



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2017 – 08:23 AM EDT

PDB ID : 5M63
Title : Crystal structure of group B Streptococcus type III DP2 oligosaccharide bound to Fab NVS-1-19-5
Authors : Carboni, F.; Adamo, R.; Veggi, D.; Rappuoli, R.; Malito, E.; Margarit, I.R.; Berti, F.
Deposited on : unknown
Resolution : 2.74 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-20029824
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-20029824

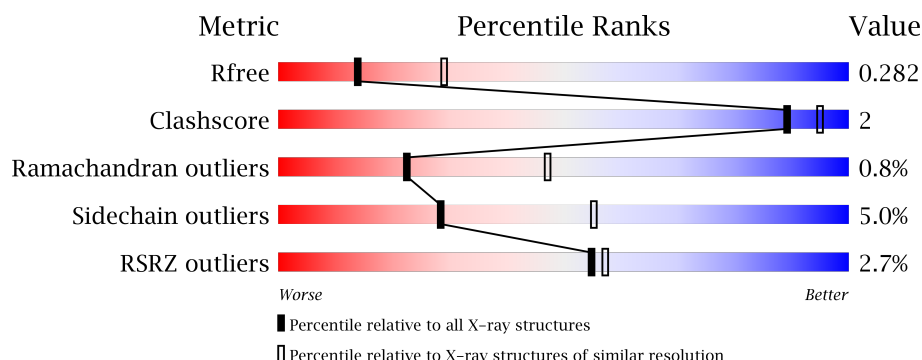
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	3342 (2.78-2.70)
Clashscore	112137	3731 (2.78-2.70)
Ramachandran outliers	110173	3670 (2.78-2.70)
Sidechain outliers	110143	3671 (2.78-2.70)
RSRZ outliers	101464	3362 (2.78-2.70)

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	H	248	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	M	248	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>9%</div> </div> </div>
2	L	239	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>10%</div> </div> </div>
2	N	239	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>10%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	H	301	-	-	-	X
3	EDO	L	309	-	-	-	X
3	EDO	M	305	-	-	-	X
3	EDO	N	308	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6930 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.

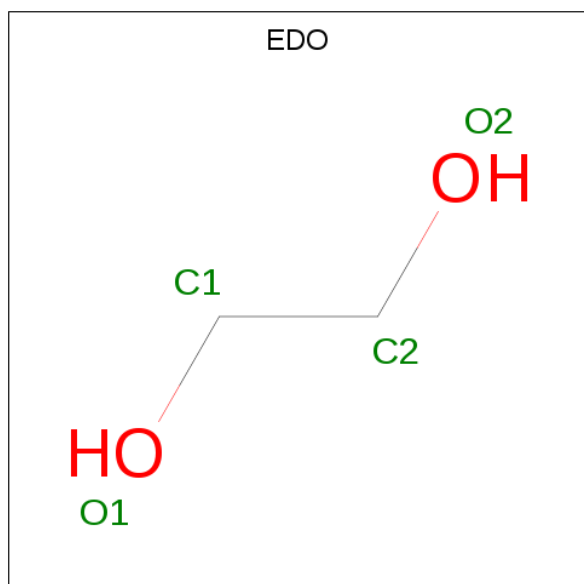
- Molecule 1 is a protein called H chain of Fab NVS-1-19-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	222	Total	C	N	O	S	0	0	0
			1639	1037	269	323	10			
1	M	226	Total	C	N	O	S	0	0	0
			1664	1050	273	330	11			

- Molecule 2 is a protein called L chain of Fab NVS-1-19-5.

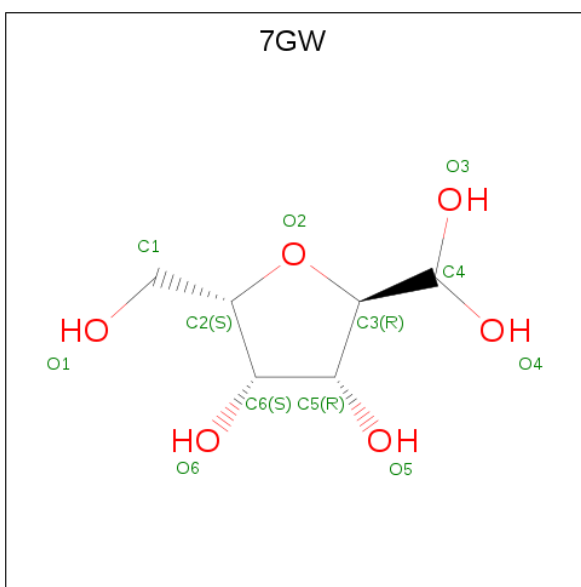
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1586	985	261	333	7			
2	N	216	Total	C	N	O	S	0	0	0
			1591	988	262	334	7			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



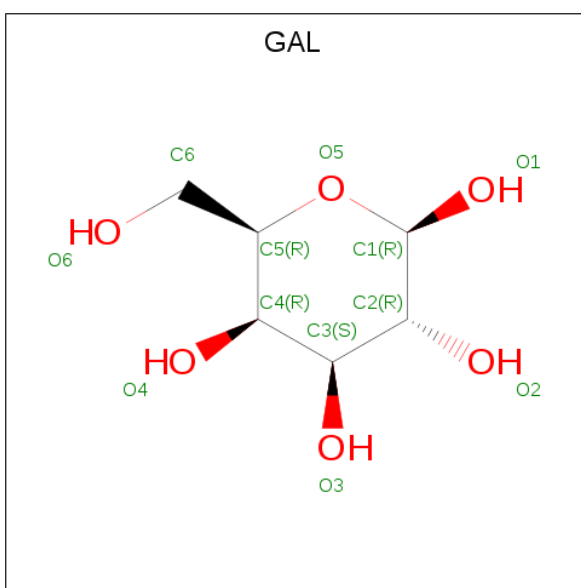
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	M	1	Total C O 4 2 2	0	0
3	M	1	Total C O 4 2 2	0	0
3	N	1	Total C O 4 2 2	0	0
3	N	1	Total C O 4 2 2	0	0
3	N	1	Total C O 4 2 2	0	0
3	N	1	Total C O 4 2 2	0	0

- Molecule 4 is (2 {R},3 {R},4 {S},5 {S})-2-[bis(oxidanyl)methyl]-5-(hydroxymethyl)oxolane-3,4-diol (three-letter code: 7GW) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			12	6	6		
4	M	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



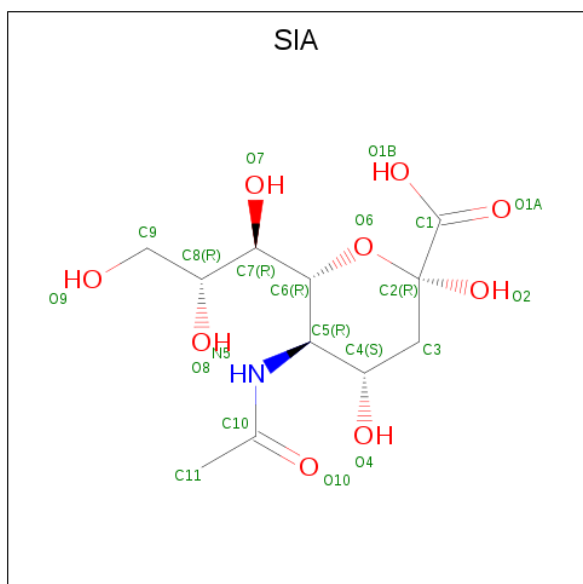
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			11	6	5		
5	L	1	Total	C	O	0	0
			11	6	5		

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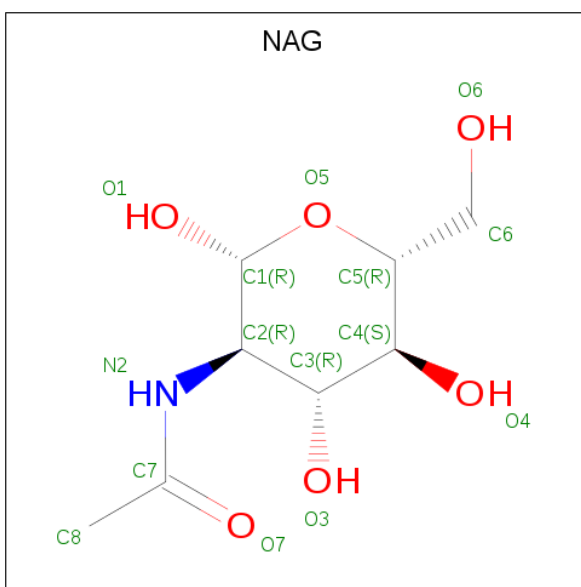
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			11	6	5		
5	L	1	Total	C	O	0	0
			11	6	5		
5	M	1	Total	C	O	0	0
			11	6	5		
5	N	1	Total	C	O	0	0
			11	6	5		
5	N	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is O-SIALIC ACID (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



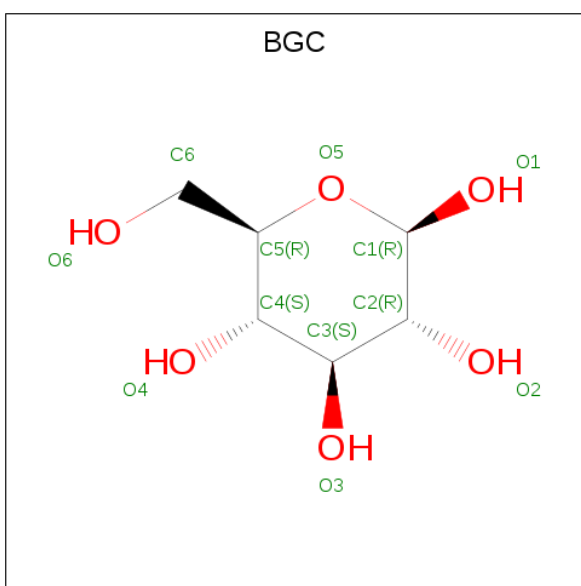
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			20	11	1	8		
6	L	1	Total	C	N	O	0	0
			20	11	1	8		
6	M	1	Total	C	N	O	0	0
			20	11	1	8		
6	N	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			14	8	1	5		
7	N	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			11	6	5		
8	L	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	C	O	0	0
			11	6	5		
8	N	1	Total	C	O	0	0
			11	6	5		

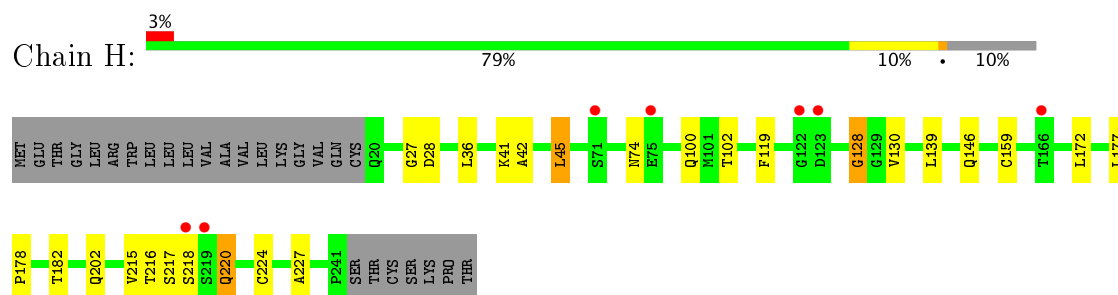
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	27	Total	O	0	0
			27	27		
9	L	27	Total	O	0	0
			27	27		
9	M	45	Total	O	0	0
			45	45		
9	N	35	Total	O	0	0
			35	35		

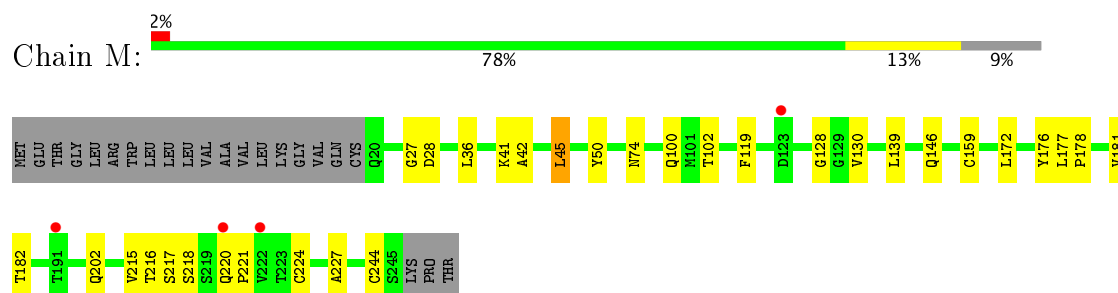
3 Residue-property plots [i](#)

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.

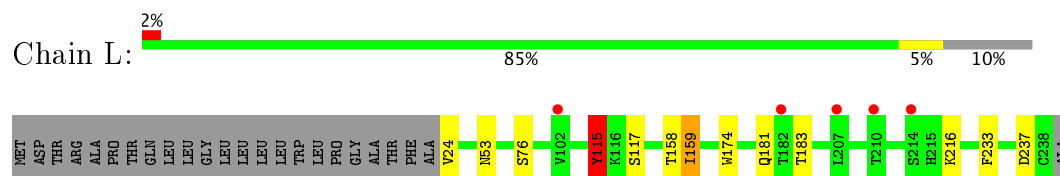
- Molecule 1: H chain of Fab NVS-1-19-5



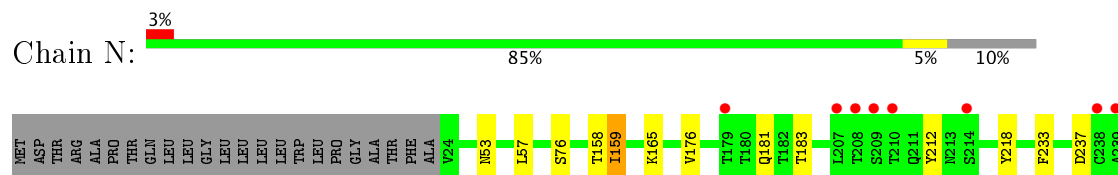
- Molecule 1: H chain of Fab NVS-1-19-5



- Molecule 2: L chain of Fab NVS-1-19-5



- Molecule 2: L chain of Fab NVS-1-19-5



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	135.34Å 142.23Å 144.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 2.74 49.02 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.02-2.74) 99.2 (49.02-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.236 , 0.282 0.236 , 0.282	Depositor DCC
R_{free} test set	1834 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.056 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6930	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.64 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.0901e-04.*

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: BGC, NAG, SIA, EDO, 7GW, GAL

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	H	0.52	1/1680 (0.1%)	0.72	0/2298
1	M	0.58	1/1705 (0.1%)	0.76	1/2332 (0.0%)
2	L	0.54	1/1616 (0.1%)	0.66	0/2212
2	N	0.53	0/1621	0.66	0/2219
All	All	0.54	3/6622 (0.0%)	0.70	1/9061 (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
1	H	0	1
1	M	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	115	TYR	CE1-CZ	-7.09	1.29	1.38
1	M	28	ASP	CB-CG	6.90	1.66	1.51
1	H	28	ASP	CB-CG	5.43	1.63	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	28	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	220	GLN	Peptide
1	M	220	GLN	Peptide

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	H	1639	0	1606	11	0
1	M	1664	0	1627	9	1
2	L	1586	0	1529	8	0
2	N	1591	0	1533	6	0
3	H	12	0	18	0	0
3	L	16	0	24	0	0
3	M	8	0	12	0	0
3	N	16	0	24	0	0
4	H	12	0	0	0	0
4	M	12	0	0	0	0
5	H	11	0	9	0	0
5	L	33	0	28	0	0
5	M	11	0	9	0	0
5	N	33	0	28	0	0
6	H	20	0	17	0	0
6	L	20	0	17	0	0
6	M	20	0	17	0	0
6	N	20	0	17	0	0
7	L	14	0	11	0	0
7	N	14	0	11	0	0
8	L	22	0	18	0	0
8	N	22	0	18	0	0
9	H	27	0	0	0	0
9	L	27	0	0	0	0
9	M	45	0	0	0	0
9	N	35	0	0	0	0
All	All	6930	0	6573	30	1

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 2.

All (30) 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:M:182:THR:HG22	1:M:227:ALA:HB3	1.71	0.72
1:H:182:THR:HG22	1:H:227:ALA:HB3	1.74	0.69
1:H:128:GLY:HA2	2:L:115:TYR:CD2	2.27	0.68
2:N:176:VAL:HG22	2:N:181:GLN:HE21	1.60	0.66
1:H:27:GLY:HA2	1:H:36:LEU:HD21	1.81	0.62
2:N:176:VAL:CG2	2:N:181:GLN:HE21	2.15	0.59
1:H:177:LEU:HD12	1:H:178:PRO:HA	1.85	0.59
1:M:27:GLY:HA2	1:M:36:LEU:HD21	1.87	0.56
1:M:177:LEU:HD12	1:M:178:PRO:HA	1.88	0.55
1:H:119:PHE:HB3	1:H:130:VAL:HG11	1.91	0.51
1:H:182:THR:CG2	1:H:227:ALA:HB3	2.41	0.50
1:H:27:GLY:CA	1:H:36:LEU:HD21	2.44	0.46
2:N:159:ILE:HD11	2:N:233:PHE:HZ	1.82	0.45
2:N:212:TYR:HA	2:N:218:TYR:OH	2.16	0.45
1:M:27:GLY:CA	1:M:36:LEU:HD21	2.47	0.45
2:L:181:GLN:OE1	2:L:181:GLN:HA	2.17	0.44
2:L:159:ILE:HD11	2:L:233:PHE:HZ	1.83	0.44
1:M:176:TYR:CE1	1:M:181:VAL:HG13	2.53	0.44
1:M:216:THR:O	1:M:218:SER:N	2.51	0.44
1:H:216:THR:O	1:H:218:SER:N	2.51	0.43
1:H:172:LEU:HD21	2:L:158:THR:HG23	2.01	0.43
1:M:119:PHE:HB3	1:M:130:VAL:HG11	2.00	0.43
1:H:172:LEU:HD21	2:L:158:THR:CG2	2.49	0.42
1:M:172:LEU:HD21	2:N:158:THR:CG2	2.50	0.42
2:L:115:TYR:CD1	2:L:115:TYR:C	2.93	0.42
1:M:42:ALA:HB1	1:M:45:LEU:HD23	2.03	0.41
2:L:159:ILE:CG2	2:L:174:TRP:CZ3	3.04	0.40
2:N:181:GLN:OE1	2:N:181:GLN:HA	2.21	0.40
1:H:42:ALA:HB1	1:H:45:LEU:HD23	2.04	0.40
2:L:115:TYR:CE1	2:L:117:SER:HA	2.56	0.40

All (1) 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)
1:M:50:TYR:OH	1:M:50:TYR:OH[3_655]	1.65	0.55

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	H	220/248 (89%)	211 (96%)	7 (3%)	2 (1%)	20	44
1	M	224/248 (90%)	214 (96%)	8 (4%)	2 (1%)	20	44
2	L	213/239 (89%)	196 (92%)	16 (8%)	1 (0%)	32	59
2	N	214/239 (90%)	196 (92%)	16 (8%)	2 (1%)	20	44
All	All	871/974 (89%)	817 (94%)	47 (5%)	7 (1%)	22	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	217	SER
1	M	217	SER
2	L	76	SER
2	N	76	SER
2	N	165	LYS
1	H	128	GLY
1	M	128	GLY

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	H	186/209 (89%)	174 (94%)	12 (6%)	20	42
1	M	190/209 (91%)	177 (93%)	13 (7%)	18	39
2	L	181/199 (91%)	174 (96%)	7 (4%)	37	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	N	181/199 (91%)	176 (97%)	5 (3%)	49 77
All	All	738/816 (90%)	701 (95%)	37 (5%)	28 55

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	41	LYS
1	H	45	LEU
1	H	74	ASN
1	H	100	GLN
1	H	102	THR
1	H	139	LEU
1	H	146	GLN
1	H	159	CYS
1	H	202	GLN
1	H	215	VAL
1	H	220	GLN
1	H	224	CYS
2	L	24	VAL
2	L	53	ASN
2	L	115	TYR
2	L	159	ILE
2	L	183	THR
2	L	216	LYS
2	L	237	ASP
1	M	41	LYS
1	M	45	LEU
1	M	74	ASN
1	M	100	GLN
1	M	102	THR
1	M	139	LEU
1	M	146	GLN
1	M	159	CYS
1	M	202	GLN
1	M	215	VAL
1	M	221	PRO
1	M	224	CYS
1	M	244	CYS
2	N	53	ASN
2	N	57	LEU
2	N	159	ILE
2	N	183	THR

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Mol	Chain	Res	Type
2	N	237	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	N	181	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 ⓘ

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	H	301	-	3,3,3	0.53	0	2,2,2	0.32	0
3	EDO	H	302	-	3,3,3	0.63	0	2,2,2	0.12	0
3	EDO	H	303	-	3,3,3	0.51	0	2,2,2	0.22	0
4	7GW	H	304	8,5	11,12,12	5.23	7 (63%)	15,17,17	1.30	1 (6%)
5	GAL	H	305	4,6	11,11,12	0.71	0	13,15,17	1.27	1 (7%)
6	SIA	H	306	5	17,20,21	0.57	0	19,28,31	1.37	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GAL	L	301	7,6	11,11,12	0.80	0	13,15,17	1.29	1 (7%)
7	NAG	L	302	8,5	14,14,15	0.65	0	15,19,21	1.13	1 (6%)
8	BGC	L	303	5,7	11,11,12	0.91	0	13,15,17	1.83	5 (38%)
5	GAL	L	304	8	11,11,12	0.84	0	13,15,17	1.53	3 (23%)
5	GAL	L	305	8,7	11,11,12	0.63	0	13,15,17	1.54	2 (15%)
8	BGC	L	306	5,4	11,11,12	0.55	0	13,15,17	1.70	3 (23%)
6	SIA	L	307	5	17,20,21	0.50	0	19,28,31	1.08	2 (10%)
3	EDO	L	308	-	3,3,3	0.56	0	2,2,2	0.09	0
3	EDO	L	309	-	3,3,3	0.58	0	2,2,2	0.07	0
3	EDO	L	310	-	3,3,3	0.54	0	2,2,2	0.13	0
3	EDO	L	311	-	3,3,3	0.48	0	2,2,2	0.35	0
3	EDO	M	301	-	3,3,3	0.42	0	2,2,2	0.46	0
4	7GW	M	302	8,5	11,12,12	5.10	7 (63%)	15,17,17	1.36	1 (6%)
5	GAL	M	303	4,6	11,11,12	0.48	0	13,15,17	1.57	3 (23%)
6	SIA	M	304	5	17,20,21	0.64	0	19,28,31	1.35	2 (10%)
3	EDO	M	305	-	3,3,3	0.59	0	2,2,2	0.33	0
5	GAL	N	301	7,6	11,11,12	0.55	0	13,15,17	1.26	2 (15%)
7	NAG	N	302	8,5	14,14,15	0.47	0	15,19,21	1.31	2 (13%)
8	BGC	N	303	5,7	11,11,12	0.68	0	13,15,17	1.21	2 (15%)
5	GAL	N	304	8	11,11,12	0.70	0	13,15,17	1.46	2 (15%)
5	GAL	N	305	8,7	11,11,12	0.64	0	13,15,17	1.88	3 (23%)
8	BGC	N	306	5,4	11,11,12	0.66	0	13,15,17	1.97	3 (23%)
6	SIA	N	307	5	17,20,21	0.54	0	19,28,31	1.14	1 (5%)
3	EDO	N	308	-	3,3,3	0.74	0	2,2,2	0.08	0
3	EDO	N	309	-	3,3,3	0.51	0	2,2,2	0.24	0
3	EDO	N	310	-	3,3,3	0.56	0	2,2,2	0.23	0
3	EDO	N	311	-	3,3,3	0.53	0	2,2,2	0.24	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
3	EDO	H	301	-	-	0/1/1/1	0/0/0/0
3	EDO	H	302	-	-	0/1/1/1	0/0/0/0
3	EDO	H	303	-	-	0/1/1/1	0/0/0/0
4	7GW	H	304	8,5	-	0/6/22/22	0/1/1/1
5	GAL	H	305	4,6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SIA	H	306	5	-	0/14/34/38	0/1/1/1
5	GAL	L	301	7,6	-	0/2/19/22	0/1/1/1
7	NAG	L	302	8,5	-	0/6/23/26	0/1/1/1
8	BGC	L	303	5,7	-	0/2/19/22	0/1/1/1
5	GAL	L	304	8	-	0/2/19/22	0/1/1/1
5	GAL	L	305	8,7	-	0/2/19/22	0/1/1/1
8	BGC	L	306	5,4	-	0/2/19/22	0/1/1/1
6	SIA	L	307	5	-	0/14/34/38	0/1/1/1
3	EDO	L	308	-	-	0/1/1/1	0/0/0/0
3	EDO	L	309	-	-	0/1/1/1	0/0/0/0
3	EDO	L	310	-	-	0/1/1/1	0/0/0/0
3	EDO	L	311	-	-	0/1/1/1	0/0/0/0
3	EDO	M	301	-	-	0/1/1/1	0/0/0/0
4	7GW	M	302	8,5	-	0/6/22/22	0/1/1/1
5	GAL	M	303	4,6	-	0/2/19/22	0/1/1/1
6	SIA	M	304	5	-	0/14/34/38	0/1/1/1
3	EDO	M	305	-	-	0/1/1/1	0/0/0/0
5	GAL	N	301	7,6	-	0/2/19/22	0/1/1/1
7	NAG	N	302	8,5	-	0/6/23/26	0/1/1/1
8	BGC	N	303	5,7	-	0/2/19/22	0/1/1/1
5	GAL	N	304	8	-	0/2/19/22	0/1/1/1
5	GAL	N	305	8,7	-	0/2/19/22	0/1/1/1
8	BGC	N	306	5,4	-	0/2/19/22	0/1/1/1
6	SIA	N	307	5	-	0/14/34/38	0/1/1/1
3	EDO	N	308	-	-	0/1/1/1	0/0/0/0
3	EDO	N	309	-	-	0/1/1/1	0/0/0/0
3	EDO	N	310	-	-	0/1/1/1	0/0/0/0
3	EDO	N	311	-	-	0/1/1/1	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	304	7GW	O2-C3	-10.39	1.28	1.44
4	M	302	7GW	O2-C3	-10.25	1.29	1.44
4	H	304	7GW	C5-C6	-9.34	1.28	1.53
4	M	302	7GW	C5-C6	-8.71	1.30	1.53
4	M	302	7GW	C1-C2	-3.61	1.39	1.51
4	H	304	7GW	C1-C2	-3.58	1.39	1.51
4	M	302	7GW	C6-C2	2.08	1.58	1.53
4	H	304	7GW	C6-C2	2.40	1.59	1.53
4	M	302	7GW	O6-C6	3.77	1.51	1.43
4	H	304	7GW	O6-C6	4.20	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	302	7GW	O2-C2	4.85	1.56	1.45
4	H	304	7GW	O2-C2	4.86	1.56	1.45
4	H	304	7GW	C5-C3	6.64	1.67	1.53
4	M	302	7GW	C5-C3	6.88	1.68	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	304	GAL	O5-C1-C2	-3.41	105.45	110.79
8	L	303	BGC	O5-C1-C2	-3.38	105.50	110.79
8	N	306	BGC	C3-C4-C5	-3.34	104.33	110.22
7	N	302	NAG	O5-C1-C2	-2.96	107.35	111.47
5	N	305	GAL	O5-C1-C2	-2.95	106.17	110.79
6	H	306	SIA	O6-C2-C3	-2.91	104.58	109.82
7	N	302	NAG	C4-C3-C2	-2.91	106.75	111.02
6	M	304	SIA	O6-C2-C3	-2.83	104.72	109.82
5	L	304	GAL	O5-C1-C2	-2.63	106.66	110.79
6	L	307	SIA	C3-C4-C5	-2.59	108.33	111.46
8	L	306	BGC	C3-C4-C5	-2.53	105.75	110.22
8	L	303	BGC	C6-C5-C4	-2.49	107.17	113.00
5	N	301	GAL	C2-C3-C4	-2.47	106.56	110.88
8	N	303	BGC	O5-C1-C2	-2.45	106.95	110.79
8	L	303	BGC	O2-C2-C3	-2.43	105.41	110.17
5	M	303	GAL	C3-C4-C5	-2.35	106.07	110.22
6	M	304	SIA	C8-C7-C6	-2.28	108.61	113.04
6	H	306	SIA	O9-C9-C8	-2.14	106.39	111.11
5	N	305	GAL	O2-C2-C3	-2.11	106.02	110.17
8	N	306	BGC	O2-C2-C1	2.16	113.58	109.18
5	N	301	GAL	C1-O5-C5	2.20	115.20	112.17
5	N	304	GAL	O2-C2-C1	2.34	113.94	109.18
6	N	307	SIA	C11-C10-N5	2.39	120.42	116.11
5	L	304	GAL	C2-C3-C4	2.39	115.05	110.88
8	N	303	BGC	O2-C2-C1	2.44	114.15	109.18
7	L	302	NAG	C1-O5-C5	2.50	115.61	112.17
5	M	303	GAL	C1-C2-C3	2.52	112.84	109.65
5	L	305	GAL	C1-O5-C5	2.56	115.70	112.17
6	L	307	SIA	C11-C10-N5	2.67	120.94	116.11
8	L	306	BGC	C1-C2-C3	2.83	113.24	109.65
5	L	304	GAL	C1-O5-C5	2.98	116.28	112.17
5	L	301	GAL	C1-O5-C5	3.04	116.36	112.17
8	L	303	BGC	C1-O5-C5	3.05	116.37	112.17
8	L	303	BGC	O2-C2-C1	3.05	115.38	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	303	GAL	C1-O5-C5	3.37	116.82	112.17
8	L	306	BGC	O4-C4-C3	3.79	118.61	110.36
4	M	302	7GW	C6-C5-C3	3.83	107.97	102.45
5	L	305	GAL	C1-C2-C3	3.89	114.58	109.65
5	H	305	GAL	C1-C2-C3	3.91	114.61	109.65
4	H	304	7GW	C6-C5-C3	4.10	108.37	102.45
8	N	306	BGC	O4-C4-C3	4.11	119.31	110.36
5	N	305	GAL	C1-C2-C3	4.91	115.87	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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, 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	H	222/248 (89%)	0.43	7 (3%) 48 50	47, 67, 110, 132	0
1	M	226/248 (91%)	0.25	4 (1%) 69 72	39, 62, 101, 130	0
2	L	215/239 (89%)	0.40	5 (2%) 61 63	52, 73, 112, 123	0
2	N	216/239 (90%)	0.32	8 (3%) 42 43	44, 63, 102, 135	0
All	All	879/974 (90%)	0.35	24 (2%) 55 57	39, 66, 107, 135	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	238	CYS	7.6
2	N	239	ALA	5.0
2	L	210	THR	3.7
2	N	210	THR	3.6
2	N	207	LEU	3.2
1	H	219	SER	3.1
2	L	182	THR	3.1
1	H	218	SER	3.1
1	H	122	GLY	2.9
2	L	214	SER	2.8
1	M	191	THR	2.7
1	H	123	ASP	2.6
2	N	179	THR	2.6
1	H	166	THR	2.5
2	L	102	VAL	2.4
2	L	207	LEU	2.3
1	M	123	ASP	2.3
2	N	209	SER	2.3
1	H	71	SER	2.2
1	H	75	GLU	2.2
1	M	222	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	208	THR	2.2
2	N	214	SER	2.2
1	M	220	GLN	2.2

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 [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	EDO	N	308	4/4	0.91	0.24	4.08	46,48,49,50	0
3	EDO	H	301	4/4	0.86	0.31	3.39	61,63,64,66	0
3	EDO	L	309	4/4	0.90	0.23	2.64	60,62,62,62	0
3	EDO	M	305	4/4	0.89	0.23	2.05	54,56,56,57	0
3	EDO	L	308	4/4	0.90	0.23	1.93	52,53,54,55	0
3	EDO	N	309	4/4	0.90	0.19	1.27	69,69,69,70	0
3	EDO	L	310	4/4	0.94	0.22	0.79	65,65,65,65	0
3	EDO	H	303	4/4	0.95	0.19	0.51	68,68,69,69	0
3	EDO	N	311	4/4	0.87	0.30	0.17	83,85,85,85	0
6	SIA	M	304	20/21	0.94	0.20	-0.24	56,63,71,74	0
7	NAG	N	302	14/15	0.96	0.16	-1.29	67,74,80,84	0
6	SIA	H	306	20/21	0.92	0.16	-1.68	66,72,78,79	0
7	NAG	L	302	14/15	0.91	0.15	-2.02	76,90,103,106	0
6	SIA	N	307	20/21	0.77	0.53	-	121,143,150,152	0
5	GAL	N	305	11/12	0.93	0.16	-	67,69,71,72	0
8	BGC	N	306	11/12	0.94	0.15	-	64,64,66,66	0
4	7GW	H	304	12/12	0.93	0.15	-	87,96,101,101	0
3	EDO	H	302	4/4	0.78	0.28	-	67,67,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GAL	L	305	11/12	0.92	0.20	-	76,79,81,81	0
3	EDO	N	310	4/4	0.87	0.15	-	61,62,63,65	0
5	GAL	H	305	11/12	0.95	0.12	-	80,84,86,87	0
5	GAL	N	304	11/12	0.79	0.35	-	92,97,100,100	0
3	EDO	M	301	4/4	0.83	0.37	-	85,85,87,89	0
5	GAL	N	301	11/12	0.92	0.22	-	92,96,101,109	0
8	BGC	N	303	11/12	0.89	0.30	-	83,86,89,93	0
5	GAL	L	301	11/12	0.84	0.22	-	106,116,124,133	0
3	EDO	L	311	4/4	0.65	0.39	-	92,93,93,94	0
5	GAL	L	304	11/12	0.60	0.53	-	118,123,125,127	0
6	SIA	L	307	20/21	0.81	0.48	-	146,151,155,155	0
4	7GW	M	302	12/12	0.93	0.14	-	66,69,73,74	0
5	GAL	M	303	11/12	0.96	0.12	-	66,67,68,69	0
8	BGC	L	303	11/12	0.79	0.50	-	111,115,117,119	0
8	BGC	L	306	11/12	0.96	0.17	-	78,79,82,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.