



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:08 pm GMT

PDB ID : 2NQN  
Title : MoeA T100W  
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Deposited on : 2006-10-31  
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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

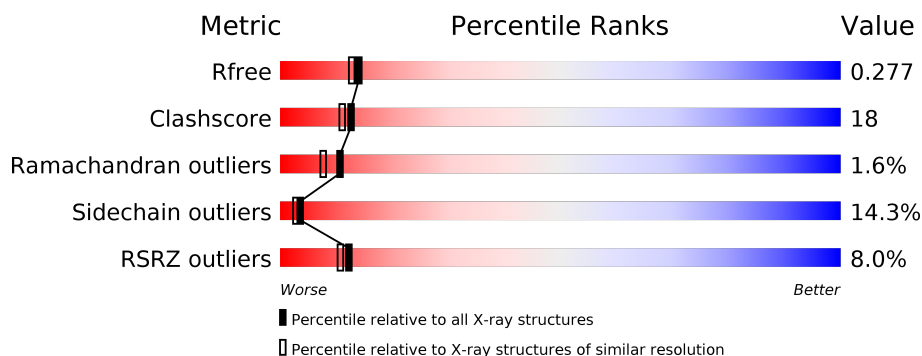
# 1 Overall quality at a glance

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))
$R_{free}$	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (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	411	
1	B	411	

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
2	GOL	A	511	-	-	-	X
2	GOL	A	518	-	-	-	X
2	GOL	B	525	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6758 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 Molybdopterin biosynthesis protein moeA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3055	1929	534	579	13			
1	B	405	Total	C	N	O	S	0	0	0
			3055	1929	534	579	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	TRP	THR	ENGINEERED	UNP P12281
B	100	TRP	THR	ENGINEERED	UNP P12281

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

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

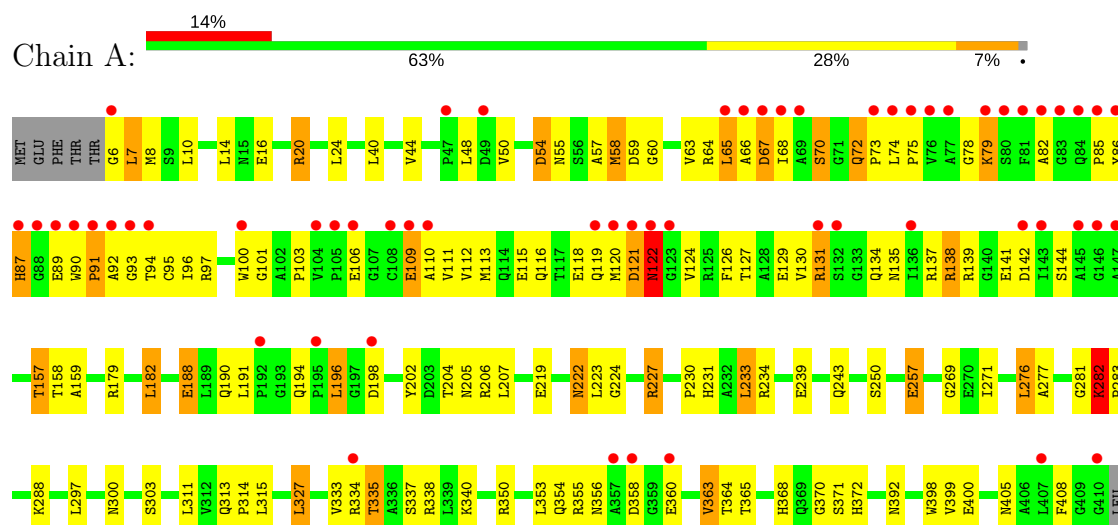
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	216	Total	O	0	0
			216	216		
3	B	258	Total	O	0	0
			258	258		

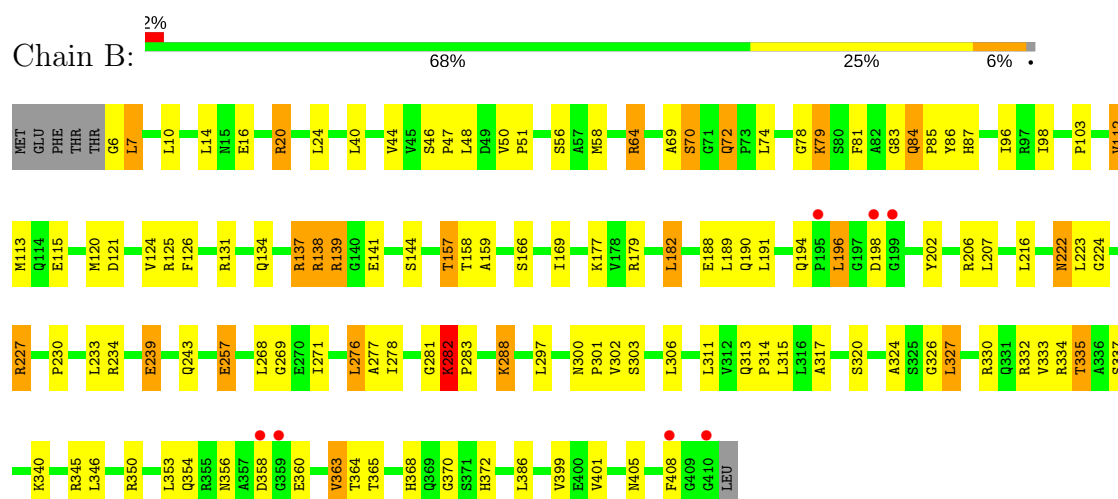
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Molybdopterin biosynthesis protein moeA



#### • Molecule 1: Molybdopterin biosynthesis protein moeA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.08Å 98.66Å 159.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.20 49.33 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.39-2.20) 97.1 (49.33-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.225 , 0.274 0.228 , 0.277	Depositor DCC
$R_{free}$ test set	2786 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6758	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0.37	0/3116	0.62	1/4235 (0.0%)
1	B	0.37	0/3116	0.63	1/4235 (0.0%)
All	All	0.37	0/6232	0.62	2/8470 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	LEU	CA-CB-CG	5.92	128.92	115.30
1	B	182	LEU	CA-CB-CG	5.37	127.66	115.30

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	3055	0	3046	131	1
1	B	3055	0	3046	97	1
2	A	78	0	104	5	0
2	B	96	0	128	12	0
3	A	216	0	0	12	0
3	B	258	0	0	13	0
All	All	6758	0	6324	226	1

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 18.

All (226) 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:72:GLN:HG2	1:A:73:PRO:HD2	1.42	0.99
1:A:157:THR:HG22	1:A:159:ALA:H	1.27	0.99
1:B:157:THR:HG22	1:B:159:ALA:H	1.29	0.93
1:B:368:HIS:HD2	1:B:370:GLY:H	1.16	0.93
1:B:177:LYS:HA	2:B:501:GOL:H11	1.51	0.90
1:B:190:GLN:HG3	1:B:194:GLN:HE21	1.35	0.88
1:A:190:GLN:HG3	1:A:194:GLN:HE21	1.36	0.88
1:B:368:HIS:CD2	1:B:370:GLY:H	1.92	0.87
1:B:6:GLY:O	1:B:7:LEU:HB2	1.72	0.87
1:A:368:HIS:HD2	1:A:370:GLY:H	1.18	0.86
1:A:368:HIS:CD2	1:A:370:GLY:H	1.94	0.84
2:A:517:GOL:H12	1:B:166:SER:HB2	1.62	0.81
1:B:216:LEU:HD22	2:B:509:GOL:H2	1.64	0.80
1:A:72:GLN:HG2	1:A:73:PRO:CD	2.12	0.79
1:A:353:LEU:HD13	1:A:363:VAL:HG13	1.67	0.77
1:A:138:ARG:O	1:A:141:GLU:HB2	1.85	0.76
1:A:100:TRP:HE1	1:A:137:ARG:HH12	1.33	0.76
1:B:300:ASN:HD22	1:B:303:SER:H	1.34	0.75
1:A:68:ILE:HD11	1:A:126:PHE:HB2	1.68	0.75
1:B:313:GLN:HE22	1:B:405:ASN:HD21	1.35	0.75
1:A:6:GLY:O	1:A:7:LEU:HB2	1.87	0.75
1:A:300:ASN:HD22	1:A:303:SER:H	1.35	0.74
1:B:353:LEU:HD13	1:B:363:VAL:HG13	1.70	0.74
1:A:313:GLN:HE22	1:A:405:ASN:HD21	1.33	0.73
1:B:222:ASN:HD22	1:B:224:GLY:H	1.36	0.73
1:B:335:THR:HG22	1:B:337:SER:H	1.55	0.71
1:B:324:ALA:HB2	2:B:514:GOL:H2	1.71	0.70
1:A:335:THR:HG22	1:A:337:SER:H	1.56	0.70
1:A:282:LYS:HB3	1:A:283:PRO:HD3	1.72	0.69
1:A:353:LEU:CD1	1:A:363:VAL:HG13	2.23	0.68
1:A:55:ASN:HD22	1:A:101:GLY:HA2	1.57	0.68
1:B:7:LEU:HD12	3:B:559:HOH:O	1.93	0.68
1:B:282:LYS:HB3	1:B:283:PRO:HD3	1.74	0.68
1:A:222:ASN:HD22	1:A:224:GLY:H	1.40	0.67
1:B:353:LEU:CD1	1:B:363:VAL:HG13	2.23	0.67
1:B:137:ARG:HG2	3:B:541:HOH:O	1.95	0.67
1:B:179:ARG:HD2	3:B:771:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:HG23	1:A:158:THR:N	2.10	0.66
1:A:157:THR:CG2	1:A:158:THR:N	2.58	0.65
1:A:65:LEU:O	1:A:68:ILE:HG22	1.96	0.65
1:A:111:VAL:HB	1:A:135:ASN:HB2	1.79	0.64
2:B:501:GOL:H12	3:B:534:HOH:O	1.97	0.64
1:A:6:GLY:HA2	1:A:277:ALA:HA	1.80	0.63
1:A:129:GLU:HG3	1:A:130:VAL:N	2.14	0.63
1:A:157:THR:HG23	1:A:158:THR:H	1.64	0.63
1:A:75:PRO:O	1:A:94:THR:HB	1.99	0.62
1:B:317:ALA:HA	2:B:509:GOL:H31	1.82	0.62
1:B:157:THR:CG2	1:B:158:THR:N	2.62	0.62
1:B:222:ASN:ND2	1:B:224:GLY:H	1.98	0.62
1:B:157:THR:HG23	1:B:158:THR:N	2.15	0.62
1:B:189:LEU:HD21	2:B:502:GOL:H31	1.83	0.61
1:A:122:ASN:HD22	1:A:122:ASN:C	2.04	0.61
1:A:219:GLU:HG2	3:A:724:HOH:O	1.99	0.61
1:A:50:VAL:O	1:A:142:ASP:HB2	2.00	0.60
1:B:368:HIS:HD2	1:B:370:GLY:N	1.94	0.60
1:A:73:PRO:HB3	1:A:120:MET:HE3	1.83	0.60
1:B:206:ARG:HH11	1:B:222:ASN:HD21	1.49	0.60
1:A:67:ASP:O	1:A:74:LEU:HD21	2.00	0.60
1:A:115:GLU:H	1:A:115:GLU:CD	2.03	0.60
1:A:58:MET:HA	1:A:100:TRP:HB2	1.84	0.60
1:A:281:GLY:O	1:A:282:LYS:HB2	2.02	0.60
1:A:115:GLU:N	1:A:115:GLU:CD	2.55	0.60
1:A:137:ARG:HG2	1:A:141:GLU:OE2	2.02	0.60
1:A:188:GLU:HB3	1:B:83:GLY:HA2	1.83	0.60
1:B:115:GLU:H	1:B:115:GLU:CD	2.05	0.60
1:B:281:GLY:O	1:B:282:LYS:HB2	2.02	0.60
1:A:368:HIS:HD2	1:A:370:GLY:N	1.96	0.59
1:A:206:ARG:HH11	1:A:222:ASN:HD21	1.51	0.58
1:A:227:ARG:HD3	3:A:615:HOH:O	2.02	0.58
1:B:157:THR:HG23	1:B:158:THR:H	1.69	0.58
1:A:72:GLN:OE1	1:A:74:LEU:HD23	2.04	0.58
1:B:257:GLU:HB2	3:B:561:HOH:O	2.03	0.57
1:B:179:ARG:NH2	3:B:685:HOH:O	2.36	0.57
1:A:138:ARG:O	1:A:141:GLU:CB	2.51	0.57
1:A:222:ASN:ND2	1:A:224:GLY:H	2.02	0.57
1:B:138:ARG:O	1:B:141:GLU:HG2	2.05	0.57
1:B:6:GLY:HA3	1:B:277:ALA:HA	1.86	0.56
1:B:85:PRO:HB3	1:B:103:PRO:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:HB2	1:A:115:GLU:OE1	2.05	0.56
2:B:504:GOL:H2	3:B:640:HOH:O	2.06	0.56
1:A:313:GLN:HE22	1:A:405:ASN:ND2	2.04	0.54
1:B:288:LYS:NZ	3:B:777:HOH:O	2.39	0.54
1:A:311:LEU:O	1:A:314:PRO:HD2	2.08	0.53
1:B:113:MET:HG2	3:B:605:HOH:O	2.07	0.53
1:A:392:ASN:HB3	3:A:620:HOH:O	2.08	0.53
1:A:179:ARG:NH1	1:A:243:GLN:O	2.42	0.53
1:B:112:VAL:HG21	1:B:126:PHE:HD2	1.74	0.53
1:A:313:GLN:HB3	1:A:314:PRO:HD3	1.91	0.52
1:B:169:ILE:HA	2:B:525:GOL:H32	1.91	0.52
1:A:243:GLN:HE22	2:A:526:GOL:H2	1.73	0.52
1:A:68:ILE:HD11	1:A:126:PHE:CB	2.38	0.52
1:A:311:LEU:C	1:A:314:PRO:HD2	2.30	0.52
1:B:353:LEU:HD13	1:B:363:VAL:CG1	2.38	0.52
1:A:157:THR:CG2	1:A:159:ALA:H	2.12	0.52
1:B:230:PRO:O	1:B:234:ARG:HG3	2.10	0.52
1:A:100:TRP:HE1	1:A:137:ARG:NH1	2.05	0.52
1:A:230:PRO:O	1:A:234:ARG:HG3	2.09	0.52
1:B:311:LEU:C	1:B:314:PRO:HD2	2.29	0.52
1:A:79:LYS:HA	1:A:97:ARG:O	2.11	0.51
1:A:206:ARG:HD2	1:A:222:ASN:HD21	1.76	0.51
1:B:222:ASN:HD22	1:B:222:ASN:C	2.14	0.51
1:A:54:ASP:HA	1:A:137:ARG:O	2.11	0.51
1:B:311:LEU:O	1:B:314:PRO:HD2	2.10	0.51
1:B:332:ARG:NH1	3:B:722:HOH:O	2.44	0.51
1:A:353:LEU:HD13	1:A:363:VAL:CG1	2.37	0.51
1:B:313:GLN:HB3	1:B:314:PRO:HD3	1.92	0.51
1:B:227:ARG:HG2	3:B:622:HOH:O	2.11	0.51
1:B:7:LEU:HD23	3:B:757:HOH:O	2.12	0.50
1:A:67:ASP:HB3	1:A:74:LEU:HD22	1.92	0.50
1:A:78:GLY:C	1:A:96:ILE:HG23	2.31	0.50
1:A:314:PRO:HG3	1:A:327:LEU:CD1	2.42	0.50
1:B:313:GLN:HE22	1:B:405:ASN:ND2	2.06	0.50
1:A:222:ASN:HD22	1:A:222:ASN:C	2.16	0.50
1:A:334:ARG:HG2	1:A:334:ARG:HH11	1.78	0.49
1:A:57:ALA:O	1:A:58:MET:HB3	2.11	0.49
1:B:74:LEU:HD12	1:B:126:PHE:CE1	2.46	0.49
1:B:179:ARG:NH1	1:B:243:GLN:O	2.45	0.49
1:B:356:ASN:ND2	1:B:360:GLU:HB3	2.27	0.49
1:B:326:GLY:HA3	2:B:509:GOL:H11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:PRO:HG2	1:B:87:HIS:CE1	2.46	0.49
1:A:60:GLY:HA3	1:A:112:VAL:O	2.13	0.49
1:B:206:ARG:HD2	1:B:222:ASN:HD21	1.77	0.49
1:B:314:PRO:HG3	1:B:327:LEU:CD1	2.42	0.49
1:B:78:GLY:HA3	1:B:86:TYR:CE2	2.46	0.49
1:A:40:LEU:HD11	1:A:44:VAL:HG23	1.94	0.49
1:B:320:SER:HB2	2:B:501:GOL:H2	1.93	0.49
1:A:85:PRO:HB3	1:A:103:PRO:CG	2.43	0.49
1:A:400:GLU:HG2	2:A:516:GOL:C1	2.42	0.49
1:A:85:PRO:HG2	1:A:87:HIS:HE1	1.77	0.49
1:A:75:PRO:HD2	1:A:94:THR:HG22	1.95	0.49
1:B:139:ARG:HG3	1:B:139:ARG:O	2.12	0.49
1:A:227:ARG:NH1	3:A:615:HOH:O	2.37	0.48
1:A:356:ASN:ND2	1:A:360:GLU:HB3	2.28	0.48
1:A:408:PHE:HA	1:B:157:THR:CG2	2.44	0.48
1:B:112:VAL:HG21	1:B:126:PHE:CD2	2.48	0.48
1:A:96:ILE:HG22	1:A:97:ARG:O	2.13	0.48
1:B:40:LEU:HD11	1:B:44:VAL:HG23	1.95	0.48
1:A:70:SER:OG	1:A:72:GLN:HB3	2.14	0.48
1:A:63:VAL:HG12	1:A:95:CYS:HB2	1.95	0.48
1:B:56:SER:HB2	1:B:98:ILE:HD13	1.96	0.48
1:A:113:MET:HG2	1:A:116:GLN:HG3	1.96	0.48
1:B:278:ILE:O	1:B:345:ARG:HD2	2.14	0.47
1:A:368:HIS:CD2	1:A:370:GLY:N	2.74	0.47
1:A:300:ASN:HD21	1:A:371:SER:HB2	1.79	0.47
1:B:157:THR:CG2	1:B:159:ALA:H	2.14	0.47
1:B:334:ARG:HG2	1:B:334:ARG:HH11	1.79	0.46
1:A:408:PHE:C	1:B:157:THR:HG21	2.36	0.46
1:A:65:LEU:HD22	1:A:65:LEU:O	2.14	0.46
1:B:50:VAL:HA	1:B:51:PRO:C	2.32	0.46
1:A:334:ARG:NH2	1:A:398:TRP:CZ2	2.83	0.46
1:A:138:ARG:H	1:A:138:ARG:HG2	1.49	0.46
1:A:405:ASN:HB2	3:A:577:HOH:O	2.15	0.46
1:A:227:ARG:HG2	3:A:542:HOH:O	2.16	0.46
1:A:110:ALA:HB1	1:A:134:GLN:HG2	1.99	0.45
1:B:190:GLN:HG3	1:B:194:GLN:NE2	2.17	0.45
1:A:120:MET:O	1:A:122:ASN:N	2.50	0.45
1:A:334:ARG:CG	1:A:334:ARG:HH11	2.29	0.45
1:A:355:ARG:HD2	1:B:330:ARG:O	2.16	0.45
1:A:6:GLY:O	1:A:7:LEU:CB	2.62	0.45
1:B:74:LEU:HD12	1:B:126:PHE:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:H	1:A:194:GLN:NE2	2.15	0.45
1:A:190:GLN:HG3	1:A:194:GLN:NE2	2.18	0.45
1:A:233:LEU:HG	3:A:713:HOH:O	2.17	0.45
1:A:64:ARG:HA	1:A:109:GLU:HB2	1.99	0.44
1:B:69:ALA:O	1:B:70:SER:C	2.56	0.44
1:B:86:TYR:CD1	1:B:96:ILE:HD13	2.52	0.44
1:A:78:GLY:HA3	1:A:86:TYR:CE1	2.52	0.44
1:A:257:GLU:HB2	3:A:553:HOH:O	2.18	0.44
1:B:368:HIS:CD2	1:B:370:GLY:N	2.72	0.44
1:A:118:GLU:HG3	3:A:612:HOH:O	2.17	0.44
1:A:121:ASP:O	1:A:122:ASN:HB3	2.18	0.44
1:A:338:ARG:HG3	3:A:620:HOH:O	2.16	0.44
1:B:16:GLU:O	1:B:20:ARG:HG3	2.18	0.44
1:A:7:LEU:HB3	1:A:8:MET:H	1.66	0.43
1:B:64:ARG:HB2	1:B:64:ARG:HE	1.48	0.43
1:A:276:LEU:HD21	1:A:311:LEU:HD11	2.01	0.43
1:A:85:PRO:HB3	1:A:103:PRO:HG2	1.99	0.43
1:A:91:PRO:C	1:A:93:GLY:H	2.22	0.43
1:A:113:MET:CG	1:A:116:GLN:HG3	2.48	0.43
1:A:91:PRO:O	1:A:93:GLY:N	2.52	0.43
1:B:276:LEU:HD21	1:B:311:LEU:HD11	2.01	0.43
1:A:333:VAL:HG12	1:A:334:ARG:N	2.34	0.43
1:A:400:GLU:HG2	2:A:516:GOL:H11	1.99	0.43
1:A:72:GLN:HG2	1:A:73:PRO:N	2.33	0.43
1:A:130:VAL:HG13	1:A:134:GLN:CD	2.39	0.42
1:B:196:LEU:HD13	1:B:202:TYR:CZ	2.54	0.42
1:B:46:SER:HA	1:B:47:PRO:HD3	1.92	0.42
1:B:6:GLY:O	1:B:7:LEU:CB	2.54	0.42
1:B:72:GLN:H	1:B:72:GLN:HG2	1.53	0.42
1:B:269:GLY:C	1:B:271:ILE:HD12	2.39	0.42
1:B:191:LEU:H	1:B:194:GLN:NE2	2.17	0.42
1:A:338:ARG:CZ	3:A:620:HOH:O	2.67	0.42
1:B:363:VAL:HG11	1:B:401:VAL:HG21	2.02	0.42
1:A:16:GLU:O	1:A:20:ARG:HG3	2.20	0.42
1:B:364:THR:HG22	1:B:365:THR:O	2.19	0.42
1:A:90:TRP:O	1:A:91:PRO:C	2.58	0.42
1:A:131:ARG:O	1:A:134:GLN:HB3	2.19	0.42
1:A:269:GLY:C	1:A:271:ILE:HD12	2.40	0.41
1:A:334:ARG:NH1	1:A:334:ARG:CG	2.83	0.41
1:A:364:THR:HG22	1:A:365:THR:O	2.20	0.41
2:B:512:GOL:H2	3:B:589:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLY:O	1:A:282:LYS:CB	2.68	0.41
1:A:196:LEU:HD13	1:A:202:TYR:CZ	2.55	0.41
1:A:368:HIS:CD2	1:A:372:HIS:HE1	2.38	0.41
1:A:333:VAL:CG1	1:A:334:ARG:N	2.83	0.41
1:B:300:ASN:HD21	1:B:302:VAL:HB	1.86	0.41
1:A:79:LYS:O	1:A:86:TYR:HB2	2.20	0.41
1:A:73:PRO:HA	1:A:124:VAL:O	2.20	0.41
1:B:306:LEU:HD13	1:B:306:LEU:C	2.40	0.41
1:A:205:ASN:HB2	3:A:560:HOH:O	2.21	0.41
1:B:81:PHE:HB2	1:B:84:GLN:OE1	2.21	0.41
1:B:300:ASN:HA	1:B:301:PRO:HD3	1.95	0.41
1:A:204:THR:HG21	2:A:517:GOL:H32	2.03	0.40
1:A:271:ILE:HD12	1:A:271:ILE:N	2.36	0.40
1:A:85:PRO:HG2	1:A:87:HIS:CE1	2.56	0.40
1:A:68:ILE:HD12	1:A:68:ILE:HA	1.88	0.40
1:B:134:GLN:HA	2:B:515:GOL:H2	2.03	0.40
1:B:333:VAL:HG12	1:B:334:ARG:N	2.36	0.40
1:B:346:LEU:HD12	1:B:386:LEU:O	2.21	0.40
1:A:157:THR:CG2	1:B:408:PHE:HA	2.51	0.40
1:A:65:LEU:HD13	1:A:65:LEU:C	2.42	0.40
1:B:334:ARG:CG	1:B:334:ARG:HH11	2.33	0.40
1:B:368:HIS:CD2	1:B:372:HIS:HE1	2.39	0.40
1:B:79:LYS:O	1:B:86:TYR:HB2	2.21	0.40
1:A:55:ASN:ND2	1:A:101:GLY:HA2	2.32	0.40
1:B:268:LEU:HA	1:B:268:LEU:HD23	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:HIS:O	1:B:239:GLU:OE2[3_545]	2.02	0.18

## 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	403/411 (98%)	377 (94%)	16 (4%)	10 (2%)	6	3
1	B	403/411 (98%)	389 (96%)	11 (3%)	3 (1%)	24	23
All	All	806/822 (98%)	766 (95%)	27 (3%)	13 (2%)	11	8

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	92	ALA
1	A	121	ASP
1	A	122	ASN
1	A	127	THR
1	A	282	LYS
1	B	7	LEU
1	B	282	LYS
1	A	66	ALA
1	A	198	ASP
1	B	198	ASP
1	A	82	ALA
1	A	91	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	325/331 (98%)	277 (85%)	48 (15%)	3	2
1	B	325/331 (98%)	280 (86%)	45 (14%)	4	3
All	All	650/662 (98%)	557 (86%)	93 (14%)	3	3

All (93) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	10	LEU
1	A	14	LEU
1	A	20	ARG
1	A	24	LEU
1	A	48	LEU
1	A	54	ASP
1	A	58	MET
1	A	59	ASP
1	A	65	LEU
1	A	67	ASP
1	A	70	SER
1	A	72	GLN
1	A	79	LYS
1	A	87	HIS
1	A	89	GLU
1	A	106	GLU
1	A	109	GLU
1	A	119	GLN
1	A	122	ASN
1	A	131	ARG
1	A	138	ARG
1	A	139	ARG
1	A	144	SER
1	A	157	THR
1	A	182	LEU
1	A	188	GLU
1	A	196	LEU
1	A	207	LEU
1	A	222	ASN
1	A	223	LEU
1	A	227	ARG
1	A	233	LEU
1	A	239	GLU
1	A	250	SER
1	A	257	GLU
1	A	276	LEU
1	A	282	LYS
1	A	288	LYS
1	A	297	LEU
1	A	315	LEU
1	A	327	LEU
1	A	335	THR
1	A	340	LYS

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Mol	Chain	Res	Type
1	A	350	ARG
1	A	354	GLN
1	A	358	ASP
1	A	363	VAL
1	A	399	VAL
1	B	10	LEU
1	B	14	LEU
1	B	20	ARG
1	B	24	LEU
1	B	48	LEU
1	B	58	MET
1	B	64	ARG
1	B	70	SER
1	B	72	GLN
1	B	79	LYS
1	B	84	GLN
1	B	112	VAL
1	B	120	MET
1	B	121	ASP
1	B	124	VAL
1	B	125	ARG
1	B	131	ARG
1	B	137	ARG
1	B	138	ARG
1	B	139	ARG
1	B	144	SER
1	B	157	THR
1	B	182	LEU
1	B	188	GLU
1	B	196	LEU
1	B	207	LEU
1	B	222	ASN
1	B	223	LEU
1	B	227	ARG
1	B	233	LEU
1	B	239	GLU
1	B	257	GLU
1	B	276	LEU
1	B	282	LYS
1	B	288	LYS
1	B	297	LEU
1	B	315	LEU

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Mol	Chain	Res	Type
1	B	327	LEU
1	B	335	THR
1	B	340	LYS
1	B	350	ARG
1	B	354	GLN
1	B	358	ASP
1	B	363	VAL
1	B	399	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	87	HIS
1	A	119	GLN
1	A	122	ASN
1	A	194	GLN
1	A	210	HIS
1	A	222	ASN
1	A	243	GLN
1	A	300	ASN
1	A	313	GLN
1	A	368	HIS
1	B	87	HIS
1	B	135	ASN
1	B	194	GLN
1	B	210	HIS
1	B	222	ASN
1	B	243	GLN
1	B	300	ASN
1	B	313	GLN
1	B	331	GLN
1	B	368	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

29 ligands are modelled in this entry.

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	$\# Z  > 2$
2	GOL	A	505	-	5,5,5	0.57	0	5,5,5	0.50	0
2	GOL	A	506	-	5,5,5	0.48	0	5,5,5	0.51	0
2	GOL	A	508	-	5,5,5	0.45	0	5,5,5	0.52	0
2	GOL	A	510	-	5,5,5	0.36	0	5,5,5	0.46	0
2	GOL	A	511	-	5,5,5	0.42	0	5,5,5	0.48	0
2	GOL	A	516	-	5,5,5	0.39	0	5,5,5	0.48	0
2	GOL	A	517	-	5,5,5	0.47	0	5,5,5	0.44	0
2	GOL	A	518	-	5,5,5	0.47	0	5,5,5	0.52	0
2	GOL	A	519	-	5,5,5	0.35	0	5,5,5	0.42	0
2	GOL	A	522	-	5,5,5	0.48	0	5,5,5	0.56	0
2	GOL	A	523	-	5,5,5	0.45	0	5,5,5	0.50	0
2	GOL	A	526	-	5,5,5	0.41	0	5,5,5	0.43	0
2	GOL	A	527	-	5,5,5	0.46	0	5,5,5	0.53	0
2	GOL	B	501	-	5,5,5	0.53	0	5,5,5	0.56	0
2	GOL	B	502	-	5,5,5	0.35	0	5,5,5	0.39	0
2	GOL	B	503	-	5,5,5	0.45	0	5,5,5	0.50	0
2	GOL	B	504	-	5,5,5	0.28	0	5,5,5	0.49	0
2	GOL	B	507	-	5,5,5	0.31	0	5,5,5	0.50	0
2	GOL	B	509	-	5,5,5	0.45	0	5,5,5	0.45	0
2	GOL	B	512	-	5,5,5	0.32	0	5,5,5	0.52	0
2	GOL	B	513	-	5,5,5	0.39	0	5,5,5	0.46	0
2	GOL	B	514	-	5,5,5	0.48	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	B	515	-	5,5,5	0.41	0	5,5,5	0.45	0
2	GOL	B	520	-	5,5,5	0.37	0	5,5,5	0.50	0
2	GOL	B	521	-	5,5,5	0.41	0	5,5,5	0.50	0
2	GOL	B	524	-	5,5,5	0.38	0	5,5,5	0.50	0
2	GOL	B	525	-	5,5,5	0.35	0	5,5,5	0.45	0
2	GOL	B	528	-	5,5,5	0.48	0	5,5,5	0.52	0
2	GOL	B	529	-	5,5,5	0.48	0	5,5,5	0.53	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
2	GOL	A	505	-	-	0/4/4/4	0/0/0/0
2	GOL	A	506	-	-	0/4/4/4	0/0/0/0
2	GOL	A	508	-	-	0/4/4/4	0/0/0/0
2	GOL	A	510	-	-	0/4/4/4	0/0/0/0
2	GOL	A	511	-	-	0/4/4/4	0/0/0/0
2	GOL	A	516	-	-	0/4/4/4	0/0/0/0
2	GOL	A	517	-	-	0/4/4/4	0/0/0/0
2	GOL	A	518	-	-	0/4/4/4	0/0/0/0
2	GOL	A	519	-	-	0/4/4/4	0/0/0/0
2	GOL	A	522	-	-	0/4/4/4	0/0/0/0
2	GOL	A	523	-	-	0/4/4/4	0/0/0/0
2	GOL	A	526	-	-	0/4/4/4	0/0/0/0
2	GOL	A	527	-	-	0/4/4/4	0/0/0/0
2	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	GOL	B	502	-	-	0/4/4/4	0/0/0/0
2	GOL	B	503	-	-	0/4/4/4	0/0/0/0
2	GOL	B	504	-	-	0/4/4/4	0/0/0/0
2	GOL	B	507	-	-	0/4/4/4	0/0/0/0
2	GOL	B	509	-	-	0/4/4/4	0/0/0/0
2	GOL	B	512	-	-	0/4/4/4	0/0/0/0
2	GOL	B	513	-	-	0/4/4/4	0/0/0/0
2	GOL	B	514	-	-	0/4/4/4	0/0/0/0
2	GOL	B	515	-	-	0/4/4/4	0/0/0/0
2	GOL	B	520	-	-	0/4/4/4	0/0/0/0
2	GOL	B	521	-	-	0/4/4/4	0/0/0/0
2	GOL	B	524	-	-	0/4/4/4	0/0/0/0
2	GOL	B	525	-	-	0/4/4/4	0/0/0/0
2	GOL	B	528	-	-	0/4/4/4	0/0/0/0
2	GOL	B	529	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	516	GOL	2	0
2	A	517	GOL	2	0
2	A	526	GOL	1	0
2	B	501	GOL	3	0
2	B	502	GOL	1	0
2	B	504	GOL	1	0
2	B	509	GOL	3	0
2	B	512	GOL	1	0
2	B	514	GOL	1	0
2	B	515	GOL	1	0
2	B	525	GOL	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	405/411 (98%)	0.66	58 (14%) <b>2</b> <b>2</b>	26, 43, 89, 100	0
1	B	405/411 (98%)	0.03	7 (1%) 70 68	26, 41, 71, 86	0
All	All	810/822 (98%)	0.35	65 (8%) <b>12</b> <b>11</b>	26, 42, 81, 100	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	GLY	9.6
1	A	81	PHE	7.1
1	A	92	ALA	6.6
1	A	87	HIS	5.9
1	A	88	GLY	5.6
1	A	68	ILE	5.5
1	A	131	ARG	5.3
1	A	145	ALA	5.3
1	B	410	GLY	5.3
1	A	65	LEU	5.0
1	A	66	ALA	4.9
1	A	146	GLY	4.7
1	A	358	ASP	4.6
1	A	90	TRP	4.3
1	A	119	GLN	4.1
1	A	69	ALA	4.0
1	A	410	GLY	3.9
1	A	132	SER	3.9
1	B	199	GLY	3.8
1	A	91	PRO	3.8
1	A	75	PRO	3.7
1	A	86	TYR	3.6
1	A	89	GLU	3.3
1	A	93	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	82	ALA	3.2
1	A	76	VAL	3.2
1	A	360	GLU	3.2
1	A	198	ASP	3.2
1	A	94	THR	3.2
1	A	83	GLY	3.1
1	A	122	ASN	3.1
1	A	80	SER	3.0
1	B	359	GLY	3.0
1	A	109	GLU	2.9
1	A	334	ARG	2.8
1	A	121	ASP	2.8
1	B	198	ASP	2.8
1	A	79	LYS	2.8
1	A	84	GLN	2.8
1	A	100	TRP	2.8
1	A	195	PRO	2.7
1	A	120	MET	2.6
1	A	108	CYS	2.6
1	A	74	LEU	2.6
1	A	357	ALA	2.6
1	A	106	GLU	2.5
1	A	67	ASP	2.5
1	A	85	PRO	2.5
1	A	142	ASP	2.4
1	B	195	PRO	2.4
1	A	143	ILE	2.3
1	A	6	GLY	2.3
1	A	136	ILE	2.3
1	A	105	PRO	2.3
1	B	408	PHE	2.2
1	A	49	ASP	2.2
1	A	104	VAL	2.2
1	A	110	ALA	2.2
1	B	358	ASP	2.2
1	A	192	PRO	2.2
1	A	147	ALA	2.1
1	A	407	LEU	2.1
1	A	77	ALA	2.1
1	A	73	PRO	2.1
1	A	47	PRO	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	511	6/6	-0.26	0.50	93,99,100,100	0
2	GOL	B	514	6/6	0.43	0.35	48,76,80,80	0
2	GOL	A	510	6/6	0.46	0.36	82,85,89,89	0
2	GOL	B	503	6/6	0.59	0.34	59,82,86,89	0
2	GOL	B	524	6/6	0.60	0.35	87,90,91,91	0
2	GOL	A	526	6/6	0.61	0.29	79,84,87,87	0
2	GOL	B	520	6/6	0.67	0.23	78,87,87,87	0
2	GOL	B	521	6/6	0.69	0.28	67,75,78,84	0
2	GOL	B	525	6/6	0.71	0.53	92,95,96,97	0
2	GOL	A	505	6/6	0.71	0.24	44,57,61,65	0
2	GOL	B	528	6/6	0.72	0.19	53,60,64,66	0
2	GOL	A	506	6/6	0.72	0.18	55,60,67,67	0
2	GOL	A	518	6/6	0.74	0.44	85,90,92,92	0
2	GOL	B	504	6/6	0.77	0.23	64,66,69,73	0
2	GOL	A	516	6/6	0.79	0.28	72,87,89,89	0
2	GOL	A	527	6/6	0.80	0.51	65,71,73,75	0
2	GOL	A	522	6/6	0.80	0.32	64,74,77,77	0
2	GOL	B	509	6/6	0.80	0.24	44,57,62,64	0
2	GOL	B	529	6/6	0.80	0.17	53,59,64,64	0
2	GOL	A	517	6/6	0.81	0.23	70,73,73,74	0
2	GOL	B	512	6/6	0.81	0.29	75,83,88,88	0
2	GOL	A	508	6/6	0.82	0.14	50,68,71,75	0
2	GOL	B	513	6/6	0.85	0.16	71,78,78,80	0
2	GOL	B	515	6/6	0.87	0.27	75,79,79,81	0
2	GOL	B	501	6/6	0.88	0.15	39,51,59,70	0
2	GOL	B	507	6/6	0.91	0.23	42,58,61,61	0
2	GOL	A	523	6/6	0.91	0.16	61,61,63,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	519	6/6	0.91	0.16	44,61,70,76	0
2	GOL	B	502	6/6	0.93	0.16	44,59,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.