wwPDB X-ray Structure Validation Summary Report (i)

Mar 7, 2026 – 01:12 AM UTC

PDB ID	:	8D0Y / pdb_00008d0y
Title	:	Crystal Structure of HIV-1 BG505 SOSIPv8 Trimer in Complex with CD4bs targeting antibody 21N13 and interface targeting antibody 35O22 at 4.7 Angstrom
Authors	:	Xian, Y.; Wilson, I.A.
Deposited on	:	2022-05-26
Resolution	:	4.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

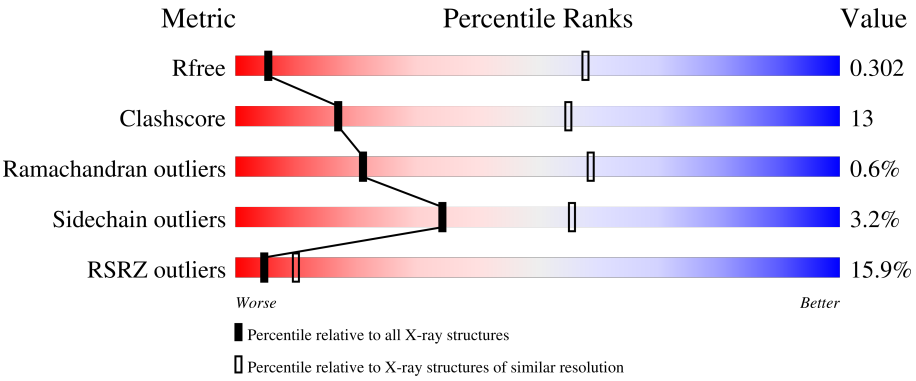
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.70 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	1020 (5.48-3.92)
Clashscore	190562	1005 (5.40-3.96)
Ramachandran outliers	187476	1095 (5.50-3.90)
Sidechain outliers	187428	1077 (5.50-3.90)
RSRZ outliers	180081	1015 (5.48-3.92)

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	D	128	16% 73% 25% ·
2	E	111	11% 72% 25% ·
3	H	225	9% 78% 21% ·
4	L	213	10% 83% 17%
5	G	455	20% 58% 40% ·

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Mol	Chain	Length	Quality of chain
6	B	146	25% 72% 28%
7	A	7	29% 71%
8	C	2	100%
8	K	2	50% 50%
9	F	7	14% 43% 43%
10	I	6	67% 33%
11	J	5	20% 80%
11	M	5	40% 40% 20%
11	N	5	40% 60%
11	O	5	40% 60%
12	P	4	50% 50%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 10622 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 35O22scFv Heavy Chain Variable.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	128	Total	C	N	O	S	0	0	0
			994	628	169	192	5			

- Molecule 2 is a protein called 35O22scFv Light Chain Variable.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	111	Total	C	N	O	S	0	0	0
			845	530	140	169	6			

- Molecule 3 is a protein called 21N13 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	225	Total	C	N	O	S	0	0	0
			1715	1086	288	335	6			

- Molecule 4 is a protein called 21N13 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	0	0
			1643	1022	279	335	7			

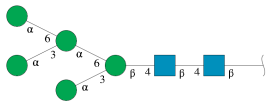
- Molecule 5 is a protein called BG505SOSIPv8 gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	455	Total	C	N	O	S	0	0	0
			3587	2255	631	673	28			

- Molecule 6 is a protein called BG505SOSIPv8 gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	146	Total	C	N	O	S	0	0	0
			1166	735	205	219	7			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



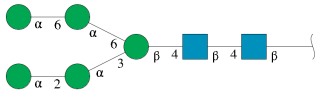
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	A	7	Total C N O 83 46 2 35	0	0	0

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



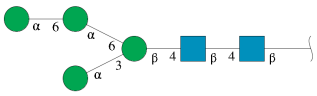
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	C	2	Total C N O 28 16 2 10	0	0	0
8	K	2	Total C N O 28 16 2 10	0	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



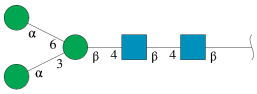
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	F	7	Total C N O 83 46 2 35	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
10	I	6	Total C N O 72 40 2 30	0	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



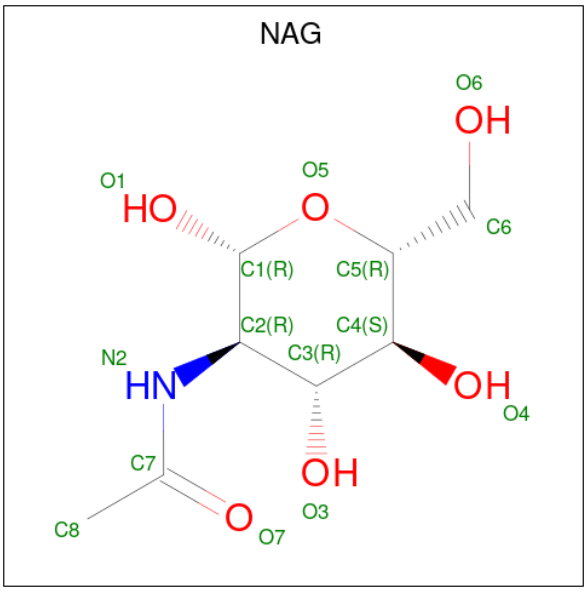
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	J	5	Total C N O 61 34 2 25	0	0	0
11	M	5	Total C N O 61 34 2 25	0	0	0
11	N	5	Total C N O 61 34 2 25	0	0	0
11	O	5	Total C N O 61 34 2 25	0	0	0

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
12	P	4	Total C N O 50 28 2 20	0	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



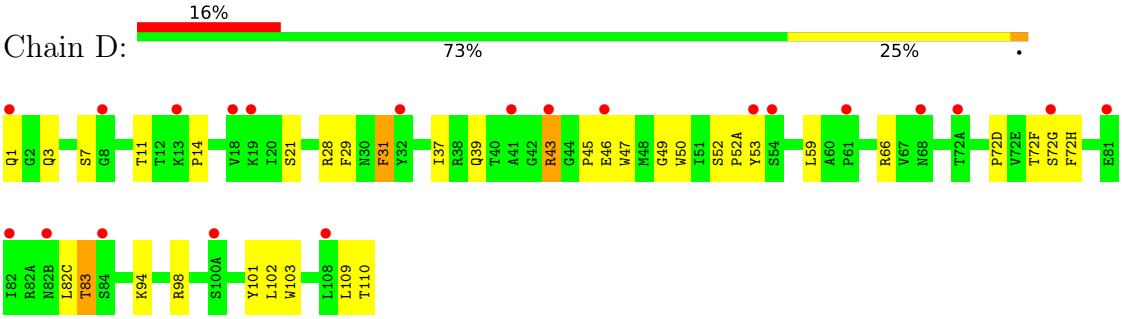
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	B	1	Total C N O 14 8 1 5	0	0

3 Residue-property plots (i)

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.

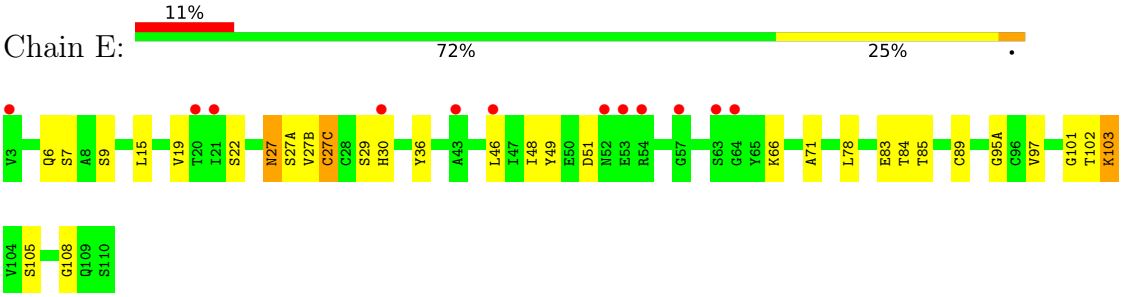
• Molecule 1: 35O22scFv Heavy Chain Variable

Chain D:



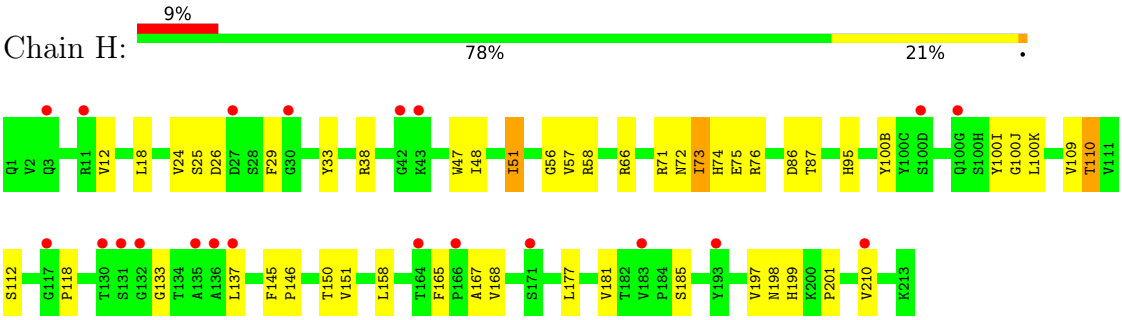
• Molecule 2: 35O22scFv Light Chain Variable

Chain E:



• Molecule 3: 21N13 Fab Heavy Chain

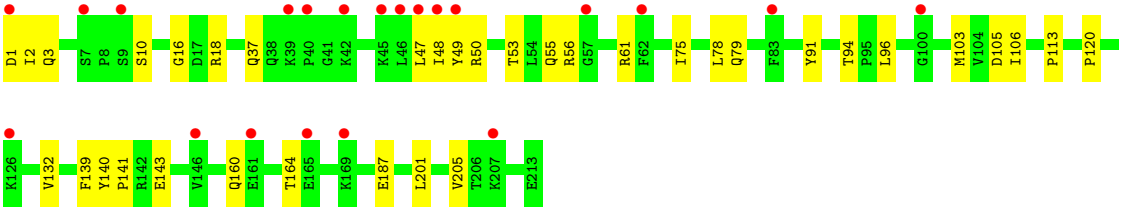
Chain H:



• Molecule 4: 21N13 Fab Light Chain

Chain L:

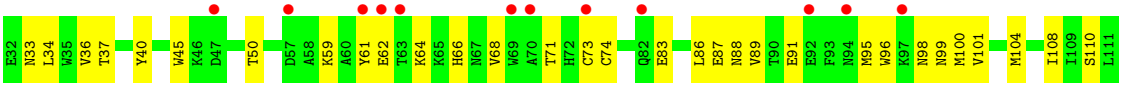


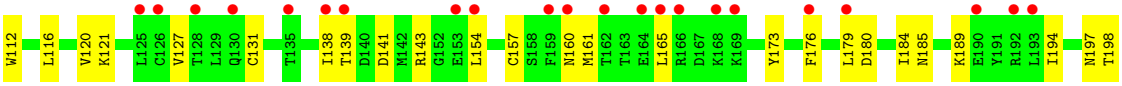


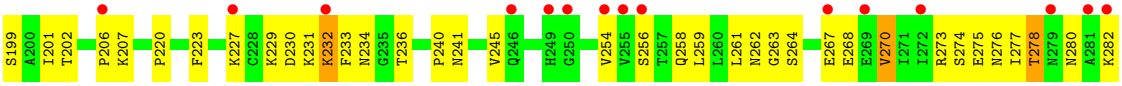
• Molecule 5: BG505SOSIPv8 gp120

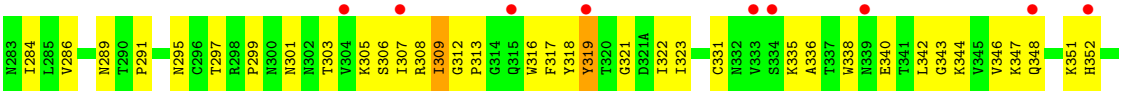
Chain G:

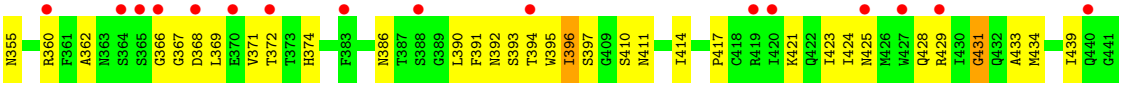


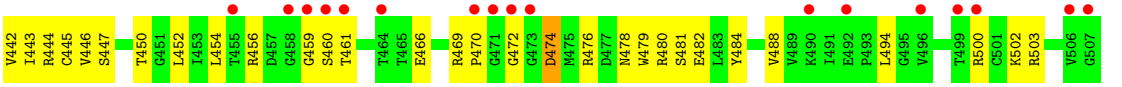








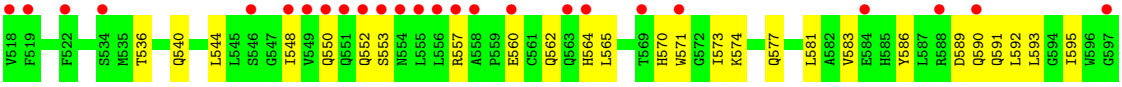


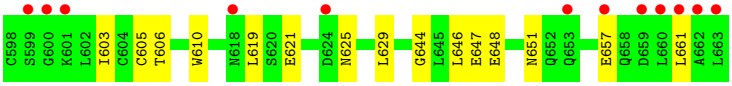


• Molecule 6: BG505SOSIPv8 gp41

Chain B:







• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

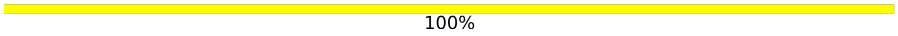
Chain A:





• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:





• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

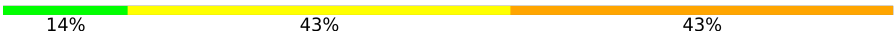
Chain K:





• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:





• Molecule 10: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:





• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

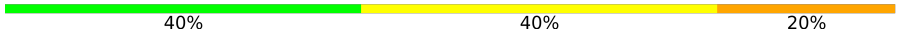
Chain J:





• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

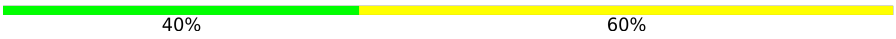
Chain M:





• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

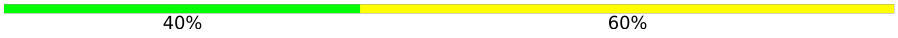
Chain N:





• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:





• Molecule 12: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	264.67Å 264.67Å 264.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.63 – 4.70 43.63 – 4.70	Depositor EDS
% Data completeness (in resolution range)	96.3 (43.63-4.70) 85.0 (43.63-4.70)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.25 (at 4.64Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.268 , 0.298 0.272 , 0.302	Depositor DCC
R_{free} test set	1573 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	212.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 393.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.055 for l,-k,h	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10622	wwPDB-VP
Average B, all atoms (Å^2)	364.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 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	D	0.11	0/1021	0.25	0/1390
2	E	0.12	0/869	0.31	0/1187
3	H	0.11	0/1762	0.30	0/2405
4	L	0.11	0/1677	0.28	0/2277
5	G	0.22	0/3663	0.75	3/4975 (0.1%)
6	B	0.20	0/1189	0.68	0/1614
All	All	0.17	0/10181	0.55	3/13848 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	431	GLY	N-CA-C	6.05	127.51	113.18
5	G	309	ILE	CA-C-N	5.95	131.21	121.87
5	G	309	ILE	C-N-CA	5.95	131.21	121.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	994	0	953	23	0
2	E	845	0	795	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1715	0	1651	39	0
4	L	1643	0	1592	23	0
5	G	3587	0	3526	157	0
6	B	1166	0	1142	28	0
7	A	83	0	70	1	0
8	C	28	0	25	4	0
8	K	28	0	25	1	0
9	F	83	0	70	4	0
10	I	72	0	61	7	0
11	J	61	0	52	1	0
11	M	61	0	52	1	0
11	N	61	0	52	0	0
11	O	61	0	52	2	0
12	P	50	0	43	1	0
13	B	14	0	13	0	0
13	G	70	0	65	6	0
All	All	10622	0	10239	264	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 13.

The worst 5 of 264 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)
5:G:392:ASN:HD22	5:G:395:TRP:HD1	1.14	0.92
5:G:280:ASN:H	5:G:456:ARG:HD2	1.38	0.87
5:G:101:VAL:HG13	5:G:479:TRP:HB2	1.58	0.84
5:G:83:GLU:HG3	5:G:245:VAL:HG12	1.60	0.81
5:G:231:LYS:HE2	5:G:267:GLU:HG2	1.61	0.81

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	D	126/128 (98%)	115 (91%)	11 (9%)	0	100 100
2	E	109/111 (98%)	101 (93%)	8 (7%)	0	100 100
3	H	221/225 (98%)	211 (96%)	9 (4%)	1 (0%)	24 63
4	L	211/213 (99%)	206 (98%)	5 (2%)	0	100 100
5	G	449/455 (99%)	405 (90%)	38 (8%)	6 (1%)	9 41
6	B	144/146 (99%)	136 (94%)	7 (5%)	1 (1%)	18 55
All	All	1260/1278 (99%)	1174 (93%)	78 (6%)	8 (1%)	21 59

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	429	ARG
5	G	466	GLU
6	B	565	LEU
5	G	460	SER
5	G	154	LEU

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	D	107/107 (100%)	103 (96%)	4 (4%)	30 51
2	E	97/97 (100%)	88 (91%)	9 (9%)	8 27
3	H	190/190 (100%)	188 (99%)	2 (1%)	65 74
4	L	189/189 (100%)	186 (98%)	3 (2%)	55 69
5	G	408/408 (100%)	393 (96%)	15 (4%)	30 51
6	B	127/127 (100%)	124 (98%)	3 (2%)	43 63
All	All	1118/1118 (100%)	1082 (97%)	36 (3%)	34 56

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	G	319	TYR
6	B	603	ILE
5	G	352	HIS
5	G	396	ILE
2	E	103	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	196	ASN
5	G	72	HIS
5	G	377	ASN
5	G	258	GLN
3	H	3	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

48 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	$\#\|Z\| > 2$
7	NAG	A	1	5,7	14,14,15	0.40	0	17,19,21	0.69	0
7	NAG	A	2	7	14,14,15	0.25	0	17,19,21	0.49	0
7	BMA	A	3	7	11,11,12	0.67	0	15,15,17	0.82	0
7	MAN	A	4	7	11,11,12	1.31	3 (27%)	15,15,17	1.57	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	A	5	7	11,11,12	0.87	0	15,15,17	1.41	2 (13%)
7	MAN	A	6	7	11,11,12	0.63	0	15,15,17	1.15	2 (13%)
7	MAN	A	7	7	11,11,12	1.57	3 (27%)	15,15,17	2.09	3 (20%)
8	NAG	C	1	5,8	14,14,15	0.40	0	17,19,21	0.51	0
8	NAG	C	2	8	14,14,15	0.31	0	17,19,21	0.39	0
9	NAG	F	1	5,9	14,14,15	0.68	1 (7%)	17,19,21	0.64	0
9	NAG	F	2	9	14,14,15	0.19	0	17,19,21	0.74	0
9	BMA	F	3	9	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
9	MAN	F	4	9	11,11,12	0.65	0	15,15,17	1.07	2 (13%)
9	MAN	F	5	9	11,11,12	0.73	0	15,15,17	0.91	1 (6%)
9	MAN	F	6	9	11,11,12	0.63	0	15,15,17	1.06	2 (13%)
9	MAN	F	7	9	11,11,12	0.66	0	15,15,17	1.00	2 (13%)
10	NAG	I	1	5,10	14,14,15	0.20	0	17,19,21	0.79	0
10	NAG	I	2	10	14,14,15	0.23	0	17,19,21	0.44	0
10	BMA	I	3	10	11,11,12	0.66	0	15,15,17	0.74	0
10	MAN	I	4	10	11,11,12	0.91	1 (9%)	15,15,17	0.88	1 (6%)
10	MAN	I	5	10	11,11,12	0.61	0	15,15,17	1.00	2 (13%)
10	MAN	I	6	10	11,11,12	0.68	0	15,15,17	1.01	2 (13%)
11	NAG	J	1	5,11	14,14,15	0.23	0	17,19,21	0.50	0
11	NAG	J	2	11	14,14,15	0.27	0	17,19,21	0.53	0
11	BMA	J	3	11	11,11,12	0.99	0	15,15,17	0.95	0
11	MAN	J	4	11	11,11,12	0.83	0	15,15,17	1.07	2 (13%)
11	MAN	J	5	11	11,11,12	0.66	0	15,15,17	1.10	2 (13%)
8	NAG	K	1	5,8	14,14,15	0.98	1 (7%)	17,19,21	0.78	0
8	NAG	K	2	8	14,14,15	0.34	0	17,19,21	0.46	0
11	NAG	M	1	11	14,14,15	0.62	1 (7%)	17,19,21	0.55	0
11	NAG	M	2	11	14,14,15	0.24	0	17,19,21	0.41	0
11	BMA	M	3	11	11,11,12	0.66	0	15,15,17	0.65	0
11	MAN	M	4	11	11,11,12	0.66	0	15,15,17	1.08	2 (13%)
11	MAN	M	5	11	11,11,12	0.73	0	15,15,17	1.00	2 (13%)
11	NAG	N	1	5,11	14,14,15	0.90	1 (7%)	17,19,21	0.54	0
11	NAG	N	2	11	14,14,15	0.41	0	17,19,21	0.38	0
11	BMA	N	3	11	11,11,12	0.58	0	15,15,17	0.63	0
11	MAN	N	4	11	11,11,12	0.76	0	15,15,17	1.24	2 (13%)
11	MAN	N	5	11	11,11,12	0.69	0	15,15,17	0.96	2 (13%)
11	NAG	O	1	5,11	14,14,15	0.34	0	17,19,21	0.56	0
11	NAG	O	2	11	14,14,15	0.33	0	17,19,21	0.42	0
11	BMA	O	3	11	11,11,12	0.73	0	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	MAN	O	4	11	11,11,12	0.74	1 (9%)	15,15,17	1.19	2 (13%)
11	MAN	O	5	11	11,11,12	0.72	0	15,15,17	0.99	2 (13%)
12	NAG	P	1	5,12	14,14,15	0.33	0	17,19,21	0.67	0
12	NAG	P	2	12	14,14,15	0.25	0	17,19,21	0.46	0
12	BMA	P	3	12	11,11,12	0.69	0	15,15,17	0.67	0
12	MAN	P	4	12	11,11,12	0.69	0	15,15,17	1.13	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
7	NAG	A	1	5,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	3/6/23/26	0/1/1/1
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	0/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
7	MAN	A	7	7	-	2/2/19/22	0/1/1/1
8	NAG	C	1	5,8	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
9	NAG	F	1	5,9	-	2/6/23/26	0/1/1/1
9	NAG	F	2	9	-	0/6/23/26	0/1/1/1
9	BMA	F	3	9	-	2/2/19/22	0/1/1/1
9	MAN	F	4	9	-	0/2/19/22	0/1/1/1
9	MAN	F	5	9	-	1/2/19/22	0/1/1/1
9	MAN	F	6	9	-	0/2/19/22	0/1/1/1
9	MAN	F	7	9	-	0/2/19/22	0/1/1/1
10	NAG	I	1	5,10	-	2/6/23/26	0/1/1/1
10	NAG	I	2	10	-	4/6/23/26	0/1/1/1
10	BMA	I	3	10	-	1/2/19/22	0/1/1/1
10	MAN	I	4	10	-	0/2/19/22	0/1/1/1
10	MAN	I	5	10	-	0/2/19/22	0/1/1/1
10	MAN	I	6	10	-	0/2/19/22	0/1/1/1
11	NAG	J	1	5,11	-	2/6/23/26	0/1/1/1
11	NAG	J	2	11	-	0/6/23/26	0/1/1/1
11	BMA	J	3	11	-	1/2/19/22	0/1/1/1
11	MAN	J	4	11	-	1/2/19/22	0/1/1/1
11	MAN	J	5	11	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	K	1	5,8	-	0/6/23/26	0/1/1/1
8	NAG	K	2	8	-	1/6/23/26	0/1/1/1
11	NAG	M	1	11	-	2/6/23/26	0/1/1/1
11	NAG	M	2	11	-	2/6/23/26	0/1/1/1
11	BMA	M	3	11	-	0/2/19/22	0/1/1/1
11	MAN	M	4	11	-	0/2/19/22	0/1/1/1
11	MAN	M	5	11	-	1/2/19/22	0/1/1/1
11	NAG	N	1	5,11	-	3/6/23/26	0/1/1/1
11	NAG	N	2	11	-	0/6/23/26	0/1/1/1
11	BMA	N	3	11	-	0/2/19/22	0/1/1/1
11	MAN	N	4	11	-	0/2/19/22	0/1/1/1
11	MAN	N	5	11	-	0/2/19/22	0/1/1/1
11	NAG	O	1	5,11	-	2/6/23/26	0/1/1/1
11	NAG	O	2	11	-	0/6/23/26	0/1/1/1
11	BMA	O	3	11	-	0/2/19/22	0/1/1/1
11	MAN	O	4	11	-	0/2/19/22	0/1/1/1
11	MAN	O	5	11	-	0/2/19/22	0/1/1/1
12	NAG	P	1	5,12	-	1/6/23/26	0/1/1/1
12	NAG	P	2	12	-	2/6/23/26	0/1/1/1
12	BMA	P	3	12	-	1/2/19/22	0/1/1/1
12	MAN	P	4	12	-	0/2/19/22	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	1	NAG	O5-C1	-3.52	1.37	1.43
7	A	7	MAN	C1-C2	3.49	1.60	1.52
7	A	7	MAN	O5-C1	3.18	1.49	1.43
11	N	1	NAG	O5-C1	-3.05	1.38	1.43
7	A	4	MAN	O5-C5	2.50	1.48	1.43

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	7	MAN	C1-O5-C5	6.86	121.37	112.19
7	A	5	MAN	C1-O5-C5	4.60	118.35	112.19
7	A	4	MAN	C1-O5-C5	4.19	117.81	112.19
7	A	4	MAN	O3-C3-C2	4.06	118.33	110.05
11	N	4	MAN	C1-O5-C5	3.75	117.21	112.19

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	J	1	NAG	O5-C5-C6-O6
11	M	1	NAG	O5-C5-C6-O6
11	N	1	NAG	O5-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
11	N	1	NAG	C4-C5-C6-O6

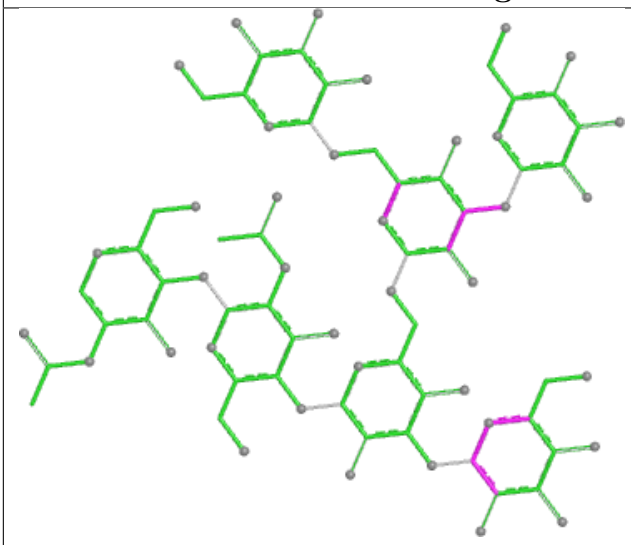
There are no ring outliers.

18 monomers are involved in 22 short contacts:

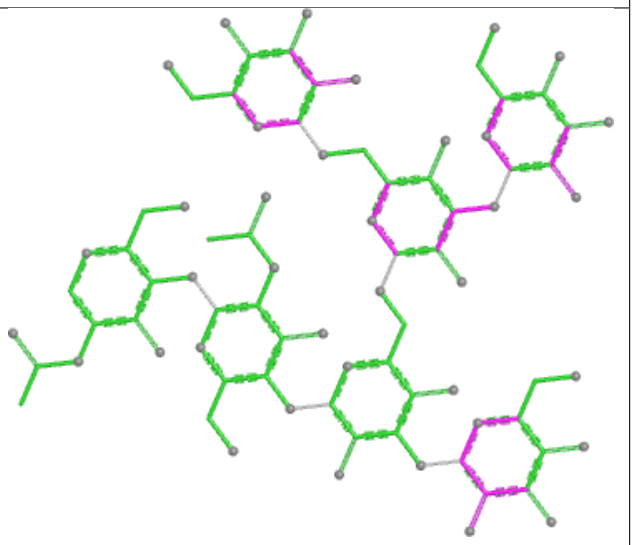
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	4	MAN	1	0
9	F	5	MAN	1	0
10	I	2	NAG	2	0
8	C	1	NAG	4	0
8	C	2	NAG	1	0
10	I	3	BMA	2	0
11	J	2	NAG	1	0
11	J	3	BMA	1	0
12	P	1	NAG	1	0
10	I	5	MAN	1	0
10	I	4	MAN	3	0
7	A	2	NAG	1	0
9	F	1	NAG	3	0
10	I	1	NAG	3	0
11	O	1	NAG	2	0
11	M	1	NAG	1	0
8	K	2	NAG	1	0
8	K	1	NAG	1	0

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

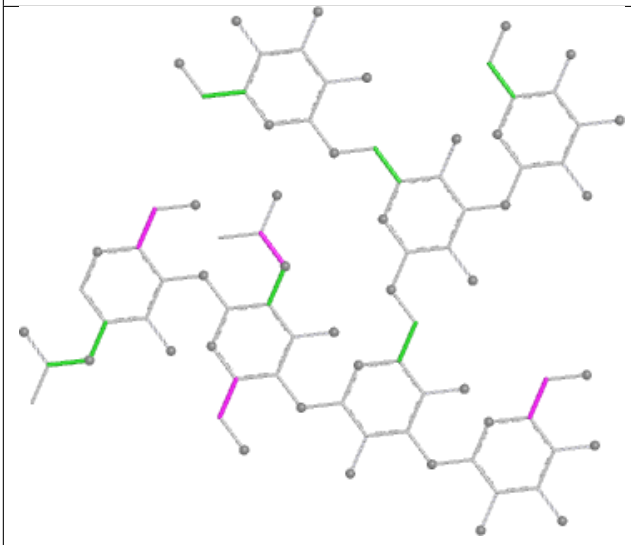
Oligosaccharide Chain A



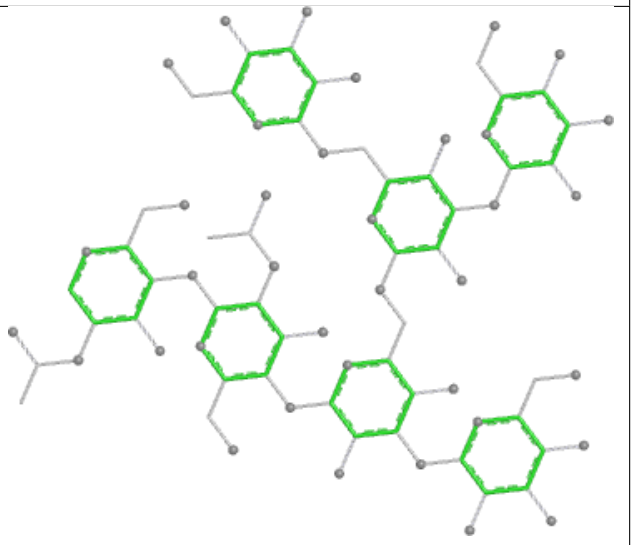
Bond lengths



Bond angles

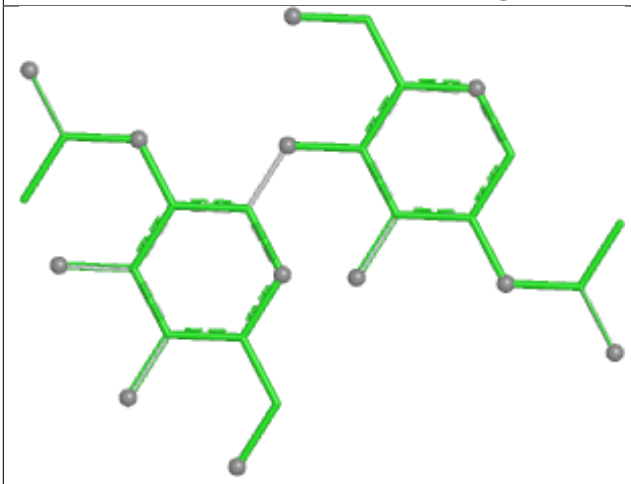


Torsions

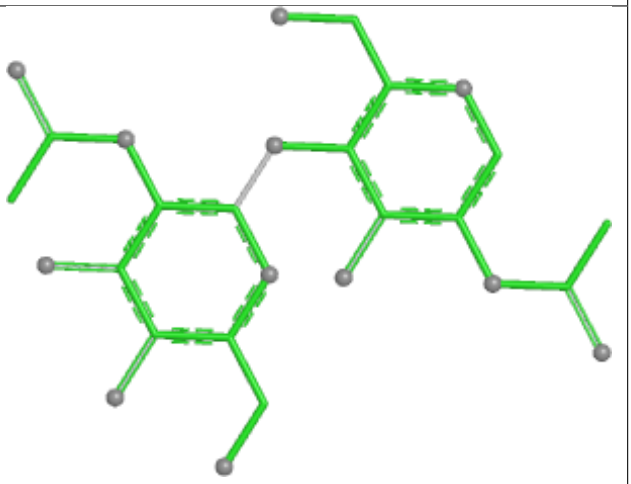


Rings

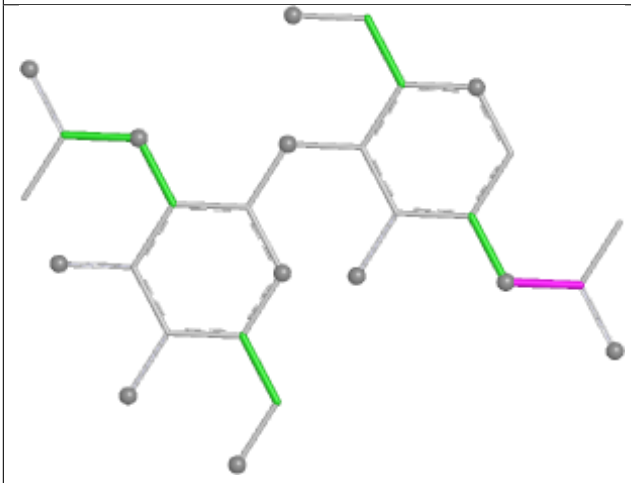
Oligosaccharide Chain C



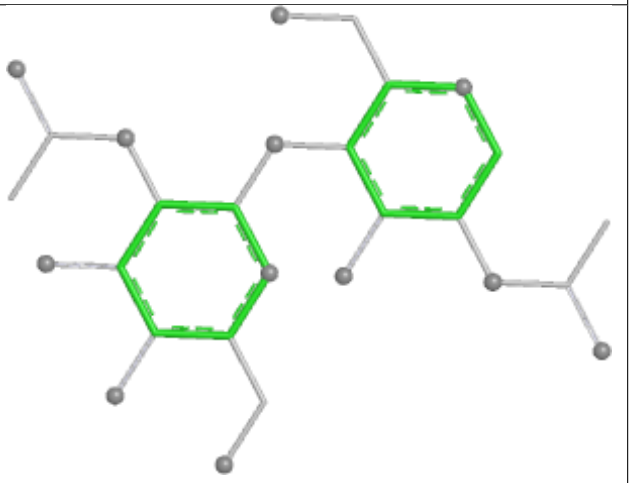
Bond lengths



Bond angles

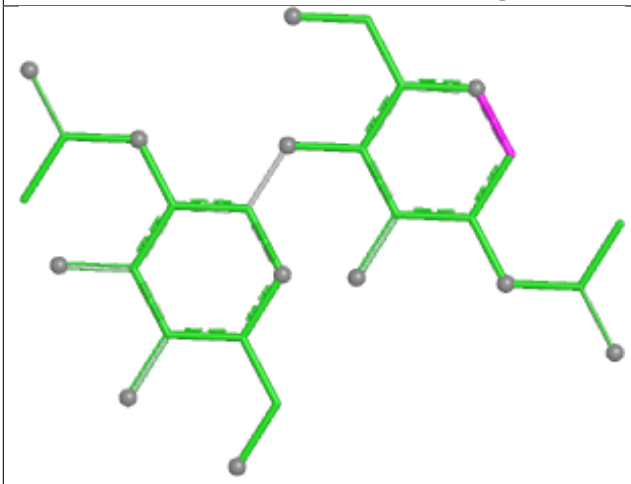


Torsions

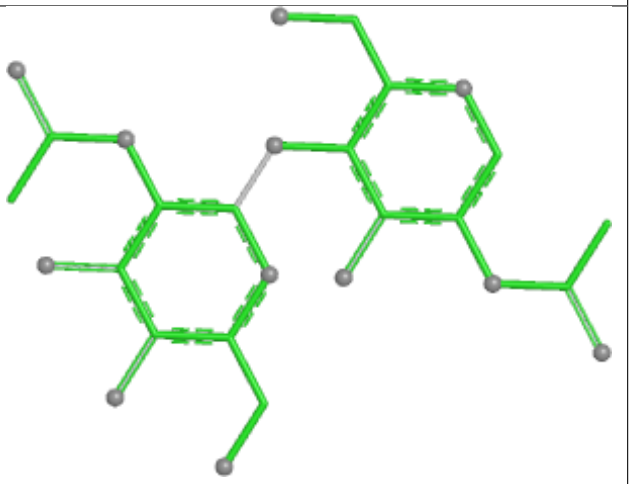


Rings

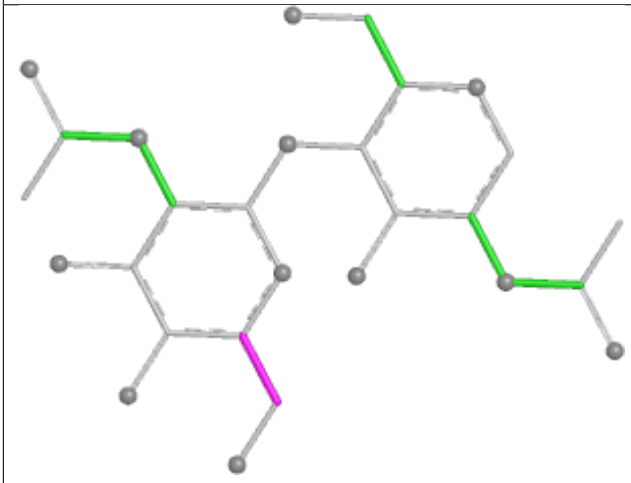
Oligosaccharide Chain K



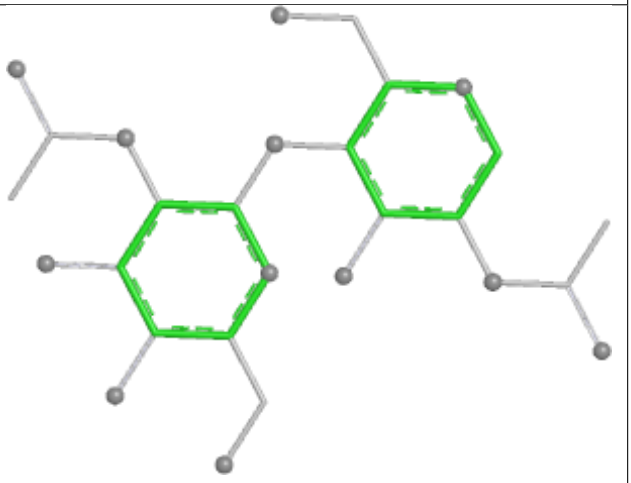
Bond lengths



Bond angles

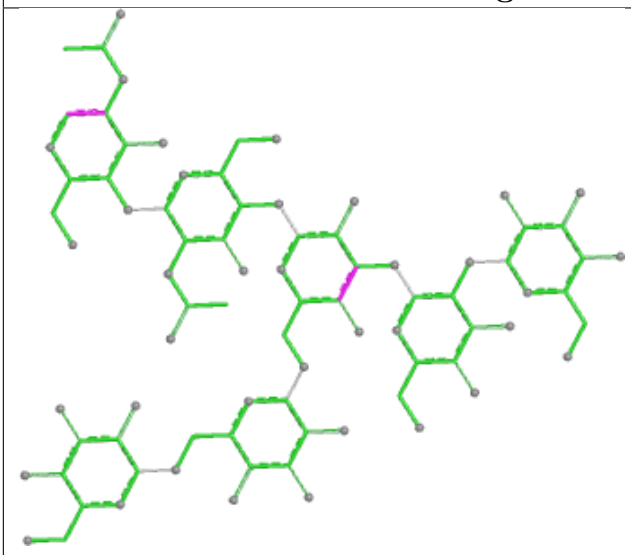


Torsions

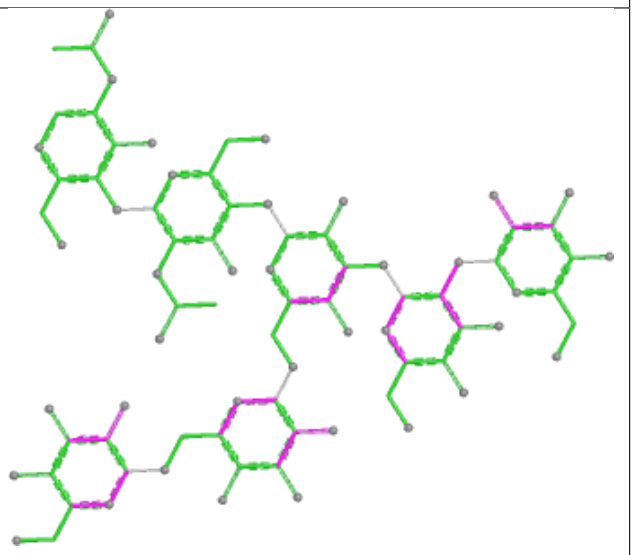


Rings

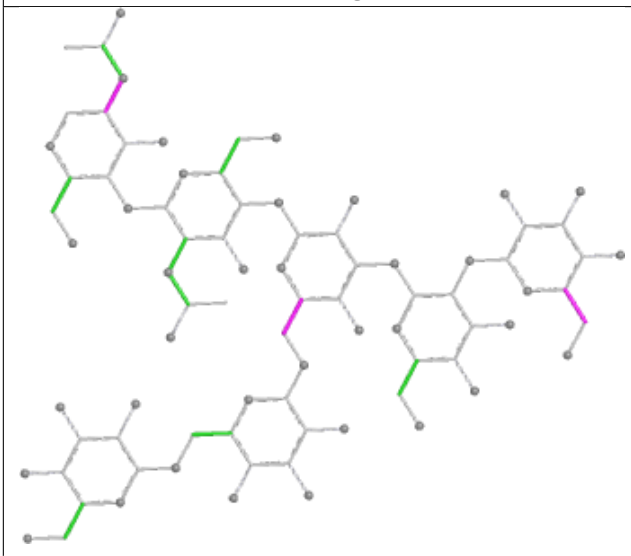
Oligosaccharide Chain F



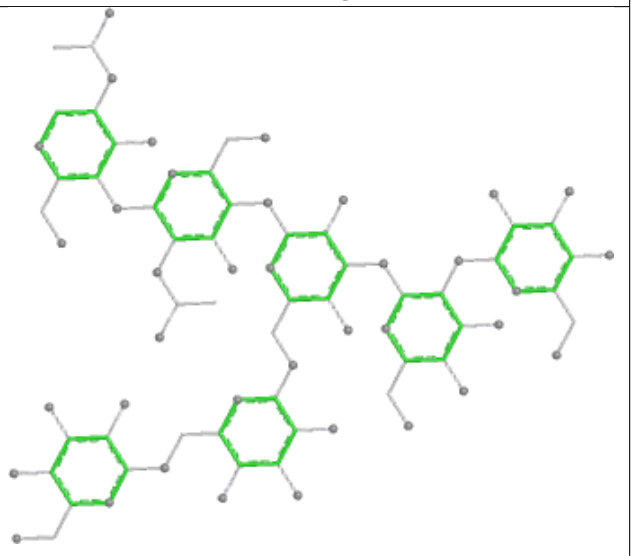
Bond lengths



Bond angles

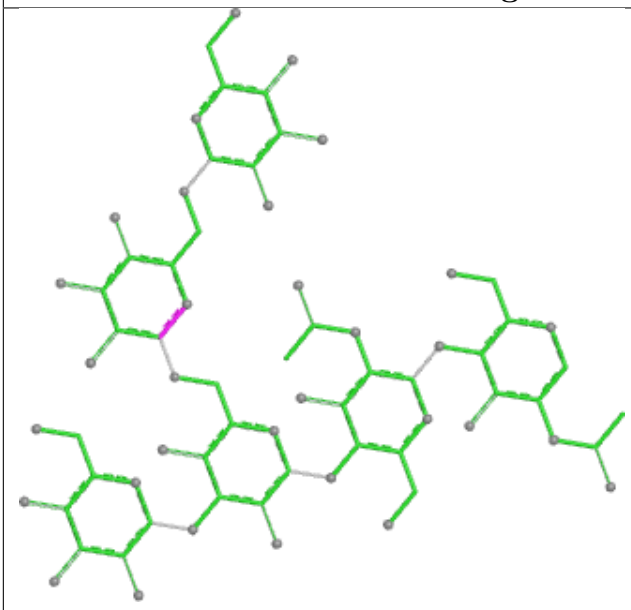


Torsions

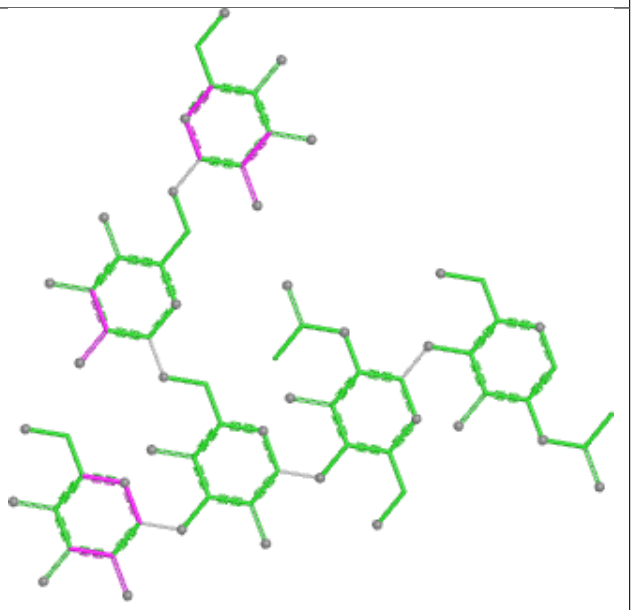


Rings

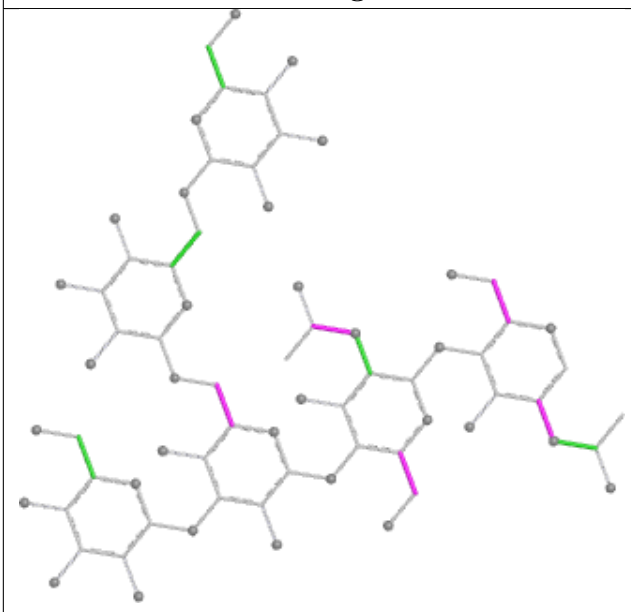
Oligosaccharide Chain I



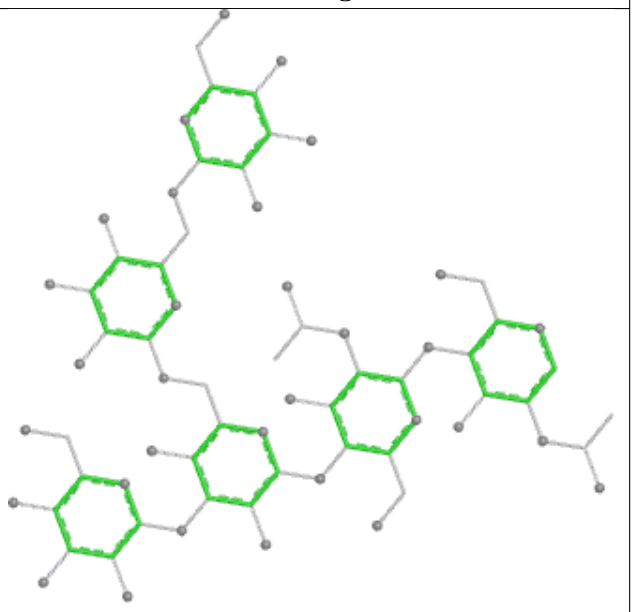
Bond lengths



Bond angles

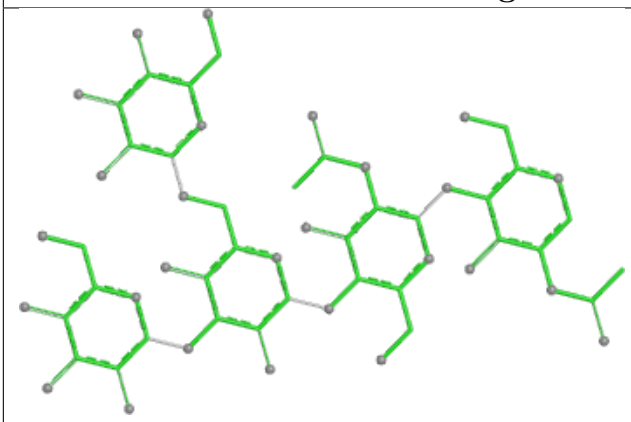


Torsions

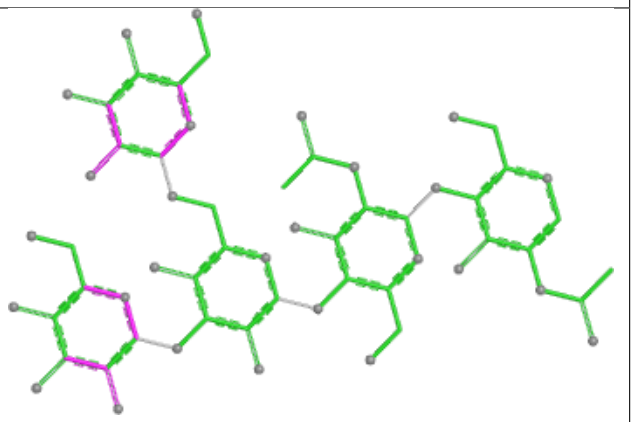


Rings

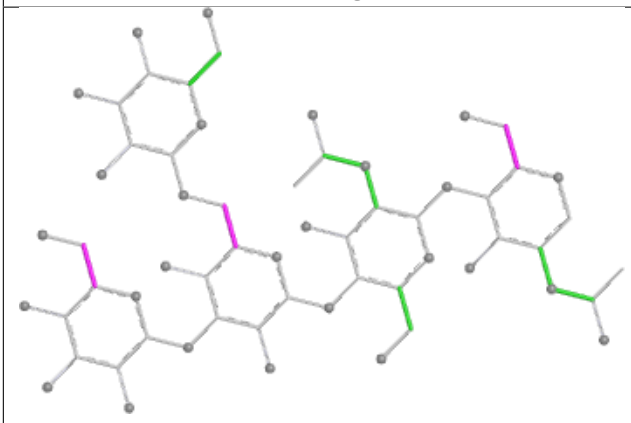
Oligosaccharide Chain J



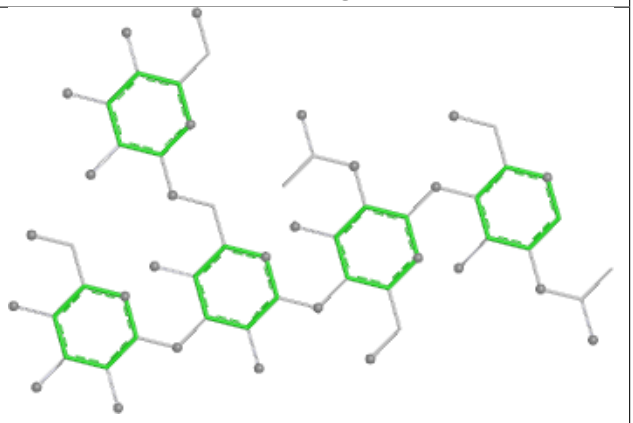
Bond lengths



Bond angles

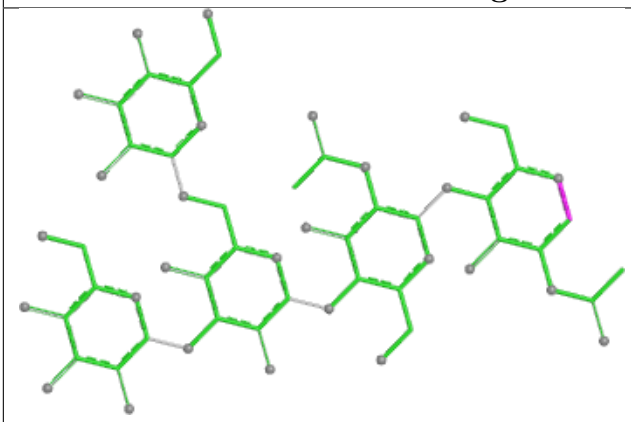


Torsions

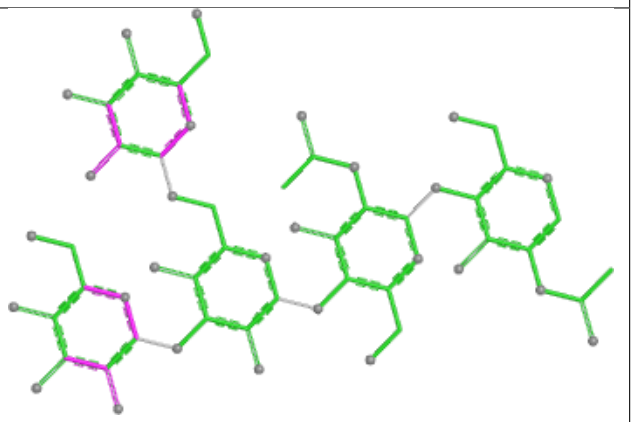


Rings

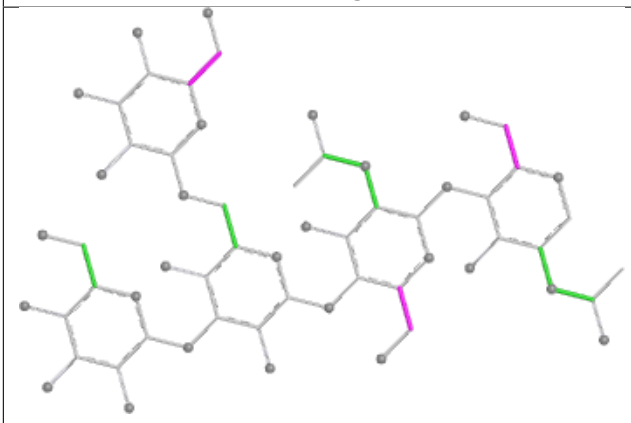
Oligosaccharide Chain M



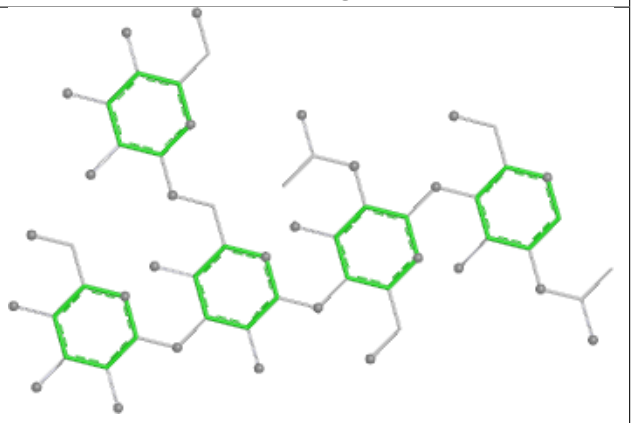
Bond lengths



Bond angles

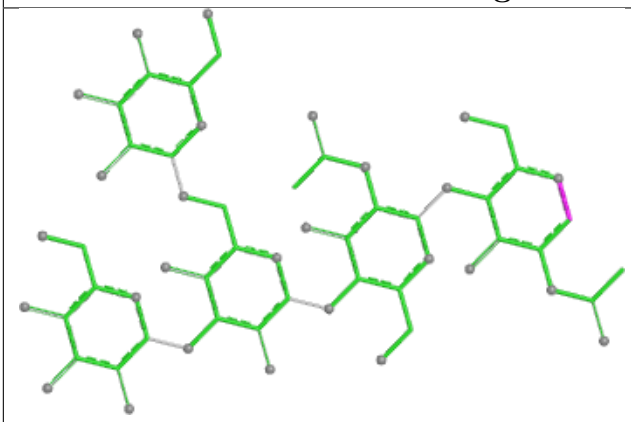


Torsions

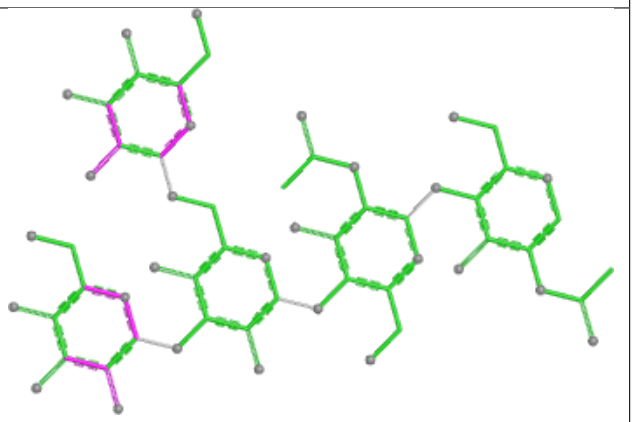


Rings

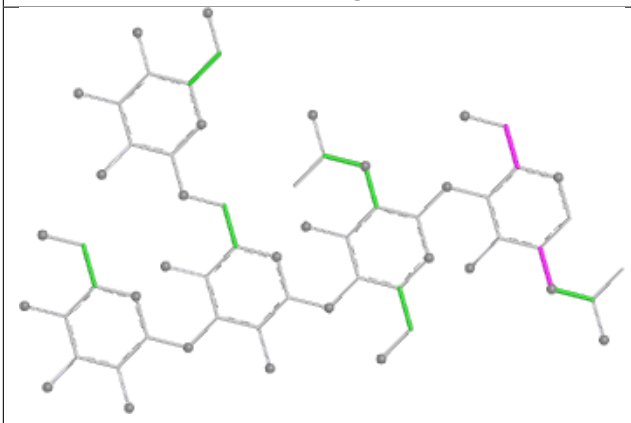
Oligosaccharide Chain N



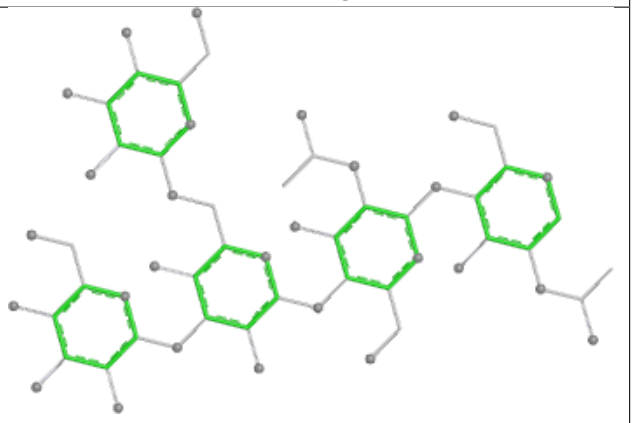
Bond lengths



Bond angles

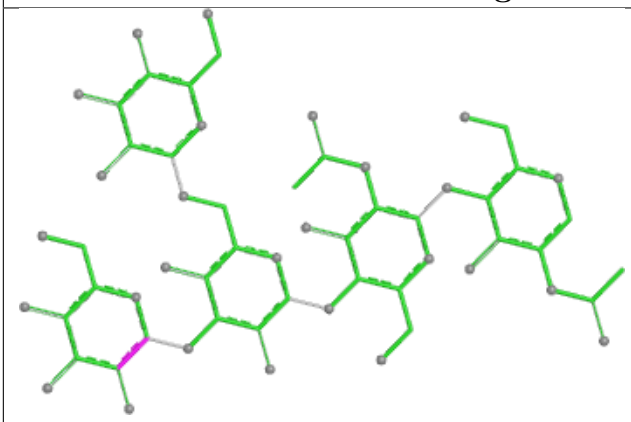


Torsions

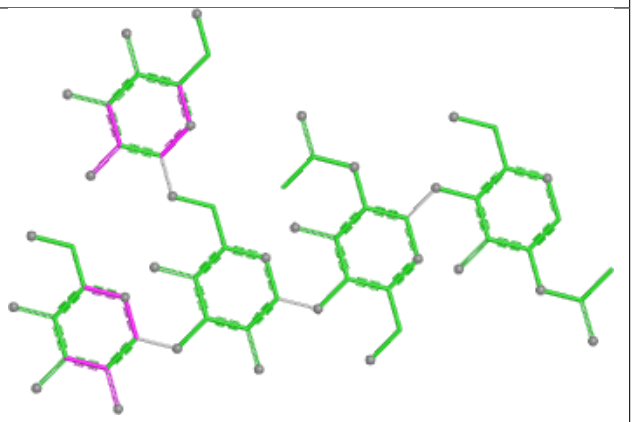


Rings

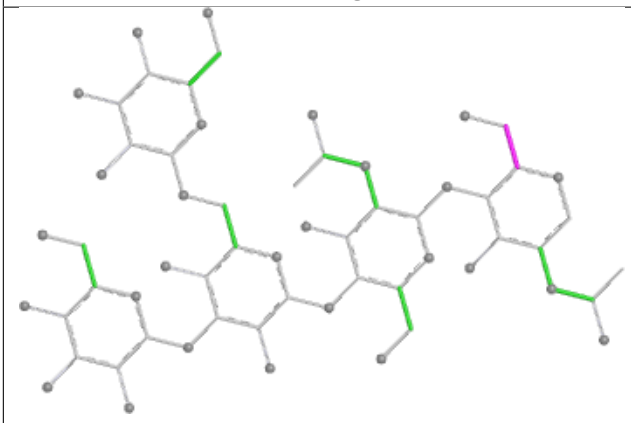
Oligosaccharide Chain O



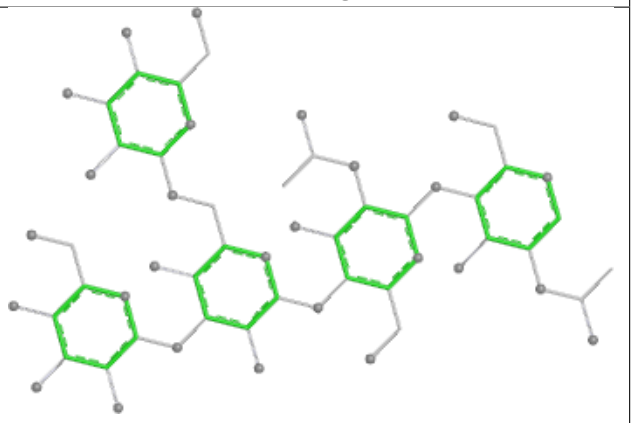
Bond lengths



Bond angles

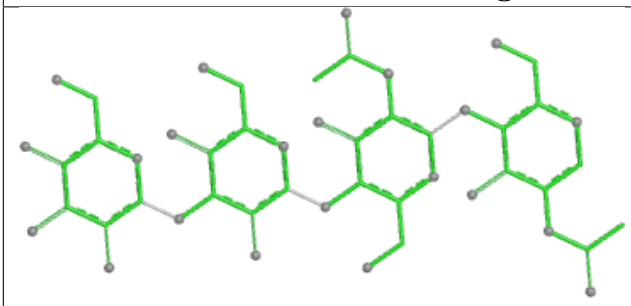


Torsions

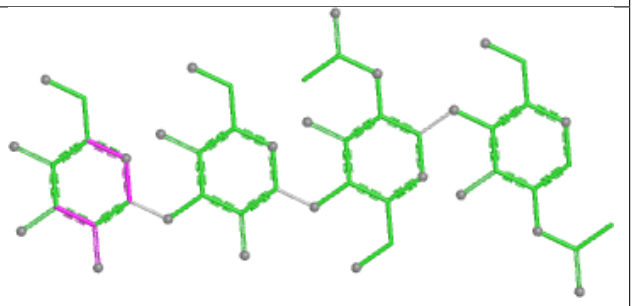


Rings

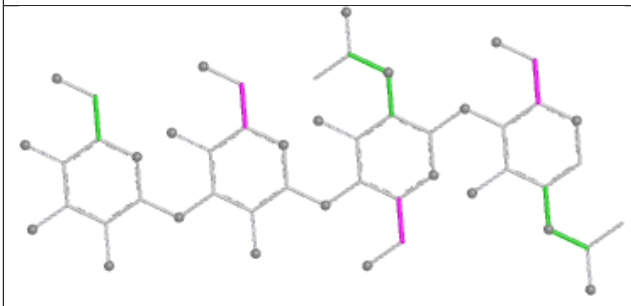
Oligosaccharide Chain P



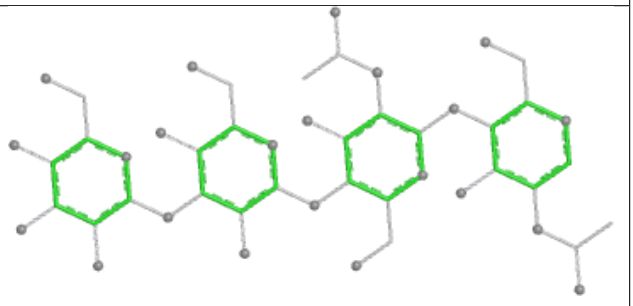
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
13	NAG	G	601	-	14,14,15	0.26	0	17,19,21	0.44	0
13	NAG	G	604	5	14,14,15	0.56	0	17,19,21	0.62	0
13	NAG	G	603	5	14,14,15	0.19	0	17,19,21	0.66	1 (5%)
13	NAG	G	602	5	14,14,15	0.57	0	17,19,21	0.51	0
13	NAG	G	605	5	14,14,15	0.32	0	17,19,21	0.46	0
13	NAG	B	701	6	14,14,15	0.24	0	17,19,21	0.37	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
13	NAG	G	601	-	-	4/6/23/26	0/1/1/1
13	NAG	G	604	5	-	2/6/23/26	0/1/1/1
13	NAG	G	603	5	-	2/6/23/26	0/1/1/1
13	NAG	G	602	5	-	2/6/23/26	0/1/1/1
13	NAG	G	605	5	-	0/6/23/26	0/1/1/1
13	NAG	B	701	6	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	603	NAG	C1-O5-C5	2.22	115.16	112.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	602	NAG	O5-C5-C6-O6
13	G	601	NAG	O5-C5-C6-O6
13	G	602	NAG	C4-C5-C6-O6
13	G	603	NAG	O5-C5-C6-O6
13	G	601	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	601	NAG	1	0
13	G	604	NAG	1	0
13	G	602	NAG	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	G	2
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	397:SER	C	409:GLY	N	6.35
1	H	125:PRO	C	130:THR	N	4.59
1	G	143:ARG	C	152:GLY	N	3.06

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	D	128/128 (100%)	0.79	21 (16%) 4 10	320, 381, 430, 447	0
2	E	111/111 (100%)	0.66	12 (10%) 11 15	318, 372, 411, 428	0
3	H	225/225 (100%)	0.45	21 (9%) 14 18	264, 345, 405, 445	0
4	L	213/213 (100%)	0.58	21 (9%) 13 17	274, 353, 397, 447	0
5	G	455/455 (100%)	1.12	91 (20%) 3 7	260, 349, 459, 544	0
6	B	146/146 (100%)	1.41	37 (25%) 1 5	268, 337, 462, 504	0
All	All	1278/1278 (100%)	0.87	203 (15%) 5 10	260, 356, 438, 544	0

The worst 5 of 203 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	G	507	GLY	8.4
5	G	364	SER	8.1
6	B	601	LYS	6.0
6	B	546	SER	6.0
6	B	663	LEU	5.9

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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
7	NAG	A	1	14/15	-	-	291,365,390,442	0
7	NAG	A	2	14/15	-	-	335,380,428,475	0
7	BMA	A	3	11/12	-	-	333,381,439,491	0
7	MAN	A	4	11/12	-	-	380,421,455,486	0
7	MAN	A	5	11/12	-	-	330,396,499,511	0
7	MAN	A	6	11/12	-	-	305,421,468,521	0
7	MAN	A	7	11/12	-	-	262,365,470,475	0
8	NAG	C	1	14/15	-	-	281,419,481,529	0
8	NAG	C	2	14/15	-	-	353,384,441,450	0
10	MAN	I	6	11/12	0.04	0.17	339,364,451,493	0
11	MAN	J	4	11/12	0.17	0.21	414,473,552,566	0
9	NAG	F	1	14/15	-	-	341,403,549,549	0
9	NAG	F	2	14/15	-	-	395,425,543,556	0
9	BMA	F	3	11/12	-	-	475,519,556,583	0
9	MAN	F	4	11/12	-	-	501,532,557,561	0
9	MAN	F	5	11/12	-	-	407,476,533,537	0
9	MAN	F	6	11/12	-	-	438,466,551,574	0
9	MAN	F	7	11/12	-	-	465,531,569,582	0
10	BMA	I	3	11/12	0.29	0.12	332,380,447,460	0
11	NAG	O	2	14/15	0.33	0.16	374,453,512,642	0
12	BMA	P	3	11/12	0.35	0.13	350,454,547,591	0
10	MAN	I	5	11/12	0.36	0.15	422,487,555,576	0
11	BMA	O	3	11/12	0.44	0.13	483,528,564,574	0
11	MAN	M	4	11/12	0.49	0.14	374,409,521,701	0
11	MAN	N	5	11/12	0.53	0.12	379,452,504,514	0
11	NAG	N	2	14/15	0.54	0.21	371,476,569,771	0
11	NAG	O	1	14/15	0.57	0.23	302,400,467,480	0
8	NAG	K	2	14/15	0.61	0.13	274,409,464,516	0
11	MAN	O	4	11/12	0.64	0.11	447,503,575,590	0
11	MAN	M	5	11/12	0.65	0.26	412,435,476,491	0
11	BMA	N	3	11/12	0.65	0.08	461,507,551,590	0
11	MAN	O	5	11/12	0.66	0.17	359,482,504,537	0
11	MAN	N	4	11/12	0.69	0.10	441,503,566,572	0
12	MAN	P	4	11/12	0.69	0.09	389,468,554,586	0
11	NAG	M	2	14/15	0.71	0.19	348,424,459,717	0
10	MAN	I	4	11/12	0.71	0.15	336,468,517,521	0
10	NAG	I	2	14/15	0.72	0.17	297,346,411,440	0
8	NAG	K	1	14/15	0.74	0.16	295,374,407,413	0
10	NAG	I	1	14/15	0.80	0.18	277,305,398,430	0
11	MAN	J	5	11/12	0.80	0.16	434,453,480,496	0
11	NAG	N	1	14/15	0.81	0.27	370,426,514,562	0
12	NAG	P	2	14/15	0.82	0.23	344,443,549,815	0
11	BMA	J	3	11/12	0.84	0.13	444,542,560,585	0

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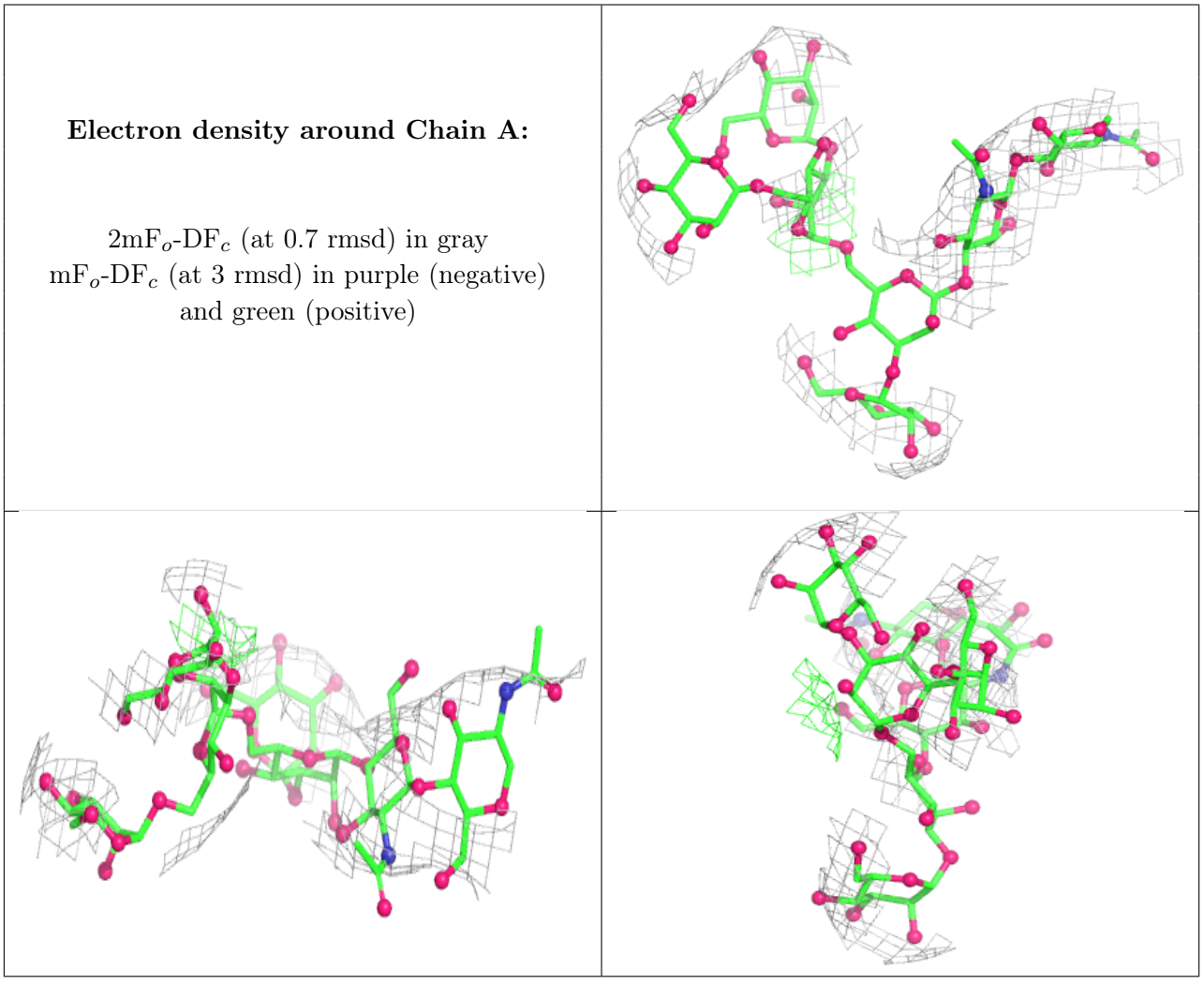
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	BMA	M	3	11/12	0.87	0.10	403,430,509,570	0
11	NAG	M	1	14/15	0.88	0.21	262,354,506,523	0
11	NAG	J	2	14/15	0.91	0.16	389,491,532,547	0
11	NAG	J	1	14/15	0.93	0.17	306,430,476,521	0
12	NAG	P	1	14/15	0.95	0.15	321,402,480,490	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.

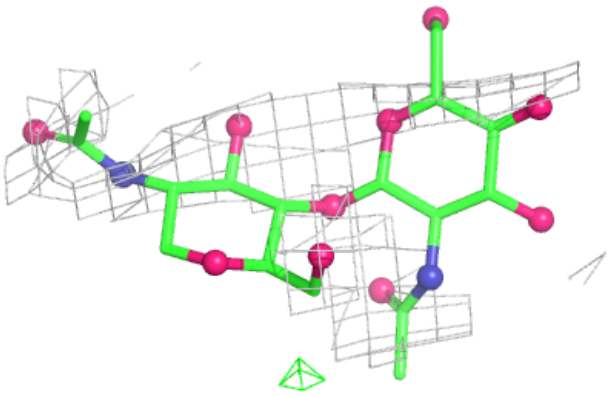
Electron density around Chain A:

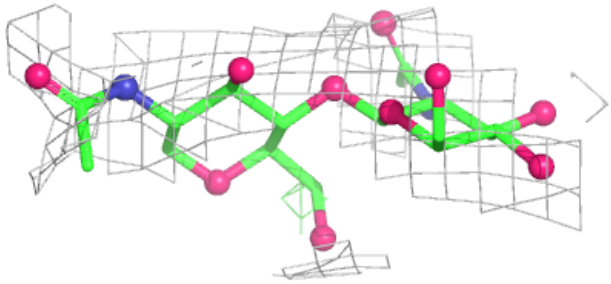
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

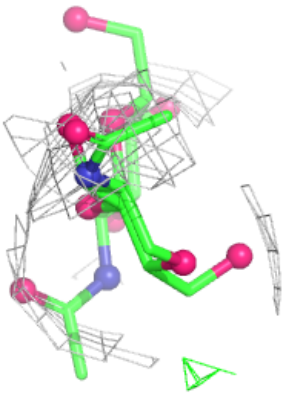


Electron density around Chain C:

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

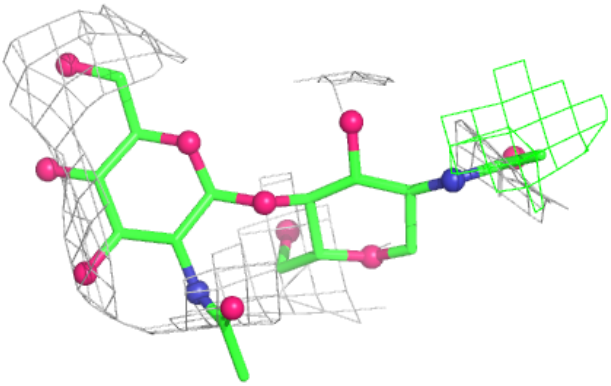


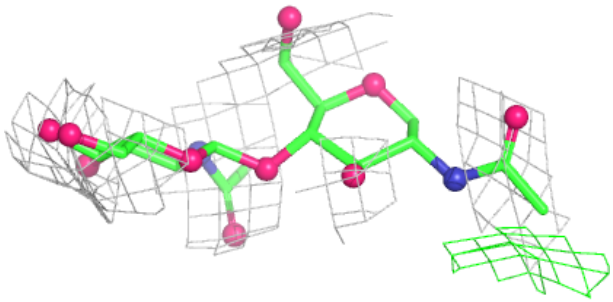


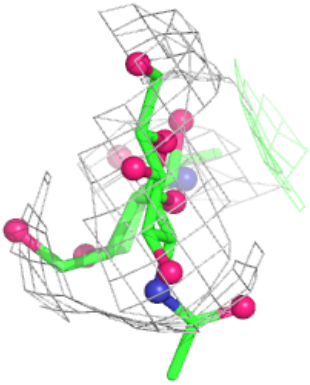


Electron density around Chain K:

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

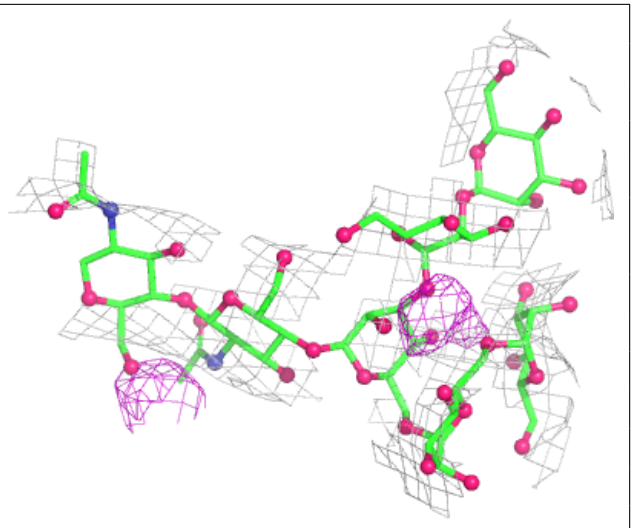


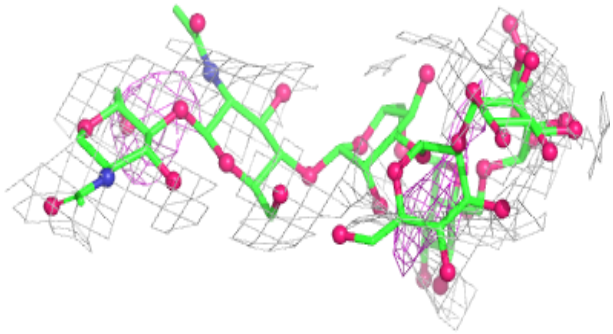


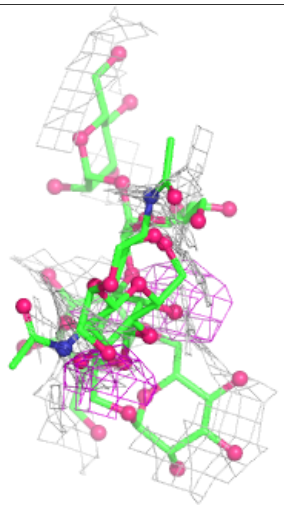


Electron density around Chain F:

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

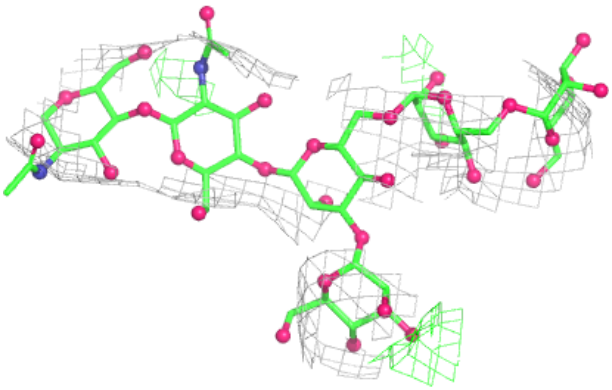


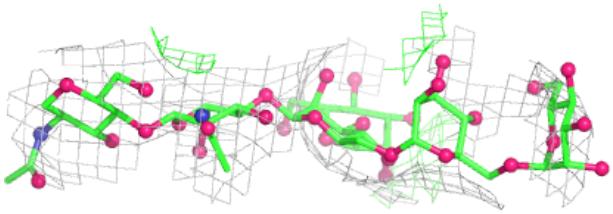


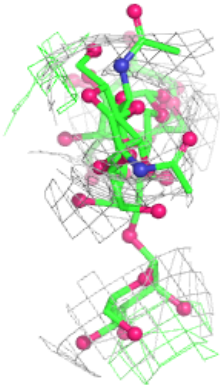


Electron density around Chain I:

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

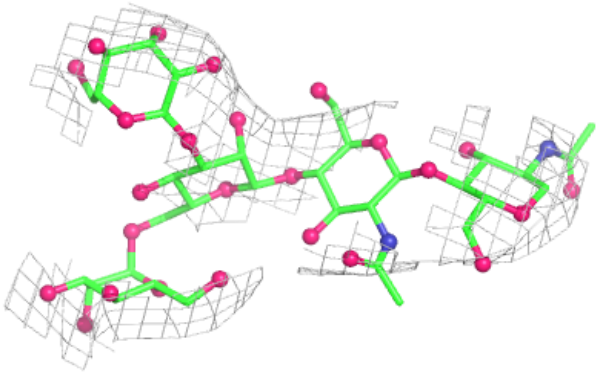


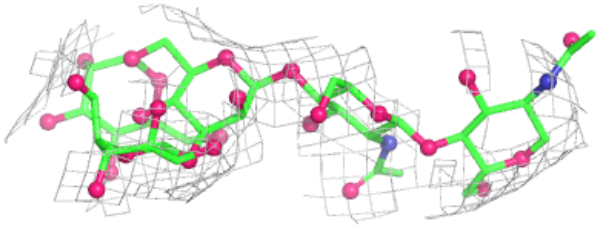


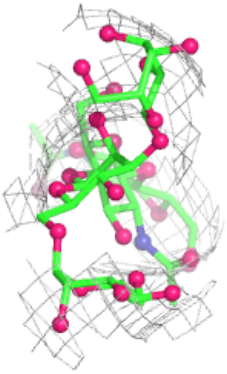


Electron density around Chain J:

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

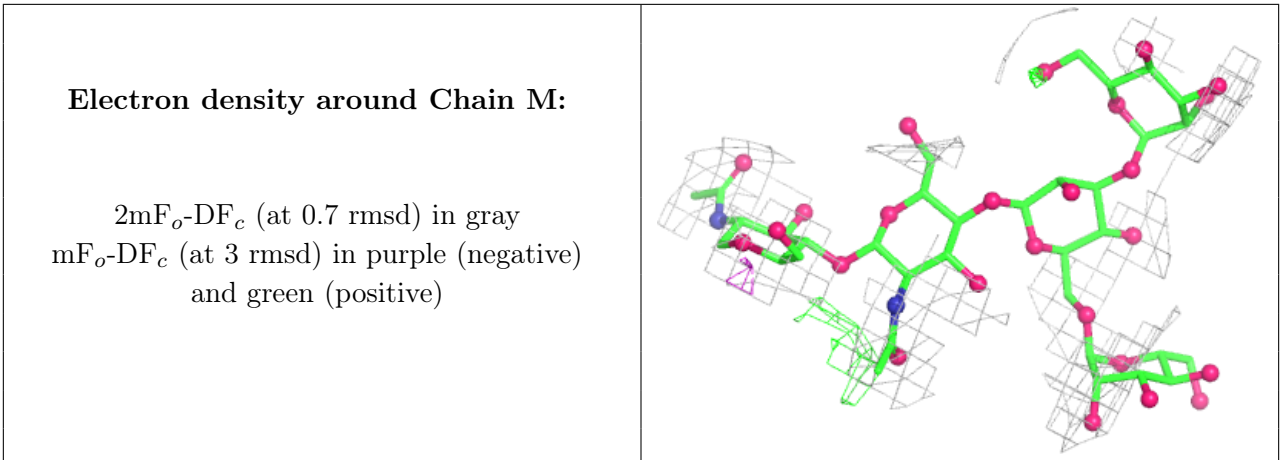


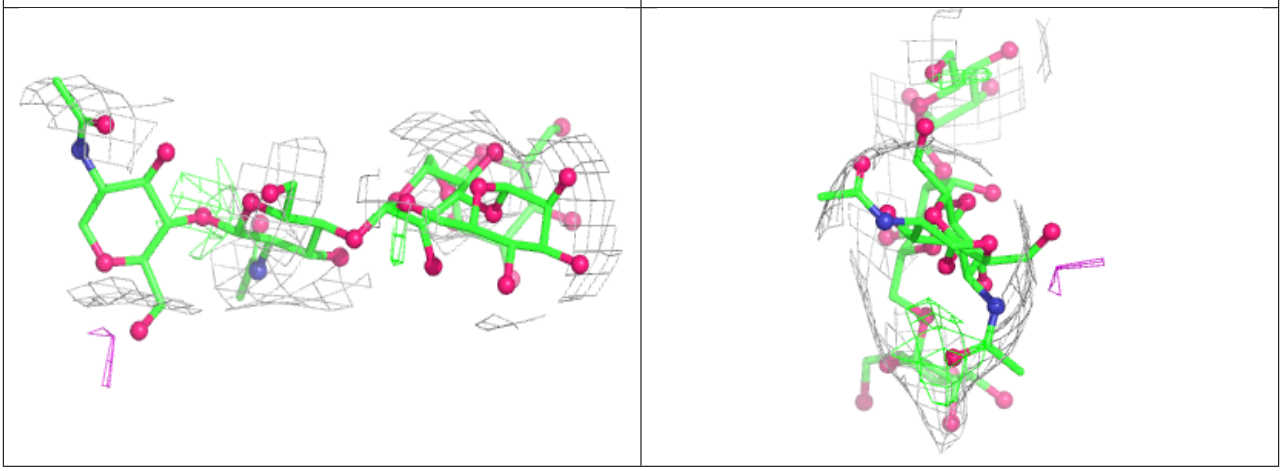




Electron density around Chain M:

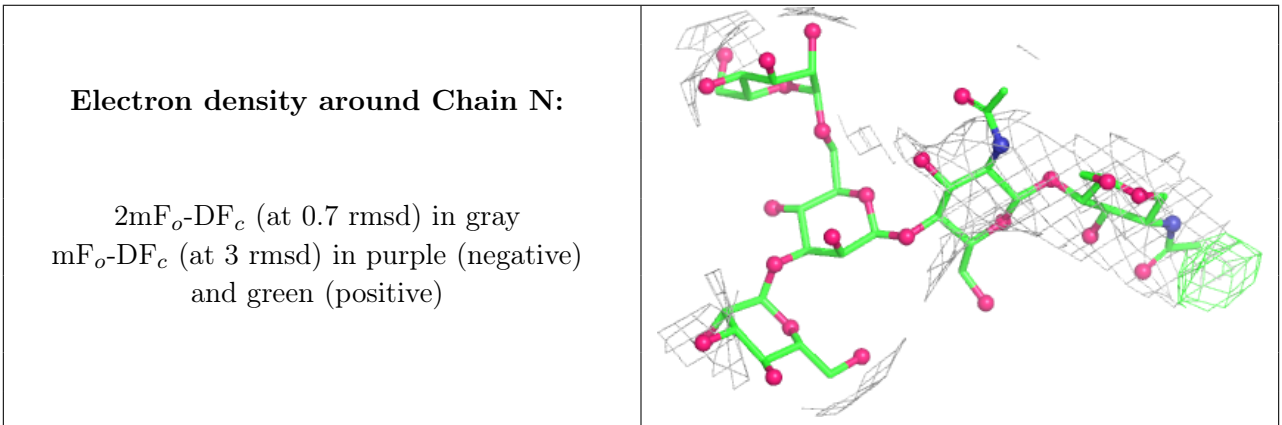
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

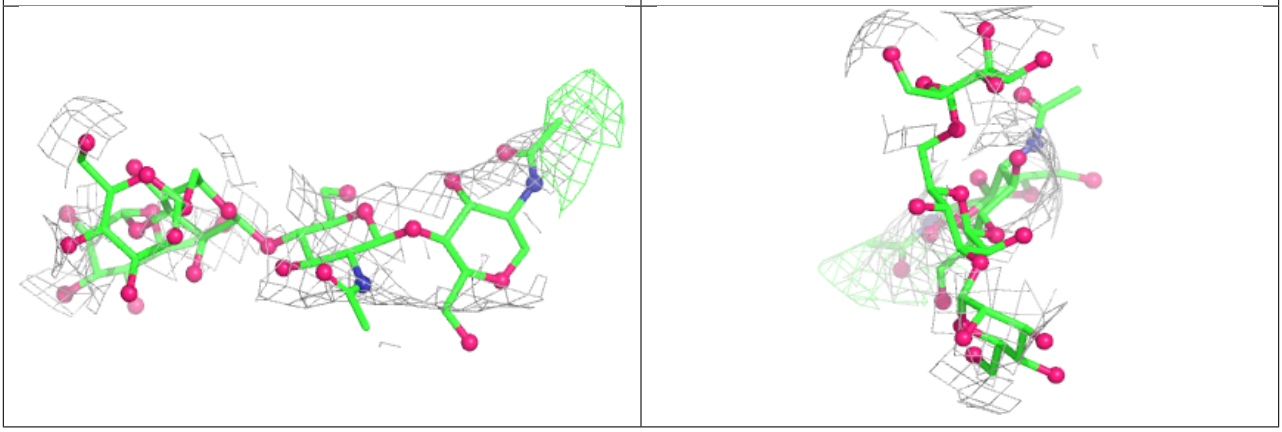




Electron density around Chain N:

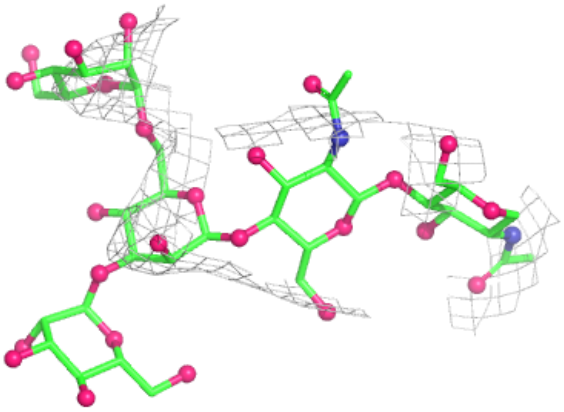
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

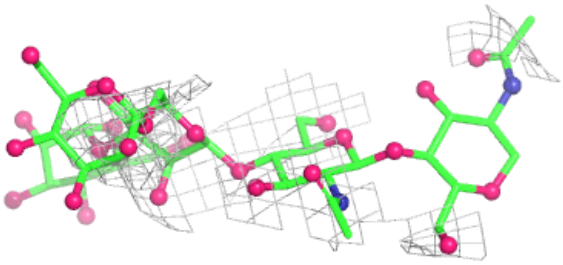


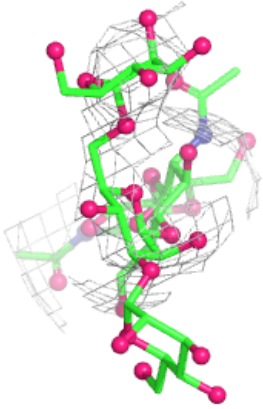


Electron density around Chain O:

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

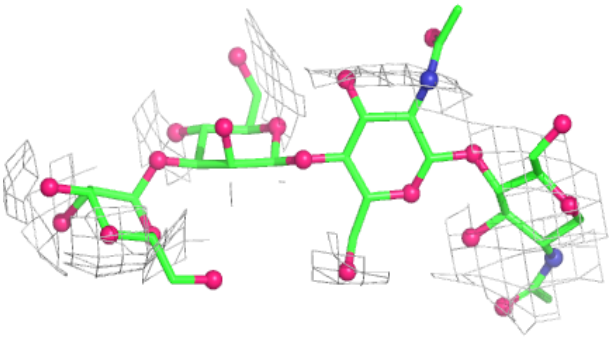


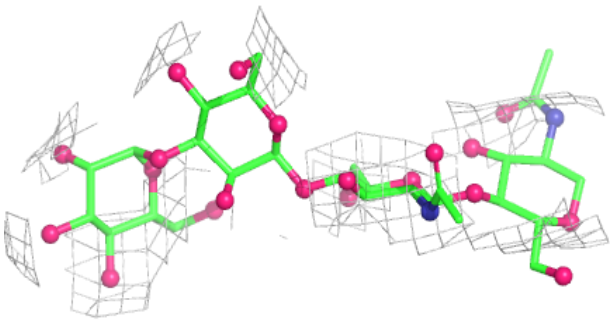


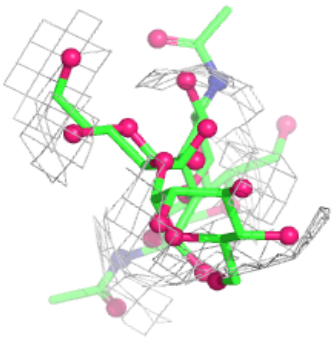


Electron density around Chain P:

$2mF_o$-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, 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
13	NAG	G	605	14/15	0.37	0.13	353,500,528,530	0
13	NAG	G	604	14/15	0.60	0.19	369,441,500,504	0
13	NAG	G	603	14/15	0.60	0.18	304,397,434,449	0
13	NAG	G	601	14/15	0.75	0.17	376,414,478,494	0
13	NAG	G	602	14/15	0.80	0.27	297,449,488,493	0
13	NAG	B	701	14/15	0.81	0.13	312,385,476,484	0

6.5 Other polymers

There are no such residues in this entry.