wwPDB X-ray Structure Validation Summary Report (i)

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 wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

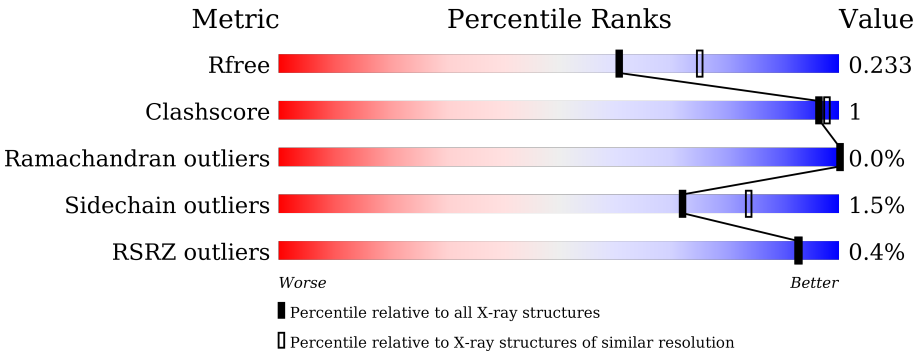
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	857	93%
1	B	857	91% 6%
1	C	857	92% 5%
1	D	857	92% 5%

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 crite-

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

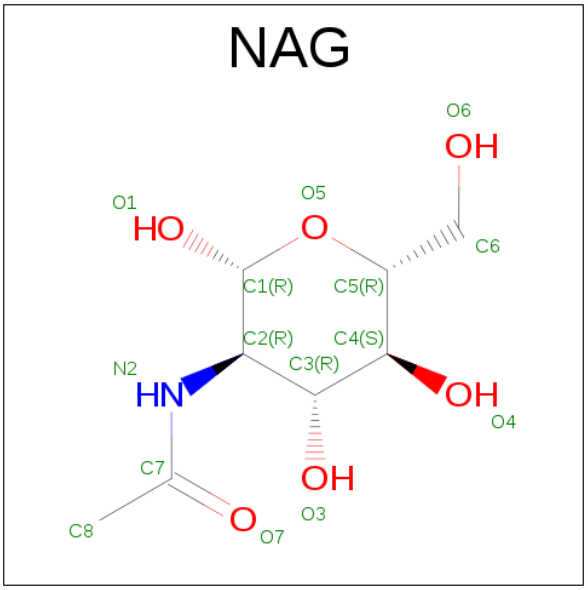
There are 7 unique types of molecules in this entry. The entry contains 29503 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: $C_8H_{15}NO_6$).



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 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0

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

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

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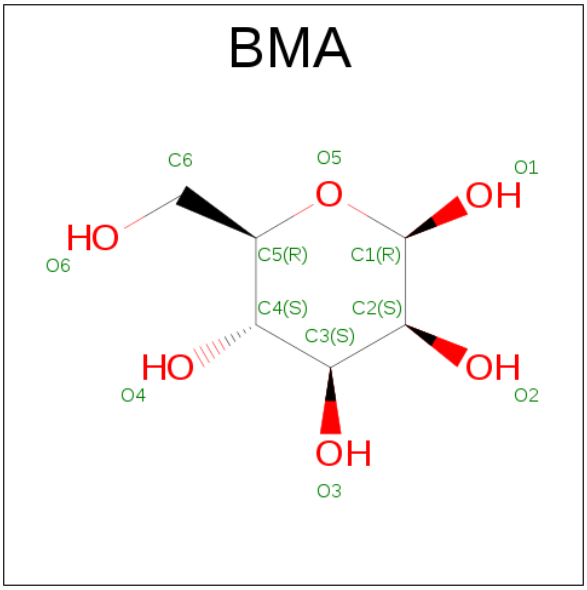
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0

- 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 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0

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

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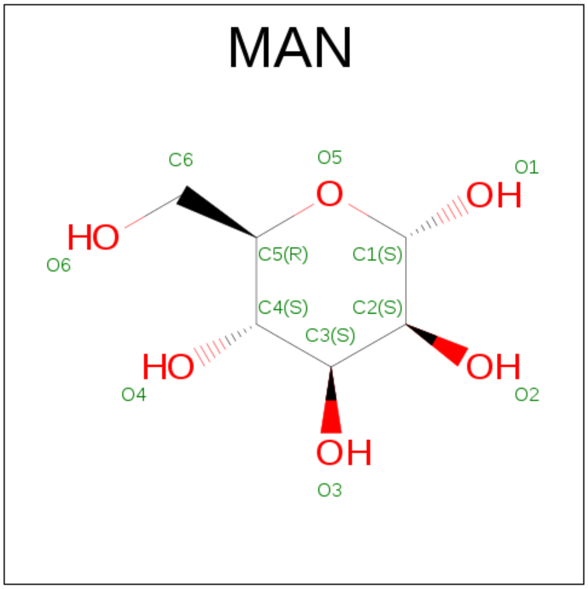
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 11 6 5	0	0

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (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	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	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	A	1	Total C O 11 6 5	0	0

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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	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	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	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
4	B	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
4	B	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
4	B	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

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

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

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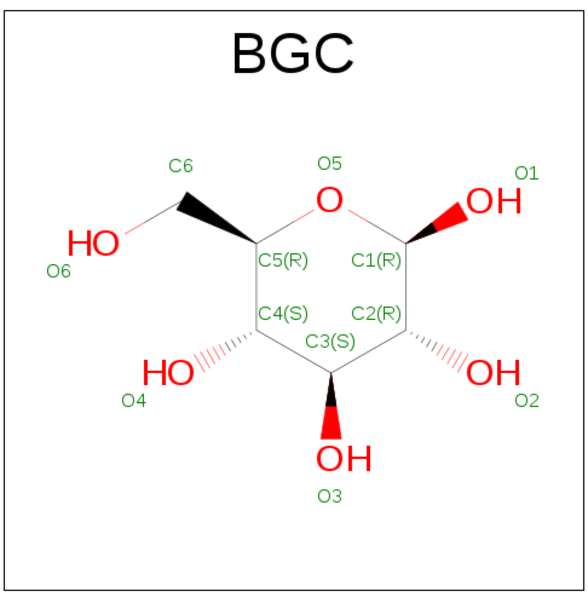
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11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

- 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 12 6 6	0	0

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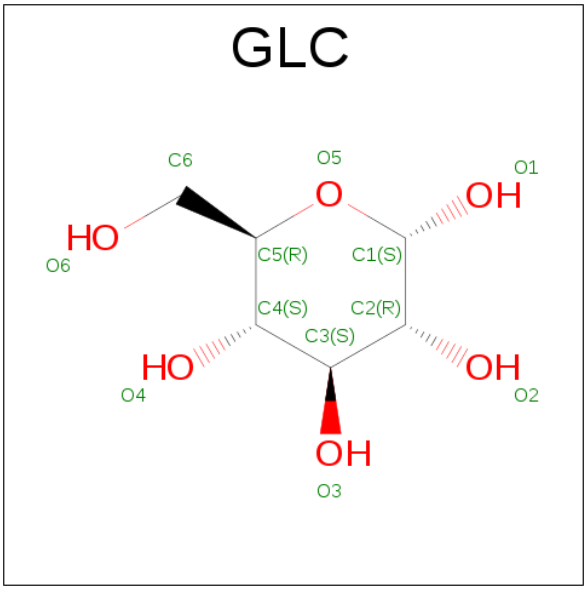
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 12 6 6	0	0
5	C	1	Total C O 12 6 6	0	0
5	D	1	Total C O 12 6 6	0	0

- Molecule 6 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



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

- Molecule 7 is water.

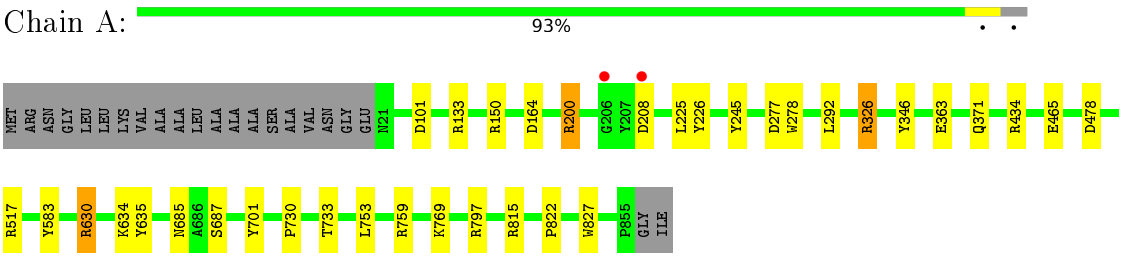
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	431	Total O 431 431	0	0
7	B	399	Total O 400 400	0	1
7	C	441	Total O 441 441	0	0
7	D	432	Total O 432 432	0	0

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.

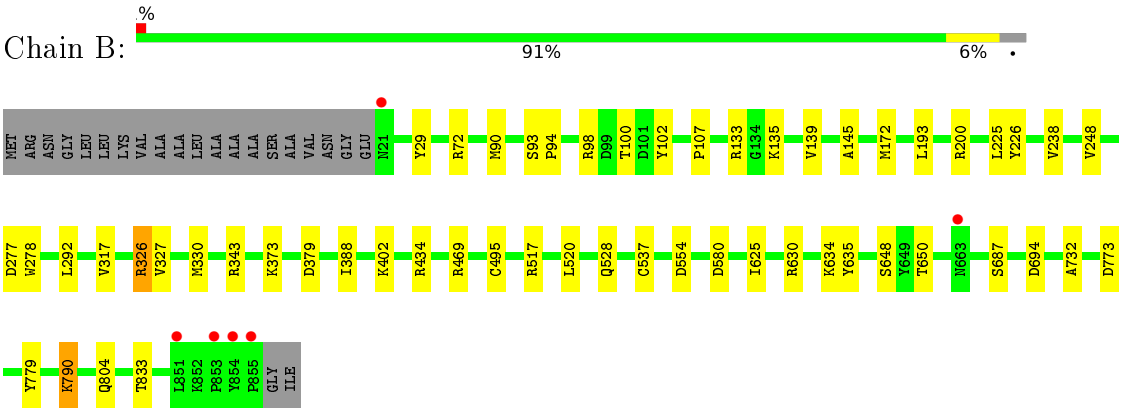
- Molecule 1: Beta-glucosidase

Chain A:



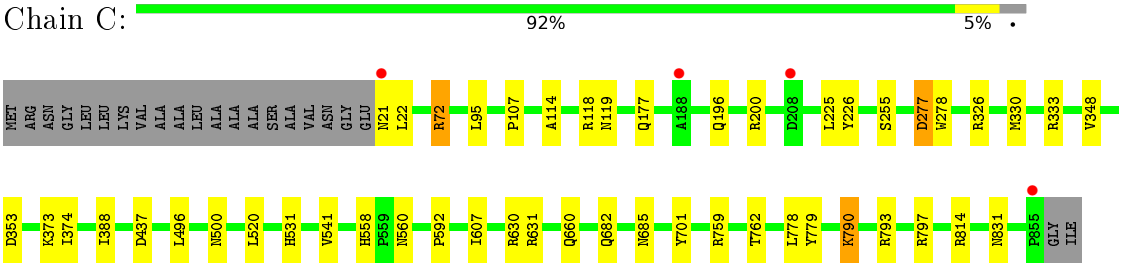
- Molecule 1: Beta-glucosidase

Chain B:



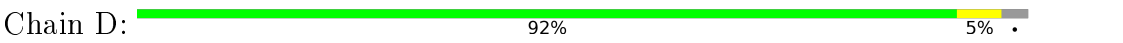
- Molecule 1: Beta-glucosidase

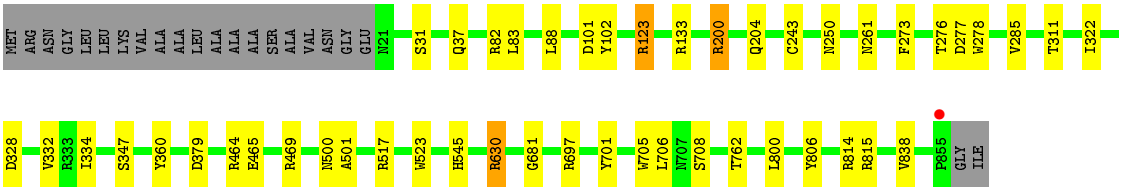
Chain C:



- Molecule 1: Beta-glucosidase

Chain D:




MET
ARG
ASN
GLY
LEU
LEU
LYS
VAL
ALA
ALA
LEU
ALA
ALA
ALA
SER
ALA
VAL
ASN
GLY
GLU
M21
S31
Q37
R82
L83
L88
D101
Y102
R123
R133
R200
Q204
C243
M250
M261
F273
T276
D277
W278
V285
T311
I322
D328
V332
R333
I334
S347
Y360
D379
R464
E465
R469
N500
A501
R517
W523
H545
R630
G681
R697
Y701
W705
L706
N707
S708
T762
L800
Y806
R814
R815
V838
P855
GLY
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	137.29Å 148.63Å 196.39Å 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
$< I/\sigma(I) >$ [1]	3.64 (at 2.20Å)	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^2)	22.4	Xtriage
Anisotropy	0.990	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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
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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	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

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	72	ARG
1	C	278	TRP
1	D	278	TRP
1	C	95	LEU
1	C	177	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	119	ASN
1	C	261	ASN
1	D	618	GLN
1	C	140	GLN
1	C	463	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	940	NAG	O4-C4	2.00	1.47	1.43

The worst 5 of 362 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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^{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	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%)

The worst 5 of 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

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^{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
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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 (i)

There are no such residues in this entry.