



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:56 AM UTC

PDB ID : 8BEQ / pdb_00008beq
Title : Structure of fructofuranosidase from *Rhodotorula dairenensis*
Authors : Jimenez-Ortega, E.; Sanz-Aparicio, J.
Deposited on : 2022-10-21
Resolution : 2.07 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

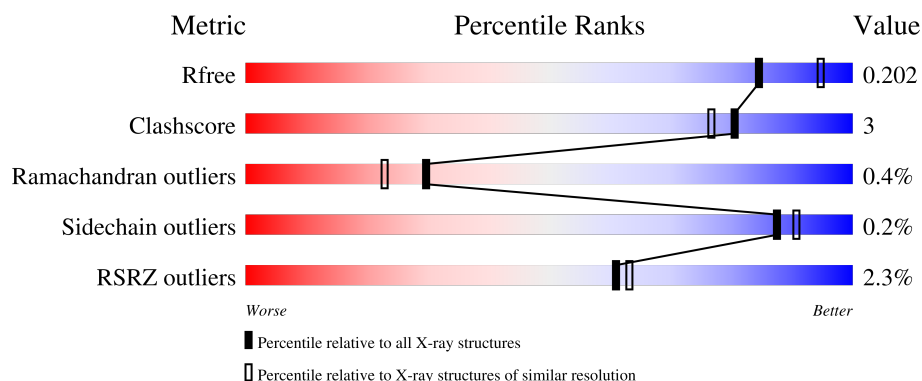
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	675	2% 73% 6% 21%
1	B	675	2% 74% 5% 21%
2	C	3	33% 67%
2	F	3	67% 33%
3	D	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	E	2	

2 Entry composition [i](#)

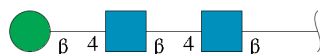
There are 9 unique types of molecules in this entry. The entry contains 9244 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fructofuranosidase from *Rhodotorula dairenensis*.

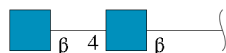
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	1	0
			4096	2601	668	816	11			
1	B	532	Total	C	N	O	S	0	0	0
			4076	2591	664	810	11			

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



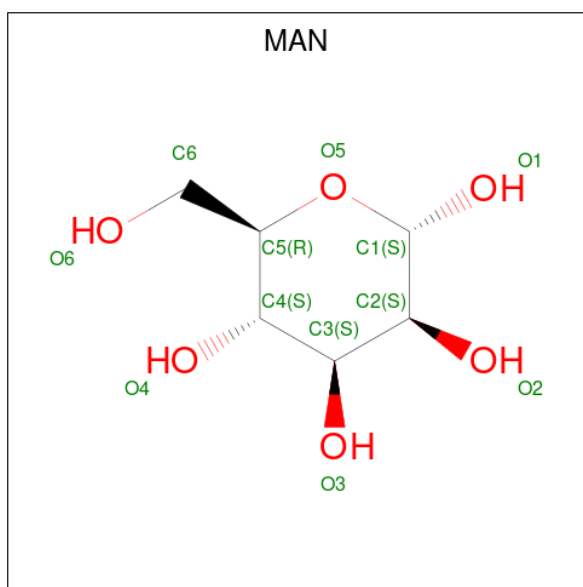
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



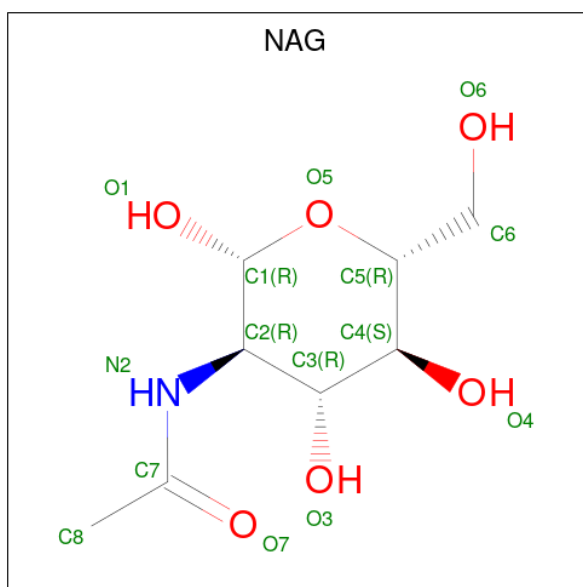
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



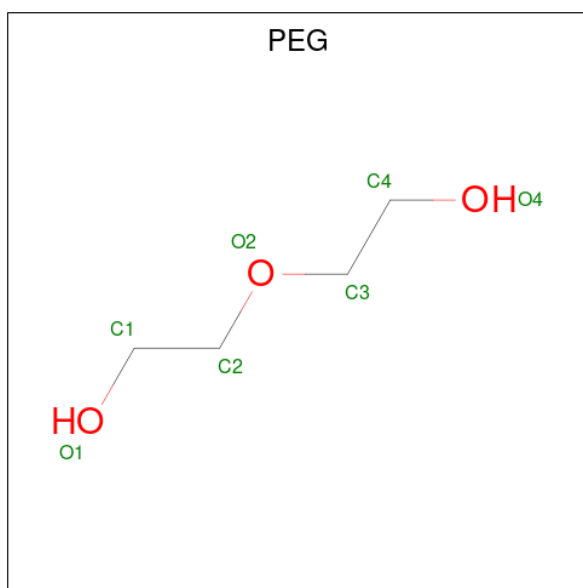
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



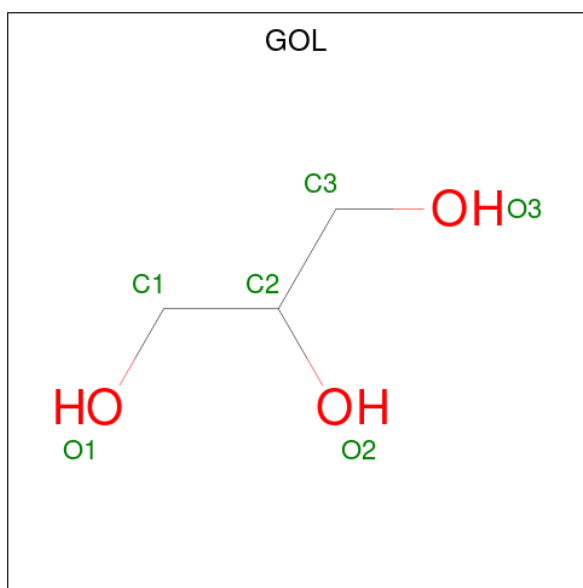
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



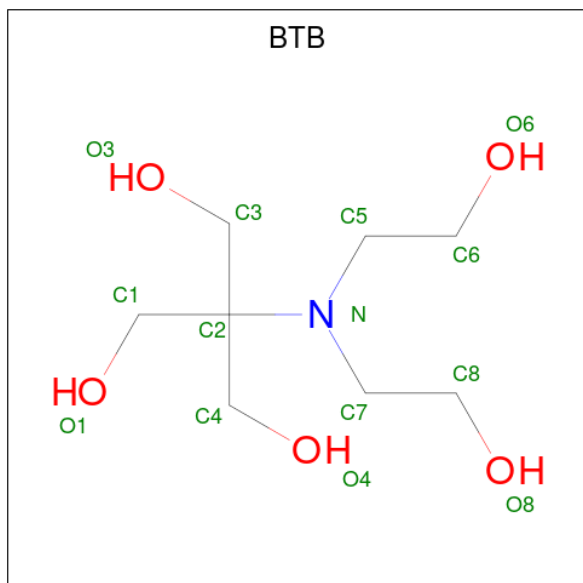
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



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

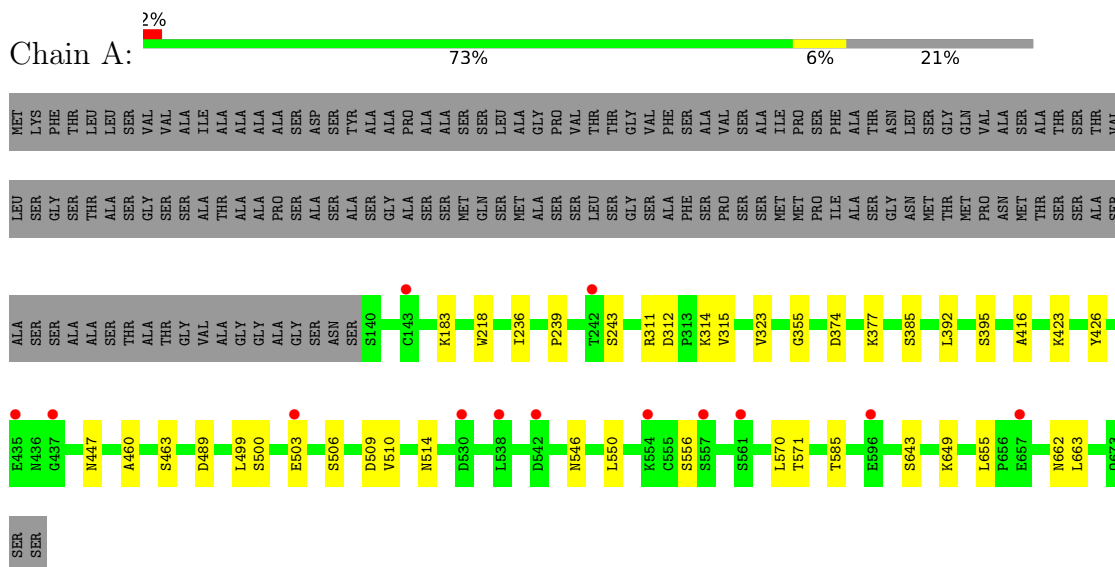
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	298	Total	O	0	0
			298	298		
9	B	300	Total	O	0	0
			300	300		

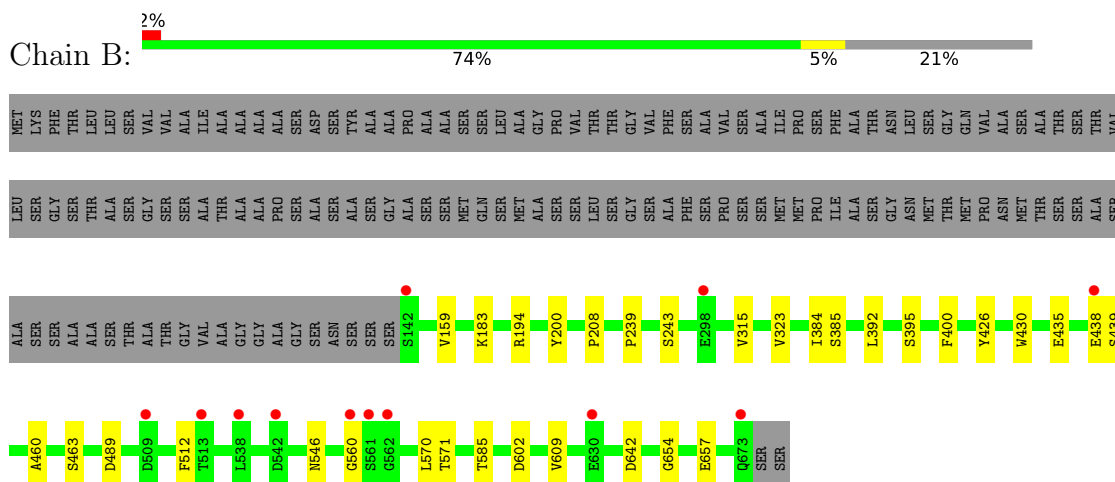
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Fructofuranosidase from *Rhodotorula dairenensis*



- Molecule 1: Fructofuranosidase from *Rhodotorula dairenensis*



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	103.38Å 108.23Å 196.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.45 – 2.07 47.45 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.45-2.07) 99.3 (47.45-2.07)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.172 , 0.209 (Not available) , 0.202	Depositor DCC
R_{free} test set	3307 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9244	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: PEG, GOL, BTB, BMA, 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	0.90	0/4225	1.02	0/5809
1	B	0.93	0/4205	1.02	3/5782 (0.1%)
All	All	0.91	0/8430	1.02	3/11591 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	602	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	512	PHE	CA-CB-CG	5.27	119.07	113.80
1	B	609	VAL	N-CA-C	-5.00	106.80	111.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4096	0	3801	25	0
1	B	4076	0	3781	19	0
2	C	39	0	34	0	0
2	F	39	0	34	0	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	33	0	30	0	0
4	B	66	0	60	0	0
5	A	84	0	78	2	0
5	B	112	0	104	3	0
6	A	7	0	10	2	0
7	A	12	0	16	1	0
7	B	12	0	16	0	0
8	B	14	0	19	0	0
9	A	298	0	0	3	0
9	B	300	0	0	0	0
All	All	9244	0	8033	44	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (44) 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:392:LEU:HD23	1:B:392:LEU:HD23	1.68	0.75
1:A:312:ASP:OD2	6:A:710:PEG:H12	1.91	0.70
1:A:385:SER:HB3	1:A:426:TYR:CE1	2.28	0.69
1:B:385:SER:HB3	1:B:426:TYR:CE1	2.26	0.69
1:A:662[A]:ASN:ND2	5:A:709:NAG:O7	2.30	0.63
1:B:395:SER:HB2	1:B:426:TYR:CD1	2.34	0.62
1:A:395:SER:HB2	1:A:426:TYR:CD1	2.35	0.61
1:A:546:ASN:OD1	1:A:571:THR:HG23	2.02	0.60
1:B:657:GLU:HG3	5:B:713:NAG:O3	2.06	0.56
1:A:550:LEU:HD11	1:A:649:LYS:HD2	1.88	0.56
1:B:546:ASN:OD1	1:B:571:THR:HG23	2.07	0.54
1:B:194:ARG:HD3	1:B:200:TYR:CZ	2.42	0.54
1:A:499:LEU:HD13	1:A:510:VAL:HG22	1.89	0.54
1:A:239:PRO:HD2	1:A:243:SER:OG	2.08	0.54
1:B:560:GLY:HA3	1:B:642:ASP:HB3	1.91	0.53
1:A:374:ASP:OD2	1:A:377:LYS:HD2	2.10	0.52
1:B:654:GLY:HA2	5:B:713:NAG:H62	1.92	0.52
1:B:435:GLU:CD	1:B:438:GLU:HG3	2.35	0.51
1:B:194:ARG:HD3	1:B:200:TYR:CE1	2.46	0.51
1:A:314:LYS:HG3	9:A:1024:HOH:O	2.10	0.51
7:A:712:GOL:H2	9:A:938:HOH:O	2.09	0.51
1:A:311:ARG:HD2	6:A:710:PEG:H21	1.96	0.47
1:B:239:PRO:HD2	1:B:243:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:VAL:HA	1:B:323:VAL:O	2.16	0.46
1:A:183:LYS:HA	1:A:460:ALA:O	2.14	0.46
1:A:570:LEU:C	1:A:570:LEU:HD23	2.42	0.44
1:A:355:GLY:HA2	1:A:416:ALA:HB2	2.00	0.44
1:A:556:SER:HB2	1:A:643:SER:HB3	1.98	0.44
1:B:183:LYS:HA	1:B:460:ALA:O	2.18	0.44
1:A:514:ASN:HB2	9:A:1008:HOH:O	2.18	0.43
1:A:218:TRP:CE3	1:A:236:ILE:HD12	2.53	0.43
1:A:315:VAL:HA	1:A:323:VAL:O	2.18	0.43
1:B:430:TRP:CD1	1:B:439:SER:HG	2.37	0.43
1:B:570:LEU:C	1:B:570:LEU:HD23	2.44	0.43
1:A:509:ASP:OD2	1:A:649:LYS:HE3	2.18	0.43
1:B:385:SER:HB3	1:B:426:TYR:CZ	2.53	0.42
1:A:385:SER:HB3	1:A:426:TYR:CZ	2.54	0.42
1:B:239:PRO:HG2	5:B:708:NAG:O6	2.19	0.42
1:A:500:SER:HA	1:A:663:LEU:O	2.20	0.41
1:B:384:ILE:HD12	1:B:400:PHE:HE1	1.86	0.41
1:A:423:LYS:HG2	1:A:447:ASN:ND2	2.36	0.40
1:A:503:GLU:HG2	1:A:506:SER:HB3	2.02	0.40
1:A:655:LEU:O	5:A:708:NAG:H3	2.21	0.40
1:B:159:VAL:HG22	1:B:208:PRO:HG2	2.03	0.40

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	533/675 (79%)	510 (96%)	21 (4%)	2 (0%)	30	23
1	B	530/675 (78%)	506 (96%)	22 (4%)	2 (0%)	30	23
All	All	1063/1350 (79%)	1016 (96%)	43 (4%)	4 (0%)	30	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	SER
1	B	463	SER
1	A	489	ASP
1	B	489	ASP

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	450/546 (82%)	449 (100%)	1 (0%)	87	91
1	B	447/546 (82%)	446 (100%)	1 (0%)	87	91
All	All	897/1092 (82%)	895 (100%)	2 (0%)	87	91

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

Mol	Chain	Res	Type
1	A	585	THR
1	B	585	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	449	GLN
1	A	471	ASN
1	B	187	ASN
1	B	354	HIS
1	B	449	GLN
1	B	471	ASN
1	B	664	GLN
1	B	666	ASN

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 ⓘ

10 monosaccharides 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	C	1	1,2	14,14,15	0.63	0	17,19,21	0.74	0
2	NAG	C	2	2	14,14,15	0.36	0	17,19,21	0.93	1 (5%)
2	BMA	C	3	2	11,11,12	0.43	0	15,15,17	1.43	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.37	0	17,19,21	0.81	0
3	NAG	D	2	3	14,14,15	0.46	0	17,19,21	1.08	1 (5%)
3	NAG	E	1	1,3	14,14,15	0.46	0	17,19,21	0.92	1 (5%)
3	NAG	E	2	3	14,14,15	0.58	0	17,19,21	0.80	0
2	NAG	F	1	1,2	14,14,15	0.44	0	17,19,21	0.62	0
2	NAG	F	2	2	14,14,15	0.41	0	17,19,21	1.24	2 (11%)
2	BMA	F	3	2	11,11,12	0.44	0	15,15,17	0.91	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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C1-O5-C5	3.40	116.74	112.19
2	C	3	BMA	C1-C2-C3	3.36	114.54	109.64
2	C	3	BMA	C1-O5-C5	3.31	116.63	112.19
2	F	2	NAG	O5-C1-C2	2.82	115.66	111.29
3	D	2	NAG	C1-O5-C5	2.63	115.72	112.19
3	E	1	NAG	C1-O5-C5	2.20	115.13	112.19
2	C	2	NAG	C3-C4-C5	2.16	114.14	110.23

There are no chirality outliers.

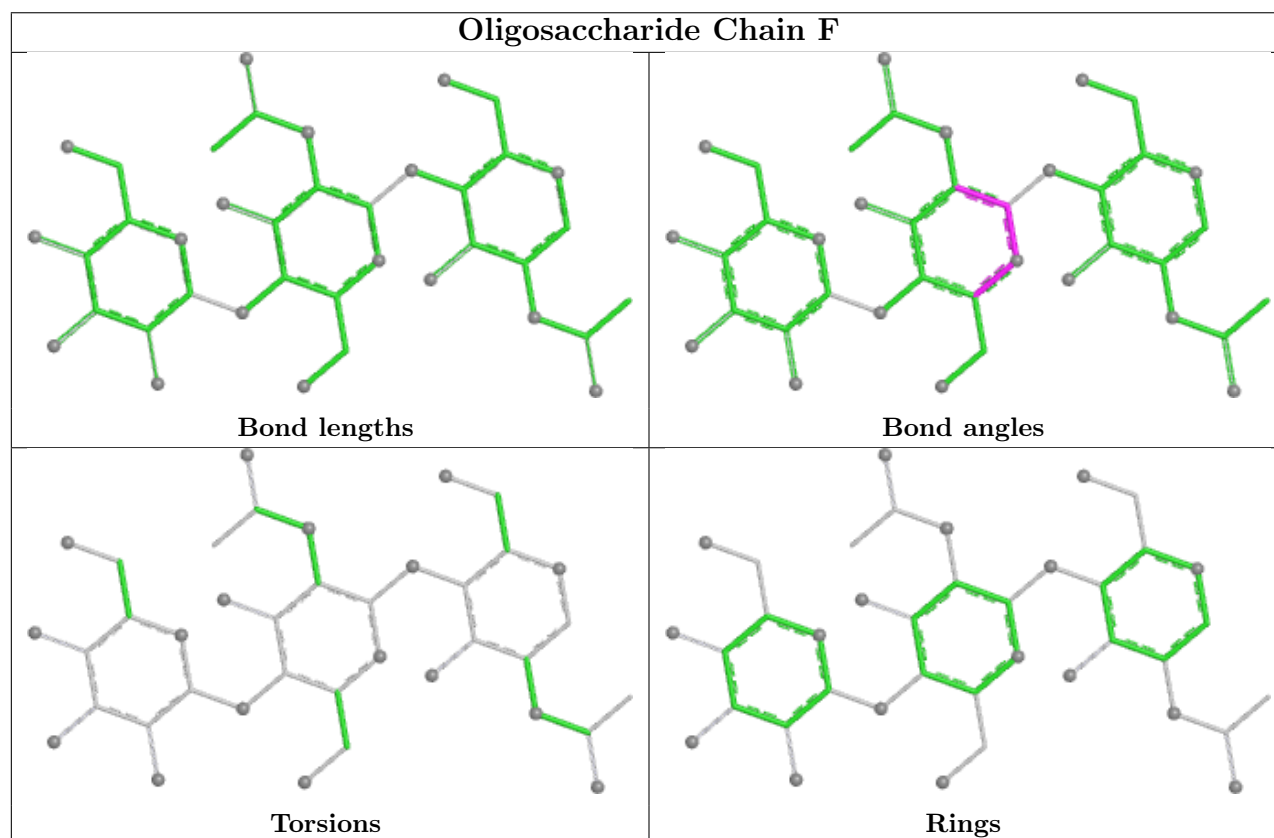
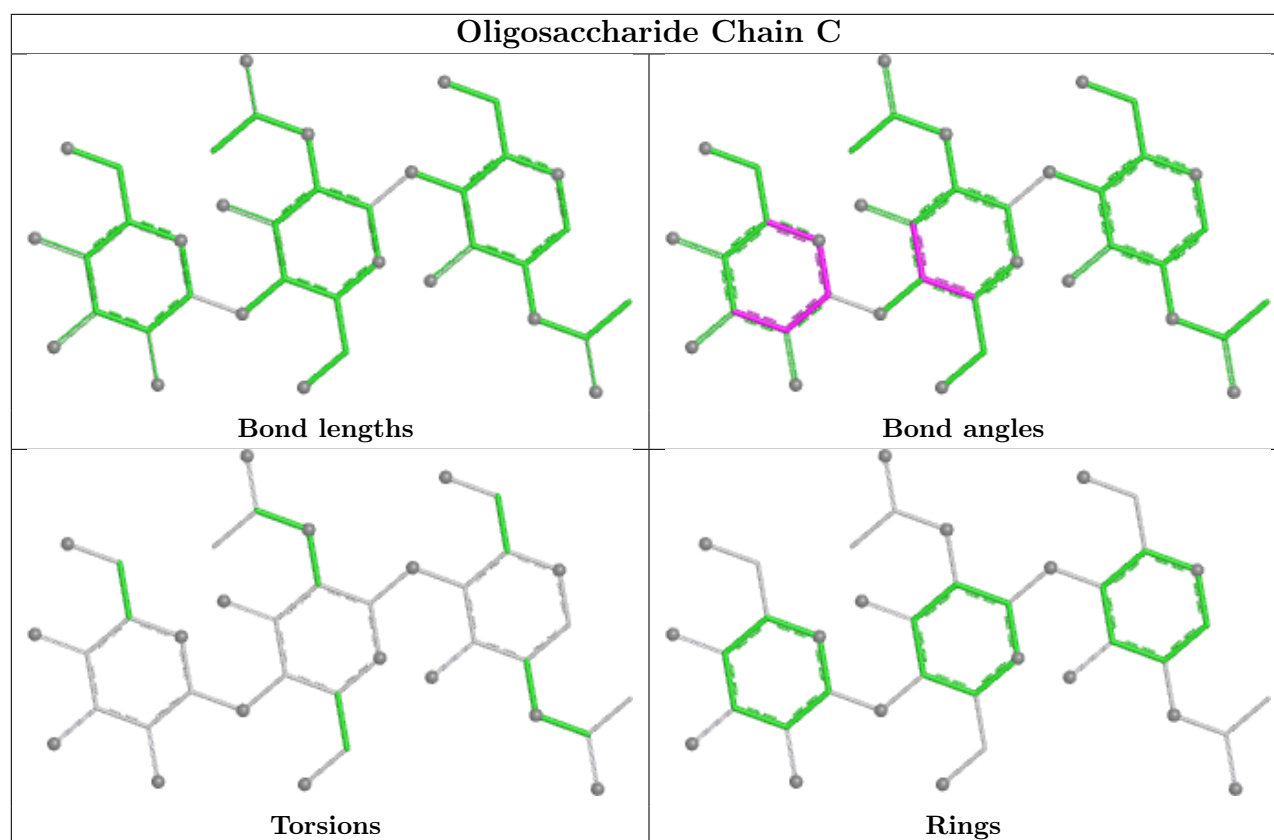
All (1) torsion outliers are listed below:

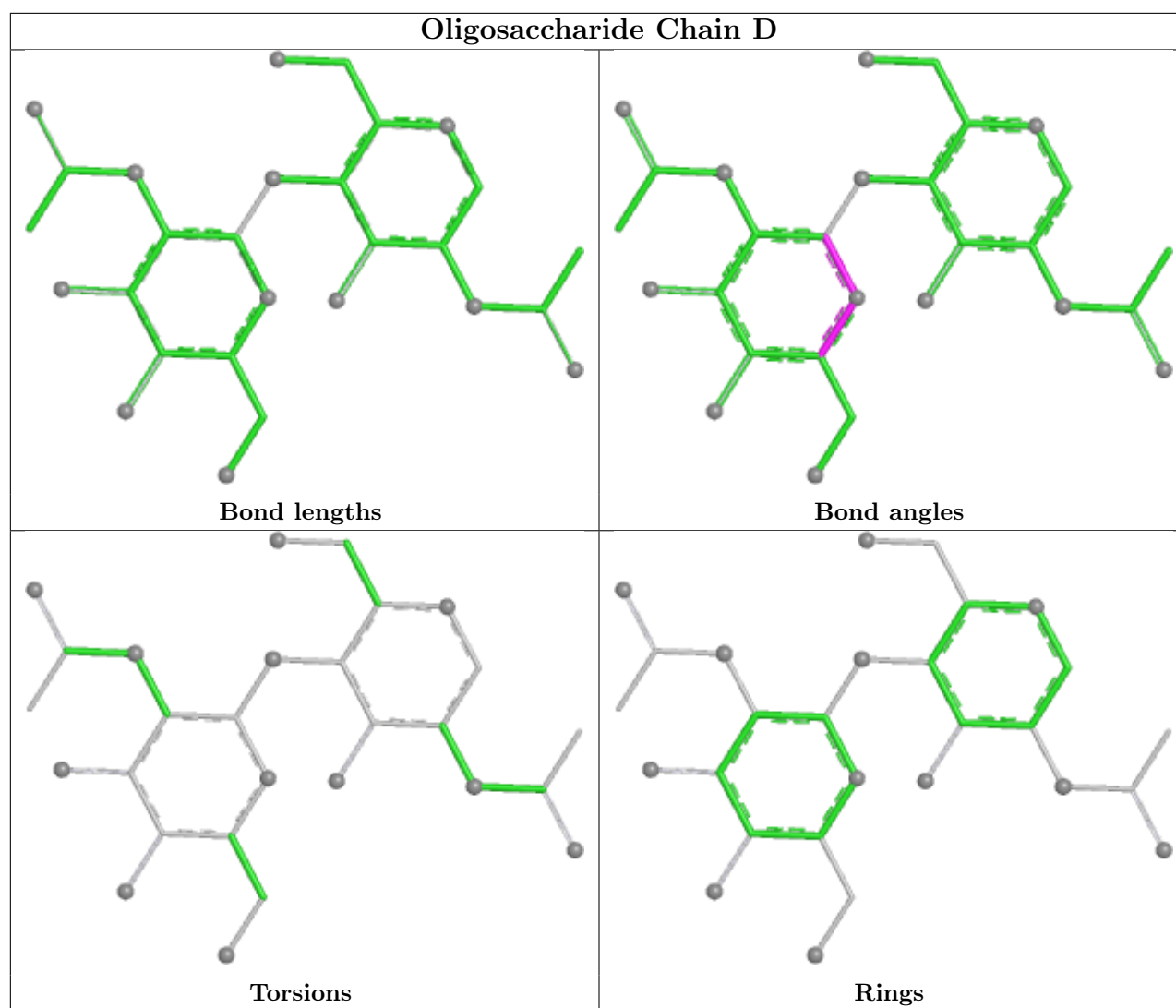
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C1-C2-N2-C7

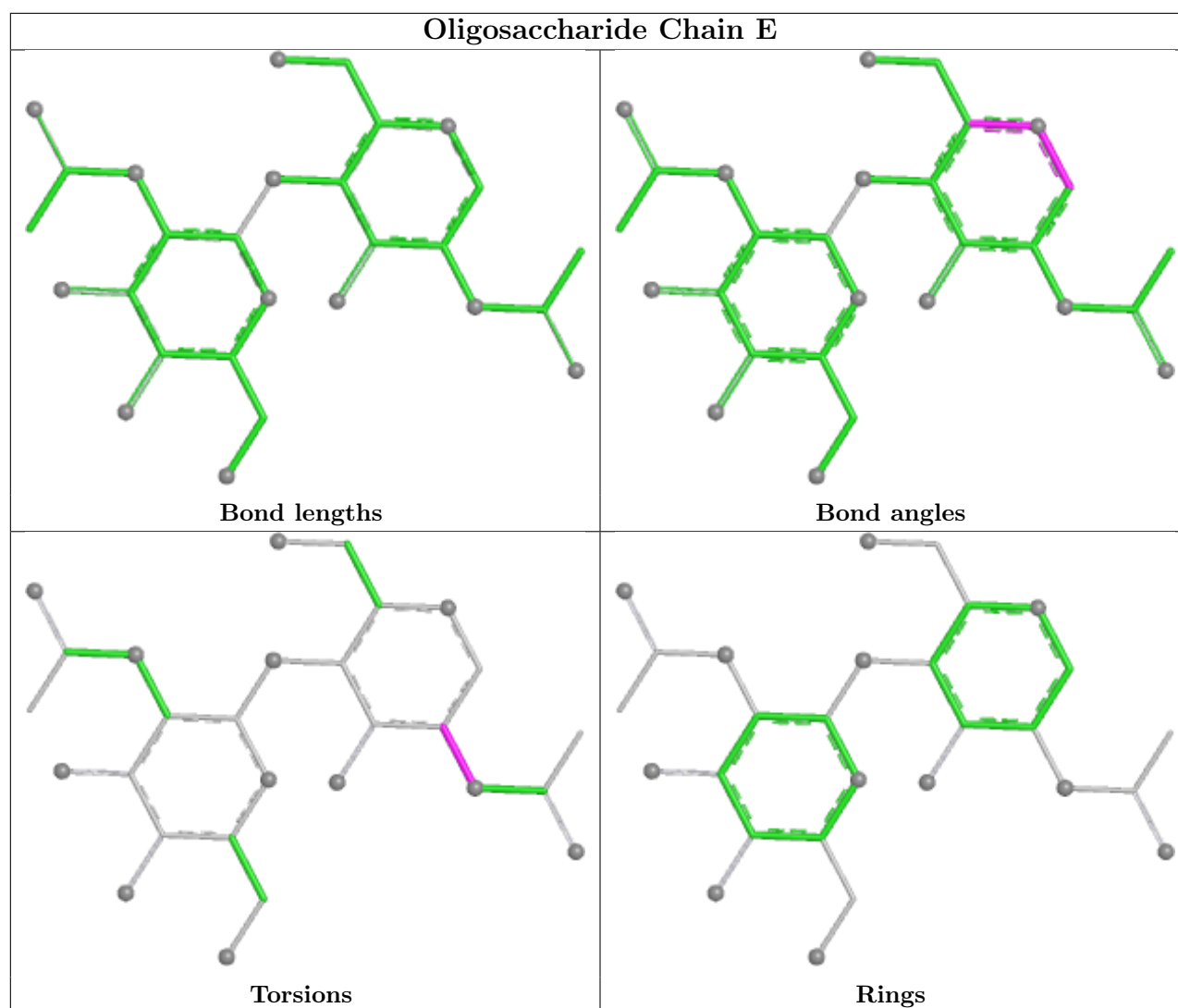
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry [i](#)

29 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	$\# Z > 2$
4	MAN	A	702	1	11,11,12	0.38	0	15,15,17	0.85	1 (6%)
4	MAN	B	704	1	11,11,12	0.49	0	15,15,17	1.14	2 (13%)
5	NAG	B	712	1	14,14,15	0.72	0	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	B	705	1	11,11,12	0.60	0	15,15,17	0.92	1 (6%)
5	NAG	B	707	1	14,14,15	0.39	0	17,19,21	0.65	0
5	NAG	A	709	1	14,14,15	0.48	0	17,19,21	0.80	1 (5%)
5	NAG	B	714	1	14,14,15	0.43	0	17,19,21	0.47	0
4	MAN	A	701	1	11,11,12	0.65	0	15,15,17	1.20	1 (6%)
5	NAG	A	707	1	14,14,15	0.31	0	17,19,21	0.71	0
8	BTB	B	716	-	13,13,13	1.25	2 (15%)	7,16,16	0.32	0
7	GOL	B	717	-	5,5,5	0.22	0	5,5,5	0.41	0
5	NAG	B	711	1	14,14,15	0.67	0	17,19,21	0.83	1 (5%)
4	MAN	B	702	1	11,11,12	0.40	0	15,15,17	1.60	4 (26%)
7	GOL	A	711	-	5,5,5	0.16	0	5,5,5	0.48	0
4	MAN	A	703	1	11,11,12	0.62	0	15,15,17	0.90	0
5	NAG	B	708	1	14,14,15	0.42	0	17,19,21	0.82	0
5	NAG	A	706	1	14,14,15	0.73	0	17,19,21	0.80	0
5	NAG	A	708	1	14,14,15	0.32	0	17,19,21	1.04	1 (5%)
4	MAN	B	703	1	11,11,12	0.42	0	15,15,17	0.81	0
4	MAN	B	701	1	11,11,12	0.42	0	15,15,17	1.28	2 (13%)
4	MAN	B	706	1	11,11,12	0.34	0	15,15,17	0.94	1 (6%)
5	NAG	B	713	1	14,14,15	0.42	0	17,19,21	1.28	2 (11%)
5	NAG	A	704	1	14,14,15	0.25	0	17,19,21	0.55	0
7	GOL	B	715	-	5,5,5	0.15	0	5,5,5	0.35	0
5	NAG	B	710	1	14,14,15	0.64	1 (7%)	17,19,21	0.98	1 (5%)
6	PEG	A	710	-	6,6,6	0.18	0	5,5,5	0.23	0
5	NAG	A	705	1	14,14,15	0.41	0	17,19,21	0.90	1 (5%)
5	NAG	B	709	1	14,14,15	0.30	0	17,19,21	1.05	0
7	GOL	A	712	-	5,5,5	0.18	0	5,5,5	0.50	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
4	MAN	A	702	1	-	0/2/19/22	0/1/1/1
4	MAN	B	704	1	-	0/2/19/22	0/1/1/1
5	NAG	B	712	1	-	1/6/23/26	0/1/1/1
4	MAN	B	705	1	-	2/2/19/22	0/1/1/1
5	NAG	B	707	1	-	1/6/23/26	0/1/1/1
5	NAG	A	709	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	714	1	-	2/6/23/26	0/1/1/1
4	MAN	A	701	1	-	1/2/19/22	0/1/1/1
5	NAG	A	707	1	-	0/6/23/26	0/1/1/1
8	BTB	B	716	-	-	1/21/21/21	-
7	GOL	B	717	-	-	3/4/4/4	-
5	NAG	B	711	1	-	0/6/23/26	0/1/1/1
4	MAN	B	702	1	-	2/2/19/22	0/1/1/1
7	GOL	A	711	-	-	0/4/4/4	-
4	MAN	A	703	1	-	0/2/19/22	0/1/1/1
5	NAG	B	708	1	-	1/6/23/26	0/1/1/1
5	NAG	A	706	1	-	0/6/23/26	0/1/1/1
5	NAG	A	708	1	-	0/6/23/26	0/1/1/1
4	MAN	B	703	1	-	0/2/19/22	0/1/1/1
4	MAN	B	701	1	-	2/2/19/22	0/1/1/1
4	MAN	B	706	1	-	1/2/19/22	0/1/1/1
5	NAG	B	713	1	-	0/6/23/26	0/1/1/1
5	NAG	A	704	1	-	0/6/23/26	0/1/1/1
7	GOL	B	715	-	-	2/4/4/4	-
5	NAG	B	710	1	-	0/6/23/26	0/1/1/1
6	PEG	A	710	-	-	1/4/4/4	-
5	NAG	A	705	1	-	0/6/23/26	0/1/1/1
5	NAG	B	709	1	-	0/6/23/26	0/1/1/1
7	GOL	A	712	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	716	BTB	C2-N	2.86	1.54	1.48
8	B	716	BTB	C5-N	2.38	1.51	1.48
5	B	710	NAG	C1-C2	2.10	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	MAN	C1-O5-C5	-3.89	106.98	112.19
5	B	710	NAG	C1-C2-N2	3.01	115.18	110.43
4	B	705	MAN	C1-O5-C5	2.91	116.09	112.19
5	A	708	NAG	C1-O5-C5	2.61	115.69	112.19
5	B	713	NAG	O5-C5-C4	-2.61	104.48	110.83
4	B	704	MAN	O3-C3-C4	2.57	116.43	110.38
5	B	713	NAG	C4-C3-C2	2.56	114.77	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	MAN	C1-O5-C5	2.54	115.59	112.19
4	B	702	MAN	C1-O5-C5	-2.47	108.88	112.19
4	B	702	MAN	C3-C4-C5	2.34	114.48	110.23
4	B	704	MAN	C1-C2-C3	-2.33	106.25	109.64
4	A	702	MAN	C3-C4-C5	2.22	114.26	110.23
4	B	706	MAN	O5-C1-C2	-2.16	105.63	110.79
4	B	702	MAN	C6-C5-C4	-2.15	107.75	113.02
4	B	701	MAN	O5-C1-C2	-2.09	105.81	110.79
4	B	702	MAN	O6-C6-C5	-2.06	104.33	111.33
5	B	711	NAG	O5-C1-C2	-2.04	108.14	111.29
5	A	709	NAG	C1-O5-C5	-2.02	109.48	112.19
5	A	705	NAG	O4-C4-C5	2.00	114.26	109.32

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	717	GOL	C1-C2-C3-O3
4	B	702	MAN	O5-C5-C6-O6
4	B	705	MAN	O5-C5-C6-O6
4	B	701	MAN	O5-C5-C6-O6
4	B	701	MAN	C4-C5-C6-O6
5	B	714	NAG	C4-C5-C6-O6
6	A	710	PEG	O2-C3-C4-O4
8	B	716	BTB	N-C5-C6-O6
5	B	714	NAG	O5-C5-C6-O6
7	A	712	GOL	O1-C1-C2-C3
7	B	715	GOL	C1-C2-C3-O3
7	B	717	GOL	O1-C1-C2-C3
7	B	715	GOL	O2-C2-C3-O3
7	B	717	GOL	O2-C2-C3-O3
4	B	702	MAN	C4-C5-C6-O6
4	A	701	MAN	O5-C5-C6-O6
7	A	712	GOL	O1-C1-C2-O2
4	B	706	MAN	O5-C5-C6-O6
4	B	705	MAN	C4-C5-C6-O6
5	A	709	NAG	C8-C7-N2-C2
5	B	708	NAG	O5-C5-C6-O6
5	B	707	NAG	C4-C5-C6-O6
5	B	712	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	709	NAG	1	0
5	B	708	NAG	1	0
5	A	708	NAG	1	0
5	B	713	NAG	2	0
6	A	710	PEG	2	0
7	A	712	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	A	534/675 (79%)	0.05	13 (2%) 59 61	13, 22, 44, 68	1 (0%)
1	B	532/675 (78%)	0.05	12 (2%) 61 63	12, 21, 44, 66	0
All	All	1066/1350 (78%)	0.05	25 (2%) 61 63	12, 21, 44, 68	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	561	SER	4.5
1	A	561	SER	3.1
1	A	542	ASP	3.0
1	B	542	ASP	3.0
1	B	562	GLY	2.9
1	A	530	ASP	2.7
1	B	560	GLY	2.6
1	B	513	THR	2.6
1	A	435	GLU	2.5
1	B	438	GLU	2.5
1	A	596	GLU	2.4
1	B	673	GLN	2.3
1	B	142	SER	2.3
1	A	538	LEU	2.3
1	B	538	LEU	2.3
1	B	630	GLU	2.2
1	B	509	ASP	2.2
1	A	557	SER	2.2
1	A	503	GLU	2.1
1	A	143	CYS	2.1
1	A	657	GLU	2.1
1	B	298	GLU	2.1
1	A	242	THR	2.1
1	A	437	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	554	LYS	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](#)

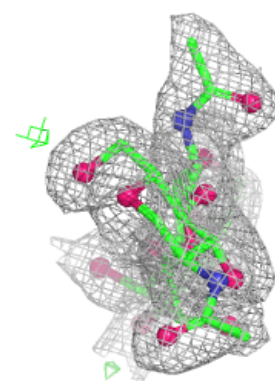
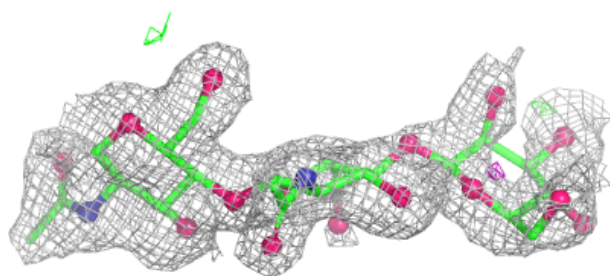
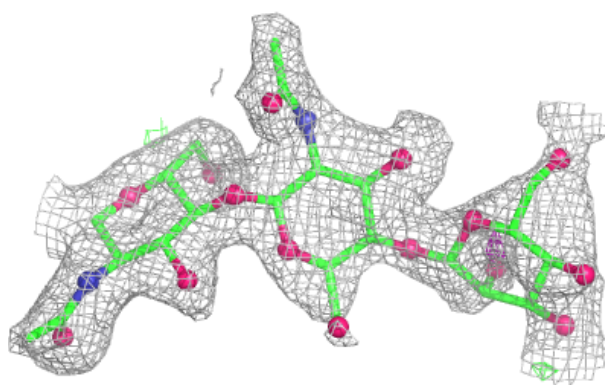
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	C	3	11/12	0.59	0.14	57,60,62,62	0
2	BMA	F	3	11/12	0.61	0.14	63,69,72,75	0
3	NAG	D	2	14/15	0.63	0.17	53,58,63,65	0
2	NAG	F	2	14/15	0.78	0.12	43,53,59,59	0
3	NAG	E	2	14/15	0.82	0.12	39,43,50,54	0
2	NAG	C	2	14/15	0.84	0.10	37,43,52,53	0
3	NAG	D	1	14/15	0.87	0.10	35,42,50,53	0
2	NAG	F	1	14/15	0.89	0.09	39,42,46,47	0
3	NAG	E	1	14/15	0.93	0.07	21,26,28,31	0
2	NAG	C	1	14/15	0.94	0.07	25,27,30,34	0

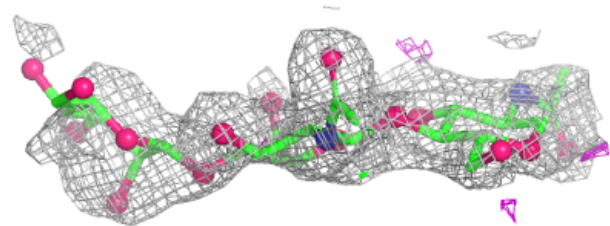
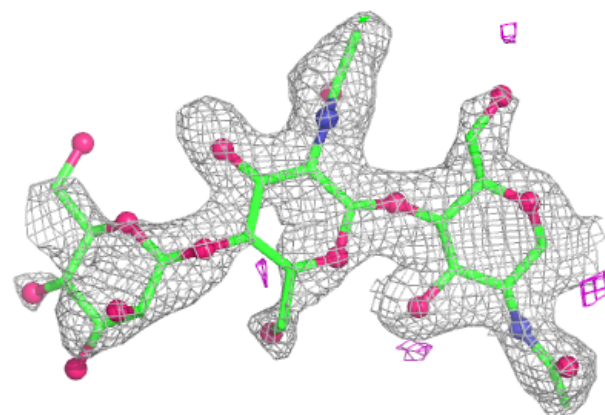
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

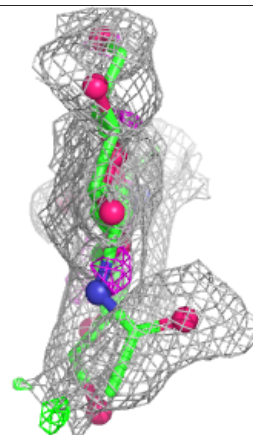
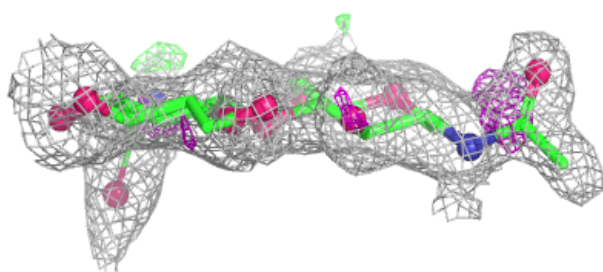
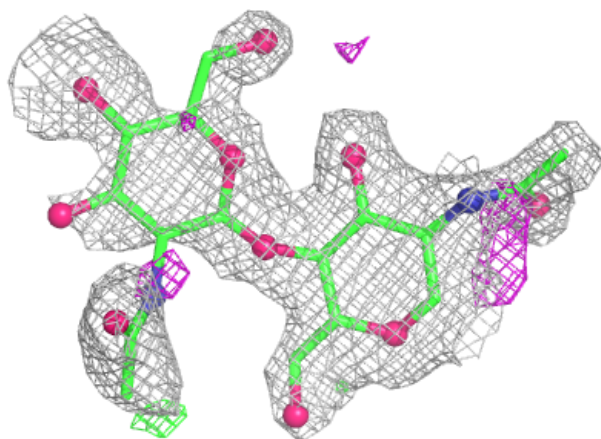
**Electron density around Chain F:**

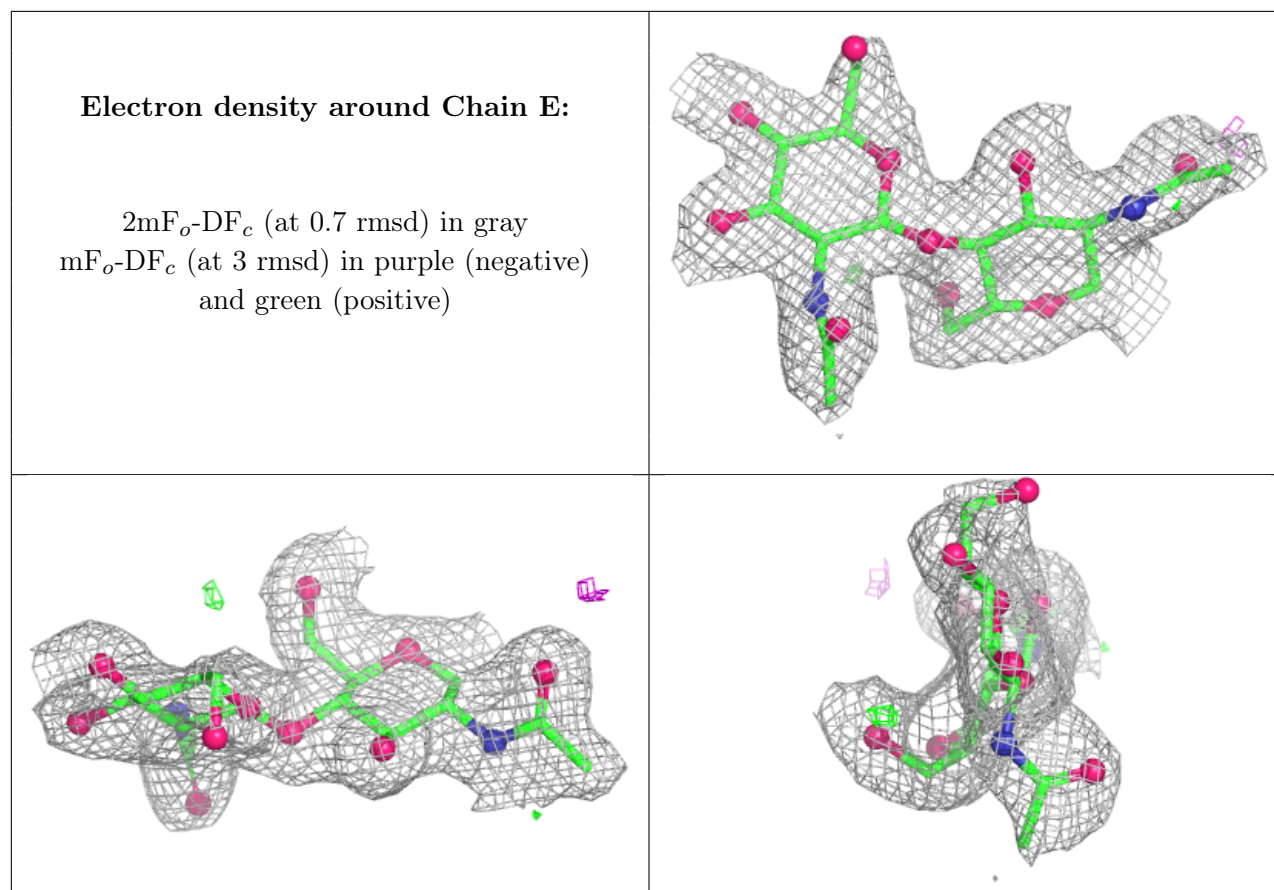
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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. 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	B-factors(Å ²)	Q<0.9
4	MAN	B	705	11/12	0.63	0.15	50,53,57,59	0
4	MAN	B	706	11/12	0.65	0.14	53,59,64,64	0
5	NAG	B	709	14/15	0.65	0.16	58,66,71,71	0
5	NAG	A	709	14/15	0.66	0.14	50,54,58,63	0
4	MAN	B	703	11/12	0.67	0.15	56,60,64,68	0
4	MAN	B	702	11/12	0.71	0.14	55,61,67,67	0
4	MAN	A	702	11/12	0.75	0.12	44,47,55,55	0
5	NAG	B	714	14/15	0.76	0.11	41,46,53,54	0
4	MAN	B	701	11/12	0.78	0.13	48,52,58,60	0
6	PEG	A	710	7/7	0.78	0.17	37,38,41,44	0
5	NAG	A	708	14/15	0.79	0.12	44,48,50,54	0
5	NAG	B	710	14/15	0.81	0.11	33,38,43,43	0
5	NAG	B	713	14/15	0.81	0.11	47,50,54,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	708	14/15	0.81	0.13	44,50,53,58	0
4	MAN	A	701	11/12	0.81	0.13	39,43,53,54	0
7	GOL	A	712	6/6	0.81	0.12	28,29,31,32	0
4	MAN	B	704	11/12	0.83	0.11	44,47,51,52	0
4	MAN	A	703	11/12	0.83	0.11	42,43,45,46	0
7	GOL	B	715	6/6	0.83	0.14	26,33,36,40	0
5	NAG	A	704	14/15	0.86	0.11	47,52,56,57	0
5	NAG	A	705	14/15	0.87	0.10	35,40,42,47	0
5	NAG	B	712	14/15	0.89	0.09	25,26,33,38	0
8	BTB	B	716	14/14	0.90	0.10	20,30,34,38	0
7	GOL	A	711	6/6	0.91	0.10	21,26,27,29	0
5	NAG	B	707	14/15	0.91	0.10	28,33,40,42	0
7	GOL	B	717	6/6	0.92	0.11	19,28,30,31	0
5	NAG	A	706	14/15	0.93	0.08	17,20,23,25	0
5	NAG	A	707	14/15	0.93	0.07	21,27,36,36	0
5	NAG	B	711	14/15	0.93	0.08	18,19,22,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.