wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:29 PM GMT

PDB ID	:	4IIE
Title	:	Crystal structure of beta-glucosidase 1 from Aspergillus aculeatus in complex with calystegine B(2)
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 (i) symbol.

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

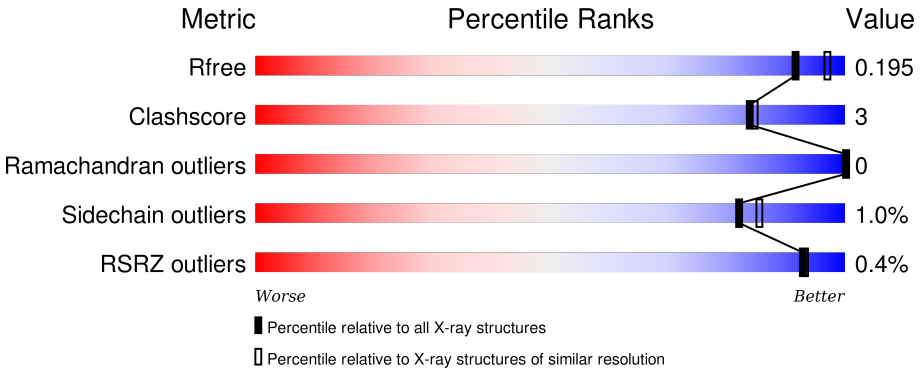
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 <=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	93% 6%
1	B	841	90% 8%

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	CGB	A	943	-	-	X	-
10	CGB	B	952	-	-	X	-
12	MAN	B	942	-	-	-	X
3	NAG	B	947	-	-	-	X
4	NAG	A	907	-	-	-	X
4	NAG	B	916	-	-	-	X
7	NAG	A	924	-	-	-	X
7	MAN	A	930	-	-	-	X
7	MAN	A	935	-	-	-	X
7	NAG	B	931	-	-	-	X
8	MRD	A	940	-	-	X	X
8	MRD	A	941	-	-	-	X
8	MRD	B	948	-	-	-	X
8	MRD	B	949	-	-	-	X
8	MRD	B	950	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 15193 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.

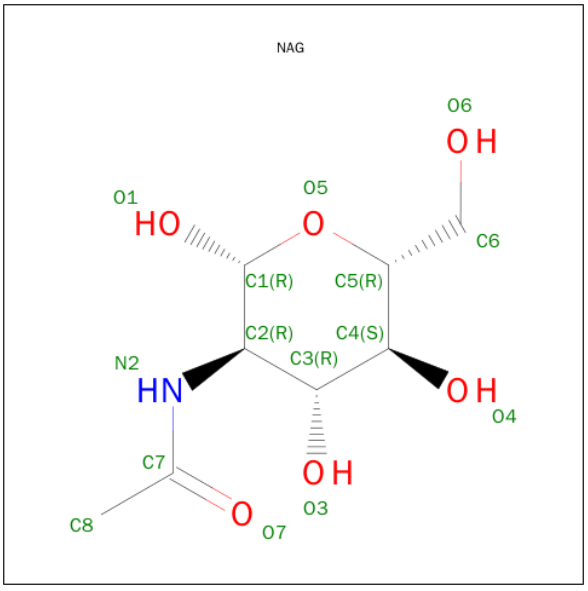
- Molecule 1 is a protein called Beta-glucosidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	834	Total	C	N	O	S	0	0	0
			6387	4031	1097	1241	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		

- 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		

Continued on next page...

Continued from previous page...

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

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

- 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 28 16 2 10	0	0

- 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 116 64 2 50	0	0
6	B	10	Total C N O 116 64 2 50	0	0

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

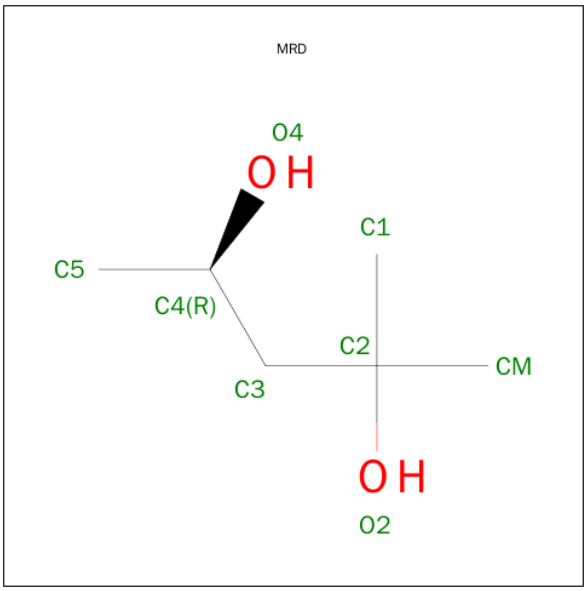
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	7	Total C N O 83 46 2 35	0	0
7	A	7	Total C N O 83 46 2 35	0	0

Continued on next page...

Continued from previous page...

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

- 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 8 6 2	0	0
8	A	1	Total C O 8 6 2	0	0
8	A	1	Total C O 8 6 2	0	0
8	B	1	Total C O 8 6 2	0	0
8	B	1	Total C O 8 6 2	0	0
8	B	1	Total C O 8 6 2	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

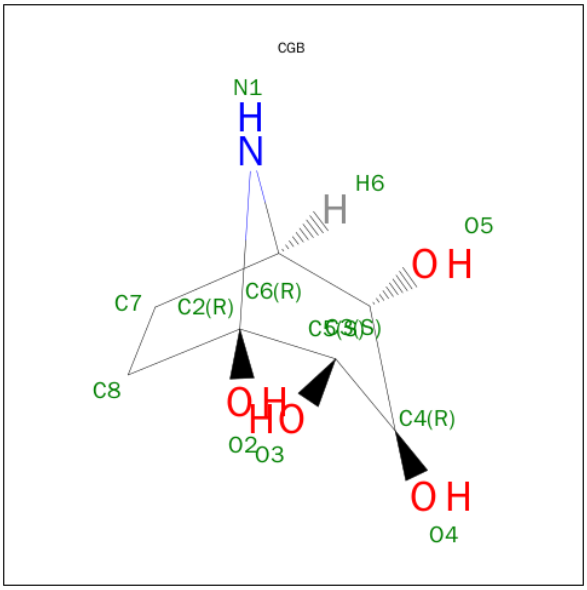
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Na 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Na 1 1	0	0

- Molecule 10 is CALYSTEGINE B2 (three-letter code: CGB) (formula: $C_7H_{13}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N O 12 7 1 4	0	0
10	B	1	Total C N O 12 7 1 4	0	0

- Molecule 11 is a polymer of unknown type called SUGAR (6-MER).

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

- 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 94 52 2 40	0	0

- Molecule 13 is water.

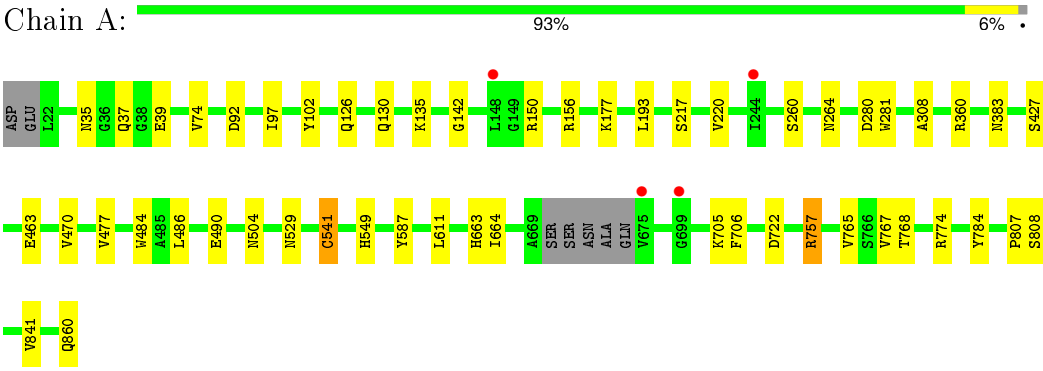
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	610	Total O 610 610	0	0
13	B	713	Total O 713 713	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

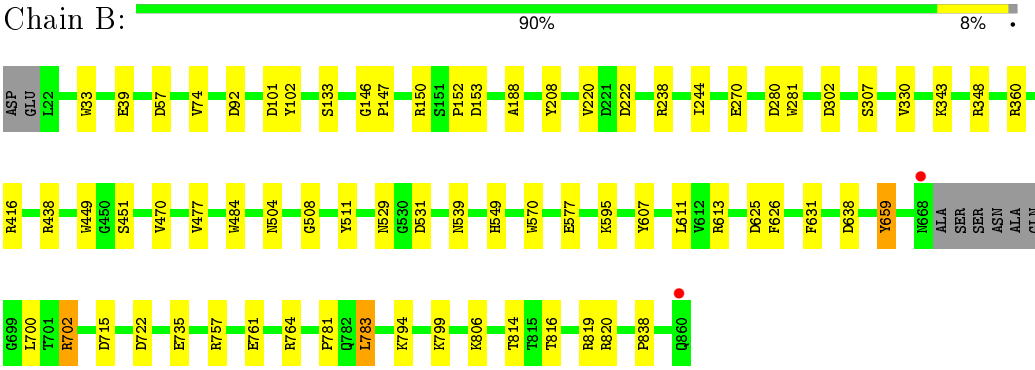
- Molecule 1: Beta-glucosidase 1

Chain A:



- Molecule 1: Beta-glucosidase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.13Å 122.15Å 222.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.07 – 2.00 39.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.07-2.00) 99.4 (39.07-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.149 , 0.193 0.151 , 0.195	Depositor DCC
R_{free} test set	7597 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 150914 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15193	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: BMA, NAG, NA, CGB, 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	1.21	6/6550 (0.1%)	1.02	10/8930 (0.1%)
1	B	1.32	9/6538 (0.1%)	1.08	25/8913 (0.3%)
All	All	1.27	15/13088 (0.1%)	1.05	35/17843 (0.2%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455	GLU	CD-OE2	5.76	1.31	1.25
1	B	270	GLU	CD-OE2	5.63	1.31	1.25
1	B	348	ARG	CZ-NH1	5.55	1.40	1.33
1	B	511	TYR	CG-CD2	5.45	1.46	1.39
1	B	761	GLU	CD-OE2	-5.43	1.19	1.25

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	702	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	B	348	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	B	348	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	B	702	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	B	438	ARG	NE-CZ-NH1	-7.52	116.54	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	6387	0	6097	34	0
1	B	6375	0	6082	33	0
2	A	50	0	43	1	0
3	A	28	0	26	0	0
3	B	42	0	39	0	0
4	A	78	0	68	2	0
4	B	78	0	68	0	0
5	A	28	0	24	0	0
6	A	116	0	97	0	0
6	B	116	0	97	0	0
7	A	166	0	139	2	0
7	B	166	0	139	2	0
8	A	24	0	42	8	0
8	B	24	0	42	5	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	12	0	13	7	0
10	B	12	0	12	7	0
11	B	72	0	61	2	0
12	B	94	0	78	1	0
13	A	610	0	0	4	0
13	B	713	0	0	7	0
All	All	15193	0	13167	81	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 81 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:92:ASP:OD2	10:A:943:CGB:H7C1	1.71	0.90
1:B:92:ASP:OD2	10:B:952:CGB:H7C1	1.75	0.86
1:A:280:ASP:OD1	10:A:943:CGB:H3	1.78	0.82
1:A:360:ARG:HH11	8:A:940:MRD:HMC3	1.44	0.82
1:A:819:ARG:HH12	1:A:860:GLN:C	1.82	0.82

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	830/841 (99%)	798 (96%)	32 (4%)	0	100	100
1	B	828/841 (98%)	803 (97%)	25 (3%)	0	100	100
All	All	1658/1682 (99%)	1601 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	661 (99%)	9 (1%)	76	79
All	All	1341/1354 (99%)	1328 (99%)	13 (1%)	82	85

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	74	VAL
1	B	281	TRP
1	B	700	LEU
1	B	33	TRP
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

80 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	1.09	1 (7%)	15,19,21	1.42	1 (6%)
2	NAG	A	902	2	14,14,15	0.90	1 (7%)	15,19,21	2.11	6 (40%)
2	BMA	A	903	2	11,11,12	1.25	1 (9%)	14,15,17	2.12	6 (42%)
2	MAN	A	904	2	11,11,12	0.96	0	14,15,17	2.61	6 (42%)
4	NAG	A	906	1,4	14,14,15	1.00	1 (7%)	15,19,21	1.36	2 (13%)
4	NAG	A	907	4	14,14,15	1.13	1 (7%)	15,19,21	1.42	2 (13%)
4	BMA	A	908	4	11,11,12	1.11	0	14,15,17	2.81	9 (64%)
5	NAG	A	909	1,5	14,14,15	0.94	0	15,19,21	1.80	4 (26%)
5	NAG	A	910	5	14,14,15	1.01	1 (7%)	15,19,21	2.41	3 (20%)
6	NAG	A	911	1,6	14,14,15	1.51	2 (14%)	15,19,21	1.64	5 (33%)
6	NAG	A	912	6	14,14,15	0.97	1 (7%)	15,19,21	0.95	0
6	BMA	A	913	6	11,11,12	1.07	1 (9%)	14,15,17	1.30	1 (7%)
6	MAN	A	914	6	11,11,12	1.07	1 (9%)	14,15,17	1.67	3 (21%)
6	MAN	A	915	6	11,11,12	1.51	3 (27%)	14,15,17	2.47	5 (35%)
6	MAN	A	916	6	11,11,12	0.59	0	14,15,17	1.69	5 (35%)
6	MAN	A	917	6	11,11,12	0.99	0	14,15,17	1.30	1 (7%)
6	MAN	A	918	6	11,11,12	1.08	1 (9%)	14,15,17	1.88	5 (35%)
6	MAN	A	919	6	11,11,12	1.22	1 (9%)	14,15,17	1.37	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	A	920	6	11,11,12	0.84	0	14,15,17	1.58	2 (14%)
4	NAG	A	921	1,4	14,14,15	0.94	1 (7%)	15,19,21	1.00	0
4	NAG	A	922	4	14,14,15	0.93	1 (7%)	15,19,21	1.40	3 (20%)
4	BMA	A	923	4	11,11,12	1.03	1 (9%)	14,15,17	2.57	3 (21%)
7	NAG	A	924	1,7	14,14,15	0.86	0	15,19,21	1.66	3 (20%)
7	NAG	A	925	7	14,14,15	0.88	0	15,19,21	2.31	5 (33%)
7	BMA	A	926	7	11,11,12	0.88	0	14,15,17	1.25	2 (14%)
7	MAN	A	927	7	11,11,12	0.85	1 (9%)	14,15,17	2.29	6 (42%)
7	MAN	A	928	7	11,11,12	0.67	0	14,15,17	1.65	5 (35%)
7	MAN	A	929	7	11,11,12	1.31	2 (18%)	14,15,17	2.06	5 (35%)
7	MAN	A	930	7	11,11,12	1.14	0	14,15,17	1.30	2 (14%)
7	NAG	A	931	1,9,7	14,14,15	1.11	0	15,19,21	1.80	5 (33%)
7	NAG	A	932	7	14,14,15	1.18	2 (14%)	15,19,21	1.39	2 (13%)
7	BMA	A	933	7	11,11,12	0.84	0	14,15,17	2.14	2 (14%)
7	MAN	A	934	7	11,11,12	1.13	1 (9%)	14,15,17	1.37	1 (7%)
7	MAN	A	935	7	11,11,12	1.35	2 (18%)	14,15,17	2.29	6 (42%)
7	MAN	A	936	7	11,11,12	0.81	0	14,15,17	1.91	5 (35%)
7	MAN	A	937	7	11,11,12	1.14	1 (9%)	14,15,17	2.48	6 (42%)
7	NAG	B	901	1,7	14,14,15	1.60	1 (7%)	15,19,21	1.39	3 (20%)
7	NAG	B	902	7	14,14,15	1.02	1 (7%)	15,19,21	1.57	2 (13%)
7	BMA	B	903	7	11,11,12	1.11	1 (9%)	14,15,17	2.10	5 (35%)
7	MAN	B	904	7	11,11,12	0.63	0	14,15,17	1.96	6 (42%)
7	MAN	B	905	7	11,11,12	1.06	1 (9%)	14,15,17	1.69	3 (21%)
7	MAN	B	906	7	11,11,12	0.94	0	14,15,17	1.69	4 (28%)
7	MAN	B	907	7	11,11,12	0.68	0	14,15,17	2.03	5 (35%)
11	NAG	B	909	1,11	14,14,15	1.12	1 (7%)	15,19,21	1.53	4 (26%)
11	NAG	B	910	11	14,14,15	1.17	2 (14%)	15,19,21	1.45	2 (13%)
11	BMA	B	911	11	11,11,12	0.77	0	14,15,17	1.74	4 (28%)
11	MAN	B	912	11	11,11,12	1.69	1 (9%)	14,15,17	2.41	5 (35%)
11	MAN	B	913	11	11,11,12	0.65	0	14,15,17	1.68	5 (35%)
11	MAN	B	914	11	11,11,12	0.70	0	14,15,17	1.46	3 (21%)
4	NAG	B	915	1,4	14,14,15	0.64	0	15,19,21	1.79	4 (26%)
4	NAG	B	916	4	14,14,15	0.53	0	15,19,21	1.77	5 (33%)
4	BMA	B	917	4	11,11,12	0.82	0	14,15,17	1.94	5 (35%)
6	NAG	B	918	1,6	14,14,15	1.12	2 (14%)	15,19,21	1.80	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	B	919	6	14,14,15	1.34	3 (21%)	15,19,21	1.25	1 (6%)
6	BMA	B	920	6	11,11,12	1.07	1 (9%)	14,15,17	1.52	4 (28%)
6	MAN	B	921	6	11,11,12	0.78	0	14,15,17	1.60	2 (14%)
6	MAN	B	922	6	11,11,12	1.06	0	14,15,17	1.87	5 (35%)
6	MAN	B	923	6	11,11,12	0.80	0	14,15,17	1.83	5 (35%)
6	MAN	B	924	6	11,11,12	0.73	0	14,15,17	2.64	6 (42%)
6	MAN	B	925	6	11,11,12	0.73	0	14,15,17	1.46	4 (28%)
6	MAN	B	926	6	11,11,12	1.26	1 (9%)	14,15,17	2.43	2 (14%)
6	MAN	B	927	6	11,11,12	1.38	1 (9%)	14,15,17	2.16	6 (42%)
4	NAG	B	928	1,4	14,14,15	0.61	0	15,19,21	1.00	1 (6%)
4	NAG	B	929	4	14,14,15	0.84	0	15,19,21	1.17	0
4	BMA	B	930	4	11,11,12	0.89	0	14,15,17	1.31	2 (14%)
7	NAG	B	931	1,7	14,14,15	1.04	1 (7%)	15,19,21	1.96	4 (26%)
7	NAG	B	932	7	14,14,15	1.04	0	15,19,21	1.61	4 (26%)
7	BMA	B	933	7	11,11,12	1.06	0	14,15,17	1.82	3 (21%)
7	MAN	B	934	7	11,11,12	0.91	0	14,15,17	2.14	7 (50%)
7	MAN	B	935	7	11,11,12	1.00	0	14,15,17	1.67	4 (28%)
7	MAN	B	936	7	11,11,12	1.23	1 (9%)	14,15,17	2.24	6 (42%)
7	MAN	B	937	7	11,11,12	0.80	1 (9%)	14,15,17	1.65	3 (21%)
12	NAG	B	938	1,9,12	14,14,15	1.18	1 (7%)	15,19,21	1.54	3 (20%)
12	NAG	B	939	12	14,14,15	0.75	0	15,19,21	1.55	3 (20%)
12	BMA	B	940	12	11,11,12	1.43	2 (18%)	14,15,17	4.41	8 (57%)
12	MAN	B	941	12	11,11,12	0.95	0	14,15,17	2.05	6 (42%)
12	MAN	B	942	12	11,11,12	1.02	1 (9%)	14,15,17	2.08	4 (28%)
12	MAN	B	943	12	11,11,12	1.04	0	14,15,17	1.91	4 (28%)
12	MAN	B	944	12	11,11,12	0.65	0	14,15,17	2.74	7 (50%)
12	MAN	B	945	12	11,11,12	0.98	1 (9%)	14,15,17	1.69	2 (14%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
7	NAG	A	931	1,9,7	-	0/6/23/26	0/1/1/1
7	NAG	A	932	7	-	0/6/23/26	0/1/1/1
7	BMA	A	933	7	-	0/2/19/22	0/1/1/1
7	MAN	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	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
11	NAG	B	909	1,11	-	0/6/23/26	0/1/1/1
11	NAG	B	910	11	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BMA	B	911	11	-	0/2/19/22	0/1/1/1
11	MAN	B	912	11	-	0/2/19/22	0/1/1/1
11	MAN	B	913	11	-	0/2/19/22	0/1/1/1
11	MAN	B	914	11	-	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
7	NAG	B	931	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	932	7	-	0/6/23/26	0/1/1/1
7	BMA	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
7	MAN	B	936	7	-	0/2/19/22	0/1/1/1
7	MAN	B	937	7	-	0/2/19/22	0/1/1/1
12	NAG	B	938	1,9,12	-	0/6/23/26	0/1/1/1
12	NAG	B	939	12	-	0/6/23/26	0/1/1/1
12	BMA	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
12	MAN	B	943	12	-	0/2/19/22	0/1/1/1
12	MAN	B	944	12	-	0/2/19/22	0/1/1/1
12	MAN	B	945	12	-	0/2/19/22	0/1/1/1

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	919	MAN	O5-C1	-3.06	1.38	1.43
7	A	932	NAG	O5-C1	-3.05	1.38	1.43
6	B	926	MAN	O5-C1	-2.98	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	910	NAG	O3-C3	-2.84	1.36	1.43
6	A	915	MAN	O5-C1	-2.80	1.39	1.43

The worst 5 of 304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	940	BMA	C6-C5-C4	-7.99	93.32	113.02
5	A	910	NAG	C3-C4-C5	-7.21	97.63	110.20
6	B	924	MAN	O6-C6-C5	-5.93	91.74	111.33
7	A	925	NAG	C2-N2-C7	-5.85	115.52	123.04
7	B	903	BMA	C1-C2-C3	-5.23	103.36	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	NAG	1	0
4	A	907	NAG	1	0
4	A	908	BMA	1	0
7	A	926	BMA	2	0
11	B	909	NAG	2	0
7	B	933	BMA	2	0
7	B	935	MAN	1	0
12	B	940	BMA	1	0
12	B	942	MAN	1	0

5.6 Ligand geometry (i)

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	905	1	14,14,15	0.94	1 (7%)	15,19,21	1.09	2 (13%)
3	NAG	A	938	1	14,14,15	0.82	1 (7%)	15,19,21	2.02	5 (33%)
8	MRD	A	939	-	6,7,7	1.15	0	7,10,10	0.34	0
8	MRD	A	940	-	6,7,7	1.39	0	7,10,10	1.13	1 (14%)
8	MRD	A	941	-	6,7,7	0.95	0	7,10,10	1.11	1 (14%)
10	CGB	A	943	-	12,13,13	2.24	5 (41%)	12,21,21	4.16	11 (91%)
3	NAG	B	908	1	14,14,15	0.92	1 (7%)	15,19,21	2.38	7 (46%)
3	NAG	B	946	1	14,14,15	0.99	0	15,19,21	1.87	3 (20%)
3	NAG	B	947	1	14,14,15	1.03	0	15,19,21	2.16	5 (33%)
8	MRD	B	948	-	6,7,7	1.04	0	7,10,10	2.72	6 (85%)
8	MRD	B	949	-	6,7,7	0.86	0	7,10,10	1.33	2 (28%)
8	MRD	B	950	-	6,7,7	1.02	0	7,10,10	0.64	0
10	CGB	B	952	-	12,13,13	2.69	4 (33%)	12,21,21	3.80	10 (83%)

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	938	1	-	0/6/23/26	0/1/1/1
8	MRD	A	939	-	-	0/5/5/5	0/0/0/0
8	MRD	A	940	-	-	0/5/5/5	0/0/0/0
8	MRD	A	941	-	-	0/5/5/5	0/0/0/0
10	CGB	A	943	-	-	0/0/29/29	0/0/2/2
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
8	MRD	B	948	-	-	0/5/5/5	0/0/0/0
8	MRD	B	949	-	-	0/5/5/5	0/0/0/0
8	MRD	B	950	-	-	0/5/5/5	0/0/0/0
10	CGB	B	952	-	-	0/0/29/29	0/0/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	952	CGB	C8-C2	-5.75	1.45	1.54
10	A	943	CGB	C8-C2	-5.72	1.45	1.54
10	B	952	CGB	O4-C4	-3.09	1.35	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	943	CGB	C4-C3	-2.70	1.48	1.53
3	A	938	NAG	O3-C3	-2.10	1.37	1.43

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	943	CGB	C2-C3-C4	-6.09	99.70	111.13
3	B	947	NAG	C1-O5-C5	-5.50	105.27	112.25
10	B	952	CGB	C2-C3-C4	-5.39	101.01	111.13
10	B	952	CGB	C4-C5-C6	-4.77	103.81	111.23
3	A	938	NAG	C2-N2-C7	-4.51	117.24	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	939	MRD	2	0
8	A	940	MRD	6	0
10	A	943	CGB	7	0
8	B	948	MRD	1	0
8	B	949	MRD	1	0
8	B	950	MRD	3	0
10	B	952	CGB	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	834/841 (99%)	-0.50	4 (0%)	91	92	11, 20, 34, 63	0
1	B	832/841 (98%)	-0.67	2 (0%)	95	95	9, 16, 28, 53	0
All	All	1666/1682 (99%)	-0.58	6 (0%)	93	93	9, 17, 31, 63	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	675	VAL	2.6
1	A	148	LEU	2.5
1	B	860	GLN	2.3
1	A	699	GLY	2.1
1	B	668	ASN	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	MAN	B	942	11/12	0.91	0.17	5.23	31,34,43,48	0
7	NAG	A	924	14/15	0.95	0.13	4.87	20,22,41,47	0
7	MAN	A	930	11/12	0.97	0.13	3.85	21,24,37,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	B	916	14/15	0.95	0.10	3.37	19,26,41,45	0
7	MAN	A	935	11/12	0.95	0.11	3.36	28,34,44,44	0
7	NAG	B	931	14/15	0.95	0.10	3.19	16,21,36,38	0
4	NAG	A	907	14/15	0.93	0.12	2.21	25,29,34,37	0
7	MAN	B	906	11/12	0.95	0.11	1.71	26,30,35,42	0
7	MAN	A	934	11/12	0.94	0.09	1.65	24,30,38,45	0
7	MAN	B	937	11/12	0.97	0.09	1.44	20,24,30,34	0
11	NAG	B	910	14/15	0.96	0.07	0.53	20,27,31,35	0
6	NAG	A	911	14/15	0.96	0.09	0.24	26,28,33,35	0
12	NAG	B	938	14/15	0.97	0.07	-0.27	19,21,23,24	0
4	NAG	A	921	14/15	0.97	0.07	-0.36	25,29,36,38	0
6	NAG	B	919	14/15	0.98	0.07	-0.40	12,16,18,18	0
6	MAN	B	927	11/12	0.98	0.06	-0.41	17,19,20,24	0
2	NAG	A	901	14/15	0.97	0.07	-0.45	17,23,26,27	0
2	NAG	A	902	14/15	0.96	0.08	-0.53	24,32,43,48	0
4	NAG	A	906	14/15	0.96	0.07	-0.54	22,25,27,27	0
6	MAN	B	926	11/12	0.98	0.07	-0.60	16,18,18,19	0
6	MAN	A	919	11/12	0.95	0.07	-0.62	23,30,33,42	0
4	NAG	B	915	14/15	0.98	0.06	-0.66	13,17,21,21	0
11	NAG	B	909	14/15	0.96	0.06	-0.66	17,20,22,24	0
7	NAG	B	901	14/15	0.98	0.06	-0.68	14,16,18,19	0
7	NAG	A	931	14/15	0.96	0.06	-0.68	21,23,25,26	0
6	NAG	B	918	14/15	0.97	0.06	-0.83	16,17,24,24	0
7	NAG	B	902	14/15	0.98	0.05	-0.90	15,18,23,29	0
6	NAG	A	912	14/15	0.97	0.07	-1.15	21,23,27,27	0
4	NAG	B	928	14/15	0.97	0.05	-1.28	22,28,32,33	0
6	MAN	A	918	11/12	0.98	0.06	-1.39	23,24,26,26	0
6	MAN	B	924	11/12	0.97	0.06	-1.44	18,22,25,33	0
6	MAN	A	917	11/12	0.96	0.06	-1.49	20,22,25,26	0
5	NAG	A	909	14/15	0.98	0.06	-1.54	19,23,27,28	0
2	BMA	A	903	11/12	0.86	0.12	-	36,44,48,53	0
7	MAN	B	905	11/12	0.95	0.13	-	28,34,42,49	0
6	BMA	A	913	11/12	0.96	0.08	-	24,26,29,32	0
6	MAN	B	925	11/12	0.94	0.09	-	24,29,33,36	0
7	MAN	A	927	11/12	0.84	0.34	-	54,60,65,69	0
7	BMA	B	903	11/12	0.96	0.06	-	20,24,26,27	0
12	BMA	B	940	11/12	0.86	0.19	-	37,41,54,60	0
6	MAN	A	915	11/12	0.94	0.13	-	39,40,50,51	0
7	BMA	A	933	11/12	0.86	0.13	-	30,41,52,63	0
11	BMA	B	911	11/12	0.93	0.16	-	40,44,54,60	0
12	MAN	B	943	11/12	0.95	0.13	-	28,35,42,47	0
4	BMA	B	930	11/12	0.86	0.19	-	43,52,60,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	MAN	B	912	11/12	0.47	0.30	-	57,62,68,68	0
4	NAG	A	922	14/15	0.88	0.20	-	42,50,61,69	0
7	BMA	B	933	11/12	0.93	0.14	-	23,27,34,46	0
6	MAN	A	920	11/12	0.93	0.14	-	33,38,43,44	0
7	NAG	A	932	14/15	0.95	0.10	-	23,27,36,42	0
7	NAG	A	925	14/15	0.93	0.15	-	20,26,32,40	0
7	MAN	B	936	11/12	0.98	0.09	-	21,22,29,34	0
7	MAN	B	904	11/12	0.97	0.11	-	27,32,39,43	0
7	MAN	B	935	11/12	0.96	0.10	-	25,27,37,39	0
7	MAN	B	907	11/12	0.91	0.09	-	27,31,36,38	0
7	MAN	A	928	11/12	0.93	0.14	-	27,30,40,43	0
12	MAN	B	944	11/12	0.80	0.27	-	49,52,56,61	0
7	MAN	A	937	11/12	0.79	0.21	-	50,54,60,73	0
11	MAN	B	914	11/12	0.85	0.31	-	68,74,76,85	0
6	MAN	B	921	11/12	0.98	0.06	-	19,21,25,29	0
6	BMA	B	920	11/12	0.98	0.05	-	17,18,19,20	0
6	MAN	B	923	11/12	0.99	0.07	-	16,18,19,19	0
7	MAN	A	929	11/12	0.95	0.12	-	21,24,34,41	0
7	NAG	B	932	14/15	0.95	0.10	-	19,24,32,33	0
5	NAG	A	910	14/15	0.96	0.10	-	30,33,48,53	0
4	BMA	A	923	11/12	0.65	0.32	-	46,60,73,77	0
6	MAN	A	914	11/12	0.96	0.11	-	27,31,34,36	0
12	MAN	B	941	11/12	0.79	0.25	-	58,71,82,84	0
12	NAG	B	939	14/15	0.95	0.12	-	26,30,37,39	0
12	MAN	B	945	11/12	0.81	0.22	-	47,56,66,68	0
7	MAN	A	936	11/12	0.86	0.26	-	54,58,62,66	0
7	BMA	A	926	11/12	0.93	0.18	-	23,27,34,43	0
4	BMA	A	908	11/12	0.84	0.23	-	42,48,57,62	0
6	MAN	B	922	11/12	0.90	0.10	-	30,37,41,42	0
4	BMA	B	917	11/12	0.82	0.28	-	55,65,76,80	0
6	MAN	A	916	11/12	0.97	0.06	-	20,24,26,28	0
7	MAN	B	934	11/12	0.71	0.29	-	62,71,74,79	0
2	MAN	A	904	11/12	0.90	0.18	-	45,52,65,71	0
4	NAG	B	929	14/15	0.95	0.15	-	31,33,46,48	0
11	MAN	B	913	11/12	0.86	0.25	-	56,66,70,70	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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	MRD	A	940	8/8	0.85	0.20	22.27	21,29,41,43	0
8	MRD	B	950	8/8	0.93	0.13	8.64	33,43,45,48	0
8	MRD	B	949	8/8	0.94	0.10	6.02	21,28,35,39	0
8	MRD	A	941	8/8	0.76	0.24	4.45	34,40,45,47	0
3	NAG	B	947	14/15	0.96	0.17	4.22	25,31,36,38	0
8	MRD	B	948	8/8	0.83	0.19	3.15	31,44,52,53	0
10	CGB	A	943	12/12	0.91	0.21	1.01	21,28,33,34	0
10	CGB	B	952	12/12	0.95	0.16	0.78	15,23,29,29	0
3	NAG	A	938	14/15	0.95	0.13	0.60	33,42,49,50	0
8	MRD	A	939	8/8	0.96	0.07	0.60	20,25,29,31	0
3	NAG	A	905	14/15	0.83	0.33	-	51,58,69,75	0
9	NA	A	942	1/1	0.96	0.13	-	29,29,29,29	0
3	NAG	B	908	14/15	0.84	0.31	-	43,53,59,63	0
9	NA	B	951	1/1	0.90	0.12	-	32,32,32,32	0
3	NAG	B	946	14/15	0.91	0.24	-	38,50,53,55	0

6.5 Other polymers (i)

There are no such residues in this entry.