



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:29 PM GMT

PDB ID : 4IIH
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus* in complex with thiocellobiose
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on : 2012-12-20
Resolution : 2.00 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 ⓘ symbol.

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

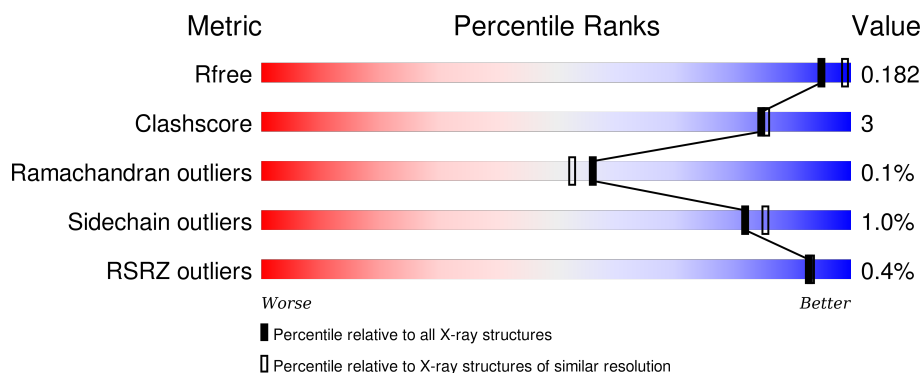
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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	
1	B	841	

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	MAN	B	942	-	-	-	X
2	MAN	A	906	-	-	-	X
2	NAG	A	927	-	-	-	X
2	MAN	A	933	-	-	-	X
2	MAN	A	937	-	-	-	X
2	MAN	A	938	-	-	-	X
2	MAN	B	906	-	-	-	X
2	MAN	B	937	-	-	-	X
3	NAG	B	947	-	-	-	X
4	NAG	A	910	-	-	-	X
7	MRD	A	943	-	-	X	X
7	MRD	B	948	-	-	-	X
7	MRD	B	949	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15509 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
			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 (7-MER).

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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		
4	B	3	Total	C	N	O	0	0
			39	22	2	15		

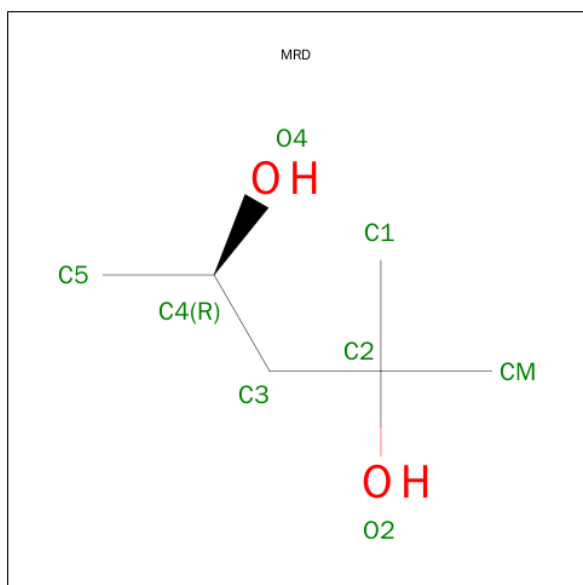
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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).

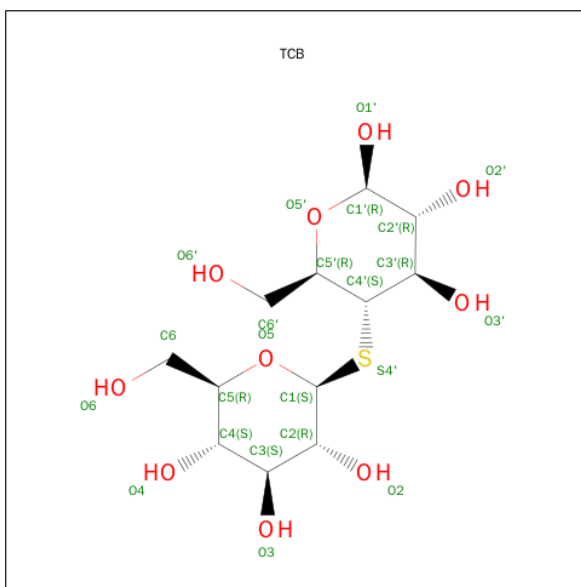
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	10	Total	C	N	O	0	0
			116	64	2	50		
6	B	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



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

- Molecule 8 is SUGAR (THIOCELLOBIOSE) (three-letter code: TCB) (formula: $C_{12}H_{22}O_{10}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	S	0	0
			23	12	10	1		
8	B	1	Total	C	O	S	0	0
			23	12	10	1		

- Molecule 9 is a polymer of unknown type called SUGAR (6-MER).

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

- Molecule 10 is a polymer of unknown type called SUGAR (8-MER).

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

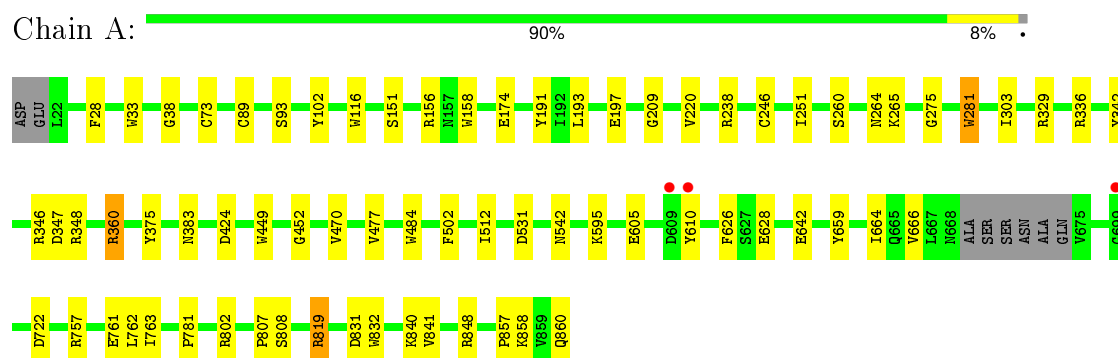
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	748	Total	O	0	0
			748	748		
11	B	859	Total	O	0	0
			859	859		

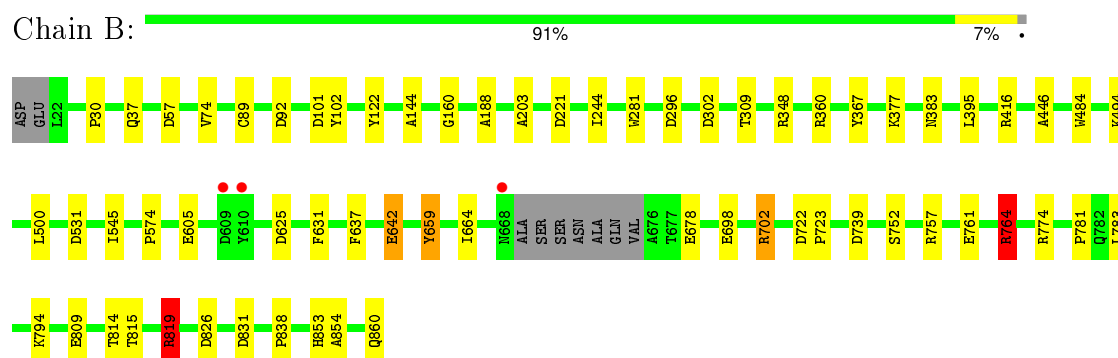
3 Residue-property plots

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



• 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, α , β , γ	82.08Å 122.39Å 221.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.07 – 2.00 41.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.07-2.00) 99.6 (41.07-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.140 , 0.181 0.141 , 0.182	Depositor DCC
R_{free} test set	7569 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 150300 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15509	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, BMA, TCB, NAG, 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	1.29	11/6545 (0.2%)	1.07	18/8923 (0.2%)
1	B	1.35	10/6538 (0.2%)	1.11	24/8913 (0.3%)
All	All	1.32	21/13083 (0.2%)	1.09	42/17836 (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	642	GLU	CD-OE1	8.91	1.35	1.25
1	B	761	GLU	CD-OE2	-7.47	1.17	1.25
1	A	281	TRP	CB-CG	7.21	1.63	1.50
1	A	761	GLU	CD-OE2	-6.17	1.18	1.25
1	B	605	GLU	CG-CD	6.00	1.60	1.51

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	B	702	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	757	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	B	757	ARG	NE-CZ-NH1	-9.23	115.69	120.30
1	B	774	ARG	NE-CZ-NH2	-9.10	115.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	6382	0	6092	31	0
1	B	6375	0	6082	32	0
2	A	249	0	210	2	0
2	B	166	0	139	4	0
3	A	28	0	26	0	0
3	B	42	0	39	0	0
4	A	78	0	67	2	0
4	B	78	0	68	0	0
5	A	28	0	25	3	0
6	A	116	0	96	0	0
6	B	116	0	97	0	0
7	A	16	0	28	9	0
7	B	16	0	28	4	0
8	A	23	0	22	0	0
8	B	23	0	22	4	0
9	B	72	0	61	0	0
10	B	94	0	79	4	0
11	A	748	0	0	3	0
11	B	859	0	0	11	0
All	All	15509	0	13181	79	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 3.

The worst 5 of 79 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:A:819:ARG:HH12	1:A:860:GLN:C	1.51	1.12
1:B:815:THR:HG22	11:B:1525:HOH:O	1.70	0.89
1:A:819:ARG:NH1	1:A:860:GLN:C	2.31	0.84
7:A:942:MRD:H5C2	11:A:1191:HOH:O	1.77	0.84
5:A:913:NAG:H83	5:A:913:NAG:H3	1.63	0.81

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%)	803 (97%)	25 (3%)	1 (0%)	56	53
1	B	828/841 (98%)	804 (97%)	24 (3%)	0	100	100
All	All	1657/1682 (98%)	1607 (97%)	49 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	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	671/677 (99%)	667 (99%)	4 (1%)	90	93
1	B	670/677 (99%)	660 (98%)	10 (2%)	72	75
All	All	1341/1354 (99%)	1327 (99%)	14 (1%)	82	85

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	281	TRP
1	B	302	ASP
1	B	764	ARG
1	B	92	ASP
1	B	698	GLU

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

83 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	1.17	2 (14%)	15,19,21	1.15	1 (6%)
2	NAG	A	902	2	14,14,15	1.11	1 (7%)	15,19,21	1.35	2 (13%)
2	BMA	A	903	2	11,11,12	0.71	0	14,15,17	2.01	3 (21%)
2	MAN	A	904	2	11,11,12	0.96	1 (9%)	14,15,17	2.55	8 (57%)
2	MAN	A	905	2	11,11,12	0.87	0	14,15,17	2.17	5 (35%)
2	MAN	A	906	2	11,11,12	1.01	0	14,15,17	2.13	6 (42%)
2	MAN	A	907	2	11,11,12	0.85	0	14,15,17	1.07	1 (7%)
4	NAG	A	909	1,4	14,14,15	1.02	0	15,19,21	1.22	2 (13%)
4	NAG	A	910	4	14,14,15	1.41	2 (14%)	15,19,21	1.93	6 (40%)
4	BMA	A	911	4	11,11,12	1.24	0	14,15,17	2.87	7 (50%)
5	NAG	A	912	1,5	14,14,15	1.27	2 (14%)	15,19,21	1.86	3 (20%)
5	NAG	A	913	5	14,14,15	1.08	2 (14%)	15,19,21	1.78	6 (40%)
6	NAG	A	914	1,6	14,14,15	1.45	3 (21%)	15,19,21	1.22	1 (6%)
6	NAG	A	915	6	14,14,15	1.02	0	15,19,21	1.60	3 (20%)
6	BMA	A	916	6	11,11,12	0.65	0	14,15,17	1.38	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	A	917	6	11,11,12	1.56	4 (36%)	14,15,17	1.96	5 (35%)
6	MAN	A	918	6	11,11,12	1.23	1 (9%)	14,15,17	2.49	6 (42%)
6	MAN	A	919	6	11,11,12	0.83	1 (9%)	14,15,17	1.10	2 (14%)
6	MAN	A	920	6	11,11,12	1.41	3 (27%)	14,15,17	1.58	2 (14%)
6	MAN	A	921	6	11,11,12	0.88	0	14,15,17	1.04	1 (7%)
6	MAN	A	922	6	11,11,12	1.30	2 (18%)	14,15,17	1.30	3 (21%)
6	MAN	A	923	6	11,11,12	0.83	0	14,15,17	1.38	3 (21%)
4	NAG	A	924	1,4	14,14,15	1.01	1 (7%)	15,19,21	1.69	3 (20%)
4	NAG	A	925	4	14,14,15	0.80	0	15,19,21	1.75	2 (13%)
4	BMA	A	926	4	11,11,12	1.28	2 (18%)	14,15,17	2.03	5 (35%)
2	NAG	A	927	1,2	14,14,15	1.09	1 (7%)	15,19,21	1.70	3 (20%)
2	NAG	A	928	2	14,14,15	0.78	0	15,19,21	1.51	3 (20%)
2	BMA	A	929	2	11,11,12	1.35	1 (9%)	14,15,17	1.84	4 (28%)
2	MAN	A	930	2	11,11,12	0.82	0	14,15,17	1.72	4 (28%)
2	MAN	A	931	2	11,11,12	0.65	0	14,15,17	1.55	1 (7%)
2	MAN	A	932	2	11,11,12	0.81	0	14,15,17	2.28	6 (42%)
2	MAN	A	933	2	11,11,12	1.57	1 (9%)	14,15,17	1.67	3 (21%)
2	NAG	A	934	1,2	14,14,15	0.99	0	15,19,21	1.15	2 (13%)
2	NAG	A	935	2	14,14,15	1.29	2 (14%)	15,19,21	1.08	1 (6%)
2	BMA	A	936	2	11,11,12	1.44	1 (9%)	14,15,17	1.90	3 (21%)
2	MAN	A	937	2	11,11,12	1.18	0	14,15,17	1.23	1 (7%)
2	MAN	A	938	2	11,11,12	1.23	0	14,15,17	2.39	6 (42%)
2	MAN	A	939	2	11,11,12	1.00	1 (9%)	14,15,17	1.90	4 (28%)
2	MAN	A	940	2	11,11,12	1.98	2 (18%)	14,15,17	1.26	1 (7%)
2	NAG	B	901	1,2	14,14,15	1.38	3 (21%)	15,19,21	1.89	3 (20%)
2	NAG	B	902	2	14,14,15	0.88	0	15,19,21	2.13	5 (33%)
2	BMA	B	903	2	11,11,12	1.86	2 (18%)	14,15,17	1.80	4 (28%)
2	MAN	B	904	2	11,11,12	0.68	0	14,15,17	1.76	4 (28%)
2	MAN	B	905	2	11,11,12	1.06	1 (9%)	14,15,17	1.13	0
2	MAN	B	906	2	11,11,12	0.87	0	14,15,17	1.41	2 (14%)
2	MAN	B	907	2	11,11,12	0.67	0	14,15,17	1.95	5 (35%)
9	NAG	B	909	1,9	14,14,15	0.88	0	15,19,21	1.50	2 (13%)
9	NAG	B	910	9	14,14,15	1.62	6 (42%)	15,19,21	1.84	6 (40%)
9	BMA	B	911	9	11,11,12	1.13	1 (9%)	14,15,17	2.00	5 (35%)
9	MAN	B	912	9	11,11,12	1.27	1 (9%)	14,15,17	1.39	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	B	913	9	11,11,12	0.82	0	14,15,17	1.68	3 (21%)
9	MAN	B	914	9	11,11,12	0.84	0	14,15,17	2.19	3 (21%)
4	NAG	B	915	1,4	14,14,15	0.85	0	15,19,21	0.93	1 (6%)
4	NAG	B	916	4	14,14,15	0.80	0	15,19,21	1.73	4 (26%)
4	BMA	B	917	4	11,11,12	0.91	0	14,15,17	2.00	5 (35%)
6	NAG	B	918	1,6	14,14,15	1.28	1 (7%)	15,19,21	1.28	1 (6%)
6	NAG	B	919	6	14,14,15	1.53	2 (14%)	15,19,21	1.45	2 (13%)
6	BMA	B	920	6	11,11,12	1.15	1 (9%)	14,15,17	1.28	1 (7%)
6	MAN	B	921	6	11,11,12	0.91	1 (9%)	14,15,17	2.50	6 (42%)
6	MAN	B	922	6	11,11,12	1.12	1 (9%)	14,15,17	2.30	4 (28%)
6	MAN	B	923	6	11,11,12	0.90	0	14,15,17	1.28	2 (14%)
6	MAN	B	924	6	11,11,12	0.93	0	14,15,17	2.11	5 (35%)
6	MAN	B	925	6	11,11,12	1.16	0	14,15,17	1.98	5 (35%)
6	MAN	B	926	6	11,11,12	0.80	0	14,15,17	2.12	4 (28%)
6	MAN	B	927	6	11,11,12	1.16	1 (9%)	14,15,17	1.51	1 (7%)
4	NAG	B	928	1,4	14,14,15	1.14	1 (7%)	15,19,21	1.48	4 (26%)
4	NAG	B	929	4	14,14,15	1.35	3 (21%)	15,19,21	3.15	8 (53%)
4	BMA	B	930	4	11,11,12	1.38	1 (9%)	14,15,17	3.05	8 (57%)
2	NAG	B	931	1,2	14,14,15	1.03	1 (7%)	15,19,21	0.82	0
2	NAG	B	932	2	14,14,15	1.13	1 (7%)	15,19,21	1.65	4 (26%)
2	BMA	B	933	2	11,11,12	1.33	2 (18%)	14,15,17	2.17	4 (28%)
2	MAN	B	934	2	11,11,12	1.26	2 (18%)	14,15,17	2.37	6 (42%)
2	MAN	B	935	2	11,11,12	0.86	0	14,15,17	1.75	5 (35%)
2	MAN	B	936	2	11,11,12	1.21	1 (9%)	14,15,17	1.81	5 (35%)
2	MAN	B	937	2	11,11,12	0.96	0	14,15,17	1.85	6 (42%)
10	NAG	B	938	1,10	14,14,15	0.96	1 (7%)	15,19,21	1.92	3 (20%)
10	NAG	B	939	10	14,14,15	0.79	0	15,19,21	1.00	1 (6%)
10	BMA	B	940	10	11,11,12	1.27	2 (18%)	14,15,17	3.56	6 (42%)
10	MAN	B	941	10	11,11,12	1.09	1 (9%)	14,15,17	2.26	6 (42%)
10	MAN	B	942	10	11,11,12	1.04	1 (9%)	14,15,17	2.13	5 (35%)
10	MAN	B	943	10	11,11,12	1.07	0	14,15,17	1.86	3 (21%)
10	MAN	B	944	10	11,11,12	0.86	0	14,15,17	3.74	8 (57%)
10	MAN	B	945	10	11,11,12	1.02	1 (9%)	14,15,17	2.88	8 (57%)

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
2	MAN	A	905	2	-	0/2/19/22	0/1/1/1
2	MAN	A	906	2	-	0/2/19/22	0/1/1/1
2	MAN	A	907	2	-	0/2/19/22	0/1/1/1
4	NAG	A	909	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	910	4	-	0/6/23/26	0/1/1/1
4	BMA	A	911	4	-	0/2/19/22	0/1/1/1
5	NAG	A	912	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	913	5	-	0/6/23/26	0/1/1/1
6	NAG	A	914	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	915	6	-	0/6/23/26	0/1/1/1
6	BMA	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
6	MAN	A	922	6	-	0/2/19/22	0/1/1/1
6	MAN	A	923	6	-	0/2/19/22	0/1/1/1
4	NAG	A	924	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	925	4	-	0/6/23/26	0/1/1/1
4	BMA	A	926	4	-	0/2/19/22	0/1/1/1
2	NAG	A	927	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	928	2	-	0/6/23/26	0/1/1/1
2	BMA	A	929	2	-	0/2/19/22	0/1/1/1
2	MAN	A	930	2	-	0/2/19/22	0/1/1/1
2	MAN	A	931	2	-	0/2/19/22	0/1/1/1
2	MAN	A	932	2	-	0/2/19/22	0/1/1/1
2	MAN	A	933	2	-	0/2/19/22	0/1/1/1
2	NAG	A	934	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	935	2	-	0/6/23/26	0/1/1/1
2	BMA	A	936	2	-	0/2/19/22	0/1/1/1
2	MAN	A	937	2	-	0/2/19/22	0/1/1/1
2	MAN	A	938	2	-	0/2/19/22	0/1/1/1
2	MAN	A	939	2	-	0/2/19/22	0/1/1/1
2	MAN	A	940	2	-	0/2/19/22	0/1/1/1
2	NAG	B	901	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	902	2	-	0/6/23/26	0/1/1/1
2	BMA	B	903	2	-	0/2/19/22	0/1/1/1
2	MAN	B	904	2	-	0/2/19/22	0/1/1/1
2	MAN	B	905	2	-	0/2/19/22	0/1/1/1
2	MAN	B	906	2	-	0/2/19/22	0/1/1/1
2	MAN	B	907	2	-	0/2/19/22	0/1/1/1
9	NAG	B	909	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	910	9	-	0/6/23/26	0/1/1/1
9	BMA	B	911	9	-	0/2/19/22	0/1/1/1
9	MAN	B	912	9	-	0/2/19/22	0/1/1/1
9	MAN	B	913	9	-	0/2/19/22	0/1/1/1
9	MAN	B	914	9	-	0/2/19/22	0/1/1/1
4	NAG	B	915	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	916	4	-	0/6/23/26	0/1/1/1
4	BMA	B	917	4	-	0/2/19/22	0/1/1/1
6	NAG	B	918	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	919	6	-	0/6/23/26	0/1/1/1
6	BMA	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
6	MAN	B	926	6	-	0/2/19/22	0/1/1/1
6	MAN	B	927	6	-	0/2/19/22	0/1/1/1
4	NAG	B	928	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	929	4	-	0/6/23/26	0/1/1/1
4	BMA	B	930	4	-	0/2/19/22	0/1/1/1
2	NAG	B	931	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	932	2	-	0/6/23/26	0/1/1/1
2	BMA	B	933	2	-	0/2/19/22	0/1/1/1
2	MAN	B	934	2	-	0/2/19/22	0/1/1/1
2	MAN	B	935	2	-	0/2/19/22	0/1/1/1
2	MAN	B	936	2	-	0/2/19/22	0/1/1/1
2	MAN	B	937	2	-	0/2/19/22	0/1/1/1
10	NAG	B	938	1,10	-	0/6/23/26	0/1/1/1
10	NAG	B	939	10	-	0/6/23/26	0/1/1/1
10	BMA	B	940	10	-	0/2/19/22	0/1/1/1
10	MAN	B	941	10	-	0/2/19/22	0/1/1/1
10	MAN	B	942	10	-	0/2/19/22	0/1/1/1
10	MAN	B	943	10	-	0/2/19/22	0/1/1/1
10	MAN	B	944	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	B	945	10	-	0/2/19/22	0/1/1/1

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	940	MAN	O5-C1	-4.90	1.35	1.43
2	A	936	BMA	O5-C1	-3.74	1.37	1.43
2	A	935	NAG	O5-C1	-2.98	1.38	1.43
2	A	927	NAG	O5-C5	-2.84	1.37	1.43
6	A	922	MAN	O3-C3	-2.71	1.36	1.43

The worst 5 of 306 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	929	NAG	C1-O5-C5	-8.67	101.25	112.25
10	B	940	BMA	C6-C5-C4	-7.37	94.84	113.02
2	A	904	MAN	O2-C2-C3	-5.08	99.91	110.12
4	B	930	BMA	O5-C1-C2	-5.01	102.74	110.86
10	B	942	MAN	O2-C2-C1	-4.77	99.65	109.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	903	BMA	1	0
2	A	907	MAN	1	0
4	A	909	NAG	2	0
5	A	913	NAG	3	0
2	A	929	BMA	1	0
2	B	902	NAG	1	0
2	B	933	BMA	3	0
2	B	935	MAN	1	0
10	B	940	BMA	3	0
10	B	942	MAN	2	0
10	B	945	MAN	1	0

5.6 Ligand geometry

11 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	908	1	14,14,15	1.13	1 (7%)	15,19,21	1.02	2 (13%)
3	NAG	A	941	1	14,14,15	0.87	0	15,19,21	2.13	6 (40%)
7	MRD	A	942	-	6,7,7	1.17	1 (16%)	7,10,10	1.02	0
7	MRD	A	943	-	6,7,7	0.82	0	7,10,10	1.05	0
8	TCB	A	944	-	24,24,24	1.82	5 (20%)	28,35,35	1.75	8 (28%)
3	NAG	B	908	1	14,14,15	1.11	2 (14%)	15,19,21	3.34	8 (53%)
3	NAG	B	946	1	14,14,15	1.13	2 (14%)	15,19,21	1.62	2 (13%)
3	NAG	B	947	1	14,14,15	0.84	0	15,19,21	1.12	0
7	MRD	B	948	-	6,7,7	0.52	0	7,10,10	1.05	0
7	MRD	B	949	-	6,7,7	1.10	1 (16%)	7,10,10	0.71	0
8	TCB	B	950	-	24,24,24	2.34	6 (25%)	28,35,35	2.54	10 (35%)

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	908	1	-	0/6/23/26	0/1/1/1
3	NAG	A	941	1	-	0/6/23/26	0/1/1/1
7	MRD	A	942	-	-	0/5/5/5	0/0/0/0
7	MRD	A	943	-	-	0/5/5/5	0/0/0/0
8	TCB	A	944	-	-	0/8/48/48	0/2/2/2
3	NAG	B	908	1	-	0/6/23/26	0/1/1/1
3	NAG	B	946	1	-	0/6/23/26	0/1/1/1
3	NAG	B	947	1	-	0/6/23/26	0/1/1/1
7	MRD	B	948	-	-	0/5/5/5	0/0/0/0
7	MRD	B	949	-	-	0/5/5/5	0/0/0/0
8	TCB	B	950	-	-	0/8/48/48	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	908	NAG	O5-C1	-2.96	1.38	1.43
3	B	908	NAG	O5-C1	-2.78	1.39	1.43
8	A	944	TCB	C3'-C4'	-2.64	1.50	1.53
7	B	949	MRD	O2-C2	-2.29	1.38	1.44
3	B	908	NAG	O3-C3	-2.23	1.37	1.43

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	908	NAG	C4-C3-C2	-7.05	100.27	111.23
8	B	950	TCB	O1'-C1'-C2'	-5.26	95.10	109.21
8	B	950	TCB	O5-C1-S4'	-4.80	97.84	110.01
3	B	908	NAG	C6-C5-C4	-3.99	103.17	113.02
3	B	946	NAG	O3-C3-C4	-3.72	101.96	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	942	MRD	3	0
7	A	943	MRD	6	0
7	B	948	MRD	2	0
7	B	949	MRD	2	0
8	B	950	TCB	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.74	3 (0%)	93 93	5, 12, 24, 50	0
1	B	832/841 (98%)	-0.91	3 (0%)	93 93	4, 9, 20, 52	0
All	All	1665/1682 (98%)	-0.83	6 (0%)	93 93	4, 10, 23, 52	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	699	GLY	3.2
1	A	610	TYR	2.6
1	B	668	ASN	2.5
1	A	609	ASP	2.4
1	B	610	TYR	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MAN	A	933	11/12	0.91	0.26	16.68	23,29,41,44	0
2	MAN	B	937	11/12	0.91	0.17	9.44	23,31,39,40	0
2	MAN	A	906	11/12	0.85	0.20	7.59	32,38,48,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	927	14/15	0.95	0.10	6.89	12,16,35,39	0
10	MAN	B	942	11/12	0.93	0.13	4.19	22,24,33,45	0
2	MAN	A	938	11/12	0.96	0.12	3.34	19,24,30,32	0
4	NAG	A	910	14/15	0.96	0.13	3.01	16,21,23,29	0
2	MAN	B	906	11/12	0.96	0.10	2.12	15,17,21,28	0
2	MAN	A	937	11/12	0.94	0.11	2.03	17,23,28,38	0
10	MAN	B	943	11/12	0.95	0.10	1.56	23,23,30,38	0
4	NAG	A	924	14/15	0.96	0.07	1.06	19,25,34,42	0
9	NAG	B	909	14/15	0.94	0.09	0.89	10,12,13,14	0
2	NAG	B	931	14/15	0.96	0.07	0.81	12,15,29,30	0
9	NAG	B	910	14/15	0.97	0.07	0.71	12,16,24,25	0
6	NAG	A	914	14/15	0.97	0.10	0.70	15,17,20,21	0
4	NAG	A	909	14/15	0.97	0.07	-0.06	13,14,16,16	0
4	NAG	B	928	14/15	0.97	0.06	-0.10	16,20,30,32	0
10	NAG	B	938	14/15	0.98	0.06	-0.34	12,14,15,16	0
6	MAN	A	922	11/12	0.96	0.06	-0.46	17,19,24,31	0
2	NAG	A	901	14/15	0.98	0.06	-0.50	13,14,15,15	0
2	NAG	A	902	14/15	0.96	0.07	-0.50	15,22,31,33	0
2	NAG	A	934	14/15	0.98	0.05	-0.52	13,15,17,18	0
6	MAN	B	926	11/12	0.98	0.06	-0.53	9,10,11,11	0
2	NAG	B	901	14/15	0.99	0.05	-0.60	8,9,10,10	0
6	NAG	B	919	14/15	0.97	0.06	-0.67	8,9,10,11	0
5	NAG	A	912	14/15	0.98	0.06	-0.75	12,13,17,18	0
6	MAN	B	924	11/12	0.97	0.06	-0.76	12,14,18,24	0
6	NAG	B	918	14/15	0.98	0.05	-0.89	9,11,14,15	0
6	MAN	B	927	11/12	0.99	0.05	-0.98	11,11,14,17	0
6	NAG	A	915	14/15	0.98	0.06	-1.12	12,13,14,14	0
4	NAG	B	915	14/15	0.99	0.05	-1.16	8,10,11,12	0
6	MAN	A	921	11/12	0.98	0.05	-1.33	13,14,15,19	0
6	MAN	A	920	11/12	0.98	0.05	-1.49	12,13,15,15	0
2	NAG	B	902	14/15	0.98	0.04	-1.56	9,12,15,21	0
4	BMA	B	930	11/12	0.79	0.20	-	42,51,62,68	0
2	MAN	A	930	11/12	0.79	0.31	-	52,58,67,68	0
4	NAG	B	929	14/15	0.91	0.15	-	25,32,36,44	0
9	BMA	B	911	11/12	0.93	0.12	-	22,25,29,33	0
6	BMA	B	920	11/12	0.99	0.04	-	10,11,12,13	0
9	MAN	B	912	11/12	0.80	0.21	-	37,42,50,51	0
6	MAN	A	917	11/12	0.97	0.09	-	16,18,23,24	0
10	MAN	B	941	11/12	0.82	0.22	-	51,60,65,66	0
4	NAG	B	916	14/15	0.94	0.09	-	13,17,28,32	0
2	BMA	B	903	11/12	0.96	0.07	-	12,17,19,20	0
10	NAG	B	939	14/15	0.96	0.10	-	17,22,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	935	14/15	0.96	0.10	-	14,18,24,29	0
2	MAN	A	939	11/12	0.85	0.24	-	36,39,46,47	0
6	MAN	A	923	11/12	0.95	0.13	-	22,24,28,31	0
9	MAN	B	914	11/12	0.91	0.21	-	37,39,46,54	0
2	NAG	A	928	14/15	0.94	0.12	-	15,19,23,26	0
2	MAN	A	907	11/12	0.80	0.14	-	45,53,59,60	0
6	MAN	B	922	11/12	0.95	0.11	-	22,32,38,39	0
5	NAG	A	913	14/15	0.94	0.12	-	15,23,32,33	0
2	MAN	B	905	11/12	0.96	0.09	-	16,23,32,37	0
10	BMA	B	940	11/12	0.87	0.12	-	25,31,38,45	0
2	MAN	B	907	11/12	0.95	0.09	-	20,27,30,31	0
2	MAN	A	904	11/12	0.83	0.27	-	52,58,63,65	0
10	MAN	B	944	11/12	0.80	0.23	-	44,50,62,64	0
2	NAG	B	932	14/15	0.93	0.11	-	14,17,23,24	0
2	MAN	B	934	11/12	0.73	0.25	-	56,65,71,77	0
9	MAN	B	913	11/12	0.91	0.17	-	33,35,41,41	0
2	BMA	A	929	11/12	0.94	0.17	-	20,24,31,40	0
6	MAN	A	919	11/12	0.98	0.05	-	13,14,16,18	0
2	MAN	A	940	11/12	0.78	0.26	-	49,53,62,70	0
6	MAN	B	925	11/12	0.96	0.08	-	19,21,25,26	0
6	MAN	A	918	11/12	0.95	0.12	-	25,32,46,53	0
2	BMA	B	933	11/12	0.95	0.11	-	23,26,31,41	0
2	MAN	B	904	11/12	0.96	0.10	-	18,25,31,32	0
2	MAN	B	936	11/12	0.92	0.14	-	22,27,31,34	0
2	MAN	A	931	11/12	0.92	0.14	-	27,31,39,43	0
4	BMA	A	911	11/12	0.83	0.17	-	25,34,40,46	0
2	MAN	A	905	11/12	0.80	0.26	-	55,60,62,63	0
4	NAG	A	925	14/15	0.81	0.18	-	40,48,59,62	0
10	MAN	B	945	11/12	0.76	0.22	-	48,54,66,71	0
2	MAN	A	932	11/12	0.94	0.16	-	20,26,34,48	0
6	MAN	B	921	11/12	0.98	0.04	-	12,14,18,19	0
2	MAN	B	935	11/12	0.93	0.12	-	27,28,38,40	0
6	BMA	A	916	11/12	0.98	0.05	-	14,15,17,18	0
2	BMA	A	903	11/12	0.86	0.17	-	35,60,65,67	0
4	BMA	A	926	11/12	0.62	0.32	-	45,66,75,79	0
4	BMA	B	917	11/12	0.81	0.23	-	45,59,70,74	0
2	BMA	A	936	11/12	0.93	0.16	-	21,29,41,45	0
6	MAN	B	923	11/12	0.99	0.06	-	9,9,10,12	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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	MRD	A	943	8/8	0.82	0.20	14.84	15,26,33,39	0
7	MRD	B	949	8/8	0.92	0.17	8.19	35,39,42,43	0
7	MRD	B	948	8/8	0.94	0.13	6.47	15,19,33,35	0
3	NAG	B	947	14/15	0.96	0.13	3.36	22,24,28,31	0
8	TCB	B	950	23/23	0.87	0.15	1.72	16,41,59,60	0
3	NAG	A	941	14/15	0.94	0.15	1.34	24,32,36,36	0
7	MRD	A	942	8/8	0.94	0.09	1.11	16,17,20,27	0
8	TCB	A	944	23/23	0.88	0.14	0.76	23,44,55,57	0
3	NAG	A	908	14/15	0.83	0.38	-	39,53,62,67	0
3	NAG	B	908	14/15	0.90	0.21	-	34,39,46,46	0
3	NAG	B	946	14/15	0.90	0.20	-	34,50,55,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.