



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:39 PM GMT

PDB ID : 1UN1
Title : XYLOGLUCAN ENDOTRANSGLYCOSYLASE NATIVE STRUCTURE.
Authors : Johansson, P.; Brumer, H.; Kallas, A.; Henriksson, H.; Denman, S.; Teeri, T.T.; Jones, T.A.
Deposited on : 2003-09-03
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

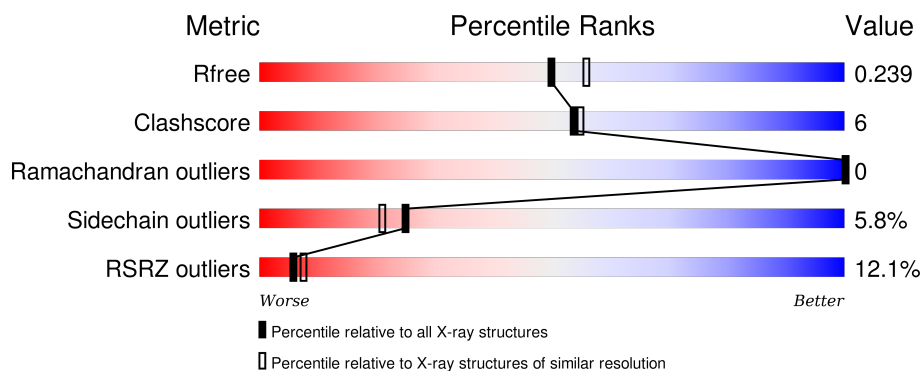
1 Overall quality at a glance

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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	278	<div> <div>14%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	278	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 5%</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
3	AU	B	1276	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4695 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 XYLOGLUCAN ENDOTRANSGLYCOSYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	27	0	0
			2220	1432	373	404	11			
1	B	264	Total	C	N	O	S	12	1	0
			2206	1426	371	398	11			

- 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		
2	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Au	0	0
			1	1		

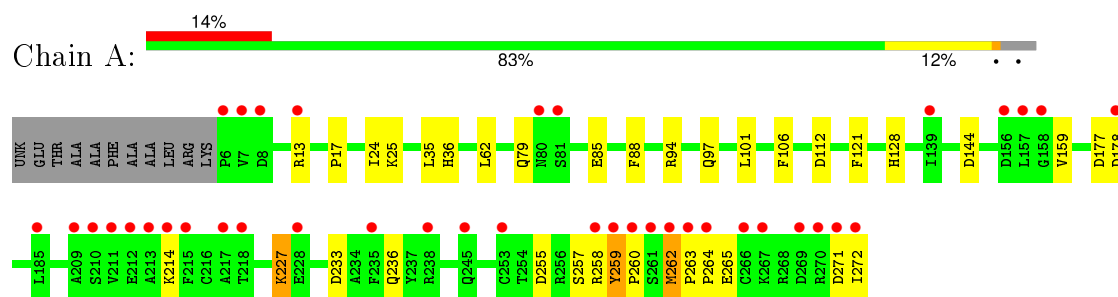
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	103	Total	O	0	0
			103	103		

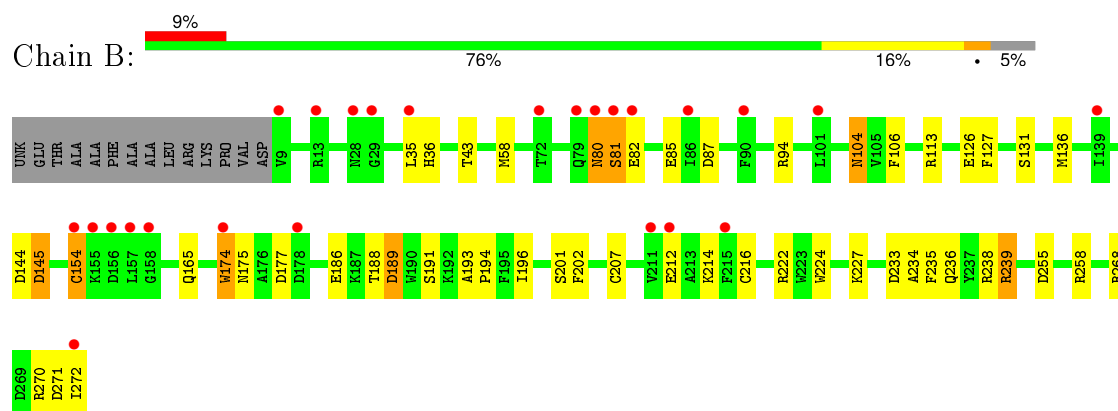
3 Residue-property plots [i](#)

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

• Molecule 1: XYLOGLUCAN ENDOTRANSGLYCOSYLASE



• Molecule 1: XYLOGLUCAN ENDOTRANSGLYCOSYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	188.76 Å 188.76 Å 45.97 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.77 – 2.10 24.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.77-2.10) 99.9 (24.93-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.206 , 0.232 0.215 , 0.239	Depositor DCC
R_{free} test set	2798 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 59.5	EDS
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55193 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4695	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, AU, NAG

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	0.65	0/2293	0.85	8/3104 (0.3%)
1	B	0.67	0/2285	0.86	9/3095 (0.3%)
All	All	0.66	0/4578	0.86	17/6199 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	94	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	145	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	144	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	189	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	144	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	227	LYS	N-CA-CB	-5.71	100.33	110.60
1	B	258	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	112	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	271	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	227	LYS	CB-CA-C	5.32	121.05	110.40
1	B	258	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	271	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	94	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	255	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	255	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	239	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	2220	0	2085	29	0
1	B	2206	0	2070	27	0
2	A	39	0	34	2	0
2	B	39	0	34	0	0
3	B	1	0	0	2	0
4	A	87	0	0	2	1
4	B	103	0	0	1	1
All	All	4695	0	4223	56	1

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 6.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:CYS:SG	3:B:1276:AU:AU	1.62	1.25
1:B:154:CYS:SG	1:B:268:ARG:NH1	2.14	1.19
1:A:260:PRO:O	4:A:2083:HOH:O	1.67	1.09
1:B:154:CYS:SG	1:B:268:ARG:HD2	2.05	0.97
1:B:207:CYS:HG	1:B:216:CYS:HG	0.92	0.92
1:A:262:MET:HE3	1:A:263:PRO:C	1.99	0.81
1:A:121:PHE:CE1	1:A:128:HIS:CD2	2.71	0.79
1:A:262:MET:HE3	1:A:262:MET:C	2.03	0.79
1:B:104:ASN:HD21	1:B:113:ARG:H	1.40	0.70
1:A:262:MET:HG2	1:A:263:PRO:HD2	1.74	0.69
1:B:80:ASN:HD22	1:B:80:ASN:H	1.41	0.67
1:A:25:LYS:NZ	1:A:36:HIS:CE1	2.66	0.64
1:A:262:MET:HE3	1:A:262:MET:O	1.98	0.63
1:A:121:PHE:CD1	1:A:128:HIS:CD2	2.86	0.63
1:A:25:LYS:HZ2	1:A:36:HIS:CE1	2.17	0.63
1:B:36:HIS:CD2	1:B:196:ILE:HG12	2.35	0.61
1:A:17:PRO:HB3	1:A:24:ILE:HD12	1.86	0.58
1:A:262:MET:CE	1:A:263:PRO:O	2.51	0.58
1:A:262:MET:HE3	1:A:263:PRO:O	2.05	0.56
1:B:233:ASP:H	1:B:236:GLN:HE21	1.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:MET:CE	1:A:262:MET:C	2.74	0.55
1:A:62:LEU:HD12	4:A:2048:HOH:O	2.06	0.55
1:A:97:GLN:HE21	2:A:1273:NAG:C6	2.21	0.54
1:A:97:GLN:NE2	2:A:1273:NAG:O6	2.41	0.54
1:A:262:MET:HG2	1:A:263:PRO:CD	2.37	0.54
1:A:262:MET:CE	1:A:262:MET:O	2.55	0.54
1:A:262:MET:CE	1:A:263:PRO:C	2.74	0.53
1:B:174[A]:TRP:HD1	4:B:2068:HOH:O	1.91	0.53
1:B:35:LEU:HG	1:B:43:THR:HG23	1.91	0.52
1:B:81:SER:O	1:B:82:GLU:HB2	2.11	0.51
1:B:154:CYS:HG	3:B:1276:AU:AU	0.45	0.50
1:A:259:TYR:CE1	1:A:263:PRO:HG3	2.46	0.50
1:B:222:ARG:HG3	1:B:224:TRP:CZ2	2.47	0.50
1:B:234:ALA:O	1:B:238:ARG:HG3	2.12	0.49
1:B:207:CYS:CB	1:B:216:CYS:HG	2.26	0.48
1:A:88:PHE:HD2	1:A:101:LEU:HD11	1.79	0.48
1:A:262:MET:HE3	1:A:263:PRO:N	2.27	0.48
1:B:80:ASN:ND2	1:B:165:GLN:OE1	2.41	0.48
1:B:126:GLU:HG3	1:B:127:PHE:N	2.29	0.48
1:B:189:ASP:OD1	1:B:191:SER:OG	2.32	0.47
1:B:235:PHE:O	1:B:239:ARG:HD2	2.14	0.47
1:B:80:ASN:N	1:B:80:ASN:HD22	2.11	0.46
1:A:121:PHE:CD1	1:A:128:HIS:NE2	2.85	0.44
1:B:233:ASP:H	1:B:236:GLN:NE2	2.15	0.44
1:A:233:ASP:H	1:A:236:GLN:HE21	1.66	0.44
1:B:175:ASN:ND2	1:B:188:THR:OG1	2.51	0.43
1:B:94:ARG:HD2	1:B:186:GLU:OE1	2.19	0.43
1:A:159:VAL:HG21	1:A:264:PRO:HB2	2.00	0.43
1:A:24:ILE:HG12	1:A:35:LEU:HD22	2.00	0.43
1:A:85:GLU:HB3	1:A:106:PHE:HB2	2.00	0.42
1:B:201:SER:O	1:B:202:PHE:C	2.59	0.41
1:B:193:ALA:HB1	1:B:194:PRO:HA	2.03	0.41
1:A:259:TYR:CZ	1:A:263:PRO:HG3	2.56	0.41
1:A:262:MET:HE1	1:A:264:PRO:HA	2.03	0.41
1:B:85:GLU:HB3	1:B:106:PHE:HB2	2.02	0.41
1:B:85:GLU:OE2	1:B:87:ASP:OD1	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2014:HOH:O	4:B:2096:HOH:O[6_655]	1.93	0.27

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	265/278 (95%)	251 (95%)	14 (5%)	0	100	100
1	B	263/278 (95%)	252 (96%)	11 (4%)	0	100	100
All	All	528/556 (95%)	503 (95%)	25 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	235/241 (98%)	223 (95%)	12 (5%)	29	26
1	B	233/241 (97%)	217 (93%)	16 (7%)	19	15
All	All	468/482 (97%)	440 (94%)	28 (6%)	25	20

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	79	GLN
1	A	177	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	178	ASP
1	A	214	LYS
1	A	227	LYS
1	A	257	SER
1	A	258	ARG
1	A	259	TYR
1	A	262	MET
1	A	265	GLU
1	A	272	ILE
1	B	58	MET
1	B	80	ASN
1	B	81	SER
1	B	104	ASN
1	B	131	SER
1	B	136	MET
1	B	145	ASP
1	B	154	CYS
1	B	174[A]	TRP
1	B	174[B]	TRP
1	B	177	ASP
1	B	212	GLU
1	B	214	LYS
1	B	227	LYS
1	B	270	ARG
1	B	272	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	46	GLN
1	A	97	GLN
1	A	128	HIS
1	A	175	ASN
1	A	236	GLN
1	B	36	HIS
1	B	79	GLN
1	B	97	GLN
1	B	104	ASN
1	B	175	ASN
1	B	219	GLN
1	B	236	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	245	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 ⓘ

6 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	1273	1,2	14,14,15	0.63	0	15,19,21	1.00	0
2	NAG	A	1274	2	14,14,15	0.78	1 (7%)	15,19,21	0.95	1 (6%)
2	BMA	A	1275	2	11,11,12	0.57	0	14,15,17	0.94	0
2	NAG	B	1273	1,2	14,14,15	0.49	0	15,19,21	1.10	1 (6%)
2	NAG	B	1274	2	14,14,15	0.71	0	15,19,21	0.61	0
2	BMA	B	1275	2	11,11,12	0.70	0	14,15,17	1.40	4 (28%)

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	1273	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1274	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1275	2	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1273	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1274	2	-	0/6/23/26	0/1/1/1
2	BMA	B	1275	2	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1274	NAG	O5-C1	-2.02	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1273	NAG	O6-C6-C5	-2.14	104.28	111.33
2	B	1275	BMA	C6-C5-C4	-2.13	107.76	113.02
2	A	1274	NAG	O4-C4-C3	-2.01	105.81	110.34
2	B	1275	BMA	C1-C2-C3	2.27	112.22	109.54
2	B	1275	BMA	C3-C4-C5	2.41	114.40	110.20
2	B	1275	BMA	C1-O5-C5	2.51	115.44	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1273	NAG	2	0

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	267/278 (96%)	0.69	39 (14%) 3 5	23, 38, 77, 86	7 (2%)
1	B	264/278 (94%)	0.40	25 (9%) 10 14	23, 38, 54, 63	3 (1%)
All	All	531/556 (95%)	0.55	64 (12%) 6 7	23, 38, 63, 86	10 (1%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	272	ILE	11.4
1	A	211	VAL	10.2
1	B	9	VAL	8.0
1	B	154	CYS	7.5
1	A	262	MET	6.4
1	A	259	TYR	6.3
1	A	215	PHE	6.1
1	A	212	GLU	6.1
1	A	210	SER	5.8
1	B	156	ASP	5.3
1	A	7	VAL	5.1
1	B	174[A]	TRP	5.0
1	A	213	ALA	4.8
1	A	6	PRO	4.8
1	A	261	SER	4.6
1	A	214	LYS	4.6
1	A	8	ASP	4.4
1	A	156	ASP	4.4
1	A	266	CYS	4.1
1	A	217	ALA	4.1
1	A	80	ASN	4.0
1	A	271	ASP	3.9
1	A	81	SER	3.8
1	B	157	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	270	ARG	3.8
1	A	235	PHE	3.7
1	B	272	ILE	3.7
1	A	253	CYS	3.7
1	B	13	ARG	3.4
1	B	28	ASN	3.3
1	B	81	SER	3.3
1	B	80	ASN	3.2
1	A	260	PRO	3.1
1	A	263	PRO	3.1
1	A	157	LEU	3.0
1	B	158	GLY	2.9
1	A	269	ASP	2.9
1	B	211	VAL	2.9
1	B	155	LYS	2.9
1	A	264	PRO	2.8
1	A	245	GLN	2.8
1	A	139	ILE	2.8
1	B	101	LEU	2.7
1	A	178	ASP	2.6
1	A	13	ARG	2.6
1	A	238	ARG	2.6
1	B	178	ASP	2.6
1	A	267	LYS	2.5
1	A	228	GLU	2.5
1	B	215	PHE	2.4
1	A	185	LEU	2.4
1	B	86	ILE	2.4
1	B	139	ILE	2.4
1	B	29	GLY	2.4
1	B	90	PHE	2.3
1	A	218	THR	2.3
1	B	35	LEU	2.3
1	A	209	ALA	2.3
1	B	82	GLU	2.3
1	B	212	GLU	2.2
1	A	258	ARG	2.2
1	A	158	GLY	2.1
1	B	72	THR	2.0
1	B	79	GLN	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
2	NAG	A	1273	14/15	0.90	0.11	-0.38	36,39,43,43	0
2	NAG	B	1273	14/15	0.95	0.09	-0.96	31,33,39,40	0
2	BMA	A	1275	11/12	0.87	0.26	-	60,62,64,65	0
2	NAG	B	1274	14/15	0.88	0.17	-	38,41,44,46	0
2	NAG	A	1274	14/15	0.91	0.15	-	44,47,51,56	0
2	BMA	B	1275	11/12	0.86	0.21	-	49,53,57,57	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
3	AU	B	1276	1/1	0.84	0.39	-	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.