Full wwPDB X-ray Structure Validation Report (i)

Mar 31, 2016 – 07:16 PM EDT

PDB ID	:	5FIX
Title	:	Structure of D80A-fructofuranosidase from Xanthophyllomyces dendrorhous complexed with sucrose
Authors	:	Ramirez-Escudero, M.; Sanz-Aparicio, J.
Deposited on	:	2015-10-02
Resolution	:	2.01 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 (i) symbol.

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

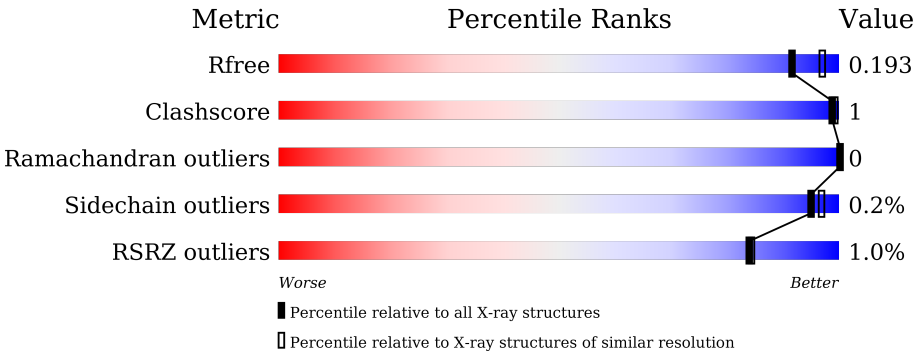
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	665	92% · 6%
1	B	665	2% 91% · 6%

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	SUC	A	1001	-	-	-	X
2	SUC	B	1001	-	-	-	X
3	NAG	A	1236	-	-	-	X
3	NAG	A	1539	-	-	-	X
3	NAG	A	1606	-	-	-	X
3	NAG	A	1644	-	-	-	X
3	NAG	B	1357	-	-	-	X
3	NAG	B	1539	X	-	-	X
3	NAG	B	1644	-	-	-	X
4	MAN	A	1062	-	-	-	X
5	MAN	B	1115	X	-	-	-
7	MAN	B	1062	X	-	-	-
7	MAN	B	1063	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12034 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.

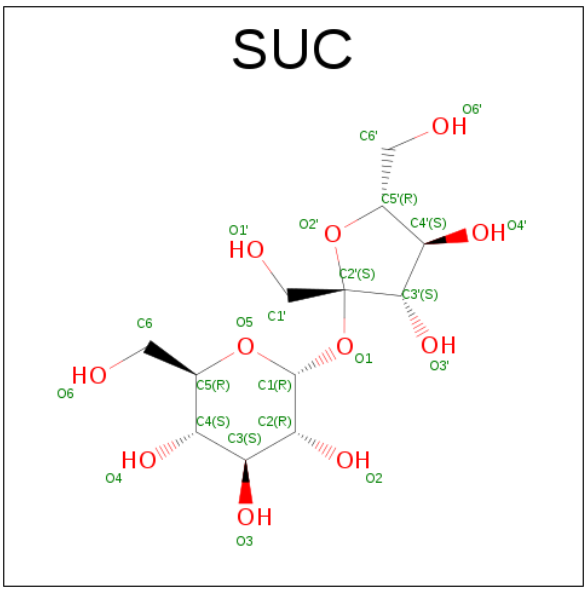
- Molecule 1 is a protein called BETA-FRUCTOFURANOSIDASE.

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:

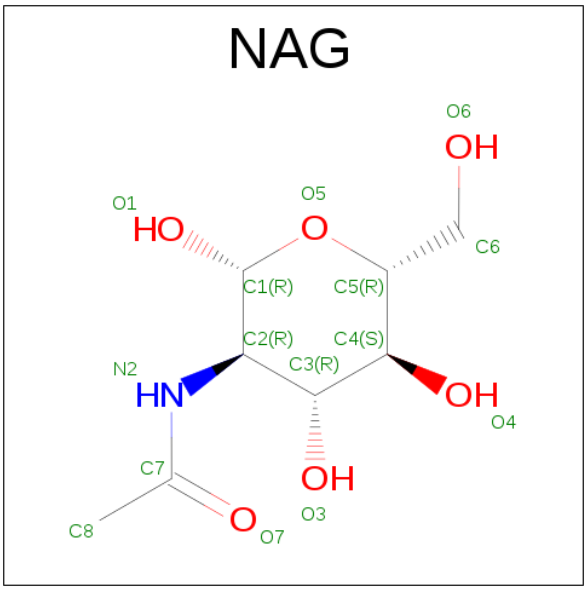
Chain	Residue	Modelled	Actual	Comment	Reference
A	663	ALA	SER	CONFLICT	UNP J7HDY4
A	665	TYR	ARG	CONFLICT	UNP J7HDY4
A	80	ALA	ASP	ENGINEERED MUTATION	UNP J7HDY4
B	663	ALA	SER	CONFLICT	UNP J7HDY4
B	665	TYR	ARG	CONFLICT	UNP J7HDY4
B	80	ALA	ASP	ENGINEERED MUTATION	UNP J7HDY4

- Molecule 2 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 23 12 11	0	0
2	A	1	Total C O 23 12 11	0	0
2	B	1	Total C O 23 12 11	0	0
2	B	1	Total C O 23 12 11	0	0

- 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 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0

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

- Molecule 4 is a polymer of unknown type called SUGAR (7-MER).

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

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

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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is a polymer of unknown type called SUGAR (6-MER).

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

- Molecule 8 is water.

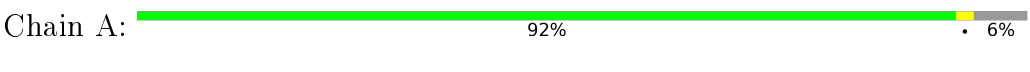
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	854	Total	O	0	0
			854	854		
8	B	657	Total	O	0	0
			657	657		

3 Residue-property plots (i)

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

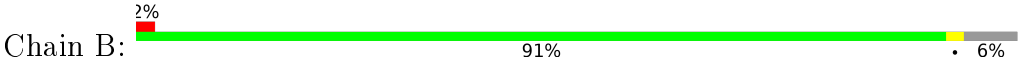
- Molecule 1: BETA-FRUCTOFURANOSIDASE

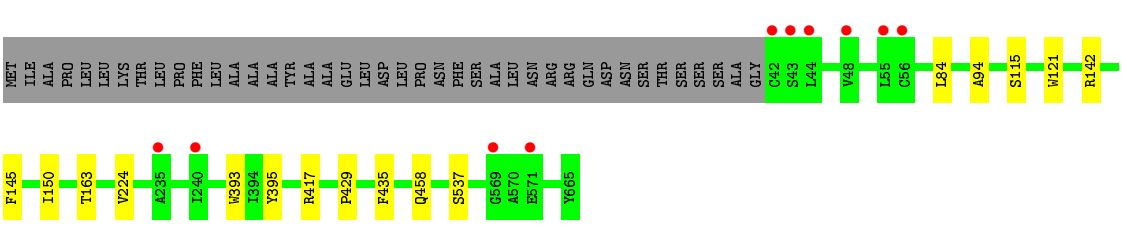
Chain A:



- Molecule 1: BETA-FRUCTOFURANOSIDASE

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	74.73Å 205.22Å 146.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.00 – 2.01 48.41 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.7 (119.00-2.01) 98.7 (48.41-2.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.166 , 0.185 0.176 , 0.193	Depositor DCC
R_{free} test set	7326 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.865	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 147986 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12034	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, SUC, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.44	0/4940	0.65	0/6754
1	B	0.42	0/4940	0.64	0/6754
All	All	0.43	0/9880	0.64	0/13508

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	B	1	0
7	B	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	1062	MAN	C1
5	B	1115	MAN	C1

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	7	0
1	B	4805	0	4503	9	0
2	A	46	0	44	0	0
2	B	46	0	44	0	0
3	A	210	0	195	0	0
3	B	168	0	156	3	0
4	A	83	0	70	1	0
5	A	116	0	97	0	1
5	B	116	0	97	0	0
6	A	28	0	25	0	0
6	B	28	0	25	0	0
7	B	72	0	61	0	0
8	A	854	0	0	2	1
8	B	657	0	0	0	1
All	All	12034	0	9817	17	3

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 (17) 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:B:150:ILE:HG12	1:B:224:VAL:HG11	1.85	0.59
1:A:150:ILE:HG12	1:A:224:VAL:HG11	1.86	0.57
4:A:1059:NAG:H83	8:A:2767:HOH:O	2.08	0.53
1:B:537:SER:HB3	3:B:1539:NAG:H82	1.92	0.52
1:A:393:TRP:CZ2	1:A:395:TYR:HB3	2.52	0.45
1:B:429:PRO:HB3	3:B:1444:NAG:H62	1.98	0.45
1:A:417:ARG:HH11	1:A:458:GLN:HE22	1.64	0.45
1:B:417:ARG:HH11	1:B:458:GLN:HE22	1.65	0.44
1:B:84:LEU:HD23	1:B:94:ALA:HA	2.00	0.43
1:B:393:TRP:CZ2	1:B:395:TYR:HB3	2.53	0.43
1:B:145:PHE:HB2	1:B:163:THR:HB	2.00	0.43
1:A:145:PHE:HB2	1:A:163:THR:HB	2.01	0.43
1:B:115:SER:HB2	1:B:121:TRP:CD2	2.53	0.43
1:A:84:LEU:HD23	1:A:94:ALA:HA	2.01	0.42
1:A:237:THR:HG23	8:A:2317:HOH:O	2.20	0.41
1:A:115:SER:HB2	1:A:121:TRP:CD2	2.56	0.41
1:B:435:PHE:CZ	3:B:1444:NAG:H5	2.57	0.40

All (3) 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)
8:A:2817:HOH:O	8:A:2817:HOH:O[2_555]	1.85	0.35
5:A:1112:MAN:O4	5:A:1112:MAN:O4[2_555]	1.92	0.28
8:B:2642:HOH:O	8:B:2642:HOH:O[2_555]	2.19	0.01

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	623/665 (94%)	596 (96%)	27 (4%)	0	100	100
1	B	623/665 (94%)	596 (96%)	27 (4%)	0	100	100
All	All	1246/1330 (94%)	1192 (96%)	54 (4%)	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	498/529 (94%)	497 (100%)	1 (0%)	95	97
1	B	498/529 (94%)	497 (100%)	1 (0%)	95	97
All	All	996/1058 (94%)	994 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

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

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	268	HIS
1	A	341	GLN
1	A	458	GLN
1	B	204	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

37 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	$\#\|Z\| > 2$
4	NAG	A	1058	1,4	14,14,15	0.36	0	15,19,21	1.02	1 (6%)
4	NAG	A	1059	4	14,14,15	0.84	1 (7%)	15,19,21	1.67	4 (26%)
4	BMA	A	1060	4	11,11,12	0.40	0	15,15,17	2.07	3 (20%)
4	MAN	A	1061	4	11,11,12	0.82	0	15,15,17	1.13	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	A	1062	4	11,11,12	0.47	0	15,15,17	0.89	1 (6%)
4	MAN	A	1063	4	11,11,12	0.65	0	15,15,17	1.55	4 (26%)
4	MAN	A	1064	4	11,11,12	0.58	0	15,15,17	2.19	3 (20%)
5	NAG	A	1107	1,5	14,14,15	1.01	1 (7%)	15,19,21	0.93	1 (6%)
5	NAG	A	1108	5	14,14,15	0.36	0	15,19,21	0.94	1 (6%)
5	BMA	A	1109	5	11,11,12	0.42	0	15,15,17	1.47	1 (6%)
5	MAN	A	1110	5	11,11,12	0.44	0	15,15,17	0.87	1 (6%)
5	MAN	A	1111	5	11,11,12	0.32	0	15,15,17	0.68	0
5	MAN	A	1112	5	11,11,12	0.69	0	15,15,17	1.20	3 (20%)
5	MAN	A	1113	5	11,11,12	0.53	0	15,15,17	0.98	0
5	MAN	A	1114	5	11,11,12	0.53	0	15,15,17	1.62	2 (13%)
5	MAN	A	1115	5	11,11,12	0.36	0	15,15,17	1.47	2 (13%)
5	MAN	A	1116	5	11,11,12	0.33	0	15,15,17	0.96	1 (6%)
6	NAG	A	1576	1,6	14,14,15	0.34	0	15,19,21	0.92	0
6	NAG	A	1577	6	14,14,15	0.50	0	15,19,21	1.77	3 (20%)
7	NAG	B	1058	1,7	14,14,15	0.45	0	15,19,21	1.19	2 (13%)
7	NAG	B	1059	7	14,14,15	0.58	0	15,19,21	0.82	0
7	BMA	B	1060	7	11,11,12	0.17	0	15,15,17	1.79	4 (26%)
7	MAN	B	1061	7	11,11,12	0.41	0	15,15,17	1.14	1 (6%)
7	MAN	B	1062	7	11,11,12	0.73	0	15,15,17	2.50	5 (33%)
7	MAN	B	1063	7	11,11,12	0.40	0	15,15,17	0.93	1 (6%)
5	NAG	B	1107	1,5	14,14,15	0.96	1 (7%)	15,19,21	0.96	0
5	NAG	B	1108	5	14,14,15	0.45	0	15,19,21	1.01	1 (6%)
5	BMA	B	1109	5	11,11,12	0.43	0	15,15,17	1.23	1 (6%)
5	MAN	B	1110	5	11,11,12	0.33	0	15,15,17	0.91	1 (6%)
5	MAN	B	1111	5	11,11,12	0.43	0	15,15,17	0.87	0
5	MAN	B	1112	5	11,11,12	0.48	0	15,15,17	1.31	1 (6%)
5	MAN	B	1113	5	11,11,12	0.64	0	15,15,17	1.01	0
5	MAN	B	1114	5	11,11,12	0.49	0	15,15,17	0.74	0
5	MAN	B	1115	5	11,11,12	0.70	0	15,15,17	1.55	2 (13%)
5	MAN	B	1116	5	11,11,12	0.59	0	15,15,17	0.94	0
6	NAG	B	1576	1,6	14,14,15	0.30	0	15,19,21	0.92	1 (6%)
6	NAG	B	1577	6	14,14,15	0.40	0	15,19,21	1.46	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
4	NAG	A	1058	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1059	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1060	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1061	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1062	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1063	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1064	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1107	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1108	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1109	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1110	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1111	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1112	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1113	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1114	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1115	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1116	5	-	0/2/19/22	0/1/1/1
6	NAG	A	1576	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1577	6	-	0/6/23/26	0/1/1/1
7	NAG	B	1058	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	1059	7	-	0/6/23/26	0/1/1/1
7	BMA	B	1060	7	-	0/2/19/22	0/1/1/1
7	MAN	B	1061	7	-	0/2/19/22	0/1/1/1
7	MAN	B	1062	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	B	1063	7	-	0/2/19/22	0/1/1/1
5	NAG	B	1107	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1108	5	-	0/6/23/26	0/1/1/1
5	BMA	B	1109	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1110	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1111	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1112	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1113	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1114	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1115	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	B	1116	5	-	0/2/19/22	0/1/1/1
6	NAG	B	1576	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1577	6	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1059	NAG	O5-C1	-2.26	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1107	NAG	C1-C2	3.38	1.57	1.52
5	A	1107	NAG	C1-C2	3.58	1.57	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1109	BMA	O3-C3-C4	-4.39	100.45	110.36
4	A	1060	BMA	O3-C3-C4	-3.70	102.01	110.36
5	B	1109	BMA	O6-C6-C5	-2.71	102.24	111.30
5	B	1115	MAN	O4-C4-C3	-2.34	105.09	110.36
5	A	1108	NAG	O5-C5-C4	-2.23	106.44	110.13
4	A	1059	NAG	C4-C3-C2	-2.20	107.92	111.34
4	A	1063	MAN	O2-C2-C3	-2.14	105.88	110.19
7	B	1062	MAN	O4-C4-C3	-2.12	105.58	110.36
5	A	1112	MAN	O2-C2-C3	-2.09	105.97	110.19
5	A	1112	MAN	O4-C4-C3	-2.09	105.65	110.36
7	B	1060	BMA	C6-C5-C4	-2.04	107.87	112.99
5	A	1107	NAG	C1-O5-C5	-2.04	109.15	112.14
5	A	1110	MAN	O5-C5-C6	2.00	111.63	107.34
5	A	1115	MAN	O5-C5-C4	2.03	113.49	110.13
4	A	1061	MAN	C1-O5-C5	2.13	115.27	112.14
4	A	1061	MAN	C1-C2-C3	2.19	112.20	109.55
7	B	1058	NAG	O4-C4-C5	2.19	115.00	109.23
6	B	1576	NAG	C1-O5-C5	2.27	115.48	112.14
7	B	1060	BMA	C3-C4-C5	2.31	114.35	110.23
4	A	1060	BMA	C1-O5-C5	2.33	115.57	112.14
6	A	1577	NAG	C2-N2-C7	2.41	126.24	123.11
4	A	1062	MAN	C1-O5-C5	2.49	115.80	112.14
7	B	1061	MAN	C3-C4-C5	2.51	114.71	110.23
4	A	1058	NAG	C1-O5-C5	2.54	115.88	112.14
7	B	1060	BMA	O5-C5-C4	2.62	114.47	110.13
4	A	1063	MAN	O5-C5-C4	2.66	114.53	110.13
5	B	1110	MAN	C1-O5-C5	2.69	116.09	112.14
4	A	1063	MAN	C1-O5-C5	2.71	116.12	112.14
7	B	1058	NAG	C1-O5-C5	2.73	116.16	112.14
4	A	1059	NAG	C8-C7-N2	2.74	121.34	116.10
5	B	1108	NAG	C2-N2-C7	2.75	126.69	123.11
7	B	1063	MAN	C1-O5-C5	2.86	116.35	112.14
5	A	1112	MAN	C3-C4-C5	2.94	115.46	110.23
4	A	1059	NAG	C1-O5-C5	3.00	116.55	112.14
4	A	1064	MAN	O5-C1-C2	3.02	115.73	110.89
5	A	1116	MAN	C1-O5-C5	3.03	116.60	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1063	MAN	C3-C4-C5	3.08	115.71	110.23
6	A	1577	NAG	C8-C7-N2	3.11	122.05	116.10
4	A	1064	MAN	C1-C2-C3	3.34	113.60	109.55
5	A	1114	MAN	O5-C5-C4	3.40	115.76	110.13
5	A	1114	MAN	C3-C4-C5	3.52	116.51	110.23
4	A	1059	NAG	C2-N2-C7	3.69	127.91	123.11
5	B	1112	MAN	C1-C2-C3	3.93	114.31	109.55
5	B	1115	MAN	C3-C4-C5	4.04	117.43	110.23
7	B	1062	MAN	C3-C4-C5	4.29	117.87	110.23
6	A	1577	NAG	C1-O5-C5	4.29	118.45	112.14
6	B	1577	NAG	C1-O5-C5	4.32	118.50	112.14
7	B	1062	MAN	O5-C1-C2	4.34	117.84	110.89
7	B	1060	BMA	C1-O5-C5	4.43	118.66	112.14
5	A	1115	MAN	C1-O5-C5	4.67	119.01	112.14
7	B	1062	MAN	O5-C5-C4	4.79	118.06	110.13
7	B	1062	MAN	C1-O5-C5	5.24	119.85	112.14
4	A	1060	BMA	O3-C3-C2	5.36	119.83	110.01
4	A	1064	MAN	C1-O5-C5	6.80	122.14	112.14

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1115	MAN	C1
7	B	1062	MAN	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1059	NAG	1	0
5	A	1112	MAN	0	1

5.6 Ligand geometry (i)

31 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	SUC	A	1000	-	24,24,24	0.37	0	36,36,36	0.80	0
2	SUC	A	1001	-	24,24,24	0.46	0	36,36,36	0.75	0
3	NAG	A	1052	1	14,14,15	0.22	0	15,19,21	1.32	2 (13%)
3	NAG	A	1125	1	14,14,15	0.66	0	15,19,21	1.12	1 (6%)
3	NAG	A	1215	1	14,14,15	0.70	0	15,19,21	2.06	3 (20%)
3	NAG	A	1236	1	14,14,15	0.36	0	15,19,21	0.85	0
3	NAG	A	1242	1	14,14,15	0.25	0	15,19,21	1.17	1 (6%)
3	NAG	A	1319	1	14,14,15	0.41	0	15,19,21	1.14	2 (13%)
3	NAG	A	1357	1	14,14,15	0.31	0	15,19,21	1.23	2 (13%)
3	NAG	A	1444	1	14,14,15	0.57	0	15,19,21	1.08	1 (6%)
3	NAG	A	1471	1	14,14,15	0.29	0	15,19,21	1.34	3 (20%)
3	NAG	A	1483	1	14,14,15	0.36	0	15,19,21	1.09	1 (6%)
3	NAG	A	1512	1	14,14,15	0.28	0	15,19,21	1.17	2 (13%)
3	NAG	A	1539	1	14,14,15	0.67	0	15,19,21	1.59	1 (6%)
3	NAG	A	1555	1	14,14,15	0.32	0	15,19,21	1.16	1 (6%)
3	NAG	A	1606	1	14,14,15	0.44	0	15,19,21	1.92	3 (20%)
3	NAG	A	1644	1	14,14,15	0.45	0	15,19,21	0.66	0
2	SUC	B	1000	-	24,24,24	0.40	0	36,36,36	1.06	3 (8%)
2	SUC	B	1001	-	24,24,24	0.50	0	36,36,36	0.90	2 (5%)
3	NAG	B	1052	1	14,14,15	0.31	0	15,19,21	0.79	0
3	NAG	B	1125	1	14,14,15	0.59	0	15,19,21	1.08	1 (6%)
3	NAG	B	1215	1	14,14,15	0.52	0	15,19,21	1.06	1 (6%)
3	NAG	B	1242	1	14,14,15	0.32	0	15,19,21	1.27	2 (13%)
3	NAG	B	1319	1	14,14,15	0.44	0	15,19,21	1.26	1 (6%)
3	NAG	B	1357	1	14,14,15	0.34	0	15,19,21	0.90	0
3	NAG	B	1444	1	14,14,15	0.48	0	15,19,21	1.45	2 (13%)
3	NAG	B	1471	1	14,14,15	0.33	0	15,19,21	0.79	1 (6%)
3	NAG	B	1483	1	14,14,15	0.24	0	15,19,21	0.86	0
3	NAG	B	1539	1	14,14,15	0.72	0	15,19,21	1.40	2 (13%)
3	NAG	B	1555	1	14,14,15	0.49	0	15,19,21	0.79	0
3	NAG	B	1644	1	14,14,15	0.45	0	15,19,21	0.77	0

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	SUC	A	1000	-	-	0/12/51/51	0/2/2/2
2	SUC	A	1001	-	-	0/12/51/51	0/2/2/2
3	NAG	A	1052	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1125	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1215	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1236	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1242	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1319	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1357	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1444	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1471	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1483	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1512	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1539	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1555	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1606	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1644	1	-	0/6/23/26	0/1/1/1
2	SUC	B	1000	-	-	0/12/51/51	0/2/2/2
2	SUC	B	1001	-	-	0/12/51/51	0/2/2/2
3	NAG	B	1052	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1125	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1215	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1242	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1319	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1357	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1444	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1471	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1483	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1539	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	1555	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1644	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1606	NAG	O7-C7-C8	-2.70	117.11	122.07
3	A	1319	NAG	O5-C5-C4	-2.61	105.81	110.13
3	B	1215	NAG	O5-C5-C4	-2.55	105.91	110.13
3	A	1052	NAG	C4-C3-C2	-2.46	107.52	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1215	NAG	C4-C3-C2	-2.24	107.86	111.34
3	B	1125	NAG	O5-C5-C4	-2.03	106.77	110.13
2	B	1000	SUC	C1'-C2'-C3'	-2.03	107.57	114.44
3	B	1471	NAG	C1-O5-C5	2.05	115.15	112.14
3	A	1319	NAG	C2-N2-C7	2.09	125.83	123.11
3	A	1125	NAG	O5-C5-C6	2.16	111.96	107.34
3	A	1471	NAG	C1-O5-C5	2.17	115.33	112.14
2	B	1000	SUC	O2'-C2'-C1'	2.20	114.23	108.05
2	B	1001	SUC	O2'-C5'-C6'	2.25	115.32	108.40
3	A	1471	NAG	C2-N2-C7	2.26	126.05	123.11
3	B	1539	NAG	O5-C5-C4	2.32	113.97	110.13
3	A	1215	NAG	O5-C5-C4	2.36	114.05	110.13
3	A	1444	NAG	C3-C4-C5	2.44	114.57	110.23
3	A	1471	NAG	C8-C7-N2	2.49	120.87	116.10
3	A	1357	NAG	C1-O5-C5	2.50	115.81	112.14
2	B	1001	SUC	O2'-C2'-C1'	2.52	115.13	108.05
3	A	1512	NAG	C8-C7-N2	2.54	120.97	116.10
3	A	1052	NAG	C8-C7-N2	2.56	121.00	116.10
3	B	1242	NAG	C2-N2-C7	2.64	126.54	123.11
3	A	1512	NAG	C2-N2-C7	2.65	126.55	123.11
3	A	1357	NAG	C2-N2-C7	2.68	126.58	123.11
3	A	1555	NAG	C8-C7-N2	2.75	121.36	116.10
3	B	1242	NAG	C8-C7-N2	2.75	121.37	116.10
3	A	1242	NAG	C1-O5-C5	2.96	116.50	112.14
3	B	1444	NAG	O5-C5-C4	2.97	115.05	110.13
2	B	1000	SUC	C1-O5-C5	3.01	119.66	113.74
3	A	1606	NAG	C8-C7-N2	3.52	122.84	116.10
3	A	1483	NAG	C1-O5-C5	3.57	117.39	112.14
3	B	1444	NAG	C1-O5-C5	4.07	118.12	112.14
3	B	1319	NAG	C1-O5-C5	4.26	118.40	112.14
3	B	1539	NAG	C1-O5-C5	4.26	118.40	112.14
3	A	1606	NAG	C2-N2-C7	5.09	129.72	123.11
3	A	1539	NAG	C1-O5-C5	5.52	120.25	112.14
3	A	1215	NAG	C1-O5-C5	6.54	121.76	112.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1539	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1444	NAG	2	0
3	B	1539	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	624/665 (93%)	-0.32	3 (0%) 91 92	16, 25, 38, 57	0
1	B	624/665 (93%)	-0.14	10 (1%) 74 75	19, 33, 50, 59	0
All	All	1248/1330 (93%)	-0.23	13 (1%) 84 84	16, 29, 46, 59	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	CYS	4.0
1	B	240	ILE	3.3
1	B	43	SER	3.0
1	A	42	CYS	2.9
1	B	44	LEU	2.9
1	B	571	GLU	2.7
1	A	43	SER	2.6
1	B	55	LEU	2.6
1	B	48	VAL	2.2
1	B	56	CYS	2.1
1	A	44	LEU	2.1
1	B	235	ALA	2.1
1	B	569	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	MAN	B	1063	11/12	0.85	0.41	21.64	74,78,79,79	0
4	MAN	A	1062	11/12	0.76	0.32	16.57	59,63,64,67	0
4	NAG	A	1058	14/15	0.96	0.11	1.44	21,24,31,31	0
7	NAG	B	1058	14/15	0.96	0.11	-0.03	28,30,35,37	0
5	NAG	B	1108	14/15	0.98	0.08	-0.22	24,25,27,28	0
5	NAG	A	1107	14/15	0.97	0.08	-0.67	18,18,22,22	0
5	NAG	B	1107	14/15	0.97	0.08	-0.79	21,22,24,25	0
5	NAG	A	1108	14/15	0.97	0.08	-0.95	20,21,23,23	0
7	NAG	B	1059	14/15	0.95	0.15	-	32,33,36,39	0
5	MAN	A	1112	11/12	0.90	0.13	-	44,48,54,56	0
5	MAN	B	1115	11/12	0.88	0.13	-	48,49,53,56	0
7	MAN	B	1062	11/12	0.75	0.45	-	72,76,80,81	0
5	MAN	B	1111	11/12	0.89	0.20	-	61,64,74,77	0
5	MAN	A	1113	11/12	0.83	0.17	-	62,68,74,74	0
4	BMA	A	1060	11/12	0.93	0.13	-	32,37,46,48	0
7	BMA	B	1060	11/12	0.91	0.18	-	45,49,58,63	0
6	NAG	B	1576	14/15	0.93	0.14	-	52,57,63,75	0
7	MAN	B	1061	11/12	0.74	0.32	-	66,72,75,79	0
5	MAN	A	1115	11/12	0.88	0.18	-	61,64,67,75	0
5	MAN	B	1114	11/12	0.98	0.10	-	22,22,23,24	0
5	MAN	A	1114	11/12	0.91	0.14	-	42,47,55,60	0
5	MAN	A	1116	11/12	0.70	0.50	-	88,94,101,102	0
5	MAN	B	1112	11/12	0.76	0.47	-	86,92,94,94	0
5	MAN	B	1113	11/12	0.95	0.10	-	25,28,36,43	0
6	NAG	A	1577	14/15	0.71	0.40	-	80,90,95,97	0
4	MAN	A	1064	11/12	0.58	0.37	-	85,91,99,103	0
6	NAG	A	1576	14/15	0.94	0.12	-	47,51,61,76	0
5	MAN	A	1110	11/12	0.96	0.10	-	23,25,33,40	0
5	MAN	B	1110	11/12	0.95	0.13	-	43,48,54,55	0
5	MAN	A	1111	11/12	0.98	0.09	-	18,20,20,21	0
6	NAG	B	1577	14/15	0.68	0.36	-	78,91,98,100	0
4	MAN	A	1063	11/12	0.87	0.23	-	56,66,72,74	0
4	MAN	A	1061	11/12	0.79	0.41	-	52,59,63,67	0
5	BMA	A	1109	11/12	0.97	0.07	-	24,25,28,34	0
4	NAG	A	1059	14/15	0.97	0.12	-	24,25,29,35	0
5	BMA	B	1109	11/12	0.96	0.08	-	28,29,32,37	0
5	MAN	B	1116	11/12	0.82	0.18	-	62,67,68,69	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	1606	14/15	0.70	0.34	6.00	57,66,71,73	0
3	NAG	B	1539	14/15	0.71	0.32	5.53	63,75,78,78	0
3	NAG	A	1539	14/15	0.83	0.18	5.35	50,57,60,62	0
2	SUC	B	1001	23/23	0.85	0.23	3.50	52,60,65,69	0
3	NAG	B	1644	14/15	0.94	0.17	3.06	32,35,38,42	0
3	NAG	A	1644	14/15	0.95	0.15	2.86	27,30,39,41	0
2	SUC	A	1001	23/23	0.89	0.22	2.30	47,51,62,66	0
3	NAG	A	1236	14/15	0.91	0.16	2.23	34,43,47,48	0
3	NAG	B	1357	14/15	0.94	0.19	2.06	47,51,57,57	0
3	NAG	B	1471	14/15	0.94	0.12	1.22	33,35,37,38	0
3	NAG	A	1357	14/15	0.95	0.11	0.38	37,39,43,44	0
2	SUC	A	1000	23/23	0.98	0.10	-0.10	16,20,23,24	0
2	SUC	B	1000	23/23	0.96	0.11	-0.20	22,27,30,34	0
3	NAG	A	1444	14/15	0.94	0.09	-0.32	32,35,40,44	0
3	NAG	A	1471	14/15	0.95	0.09	-0.45	30,32,38,46	0
3	NAG	B	1444	14/15	0.93	0.11	-0.86	37,39,41,42	0
3	NAG	A	1242	14/15	0.86	0.34	-	63,65,69,70	0
3	NAG	A	1125	14/15	0.82	0.29	-	64,71,77,77	0
3	NAG	B	1483	14/15	0.87	0.18	-	60,65,71,74	0
3	NAG	A	1512	14/15	0.87	0.22	-	59,67,87,91	0
3	NAG	A	1319	14/15	0.79	0.44	-	73,83,87,90	0
3	NAG	B	1555	14/15	0.85	0.20	-	42,48,53,53	0
3	NAG	B	1242	14/15	0.84	0.43	-	79,83,87,91	0
3	NAG	A	1483	14/15	0.93	0.15	-	42,47,49,51	0
3	NAG	B	1125	14/15	0.66	0.30	-	65,71,76,78	0
3	NAG	B	1052	14/15	0.74	0.34	-	73,80,84,84	0
3	NAG	A	1052	14/15	0.84	0.31	-	59,65,68,75	0
3	NAG	B	1215	14/15	0.83	0.45	-	78,83,87,92	0
3	NAG	A	1215	14/15	0.79	0.33	-	64,76,79,83	0
3	NAG	A	1555	14/15	0.79	0.24	-	66,75,79,80	0
3	NAG	B	1319	14/15	0.82	0.51	-	85,92,93,94	0

6.5 Other polymers (i)

There are no such residues in this entry.