



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:31 PM GMT

PDB ID : 4IIB
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus*
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on : 2012-12-20
Resolution : 1.80 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

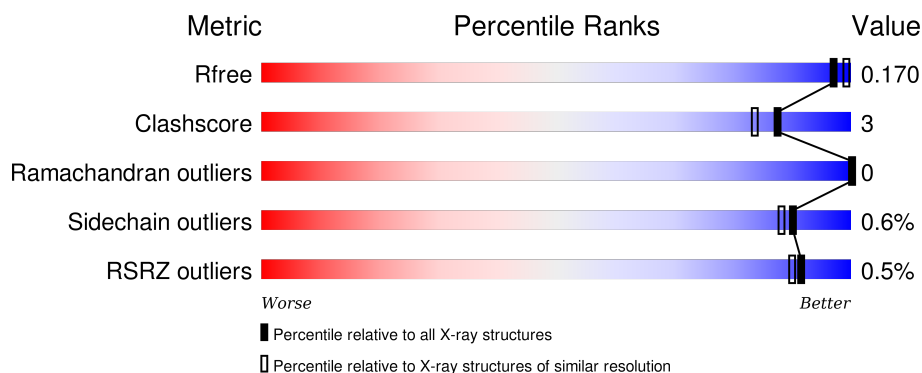
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 10px; right: 0;">91%</div> <div style="position: absolute; top: 10px; right: 10px;">7% .</div> </div> </div>
1	B	841	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 10px; right: 0;">90%</div> <div style="position: absolute; top: 10px; right: 10px;">8% ..</div> </div> </div>

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	MRD	A	942	-	-	-	X
10	MRD	A	943	-	-	-	X
10	MRD	B	947	-	-	-	X
10	MRD	B	948	-	-	-	X
10	MRD	B	949	-	-	-	X
14	MAN	B	942	-	-	-	X
2	MAN	A	904	-	-	X	-
2	NAG	B	910	-	-	-	X
3	NAG	B	946	-	-	-	X
4	NAG	A	909	-	-	-	X
7	MAN	B	907	-	-	-	X
8	NAG	A	926	-	-	-	X
8	MAN	A	932	-	-	-	X
8	MAN	A	936	-	-	-	X
8	MAN	B	937	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 15992 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.

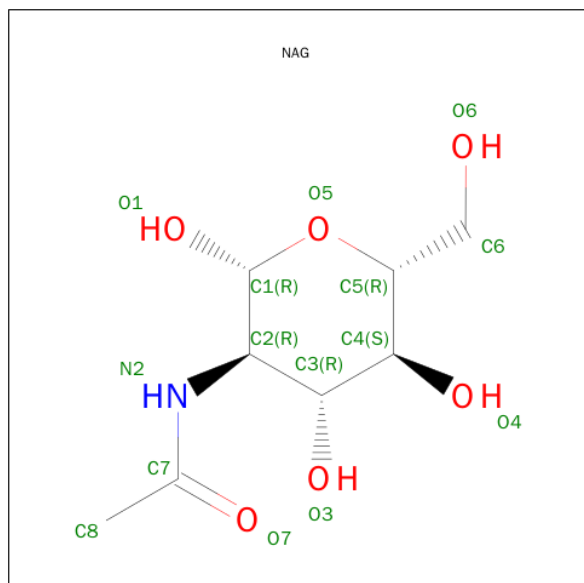
- Molecule 1 is a protein called Beta-glucosidase 1.

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 (6-MER).

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

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



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

- 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 (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 7 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is a polymer of unknown type called SUGAR (7-MER).

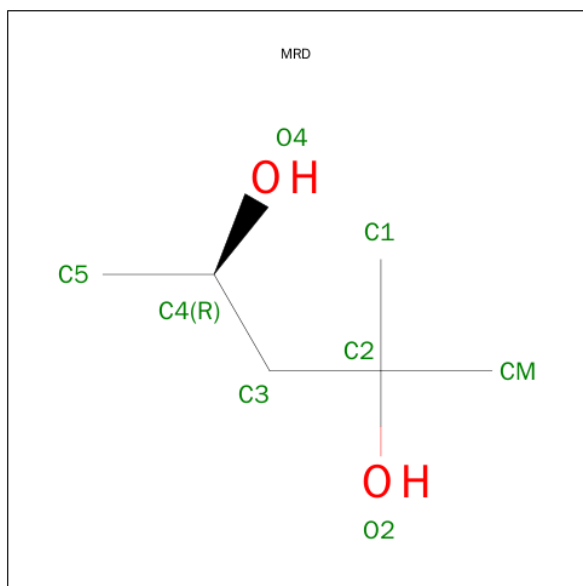
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	7	Total	C	N	O	0	0
			83	46	2	35		
8	A	7	Total	C	N	O	0	0
			83	46	2	35		
8	B	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 10 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



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

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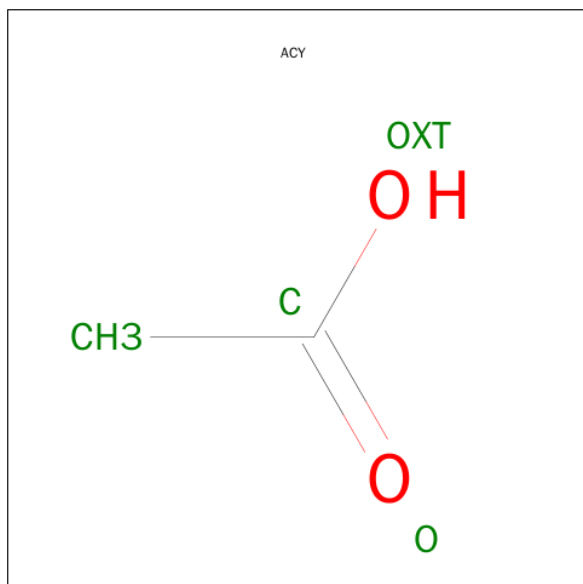
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			8	6	2		
10	B	1	Total	C	O	0	0
			8	6	2		
10	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 12 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			4	2	2		
12	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 13 is a polymer of unknown type called SUGAR (10-MER).

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

- Molecule 14 is a polymer of unknown type called SUGAR (8-MER).

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

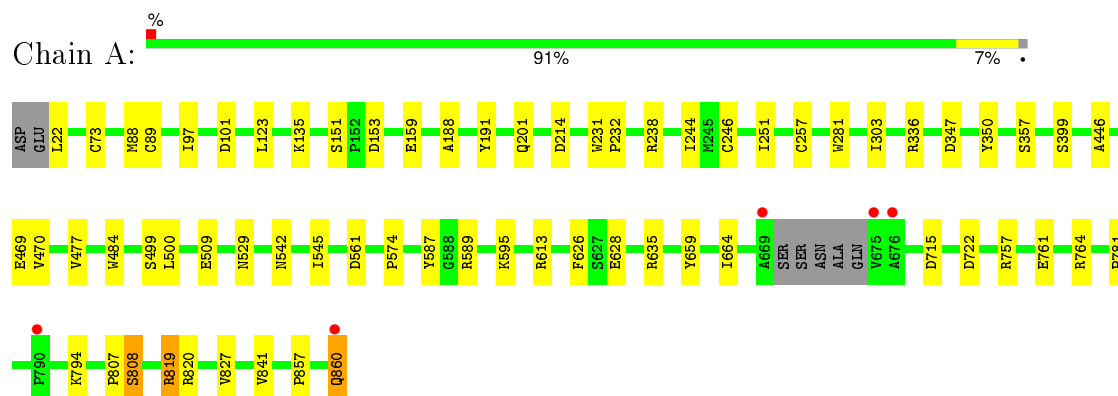
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1027	Total	O	0	0
			1027	1027		
15	B	1103	Total	O	0	0
			1103	1103		

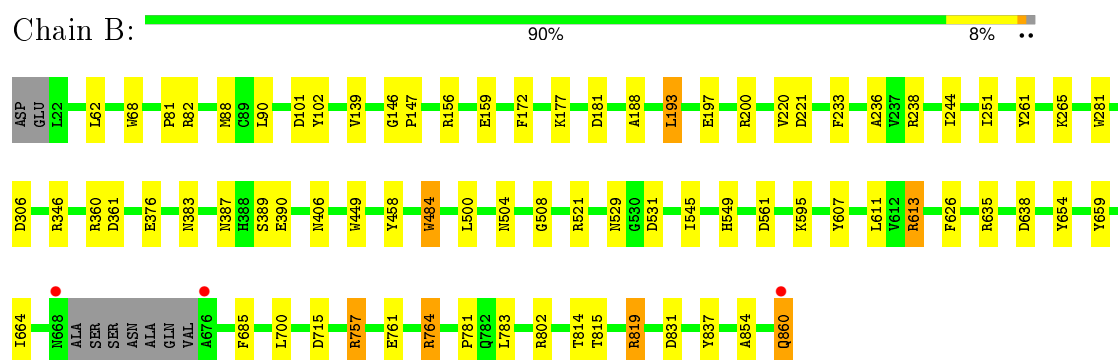
3 Residue-property plots [i](#)

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	82.16Å 123.02Å 222.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.49 – 1.80 34.49 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.49-1.80) 99.9 (34.49-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.58 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.137 , 0.169 0.137 , 0.170	Depositor DCC
R_{free} test set	10460 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 207752 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15992	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 2.53% 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, NA, MRD, ACY, 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	1.48	18/6550 (0.3%)	1.22	28/8930 (0.3%)
1	B	1.48	16/6538 (0.2%)	1.25	33/8913 (0.4%)
All	All	1.48	34/13088 (0.3%)	1.23	61/17843 (0.3%)

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	GLU	CD-OE2	-7.73	1.17	1.25
1	A	761	GLU	CD-OE2	-7.13	1.17	1.25
1	B	761	GLU	CD-OE2	-6.91	1.18	1.25
1	B	458	TYR	CG-CD2	6.30	1.47	1.39
1	A	561	ASP	CG-OD2	5.94	1.39	1.25

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	819	ARG	NE-CZ-NH1	-12.85	113.87	120.30
1	B	764	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	A	336	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	764	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	589	ARG	NE-CZ-NH2	-8.61	116.00	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	6387	0	6097	22	0
1	B	6375	0	6083	26	0
2	A	72	0	61	6	0
2	B	144	0	121	3	0
3	A	28	0	26	0	0
3	B	28	0	26	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	105	0	88	3	0
7	A	11	0	10	3	0
7	B	11	0	10	2	0
8	A	166	0	138	2	0
8	B	83	0	69	1	0
9	A	8	0	14	0	0
10	A	16	0	28	2	0
10	B	24	0	42	5	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
12	A	4	0	3	0	0
12	B	4	0	3	0	0
13	B	116	0	97	0	0
14	B	94	0	77	0	0
15	A	1027	0	0	7	0
15	B	1103	0	0	8	0
All	All	15992	0	13153	69	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 69 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)
2:A:903:BMA:C3	2:A:904:MAN:H5	1.82	1.09
2:A:903:BMA:H3	2:A:904:MAN:H5	1.36	1.07
2:A:903:BMA:H3	2:A:904:MAN:C5	1.84	1.07
2:A:903:BMA:C3	2:A:904:MAN:C5	2.45	0.94
1:A:819:ARG:HH12	1:A:860:GLN:C	1.71	0.92

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%)	807 (97%)	23 (3%)	0	100	100
1	B	828/841 (98%)	802 (97%)	26 (3%)	0	100	100
All	All	1658/1682 (99%)	1609 (97%)	49 (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%)	668 (100%)	3 (0%)	93	92
1	B	670/677 (99%)	665 (99%)	5 (1%)	88	86
All	All	1341/1354 (99%)	1333 (99%)	8 (1%)	90	88

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	PRO
1	B	860	GLN
1	B	700	LEU
1	A	860	GLN
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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	1.53	3 (21%)	15,19,21	1.98	5 (33%)
2	NAG	A	902	2	14,14,15	1.00	2 (14%)	15,19,21	2.32	9 (60%)
2	BMA	A	903	2	11,11,12	0.94	1 (9%)	14,15,17	2.96	5 (35%)
2	MAN	A	904	2	11,11,12	1.81	3 (27%)	14,15,17	4.18	10 (71%)
2	MAN	A	905	2	11,11,12	0.70	0	14,15,17	1.87	4 (28%)
2	MAN	A	906	2	11,11,12	0.77	0	14,15,17	2.09	6 (42%)
4	NAG	A	908	1,4	14,14,15	1.65	2 (14%)	15,19,21	1.97	4 (26%)
4	NAG	A	909	4	14,14,15	1.53	2 (14%)	15,19,21	2.71	6 (40%)
4	BMA	A	910	4	11,11,12	1.17	1 (9%)	14,15,17	3.12	6 (42%)
5	NAG	A	911	1,5	14,14,15	0.95	1 (7%)	15,19,21	1.94	4 (26%)
5	NAG	A	912	5	14,14,15	1.59	2 (14%)	15,19,21	2.26	6 (40%)
6	NAG	A	913	1,6	14,14,15	1.53	3 (21%)	15,19,21	1.57	3 (20%)
6	NAG	A	914	6	14,14,15	1.93	1 (7%)	15,19,21	1.57	2 (13%)
6	BMA	A	915	6	11,11,12	1.27	2 (18%)	14,15,17	1.73	4 (28%)
6	MAN	A	916	6	11,11,12	1.12	1 (9%)	14,15,17	2.13	5 (35%)

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	1.49	2 (18%)	14,15,17	2.59	8 (57%)
6	MAN	A	918	6	11,11,12	0.79	0	14,15,17	1.27	2 (14%)
6	MAN	A	919	6	11,11,12	1.49	2 (18%)	14,15,17	1.35	2 (14%)
6	MAN	A	920	6	11,11,12	1.27	1 (9%)	14,15,17	1.48	1 (7%)
6	MAN	A	921	7,6	11,11,12	1.28	2 (18%)	14,15,17	1.88	5 (35%)
4	NAG	A	923	1,4	14,14,15	0.95	1 (7%)	15,19,21	1.75	5 (33%)
4	NAG	A	924	4	14,14,15	1.11	2 (14%)	15,19,21	1.57	4 (26%)
4	BMA	A	925	4	11,11,12	0.92	1 (9%)	14,15,17	2.28	5 (35%)
8	NAG	A	926	1,8	14,14,15	1.45	2 (14%)	15,19,21	2.26	6 (40%)
8	NAG	A	927	8	14,14,15	0.98	0	15,19,21	2.27	5 (33%)
8	BMA	A	928	8	11,11,12	1.21	1 (9%)	14,15,17	1.20	1 (7%)
8	MAN	A	929	8	11,11,12	0.84	0	14,15,17	2.07	6 (42%)
8	MAN	A	930	8	11,11,12	0.99	1 (9%)	14,15,17	2.32	7 (50%)
8	MAN	A	931	8	11,11,12	1.07	1 (9%)	14,15,17	2.85	7 (50%)
8	MAN	A	932	8	11,11,12	1.13	1 (9%)	14,15,17	1.27	1 (7%)
8	NAG	A	933	1,8,11	14,14,15	0.79	0	15,19,21	1.57	3 (20%)
8	NAG	A	934	8	14,14,15	1.26	2 (14%)	15,19,21	1.62	4 (26%)
8	BMA	A	935	8	11,11,12	0.96	0	14,15,17	2.21	4 (28%)
8	MAN	A	936	8	11,11,12	1.29	1 (9%)	14,15,17	1.60	2 (14%)
8	MAN	A	937	8	11,11,12	1.21	1 (9%)	14,15,17	1.44	3 (21%)
8	MAN	A	938	8	11,11,12	1.12	0	14,15,17	2.67	5 (35%)
8	MAN	A	939	8	11,11,12	1.18	2 (18%)	14,15,17	1.71	2 (14%)
2	NAG	B	901	1,2	14,14,15	1.66	3 (21%)	15,19,21	1.97	6 (40%)
2	NAG	B	902	2	14,14,15	1.06	1 (7%)	15,19,21	2.43	6 (40%)
2	BMA	B	903	2	11,11,12	1.73	3 (27%)	14,15,17	3.22	5 (35%)
2	MAN	B	904	2	11,11,12	1.14	1 (9%)	14,15,17	1.85	5 (35%)
2	MAN	B	905	2,7	11,11,12	1.09	0	14,15,17	2.25	6 (42%)
2	MAN	B	906	2	11,11,12	0.87	0	14,15,17	2.61	6 (42%)
2	NAG	B	909	1,2	14,14,15	1.03	1 (7%)	15,19,21	1.61	3 (20%)
2	NAG	B	910	2	14,14,15	1.95	6 (42%)	15,19,21	2.44	7 (46%)
2	BMA	B	911	2	11,11,12	0.96	1 (9%)	14,15,17	1.39	2 (14%)
2	MAN	B	912	2	11,11,12	1.47	1 (9%)	14,15,17	1.92	2 (14%)
2	MAN	B	913	2	11,11,12	0.77	0	14,15,17	1.95	3 (21%)
2	MAN	B	914	2	11,11,12	1.22	1 (9%)	14,15,17	1.19	1 (7%)
4	NAG	B	915	1,4	14,14,15	1.33	1 (7%)	15,19,21	1.30	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	916	4	14,14,15	1.07	1 (7%)	15,19,21	1.74	5 (33%)
4	BMA	B	917	4	11,11,12	0.88	0	14,15,17	2.45	5 (35%)
13	NAG	B	918	1,13	14,14,15	0.97	0	15,19,21	1.91	3 (20%)
13	NAG	B	919	13	14,14,15	1.31	1 (7%)	15,19,21	1.81	2 (13%)
13	BMA	B	920	13	11,11,12	1.27	1 (9%)	14,15,17	2.29	7 (50%)
13	MAN	B	921	13	11,11,12	1.11	0	14,15,17	2.36	6 (42%)
13	MAN	B	922	13	11,11,12	0.77	0	14,15,17	2.04	4 (28%)
13	MAN	B	923	13	11,11,12	0.95	0	14,15,17	1.71	3 (21%)
13	MAN	B	924	13	11,11,12	1.41	1 (9%)	14,15,17	2.93	9 (64%)
13	MAN	B	925	13	11,11,12	1.14	0	14,15,17	1.45	4 (28%)
13	MAN	B	926	13	11,11,12	1.62	2 (18%)	14,15,17	2.59	6 (42%)
13	MAN	B	927	13	11,11,12	1.45	3 (27%)	14,15,17	1.77	4 (28%)
4	NAG	B	928	1,4	14,14,15	1.06	1 (7%)	15,19,21	2.12	3 (20%)
4	NAG	B	929	4	14,14,15	1.18	2 (14%)	15,19,21	2.08	4 (26%)
4	BMA	B	930	4	11,11,12	1.25	1 (9%)	14,15,17	2.30	6 (42%)
8	NAG	B	931	1,8	14,14,15	1.49	4 (28%)	15,19,21	1.82	6 (40%)
8	NAG	B	932	8	14,14,15	0.88	0	15,19,21	2.04	6 (40%)
8	BMA	B	933	8	11,11,12	1.06	1 (9%)	14,15,17	2.35	4 (28%)
8	MAN	B	934	8	11,11,12	1.15	1 (9%)	14,15,17	2.46	5 (35%)
8	MAN	B	935	8	11,11,12	1.59	2 (18%)	14,15,17	2.46	7 (50%)
8	MAN	B	936	8	11,11,12	1.42	2 (18%)	14,15,17	2.34	5 (35%)
8	MAN	B	937	8	11,11,12	1.34	2 (18%)	14,15,17	2.10	7 (50%)
14	NAG	B	938	1,11,14	14,14,15	1.32	2 (14%)	15,19,21	1.95	6 (40%)
14	NAG	B	939	14	14,14,15	1.03	0	15,19,21	1.71	5 (33%)
14	BMA	B	940	14	11,11,12	1.10	2 (18%)	14,15,17	1.36	3 (21%)
14	MAN	B	941	14	11,11,12	1.18	0	14,15,17	2.56	8 (57%)
14	MAN	B	942	14	11,11,12	1.42	1 (9%)	14,15,17	2.21	7 (50%)
14	MAN	B	943	14	11,11,12	1.22	1 (9%)	14,15,17	1.56	3 (21%)
14	MAN	B	944	14	11,11,12	1.00	1 (9%)	14,15,17	1.54	4 (28%)
14	MAN	B	945	14	11,11,12	1.36	2 (18%)	14,15,17	2.48	5 (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
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
4	NAG	A	908	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	909	4	-	0/6/23/26	0/1/1/1
4	BMA	A	910	4	-	0/2/19/22	0/1/1/1
5	NAG	A	911	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	912	5	-	0/6/23/26	0/1/1/1
6	NAG	A	913	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	914	6	-	0/6/23/26	0/1/1/1
6	BMA	A	915	6	-	0/2/19/22	0/1/1/1
6	MAN	A	916	6	-	0/2/19/22	0/1/1/1
6	MAN	A	917	6	-	0/2/19/22	0/1/1/1
6	MAN	A	918	6	-	0/2/19/22	0/1/1/1
6	MAN	A	919	6	-	0/2/19/22	0/1/1/1
6	MAN	A	920	6	-	0/2/19/22	0/1/1/1
6	MAN	A	921	7,6	-	0/2/19/22	0/1/1/1
4	NAG	A	923	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	924	4	-	0/6/23/26	0/1/1/1
4	BMA	A	925	4	-	0/2/19/22	0/1/1/1
8	NAG	A	926	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	927	8	-	0/6/23/26	0/1/1/1
8	BMA	A	928	8	-	0/2/19/22	0/1/1/1
8	MAN	A	929	8	-	0/2/19/22	0/1/1/1
8	MAN	A	930	8	-	0/2/19/22	0/1/1/1
8	MAN	A	931	8	-	0/2/19/22	0/1/1/1
8	MAN	A	932	8	-	0/2/19/22	0/1/1/1
8	NAG	A	933	1,8,11	-	0/6/23/26	0/1/1/1
8	NAG	A	934	8	-	0/6/23/26	0/1/1/1
8	BMA	A	935	8	-	0/2/19/22	0/1/1/1
8	MAN	A	936	8	-	0/2/19/22	0/1/1/1
8	MAN	A	937	8	-	0/2/19/22	0/1/1/1
8	MAN	A	938	8	-	0/2/19/22	0/1/1/1
8	MAN	A	939	8	-	0/2/19/22	0/1/1/1
2	NAG	B	901	1,2	-	0/6/23/26	0/1/1/1
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	2,7	-	0/2/19/22	0/1/1/1
2	MAN	B	906	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	909	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	910	2	-	0/6/23/26	0/1/1/1
2	BMA	B	911	2	-	0/2/19/22	0/1/1/1
2	MAN	B	912	2	-	0/2/19/22	0/1/1/1
2	MAN	B	913	2	-	0/2/19/22	0/1/1/1
2	MAN	B	914	2	-	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
13	NAG	B	918	1,13	-	0/6/23/26	0/1/1/1
13	NAG	B	919	13	-	0/6/23/26	0/1/1/1
13	BMA	B	920	13	-	0/2/19/22	0/1/1/1
13	MAN	B	921	13	-	0/2/19/22	0/1/1/1
13	MAN	B	922	13	-	0/2/19/22	0/1/1/1
13	MAN	B	923	13	-	0/2/19/22	0/1/1/1
13	MAN	B	924	13	-	0/2/19/22	0/1/1/1
13	MAN	B	925	13	-	0/2/19/22	0/1/1/1
13	MAN	B	926	13	-	0/2/19/22	0/1/1/1
13	MAN	B	927	13	-	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
8	NAG	B	931	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	932	8	-	0/6/23/26	0/1/1/1
8	BMA	B	933	8	-	0/2/19/22	0/1/1/1
8	MAN	B	934	8	-	0/2/19/22	0/1/1/1
8	MAN	B	935	8	-	0/2/19/22	0/1/1/1
8	MAN	B	936	8	-	0/2/19/22	0/1/1/1
8	MAN	B	937	8	-	0/2/19/22	0/1/1/1
14	NAG	B	938	1,11,14	-	0/6/23/26	0/1/1/1
14	NAG	B	939	14	-	0/6/23/26	0/1/1/1
14	BMA	B	940	14	-	0/2/19/22	0/1/1/1
14	MAN	B	941	14	-	0/2/19/22	0/1/1/1
14	MAN	B	942	14	-	0/2/19/22	0/1/1/1
14	MAN	B	943	14	-	0/2/19/22	0/1/1/1
14	MAN	B	944	14	-	0/2/19/22	0/1/1/1
14	MAN	B	945	14	-	0/2/19/22	0/1/1/1

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	935	MAN	O2-C2	-4.12	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	912	NAG	C8-C7	-3.59	1.43	1.50
2	B	914	MAN	O5-C1	-3.14	1.38	1.43
2	A	904	MAN	C4-C5	-3.03	1.46	1.53
6	A	921	MAN	O5-C1	-3.03	1.38	1.43

The worst 5 of 372 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	904	MAN	C1-C2-C3	-8.56	99.41	109.54
2	B	903	BMA	C1-C2-C3	-7.90	100.20	109.54
2	A	903	BMA	O3-C3-C2	-7.72	96.04	110.00
4	A	909	NAG	C1-O5-C5	-6.87	103.53	112.25
8	B	934	MAN	O5-C1-C2	-6.58	100.18	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	903	BMA	5	0
2	A	904	MAN	6	0
4	A	908	NAG	1	0
4	A	909	NAG	1	0
5	A	912	NAG	3	0
6	A	921	MAN	3	0
8	A	926	NAG	1	0
8	A	928	BMA	1	0
2	B	905	MAN	2	0
2	B	909	NAG	1	0
8	B	933	BMA	1	0

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	907	1	14,14,15	0.94	1 (7%)	15,19,21	1.35	2 (13%)
7	MAN	A	922	6	11,11,12	0.58	0	14,15,17	2.35	4 (28%)
3	NAG	A	940	1	14,14,15	0.85	1 (7%)	15,19,21	1.40	4 (26%)
9	MPD	A	941	-	6,7,7	0.89	0	7,10,10	1.54	1 (14%)
10	MRD	A	942	-	6,7,7	1.34	1 (16%)	7,10,10	1.36	1 (14%)
10	MRD	A	943	-	6,7,7	1.05	0	7,10,10	0.27	0
12	ACY	A	945	-	1,3,3	3.88	1 (100%)	0,3,3	0.00	-
7	MAN	B	907	2	11,11,12	1.07	1 (9%)	14,15,17	2.65	6 (42%)
3	NAG	B	908	1	14,14,15	1.15	2 (14%)	15,19,21	2.67	6 (40%)
3	NAG	B	946	1	14,14,15	0.79	0	15,19,21	1.59	2 (13%)
10	MRD	B	947	-	6,7,7	1.06	1 (16%)	7,10,10	0.72	0
10	MRD	B	948	-	6,7,7	1.34	1 (16%)	7,10,10	1.27	0
10	MRD	B	949	-	6,7,7	1.08	0	7,10,10	1.56	1 (14%)
12	ACY	B	951	-	1,3,3	6.21	1 (100%)	0,3,3	0.00	-

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	907	1	-	0/6/23/26	0/1/1/1
7	MAN	A	922	6	-	0/2/19/22	0/1/1/1
3	NAG	A	940	1	-	0/6/23/26	0/1/1/1
9	MPD	A	941	-	-	0/5/5/5	0/0/0/0
10	MRD	A	942	-	-	0/5/5/5	0/0/0/0
10	MRD	A	943	-	-	0/5/5/5	0/0/0/0
12	ACY	A	945	-	-	0/0/0/0	0/0/0/0
7	MAN	B	907	2	-	0/2/19/22	0/1/1/1
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
10	MRD	B	947	-	-	0/5/5/5	0/0/0/0
10	MRD	B	948	-	-	0/5/5/5	0/0/0/0
10	MRD	B	949	-	-	0/5/5/5	0/0/0/0
12	ACY	B	951	-	-	0/0/0/0	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	907	NAG	O5-C1	-2.66	1.39	1.43
3	B	908	NAG	O5-C1	-2.17	1.40	1.43
3	A	940	NAG	C1-C2	-2.12	1.49	1.52
3	B	908	NAG	C2-N2	-2.01	1.42	1.46
10	A	942	MRD	CM-C2	2.06	1.59	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	908	NAG	C4-C3-C2	-7.21	100.01	111.23
7	B	907	MAN	O2-C2-C1	-5.03	99.12	109.21
7	A	922	MAN	O2-C2-C1	-4.25	100.69	109.21
9	A	941	MPD	CM-C2-C1	-3.81	101.94	110.24
3	B	946	NAG	C1-O5-C5	-3.75	107.49	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	922	MAN	3	0
10	A	942	MRD	2	0
7	B	907	MAN	2	0
10	B	948	MRD	4	0
10	B	949	MRD	1	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%)	-0.55	5 (0%) 90 88	5, 12, 23, 55	0
1	B	832/841 (98%)	-0.59	3 (0%) 93 91	5, 9, 20, 51	0
All	All	1666/1682 (99%)	-0.57	8 (0%) 91 90	5, 10, 22, 55	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	675	VAL	3.8
1	B	668	ASN	3.2
1	B	860	GLN	3.0
1	A	860	GLN	2.8
1	A	669	ALA	2.7

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
8	MAN	A	932	11/12	0.96	0.15	8.00	12,16,25,33	0
8	MAN	B	937	11/12	0.95	0.13	5.05	15,18,27,30	0
8	NAG	A	926	14/15	0.97	0.09	3.86	11,13,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	909	14/15	0.94	0.14	3.57	17,23,26,29	0
14	MAN	B	942	11/12	0.94	0.14	3.54	16,20,25,28	0
8	MAN	A	936	11/12	0.96	0.12	3.42	15,20,24,25	0
2	NAG	B	910	14/15	0.96	0.08	2.21	11,16,25,27	0
4	NAG	A	923	14/15	0.95	0.09	1.97	14,18,26,26	0
8	NAG	B	931	14/15	0.97	0.08	1.29	10,13,33,33	0
6	NAG	A	913	14/15	0.95	0.09	1.04	13,15,20,22	0
4	NAG	B	928	14/15	0.96	0.07	0.84	12,14,23,28	0
6	MAN	A	920	11/12	0.97	0.09	0.66	13,15,16,16	0
13	NAG	B	918	14/15	0.98	0.07	0.25	9,10,15,15	0
13	MAN	B	927	11/12	0.98	0.07	-0.05	11,13,14,15	0
2	NAG	B	909	14/15	0.97	0.07	-0.16	10,13,16,16	0
6	MAN	A	921	11/12	0.95	0.08	-0.17	12,17,19,31	0
14	NAG	B	938	14/15	0.98	0.07	-0.19	11,13,17,18	0
2	NAG	A	902	14/15	0.97	0.07	-0.29	13,18,28,33	0
2	NAG	A	901	14/15	0.97	0.07	-0.29	11,13,15,15	0
13	NAG	B	919	14/15	0.97	0.07	-0.29	8,10,11,11	0
4	NAG	A	908	14/15	0.96	0.07	-0.50	11,15,16,18	0
13	MAN	B	924	11/12	0.95	0.08	-0.53	11,13,17,24	0
13	MAN	B	926	11/12	0.98	0.07	-0.55	8,9,11,12	0
8	NAG	A	933	14/15	0.98	0.06	-0.72	11,13,16,18	0
2	NAG	B	902	14/15	0.98	0.06	-0.76	9,11,15,22	0
6	NAG	A	914	14/15	0.98	0.06	-0.79	12,13,14,15	0
5	NAG	A	911	14/15	0.97	0.06	-0.86	11,14,16,16	0
4	NAG	B	915	14/15	0.98	0.06	-0.91	9,10,12,13	0
6	MAN	A	919	11/12	0.98	0.06	-1.14	11,13,15,16	0
2	NAG	B	901	14/15	0.99	0.05	-1.21	7,9,11,11	0
2	MAN	B	904	11/12	0.96	0.13	-	20,27,33,36	0
6	BMA	A	915	11/12	0.97	0.06	-	13,15,17,18	0
14	MAN	B	943	11/12	0.94	0.11	-	18,20,25,28	0
2	BMA	B	911	11/12	0.91	0.16	-	24,27,31,31	0
2	MAN	A	905	11/12	0.85	0.24	-	25,27,32,32	0
2	MAN	B	913	11/12	0.88	0.23	-	32,36,43,44	0
8	BMA	A	928	11/12	0.93	0.16	-	15,18,25,30	0
14	NAG	B	939	14/15	0.96	0.11	-	18,22,24,29	0
8	MAN	B	935	11/12	0.96	0.12	-	17,19,28,35	0
2	MAN	B	912	11/12	0.82	0.32	-	33,37,44,45	0
14	MAN	B	945	11/12	0.89	0.22	-	26,34,37,45	0
14	MAN	B	944	11/12	0.87	0.22	-	41,49,56,61	0
4	NAG	B	916	14/15	0.93	0.12	-	13,17,26,34	0
2	MAN	B	906	11/12	0.92	0.11	-	22,26,29,36	0
14	MAN	B	941	11/12	0.76	0.23	-	48,58,65,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	NAG	A	927	14/15	0.96	0.09	-	13,16,25,27	0
14	BMA	B	940	11/12	0.93	0.14	-	20,26,29,33	0
5	NAG	A	912	14/15	0.93	0.12	-	12,22,31,38	0
6	MAN	A	917	11/12	0.93	0.17	-	31,36,46,51	0
8	MAN	A	931	11/12	0.95	0.13	-	15,16,26,34	0
8	MAN	A	929	11/12	0.80	0.30	-	52,55,61,62	0
2	BMA	B	903	11/12	0.97	0.07	-	12,14,19,19	0
8	MAN	A	939	11/12	0.90	0.23	-	25,28,34,34	0
2	MAN	B	905	11/12	0.95	0.14	-	20,29,40,58	0
13	MAN	B	923	11/12	0.99	0.06	-	9,9,12,12	0
13	MAN	B	925	11/12	0.95	0.11	-	18,21,27,32	0
2	MAN	A	904	11/12	0.73	0.31	-	28,45,54,60	0
13	BMA	B	920	11/12	0.98	0.06	-	9,10,12,12	0
4	NAG	A	924	14/15	0.85	0.21	-	26,32,39,39	0
13	MAN	B	921	11/12	0.98	0.06	-	12,14,17,18	0
4	BMA	A	925	11/12	0.79	0.29	-	30,40,51,58	0
8	MAN	A	937	11/12	0.94	0.11	-	16,21,24,26	0
4	BMA	B	917	11/12	0.75	0.29	-	53,62,81,82	0
8	MAN	A	930	11/12	0.94	0.13	-	18,23,30,30	0
4	BMA	A	910	11/12	0.85	0.21	-	31,37,46,57	0
8	BMA	B	933	11/12	0.94	0.15	-	16,18,27,28	0
2	MAN	A	906	11/12	0.92	0.15	-	26,33,39,41	0
13	MAN	B	922	11/12	0.92	0.13	-	19,25,30,32	0
4	NAG	B	929	14/15	0.92	0.16	-	20,26,42,44	0
4	BMA	B	930	11/12	0.86	0.22	-	33,40,48,56	0
2	MAN	B	914	11/12	0.86	0.26	-	34,36,43,47	0
8	MAN	B	934	11/12	0.80	0.31	-	54,63,69,71	0
6	MAN	A	916	11/12	0.97	0.07	-	17,18,22,25	0
8	MAN	B	936	11/12	0.95	0.12	-	16,19,28,34	0
6	MAN	A	918	11/12	0.99	0.05	-	11,12,14,15	0
8	NAG	A	934	14/15	0.95	0.10	-	15,20,23,25	0
8	NAG	B	932	14/15	0.94	0.12	-	12,19,25,28	0
2	BMA	A	903	11/12	0.92	0.17	-	19,24,27,30	0
8	BMA	A	935	11/12	0.92	0.14	-	20,25,30,34	0
8	MAN	A	938	11/12	0.90	0.24	-	38,49,56,67	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
10	MRD	A	942	8/8	0.92	0.13	17.18	13,16,31,33	0
10	MRD	B	949	8/8	0.88	0.19	8.09	28,39,42,42	0
10	MRD	A	943	8/8	0.88	0.15	6.67	19,23,27,28	0
10	MRD	B	947	8/8	0.89	0.15	6.56	17,21,24,24	0
10	MRD	B	948	8/8	0.94	0.10	5.45	13,19,32,35	0
3	NAG	B	946	14/15	0.97	0.16	3.66	19,23,28,32	0
7	MAN	B	907	11/12	0.94	0.13	2.54	18,21,29,35	0
3	NAG	A	940	14/15	0.96	0.16	1.93	21,28,36,39	0
9	MPD	A	941	8/8	0.95	0.08	1.05	16,18,20,22	0
12	ACY	B	951	4/4	0.94	0.10	0.45	13,16,16,18	0
12	ACY	A	945	4/4	0.95	0.10	0.04	18,18,20,21	0
11	NA	A	944	1/1	0.98	0.12	-	16,16,16,16	0
7	MAN	A	922	11/12	0.94	0.14	-	22,25,32,35	0
11	NA	B	950	1/1	0.97	0.11	-	20,20,20,20	0
3	NAG	B	908	14/15	0.88	0.26	-	30,40,47,51	0
3	NAG	A	907	14/15	0.83	0.33	-	37,48,55,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.