HA	1:A:140:ILE:HG12	1.95	0.47
1:A:111:LEU:HG	1:A:470:ILE:HD13	1.97	0.47
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.97	0.46
1:A:243:PHE:O	1:A:352:ALA:HB2	2.14	0.46
1:B:251:VAL:O	1:B:252:ARG:HD2	2.15	0.46
1:B:281:TRP:O	1:B:283:PRO:HD3	2.14	0.46
1:B:226:LEU:HD12	1:B:226:LEU:N	2.31	0.46
1:B:114:ARG:HH11	1:B:115:PRO:HD3	1.81	0.46
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.51	0.46
1:A:267:PRO:O	1:A:270:VAL:HG23	2.16	0.46
1:B:324:TRP:HB2	7:B:951:CAD:C1	2.46	0.46
1:B:251:VAL:HA	9:B:1009:HOH:O	2.15	0.46
1:A:234:PRO:HB2	1:A:243:PHE:CD1	2.51	0.46
1:A:252:ARG:HD2	1:A:252:ARG:HA	1.75	0.46
4:B:500:HEM:HBC2	4:B:500:HEM:CMC	2.45	0.45
4:B:500:HEM:O2A	5:B:821:3BT:HCD2	2.16	0.45
1:B:146:GLN:O	1:B:150:GLU:HG3	2.16	0.45
1:A:366:THR:HG21	1:A:454:ILE:HG23	1.98	0.45
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.51	0.45
1:A:363:GLU:OE2	5:A:820:3BT:N2	2.50	0.45
1:B:69:LYS:HB2	1:B:69:LYS:HZ1	1.82	0.45
1:B:151:ARG:O	1:B:155:VAL:HG23	2.16	0.45
1:B:371:ASP:HB2	1:B:374:ARG:CG	2.47	0.45
1:B:244:ARG:CZ	1:B:481:PRO:HD3	2.46	0.45
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.53	0.44
1:B:182:ASN:O	1:B:184:PRO:HD3	2.16	0.44
1:A:294:LEU:CD2	1:A:304:LEU:HD13	2.48	0.44
1:A:196:GLN:HG2	1:A:219:TYR:CE1	2.53	0.44
1:A:233:PHE:HB3	1:A:234:PRO:HD2	1.99	0.44
1:B:338:VAL:HG23	5:B:821:3BT:C1	2.48	0.43
1:B:112:GLN:HG3	1:B:113:THR:N	2.29	0.43
1:A:92:GLN:HE22	1:A:111:LEU:HA	1.84	0.43
1:A:281:TRP:O	1:A:283:PRO:HD3	2.18	0.43
1:B:336:PRO:HB2	5:B:821:3BT:H61	1.99	0.43
1:A:159:VAL:HA	1:A:164:THR:O	2.19	0.43
1:A:337:ALA:HB2	1:A:356:SER:HB3	2.00	0.43
1:B:140:ILE:O	1:B:142:ARG:HG2	2.18	0.43
1:A:109:ARG:NH1	1:A:109:ARG:HG2	2.34	0.43
1:A:216:HIS:C	1:A:216:HIS:CD2	2.92	0.43
1:B:381:VAL:HG21	1:B:404:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HD3	1:B:449:TRP:CE3	2.54	0.42
1:A:167:LEU:HG	1:A:348:LEU:HD12	2.01	0.42
1:B:431:LYS:HE3	9:B:1069:HOH:O	2.19	0.42
1:B:252:ARG:HB2	1:B:291:LEU:HD12	2.00	0.42
1:A:92:GLN:OE1	1:A:476:ARG:NH1	2.52	0.42
1:A:376:ASN:ND2	9:A:1088:HOH:O	2.42	0.42
1:B:69:LYS:NZ	1:B:69:LYS:CB	2.81	0.42
1:B:71:PRO:HG2	1:B:84:ASP:HB3	2.01	0.42
1:A:99:ARG:NH1	1:A:99:ARG:CG	2.81	0.41
1:B:313:LEU:HD12	1:B:314:GLU:N	2.33	0.41
4:B:500:HEM:HMC1	4:B:500:HEM:CBC	2.49	0.41
1:A:158:GLU:HG2	1:A:165:TYR:HA	2.02	0.41
1:A:392:THR:HB	1:B:423:HIS:HB2	2.02	0.41
1:A:114:ARG:HA	1:A:479:PRO:HG2	2.02	0.41
1:A:360:MET:HA	1:A:420:VAL:O	2.19	0.41
1:A:338:VAL:HB	1:A:355:PHE:CZ	2.56	0.41
1:B:110:LYS:O	1:B:112:GLN:N	2.53	0.41
1:A:338:VAL:HG11	1:A:341:MET:CG	2.45	0.41
1:B:231:THR:O	1:B:353:ALA:HA	2.21	0.41
1:B:254:ALA:HB2	1:B:291:LEU:CD2	2.50	0.41
1:B:112:GLN:NE2	1:B:478:GLN:HA	2.35	0.41
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.91	0.41
1:A:423:HIS:HB2	1:B:392:THR:HB	2.02	0.41
1:A:246:TRP:HB2	1:A:294:LEU:HB2	2.04	0.40
1:A:129:ALA:HB2	1:A:165:TYR:CE2	2.56	0.40
1:B:371:ASP:HB2	1:B:374:ARG:HG2	2.02	0.40
1:B:423:HIS:O	1:B:427:VAL:HG23	2.21	0.40
1:B:307:LEU:HA	1:B:308:PRO:HD3	1.96	0.40
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.96	0.40
1:B:117:PRO:HA	1:B:239:GLY:N	2.36	0.40
1:B:389:THR:HA	1:B:396:TRP:CD1	2.57	0.40
1:A:390:ARG:HE	1:A:390:ARG:HB2	1.57	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%)	23 (6%)	3 (1%)	26	25
1	B	412/444 (93%)	379 (92%)	29 (7%)	4 (1%)	19	16
All	All	826/888 (93%)	767 (93%)	52 (6%)	7 (1%)	24	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	A	112	GLN
1	B	111	LEU
1	B	145	SER
1	A	117	PRO
1	B	115	PRO
1	A	121	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%)	347 (98%)	7 (2%)	63	76
1	B	353/377 (94%)	347 (98%)	6 (2%)	68	81
All	All	707/754 (94%)	694 (98%)	13 (2%)	66	79

All (13) 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	259	GLN
1	A	285	ASN

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Mol	Chain	Res	Type
1	A	414	LEU
1	A	468	ASN
1	B	99	ARG
1	B	100	ARG
1	B	114	ARG
1	B	225	ASN
1	B	323	GLU
1	B	398	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	153	GLN
1	A	191	GLN
1	A	259	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	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 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 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
4	HEM	A	500	1	30,50,50	2.96	11 (36%)	24,82,82	2.18	8 (33%)
5	3BT	A	820	-	16,18,18	3.16	7 (43%)	18,22,22	1.79	3 (16%)
2	ACT	A	850	-	1,3,3	2.73	1 (100%)	0,3,3	0.00	-
2	ACT	A	860	-	1,3,3	2.24	1 (100%)	0,3,3	0.00	-
6	EDO	A	870	-	3,3,3	0.45	0	2,2,2	0.34	0
8	GOL	A	881	-	5,5,5	0.33	0	5,5,5	0.19	0
8	GOL	A	890	-	5,5,5	0.21	0	5,5,5	0.32	0
7	CAD	A	950	1	0,2,4	0.00	-	0,1,6	0.00	-
4	HEM	B	500	1	30,50,50	2.57	9 (30%)	24,82,82	2.08	8 (33%)
5	3BT	B	821	-	16,18,18	3.31	7 (43%)	18,22,22	1.71	3 (16%)
2	ACT	B	851	-	1,3,3	4.15	1 (100%)	0,3,3	0.00	-
2	ACT	B	861	-	1,3,3	1.79	0	0,3,3	0.00	-
6	EDO	B	871	-	3,3,3	0.54	0	2,2,2	0.33	0
8	GOL	B	891	-	5,5,5	0.21	0	5,5,5	0.13	0
7	CAD	B	951	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
4	HEM	A	500	1	-	0/10/54/54	0/0/8/8
5	3BT	A	820	-	-	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
6	EDO	A	870	-	-	0/1/1/1	0/0/0/0
8	GOL	A	881	-	-	0/4/4/4	0/0/0/0
8	GOL	A	890	-	-	0/4/4/4	0/0/0/0
7	CAD	A	950	1	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	B	500	1	-	0/10/54/54	0/0/8/8
5	3BT	B	821	-	-	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
6	EDO	B	871	-	-	0/1/1/1	0/0/0/0
8	GOL	B	891	-	-	0/4/4/4	0/0/0/0
7	CAD	B	951	1	-	0/0/0/0	0/0/0/0

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	HEM	C2D-C3D	-6.78	1.34	1.54
4	B	500	HEM	C3B-C4B	-6.29	1.46	1.51
4	A	500	HEM	C3B-CAB	-6.21	1.39	1.51
4	B	500	HEM	C2D-C3D	-6.00	1.36	1.54
4	A	500	HEM	C3B-C4B	-5.43	1.47	1.51
4	B	500	HEM	C3B-CAB	-5.30	1.41	1.51
4	A	500	HEM	C3D-C4D	-5.27	1.44	1.51
4	B	500	HEM	C3D-C4D	-5.05	1.45	1.51
4	A	500	HEM	C3C-CAC	-5.03	1.41	1.51
4	B	500	HEM	C3C-CAC	-4.38	1.43	1.51
4	B	500	HEM	C2C-C1C	-4.22	1.44	1.52
4	A	500	HEM	C2C-C1C	-3.63	1.45	1.52
4	A	500	HEM	C2B-C1B	-2.46	1.43	1.51
4	B	500	HEM	C2B-C1B	-2.27	1.44	1.51
5	B	821	3BT	C5-C4	2.09	1.43	1.38
4	A	500	HEM	CHD-C4C	2.10	1.41	1.36
4	B	500	HEM	C1C-NC	2.14	1.38	1.36
5	A	820	3BT	C5-C4	2.19	1.43	1.38
2	A	860	ACT	CH3-C	2.24	1.51	1.48
4	A	500	HEM	CHC-C1C	2.33	1.41	1.36
5	B	821	3BT	C6-C1	2.37	1.43	1.38
5	A	820	3BT	C6-C1	2.38	1.43	1.38
2	A	850	ACT	CH3-C	2.73	1.52	1.48
4	B	500	HEM	C4C-NC	3.30	1.40	1.36
5	B	821	3BT	C-N2	3.43	1.40	1.28
5	A	820	3BT	C-N2	3.70	1.41	1.28
5	A	820	3BT	C-N1	3.72	1.42	1.34
5	A	820	3BT	C'-N1'	3.98	1.42	1.34
5	B	821	3BT	C-N1	3.98	1.42	1.34
5	B	821	3BT	C'-N2'	4.05	1.43	1.28
2	B	851	ACT	CH3-C	4.15	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	820	3BT	C'-N2'	4.20	1.43	1.28
4	A	500	HEM	C1C-NC	4.30	1.41	1.36
5	B	821	3BT	C'-N1'	4.37	1.43	1.34
4	A	500	HEM	C4C-NC	5.53	1.42	1.36
5	A	820	3BT	C2-C3	9.02	1.55	1.39
5	B	821	3BT	C2-C3	9.43	1.56	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	500	HEM	CBA-CAA-C2A	-3.85	105.63	112.53
5	A	820	3BT	C1-C2-C3	-2.08	118.55	121.25
5	B	821	3BT	C1-C2-C3	-2.01	118.65	121.25
4	B	500	HEM	C3C-CAC-CBC	2.02	127.56	124.46
4	A	500	HEM	CMD-C2D-C3D	2.06	123.44	114.35
4	B	500	HEM	CMD-C2D-C3D	2.20	124.08	114.35
4	A	500	HEM	C3B-CAB-CBB	2.24	127.89	124.46
4	A	500	HEM	C3C-CAC-CBC	2.30	127.99	124.46
4	B	500	HEM	C2D-C3D-C4D	2.32	105.44	101.50
4	B	500	HEM	CMC-C2C-C3C	3.28	124.71	116.53
4	B	500	HEM	CMB-C2B-C3B	3.70	125.78	116.53
5	A	820	3BT	CC-S'-C'	3.84	108.72	100.77
4	A	500	HEM	C2D-C3D-C4D	3.93	108.16	101.50
4	A	500	HEM	CAD-C3D-C4D	3.95	126.41	112.47
4	B	500	HEM	CAD-C3D-C4D	3.97	126.47	112.47
4	A	500	HEM	CAD-C3D-C2D	4.24	125.41	113.22
5	B	821	3BT	CA-S-C	4.35	109.77	100.77
5	B	821	3BT	CC-S'-C'	4.44	109.97	100.77
4	A	500	HEM	CMC-C2C-C3C	4.47	127.69	116.53
4	A	500	HEM	CMB-C2B-C3B	4.66	128.16	116.53
4	B	500	HEM	CAD-C3D-C2D	5.14	127.99	113.22
5	A	820	3BT	CA-S-C	5.59	112.35	100.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	820	3BT	2	0
8	A	890	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	500	HEM	4	0
5	B	821	3BT	3	0
8	B	891	GOL	1	0
7	B	951	CAD	1	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%)	0.44	38 (9%) 11 11	30, 45, 78, 100	0
1	B	414/444 (93%)	0.56	38 (9%) 11 10	31, 50, 79, 100	0
All	All	830/888 (93%)	0.50	76 (9%) 11 10	30, 47, 79, 100	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	PRO	13.2
1	B	115	PRO	11.5
1	B	118	GLY	10.8
1	A	113	THR	10.5
1	B	111	LEU	10.4
1	B	119	PRO	10.3
1	B	120	PRO	10.2
1	A	119	PRO	10.1
1	B	116	SER	9.9
1	A	117	PRO	9.5
1	B	113	THR	9.2
1	A	115	PRO	8.9
1	A	111	LEU	7.8
1	B	110	LYS	7.7
1	B	112	GLN	7.5
1	A	114	ARG	7.2
1	B	114	ARG	7.0
1	A	118	GLY	6.9
1	A	110	LYS	6.8
1	A	109	ARG	6.7
1	B	121	PRO	5.8
1	A	116	SER	5.7
1	A	112	GLN	5.2
1	B	122	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	4.6
1	A	99	ARG	4.6
1	B	260	ASP	4.4
1	B	259	GLN	4.1
1	A	120	PRO	4.1
1	A	259	GLN	3.9
1	B	94	GLY	3.6
1	A	239	GLY	3.5
1	B	146	GLN	3.5
1	A	107	LEU	3.5
1	A	69	LYS	3.2
1	B	108	PRO	3.2
1	A	390	ARG	3.1
1	A	146	GLN	2.9
1	B	141	LYS	2.9
1	A	121	PRO	2.8
1	A	123	GLU	2.8
1	A	337	ALA	2.8
1	B	147	ALA	2.8
1	A	67	GLY	2.7
1	B	337	ALA	2.7
1	A	91	GLN	2.7
1	B	143	SER	2.6
1	A	257	ARG	2.6
1	A	338	VAL	2.6
1	B	109	ARG	2.5
1	B	261	GLY	2.5
1	A	270	VAL	2.5
1	B	123	GLU	2.4
1	B	239	GLY	2.4
1	A	277	ILE	2.4
1	B	353	ALA	2.4
1	A	98	PRO	2.3
1	B	354	PRO	2.3
1	A	482	TRP	2.3
1	B	258	GLN	2.3
1	B	233	PHE	2.2
1	B	390	ARG	2.2
1	A	414	LEU	2.2
1	B	69	LYS	2.2
1	B	223	ARG	2.2
1	B	482	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	92	GLN	2.1
1	B	70	PHE	2.1
1	A	122	ALA	2.1
1	B	280	GLY	2.1
1	B	282	THR	2.1
1	A	160	ALA	2.1
1	A	260	ASP	2.0
1	A	163	GLY	2.0
1	B	203	CYS	2.0
1	A	223	ARG	2.0

## 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
8	GOL	A	890	6/6	0.94	0.24	5.26	55,55,57,59	0
8	GOL	B	891	6/6	0.90	0.26	3.77	56,56,57,58	0
5	3BT	B	821	18/18	0.91	0.24	1.25	49,60,63,63	0
6	EDO	A	870	4/4	0.86	0.16	1.20	52,54,55,55	0
5	3BT	A	820	18/18	0.90	0.24	1.16	44,55,58,60	0
8	GOL	A	881	6/6	0.91	0.18	0.97	53,55,56,56	0
6	EDO	B	871	4/4	0.83	0.16	0.89	55,56,57,59	0
4	HEM	A	500	43/43	0.97	0.17	0.72	28,34,48,54	0
2	ACT	B	861	4/4	0.94	0.12	0.13	50,51,52,54	0
4	HEM	B	500	43/43	0.97	0.15	-0.06	29,32,45,46	0
2	ACT	A	860	4/4	0.95	0.11	-0.19	45,46,46,47	0

*Continued on next page...*



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CAD	B	951	3/5	0.98	0.15	-0.30	83,83,83,88	0
7	CAD	A	950	3/5	0.98	0.10	-0.37	53,53,54,59	0
2	ACT	A	850	4/4	0.95	0.13	-0.58	53,55,56,56	0
2	ACT	B	851	4/4	0.96	0.11	-1.27	48,49,50,51	0
3	ZN	B	900	1/1	0.98	0.03	-2.80	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.