



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:29 PM GMT

PDB ID : 4IIF  
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus* in complex with castanospermine  
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.  
Deposited on : 2012-12-20  
Resolution : 2.45 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](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

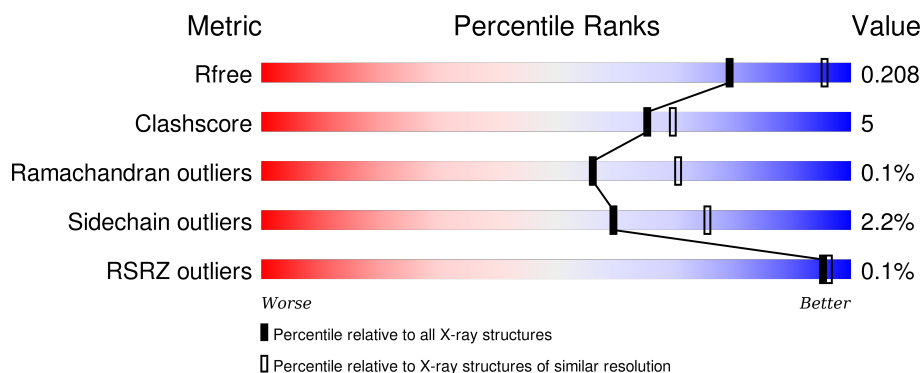
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	841	 89% 9% .
1	B	841	 87% 11% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MPD	A	939	-	-	-	X
10	MPD	A	940	-	-	-	X
4	NAG	A	907	-	-	-	X
7	NAG	A	924	-	-	-	X
7	MAN	A	930	-	-	-	X
7	MAN	B	906	-	-	-	X
9	MRD	B	945	-	-	-	X
9	MRD	B	946	-	-	-	X
9	MRD	B	947	-	-	-	X

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 14647 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.

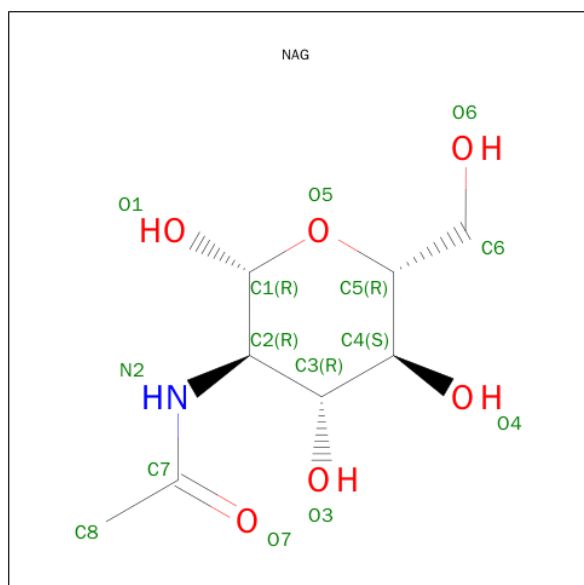
- Molecule 1 is a protein called Beta-glucosidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6378	4026	1095	1239	18			
1	B	832	Total	C	N	O	S	0	0	0
			6375	4023	1095	1239	18			

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			50	28	2	20		
2	B	4	Total	C	N	O	0	0
			50	28	2	20		

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



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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

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

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

- Molecule 6 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	10	Total	C	N	O	0	0
			116	64	2	50		
6	B	10	Total	C	N	O	0	0
			116	64	2	50		

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

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

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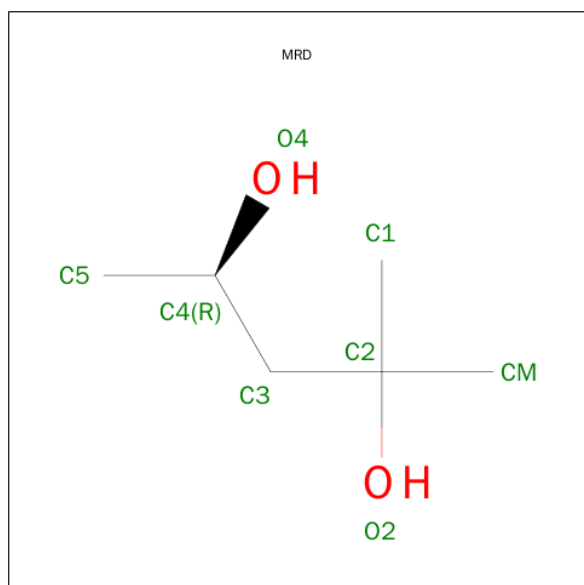
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	7	Total	C	N	O	0	0
			83	46	2	35		
7	B	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

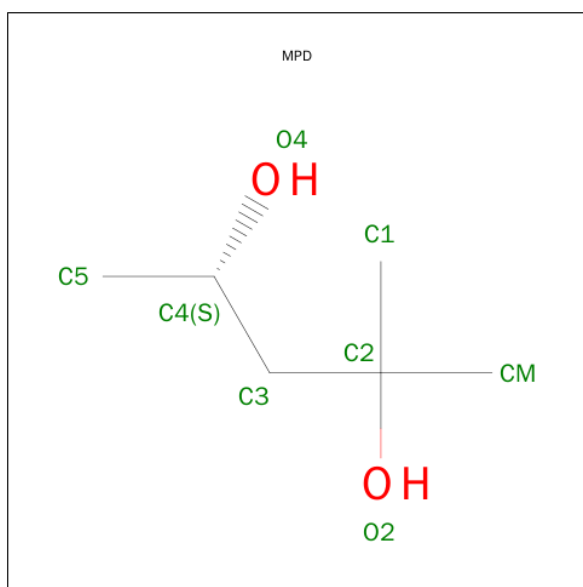
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



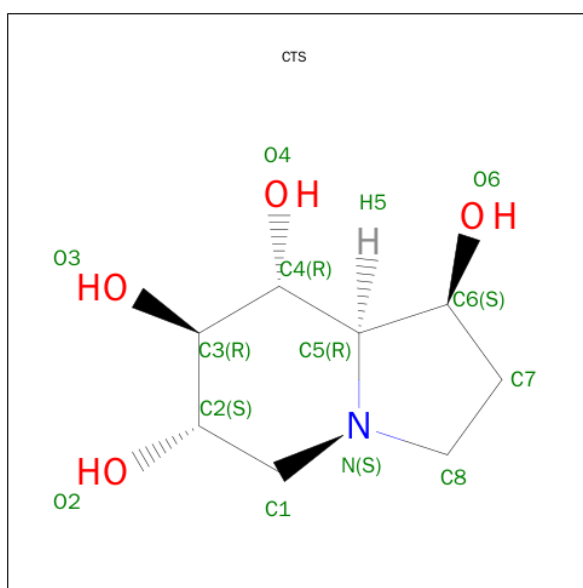
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			8	6	2		
9	B	1	Total	C	O	0	0
			8	6	2		
9	B	1	Total	C	O	0	0
			8	6	2		
9	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 10 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			8	6	2		
10	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 11 is CASTANOSPERMINE (three-letter code: CTS) (formula:  $C_8H_{15}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			13	8	1	4		
11	B	1	Total	C	N	O	0	0
			13	8	1	4		

- Molecule 12 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 13 is water.

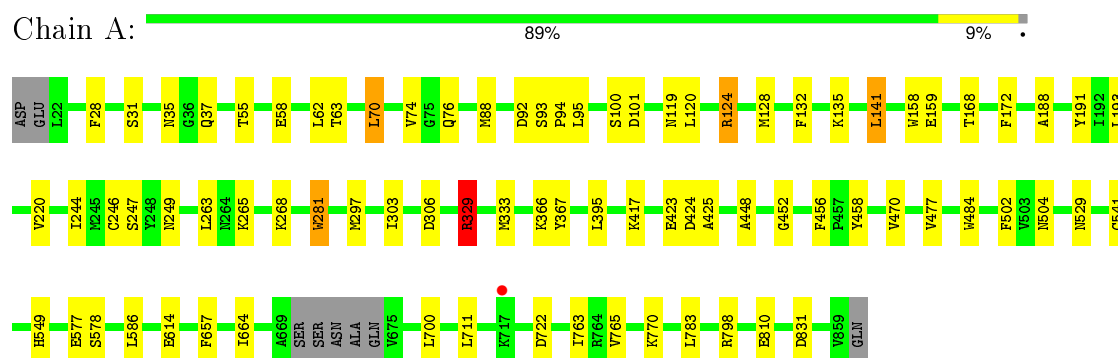
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	380	Total	O	0	0
			380	380		
13	B	450	Total	O	0	0
			450	450		



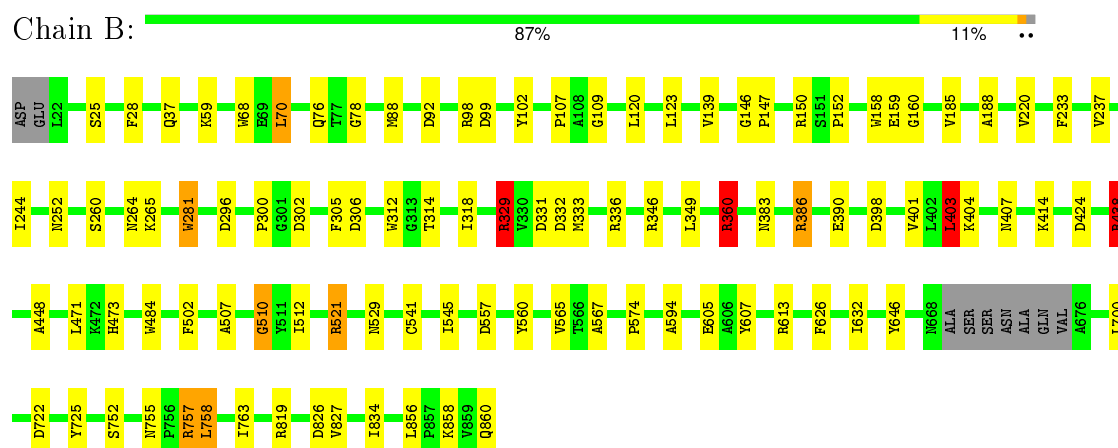
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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 1



#### • Molecule 1: Beta-glucosidase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.38Å 122.24Å 222.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 2.45 49.08 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.08-2.45) 99.4 (49.08-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.154 , 0.205 0.157 , 0.208	Depositor DCC
$R_{free}$ test set	4152 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 82518 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, BMA, NAG, CTS, MRD, 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	0.83	3/6541 (0.0%)	0.89	8/8918 (0.1%)
1	B	0.89	2/6538 (0.0%)	0.95	17/8913 (0.2%)
All	All	0.86	5/13079 (0.0%)	0.92	25/17831 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	CYS	CB-SG	6.83	1.93	1.82
1	B	541	CYS	CB-SG	5.52	1.91	1.82
1	B	541	CYS	CA-CB	5.48	1.66	1.53
1	A	423	GLU	CD-OE1	5.33	1.31	1.25
1	A	541	CYS	CA-CB	5.08	1.65	1.53

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	ARG	NE-CZ-NH2	-14.40	113.10	120.30
1	B	521	ARG	NE-CZ-NH2	-13.86	113.37	120.30
1	B	329	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	B	521	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	B	438	ARG	NE-CZ-NH1	-10.72	114.94	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	6378	0	6089	52	0
1	B	6375	0	6082	75	0
2	A	50	0	43	0	0
2	B	50	0	43	3	0
3	A	28	0	26	0	0
3	B	42	0	39	0	0
4	A	78	0	68	0	0
4	B	39	0	34	0	0
5	A	28	0	25	2	0
5	B	28	0	25	0	0
6	A	116	0	97	0	0
6	B	116	0	97	0	0
7	A	83	0	70	2	0
7	B	166	0	140	3	0
8	A	72	0	61	0	0
9	A	8	0	14	1	0
9	B	24	0	42	6	0
10	A	16	0	28	1	0
11	A	13	0	15	2	0
11	B	13	0	15	2	0
12	B	94	0	79	0	0
13	A	380	0	0	4	0
13	B	450	0	0	7	0
All	All	14647	0	13132	135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 135 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:LEU:HD23	1:B:758:LEU:H	1.22	1.02
1:B:755:ASN:O	1:B:758:LEU:HD23	1.61	0.99
9:B:946:MRD:H1C2	9:B:946:MRD:H5C3	1.47	0.95
1:A:63:THR:HG21	1:A:333:MET:HE2	1.51	0.90
9:B:946:MRD:H1C2	9:B:946:MRD:C5	2.01	0.89

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	829/841 (99%)	798 (96%)	31 (4%)	0	100	100
1	B	828/841 (98%)	797 (96%)	30 (4%)	1 (0%)	56	71
All	All	1657/1682 (98%)	1595 (96%)	61 (4%)	1 (0%)	56	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	510	GLY

### 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	670/677 (99%)	657 (98%)	13 (2%)	65	79
1	B	670/677 (99%)	653 (98%)	17 (2%)	55	72
All	All	1340/1354 (99%)	1310 (98%)	30 (2%)	60	75

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	70	LEU
1	B	281	TRP
1	B	757	ARG
1	B	123	LEU
1	B	329	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	658	ASN
1	B	37	GLN
1	B	473	HIS

### 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 ⓘ

76 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAG	A	901	1,2	14,14,15	0.75	0	15,19,21	0.94	0
2	NAG	A	902	2	14,14,15	0.71	0	15,19,21	1.77	2 (13%)
2	BMA	A	903	2	11,11,12	1.17	0	14,15,17	2.65	6 (42%)
2	MAN	A	904	2	11,11,12	0.92	0	14,15,17	2.83	7 (50%)
4	NAG	A	906	1,4	14,14,15	1.03	1 (7%)	15,19,21	0.96	1 (6%)
4	NAG	A	907	4	14,14,15	0.63	0	15,19,21	1.42	1 (6%)
4	BMA	A	908	4	11,11,12	0.77	0	14,15,17	2.74	10 (71%)
5	NAG	A	909	1,5	14,14,15	0.61	0	15,19,21	1.81	2 (13%)
5	NAG	A	910	5	14,14,15	0.65	1 (7%)	15,19,21	1.69	4 (26%)
6	NAG	A	911	1,6	14,14,15	0.71	0	15,19,21	0.95	0
6	NAG	A	912	6	14,14,15	0.96	1 (7%)	15,19,21	1.53	3 (20%)
6	BMA	A	913	6	11,11,12	1.03	1 (9%)	14,15,17	1.12	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	A	914	6	11,11,12	0.84	0	14,15,17	1.09	2 (14%)
6	MAN	A	915	6	11,11,12	1.05	1 (9%)	14,15,17	1.71	2 (14%)
6	MAN	A	916	6	11,11,12	0.68	0	14,15,17	1.60	3 (21%)
6	MAN	A	917	6	11,11,12	1.01	1 (9%)	14,15,17	1.58	5 (35%)
6	MAN	A	918	6	11,11,12	0.73	0	14,15,17	1.74	3 (21%)
6	MAN	A	919	6	11,11,12	1.17	1 (9%)	14,15,17	1.98	4 (28%)
6	MAN	A	920	6	11,11,12	0.77	0	14,15,17	1.44	3 (21%)
4	NAG	A	921	1,4	14,14,15	0.74	0	15,19,21	1.73	1 (6%)
4	NAG	A	922	4	14,14,15	0.80	0	15,19,21	1.55	4 (26%)
4	BMA	A	923	4	11,11,12	0.81	0	14,15,17	1.78	4 (28%)
7	NAG	A	924	1,7	14,14,15	0.71	0	15,19,21	1.70	4 (26%)
7	NAG	A	925	7	14,14,15	0.95	1 (7%)	15,19,21	2.14	4 (26%)
7	BMA	A	926	7	11,11,12	0.76	0	14,15,17	1.77	3 (21%)
7	MAN	A	927	7	11,11,12	0.75	0	14,15,17	2.06	4 (28%)
7	MAN	A	928	7	11,11,12	1.04	1 (9%)	14,15,17	1.78	4 (28%)
7	MAN	A	929	7	11,11,12	0.82	1 (9%)	14,15,17	2.40	6 (42%)
7	MAN	A	930	7	11,11,12	0.83	0	14,15,17	1.57	3 (21%)
8	NAG	A	931	1,8	14,14,15	0.89	1 (7%)	15,19,21	2.11	3 (20%)
8	NAG	A	932	8	14,14,15	0.85	1 (7%)	15,19,21	1.44	2 (13%)
8	BMA	A	933	8	11,11,12	0.66	0	14,15,17	1.97	4 (28%)
8	MAN	A	934	8	11,11,12	1.10	0	14,15,17	2.24	9 (64%)
8	MAN	A	935	8	11,11,12	1.25	1 (9%)	14,15,17	2.13	6 (42%)
8	MAN	A	936	8	11,11,12	0.79	0	14,15,17	1.43	3 (21%)
7	NAG	B	901	1,7	14,14,15	1.15	1 (7%)	15,19,21	1.54	2 (13%)
7	NAG	B	902	7	14,14,15	0.84	0	15,19,21	1.69	3 (20%)
7	BMA	B	903	7	11,11,12	0.84	0	14,15,17	1.66	2 (14%)
7	MAN	B	904	7	11,11,12	0.74	0	14,15,17	1.14	2 (14%)
7	MAN	B	905	7	11,11,12	0.73	0	14,15,17	1.55	2 (14%)
7	MAN	B	906	7	11,11,12	0.73	0	14,15,17	1.21	3 (21%)
7	MAN	B	907	7	11,11,12	1.00	1 (9%)	14,15,17	2.12	6 (42%)
2	NAG	B	909	1,2	14,14,15	1.14	2 (14%)	15,19,21	1.66	4 (26%)
2	NAG	B	910	2	14,14,15	0.77	0	15,19,21	0.91	0
2	BMA	B	911	2	11,11,12	0.78	0	14,15,17	1.27	2 (14%)
2	MAN	B	912	2	11,11,12	1.28	1 (9%)	14,15,17	2.20	5 (35%)
5	NAG	B	913	1,5	14,14,15	0.92	0	15,19,21	1.61	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	914	5	14,14,15	0.77	0	15,19,21	1.83	4 (26%)
6	NAG	B	915	1,6	14,14,15	0.79	0	15,19,21	1.83	4 (26%)
6	NAG	B	916	6	14,14,15	0.76	0	15,19,21	0.98	0
6	BMA	B	917	6	11,11,12	1.08	1 (9%)	14,15,17	1.29	2 (14%)
6	MAN	B	918	6	11,11,12	0.64	0	14,15,17	1.78	4 (28%)
6	MAN	B	919	6	11,11,12	1.04	1 (9%)	14,15,17	2.53	6 (42%)
6	MAN	B	920	6	11,11,12	0.74	0	14,15,17	2.17	6 (42%)
6	MAN	B	921	6	11,11,12	0.90	0	14,15,17	2.10	4 (28%)
6	MAN	B	922	6	11,11,12	0.84	0	14,15,17	1.60	2 (14%)
6	MAN	B	923	6	11,11,12	0.85	0	14,15,17	1.64	2 (14%)
6	MAN	B	924	6	11,11,12	0.79	0	14,15,17	1.77	2 (14%)
4	NAG	B	925	1,4	14,14,15	0.80	0	15,19,21	1.51	4 (26%)
4	NAG	B	926	4	14,14,15	0.97	1 (7%)	15,19,21	1.12	1 (6%)
4	BMA	B	927	4	11,11,12	0.77	0	14,15,17	2.22	3 (21%)
7	NAG	B	928	1,7	14,14,15	1.05	1 (7%)	15,19,21	1.34	1 (6%)
7	NAG	B	929	7	14,14,15	1.11	2 (14%)	15,19,21	1.68	2 (13%)
7	BMA	B	930	7	11,11,12	0.66	0	14,15,17	1.31	2 (14%)
7	MAN	B	931	7	11,11,12	0.93	0	14,15,17	2.42	5 (35%)
7	MAN	B	932	7	11,11,12	1.07	0	14,15,17	1.85	3 (21%)
7	MAN	B	933	7	11,11,12	0.69	0	14,15,17	1.76	3 (21%)
7	MAN	B	934	7	11,11,12	0.73	0	14,15,17	2.04	3 (21%)
12	NAG	B	935	1,12	14,14,15	0.96	1 (7%)	15,19,21	1.79	3 (20%)
12	NAG	B	936	12	14,14,15	0.86	1 (7%)	15,19,21	1.72	3 (20%)
12	BMA	B	937	12	11,11,12	1.08	1 (9%)	14,15,17	1.59	2 (14%)
12	MAN	B	938	12	11,11,12	0.94	0	14,15,17	2.24	7 (50%)
12	MAN	B	939	12	11,11,12	0.65	0	14,15,17	1.86	4 (28%)
12	MAN	B	940	12	11,11,12	0.85	0	14,15,17	1.54	2 (14%)
12	MAN	B	941	12	11,11,12	0.83	1 (9%)	14,15,17	1.67	2 (14%)
12	MAN	B	942	12	11,11,12	0.88	1 (9%)	14,15,17	2.16	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	902	2	-	0/6/23/26	0/1/1/1
2	BMA	A	903	2	-	0/2/19/22	0/1/1/1
2	MAN	A	904	2	-	0/2/19/22	0/1/1/1
4	NAG	A	906	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	907	4	-	0/6/23/26	0/1/1/1
4	BMA	A	908	4	-	0/2/19/22	0/1/1/1
5	NAG	A	909	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	910	5	-	0/6/23/26	0/1/1/1
6	NAG	A	911	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	912	6	-	0/6/23/26	0/1/1/1
6	BMA	A	913	6	-	0/2/19/22	0/1/1/1
6	MAN	A	914	6	-	0/2/19/22	0/1/1/1
6	MAN	A	915	6	-	0/2/19/22	0/1/1/1
6	MAN	A	916	6	-	0/2/19/22	0/1/1/1
6	MAN	A	917	6	-	0/2/19/22	0/1/1/1
6	MAN	A	918	6	-	0/2/19/22	0/1/1/1
6	MAN	A	919	6	-	0/2/19/22	0/1/1/1
6	MAN	A	920	6	-	0/2/19/22	0/1/1/1
4	NAG	A	921	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	922	4	-	0/6/23/26	0/1/1/1
4	BMA	A	923	4	-	0/2/19/22	0/1/1/1
7	NAG	A	924	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	925	7	-	0/6/23/26	0/1/1/1
7	BMA	A	926	7	-	0/2/19/22	0/1/1/1
7	MAN	A	927	7	-	0/2/19/22	0/1/1/1
7	MAN	A	928	7	-	0/2/19/22	0/1/1/1
7	MAN	A	929	7	-	0/2/19/22	0/1/1/1
7	MAN	A	930	7	-	0/2/19/22	0/1/1/1
8	NAG	A	931	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	932	8	-	0/6/23/26	0/1/1/1
8	BMA	A	933	8	-	0/2/19/22	0/1/1/1
8	MAN	A	934	8	-	0/2/19/22	0/1/1/1
8	MAN	A	935	8	-	0/2/19/22	0/1/1/1
8	MAN	A	936	8	-	0/2/19/22	0/1/1/1
7	NAG	B	901	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	902	7	-	0/6/23/26	0/1/1/1
7	BMA	B	903	7	-	0/2/19/22	0/1/1/1
7	MAN	B	904	7	-	0/2/19/22	0/1/1/1
7	MAN	B	905	7	-	0/2/19/22	0/1/1/1
7	MAN	B	906	7	-	0/2/19/22	0/1/1/1
7	MAN	B	907	7	-	0/2/19/22	0/1/1/1
2	NAG	B	909	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	910	2	-	0/6/23/26	0/1/1/1
2	BMA	B	911	2	-	0/2/19/22	0/1/1/1
2	MAN	B	912	2	-	0/2/19/22	0/1/1/1
5	NAG	B	913	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	914	5	-	0/6/23/26	0/1/1/1
6	NAG	B	915	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	916	6	-	0/6/23/26	0/1/1/1
6	BMA	B	917	6	-	0/2/19/22	0/1/1/1
6	MAN	B	918	6	-	0/2/19/22	0/1/1/1
6	MAN	B	919	6	-	0/2/19/22	0/1/1/1
6	MAN	B	920	6	-	0/2/19/22	0/1/1/1
6	MAN	B	921	6	-	0/2/19/22	0/1/1/1
6	MAN	B	922	6	-	0/2/19/22	0/1/1/1
6	MAN	B	923	6	-	0/2/19/22	0/1/1/1
6	MAN	B	924	6	-	0/2/19/22	0/1/1/1
4	NAG	B	925	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	926	4	-	0/6/23/26	0/1/1/1
4	BMA	B	927	4	-	0/2/19/22	0/1/1/1
7	NAG	B	928	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	929	7	-	0/6/23/26	0/1/1/1
7	BMA	B	930	7	-	0/2/19/22	0/1/1/1
7	MAN	B	931	7	-	0/2/19/22	0/1/1/1
7	MAN	B	932	7	-	0/2/19/22	0/1/1/1
7	MAN	B	933	7	-	0/2/19/22	0/1/1/1
7	MAN	B	934	7	-	0/2/19/22	0/1/1/1
12	NAG	B	935	1,12	-	0/6/23/26	0/1/1/1
12	NAG	B	936	12	-	0/6/23/26	0/1/1/1
12	BMA	B	937	12	-	0/2/19/22	0/1/1/1
12	MAN	B	938	12	-	0/2/19/22	0/1/1/1
12	MAN	B	939	12	-	0/2/19/22	0/1/1/1
12	MAN	B	940	12	-	0/2/19/22	0/1/1/1
12	MAN	B	941	12	-	0/2/19/22	0/1/1/1
12	MAN	B	942	12	-	0/2/19/22	0/1/1/1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	901	NAG	O5-C1	-2.98	1.38	1.43
7	B	928	NAG	O5-C1	-2.84	1.39	1.43
4	A	906	NAG	O5-C1	-2.78	1.39	1.43
8	A	935	MAN	O5-C1	-2.75	1.39	1.43
6	A	919	MAN	O5-C1	-2.61	1.39	1.43

The worst 5 of 247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	931	MAN	C1-O5-C5	-6.58	103.90	112.25
7	A	925	NAG	C2-N2-C7	-5.91	115.45	123.04
2	A	903	BMA	O5-C5-C6	-5.22	96.05	107.35
5	B	914	NAG	C3-C4-C5	-4.80	101.83	110.20
7	A	927	MAN	O5-C1-C2	-4.69	103.25	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	910	NAG	2	0
7	A	926	BMA	2	0
7	B	901	NAG	2	0
2	B	909	NAG	1	0
2	B	910	NAG	2	0
7	B	930	BMA	1	0

## 5.6 Ligand geometry

13 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$
3	NAG	A	905	1	14,14,15	0.72	0	15,19,21	1.35	1 (6%)
3	NAG	A	937	1	14,14,15	0.97	0	15,19,21	1.94	4 (26%)
9	MRD	A	938	-	6,7,7	0.28	0	7,10,10	0.69	0
10	MPD	A	939	-	6,7,7	0.35	0	7,10,10	0.60	0
10	MPD	A	940	-	6,7,7	0.45	0	7,10,10	0.91	0
11	CTS	A	941	-	14,14,14	1.34	1 (7%)	15,21,21	1.27	3 (20%)
3	NAG	B	908	1	14,14,15	1.04	1 (7%)	15,19,21	1.47	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	943	1	14,14,15	0.71	0	15,19,21	1.35	1 (6%)
3	NAG	B	944	1	14,14,15	0.69	0	15,19,21	1.60	2 (13%)
9	MRD	B	945	-	6,7,7	0.54	0	7,10,10	0.40	0
9	MRD	B	946	-	6,7,7	0.73	0	7,10,10	1.02	1 (14%)
9	MRD	B	947	-	6,7,7	0.53	0	7,10,10	0.40	0
11	CTS	B	948	-	14,14,14	1.06	1 (7%)	15,21,21	1.29	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	905	1	-	0/6/23/26	0/1/1/1
3	NAG	A	937	1	-	0/6/23/26	0/1/1/1
9	MRD	A	938	-	-	0/5/5/5	0/0/0/0
10	MPD	A	939	-	-	0/5/5/5	0/0/0/0
10	MPD	A	940	-	-	0/5/5/5	0/0/0/0
11	CTS	A	941	-	-	0/0/29/29	0/2/2/2
3	NAG	B	908	1	-	0/6/23/26	0/1/1/1
3	NAG	B	943	1	-	0/6/23/26	0/1/1/1
3	NAG	B	944	1	-	0/6/23/26	0/1/1/1
9	MRD	B	945	-	-	0/5/5/5	0/0/0/0
9	MRD	B	946	-	-	0/5/5/5	0/0/0/0
9	MRD	B	947	-	-	0/5/5/5	0/0/0/0
11	CTS	B	948	-	-	0/0/29/29	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	941	CTS	C6-C5	-4.36	1.49	1.54
3	B	908	NAG	O5-C1	-2.64	1.39	1.43
11	B	948	CTS	C1-C2	2.88	1.56	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	937	NAG	C2-N2-C7	-4.95	116.68	123.04
3	A	905	NAG	C4-C3-C2	-3.72	105.45	111.23
3	A	937	NAG	C3-C4-C5	-2.91	105.12	110.20
11	A	941	CTS	O2-C2-C3	-2.34	105.41	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	908	NAG	O7-C7-C8	-2.27	117.90	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	938	MRD	1	0
10	A	939	MPD	1	0
11	A	941	CTS	2	0
9	B	945	MRD	1	0
9	B	946	MRD	3	0
9	B	947	MRD	2	0
11	B	948	CTS	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	833/841 (99%)	-0.51	1 (0%) 95 96	17, 26, 42, 72	0
1	B	832/841 (98%)	-0.66	0 100 100	16, 23, 35, 58	0
All	All	1665/1682 (98%)	-0.58	1 (0%) 95 96	16, 24, 39, 72	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	LYS	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 ⓘ

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
7	MAN	A	930	11/12	0.96	0.12	2.87	32,36,44,45	0
7	NAG	A	924	14/15	0.95	0.15	2.72	26,33,47,49	0
4	NAG	A	907	14/15	0.95	0.13	2.64	27,35,37,37	0
7	MAN	B	906	11/12	0.95	0.19	2.64	31,37,41,48	0
12	MAN	B	939	11/12	0.97	0.19	1.88	30,38,52,60	0
7	MAN	B	934	11/12	0.96	0.16	1.48	30,39,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	921	14/15	0.95	0.12	0.80	35,39,47,49	0
8	MAN	A	935	11/12	0.95	0.13	0.79	33,40,46,48	0
6	MAN	B	921	11/12	0.96	0.10	0.56	27,28,33,37	0
7	NAG	B	928	14/15	0.96	0.10	0.40	22,33,45,46	0
6	MAN	A	919	11/12	0.96	0.09	0.35	29,30,37,45	0
8	MAN	A	934	11/12	0.93	0.14	0.17	35,37,41,43	0
6	MAN	A	918	11/12	0.97	0.11	-0.01	28,29,34,35	0
6	NAG	A	911	14/15	0.97	0.16	-0.02	27,32,39,40	0
6	NAG	B	916	14/15	0.97	0.11	-0.20	19,22,26,30	0
8	NAG	A	931	14/15	0.97	0.12	-0.34	26,29,33,37	0
7	NAG	B	901	14/15	0.99	0.10	-0.36	19,20,24,28	0
6	NAG	A	912	14/15	0.97	0.13	-0.37	28,31,34,39	0
6	NAG	B	915	14/15	0.98	0.10	-0.38	22,26,29,30	0
4	NAG	B	925	14/15	0.96	0.10	-0.41	28,33,41,43	0
4	NAG	A	906	14/15	0.96	0.10	-0.47	26,30,32,34	0
12	NAG	B	935	14/15	0.97	0.11	-0.49	23,25,29,34	0
2	NAG	A	901	14/15	0.98	0.09	-0.64	25,32,35,36	0
6	MAN	A	917	11/12	0.97	0.10	-0.73	28,31,33,35	0
2	NAG	A	902	14/15	0.97	0.11	-0.79	31,41,51,61	0
5	NAG	A	909	14/15	0.97	0.11	-0.85	25,28,32,33	0
5	NAG	B	913	14/15	0.98	0.09	-0.87	18,22,26,27	0
7	NAG	B	902	14/15	0.98	0.10	-1.69	21,26,30,31	0
2	NAG	B	910	14/15	0.96	0.08	-1.70	25,34,39,41	0
2	NAG	B	909	14/15	0.97	0.08	-1.94	22,26,28,32	0
6	MAN	B	924	11/12	0.97	0.08	-1.99	26,28,30,31	0
6	MAN	B	923	11/12	0.98	0.08	-2.38	19,21,23,24	0
6	MAN	A	920	11/12	0.93	0.12	-	38,41,46,48	0
12	MAN	B	942	11/12	0.85	0.26	-	53,67,74,75	0
12	MAN	B	938	11/12	0.83	0.26	-	62,71,81,81	0
4	NAG	A	922	14/15	0.87	0.24	-	53,63,73,84	0
7	MAN	B	932	11/12	0.91	0.14	-	33,35,40,46	0
6	MAN	A	916	11/12	0.99	0.08	-	22,26,28,30	0
7	BMA	B	930	11/12	0.92	0.18	-	40,47,56,68	0
7	MAN	A	928	11/12	0.95	0.15	-	35,40,47,48	0
4	BMA	A	908	11/12	0.89	0.25	-	39,48,55,56	0
5	NAG	B	914	14/15	0.91	0.15	-	30,38,49,52	0
7	NAG	B	929	14/15	0.94	0.16	-	23,32,39,40	0
6	BMA	B	917	11/12	0.98	0.10	-	24,25,27,30	0
2	MAN	A	904	11/12	0.80	0.15	-	54,63,71,71	0
7	MAN	B	931	11/12	0.77	0.28	-	70,80,84,88	0
2	BMA	A	903	11/12	0.83	0.13	-	40,53,60,60	0
8	BMA	A	933	11/12	0.92	0.13	-	43,49,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BMA	B	911	11/12	0.90	0.13	-	49,53,58,59	0
6	MAN	A	914	11/12	0.97	0.11	-	35,38,43,44	0
12	NAG	B	936	14/15	0.93	0.15	-	29,36,45,45	0
7	NAG	A	925	14/15	0.94	0.15	-	27,33,39,42	0
6	MAN	B	920	11/12	0.99	0.09	-	19,21,24,25	0
6	MAN	B	922	11/12	0.94	0.16	-	36,41,44,44	0
6	MAN	B	919	11/12	0.86	0.15	-	39,49,55,55	0
12	MAN	B	941	11/12	0.93	0.29	-	61,66,71,72	0
12	MAN	B	940	11/12	0.94	0.18	-	39,42,48,50	0
8	NAG	A	932	14/15	0.96	0.17	-	26,35,48,51	0
5	NAG	A	910	14/15	0.96	0.12	-	33,38,50,56	0
8	MAN	A	936	11/12	0.88	0.21	-	50,55,65,70	0
4	NAG	B	926	14/15	0.94	0.10	-	38,40,45,50	0
4	BMA	B	927	11/12	0.89	0.20	-	51,63,70,72	0
7	MAN	A	929	11/12	0.97	0.10	-	26,29,37,43	0
2	MAN	B	912	11/12	0.84	0.23	-	56,69,79,79	0
12	BMA	B	937	11/12	0.93	0.20	-	42,48,58,67	0
7	MAN	B	904	11/12	0.96	0.14	-	38,44,52,56	0
7	MAN	B	907	11/12	0.90	0.16	-	30,38,44,49	0
6	MAN	B	918	11/12	0.96	0.10	-	28,30,33,42	0
7	MAN	B	933	11/12	0.97	0.17	-	30,34,38,47	0
6	BMA	A	913	11/12	0.97	0.10	-	28,33,34,38	0
6	MAN	A	915	11/12	0.94	0.14	-	43,49,59,59	0
7	MAN	A	927	11/12	0.77	0.27	-	60,63,68,68	0
7	BMA	B	903	11/12	0.95	0.10	-	32,35,39,40	0
7	BMA	A	926	11/12	0.91	0.16	-	35,44,50,55	0
7	MAN	B	905	11/12	0.97	0.17	-	39,46,51,59	0
4	BMA	A	923	11/12	0.61	0.36	-	66,80,85,85	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
10	MPD	A	939	8/8	0.93	0.19	7.49	34,42,48,49	0
9	MRD	B	947	8/8	0.90	0.18	6.19	54,59,63,70	0
10	MPD	A	940	8/8	0.86	0.22	5.38	49,58,69,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MRD	B	946	8/8	0.96	0.15	5.24	32,38,42,44	0
9	MRD	B	945	8/8	0.84	0.29	4.87	46,66,73,75	0
3	NAG	B	944	14/15	0.97	0.21	1.63	35,39,42,46	0
11	CTS	B	948	13/13	0.99	0.17	1.09	20,23,27,28	0
9	MRD	A	938	8/8	0.96	0.14	1.00	38,40,42,43	0
3	NAG	A	937	14/15	0.96	0.24	1.00	39,44,47,52	0
11	CTS	A	941	13/13	0.99	0.15	-0.16	24,26,29,29	0
3	NAG	B	908	14/15	0.87	0.23	-	50,64,80,82	0
3	NAG	B	943	14/15	0.90	0.23	-	54,68,84,84	0
3	NAG	A	905	14/15	0.91	0.22	-	55,67,69,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.