



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 02:50 PM EST

PDB ID : 5FKB
Title : Structure of D80A-fructofuranosidase from Xanthophyllomyces dendrorhous complexed with 1-Kestose
Authors : Ramirez-Escudero, M.; Sanz-Aparicio, J.
Deposited on : 2015-10-15
Resolution : 1.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

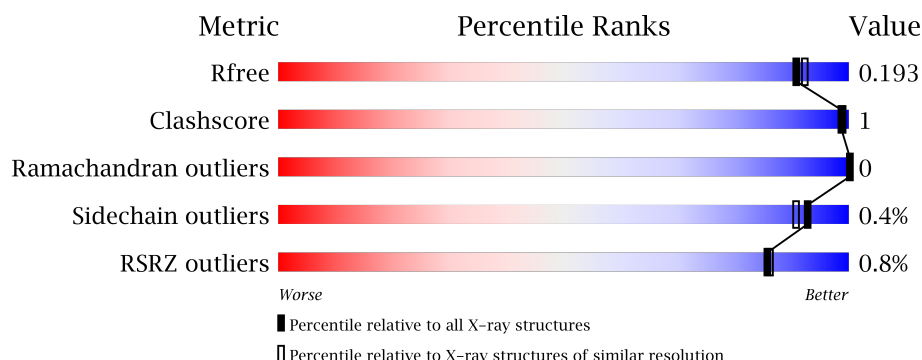
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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}	100719	7172 (1.80-1.76)
Clashscore	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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	663	
1	B	663	

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
2	NAG	A	1471	-	-	-	X
2	NAG	A	1539	-	-	-	X
2	NAG	A	1606	-	-	-	X
2	NAG	B	1052	X	-	-	-
2	NAG	B	1471	-	-	-	X
2	NAG	B	1539	-	-	-	X
4	MAN	A	1062	-	-	-	X
4	MAN	A	1063	X	-	-	-
4	MAN	B	1062	X	-	-	-
6	FRU	A	3002	-	-	-	X
6	FRU	B	3002	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12140 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.

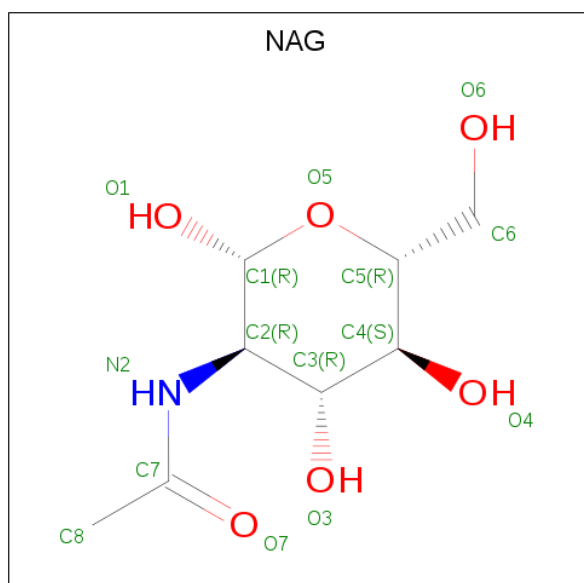
- Molecule 1 is a protein called BETA-FRUCTOFURANOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	1	0
			4805	3063	784	951	7			
1	B	624	Total	C	N	O	S	0	1	0
			4805	3063	784	951	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	663	ALA	SER	conflict	UNP J7HDY4
A	665	TYR	ARG	conflict	UNP J7HDY4
A	80	ALA	ASP	engineered mutation	UNP J7HDY4
B	663	ALA	SER	conflict	UNP J7HDY4
B	665	TYR	ARG	conflict	UNP J7HDY4
B	80	ALA	ASP	engineered mutation	UNP J7HDY4

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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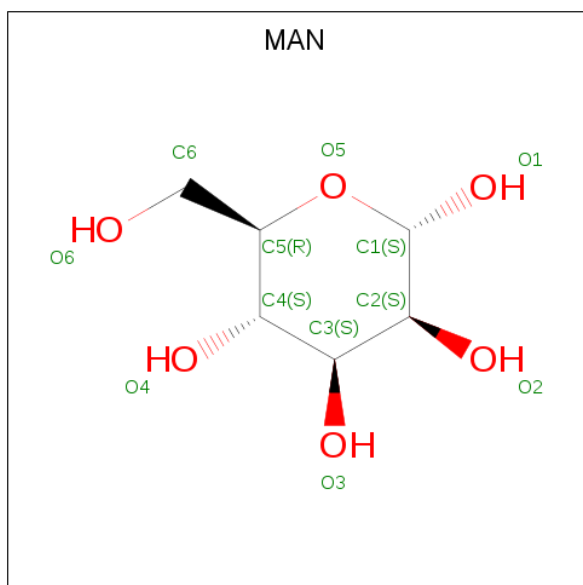
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1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

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



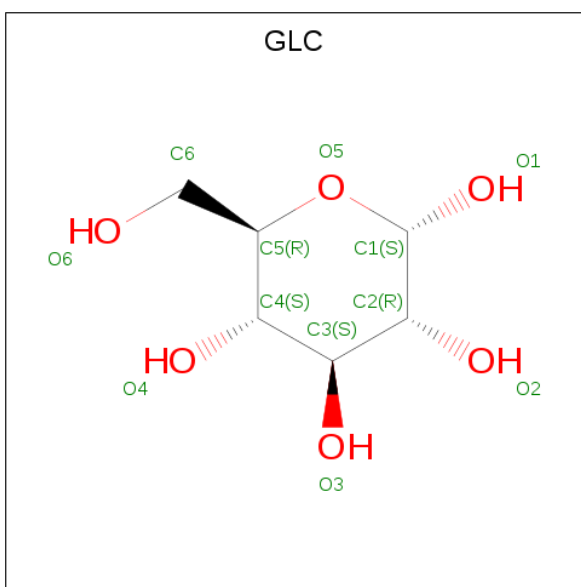
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



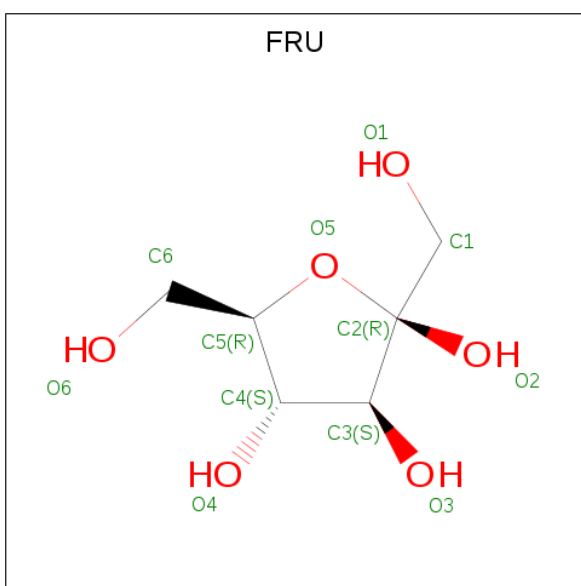
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4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

- Molecule 5 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C₆H₁₂O₆).



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

- Molecule 6 is FRUCTOSE (three-letter code: FRU) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	6	6		
6	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			12	6	6		
6	B	1	Total	C	O	0	0
			11	6	5		

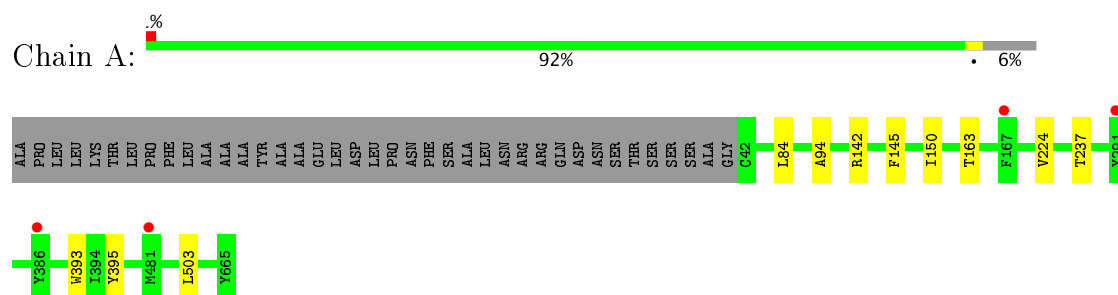
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	916	Total	O	0	0
			916	916		
7	B	725	Total	O	0	0
			725	725		

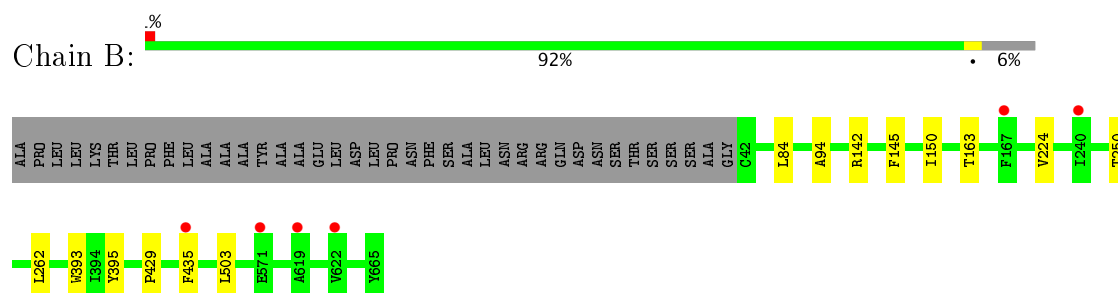
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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-FRUCTOFURANOSIDASE



• Molecule 1: BETA-FRUCTOFURANOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.53Å 205.02Å 145.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.92 – 1.78 118.92 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (118.92-1.78) 99.9 (118.92-1.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.170 , 0.184 0.180 , 0.193	Depositor DCC
R_{free} test set	10689 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12140	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.21% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GLC, BMA, NAG, FRU, 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	0.39	0/4940	0.62	0/6754
1	B	0.37	0/4940	0.61	0/6754
All	All	0.38	0/9880	0.62	0/13508

There are no bond length outliers.

There are no bond angle outliers.

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	4805	0	4500	5	0
1	B	4805	0	4503	7	0
2	A	294	0	268	1	0
2	B	252	0	229	2	0
3	A	22	0	16	0	0
3	B	22	0	16	0	0
4	A	121	0	103	0	1
4	B	110	0	94	0	1
5	A	11	0	10	0	0
5	B	11	0	10	0	0
6	A	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	23	0	21	0	0
7	A	916	0	0	2	1
7	B	725	0	0	0	1
All	All	12140	0	9791	13	4

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 1.

All (13) 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:237:THR:HG23	7:A:2352:HOH:O	2.07	0.54
2:A:1059:NAG:H83	7:A:2827:HOH:O	2.08	0.53
1:B:150:ILE:HG12	1:B:224:VAL:HG11	1.91	0.52
1:A:150:ILE:HG12	1:A:224:VAL:HG11	1.91	0.52
1:A:393:TRP:CZ2	1:A:395:TYR:HB3	2.52	0.45
1:B:145:PHE:HB2	1:B:163:THR:HB	2.00	0.44
1:A:145:PHE:HB2	1:A:163:THR:HB	2.01	0.43
1:B:393:TRP:CZ2	1:B:395:TYR:HB3	2.54	0.43
1:B:84:LEU:HD23	1:B:94:ALA:HA	2.01	0.43
1:B:429:PRO:HB3	2:B:1444:NAG:H62	1.99	0.42
1:A:84:LEU:HD23	1:A:94:ALA:HA	2.01	0.42
1:B:435:PHE:CZ	2:B:1444:NAG:H5	2.55	0.41
1:B:250:THR:HB	1:B:262:LEU:HD11	2.02	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2876:HOH:O	7:A:2876:HOH:O[2_555]	1.73	0.47
7:B:2710:HOH:O	7:B:2710:HOH:O[2_555]	1.94	0.26
4:A:1112:MAN:O4	4:A:1112:MAN:O4[2_555]	2.08	0.12
4:B:1115:MAN:O4	4:B:1115:MAN:O4[2_555]	2.15	0.05

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	623/663 (94%)	597 (96%)	26 (4%)	0	100	100
1	B	623/663 (94%)	597 (96%)	26 (4%)	0	100	100
All	All	1246/1326 (94%)	1194 (96%)	52 (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	498/527 (94%)	496 (100%)	2 (0%)	93	91
1	B	498/527 (94%)	496 (100%)	2 (0%)	93	91
All	All	996/1054 (94%)	992 (100%)	4 (0%)	93	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ARG
1	A	503	LEU
1	B	142	ARG
1	B	503	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	268	HIS
1	A	341	GLN
1	A	458	GLN
1	B	268	HIS
1	B	341	GLN
1	B	458	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

70 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	$\# Z > 2$
2	NAG	A	1052	1	14,14,15	0.24	0	15,19,21	1.17	3 (20%)
2	NAG	A	1058	1,2	14,14,15	0.35	0	15,19,21	1.29	1 (6%)
2	NAG	A	1059	3,2	14,14,15	0.58	0	15,19,21	1.47	3 (20%)
3	BMA	A	1060	2,4	11,11,12	0.37	0	13,15,17	2.03	3 (23%)
4	MAN	A	1061	3,4	11,11,12	0.57	0	13,15,17	0.77	0
4	MAN	A	1062	4	11,11,12	0.38	0	13,15,17	0.82	0
4	MAN	A	1063	3,4	11,11,12	0.61	0	13,15,17	1.52	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	A	1064	4	11,11,12	0.51	0	13,15,17	1.29	2 (15%)
2	NAG	A	1107	1,2	14,14,15	0.93	1 (7%)	15,19,21	0.88	0
2	NAG	A	1108	3,2	14,14,15	0.30	0	15,19,21	0.78	0
3	BMA	A	1109	2,4	11,11,12	0.45	0	13,15,17	1.44	1 (7%)
4	MAN	A	1110	3,4	11,11,12	0.42	0	13,15,17	0.69	0
4	MAN	A	1111	4	11,11,12	0.38	0	13,15,17	0.73	1 (7%)
4	MAN	A	1112	4	11,11,12	0.32	0	13,15,17	0.75	0
4	MAN	A	1113	4	11,11,12	0.42	0	13,15,17	0.82	0
4	MAN	A	1114	3,4	11,11,12	0.55	0	13,15,17	1.35	1 (7%)
4	MAN	A	1115	4	11,11,12	0.39	0	13,15,17	1.29	1 (7%)
4	MAN	A	1116	4	11,11,12	0.39	0	13,15,17	0.64	0
2	NAG	A	1125	1	14,14,15	0.42	0	15,19,21	1.23	2 (13%)
2	NAG	A	1215	1	14,14,15	0.53	0	15,19,21	2.16	3 (20%)
2	NAG	A	1236	1	14,14,15	0.42	0	15,19,21	0.94	0
2	NAG	A	1242	1	14,14,15	0.26	0	15,19,21	1.26	2 (13%)
2	NAG	A	1319	1	14,14,15	0.37	0	15,19,21	0.78	0
2	NAG	A	1357	1	14,14,15	0.28	0	15,19,21	1.28	4 (26%)
2	NAG	A	1444	1	14,14,15	0.53	0	15,19,21	0.87	1 (6%)
2	NAG	A	1471	1	14,14,15	0.35	0	15,19,21	1.33	2 (13%)
2	NAG	A	1483	1	14,14,15	0.28	0	15,19,21	0.98	1 (6%)
2	NAG	A	1512	1	14,14,15	0.31	0	15,19,21	1.18	2 (13%)
2	NAG	A	1539	1	14,14,15	0.49	0	15,19,21	1.37	2 (13%)
2	NAG	A	1555	1	14,14,15	0.34	0	15,19,21	1.34	2 (13%)
2	NAG	A	1576	1,2	14,14,15	0.31	0	15,19,21	0.97	0
2	NAG	A	1577	2	14,14,15	0.29	0	15,19,21	1.31	2 (13%)
2	NAG	A	1606	1	14,14,15	0.48	0	15,19,21	2.17	6 (40%)
2	NAG	A	1644	1	14,14,15	0.44	0	15,19,21	0.65	0
5	GLC	A	3001	6	11,11,12	0.51	0	13,15,17	1.55	1 (7%)
6	FRU	A	3002	5,6	11,12,12	0.83	1 (9%)	10,18,18	0.93	1 (10%)
6	FRU	A	3003	6	11,11,12	0.45	0	15,15,18	1.18	2 (13%)
2	NAG	B	1052	1	14,14,15	0.39	0	15,19,21	0.81	1 (6%)
2	NAG	B	1058	1,2	14,14,15	0.39	0	15,19,21	1.18	3 (20%)
2	NAG	B	1059	3,2	14,14,15	0.53	0	15,19,21	0.80	0
3	BMA	B	1060	2,4	11,11,12	0.27	0	13,15,17	1.77	4 (30%)
4	MAN	B	1061	3	11,11,12	0.40	0	13,15,17	0.88	1 (7%)
4	MAN	B	1062	3,4	11,11,12	0.67	0	13,15,17	1.49	2 (15%)
4	MAN	B	1063	4	11,11,12	0.35	0	13,15,17	0.80	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1107	1,2	14,14,15	0.77	1 (7%)	15,19,21	1.00	1 (6%)
2	NAG	B	1108	3,2	14,14,15	0.37	0	15,19,21	0.71	0
3	BMA	B	1109	2,4	11,11,12	0.41	0	13,15,17	1.04	1 (7%)
4	MAN	B	1110	3,4	11,11,12	0.34	0	13,15,17	1.03	1 (7%)
4	MAN	B	1111	4	11,11,12	0.41	0	13,15,17	0.70	0
4	MAN	B	1112	4	11,11,12	0.36	0	13,15,17	0.81	1 (7%)
4	MAN	B	1113	3,4	11,11,12	0.46	0	13,15,17	1.01	1 (7%)
4	MAN	B	1114	4	11,11,12	0.37	0	13,15,17	0.82	0
4	MAN	B	1115	4	11,11,12	0.38	0	13,15,17	0.83	0
4	MAN	B	1116	4	11,11,12	0.46	0	13,15,17	0.90	0
2	NAG	B	1125	1	14,14,15	0.43	0	15,19,21	1.00	1 (6%)
2	NAG	B	1215	1	14,14,15	0.40	0	15,19,21	1.13	1 (6%)
2	NAG	B	1242	1	14,14,15	0.29	0	15,19,21	1.40	3 (20%)
2	NAG	B	1319	1	14,14,15	0.39	0	15,19,21	1.02	1 (6%)
2	NAG	B	1357	1	14,14,15	0.30	0	15,19,21	0.89	0
2	NAG	B	1444	1	14,14,15	0.50	0	15,19,21	1.26	1 (6%)
2	NAG	B	1471	1	14,14,15	0.37	0	15,19,21	0.78	0
2	NAG	B	1483	1	14,14,15	0.28	0	15,19,21	0.94	1 (6%)
2	NAG	B	1539	1	14,14,15	0.47	0	15,19,21	1.12	1 (6%)
2	NAG	B	1555	1	14,14,15	0.40	0	15,19,21	0.85	0
2	NAG	B	1576	1,2	14,14,15	0.33	0	15,19,21	0.99	0
2	NAG	B	1577	2	14,14,15	0.29	0	15,19,21	0.96	1 (6%)
2	NAG	B	1644	1	14,14,15	0.46	0	15,19,21	0.60	0
5	GLC	B	3001	6	11,11,12	0.38	0	13,15,17	1.38	1 (7%)
6	FRU	B	3002	5,6	11,12,12	0.79	1 (9%)	10,18,18	0.90	0
6	FRU	B	3003	6	11,11,12	0.41	0	15,15,18	1.09	1 (6%)

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	1052	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1058	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1059	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1060	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1061	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1062	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	1063	3,4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	1064	4	-	0/2/19/22	1/1/1/1
2	NAG	A	1107	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1108	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1109	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1110	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1111	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1112	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1113	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1114	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1115	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1116	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1125	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1215	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1236	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1242	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1319	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1357	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1444	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1471	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1483	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1512	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1539	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1555	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1576	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1577	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1606	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1644	1	-	0/6/23/26	0/1/1/1
5	GLC	A	3001	6	-	0/2/19/22	0/1/1/1
6	FRU	A	3002	5,6	-	0/5/24/24	0/1/1/1
6	FRU	A	3003	6	-	0/4/20/24	0/1/1/1
2	NAG	B	1052	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	1058	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1059	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1060	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1061	3	-	0/2/19/22	0/1/1/1
4	MAN	B	1062	3,4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	1063	4	-	0/2/19/22	0/1/1/1
2	NAG	B	1107	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1108	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1109	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1110	3,4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	B	1111	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1112	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1113	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1114	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1115	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1116	4	-	0/2/19/22	0/1/1/1
2	NAG	B	1125	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1215	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1242	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1319	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1357	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1444	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1471	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1483	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1539	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1555	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1576	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1577	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1644	1	-	0/6/23/26	0/1/1/1
5	GLC	B	3001	6	-	0/2/19/22	0/1/1/1
6	FRU	B	3002	5,6	-	0/5/24/24	0/1/1/1
6	FRU	B	3003	6	-	0/4/20/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3002	FRU	O2-C2	2.46	1.45	1.40
2	B	1107	NAG	C1-C2	2.51	1.55	1.52
6	A	3002	FRU	O2-C2	2.57	1.45	1.40
2	A	1107	NAG	C1-C2	3.05	1.56	1.52

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1109	BMA	O3-C3-C4	-4.40	100.79	110.36
3	A	1060	BMA	O3-C3-C4	-3.25	103.28	110.36
2	A	1058	NAG	O5-C1-C2	-3.08	107.19	111.47
2	A	1242	NAG	O5-C1-C2	-3.03	107.25	111.47
6	B	3003	FRU	C1-C2-C3	-3.00	107.80	115.05
6	A	3003	FRU	C1-C2-C3	-2.99	107.82	115.05
2	A	1606	NAG	O5-C1-C2	-2.84	107.53	111.47
2	A	1125	NAG	O5-C1-C2	-2.83	107.53	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1215	NAG	O5-C1-C2	-2.60	107.86	111.47
2	A	1555	NAG	O5-C1-C2	-2.59	107.87	111.47
2	B	1483	NAG	O5-C1-C2	-2.35	108.20	111.47
2	A	1606	NAG	C4-C3-C2	-2.22	107.77	111.02
2	A	1606	NAG	O7-C7-C8	-2.20	118.06	122.06
2	A	1052	NAG	O5-C1-C2	-2.18	108.44	111.47
3	B	1060	BMA	C6-C5-C4	-2.15	107.96	113.00
2	B	1058	NAG	O5-C1-C2	-2.15	108.49	111.47
4	B	1113	MAN	C1-C2-C3	-2.12	106.96	109.65
3	B	1109	BMA	O6-C6-C5	-2.12	104.20	111.34
3	B	1060	BMA	O3-C3-C4	-2.07	105.86	110.36
2	B	1107	NAG	O5-C1-C2	-2.04	108.64	111.47
2	A	1357	NAG	O5-C1-C2	-2.01	108.67	111.47
4	B	1061	MAN	C1-O5-C5	2.04	114.97	112.17
2	A	1444	NAG	C1-O5-C5	2.07	115.02	112.17
2	A	1059	NAG	C8-C7-N2	2.09	119.88	116.11
4	B	1112	MAN	C1-C2-C3	2.10	112.31	109.65
2	A	1242	NAG	C1-O5-C5	2.10	115.07	112.17
2	A	1052	NAG	C2-N2-C7	2.11	126.01	122.94
2	B	1058	NAG	O4-C4-C5	2.12	114.62	109.28
2	A	1357	NAG	C1-O5-C5	2.14	115.12	112.17
4	A	1111	MAN	C1-O5-C5	2.14	115.12	112.17
6	A	3002	FRU	O2-C2-O5	2.15	113.73	109.45
4	B	1063	MAN	C1-O5-C5	2.24	115.25	112.17
2	A	1357	NAG	C8-C7-N2	2.26	120.19	116.11
2	B	1242	NAG	C2-N2-C7	2.26	126.24	122.94
3	A	1060	BMA	C1-O5-C5	2.29	115.32	112.17
2	A	1052	NAG	C8-C7-N2	2.29	120.25	116.11
6	A	3003	FRU	O5-C2-C1	2.37	114.23	109.16
2	B	1125	NAG	C1-O5-C5	2.39	115.47	112.17
2	A	1512	NAG	C8-C7-N2	2.40	120.44	116.11
2	A	1471	NAG	C8-C7-N2	2.41	120.47	116.11
2	A	1539	NAG	C1-C2-N2	2.46	114.69	110.49
4	A	1064	MAN	C1-C2-C3	2.50	112.82	109.65
2	A	1125	NAG	C1-O5-C5	2.50	115.61	112.17
2	A	1512	NAG	C2-N2-C7	2.52	126.62	122.94
2	A	1059	NAG	C1-O5-C5	2.52	115.64	112.17
2	A	1555	NAG	C8-C7-N2	2.54	120.69	116.11
2	B	1215	NAG	C1-O5-C5	2.54	115.67	112.17
2	B	1242	NAG	C8-C7-N2	2.54	120.69	116.11
2	B	1052	NAG	C1-O5-C5	2.56	115.69	112.17
2	B	1058	NAG	C1-O5-C5	2.56	115.70	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1577	NAG	C8-C7-N2	2.62	120.83	116.11
2	A	1471	NAG	C2-N2-C7	2.67	126.84	122.94
2	A	1577	NAG	C2-N2-C7	2.69	126.87	122.94
3	B	1060	BMA	C3-C4-C5	2.74	115.04	110.22
2	A	1357	NAG	C2-N2-C7	2.74	126.94	122.94
4	A	1063	MAN	C3-C4-C5	2.85	115.25	110.22
2	B	1242	NAG	C1-O5-C5	2.90	116.16	112.17
2	A	1059	NAG	C2-N2-C7	2.91	127.18	122.94
4	B	1110	MAN	C1-O5-C5	3.00	116.30	112.17
4	A	1114	MAN	C3-C4-C5	3.04	115.58	110.22
2	A	1215	NAG	C1-C2-N2	3.16	115.89	110.49
2	A	1606	NAG	C8-C7-N2	3.18	121.84	116.11
2	B	1577	NAG	C1-O5-C5	3.19	116.56	112.17
4	B	1062	MAN	C1-O5-C5	3.20	116.58	112.17
2	A	1483	NAG	C1-O5-C5	3.27	116.68	112.17
2	B	1539	NAG	C1-O5-C5	3.42	116.89	112.17
2	A	1606	NAG	C1-C2-N2	3.43	116.34	110.49
2	B	1319	NAG	C1-O5-C5	3.44	116.91	112.17
4	A	1063	MAN	C1-O5-C5	3.47	116.95	112.17
4	A	1064	MAN	C1-O5-C5	3.64	117.18	112.17
4	B	1062	MAN	O5-C1-C2	3.78	116.71	110.79
5	B	3001	GLC	C1-O5-C5	3.81	117.41	112.17
4	A	1115	MAN	C1-O5-C5	3.82	117.44	112.17
2	A	1539	NAG	C1-O5-C5	4.03	117.72	112.17
2	B	1444	NAG	C1-O5-C5	4.32	118.12	112.17
3	B	1060	BMA	C1-O5-C5	4.42	118.26	112.17
5	A	3001	GLC	C1-O5-C5	4.84	118.84	112.17
2	A	1606	NAG	C2-N2-C7	5.13	130.42	122.94
3	A	1060	BMA	O3-C3-C2	5.22	119.52	110.02
2	A	1215	NAG	C1-O5-C5	6.45	121.05	112.17

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1052	NAG	C1
4	B	1062	MAN	C1
4	A	1063	MAN	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1064	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1059	NAG	1	0
4	A	1112	MAN	0	1
4	B	1115	MAN	0	1
2	B	1444	NAG	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	624/663 (94%)	0.13	4 (0%) 89 89	13, 21, 32, 43	0
1	B	624/663 (94%)	0.13	6 (0%) 82 83	15, 27, 42, 52	0
All	All	1248/1326 (94%)	0.13	10 (0%) 86 86	13, 24, 39, 52	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	167[A]	PHE	3.7
1	B	619	ALA	3.3
1	A	386	TYR	2.9
1	A	167[A]	PHE	2.9
1	B	435	PHE	2.8
1	B	240	ILE	2.8
1	B	622	VAL	2.6
1	A	481	MET	2.3
1	A	291	TYR	2.1
1	B	571	GLU	2.0

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](#)

There are no carbohydrates in this entry.

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
4	MAN	A	1062	11/12	0.77	0.26	12.67	48,50,53,53	0
2	NAG	B	1539	14/15	0.73	0.31	7.76	53,58,63,64	0
2	NAG	A	1539	14/15	0.75	0.21	6.60	42,47,51,51	0
2	NAG	A	1606	14/15	0.60	0.27	5.54	44,48,53,58	0
2	NAG	B	1471	14/15	0.90	0.18	5.10	31,35,40,40	0
6	FRU	A	3002	12/12	0.92	0.13	4.12	22,33,36,37	0
2	NAG	A	1471	14/15	0.91	0.14	3.04	29,32,37,43	0
6	FRU	B	3002	12/12	0.91	0.12	2.90	29,40,44,45	0
2	NAG	A	1236	14/15	0.86	0.12	1.72	30,36,39,39	0
6	FRU	B	3003	11/12	0.98	0.10	1.55	21,22,25,26	0
2	NAG	B	1644	14/15	0.92	0.11	1.28	26,28,34,37	0
2	NAG	B	1357	14/15	0.91	0.14	1.05	43,46,49,51	0
6	FRU	A	3003	11/12	0.97	0.11	1.02	15,16,20,23	0
2	NAG	A	1107	14/15	0.98	0.10	0.35	15,16,17,17	0
2	NAG	B	1107	14/15	0.96	0.09	-0.04	19,19,21,21	0
2	NAG	A	1357	14/15	0.94	0.11	-0.06	33,35,39,42	0
2	NAG	A	1058	14/15	0.96	0.10	-0.17	18,20,25,26	0
2	NAG	B	1444	14/15	0.92	0.12	-0.22	33,34,36,36	0
2	NAG	B	1058	14/15	0.97	0.09	-0.38	24,27,31,32	0
2	NAG	A	1644	14/15	0.94	0.10	-0.39	22,25,32,33	0
2	NAG	A	1444	14/15	0.94	0.10	-0.65	28,29,32,36	0
2	NAG	B	1108	14/15	0.98	0.08	-1.62	19,20,21,22	0
2	NAG	A	1108	14/15	0.97	0.09	-3.27	17,18,18,19	0
4	MAN	A	1115	11/12	0.83	0.17	-	48,50,53,61	0
2	NAG	B	1052	14/15	0.65	0.30	-	64,70,71,74	0
4	MAN	B	1062	11/12	0.69	0.30	-	61,64,67,69	0
3	BMA	A	1060	11/12	0.90	0.13	-	28,33,42,42	0
4	MAN	B	1111	11/12	0.81	0.20	-	55,56,59,66	0
5	GLC	B	3001	11/12	0.64	0.33	-	52,61,66,67	0
2	NAG	A	1319	14/15	0.81	0.29	-	60,67,70,71	0
4	MAN	B	1116	11/12	0.75	0.25	-	50,52,55,56	0
2	NAG	A	1512	14/15	0.82	0.23	-	52,57,69,70	0
4	MAN	A	1114	11/12	0.90	0.14	-	34,39,43,49	0
3	BMA	B	1060	11/12	0.89	0.10	-	39,45,51,55	0
2	NAG	A	1555	14/15	0.65	0.22	-	54,62,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	1215	14/15	0.73	0.31	-	55,64,67,72	0
2	NAG	B	1319	14/15	0.85	0.37	-	71,78,79,80	0
4	MAN	B	1063	11/12	0.78	0.28	-	64,66,67,67	0
4	MAN	A	1110	11/12	0.96	0.09	-	17,20,25,28	0
4	MAN	B	1061	11/12	0.64	0.24	-	59,64,66,68	0
4	MAN	B	1114	11/12	0.98	0.08	-	17,19,19,19	0
2	NAG	A	1576	14/15	0.93	0.10	-	39,43,49,59	0
3	BMA	B	1109	11/12	0.95	0.09	-	23,24,26,31	0
2	NAG	A	1242	14/15	0.84	0.20	-	52,56,59,61	0
2	NAG	A	1577	14/15	0.76	0.24	-	68,72,77,78	0
4	MAN	B	1115	11/12	0.88	0.18	-	36,38,43,44	0
4	MAN	A	1064	11/12	0.62	0.34	-	74,79,81,83	0
4	MAN	A	1111	11/12	0.98	0.10	-	15,16,16,16	0
4	MAN	A	1112	11/12	0.87	0.18	-	33,35,39,42	0
4	MAN	B	1110	11/12	0.91	0.14	-	37,42,47,48	0
2	NAG	A	1125	14/15	0.79	0.33	-	48,54,58,61	0
2	NAG	B	1555	14/15	0.80	0.17	-	39,41,43,45	0
4	MAN	A	1116	11/12	0.80	0.46	-	72,78,80,80	0
2	NAG	B	1125	14/15	0.67	0.35	-	50,55,59,60	0
5	GLC	A	3001	11/12	0.71	0.29	-	41,45,49,49	0
4	MAN	A	1063	11/12	0.80	0.20	-	51,59,63,63	0
3	BMA	A	1109	11/12	0.96	0.09	-	20,20,22,27	0
2	NAG	A	1052	14/15	0.84	0.18	-	47,53,56,57	0
2	NAG	B	1483	14/15	0.88	0.19	-	52,56,60,62	0
2	NAG	B	1242	14/15	0.75	0.28	-	67,72,73,74	0
2	NAG	B	1576	14/15	0.91	0.10	-	44,50,54,63	0
4	MAN	B	1113	11/12	0.95	0.09	-	20,22,27,30	0
2	NAG	B	1215	14/15	0.75	0.39	-	67,73,77,80	0
2	NAG	B	1577	14/15	0.69	0.26	-	67,75,79,80	0
4	MAN	A	1061	11/12	0.71	0.30	-	47,49,53,56	0
2	NAG	A	1483	14/15	0.89	0.13	-	37,41,44,46	0
4	MAN	B	1112	11/12	0.78	0.43	-	75,81,84,86	0
2	NAG	A	1059	14/15	0.95	0.12	-	20,22,26,33	0
2	NAG	B	1059	14/15	0.95	0.09	-	27,29,31,34	0
4	MAN	A	1113	11/12	0.82	0.28	-	47,51,56,57	0

6.5 Other polymers

There are no such residues in this entry.