Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:39 AM GMT

PDB ID	:	2NQS
Title	:	MoeA E188A
Authors	:	Nicolas, J.; Xiang, S.; Schindelin, H.; Rajagopalan, K.V.
Deposited on	:	2006-10-31
Resolution	:	2.50 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

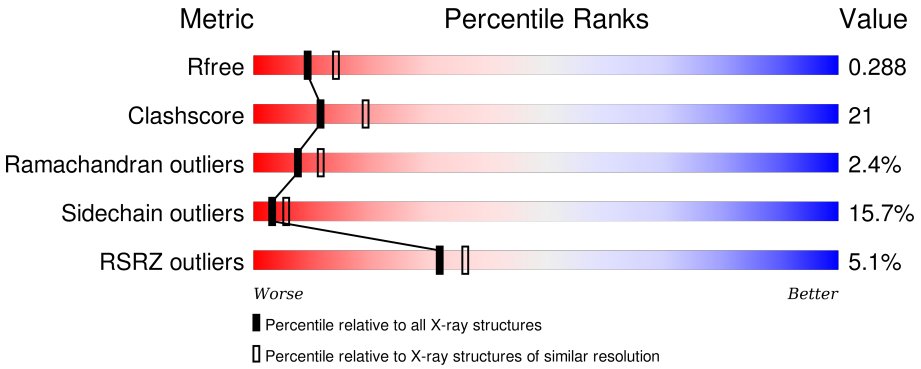
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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 <=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	9% 59% 31% 7% •
1	B	411	% 60% 31% 7% •

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	905	-	-	-	X
2	GOL	A	906	-	-	-	X
2	GOL	A	908	-	-	-	X
2	GOL	A	910	-	-	-	X
2	GOL	B	901	-	-	-	X
2	GOL	B	907	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6371 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.

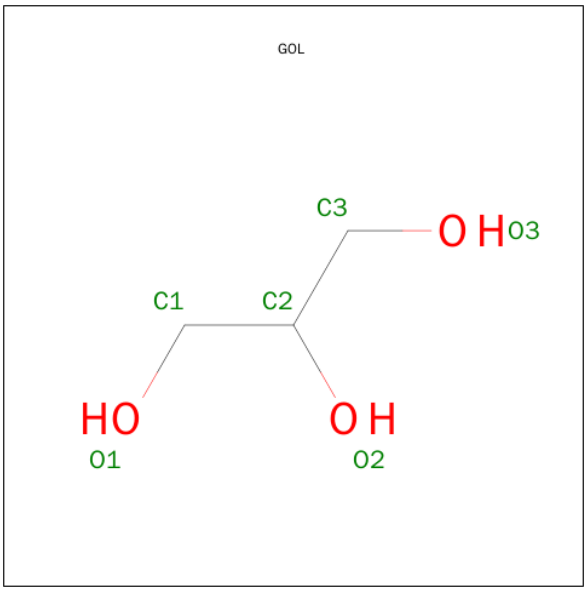
- Molecule 1 is a protein called Molybdopterin biosynthesis protein moeA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3036	1916	531	576	13			
1	B	403	Total	C	N	O	S	0	0	0
			3036	1916	531	576	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	ALA	GLU	ENGINEERED	UNP P12281
B	188	ALA	GLU	ENGINEERED	UNP P12281

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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	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	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		

- Molecule 3 is water.

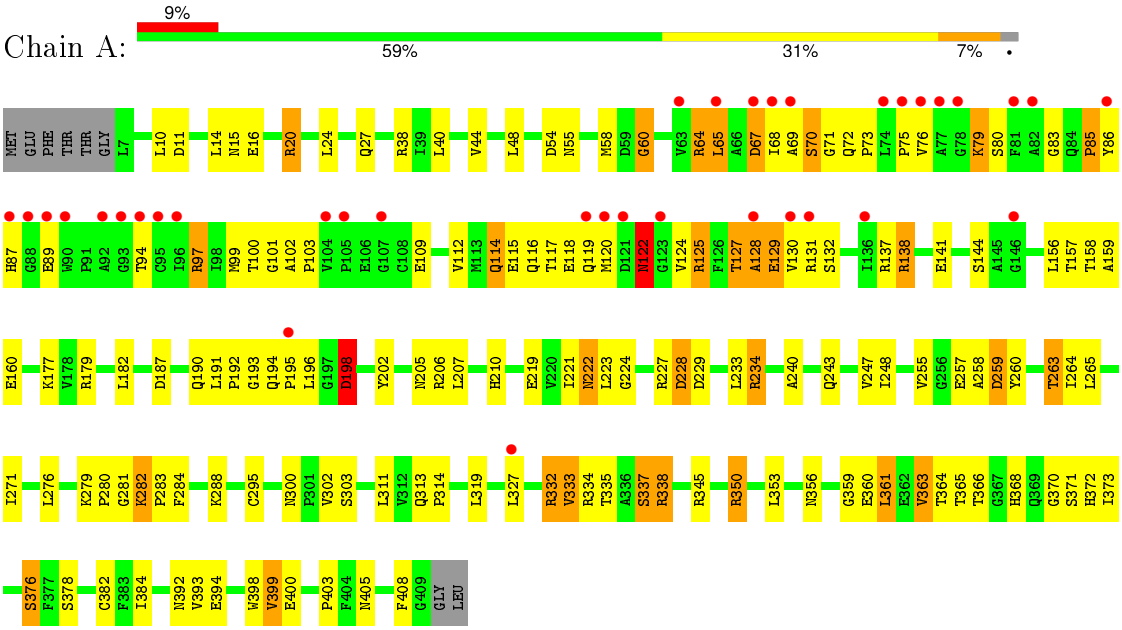
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	137	Total	O	0	0
			137	137		

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 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.

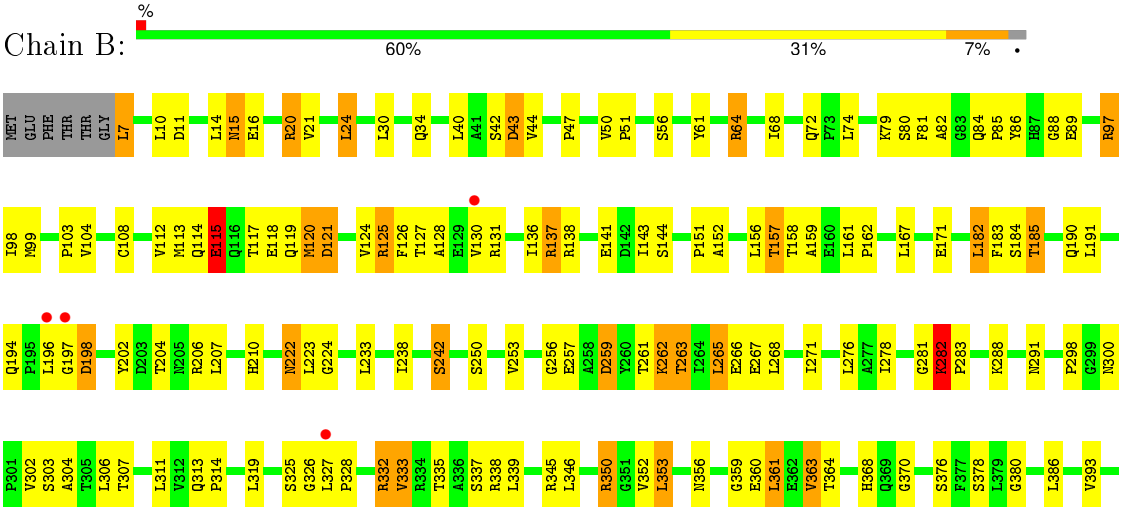
- Molecule 1: Molybdopterin biosynthesis protein moeA

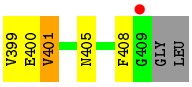
Chain A:



- Molecule 1: Molybdopterin biosynthesis protein moeA

Chain B:




V399
E400
V401
N405
F408
G409
GLY
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.43Å 98.19Å 161.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.50 49.09 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.39-2.50) 98.1 (49.09-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.225 , 0.293 0.220 , 0.288	Depositor DCC
R_{free} test set	1884 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	48.7	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 37250 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6371	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.38	0/3095	0.64	0/4207
1	B	0.39	0/3095	0.64	0/4207
All	All	0.38	0/6190	0.64	0/8414

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3036	0	3036	123	0
1	B	3036	0	3036	133	0
2	A	36	0	48	2	0
2	B	24	0	32	3	0
3	A	102	0	0	10	0
3	B	137	0	0	4	0
All	All	6371	0	6152	252	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 21.

All (252) 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:327:LEU:HD12	1:B:328:PRO:HD2	1.36	1.05
1:B:157:THR:HG22	1:B:159:ALA:H	1.18	1.02
1:A:157:THR:HG22	1:A:159:ALA:H	1.31	0.94
1:B:368:HIS:HD2	1:B:370:GLY:H	0.98	0.94
1:B:300:ASN:HD22	1:B:303:SER:H	1.15	0.91
1:B:368:HIS:CD2	1:B:370:GLY:H	1.89	0.90
1:B:119:GLN:HE21	1:B:120:MET:H	1.17	0.90
1:A:368:HIS:HD2	1:A:370:GLY:H	1.21	0.87
1:B:265:LEU:HD22	1:B:271:ILE:HG13	1.61	0.82
1:B:378:SER:O	2:B:902:GOL:H31	1.80	0.82
1:B:119:GLN:NE2	1:B:120:MET:H	1.78	0.80
1:B:368:HIS:HD2	1:B:370:GLY:N	1.78	0.79
1:A:138:ARG:O	1:A:141:GLU:HB2	1.83	0.79
1:A:85:PRO:HB3	1:A:103:PRO:HG2	1.65	0.78
1:B:104:VAL:HG13	1:B:108:CYS:HB3	1.66	0.77
1:B:222:ASN:HD22	1:B:224:GLY:H	1.30	0.76
1:A:265:LEU:HD22	1:A:271:ILE:HG13	1.66	0.75
1:B:380:GLY:O	2:B:902:GOL:H32	1.87	0.75
1:B:137:ARG:HD2	3:B:977:HOH:O	1.87	0.75
1:B:222:ASN:ND2	1:B:224:GLY:H	1.85	0.74
1:B:325:SER:HB3	3:B:931:HOH:O	1.87	0.74
1:A:55:ASN:HD22	1:A:101:GLY:HA2	1.52	0.74
1:A:194:GLN:HB2	1:A:195:PRO:HD2	1.70	0.73
1:A:60:GLY:HA3	1:A:112:VAL:O	1.89	0.72
1:B:74:LEU:H	1:B:124:VAL:H	1.37	0.72
1:B:113:MET:HG3	1:B:115:GLU:HG2	1.73	0.71
1:B:278:ILE:O	1:B:345:ARG:HD2	1.91	0.70
1:A:313:GLN:HE22	1:A:405:ASN:HD21	1.39	0.70
1:B:313:GLN:HB3	1:B:314:PRO:HD3	1.72	0.70
1:A:394:GLU:HB3	3:A:973:HOH:O	1.92	0.69
1:B:157:THR:CG2	1:B:158:THR:N	2.57	0.68
1:B:157:THR:HG23	1:B:158:THR:N	2.07	0.68
1:B:97:ARG:HH12	1:B:99:MET:HE1	1.58	0.68
1:B:335:THR:HG22	1:B:337:SER:H	1.58	0.68
1:B:7:LEU:N	3:B:944:HOH:O	2.25	0.68
1:B:356:ASN:HD21	1:B:360:GLU:HB2	1.58	0.68
1:A:234:ARG:HH11	1:A:234:ARG:HB3	1.58	0.68
1:A:157:THR:CG2	1:A:158:THR:N	2.57	0.67
1:B:97:ARG:HH12	1:B:99:MET:CE	2.08	0.67
1:A:313:GLN:HB3	1:A:314:PRO:HD3	1.75	0.67
1:B:80:SER:HB3	1:B:98:ILE:HG13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:THR:CG2	1:B:159:ALA:H	2.03	0.66
1:B:85:PRO:HB3	1:B:103:PRO:HG2	1.78	0.66
1:B:307:THR:HG23	1:B:311:LEU:HD12	1.77	0.65
1:B:263:THR:O	1:B:267:GLU:HG2	1.97	0.65
1:A:206:ARG:HH11	1:A:222:ASN:HD21	1.44	0.65
1:A:55:ASN:ND2	1:A:101:GLY:HA2	2.11	0.64
1:A:350:ARG:HD2	1:A:376:SER:HB2	1.78	0.64
1:B:350:ARG:HD2	1:B:376:SER:OG	1.98	0.64
1:B:157:THR:HG23	1:B:158:THR:H	1.62	0.64
1:A:279:LYS:HD2	1:A:345:ARG:NH2	2.13	0.64
1:A:282:LYS:HB3	1:A:283:PRO:HD3	1.79	0.64
1:B:81:PHE:HD2	1:B:99:MET:HG3	1.63	0.63
1:A:222:ASN:HD22	1:A:224:GLY:H	1.43	0.63
1:B:313:GLN:HE22	1:B:405:ASN:HD21	1.45	0.63
1:A:335:THR:HG22	1:A:337:SER:H	1.64	0.63
1:B:81:PHE:HB2	1:B:84:GLN:HB3	1.81	0.63
1:B:300:ASN:ND2	1:B:303:SER:H	1.91	0.63
1:A:69:ALA:HA	3:A:979:HOH:O	1.98	0.62
1:B:256:GLY:O	1:B:262:LYS:HE2	2.00	0.62
1:A:72:GLN:HB3	1:A:73:PRO:HD2	1.83	0.61
1:B:333:VAL:CG1	1:B:363:VAL:HG22	2.30	0.61
1:B:184:SER:HB3	1:B:250:SER:OG	2.01	0.61
1:B:56:SER:HB2	1:B:98:ILE:HD13	1.83	0.61
1:A:300:ASN:HD21	1:A:371:SER:HB2	1.66	0.61
1:B:356:ASN:OD1	1:B:359:GLY:N	2.35	0.60
1:B:202:TYR:O	1:B:204:THR:HG23	2.01	0.60
1:A:300:ASN:ND2	1:A:371:SER:HB2	2.16	0.60
1:B:327:LEU:HD12	1:B:328:PRO:CD	2.23	0.60
1:B:353:LEU:CD1	1:B:363:VAL:HG13	2.32	0.60
1:B:206:ARG:HH11	1:B:222:ASN:HD21	1.49	0.59
1:B:222:ASN:HD22	1:B:222:ASN:C	2.06	0.59
1:A:120:MET:HB2	1:A:122:ASN:ND2	2.17	0.59
1:A:221:ILE:HG21	1:A:243:GLN:HE21	1.67	0.58
1:A:187:ASP:OD2	1:A:228:ASP:HB2	2.03	0.58
1:B:114:GLN:O	1:B:117:THR:HB	2.04	0.58
1:A:205:ASN:HB2	3:A:943:HOH:O	2.03	0.58
1:A:70:SER:OG	1:A:72:GLN:HB2	2.03	0.58
1:B:74:LEU:N	1:B:124:VAL:H	2.02	0.58
1:B:185:THR:CG2	1:B:253:VAL:HG23	2.33	0.57
1:B:259:ASP:OD1	1:B:261:THR:N	2.33	0.57
1:B:81:PHE:CD2	1:B:99:MET:HG3	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ILE:HG21	1:A:243:GLN:NE2	2.19	0.56
1:A:353:LEU:HD13	1:A:363:VAL:HG13	1.87	0.56
1:A:38:ARG:HD2	3:A:937:HOH:O	2.05	0.56
1:A:300:ASN:HB3	1:A:303:SER:HB2	1.86	0.56
1:B:300:ASN:HD21	1:B:302:VAL:HB	1.69	0.56
1:A:378:SER:O	2:A:905:GOL:H12	2.06	0.56
1:A:120:MET:CB	1:A:122:ASN:HD21	2.19	0.55
1:B:119:GLN:O	1:B:120:MET:SD	2.64	0.55
1:A:177:LYS:HE2	3:A:950:HOH:O	2.06	0.55
3:A:1005:HOH:O	1:B:34:GLN:HG2	2.05	0.55
1:A:157:THR:HG22	1:A:158:THR:N	2.21	0.55
1:B:104:VAL:CG1	1:B:108:CYS:HB3	2.34	0.55
1:B:182:LEU:HD22	1:B:206:ARG:HG3	1.88	0.55
1:A:384:ILE:HG23	1:A:399:VAL:HG11	1.89	0.54
1:A:368:HIS:CD2	1:A:370:GLY:H	2.13	0.54
1:A:282:LYS:HB3	1:A:283:PRO:CD	2.37	0.54
1:A:353:LEU:HG	1:A:361:LEU:HG	1.88	0.54
1:A:260:TYR:HA	1:A:263:THR:HG23	1.90	0.54
1:B:61:TYR:HE1	1:B:117:THR:HG21	1.73	0.54
1:B:121:ASP:HA	3:B:953:HOH:O	2.08	0.53
1:B:42:SER:HA	1:B:152:ALA:HB2	1.90	0.53
1:B:196:LEU:HD22	1:B:202:TYR:CE1	2.44	0.53
1:A:119:GLN:HG3	1:A:124:VAL:HG13	1.91	0.53
1:B:157:THR:HG22	1:B:159:ALA:N	2.04	0.53
1:A:190:GLN:NE2	1:A:194:GLN:HE21	2.07	0.53
1:A:120:MET:HB2	1:A:122:ASN:HD21	1.74	0.53
1:A:128:ALA:O	1:A:129:GLU:C	2.47	0.52
1:A:80:SER:HB2	1:A:86:TYR:HB2	1.90	0.52
1:B:337:SER:OG	1:B:364:THR:HG23	2.08	0.52
1:B:353:LEU:HD11	1:B:401:VAL:HG11	1.92	0.52
1:A:157:THR:HG21	1:B:408:PHE:C	2.29	0.52
1:B:210:HIS:HD2	1:B:222:ASN:OD1	1.93	0.52
1:B:185:THR:HG21	1:B:253:VAL:HG23	1.91	0.52
1:B:74:LEU:HD12	1:B:126:PHE:CE1	2.45	0.52
1:A:157:THR:CG2	1:B:408:PHE:HA	2.39	0.52
1:A:157:THR:HG21	1:B:408:PHE:HA	1.92	0.52
1:B:352:VAL:HG22	1:B:380:GLY:HA2	1.91	0.52
1:A:280:PRO:HG3	1:A:302:VAL:HG12	1.91	0.51
1:B:104:VAL:HG13	1:B:108:CYS:CB	2.38	0.51
1:A:54:ASP:HA	1:A:137:ARG:O	2.11	0.51
1:A:314:PRO:HG3	1:A:327:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:HG23	1:A:158:THR:H	1.76	0.51
1:B:313:GLN:HE22	1:B:405:ASN:ND2	2.08	0.51
1:A:222:ASN:ND2	1:A:224:GLY:H	2.08	0.51
1:B:138:ARG:HG2	1:B:138:ARG:HH11	1.75	0.50
1:A:258:ALA:O	1:A:259:ASP:HB3	2.11	0.50
1:B:117:THR:HG23	1:B:124:VAL:HG13	1.94	0.50
1:B:138:ARG:N	1:B:141:GLU:OE2	2.43	0.49
1:A:350:ARG:O	1:A:366:THR:HG23	2.13	0.49
1:A:234:ARG:HH11	1:A:234:ARG:CB	2.25	0.49
1:A:384:ILE:HG23	1:A:399:VAL:CG1	2.43	0.49
1:B:182:LEU:HD21	1:B:250:SER:HB3	1.94	0.48
1:A:40:LEU:CD1	1:A:44:VAL:HG23	2.44	0.48
1:B:47:PRO:HD2	1:B:167:LEU:HB3	1.94	0.48
1:A:408:PHE:C	1:B:157:THR:HG21	2.34	0.48
1:B:368:HIS:CD2	1:B:370:GLY:N	2.66	0.48
1:B:61:TYR:CE2	1:B:97:ARG:HD2	2.49	0.48
1:B:86:TYR:CZ	1:B:88:GLY:HA3	2.48	0.48
1:B:262:LYS:O	1:B:266:GLU:HG3	2.13	0.48
1:B:291:ASN:O	2:B:907:GOL:H31	2.13	0.48
1:B:74:LEU:HD12	1:B:126:PHE:HE1	1.79	0.48
1:B:332:ARG:HD2	1:B:400:GLU:OE1	2.14	0.48
1:B:353:LEU:HD13	1:B:363:VAL:HG13	1.96	0.48
1:B:353:LEU:HD12	1:B:363:VAL:HG13	1.96	0.48
1:A:338:ARG:HD3	1:A:393:VAL:O	2.15	0.47
1:A:311:LEU:C	1:A:314:PRO:HD2	2.34	0.47
1:B:327:LEU:CD1	1:B:328:PRO:HD2	2.26	0.47
1:A:333:VAL:CG1	1:A:363:VAL:HG22	2.44	0.47
1:A:194:GLN:CB	1:A:195:PRO:HD2	2.42	0.47
1:B:333:VAL:HG22	1:B:361:LEU:O	2.14	0.47
1:A:364:THR:HG22	1:A:365:THR:O	2.14	0.47
1:B:115:GLU:H	1:B:115:GLU:CD	2.13	0.47
1:B:333:VAL:HG11	1:B:363:VAL:HG22	1.96	0.47
1:A:333:VAL:HG12	1:A:363:VAL:HG22	1.96	0.47
1:A:210:HIS:HD2	1:A:222:ASN:OD1	1.98	0.47
2:A:906:GOL:H12	3:A:936:HOH:O	2.15	0.47
1:A:137:ARG:HD3	3:A:916:HOH:O	2.14	0.46
1:A:65:LEU:HB2	1:A:109:GLU:OE2	2.15	0.46
1:A:157:THR:HB	1:A:160:GLU:OE2	2.16	0.46
1:B:61:TYR:CE1	1:B:117:THR:HG21	2.49	0.46
1:A:368:HIS:HD2	1:A:370:GLY:N	2.02	0.46
1:A:219:GLU:HG3	3:A:963:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:HD2	1:A:222:ASN:HD21	1.81	0.46
1:B:40:LEU:HG	1:B:156:LEU:HD21	1.98	0.46
1:B:307:THR:O	1:B:311:LEU:HB2	2.16	0.46
1:B:61:TYR:HE2	1:B:97:ARG:HD2	1.81	0.45
1:A:70:SER:O	1:A:72:GLN:N	2.49	0.45
1:A:382:CYS:CB	1:A:403:PRO:HA	2.47	0.45
1:B:11:ASP:O	1:B:15:ASN:HB2	2.16	0.45
1:B:206:ARG:NH1	1:B:224:GLY:HA2	2.32	0.45
1:A:72:GLN:CB	1:A:73:PRO:HD2	2.46	0.45
1:B:50:VAL:HB	1:B:143:ILE:HB	1.98	0.45
1:B:183:PHE:C	1:B:183:PHE:CD1	2.89	0.45
1:A:281:GLY:O	1:A:282:LYS:HB2	2.16	0.45
1:A:99:MET:O	1:A:102:ALA:CB	2.65	0.45
1:B:43:ASP:OD1	1:B:151:PRO:HA	2.16	0.45
1:B:196:LEU:HA	1:B:196:LEU:HD12	1.74	0.44
1:A:313:GLN:HE22	1:A:405:ASN:ND2	2.10	0.44
1:A:127:THR:HB	1:A:128:ALA:H	1.65	0.44
1:A:332:ARG:HG3	1:A:400:GLU:OE1	2.17	0.44
1:B:339:LEU:HB2	1:B:393:VAL:HB	1.99	0.44
1:A:191:LEU:O	1:A:193:GLY:N	2.51	0.44
1:A:114:GLN:OE1	1:A:115:GLU:HG3	2.17	0.44
1:B:127:THR:OG1	1:B:128:ALA:N	2.50	0.44
1:B:196:LEU:HD22	1:B:202:TYR:CZ	2.52	0.44
1:B:283:PRO:HG2	1:B:298:PRO:HB3	1.98	0.44
1:A:64:ARG:HB2	1:A:67:ASP:OD1	2.18	0.44
1:A:260:TYR:HD1	1:A:264:ILE:HD12	1.82	0.44
1:B:21:VAL:HG11	1:B:319:LEU:HG	2.00	0.44
1:B:191:LEU:O	1:B:194:GLN:HB2	2.18	0.44
1:B:119:GLN:HE21	1:B:120:MET:N	2.00	0.44
1:A:72:GLN:HB3	1:A:73:PRO:CD	2.46	0.43
1:A:350:ARG:C	1:A:366:THR:HG23	2.39	0.43
1:B:16:GLU:OE2	1:B:20:ARG:NE	2.49	0.43
1:A:248:ILE:HG12	1:A:295:CYS:HB2	2.01	0.43
1:A:372:HIS:O	1:A:373:ILE:HG23	2.18	0.43
1:B:307:THR:CG2	1:B:311:LEU:HD12	2.47	0.43
1:A:40:LEU:HD13	1:A:44:VAL:HG23	2.00	0.43
1:B:346:LEU:HD12	1:B:386:LEU:O	2.18	0.43
1:A:97:ARG:HG3	1:A:97:ARG:NH1	2.33	0.43
1:B:64:ARG:NH1	1:B:64:ARG:HG3	2.34	0.43
1:A:240:ALA:HB1	1:A:247:VAL:HG22	2.00	0.43
1:A:196:LEU:HD13	1:A:202:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:CD1	1:B:44:VAL:HG23	2.49	0.43
1:B:298:PRO:O	1:B:304:ALA:HB2	2.18	0.43
1:A:68:ILE:HG12	1:A:130:VAL:HG21	2.01	0.43
1:A:234:ARG:HH11	1:A:234:ARG:CG	2.31	0.43
1:A:281:GLY:O	1:A:282:LYS:CB	2.66	0.43
1:B:353:LEU:CD1	1:B:401:VAL:HG11	2.49	0.43
1:B:114:GLN:O	1:B:117:THR:N	2.52	0.42
1:B:190:GLN:OE1	1:B:194:GLN:NE2	2.52	0.42
1:A:284:PHE:CE2	1:A:311:LEU:HD13	2.53	0.42
1:A:79:LYS:O	1:A:86:TYR:HD1	2.02	0.42
1:A:65:LEU:HD13	1:A:65:LEU:HA	1.86	0.42
1:A:120:MET:SD	1:A:125:ARG:HD2	2.59	0.42
1:A:120:MET:SD	1:A:125:ARG:CD	3.07	0.42
1:A:40:LEU:HG	1:A:156:LEU:HD21	2.01	0.42
1:A:198:ASP:CB	3:A:947:HOH:O	2.68	0.42
1:A:280:PRO:HG3	1:A:302:VAL:CG1	2.50	0.42
1:A:75:PRO:O	1:A:94:THR:HB	2.19	0.42
1:A:356:ASN:OD1	1:A:359:GLY:N	2.53	0.42
1:A:65:LEU:O	1:A:68:ILE:HG22	2.20	0.42
1:B:24:LEU:HD13	1:B:319:LEU:CD2	2.50	0.42
1:A:157:THR:HG21	1:B:408:PHE:CA	2.50	0.42
1:A:300:ASN:HD22	1:A:303:SER:H	1.68	0.42
1:B:136:ILE:HG22	1:B:138:ARG:HD3	2.00	0.42
1:B:68:ILE:HD12	1:B:130:VAL:HG21	2.02	0.42
1:A:40:LEU:HD11	1:A:44:VAL:CG2	2.50	0.42
1:A:196:LEU:HA	1:A:196:LEU:HD12	1.84	0.42
1:A:311:LEU:O	1:A:314:PRO:HD2	2.19	0.41
1:A:72:GLN:CB	1:A:73:PRO:CD	2.98	0.41
1:B:42:SER:O	1:B:43:ASP:C	2.58	0.41
1:B:281:GLY:O	1:B:282:LYS:CB	2.68	0.41
1:B:118:GLU:OE1	1:B:125:ARG:NH1	2.53	0.41
1:A:16:GLU:O	1:A:20:ARG:HG3	2.20	0.41
1:B:333:VAL:HG21	1:B:361:LEU:HB3	2.02	0.41
1:A:112:VAL:HG22	1:A:130:VAL:HG13	2.03	0.41
1:B:97:ARG:NH1	1:B:99:MET:HE3	2.36	0.41
1:A:334:ARG:CZ	1:A:398:TRP:CZ2	3.03	0.41
1:A:79:LYS:HD2	1:A:79:LYS:O	2.21	0.41
1:B:161:LEU:N	1:B:162:PRO:CD	2.84	0.41
1:B:50:VAL:HA	1:B:51:PRO:C	2.41	0.41
1:A:114:GLN:C	1:A:116:GLN:H	2.24	0.41
1:B:326:GLY:O	1:B:327:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:MET:CB	1:A:122:ASN:ND2	2.82	0.40
1:A:334:ARG:NH2	1:A:398:TRP:CZ2	2.89	0.40
1:A:333:VAL:CG1	1:A:334:ARG:N	2.84	0.40
1:B:112:VAL:HG21	1:B:126:PHE:HD2	1.87	0.40
1:A:76:VAL:O	1:A:76:VAL:HG23	2.21	0.40
1:B:238:ILE:O	1:B:242:SER:HB3	2.22	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	401/411 (98%)	357 (89%)	31 (8%)	13 (3%)	5 6
1	B	401/411 (98%)	376 (94%)	19 (5%)	6 (2%)	13 22
All	All	802/822 (98%)	733 (91%)	50 (6%)	19 (2%)	7 11

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	282	LYS
1	B	282	LYS
1	A	60	GLY
1	A	100	THR
1	A	122	ASN
1	A	392	ASN
1	B	43	ASP
1	A	71	GLY
1	A	85	PRO
1	B	82	ALA
1	B	115	GLU

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Mol	Chain	Res	Type
1	B	197	GLY
1	B	198	ASP
1	A	129	GLU
1	A	128	ALA
1	A	259	ASP
1	A	83	GLY
1	A	192	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	324/330 (98%)	270 (83%)	54 (17%)	3 5
1	B	324/330 (98%)	276 (85%)	48 (15%)	4 7
All	All	648/660 (98%)	546 (84%)	102 (16%)	3 5

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	11	ASP
1	A	14	LEU
1	A	15	ASN
1	A	20	ARG
1	A	24	LEU
1	A	27	GLN
1	A	48	LEU
1	A	58	MET
1	A	64	ARG
1	A	65	LEU
1	A	67	ASP
1	A	70	SER
1	A	79	LYS
1	A	87	HIS
1	A	89	GLU

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Mol	Chain	Res	Type
1	A	97	ARG
1	A	114	GLN
1	A	117	THR
1	A	118	GLU
1	A	122	ASN
1	A	125	ARG
1	A	127	THR
1	A	131	ARG
1	A	132	SER
1	A	138	ARG
1	A	144	SER
1	A	179	ARG
1	A	182	LEU
1	A	198	ASP
1	A	207	LEU
1	A	222	ASN
1	A	223	LEU
1	A	227	ARG
1	A	228	ASP
1	A	229	ASP
1	A	233	LEU
1	A	234	ARG
1	A	255	VAL
1	A	257	GLU
1	A	263	THR
1	A	276	LEU
1	A	288	LYS
1	A	319	LEU
1	A	332	ARG
1	A	333	VAL
1	A	337	SER
1	A	338	ARG
1	A	350	ARG
1	A	360	GLU
1	A	361	LEU
1	A	363	VAL
1	A	376	SER
1	A	399	VAL
1	B	7	LEU
1	B	10	LEU
1	B	14	LEU
1	B	15	ASN

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Mol	Chain	Res	Type
1	B	20	ARG
1	B	24	LEU
1	B	30	LEU
1	B	64	ARG
1	B	72	GLN
1	B	79	LYS
1	B	89	GLU
1	B	97	ARG
1	B	115	GLU
1	B	120	MET
1	B	121	ASP
1	B	125	ARG
1	B	131	ARG
1	B	137	ARG
1	B	144	SER
1	B	157	THR
1	B	171	GLU
1	B	182	LEU
1	B	185	THR
1	B	198	ASP
1	B	207	LEU
1	B	222	ASN
1	B	223	LEU
1	B	233	LEU
1	B	242	SER
1	B	257	GLU
1	B	259	ASP
1	B	262	LYS
1	B	263	THR
1	B	265	LEU
1	B	268	LEU
1	B	276	LEU
1	B	282	LYS
1	B	288	LYS
1	B	306	LEU
1	B	332	ARG
1	B	333	VAL
1	B	338	ARG
1	B	350	ARG
1	B	353	LEU
1	B	361	LEU
1	B	363	VAL

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Mol	Chain	Res	Type
1	B	399	VAL
1	B	401	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
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	354	GLN
1	A	368	HIS
1	B	27	GLN
1	B	119	GLN
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	354	GLN
1	B	368	HIS

5.3.3 RNA (i)

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)

10 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	904	-	5,5,5	0.52	0	5,5,5	0.55	0
2	GOL	A	905	-	5,5,5	0.43	0	5,5,5	0.40	0
2	GOL	A	906	-	5,5,5	0.46	0	5,5,5	0.37	0
2	GOL	A	908	-	5,5,5	0.52	0	5,5,5	0.51	0
2	GOL	A	909	-	5,5,5	0.39	0	5,5,5	0.47	0
2	GOL	A	910	-	5,5,5	0.40	0	5,5,5	0.45	0
2	GOL	B	901	-	5,5,5	0.47	0	5,5,5	0.44	0
2	GOL	B	902	-	5,5,5	0.50	0	5,5,5	0.52	0
2	GOL	B	903	-	5,5,5	0.47	0	5,5,5	0.45	0
2	GOL	B	907	-	5,5,5	0.43	0	5,5,5	0.40	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	904	-	-	0/4/4/4	0/0/0/0
2	GOL	A	905	-	-	0/4/4/4	0/0/0/0
2	GOL	A	906	-	-	0/4/4/4	0/0/0/0
2	GOL	A	908	-	-	0/4/4/4	0/0/0/0
2	GOL	A	909	-	-	0/4/4/4	0/0/0/0
2	GOL	A	910	-	-	0/4/4/4	0/0/0/0
2	GOL	B	901	-	-	0/4/4/4	0/0/0/0
2	GOL	B	902	-	-	0/4/4/4	0/0/0/0
2	GOL	B	903	-	-	0/4/4/4	0/0/0/0
2	GOL	B	907	-	-	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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	905	GOL	1	0
2	A	906	GOL	1	0
2	B	902	GOL	2	0
2	B	907	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^{th} 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	403/411 (98%)	0.51	36 (8%) 12 13	30, 51, 97, 100	0
1	B	403/411 (98%)	0.06	5 (1%) 81 83	27, 45, 76, 96	0
All	All	806/822 (98%)	0.29	41 (5%) 32 36	27, 48, 93, 100	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	VAL	7.8
1	A	87	HIS	7.4
1	A	68	ILE	7.1
1	A	88	GLY	5.0
1	A	93	GLY	5.0
1	A	81	PHE	4.7
1	A	65	LEU	4.3
1	A	121	ASP	4.3
1	A	86	TYR	4.2
1	A	119	GLN	4.1
1	A	123	GLY	3.9
1	B	409	GLY	3.9
1	A	94	THR	3.8
1	A	69	ALA	3.7
1	A	75	PRO	3.6
1	A	63	VAL	3.5
1	A	89	GLU	3.5
1	A	146	GLY	3.2
1	A	96	ILE	3.0
1	A	77	ALA	2.8
1	A	90	TRP	2.7
1	A	120	MET	2.7
1	A	78	GLY	2.6
1	A	131	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	327	LEU	2.5
1	A	128	ALA	2.5
1	B	130	VAL	2.5
1	A	195	PRO	2.5
1	A	74	LEU	2.4
1	B	197	GLY	2.4
1	A	104	VAL	2.4
1	A	76	VAL	2.3
1	B	196	LEU	2.3
1	A	82	ALA	2.3
1	A	327	LEU	2.3
1	A	92	ALA	2.2
1	A	67	ASP	2.2
1	A	136	ILE	2.2
1	A	95	CYS	2.2
1	A	107	GLY	2.1
1	A	105	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. 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^{th} 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^2)	Q<0.9
2	GOL	A	908	6/6	0.83	0.49	9.50	50,60,65,66	0
2	GOL	A	905	6/6	0.81	0.34	6.19	62,63,69,70	0
2	GOL	B	907	6/6	0.72	0.19	2.91	69,76,77,79	0
2	GOL	A	906	6/6	0.76	0.28	2.69	53,55,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	B	901	6/6	0.85	0.21	2.61	41,55,61,64	0
2	GOL	A	910	6/6	0.78	0.35	2.32	87,93,94,97	0
2	GOL	B	902	6/6	0.84	0.32	1.54	56,57,63,66	0
2	GOL	A	904	6/6	0.84	0.12	-0.75	55,69,70,72	0
2	GOL	A	909	6/6	0.65	0.22	-0.97	95,97,100,100	0
2	GOL	B	903	6/6	0.86	0.14	-1.39	63,70,74,79	0

6.5 Other polymers

There are no such residues in this entry.