



Full wwPDB X-ray Structure Validation Report

May 19, 2014 – 09:58 PM EDT

PDB ID : 4JKX
Title : Crystal structure Mistletoe Lectin I from Viscum album in complex with kinetin at 2.35 Å resolution.
Authors : Prokofev, I.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Meyer, A.; Barciszewski, J.; Betzel, C.; Mikhailov, A.M.
Deposited on : 2013-03-12
Resolution : 2.35 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>

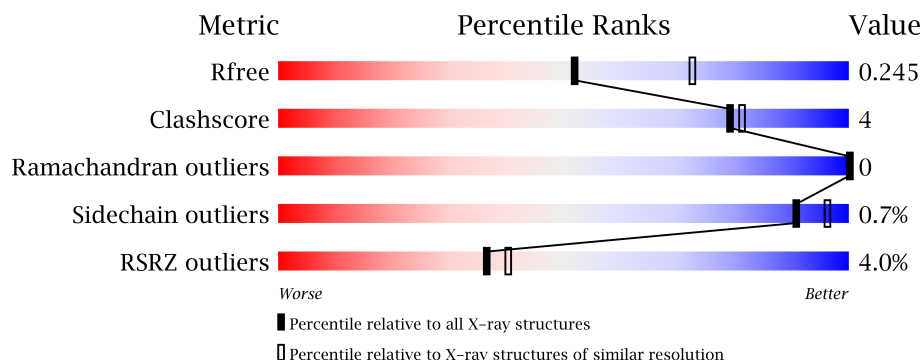
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
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) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.35 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	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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	249	
2	B	263	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	B	313	-	X
5	GOL	B	315	-	X
5	GOL	B	317	-	X
5	GOL	B	318	-	X
5	GOL	B	319	-	X
6	H35	A	305	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
7	EDO	B	309	-	X
9	AZI	B	301	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 4402 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 Beta-galactoside-specific lectin 1 A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	1	0
			1949	1234	339	372	4			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ALA	GLU	SEE REMARK 999	UNP P81446
A	19	SER	ARG	SEE REMARK 999	UNP P81446
A	36	GLN	GLU	SEE REMARK 999	UNP P81446
A	49	GLU	ASP	SEE REMARK 999	UNP P81446
A	50	GLY	ALA	SEE REMARK 999	UNP P81446
A	61	ALA	GLU	SEE REMARK 999	UNP P81446
A	90	LYS	ARG	SEE REMARK 999	UNP P81446
A	94	ALA	ARG	SEE REMARK 999	UNP P81446
A	99	GLN	HIS	SEE REMARK 999	UNP P81446
A	100	ASP	LEU	SEE REMARK 999	UNP P81446
A	208	HIS	GLN	SEE REMARK 999	UNP P81446
A	222	LEU	ILE	SEE REMARK 999	UNP P81446
A	223	ALA	PRO	SEE REMARK 999	UNP P81446
A	225	ALA	GLY	SEE REMARK 999	UNP P81446
A	227	ILE	PHE	SEE REMARK 999	UNP P81446

- Molecule 2 is a protein called Beta-galactoside-specific lectin 1 B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	263	Total	C	N	O	S	0	1	0
			2009	1244	356	396	13			

There are 9 discrepancies between the modelled and reference sequences:

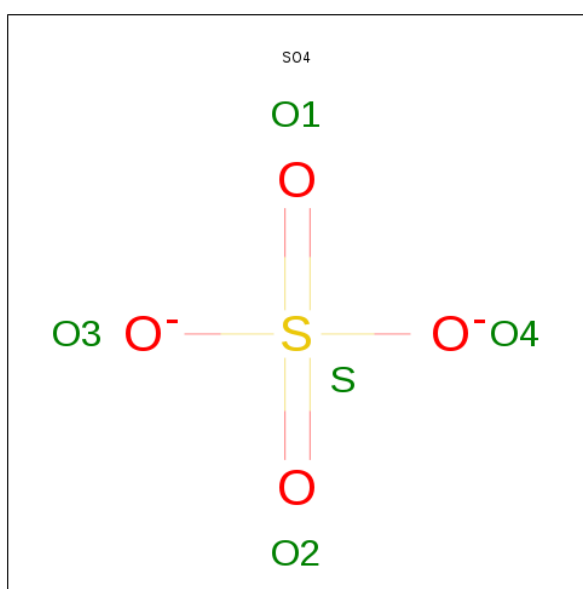
Chain	Residue	Modelled	Actual	Comment	Reference
B	21	THR	CYS	SEE REMARK 999	UNP P81446

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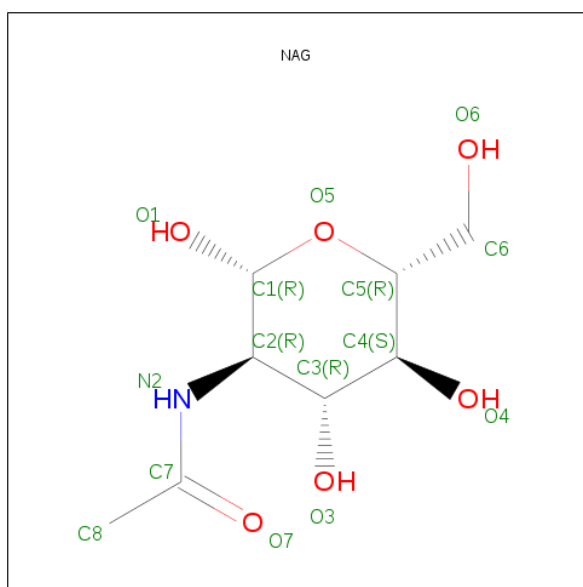
Chain	Residue	Modelled	Actual	Comment	Reference
B	54	LYS	ARG	SEE REMARK 999	UNP P81446
B	90	ILE	LEU	SEE REMARK 999	UNP P81446
B	167	ALA	ILE	SEE REMARK 999	UNP P81446
B	189	SER	ASP	SEE REMARK 999	UNP P81446
B	222	ALA	GLU	SEE REMARK 999	UNP P81446
B	242	SER	LYS	SEE REMARK 999	UNP P81446
B	244	GLN	ARG	SEE REMARK 999	UNP P81446
B	254	ASN	LYS	SEE REMARK 999	UNP P81446

- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



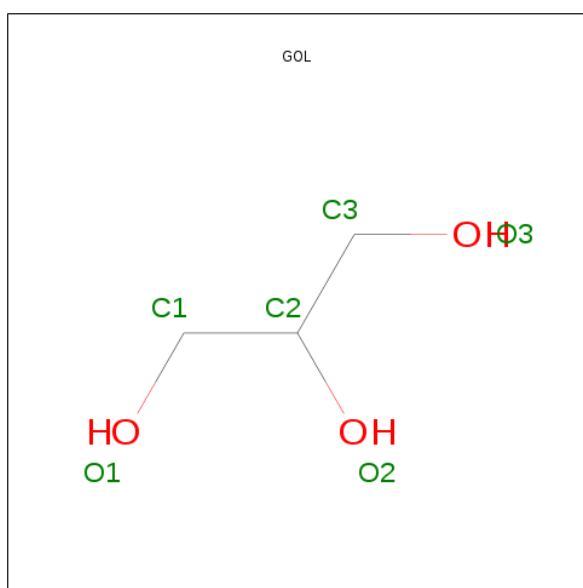
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



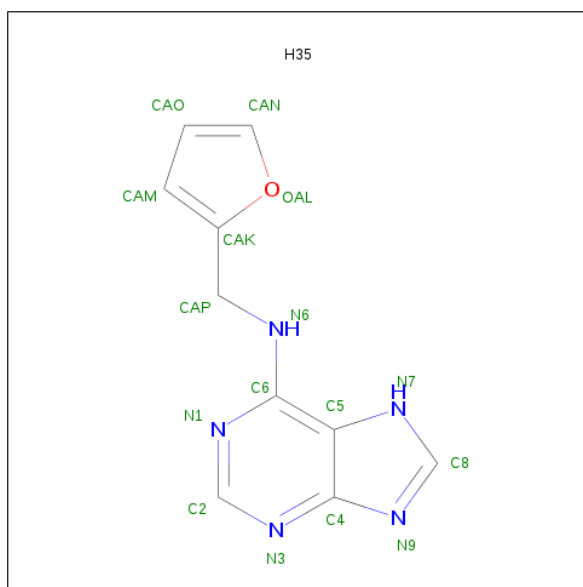
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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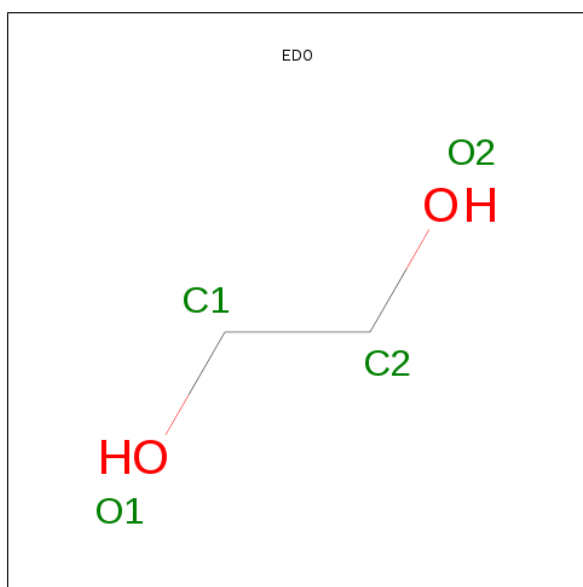
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is N-(FURAN-2-YLMETHYL)-7H-PURIN-6-AMINE (three-letter code: H35) (formula: C₁₀H₉N₅O).



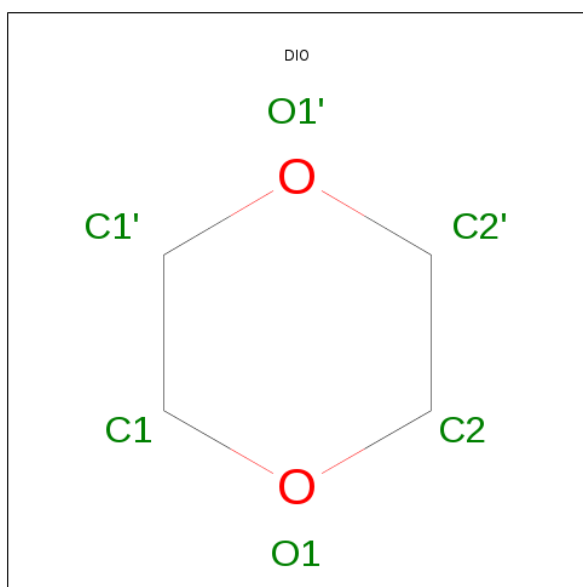
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			16	10	5	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



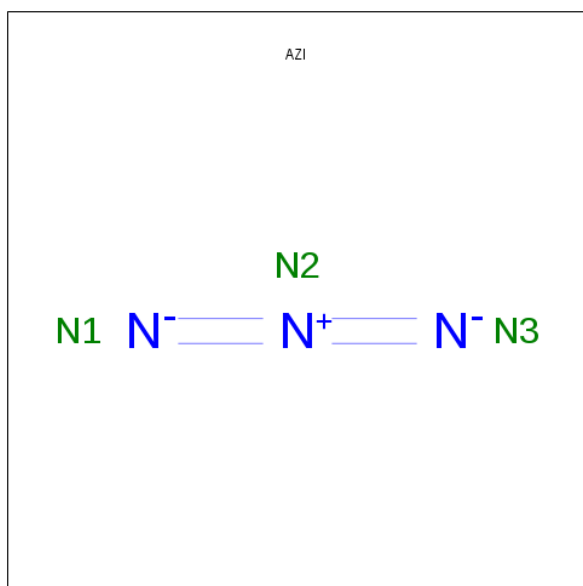
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 9 is AZIDE ION (three-letter code: AZI) (formula: N_3).



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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Cl 1 1	0	0
10	A	1	Total Cl 1 1	0	0

- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	2	Total C N O 28 16 2 10	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	THR	CYS	SEE REMARK 999	UNP P81446
B	54	LYS	ARG	SEE REMARK 999	UNP P81446
B	90	ILE	LEU	SEE REMARK 999	UNP P81446
B	167	ALA	ILE	SEE REMARK 999	UNP P81446
B	189	SER	ASP	SEE REMARK 999	UNP P81446
B	222	ALA	GLU	SEE REMARK 999	UNP P81446
B	242	SER	LYS	SEE REMARK 999	UNP P81446
B	244	GLN	ARG	SEE REMARK 999	UNP P81446
B	254	ASN	LYS	SEE REMARK 999	UNP P81446

- Molecule 12 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	3	Total C N O 42 24 3 15	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	THR	CYS	SEE REMARK 999	UNP P81446
B	54	LYS	ARG	SEE REMARK 999	UNP P81446
B	90	ILE	LEU	SEE REMARK 999	UNP P81446
B	167	ALA	ILE	SEE REMARK 999	UNP P81446
B	189	SER	ASP	SEE REMARK 999	UNP P81446
B	222	ALA	GLU	SEE REMARK 999	UNP P81446
B	242	SER	LYS	SEE REMARK 999	UNP P81446
B	244	GLN	ARG	SEE REMARK 999	UNP P81446
B	254	ASN	LYS	SEE REMARK 999	UNP P81446

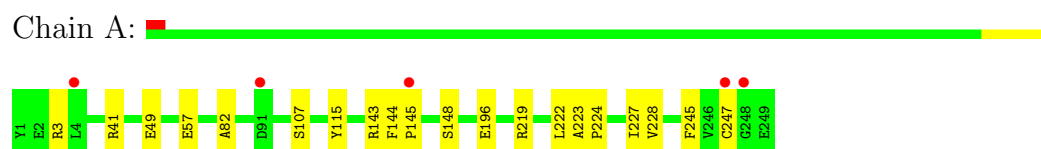
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	137	Total 137	O 137	0	0
13	A	73	Total 73	O 73	0	0

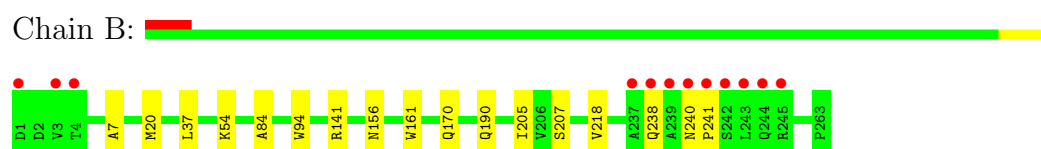
3 Residue-property plots

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: Beta-galactoside-specificlectin 1 A chain



- Molecule 2: Beta-galactoside-specificlectin 1 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	107.01Å 107.01Å 312.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.70 – 2.35 79.70 – 2.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (79.70-2.35) 98.8 (79.70-2.08)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.248 0.227 , 0.245	Depositor DCC
R_{free} test set	3177 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 63529 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4402	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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: AZI, GOL, DIO, NAG, CL, EDO, SO4, H35

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	0.41	0/1991	0.53	0/2711
2	B	0.43	0/2052	0.57	0/2800
All	All	0.42	0/4043	0.55	0/5511

There are no bond length outliers.

There are no bond angle outliers.

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	1949	0	1933	16	0
2	B	2009	0	1939	12	0
3	A	25	0	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	1	0
5	A	18	0	24	1	0
5	B	42	0	56	4	0
6	A	16	0	9	7	0
7	A	4	0	6	0	0
7	B	20	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	6	0	8	1	0
9	B	3	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	B	28	0	25	1	0
12	B	42	0	37	0	0
13	A	73	0	0	0	0
13	B	137	0	0	1	0
All	All	4402	0	4093	29	0

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 4.

All (29) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148:SER:HB2	5:A:303:GOL:H2	1.75	0.69
1:A:245:PHE:HE1	1:A:247:CYS:O	1.77	0.66
1:A:222:LEU:HD11	1:A:228:VAL:HG13	1.77	0.66
1:A:115:TYR:HB2	6:A:305:H35:N7	2.12	0.65
1:A:115:TYR:N	6:A:305:H35:H7	1.95	0.64
2:B:170:GLN:HB2	5:B:318:GOL:H32	1.78	0.64
2:B:141:ARG:HD3	7:B:309:EDO:H12	1.85	0.59
4:B:307:NAG:H62	13:B:528:HOH:O	2.05	0.56
2:B:20:MET:HB2	2:B:37:LEU:HG	1.89	0.53
2:B:207:SER:H	7:B:311:EDO:H11	1.72	0.53
1:A:219:ARG:HH21	1:A:227:ILE:HG21	1.77	0.49
2:B:156:ASN:HD22	2:B:161:TRP:HD1	1.59	0.48
2:B:7:ALA:HB1	2:B:54:LYS:HD3	1.97	0.47
1:A:115:TYR:HB2	6:A:305:H35:H7	1.80	0.45
2:B:84:ALA:HA	5:B:315:GOL:H31	1.97	0.45
1:A:144:PHE:HA	1:A:145:PRO:HD3	1.85	0.45
1:A:82:ALA:HB1	1:A:143:ARG:HA	1.98	0.45
1:A:196:GLU:HB3	6:A:305:H35:N1	2.31	0.45
1:A:115:TYR:H	6:A:305:H35:H7	1.63	0.44
1:A:41:ARG:HE	8:A:307:DIO:H1'2	1.83	0.43
2:B:190:GLN:HB3	2:B:205:ILE:HG22	2.01	0.43
1:A:3:ARG:NH1	1:A:57:GLU:OE1	2.49	0.42
2:B:94:TRP:CG	11:B:302:NAG:H62	2.55	0.42
1:A:115:TYR:CB	6:A:305:H35:H7	2.32	0.42
1:A:115:TYR:N	6:A:305:H35:N7	2.63	0.42
2:B:170:GLN:HG2	5:B:318:GOL:H11	2.02	0.41
2:B:240:ASN:HA	2:B:241:PRO:HD2	1.96	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:ALA:HB3	1:A:224:PRO:HD3	2.03	0.41
2:B:218:VAL:HG11	5:B:319:GOL:H12	2.04	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	248/249 (100%)	239 (96%)	9 (4%)	0	100	100
2	B	262/263 (100%)	249 (95%)	13 (5%)	0	100	100
All	All	510/512 (100%)	488 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	212/211 (100%)	210 (99%)	2 (1%)	87	94
2	B	222/221 (100%)	221 (100%)	1 (0%)	94	98
All	All	434/432 (100%)	431 (99%)	3 (1%)	91	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLU
1	A	107	SER
2	B	238	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

5 carbohydrates 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	$\# Z > 2$
11	NAG	B	302	11,2	12,14,15	0.66	0	15,19,21	1.16	2 (13%)
11	NAG	B	303	11	12,14,15	0.69	1 (8%)	15,19,21	0.76	0
12	NAG	B	304	12,2	12,14,15	0.83	1 (8%)	15,19,21	1.04	1 (6%)
12	NAG	B	305	12	12,14,15	0.77	1 (8%)	15,19,21	1.15	1 (6%)
12	NAG	B	306	12	12,14,15	0.57	0	15,19,21	1.18	2 (13%)

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
11	NAG	B	302	11,2	-	0/6/23/26	0/1/1/1
11	NAG	B	303	11	-	0/6/23/26	0/1/1/1
12	NAG	B	304	12,2	-	0/6/23/26	0/1/1/1
12	NAG	B	305	12	-	0/6/23/26	0/1/1/1
12	NAG	B	306	12	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	304	NAG	O5-C5	-2.33	1.41	1.45
12	B	305	NAG	O5-C5	-2.22	1.42	1.45
11	B	303	NAG	O5-C5	-2.03	1.42	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	305	NAG	O4-C4-C3	3.03	117.13	110.36
11	B	302	NAG	O5-C5-C6	2.81	109.93	106.98
12	B	304	NAG	C3-C2-N2	-2.80	107.42	111.62
12	B	306	NAG	O5-C5-C6	2.21	109.30	106.98
11	B	302	NAG	C2-N2-C7	2.21	126.07	123.39
12	B	306	NAG	O5-C5-C4	2.17	113.41	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 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$
3	SO4	A	301	-	4,4,4	0.17	0	6,6,6	0.14	0
4	NAG	A	302	1	12,14,15	0.75	1 (8%)	15,19,21	1.11	1 (6%)
5	GOL	A	303	-	5,5,5	0.37	0	5,5,5	0.21	0
5	GOL	A	304	-	5,5,5	0.38	0	5,5,5	0.26	0
6	H35	A	305	-	18,18,18	5.23	7 (38%)	21,24,24	2.73	8 (38%)
7	EDO	A	306	-	3,3,3	0.51	0	2,2,2	0.48	0
8	DIO	A	307	-	6,6,6	0.50	0	6,6,6	0.70	0
5	GOL	A	308	-	5,5,5	0.37	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	309	-	4,4,4	0.22	0	6,6,6	0.12	0
3	SO4	A	310	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	311	-	4,4,4	0.22	0	6,6,6	0.09	0
3	SO4	A	312	-	4,4,4	0.22	0	6,6,6	0.11	0
9	AZI	B	301	-	2,2,2	1.17	0	0,1,1	0.00	-
4	NAG	B	307	2	12,14,15	0.81	0	15,19,21	1.92	6 (40%)
7	EDO	B	308	-	3,3,3	0.54	0	2,2,2	0.23	0
7	EDO	B	309	-	3,3,3	0.55	0	2,2,2	0.30	0
7	EDO	B	310	-	3,3,3	0.53	0	2,2,2	0.38	0
7	EDO	B	311	-	3,3,3	0.50	0	2,2,2	0.46	0
7	EDO	B	312	-	3,3,3	0.47	0	2,2,2	0.50	0
5	GOL	B	313	-	5,5,5	0.49	0	5,5,5	0.63	0
5	GOL	B	314	-	5,5,5	0.38	0	5,5,5	0.14	0
5	GOL	B	315	-	5,5,5	0.39	0	5,5,5	0.35	0
5	GOL	B	316	-	5,5,5	0.33	0	5,5,5	0.21	0
5	GOL	B	317	-	5,5,5	0.33	0	5,5,5	0.22	0
5	GOL	B	318	-	5,5,5	0.38	0	5,5,5	0.21	0
5	GOL	B	319	-	5,5,5	0.33	0	5,5,5	0.21	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
3	SO4	A	301	-	-	0/0/0/0	0/0/0/0
4	NAG	A	302	1	-	0/6/23/26	0/1/1/1
5	GOL	A	303	-	-	0/4/4/4	0/0/0/0
5	GOL	A	304	-	-	0/4/4/4	0/0/0/0
6	H35	A	305	-	-	0/4/5/5	0/3/3/3
7	EDO	A	306	-	-	0/1/1/1	0/0/0/0
8	DIO	A	307	-	-	0/0/6/6	0/1/1/1
5	GOL	A	308	-	-	0/4/4/4	0/0/0/0
3	SO4	A	309	-	-	0/0/0/0	0/0/0/0
3	SO4	A	310	-	-	0/0/0/0	0/0/0/0
3	SO4	A	311	-	-	0/0/0/0	0/0/0/0
3	SO4	A	312	-	-	0/0/0/0	0/0/0/0
9	AZI	B	301	-	-	0/0/0/0	0/0/0/0
4	NAG	B	307	2	-	0/6/23/26	0/1/1/1
7	EDO	B	308	-	-	0/1/1/1	0/0/0/0
7	EDO	B	309	-	-	0/1/1/1	0/0/0/0
7	EDO	B	310	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	311	-	-	0/1/1/1	0/0/0/0
7	EDO	B	312	-	-	0/1/1/1	0/0/0/0
5	GOL	B	313	-	-	0/4/4/4	0/0/0/0
5	GOL	B	314	-	-	0/4/4/4	0/0/0/0
5	GOL	B	315	-	-	0/4/4/4	0/0/0/0
5	GOL	B	316	-	-	0/4/4/4	0/0/0/0
5	GOL	B	317	-	-	0/4/4/4	0/0/0/0
5	GOL	B	318	-	-	0/4/4/4	0/0/0/0
5	GOL	B	319	-	-	0/4/4/4	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	305	H35	C8-N7	17.67	1.54	1.34
6	A	305	H35	C5-C4	-8.98	1.27	1.39
6	A	305	H35	C8-N9	5.40	1.45	1.34
6	A	305	H35	C6-N6	5.36	1.44	1.34
6	A	305	H35	OAL-CAN	3.95	1.43	1.35
6	A	305	H35	OAL-CAK	2.88	1.43	1.36
6	A	305	H35	C4-N9	2.66	1.39	1.35
4	A	302	NAG	O5-C5	-2.30	1.41	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	305	H35	C4-C5-N7	6.79	113.38	106.02
6	A	305	H35	CAN-OAL-CAK	-5.58	105.23	106.52
6	A	305	H35	C8-N7-C5	-4.70	105.17	108.52
4	B	307	NAG	O5-C5-C4	4.01	115.74	110.65
6	A	305	H35	N7-C8-N9	-3.70	103.13	111.66
6	A	305	H35	C6-C5-C4	3.41	121.35	117.48
6	A	305	H35	OAL-CAK-CAP	3.21	124.62	116.30
4	B	307	NAG	C2-N2-C7	-2.85	119.95	123.39
4	B	307	NAG	O5-C5-C6	2.81	109.93	106.98
4	B	307	NAG	C6-C5-C4	-2.50	106.93	113.04
4	B	307	NAG	C3-C4-C5	2.35	114.38	110.17
4	A	302	NAG	O5-C5-C6	2.33	109.42	106.98
6	A	305	H35	OAL-CAN-CAO	-2.23	109.60	111.35
4	B	307	NAG	C4-C3-C2	-2.19	106.14	110.74
6	A	305	H35	C5-C4-N3	-2.02	123.05	125.86

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	249/249 (100%)	0.48	5 (2%) 62 65	38, 52, 71, 79	0
2	B	263/263 (100%)	0.60	12 (4%) 31 35	32, 44, 70, 85	0
All	All	512/512 (100%)	0.54	17 (3%) 36 48	32, 49, 72, 85	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	238	GLN	5.5
2	B	240	ASN	4.9
1	A	248	GLY	4.8
2	B	239	ALA	4.6
1	A	247	CYS	3.9
2	B	241	PRO	2.9
2	B	237	ALA	2.9
2	B	1	ASP	2.9
2	B	243	LEU	2.8
2	B	245	ARG	2.8
2	B	242	SER	2.6
2	B	4	THR	2.5
2	B	3	VAL	2.4
1	A	91	ASP	2.1
2	B	244	GLN	2.1
1	A	145	PRO	2.0
1	A	4	LEU	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

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
11	NAG	B	302	14/15	0.17	1.36	63,69,71,76	0
11	NAG	B	303	14/15	0.18	-0.20	80,82,84,85	0
12	NAG	B	304	14/15	0.15	-0.33	49,54,60,65	0
12	NAG	B	305	14/15	0.14	-1.16	72,75,80,85	0
12	NAG	B	306	14/15	0.25	-	89,91,93,93	0

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
5	GOL	B	319	6/6	0.41	20.11	60,60,61,61	6
7	EDO	B	309	4/4	0.44	12.28	60,62,62,63	0
6	H35	A	305	16/16	0.41	10.67	112,113,113,113	16
5	GOL	B	313	6/6	0.27	7.95	63,64,65,65	0
9	AZI	B	301	3/3	0.30	7.88	72,72,72,73	0
5	GOL	B	318	6/6	0.34	4.85	102,102,102,103	0
5	GOL	B	315	6/6	0.19	2.80	50,53,56,58	0
5	GOL	B	317	6/6	0.30	2.60	93,93,93,93	0
5	GOL	B	316	6/6	0.41	1.58	104,104,104,104	0
5	GOL	A	303	6/6	0.20	1.54	71,71,72,73	0
7	EDO	B	312	4/4	0.21	1.49	68,69,70,70	4
7	EDO	A	306	4/4	0.18	1.38	79,79,79,79	0
5	GOL	A	304	6/6	0.18	1.36	69,69,70,70	0
3	SO4	A	310	5/5	0.21	1.24	74,74,74,74	5
8	DIO	A	307	6/6	0.16	1.09	83,83,84,84	0
4	NAG	B	307	14/15	0.18	0.50	66,70,71,72	0
3	SO4	A	301	5/5	0.15	0.20	56,57,58,58	0
3	SO4	A	311	5/5	0.15	0.14	56,56,57,57	5

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	EDO	B	310	4/4	0.14	-0.22	81,82,82,82	0
5	GOL	B	314	6/6	0.15	-0.36	55,55,56,56	0
5	GOL	A	308	6/6	0.15	-0.47	73,73,74,74	0
3	SO4	A	312	5/5	0.13	-0.71	112,112,113,113	0
10	CL	B	320	1/1	0.15	-0.74	70,70,70,70	0
4	NAG	A	302	14/15	0.14	-1.05	72,75,77,78	0
7	EDO	B	311	4/4	0.13	-1.05	80,81,81,81	0
3	SO4	A	309	5/5	0.13	-1.52	105,105,105,106	0
10	CL	A	313	1/1	0.07	-3.92	88,88,88,88	0
7	EDO	B	308	4/4	0.09	-5.03	51,52,53,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.