



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2016 – 05:08 PM EDT

PDB ID : 5JU6  
Title : Structural and Functional Studies of Glycoside Hydrolase Family 3 beta-Glucosidase Cel3A from the Moderately Thermophilic Fungus *Rasamsonia emersonii*  
Authors : Gudmundsson, M.; Sandgren, M.; Karkehabadi, S.  
Deposited on : 2016-05-10  
Resolution : 2.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
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) : rb-20027790

**i**

## X-RAY DIFFRACTION

A.

 $R_{free}$ 1

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	930	-	-	-	X
2	NAG	A	940	-	-	-	X
2	NAG	A	942	-	-	-	X
2	NAG	B	941	-	-	-	X
2	NAG	B	944	-	-	-	X
2	NAG	C	935	-	-	-	X
2	NAG	C	944	-	-	-	X
2	NAG	C	947	-	-	-	X
2	NAG	D	940	-	-	-	X
2	NAG	D	942	-	-	-	X
4	MAN	A	925	-	-	-	X
4	MAN	A	939	-	-	-	X
4	MAN	B	939	-	-	-	X
4	MAN	C	943	-	-	-	X
4	MAN	D	928	-	-	-	X
4	MAN	D	939	-	-	-	X
5	BGC	A	946	-	-	-	X
5	BGC	B	945	-	-	-	X
5	BGC	C	951	-	-	-	X

## 2 Entry composition [i](#)

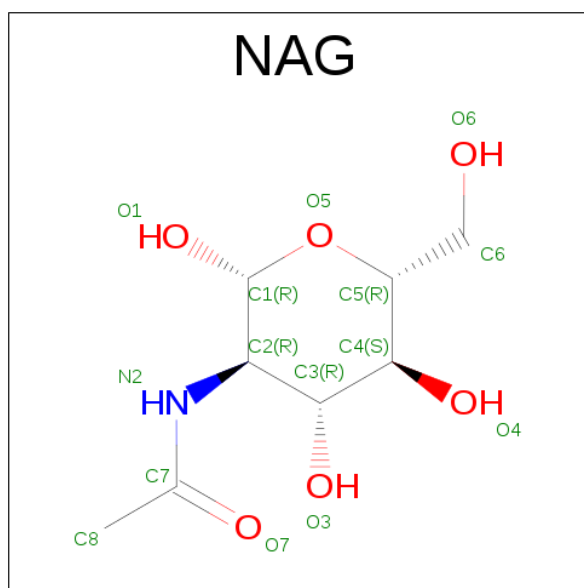
There are 7 unique types of molecules in this entry. The entry contains 29503 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total	C	N	O	S	0	0	0
			6373	4018	1093	1239	23			
1	B	835	Total	C	N	O	S	0	1	0
			6379	4021	1094	1241	23			
1	C	835	Total	C	N	O	S	0	3	0
			6388	4028	1095	1242	23			
1	D	835	Total	C	N	O	S	0	2	0
			6382	4023	1094	1241	24			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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

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

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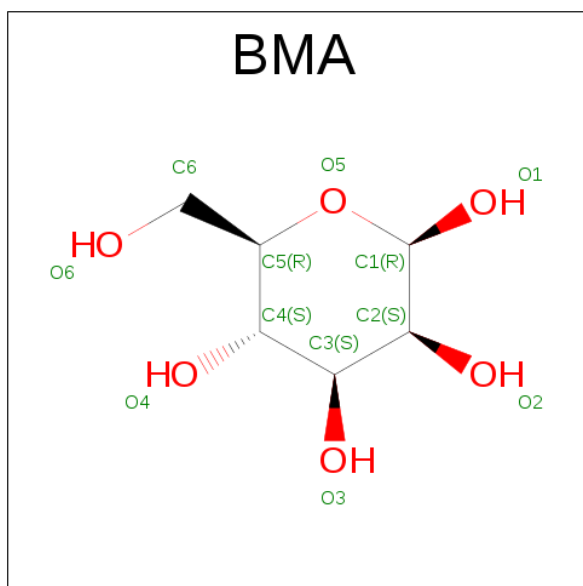
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



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

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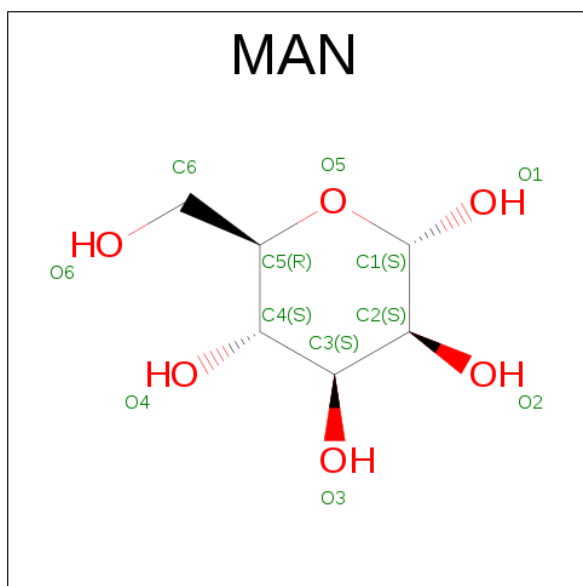
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

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

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

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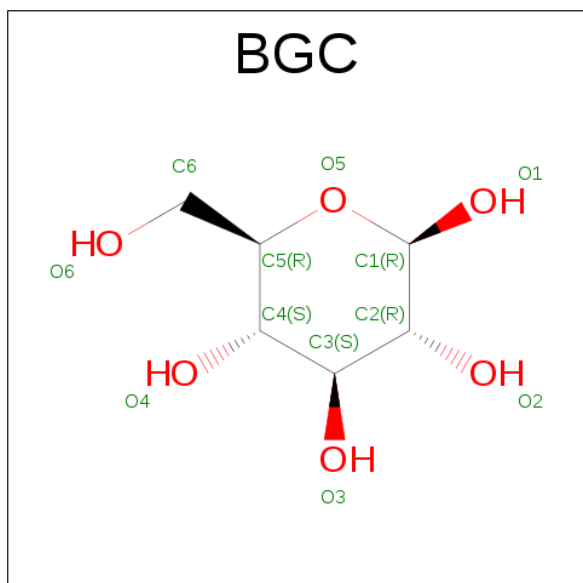
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4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

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

- Molecule 5 is BETA-D-GLUCOSE (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



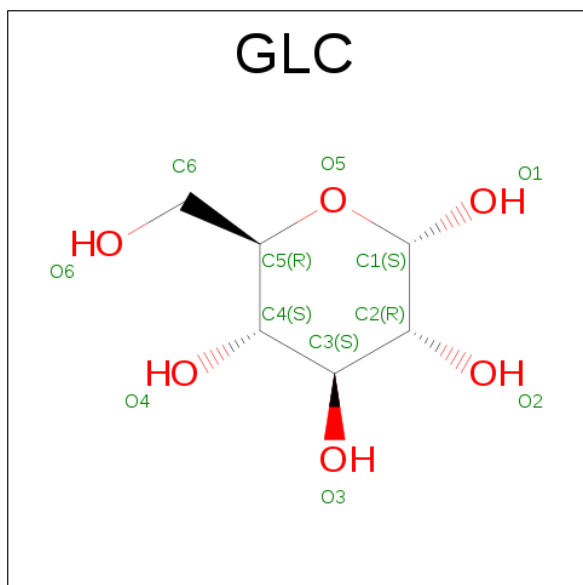
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			12	6	6		
5	C	1	Total	C	O	0	0
			12	6	6		
5	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

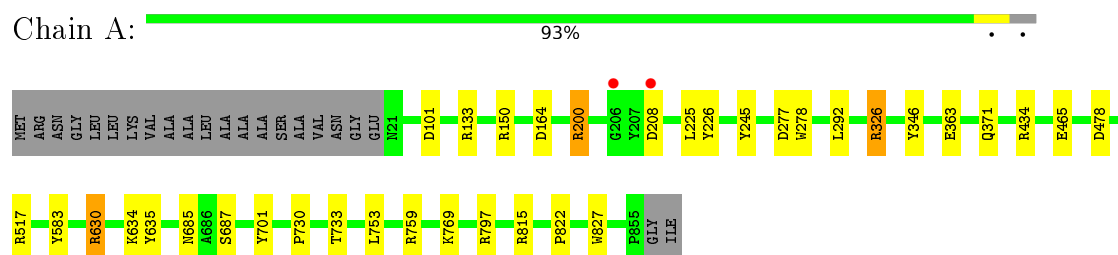
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	431	Total	O	0	0
			431	431		
7	B	399	Total	O	0	1
			400	400		
7	C	441	Total	O	0	0
			441	441		
7	D	432	Total	O	0	0
			432	432		

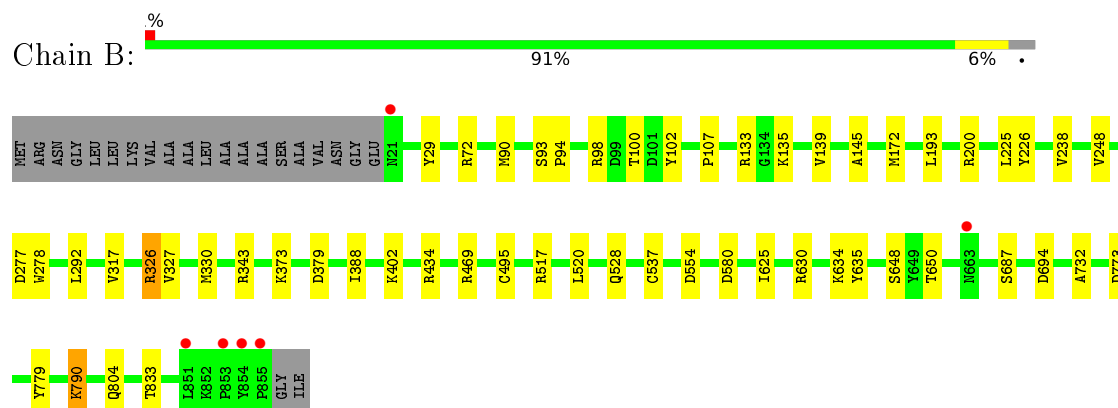
### 3 Residue-property plots [i](#)

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.

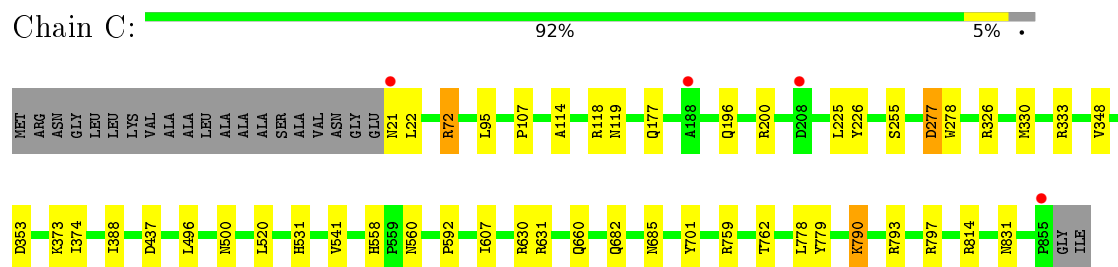
- Molecule 1: Beta-glucosidase



- Molecule 1: Beta-glucosidase



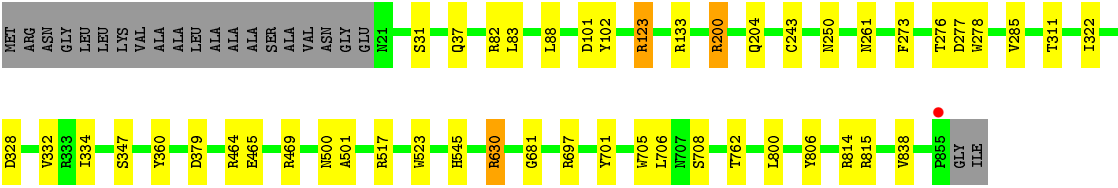
- Molecule 1: Beta-glucosidase



- Molecule 1: Beta-glucosidase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.29 Å   148.63 Å   196.39 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	118.51 – 2.20 48.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (118.51-2.20) 99.9 (48.04-2.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.173   ,   0.228 0.180   ,   0.233	Depositor DCC
$R_{free}$ test set	10210 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.990	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	29503	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, BGC, NAG, BMA, 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	0.74	0/6549	0.86	16/8954 (0.2%)
1	B	0.73	0/6555	0.87	14/8962 (0.2%)
1	C	0.74	0/6574	0.85	11/8988 (0.1%)
1	D	0.77	0/6561	0.86	14/8970 (0.2%)
All	All	0.74	0/26239	0.86	55/35874 (0.2%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	ARG	NE-CZ-NH2	-10.85	114.87	120.30
1	A	326	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	B	326	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	B	72	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	326	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	D	630	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	630	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	C	814	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	C	118	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	759	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	434	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	630	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	464	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	B	517	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	343	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	D	517	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	517	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	434	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	D	133	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	631	ARG	NE-CZ-NH2	-6.08	117.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	797	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	434	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	814	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	133	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	517	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	200	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	D	200	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	101	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	469	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	D	133	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	815	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	580	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	793	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	D	200	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	D	123	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	200	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	98	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	814	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	630	ARG	CG-CD-NE	-5.44	100.37	111.80
1	A	815	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	B	98	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	101	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	200	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	C	277	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	478	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	150	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	82	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	C	333	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	773	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	631	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	517	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	200	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	517	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	C	797	ARG	NE-CZ-NH2	-5.01	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	6373	0	6031	12	0
1	B	6379	0	6039	22	0
1	C	6388	0	6048	20	0
1	D	6382	0	6040	20	0
2	A	266	0	234	2	0
2	B	238	0	208	0	0
2	C	266	0	232	1	0
2	D	238	0	209	1	0
3	A	66	0	51	0	0
3	B	77	0	61	0	0
3	C	77	0	60	0	0
3	D	66	0	51	0	0
4	A	220	0	189	0	0
4	B	220	0	189	1	0
4	C	253	0	216	0	0
4	D	220	0	188	0	0
5	A	12	0	12	1	0
5	B	12	0	12	1	0
5	C	12	0	12	1	0
5	D	12	0	12	1	0
6	C	11	0	10	0	0
6	D	11	0	10	0	0
7	A	431	0	0	1	0
7	B	400	0	0	2	0
7	C	441	0	0	5	0
7	D	432	0	0	6	0
All	All	29503	0	26114	74	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 1.

All (74) 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:C:196:GLN:HE22	1:C:607:ILE:H	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:GLN:HE22	1:C:348:VAL:HG12	1.54	0.73
4:B:904:MAN:O2	4:B:905:MAN:C1	2.41	0.68
1:D:360:TYR:O	7:D:1001:HOH:O	2.13	0.67
1:B:225:LEU:HD23	1:B:226:TYR:CZ	2.31	0.65
1:C:119:ASN:ND2	7:C:1002:HOH:O	2.28	0.65
1:A:277:ASP:OD1	5:A:946:BGC:H1	1.96	0.64
1:C:660:GLN:NE2	7:C:1003:HOH:O	2.31	0.63
1:A:465:GLU:HG2	1:A:583:TYR:CE2	2.34	0.62
1:D:277:ASP:OD1	5:D:945:BGC:H1	2.02	0.60
1:D:311:THR:OG1	1:D:705:TRP:O	2.17	0.59
1:B:225:LEU:HD23	1:B:226:TYR:CE2	2.38	0.57
1:A:164:ASP:OD1	1:A:630:ARG:NH2	2.38	0.57
1:D:762:THR:HG21	1:D:838:VAL:HG11	1.87	0.56
1:C:630:ARG:NH1	7:C:1001:HOH:O	2.22	0.56
1:B:277:ASP:OD1	5:B:945:BGC:H1	2.06	0.55
1:B:193:LEU:HD12	1:B:248:VAL:HG13	1.87	0.55
1:C:558:HIS:HD2	1:C:560:ASN:H	1.52	0.55
1:B:648:SER:OG	1:B:650:THR:O	2.25	0.54
1:D:102:TYR:HB3	1:D:379:ASP:HA	1.90	0.53
1:D:500:ASN:HB2	1:D:545:HIS:O	2.09	0.52
1:D:800:LEU:HD21	1:D:806:TYR:HB2	1.91	0.52
1:C:701:TYR:CZ	2:C:902:NAG:H82	2.46	0.51
1:D:630:ARG:HD3	7:D:1003:HOH:O	2.10	0.50
1:C:496:LEU:HD23	1:C:541:VAL:HB	1.94	0.49
1:D:681:GLY:HA3	7:D:1128:HOH:O	2.12	0.49
1:D:697:ARG:HD3	7:D:1291:HOH:O	2.12	0.49
1:C:225:LEU:HD23	1:C:226:TYR:CE2	2.48	0.49
1:C:277:ASP:OD1	5:C:951:BGC:H1	2.13	0.49
1:D:285:VAL:HA	1:D:322:ILE:HD11	1.95	0.49
1:B:495:CYS:HG	1:B:537:CYS:CB	2.27	0.48
1:C:107:PRO:HD3	1:C:388:ILE:HG23	1.95	0.48
1:B:495:CYS:SG	1:B:537:CYS:SG	3.00	0.47
1:A:225:LEU:HD23	1:A:226:TYR:CE2	2.49	0.47
1:B:528:GLN:HB2	7:B:1372:HOH:O	2.15	0.47
1:C:778:LEU:HD23	1:C:778:LEU:C	2.35	0.47
1:B:634:LYS:HD3	1:B:635:TYR:CE1	2.50	0.46
1:D:273:PHE:CD1	1:D:334:ILE:HA	2.50	0.46
1:B:625:ILE:O	1:B:630:ARG:HD3	2.16	0.46
1:C:779:TYR:HB3	1:C:790:LYS:HB2	1.99	0.45
1:A:634:LYS:HD3	1:A:635:TYR:CE2	2.52	0.45
1:B:93:SER:HB2	1:B:94:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:TYR:HB3	1:B:790:LYS:HB2	1.99	0.45
1:D:701:TYR:CZ	2:D:902:NAG:H82	2.52	0.45
1:B:292:LEU:O	1:B:326:ARG:NH2	2.50	0.44
1:D:37:GLN:NE2	7:D:1023:HOH:O	2.49	0.44
1:B:29:TYR:HB3	1:B:732:ALA:HA	2.00	0.44
1:A:730:PRO:HB3	2:A:945:NAG:H82	2.00	0.44
1:D:243[B]:CYS:SG	1:D:276:THR:HA	2.58	0.43
1:B:145:ALA:HB2	1:B:172:MET:SD	2.58	0.43
1:B:326:ARG:O	1:B:330:MET:HG3	2.18	0.43
1:D:465:GLU:OE1	1:D:469:ARG:NH2	2.51	0.43
1:A:701:TYR:CZ	2:A:902:NAG:H82	2.54	0.43
7:B:1313:HOH:O	1:C:759:ARG:HD3	2.18	0.43
1:D:31:SER:HA	1:D:261:ASN:ND2	2.34	0.43
1:A:733:THR:CG2	7:A:1351:HOH:O	2.66	0.43
1:B:90:MET:HG3	1:B:139:VAL:HB	2.00	0.43
1:B:107:PRO:HD3	1:B:388:ILE:HG23	2.01	0.43
1:C:630:ARG:HD2	7:C:1001:HOH:O	2.18	0.43
1:A:292:LEU:O	1:A:326:ARG:NH2	2.52	0.42
1:C:353:ASP:HB2	1:C:374:ILE:HB	2.01	0.42
1:D:328:ASP:O	1:D:332:VAL:HG23	2.18	0.42
1:C:21:ASN:HB3	7:C:1322:HOH:O	2.20	0.42
1:B:317:VAL:HG21	1:B:327:VAL:HG21	2.02	0.42
1:D:250:ASN:ND2	7:D:1011:HOH:O	2.44	0.42
1:B:102:TYR:HB3	1:B:379:ASP:HA	2.02	0.41
1:A:753:LEU:HD21	1:A:827:TRP:HB2	2.01	0.41
1:A:200:ARG:O	1:A:245:TYR:HB3	2.19	0.41
1:C:437:ASP:OD2	1:C:500:ASN:OD1	2.39	0.41
1:C:114:ALA:HB2	1:C:592:PRO:HD3	2.02	0.41
1:D:501:ALA:HA	1:D:523:TRP:CD1	2.55	0.40
1:B:100:THR:HG21	1:B:135:LYS:HE3	2.04	0.40
1:A:133:ARG:HD2	1:A:346:TYR:CD1	2.56	0.40
1:C:326:ARG:O	1:C:330:MET:HG3	2.21	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	833/857 (97%)	804 (96%)	29 (4%)	0	100	100
1	B	834/857 (97%)	802 (96%)	31 (4%)	1 (0%)	56	64
1	C	836/857 (98%)	807 (96%)	29 (4%)	0	100	100
1	D	835/857 (97%)	800 (96%)	35 (4%)	0	100	100
All	All	3338/3428 (97%)	3213 (96%)	124 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	694	ASP

### 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	672/685 (98%)	664 (99%)	8 (1%)	78	88
1	B	673/685 (98%)	664 (99%)	9 (1%)	76	87
1	C	675/685 (98%)	660 (98%)	15 (2%)	60	72
1	D	674/685 (98%)	665 (99%)	9 (1%)	76	87
All	All	2694/2740 (98%)	2653 (98%)	41 (2%)	72	84

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	ASP
1	A	278	TRP
1	A	363	GLU
1	A	371	GLN
1	A	685	ASN

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Mol	Chain	Res	Type
1	A	687	SER
1	A	769	LYS
1	A	822	PRO
1	B	238	VAL
1	B	278	TRP
1	B	373	LYS
1	B	402	LYS
1	B	520	LEU
1	B	554	ASP
1	B	687	SER
1	B	790	LYS
1	B	833	THR
1	C	22	LEU
1	C	72	ARG
1	C	95	LEU
1	C	177	GLN
1	C	255	SER
1	C	278	TRP
1	C	373	LYS
1	C	520	LEU
1	C	531[A]	HIS
1	C	531[B]	HIS
1	C	682	GLN
1	C	685	ASN
1	C	762	THR
1	C	790	LYS
1	C	831	ASN
1	D	83	LEU
1	D	88	LEU
1	D	123	ARG
1	D	200	ARG
1	D	204	GLN
1	D	278	TRP
1	D	347	SER
1	D	706	LEU
1	D	708	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	157	ASN

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Mol	Chain	Res	Type
1	A	246	ASN
1	A	369	GLN
1	A	371	GLN
1	A	460	GLN
1	A	539	ASN
1	A	558	HIS
1	A	612	ASN
1	A	636	ASN
1	A	777	GLN
1	A	844	ASN
1	B	45	GLN
1	B	91	GLN
1	B	157	ASN
1	B	261	ASN
1	B	369	GLN
1	B	463	GLN
1	B	619	GLN
1	B	716	ASN
1	B	804	GLN
1	B	844	ASN
1	C	37	GLN
1	C	119	ASN
1	C	132	HIS
1	C	140	GLN
1	C	177	GLN
1	C	196	GLN
1	C	261	ASN
1	C	463	GLN
1	C	491	GLN
1	C	539	ASN
1	C	558	HIS
1	C	612	ASN
1	C	618	GLN
1	C	660	GLN
1	D	37	GLN
1	D	45	GLN
1	D	132	HIS
1	D	216	ASN
1	D	250	ASN
1	D	261	ASN
1	D	282	HIS
1	D	371	GLN

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Mol	Chain	Res	Type
1	D	463	GLN
1	D	470	ASN
1	D	491	GLN
1	D	618	GLN
1	D	656	GLN
1	D	716	ASN
1	D	805	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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

187 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAG	A	901	1,2	14,14,15	0.49	0	15,19,21	0.90	0
2	NAG	A	902	3,2	14,14,15	0.63	0	15,19,21	1.16	1 (6%)
3	BMA	A	903	2,4	11,11,12	1.07	1 (9%)	15,15,17	1.69	4 (26%)
4	MAN	A	904	3,4	11,11,12	0.42	0	15,15,17	1.48	3 (20%)
4	MAN	A	905	4	11,11,12	0.65	0	15,15,17	0.85	0
2	NAG	A	906	1,2	14,14,15	0.75	0	15,19,21	1.30	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	907	3,2	14,14,15	0.52	0	15,19,21	0.65	0
3	BMA	A	908	2,4	11,11,12	0.23	0	15,15,17	1.35	1 (6%)
4	MAN	A	909	3,4	11,11,12	0.92	1 (9%)	15,15,17	1.33	2 (13%)
4	MAN	A	910	4	11,11,12	0.79	0	15,15,17	1.40	1 (6%)
4	MAN	A	911	4	11,11,12	0.76	0	15,15,17	1.12	1 (6%)
4	MAN	A	912	3	11,11,12	1.38	2 (18%)	15,15,17	2.02	7 (46%)
2	NAG	A	913	1,2	14,14,15	0.66	0	15,19,21	1.29	1 (6%)
2	NAG	A	914	3,2	14,14,15	0.59	0	15,19,21	1.26	1 (6%)
3	BMA	A	915	2,4	11,11,12	0.59	0	15,15,17	2.40	7 (46%)
4	MAN	A	916	3	11,11,12	0.94	0	15,15,17	1.56	2 (13%)
2	NAG	A	917	1,2	14,14,15	0.39	0	15,19,21	0.79	0
2	NAG	A	918	3,2	14,14,15	0.92	1 (7%)	15,19,21	1.03	0
3	BMA	A	919	2,4	11,11,12	0.66	0	15,15,17	0.93	0
4	MAN	A	920	3,4	11,11,12	0.60	0	15,15,17	1.73	4 (26%)
4	MAN	A	921	4	11,11,12	0.99	1 (9%)	15,15,17	1.37	2 (13%)
4	MAN	A	922	3,4	11,11,12	0.49	0	15,15,17	1.40	2 (13%)
4	MAN	A	923	4	11,11,12	1.02	0	15,15,17	1.67	4 (26%)
4	MAN	A	924	4	11,11,12	0.59	0	15,15,17	1.40	3 (20%)
4	MAN	A	925	4	11,11,12	0.70	0	15,15,17	1.41	3 (20%)
2	NAG	A	926	1,2	14,14,15	0.76	0	15,19,21	0.89	0
2	NAG	A	927	3,2	14,14,15	0.58	0	15,19,21	1.70	2 (13%)
3	BMA	A	928	2,4	11,11,12	0.78	0	15,15,17	1.24	3 (20%)
4	MAN	A	929	3	11,11,12	0.87	0	15,15,17	1.42	2 (13%)
2	NAG	A	930	1	14,14,15	0.64	0	15,19,21	1.34	3 (20%)
2	NAG	A	931	1,2	14,14,15	0.64	0	15,19,21	0.93	0
2	NAG	A	932	3,2	14,14,15	0.44	0	15,19,21	1.34	2 (13%)
3	BMA	A	933	2,4	11,11,12	0.68	0	15,15,17	1.48	4 (26%)
4	MAN	A	934	3,4	11,11,12	0.45	0	15,15,17	1.44	3 (20%)
4	MAN	A	935	4	11,11,12	1.03	0	15,15,17	1.43	3 (20%)
4	MAN	A	936	4	11,11,12	0.92	1 (9%)	15,15,17	0.93	0
4	MAN	A	937	3,4	11,11,12	0.92	0	15,15,17	1.61	1 (6%)
4	MAN	A	938	4	11,11,12	0.52	0	15,15,17	1.59	3 (20%)
4	MAN	A	939	4	11,11,12	0.56	0	15,15,17	1.21	1 (6%)
2	NAG	A	940	1	14,14,15	0.84	0	15,19,21	1.26	1 (6%)
2	NAG	A	941	1	14,14,15	0.54	0	15,19,21	1.09	1 (6%)
2	NAG	A	942	1,2	14,14,15	0.40	0	15,19,21	1.28	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	943	2	14,14,15	0.48	0	15,19,21	1.01	0
2	NAG	A	944	1	14,14,15	0.70	0	15,19,21	1.51	2 (13%)
2	NAG	A	945	1	14,14,15	0.70	0	15,19,21	1.50	3 (20%)
5	BGC	A	946	-	12,12,12	1.07	1 (8%)	17,17,17	1.13	2 (11%)
2	NAG	B	901	1,2	14,14,15	0.60	0	15,19,21	0.93	0
2	NAG	B	902	3,2	14,14,15	0.49	0	15,19,21	1.07	1 (6%)
3	BMA	B	903	2,4	11,11,12	0.38	0	15,15,17	1.13	1 (6%)
4	MAN	B	904	3	11,11,12	0.70	0	15,15,17	1.37	3 (20%)
4	MAN	B	905	-	11,11,12	0.78	0	15,15,17	1.64	4 (26%)
2	NAG	B	906	1,2	14,14,15	0.39	0	15,19,21	1.56	3 (20%)
2	NAG	B	907	3,2	14,14,15	0.50	0	15,19,21	0.89	1 (6%)
3	BMA	B	908	2,4	11,11,12	0.46	0	15,15,17	1.73	3 (20%)
4	MAN	B	909	3,4	11,11,12	0.95	1 (9%)	15,15,17	1.59	4 (26%)
4	MAN	B	910	4	11,11,12	0.87	1 (9%)	15,15,17	1.80	6 (40%)
2	NAG	B	911	1,2	14,14,15	0.72	0	15,19,21	1.05	1 (6%)
2	NAG	B	912	3,2	14,14,15	0.63	0	15,19,21	1.99	4 (26%)
3	BMA	B	913	2,4	11,11,12	0.87	0	15,15,17	1.26	3 (20%)
4	MAN	B	914	3	11,11,12	0.90	0	15,15,17	1.23	2 (13%)
2	NAG	B	915	1,2	14,14,15	0.71	0	15,19,21	1.20	2 (13%)
2	NAG	B	916	3,2	14,14,15	0.61	0	15,19,21	0.87	0
3	BMA	B	917	2,4	11,11,12	0.45	0	15,15,17	0.88	0
4	MAN	B	918	3,4	11,11,12	0.62	0	15,15,17	1.00	0
4	MAN	B	919	4	11,11,12	1.03	1 (9%)	15,15,17	1.64	5 (33%)
4	MAN	B	920	3,4	11,11,12	0.52	0	15,15,17	1.08	2 (13%)
4	MAN	B	921	4	11,11,12	1.04	0	15,15,17	1.54	3 (20%)
4	MAN	B	922	4	11,11,12	0.92	0	15,15,17	1.14	2 (13%)
4	MAN	B	923	4	11,11,12	0.77	0	15,15,17	1.20	1 (6%)
4	MAN	B	924	4	11,11,12	0.60	0	15,15,17	1.78	5 (33%)
2	NAG	B	925	1,2	14,14,15	0.65	0	15,19,21	1.13	3 (20%)
2	NAG	B	926	3,2	14,14,15	0.64	0	15,19,21	0.99	0
3	BMA	B	927	3,2,4	11,11,12	0.67	0	15,15,17	1.36	2 (13%)
3	BMA	B	928	3	11,11,12	0.90	0	15,15,17	1.37	1 (6%)
4	MAN	B	929	3	11,11,12	0.95	1 (9%)	15,15,17	1.39	3 (20%)
2	NAG	B	930	1,2	14,14,15	0.55	0	15,19,21	1.05	0
2	NAG	B	931	3,2	14,14,15	0.61	0	15,19,21	1.15	1 (6%)
3	BMA	B	932	2,4	11,11,12	0.67	0	15,15,17	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	B	933	3,4	11,11,12	0.61	0	15,15,17	1.41	2 (13%)
4	MAN	B	934	4	11,11,12	0.91	1 (9%)	15,15,17	1.45	3 (20%)
4	MAN	B	935	4	11,11,12	0.76	0	15,15,17	1.14	0
4	MAN	B	936	3,4	11,11,12	0.71	0	15,15,17	2.24	7 (46%)
4	MAN	B	937	4	11,11,12	0.78	0	15,15,17	1.45	4 (26%)
4	MAN	B	938	4	11,11,12	0.61	0	15,15,17	1.23	2 (13%)
4	MAN	B	939	4	11,11,12	0.97	0	15,15,17	1.08	0
2	NAG	B	940	1	14,14,15	0.91	0	15,19,21	1.41	3 (20%)
2	NAG	B	941	1,2	14,14,15	0.73	0	15,19,21	1.52	2 (13%)
2	NAG	B	942	2	14,14,15	0.69	0	15,19,21	1.41	2 (13%)
2	NAG	B	943	1	14,14,15	0.55	0	15,19,21	1.19	1 (6%)
2	NAG	B	944	1	14,14,15	0.38	0	15,19,21	1.18	3 (20%)
5	BGC	B	945	-	12,12,12	1.22	0	17,17,17	1.13	1 (5%)
2	NAG	C	901	1,2	14,14,15	0.44	0	15,19,21	1.10	1 (6%)
2	NAG	C	902	3,2	14,14,15	0.45	0	15,19,21	1.23	2 (13%)
3	BMA	C	903	2,4	11,11,12	0.59	0	15,15,17	1.32	2 (13%)
4	MAN	C	904	3,4	11,11,12	0.54	0	15,15,17	0.78	0
4	MAN	C	905	4	11,11,12	0.75	0	15,15,17	1.46	3 (20%)
4	MAN	C	906	4	11,11,12	1.10	1 (9%)	15,15,17	1.69	5 (33%)
4	MAN	C	907	3,4	11,11,12	1.07	1 (9%)	15,15,17	1.29	2 (13%)
4	MAN	C	908	4	11,11,12	0.93	0	15,15,17	1.18	1 (6%)
4	MAN	C	909	4	11,11,12	0.95	1 (9%)	15,15,17	1.16	1 (6%)
2	NAG	C	910	1,2	14,14,15	0.68	0	15,19,21	1.74	4 (26%)
2	NAG	C	911	3,2	14,14,15	0.74	0	15,19,21	0.87	0
3	BMA	C	912	2,4	11,11,12	0.57	0	15,15,17	1.81	5 (33%)
4	MAN	C	913	3,4	11,11,12	0.56	0	15,15,17	1.06	0
4	MAN	C	914	4	11,11,12	0.76	0	15,15,17	1.15	0
4	MAN	C	915	4,6	11,11,12	1.38	1 (9%)	15,15,17	1.58	2 (13%)
6	GLC	C	916	4	11,11,12	1.05	1 (9%)	15,15,17	1.79	2 (13%)
4	MAN	C	917	3	11,11,12	1.26	2 (18%)	15,15,17	1.65	4 (26%)
2	NAG	C	918	1,2	14,14,15	0.44	0	15,19,21	1.18	2 (13%)
2	NAG	C	919	3,2	14,14,15	0.44	0	15,19,21	1.60	3 (20%)
3	BMA	C	920	2,4	11,11,12	0.68	0	15,15,17	1.09	0
4	MAN	C	921	3	11,11,12	0.60	0	15,15,17	1.02	0
4	MAN	C	922	3	11,11,12	1.04	1 (9%)	15,15,17	1.44	3 (20%)
2	NAG	C	923	1,2	14,14,15	0.47	0	15,19,21	1.23	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	924	3,2	14,14,15	0.46	0	15,19,21	0.98	0
3	BMA	C	925	2,4	11,11,12	0.80	1 (9%)	15,15,17	1.02	0
4	MAN	C	926	3,4	11,11,12	0.60	0	15,15,17	1.39	3 (20%)
4	MAN	C	927	4	11,11,12	1.03	1 (9%)	15,15,17	1.29	2 (13%)
4	MAN	C	928	3,4	11,11,12	0.69	0	15,15,17	1.10	1 (6%)
4	MAN	C	929	4	11,11,12	0.68	0	15,15,17	1.34	2 (13%)
4	MAN	C	930	4	11,11,12	0.58	0	15,15,17	1.15	1 (6%)
4	MAN	C	931	4	11,11,12	0.61	0	15,15,17	1.17	2 (13%)
2	NAG	C	932	1,2	14,14,15	0.62	0	15,19,21	1.53	4 (26%)
2	NAG	C	933	3,2	14,14,15	0.53	0	15,19,21	1.46	2 (13%)
3	BMA	C	934	2	11,11,12	0.66	0	15,15,17	1.12	0
2	NAG	C	935	1	14,14,15	0.76	0	15,19,21	1.42	3 (20%)
2	NAG	C	936	1,2	14,14,15	0.74	0	15,19,21	1.95	7 (46%)
2	NAG	C	937	3,2	14,14,15	0.41	0	15,19,21	1.57	3 (20%)
3	BMA	C	938	2,4	11,11,12	0.65	0	15,15,17	1.43	3 (20%)
4	MAN	C	939	3,4	11,11,12	0.62	0	15,15,17	0.87	0
4	MAN	C	940	4	11,11,12	1.18	1 (9%)	15,15,17	1.76	4 (26%)
4	MAN	C	941	3,4	11,11,12	0.66	0	15,15,17	1.00	0
4	MAN	C	942	4	11,11,12	0.78	0	15,15,17	1.51	2 (13%)
4	MAN	C	943	4	11,11,12	0.71	0	15,15,17	0.95	1 (6%)
2	NAG	C	944	1	14,14,15	0.90	0	15,19,21	1.98	4 (26%)
2	NAG	C	945	1,2	14,14,15	0.40	0	15,19,21	0.98	0
2	NAG	C	946	2	14,14,15	0.69	0	15,19,21	1.37	2 (13%)
2	NAG	C	947	1,2	14,14,15	0.62	0	15,19,21	1.70	4 (26%)
2	NAG	C	948	3,2	14,14,15	0.66	0	15,19,21	1.52	3 (20%)
3	BMA	C	949	2	11,11,12	0.87	0	15,15,17	1.06	2 (13%)
2	NAG	C	950	1	14,14,15	0.65	0	15,19,21	0.82	1 (6%)
5	BGC	C	951	-	12,12,12	1.20	1 (8%)	17,17,17	1.44	2 (11%)
2	NAG	D	901	1,2	14,14,15	0.58	0	15,19,21	1.28	2 (13%)
2	NAG	D	902	3,2	14,14,15	0.41	0	15,19,21	1.22	2 (13%)
3	BMA	D	903	2,4	11,11,12	0.59	0	15,15,17	1.07	2 (13%)
4	MAN	D	904	3,4	11,11,12	0.63	0	15,15,17	1.45	2 (13%)
4	MAN	D	905	4	11,11,12	0.81	0	15,15,17	0.98	0
4	MAN	D	906	3	11,11,12	0.63	0	15,15,17	0.77	0
2	NAG	D	907	1,2	14,14,15	0.74	1 (7%)	15,19,21	1.04	1 (6%)
2	NAG	D	908	3,2	14,14,15	0.55	0	15,19,21	1.11	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	D	909	2,4	11,11,12	0.64	0	15,15,17	1.34	3 (20%)
4	MAN	D	910	3,4	11,11,12	1.04	0	15,15,17	1.03	1 (6%)
4	MAN	D	911	4	11,11,12	0.56	0	15,15,17	1.15	1 (6%)
4	MAN	D	912	4,6	11,11,12	0.85	1 (9%)	15,15,17	1.39	2 (13%)
6	GLC	D	913	4	11,11,12	0.71	0	15,15,17	1.27	0
4	MAN	D	914	3	11,11,12	1.29	1 (9%)	15,15,17	1.63	4 (26%)
2	NAG	D	915	1,2	14,14,15	0.56	0	15,19,21	1.22	1 (6%)
2	NAG	D	916	3,2	14,14,15	0.83	0	15,19,21	1.85	3 (20%)
3	BMA	D	917	2,4	11,11,12	0.70	0	15,15,17	1.85	6 (40%)
4	MAN	D	918	3	11,11,12	0.77	0	15,15,17	0.97	1 (6%)
2	NAG	D	919	1,2	14,14,15	0.53	0	15,19,21	1.33	2 (13%)
2	NAG	D	920	3,2	14,14,15	0.74	0	15,19,21	0.94	0
3	BMA	D	921	2,4	11,11,12	0.79	0	15,15,17	1.05	0
4	MAN	D	922	3,4	11,11,12	0.59	0	15,15,17	1.34	2 (13%)
4	MAN	D	923	4	11,11,12	0.73	0	15,15,17	1.32	2 (13%)
4	MAN	D	924	3,4	11,11,12	0.52	0	15,15,17	1.01	0
4	MAN	D	925	4	11,11,12	0.74	0	15,15,17	1.27	1 (6%)
4	MAN	D	926	4	11,11,12	0.67	0	15,15,17	0.99	1 (6%)
4	MAN	D	927	4	11,11,12	0.90	0	15,15,17	1.13	2 (13%)
4	MAN	D	928	4	11,11,12	0.61	0	15,15,17	1.38	2 (13%)
2	NAG	D	929	1,2	14,14,15	0.74	0	15,19,21	1.23	3 (20%)
2	NAG	D	930	3,2	14,14,15	0.48	0	15,19,21	1.30	2 (13%)
3	BMA	D	931	2	11,11,12	0.65	0	15,15,17	1.23	3 (20%)
2	NAG	D	932	1,2	14,14,15	0.50	0	15,19,21	1.26	3 (20%)
2	NAG	D	933	3,2	14,14,15	0.87	1 (7%)	15,19,21	1.17	2 (13%)
3	BMA	D	934	2,4	11,11,12	0.49	0	15,15,17	0.94	0
4	MAN	D	935	3,4	11,11,12	0.78	0	15,15,17	0.99	1 (6%)
4	MAN	D	936	4	11,11,12	0.60	0	15,15,17	1.45	3 (20%)
4	MAN	D	937	3,4	11,11,12	0.66	0	15,15,17	0.89	0
4	MAN	D	938	4	11,11,12	0.90	1 (9%)	15,15,17	1.44	1 (6%)
4	MAN	D	939	4	11,11,12	0.84	0	15,15,17	1.35	2 (13%)
2	NAG	D	940	1	14,14,15	0.76	1 (7%)	15,19,21	1.05	1 (6%)
2	NAG	D	941	1	14,14,15	0.51	0	15,19,21	0.98	0
2	NAG	D	942	1	14,14,15	0.97	0	15,19,21	1.34	4 (26%)
2	NAG	D	943	1	14,14,15	0.58	0	15,19,21	1.50	3 (20%)
2	NAG	D	944	1	14,14,15	0.97	1 (7%)	15,19,21	1.74	3 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BGC	D	945	-	12,12,12	0.80	0	17,17,17	1.27	2 (11%)

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	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	902	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	903	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	904	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	905	4	-	0/2/19/22	0/1/1/1
2	NAG	A	906	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	907	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	908	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	909	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	910	4	-	0/2/19/22	0/1/1/1
4	MAN	A	911	4	-	0/2/19/22	0/1/1/1
4	MAN	A	912	3	-	0/2/19/22	0/1/1/1
2	NAG	A	913	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	914	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	915	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	916	3	-	0/2/19/22	0/1/1/1
2	NAG	A	917	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	918	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	919	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	920	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	921	4	-	0/2/19/22	0/1/1/1
4	MAN	A	922	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	923	4	-	0/2/19/22	0/1/1/1
4	MAN	A	924	4	-	0/2/19/22	0/1/1/1
4	MAN	A	925	4	-	0/2/19/22	0/1/1/1
2	NAG	A	926	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	927	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	928	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	929	3	-	0/2/19/22	0/1/1/1
2	NAG	A	930	1	-	0/6/23/26	0/1/1/1
2	NAG	A	931	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	932	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	933	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	934	3,4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	935	4	-	0/2/19/22	0/1/1/1
4	MAN	A	936	4	-	0/2/19/22	0/1/1/1
4	MAN	A	937	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	938	4	-	0/2/19/22	0/1/1/1
4	MAN	A	939	4	-	0/2/19/22	0/1/1/1
2	NAG	A	940	1	-	0/6/23/26	0/1/1/1
2	NAG	A	941	1	-	0/6/23/26	0/1/1/1
2	NAG	A	942	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	943	2	-	0/6/23/26	0/1/1/1
2	NAG	A	944	1	-	0/6/23/26	0/1/1/1
2	NAG	A	945	1	-	0/6/23/26	0/1/1/1
5	BGC	A	946	-	-	0/2/22/22	0/1/1/1
2	NAG	B	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	902	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	903	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	904	3	-	0/2/19/22	0/1/1/1
4	MAN	B	905	-	-	0/2/19/22	0/1/1/1
2	NAG	B	906	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	907	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	908	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	909	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	910	4	-	0/2/19/22	0/1/1/1
2	NAG	B	911	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	912	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	913	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	914	3	-	0/2/19/22	0/1/1/1
2	NAG	B	915	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	916	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	917	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	918	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	919	4	-	0/2/19/22	0/1/1/1
4	MAN	B	920	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	921	4	-	0/2/19/22	0/1/1/1
4	MAN	B	922	4	-	0/2/19/22	0/1/1/1
4	MAN	B	923	4	-	0/2/19/22	0/1/1/1
4	MAN	B	924	4	-	0/2/19/22	0/1/1/1
2	NAG	B	925	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	926	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	927	3,2,4	-	0/2/19/22	0/1/1/1
3	BMA	B	928	3	-	0/2/19/22	0/1/1/1
4	MAN	B	929	3	-	0/2/19/22	0/1/1/1
2	NAG	B	930	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	931	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	932	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	933	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	934	4	-	0/2/19/22	0/1/1/1
4	MAN	B	935	4	-	0/2/19/22	0/1/1/1
4	MAN	B	936	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	937	4	-	0/2/19/22	0/1/1/1
4	MAN	B	938	4	-	0/2/19/22	0/1/1/1
4	MAN	B	939	4	-	0/2/19/22	0/1/1/1
2	NAG	B	940	1	-	0/6/23/26	0/1/1/1
2	NAG	B	941	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	942	2	-	0/6/23/26	0/1/1/1
2	NAG	B	943	1	-	0/6/23/26	0/1/1/1
2	NAG	B	944	1	-	0/6/23/26	0/1/1/1
5	BGC	B	945	-	-	0/2/22/22	0/1/1/1
2	NAG	C	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	902	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	903	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	904	3,4	-	0/2/19/22	0/1/1/1
4	MAN	C	905	4	-	0/2/19/22	0/1/1/1
4	MAN	C	906	4	-	0/2/19/22	0/1/1/1
4	MAN	C	907	3,4	-	0/2/19/22	0/1/1/1
4	MAN	C	908	4	-	0/2/19/22	0/1/1/1
4	MAN	C	909	4	-	0/2/19/22	0/1/1/1
2	NAG	C	910	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	911	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	912	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	913	3,4	-	0/2/19/22	0/1/1/1
4	MAN	C	914	4	-	0/2/19/22	0/1/1/1
4	MAN	C	915	4,6	-	0/2/19/22	0/1/1/1
6	GLC	C	916	4	-	0/2/19/22	0/1/1/1
4	MAN	C	917	3	-	0/2/19/22	0/1/1/1
2	NAG	C	918	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	919	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	920	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	921	3	-	0/2/19/22	0/1/1/1
4	MAN	C	922	3	-	0/2/19/22	0/1/1/1
2	NAG	C	923	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	924	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	925	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	926	3,4	-	0/2/19/22	0/1/1/1
4	MAN	C	927	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	C	928	3,4	-	0/2/19/22	0/1/1/1
4	MAN	C	929	4	-	0/2/19/22	0/1/1/1
4	MAN	C	930	4	-	0/2/19/22	0/1/1/1
4	MAN	C	931	4	-	0/2/19/22	0/1/1/1
2	NAG	C	932	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	933	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	934	2	-	0/2/19/22	0/1/1/1
2	NAG	C	935	1	-	0/6/23/26	0/1/1/1
2	NAG	C	936	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	937	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	938	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	939	3,4	-	0/2/19/22	0/1/1/1
4	MAN	C	940	4	-	0/2/19/22	0/1/1/1
4	MAN	C	941	3,4	-	0/2/19/22	0/1/1/1
4	MAN	C	942	4	-	0/2/19/22	0/1/1/1
4	MAN	C	943	4	-	0/2/19/22	0/1/1/1
2	NAG	C	944	1	-	0/6/23/26	0/1/1/1
2	NAG	C	945	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	946	2	-	0/6/23/26	0/1/1/1
2	NAG	C	947	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	948	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	949	2	-	0/2/19/22	0/1/1/1
2	NAG	C	950	1	-	0/6/23/26	0/1/1/1
5	BGC	C	951	-	-	0/2/22/22	0/1/1/1
2	NAG	D	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	902	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	903	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	904	3,4	-	0/2/19/22	0/1/1/1
4	MAN	D	905	4	-	0/2/19/22	0/1/1/1
4	MAN	D	906	3	-	0/2/19/22	0/1/1/1
2	NAG	D	907	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	908	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	909	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	910	3,4	-	0/2/19/22	0/1/1/1
4	MAN	D	911	4	-	0/2/19/22	0/1/1/1
4	MAN	D	912	4,6	-	0/2/19/22	0/1/1/1
6	GLC	D	913	4	-	0/2/19/22	0/1/1/1
4	MAN	D	914	3	-	0/2/19/22	0/1/1/1
2	NAG	D	915	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	916	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	917	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	918	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	919	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	920	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	921	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	922	3,4	-	0/2/19/22	0/1/1/1
4	MAN	D	923	4	-	0/2/19/22	0/1/1/1
4	MAN	D	924	3,4	-	0/2/19/22	0/1/1/1
4	MAN	D	925	4	-	0/2/19/22	0/1/1/1
4	MAN	D	926	4	-	0/2/19/22	0/1/1/1
4	MAN	D	927	4	-	0/2/19/22	0/1/1/1
4	MAN	D	928	4	-	0/2/19/22	0/1/1/1
2	NAG	D	929	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	930	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	931	2	-	0/2/19/22	0/1/1/1
2	NAG	D	932	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	933	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	934	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	935	3,4	-	0/2/19/22	0/1/1/1
4	MAN	D	936	4	-	0/2/19/22	0/1/1/1
4	MAN	D	937	3,4	-	0/2/19/22	0/1/1/1
4	MAN	D	938	4	-	0/2/19/22	0/1/1/1
4	MAN	D	939	4	-	0/2/19/22	0/1/1/1
2	NAG	D	940	1	-	0/6/23/26	0/1/1/1
2	NAG	D	941	1	-	0/6/23/26	0/1/1/1
2	NAG	D	942	1	-	0/6/23/26	0/1/1/1
2	NAG	D	943	1	-	0/6/23/26	0/1/1/1
2	NAG	D	944	1	-	0/6/23/26	0/1/1/1
5	BGC	D	945	-	-	0/2/22/22	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	933	NAG	C1-C2	-2.46	1.49	1.52
2	A	918	NAG	O5-C1	-2.18	1.40	1.43
3	C	925	BMA	O5-C1	-2.16	1.40	1.43
2	D	907	NAG	O5-C1	-2.15	1.40	1.43
2	D	940	NAG	O4-C4	2.00	1.47	1.43
4	D	938	MAN	C2-C3	2.03	1.55	1.52
6	C	916	GLC	C2-C3	2.06	1.55	1.52
4	B	929	MAN	C2-C3	2.10	1.55	1.52
4	B	919	MAN	C2-C3	2.10	1.55	1.52
4	A	912	MAN	C4-C5	2.12	1.57	1.53
4	B	934	MAN	C2-C3	2.17	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	917	MAN	C1-C2	2.19	1.57	1.52
4	C	907	MAN	C2-C3	2.20	1.55	1.52
4	A	909	MAN	C2-C3	2.20	1.55	1.52
4	A	936	MAN	C2-C3	2.22	1.55	1.52
4	A	912	MAN	C2-C3	2.22	1.55	1.52
5	A	946	BGC	C1-C2	2.27	1.57	1.52
4	C	909	MAN	C2-C3	2.35	1.55	1.52
4	C	917	MAN	C2-C3	2.37	1.55	1.52
4	D	912	MAN	C2-C3	2.42	1.55	1.52
4	B	910	MAN	C2-C3	2.43	1.55	1.52
5	C	951	BGC	C1-C2	2.45	1.58	1.52
4	C	940	MAN	C2-C3	2.48	1.55	1.52
4	A	921	MAN	C2-C3	2.54	1.55	1.52
4	C	922	MAN	C2-C3	2.57	1.56	1.52
3	A	903	BMA	C2-C3	2.61	1.56	1.52
4	B	909	MAN	C2-C3	2.63	1.56	1.52
4	C	927	MAN	C2-C3	2.68	1.56	1.52
4	D	914	MAN	C2-C3	2.86	1.56	1.52
2	D	944	NAG	C1-C2	2.88	1.56	1.52
4	C	906	MAN	C2-C3	3.01	1.56	1.52
4	C	915	MAN	C2-C3	3.94	1.57	1.52

All (362) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	933	MAN	O5-C1-C2	-4.22	104.14	110.89
2	B	912	NAG	O4-C4-C3	-4.08	101.17	110.36
4	C	940	MAN	C1-C2-C3	-3.95	104.76	109.55
2	C	937	NAG	O4-C4-C3	-3.71	101.99	110.36
2	C	944	NAG	C3-C4-C5	-3.69	103.66	110.23
3	B	908	BMA	O5-C1-C2	-3.58	105.17	110.89
4	A	923	MAN	C1-C2-C3	-3.48	105.33	109.55
3	A	915	BMA	O5-C5-C6	-3.47	99.90	107.34
2	C	947	NAG	O3-C3-C2	-3.45	102.00	109.37
2	D	916	NAG	C8-C7-N2	-3.44	109.50	116.10
2	B	912	NAG	C8-C7-N2	-3.43	109.53	116.10
4	D	922	MAN	O4-C4-C3	-3.42	102.64	110.36
4	D	928	MAN	O5-C1-C2	-3.42	105.43	110.89
4	B	924	MAN	C6-C5-C4	-3.39	104.48	112.99
2	C	923	NAG	O3-C3-C2	-3.38	102.13	109.37
4	B	936	MAN	O5-C5-C4	-3.37	104.55	110.13
4	C	905	MAN	O2-C2-C3	-3.36	103.41	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	951	BGC	O1-C1-O5	-3.36	100.97	110.33
3	C	903	BMA	O5-C5-C4	-3.32	104.64	110.13
4	A	938	MAN	O5-C1-C2	-3.27	105.67	110.89
2	C	936	NAG	O3-C3-C2	-3.26	102.40	109.37
3	C	938	BMA	O5-C1-C2	-3.21	105.75	110.89
2	D	919	NAG	O4-C4-C5	-3.20	100.78	109.23
3	D	917	BMA	O4-C4-C3	-3.20	103.15	110.36
4	A	920	MAN	C6-C5-C4	-3.16	105.06	112.99
3	A	915	BMA	O4-C4-C3	-3.12	103.33	110.36
3	A	915	BMA	O3-C3-C4	-3.12	103.33	110.36
4	B	924	MAN	O3-C3-C4	-3.11	103.35	110.36
4	B	936	MAN	C1-C2-C3	-3.10	105.79	109.55
4	B	929	MAN	O5-C1-C2	-3.06	106.01	110.89
3	A	908	BMA	O5-C1-C2	-3.05	106.01	110.89
4	B	936	MAN	C3-C4-C5	-3.02	104.84	110.23
3	C	912	BMA	O5-C5-C4	-3.02	105.13	110.13
4	A	934	MAN	O2-C2-C3	-2.98	104.18	110.19
2	A	902	NAG	O3-C3-C2	-2.98	103.00	109.37
2	D	915	NAG	C4-C3-C2	-2.97	106.73	111.34
4	A	925	MAN	O5-C1-C2	-2.97	106.15	110.89
3	B	928	BMA	O5-C1-C2	-2.96	106.16	110.89
3	D	909	BMA	O4-C4-C3	-2.96	103.69	110.36
4	A	939	MAN	O5-C1-C2	-2.95	106.17	110.89
4	A	934	MAN	O5-C1-C2	-2.91	106.24	110.89
2	C	936	NAG	O4-C4-C5	-2.90	101.57	109.23
3	A	928	BMA	O5-C5-C4	-2.90	105.33	110.13
4	C	909	MAN	O5-C1-C2	-2.89	106.27	110.89
2	C	935	NAG	O5-C5-C4	-2.87	105.37	110.13
4	C	929	MAN	O5-C1-C2	-2.86	106.32	110.89
3	A	903	BMA	O5-C5-C4	-2.86	105.40	110.13
5	D	945	BGC	O1-C1-O5	-2.80	102.51	110.33
2	C	910	NAG	C4-C3-C2	-2.79	107.00	111.34
2	C	947	NAG	O5-C5-C4	-2.79	105.52	110.13
2	B	902	NAG	O4-C4-C5	-2.79	101.89	109.23
4	A	904	MAN	O5-C1-C2	-2.77	106.47	110.89
2	D	902	NAG	O3-C3-C2	-2.76	103.46	109.37
4	D	927	MAN	O5-C1-C2	-2.76	106.48	110.89
4	C	940	MAN	O5-C1-C2	-2.76	106.49	110.89
4	D	918	MAN	O5-C1-C2	-2.76	106.49	110.89
3	C	912	BMA	O4-C4-C3	-2.76	104.15	110.36
2	A	932	NAG	O4-C4-C3	-2.74	104.18	110.36
2	A	945	NAG	O4-C4-C3	-2.72	104.22	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	932	NAG	O3-C3-C2	-2.72	103.55	109.37
4	B	909	MAN	O2-C2-C1	-2.71	103.81	109.23
4	C	906	MAN	O2-C2-C1	-2.67	103.89	109.23
4	A	922	MAN	O6-C6-C5	-2.67	102.39	111.30
2	C	948	NAG	C4-C3-C2	-2.65	107.22	111.34
2	B	940	NAG	C3-C4-C5	-2.64	105.53	110.23
4	D	912	MAN	O5-C1-C2	-2.63	106.69	110.89
4	D	928	MAN	C6-C5-C4	-2.62	106.41	112.99
4	B	922	MAN	O5-C1-C2	-2.61	106.72	110.89
2	C	936	NAG	O7-C7-C8	-2.60	117.29	122.07
4	B	938	MAN	O4-C4-C3	-2.59	104.52	110.36
2	C	902	NAG	C2-N2-C7	-2.59	119.74	123.11
2	D	932	NAG	O4-C4-C5	-2.57	102.46	109.23
3	B	927	BMA	O5-C1-C2	-2.56	106.80	110.89
2	A	930	NAG	C6-C5-C4	-2.56	106.58	112.99
2	D	901	NAG	O4-C4-C5	-2.55	102.50	109.23
2	C	910	NAG	O7-C7-C8	-2.55	117.38	122.07
3	B	903	BMA	O5-C5-C4	-2.54	105.92	110.13
4	B	937	MAN	C1-O5-C5	-2.53	108.42	112.14
2	B	915	NAG	O4-C4-C5	-2.51	102.61	109.23
2	D	933	NAG	O4-C4-C3	-2.50	104.72	110.36
3	D	931	BMA	C1-C2-C3	-2.49	106.53	109.55
3	B	908	BMA	O4-C4-C3	-2.49	104.75	110.36
2	D	902	NAG	O4-C4-C5	-2.47	102.71	109.23
3	D	917	BMA	O2-C2-C1	-2.47	104.30	109.23
4	C	905	MAN	O4-C4-C3	-2.46	104.81	110.36
3	D	909	BMA	O5-C5-C4	-2.44	106.08	110.13
4	D	926	MAN	O5-C1-C2	-2.43	107.01	110.89
4	A	912	MAN	O5-C5-C4	-2.43	106.11	110.13
4	D	914	MAN	O5-C1-C2	-2.43	107.01	110.89
4	A	912	MAN	C2-C3-C4	-2.43	106.82	111.05
4	C	906	MAN	O5-C1-C2	-2.42	107.03	110.89
4	A	924	MAN	O5-C1-C2	-2.41	107.04	110.89
4	C	928	MAN	O6-C6-C5	-2.38	103.36	111.30
2	A	913	NAG	C4-C3-C2	-2.37	107.66	111.34
4	B	905	MAN	O5-C5-C4	-2.35	106.24	110.13
4	B	923	MAN	O2-C2-C3	-2.35	105.45	110.19
4	C	931	MAN	O5-C1-C2	-2.35	107.14	110.89
3	A	915	BMA	O2-C2-C1	-2.34	104.56	109.23
4	A	925	MAN	O2-C2-C3	-2.33	105.50	110.19
2	B	931	NAG	O4-C4-C3	-2.32	105.12	110.36
2	C	932	NAG	O5-C5-C4	-2.31	106.30	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	940	NAG	O3-C3-C2	-2.31	104.42	109.37
4	C	942	MAN	O2-C2-C3	-2.31	105.54	110.19
4	B	920	MAN	O6-C6-C5	-2.30	103.61	111.30
2	D	908	NAG	C4-C3-C2	-2.28	107.80	111.34
2	D	933	NAG	O5-C5-C4	-2.27	106.38	110.13
4	A	924	MAN	O2-C2-C3	-2.26	105.64	110.19
2	C	935	NAG	O3-C3-C2	-2.25	104.56	109.37
2	C	937	NAG	C1-O5-C5	-2.25	108.83	112.14
4	C	931	MAN	C6-C5-C4	-2.25	107.35	112.99
2	B	906	NAG	C4-C3-C2	-2.25	107.85	111.34
4	B	924	MAN	O5-C1-C2	-2.24	107.31	110.89
3	D	903	BMA	O5-C5-C4	-2.23	106.45	110.13
4	B	937	MAN	O4-C4-C3	-2.22	105.35	110.36
4	D	936	MAN	C1-O5-C5	-2.22	108.88	112.14
4	B	910	MAN	C6-C5-C4	-2.20	107.47	112.99
2	D	943	NAG	C3-C4-C5	-2.20	106.31	110.23
2	D	929	NAG	O3-C3-C4	-2.20	105.41	110.36
4	A	920	MAN	O4-C4-C3	-2.20	105.41	110.36
2	C	919	NAG	O4-C4-C5	-2.18	103.47	109.23
4	B	933	MAN	O2-C2-C3	-2.18	105.79	110.19
5	D	945	BGC	O3-C3-C4	-2.16	105.48	110.36
2	A	945	NAG	C6-C5-C4	-2.16	107.56	112.99
4	B	909	MAN	O5-C5-C4	-2.16	106.56	110.13
3	C	938	BMA	O6-C6-C5	-2.16	104.09	111.30
2	B	944	NAG	O6-C6-C5	-2.15	104.11	111.30
4	B	921	MAN	C1-C2-C3	-2.15	106.95	109.55
4	D	939	MAN	C2-C3-C4	-2.15	107.30	111.05
2	C	902	NAG	C4-C3-C2	-2.15	108.01	111.34
3	B	913	BMA	O5-C1-C2	-2.14	107.47	110.89
4	D	904	MAN	O3-C3-C4	-2.14	105.53	110.36
2	D	908	NAG	O3-C3-C2	-2.14	104.80	109.37
4	C	926	MAN	O4-C4-C3	-2.13	105.55	110.36
2	B	942	NAG	O3-C3-C4	-2.13	105.56	110.36
2	D	907	NAG	C4-C3-C2	-2.12	108.05	111.34
3	A	933	BMA	O5-C5-C4	-2.12	106.63	110.13
3	B	908	BMA	O3-C3-C4	-2.11	105.59	110.36
3	A	933	BMA	O2-C2-C1	-2.11	105.00	109.23
4	B	920	MAN	O3-C3-C4	-2.11	105.59	110.36
3	D	909	BMA	O3-C3-C2	-2.11	106.14	110.01
4	D	936	MAN	O4-C4-C5	-2.11	103.66	109.23
4	B	910	MAN	O5-C5-C4	-2.11	106.65	110.13
3	C	949	BMA	O5-C1-C2	-2.10	107.53	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	929	MAN	C1-C2-C3	-2.10	107.01	109.55
4	B	919	MAN	O3-C3-C2	-2.10	106.17	110.01
4	C	926	MAN	O5-C1-C2	-2.09	107.55	110.89
2	C	918	NAG	O4-C4-C5	-2.09	103.72	109.23
4	A	909	MAN	O2-C2-C1	-2.09	105.06	109.23
2	D	942	NAG	C3-C4-C5	-2.08	106.51	110.23
4	D	925	MAN	O5-C1-C2	-2.08	107.57	110.89
2	C	946	NAG	C6-C5-C4	-2.08	107.78	112.99
4	B	904	MAN	O3-C3-C4	-2.07	105.69	110.36
4	A	916	MAN	O5-C1-C2	-2.07	107.59	110.89
4	A	934	MAN	O4-C4-C3	-2.07	105.70	110.36
2	A	944	NAG	C3-C4-C5	-2.05	106.56	110.23
4	D	911	MAN	C2-C3-C4	-2.05	107.47	111.05
2	A	932	NAG	O6-C6-C5	-2.04	104.47	111.30
2	B	944	NAG	C3-C4-C5	-2.03	106.60	110.23
4	B	921	MAN	O5-C1-C2	-2.03	107.65	110.89
4	A	909	MAN	O5-C1-C2	-2.03	107.65	110.89
2	B	925	NAG	O3-C3-C4	-2.02	105.81	110.36
6	C	916	GLC	O2-C2-C3	-2.02	106.12	110.19
2	D	929	NAG	O5-C5-C4	-2.02	106.80	110.13
2	C	937	NAG	O7-C7-C8	-2.01	118.36	122.07
2	B	915	NAG	O3-C3-C2	-2.01	105.07	109.37
3	B	913	BMA	O4-C4-C3	-2.01	105.82	110.36
2	C	932	NAG	C8-C7-N2	-2.01	112.24	116.10
2	B	907	NAG	O4-C4-C3	-2.01	105.83	110.36
4	B	919	MAN	O5-C5-C4	-2.00	106.82	110.13
2	C	936	NAG	C3-C4-C5	2.00	113.79	110.23
4	B	904	MAN	O2-C2-C3	2.01	114.23	110.19
4	A	929	MAN	C1-C2-C3	2.01	111.99	109.55
3	B	927	BMA	O3-C3-C4	2.01	114.89	110.36
4	B	938	MAN	O2-C2-C1	2.01	113.27	109.23
2	B	925	NAG	C1-O5-C5	2.01	115.10	112.14
2	C	936	NAG	O4-C4-C3	2.01	114.90	110.36
2	D	930	NAG	O3-C3-C4	2.02	114.91	110.36
3	D	931	BMA	O3-C3-C4	2.02	114.92	110.36
4	B	914	MAN	O5-C5-C6	2.03	111.69	107.34
4	C	917	MAN	O3-C3-C2	2.03	113.73	110.01
2	B	911	NAG	C1-O5-C5	2.04	115.13	112.14
4	A	904	MAN	O3-C3-C4	2.04	114.95	110.36
2	D	942	NAG	O4-C4-C3	2.04	114.96	110.36
3	A	928	BMA	C1-C2-C3	2.05	112.03	109.55
5	A	946	BGC	O1-C1-C2	2.05	114.73	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	932	NAG	O3-C3-C4	2.06	115.01	110.36
4	B	929	MAN	C1-O5-C5	2.06	115.17	112.14
5	A	946	BGC	O2-C2-C1	2.07	114.27	109.74
2	D	944	NAG	O4-C4-C5	2.08	114.70	109.23
4	A	920	MAN	O2-C2-C1	2.09	113.41	109.23
4	C	908	MAN	O2-C2-C1	2.09	113.42	109.23
3	A	933	BMA	C1-O5-C5	2.10	115.22	112.14
4	A	925	MAN	C1-O5-C5	2.10	115.22	112.14
3	D	917	BMA	C1-O5-C5	2.10	115.22	112.14
2	A	945	NAG	C3-C4-C5	2.10	113.97	110.23
4	D	923	MAN	C3-C4-C5	2.10	113.97	110.23
2	D	919	NAG	O3-C3-C4	2.10	115.10	110.36
2	C	950	NAG	C2-N2-C7	2.10	125.84	123.11
4	A	938	MAN	O3-C3-C2	2.10	113.86	110.01
4	C	943	MAN	C3-C4-C5	2.11	114.00	110.23
2	B	912	NAG	O4-C4-C5	2.12	114.81	109.23
5	B	945	BGC	O4-C4-C5	2.13	114.83	109.23
4	C	922	MAN	O4-C4-C5	2.14	114.86	109.23
3	D	917	BMA	O3-C3-C2	2.14	113.93	110.01
4	A	924	MAN	O2-C2-C1	2.14	113.52	109.23
4	B	922	MAN	C1-C2-C3	2.14	112.15	109.55
2	C	947	NAG	O7-C7-N2	2.15	126.22	121.84
2	C	936	NAG	O7-C7-N2	2.15	126.23	121.84
2	D	929	NAG	C1-O5-C5	2.15	115.31	112.14
3	C	912	BMA	O2-C2-C3	2.16	114.53	110.19
4	A	935	MAN	O3-C3-C4	2.16	115.22	110.36
4	B	924	MAN	O4-C4-C5	2.17	114.94	109.23
3	C	949	BMA	O5-C5-C6	2.17	111.99	107.34
4	A	904	MAN	C1-O5-C5	2.17	115.34	112.14
4	B	937	MAN	O2-C2-C3	2.18	114.57	110.19
4	C	906	MAN	O2-C2-C3	2.18	114.58	110.19
4	B	934	MAN	C1-O5-C5	2.18	115.35	112.14
3	C	903	BMA	O5-C5-C6	2.19	112.03	107.34
4	A	935	MAN	C1-O5-C5	2.19	115.36	112.14
4	B	919	MAN	O2-C2-C3	2.22	114.66	110.19
4	D	927	MAN	C1-O5-C5	2.23	115.42	112.14
3	D	931	BMA	O2-C2-C1	2.23	113.71	109.23
4	C	922	MAN	O3-C3-C2	2.24	114.11	110.01
3	C	938	BMA	C1-O5-C5	2.24	115.43	112.14
4	A	911	MAN	O3-C3-C2	2.24	114.12	110.01
4	B	919	MAN	C2-C3-C4	2.25	114.97	111.05
2	D	901	NAG	C2-N2-C7	2.26	126.04	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	925	NAG	C2-N2-C7	2.26	126.05	123.11
2	B	941	NAG	C2-N2-C7	2.27	126.06	123.11
3	C	912	BMA	C1-O5-C5	2.28	115.49	112.14
4	A	912	MAN	C6-C5-C4	2.28	118.70	112.99
2	C	933	NAG	O7-C7-N2	2.28	126.49	121.84
2	C	919	NAG	O7-C7-N2	2.28	126.50	121.84
2	C	918	NAG	C1-O5-C5	2.31	115.54	112.14
3	D	903	BMA	C3-C4-C5	2.31	114.35	110.23
2	C	948	NAG	O4-C4-C5	2.31	115.32	109.23
4	A	921	MAN	O2-C2-C3	2.32	114.86	110.19
4	C	917	MAN	O2-C2-C1	2.32	113.89	109.23
3	A	928	BMA	O5-C5-C6	2.33	112.33	107.34
2	A	930	NAG	C2-N2-C7	2.34	126.14	123.11
3	A	933	BMA	C1-C2-C3	2.35	112.39	109.55
4	B	905	MAN	C2-C3-C4	2.35	115.14	111.05
2	D	942	NAG	C1-O5-C5	2.35	115.60	112.14
4	B	936	MAN	C1-O5-C5	2.36	115.61	112.14
4	C	906	MAN	C1-C2-C3	2.36	112.42	109.55
4	B	934	MAN	O3-C3-C2	2.37	114.35	110.01
2	D	943	NAG	C2-N2-C7	2.38	126.21	123.11
4	B	904	MAN	O5-C5-C6	2.39	112.46	107.34
4	C	940	MAN	O5-C5-C6	2.40	112.48	107.34
3	A	903	BMA	C6-C5-C4	2.40	119.01	112.99
2	D	930	NAG	C2-N2-C7	2.41	126.24	123.11
4	A	923	MAN	O3-C3-C4	2.42	115.81	110.36
4	A	912	MAN	O3-C3-C2	2.42	114.44	110.01
3	D	917	BMA	C3-C4-C5	2.43	114.55	110.23
2	A	941	NAG	C1-O5-C5	2.43	115.71	112.14
4	B	905	MAN	O5-C1-C2	2.43	114.78	110.89
4	A	912	MAN	O5-C5-C6	2.44	112.57	107.34
4	B	934	MAN	O4-C4-C5	2.45	115.67	109.23
4	C	907	MAN	O5-C5-C6	2.45	112.59	107.34
4	B	929	MAN	O3-C3-C2	2.46	114.51	110.01
2	B	906	NAG	C2-N2-C7	2.46	126.30	123.11
4	C	907	MAN	O2-C2-C3	2.48	115.18	110.19
4	C	915	MAN	O3-C3-C2	2.49	114.57	110.01
2	A	927	NAG	O7-C7-N2	2.52	126.98	121.84
4	B	910	MAN	C1-O5-C5	2.53	115.86	112.14
2	A	940	NAG	C1-O5-C5	2.54	115.87	112.14
2	A	914	NAG	C2-N2-C7	2.54	126.41	123.11
2	B	912	NAG	C4-C3-C2	2.56	115.31	111.34
2	C	935	NAG	O5-C5-C6	2.57	112.85	107.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	914	MAN	C1-C2-C3	2.57	112.67	109.55
2	A	930	NAG	C1-O5-C5	2.58	115.94	112.14
4	D	914	MAN	C1-C2-C3	2.59	112.69	109.55
2	B	943	NAG	C1-O5-C5	2.59	115.95	112.14
4	B	909	MAN	O3-C3-C2	2.62	114.81	110.01
4	D	922	MAN	C1-C2-C3	2.62	112.73	109.55
4	C	905	MAN	O2-C2-C1	2.65	114.53	109.23
2	C	944	NAG	O5-C5-C6	2.67	113.06	107.34
4	B	936	MAN	O2-C2-C3	2.67	115.57	110.19
2	D	942	NAG	O4-C4-C5	2.69	116.31	109.23
2	B	942	NAG	C1-O5-C5	2.70	116.11	112.14
3	A	903	BMA	O2-C2-C1	2.70	114.64	109.23
2	B	940	NAG	O5-C5-C6	2.72	113.17	107.34
2	B	944	NAG	C1-O5-C5	2.72	116.15	112.14
2	C	901	NAG	C2-N2-C7	2.73	126.66	123.11
4	D	939	MAN	O4-C4-C5	2.73	116.42	109.23
3	A	903	BMA	O5-C5-C6	2.75	113.22	107.34
4	D	912	MAN	O2-C2-C3	2.75	115.72	110.19
4	A	921	MAN	C2-C3-C4	2.76	115.87	111.05
4	C	927	MAN	C1-O5-C5	2.78	116.23	112.14
4	A	912	MAN	O4-C4-C5	2.78	116.55	109.23
2	C	932	NAG	O7-C7-N2	2.78	127.52	121.84
5	C	951	BGC	C1-O5-C5	2.79	118.89	113.54
4	B	910	MAN	O5-C5-C6	2.80	113.33	107.34
4	C	940	MAN	O2-C2-C3	2.80	115.83	110.19
4	C	930	MAN	C1-O5-C5	2.80	116.26	112.14
4	A	923	MAN	O2-C2-C1	2.80	114.85	109.23
4	D	910	MAN	O5-C5-C6	2.82	113.37	107.34
2	B	940	NAG	C1-O5-C5	2.82	116.28	112.14
2	C	932	NAG	C2-N2-C7	2.85	126.81	123.11
4	A	923	MAN	O2-C2-C3	2.86	115.95	110.19
4	A	922	MAN	O2-C2-C1	2.87	114.98	109.23
4	C	922	MAN	C1-C2-C3	2.89	113.05	109.55
4	B	910	MAN	O3-C3-C2	2.89	115.31	110.01
4	C	927	MAN	O2-C2-C3	2.89	116.02	110.19
4	D	923	MAN	O2-C2-C3	2.90	116.02	110.19
2	D	943	NAG	C1-O5-C5	2.90	116.40	112.14
4	B	937	MAN	C3-C4-C5	2.91	115.41	110.23
4	B	909	MAN	O2-C2-C3	2.92	116.06	110.19
4	D	936	MAN	C3-C4-C5	2.92	115.43	110.23
2	C	910	NAG	O7-C7-N2	2.93	127.81	121.84
4	A	938	MAN	C1-O5-C5	2.94	116.46	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	920	MAN	C1-O5-C5	2.96	116.49	112.14
2	C	910	NAG	C2-N2-C7	2.98	126.98	123.11
4	A	935	MAN	O2-C2-C1	2.99	115.23	109.23
2	C	944	NAG	C1-O5-C5	2.99	116.54	112.14
3	B	913	BMA	C3-C4-C5	3.00	115.57	110.23
4	B	921	MAN	O5-C5-C6	3.02	113.80	107.34
4	B	936	MAN	O3-C3-C2	3.02	115.54	110.01
4	D	914	MAN	O5-C5-C6	3.04	113.86	107.34
2	C	936	NAG	C2-N2-C7	3.11	127.15	123.11
4	D	935	MAN	O2-C2-C1	3.12	115.47	109.23
4	A	910	MAN	C1-O5-C5	3.12	116.73	112.14
4	C	926	MAN	O2-C2-C3	3.15	116.53	110.19
2	C	947	NAG	C1-O5-C5	3.16	116.79	112.14
4	D	914	MAN	C1-O5-C5	3.19	116.84	112.14
4	C	917	MAN	C1-O5-C5	3.20	116.85	112.14
3	D	917	BMA	O2-C2-C3	3.21	116.66	110.19
4	B	919	MAN	C3-C4-C5	3.22	115.97	110.23
2	D	916	NAG	O7-C7-N2	3.23	128.43	121.84
2	C	944	NAG	O4-C4-C5	3.26	117.81	109.23
4	C	917	MAN	C1-C2-C3	3.29	113.53	109.55
4	B	905	MAN	O2-C2-C3	3.29	116.81	110.19
4	C	906	MAN	O3-C3-C2	3.30	116.05	110.01
2	C	933	NAG	C2-N2-C7	3.33	127.44	123.11
3	A	915	BMA	C1-O5-C5	3.35	117.07	112.14
4	B	910	MAN	O2-C2-C3	3.38	117.00	110.19
2	D	944	NAG	C2-N2-C7	3.39	127.52	123.11
2	A	906	NAG	C2-N2-C7	3.40	127.53	123.11
4	D	904	MAN	C1-O5-C5	3.47	117.25	112.14
2	C	946	NAG	C1-O5-C5	3.49	117.27	112.14
2	C	948	NAG	C1-O5-C5	3.61	117.45	112.14
3	A	915	BMA	C3-C4-C5	3.64	116.72	110.23
4	B	924	MAN	C1-O5-C5	3.66	117.52	112.14
4	B	936	MAN	O5-C5-C6	3.69	115.25	107.34
4	A	937	MAN	C1-C2-C3	3.76	114.11	109.55
4	D	938	MAN	O2-C2-C1	3.78	116.81	109.23
2	D	916	NAG	C2-N2-C7	3.79	128.04	123.11
4	A	912	MAN	C1-C2-C3	3.81	114.17	109.55
3	A	915	BMA	C1-C2-C3	3.88	114.26	109.55
4	A	929	MAN	C1-O5-C5	3.92	117.90	112.14
2	D	944	NAG	C1-O5-C5	4.07	118.12	112.14
3	C	912	BMA	O5-C5-C6	4.13	116.17	107.34
2	B	906	NAG	C1-O5-C5	4.14	118.23	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	919	NAG	C1-O5-C5	4.14	118.23	112.14
2	A	942	NAG	C1-O5-C5	4.32	118.49	112.14
2	A	944	NAG	C1-O5-C5	4.38	118.58	112.14
2	B	941	NAG	C1-O5-C5	4.42	118.64	112.14
4	A	916	MAN	C1-O5-C5	4.50	118.76	112.14
4	C	915	MAN	O2-C2-C3	4.68	119.62	110.19
4	C	942	MAN	O2-C2-C1	4.74	118.73	109.23
2	A	927	NAG	C2-N2-C7	5.33	130.04	123.11
6	C	916	GLC	C1-C2-C3	5.95	116.76	109.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	NAG	1	0
2	A	945	NAG	1	0
5	A	946	BGC	1	0
4	B	904	MAN	1	0
4	B	905	MAN	1	0
5	B	945	BGC	1	0
2	C	902	NAG	1	0
5	C	951	BGC	1	0
2	D	902	NAG	1	0
5	D	945	BGC	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	835/857 (97%)	-0.48	2 (0%) 95 95	14, 25, 41, 69	7 (0%)
1	B	835/857 (97%)	-0.38	6 (0%) 89 88	16, 26, 43, 77	9 (1%)
1	C	835/857 (97%)	-0.38	4 (0%) 91 91	14, 24, 40, 75	11 (1%)
1	D	835/857 (97%)	-0.39	1 (0%) 95 95	12, 23, 39, 79	8 (0%)
All	All	3340/3428 (97%)	-0.41	13 (0%) 93 93	12, 25, 41, 79	35 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	854	TYR	3.6
1	B	853	PRO	3.5
1	A	208	ASP	3.4
1	A	206	GLY	3.0
1	D	855	PRO	2.7
1	B	855	PRO	2.6
1	B	663	ASN	2.6
1	C	855	PRO	2.2
1	B	851	LEU	2.2
1	C	21	ASN	2.2
1	B	21	ASN	2.1
1	C	208	ASP	2.0
1	C	188	ALA	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 ⓘ

There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	MAN	D	939	11/12	0.90	0.20	17.26	39,43,46,47	0
2	NAG	C	947	14/15	0.95	0.17	6.37	31,36,42,55	0
5	BGC	B	945	12/12	0.77	0.28	6.11	39,47,55,63	0
2	NAG	B	944	14/15	0.80	0.19	5.52	54,65,70,76	0
4	MAN	B	939	11/12	0.90	0.17	5.20	35,43,48,53	0
2	NAG	C	935	14/15	0.81	0.21	4.19	61,72,85,87	0
5	BGC	C	951	12/12	0.69	0.27	4.18	44,58,64,67	0
4	MAN	A	939	11/12	0.90	0.17	3.45	43,49,51,52	0
4	MAN	C	943	11/12	0.95	0.19	3.37	34,39,43,44	0
4	MAN	D	928	11/12	0.93	0.12	3.28	29,31,33,38	0
2	NAG	D	940	14/15	0.74	0.21	3.02	58,63,68,73	0
2	NAG	A	930	14/15	0.83	0.17	2.94	57,62,65,72	0
5	BGC	A	946	12/12	0.87	0.20	2.94	36,46,49,53	0
2	NAG	A	940	14/15	0.93	0.19	2.93	41,51,56,57	0
4	MAN	A	925	11/12	0.94	0.12	2.89	28,30,32,37	0
2	NAG	B	941	14/15	0.94	0.19	2.88	29,38,41,53	0
2	NAG	C	944	14/15	0.89	0.17	2.78	41,47,50,51	0
2	NAG	D	942	14/15	0.92	0.18	2.51	32,34,35,38	0
2	NAG	A	942	14/15	0.94	0.20	2.35	37,43,46,54	0
2	NAG	A	907	14/15	0.96	0.12	1.80	29,32,37,40	0
2	NAG	D	908	14/15	0.93	0.15	1.51	29,32,38,38	0
2	NAG	A	945	14/15	0.91	0.13	1.40	46,52,54,62	0
2	NAG	D	943	14/15	0.96	0.11	1.39	25,28,36,36	0
5	BGC	D	945	12/12	0.88	0.21	1.23	46,52,57,61	0
2	NAG	A	931	14/15	0.92	0.12	1.22	26,30,32,33	0
2	NAG	A	944	14/15	0.92	0.13	1.19	29,32,37,40	0
2	NAG	D	933	14/15	0.94	0.12	0.69	22,25,30,33	0
2	NAG	D	902	14/15	0.94	0.13	0.61	22,28,34,41	0
2	NAG	C	932	14/15	0.95	0.10	0.54	30,33,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	D	907	14/15	0.95	0.11	0.49	22,24,27,28	0
2	NAG	D	919	14/15	0.96	0.10	0.35	20,24,27,28	0
2	NAG	B	925	14/15	0.91	0.11	0.32	32,38,42,45	0
2	NAG	A	906	14/15	0.95	0.10	0.25	25,27,29,30	0
2	NAG	C	902	14/15	0.95	0.15	0.24	31,35,39,46	0
4	MAN	C	930	11/12	0.96	0.10	0.12	22,24,26,29	0
2	NAG	D	929	14/15	0.95	0.10	0.08	31,32,34,37	0
2	NAG	D	932	14/15	0.96	0.10	-0.00	23,25,30,30	0
4	MAN	B	924	11/12	0.97	0.09	-0.05	26,27,31,36	0
2	NAG	B	931	14/15	0.93	0.10	-0.08	22,24,26,27	0
2	NAG	B	901	14/15	0.95	0.10	-0.20	22,28,29,30	0
2	NAG	A	926	14/15	0.95	0.10	-0.23	26,31,34,34	0
2	NAG	C	910	14/15	0.96	0.10	-0.29	18,21,23,24	0
4	MAN	D	927	11/12	0.96	0.09	-0.34	20,24,26,27	0
2	NAG	A	914	14/15	0.95	0.11	-0.34	29,35,41,46	0
2	NAG	B	906	14/15	0.94	0.09	-0.36	27,28,29,31	0
2	NAG	B	916	14/15	0.96	0.10	-0.40	23,26,27,27	0
2	NAG	A	902	14/15	0.95	0.09	-0.46	21,27,38,40	0
2	NAG	C	901	14/15	0.97	0.10	-0.48	24,25,28,28	0
2	NAG	C	923	14/15	0.96	0.11	-0.49	25,27,32,34	0
4	MAN	B	923	11/12	0.96	0.09	-0.50	24,25,29,29	0
2	NAG	B	930	14/15	0.94	0.10	-0.52	24,27,32,33	0
2	NAG	B	907	14/15	0.95	0.09	-0.58	34,37,41,45	0
2	NAG	A	917	14/15	0.97	0.09	-0.63	24,25,28,29	0
2	NAG	A	913	14/15	0.96	0.09	-0.66	20,22,27,27	0
2	NAG	A	918	14/15	0.97	0.08	-0.68	21,24,30,31	0
2	NAG	C	936	14/15	0.96	0.09	-0.71	23,25,28,30	0
2	NAG	B	902	14/15	0.96	0.09	-0.73	30,33,38,45	0
2	NAG	B	915	14/15	0.96	0.09	-0.79	25,26,27,28	0
2	NAG	C	937	14/15	0.96	0.08	-0.79	22,24,28,28	0
4	MAN	C	931	11/12	0.96	0.08	-0.82	25,27,29,33	0
4	MAN	A	924	11/12	0.98	0.08	-0.90	18,21,23,24	0
2	NAG	C	924	14/15	0.96	0.10	-0.98	21,26,29,29	0
2	NAG	C	911	14/15	0.96	0.08	-1.07	25,27,30,31	0
2	NAG	D	901	14/15	0.97	0.07	-1.14	21,23,25,26	0
2	NAG	D	915	14/15	0.97	0.08	-1.14	19,20,22,27	0
2	NAG	B	911	14/15	0.97	0.08	-1.16	22,25,27,30	0
2	NAG	C	918	14/15	0.96	0.10	-1.36	24,29,32,34	0
2	NAG	A	901	14/15	0.98	0.08	-1.36	22,24,27,30	0
2	NAG	D	920	14/15	0.97	0.07	-1.52	20,21,24,24	0
2	NAG	A	932	14/15	0.96	0.08	-2.06	24,28,31,32	0
4	MAN	C	939	11/12	0.92	0.20	-	46,49,52,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	948	14/15	0.82	0.35	-	55,77,93,106	0
4	MAN	B	909	11/12	0.77	0.17	-	67,75,78,81	0
3	BMA	B	908	11/12	0.88	0.13	-	45,54,57,67	0
4	MAN	D	926	11/12	0.83	0.41	-	56,61,64,70	0
4	MAN	A	935	11/12	0.84	0.20	-	57,65,70,71	0
4	MAN	D	906	11/12	0.79	0.23	-	67,78,86,89	0
2	NAG	D	941	14/15	0.90	0.34	-	64,79,84,85	0
4	MAN	C	907	11/12	0.88	0.26	-	57,63,65,71	0
3	BMA	A	928	11/12	0.77	0.21	-	71,77,91,102	0
2	NAG	D	944	14/15	0.72	0.23	-	62,80,88,88	0
3	BMA	D	909	11/12	0.93	0.12	-	38,39,52,70	0
2	NAG	C	919	14/15	0.92	0.13	-	39,43,46,52	0
4	MAN	D	924	11/12	0.96	0.11	-	22,25,27,29	0
3	BMA	C	912	11/12	0.93	0.11	-	33,33,44,61	0
3	BMA	A	933	11/12	0.90	0.10	-	33,34,37,38	0
3	BMA	A	919	11/12	0.97	0.10	-	26,28,31,40	0
4	MAN	B	910	11/12	0.87	0.20	-	55,67,79,86	0
4	MAN	B	937	11/12	0.76	0.24	-	64,70,73,76	0
4	MAN	D	904	11/12	0.87	0.21	-	71,79,88,90	0
4	MAN	B	935	11/12	0.79	0.31	-	75,79,86,86	0
4	MAN	D	923	11/12	0.75	0.23	-	77,84,86,87	0
2	NAG	B	940	14/15	0.88	0.17	-	42,58,66,71	0
3	BMA	B	917	11/12	0.95	0.09	-	27,28,31,35	0
4	MAN	D	922	11/12	0.92	0.12	-	38,48,53,64	0
4	MAN	C	926	11/12	0.88	0.17	-	46,48,56,72	0
6	GLC	D	913	11/12	0.69	0.28	-	66,88,96,99	0
4	MAN	C	928	11/12	0.96	0.09	-	25,31,35,40	0
4	MAN	B	936	11/12	0.95	0.08	-	38,40,46,54	0
4	MAN	C	909	11/12	0.70	0.32	-	73,89,92,94	0
3	BMA	D	921	11/12	0.97	0.09	-	22,24,29,35	0
2	NAG	C	950	14/15	0.80	0.31	-	62,72,82,88	0
4	MAN	C	908	11/12	0.85	0.20	-	72,76,79,84	0
4	MAN	A	904	11/12	0.89	0.15	-	60,70,76,77	0
4	MAN	D	905	11/12	0.62	0.26	-	74,94,99,100	0
4	MAN	B	919	11/12	0.80	0.18	-	59,65,70,71	0
3	BMA	A	903	11/12	0.88	0.23	-	50,59,67,73	0
3	BMA	A	908	11/12	0.89	0.10	-	43,48,58,64	0
4	MAN	C	915	11/12	0.92	0.14	-	45,50,55,66	0
3	BMA	D	903	11/12	0.89	0.21	-	44,65,82,84	0
3	BMA	D	934	11/12	0.95	0.11	-	29,34,37,42	0
2	NAG	B	926	14/15	0.90	0.14	-	45,48,54,67	0
4	MAN	D	938	11/12	0.91	0.17	-	39,43,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	943	14/15	0.82	0.22	-	64,74,84,84	0
6	GLC	C	916	11/12	0.80	0.24	-	58,67,73,74	0
4	MAN	A	905	11/12	0.78	0.26	-	92,94,96,97	0
2	NAG	C	933	14/15	0.95	0.17	-	40,44,50,64	0
2	NAG	B	912	14/15	0.91	0.15	-	36,43,50,59	0
4	MAN	B	905	11/12	0.68	0.20	-	63,88,99,102	0
2	NAG	C	945	14/15	0.87	0.29	-	56,66,73,77	0
4	MAN	A	920	11/12	0.91	0.18	-	47,55,60,67	0
4	MAN	B	918	11/12	0.92	0.12	-	42,45,47,52	0
4	MAN	D	925	11/12	0.96	0.19	-	35,39,42,45	0
4	MAN	A	916	11/12	0.72	0.28	-	69,85,86,87	0
4	MAN	A	912	11/12	0.72	0.27	-	56,75,83,84	0
2	NAG	D	930	14/15	0.90	0.14	-	36,43,49,60	0
4	MAN	B	929	11/12	0.69	0.29	-	92,101,109,109	0
4	MAN	A	922	11/12	0.97	0.10	-	27,29,33,40	0
3	BMA	C	925	11/12	0.95	0.10	-	26,30,33,37	0
3	BMA	C	949	11/12	0.57	0.35	-	82,110,119,119	0
4	MAN	C	929	11/12	0.89	0.19	-	47,52,53,60	0
4	MAN	C	904	11/12	0.93	0.10	-	52,58,63,63	0
3	BMA	B	928	11/12	0.67	0.38	-	78,85,94,99	0
4	MAN	C	906	11/12	0.83	0.20	-	59,68,74,76	0
4	MAN	C	905	11/12	0.92	0.15	-	48,50,53,56	0
4	MAN	D	918	11/12	0.52	0.29	-	87,104,110,111	0
4	MAN	D	911	11/12	0.95	0.10	-	40,43,46,54	0
2	NAG	A	927	14/15	0.94	0.12	-	40,43,48,58	0
4	MAN	D	936	11/12	0.61	0.30	-	70,83,92,93	0
3	BMA	D	917	11/12	0.79	0.21	-	58,69,76,90	0
4	MAN	B	914	11/12	0.61	0.41	-	81,99,110,115	0
3	BMA	B	913	11/12	0.71	0.33	-	73,84,91,102	0
4	MAN	B	904	11/12	0.82	0.13	-	66,72,76,79	0
4	MAN	C	942	11/12	0.91	0.23	-	35,40,44,48	0
4	MAN	A	929	11/12	0.69	0.38	-	89,98,103,106	0
4	MAN	A	910	11/12	0.83	0.18	-	76,82,85,100	0
4	MAN	B	921	11/12	0.93	0.20	-	39,42,45,51	0
4	MAN	C	927	11/12	0.65	0.31	-	84,91,100,101	0
4	MAN	D	935	11/12	0.83	0.21	-	55,59,65,67	0
3	BMA	B	903	11/12	0.90	0.14	-	55,66,73,73	0
2	NAG	A	943	14/15	0.86	0.29	-	65,70,78,78	0
4	MAN	C	914	11/12	0.94	0.12	-	31,36,40,43	0
4	MAN	A	909	11/12	0.81	0.20	-	73,79,86,87	0
4	MAN	D	914	11/12	0.64	0.40	-	88,102,108,109	0
4	MAN	B	920	11/12	0.96	0.10	-	27,28,34,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	BMA	C	934	11/12	0.78	0.26	-	75,85,92,95	0
4	MAN	D	937	11/12	0.88	0.13	-	39,42,46,47	0
4	MAN	A	911	11/12	0.82	0.22	-	77,90,96,98	0
2	NAG	A	941	14/15	0.84	0.26	-	59,66,69,70	0
4	MAN	A	934	11/12	0.92	0.13	-	43,49,57,57	0
4	MAN	B	938	11/12	0.93	0.18	-	43,49,53,57	0
4	MAN	D	910	11/12	0.91	0.14	-	40,43,45,46	0
4	MAN	C	941	11/12	0.94	0.13	-	30,36,42,43	0
3	BMA	C	938	11/12	0.94	0.12	-	30,32,37,40	0
2	NAG	C	946	14/15	0.77	0.39	-	67,82,96,100	0
4	MAN	A	923	11/12	0.91	0.20	-	43,53,59,65	0
4	MAN	A	937	11/12	0.91	0.10	-	37,40,42,42	0
4	MAN	D	912	11/12	0.87	0.12	-	53,63,67,81	0
2	NAG	B	942	14/15	0.80	0.28	-	53,66,79,80	0
4	MAN	C	913	11/12	0.94	0.12	-	34,38,41,41	0
4	MAN	A	938	11/12	0.92	0.11	-	40,44,47,47	0
2	NAG	D	916	14/15	0.92	0.13	-	29,36,43,46	0
3	BMA	B	932	11/12	0.95	0.09	-	29,32,36,44	0
3	BMA	A	915	11/12	0.86	0.22	-	60,70,79,81	0
4	MAN	C	921	11/12	0.71	0.20	-	91,94,99,104	0
4	MAN	B	933	11/12	0.91	0.17	-	45,51,55,63	0
4	MAN	A	921	11/12	0.73	0.31	-	70,88,92,93	0
4	MAN	C	922	11/12	0.81	0.22	-	77,90,95,95	0
3	BMA	C	903	11/12	0.90	0.17	-	44,54,61,62	0
4	MAN	C	917	11/12	0.63	0.37	-	82,88,94,96	0
3	BMA	C	920	11/12	0.89	0.12	-	62,70,78,83	0
3	BMA	D	931	11/12	0.71	0.27	-	72,81,84,86	0
4	MAN	B	922	11/12	0.91	0.34	-	50,57,60,60	0
4	MAN	B	934	11/12	0.78	0.27	-	80,82,86,87	0
3	BMA	B	927	11/12	0.81	0.20	-	77,85,90,92	0
4	MAN	C	940	11/12	0.71	0.30	-	55,70,76,79	0
4	MAN	A	936	11/12	0.77	0.27	-	76,85,89,90	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.