



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 10:09 am GMT

PDB ID : 3LRL
Title : Structure of alfa-galactosidase (MEL1) from *Saccharomyces cerevisiae* with melibiose
Authors : Fernandez-Leiro, R.; Pereira-Rodriguez, A.; Cerdan, M.E.; Becerra, M.; Sanz-Aparicio, J.
Deposited on : 2010-02-11
Resolution : 2.40 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

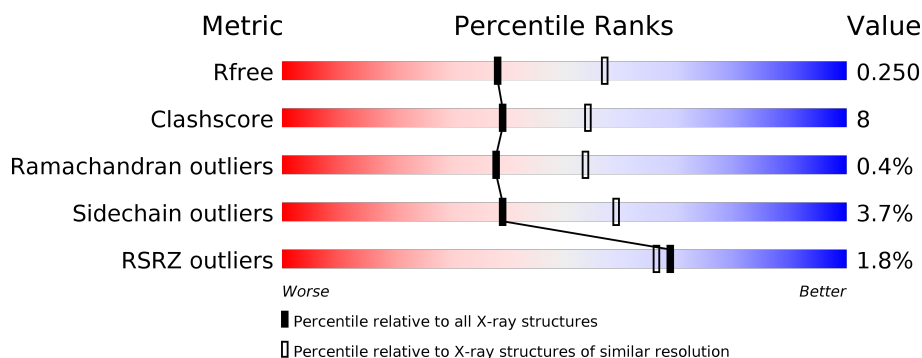
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	479	<div> <div>2%</div> <div>81%</div> <div>13%</div> <div>6%</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
2	NAG	A	6001	-	-	X	X
3	NAG	A	3001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GLC	A	480	X	-	-	X
5	GLA	A	481	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4069 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 Alpha-galactosidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3518	2204	596	697	21			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	VAL	ILE	ENGINEERED	UNP P04824
A	472	ASP	-	EXPRESSION TAG	UNP P04824
A	473	TYR	-	EXPRESSION TAG	UNP P04824
A	474	LYS	-	EXPRESSION TAG	UNP P04824
A	475	ASP	-	EXPRESSION TAG	UNP P04824
A	476	ASP	-	EXPRESSION TAG	UNP P04824
A	477	ASP	-	EXPRESSION TAG	UNP P04824
A	478	ASP	-	EXPRESSION TAG	UNP P04824
A	479	LYS	-	EXPRESSION TAG	UNP P04824

- Molecule 2 is SUGAR (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		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

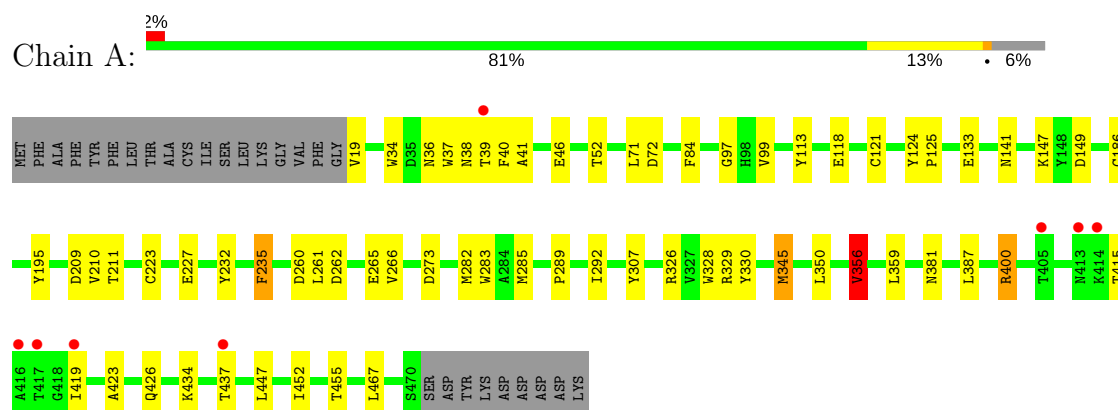
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	415	Total	O	0	0
			415	415		

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: Alpha-galactosidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.73Å 100.73Å 111.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.99 – 2.40 50.36 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (59.99-2.40) 99.5 (50.36-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.15 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.253 0.200 , 0.250	Depositor DCC
R_{free} test set	1174 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4069	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, GLC, NAG, NA

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	0.60	0/3605	0.68	2/4895 (0.0%)

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	A	1	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	261	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	356	VAL	CB-CA-C	-5.29	101.36	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	480	GLC	C1

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	3518	0	3279	58	0
2	A	56	0	52	9	0
3	A	56	0	50	1	0
4	A	1	0	0	0	0
5	A	23	0	21	9	0
6	A	415	0	0	3	0
All	All	4069	0	3402	60	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 8.

The worst 5 of 60 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:328:TRP:CH2	2:A:6001:NAG:H82	1.73	1.24
1:A:209:ASP:OD1	5:A:481:GLA:O2	1.71	1.05
1:A:118:GLU:HG3	6:A:811:HOH:O	1.59	1.01
1:A:328:TRP:CH2	2:A:6001:NAG:C8	2.49	0.96
1:A:328:TRP:CZ3	2:A:6001:NAG:H82	2.03	0.92

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	450/479 (94%)	430 (96%)	18 (4%)	2 (0%)	38 54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	262	ASP

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	376/399 (94%)	362 (96%)	14 (4%)	39 59

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

Mol	Chain	Res	Type
1	A	345	MET
1	A	356	VAL
1	A	452	ILE
1	A	283	TRP
1	A	447	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	435	ASN
1	A	355	GLN
1	A	141	ASN
1	A	426	GLN

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](#)

6 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	$\# Z > 2$
3	NAG	A	3001	1,3	14,14,15	0.84	0	15,19,21	0.84	1 (6%)
3	NAG	A	3002	3	14,14,15	1.27	1 (7%)	15,19,21	2.76	5 (33%)
5	GLC	A	480	5	12,12,12	0.57	0	17,17,17	2.01	5 (29%)
5	GLA	A	481	5	11,11,12	1.14	0	13,15,17	1.70	4 (30%)
3	NAG	A	5001	1,3	14,14,15	0.49	0	15,19,21	1.53	3 (20%)
3	NAG	A	5002	3	14,14,15	0.51	0	15,19,21	1.24	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
3	NAG	A	3001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3002	3	-	0/6/23/26	0/1/1/1
5	GLC	A	480	5	1/1/5/5	0/2/22/22	0/1/1/1
5	GLA	A	481	5	-	0/2/19/22	0/1/1/1
3	NAG	A	5001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	5002	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3002	NAG	O5-C1	-2.94	1.38	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3002	NAG	C2-N2-C7	-6.11	114.02	122.94
3	A	3002	NAG	C3-C4-C5	-5.82	99.97	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3002	NAG	O5-C1-C2	-4.37	105.39	111.47
3	A	5001	NAG	O5-C1-C2	-2.66	107.77	111.47
5	A	480	GLC	C6-C5-C4	-2.62	106.88	113.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	480	GLC	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	NAG	1	0
3	A	3002	NAG	1	0
5	A	480	GLC	1	0
5	A	481	GLA	8	0

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
2	NAG	A	1001	1	14,14,15	0.64	0	15,19,21	1.32	1 (6%)
2	NAG	A	2001	1	14,14,15	0.58	0	15,19,21	1.92	2 (13%)
2	NAG	A	4001	1	14,14,15	0.52	0	15,19,21	1.33	1 (6%)
2	NAG	A	6001	1	14,14,15	2.50	2 (14%)	15,19,21	0.84	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	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	4001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	6001	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6001	NAG	O5-C1	-6.22	1.33	1.43
2	A	6001	NAG	C1-C2	6.68	1.61	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	NAG	C6-C5-C4	-3.79	104.13	113.00
2	A	6001	NAG	C4-C3-C2	2.23	114.29	111.02
2	A	1001	NAG	C1-O5-C5	3.38	116.83	112.17
2	A	4001	NAG	C1-O5-C5	3.90	117.54	112.17
2	A	2001	NAG	C1-O5-C5	5.59	119.87	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6001	NAG	9	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	452/479 (94%)	-0.31	8 (1%) 69 66	11, 22, 48, 66	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	ILE	3.7
1	A	414	LYS	3.6
1	A	417	THR	3.3
1	A	413	ASN	2.7
1	A	416	ALA	2.4

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
3	NAG	A	3001	14/15	0.73	0.36	18.53	54,61,65,65	0
5	GLA	A	481	11/12	0.55	0.48	10.67	45,47,48,48	0
5	GLC	A	480	12/12	0.82	0.22	2.95	46,51,52,52	0
3	NAG	A	5001	14/15	0.92	0.12	-0.23	41,42,44,45	0
3	NAG	A	5002	14/15	0.93	0.11	-	37,39,40,40	0
3	NAG	A	3002	14/15	0.67	0.28	-	68,70,71,71	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, 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
2	NAG	A	6001	14/15	0.68	0.44	17.05	54,61,65,65	0
2	NAG	A	1001	14/15	0.95	0.16	0.61	29,30,32,35	0
2	NAG	A	2001	14/15	0.91	0.12	0.16	26,30,32,33	0
4	NA	A	8001	1/1	0.96	0.36	-	11,11,11,11	0
2	NAG	A	4001	14/15	0.92	0.22	-	41,42,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.