Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:27 PM GMT

PDB ID	:	4XX6
Title	:	Crystal structure of a glycosylated endo-beta-1,4-xylanase (glycoside hydrolase family 10/GH10) enzyme from Gloeophyllum trabeum
Authors	:	Stogios, P.J.; Nocek, B.; Xu, X.; Cui, H.; Lowden, M.; Savchenko, A.
Deposited on	:	2015-01-29
Resolution	:	1.95 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 ①) were used in the production of this report:

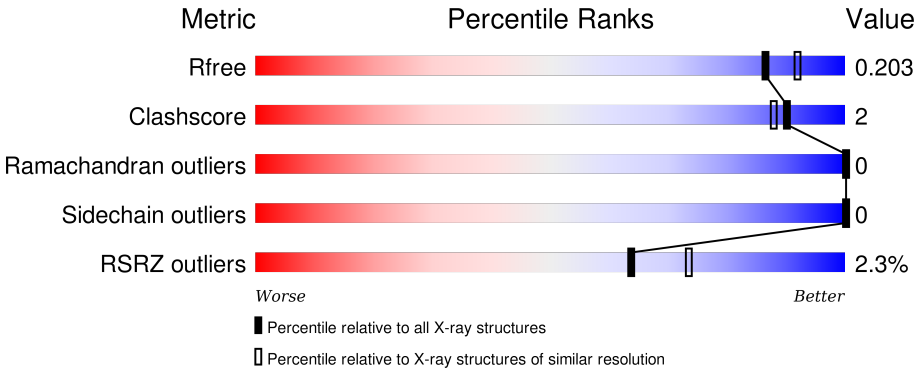
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

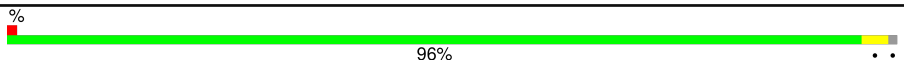
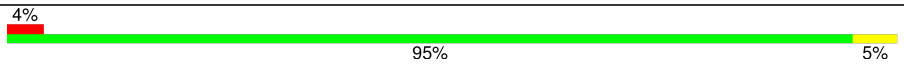
The reported resolution of this entry is 1.95 Å.

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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	321	
1	B	321	

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
2	UNX	A	401	-	-	-	X
2	UNX	B	401	-	-	-	X
3	NAG	A	423	-	-	-	X
5	MAN	A	405	-	-	-	X
5	MAN	A	406	-	-	-	X
5	MAN	A	409	-	-	-	X
5	MAN	B	405	-	-	-	X
7	PEG	A	425	-	-	-	X
7	PEG	B	422	-	-	-	X
7	PEG	B	423	-	-	-	X
8	P6G	A	427	-	-	-	X
9	GOL	A	430	-	-	-	X
9	GOL	A	431	-	-	-	X
9	GOL	B	425	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6233 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.

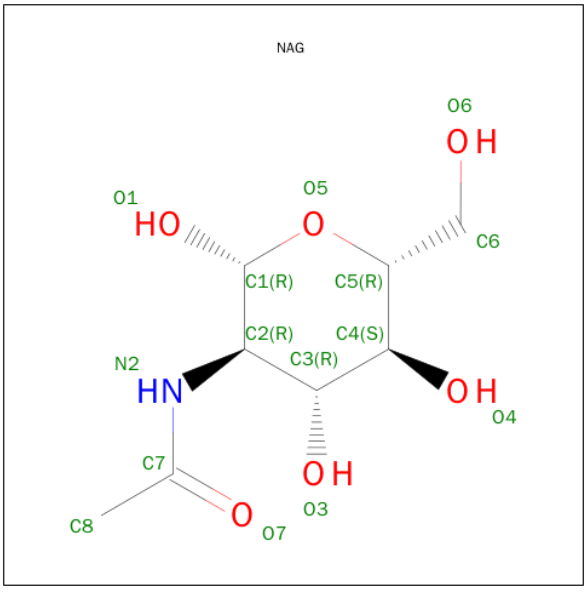
- Molecule 1 is a protein called Beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	2	0
			2515	1618	413	476	8			
1	B	321	Total	C	N	O	S	0	2	0
			2533	1627	416	482	8			

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

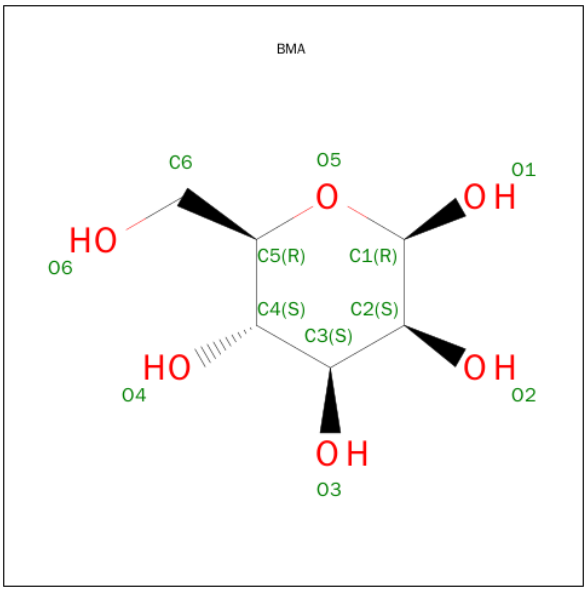
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	X	0	0
			1	1		
2	A	1	Total	X	0	0
			1	1		

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



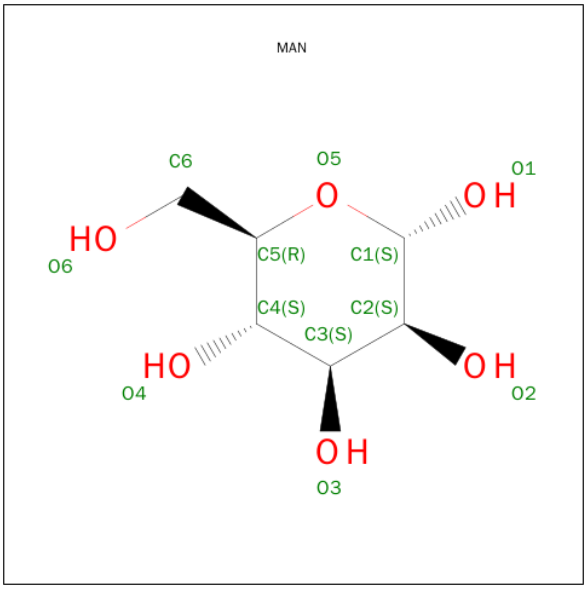
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total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

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

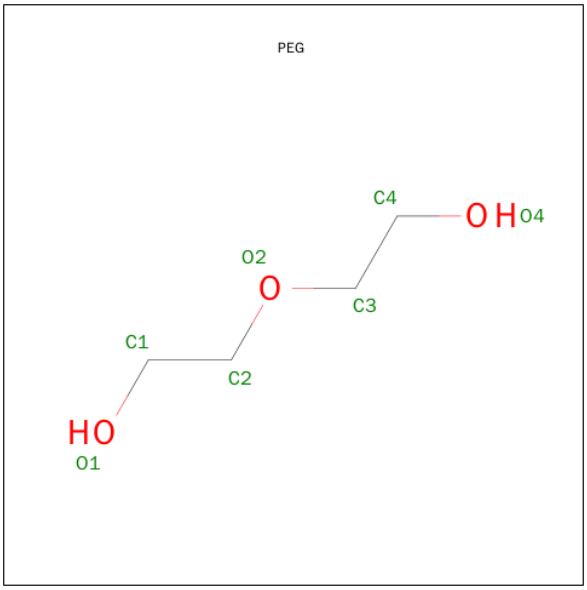


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

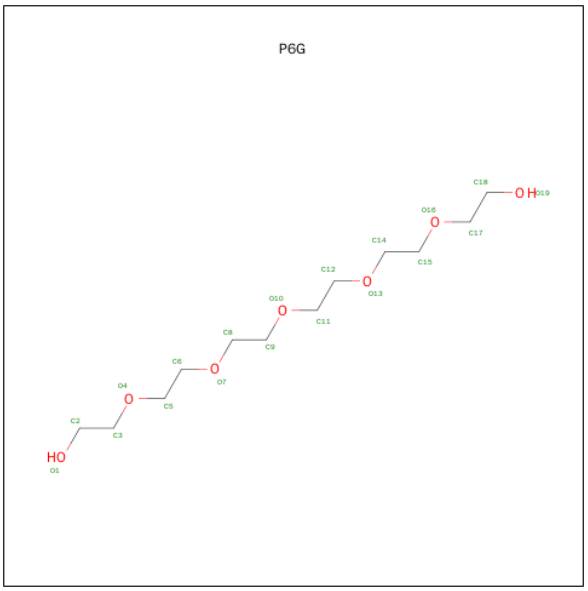
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	0	0
6	A	1	Total Mg 1 1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



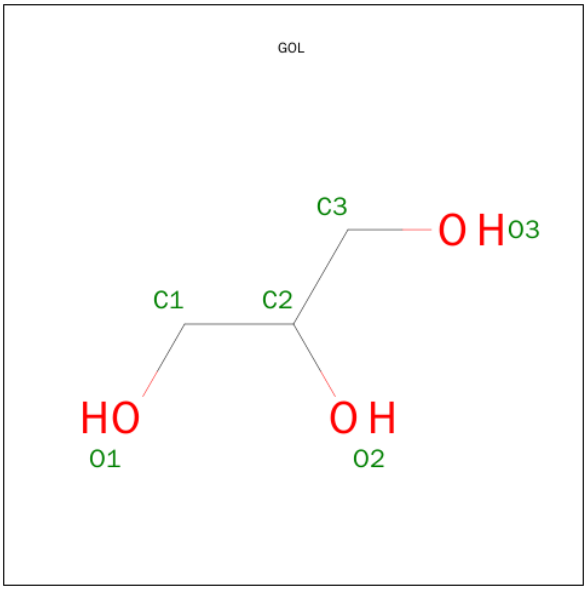
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0

- Molecule 8 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 18 12 6	0	0
8	A	1	Total C O 13 8 5	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- 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

- Molecule 11 is water.

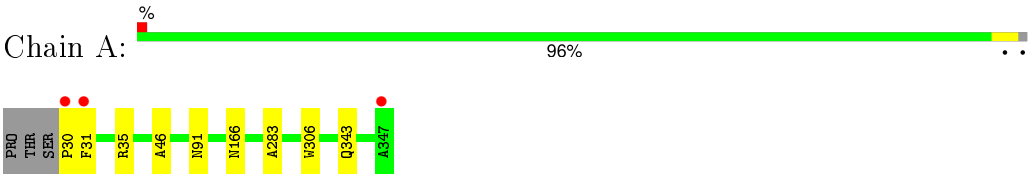
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	293	Total O 306 306	0	13
11	B	288	Total O 295 295	0	7

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.

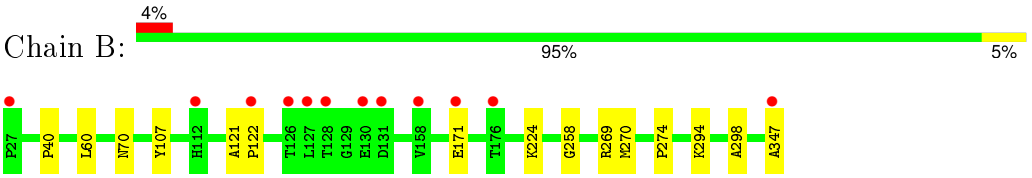
- Molecule 1: Beta-xylanase

Chain A:



- Molecule 1: Beta-xylanase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.41Å 99.34Å 147.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.20 – 1.95 30.20 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.7 (30.20-1.95) 86.6 (30.20-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	4.96 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.154 , 0.204 0.158 , 0.203	Depositor DCC
R_{free} test set	2000 reflections (4.22%)	DCC
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 66.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 51041 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6233	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: GOL, MG, BMA, NAG, CL, UNX, P6G, PEG, 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	0.40	0/2596	0.53	0/3563
1	B	0.39	0/2615	0.53	0/3589
All	All	0.40	0/5211	0.53	0/7152

There are no bond length outliers.

There are no bond angle outliers.

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	2515	0	2370	8	0
1	B	2533	0	2382	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	98	0	85	3	0
3	B	112	0	99	0	0
4	A	33	0	25	3	0
4	B	22	0	18	0	0
5	A	132	0	113	2	0
5	B	88	0	74	1	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	7	0	10	0	0
7	B	14	0	20	3	0
8	A	31	0	39	2	0
9	A	24	0	32	1	0
9	B	18	0	24	2	0
10	B	1	0	0	0	0
11	A	306	0	0	1	0
11	B	295	0	0	0	1
All	All	6233	0	5291	25	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 2.

All (25) 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:269:ARG:HH22	9:B:424:GOL:H32	1.46	0.80
1:B:298:ALA:HA	7:B:422:PEG:H22	1.69	0.75
1:A:35:ARG:HE	8:A:426:P6G:H171	1.63	0.64
1:B:171:GLU:HG3	1:B:171:GLU:O	1.98	0.61
1:B:294:LYS:NZ	1:B:347:ALA:O	2.40	0.54
1:B:269:ARG:NH2	9:B:424:GOL:H32	2.20	0.54
5:B:406:MAN:H5	5:B:407:MAN:O5	2.10	0.51
1:B:40:PRO:HG2	7:B:422:PEG:H12	1.94	0.50
1:A:30:PRO:HA	1:A:31:PHE:HA	1.69	0.48
1:A:46:ALA:HB2	1:A:306:TRP:CE3	2.50	0.47
7:B:423:PEG:H31	7:B:423:PEG:H11	1.79	0.47
3:A:420:NAG:O3	4:A:421:BMA:H2	2.15	0.47
1:A:283:ALA:HB3	9:A:428:GOL:H32	1.98	0.46
1:B:70:ASN:HA	1:B:107:TYR:CE1	2.51	0.46
4:A:412:BMA:H3	5:A:418:MAN:H2	1.84	0.45
1:A:30:PRO:HA	1:A:31:PHE:HD1	1.83	0.44
1:A:343:GLN:HG2	11:A:771:HOH:O	2.19	0.42
8:A:426:P6G:H51	8:A:426:P6G:H82	1.56	0.42
1:B:60:LEU:HA	1:B:60:LEU:HD23	1.83	0.42
1:B:270:MET:SD	1:B:274:PRO:HB3	2.61	0.41
1:A:91:ASN:HD22	3:A:410:NAG:H83	1.85	0.41
4:A:421:BMA:H3	5:A:422:MAN:H2	1.54	0.41
1:A:166:ASN:HD22	3:A:419:NAG:H83	1.86	0.41
1:B:121:ALA:HA	1:B:122:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LYS:HE3	1:B:258:GLY:O	2.21	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)
11:B:611:HOH:O	11:B:680:HOH:O[1_655]	2.19	0.01

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	318/321 (99%)	313 (98%)	5 (2%)	0	100	100
1	B	321/321 (100%)	315 (98%)	6 (2%)	0	100	100
All	All	639/642 (100%)	628 (98%)	11 (2%)	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	262/263 (100%)	262 (100%)	0	100	100
1	B	265/263 (101%)	265 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	527/526 (100%)	527 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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 molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 57 ligands modelled in this entry, 2 are unknown and 3 are monoatomic - leaving 52 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	402	1,3	14,14,15	0.29	0	15,19,21	0.55	0
3	NAG	A	403	3,4	14,14,15	0.51	0	15,19,21	0.43	0
4	BMA	A	404	3,5	11,11,12	0.58	0	14,15,17	0.88	0
5	MAN	A	405	5,4	11,11,12	0.72	0	14,15,17	0.89	0
5	MAN	A	406	5	11,11,12	0.88	1 (9%)	14,15,17	0.95	1 (7%)
5	MAN	A	407	5,4	11,11,12	1.04	0	14,15,17	1.94	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	A	408	5	11,11,12	0.67	0	14,15,17	1.12	1 (7%)
5	MAN	A	409	5	11,11,12	0.59	0	14,15,17	0.84	0
3	NAG	A	410	1,3	14,14,15	0.43	0	15,19,21	0.61	0
3	NAG	A	411	3,4	14,14,15	0.36	0	15,19,21	0.55	0
4	BMA	A	412	3,5	11,11,12	0.99	1 (9%)	14,15,17	1.00	1 (7%)
5	MAN	A	413	5,4	11,11,12	0.87	0	14,15,17	0.90	0
5	MAN	A	414	5	11,11,12	0.78	0	14,15,17	0.94	0
5	MAN	A	415	5	11,11,12	0.83	0	14,15,17	0.87	0
5	MAN	A	416	5	11,11,12	0.74	0	14,15,17	1.03	1 (7%)
5	MAN	A	417	5	11,11,12	0.62	0	14,15,17	0.81	0
5	MAN	A	418	4	11,11,12	1.00	1 (9%)	14,15,17	0.86	0
3	NAG	A	419	1,3	14,14,15	0.54	0	15,19,21	0.70	0
3	NAG	A	420	3,4	14,14,15	0.38	0	15,19,21	0.54	0
4	BMA	A	421	3,5	11,11,12	1.03	1 (9%)	14,15,17	1.51	2 (14%)
5	MAN	A	422	4	11,11,12	0.78	1 (9%)	14,15,17	0.89	0
3	NAG	A	423	1	14,14,15	0.32	0	15,19,21	0.33	0
7	PEG	A	425	-	6,6,6	0.64	0	5,5,5	0.23	0
8	P6G	A	426	-	17,17,18	0.59	0	16,16,17	1.85	4 (25%)
8	P6G	A	427	-	12,12,18	0.67	0	11,11,17	0.99	1 (9%)
9	GOL	A	428	-	5,5,5	0.31	0	5,5,5	0.29	0
9	GOL	A	429	-	5,5,5	0.30	0	5,5,5	0.29	0
9	GOL	A	430	-	5,5,5	0.34	0	5,5,5	0.26	0
9	GOL	A	431	-	5,5,5	0.31	0	5,5,5	0.21	0
3	NAG	B	402	1,3	14,14,15	0.28	0	15,19,21	0.37	0
3	NAG	B	403	3,4	14,14,15	0.60	1 (7%)	15,19,21	0.67	0
4	BMA	B	404	3,5	11,11,12	0.99	0	14,15,17	1.86	3 (21%)
5	MAN	B	405	5,4	11,11,12	0.69	0	14,15,17	0.81	0
5	MAN	B	406	5	11,11,12	1.21	2 (18%)	14,15,17	1.23	1 (7%)
5	MAN	B	407	5	11,11,12	0.84	0	14,15,17	0.87	1 (7%)
3	NAG	B	408	1,3	14,14,15	0.52	0	15,19,21	0.33	0
3	NAG	B	409	3,4	14,14,15	0.17	0	15,19,21	0.52	0
4	BMA	B	410	3,5	11,11,12	0.61	0	14,15,17	0.73	0
5	MAN	B	411	5,4	11,11,12	0.86	0	14,15,17	1.02	1 (7%)
5	MAN	B	412	5	11,11,12	0.73	0	14,15,17	0.83	0
5	MAN	B	413	5	11,11,12	0.73	0	14,15,17	0.76	0
5	MAN	B	414	5	11,11,12	0.80	0	14,15,17	1.10	2 (14%)
5	MAN	B	415	5	11,11,12	0.64	0	14,15,17	0.85	0
3	NAG	B	416	1	14,14,15	0.18	0	15,19,21	0.67	1 (6%)
3	NAG	B	417	1,3	14,14,15	0.32	0	15,19,21	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	418	3	14,14,15	0.21	0	15,19,21	0.30	0
3	NAG	B	419	1	14,14,15	0.30	0	15,19,21	0.50	0
7	PEG	B	422	-	6,6,6	0.64	0	5,5,5	0.27	0
7	PEG	B	423	-	6,6,6	0.65	0	5,5,5	0.32	0
9	GOL	B	424	-	5,5,5	0.34	0	5,5,5	0.20	0
9	GOL	B	425	-	5,5,5	0.34	0	5,5,5	0.19	0
9	GOL	B	426	-	5,5,5	0.32	0	5,5,5	0.30	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	402	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	403	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	404	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	405	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	406	5	-	0/2/19/22	0/1/1/1
5	MAN	A	407	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	408	5	-	0/2/19/22	1/1/1/1
5	MAN	A	409	5	-	0/2/19/22	0/1/1/1
3	NAG	A	410	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	411	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	412	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	413	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	414	5	-	0/2/19/22	0/1/1/1
5	MAN	A	415	5	-	0/2/19/22	0/1/1/1
5	MAN	A	416	5	-	0/2/19/22	0/1/1/1
5	MAN	A	417	5	-	0/2/19/22	0/1/1/1
5	MAN	A	418	4	-	0/2/19/22	0/1/1/1
3	NAG	A	419	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	420	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	421	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	422	4	-	0/2/19/22	0/1/1/1
3	NAG	A	423	1	-	0/6/23/26	0/1/1/1
7	PEG	A	425	-	-	0/4/4/4	0/0/0/0
8	P6G	A	426	-	-	0/15/15/16	0/0/0/0
8	P6G	A	427	-	-	0/10/10/16	0/0/0/0
9	GOL	A	428	-	-	0/4/4/4	0/0/0/0
9	GOL	A	429	-	-	0/4/4/4	0/0/0/0
9	GOL	A	430	-	-	0/4/4/4	0/0/0/0
9	GOL	A	431	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	402	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	403	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	404	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	405	5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	406	5	-	0/2/19/22	0/1/1/1
5	MAN	B	407	5	-	0/2/19/22	1/1/1/1
3	NAG	B	408	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	409	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	410	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	411	5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	412	5	-	0/2/19/22	0/1/1/1
5	MAN	B	413	5	-	0/2/19/22	0/1/1/1
5	MAN	B	414	5	-	0/2/19/22	0/1/1/1
5	MAN	B	415	5	-	0/2/19/22	0/1/1/1
3	NAG	B	416	1	-	0/6/23/26	0/1/1/1
3	NAG	B	417	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	418	3	-	0/6/23/26	0/1/1/1
3	NAG	B	419	1	-	0/6/23/26	0/1/1/1
7	PEG	B	422	-	-	0/4/4/4	0/0/0/0
7	PEG	B	423	-	-	0/4/4/4	0/0/0/0
9	GOL	B	424	-	-	0/4/4/4	0/0/0/0
9	GOL	B	425	-	-	0/4/4/4	0/0/0/0
9	GOL	B	426	-	-	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)
3	B	403	NAG	O5-C1	-2.06	1.40	1.43
5	A	422	MAN	C1-C2	2.02	1.57	1.52
5	A	418	MAN	C2-C3	2.13	1.55	1.52
5	B	406	MAN	C4-C5	2.14	1.57	1.53
5	A	406	MAN	C2-C3	2.18	1.55	1.52
4	A	421	BMA	O5-C5	2.24	1.48	1.43
4	A	412	BMA	C2-C3	2.50	1.55	1.52
5	B	406	MAN	O4-C4	2.54	1.49	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	421	BMA	C1-C2-C3	-4.30	104.46	109.54
8	A	426	P6G	O10-C9-C8	-3.61	94.32	110.36
5	A	407	MAN	C1-C2-C3	-3.23	105.72	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	426	P6G	C8-O7-C6	-3.11	99.95	113.31
5	B	414	MAN	O2-C2-C3	-2.91	104.27	110.12
5	A	416	MAN	O2-C2-C3	-2.56	104.98	110.12
4	B	404	BMA	O6-C6-C5	-2.16	104.21	111.33
8	A	426	P6G	O16-C15-C14	-2.10	101.03	110.36
5	B	411	MAN	O3-C3-C4	-2.04	105.75	110.34
5	A	407	MAN	C1-O5-C5	2.03	114.83	112.25
5	B	407	MAN	C1-O5-C5	2.03	114.83	112.25
5	B	414	MAN	C1-O5-C5	2.10	114.91	112.25
5	A	406	MAN	O3-C3-C2	2.23	114.03	110.00
8	A	427	P6G	O13-C12-C11	2.23	120.30	110.36
4	A	421	BMA	O3-C3-C2	2.37	114.28	110.00
3	B	416	NAG	C1-O5-C5	2.37	115.26	112.25
4	A	412	BMA	C1-O5-C5	2.47	115.39	112.25
4	B	404	BMA	O5-C1-C2	2.61	115.08	110.86
5	A	408	MAN	C1-O5-C5	2.86	115.87	112.25
5	B	406	MAN	C1-O5-C5	3.08	116.15	112.25
8	A	426	P6G	O7-C8-C9	4.36	129.76	110.36
4	B	404	BMA	C1-O5-C5	5.40	119.10	112.25
5	A	407	MAN	O3-C3-C2	5.68	120.25	110.00

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	408	MAN	C1-C2-C3-C4-C5-O5
5	B	407	MAN	C1-C2-C3-C4-C5-O5

14 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	410	NAG	1	0
4	A	412	BMA	1	0
5	A	418	MAN	1	0
3	A	419	NAG	1	0
3	A	420	NAG	1	0
4	A	421	BMA	2	0
5	A	422	MAN	1	0
8	A	426	P6G	2	0
9	A	428	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	406	MAN	1	0
5	B	407	MAN	1	0
7	B	422	PEG	2	0
7	B	423	PEG	1	0
9	B	424	GOL	2	0

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	318/321 (99%)	-0.09	3 (0%) 85 90	10, 19, 37, 99	0
1	B	321/321 (100%)	0.02	12 (3%) 45 56	10, 21, 41, 64	0
All	All	639/642 (99%)	-0.04	15 (2%) 64 73	10, 20, 40, 99	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	PHE	11.1
1	A	30	PRO	10.3
1	B	127	LEU	5.3
1	A	347	ALA	3.4
1	B	347	ALA	2.9
1	B	171	GLU	2.8
1	B	27	PRO	2.7
1	B	130	GLU	2.7
1	B	122	PRO	2.6
1	B	176	THR	2.6
1	B	131	ASP	2.5
1	B	126	THR	2.4
1	B	158	VAL	2.3
1	B	128	THR	2.3
1	B	112	HIS	2.1

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

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	UNX	A	401	1/1	0.84	0.72	21.05	30,30,30,30	0
2	UNX	B	401	1/1	0.90	0.63	19.86	30,30,30,30	0
9	GOL	A	431	6/6	0.48	0.30	17.80	57,69,71,74	0
7	PEG	B	422	7/7	0.92	0.24	10.67	42,50,63,67	0
5	MAN	A	406	11/12	0.88	0.20	9.62	41,46,58,64	0
9	GOL	A	430	6/6	0.69	0.33	9.62	83,85,89,90	0
3	NAG	A	423	14/15	0.74	0.31	8.20	47,57,73,73	0
9	GOL	B	425	6/6	0.61	0.29	6.13	61,78,79,85	0
5	MAN	A	405	11/12	0.92	0.16	5.60	25,31,38,38	0
7	PEG	A	425	7/7	0.91	0.26	4.82	40,47,50,53	0
8	P6G	A	427	13/19	0.91	0.18	2.81	36,44,54,56	0
5	MAN	A	409	11/12	0.95	0.12	2.74	23,31,35,39	0
7	PEG	B	423	7/7	0.80	0.28	2.69	44,58,62,66	0
5	MAN	B	405	11/12	0.92	0.13	2.40	26,32,38,41	0
9	GOL	A	428	6/6	0.73	0.23	1.94	62,63,65,68	0
5	MAN	B	406	11/12	0.88	0.18	1.74	41,50,83,88	0
9	GOL	B	424	6/6	0.87	0.12	1.64	58,59,59,60	0
5	MAN	B	412	11/12	0.92	0.16	1.12	22,24,30,35	0
8	P6G	A	426	18/19	0.67	0.28	0.95	50,66,80,81	0
3	NAG	B	402	14/15	0.96	0.12	0.34	13,21,27,42	0
3	NAG	A	402	14/15	0.96	0.08	0.00	12,17,29,33	0
3	NAG	B	409	14/15	0.96	0.09	-0.13	14,17,30,32	0
3	NAG	A	410	14/15	0.96	0.08	-0.59	10,17,30,40	0
3	NAG	B	408	14/15	0.96	0.08	-0.80	16,18,38,53	0
3	NAG	A	411	14/15	0.96	0.08	-1.63	11,15,25,26	0
3	NAG	A	419	14/15	0.91	0.14	-	24,36,52,52	0
3	NAG	B	419	14/15	0.86	0.26	-	39,54,71,77	0
5	MAN	A	417	11/12	0.89	0.31	-	55,58,62,67	0
5	MAN	A	418	11/12	0.69	0.40	-	68,83,90,92	0
9	GOL	A	429	6/6	0.77	0.33	-	58,62,62,62	0
3	NAG	B	417	14/15	0.86	0.33	-	41,59,65,68	0
5	MAN	B	415	11/12	0.90	0.21	-	43,45,55,56	0
9	GOL	B	426	6/6	0.68	0.30	-	75,76,81,84	0
5	MAN	B	414	11/12	0.94	0.19	-	28,34,46,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	420	14/15	0.84	0.28	-	27,58,68,71	0
5	MAN	B	411	11/12	0.94	0.14	-	20,26,34,34	0
6	MG	A	424	1/1	0.97	0.08	-	21,21,21,21	0
4	BMA	A	404	11/12	0.93	0.15	-	18,27,30,31	0
6	MG	B	420	1/1	0.95	0.04	-	23,23,23,23	0
4	BMA	A	412	11/12	0.93	0.17	-	23,28,41,52	0
3	NAG	B	403	14/15	0.93	0.19	-	20,25,38,39	0
4	BMA	A	421	11/12	0.60	0.30	-	62,78,84,88	0
5	MAN	A	422	11/12	0.58	0.31	-	79,88,100,101	0
3	NAG	B	416	14/15	0.90	0.39	-	40,62,68,72	0
3	NAG	B	418	14/15	0.81	0.41	-	76,82,86,92	0
5	MAN	A	416	11/12	0.93	0.23	-	36,42,55,64	0
5	MAN	A	408	11/12	0.76	0.33	-	62,70,79,86	0
5	MAN	A	415	11/12	0.72	0.33	-	48,65,74,77	0
5	MAN	B	407	11/12	0.43	0.70	-	96,100,105,106	0
4	BMA	B	410	11/12	0.94	0.14	-	23,28,40,43	0
5	MAN	A	407	11/12	0.95	0.17	-	24,30,37,45	0
5	MAN	A	414	11/12	0.89	0.13	-	27,30,36,38	0
10	CL	B	421	1/1	0.98	0.07	-	21,21,21,21	0
5	MAN	B	413	11/12	0.85	0.39	-	50,58,70,71	0
3	NAG	A	403	14/15	0.97	0.09	-	12,21,27,28	0
4	BMA	B	404	11/12	0.79	0.28	-	27,61,96,103	0
5	MAN	A	413	11/12	0.96	0.15	-	20,24,31,34	0

6.5 Other polymers (i)

There are no such residues in this entry.