W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:23 PM GMT

PDB ID	:	1TG7
Title	:	Native structure of beta-galactosidase from Penicillium sp.
Authors	:	Rojas, A.L.; Nagem, R.A.P.; Neustroev, K.N.; Arand, M.; Adamska, M.; Eneyskaya, E.V.; Kulminskaya, A.A.; Garratt, R.C.; Golubev, A.M.; Polikarpov, I.
Deposited on	:	2004-05-28
Resolution	:	1.90 Å(reported)

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

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 1.90 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.
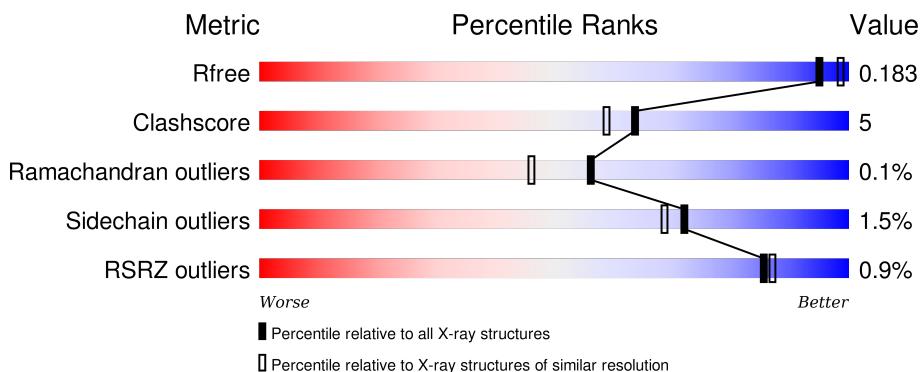
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	971	88% 11% •
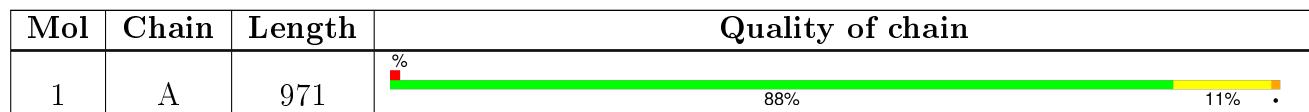
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	EDO	A	9221	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	EDO	A	9222	-	-	-	X
10	EDO	A	9223	-	-	-	X
10	EDO	A	9225	-	-	-	X
10	EDO	A	9226	-	-	-	X
10	EDO	A	9228	-	-	-	X
10	EDO	A	9229	-	-	-	X
3	NAG	A	4001	-	-	-	X
5	NAG	A	5001	-	-	-	X
9	PO4	A	9111	-	-	-	X
9	PO4	A	9112	-	-	-	X
9	PO4	A	9113	-	-	-	X
9	PO4	A	9114	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 9154 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-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	971	Total	C	N	O	S	21	3	0
			7499	4790	1241	1458	10			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
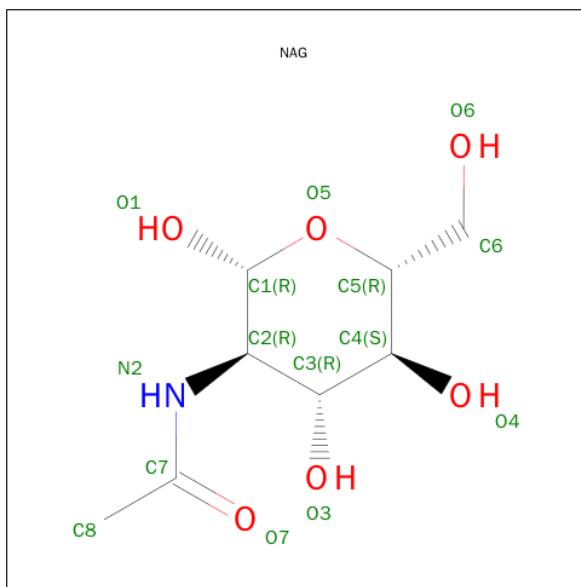
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	9	Total 105	C 58	N 2	O 45	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	5	Total 61	C 34	N 2	O 25	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	7	Total 83	C 46	N 2	O 35	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total 3	Na 3	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
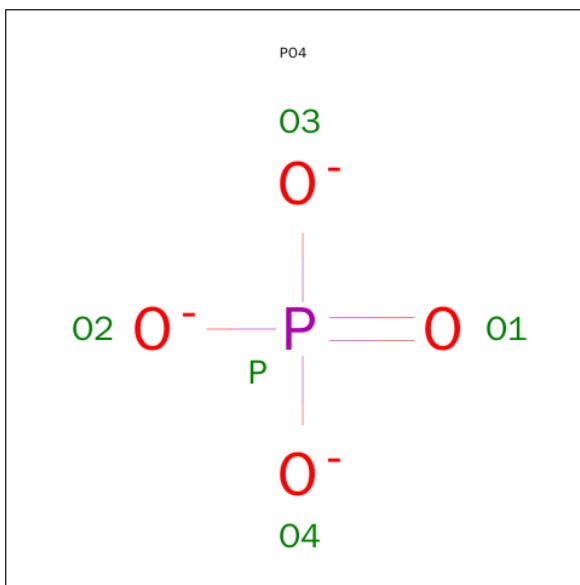
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 5	O 4	P 1	0	0
9	A	1	Total 5	O 4	P 1	0	0
9	A	1	Total 5	O 4	P 1	0	0
9	A	1	Total 5	O 4	P 1	0	0

• Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
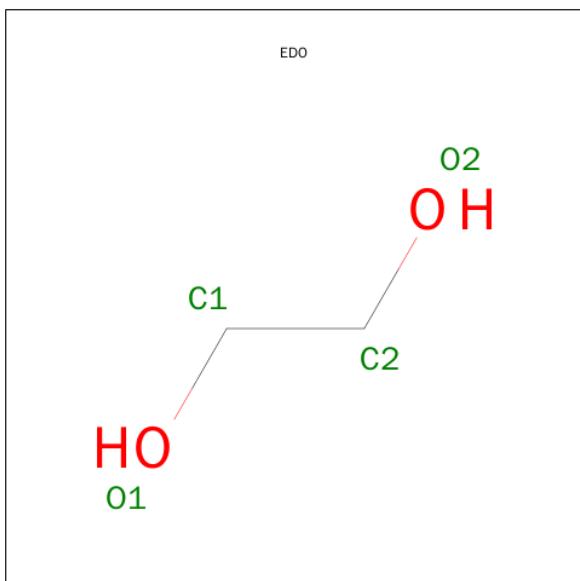
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1252	Total 1252	O 1252	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-galactosidase
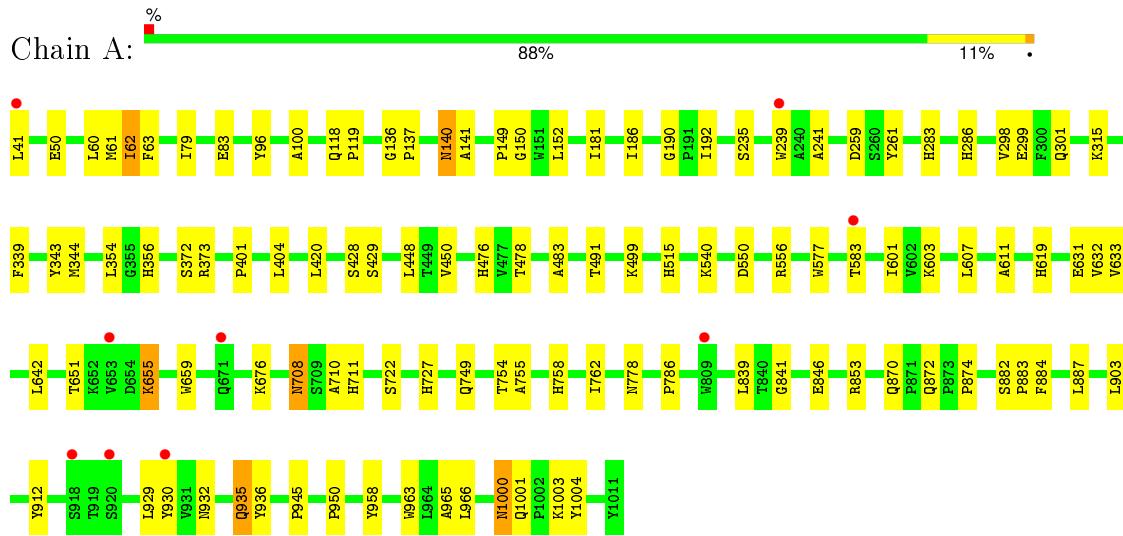
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	110.96Å 110.96Å 161.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.30 – 1.90 110.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (22.30-1.90) 99.9 (110.96-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.166 , 0.185 0.164 , 0.183	Depositor DCC
R_{free} test set	1543 reflections (1.02%)	DCC
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.9	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Outliers	0 of 152744 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9154	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NA, PO4, EDO, MAN

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	0.32	0/7726	0.64	3/10540 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	62[A]	ILE	CA-C-N	-5.49	105.13	117.20
1	A	62[B]	ILE	CA-C-N	-5.49	105.13	117.20
1	A	841	GLY	N-CA-C	-5.26	99.94	113.10

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	7499	0	7143	76	0
2	A	39	0	34	0	0
3	A	28	0	26	0	0
4	A	105	0	88	0	0
5	A	28	0	25	1	0
6	A	61	0	52	3	0
7	A	83	0	70	0	0
8	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	20	0	0	0	0
10	A	36	0	54	3	0
11	A	1252	0	0	13	0
All	All	9154	0	7492	79	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 5.

All (79) 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:778:ASN:HD21	6:A:6001:NAG:HN2	1.30	0.78
1:A:853:ARG:HH12	1:A:870:GLN:HE21	1.38	0.71
1:A:259:ASP:CG	1:A:299:GLU:HB2	2.14	0.68
1:A:708:ASN:HD22	1:A:710:ALA:H	1.46	0.62
1:A:932:ASN:ND2	1:A:963:TRP:H	1.96	0.61
1:A:778:ASN:ND2	6:A:6001:NAG:HN2	2.00	0.60
1:A:239:TRP:NE1	1:A:241:ALA:HB2	2.15	0.60
1:A:41:LEU:HD11	11:A:8281:HOH:O	2.02	0.58
1:A:428:SER:HB2	11:A:9942:HOH:O	2.05	0.55
1:A:882:SER:HB2	1:A:883:PRO:HD2	1.89	0.55
1:A:722:SER:OG	1:A:727:HIS:HD2	1.89	0.55
1:A:140:ASN:HB3	10:A:9229:EDO:H22	1.89	0.55
1:A:96:TYR:CE2	1:A:141:ALA:HB2	2.42	0.54
1:A:100:ALA:HA	1:A:149:PRO:HG3	1.90	0.54
1:A:286:HIS:HE1	11:A:9371:HOH:O	1.91	0.54
1:A:711:HIS:HE1	11:A:9444:HOH:O	1.90	0.53
1:A:286:HIS:HD2	11:A:9425:HOH:O	1.92	0.53
1:A:476:HIS:HD2	1:A:491:THR:O	1.93	0.52
1:A:261:TYR:HA	1:A:301:GLN:HB2	1.91	0.52
1:A:930[B]:TYR:HB2	1:A:965:ALA:HB3	1.91	0.52
1:A:540:LYS:HE3	11:A:8300:HOH:O	2.09	0.51
1:A:283:HIS:HE1	11:A:8255:HOH:O	1.93	0.51
1:A:749:GLN:HE21	1:A:778:ASN:HD22	1.58	0.50
1:A:283:HIS:HD2	11:A:9466:HOH:O	1.93	0.50
1:A:499:LYS:HE3	11:A:9983:HOH:O	2.12	0.49
5:A:5001:NAG:H83	11:A:8357:HOH:O	2.13	0.49
6:A:6002:NAG:H83	6:A:6004:MAN:O4	2.13	0.48
1:A:603:LYS:HB3	1:A:631:GLU:HB2	1.95	0.48
1:A:708:ASN:ND2	1:A:710:ALA:H	2.11	0.48
1:A:401:PRO:HA	1:A:420:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:GLN:HE21	1:A:778:ASN:ND2	2.12	0.48
1:A:762:ILE:O	1:A:762:ILE:HG23	2.13	0.48
1:A:874:PRO:HD3	1:A:1004:TYR:CD2	2.48	0.48
1:A:932:ASN:HD21	1:A:963:TRP:H	1.62	0.47
10:A:9228:EDO:O1	10:A:9229:EDO:H21	2.14	0.47
1:A:515:HIS:HE1	11:A:9463:HOH:O	1.96	0.47
1:A:515:HIS:HD2	1:A:550:ASP:OD1	1.97	0.47
1:A:1000:ASN:HD22	1:A:1001:GLN:N	2.12	0.46
1:A:118:GLN:HB3	1:A:119:PRO:HD3	1.97	0.46
1:A:483:ALA:HB1	1:A:499:LYS:HD2	1.97	0.46
1:A:611:ALA:HA	1:A:619:HIS:O	2.15	0.46
1:A:181:ILE:HG23	1:A:192:ILE:HD13	1.97	0.46
1:A:676:LYS:HA	1:A:884:PHE:CE2	2.50	0.46
1:A:136:GLY:HA3	1:A:137:PRO:C	2.36	0.46
1:A:930[A]:TYR:CE1	1:A:935:GLN:HB2	2.50	0.46
1:A:60:LEU:HD23	1:A:62[B]:ILE:HD11	1.98	0.46
1:A:577:TRP:CZ2	1:A:607:LEU:HA	2.52	0.45
1:A:601:ILE:HB	1:A:633:VAL:HB	1.99	0.45
1:A:727:HIS:HE1	1:A:846:GLU:OE2	2.00	0.44
1:A:708:ASN:C	1:A:708:ASN:HD22	2.22	0.43
1:A:149:PRO:HD2	1:A:152:LEU:HD23	2.00	0.43
1:A:887:LEU:N	1:A:887:LEU:HD12	2.33	0.43
1:A:655:LYS:C	1:A:655:LYS:HD3	2.38	0.43
1:A:903:LEU:HD12	1:A:958:TYR:CD2	2.54	0.43
1:A:140:ASN:HB3	1:A:141:ALA:H	1.73	0.43
1:A:872:GLN:HE22	1:A:1003:LYS:NZ	2.17	0.43
1:A:754:THR:O	1:A:755:ALA:HB3	2.19	0.42
1:A:186:ILE:HA	1:A:190:GLY:O	2.19	0.42
1:A:912:TYR:CE2	1:A:950:PRO:HB3	2.54	0.42
1:A:632:VAL:HB	1:A:659:TRP:HB2	2.02	0.42
1:A:315:LYS:HE2	11:A:8018:HOH:O	2.20	0.41
1:A:429:SER:HB2	1:A:478:THR:OG1	2.19	0.41
1:A:642:LEU:HB3	1:A:651:THR:HG21	2.03	0.41
1:A:404:LEU:HD12	1:A:404:LEU:C	2.41	0.41
1:A:79:ILE:O	1:A:83:GLU:HG3	2.21	0.41
1:A:929:LEU:HA	1:A:966:LEU:HD23	2.03	0.41
1:A:50:GLU:HG2	11:A:8348:HOH:O	2.19	0.41
1:A:727:HIS:CE1	1:A:846:GLU:OE2	2.74	0.41
1:A:150:GLY:HA3	1:A:727:HIS:CG	2.56	0.41
1:A:448:LEU:HG	1:A:450:VAL:HG13	2.03	0.41
1:A:758:HIS:C	1:A:758:HIS:CD2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD23	1:A:62[B]:ILE:CD1	2.51	0.41
1:A:372:SER:O	1:A:373:ARG:HB2	2.21	0.41
1:A:354:LEU:C	1:A:354:LEU:HD12	2.42	0.41
1:A:235:SER:O	1:A:298:VAL:HG21	2.20	0.40
1:A:343:TYR:HA	1:A:344:MET:HA	1.88	0.40
1:A:786:PRO:HG2	10:A:9226:EDO:H12	2.02	0.40
1:A:96:TYR:CD2	1:A:141:ALA:HB2	2.57	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	972/971 (100%)	939 (97%)	32 (3%)	1 (0%)	56　46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ASN

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	798/795 (100%)	786 (98%)	12 (2%)	72　69

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

Mol	Chain	Res	Type
1	A	61	MET
1	A	63	PHE
1	A	356	HIS
1	A	556	ARG
1	A	583	THR
1	A	655	LYS
1	A	708	ASN
1	A	839	LEU
1	A	935	GLN
1	A	936	TYR
1	A	945	PRO
1	A	1000	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	223	HIS
1	A	283	HIS
1	A	286	HIS
1	A	322	HIS
1	A	476	HIS
1	A	515	HIS
1	A	650	GLN
1	A	708	ASN
1	A	711	HIS
1	A	727	HIS
1	A	778	ASN
1	A	824	GLN
1	A	870	GLN
1	A	872	GLN
1	A	932	ASN
1	A	985	ASN
1	A	1000	ASN

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)

26 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	$\#|Z| > 2$
2	NAG	A	1991	1,2	14,14,15	0.55	0	15,19,21	0.79	1 (6%)
2	NAG	A	1992	2	14,14,15	0.56	0	15,19,21	0.62	0
2	BMA	A	1993	2	11,11,12	0.40	0	14,15,17	0.36	0
4	NAG	A	3001	1,4	14,14,15	0.48	0	15,19,21	0.67	0
4	NAG	A	3002	4	14,14,15	0.55	0	15,19,21	0.68	0
4	BMA	A	3003	4	11,11,12	0.50	0	14,15,17	0.37	0
4	BMA	A	3004	4	11,11,12	0.56	0	14,15,17	0.91	1 (7%)
4	MAN	A	3005	4	11,11,12	0.41	0	14,15,17	0.74	1 (7%)
4	MAN	A	3006	4	11,11,12	0.50	0	14,15,17	0.69	1 (7%)
4	MAN	A	3007	4	11,11,12	0.44	0	14,15,17	0.50	0
4	MAN	A	3008	4	11,11,12	0.42	0	14,15,17	0.65	1 (7%)
4	MAN	A	3009	4	11,11,12	0.47	0	14,15,17	0.65	1 (7%)
5	NAG	A	5001	1,5	14,14,15	0.55	0	15,19,21	0.74	1 (6%)
5	NAG	A	5002	5	14,14,15	0.48	0	15,19,21	0.73	1 (6%)
6	NAG	A	6001	1,6	14,14,15	0.47	0	15,19,21	0.72	1 (6%)
6	NAG	A	6002	6	14,14,15	0.49	0	15,19,21	0.70	1 (6%)
6	BMA	A	6003	6	11,11,12	0.46	0	14,15,17	0.34	0
6	MAN	A	6004	6	11,11,12	0.45	0	14,15,17	0.63	1 (7%)
6	MAN	A	6005	6	11,11,12	0.45	0	14,15,17	0.60	0
7	NAG	A	7001	1,8,7	14,14,15	0.48	0	15,19,21	0.73	1 (6%)
7	NAG	A	7002	7	14,14,15	0.50	0	15,19,21	0.69	0
7	BMA	A	7003	7	11,11,12	0.39	0	14,15,17	0.34	0
7	MAN	A	7004	7	11,11,12	0.46	0	14,15,17	0.51	0
7	MAN	A	7005	7	11,11,12	0.50	0	14,15,17	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
7	MAN	A	7006	7	11,11,12	0.49	0	14,15,17	0.50	0
7	MAN	A	7007	7	11,11,12	0.52	0	14,15,17	0.53	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	NAG	A	1991	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1992	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1993	2	-	0/2/19/22	0/1/1/1
4	NAG	A	3001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	3002	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3003	4	-	0/2/19/22	0/1/1/1
4	BMA	A	3004	4	-	0/2/19/22	1/1/1/1
4	MAN	A	3005	4	-	0/2/19/22	0/1/1/1
4	MAN	A	3006	4	-	0/2/19/22	0/1/1/1
4	MAN	A	3007	4	-	0/2/19/22	0/1/1/1
4	MAN	A	3008	4	-	0/2/19/22	0/1/1/1
4	MAN	A	3009	4	-	0/2/19/22	0/1/1/1
5	NAG	A	5001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	5002	5	-	0/6/23/26	0/1/1/1
6	NAG	A	6001	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	6002	6	-	0/6/23/26	0/1/1/1
6	BMA	A	6003	6	-	0/2/19/22	0/1/1/1
6	MAN	A	6004	6	-	0/2/19/22	0/1/1/1
6	MAN	A	6005	6	-	0/2/19/22	0/1/1/1
7	NAG	A	7001	1,8,7	-	0/6/23/26	0/1/1/1
7	NAG	A	7002	7	-	0/6/23/26	0/1/1/1
7	BMA	A	7003	7	-	0/2/19/22	0/1/1/1
7	MAN	A	7004	7	-	0/2/19/22	0/1/1/1
7	MAN	A	7005	7	-	0/2/19/22	0/1/1/1
7	MAN	A	7006	7	-	0/2/19/22	0/1/1/1
7	MAN	A	7007	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	5002	NAG	C2-N2-C7	-2.31	120.07	123.04
5	A	5001	NAG	C2-N2-C7	-2.19	120.23	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	6002	NAG	C2-N2-C7	-2.18	120.24	123.04
7	A	7001	NAG	C2-N2-C7	-2.16	120.26	123.04
6	A	6001	NAG	C2-N2-C7	-2.15	120.27	123.04
2	A	1991	NAG	C2-N2-C7	-2.07	120.39	123.04
6	A	6004	MAN	C1-O5-C5	2.00	114.79	112.25
4	A	3006	MAN	C1-O5-C5	2.07	114.87	112.25
4	A	3009	MAN	C1-O5-C5	2.08	114.89	112.25
4	A	3008	MAN	C1-O5-C5	2.09	114.89	112.25
4	A	3005	MAN	C1-O5-C5	2.29	115.16	112.25
4	A	3004	BMA	C1-O5-C5	2.83	115.83	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3004	BMA	C1-C2-C3-C4-C5-O5

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5001	NAG	1	0
6	A	6001	NAG	2	0
6	A	6002	NAG	1	0
6	A	6004	MAN	1	0

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 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	NAG	A	2001	1	14,14,15	0.49	0	15,19,21	0.74	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	A	4001	1	14,14,15	0.47	0	15,19,21	0.78	1 (6%)
9	PO4	A	9111	-	4,4,4	1.09	0	6,6,6	0.27	0
9	PO4	A	9112	-	4,4,4	1.11	0	6,6,6	0.27	0
9	PO4	A	9113	-	4,4,4	1.18	0	6,6,6	0.27	0
9	PO4	A	9114	-	4,4,4	1.16	0	6,6,6	0.27	0
10	EDO	A	9221	-	3,3,3	0.55	0	2,2,2	0.41	0
10	EDO	A	9222	-	3,3,3	0.55	0	2,2,2	0.42	0
10	EDO	A	9223	-	3,3,3	0.56	0	2,2,2	0.41	0
10	EDO	A	9224	-	3,3,3	0.56	0	2,2,2	0.43	0
10	EDO	A	9225	-	3,3,3	0.67	0	2,2,2	0.42	0
10	EDO	A	9226	-	3,3,3	0.56	0	2,2,2	0.42	0
10	EDO	A	9227	-	3,3,3	0.60	0	2,2,2	0.43	0
10	EDO	A	9228	-	3,3,3	0.57	0	2,2,2	0.43	0
10	EDO	A	9229	-	3,3,3	0.46	0	2,2,2	0.48	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	NAG	A	2001	1	-	0/6/23/26	0/1/1/1
3	NAG	A	4001	1	-	0/6/23/26	0/1/1/1
9	PO4	A	9111	-	-	0/0/0/0	0/0/0/0
9	PO4	A	9112	-	-	0/0/0/0	0/0/0/0
9	PO4	A	9113	-	-	0/0/0/0	0/0/0/0
9	PO4	A	9114	-	-	0/0/0/0	0/0/0/0
10	EDO	A	9221	-	-	0/1/1/1	0/0/0/0
10	EDO	A	9222	-	-	0/1/1/1	0/0/0/0
10	EDO	A	9223	-	-	0/1/1/1	0/0/0/0
10	EDO	A	9224	-	-	0/1/1/1	0/0/0/0
10	EDO	A	9225	-	-	0/1/1/1	0/0/0/0
10	EDO	A	9226	-	-	0/1/1/1	0/0/0/0
10	EDO	A	9227	-	-	0/1/1/1	0/0/0/0
10	EDO	A	9228	-	-	0/1/1/1	0/0/0/0
10	EDO	A	9229	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4001	NAG	C2-N2-C7	-2.41	119.94	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2001	NAG	C2-N2-C7	-2.27	120.12	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	9226	EDO	1	0
10	A	9228	EDO	1	0
10	A	9229	EDO	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	971/971 (100%)	0.04	9 (0%)	85	87	12, 19, 30, 42	30 (3%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	THR	5.1
1	A	809	TRP	3.6
1	A	41	LEU	3.3
1	A	671	GLN	2.5
1	A	239	TRP	2.2
1	A	653[A]	VAL	2.1
1	A	918	SER	2.0
1	A	920	SER	2.0
1	A	930[A]	TYR	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)

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(Å^2)	Q<0.9
5	NAG	A	5001	14/15	0.89	0.16	2.15	37,42,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
4	NAG	A	3001	14/15	0.97	0.12	1.97	16,20,28,29	0
6	NAG	A	6001	14/15	0.93	0.11	1.07	20,27,33,38	0
2	NAG	A	1991	14/15	0.96	0.10	0.41	16,17,18,18	0
4	NAG	A	3002	14/15	0.97	0.11	0.25	17,19,24,27	0
4	MAN	A	3007	11/12	0.97	0.10	-0.20	19,21,26,26	0
7	NAG	A	7001	14/15	0.97	0.10	-0.48	15,17,21,26	0
7	NAG	A	7002	14/15	0.97	0.11	-0.53	14,19,27,28	0
6	MAN	A	6004	11/12	0.84	0.17	-	43,44,45,46	11
7	BMA	A	7003	11/12	0.98	0.10	-	18,19,20,21	0
4	MAN	A	3008	11/12	0.94	0.10	-	28,31,32,33	0
6	BMA	A	6003	11/12	0.70	0.27	-	44,46,47,48	0
6	NAG	A	6002	14/15	0.86	0.24	-	37,42,45,46	0
4	MAN	A	3009	11/12	0.60	0.22	-	34,36,37,37	11
5	NAG	A	5002	14/15	0.74	0.23	-	41,47,48,51	14
7	MAN	A	7005	11/12	0.97	0.10	-	19,22,26,26	0
6	MAN	A	6005	11/12	0.70	0.20	-	41,43,45,47	11
4	BMA	A	3003	11/12	0.97	0.10	-	20,21,26,35	0
2	NAG	A	1992	14/15	0.95	0.10	-	18,21,29,30	0
2	BMA	A	1993	11/12	0.83	0.20	-	38,43,46,48	0
7	MAN	A	7007	11/12	0.91	0.13	-	27,32,35,37	0
4	MAN	A	3006	11/12	0.73	0.25	-	26,33,34,35	11
7	MAN	A	7006	11/12	0.94	0.11	-	27,31,32,33	0
4	BMA	A	3004	11/12	0.68	0.30	-	45,50,54,56	0
4	MAN	A	3005	11/12	0.96	0.11	-	20,21,24,29	0
7	MAN	A	7004	11/12	0.96	0.09	-	25,28,31,33	0

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($Å^2$)	Q<0.9
10	EDO	A	9223	4/4	0.95	0.22	13.61	34,36,37,40	0
9	PO4	A	9112	5/5	0.90	0.19	10.12	37,38,39,39	5
10	EDO	A	9229	4/4	0.90	0.20	7.70	23,25,26,30	0
9	PO4	A	9113	5/5	0.98	0.14	6.84	31,32,33,33	5
9	PO4	A	9114	5/5	0.92	0.18	6.11	53,54,55,55	5
10	EDO	A	9225	4/4	0.83	0.16	4.96	26,32,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	PO4	A	9111	5/5	0.93	0.15	4.36	12,15,22,22	5
10	EDO	A	9228	4/4	0.92	0.13	3.94	18,23,25,27	0
3	NAG	A	4001	14/15	0.88	0.13	3.80	26,31,36,38	0
10	EDO	A	9222	4/4	0.95	0.14	3.38	29,31,32,35	0
10	EDO	A	9226	4/4	0.94	0.15	2.14	33,33,34,37	0
10	EDO	A	9221	4/4	0.95	0.14	2.10	23,23,24,27	0
10	EDO	A	9227	4/4	0.83	0.21	-	32,38,40,43	0
8	NA	A	9001	1/1	0.99	0.15	-	16,16,16,16	0
10	EDO	A	9224	4/4	0.96	0.14	-	26,27,28,30	0
3	NAG	A	2001	14/15	0.69	0.28	-	48,50,54,55	0
8	NA	A	9003	1/1	0.97	0.12	-	23,23,23,23	0
8	NA	A	9002	1/1	0.99	0.14	-	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.