



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:06 AM GMT

PDB ID : 4IIC
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus* in complex with isofagomine
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on : 2012-12-20
Resolution : 1.90 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

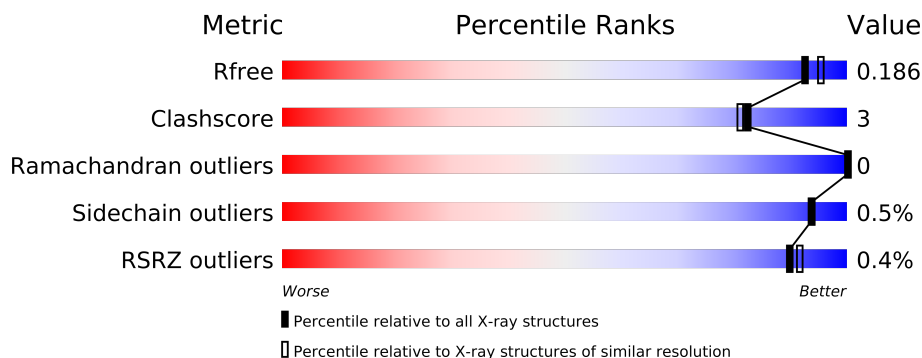
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	841	
1	B	841	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	NA	B	949	-	X
3	NAG	A	906	-	X
3	NAG	B	908	-	X
3	NAG	B	944	-	X
3	NAG	B	945	-	X
8	MRD	A	941	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
8	MRD	B	946	-	X
8	MRD	B	947	-	X
8	MRD	B	948	-	X
9	MPD	A	942	-	X

2 Entry composition i

There are 14 unique types of molecules in this entry. The entry contains 15282 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

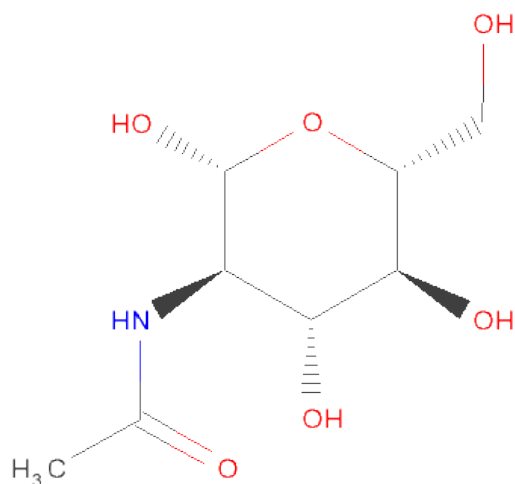
- Molecule 1 is a protein called Beta-glucosidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6382	4028	1096	1240	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 (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			61	34	2	25		

- 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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		
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		

- 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).

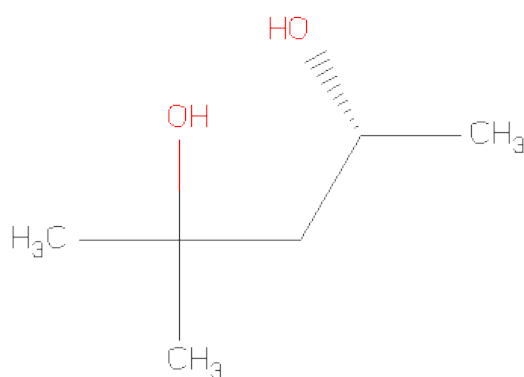
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	7	Total	C	N	O	0	0
			83	46	2	35		
7	A	7	Total	C	N	O	0	0
			83	46	2	35		

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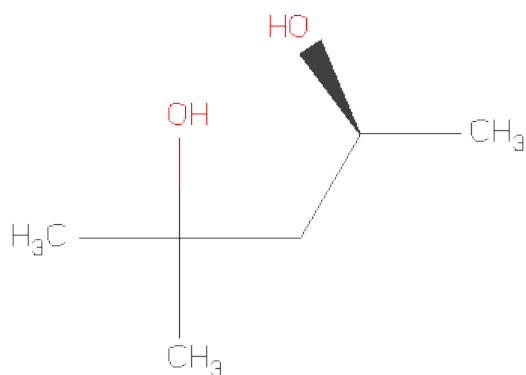
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	7	Total	C	N	O	0	0
			83	46	2	35		
7	B	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 8 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



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

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

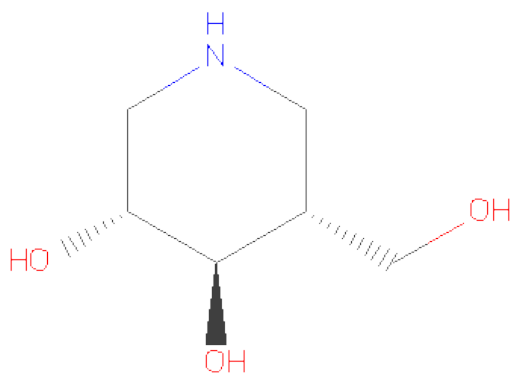


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Na	0	0
			1	1		
10	A	1	Total	Na	0	0
			1	1		

- Molecule 11 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (three-letter code: IFM) (formula: C₆H₁₃NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			10	6	1	3		
11	B	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 12 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 13 is a polymer of unknown type called SUGAR (8-MER).

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

- Molecule 14 is water.

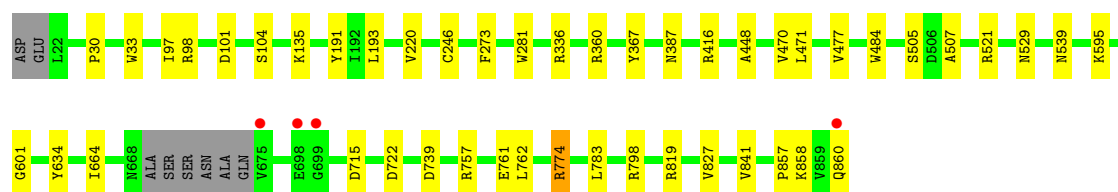
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	671	Total	O	0	0
			671	671		
14	B	761	Total	O	0	0
			761	761		

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 ($RSRZ > 2$). 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

Chain A: 



• Molecule 1: Beta-glucosidase 1

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.14Å 122.48Å 222.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.23 – 1.90 37.23 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.23-1.90) 99.7 (37.23-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.145 , 0.184 0.147 , 0.186	Depositor DCC
R_{free} test set	8816 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 176093 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15282	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, BMA, NAG, NA, MRD, IFM, 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	1.27	8/6545 (0.1%)	1.07	13/8923 (0.1%)
1	B	1.36	13/6538 (0.2%)	1.13	25/8913 (0.3%)
All	All	1.32	21/13083 (0.2%)	1.10	38/17836 (0.2%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	541	CYS	CA-CB	9.60	1.75	1.53
1	B	122	TYR	CE1-CZ	7.42	1.48	1.38
1	B	646	TYR	CG-CD1	6.77	1.48	1.39
1	A	33	TRP	CE3-CZ3	6.75	1.50	1.38
1	B	761	GLU	CD-OE2	-5.68	1.19	1.25

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	ARG	NE-CZ-NH2	-12.94	113.83	120.30
1	B	702	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	B	541	CYS	N-CA-CB	9.41	127.53	110.60
1	A	757	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	B	722	ASP	CB-CG-OD1	8.13	125.61	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts i

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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6382	0	6092	24	0
1	B	6375	0	6082	34	0
2	A	61	0	52	1	0
3	A	28	0	26	0	0
3	B	42	0	39	0	0
4	A	78	0	68	1	0
4	B	78	0	68	0	0
5	A	28	0	25	0	0
6	A	116	0	96	0	0
6	B	116	0	96	0	0
7	A	166	0	139	2	0
7	B	166	0	140	2	0
8	A	16	0	28	7	0
8	B	24	0	42	8	0
9	A	8	0	14	9	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	10	0	13	0	0
11	B	10	0	13	0	0
12	B	50	0	43	1	0
13	B	94	0	77	6	0
14	A	671	0	0	6	0
14	B	761	0	0	14	0
All	All	15282	0	13153	84	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

The worst 5 of 84 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:541:CYS:CA	1:B:541:CYS:CB	1.75	1.64
9:A:942:MPD:C1	9:A:942:MPD:H52	1.66	1.23
9:A:942:MPD:H52	9:A:942:MPD:H11	1.08	1.05
1:B:678:GLU:HG2	14:B:1593:HOH:O	1.59	1.02
9:A:942:MPD:C1	9:A:942:MPD:C5	2.33	1.01

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	829/841 (99%)	801 (97%)	28 (3%)	0	100	100
1	B	828/841 (98%)	806 (97%)	22 (3%)	0	100	100
All	All	1657/1682 (98%)	1607 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	671/677 (99%)	668 (100%)	3 (0%)	95	95
1	B	670/677 (99%)	666 (99%)	4 (1%)	92	92
All	All	1341/1354 (99%)	1334 (100%)	7 (0%)	94	94

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	281	TRP
1	B	860	GLN
1	B	449	TRP
1	A	774	ARG
1	B	700	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

79 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	12,14,15	1.02	0	15,19,21	1.67	2 (13%)
2	NAG	A	902	2	12,14,15	0.84	0	15,19,21	2.31	7 (46%)
2	BMA	A	903	2	10,11,12	1.26	1 (10%)	11,15,17	2.48	5 (45%)
2	MAN	A	904	2	10,11,12	1.02	1 (10%)	11,15,17	2.41	6 (54%)
2	MAN	A	905	2	10,11,12	0.93	0	11,15,17	1.93	3 (27%)
4	NAG	A	907	1,4	12,14,15	1.10	0	15,19,21	2.04	4 (26%)
4	NAG	A	908	4	12,14,15	1.34	1 (8%)	15,19,21	1.46	3 (20%)
4	BMA	A	909	4	10,11,12	1.02	0	11,15,17	4.19	6 (54%)
5	NAG	A	910	1,5	12,14,15	0.80	0	15,19,21	1.66	3 (20%)
5	NAG	A	911	5	12,14,15	1.04	1 (8%)	15,19,21	2.44	4 (26%)
6	NAG	A	912	1,6	12,14,15	1.56	2 (16%)	15,19,21	1.32	2 (13%)
6	NAG	A	913	6	12,14,15	1.05	0	15,19,21	1.36	3 (20%)
6	BMA	A	914	6	10,11,12	0.94	0	11,15,17	1.79	2 (18%)
6	MAN	A	915	6	10,11,12	1.23	1 (10%)	11,15,17	1.75	4 (36%)
6	MAN	A	916	6	10,11,12	0.94	1 (10%)	11,15,17	1.94	4 (36%)
6	MAN	A	917	6	10,11,12	0.67	0	11,15,17	1.63	2 (18%)
6	MAN	A	918	6	10,11,12	1.16	1 (10%)	11,15,17	1.55	2 (18%)
6	MAN	A	919	6	10,11,12	0.95	1 (10%)	11,15,17	1.88	4 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	A	920	6	10,11,12	0.60	0	11,15,17	1.83	2 (18%)
6	MAN	A	921	6	10,11,12	0.64	0	11,15,17	2.78	2 (18%)
4	NAG	A	922	1,4	12,14,15	0.75	0	15,19,21	1.76	4 (26%)
4	NAG	A	923	4	12,14,15	0.77	0	15,19,21	1.75	2 (13%)
4	BMA	A	924	4	10,11,12	0.96	0	11,15,17	2.07	4 (36%)
7	NAG	A	925	1,7	12,14,15	1.14	1 (8%)	15,19,21	2.57	2 (13%)
7	NAG	A	926	7	12,14,15	1.03	1 (8%)	15,19,21	1.86	5 (33%)
7	BMA	A	927	7	10,11,12	0.90	0	11,15,17	1.77	2 (18%)
7	MAN	A	928	7	10,11,12	0.68	0	11,15,17	1.78	5 (45%)
7	MAN	A	929	7	10,11,12	0.75	0	11,15,17	1.82	5 (45%)
7	MAN	A	930	7	10,11,12	0.96	1 (10%)	11,15,17	1.79	4 (36%)
7	MAN	A	931	7	10,11,12	1.09	1 (10%)	11,15,17	1.63	1 (9%)
7	NAG	A	932	1,10,7	12,14,15	1.07	0	15,19,21	1.61	4 (26%)
7	NAG	A	933	7	12,14,15	0.92	1 (8%)	15,19,21	1.30	2 (13%)
7	BMA	A	934	7	10,11,12	0.98	1 (10%)	11,15,17	2.12	4 (36%)
7	MAN	A	935	7	10,11,12	0.99	0	11,15,17	3.47	2 (18%)
7	MAN	A	936	7	10,11,12	0.87	0	11,15,17	2.39	5 (45%)
7	MAN	A	937	7	10,11,12	0.55	0	11,15,17	2.49	5 (45%)
7	MAN	A	938	7	10,11,12	0.70	0	11,15,17	2.07	2 (18%)
7	NAG	B	901	1,7	12,14,15	1.06	1 (8%)	15,19,21	2.22	5 (33%)
7	NAG	B	902	7	12,14,15	1.09	1 (8%)	15,19,21	1.91	4 (26%)
7	BMA	B	903	7	10,11,12	1.23	1 (10%)	11,15,17	2.57	4 (36%)
7	MAN	B	904	7	10,11,12	0.57	0	11,15,17	2.84	6 (54%)
7	MAN	B	905	7	10,11,12	0.69	0	11,15,17	1.95	1 (9%)
7	MAN	B	906	7	10,11,12	0.69	0	11,15,17	1.67	2 (18%)
7	MAN	B	907	7	10,11,12	0.53	0	11,15,17	2.30	4 (36%)
12	NAG	B	909	1,12	12,14,15	1.25	1 (8%)	15,19,21	2.04	5 (33%)
12	NAG	B	910	12	12,14,15	1.59	3 (25%)	15,19,21	1.45	3 (20%)
12	BMA	B	911	12	10,11,12	0.67	0	11,15,17	1.64	2 (18%)
12	MAN	B	912	12	10,11,12	1.07	1 (10%)	11,15,17	3.01	5 (45%)
4	NAG	B	913	1,4	12,14,15	1.17	1 (8%)	15,19,21	2.10	5 (33%)
4	NAG	B	914	4	12,14,15	0.59	0	15,19,21	1.93	5 (33%)
4	BMA	B	915	4	10,11,12	0.75	0	11,15,17	2.30	4 (36%)
6	NAG	B	916	1,6	12,14,15	1.22	1 (8%)	15,19,21	1.97	3 (20%)
6	NAG	B	917	6	12,14,15	1.25	1 (8%)	15,19,21	1.36	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	B	918	6	10,11,12	1.21	1 (10%)	11,15,17	2.57	2 (18%)
6	MAN	B	919	6	10,11,12	1.00	0	11,15,17	1.77	3 (27%)
6	MAN	B	920	6	10,11,12	1.16	1 (10%)	11,15,17	1.95	4 (36%)
6	MAN	B	921	6	10,11,12	1.00	1 (10%)	11,15,17	2.11	5 (45%)
6	MAN	B	922	6	10,11,12	0.52	0	11,15,17	2.00	3 (27%)
6	MAN	B	923	6	10,11,12	0.77	0	11,15,17	2.41	1 (9%)
6	MAN	B	924	6	10,11,12	1.20	2 (20%)	11,15,17	2.61	6 (54%)
6	MAN	B	925	6	10,11,12	0.97	0	11,15,17	2.48	2 (18%)
4	NAG	B	926	1,4	12,14,15	0.62	0	15,19,21	1.12	2 (13%)
4	NAG	B	927	4	12,14,15	0.91	0	15,19,21	1.38	2 (13%)
4	BMA	B	928	4	10,11,12	0.70	0	11,15,17	2.88	4 (36%)
7	NAG	B	929	1,7	12,14,15	0.91	0	15,19,21	2.07	4 (26%)
7	NAG	B	930	7	12,14,15	1.36	2 (16%)	15,19,21	2.12	6 (40%)
7	BMA	B	931	7	10,11,12	0.87	0	11,15,17	1.51	2 (18%)
7	MAN	B	932	7	10,11,12	0.79	0	11,15,17	2.04	3 (27%)
7	MAN	B	933	7	10,11,12	1.11	1 (10%)	11,15,17	1.87	5 (45%)
7	MAN	B	934	7	10,11,12	0.82	0	11,15,17	2.24	4 (36%)
7	MAN	B	935	7	10,11,12	0.61	0	11,15,17	1.59	3 (27%)
13	NAG	B	936	1,10,13	12,14,15	1.27	1 (8%)	15,19,21	1.70	2 (13%)
13	NAG	B	937	13	12,14,15	0.80	0	15,19,21	1.45	3 (20%)
13	BMA	B	938	13	10,11,12	0.90	0	11,15,17	3.73	6 (54%)
13	MAN	B	939	13	10,11,12	0.87	1 (10%)	11,15,17	2.43	3 (27%)
13	MAN	B	940	13	10,11,12	0.91	0	11,15,17	1.49	2 (18%)
13	MAN	B	941	13	10,11,12	0.88	0	11,15,17	2.98	7 (63%)
13	MAN	B	942	13	10,11,12	0.96	0	11,15,17	3.26	5 (45%)
13	MAN	B	943	13	10,11,12	0.91	0	11,15,17	2.75	3 (27%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	A	905	2	-	0/2/19/22	0/1/1/1
4	NAG	A	907	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	908	4	-	0/6/23/26	0/1/1/1
4	BMA	A	909	4	-	0/2/19/22	0/1/1/1
5	NAG	A	910	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	911	5	-	0/6/23/26	0/1/1/1
6	NAG	A	912	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	913	6	-	0/6/23/26	0/1/1/1
6	BMA	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
6	MAN	A	921	6	-	0/2/19/22	0/1/1/1
4	NAG	A	922	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	923	4	-	0/6/23/26	0/1/1/1
4	BMA	A	924	4	-	0/2/19/22	0/1/1/1
7	NAG	A	925	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	926	7	-	0/6/23/26	0/1/1/1
7	BMA	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
7	MAN	A	931	7	-	0/2/19/22	0/1/1/1
7	NAG	A	932	1,10,7	-	0/6/23/26	0/1/1/1
7	NAG	A	933	7	-	0/6/23/26	0/1/1/1
7	BMA	A	934	7	-	0/2/19/22	0/1/1/1
7	MAN	A	935	7	-	0/2/19/22	0/1/1/1
7	MAN	A	936	7	-	0/2/19/22	0/1/1/1
7	MAN	A	937	7	-	0/2/19/22	0/1/1/1
7	MAN	A	938	7	-	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
12	NAG	B	909	1,12	-	0/6/23/26	0/1/1/1
12	NAG	B	910	12	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BMA	B	911	12	-	0/2/19/22	0/1/1/1
12	MAN	B	912	12	-	0/2/19/22	0/1/1/1
4	NAG	B	913	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	914	4	-	0/6/23/26	0/1/1/1
4	BMA	B	915	4	-	0/2/19/22	0/1/1/1
6	NAG	B	916	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	917	6	-	0/6/23/26	0/1/1/1
6	BMA	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
6	MAN	B	925	6	-	0/2/19/22	0/1/1/1
4	NAG	B	926	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	927	4	-	0/6/23/26	0/1/1/1
4	BMA	B	928	4	-	0/2/19/22	0/1/1/1
7	NAG	B	929	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	930	7	-	0/6/23/26	0/1/1/1
7	BMA	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
7	MAN	B	935	7	-	0/2/19/22	0/1/1/1
13	NAG	B	936	1,10,13	-	0/6/23/26	0/1/1/1
13	NAG	B	937	13	-	0/6/23/26	0/1/1/1
13	BMA	B	938	13	-	0/2/19/22	0/1/1/1
13	MAN	B	939	13	-	0/2/19/22	0/1/1/1
13	MAN	B	940	13	-	0/2/19/22	0/1/1/1
13	MAN	B	941	13	-	0/2/19/22	0/1/1/1
13	MAN	B	942	13	-	0/2/19/22	0/1/1/1
13	MAN	B	943	13	-	0/2/19/22	0/1/1/1

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	910	NAG	C3-C2	3.27	1.59	1.52
13	B	936	NAG	O7-C7	3.11	1.30	1.23
12	B	909	NAG	O5-C5	-3.08	1.39	1.45
6	A	912	NAG	C2-N2	3.07	1.49	1.46
6	B	916	NAG	C2-N2	2.95	1.49	1.46

The worst 5 of 280 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	935	MAN	O5-C5-C6	10.55	118.05	106.98
4	A	909	BMA	O5-C5-C6	10.24	117.72	106.98
7	A	925	NAG	C3-C2-N2	-8.27	99.16	111.76
13	B	942	MAN	O5-C5-C6	8.15	115.53	106.98
12	B	912	MAN	O5-C5-C6	8.08	115.46	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	906	1	12,14,15	0.74	0	15,19,21	1.52	1 (6%)
3	NAG	A	939	1	12,14,15	1.15	2 (16%)	15,19,21	2.28	6 (40%)
8	MRD	A	940	-	7,7,7	1.15	0	10,10,10	0.39	0
8	MRD	A	941	-	7,7,7	1.23	0	10,10,10	1.31	3 (30%)
9	MPD	A	942	-	7,7,7	0.68	0	10,10,10	1.04	0
11	IFM	A	944	-	10,10,10	3.06	5 (50%)	13,13,13	2.24	2 (15%)
3	NAG	B	908	1	12,14,15	0.53	0	15,19,21	3.07	7 (46%)
3	NAG	B	944	1	12,14,15	0.88	0	15,19,21	2.04	5 (33%)
3	NAG	B	945	1	12,14,15	1.00	0	15,19,21	2.14	3 (20%)
8	MRD	B	946	-	7,7,7	1.15	0	10,10,10	0.50	0
8	MRD	B	947	-	7,7,7	1.02	1 (14%)	10,10,10	1.33	1 (10%)
8	MRD	B	948	-	7,7,7	0.99	1 (14%)	10,10,10	0.51	0
11	IFM	B	950	-	10,10,10	2.55	4 (40%)	13,13,13	1.57	3 (23%)

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	906	1	-	0/6/23/26	0/1/1/1
3	NAG	A	939	1	-	0/6/23/26	0/1/1/1
8	MRD	A	940	-	-	0/5/5/5	0/0/0/0
8	MRD	A	941	-	-	0/5/5/5	0/0/0/0
9	MPD	A	942	-	-	0/5/5/5	0/0/0/0
11	IFM	A	944	-	-	0/2/16/16	0/1/1/1
3	NAG	B	908	1	-	0/6/23/26	0/1/1/1
3	NAG	B	944	1	-	0/6/23/26	0/1/1/1
3	NAG	B	945	1	-	0/6/23/26	0/1/1/1
8	MRD	B	946	-	-	0/5/5/5	0/0/0/0
8	MRD	B	947	-	-	0/5/5/5	0/0/0/0
8	MRD	B	948	-	-	0/5/5/5	0/0/0/0
11	IFM	B	950	-	-	0/2/16/16	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	944	IFM	C2-C3	5.91	1.59	1.52
11	A	944	IFM	C5-C4	5.66	1.60	1.53
11	B	950	IFM	C1-C5	4.95	1.58	1.52
11	B	950	IFM	C2-C3	4.24	1.57	1.52
11	A	944	IFM	C1-N	3.07	1.53	1.46

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	908	NAG	O5-C5-C6	7.51	114.86	106.98
11	A	944	IFM	C5-C4-C3	-6.14	104.99	112.80
3	B	908	NAG	C8-C7-N2	5.19	126.26	116.11
3	A	939	NAG	O5-C5-C4	-4.89	104.45	110.65
3	B	945	NAG	O5-C5-C4	-4.72	104.67	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	833/841 (99%)	-0.36	4 (0%) 88 90	10, 17, 30, 53	0
1	B	832/841 (98%)	-0.48	3 (0%) 90 91	9, 14, 26, 53	0
All	All	1665/1682 (98%)	-0.42	7 (0%) 90 91	9, 15, 29, 53	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	860	GLN	2.6
1	A	699	GLY	2.3
1	B	698	GLU	2.2
1	A	698	GLU	2.1
1	A	675	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	BMA	A	924	11/12	0.31	62.50	41,51,62,72	0
7	MAN	A	938	11/12	0.24	47.57	50,55,60,72	0
13	MAN	B	942	11/12	0.27	18.14	47,52,60,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MAN	A	937	11/12	0.25	14.85	40,51,55,66	0
13	MAN	B	943	11/12	0.25	13.56	42,50,57,62	0
12	BMA	B	911	11/12	0.18	12.83	32,38,48,49	0
7	MAN	A	929	11/12	0.13	10.17	24,26,38,39	0
2	MAN	A	905	11/12	0.17	9.83	41,50,56,62	0
7	MAN	A	931	11/12	0.15	9.01	18,22,33,38	0
7	MAN	A	930	11/12	0.14	8.84	19,22,34,37	0
4	BMA	B	928	11/12	0.20	5.55	35,42,55,67	0
13	MAN	B	941	11/12	0.13	5.34	24,31,35,42	0
7	NAG	A	925	14/15	0.08	4.19	15,18,39,42	0
4	BMA	A	909	11/12	0.21	4.08	34,42,51,57	0
4	NAG	A	908	14/15	0.16	3.08	23,27,34,37	0
7	NAG	A	926	14/15	0.10	3.03	17,23,28,34	0
7	MAN	A	936	11/12	0.10	2.90	24,31,40,43	0
13	MAN	B	940	11/12	0.16	2.78	27,31,39,42	0
4	NAG	B	926	14/15	0.08	2.60	18,23,32,33	0
12	NAG	B	910	14/15	0.10	2.58	17,23,31,31	0
7	MAN	B	935	11/12	0.11	2.49	18,22,29,32	0
7	NAG	B	929	14/15	0.10	2.19	16,20,39,43	0
5	NAG	A	911	14/15	0.11	2.12	25,30,47,49	0
7	NAG	B	930	14/15	0.12	2.03	18,23,32,33	0
7	MAN	B	933	11/12	0.13	1.96	23,28,38,43	0
7	MAN	B	934	11/12	0.11	1.87	21,23,29,34	0
4	NAG	B	914	14/15	0.10	1.71	18,23,42,43	0
7	MAN	B	906	11/12	0.11	1.47	22,26,29,37	0
4	NAG	A	922	14/15	0.08	1.46	19,25,35,38	0
7	MAN	B	907	11/12	0.12	1.45	22,29,34,34	0
7	MAN	A	935	11/12	0.10	1.41	22,29,39,50	0
4	NAG	A	907	14/15	0.10	0.78	17,20,22,24	0
6	MAN	B	925	11/12	0.07	0.67	16,17,19,21	0
12	NAG	B	909	14/15	0.08	0.57	16,18,20,21	0
7	MAN	B	905	11/12	0.10	0.14	23,30,37,47	0
6	MAN	A	915	11/12	0.10	-0.16	24,25,32,33	0
6	MAN	A	919	11/12	0.09	-0.19	18,20,21,22	0
7	NAG	A	932	14/15	0.06	-0.37	17,20,23,24	0
6	NAG	B	916	14/15	0.06	-0.46	12,14,19,22	0
6	NAG	B	917	14/15	0.06	-0.61	12,15,15,16	0
2	NAG	A	901	14/15	0.07	-0.63	16,19,21,23	0
13	NAG	B	936	14/15	0.06	-0.66	15,18,21,22	0
2	NAG	A	902	14/15	0.08	-0.75	20,28,38,42	0
6	MAN	A	920	11/12	0.07	-0.79	20,24,30,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MAN	B	922	11/12	0.07	-0.85	18,21,22,33	0
6	MAN	B	919	11/12	0.06	-0.85	18,20,24,26	0
6	MAN	A	918	11/12	0.06	-0.90	16,18,21,22	0
6	NAG	A	912	14/15	0.07	-0.93	20,23,26,29	0
7	NAG	B	901	14/15	0.06	-0.96	12,14,17,18	0
6	NAG	A	913	14/15	0.07	-0.99	17,19,20,22	0
4	NAG	B	913	14/15	0.06	-0.99	14,16,19,19	0
7	NAG	B	902	14/15	0.06	-1.03	14,16,20,28	0
6	MAN	B	924	11/12	0.06	-1.03	13,14,16,16	0
6	BMA	B	918	11/12	0.05	-1.13	14,16,18,18	0
5	NAG	A	910	14/15	0.07	-1.18	16,19,23,25	0
6	MAN	B	921	11/12	0.05	-1.86	14,15,15,16	0
6	MAN	A	917	11/12	0.06	-1.99	17,20,22,23	0
6	BMA	A	914	11/12	0.08	-2.42	19,21,26,27	0
7	BMA	A	927	11/12	0.15	-	21,25,32,43	0
13	NAG	B	937	14/15	0.10	-	24,29,35,36	0
12	MAN	B	912	11/12	0.30	-	53,60,64,65	0
2	BMA	A	903	11/12	0.16	-	33,46,53,57	0
4	BMA	B	915	11/12	0.34	-	56,73,91,97	0
4	NAG	A	923	14/15	0.20	-	36,43,52,56	0
7	MAN	A	928	11/12	0.30	-	52,62,64,67	0
6	MAN	B	923	11/12	0.12	-	25,28,34,35	0
7	BMA	A	934	11/12	0.17	-	30,37,47,51	0
2	MAN	A	904	11/12	0.27	-	60,74,81,87	0
7	BMA	B	903	11/12	0.10	-	19,21,22,24	0
4	NAG	B	927	14/15	0.13	-	24,29,41,41	0
7	NAG	A	933	14/15	0.11	-	22,27,32,37	0
13	MAN	B	939	11/12	0.25	-	59,67,77,86	0
6	MAN	B	920	11/12	0.12	-	27,36,41,43	0
7	BMA	B	931	11/12	0.16	-	24,28,34,45	0
7	MAN	B	904	11/12	0.15	-	24,31,40,41	0
6	MAN	A	921	11/12	0.16	-	27,29,34,40	0
7	MAN	B	932	11/12	0.33	-	58,63,67,71	0
13	BMA	B	938	11/12	0.16	-	35,38,46,58	0
6	MAN	A	916	11/12	0.15	-	31,37,44,57	0

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, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	908	14/15	0.31	33.73	39,48,52,53	0
8	MRD	A	941	8/8	0.17	10.96	18,30,41,43	0
3	NAG	A	906	14/15	0.35	9.81	42,52,57,58	0
8	MRD	B	948	8/8	0.16	7.34	32,41,42,43	0
3	NAG	B	944	14/15	0.26	6.56	36,50,55,59	0
8	MRD	B	946	8/8	0.20	4.57	19,32,40,43	0
9	MPD	A	942	8/8	0.21	3.96	37,39,45,48	0
10	NA	B	949	1/1	0.23	3.67	29,29,29,29	0
8	MRD	B	947	8/8	0.10	3.56	20,25,37,37	0
3	NAG	B	945	14/15	0.15	2.54	26,29,33,34	0
10	NA	A	943	1/1	0.14	1.00	26,26,26,26	0
3	NAG	A	939	14/15	0.12	0.74	35,38,42,46	0
11	IFM	A	944	10/10	0.15	0.66	12,13,14,15	0
11	IFM	B	950	10/10	0.11	0.40	10,11,11,11	0
8	MRD	A	940	8/8	0.07	0.11	20,22,25,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.