Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 12:31 am GMT

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	:	2016-10-24
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
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:

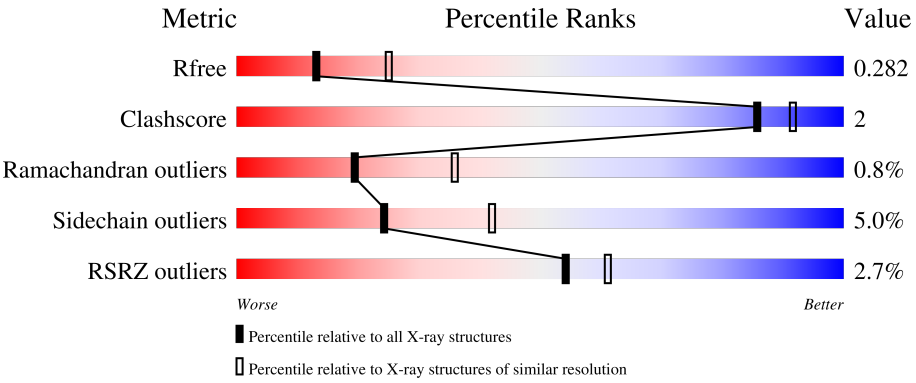
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.74 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}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 <=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	3% 79% 10% • 10%
1	M	248	2% 78% 12% 9%
2	L	239	2% 85% 5% 10%
2	N	239	3% 85% 5% 10%
3	A	2	100%

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Mol	Chain	Length	Quality of chain
3	C	2	100%
4	B	7	100%
4	D	7	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BGC	B	6	-	-	-	X
4	GAL	B	7	-	-	-	X
4	SIA	D	5	-	-	-	X

2 Entry composition (i)

There are 7 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.

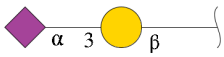
- Molecule 1 is a protein called H chain of Fab NVS-1-19-5.

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.

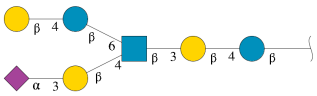
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1586	985	261	333	7			
2	N	216	Total	C	N	O	S	0	0	0
			1591	988	262	334	7			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose.



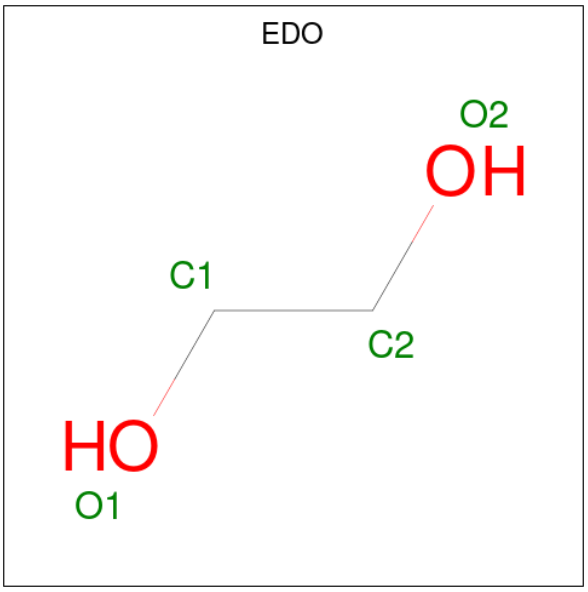
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total	C	N	O	0	0	0
			31	17	1	13			
3	C	2	Total	C	N	O	0	0	0
			31	17	1	13			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-[beta-D-galactopyranose-(1-4)-beta-D-glucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	B	7	Total C N O 89 49 2 38	0	0	0
4	D	7	Total C N O 89 49 2 38	0	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0

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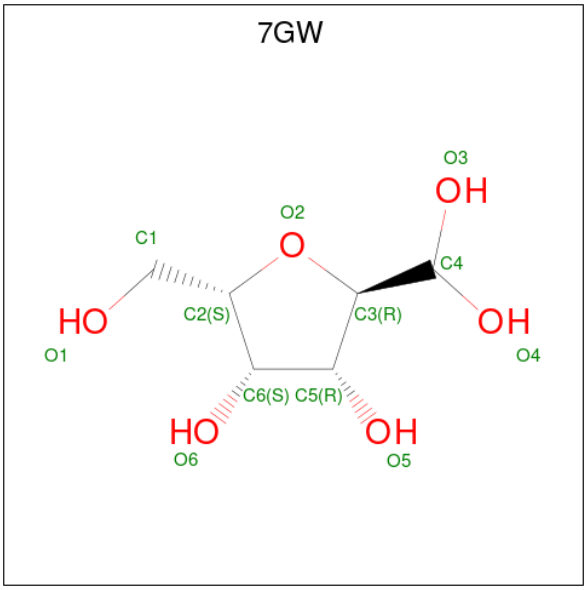
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total C O 4 2 2	0	0
5	M	1	Total C O 4 2 2	0	0
5	N	1	Total C O 4 2 2	0	0
5	N	1	Total C O 4 2 2	0	0
5	N	1	Total C O 4 2 2	0	0
5	N	1	Total C O 4 2 2	0	0

- Molecule 6 is (2 {R},3 {R},4 {S},5 {S})-2-[bis(oxidanyl)methyl]-5-(hydroxymethyl)oxolane-3,4-diol (three-letter code: 7GW) (formula: $C_6H_{12}O_6$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	27	Total O 27 27	0	0

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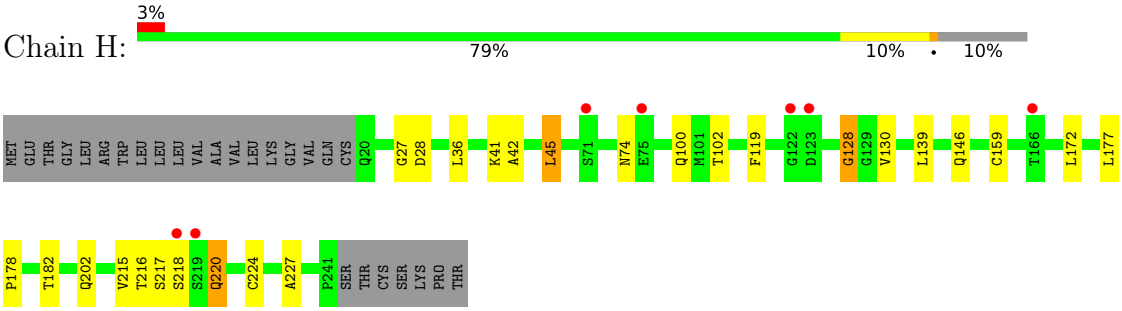
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	27	Total O 27 27	0	0
7	M	45	Total O 45 45	0	0
7	N	35	Total O 35 35	0	0

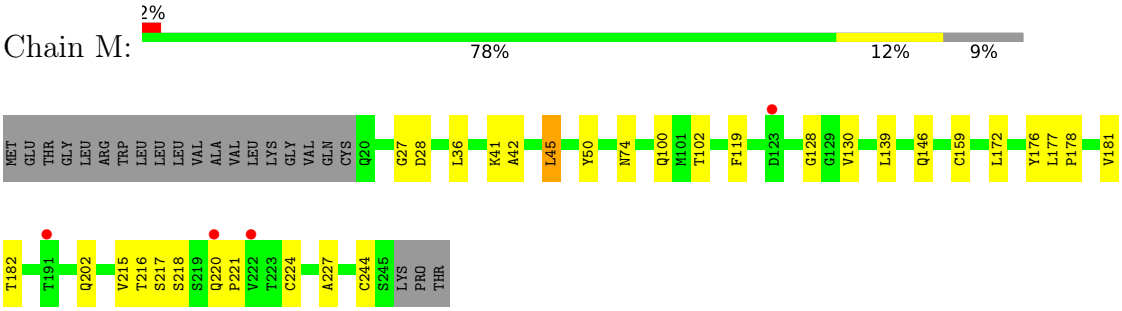
3 Residue-property plots

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.

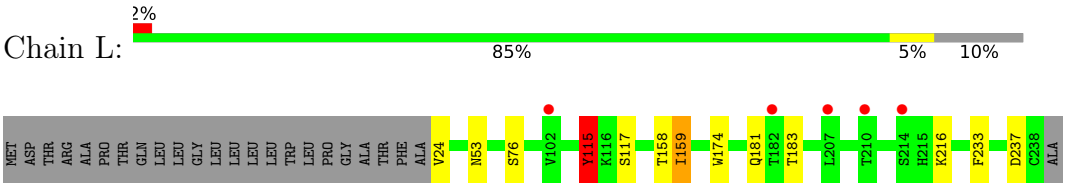
• Molecule 1: H chain of Fab NVS-1-19-5



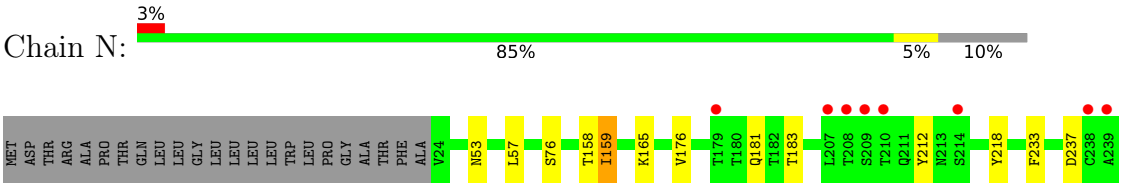
• Molecule 1: H chain of Fab NVS-1-19-5



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

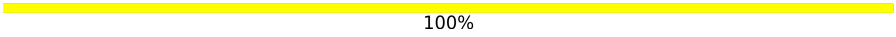


• Molecule 2: L chain of Fab NVS-1-19-5



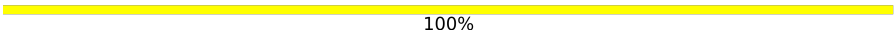
• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain A:



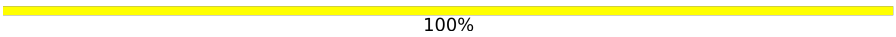
• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain C:



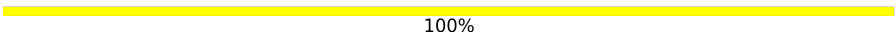
• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[beta-D-galactopyranose-(1-4)-beta-D-glucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain B:



• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[beta-D-galactopyranose-(1-4)-beta-D-glucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.00%)	wwPDB-VP
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]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, SIA, EDO, 7GW, GAL, BGC

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(^{o})	Ideal(^{o})
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 (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	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	A	31	0	26	0	0
3	C	31	0	26	0	0
4	B	89	0	74	0	0
4	D	89	0	74	0	0
5	H	12	0	18	0	0
5	L	16	0	24	0	0
5	M	8	0	12	0	0
5	N	16	0	24	0	0
6	H	12	0	0	0	0
6	M	12	0	0	0	0
7	H	27	0	0	0	0
7	L	27	0	0	0	0
7	M	45	0	0	0	0
7	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	2:L:181:GLN:OE1	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 (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	H	220/248 (89%)	211 (96%)	7 (3%)	2 (1%)	17	32
1	M	224/248 (90%)	214 (96%)	8 (4%)	2 (1%)	17	32
2	L	213/239 (89%)	196 (92%)	16 (8%)	1 (0%)	29	48
2	N	214/239 (90%)	196 (92%)	16 (8%)	2 (1%)	17	32
All	All	871/974 (89%)	817 (94%)	47 (5%)	7 (1%)	19	36

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 (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	H	186/209 (89%)	174 (94%)	12 (6%)	17	30
1	M	190/209 (91%)	177 (93%)	13 (7%)	16	28
2	L	181/199 (91%)	174 (96%)	7 (4%)	32	53
2	N	181/199 (91%)	176 (97%)	5 (3%)	43	63
All	All	738/816 (90%)	701 (95%)	37 (5%)	24	42

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

Mol	Chain	Res	Type
1	H	41	LYS

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Mol	Chain	Res	Type
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
2	N	237	ASP

Sometimes 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

18 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	$\#\|Z\| > 2$
3	GAL	A	1	3,6	11,11,12	0.70	0	15,15,17	1.37	2 (13%)
3	SIA	A	2	3	20,20,21	0.85	1 (5%)	24,28,31	1.64	4 (16%)
4	BGC	B	1	4,6	11,11,12	0.55	0	15,15,17	1.61	3 (20%)
4	GAL	B	2	4	11,11,12	0.62	0	15,15,17	1.70	4 (26%)
4	NAG	B	3	4	14,14,15	0.66	0	17,19,21	1.48	2 (11%)
4	GAL	B	4	4	11,11,12	0.80	0	15,15,17	1.22	1 (6%)
4	SIA	B	5	4	20,20,21	0.65	0	24,28,31	1.33	4 (16%)
4	BGC	B	6	4	11,11,12	0.91	0	15,15,17	1.75	5 (33%)
4	GAL	B	7	4	11,11,12	0.84	0	15,15,17	1.56	4 (26%)
3	GAL	C	1	3,6	11,11,12	0.48	0	15,15,17	1.60	4 (26%)
3	SIA	C	2	3	20,20,21	0.80	0	24,28,31	1.67	5 (20%)
4	BGC	D	1	4,6	11,11,12	0.66	0	15,15,17	1.84	4 (26%)
4	GAL	D	2	4	11,11,12	0.63	0	15,15,17	1.90	3 (20%)
4	NAG	D	3	4	14,14,15	0.47	0	17,19,21	1.17	2 (11%)
4	GAL	D	4	4	11,11,12	0.55	0	15,15,17	1.22	2 (13%)
4	SIA	D	5	4	20,20,21	0.85	1 (5%)	24,28,31	1.39	4 (16%)
4	BGC	D	6	4	11,11,12	0.68	0	15,15,17	1.16	2 (13%)
4	GAL	D	7	4	11,11,12	0.72	0	15,15,17	1.46	2 (13%)

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	GAL	A	1	3,6	-	2/2/19/22	0/1/1/1
3	SIA	A	2	3	-	2/18/34/38	0/1/1/1
4	BGC	B	1	4,6	-	1/2/19/22	0/1/1/1
4	GAL	B	2	4	-	2/2/19/22	0/1/1/1
4	NAG	B	3	4	-	0/6/23/26	0/1/1/1
4	GAL	B	4	4	-	2/2/19/22	0/1/1/1
4	SIA	B	5	4	-	3/18/34/38	0/1/1/1
4	BGC	B	6	4	-	1/2/19/22	0/1/1/1
4	GAL	B	7	4	-	0/2/19/22	0/1/1/1
3	GAL	C	1	3,6	-	2/2/19/22	0/1/1/1
3	SIA	C	2	3	-	1/18/34/38	0/1/1/1
4	BGC	D	1	4,6	-	1/2/19/22	0/1/1/1
4	GAL	D	2	4	-	0/2/19/22	0/1/1/1
4	NAG	D	3	4	-	2/6/23/26	0/1/1/1
4	GAL	D	4	4	-	1/2/19/22	0/1/1/1
4	SIA	D	5	4	-	10/18/34/38	0/1/1/1
4	BGC	D	6	4	-	1/2/19/22	0/1/1/1
4	GAL	D	7	4	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5	SIA	C2-C1	2.30	1.54	1.52
3	A	2	SIA	C2-C1	2.12	1.54	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2	GAL	C1-C2-C3	5.05	115.87	109.67
4	B	3	NAG	O5-C5-C6	4.27	113.91	107.20
3	A	2	SIA	O6-C2-C3	-4.27	104.58	110.46
3	C	2	SIA	O6-C2-C3	-4.17	104.72	110.46
3	A	1	GAL	C1-C2-C3	4.02	114.61	109.67
4	B	2	GAL	C1-C2-C3	4.00	114.58	109.67
4	D	1	BGC	O4-C4-C3	3.87	119.31	110.35
4	B	1	BGC	O4-C4-C3	3.57	118.61	110.35
4	D	7	GAL	O5-C1-C2	-3.45	105.45	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	6	BGC	O5-C1-C2	-3.42	105.50	110.77
3	C	1	GAL	C1-O5-C5	3.41	116.82	112.19
4	D	1	BGC	C3-C4-C5	-3.32	104.33	110.24
4	B	6	BGC	C1-O5-C5	3.08	116.37	112.19
4	B	4	GAL	C1-O5-C5	3.08	116.36	112.19
4	B	6	BGC	O2-C2-C1	3.05	115.38	109.15
4	B	7	GAL	C1-O5-C5	3.02	116.28	112.19
4	B	5	SIA	C6-O6-C2	3.01	117.77	111.34
4	D	2	GAL	O5-C1-C2	-2.98	106.17	110.77
4	B	1	BGC	C1-C2-C3	2.91	113.24	109.67
4	D	3	NAG	C4-C3-C2	-2.91	106.75	111.02
4	B	5	SIA	C11-C10-N5	2.86	120.94	116.10
3	C	2	SIA	O6-C2-C1	2.66	112.92	107.70
4	B	7	GAL	O5-C1-C2	-2.66	106.66	110.77
4	B	2	GAL	O5-C5-C4	-2.61	104.47	110.83
3	A	2	SIA	O1B-C1-C2	2.61	120.47	113.03
4	B	5	SIA	C3-C4-C5	-2.59	108.33	111.46
4	B	2	GAL	C1-O5-C5	2.59	115.70	112.19
3	C	1	GAL	C1-C2-C3	2.58	112.84	109.67
4	D	5	SIA	C11-C10-N5	2.55	120.42	116.10
4	B	3	NAG	C1-O5-C5	2.53	115.61	112.19
4	B	1	BGC	C3-C4-C5	-2.52	105.75	110.24
4	D	4	GAL	C2-C3-C4	-2.51	106.56	110.89
4	D	3	NAG	O5-C1-C2	-2.49	107.35	111.29
4	B	6	BGC	C6-C5-C4	-2.49	107.17	113.00
4	D	6	BGC	O5-C1-C2	-2.47	106.95	110.77
4	D	6	BGC	O2-C2-C1	2.44	114.15	109.15
3	A	1	GAL	O5-C5-C6	2.44	111.03	107.20
3	C	1	GAL	O5-C5-C6	2.40	110.97	107.20
4	B	7	GAL	C2-C3-C4	2.40	115.05	110.89
4	B	2	GAL	O5-C5-C6	2.36	110.91	107.20
4	B	6	BGC	O2-C2-C3	-2.36	105.41	110.14
4	D	7	GAL	O2-C2-C1	2.34	113.94	109.15
3	C	1	GAL	C3-C4-C5	-2.33	106.07	110.24
3	C	2	SIA	C6-O6-C2	2.33	116.33	111.34
3	C	2	SIA	C8-C7-C6	-2.33	108.61	113.03
3	C	2	SIA	O1B-C1-C2	2.33	119.69	113.03
4	D	5	SIA	C6-O6-C2	2.26	116.19	111.34
4	D	4	GAL	C1-O5-C5	2.22	115.20	112.19
4	D	1	BGC	O2-C2-C1	2.16	113.58	109.15
4	D	5	SIA	O1B-C1-C2	2.16	119.19	113.03
3	A	2	SIA	O9-C9-C8	-2.15	106.39	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	5	SIA	O1B-C1-C2	2.14	119.14	113.03
3	A	2	SIA	O6-C2-C1	2.11	111.83	107.70
4	B	7	GAL	O5-C5-C6	2.10	110.50	107.20
4	D	2	GAL	O2-C2-C3	-2.05	106.02	110.14
4	D	5	SIA	O6-C2-C1	2.01	111.63	107.70
4	D	1	BGC	C1-C2-C3	2.00	112.13	109.67

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	SIA	O1A-C1-C2-O6
4	D	5	SIA	C5-C6-C7-O7
4	D	5	SIA	O6-C6-C7-O7
4	D	3	NAG	C4-C5-C6-O6
4	D	3	NAG	O5-C5-C6-O6
3	C	1	GAL	C4-C5-C6-O6
3	C	1	GAL	O5-C5-C6-O6
4	B	4	GAL	O5-C5-C6-O6
3	A	1	GAL	C4-C5-C6-O6
4	B	5	SIA	C11-C10-N5-C5
4	B	5	SIA	O10-C10-N5-C5
4	D	5	SIA	C11-C10-N5-C5
4	D	5	SIA	O10-C10-N5-C5
4	B	4	GAL	C4-C5-C6-O6
4	D	5	SIA	C6-C7-C8-O8
4	D	5	SIA	O7-C7-C8-C9
4	D	5	SIA	C6-C7-C8-C9
4	B	2	GAL	O5-C5-C6-O6
3	A	1	GAL	O5-C5-C6-O6
4	D	5	SIA	O7-C7-C8-O8
4	D	1	BGC	O5-C5-C6-O6
4	B	2	GAL	C4-C5-C6-O6
4	B	1	BGC	O5-C5-C6-O6
4	D	4	GAL	C4-C5-C6-O6
4	B	6	BGC	C4-C5-C6-O6
4	D	5	SIA	C5-C6-C7-C8
4	D	7	GAL	C4-C5-C6-O6
4	B	5	SIA	O8-C8-C9-O9
4	D	6	BGC	C4-C5-C6-O6
3	A	2	SIA	O1B-C1-C2-O6
3	C	2	SIA	O1A-C1-C2-O6

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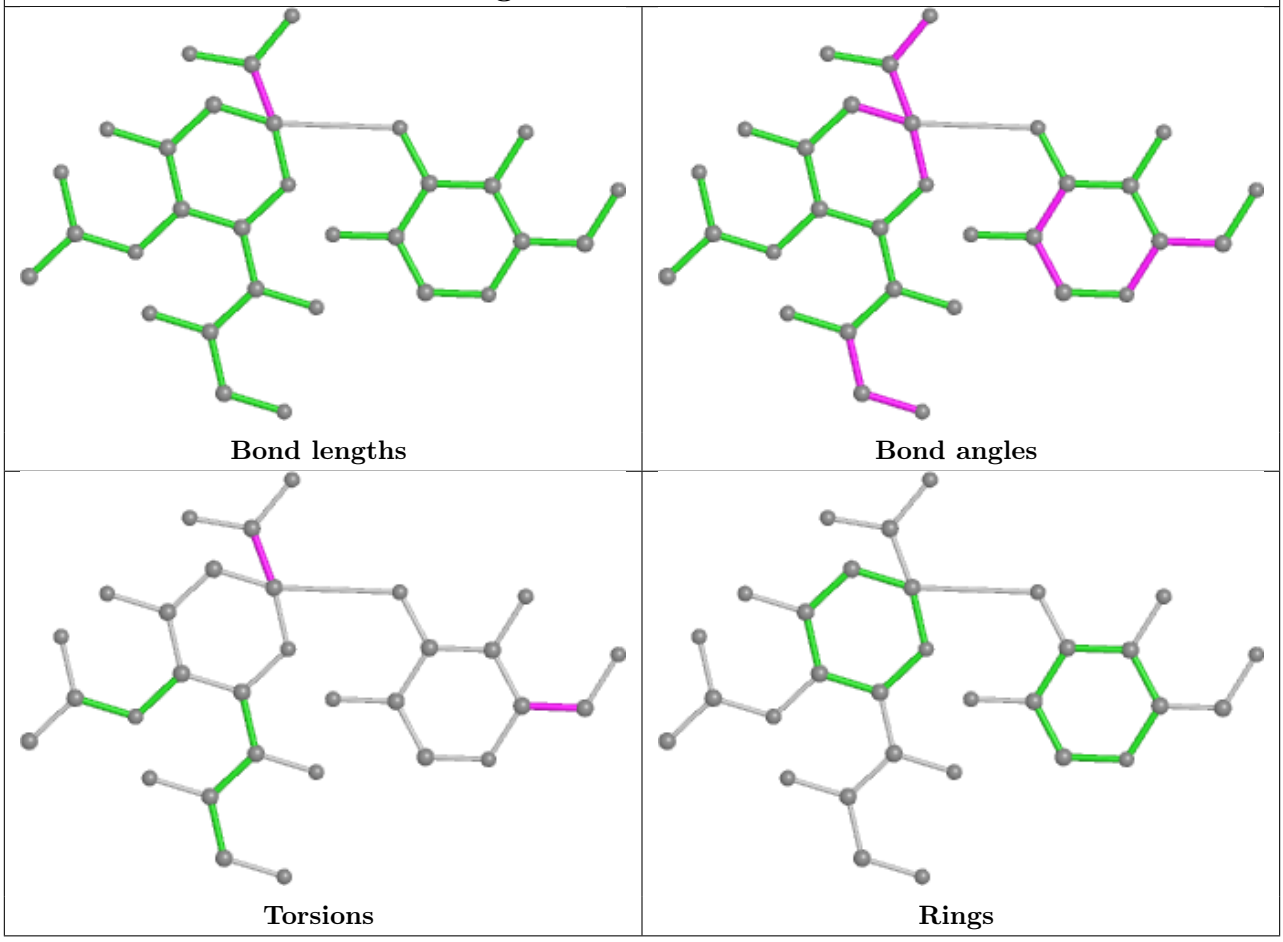
Mol	Chain	Res	Type	Atoms
4	D	5	SIA	O1A-C1-C2-O6

There are no ring outliers.

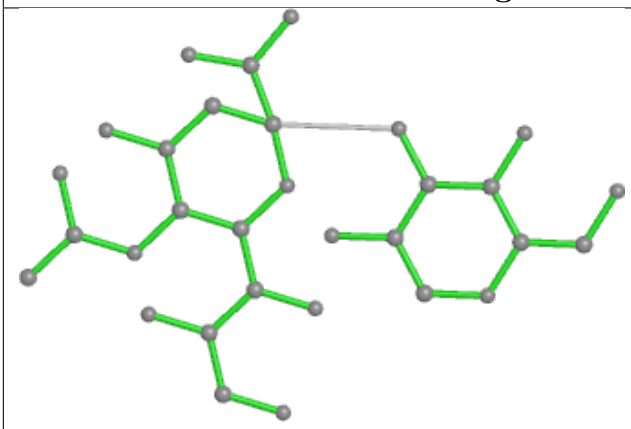
No monomer is involved in short contacts.

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

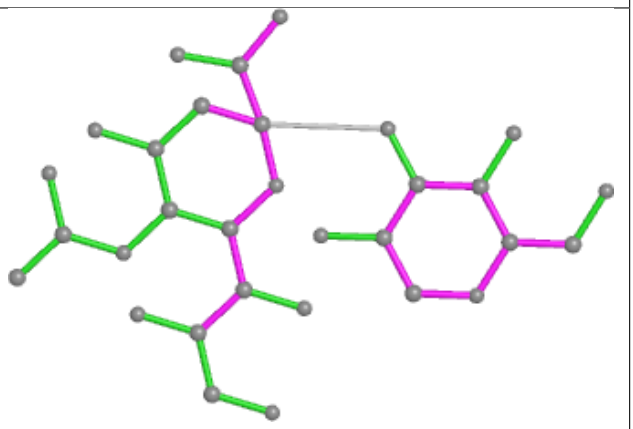
Oligosaccharide Chain A



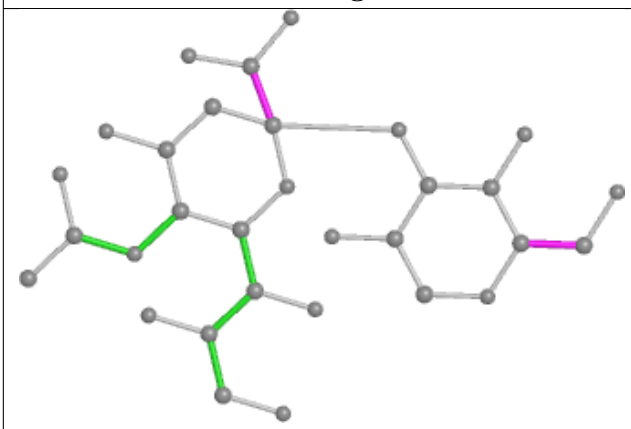
Oligosaccharide Chain C



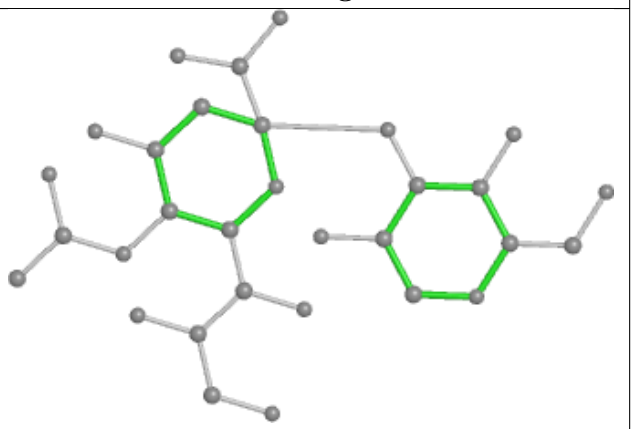
Bond lengths



Bond angles

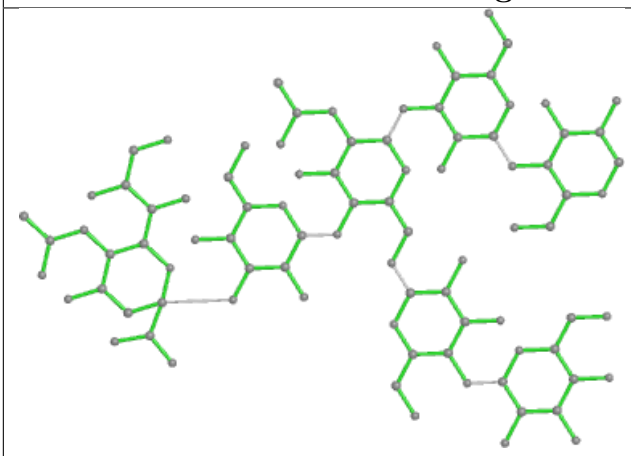


Torsions

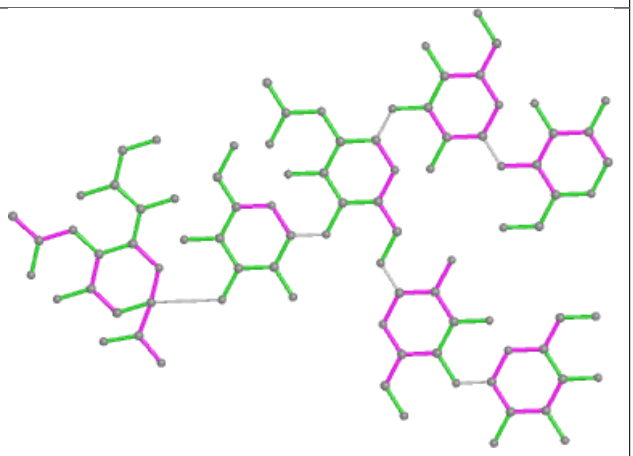


Rings

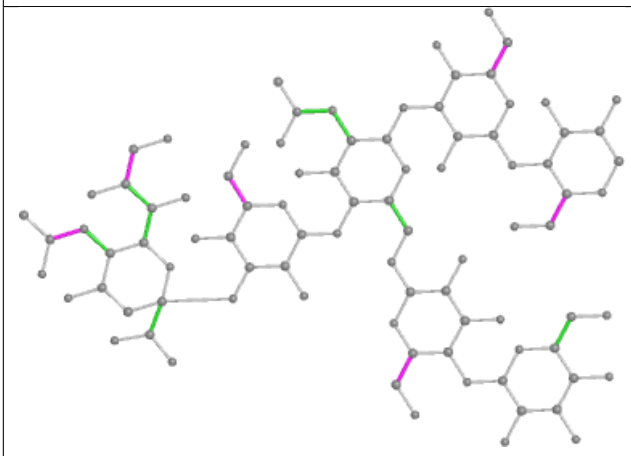
Oligosaccharide Chain B



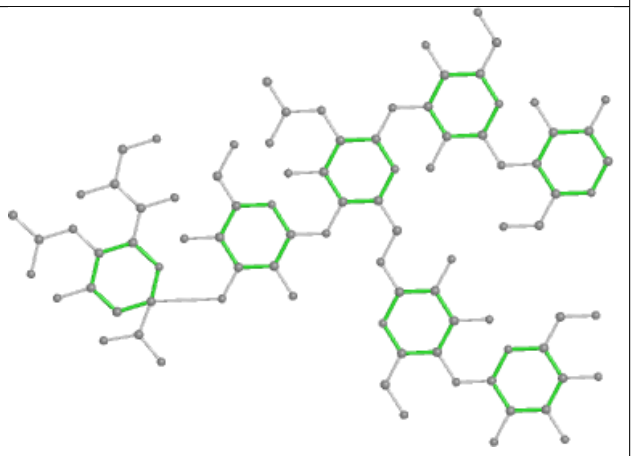
Bond lengths



Bond angles

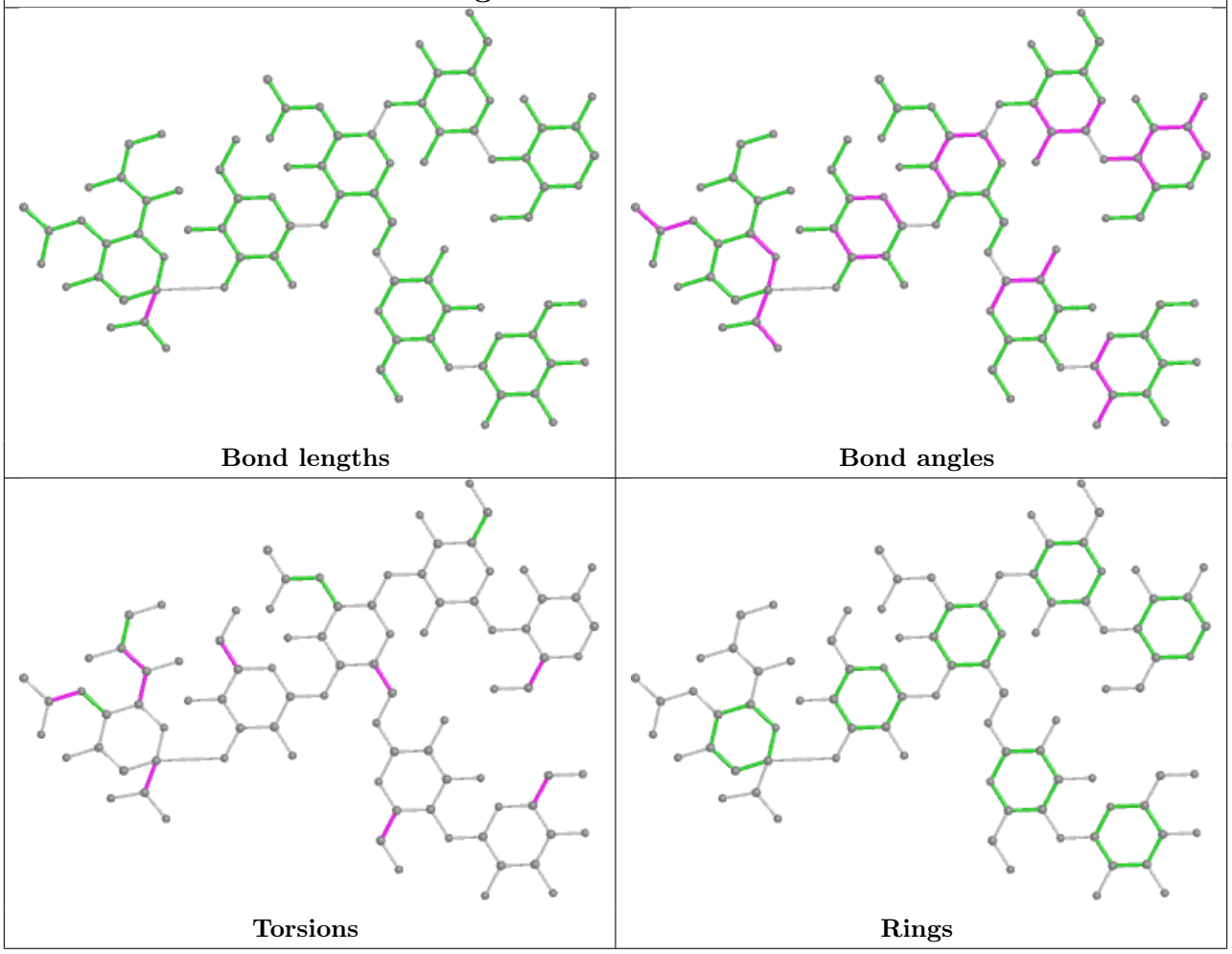


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

15 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	$\#\|Z\| > 2$
5	EDO	N	311	-	3,3,3	0.54	0	2,2,2	0.22	0
6	7GW	M	302	3,4	12,12,12	4.85	7 (58%)	15,17,17	1.35	1 (6%)
5	EDO	H	301	-	3,3,3	0.54	0	2,2,2	0.30	0
5	EDO	L	311	-	3,3,3	0.49	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	M	305	-	3,3,3	0.60	0	2,2,2	0.31	0
5	EDO	L	308	-	3,3,3	0.57	0	2,2,2	0.08	0
5	EDO	N	308	-	3,3,3	0.76	0	2,2,2	0.10	0
5	EDO	N	310	-	3,3,3	0.56	0	2,2,2	0.21	0
6	7GW	H	304	3,4	12,12,12	4.97	7 (58%)	15,17,17	1.30	1 (6%)
5	EDO	M	301	-	3,3,3	0.42	0	2,2,2	0.44	0
5	EDO	N	309	-	3,3,3	0.52	0	2,2,2	0.21	0
5	EDO	L	310	-	3,3,3	0.55	0	2,2,2	0.11	0
5	EDO	L	309	-	3,3,3	0.59	0	2,2,2	0.08	0
5	EDO	H	302	-	3,3,3	0.64	0	2,2,2	0.10	0
5	EDO	H	303	-	3,3,3	0.52	0	2,2,2	0.19	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
5	EDO	N	311	-	-	1/1/1/1	-
6	7GW	M	302	3,4	-	0/6/22/22	0/1/1/1
5	EDO	H	301	-	-	1/1/1/1	-
5	EDO	L	311	-	-	0/1/1/1	-
5	EDO	M	305	-	-	0/1/1/1	-
5	EDO	L	308	-	-	1/1/1/1	-
5	EDO	N	308	-	-	1/1/1/1	-
5	EDO	N	310	-	-	1/1/1/1	-
6	7GW	H	304	3,4	-	2/6/22/22	0/1/1/1
5	EDO	M	301	-	-	0/1/1/1	-
5	EDO	N	309	-	-	1/1/1/1	-
5	EDO	L	310	-	-	0/1/1/1	-
5	EDO	L	309	-	-	1/1/1/1	-
5	EDO	H	302	-	-	1/1/1/1	-
5	EDO	H	303	-	-	1/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	304	7GW	O2-C3	-10.38	1.28	1.44
6	M	302	7GW	O2-C3	-10.24	1.29	1.44
6	H	304	7GW	C6-C5	-9.01	1.28	1.53
6	M	302	7GW	C6-C5	-8.39	1.30	1.53
6	M	302	7GW	C5-C3	6.92	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	304	7GW	C5-C3	6.68	1.67	1.52
6	H	304	7GW	O2-C2	4.93	1.56	1.45
6	M	302	7GW	O2-C2	4.92	1.56	1.45
6	H	304	7GW	O6-C6	4.09	1.52	1.43
6	M	302	7GW	O6-C6	3.67	1.51	1.43
6	M	302	7GW	C1-C2	-3.66	1.39	1.51
6	H	304	7GW	C1-C2	-3.63	1.39	1.51
6	H	304	7GW	C6-C2	2.46	1.59	1.53
6	M	302	7GW	C6-C2	2.14	1.58	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	304	7GW	C6-C5-C3	4.10	108.37	102.45
6	M	302	7GW	C6-C5-C3	3.83	107.97	102.45

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	304	7GW	O1-C1-C2-O2
5	H	301	EDO	O1-C1-C2-O2
5	H	302	EDO	O1-C1-C2-O2
5	H	303	EDO	O1-C1-C2-O2
5	L	308	EDO	O1-C1-C2-O2
5	L	309	EDO	O1-C1-C2-O2
5	N	308	EDO	O1-C1-C2-O2
5	N	309	EDO	O1-C1-C2-O2
6	H	304	7GW	O1-C1-C2-C6
5	N	311	EDO	O1-C1-C2-O2
5	N	310	EDO	O1-C1-C2-O2

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	H	222/248 (89%)	0.43	7 (3%)	47	54	47, 67, 110, 132	0
1	M	226/248 (91%)	0.25	4 (1%)	68	74	39, 62, 101, 130	0
2	L	215/239 (89%)	0.40	5 (2%)	60	67	52, 73, 112, 123	0
2	N	216/239 (90%)	0.32	8 (3%)	41	46	44, 63, 102, 135	0
All	All	879/974 (90%)	0.35	24 (2%)	54	61	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
2	L	182	THR	3.1
1	H	219	SER	3.1
1	H	218	SER	3.1
1	H	122	GLY	2.9
2	L	214	SER	2.8
1	H	123	ASP	2.7
1	M	191	THR	2.7
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	75	GLU	2.2
1	H	71	SER	2.2
1	M	222	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	220	GLN	2.2
2	N	208	THR	2.2
2	N	214	SER	2.1

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)

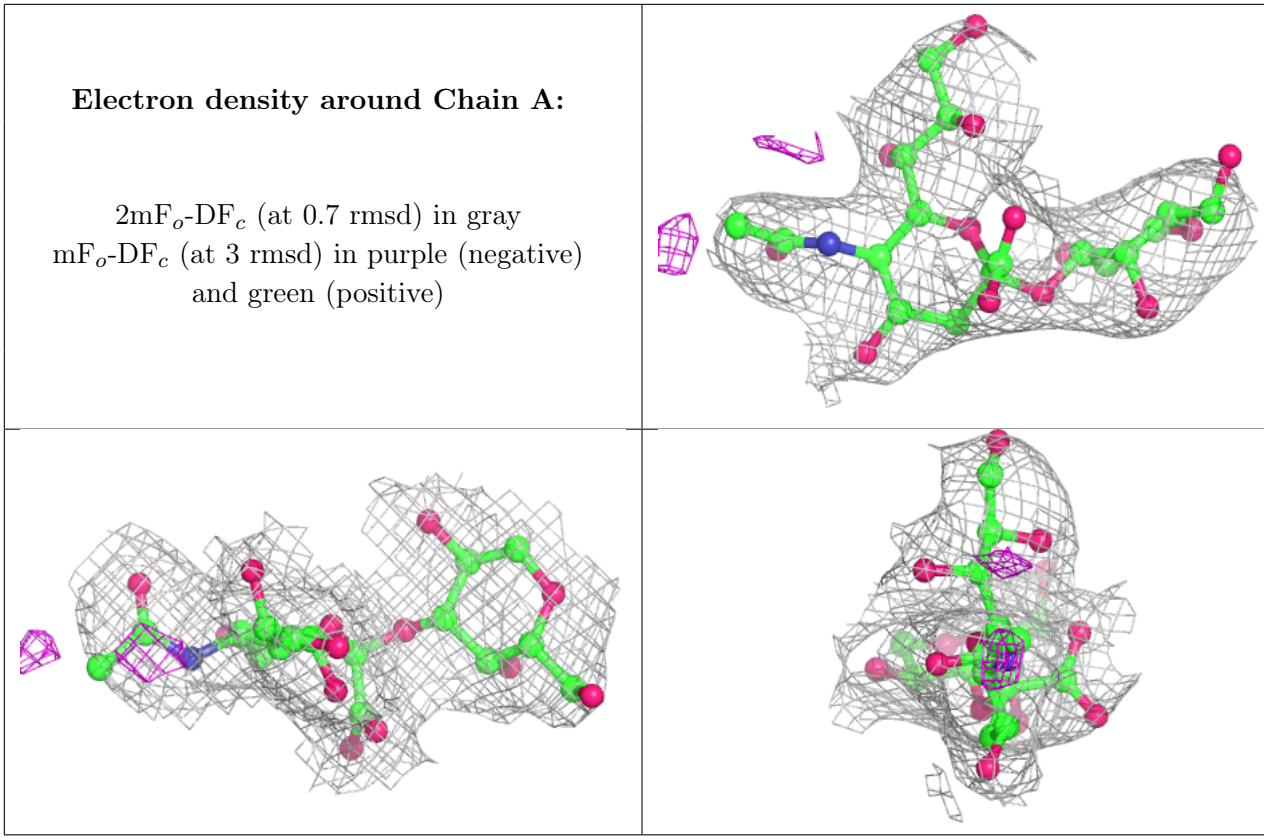
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GAL	B	7	11/12	0.60	0.53	118,123,125,127	0
4	SIA	D	5	20/21	0.77	0.53	121,143,150,152	0
4	GAL	D	7	11/12	0.79	0.35	92,97,100,100	0
4	BGC	B	6	11/12	0.80	0.50	111,115,117,119	0
4	SIA	B	5	20/21	0.81	0.48	146,151,155,155	0
4	GAL	B	4	11/12	0.84	0.22	106,116,124,133	0
4	BGC	D	6	11/12	0.88	0.30	83,86,89,93	0
4	NAG	B	3	14/15	0.91	0.15	76,90,103,106	0
4	GAL	B	2	11/12	0.92	0.20	76,79,81,81	0
3	SIA	A	2	20/21	0.92	0.16	66,72,78,79	0
4	GAL	D	4	11/12	0.92	0.22	92,96,101,109	0
4	GAL	D	2	11/12	0.93	0.16	67,69,71,72	0
4	BGC	D	1	11/12	0.94	0.15	64,64,66,66	0
3	SIA	C	2	20/21	0.94	0.20	56,63,71,74	0
3	GAL	A	1	11/12	0.95	0.12	80,84,86,87	0
4	BGC	B	1	11/12	0.96	0.17	78,79,82,84	0
4	NAG	D	3	14/15	0.96	0.16	67,74,80,84	0
3	GAL	C	1	11/12	0.96	0.12	66,67,68,69	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.

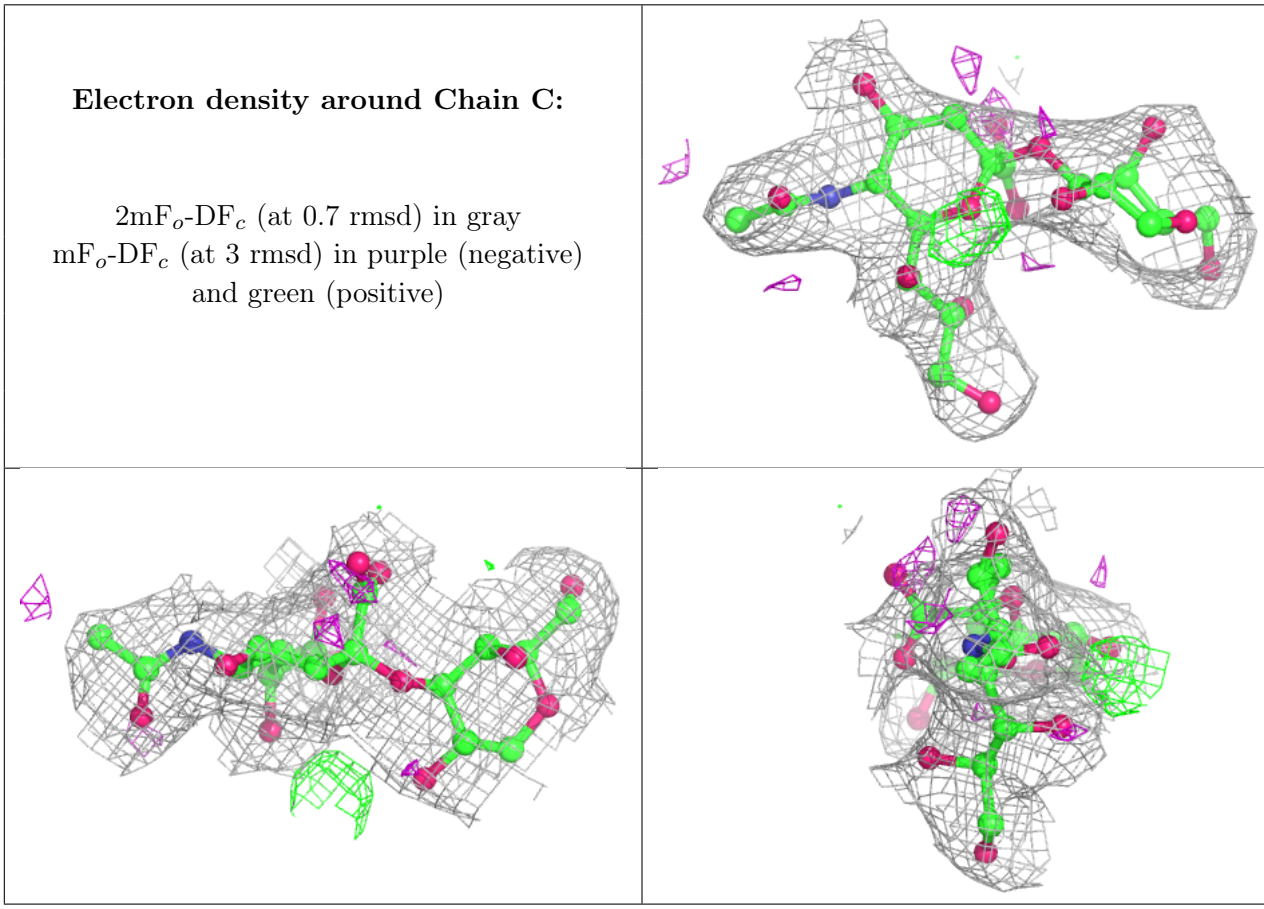
Electron density around Chain A:

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



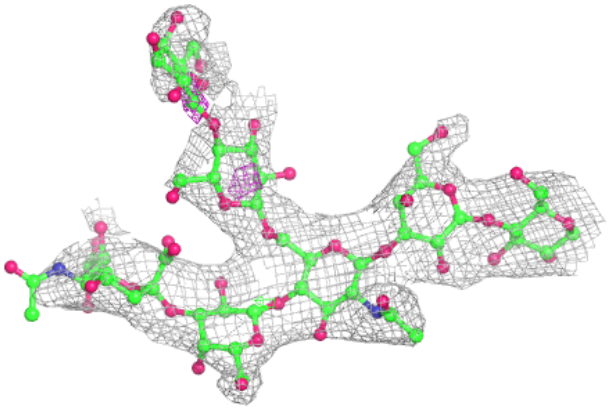
Electron density around Chain C:

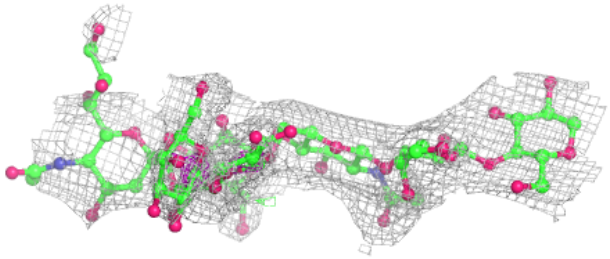
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

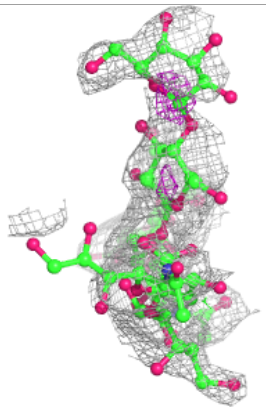


Electron density around Chain B:

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

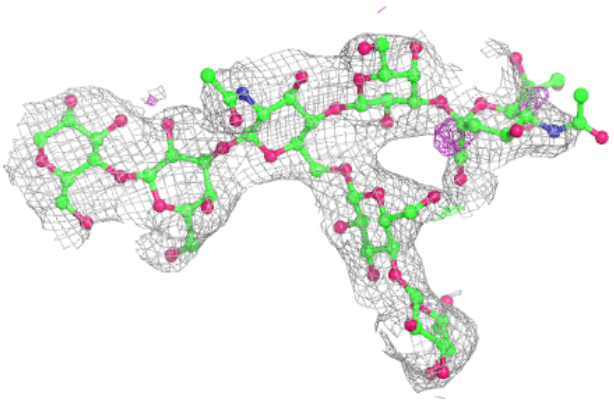


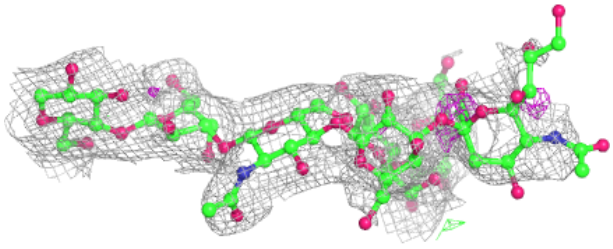


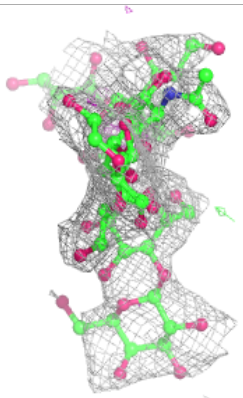


Electron density around Chain D:

$2mF_o$-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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	L	311	4/4	0.64	0.39	92,93,93,94	0
5	EDO	H	302	4/4	0.79	0.28	67,67,68,69	0
5	EDO	M	301	4/4	0.84	0.37	85,85,87,89	0
5	EDO	H	301	4/4	0.86	0.31	61,63,64,66	0
5	EDO	N	310	4/4	0.87	0.15	61,62,63,65	0
5	EDO	N	311	4/4	0.87	0.30	83,85,85,85	0
5	EDO	M	305	4/4	0.89	0.23	54,56,56,57	0
5	EDO	N	309	4/4	0.90	0.19	69,69,69,70	0
5	EDO	L	309	4/4	0.90	0.23	60,62,62,62	0
5	EDO	L	308	4/4	0.90	0.23	52,53,54,55	0
5	EDO	N	308	4/4	0.91	0.24	46,48,49,50	0
6	7GW	H	304	12/12	0.93	0.15	87,96,101,101	0
6	7GW	M	302	12/12	0.93	0.14	66,69,73,74	0
5	EDO	L	310	4/4	0.94	0.22	65,65,65,65	0
5	EDO	H	303	4/4	0.95	0.19	68,68,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.