



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:30 PM GMT

PDB ID : 4IID
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus* in complex with 1-deoxynojirimycin
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on : 2012-12-20
Resolution : 2.30 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

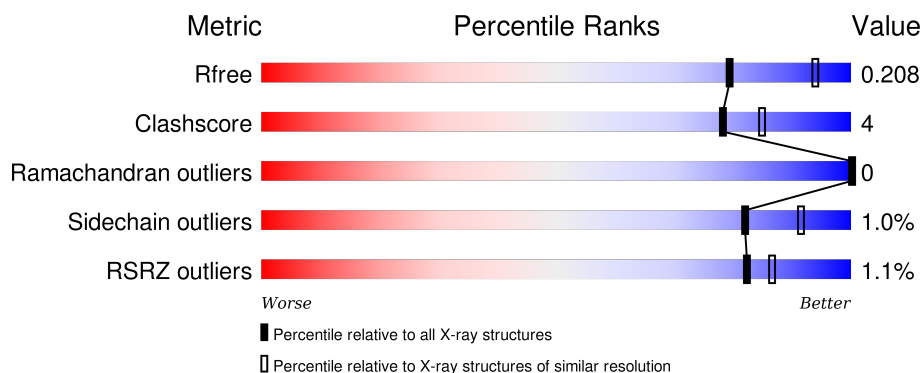
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	 2% 91% 7% •
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	NAG	B	910	-	-	-	X
11	MAN	B	941	-	-	-	X
12	MPD	B	947	-	-	-	X
3	NAG	B	946	-	-	-	X
4	NAG	A	907	-	-	-	X
7	NAG	A	923	-	-	-	X
7	MAN	A	929	-	-	-	X
8	MRD	A	939	-	-	X	X
8	MRD	B	948	-	-	-	X

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 14782 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.

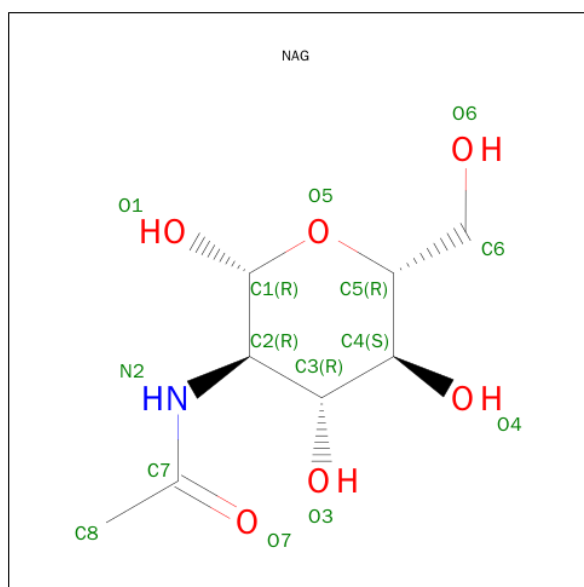
- Molecule 1 is a protein called Beta-glucosidase 1.

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		

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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	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		
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).

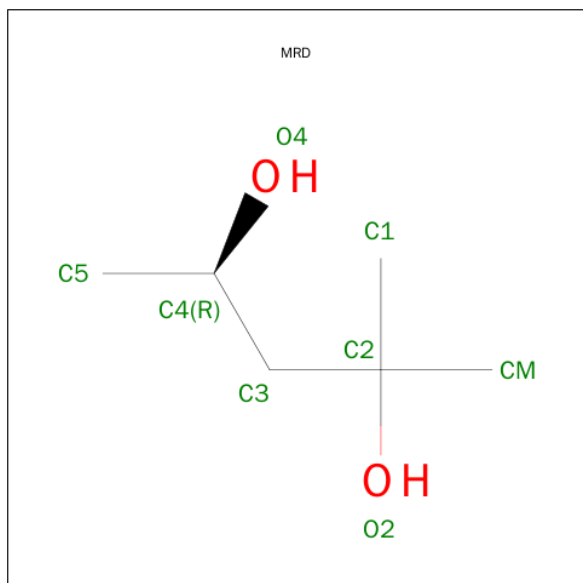
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	7	Total	C	N	O	0	0
			83	46	2	35		
7	A	7	Total	C	N	O	0	0
			83	46	2	35		

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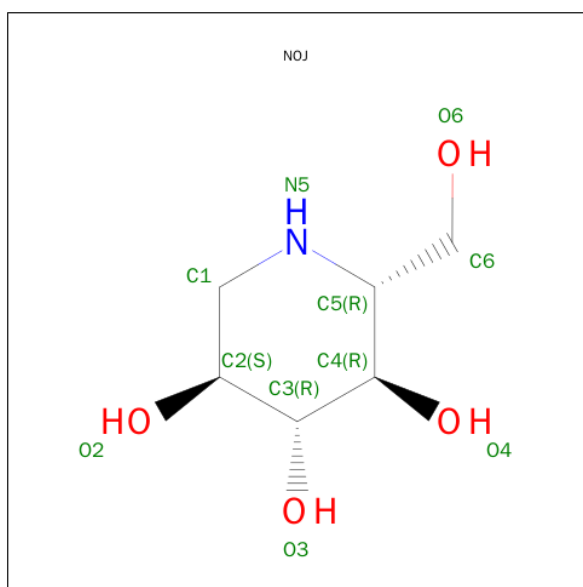
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	7	Total	C	N	O	0	0
			83	46	2	35		
7	B	7	Total	C	N	O	0	0
			83	46	2	35		

- 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		

- Molecule 9 is 1-DEOXYNOJIRIMYCIN (three-letter code: NOJ) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			11	6	1	4		
9	B	1	Total	C	N	O	0	0
			11	6	1	4		

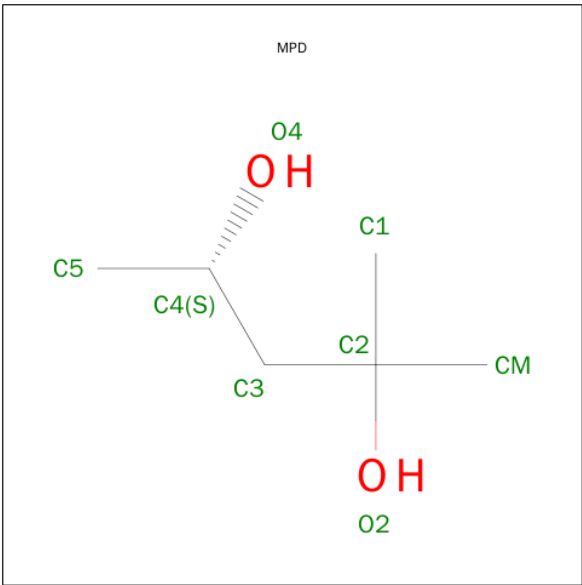
- Molecule 10 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 11 is a polymer of unknown type called SUGAR (8-MER).

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

- Molecule 12 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

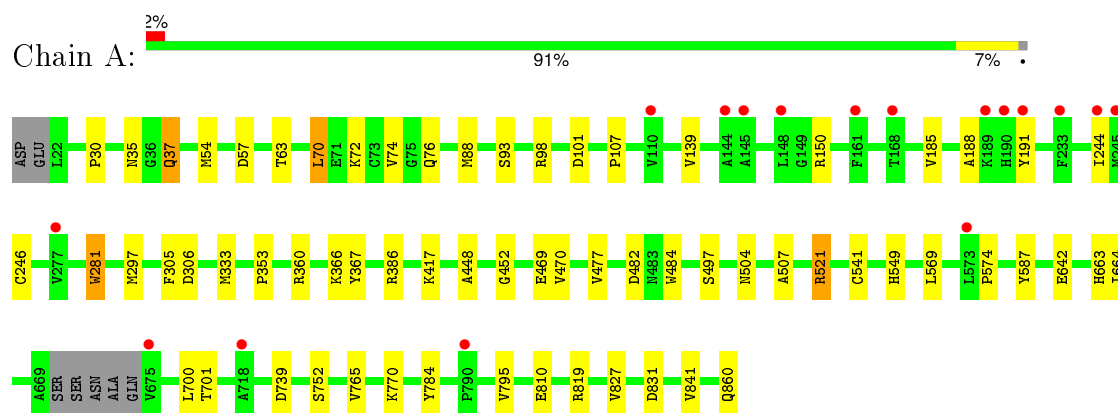
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	450	Total	O	0	0
			450	450		
13	B	504	Total	O	0	0
			504	504		

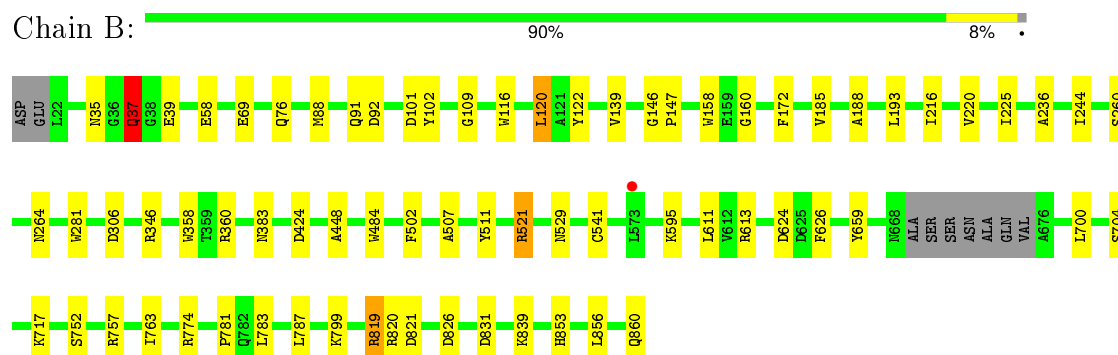
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Beta-glucosidase 1



• Molecule 1: Beta-glucosidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.45Å 121.60Å 221.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.07 – 2.30 39.07 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.07-2.30) 99.5 (39.07-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.155 , 0.207 0.157 , 0.208	Depositor DCC
R_{free} test set	4977 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 99146 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14782	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: MPD, BMA, NAG, NOJ, MRD, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.94	1/6550 (0.0%)	0.93	11/8930 (0.1%)
1	B	1.01	5/6538 (0.1%)	0.94	13/8913 (0.1%)
All	All	0.97	6/13088 (0.0%)	0.94	24/17843 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	541	CYS	CA-CB	6.87	1.69	1.53
1	A	541	CYS	CA-CB	6.63	1.68	1.53
1	B	820	ARG	CZ-NH2	6.09	1.41	1.33
1	B	511	TYR	CE1-CZ	5.67	1.46	1.38
1	B	541	CYS	CB-SG	5.49	1.91	1.82

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	521	ARG	NE-CZ-NH2	-16.07	112.27	120.30
1	A	521	ARG	NE-CZ-NH2	-15.81	112.39	120.30
1	A	521	ARG	NE-CZ-NH1	13.38	126.99	120.30
1	B	521	ARG	NE-CZ-NH1	12.77	126.69	120.30
1	A	70	LEU	CA-CB-CG	-8.84	94.98	115.30

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	6387	0	6096	51	0
1	B	6375	0	6082	34	0
2	A	50	0	43	0	0
3	A	28	0	26	0	0
3	B	42	0	39	0	0
4	A	39	0	34	1	0
4	B	78	0	68	0	0
5	A	56	0	50	1	0
6	A	116	0	97	0	0
6	B	116	0	97	0	0
7	A	166	0	140	3	0
7	B	166	0	140	3	0
8	A	16	0	28	11	0
8	B	8	0	14	2	0
9	A	11	0	13	0	0
9	B	11	0	13	0	0
10	B	61	0	52	0	0
11	B	94	0	79	0	0
12	B	8	0	14	4	0
13	A	450	0	0	0	0
13	B	504	0	0	5	0
All	All	14782	0	13125	98	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 4.

The worst 5 of 98 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)
12:B:947:MPD:C5	12:B:947:MPD:HM1	1.66	1.16
12:B:947:MPD:H53	12:B:947:MPD:CM	1.79	1.11
1:A:63:THR:HG21	1:A:333:MET:CE	1.83	1.08
1:A:63:THR:HG21	1:A:333:MET:HE2	1.33	1.06
1:A:63:THR:CG2	1:A:333:MET:CE	2.39	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	830/841 (99%)	795 (96%)	35 (4%)	0	100	100
1	B	828/841 (98%)	799 (96%)	29 (4%)	0	100	100
All	All	1658/1682 (99%)	1594 (96%)	64 (4%)	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%)	663 (99%)	8 (1%)	78	89
1	B	670/677 (99%)	664 (99%)	6 (1%)	84	93
All	All	1341/1354 (99%)	1327 (99%)	14 (1%)	82	91

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

Mol	Chain	Res	Type
1	A	700	LEU
1	A	701	THR
1	B	700	LEU
1	A	642	GLU
1	B	281	TRP

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 ⓘ

78 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	A	901	1,2	14,14,15	0.97	1 (7%)	15,19,21	1.54	2 (13%)
2	NAG	A	902	2	14,14,15	0.93	1 (7%)	15,19,21	1.74	3 (20%)
2	BMA	A	903	2	11,11,12	1.29	1 (9%)	14,15,17	2.03	3 (21%)
2	MAN	A	904	2	11,11,12	1.01	0	14,15,17	2.24	4 (28%)
4	NAG	A	906	1,4	14,14,15	1.03	1 (7%)	15,19,21	1.23	2 (13%)
4	NAG	A	907	4	14,14,15	0.81	0	15,19,21	1.60	3 (20%)
4	BMA	A	908	4	11,11,12	1.05	0	14,15,17	2.96	7 (50%)
5	NAG	A	909	1,5	14,14,15	0.59	0	15,19,21	1.34	2 (13%)
5	NAG	A	910	5	14,14,15	0.57	0	15,19,21	1.59	3 (20%)
6	NAG	A	911	1,6	14,14,15	1.20	1 (7%)	15,19,21	0.79	0
6	NAG	A	912	6	14,14,15	0.76	0	15,19,21	1.39	2 (13%)
6	BMA	A	913	6	11,11,12	0.88	0	14,15,17	1.91	4 (28%)
6	MAN	A	914	6	11,11,12	0.76	0	14,15,17	1.19	2 (14%)
6	MAN	A	915	6	11,11,12	1.16	2 (18%)	14,15,17	2.09	5 (35%)
6	MAN	A	916	6	11,11,12	0.64	0	14,15,17	1.82	3 (21%)
6	MAN	A	917	6	11,11,12	0.63	0	14,15,17	1.58	3 (21%)
6	MAN	A	918	6	11,11,12	0.60	0	14,15,17	1.65	4 (28%)
6	MAN	A	919	6	11,11,12	0.95	0	14,15,17	2.00	5 (35%)

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	0.97	1 (9%)	14,15,17	1.53	3 (21%)
5	NAG	A	921	1,5	14,14,15	0.78	0	15,19,21	1.56	2 (13%)
5	NAG	A	922	5	14,14,15	0.87	1 (7%)	15,19,21	1.31	2 (13%)
7	NAG	A	923	1,7	14,14,15	0.65	0	15,19,21	0.81	1 (6%)
7	NAG	A	924	7	14,14,15	0.91	0	15,19,21	1.70	4 (26%)
7	BMA	A	925	7	11,11,12	0.84	0	14,15,17	1.15	1 (7%)
7	MAN	A	926	7	11,11,12	0.72	0	14,15,17	1.86	2 (14%)
7	MAN	A	927	7	11,11,12	0.80	0	14,15,17	1.08	0
7	MAN	A	928	7	11,11,12	0.81	0	14,15,17	1.91	4 (28%)
7	MAN	A	929	7	11,11,12	0.63	0	14,15,17	1.66	3 (21%)
7	NAG	A	930	1,7	14,14,15	0.98	1 (7%)	15,19,21	1.83	2 (13%)
7	NAG	A	931	7	14,14,15	0.80	1 (7%)	15,19,21	1.40	2 (13%)
7	BMA	A	932	7	11,11,12	1.11	0	14,15,17	1.97	3 (21%)
7	MAN	A	933	7	11,11,12	0.92	0	14,15,17	1.43	2 (14%)
7	MAN	A	934	7	11,11,12	0.89	0	14,15,17	1.58	3 (21%)
7	MAN	A	935	7	11,11,12	0.58	0	14,15,17	2.11	5 (35%)
7	MAN	A	936	7	11,11,12	1.17	2 (18%)	14,15,17	3.84	7 (50%)
7	NAG	B	901	1,7	14,14,15	1.16	1 (7%)	15,19,21	1.55	3 (20%)
7	NAG	B	902	7	14,14,15	0.68	0	15,19,21	1.87	4 (26%)
7	BMA	B	903	7	11,11,12	0.94	0	14,15,17	1.73	2 (14%)
7	MAN	B	904	7	11,11,12	0.56	0	14,15,17	1.66	2 (14%)
7	MAN	B	905	7	11,11,12	0.87	0	14,15,17	1.33	2 (14%)
7	MAN	B	906	7	11,11,12	0.83	0	14,15,17	1.54	3 (21%)
7	MAN	B	907	7	11,11,12	0.98	0	14,15,17	2.47	8 (57%)
10	NAG	B	909	1,10	14,14,15	1.07	0	15,19,21	1.67	3 (20%)
10	NAG	B	910	10	14,14,15	0.81	0	15,19,21	1.32	2 (13%)
10	BMA	B	911	10	11,11,12	0.57	0	14,15,17	1.74	1 (7%)
10	MAN	B	912	10	11,11,12	1.14	1 (9%)	14,15,17	1.56	4 (28%)
10	MAN	B	913	10	11,11,12	0.91	0	14,15,17	1.75	3 (21%)
4	NAG	B	914	1,4	14,14,15	0.78	0	15,19,21	1.71	3 (20%)
4	NAG	B	915	4	14,14,15	0.73	0	15,19,21	1.75	4 (26%)
4	BMA	B	916	4	11,11,12	0.82	0	14,15,17	1.78	3 (21%)
6	NAG	B	917	1,6	14,14,15	1.15	2 (14%)	15,19,21	1.67	4 (26%)
6	NAG	B	918	6	14,14,15	1.01	0	15,19,21	1.08	2 (13%)
6	BMA	B	919	6	11,11,12	0.79	0	14,15,17	1.09	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	B	920	6	11,11,12	0.85	0	14,15,17	0.81	0
6	MAN	B	921	6	11,11,12	1.30	2 (18%)	14,15,17	2.10	6 (42%)
6	MAN	B	922	6	11,11,12	0.81	0	14,15,17	2.30	6 (42%)
6	MAN	B	923	6	11,11,12	0.57	0	14,15,17	2.55	6 (42%)
6	MAN	B	924	6	11,11,12	0.67	0	14,15,17	1.16	1 (7%)
6	MAN	B	925	6	11,11,12	0.94	0	14,15,17	1.45	2 (14%)
6	MAN	B	926	6	11,11,12	1.48	2 (18%)	14,15,17	2.15	4 (28%)
4	NAG	B	927	1,4	14,14,15	0.75	0	15,19,21	1.37	1 (6%)
4	NAG	B	928	4	14,14,15	0.94	0	15,19,21	1.47	4 (26%)
4	BMA	B	929	4	11,11,12	0.91	0	14,15,17	2.38	5 (35%)
7	NAG	B	930	1,7	14,14,15	0.85	0	15,19,21	1.48	3 (20%)
7	NAG	B	931	7	14,14,15	1.13	1 (7%)	15,19,21	1.82	5 (33%)
7	BMA	B	932	7	11,11,12	0.59	0	14,15,17	3.09	4 (28%)
7	MAN	B	933	7	11,11,12	1.08	1 (9%)	14,15,17	1.99	4 (28%)
7	MAN	B	934	7	11,11,12	1.34	2 (18%)	14,15,17	2.36	4 (28%)
7	MAN	B	935	7	11,11,12	0.61	0	14,15,17	1.15	0
7	MAN	B	936	7	11,11,12	0.90	0	14,15,17	1.40	2 (14%)
11	NAG	B	937	11,1	14,14,15	0.71	0	15,19,21	2.04	2 (13%)
11	NAG	B	938	11	14,14,15	0.87	1 (7%)	15,19,21	1.48	1 (6%)
11	BMA	B	939	11	11,11,12	1.02	0	14,15,17	1.23	2 (14%)
11	MAN	B	940	11	11,11,12	1.02	1 (9%)	14,15,17	1.80	4 (28%)
11	MAN	B	941	11	11,11,12	0.71	0	14,15,17	1.44	2 (14%)
11	MAN	B	942	11	11,11,12	0.72	0	14,15,17	2.25	3 (21%)
11	MAN	B	943	11	11,11,12	0.72	0	14,15,17	1.83	5 (35%)
11	MAN	B	944	11	11,11,12	1.07	1 (9%)	14,15,17	1.76	4 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	902	2	-	0/6/23/26	0/1/1/1
2	BMA	A	903	2	-	0/2/19/22	0/1/1/1
2	MAN	A	904	2	-	0/2/19/22	0/1/1/1
4	NAG	A	906	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
5	NAG	A	921	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	922	5	-	0/6/23/26	0/1/1/1
7	NAG	A	923	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	924	7	-	0/6/23/26	0/1/1/1
7	BMA	A	925	7	-	0/2/19/22	0/1/1/1
7	MAN	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	NAG	A	930	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	931	7	-	0/6/23/26	0/1/1/1
7	BMA	A	932	7	-	0/2/19/22	0/1/1/1
7	MAN	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	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
10	NAG	B	909	1,10	-	0/6/23/26	0/1/1/1
10	NAG	B	910	10	-	0/6/23/26	0/1/1/1
10	BMA	B	911	10	-	0/2/19/22	0/1/1/1
10	MAN	B	912	10	-	0/2/19/22	0/1/1/1
10	MAN	B	913	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	914	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	915	4	-	0/6/23/26	0/1/1/1
4	BMA	B	916	4	-	0/2/19/22	0/1/1/1
6	NAG	B	917	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	918	6	-	0/6/23/26	0/1/1/1
6	BMA	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
6	MAN	B	926	6	-	0/2/19/22	0/1/1/1
4	NAG	B	927	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	928	4	-	0/6/23/26	0/1/1/1
4	BMA	B	929	4	-	0/2/19/22	0/1/1/1
7	NAG	B	930	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	931	7	-	0/6/23/26	0/1/1/1
7	BMA	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
7	MAN	B	936	7	-	0/2/19/22	0/1/1/1
11	NAG	B	937	11,1	-	0/6/23/26	0/1/1/1
11	NAG	B	938	11	-	0/6/23/26	0/1/1/1
11	BMA	B	939	11	-	0/2/19/22	0/1/1/1
11	MAN	B	940	11	-	0/2/19/22	0/1/1/1
11	MAN	B	941	11	-	0/2/19/22	0/1/1/1
11	MAN	B	942	11	-	0/2/19/22	0/1/1/1
11	MAN	B	943	11	-	0/2/19/22	0/1/1/1
11	MAN	B	944	11	-	0/2/19/22	0/1/1/1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	934	MAN	O5-C1	-3.35	1.38	1.43
6	A	911	NAG	O5-C1	-3.01	1.38	1.43
7	A	930	NAG	C2-N2	-2.88	1.41	1.46
6	B	926	MAN	O5-C1	-2.64	1.39	1.43
6	B	921	MAN	O5-C1	-2.57	1.39	1.43

The worst 5 of 237 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	932	BMA	C6-C5-C4	-9.17	90.39	113.02
7	A	936	MAN	C1-C2-C3	-7.05	101.20	109.54
6	B	923	MAN	O6-C6-C5	-5.57	92.91	111.33
7	A	926	MAN	O5-C1-C2	-4.95	102.83	110.86
4	A	908	BMA	O3-C3-C2	-4.32	102.19	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	907	NAG	1	0
5	A	909	NAG	1	0
5	A	910	NAG	1	0
7	A	925	BMA	3	0
7	B	901	NAG	1	0
7	B	932	BMA	2	0
7	B	934	MAN	2	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	905	1	14,14,15	0.90	0	15,19,21	1.34	2 (13%)
3	NAG	A	937	1	14,14,15	0.56	0	15,19,21	1.78	4 (26%)
8	MRD	A	938	-	6,7,7	0.29	0	7,10,10	0.73	0
8	MRD	A	939	-	6,7,7	0.67	0	7,10,10	1.24	1 (14%)
9	NOJ	A	940	-	11,11,11	0.48	0	11,15,15	1.14	1 (9%)
3	NAG	B	908	1	14,14,15	0.80	0	15,19,21	1.25	3 (20%)
3	NAG	B	945	1	14,14,15	0.56	0	15,19,21	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	946	1	14,14,15	0.67	0	15,19,21	1.23	1 (6%)
12	MPD	B	947	-	6,7,7	0.54	0	7,10,10	1.27	1 (14%)
8	MRD	B	948	-	6,7,7	0.84	0	7,10,10	0.37	0
9	NOJ	B	949	-	11,11,11	1.53	3 (27%)	11,15,15	1.75	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
3	NAG	A	905	1	-	0/6/23/26	0/1/1/1
3	NAG	A	937	1	-	0/6/23/26	0/1/1/1
8	MRD	A	938	-	-	0/5/5/5	0/0/0/0
8	MRD	A	939	-	-	0/5/5/5	0/0/0/0
9	NOJ	A	940	-	-	0/2/19/19	0/1/1/1
3	NAG	B	908	1	-	0/6/23/26	0/1/1/1
3	NAG	B	945	1	-	0/6/23/26	0/1/1/1
3	NAG	B	946	1	-	0/6/23/26	0/1/1/1
12	MPD	B	947	-	-	0/5/5/5	0/0/0/0
8	MRD	B	948	-	-	0/5/5/5	0/0/0/0
9	NOJ	B	949	-	-	0/2/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	949	NOJ	C2-C3	2.66	1.56	1.52
9	B	949	NOJ	C5-N5	2.68	1.50	1.47
9	B	949	NOJ	C1-C2	2.71	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	937	NAG	C3-C4-C5	-3.63	103.87	110.20
3	A	937	NAG	C4-C3-C2	-3.04	106.50	111.23
9	B	949	NOJ	O2-C2-C1	-2.98	103.61	109.57
3	A	905	NAG	O7-C7-C8	-2.87	116.79	122.06
8	A	939	MRD	C2-C3-C4	-2.55	104.62	116.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	938	MRD	2	0
8	A	939	MRD	9	0
12	B	947	MPD	4	0
8	B	948	MRD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	834/841 (99%)	-0.32	17 (2%) 68 75	11, 21, 36, 74	0
1	B	832/841 (98%)	-0.48	1 (0%) 95 97	11, 18, 32, 56	0
All	All	1666/1682 (99%)	-0.40	18 (1%) 82 86	11, 20, 34, 74	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	MET	3.0
1	A	144	ALA	3.0
1	A	675	VAL	2.9
1	A	277	VAL	2.6
1	B	573	LEU	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
7	MAN	A	929	11/12	0.97	0.17	7.24	29,31,40,49	0
7	NAG	A	923	14/15	0.95	0.15	5.68	18,26,39,42	0
4	NAG	A	907	14/15	0.94	0.12	2.89	24,31,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	NAG	B	910	14/15	0.96	0.13	2.88	27,29,35,42	0
11	MAN	B	941	11/12	0.96	0.16	2.14	27,35,47,52	0
5	NAG	A	921	14/15	0.96	0.10	1.72	29,36,44,47	0
6	MAN	A	919	11/12	0.96	0.12	1.72	24,28,35,39	0
7	MAN	B	936	11/12	0.95	0.13	1.27	26,31,37,39	0
6	MAN	A	918	11/12	0.97	0.13	1.24	21,22,26,27	0
7	MAN	B	906	11/12	0.96	0.13	0.73	28,31,36,40	0
7	NAG	B	930	14/15	0.95	0.10	0.54	16,24,41,41	0
6	NAG	A	911	14/15	0.97	0.13	0.37	24,28,31,31	0
7	NAG	B	901	14/15	0.96	0.09	-0.18	14,17,20,21	0
6	MAN	B	926	11/12	0.97	0.08	-0.25	18,20,20,25	0
2	NAG	A	901	14/15	0.96	0.09	-0.28	19,25,26,27	0
6	NAG	B	918	14/15	0.96	0.09	-0.31	18,20,27,30	0
6	NAG	A	912	14/15	0.97	0.10	-0.44	26,27,31,31	0
4	NAG	B	927	14/15	0.97	0.08	-0.52	26,33,46,54	0
10	NAG	B	909	14/15	0.97	0.09	-0.55	21,24,27,28	0
7	MAN	A	933	11/12	0.95	0.10	-0.66	27,34,41,52	0
6	MAN	B	923	11/12	0.98	0.08	-0.68	21,23,30,32	0
2	NAG	A	902	14/15	0.96	0.09	-0.74	27,31,36,39	0
6	NAG	B	917	14/15	0.97	0.07	-0.78	17,20,23,25	0
11	NAG	B	937	14/15	0.97	0.07	-0.83	19,23,26,27	0
6	MAN	A	917	11/12	0.96	0.09	-0.83	23,25,27,27	0
7	NAG	A	930	14/15	0.97	0.08	-0.92	21,24,26,31	0
5	NAG	A	909	14/15	0.96	0.08	-1.02	18,24,27,29	0
4	NAG	A	906	14/15	0.96	0.08	-1.03	19,25,30,34	0
7	NAG	B	902	14/15	0.98	0.07	-1.12	16,21,25,31	0
6	MAN	B	925	11/12	0.98	0.07	-1.28	15,17,20,24	0
4	NAG	B	914	14/15	0.98	0.07	-1.36	15,19,22,23	0
4	NAG	B	915	14/15	0.94	0.14	-	20,32,45,51	0
7	MAN	B	905	11/12	0.94	0.19	-	33,37,46,61	0
7	NAG	A	931	14/15	0.95	0.13	-	26,32,42,45	0
7	MAN	B	904	11/12	0.96	0.16	-	28,34,39,41	0
4	NAG	B	928	14/15	0.93	0.18	-	39,42,50,57	0
7	BMA	B	903	11/12	0.94	0.09	-	26,28,32,32	0
11	BMA	B	939	11/12	0.93	0.15	-	37,44,55,66	0
11	MAN	B	940	11/12	0.81	0.22	-	62,72,77,79	0
6	MAN	B	924	11/12	0.92	0.13	-	29,37,42,43	0
6	MAN	A	920	11/12	0.93	0.16	-	33,38,43,43	0
6	BMA	A	913	11/12	0.98	0.09	-	24,26,29,31	0
10	MAN	B	913	11/12	0.73	0.28	-	56,66,70,73	0
2	BMA	A	903	11/12	0.92	0.09	-	32,39,46,47	0
7	MAN	A	935	11/12	0.89	0.21	-	50,56,59,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	MAN	B	922	11/12	0.98	0.08	-	17,19,20,21	0
7	NAG	A	924	14/15	0.93	0.15	-	18,26,37,39	0
11	MAN	B	943	11/12	0.89	0.24	-	51,58,63,67	0
7	MAN	B	933	11/12	0.74	0.30	-	71,76,79,85	0
7	BMA	B	932	11/12	0.92	0.17	-	34,39,47,54	0
4	BMA	B	916	11/12	0.80	0.29	-	57,75,80,91	0
4	BMA	A	908	11/12	0.93	0.25	-	38,43,52,56	0
7	MAN	A	936	11/12	0.83	0.22	-	51,57,67,69	0
5	NAG	A	910	14/15	0.96	0.13	-	32,37,42,47	0
6	MAN	A	915	11/12	0.94	0.17	-	35,45,55,58	0
11	NAG	B	938	14/15	0.94	0.13	-	25,35,42,44	0
7	MAN	A	934	11/12	0.97	0.11	-	28,35,45,49	0
7	MAN	B	935	11/12	0.97	0.14	-	27,30,34,40	0
2	MAN	A	904	11/12	0.87	0.15	-	42,50,53,58	0
7	MAN	A	927	11/12	0.94	0.17	-	30,36,41,46	0
7	MAN	A	928	11/12	0.98	0.15	-	25,27,28,32	0
11	MAN	B	944	11/12	0.78	0.22	-	45,61,66,70	0
6	MAN	A	916	11/12	0.98	0.08	-	17,20,23,23	0
7	MAN	B	907	11/12	0.93	0.11	-	34,38,42,44	0
7	BMA	A	932	11/12	0.93	0.14	-	38,43,49,53	0
11	MAN	B	942	11/12	0.96	0.13	-	26,33,38,48	0
7	MAN	B	934	11/12	0.93	0.17	-	30,35,41,41	0
4	BMA	B	929	11/12	0.85	0.25	-	56,65,69,69	0
6	MAN	B	920	11/12	0.98	0.08	-	19,22,24,31	0
7	BMA	A	925	11/12	0.91	0.19	-	32,35,43,53	0
5	NAG	A	922	14/15	0.88	0.20	-	49,56,64,65	0
7	MAN	A	926	11/12	0.82	0.34	-	66,68,75,77	0
7	NAG	B	931	14/15	0.92	0.17	-	23,28,38,38	0
6	BMA	B	919	11/12	0.97	0.07	-	20,22,25,26	0
6	MAN	A	914	11/12	0.97	0.13	-	30,34,38,41	0
6	MAN	B	921	11/12	0.91	0.12	-	32,38,45,48	0
10	MAN	B	912	11/12	0.67	0.24	-	71,78,86,88	0
10	BMA	B	911	11/12	0.92	0.16	-	47,53,62,78	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(\AA^2)	Q<0.9
8	MRD	A	939	8/8	0.92	0.15	10.23	24,28,37,37	0
12	MPD	B	947	8/8	0.93	0.15	6.89	26,32,40,44	0
8	MRD	B	948	8/8	0.95	0.17	4.78	38,45,48,52	0
3	NAG	B	946	14/15	0.96	0.22	4.36	29,35,40,43	0
9	NOJ	B	949	11/11	0.98	0.17	0.55	14,15,17,18	0
9	NOJ	A	940	11/11	0.99	0.23	0.53	17,21,22,24	0
8	MRD	A	938	8/8	0.96	0.11	0.42	36,38,40,41	0
3	NAG	A	937	14/15	0.96	0.14	-0.06	39,45,50,52	0
3	NAG	B	908	14/15	0.90	0.27	-	44,58,67,69	0
3	NAG	A	905	14/15	0.83	0.33	-	49,63,72,73	0
3	NAG	B	945	14/15	0.91	0.23	-	45,60,67,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.