



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2022 – 06:28 pm GMT

PDB ID : 8BEQ
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.31.3
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

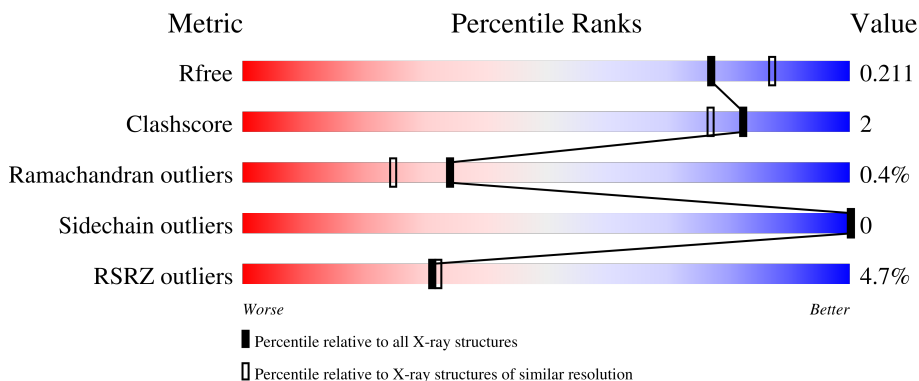
1 Overall quality at a glance

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}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (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	 5% 73% 6% 21%
1	B	675	 3% 75% 1% 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	 50% 50%

2 Entry composition [i](#)

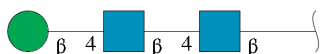
There are 9 unique types of molecules in this entry. The entry contains 9244 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
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.



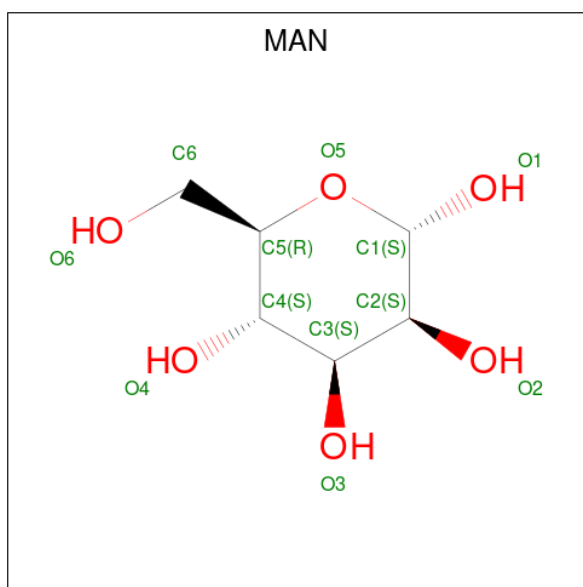
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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
			Total	C	N	O			
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 (three-letter code: MAN) (formula: C₆H₁₂O₆).



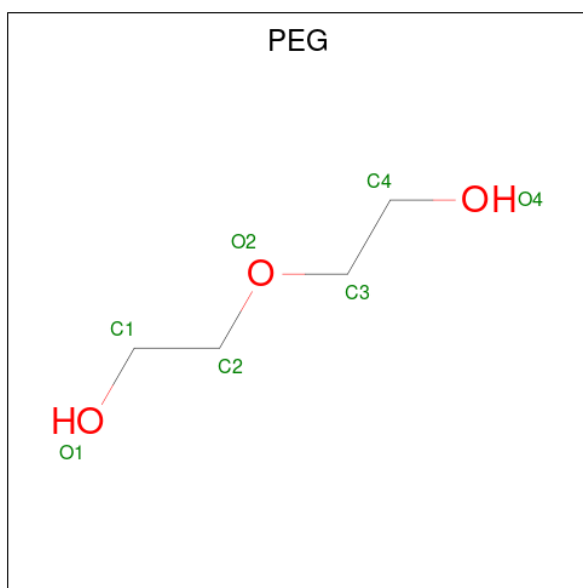
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0

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



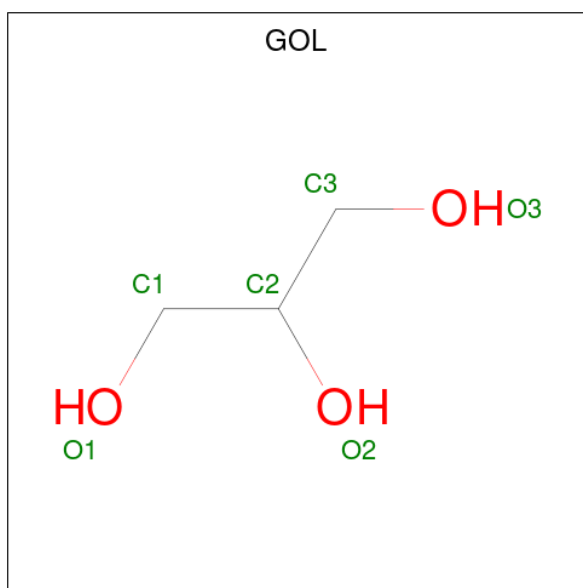
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			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 (three-letter code: 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



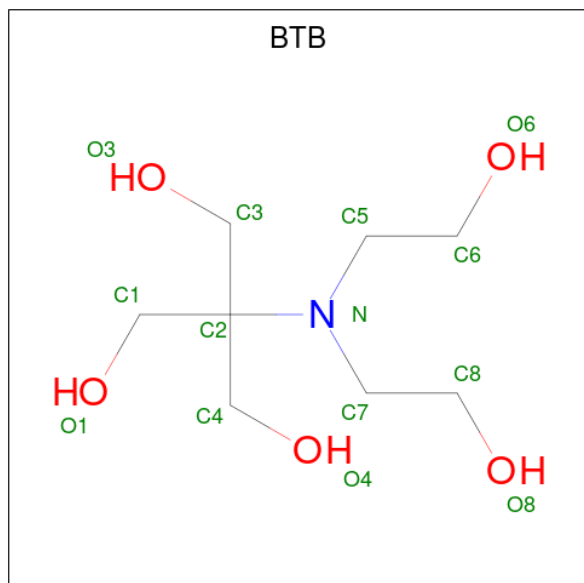
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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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		

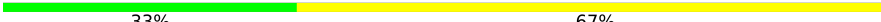
- Molecule 8 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



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		

Chain C:  33% 67%

MAG1
MAG2
BMA3

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

Chain F:  67% 33%

MAG1
MAG2
BMA3

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

Chain D:  50% 50%

MAG1
MAG2

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

Chain E:  50% 50%

MAG1
MAG2

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 47.41 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.45-2.07) 99.3 (47.41-2.07)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.07Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.172 , 0.209 0.177 , 0.211	Depositor DCC
R_{free} test set	3304 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtrriage
Anisotropy	0.310	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.026 for -k,-h,-l	Xtrriage
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

Xtrriage'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: MAN, GOL, BMA, NAG, BTB, PEG

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	0.61	0/4225	0.73	0/5809
1	B	0.63	0/4205	0.73	0/5782
All	All	0.62	0/8430	0.73	0/11591

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts 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	24	0
1	B	4076	0	3781	17	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	41	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 2.

All (41) 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: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:435:GLU:CD	1:B:438:GLU:HG3	2.35	0.47
1:B:239:PRO:HD2	1:B:243:SER:OG	2.14	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 [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	533/675 (79%)	510 (96%)	21 (4%)	2 (0%)	34 25
1	B	530/675 (78%)	506 (96%)	22 (4%)	2 (0%)	34 25
All	All	1063/1350 (79%)	1016 (96%)	43 (4%)	4 (0%)	34 25

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 [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	450/546 (82%)	450 (100%)	0	100	100
1	B	447/546 (82%)	447 (100%)	0	100	100
All	All	897/1092 (82%)	897 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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	2,1	14,14,15	0.63	0	17,19,21	0.76	0
2	NAG	C	2	2	14,14,15	0.36	0	17,19,21	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	C	3	2	11,11,12	0.44	0	15,15,17	1.57	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.39	0	17,19,21	0.86	0
3	NAG	D	2	3	14,14,15	0.47	0	17,19,21	1.08	1 (5%)
3	NAG	E	1	1,3	14,14,15	0.45	0	17,19,21	0.91	1 (5%)
3	NAG	E	2	3	14,14,15	0.57	0	17,19,21	0.85	0
2	NAG	F	1	2,1	14,14,15	0.44	0	17,19,21	0.63	0
2	NAG	F	2	2	14,14,15	0.41	0	17,19,21	1.22	2 (11%)
2	BMA	F	3	2	11,11,12	0.45	0	15,15,17	0.99	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	2,1	-	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
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	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	C	3	BMA	C1-C2-C3	3.97	114.54	109.67
2	F	2	NAG	C1-O5-C5	3.36	116.74	112.19
2	C	3	BMA	C1-O5-C5	3.27	116.63	112.19
2	F	2	NAG	O5-C1-C2	2.77	115.66	111.29
3	D	2	NAG	C1-O5-C5	2.60	115.72	112.19
2	C	2	NAG	C3-C4-C5	2.19	114.14	110.24
3	E	1	NAG	C1-O5-C5	2.17	115.13	112.19

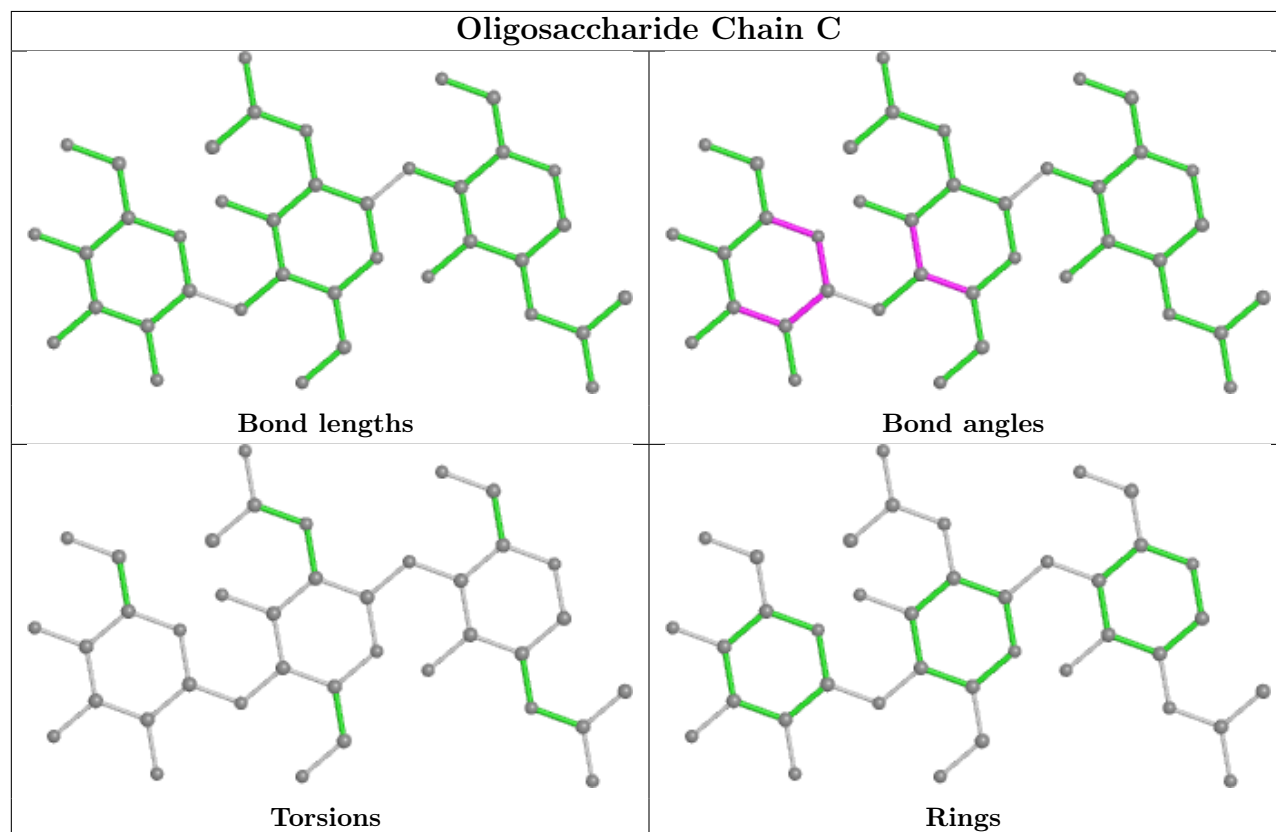
There are no chirality outliers.

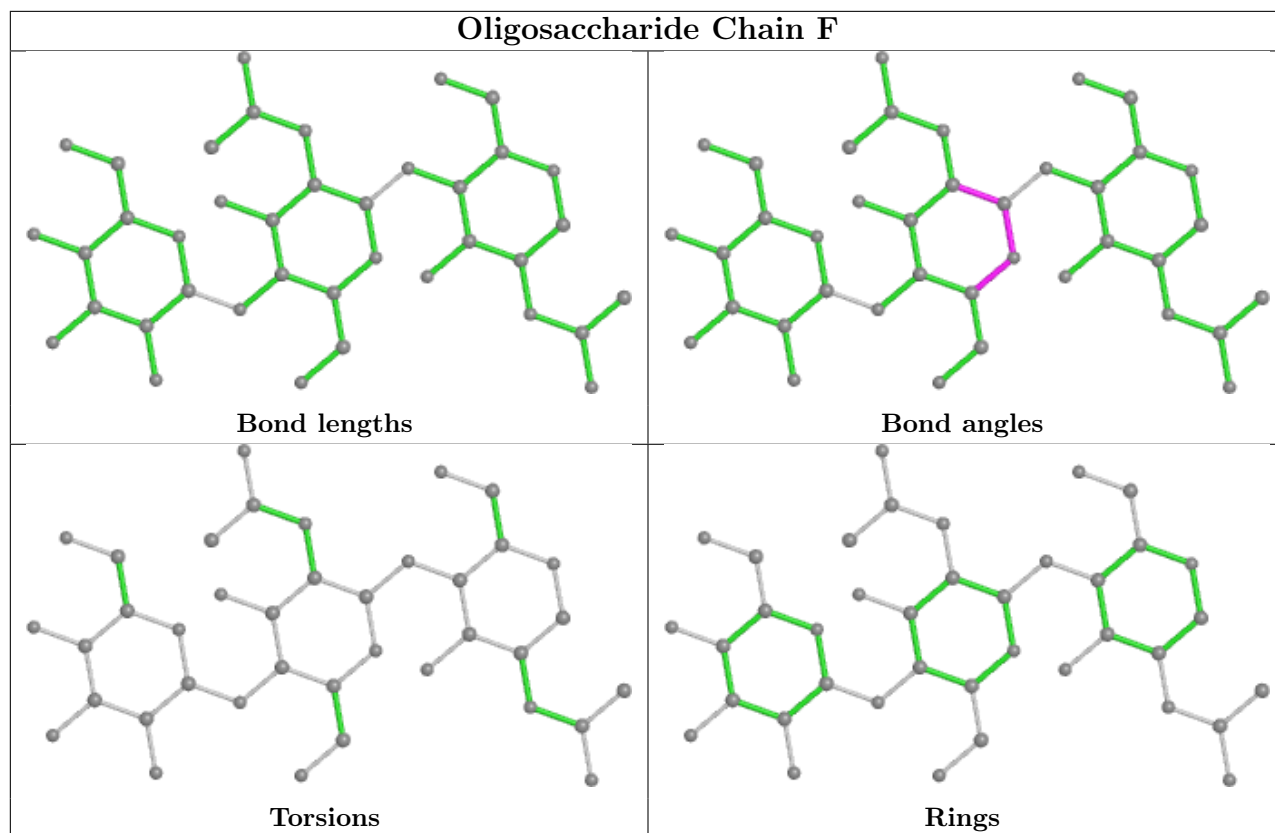
There are no torsion outliers.

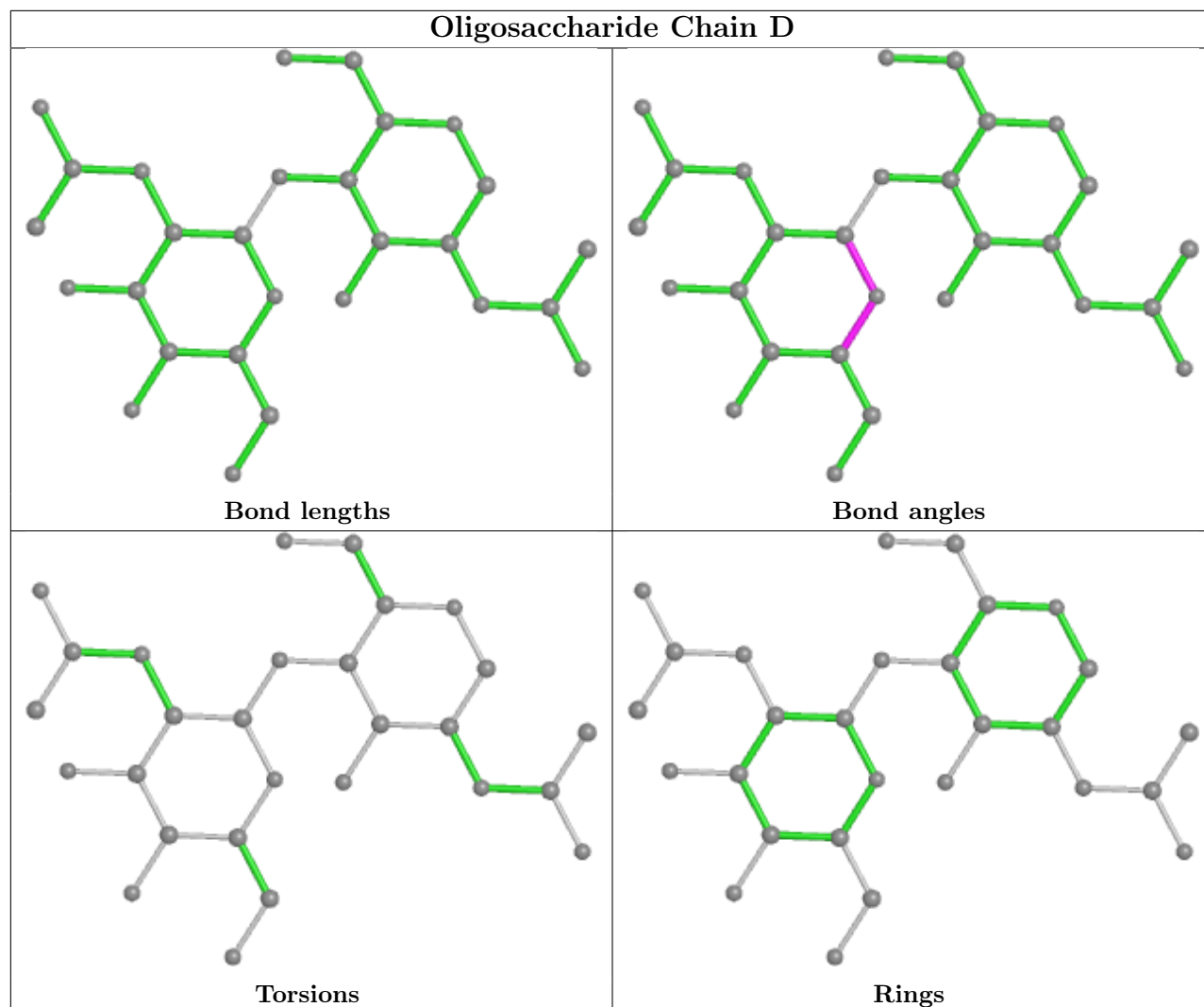
There are no ring outliers.

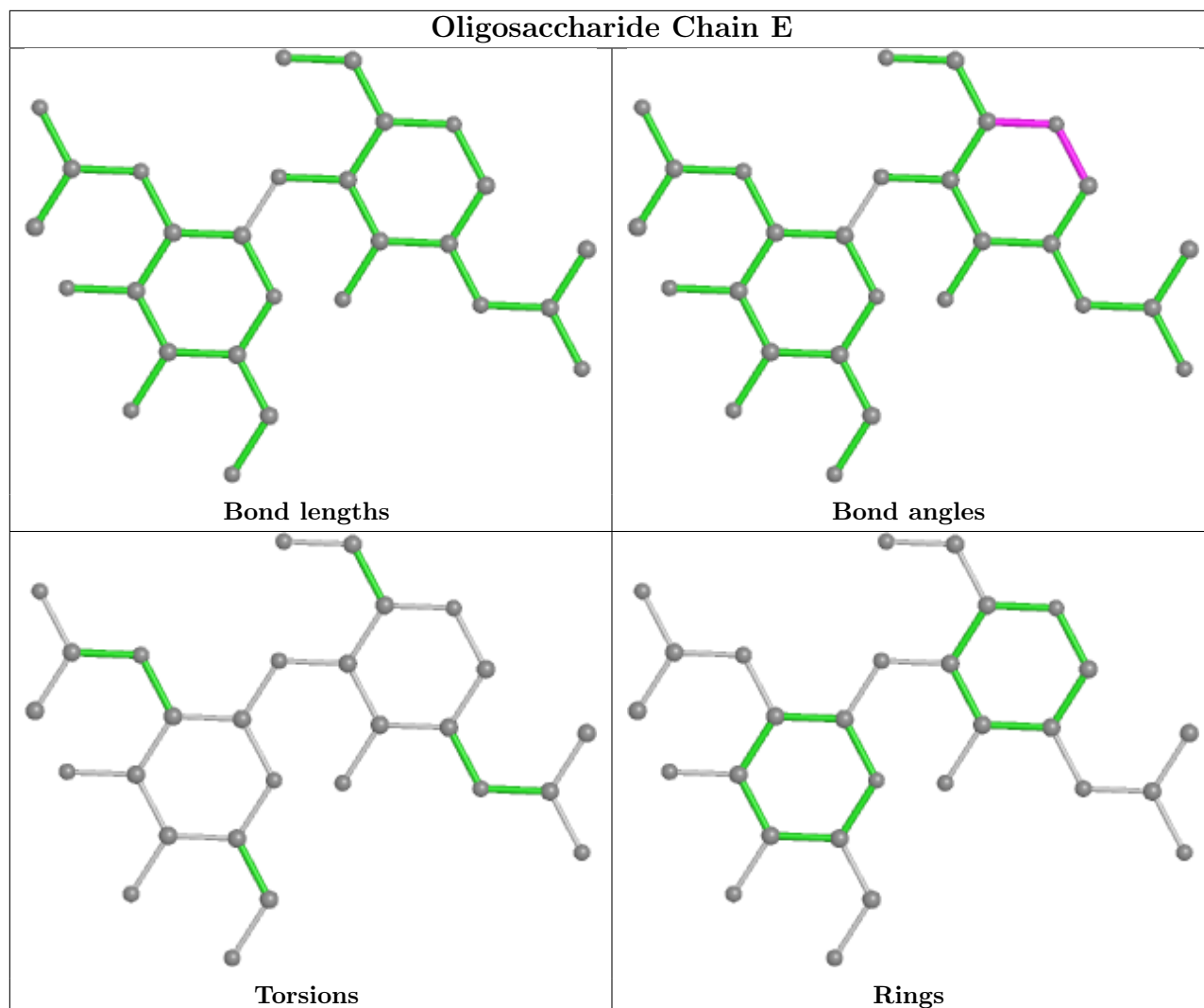
No monomer is involved in short contacts.

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	B	704	1	11,11,12	0.51	0	15,15,17	1.27	2 (13%)
5	NAG	B	712	1	14,14,15	0.71	0	17,19,21	0.71	0
4	MAN	B	706	1	11,11,12	0.36	0	15,15,17	1.17	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	713	1	14,14,15	0.43	0	17,19,21	1.27	2 (11%)
8	BTB	B	716	-	13,13,13	1.19	2 (15%)	7,16,16	0.32	0
7	GOL	A	711	-	5,5,5	0.16	0	5,5,5	0.47	0
7	GOL	B	717	-	5,5,5	0.21	0	5,5,5	0.40	0
4	MAN	A	702	1	11,11,12	0.39	0	15,15,17	0.94	1 (6%)
4	MAN	B	703	1	11,11,12	0.44	0	15,15,17	0.85	0
6	PEG	A	710	-	6,6,6	0.18	0	5,5,5	0.23	0
5	NAG	B	710	1	14,14,15	0.59	0	17,19,21	0.94	1 (5%)
4	MAN	A	703	1	11,11,12	0.64	0	15,15,17	1.05	1 (6%)
7	GOL	A	712	-	5,5,5	0.18	0	5,5,5	0.49	0
5	NAG	A	708	1	14,14,15	0.32	0	17,19,21	1.04	1 (5%)
4	MAN	B	705	1	11,11,12	0.62	0	15,15,17	0.93	1 (6%)
5	NAG	B	708	1	14,14,15	0.40	0	17,19,21	0.90	0
5	NAG	B	714	1	14,14,15	0.43	0	17,19,21	0.50	0
4	MAN	B	702	1	11,11,12	0.41	0	15,15,17	1.75	5 (33%)
5	NAG	A	704	1	14,14,15	0.26	0	17,19,21	0.58	0
5	NAG	B	709	1	14,14,15	0.30	0	17,19,21	1.06	0
5	NAG	B	707	1	14,14,15	0.38	0	17,19,21	0.73	0
7	GOL	B	715	-	5,5,5	0.15	0	5,5,5	0.34	0
5	NAG	A	706	1	14,14,15	0.71	0	17,19,21	0.82	0
5	NAG	A	709	1	14,14,15	0.49	0	17,19,21	0.79	1 (5%)
4	MAN	A	701	1	11,11,12	0.68	0	15,15,17	1.31	2 (13%)
5	NAG	A	707	1	14,14,15	0.31	0	17,19,21	0.71	0
4	MAN	B	701	1	11,11,12	0.44	0	15,15,17	1.46	2 (13%)
5	NAG	B	711	1	14,14,15	0.65	0	17,19,21	0.80	0
5	NAG	A	705	1	14,14,15	0.41	0	17,19,21	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
4	MAN	B	704	1	-	0/2/19/22	0/1/1/1
5	NAG	B	712	1	-	0/6/23/26	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
8	BTB	B	716	-	-	1/21/21/21	-
7	GOL	A	711	-	-	0/4/4/4	-
7	GOL	B	717	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	702	1	-	0/2/19/22	0/1/1/1
4	MAN	B	703	1	-	0/2/19/22	0/1/1/1
6	PEG	A	710	-	-	1/4/4/4	-
5	NAG	B	710	1	-	0/6/23/26	0/1/1/1
4	MAN	A	703	1	-	0/2/19/22	0/1/1/1
7	GOL	A	712	-	-	2/4/4/4	-
5	NAG	A	708	1	-	0/6/23/26	0/1/1/1
4	MAN	B	705	1	-	2/2/19/22	0/1/1/1
5	NAG	B	708	1	-	1/6/23/26	0/1/1/1
5	NAG	B	714	1	-	2/6/23/26	0/1/1/1
4	MAN	B	702	1	-	2/2/19/22	0/1/1/1
5	NAG	A	704	1	-	0/6/23/26	0/1/1/1
5	NAG	B	709	1	-	0/6/23/26	0/1/1/1
5	NAG	B	707	1	-	1/6/23/26	0/1/1/1
7	GOL	B	715	-	-	2/4/4/4	-
5	NAG	A	706	1	-	0/6/23/26	0/1/1/1
5	NAG	A	709	1	-	1/6/23/26	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
4	MAN	B	701	1	-	2/2/19/22	0/1/1/1
5	NAG	B	711	1	-	0/6/23/26	0/1/1/1
5	NAG	A	705	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)
8	B	716	BTB	C2-N	2.81	1.54	1.48
8	B	716	BTB	C5-N	2.31	1.51	1.48

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	MAN	C1-O5-C5	-3.85	106.98	112.19
4	B	706	MAN	O5-C1-C2	-3.33	105.63	110.77
4	B	701	MAN	O5-C1-C2	-3.22	105.81	110.77
4	B	702	MAN	O5-C1-C2	-2.91	106.28	110.77
4	B	705	MAN	C1-O5-C5	2.88	116.09	112.19
4	B	704	MAN	C1-C2-C3	-2.78	106.25	109.67
5	B	710	NAG	C1-C2-N2	2.75	115.18	110.49
4	B	704	MAN	O3-C3-C4	2.63	116.43	110.35
5	B	713	NAG	O5-C5-C4	-2.61	104.48	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	708	NAG	C1-O5-C5	2.58	115.69	112.19
5	B	713	NAG	C4-C3-C2	2.56	114.77	111.02
4	A	701	MAN	C1-O5-C5	2.50	115.59	112.19
4	B	702	MAN	C1-O5-C5	-2.45	108.88	112.19
4	B	702	MAN	C3-C4-C5	2.38	114.48	110.24
4	A	701	MAN	O5-C1-C2	-2.33	107.17	110.77
4	A	702	MAN	C3-C4-C5	2.26	114.26	110.24
4	A	703	MAN	O5-C1-C2	-2.25	107.29	110.77
4	B	702	MAN	C6-C5-C4	-2.24	107.75	113.00
4	B	702	MAN	O6-C6-C5	-2.03	104.33	111.29
5	A	709	NAG	C1-O5-C5	-2.00	109.48	112.19

There are no chirality outliers.

All (22) 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
6	A	710	PEG	O2-C3-C4-O4
5	B	714	NAG	O5-C5-C6-O6
5	B	714	NAG	C4-C5-C6-O6
8	B	716	BTB	N-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
4	B	702	MAN	C4-C5-C6-O6
7	B	715	GOL	O2-C2-C3-O3
7	B	717	GOL	O2-C2-C3-O3
4	A	701	MAN	O5-C5-C6-O6
7	A	712	GOL	O1-C1-C2-O2
4	B	705	MAN	C4-C5-C6-O6
4	B	706	MAN	O5-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

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	713	NAG	2	0
6	A	710	PEG	2	0
7	A	712	GOL	1	0
5	A	708	NAG	1	0
5	B	708	NAG	1	0
5	A	709	NAG	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%)	0.31	33 (6%) 20 21	13, 22, 44, 68	0
1	B	532/675 (78%)	0.28	17 (3%) 47 50	12, 21, 44, 66	0
All	All	1066/1350 (78%)	0.30	50 (4%) 31 32	12, 21, 44, 68	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	561	SER	6.1
1	B	538	LEU	5.1
1	A	532	ALA	4.4
1	A	530	ASP	4.2
1	A	534	GLN	4.2
1	A	436	ASN	4.0
1	B	531	ALA	3.9
1	B	542	ASP	3.8
1	A	538	LEU	3.8
1	A	533	ILE	3.7
1	B	534	GLN	3.5
1	A	435	GLU	3.4
1	A	197	ASN	3.3
1	B	535	ASN	3.0
1	A	561	SER	3.0
1	A	531	ALA	2.9
1	A	241	SER	2.9
1	A	242	THR	2.8
1	A	542	ASP	2.7
1	B	513	THR	2.6
1	B	530	ASP	2.5
1	A	437	GLY	2.5
1	A	537	SER	2.5
1	A	393	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	536	ALA	2.5
1	A	418	ILE	2.5
1	B	392	LEU	2.4
1	B	438	GLU	2.4
1	A	535	ASN	2.4
1	B	657	GLU	2.4
1	A	562	GLY	2.4
1	A	158	THR	2.3
1	B	528	LEU	2.3
1	A	373	ASP	2.3
1	A	422	ALA	2.3
1	A	392	LEU	2.3
1	A	150	ALA	2.3
1	A	154	GLU	2.3
1	B	142	SER	2.3
1	A	657	GLU	2.2
1	B	422	ALA	2.2
1	A	396	VAL	2.2
1	A	445	ALA	2.2
1	A	509	ASP	2.2
1	A	554	LYS	2.2
1	A	157	THR	2.1
1	A	196	ARG	2.1
1	A	596	GLU	2.0
1	B	630	GLU	2.0
1	B	150	ALA	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.

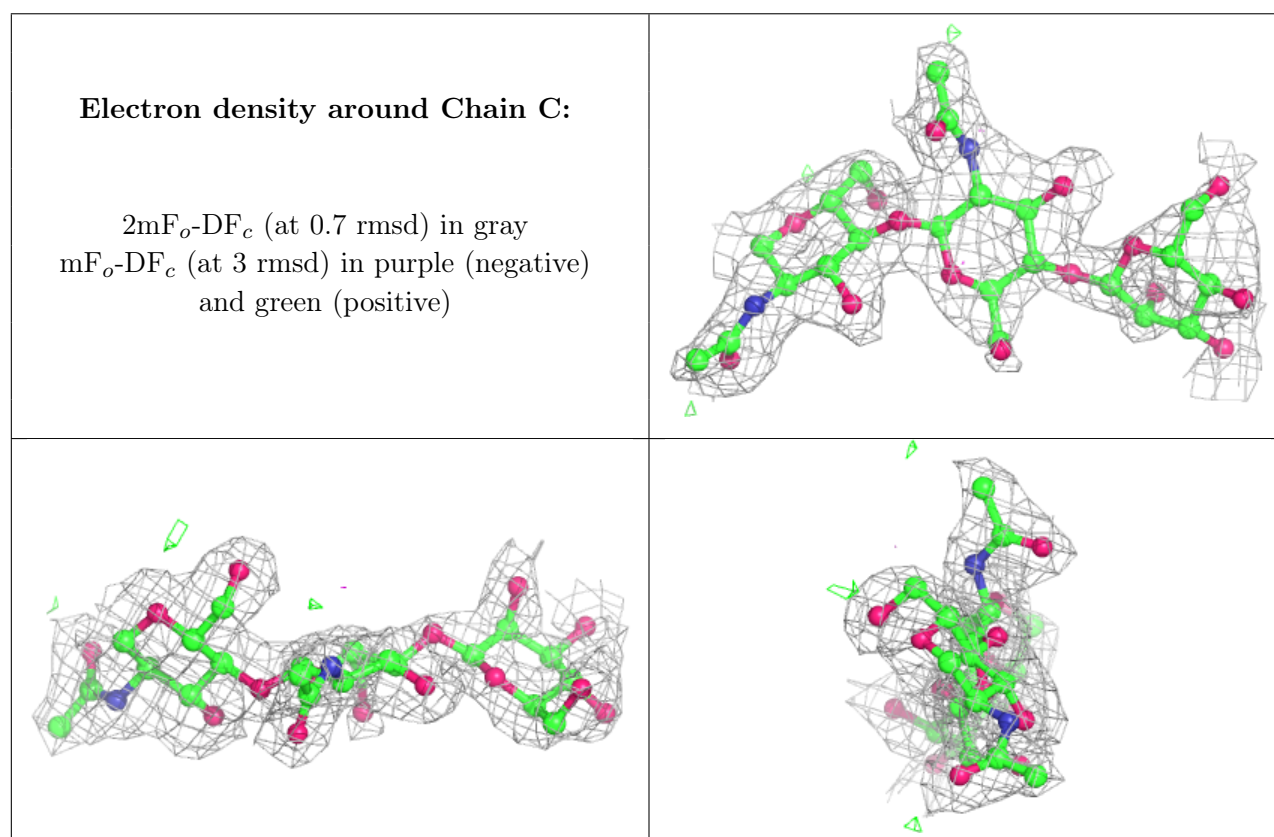
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	2	14/15	0.53	0.34	53,58,63,65	0
2	BMA	C	3	11/12	0.62	0.36	57,60,62,62	0

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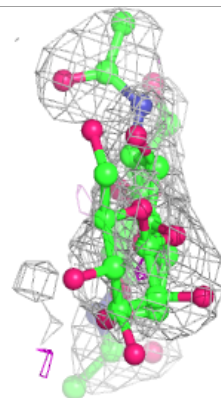
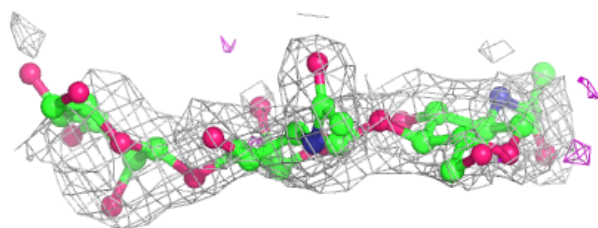
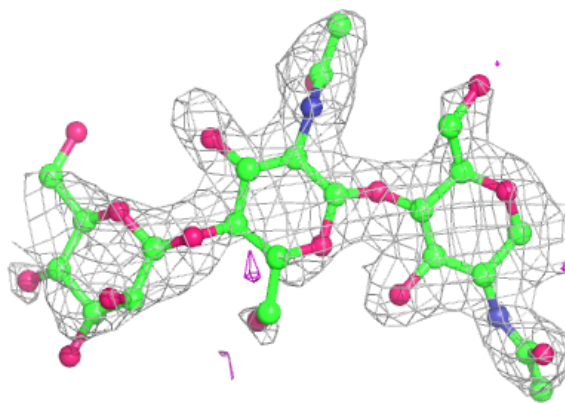
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BMA	F	3	11/12	0.72	0.34	63,69,72,75	0
2	NAG	F	2	14/15	0.75	0.24	43,53,59,59	0
2	NAG	C	2	14/15	0.82	0.28	37,43,52,53	0
3	NAG	D	1	14/15	0.85	0.20	35,42,50,53	0
3	NAG	E	2	14/15	0.85	0.25	39,43,50,54	0
2	NAG	F	1	14/15	0.91	0.17	39,42,46,47	0
3	NAG	E	1	14/15	0.94	0.09	21,26,28,31	0
2	NAG	C	1	14/15	0.94	0.12	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.

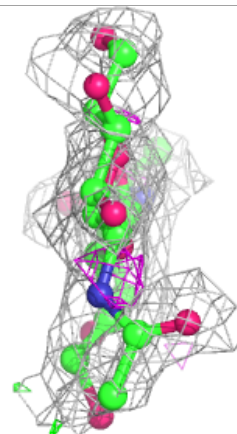
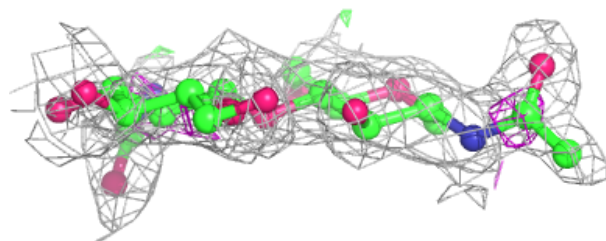
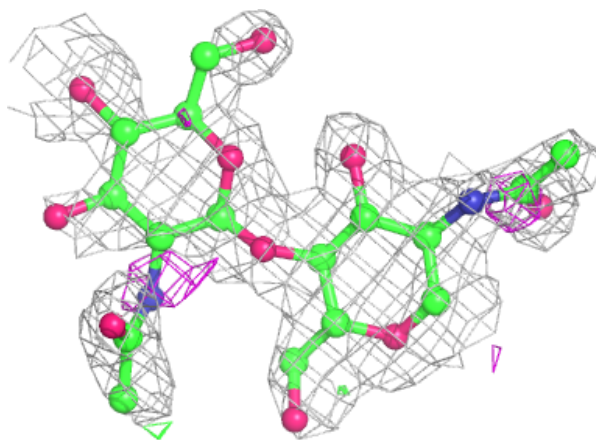


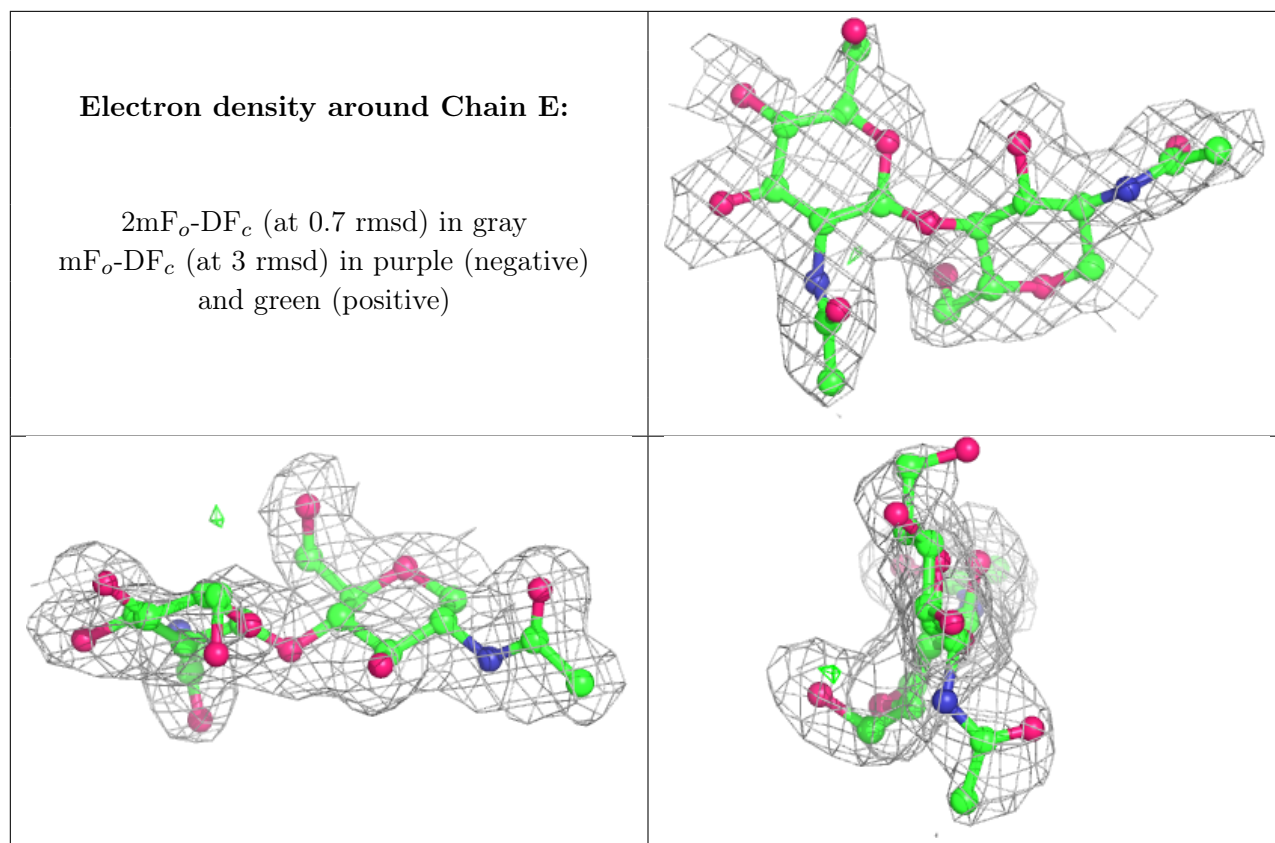
Electron density around Chain F:

$2mF_o-DF_c$ (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 [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(Å ²)	Q<0.9
4	MAN	B	703	11/12	0.68	0.28	56,60,64,68	0
5	NAG	A	709	14/15	0.72	0.30	50,54,58,63	0
4	MAN	B	705	11/12	0.75	0.24	50,53,57,59	0
4	MAN	B	702	11/12	0.76	0.28	55,61,67,67	0
4	MAN	A	702	11/12	0.76	0.31	44,47,55,55	0
6	PEG	A	710	7/7	0.76	0.24	37,38,41,44	0
5	NAG	B	709	14/15	0.77	0.32	58,66,71,71	0
7	GOL	A	712	6/6	0.79	0.19	28,29,31,32	0
5	NAG	A	708	14/15	0.81	0.25	44,48,50,54	0
4	MAN	B	706	11/12	0.84	0.20	53,59,64,64	0
4	MAN	B	701	11/12	0.84	0.18	48,52,58,60	0
5	NAG	B	714	14/15	0.85	0.31	41,46,53,54	0
4	MAN	A	703	11/12	0.86	0.20	42,43,45,46	0
5	NAG	A	704	14/15	0.86	0.24	47,52,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	B	713	14/15	0.87	0.29	47,50,54,61	0
7	GOL	B	715	6/6	0.87	0.17	26,33,36,40	0
5	NAG	B	710	14/15	0.88	0.20	33,38,43,43	0
5	NAG	A	705	14/15	0.88	0.23	35,40,42,47	0
8	BTB	B	716	14/14	0.88	0.15	20,30,34,38	0
5	NAG	B	708	14/15	0.89	0.20	44,50,53,58	0
4	MAN	A	701	11/12	0.89	0.23	39,43,53,54	0
4	MAN	B	704	11/12	0.89	0.27	44,47,51,52	0
5	NAG	B	707	14/15	0.91	0.14	28,33,40,42	0
7	GOL	B	717	6/6	0.92	0.21	19,28,30,31	0
7	GOL	A	711	6/6	0.92	0.16	21,26,27,29	0
5	NAG	A	706	14/15	0.93	0.12	17,20,23,25	0
5	NAG	B	712	14/15	0.93	0.20	25,26,33,38	0
5	NAG	A	707	14/15	0.94	0.18	21,27,36,36	0
5	NAG	B	711	14/15	0.95	0.11	18,19,22,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.