Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 12:11 PM EDT

PDB ID	:	1SZ6
Title	:	MISTLETOE LECTIN I FROM VISCUM ALBUM. CRYSTAL STRUCTURE AT 2.05 A RESOLUTION
Authors	:	Gabdoulkhakov, A.G.; Guhlistova, N.E.; Lyashenko, A.V.; Krauspenhaar, R.; Stoeva, S.; Voelter, W.; Nikonov, S.V.; Betzel, C.; Mikhailov, A.M.
Deposited on	:	2004-04-04
Resolution	:	2.05 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

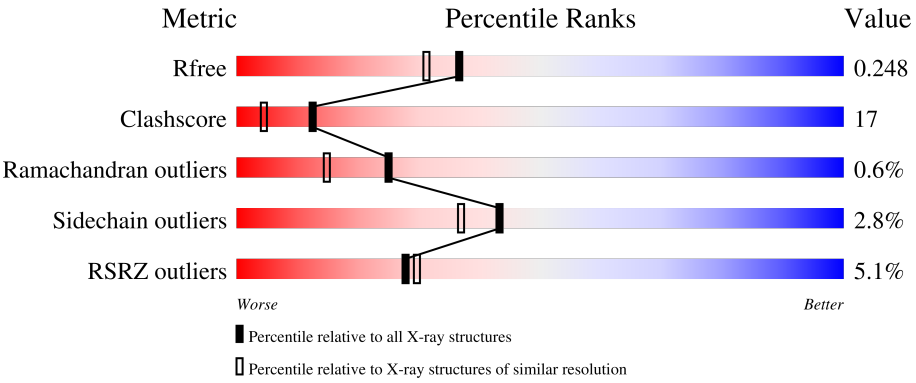
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.05 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	249	5% 59% 39%
2	B	263	5% 81% 17%

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
5	AZI	B	4005	-	-	-	X
7	GOL	A	4007	-	X	-	-
7	GOL	A	4008	-	X	-	-
7	GOL	A	4009	-	X	-	-
7	GOL	A	4010	-	X	-	-
7	GOL	A	4011	-	X	-	-
7	GOL	A	4016	-	X	-	-
7	GOL	A	4019	-	X	-	-
7	GOL	A	4020	-	X	X	-
7	GOL	B	4006	-	X	-	-
7	GOL	B	4012	-	X	-	-
7	GOL	B	4013	-	X	-	-
7	GOL	B	4014	-	X	-	-
7	GOL	B	4015	-	X	-	-
7	GOL	B	4017	-	X	-	-
7	GOL	B	4018	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4397 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.

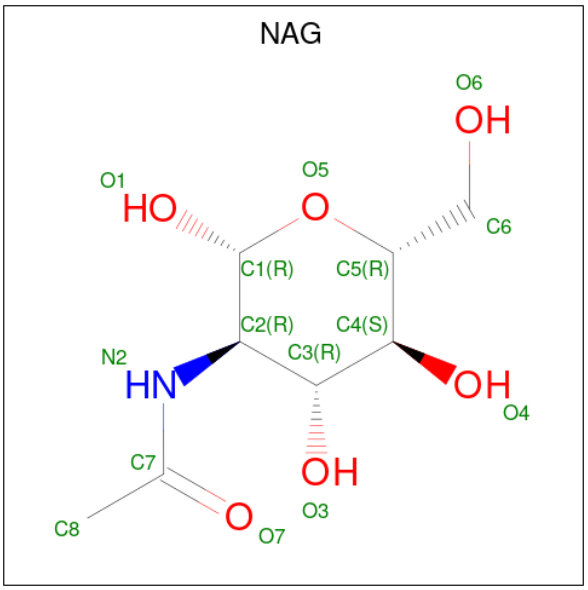
- Molecule 1 is a protein called RRNA N-GLYCOSIDASE A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1921	1218	328	371	4			

- Molecule 2 is a protein called BETA-GALACTOSIDE SPECIFIC LECTIN I B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	263	Total	C	N	O	S	0	0	0
			1996	1238	353	393	12			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



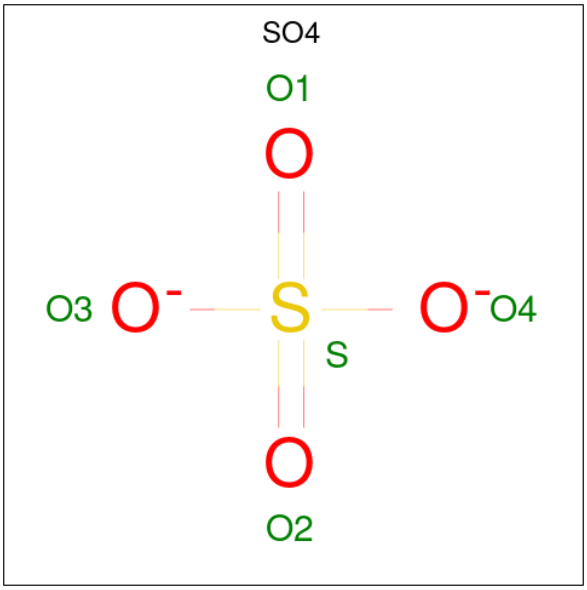
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

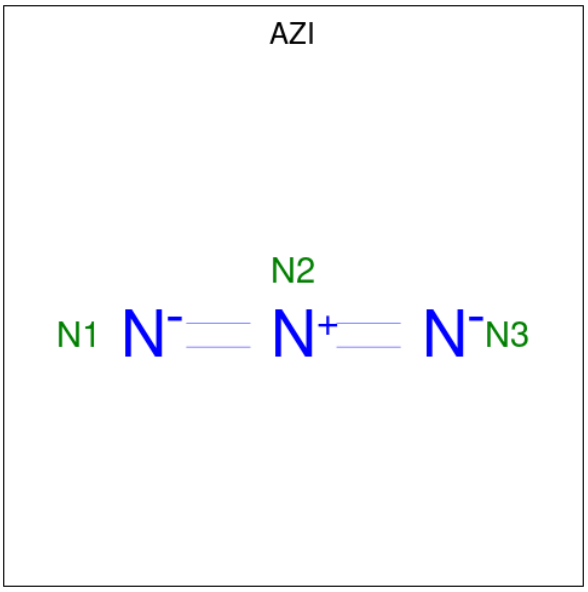
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is AZIDE ION (three-letter code: AZI) (formula: N_3).

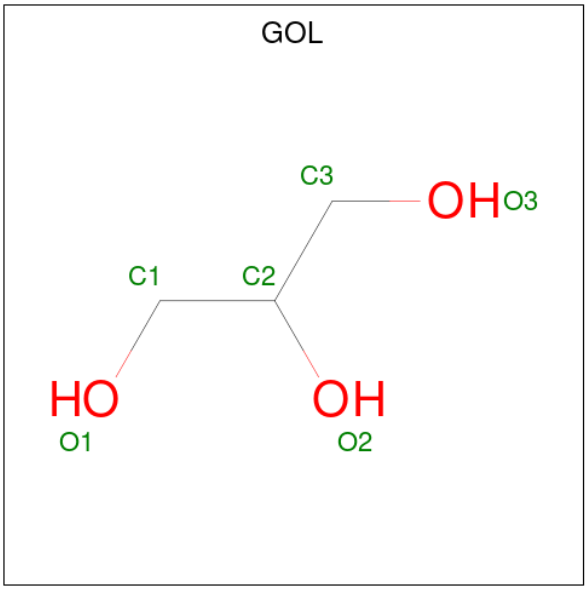


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N 3 3	0	0
5	B	1	Total N 3 3	0	0
5	B	1	Total N 3 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Cl 2 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 8 is water.

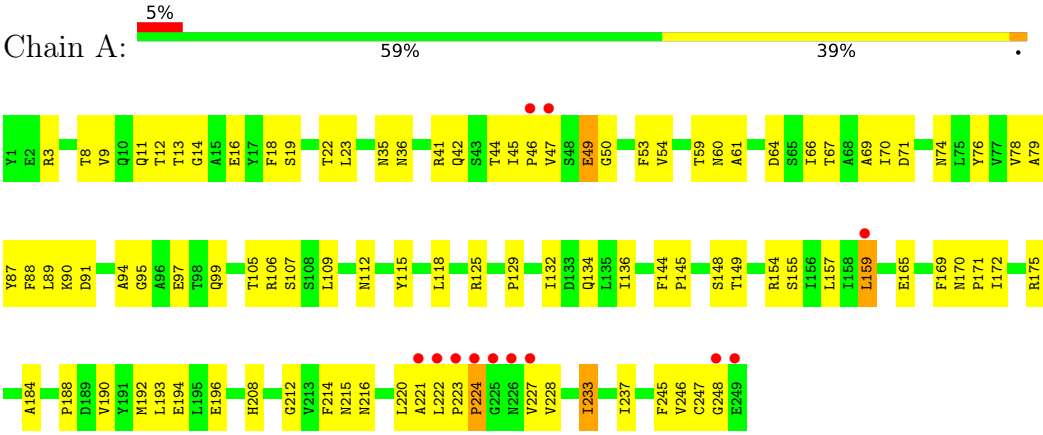
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	110	Total O 110 110	0	0
8	B	208	Total O 208 208	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

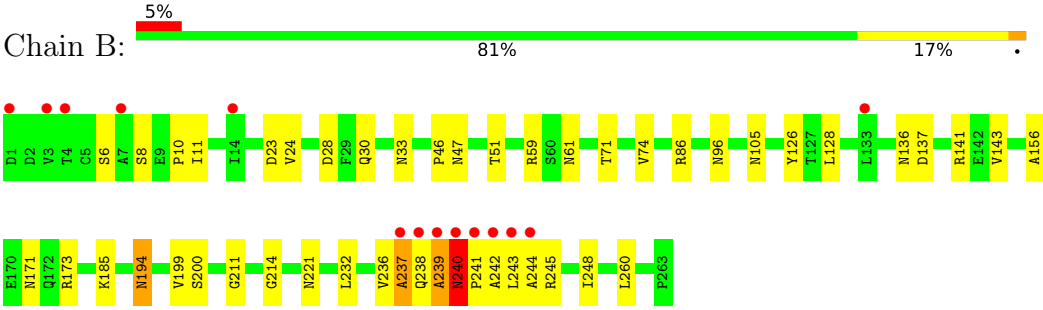
• Molecule 1: RRNA N-GLYCOSIDASE A CHAIN

Chain A:



• Molecule 2: BETA-GALACTOSIDE SPECIFIC LECTIN I B CHAIN

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	106.88Å 106.88Å 310.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.00 – 2.05 29.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.00-2.05) 98.6 (29.00-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.04Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.253 0.210 , 0.248	Depositor DCC
R_{free} test set	3238 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4397	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: SO4, NAG, CL, GOL, AZI

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	0.36	0/1960	0.60	1/2670 (0.0%)
2	B	0.40	0/2035	0.74	1/2777 (0.0%)
All	All	0.38	0/3995	0.68	2/5447 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	239	ALA	N-CA-C	-9.72	84.77	111.00
1	A	248	GLY	N-CA-C	-6.63	96.51	113.10

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	1921	0	1900	86	0
2	B	1996	0	1935	53	0
3	A	14	0	13	3	0
3	B	42	0	39	8	0
4	A	5	0	0	0	0
5	A	3	0	0	0	0
5	B	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	2	0	0	1	0
7	A	48	0	32	7	0
7	B	42	0	28	3	0
8	A	110	0	0	5	0
8	B	208	0	0	2	0
All	All	4397	0	3947	135	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 17.

All (135) 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:9:VAL:HG23	1:A:11:GLN:H	1.21	1.03
2:B:161:TRP:HB3	2:B:244:ALA:O	1.63	0.97
1:A:84:GLN:HE21	1:A:84:GLN:H	1.06	0.96
2:B:194:ASN:HD22	2:B:194:ASN:H	1.10	0.91
1:A:84:GLN:HE21	1:A:84:GLN:N	1.70	0.89
1:A:149:THR:H	7:A:4020:GOL:H11	1.42	0.82
1:A:45:ILE:HG23	1:A:49:GLU:HG3	1.64	0.80
2:B:194:ASN:HD22	2:B:194:ASN:N	1.82	0.78
1:A:112:ASN:HD21	3:A:5003:NAG:C1	1.97	0.77
2:B:61:ASN:HD21	3:B:5004:NAG:C1	1.97	0.77
1:A:9:VAL:HG23	1:A:11:GLN:N	1.99	0.74
1:A:155:SER:O	1:A:159:LEU:HD22	1.85	0.74
2:B:194:ASN:HD21	2:B:214:GLY:HA2	1.54	0.73
1:A:222:LEU:HB3	1:A:224:PRO:HD2	1.74	0.69
2:B:11:ILE:HG13	8:B:3199:HOH:O	1.91	0.69
1:A:86:SER:HB3	1:A:88:PHE:HE1	1.59	0.68
1:A:84:GLN:H	1:A:84:GLN:NE2	1.86	0.68
1:A:19:SER:O	1:A:23:LEU:HD13	1.95	0.66
1:A:13:THR:OG1	1:A:16:GLU:HG3	1.95	0.66
1:A:90:LYS:O	1:A:91:ASP:HB2	1.94	0.66
2:B:136:ASN:HD21	3:B:5001:NAG:C1	2.09	0.64
1:A:154:ARG:HD3	8:A:3288:HOH:O	1.96	0.64
2:B:11:ILE:HG12	2:B:51:THR:OG1	1.98	0.64
2:B:161:TRP:CB	2:B:244:ALA:O	2.43	0.64
1:A:112:ASN:ND2	3:A:5003:NAG:C1	2.62	0.63
2:B:194:ASN:H	2:B:194:ASN:ND2	1.91	0.63
2:B:156:ALA:HB2	2:B:161:TRP:HE1	1.63	0.63
1:A:106:ARG:HB2	1:A:106:ARG:NH1	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:GLN:NE2	2:B:238:GLN:HA	2.16	0.61
1:A:46:PRO:O	1:A:49:GLU:HB2	2.01	0.61
1:A:149:THR:N	7:A:4020:GOL:H11	2.16	0.60
2:B:136:ASN:ND2	3:B:5001:NAG:C1	2.64	0.60
1:A:49:GLU:OE1	1:A:50:GLY:N	2.35	0.60
1:A:90:LYS:O	1:A:112:ASN:HB3	2.02	0.59
1:A:95:GLY:O	1:A:99:GLN:HG2	2.02	0.59
2:B:141:ARG:HG3	7:B:4018:GOL:O1	2.03	0.59
2:B:194:ASN:HD21	2:B:214:GLY:CA	2.16	0.59
2:B:61:ASN:ND2	3:B:5004:NAG:C1	2.65	0.58
1:A:237:ILE:HD11	2:B:221:ASN:HB2	1.87	0.57
1:A:86:SER:HB3	1:A:88:PHE:CE1	2.41	0.55
1:A:59:THR:HA	1:A:64:ASP:O	2.06	0.55
1:A:61:ALA:HB3	8:A:3282:HOH:O	2.06	0.55
1:A:60:ASN:HB2	1:A:136:ILE:HG23	1.89	0.55
1:A:97:GLU:HG3	7:A:4010:GOL:H12	1.89	0.55
2:B:239:ALA:HB3	2:B:243:LEU:CD2	2.36	0.55
2:B:156:ALA:CB	2:B:161:TRP:HE1	2.20	0.55
1:A:85:GLN:NE2	1:A:105:THR:HB	2.21	0.55
1:A:84:GLN:HE21	1:A:84:GLN:CA	2.19	0.54
1:A:188:PRO:HB2	1:A:193:LEU:HD21	1.88	0.54
1:A:84:GLN:O	1:A:84:GLN:HG2	2.06	0.54
2:B:169:GLN:HG2	2:B:171:ASN:OD1	2.08	0.54
2:B:194:ASN:N	2:B:194:ASN:ND2	2.54	0.53
2:B:86:ARG:HG3	2:B:86:ARG:HH11	1.74	0.53
2:B:86:ARG:HG3	2:B:86:ARG:NH1	2.24	0.53
1:A:129:PRO:O	1:A:134:GLN:HG2	2.08	0.52
1:A:148:SER:HB2	7:A:4020:GOL:H11	1.93	0.51
1:A:71:ASP:HB3	1:A:74:ASN:OD1	2.10	0.51
2:B:96:ASN:ND2	8:B:3118:HOH:O	2.44	0.50
1:A:169:PHE:HB3	1:A:171:PRO:HD2	1.94	0.50
1:A:115:TYR:CD1	1:A:125:ARG:HD3	2.46	0.49
1:A:194:GLU:OE1	1:A:221:ALA:O	2.31	0.49
1:A:97:GLU:CG	7:A:4010:GOL:H12	2.43	0.49
1:A:41:ARG:HG3	8:A:3016:HOH:O	2.12	0.49
2:B:236:VAL:O	2:B:238:GLN:N	2.46	0.49
1:A:74:ASN:OD1	1:A:76:TYR:HB2	2.13	0.48
1:A:216:ASN:ND2	6:A:4021:CL:CL	2.82	0.48
2:B:194:ASN:ND2	2:B:214:GLY:CA	2.75	0.48
1:A:223:PRO:HB2	1:A:224:PRO:HD3	1.95	0.48
1:A:35:ASN:O	1:A:36:ASN:HB2	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:THR:O	2:B:74:VAL:HG22	2.13	0.48
2:B:61:ASN:OD1	3:B:5004:NAG:C1	2.62	0.48
1:A:18:PHE:O	1:A:22:THR:HG23	2.15	0.47
1:A:60:ASN:CB	1:A:136:ILE:HG23	2.44	0.47
1:A:170:ASN:N	1:A:171:PRO:CD	2.77	0.47
1:A:192:MET:O	1:A:196:GLU:HG3	2.16	0.46
2:B:137:ASP:HB3	2:B:141:ARG:NH2	2.29	0.46
1:A:79:ALA:HB1	1:A:87:TYR:O	2.16	0.46
1:A:171:PRO:HA	2:B:260:LEU:HD21	1.96	0.46
2:B:28:ASP:HB3	2:B:33:ASN:ND2	2.30	0.46
2:B:126:TYR:CE1	3:B:5002:NAG:H82	2.51	0.46
2:B:96:ASN:CG	3:B:5002:NAG:C1	2.85	0.45
1:A:212:GLY:HA2	1:A:233:ILE:HG23	1.98	0.45
1:A:214:PHE:HE1	1:A:233:ILE:HG22	1.80	0.45
2:B:238:GLN:HE22	2:B:241:PRO:HD3	1.80	0.45
1:A:118:LEU:HD23	1:A:157:LEU:HD13	1.99	0.45
1:A:175:ARG:HD3	8:A:3308:HOH:O	2.16	0.45
1:A:132:ILE:O	1:A:136:ILE:HG13	2.17	0.45
2:B:128:LEU:HD12	2:B:211:GLY:HA2	1.97	0.45
2:B:173:ARG:HB3	2:B:185:LYS:HD2	1.99	0.45
1:A:245:PHE:CE1	1:A:247:CYS:HB2	2.52	0.44
1:A:8:THR:O	1:A:60:ASN:HA	2.17	0.44
1:A:148:SER:HB2	7:A:4020:GOL:C1	2.47	0.44
1:A:172:ILE:HG12	1:A:192:MET:HG3	1.99	0.44
1:A:223:PRO:N	1:A:224:PRO:CD	2.80	0.44
2:B:199:VAL:O	2:B:200:SER:HB2	2.17	0.44
1:A:144:PHE:HA	1:A:145:PRO:HD3	1.86	0.44
1:A:215:ASN:OD1	2:B:10:PRO:HD3	2.18	0.44
1:A:60:ASN:ND2	1:A:64:ASP:HB2	2.33	0.44
3:A:5003:NAG:H61	8:A:3271:HOH:O	2.16	0.44
2:B:23:ASP:OD1	7:B:4012:GOL:O2	2.35	0.43
2:B:232:LEU:HD12	2:B:248:ILE:HD12	1.99	0.43
2:B:239:ALA:CB	2:B:243:LEU:HD21	2.49	0.43
1:A:42:GLN:C	1:A:44:THR:H	2.22	0.43
1:A:53:PHE:CE1	1:A:78:VAL:HG21	2.54	0.43
1:A:69:ALA:O	1:A:78:VAL:HG22	2.18	0.43
1:A:9:VAL:CG2	1:A:11:GLN:HB2	2.48	0.43
2:B:238:GLN:HA	2:B:238:GLN:HE21	1.81	0.43
2:B:96:ASN:OD1	3:B:5002:NAG:C1	2.67	0.42
1:A:14:GLY:HA3	1:A:181:ASN:ND2	2.34	0.42
2:B:59:ARG:HH22	7:B:4017:GOL:C3	2.31	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HG11	1:A:94:ALA:O	2.20	0.42
2:B:24:VAL:HB	2:B:47:ASN:HB2	2.01	0.42
1:A:165:GLU:HA	1:A:165:GLU:OE1	2.19	0.42
1:A:89:LEU:HA	1:A:109:LEU:HB2	2.02	0.42
1:A:179:TYR:HD1	1:A:184:ALA:HB3	1.85	0.42
1:A:220:LEU:HB2	1:A:228:VAL:CG1	2.49	0.42
2:B:245:ARG:HB2	2:B:245:ARG:NH1	2.35	0.42
2:B:239:ALA:HB3	2:B:243:LEU:HD21	2.01	0.41
1:A:190:VAL:HB	1:A:223:PRO:HG3	2.02	0.41
1:A:54:VAL:HG13	1:A:70:ILE:HB	2.01	0.41
1:A:220:LEU:O	1:A:228:VAL:HG12	2.20	0.41
1:A:221:ALA:HA	1:A:227:VAL:HG12	2.02	0.41
1:A:106:ARG:HB2	1:A:106:ARG:HH11	1.82	0.41
1:A:208:HIS:O	2:B:6:SER:HB2	2.20	0.41
2:B:240:ASN:C	2:B:242:ALA:H	2.23	0.41
2:B:46:PRO:HB2	2:B:61:ASN:HB2	2.01	0.41
1:A:60:ASN:HD21	1:A:64:ASP:HB2	1.85	0.41
1:A:66:ILE:HD12	1:A:66:ILE:O	2.21	0.41
2:B:161:TRP:CB	2:B:244:ALA:HB1	2.51	0.41
1:A:12:THR:HA	1:A:16:GLU:OE1	2.20	0.41
2:B:236:VAL:O	2:B:237:ALA:C	2.59	0.41
1:A:95:GLY:H	7:A:4010:GOL:C3	2.34	0.40
1:A:3:ARG:HH12	1:A:67:THR:HG21	1.86	0.40
1:A:246:VAL:HG12	1:A:246:VAL:O	2.21	0.40
1:A:208:HIS:O	2:B:6:SER:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	247/249 (99%)	236 (96%)	10 (4%)	1 (0%)	34 24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	261/263 (99%)	245 (94%)	14 (5%)	2 (1%)	19 10
All	All	508/512 (99%)	481 (95%)	24 (5%)	3 (1%)	25 15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	237	ALA
1	A	224	PRO
2	B	240	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/209 (100%)	204 (98%)	5 (2%)	49 42
2	B	217/217 (100%)	210 (97%)	7 (3%)	39 32
All	All	426/426 (100%)	414 (97%)	12 (3%)	43 37

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLU
1	A	84	GLN
1	A	107	SER
1	A	159	LEU
1	A	233	ILE
2	B	8	SER
2	B	30	GLN
2	B	105	ASN
2	B	143	VAL
2	B	161	TRP
2	B	194	ASN
2	B	240	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	36	ASN
1	A	42	GLN
1	A	84	GLN
1	A	85	GLN
1	A	112	ASN
1	A	127	GLN
2	B	44	ASN
2	B	82	ASN
2	B	105	ASN
2	B	136	ASN
2	B	194	ASN
2	B	238	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	$\#\|Z\|>2$
7	GOL	A	4016	-	5,5,5	4.54	5 (100%)	5,5,5	5.77	3 (60%)
5	AZI	B	4005	-	0,2,2	-	-	0,1,1	-	-
3	NAG	B	5001	-	14,14,15	1.99	6 (42%)	17,19,21	0.98	1 (5%)
7	GOL	B	4018	-	5,5,5	4.38	5 (100%)	5,5,5	5.79	3 (60%)
7	GOL	A	4019	-	5,5,5	4.53	5 (100%)	5,5,5	5.79	3 (60%)
7	GOL	A	4011	-	5,5,5	4.52	5 (100%)	5,5,5	5.79	3 (60%)
7	GOL	B	4017	-	5,5,5	4.46	5 (100%)	5,5,5	5.79	3 (60%)
5	AZI	A	4004	-	0,2,2	-	-	0,1,1	-	-
7	GOL	B	4014	-	5,5,5	4.54	5 (100%)	5,5,5	5.78	3 (60%)
3	NAG	B	5002	-	14,14,15	1.90	4 (28%)	17,19,21	1.05	1 (5%)
7	GOL	B	4012	-	5,5,5	4.49	5 (100%)	5,5,5	5.69	3 (60%)
7	GOL	A	4010	-	5,5,5	4.53	5 (100%)	5,5,5	5.80	3 (60%)
5	AZI	B	4003	-	0,2,2	-	-	0,1,1	-	-
3	NAG	A	5003	-	14,14,15	2.00	6 (42%)	17,19,21	1.09	1 (5%)
7	GOL	A	4008	-	5,5,5	4.56	5 (100%)	5,5,5	5.70	3 (60%)
7	GOL	A	4009	-	5,5,5	4.59	5 (100%)	5,5,5	5.77	3 (60%)
7	GOL	B	4006	-	5,5,5	4.56	5 (100%)	5,5,5	5.79	3 (60%)
7	GOL	B	4013	-	5,5,5	4.50	5 (100%)	5,5,5	5.77	3 (60%)
7	GOL	A	4020	-	5,5,5	4.50	5 (100%)	5,5,5	5.78	3 (60%)
4	SO4	A	4001	-	4,4,4	0.29	0	6,6,6	0.14	0
7	GOL	A	4007	-	5,5,5	4.48	5 (100%)	5,5,5	5.77	3 (60%)
7	GOL	B	4015	-	5,5,5	4.58	5 (100%)	5,5,5	5.75	3 (60%)
3	NAG	B	5004	-	14,14,15	1.83	5 (35%)	17,19,21	1.14	2 (11%)

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
7	GOL	A	4016	-	-	2/4/4/4	-
3	NAG	B	5001	-	-	2/6/23/26	0/1/1/1
7	GOL	B	4018	-	-	2/4/4/4	-
7	GOL	A	4019	-	-	3/4/4/4	-
7	GOL	A	4011	-	-	2/4/4/4	-
7	GOL	B	4017	-	-	2/4/4/4	-
7	GOL	B	4014	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	5002	-	-	1/6/23/26	0/1/1/1
7	GOL	B	4012	-	-	2/4/4/4	-
7	GOL	A	4010	-	-	3/4/4/4	-
3	NAG	A	5003	-	-	2/6/23/26	0/1/1/1
7	GOL	A	4008	-	-	2/4/4/4	-
7	GOL	A	4009	-	-	2/4/4/4	-
7	GOL	B	4006	-	-	2/4/4/4	-
7	GOL	B	4013	-	-	2/4/4/4	-
7	GOL	A	4020	-	-	2/4/4/4	-
7	GOL	A	4007	-	-	2/4/4/4	-
7	GOL	B	4015	-	-	2/4/4/4	-
3	NAG	B	5004	-	-	0/6/23/26	0/1/1/1

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4015	GOL	C3-C2	-7.67	1.20	1.51
7	A	4016	GOL	C3-C2	-7.59	1.20	1.51
7	A	4009	GOL	C3-C2	-7.57	1.20	1.51
7	A	4008	GOL	C3-C2	-7.55	1.20	1.51
7	B	4012	GOL	C3-C2	-7.53	1.20	1.51
7	B	4014	GOL	C3-C2	-7.41	1.21	1.51
7	A	4010	GOL	C3-C2	-7.40	1.21	1.51
7	B	4013	GOL	C3-C2	-7.40	1.21	1.51
7	A	4011	GOL	C3-C2	-7.39	1.21	1.51
7	A	4019	GOL	C3-C2	-7.37	1.21	1.51
7	B	4006	GOL	C3-C2	-7.34	1.21	1.51
7	A	4020	GOL	C3-C2	-7.28	1.21	1.51
7	A	4007	GOL	C3-C2	-7.28	1.21	1.51
7	B	4017	GOL	C3-C2	-7.25	1.21	1.51
7	B	4018	GOL	C3-C2	-7.22	1.22	1.51
7	A	4010	GOL	O1-C1	4.68	1.62	1.42
7	A	4016	GOL	O1-C1	4.67	1.62	1.42
7	A	4011	GOL	O1-C1	4.66	1.62	1.42
7	A	4008	GOL	O1-C1	4.63	1.62	1.42
7	B	4013	GOL	O1-C1	4.59	1.61	1.42
7	A	4007	GOL	O1-C1	4.58	1.61	1.42
7	A	4019	GOL	O1-C1	4.55	1.61	1.42
7	B	4017	GOL	O1-C1	4.54	1.61	1.42
7	B	4014	GOL	O1-C1	4.54	1.61	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4006	GOL	O1-C1	4.53	1.61	1.42
7	B	4015	GOL	O1-C1	4.48	1.61	1.42
7	A	4009	GOL	O1-C1	4.45	1.61	1.42
7	B	4018	GOL	O1-C1	4.43	1.61	1.42
7	B	4012	GOL	O1-C1	4.30	1.60	1.42
7	A	4020	GOL	O1-C1	4.27	1.60	1.42
3	B	5002	NAG	O7-C7	-3.66	1.15	1.23
3	B	5002	NAG	C4-C5	3.64	1.60	1.53
7	B	4018	GOL	O3-C3	3.58	1.57	1.42
3	A	5003	NAG	C4-C5	3.53	1.60	1.53
7	B	4006	GOL	O3-C3	3.47	1.57	1.42
7	A	4007	GOL	O3-C3	3.47	1.57	1.42
7	A	4020	GOL	O3-C3	3.44	1.56	1.42
7	B	4017	GOL	O3-C3	3.43	1.56	1.42
7	B	4014	GOL	O3-C3	3.43	1.56	1.42
7	B	4013	GOL	O3-C3	3.42	1.56	1.42
7	B	4012	GOL	O3-C3	3.40	1.56	1.42
7	A	4011	GOL	O3-C3	3.39	1.56	1.42
7	A	4019	GOL	O3-C3	3.39	1.56	1.42
3	A	5003	NAG	O7-C7	-3.39	1.15	1.23
3	B	5001	NAG	O7-C7	-3.38	1.15	1.23
3	B	5004	NAG	C4-C5	3.36	1.60	1.53
7	A	4009	GOL	O3-C3	3.35	1.56	1.42
7	A	4010	GOL	O3-C3	3.29	1.56	1.42
7	A	4008	GOL	O3-C3	3.24	1.56	1.42
3	B	5001	NAG	C1-C2	3.21	1.57	1.52
3	B	5004	NAG	O7-C7	-3.20	1.16	1.23
7	B	4006	GOL	O2-C2	-3.12	1.34	1.43
3	A	5003	NAG	C1-C2	3.10	1.57	1.52
7	B	4015	GOL	O3-C3	3.07	1.55	1.42
3	B	5001	NAG	O5-C5	3.06	1.49	1.43
7	A	4016	GOL	O3-C3	3.05	1.55	1.42
7	A	4020	GOL	C1-C2	-3.02	1.39	1.51
7	A	4020	GOL	O2-C2	-2.98	1.34	1.43
7	A	4009	GOL	C1-C2	-2.96	1.39	1.51
7	B	4012	GOL	O2-C2	-2.95	1.34	1.43
7	A	4009	GOL	O2-C2	-2.90	1.34	1.43
7	A	4019	GOL	C1-C2	-2.89	1.39	1.51
7	B	4015	GOL	C1-C2	-2.87	1.39	1.51
7	B	4015	GOL	O2-C2	-2.87	1.34	1.43
7	A	4010	GOL	O2-C2	-2.83	1.35	1.43
7	B	4006	GOL	C1-C2	-2.81	1.40	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4014	GOL	O2-C2	-2.81	1.35	1.43
7	B	4014	GOL	C1-C2	-2.80	1.40	1.51
7	A	4011	GOL	O2-C2	-2.78	1.35	1.43
7	A	4008	GOL	O2-C2	-2.76	1.35	1.43
7	B	4017	GOL	C1-C2	-2.75	1.40	1.51
7	A	4019	GOL	O2-C2	-2.75	1.35	1.43
3	B	5001	NAG	C4-C5	2.71	1.58	1.53
7	A	4008	GOL	C1-C2	-2.70	1.40	1.51
7	A	4007	GOL	C1-C2	-2.69	1.40	1.51
7	A	4016	GOL	O2-C2	-2.69	1.35	1.43
7	A	4016	GOL	C1-C2	-2.68	1.40	1.51
7	A	4010	GOL	C1-C2	-2.68	1.40	1.51
7	A	4007	GOL	O2-C2	-2.67	1.35	1.43
7	B	4013	GOL	O2-C2	-2.66	1.35	1.43
3	B	5002	NAG	C8-C7	-2.65	1.45	1.50
7	B	4017	GOL	O2-C2	-2.65	1.35	1.43
7	A	4011	GOL	C1-C2	-2.61	1.41	1.51
3	B	5004	NAG	C3-C2	2.60	1.58	1.52
7	B	4013	GOL	C1-C2	-2.59	1.41	1.51
7	B	4018	GOL	C1-C2	-2.58	1.41	1.51
3	B	5002	NAG	O5-C5	2.57	1.48	1.43
3	A	5003	NAG	O5-C5	2.49	1.48	1.43
3	A	5003	NAG	C8-C7	-2.38	1.45	1.50
7	B	4012	GOL	C1-C2	-2.37	1.42	1.51
3	B	5004	NAG	O5-C5	2.28	1.48	1.43
3	B	5001	NAG	C3-C2	2.27	1.57	1.52
3	A	5003	NAG	C3-C2	2.24	1.57	1.52
7	B	4018	GOL	O2-C2	-2.20	1.36	1.43
3	B	5004	NAG	C1-C2	2.06	1.55	1.52
3	B	5001	NAG	C8-C7	-2.01	1.46	1.50

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	4012	GOL	O3-C3-C2	10.74	161.70	110.20
7	A	4020	GOL	O3-C3-C2	10.60	161.03	110.20
7	B	4006	GOL	O3-C3-C2	10.60	161.02	110.20
7	B	4017	GOL	O3-C3-C2	10.56	160.85	110.20
7	A	4010	GOL	O3-C3-C2	10.55	160.80	110.20
7	A	4019	GOL	O3-C3-C2	10.53	160.71	110.20
7	A	4011	GOL	O3-C3-C2	10.51	160.57	110.20
7	B	4018	GOL	O3-C3-C2	10.49	160.51	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	4009	GOL	O3-C3-C2	10.49	160.48	110.20
7	A	4016	GOL	O3-C3-C2	10.47	160.41	110.20
7	B	4013	GOL	O3-C3-C2	10.46	160.35	110.20
7	B	4014	GOL	O3-C3-C2	10.44	160.28	110.20
7	A	4007	GOL	O3-C3-C2	10.44	160.27	110.20
7	B	4015	GOL	O3-C3-C2	10.37	159.92	110.20
7	A	4008	GOL	O3-C3-C2	10.26	159.40	110.20
7	B	4015	GOL	O2-C2-C3	6.81	139.14	109.12
7	A	4009	GOL	O2-C2-C3	6.79	139.02	109.12
7	A	4019	GOL	O2-C2-C3	6.79	139.02	109.12
7	A	4007	GOL	O2-C2-C3	6.77	138.94	109.12
7	A	4008	GOL	O2-C2-C3	6.77	138.94	109.12
7	B	4018	GOL	O2-C2-C3	6.75	138.87	109.12
7	B	4014	GOL	O2-C2-C3	6.75	138.86	109.12
7	B	4017	GOL	O2-C2-C3	6.73	138.76	109.12
7	A	4020	GOL	O2-C2-C3	6.72	138.74	109.12
7	A	4016	GOL	O2-C2-C3	6.70	138.63	109.12
7	A	4010	GOL	O2-C2-C3	6.70	138.62	109.12
7	A	4011	GOL	O2-C2-C3	6.69	138.60	109.12
7	B	4013	GOL	O2-C2-C3	6.68	138.54	109.12
7	B	4006	GOL	O2-C2-C3	6.67	138.52	109.12
7	B	4012	GOL	O2-C2-C3	6.41	137.37	109.12
7	B	4013	GOL	O1-C1-C2	3.42	126.61	110.20
7	A	4010	GOL	O1-C1-C2	3.40	126.51	110.20
7	B	4014	GOL	O1-C1-C2	3.40	126.50	110.20
7	A	4011	GOL	O1-C1-C2	3.40	126.49	110.20
7	B	4018	GOL	O1-C1-C2	3.35	126.27	110.20
7	A	4016	GOL	O1-C1-C2	3.31	126.08	110.20
7	A	4008	GOL	O1-C1-C2	3.29	125.98	110.20
7	A	4007	GOL	O1-C1-C2	3.29	125.97	110.20
7	B	4015	GOL	O1-C1-C2	3.29	125.96	110.20
7	B	4017	GOL	O1-C1-C2	3.22	125.66	110.20
7	B	4006	GOL	O1-C1-C2	3.19	125.52	110.20
7	A	4019	GOL	O1-C1-C2	3.17	125.41	110.20
7	A	4009	GOL	O1-C1-C2	3.15	125.31	110.20
7	A	4020	GOL	O1-C1-C2	3.04	124.78	110.20
3	B	5002	NAG	C4-C3-C2	-2.73	107.02	111.02
3	B	5004	NAG	C4-C3-C2	-2.70	107.06	111.02
3	A	5003	NAG	C4-C3-C2	-2.65	107.13	111.02
3	B	5001	NAG	C4-C3-C2	-2.55	107.28	111.02
7	B	4012	GOL	O1-C1-C2	2.26	121.05	110.20
3	B	5004	NAG	O5-C5-C4	-2.04	105.86	110.83

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4007	GOL	O1-C1-C2-O2
7	A	4007	GOL	C1-C2-C3-O3
7	A	4008	GOL	O1-C1-C2-C3
7	A	4008	GOL	C1-C2-C3-O3
7	A	4009	GOL	O1-C1-C2-C3
7	A	4009	GOL	C1-C2-C3-O3
7	A	4010	GOL	C1-C2-C3-O3
7	A	4011	GOL	C1-C2-C3-O3
7	A	4016	GOL	C1-C2-C3-O3
7	A	4019	GOL	O1-C1-C2-C3
7	A	4019	GOL	C1-C2-C3-O3
7	A	4020	GOL	O1-C1-C2-C3
7	A	4020	GOL	C1-C2-C3-O3
7	B	4006	GOL	C1-C2-C3-O3
7	B	4012	GOL	C1-C2-C3-O3
7	B	4013	GOL	O1-C1-C2-C3
7	B	4013	GOL	C1-C2-C3-O3
7	B	4014	GOL	O1-C1-C2-C3
7	B	4014	GOL	C1-C2-C3-O3
7	B	4015	GOL	O1-C1-C2-C3
7	B	4015	GOL	C1-C2-C3-O3
7	B	4017	GOL	O1-C1-C2-C3
7	B	4017	GOL	C1-C2-C3-O3
7	B	4018	GOL	O1-C1-C2-C3
7	B	4018	GOL	C1-C2-C3-O3
7	B	4012	GOL	O1-C1-C2-O2
3	A	5003	NAG	O5-C5-C6-O6
3	B	5001	NAG	O5-C5-C6-O6
7	A	4010	GOL	O1-C1-C2-C3
3	A	5003	NAG	C4-C5-C6-O6
7	A	4010	GOL	O1-C1-C2-O2
7	A	4011	GOL	O1-C1-C2-O2
7	A	4016	GOL	O1-C1-C2-O2
7	B	4006	GOL	O1-C1-C2-O2
3	B	5001	NAG	C4-C5-C6-O6
3	B	5002	NAG	O5-C5-C6-O6
7	A	4019	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5001	NAG	2	0
7	B	4018	GOL	1	0
7	B	4017	GOL	1	0
3	B	5002	NAG	3	0
7	B	4012	GOL	1	0
7	A	4010	GOL	3	0
3	A	5003	NAG	3	0
7	A	4020	GOL	4	0
3	B	5004	NAG	3	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	249/249 (100%)	0.10	12 (4%)	30	33	31, 48, 83, 100	0
2	B	263/263 (100%)	-0.04	14 (5%)	26	28	25, 38, 81, 100	0
All	All	512/512 (100%)	0.03	26 (5%)	28	30	25, 43, 83, 100	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	239	ALA	8.8
1	A	223	PRO	8.1
2	B	240	ASN	7.0
2	B	244	ALA	6.9
1	A	225	GLY	6.7
1	A	248	GLY	5.4
1	A	224	PRO	5.3
2	B	243	LEU	4.9
1	A	226	ASN	4.9
1	A	249	GLU	4.2
2	B	1	ASP	3.9
2	B	238	GLN	3.6
2	B	242	ALA	3.6
1	A	222	LEU	3.5
1	A	221	ALA	3.3
2	B	4	THR	3.2
2	B	14	ILE	2.9
1	A	46	PRO	2.7
2	B	237	ALA	2.7
1	A	227	VAL	2.6
2	B	241	PRO	2.3
2	B	3	VAL	2.2
2	B	133	LEU	2.2
2	B	7	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	47	VAL	2.1
1	A	159	LEU	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 monosaccharides 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^{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	B-factors(Å^2)	Q<0.9
7	GOL	B	4013	6/6	0.58	0.23	77,83,88,96	0
5	AZI	B	4005	3/3	0.67	0.44	70,70,76,78	0
3	NAG	B	5002	14/15	0.72	0.22	85,95,100,100	0
3	NAG	B	5004	14/15	0.76	0.22	63,82,92,98	0
7	GOL	A	4019	6/6	0.79	0.22	74,81,86,92	0
7	GOL	A	4010	6/6	0.79	0.12	62,71,76,77	0
7	GOL	B	4006	6/6	0.80	0.31	69,69,71,74	0
7	GOL	A	4011	6/6	0.81	0.14	71,79,80,83	0
5	AZI	B	4003	3/3	0.81	0.08	50,50,59,60	0
7	GOL	B	4018	6/6	0.81	0.47	74,79,81,83	0
7	GOL	B	4017	6/6	0.83	0.22	70,82,82,83	0
3	NAG	A	5003	14/15	0.85	0.28	85,93,100,100	0
7	GOL	A	4020	6/6	0.85	0.16	60,66,69,82	0
7	GOL	A	4016	6/6	0.88	0.21	55,61,64,73	0
7	GOL	A	4007	6/6	0.89	0.24	83,88,89,89	0
3	NAG	B	5001	14/15	0.90	0.11	30,43,54,58	0
7	GOL	B	4014	6/6	0.90	0.21	49,75,83,85	0
7	GOL	A	4009	6/6	0.91	0.19	71,72,79,82	0
7	GOL	A	4008	6/6	0.92	0.19	58,65,71,72	0
5	AZI	A	4004	3/3	0.93	0.17	54,54,59,65	0
7	GOL	B	4012	6/6	0.95	0.14	34,38,51,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	4001	5/5	0.96	0.10	69,73,76,81	0
7	GOL	B	4015	6/6	0.96	0.10	40,54,60,61	0
6	CL	A	4021	1/1	0.97	0.03	71,71,71,71	0
6	CL	A	4022	1/1	0.99	0.20	43,43,43,43	1

6.5 Other polymers (i)

There are no such residues in this entry.