



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:15 AM GMT

PDB ID : 2NQN
Title : MoeA T100W
Authors : Nicolas, J.; Xiang, S.; Schindelin, H.; Rajagopalan, K.V.
Deposited on : 2006-10-31
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

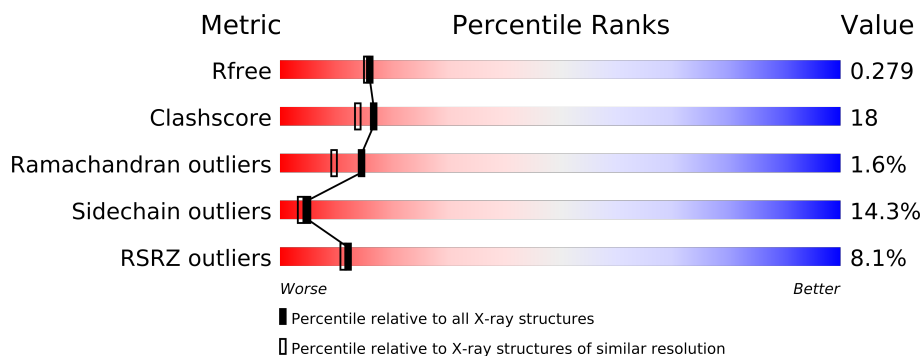
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	411	
1	B	411	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	505	-	X
2	GOL	A	510	-	X
2	GOL	A	511	-	X
2	GOL	A	517	-	X
2	GOL	A	522	-	X
2	GOL	A	523	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	527	-	X
2	GOL	B	503	-	X
2	GOL	B	504	-	X
2	GOL	B	509	-	X
2	GOL	B	512	-	X
2	GOL	B	514	-	X
2	GOL	B	515	-	X
2	GOL	B	520	-	X
2	GOL	B	524	-	X
2	GOL	B	525	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6758 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

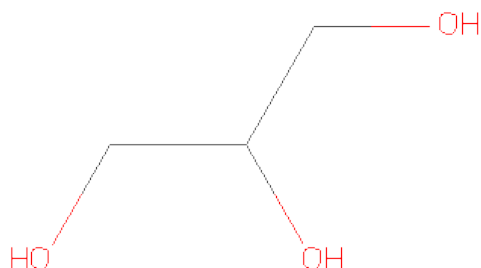
- Molecule 1 is a protein called Molybdopterin biosynthesis protein moeA.

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: C₃H₈O₃).



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

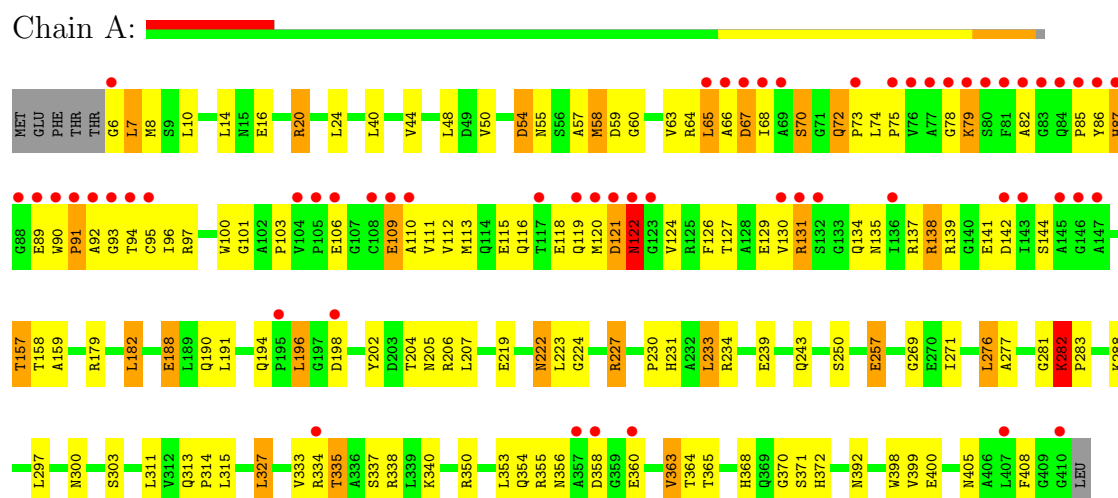
- Molecule 3 is water.

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

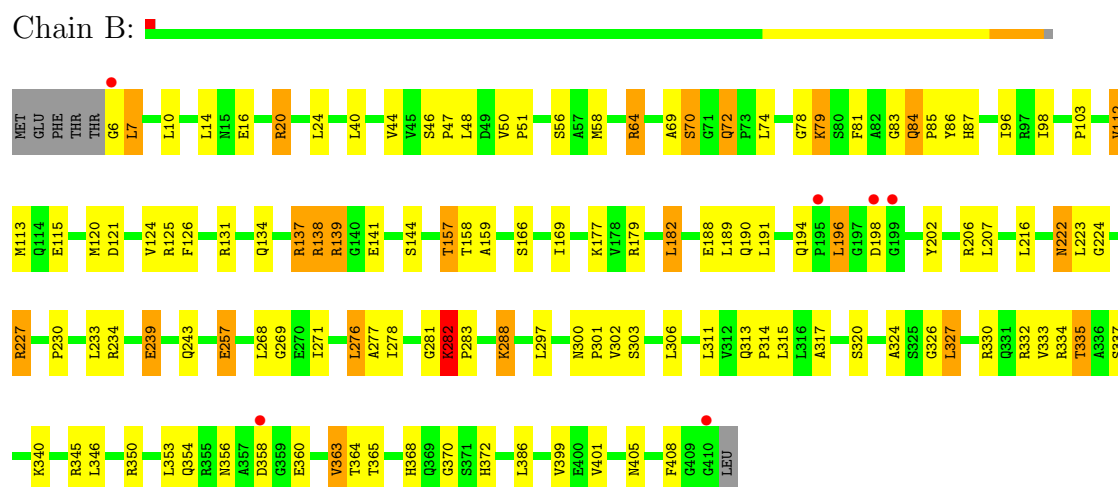
3 Residue-property plots

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: 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.225 , 0.274 0.230 , 0.279	Depositor DCC
R_{free} test set	2786 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 54368 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6758	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	258	0	0	13	0
All	All	6758	0	6324	226	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (226) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:B:222:ASN:HD22	1:B:224:GLY:H	1.36	0.73
1:A:313:GLN:HE22	1:A:405:ASN:HD21	1.33	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:B:353:LEU:CD1	1:B:363:VAL:HG13	2.23	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:222:ASN:HD22	1:A:224:GLY:H	1.40	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
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:137:ARG:HG2	1:A:141:GLU:OE2	2.02	0.60
1:A:115:GLU:N	1:A:115:GLU:CD	2.55	0.60
1:A:188:GLU:HB3	1:B:83:GLY:HA2	1.83	0.60
1:B:281:GLY:O	1:B:282:LYS:HB2	2.02	0.60
1:B:115:GLU:H	1:B:115:GLU:CD	2.05	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:B:353:LEU:HD13	1:B:363:VAL:CG1	2.38	0.52
1:A:311:LEU:C	1:A:314:PRO:HD2	2.30	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:B:311:LEU:C	1:B:314:PRO:HD2	2.29	0.52
1:A:230:PRO:O	1:A:234:ARG:HG3	2.09	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:B:313:GLN:HE22	1:B:405:ASN:ND2	2.06	0.50
1:A:314:PRO:HG3	1:A:327:LEU:CD1	2.42	0.50
1:A:222:ASN:HD22	1:A:222:ASN:C	2.16	0.50
1:A:57:ALA:O	1:A:58:MET:HB3	2.11	0.49
1:B:179:ARG:NH1	1:B:243:GLN:O	2.45	0.49
1:B:74:LEU:HD12	1:B:126:PHE:CE1	2.46	0.49
1:A:334:ARG:HG2	1:A:334:ARG:HH11	1.78	0.49
1:B:356:ASN:ND2	1:B:360:GLU:HB3	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:326:GLY:HA3	2:B:509:GOL:H11	1.95	0.49
1:B:85:PRO:HG2	1:B:87:HIS:CE1	2.46	0.49
1:B:314:PRO:HG3	1:B:327:LEU:CD1	2.42	0.49
1:B:206:ARG:HD2	1:B:222:ASN:HD21	1.77	0.49
1:B:78:GLY:HA3	1:B:86:TYR:CE2	2.46	0.49
1:A:60:GLY:HA3	1:A:112:VAL:O	2.13	0.49
1:B:320:SER:HB2	2:B:501:GOL:H2	1.93	0.49
1:A:40:LEU:HD11	1:A:44:VAL:HG23	1.94	0.49
1:A:400:GLU:HG2	2:A:516:GOL:C1	2.42	0.49
1:A:85:PRO:HB3	1:A:103:PRO:CG	2.43	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:HH11	1:B:334:ARG:HG2	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:HG2	1:A:138:ARG:H	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:B:190:GLN:HG3	1:B:194:GLN:NE2	2.17	0.45
1:A:110:ALA:HB1	1:A:134:GLN:HG2	1.99	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	Distance(Å)	Clash(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:B:86:TYR:CD1	1:B:96:ILE:HD13	2.52	0.44
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:A:78:GLY:HA3	1:A:86:TYR:CE1	2.52	0.44
1:B:368:HIS:CD2	1:B:370:GLY:N	2.72	0.44
1:A:257:GLU:HB2	3:A:553:HOH:O	2.18	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:118:GLU:HG3	3:A:612:HOH:O	2.17	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:72:GLN:HG2	1:A:73:PRO:N	2.33	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: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:6:GLY:O	1:B:7:LEU:CB	2.54	0.42
1:B:46:SER:HA	1:B:47:PRO:HD3	1.92	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:B:363:VAL:HG11	1:B:401:VAL:HG21	2.02	0.42
1:A:338:ARG:CZ	3:A:620:HOH:O	2.67	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:334:ARG:NH1	1:A:334:ARG:CG	2.83	0.41
2:B:512:GOL:H2	3:B:589:HOH:O	2.19	0.41
1:A:364:THR:HG22	1:A:365:THR:O	2.20	0.41
1:A:269:GLY:C	1:A:271:ILE:HD12	2.40	0.41
1:A:281:GLY:O	1:A:282:LYS:CB	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:368:HIS:CD2	1:A:372:HIS:HE1	2.38	0.41
1:A:196:LEU:HD13	1:A:202:TYR:CZ	2.55	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:85:PRO:HG2	1:A:87:HIS:CE1	2.56	0.40
1:A:271:ILE:HD12	1:A:271:ILE:N	2.36	0.40
1:A:68:ILE:HD12	1:A:68:ILE:HA	1.88	0.40
1:B:333:VAL:HG12	1:B:334:ARG:N	2.36	0.40
1:B:134:GLN:HA	2:B:515:GOL:H2	2.03	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:B:368:HIS:CD2	1:B:372:HIS:HE1	2.39	0.40
1:A:65:LEU:HD13	1:A:65:LEU:C	2.42	0.40
1:B:79:LYS:O	1:B:86:TYR:HB2	2.21	0.40
1:B:334:ARG:CG	1:B:334:ARG:HH11	2.33	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	Distance(Å)	Clash(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%)	9	4
1	B	403/411 (98%)	389 (96%)	11 (3%)	3 (1%)	30	28
All	All	806/822 (98%)	766 (95%)	27 (3%)	13 (2%)	14	9

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%)	4	3
1	B	325/331 (98%)	280 (86%)	45 (14%)	5	4
All	All	650/662 (98%)	557 (86%)	93 (14%)	5	4

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

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Mol	Chain	Res	Type
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
1	A	350	ARG
1	A	354	GLN
1	A	358	ASP

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Mol	Chain	Res	Type
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
1	B	327	LEU
1	B	335	THR
1	B	340	LYS

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Mol	Chain	Res	Type
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 chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.49	0	5,5,5	0.56	0
2	GOL	A	506	-	5,5,5	0.42	0	5,5,5	0.56	0
2	GOL	A	508	-	5,5,5	0.39	0	5,5,5	0.58	0
2	GOL	A	510	-	5,5,5	0.33	0	5,5,5	0.50	0
2	GOL	A	511	-	5,5,5	0.37	0	5,5,5	0.53	0
2	GOL	A	516	-	5,5,5	0.34	0	5,5,5	0.53	0
2	GOL	A	517	-	5,5,5	0.44	0	5,5,5	0.48	0
2	GOL	A	518	-	5,5,5	0.41	0	5,5,5	0.60	0
2	GOL	A	519	-	5,5,5	0.32	0	5,5,5	0.46	0
2	GOL	A	522	-	5,5,5	0.42	0	5,5,5	0.61	0
2	GOL	A	523	-	5,5,5	0.40	0	5,5,5	0.55	0
2	GOL	A	526	-	5,5,5	0.36	0	5,5,5	0.48	0
2	GOL	A	527	-	5,5,5	0.41	0	5,5,5	0.59	0
2	GOL	B	501	-	5,5,5	0.48	0	5,5,5	0.61	0
2	GOL	B	502	-	5,5,5	0.30	0	5,5,5	0.44	0
2	GOL	B	503	-	5,5,5	0.39	0	5,5,5	0.54	0
2	GOL	B	504	-	5,5,5	0.28	0	5,5,5	0.53	0
2	GOL	B	507	-	5,5,5	0.27	0	5,5,5	0.54	0
2	GOL	B	509	-	5,5,5	0.41	0	5,5,5	0.51	0
2	GOL	B	512	-	5,5,5	0.30	0	5,5,5	0.56	0
2	GOL	B	513	-	5,5,5	0.34	0	5,5,5	0.52	0
2	GOL	B	514	-	5,5,5	0.41	0	5,5,5	0.53	0
2	GOL	B	515	-	5,5,5	0.36	0	5,5,5	0.52	0
2	GOL	B	520	-	5,5,5	0.33	0	5,5,5	0.54	0
2	GOL	B	521	-	5,5,5	0.36	0	5,5,5	0.55	0
2	GOL	B	524	-	5,5,5	0.35	0	5,5,5	0.54	0
2	GOL	B	525	-	5,5,5	0.31	0	5,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	528	-	5,5,5	0.41	0	5,5,5	0.57	0
2	GOL	B	529	-	5,5,5	0.43	0	5,5,5	0.58	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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	405/411 (98%)	0.69	57 (14%) 3 3	26, 43, 89, 100	0
1	B	405/411 (98%)	0.05	6 (1%) 70 71	26, 41, 71, 86	0
All	All	810/822 (98%)	0.37	63 (7%) 12 12	26, 42, 81, 100	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	GLY	9.4
1	A	92	ALA	7.5
1	A	81	PHE	6.7
1	A	88	GLY	6.7
1	B	199	GLY	6.0
1	A	65	LEU	5.6
1	A	66	ALA	5.3
1	A	122	ASN	5.0
1	A	358	ASP	5.0
1	A	87	HIS	4.9
1	A	76	VAL	4.8
1	A	89	GLU	4.7
1	A	68	ILE	4.7
1	A	90	TRP	4.5
1	B	410	GLY	4.3
1	A	146	GLY	4.2
1	A	75	PRO	4.1
1	A	145	ALA	4.1
1	A	83	GLY	4.0
1	A	131	ARG	3.9
1	A	106	GLU	3.9
1	A	360	GLU	3.8
1	A	69	ALA	3.8
1	A	132	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	86	TYR	3.7
1	A	77	ALA	3.6
1	A	143	ILE	3.6
1	A	91	PRO	3.6
1	A	410	GLY	3.5
1	A	357	ALA	3.3
1	A	82	ALA	3.2
1	B	195	PRO	3.2
1	A	198	ASP	3.1
1	A	78	GLY	3.1
1	A	104	VAL	3.1
1	A	93	GLY	3.0
1	B	198	ASP	3.0
1	A	80	SER	3.0
1	A	95	CYS	2.9
1	A	334	ARG	2.8
1	A	105	PRO	2.8
1	A	136	ILE	2.8
1	A	119	GLN	2.8
1	A	121	ASP	2.8
1	A	109	GLU	2.8
1	A	94	THR	2.8
1	A	79	LYS	2.7
1	A	142	ASP	2.4
1	A	108	CYS	2.4
1	A	84	GLN	2.3
1	A	73	PRO	2.2
1	A	407	LEU	2.2
1	A	120	MET	2.2
1	A	85	PRO	2.2
1	A	195	PRO	2.2
1	A	6	GLY	2.1
1	A	117	THR	2.1
1	A	110	ALA	2.1
1	A	67	ASP	2.1
1	B	6	GLY	2.1
1	A	130	VAL	2.0
1	A	147	ALA	2.0
1	B	358	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	A	522	6/6	0.37	14.56	64,74,77,77	0
2	GOL	B	525	6/6	0.66	14.23	92,95,96,97	0
2	GOL	B	514	6/6	0.41	13.87	48,76,80,80	0
2	GOL	B	524	6/6	0.38	7.40	87,90,91,91	0
2	GOL	B	503	6/6	0.29	6.77	59,82,86,89	0
2	GOL	A	510	6/6	0.42	5.87	82,85,89,89	0
2	GOL	A	527	6/6	0.44	4.95	65,71,73,75	0
2	GOL	B	520	6/6	0.30	4.25	78,87,87,87	0
2	GOL	A	511	6/6	0.41	4.00	93,99,100,100	0
2	GOL	A	517	6/6	0.21	3.49	70,73,73,74	0
2	GOL	B	509	6/6	0.28	3.45	44,57,62,64	0
2	GOL	B	515	6/6	0.32	3.31	75,79,79,81	0
2	GOL	B	504	6/6	0.26	3.00	64,66,69,73	0
2	GOL	B	512	6/6	0.23	2.41	75,83,88,88	0
2	GOL	A	505	6/6	0.23	2.21	44,57,61,65	0
2	GOL	A	523	6/6	0.16	2.11	61,61,63,67	0
2	GOL	B	501	6/6	0.16	1.92	39,51,59,70	0
2	GOL	A	516	6/6	0.25	1.86	72,87,89,89	0
2	GOL	A	526	6/6	0.27	1.31	79,84,87,87	0
2	GOL	B	521	6/6	0.24	0.99	67,75,78,84	0
2	GOL	A	506	6/6	0.16	0.58	55,60,67,67	0
2	GOL	B	528	6/6	0.19	0.47	53,60,64,66	0
2	GOL	B	507	6/6	0.20	0.43	42,58,61,61	0
2	GOL	A	519	6/6	0.15	0.41	44,61,70,76	0
2	GOL	B	529	6/6	0.17	0.35	53,59,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	B	502	6/6	0.15	0.08	44,59,64,64	0
2	GOL	B	513	6/6	0.12	-0.09	71,78,78,80	0
2	GOL	A	508	6/6	0.13	-1.00	50,68,71,75	0
2	GOL	A	518	6/6	0.46	-	85,90,92,92	0

6.5 Other polymers ⓘ

There are no such residues in this entry.