



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:32 pm GMT

PDB ID : 1ONK
Title : Mistletoe lectin I from viscum album
Authors : Gabdoulkhakov, A.G.; Savoshkina, Y.; Krauspenhaar, R.; Stoeva, S.;
Konareva, N.; Kornilov, V.; Kornev, A.N.; Voelter, W.; Nikonov, S.V.; Betzel,
C.; Mikhailov, A.M.
Deposited on : 2003-02-28
Resolution : 2.10 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

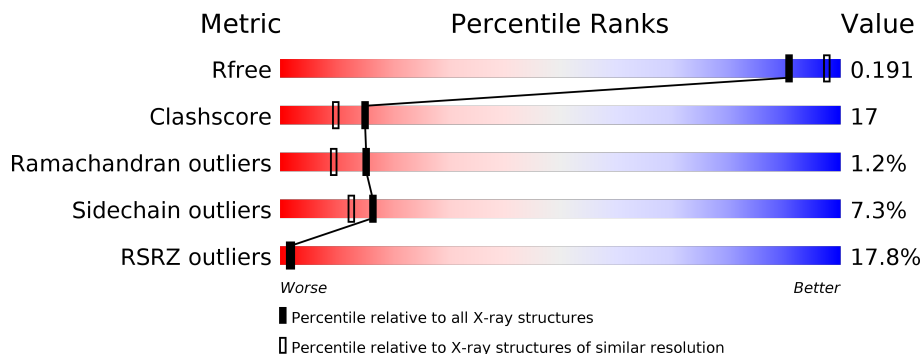
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	254	<div> <div>19%</div> <div>69%</div> <div>25%</div> <div>• •</div> </div>
2	B	263	<div> <div>17%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	4001	-	-	X	-
5	AZI	A	4006	-	-	-	X
5	AZI	A	4009	-	-	X	X
5	AZI	B	4005	-	-	-	X
5	AZI	B	4007	-	-	-	X
5	AZI	B	4008	-	-	-	X
6	GOL	A	4012	-	-	X	-
6	GOL	A	4013	-	-	X	-
6	GOL	B	4016	-	-	-	X
6	GOL	B	4017	-	-	-	X
6	GOL	B	4018	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4453 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 Beta-galactoside specific lectin I A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1975	1251	346	374	4			

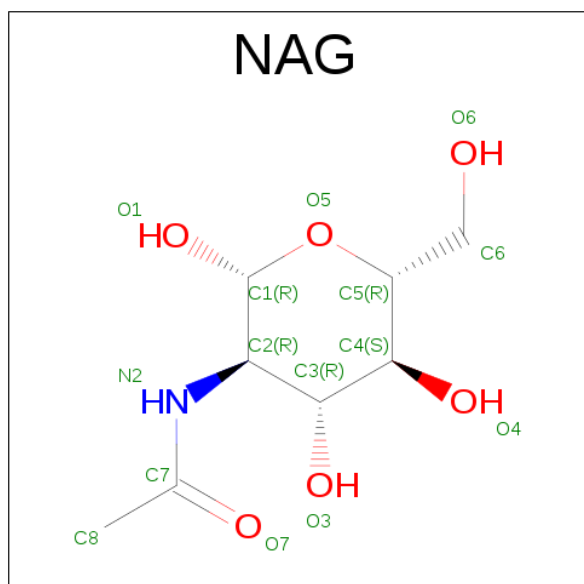
- Molecule 2 is a protein called Galactose specific lectin I B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	263	Total	C	N	O	S	0	0	0
			2029	1258	362	397	12			

There is a discrepancy between the modelled and reference sequences:

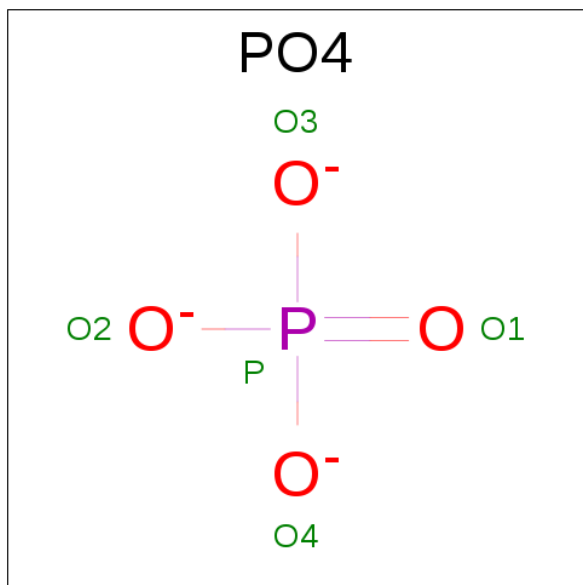
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	SEE REMARK 999	UNP P81830

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



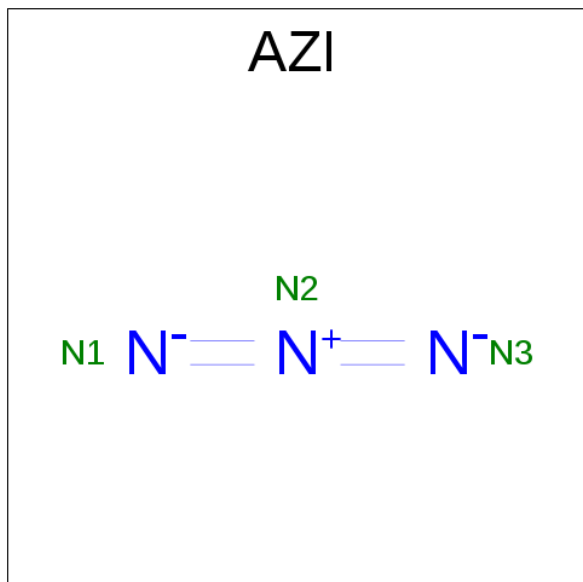
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



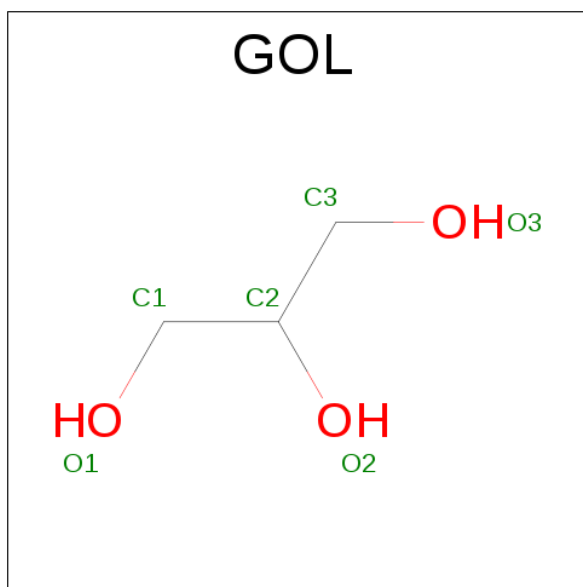
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

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



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

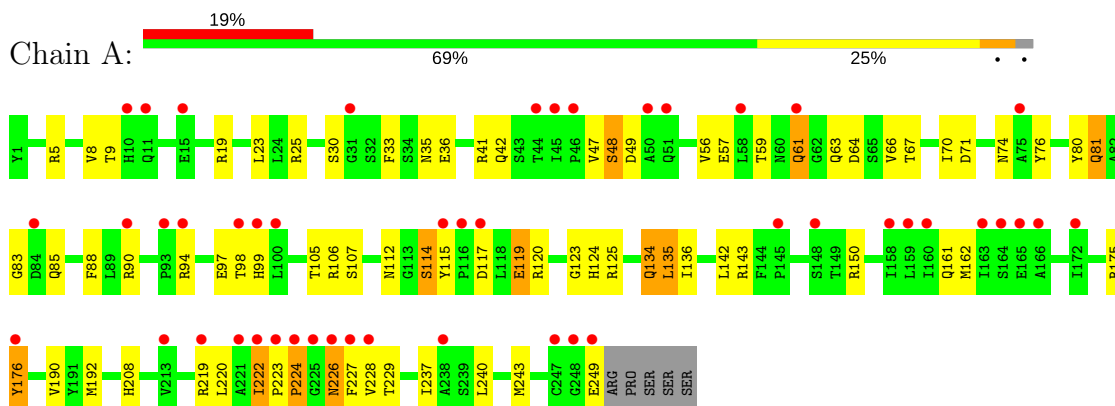
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	127	Total	O	0	0
			127	127		
7	B	214	Total	O	0	0
			214	214		

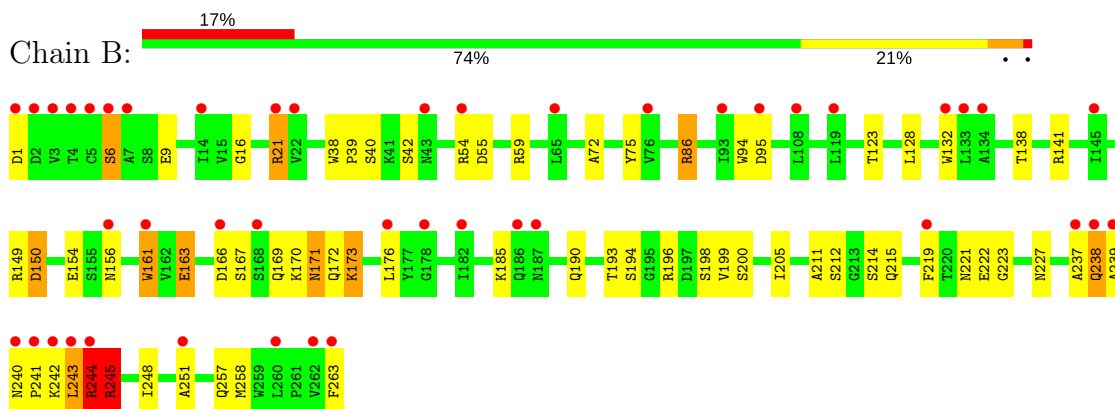
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Beta-galactoside specific lectin I A chain



- Molecule 2: Galactose specific lectin I B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	107.28Å 107.28Å 311.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.10 29.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.9 (8.00-2.10) 99.9 (29.10-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.160 , 0.223 0.179 , 0.191	Depositor DCC
R_{free} test set	3162 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 118.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4453	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, PO4, NAG, 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	0/2018	1.15	2/2748 (0.1%)
2	B	0.39	0/2069	1.21	6/2817 (0.2%)
All	All	0.38	0/4087	1.18	8/5565 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	238	GLN	C-N-CA	15.85	161.32	121.70
1	A	176	TYR	CD1-CE1-CZ	6.44	125.60	119.80
2	B	196	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	B	59	ARG	NE-CZ-NH1	-5.90	117.35	120.30
2	B	212	SER	C-N-CA	5.52	133.89	122.30
1	A	176	TYR	CG-CD1-CE1	-5.43	116.96	121.30
2	B	21	ARG	CG-CD-NE	5.36	123.05	111.80
2	B	173	LYS	CA-CB-CG	5.27	124.99	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1975	0	1944	72	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2029	0	1965	64	0
3	B	28	0	26	0	0
4	A	5	0	0	2	0
5	A	12	0	0	4	0
5	B	15	0	0	1	0
6	A	30	0	40	11	0
6	B	18	0	24	4	0
7	A	127	0	0	5	0
7	B	214	0	0	10	0
All	All	4453	0	3999	136	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 (136) 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)
2:B:128:LEU:HB2	2:B:211:ALA:HB1	1.43	0.98
1:A:119:GLU:OE2	4:A:4001:PO4:O2	1.88	0.91
1:A:143:ARG:HH21	6:A:4013:GOL:H11	1.32	0.90
2:B:238:GLN:HE22	2:B:241:PRO:HD3	1.34	0.89
6:B:4018:GOL:H32	7:B:3187:HOH:O	1.73	0.87
1:A:41:ARG:HG2	6:A:4012:GOL:C1	2.06	0.85
1:A:134:GLN:NE2	1:A:134:GLN:H	1.82	0.78
1:A:41:ARG:HG2	6:A:4012:GOL:H12	1.64	0.78
1:A:208:HIS:O	2:B:6:SER:HB3	1.85	0.75
1:A:42:GLN:HB2	6:A:4012:GOL:H32	1.69	0.74
2:B:211:ALA:HB2	7:B:3068:HOH:O	1.88	0.72
1:A:222:ILE:HG22	1:A:224:PRO:HG2	1.70	0.72
1:A:224:PRO:HB2	1:A:226:ASN:HD21	1.54	0.71
2:B:237:ALA:HB3	2:B:243:LEU:HD21	1.73	0.71
1:A:61:GLN:NE2	1:A:136:ILE:HD13	2.08	0.69
1:A:5:ARG:HG2	1:A:57:GLU:HB3	1.76	0.67
2:B:240:ASN:OD1	2:B:241:PRO:HD2	1.94	0.67
7:A:3063:HOH:O	2:B:258:MET:HE3	1.93	0.67
2:B:21:ARG:HD3	2:B:40:SER:N	2.10	0.66
1:A:9:THR:HB	1:A:61:GLN:HG2	1.77	0.65
2:B:214:SER:HA	2:B:227:ASN:HD21	1.60	0.65
1:A:162:MET:HA	1:A:176:TYR:CE1	2.32	0.65
1:A:223:PRO:HA	7:A:3322:HOH:O	1.96	0.65
1:A:134:GLN:H	1:A:134:GLN:HE21	1.46	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:SER:HB2	6:A:4012:GOL:H11	1.78	0.64
1:A:119:GLU:HG3	1:A:123:GLY:O	1.99	0.63
1:A:143:ARG:NH2	6:A:4013:GOL:H11	2.11	0.62
1:A:42:GLN:HB2	6:A:4012:GOL:C3	2.30	0.62
2:B:166:ASP:HB3	2:B:169:GLN:HB2	1.83	0.61
2:B:72:ALA:HB1	6:B:4018:GOL:H12	1.83	0.60
2:B:21:ARG:NH1	2:B:40:SER:H	1.99	0.60
1:A:162:MET:HG2	1:A:176:TYR:CE2	2.38	0.59
2:B:169:GLN:HG2	2:B:171:ASN:ND2	2.16	0.59
1:A:106:ARG:HH11	1:A:106:ARG:HB2	1.67	0.59
1:A:224:PRO:HB2	1:A:226:ASN:ND2	2.17	0.59
2:B:21:ARG:NE	2:B:40:SER:HB2	2.18	0.58
2:B:166:ASP:HB3	2:B:169:GLN:CB	2.34	0.58
1:A:143:ARG:HH21	6:A:4013:GOL:C1	2.10	0.57
1:A:33:PHE:HB2	2:B:1:ASP:O	2.03	0.57
2:B:21:ARG:N	2:B:21:ARG:HD2	2.19	0.57
1:A:175:ARG:NH1	1:A:192:MET:HB2	2.21	0.56
1:A:48:SER:HA	1:A:99:HIS:NE2	2.21	0.56
1:A:222:ILE:HG22	1:A:224:PRO:CG	2.36	0.55
1:A:9:THR:CB	1:A:61:GLN:HG2	2.37	0.54
2:B:161:TRP:HE3	2:B:244:ARG:HB3	1.73	0.54
1:A:190:VAL:HB	1:A:223:PRO:HD3	1.90	0.53
2:B:243:LEU:O	2:B:244:ARG:HB2	2.07	0.53
1:A:112:ASN:ND2	5:A:4003:AZI:N1	2.54	0.53
2:B:237:ALA:CB	2:B:243:LEU:HD21	2.39	0.53
1:A:162:MET:HA	1:A:176:TYR:CZ	2.45	0.52
1:A:67:THR:HB	1:A:81:GLN:HE21	1.73	0.52
1:A:112:ASN:OD1	1:A:114:SER:HB3	2.10	0.52
2:B:170:LYS:HG2	7:B:3267:HOH:O	2.10	0.50
2:B:72:ALA:CB	6:B:4018:GOL:H12	2.41	0.50
2:B:238:GLN:HE22	2:B:241:PRO:CD	2.16	0.50
5:A:4009:AZI:N3	2:B:150:ASP:OD2	2.45	0.50
1:A:150:ARG:HG3	1:A:150:ARG:HH11	1.76	0.50
2:B:156:ASN:CG	2:B:161:TRP:HE1	2.16	0.49
2:B:241:PRO:O	2:B:244:ARG:HA	2.12	0.49
1:A:219:ARG:HD3	1:A:229:THR:OG1	2.13	0.49
2:B:199:VAL:O	2:B:200:SER:HB2	2.13	0.49
2:B:161:TRP:CE3	2:B:244:ARG:HB3	2.48	0.48
2:B:194:SER:OG	2:B:214:SER:HB2	2.13	0.48
2:B:21:ARG:HH11	2:B:39:PRO:HA	1.77	0.48
2:B:141:ARG:HB2	2:B:176:LEU:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:SER:CB	2:B:248:ILE:HD13	2.42	0.48
1:A:161:GLN:HB3	1:A:176:TYR:OH	2.14	0.47
1:A:88:PHE:CD2	1:A:97:GLU:HG2	2.49	0.47
2:B:240:ASN:O	2:B:243:LEU:HD22	2.15	0.47
1:A:240:LEU:HD21	1:A:243:MET:HG2	1.97	0.47
2:B:21:ARG:HE	2:B:138:THR:HB	1.79	0.47
1:A:175:ARG:HH12	1:A:192:MET:HB2	1.78	0.47
2:B:243:LEU:HG	2:B:245:ARG:NH1	2.30	0.46
2:B:190:GLN:HB3	2:B:205:ILE:CG2	2.45	0.46
1:A:134:GLN:NE2	1:A:134:GLN:N	2.58	0.46
1:A:41:ARG:HG2	6:A:4012:GOL:H11	1.94	0.46
1:A:5:ARG:HD3	1:A:57:GLU:OE1	2.16	0.46
1:A:42:GLN:CB	6:A:4012:GOL:H32	2.44	0.45
2:B:154:GLU:HG2	2:B:156:ASN:OD1	2.15	0.45
2:B:21:ARG:NH2	7:B:3139:HOH:O	2.49	0.45
2:B:94:TRP:HB3	7:B:3238:HOH:O	2.17	0.45
1:A:115:TYR:CE1	1:A:125:ARG:HD3	2.51	0.45
6:A:4013:GOL:O2	7:A:3042:HOH:O	2.21	0.45
5:A:4009:AZI:N1	7:A:3340:HOH:O	2.33	0.45
1:A:8:VAL:O	1:A:8:VAL:HG23	2.17	0.45
1:A:117:ASP:O	1:A:120:ARG:HB2	2.17	0.45
1:A:83:GLY:HA3	5:A:4010:AZI:N1	2.31	0.45
1:A:115:TYR:O	1:A:119:GLU:HB2	2.17	0.44
2:B:166:ASP:N	2:B:172:GLN:OE1	2.50	0.44
2:B:75:TYR:HD1	7:B:3110:HOH:O	1.99	0.44
1:A:42:GLN:NE2	1:A:249:GLU:HA	2.32	0.44
1:A:59:THR:HA	1:A:64:ASP:O	2.18	0.44
2:B:222:GLU:HB3	7:B:3202:HOH:O	2.16	0.44
1:A:85:GLN:NE2	1:A:105:THR:HB	2.33	0.44
2:B:237:ALA:O	2:B:243:LEU:HD22	2.17	0.43
1:A:220:LEU:HB2	1:A:228:VAL:HG13	1.99	0.43
1:A:56:VAL:HG23	1:A:56:VAL:O	2.19	0.43
1:A:106:ARG:NH1	1:A:106:ARG:HB2	2.33	0.43
1:A:223:PRO:HG2	1:A:224:PRO:HD2	2.01	0.43
1:A:61:GLN:H	1:A:61:GLN:HG3	1.21	0.43
2:B:190:GLN:HE21	2:B:205:ILE:HG22	1.83	0.43
2:B:163:GLU:OE1	2:B:244:ARG:NH1	2.52	0.42
1:A:48:SER:HA	1:A:99:HIS:CD2	2.54	0.42
2:B:141:ARG:HB3	2:B:263:PHE:CE2	2.54	0.42
2:B:251:ALA:HA	2:B:257:GLN:OE1	2.20	0.42
1:A:224:PRO:CB	1:A:226:ASN:HD21	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:HB3	1:A:74:ASN:OD1	2.20	0.42
2:B:193:THR:HA	2:B:214:SER:O	2.20	0.42
2:B:170:LYS:HZ3	2:B:185:LYS:HZ3	1.66	0.42
1:A:135:LEU:HA	1:A:135:LEU:HD12	1.83	0.42
2:B:222:GLU:HA	7:B:3202:HOH:O	2.19	0.42
1:A:124:HIS:HB3	4:A:4001:PO4:O4	2.20	0.42
2:B:240:ASN:O	2:B:243:LEU:HB3	2.19	0.42
2:B:243:LEU:CD1	2:B:245:ARG:HH12	2.33	0.42
1:A:90:ARG:O	1:A:112:ASN:HB3	2.20	0.41
1:A:90:ARG:NH2	7:A:3308:HOH:O	2.52	0.41
1:A:35:ASN:O	1:A:36:GLU:HB2	2.21	0.41
1:A:70:ILE:HA	1:A:76:TYR:O	2.20	0.41
1:A:47:VAL:HG21	1:A:94:ARG:O	2.21	0.41
2:B:211:ALA:HA	2:B:215:GLN:OE1	2.20	0.41
2:B:9:GLU:OE2	2:B:54:ARG:HB2	2.20	0.41
2:B:194:SER:O	2:B:214:SER:OG	2.35	0.41
2:B:219:PHE:O	5:B:4007:AZI:N1	2.53	0.41
1:A:80:TYR:CZ	1:A:142:LEU:HD22	2.56	0.41
2:B:194:SER:HB2	2:B:248:ILE:HD13	2.02	0.41
1:A:237:ILE:O	2:B:221:ASN:HA	2.20	0.41
2:B:223:GLY:HA2	7:B:3263:HOH:O	2.20	0.41
1:A:150:ARG:HG3	1:A:150:ARG:NH1	2.34	0.41
2:B:123:THR:OG1	6:B:4018:GOL:H2	2.21	0.41
2:B:55:ASP:HB2	2:B:86:ARG:HH12	1.86	0.40
1:A:88:PHE:CG	1:A:97:GLU:HG2	2.56	0.40
2:B:16:GLY:HA3	2:B:132:TRP:CE3	2.56	0.40
1:A:88:PHE:CZ	1:A:97:GLU:HA	2.57	0.40
2:B:75:TYR:HB3	7:B:3110:HOH:O	2.21	0.40
2:B:38:TRP:CG	2:B:39:PRO:HD2	2.57	0.40
1:A:115:TYR:O	1:A:119:GLU:OE1	2.39	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	247/254 (97%)	236 (96%)	8 (3%)	3 (1%)	15	9
2	B	261/263 (99%)	247 (95%)	11 (4%)	3 (1%)	17	11
All	All	508/517 (98%)	483 (95%)	19 (4%)	6 (1%)	15	9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
2	B	239	ALA
2	B	244	ARG
2	B	245	ARG
1	A	48	SER
1	A	224	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	216/221 (98%)	200 (93%)	16 (7%)	16	12
2	B	224/224 (100%)	208 (93%)	16 (7%)	17	13
All	All	440/445 (99%)	408 (93%)	32 (7%)	16	13

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	23	LEU
1	A	25	ARG
1	A	61	GLN
1	A	63	GLN
1	A	66	VAL
1	A	81	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	98	THR
1	A	107	SER
1	A	114	SER
1	A	119	GLU
1	A	134	GLN
1	A	135	LEU
1	A	222	ILE
1	A	226	ASN
1	A	227	PHE
2	B	6	SER
2	B	42	SER
2	B	86	ARG
2	B	95	ASP
2	B	149	ARG
2	B	150	ASP
2	B	161	TRP
2	B	163	GLU
2	B	167	SER
2	B	171	ASN
2	B	173	LYS
2	B	198	SER
2	B	242	LYS
2	B	243	LEU
2	B	244	ARG
2	B	245	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	42	GLN
1	A	61	GLN
1	A	81	GLN
1	A	85	GLN
1	A	127	GLN
1	A	134	GLN
1	A	152	GLN
1	A	208	HIS
1	A	226	ASN
2	B	30	HIS
2	B	44	ASN
2	B	61	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	169	GLN
2	B	171	ASN
2	B	190	GLN
2	B	238	GLN

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](#)

20 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	$\# Z > 2$
4	PO4	A	4001	-	4,4,4	0.67	0	6,6,6	0.81	0
5	AZI	A	4003	-	0,2,2	0.00	-	0,1,1	0.00	-
5	AZI	A	4006	-	0,2,2	0.00	-	0,1,1	0.00	-
5	AZI	A	4009	-	0,2,2	0.00	-	0,1,1	0.00	-
5	AZI	A	4010	-	0,2,2	0.00	-	0,1,1	0.00	-
6	GOL	A	4011	-	5,5,5	0.93	0	5,5,5	0.99	0
6	GOL	A	4012	-	5,5,5	0.69	0	5,5,5	1.65	2 (40%)
6	GOL	A	4013	-	5,5,5	0.59	0	5,5,5	0.66	0
6	GOL	A	4014	-	5,5,5	0.22	0	5,5,5	0.98	0
6	GOL	A	4015	-	5,5,5	0.55	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	AZI	B	4002	-	0,2,2	0.00	-	0,1,1	0.00	-
5	AZI	B	4004	-	0,2,2	0.00	-	0,1,1	0.00	-
5	AZI	B	4005	-	0,2,2	0.00	-	0,1,1	0.00	-
5	AZI	B	4007	-	0,2,2	0.00	-	0,1,1	0.00	-
5	AZI	B	4008	-	0,2,2	0.00	-	0,1,1	0.00	-
6	GOL	B	4016	-	5,5,5	1.17	0	5,5,5	1.44	1 (20%)
6	GOL	B	4017	-	5,5,5	0.68	0	5,5,5	1.08	0
6	GOL	B	4018	-	5,5,5	0.67	0	5,5,5	1.91	2 (40%)
3	NAG	B	5001	2	14,14,15	1.18	2 (14%)	15,19,21	1.91	6 (40%)
3	NAG	B	5002	2	14,14,15	1.27	2 (14%)	15,19,21	2.38	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PO4	A	4001	-	-	0/0/0/0	0/0/0/0
5	AZI	A	4003	-	-	0/0/0/0	0/0/0/0
5	AZI	A	4006	-	-	0/0/0/0	0/0/0/0
5	AZI	A	4009	-	-	0/0/0/0	0/0/0/0
5	AZI	A	4010	-	-	0/0/0/0	0/0/0/0
6	GOL	A	4011	-	-	0/4/4/4	0/0/0/0
6	GOL	A	4012	-	-	0/4/4/4	0/0/0/0
6	GOL	A	4013	-	-	0/4/4/4	0/0/0/0
6	GOL	A	4014	-	-	0/4/4/4	0/0/0/0
6	GOL	A	4015	-	-	0/4/4/4	0/0/0/0
5	AZI	B	4002	-	-	0/0/0/0	0/0/0/0
5	AZI	B	4004	-	-	0/0/0/0	0/0/0/0
5	AZI	B	4005	-	-	0/0/0/0	0/0/0/0
5	AZI	B	4007	-	-	0/0/0/0	0/0/0/0
5	AZI	B	4008	-	-	0/0/0/0	0/0/0/0
6	GOL	B	4016	-	-	0/4/4/4	0/0/0/0
6	GOL	B	4017	-	-	0/4/4/4	0/0/0/0
6	GOL	B	4018	-	-	0/4/4/4	0/0/0/0
3	NAG	B	5001	2	-	0/6/23/26	0/1/1/1
3	NAG	B	5002	2	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5001	NAG	O5-C1	-2.75	1.39	1.43
3	B	5001	NAG	O7-C7	-2.28	1.17	1.23
3	B	5002	NAG	C1-C2	2.15	1.55	1.52
3	B	5002	NAG	O7-C7	3.04	1.30	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5001	NAG	O7-C7-N2	-3.33	115.50	121.92
3	B	5002	NAG	C8-C7-N2	-3.27	110.19	116.11
6	B	4018	GOL	C3-C2-C1	-2.81	100.37	111.52
3	B	5001	NAG	C3-C4-C5	-2.69	105.48	110.22
3	B	5001	NAG	O5-C1-C2	-2.55	107.92	111.47
6	A	4012	GOL	O1-C1-C2	-2.07	99.65	110.07
3	B	5001	NAG	O4-C4-C5	2.27	115.01	109.28
3	B	5001	NAG	C8-C7-N2	2.30	120.26	116.11
6	B	4018	GOL	O3-C3-C2	2.34	121.85	110.07
3	B	5002	NAG	O4-C4-C5	2.55	115.71	109.28
6	A	4012	GOL	O2-C2-C3	2.62	121.19	108.84
6	B	4016	GOL	O3-C3-C2	2.74	123.86	110.07
3	B	5002	NAG	O7-C7-N2	2.85	127.40	121.92
3	B	5001	NAG	O4-C4-C3	3.13	117.17	110.36
3	B	5002	NAG	C1-O5-C5	7.03	121.85	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4001	PO4	2	0
5	A	4003	AZI	1	0
5	A	4009	AZI	2	0
5	A	4010	AZI	1	0
6	A	4012	GOL	7	0
6	A	4013	GOL	4	0
5	B	4007	AZI	1	0
6	B	4018	GOL	4	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, 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	249/254 (98%)	1.03	47 (18%)	1 1	43, 61, 106, 138	0
2	B	263/263 (100%)	0.84	44 (16%)	2 2	35, 50, 96, 137	0
All	All	512/517 (99%)	0.93	91 (17%)	2 2	35, 55, 102, 138	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	239	ALA	8.6
1	A	225	GLY	8.0
2	B	243	LEU	7.7
2	B	5	CYS	7.4
1	A	226	ASN	7.2
1	A	98	THR	6.8
2	B	240	ASN	6.8
1	A	227	PHE	6.4
1	A	222	ILE	6.0
1	A	224	PRO	5.8
1	A	145	PRO	5.1
2	B	1	ASP	5.1
2	B	263	PHE	4.8
1	A	249	GLU	4.8
2	B	156	ASN	4.8
1	A	223	PRO	4.7
1	A	46	PRO	4.6
1	A	99	HIS	4.5
1	A	50	ALA	4.4
2	B	14	ILE	4.4
2	B	242	LYS	4.4
2	B	168	SER	4.3
1	A	115	TYR	4.2
1	A	248	GLY	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	247	CYS	3.8
2	B	22	VAL	3.8
1	A	172	ILE	3.8
2	B	6	SER	3.7
1	A	15	GLU	3.5
2	B	244	ARG	3.4
1	A	116	PRO	3.3
1	A	158	ILE	3.3
2	B	182	ILE	3.2
2	B	7	ALA	3.2
1	A	219	ARG	3.2
1	A	238	ALA	3.2
2	B	21	ARG	3.2
1	A	44	THR	3.2
1	A	148	SER	3.1
1	A	159	LEU	3.1
2	B	176	LEU	3.1
2	B	260	LEU	3.1
1	A	11	GLN	3.0
2	B	132	TRP	3.0
1	A	45	ILE	2.9
2	B	2	ASP	2.9
1	A	176	TYR	2.9
1	A	221	ALA	2.9
1	A	51	GLN	2.8
2	B	238	GLN	2.8
1	A	160	ILE	2.8
2	B	95	ASP	2.7
1	A	94	ARG	2.7
2	B	93	ILE	2.7
2	B	166	ASP	2.7
2	B	241	PRO	2.7
2	B	4	THR	2.6
1	A	166	ALA	2.6
2	B	54	ARG	2.5
2	B	237	ALA	2.5
2	B	251	ALA	2.5
1	A	31	GLY	2.5
1	A	10	HIS	2.5
2	B	43	ASN	2.5
2	B	108	LEU	2.4
2	B	133	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	3	VAL	2.4
2	B	187	ASN	2.4
2	B	76	VAL	2.4
1	A	90	ARG	2.4
1	A	164	SER	2.3
1	A	117	ASP	2.3
2	B	262	VAL	2.3
2	B	186	GLN	2.3
1	A	58	LEU	2.3
1	A	228	VAL	2.3
1	A	61	GLN	2.3
2	B	65	LEU	2.3
1	A	75	ALA	2.3
2	B	145	ILE	2.3
2	B	119	LEU	2.2
1	A	84	ASP	2.2
2	B	134	ALA	2.2
1	A	163	ILE	2.1
1	A	213	VAL	2.1
2	B	219	PHE	2.1
1	A	165	GLU	2.1
2	B	161	TRP	2.1
2	B	178	GLY	2.1
1	A	100	LEU	2.0
1	A	93	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, 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	AZI	B	4005	3/3	0.86	0.56	16.15	60,60,78,80	0
5	AZI	A	4009	3/3	0.85	0.68	12.14	88,88,94,96	0
5	AZI	A	4006	3/3	0.80	0.81	11.30	90,90,90,99	0
5	AZI	B	4007	3/3	0.57	0.82	9.68	89,89,93,93	0
5	AZI	B	4008	3/3	0.02	0.61	5.66	111,111,113,113	0
6	GOL	B	4016	6/6	0.95	0.20	3.68	59,62,70,75	0
6	GOL	B	4017	6/6	0.80	0.17	2.00	94,98,100,106	0
4	PO4	A	4001	5/5	0.94	0.21	1.53	95,95,97,99	0
6	GOL	A	4015	6/6	0.79	0.28	0.33	104,107,109,110	0
6	GOL	A	4012	6/6	0.89	0.21	-0.24	104,106,107,110	0
3	NAG	B	5001	14/15	0.92	0.14	-0.45	70,77,83,85	0
5	AZI	A	4003	3/3	0.76	0.15	-1.51	102,102,103,105	0
6	GOL	A	4014	6/6	0.86	0.10	-	114,115,116,123	0
6	GOL	A	4011	6/6	0.36	0.30	-	112,119,120,120	0
5	AZI	A	4010	3/3	0.28	0.46	-	128,128,132,134	0
6	GOL	A	4013	6/6	0.66	0.30	-	116,120,123,127	0
3	NAG	B	5002	14/15	0.70	0.30	-	92,102,109,114	0
6	GOL	B	4018	6/6	0.83	0.27	-	72,78,88,91	0
5	AZI	B	4002	3/3	0.74	0.39	-	124,124,128,131	0
5	AZI	B	4004	3/3	0.94	0.22	-	82,82,86,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.