wwPDB X-ray Structure Validation Summary Report (i)

May 27, 2024 – 08:25 PM EDT

PDB ID	:	6MCO
Title	:	Crystal structure of the B41 SOSIP.664 Env trimer with PGT124 and 35O22 Fabs, in P23 space group
Authors	:	Kumar, S.; Sarkar, A.; Wilson, I.A.
Deposited on	:	2018-08-31
Resolution	:	3.53 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:

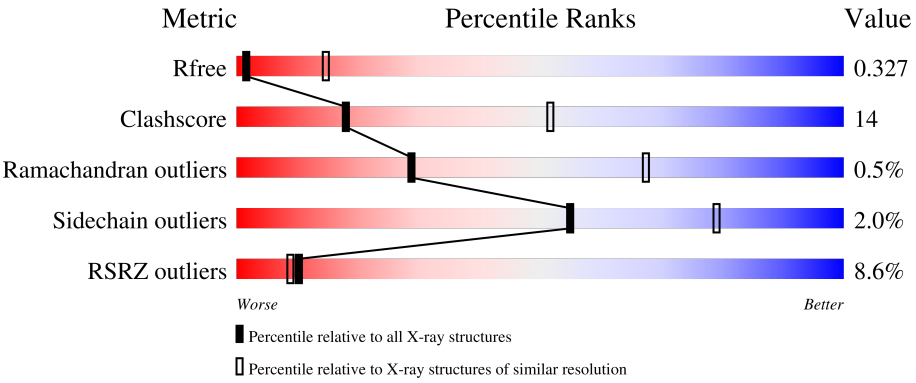
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.53 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	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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	B	153	3% 66% 20% • 13%
2	D	243	14% 79% 20% •
3	E	216	5% 84% 14% ••
4	G	482	4% 70% 22% • 5%
5	H	236	14% 69% 28% •

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Mol	Chain	Length	Quality of chain
6	L	214	11% 78% 20%
7	A	6	17% 67% 17%
8	C	2	100%
8	I	2	100%
8	Q	2	50% 50%
9	F	7	86% 14%
10	J	4	50% 50%
10	M	4	75% 25%
11	K	3	33% 33% 33%
11	N	3	33% 33% 33%
11	O	3	33% 33% 33%
11	U	3	100%
12	P	8	12% 62% 25%
13	R	4	100%
14	S	5	40% 60%
15	T	3	67% 33%

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
12	MAN	P	8	-	-	-	X
16	NAG	G	650	-	-	-	X
7	MAN	A	4	-	-	-	X
7	MAN	A	5	-	-	-	X
8	NAG	C	1	-	-	-	X
8	NAG	C	2	-	-	-	X
8	NAG	Q	2	-	-	-	X
9	NAG	F	2	-	-	-	X
9	MAN	F	6	-	-	-	X

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 12268 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 Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	133	Total	C	N	O	S	0	0	0
			1058	675	178	198	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP B3UF08

- Molecule 2 is a protein called 35O22 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 3 is a protein called 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 4 is a protein called Surface protein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	456	Total	C	N	O	S	0	0	0
			3576	2244	632	674	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP B3UES2

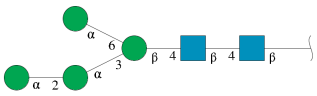
- Molecule 5 is a protein called PGT124 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	231	Total	C	N	O	S	0	0	0
			1754	1111	293	345	5			

- Molecule 6 is a protein called PGT124 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1601	1008	271	317	5			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.

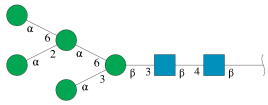


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	6	Total	C	N	O	0	0	0
			72	40	2	30			

- 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	0	0	0
			28	16	2	10			
8	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

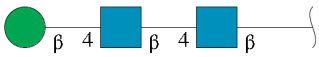


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 10 is an oligosaccharide called 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.

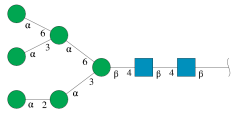
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	4	Total	C	N	O	0	0	0
			50	28	2	20			
10	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 11 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.

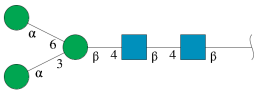


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	P	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 13 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.

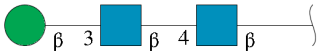
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 14 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.



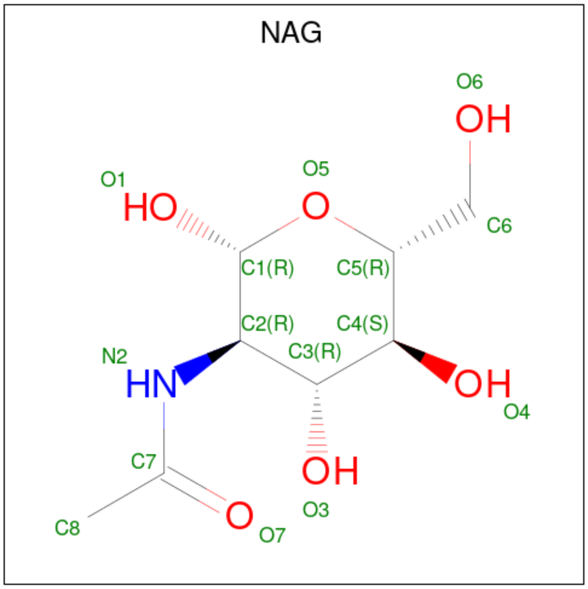
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 15 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



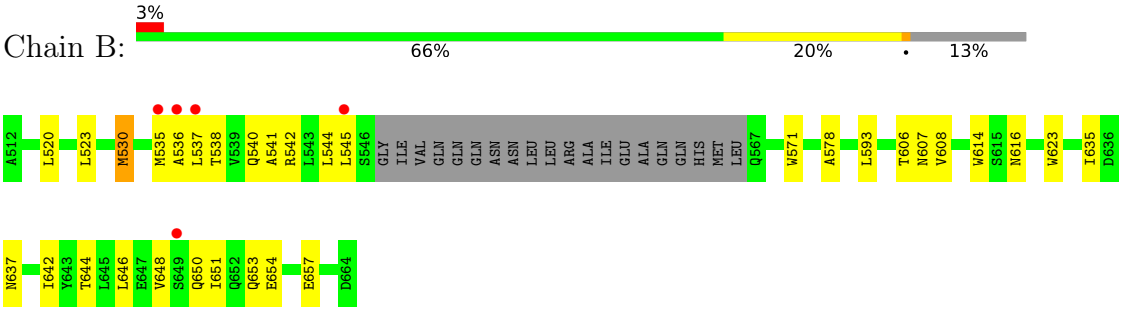
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total C N O 14 8 1 5	0	0
16	B	1	Total C N O 14 8 1 5	0	0
16	G	1	Total C N O 14 8 1 5	0	0
16	G	1	Total C N O 14 8 1 5	0	0
16	G	1	Total C N O 14 8 1 5	0	0
16	G	1	Total C N O 14 8 1 5	0	0
16	G	1	Total C N O 14 8 1 5	0	0
16	G	1	Total C N O 14 8 1 5	0	0

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.

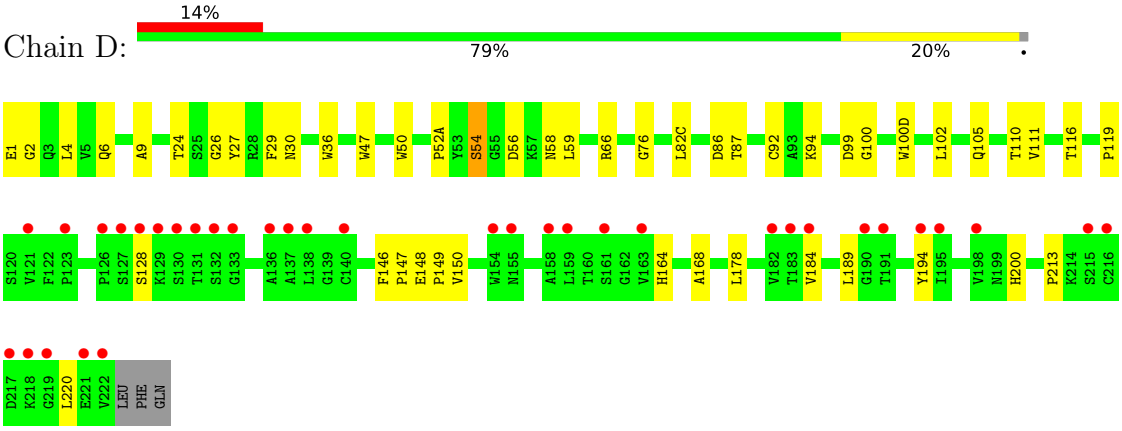
• Molecule 1: Transmembrane protein gp41

Chain B:



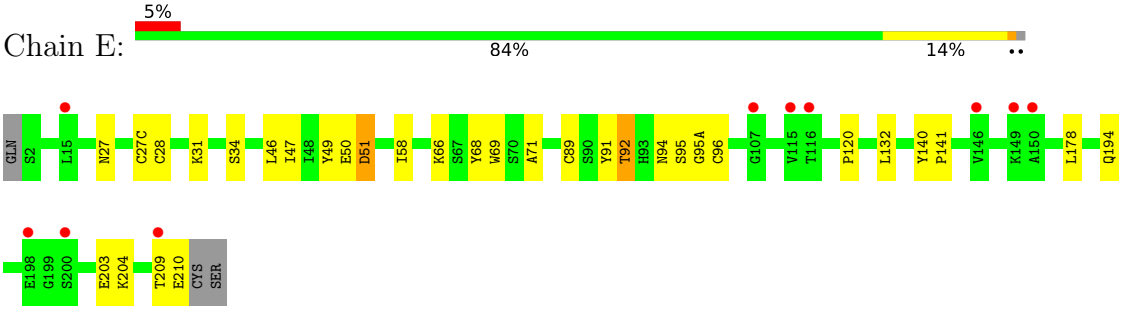
• Molecule 2: 35O22 Fab heavy chain

Chain D:



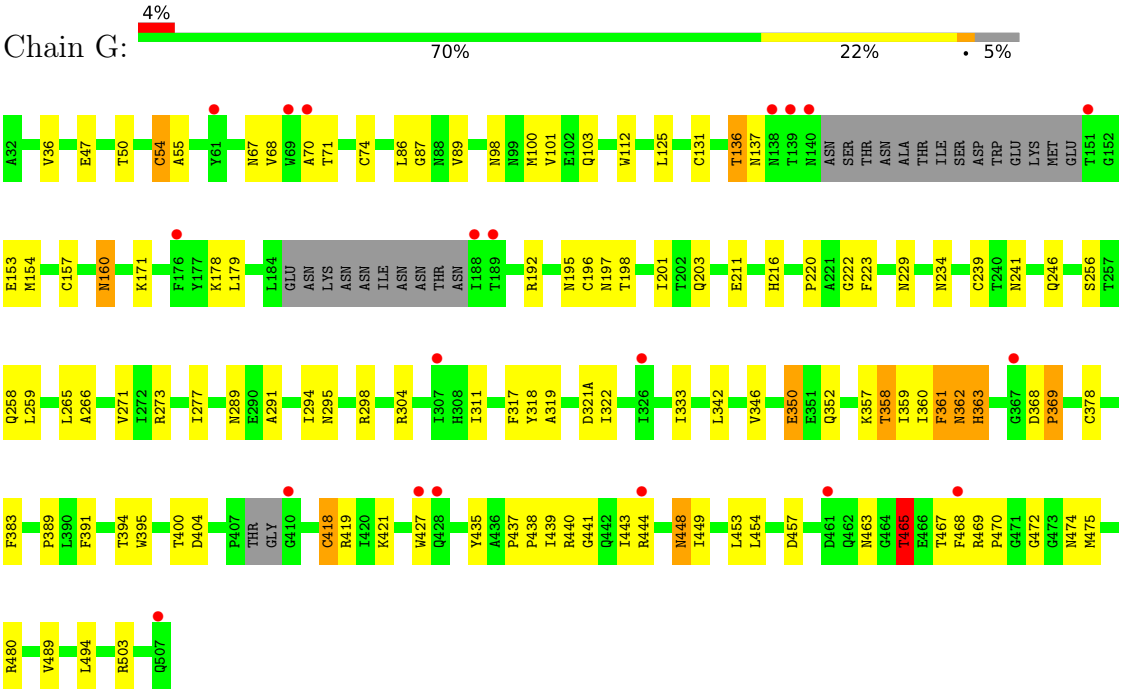
• Molecule 3: 35O22 Fab light chain

Chain E:



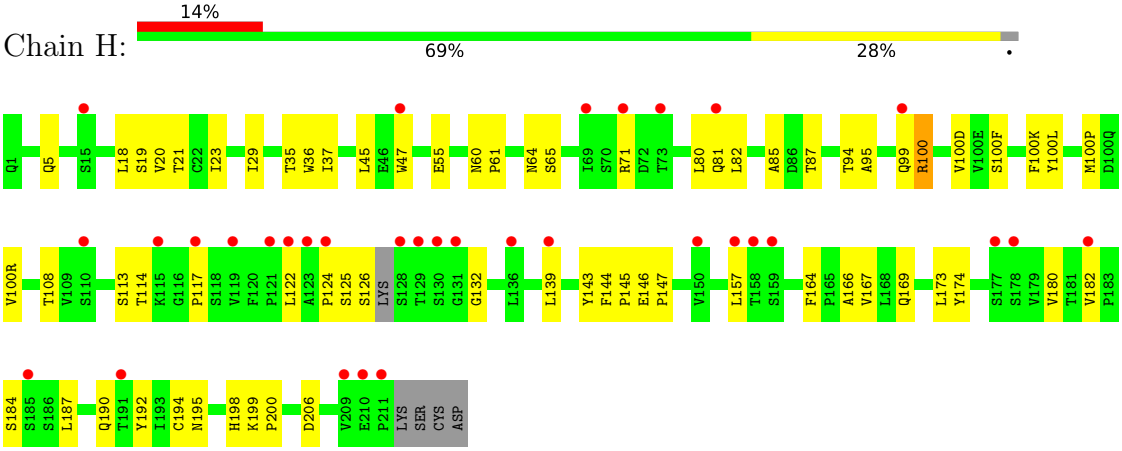
• Molecule 4: Surface protein gp120

Chain G:



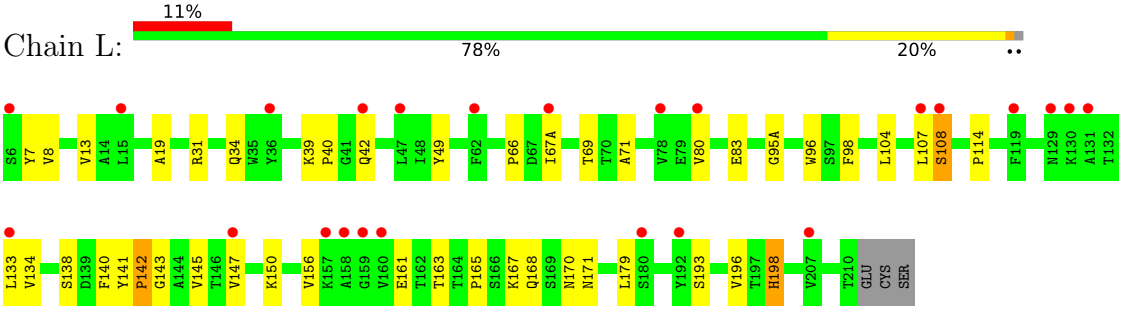
• Molecule 5: PGT124 Fab heavy chain

Chain H:



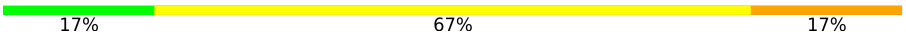
• Molecule 6: PGT124 Fab light chain

Chain L:



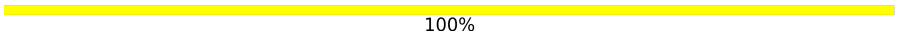
• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:



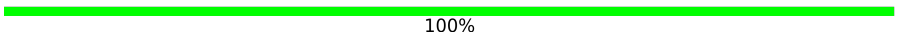
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain I:



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

Chain Q:

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

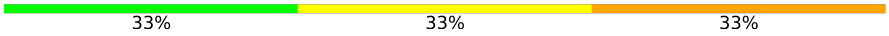
Chain J:

• Molecule 10: 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:

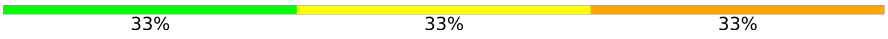
• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



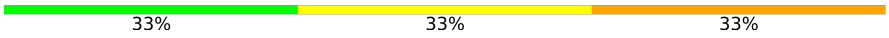
• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



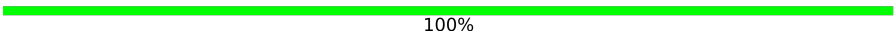
• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

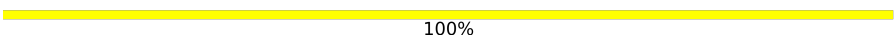


• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

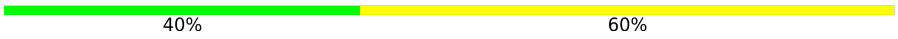
• Molecule 13: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 14: 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 S:



• Molecule 15: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α, β, γ	212.33Å 212.33Å 212.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.05 – 3.53 50.05 – 3.53	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.05-3.53) 99.7 (50.05-3.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.306 , 0.322 0.318 , 0.327	Depositor DCC
R_{free} test set	1951 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	106.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	12268	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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: NAG, MAN, BMA

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	B	0.27	0/1077	0.49	0/1461
2	D	0.26	0/1860	0.46	0/2533
3	E	0.27	0/1659	0.47	0/2269
4	G	0.26	0/3651	0.47	0/4965
5	H	0.27	0/1797	0.58	1/2453 (0.0%)
6	L	0.28	0/1644	0.51	1/2246 (0.0%)
All	All	0.27	0/11688	0.50	2/15927 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	71	ALA	N-CA-CB	-6.93	100.40	110.10
5	H	100	ARG	NE-CZ-NH1	-6.25	117.17	120.30

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	B	1058	0	1042	36	0
2	D	1813	0	1784	33	0
3	E	1615	0	1544	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	3576	0	3493	120	0
5	H	1754	0	1719	84	0
6	L	1601	0	1546	47	0
7	A	72	0	61	3	0
8	C	28	0	25	0	0
8	I	28	0	25	0	0
8	Q	28	0	25	2	0
9	F	83	0	69	1	0
10	J	50	0	43	0	0
10	M	50	0	43	0	0
11	K	39	0	34	5	0
11	N	39	0	34	2	0
11	O	39	0	34	2	0
11	U	39	0	34	0	0
12	P	94	0	79	7	0
13	R	50	0	43	0	0
14	S	61	0	52	1	0
15	T	39	0	34	0	0
16	B	28	0	26	1	0
16	G	84	0	78	5	0
All	All	12268	0	11867	326	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 14.

The worst 5 of 326 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)
4:G:360:ILE:CG1	4:G:395:TRP:H	1.26	1.47
4:G:360:ILE:HG13	4:G:395:TRP:N	1.31	1.44
1:B:545:LEU:O	1:B:545:LEU:HD23	1.43	1.16
5:H:94:THR:HG22	5:H:100(R):VAL:HB	1.35	1.07
5:H:29:ILE:HB	5:H:71:ARG:HD2	1.11	1.07

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	B	129/153 (84%)	116 (90%)	12 (9%)	1 (1%)	19 59
2	D	238/243 (98%)	226 (95%)	12 (5%)	0	100 100
3	E	211/216 (98%)	198 (94%)	13 (6%)	0	100 100
4	G	448/482 (93%)	413 (92%)	31 (7%)	4 (1%)	17 57
5	H	227/236 (96%)	211 (93%)	15 (7%)	1 (0%)	34 71
6	L	209/214 (98%)	194 (93%)	13 (6%)	2 (1%)	15 54
All	All	1462/1544 (95%)	1358 (93%)	96 (7%)	8 (0%)	29 67

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	358	THR
4	G	369	PRO
5	H	125	SER
6	L	142	PRO
6	L	108	SER

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	B	113/130 (87%)	112 (99%)	1 (1%)	78 90
2	D	203/206 (98%)	201 (99%)	2 (1%)	76 88
3	E	186/189 (98%)	183 (98%)	3 (2%)	62 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	G	403/427 (94%)	387 (96%)	16 (4%)	31 64
5	H	199/204 (98%)	197 (99%)	2 (1%)	76 88
6	L	177/180 (98%)	175 (99%)	2 (1%)	73 87
All	All	1281/1336 (96%)	1255 (98%)	26 (2%)	55 79

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	362	ASN
4	G	404	ASP
6	L	145	VAL
4	G	378	CYS
4	G	418	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	G	195	ASN
4	G	229	ASN
4	G	330	HIS
6	L	42	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

59 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	7,1	14,14,15	0.33	0	17,19,21	1.05	2 (11%)
7	NAG	A	2	7	14,14,15	0.28	0	17,19,21	1.31	1 (5%)
7	BMA	A	3	7	11,11,12	0.51	0	15,15,17	1.86	6 (40%)
7	MAN	A	4	7	11,11,12	1.27	1 (9%)	15,15,17	0.92	1 (6%)
7	MAN	A	5	7	11,11,12	1.22	0	15,15,17	0.86	0
7	MAN	A	6	7	11,11,12	0.79	0	15,15,17	1.19	2 (13%)
8	NAG	C	1	8,1	14,14,15	0.40	0	17,19,21	1.40	2 (11%)
8	NAG	C	2	8	14,14,15	0.34	0	17,19,21	0.65	1 (5%)
9	NAG	F	1	4,9	14,14,15	0.37	0	17,19,21	1.08	1 (5%)
9	NAG	F	2	2,9	14,14,15	0.64	0	17,19,21	1.11	1 (5%)
9	BMA	F	3	9	11,11,12	0.45	0	15,15,17	1.19	1 (6%)
9	MAN	F	4	9	11,11,12	2.12	4 (36%)	15,15,17	1.68	4 (26%)
9	MAN	F	5	9	11,11,12	0.81	1 (9%)	15,15,17	1.25	2 (13%)
9	MAN	F	6	9	11,11,12	0.56	0	15,15,17	1.25	2 (13%)
9	MAN	F	7	9	11,11,12	0.71	0	15,15,17	0.91	1 (6%)
8	NAG	I	1	8,4	14,14,15	0.30	0	17,19,21	0.73	0
8	NAG	I	2	8	14,14,15	0.29	0	17,19,21	0.69	0
10	NAG	J	1	10,4	14,14,15	0.34	0	17,19,21	0.86	0
10	NAG	J	2	10	14,14,15	0.42	0	17,19,21	1.67	3 (17%)
10	BMA	J	3	10	11,11,12	0.30	0	15,15,17	0.76	0
10	MAN	J	4	10	11,11,12	0.73	0	15,15,17	0.96	2 (13%)
11	NAG	K	1	11,4	14,14,15	0.35	0	17,19,21	0.86	0
11	NAG	K	2	11	14,14,15	0.48	0	17,19,21	1.50	2 (11%)
11	BMA	K	3	11	11,11,12	0.23	0	15,15,17	0.66	0
10	NAG	M	1	10,4	14,14,15	0.30	0	17,19,21	0.75	0
10	NAG	M	2	10	14,14,15	0.33	0	17,19,21	0.79	0
10	BMA	M	3	10	11,11,12	0.28	0	15,15,17	0.66	0
10	MAN	M	4	10	11,11,12	0.83	0	15,15,17	1.15	2 (13%)
11	NAG	N	1	11,4	14,14,15	0.35	0	17,19,21	0.93	1 (5%)
11	NAG	N	2	11	14,14,15	0.32	0	17,19,21	0.73	0
11	BMA	N	3	11	11,11,12	0.27	0	15,15,17	0.82	0
11	NAG	O	1	11,4	14,14,15	0.28	0	17,19,21	0.59	0
11	NAG	O	2	11	14,14,15	0.28	0	17,19,21	0.92	1 (5%)
11	BMA	O	3	11	11,11,12	0.30	0	15,15,17	0.83	0
12	NAG	P	1	12,4	14,14,15	0.29	0	17,19,21	1.24	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	NAG	P	2	12	14,14,15	0.34	0	17,19,21	1.17	2 (11%)
12	BMA	P	3	12	11,11,12	0.66	0	15,15,17	1.74	3 (20%)
12	MAN	P	4	12	11,11,12	0.87	1 (9%)	15,15,17	1.72	3 (20%)
12	MAN	P	5	12	11,11,12	1.02	0	15,15,17	1.52	2 (13%)
12	MAN	P	6	12	11,11,12	0.77	0	15,15,17	1.13	2 (13%)
12	MAN	P	7	12	11,11,12	0.80	0	15,15,17	0.90	1 (6%)
12	MAN	P	8	12	11,11,12	0.92	0	15,15,17	0.99	0
8	NAG	Q	1	8,4	14,14,15	0.35	0	17,19,21	1.06	2 (11%)
8	NAG	Q	2	8	14,14,15	0.29	0	17,19,21	0.93	0
13	NAG	R	1	13,4	14,14,15	0.30	0	17,19,21	0.99	2 (11%)
13	NAG	R	2	13	14,14,15	0.40	0	17,19,21	0.88	1 (5%)
13	BMA	R	3	13	11,11,12	0.43	0	15,15,17	0.97	1 (6%)
13	MAN	R	4	13	11,11,12	0.87	0	15,15,17	0.96	2 (13%)
14	NAG	S	1	4,14	14,14,15	0.27	0	17,19,21	0.66	0
14	NAG	S	2	14	14,14,15	0.33	0	17,19,21	0.66	0
14	BMA	S	3	14	11,11,12	0.33	0	15,15,17	0.88	0
14	MAN	S	4	14	11,11,12	0.77	0	15,15,17	0.88	1 (6%)
14	MAN	S	5	14	11,11,12	0.63	0	15,15,17	1.08	2 (13%)
15	NAG	T	1	15,4	14,14,15	0.38	0	17,19,21	0.93	0
15	NAG	T	2	15	14,14,15	0.55	0	17,19,21	1.99	4 (23%)
15	BMA	T	3	15	11,11,12	0.29	0	15,15,17	0.85	0
11	NAG	U	1	11,4	14,14,15	0.31	0	17,19,21	0.77	0
11	NAG	U	2	11	14,14,15	0.29	0	17,19,21	0.71	0
11	BMA	U	3	11	11,11,12	0.28	0	15,15,17	0.84	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
7	NAG	A	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	2/6/23/26	0/1/1/1
7	BMA	A	3	7	-	1/2/19/22	0/1/1/1
7	MAN	A	4	7	-	2/2/19/22	0/1/1/1
7	MAN	A	5	7	-	2/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	8,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
9	NAG	F	1	4,9	-	4/6/23/26	0/1/1/1
9	NAG	F	2	2,9	-	2/6/23/26	0/1/1/1
9	BMA	F	3	9	-	1/2/19/22	0/1/1/1
9	MAN	F	4	9	-	2/2/19/22	0/1/1/1
9	MAN	F	5	9	-	0/2/19/22	0/1/1/1
9	MAN	F	6	9	-	1/2/19/22	0/1/1/1
9	MAN	F	7	9	-	2/2/19/22	0/1/1/1
8	NAG	I	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	1/6/23/26	0/1/1/1
10	NAG	J	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	J	2	10	-	4/6/23/26	0/1/1/1
10	BMA	J	3	10	-	2/2/19/22	0/1/1/1
10	MAN	J	4	10	-	2/2/19/22	0/1/1/1
11	NAG	K	1	11,4	-	3/6/23/26	0/1/1/1
11	NAG	K	2	11	-	6/6/23/26	0/1/1/1
11	BMA	K	3	11	-	0/2/19/22	0/1/1/1
10	NAG	M	1	10,4	-	1/6/23/26	0/1/1/1
10	NAG	M	2	10	-	0/6/23/26	0/1/1/1
10	BMA	M	3	10	-	2/2/19/22	0/1/1/1
10	MAN	M	4	10	-	1/2/19/22	0/1/1/1
11	NAG	N	1	11,4	-	4/6/23/26	0/1/1/1
11	NAG	N	2	11	-	3/6/23/26	0/1/1/1
11	BMA	N	3	11	-	0/2/19/22	0/1/1/1
11	NAG	O	1	11,4	-	0/6/23/26	0/1/1/1
11	NAG	O	2	11	-	4/6/23/26	0/1/1/1
11	BMA	O	3	11	-	0/2/19/22	0/1/1/1
12	NAG	P	1	12,4	-	3/6/23/26	0/1/1/1
12	NAG	P	2	12	-	1/6/23/26	0/1/1/1
12	BMA	P	3	12	-	0/2/19/22	0/1/1/1
12	MAN	P	4	12	-	2/2/19/22	0/1/1/1
12	MAN	P	5	12	-	0/2/19/22	0/1/1/1
12	MAN	P	6	12	-	2/2/19/22	0/1/1/1
12	MAN	P	7	12	-	2/2/19/22	0/1/1/1
12	MAN	P	8	12	-	0/2/19/22	0/1/1/1
8	NAG	Q	1	8,4	-	3/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	4/6/23/26	0/1/1/1
13	NAG	R	1	13,4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	R	2	13	-	2/6/23/26	0/1/1/1
13	BMA	R	3	13	-	1/2/19/22	0/1/1/1
13	MAN	R	4	13	-	1/2/19/22	0/1/1/1
14	NAG	S	1	4,14	-	2/6/23/26	0/1/1/1
14	NAG	S	2	14	-	2/6/23/26	0/1/1/1
14	BMA	S	3	14	-	2/2/19/22	0/1/1/1
14	MAN	S	4	14	-	0/2/19/22	0/1/1/1
14	MAN	S	5	14	-	0/2/19/22	0/1/1/1
15	NAG	T	1	15,4	-	2/6/23/26	0/1/1/1
15	NAG	T	2	15	-	5/6/23/26	0/1/1/1
15	BMA	T	3	15	-	2/2/19/22	0/1/1/1
11	NAG	U	1	11,4	-	1/6/23/26	0/1/1/1
11	NAG	U	2	11	-	0/6/23/26	0/1/1/1
11	BMA	U	3	11	-	0/2/19/22	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	4	MAN	O2-C2	4.24	1.52	1.43
9	F	4	MAN	O5-C1	-3.35	1.38	1.43
9	F	4	MAN	C2-C3	3.17	1.57	1.52
7	A	4	MAN	O5-C1	-3.03	1.38	1.43
9	F	5	MAN	C1-C2	2.57	1.58	1.52

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	2	NAG	C2-N2-C7	5.67	130.98	122.90
10	J	2	NAG	C2-N2-C7	5.08	130.14	122.90
12	P	3	BMA	O3-C3-C2	-4.70	101.00	109.99
12	P	4	MAN	C1-O5-C5	4.41	118.17	112.19
12	P	5	MAN	C1-C2-C3	-4.22	104.48	109.67

There are no chirality outliers.

5 of 99 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	Q	1	NAG	O7-C7-N2-C2
8	Q	2	NAG	C3-C2-N2-C7
10	J	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
10	J	2	NAG	C8-C7-N2-C2
10	J	2	NAG	O7-C7-N2-C2

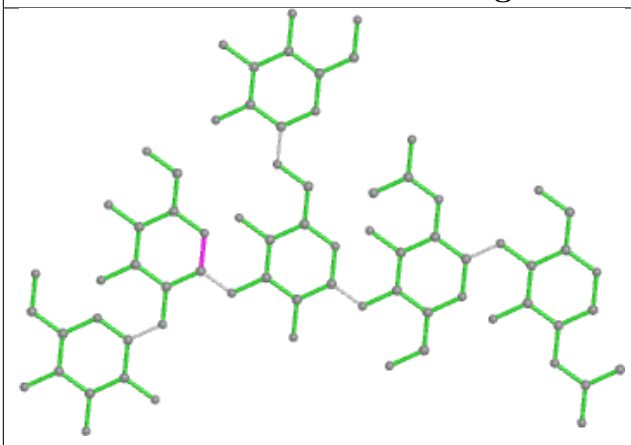
There are no ring outliers.

13 monomers are involved in 23 short contacts:

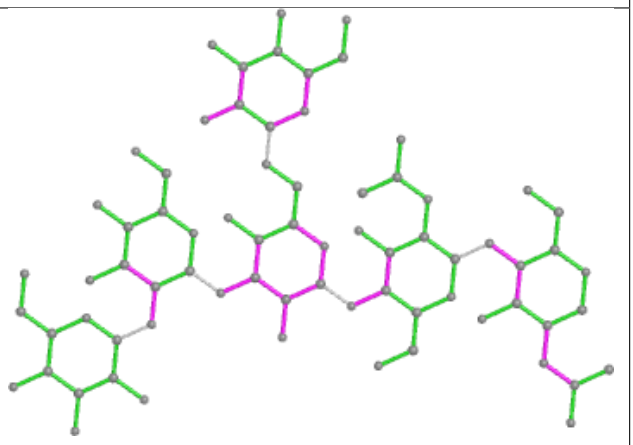
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	2	NAG	2	0
12	P	1	NAG	4	0
9	F	6	MAN	1	0
12	P	5	MAN	3	0
11	N	1	NAG	2	0
7	A	2	NAG	3	0
11	K	1	NAG	4	0
8	Q	1	NAG	2	0
11	O	1	NAG	2	0
11	N	2	NAG	1	0
14	S	1	NAG	1	0
8	Q	2	NAG	1	0
11	O	2	NAG	2	0

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

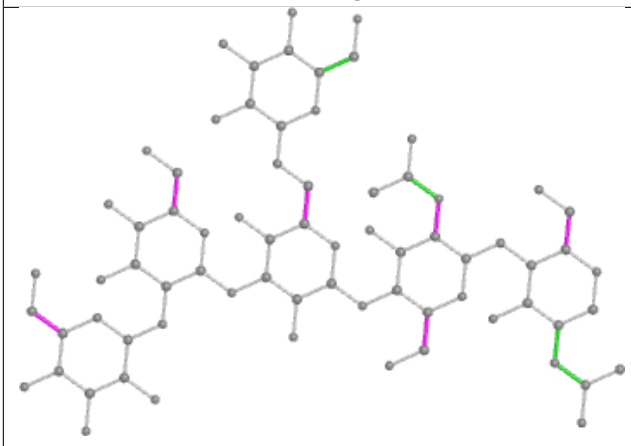
Oligosaccharide Chain A



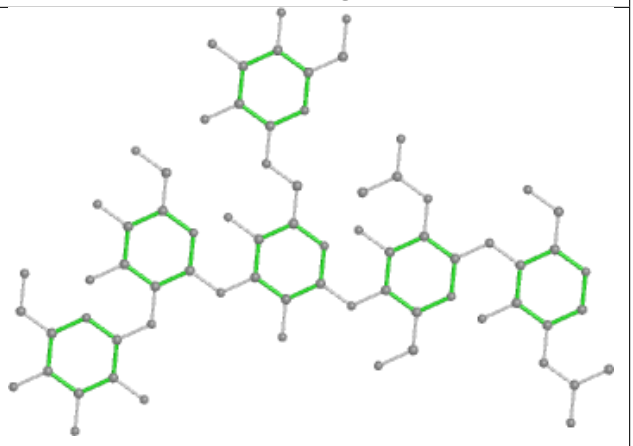
Bond lengths



Bond angles

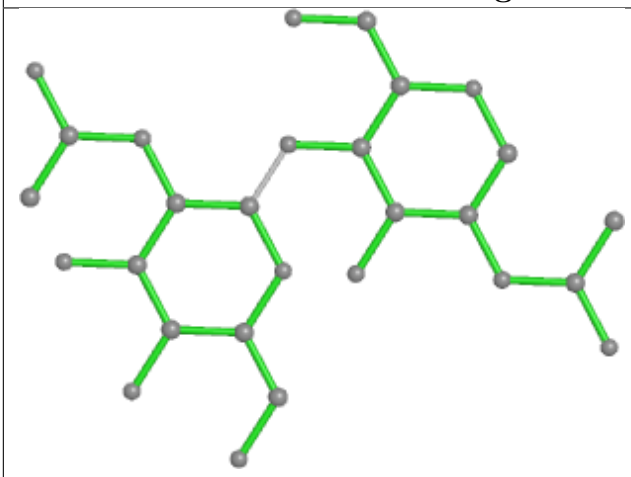


Torsions

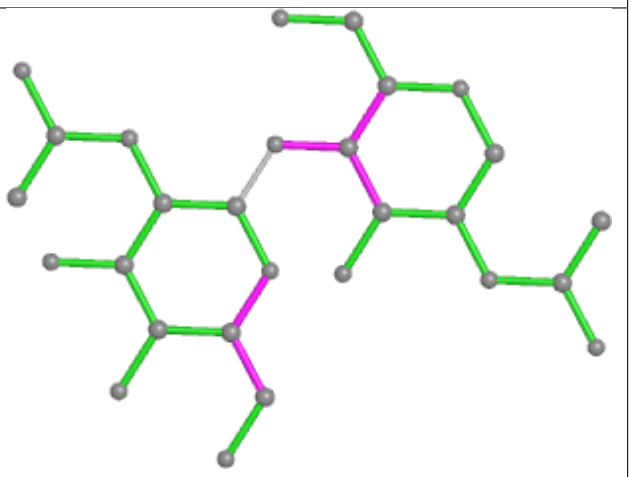


Rings

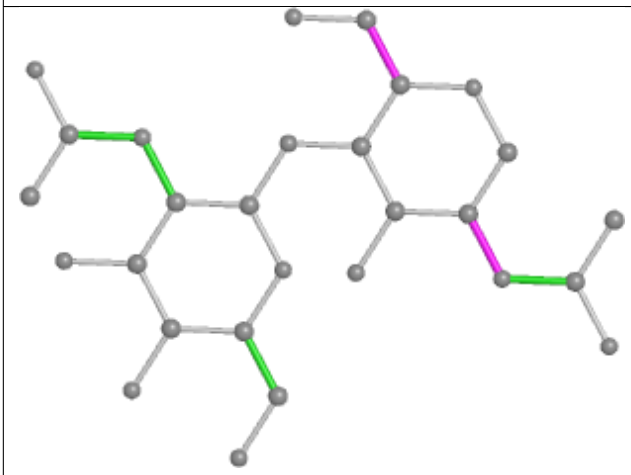
Oligosaccharide Chain C



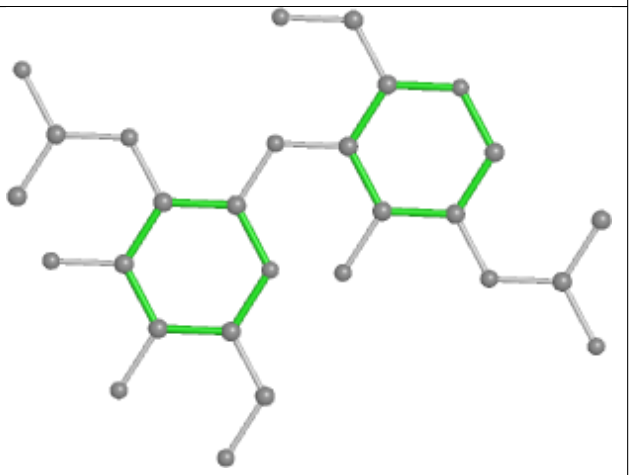
Bond lengths



Bond angles

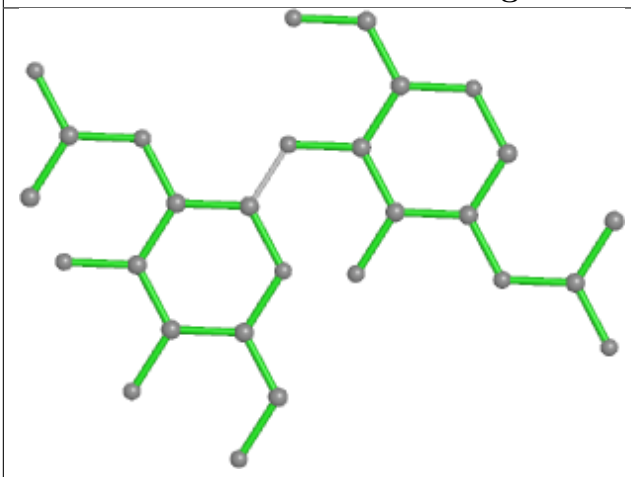


Torsions

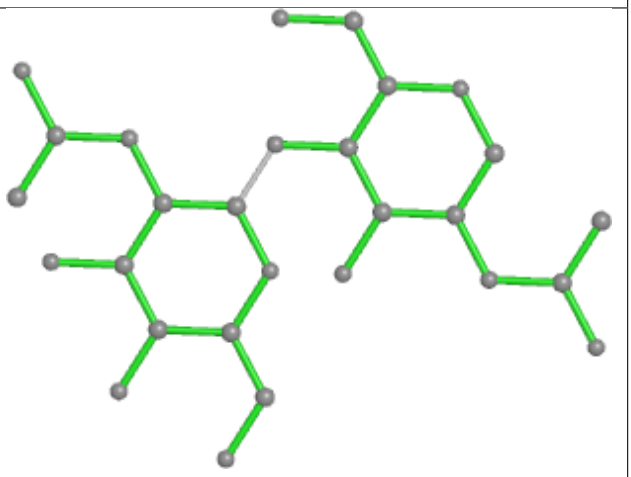


Rings

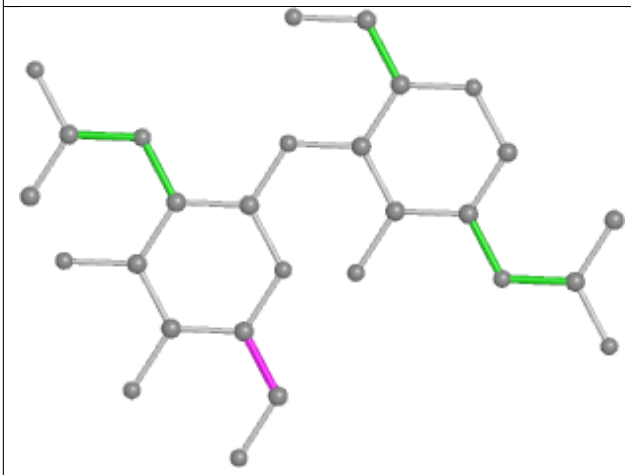
Oligosaccharide Chain I



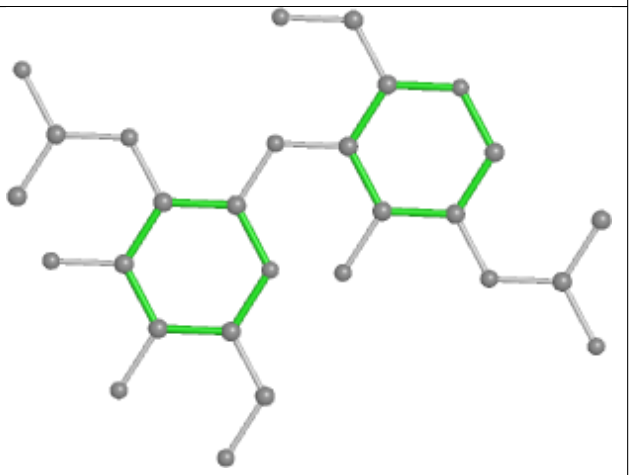
Bond lengths



Bond angles

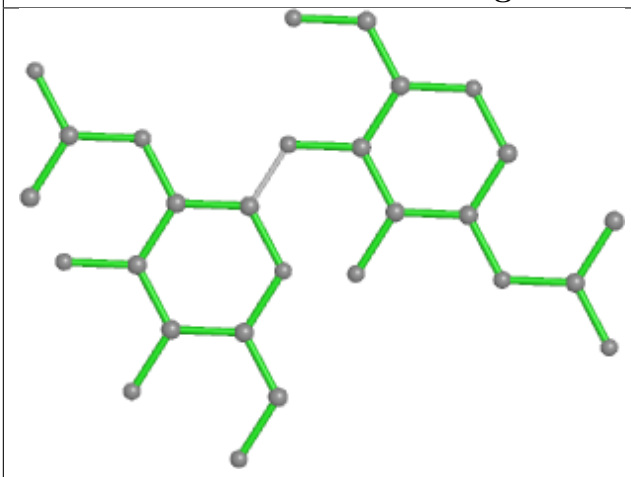


Torsions

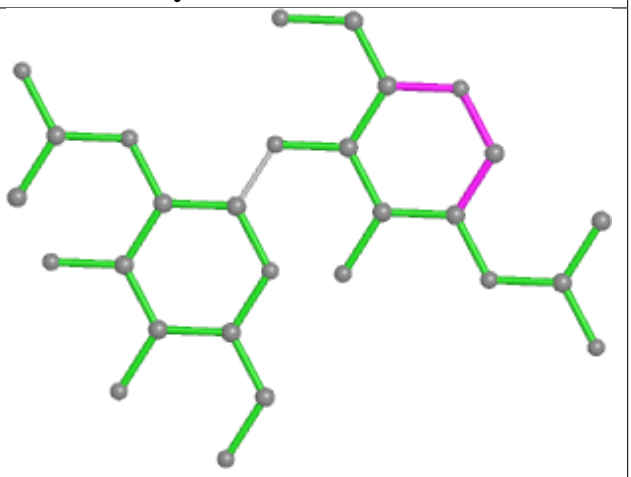


Rings

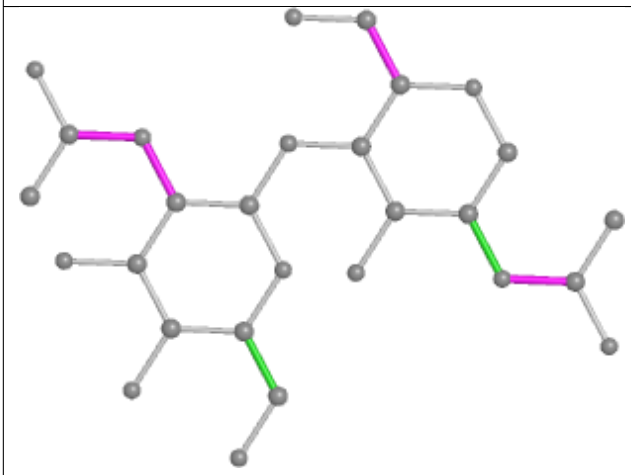
Oligosaccharide Chain Q



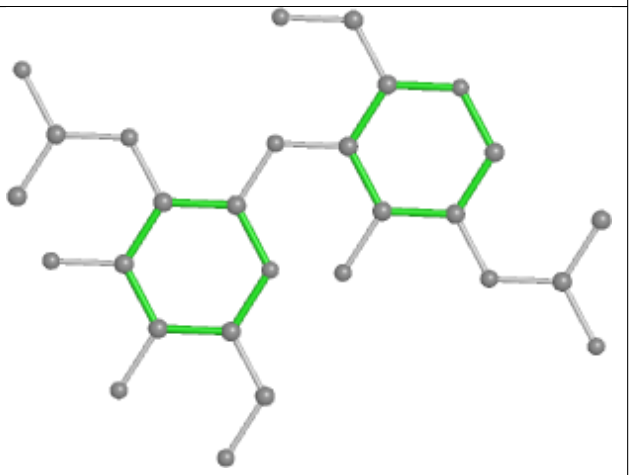
Bond lengths



Bond angles

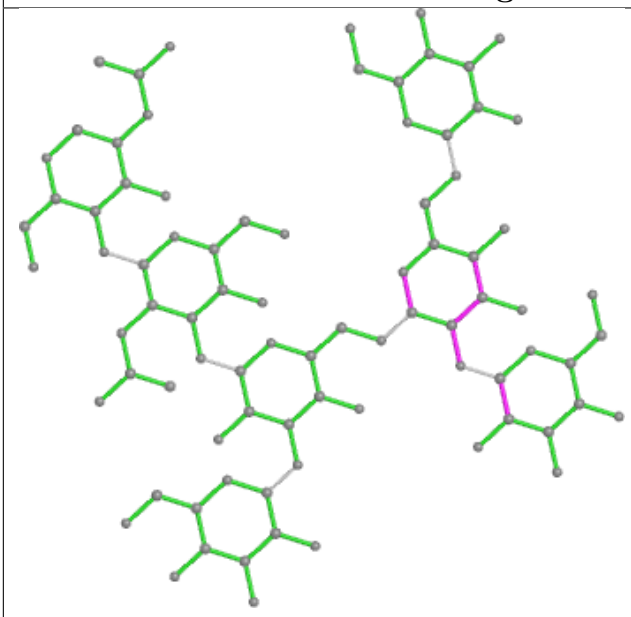


Torsions

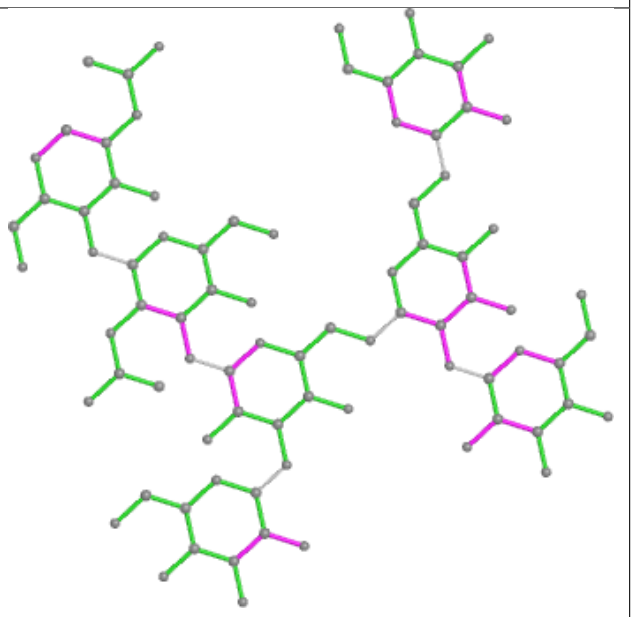


Rings

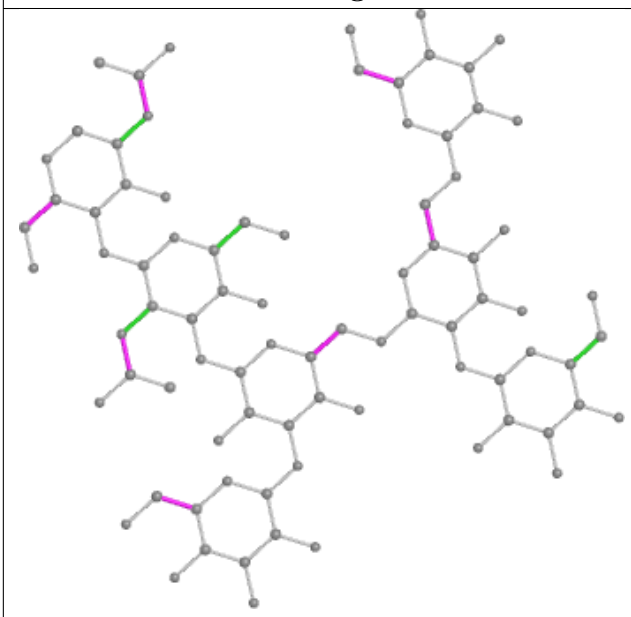
Oligosaccharide Chain F



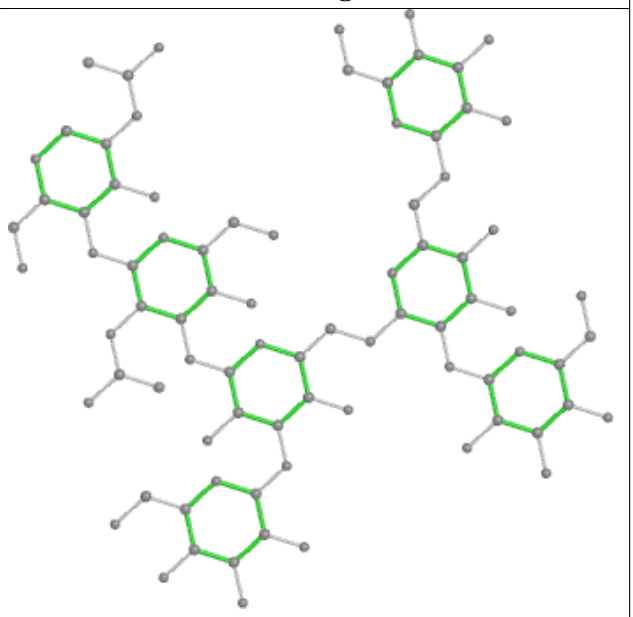
Bond lengths



Bond angles

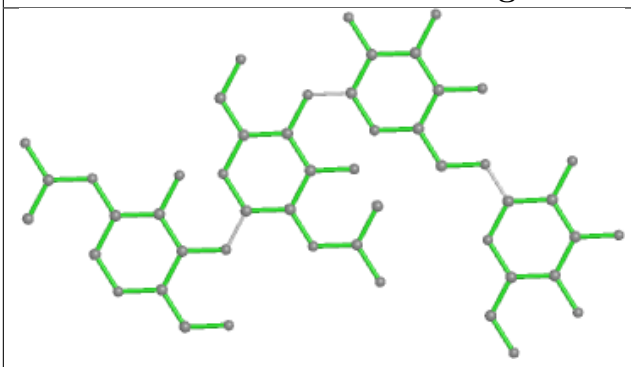


Torsions

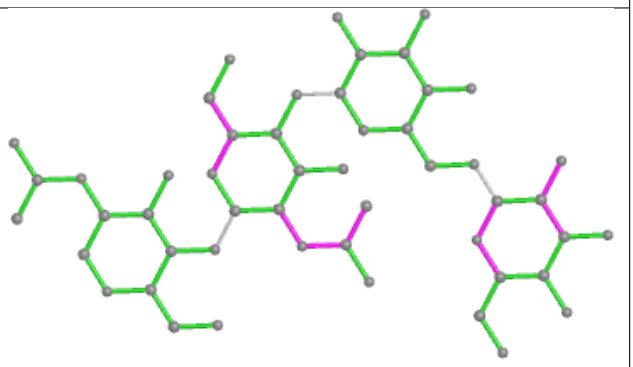


Rings

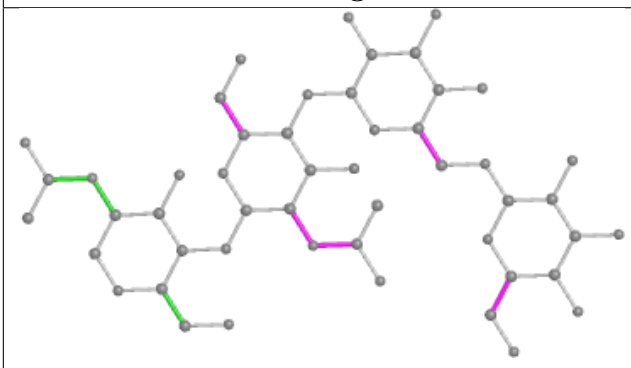
Oligosaccharide Chain J



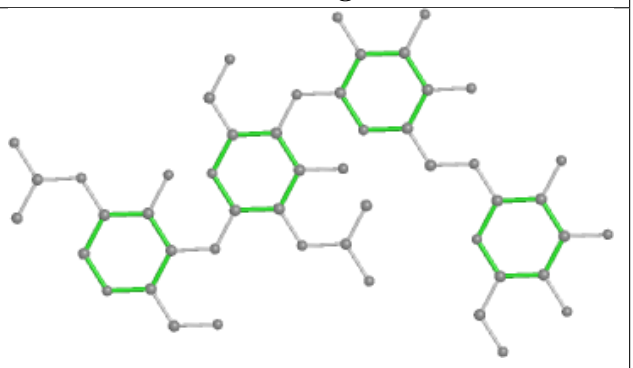
Bond lengths



Bond angles

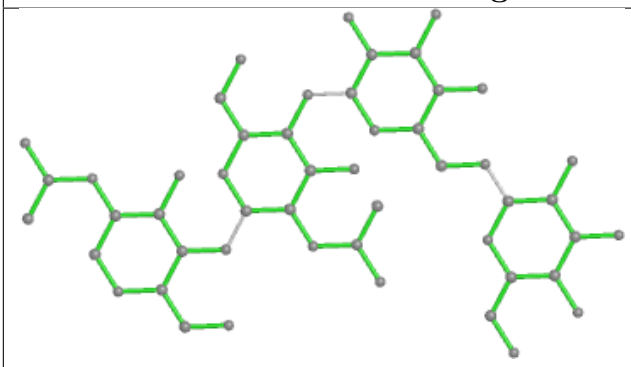


Torsions

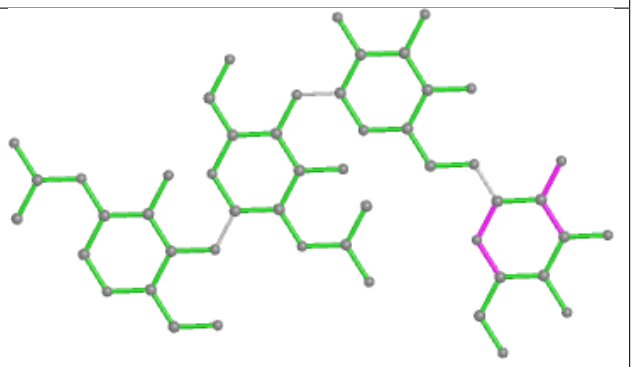


Rings

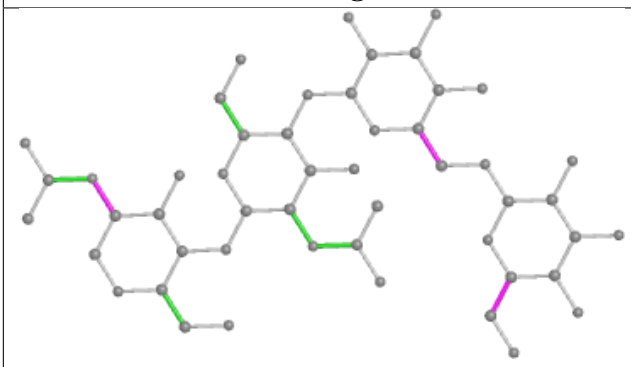
Oligosaccharide Chain M



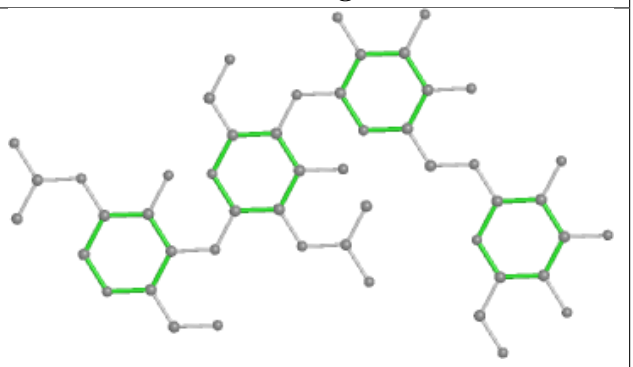
Bond lengths



Bond angles

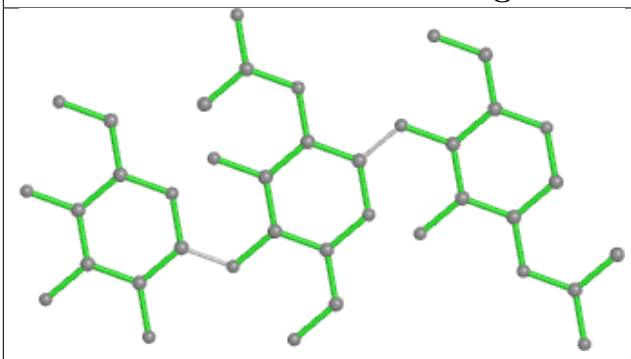


Torsions

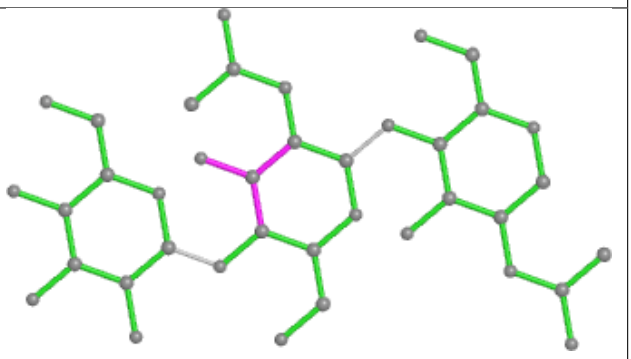


Rings

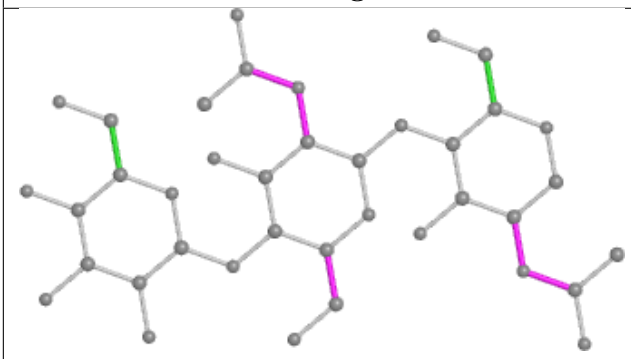
Oligosaccharide Chain K



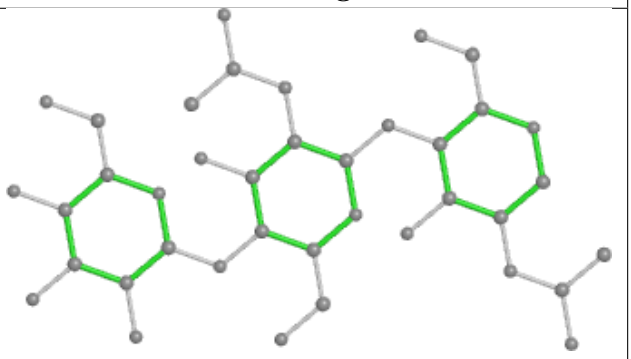
Bond lengths



Bond angles

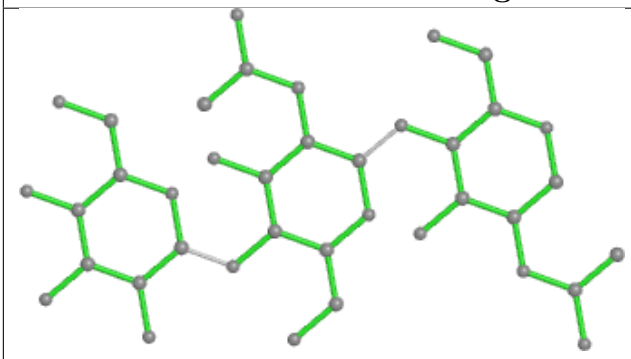


Torsions

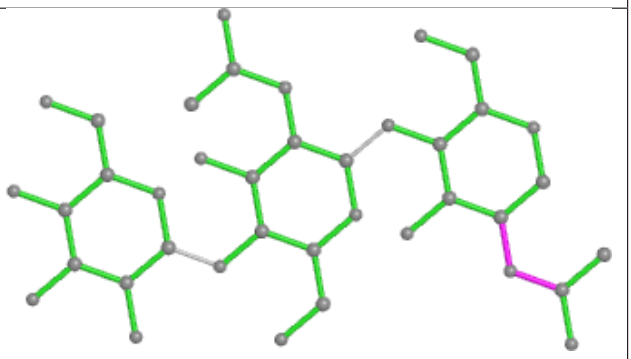


Rings

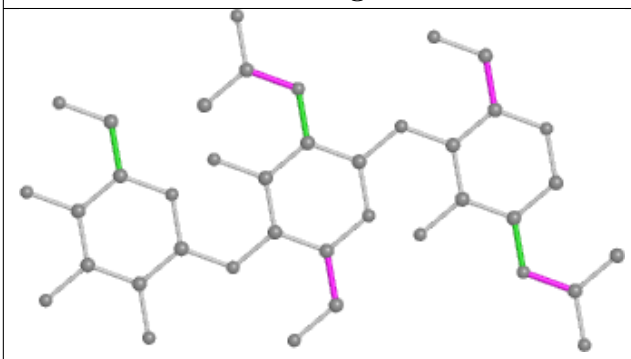
Oligosaccharide Chain N



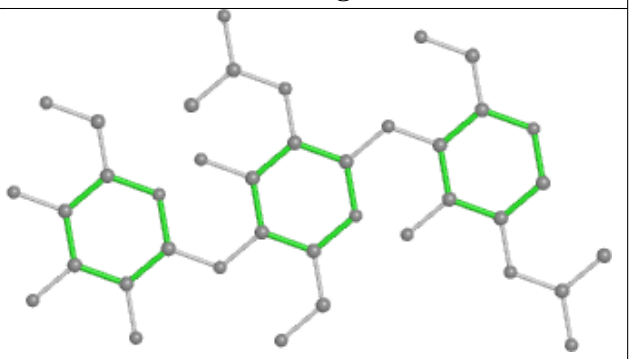
Bond lengths



Bond angles

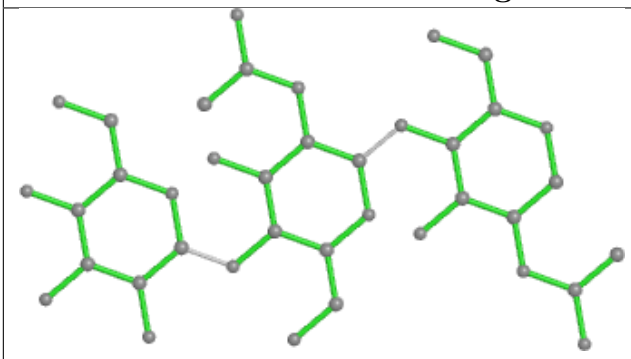


Torsions

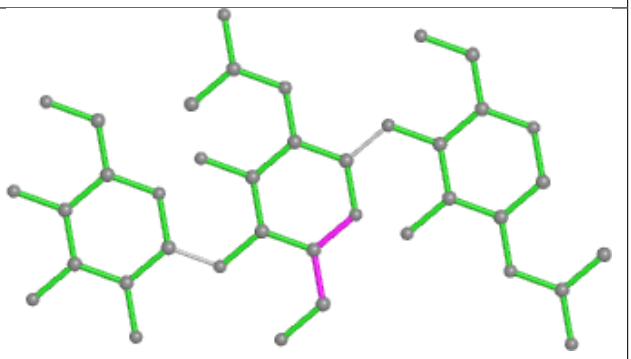


Rings

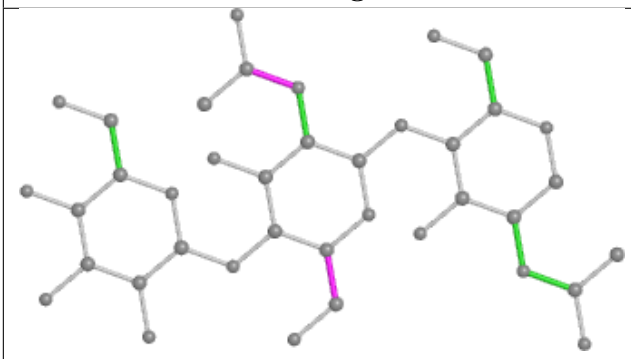
Oligosaccharide Chain O



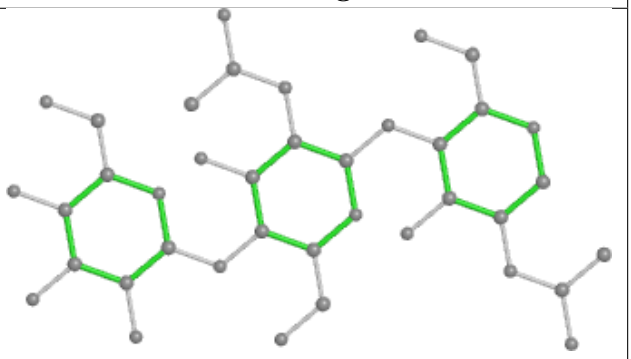
Bond lengths



Bond angles

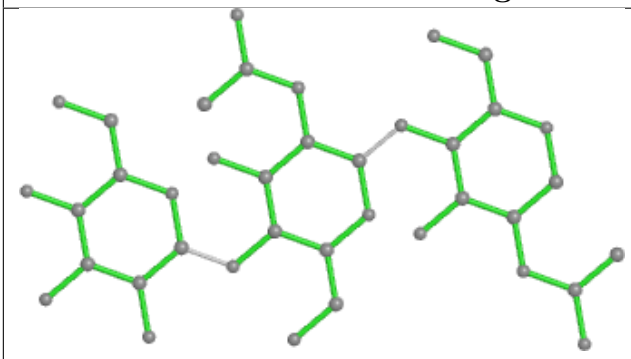


Torsions

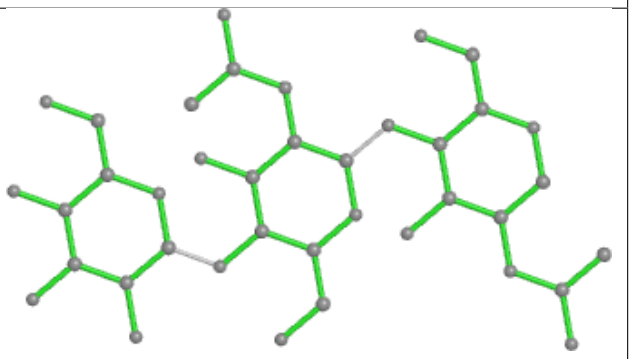


Rings

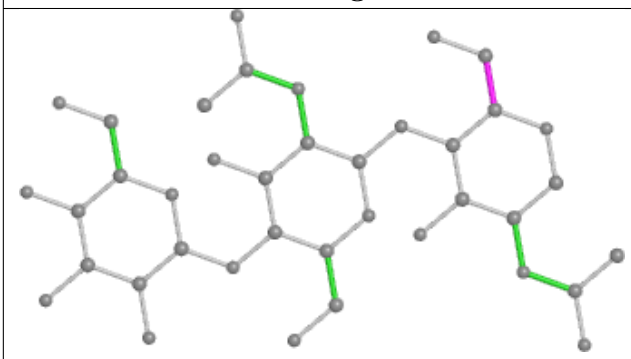
Oligosaccharide Chain U



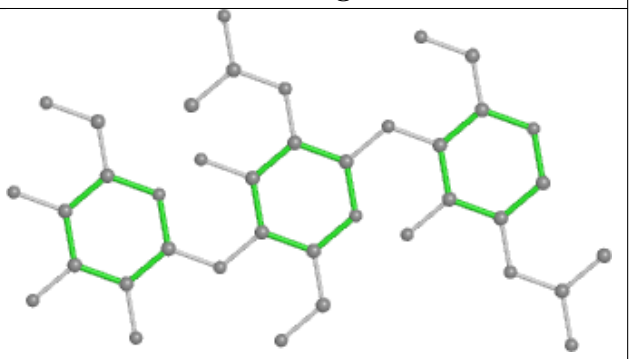
Bond lengths



Bond angles

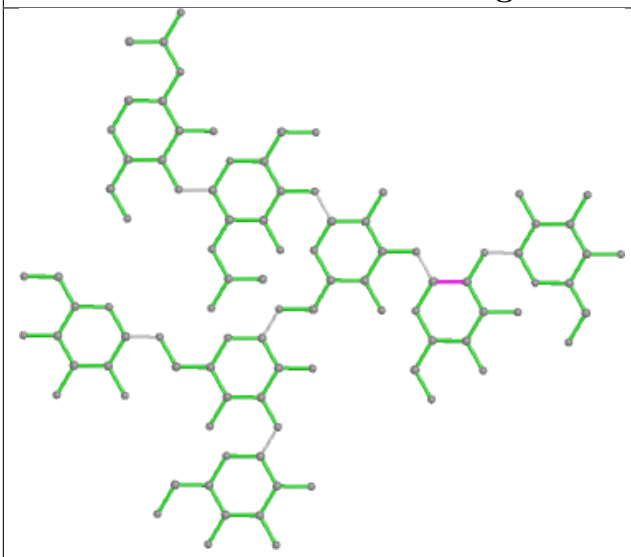


Torsions

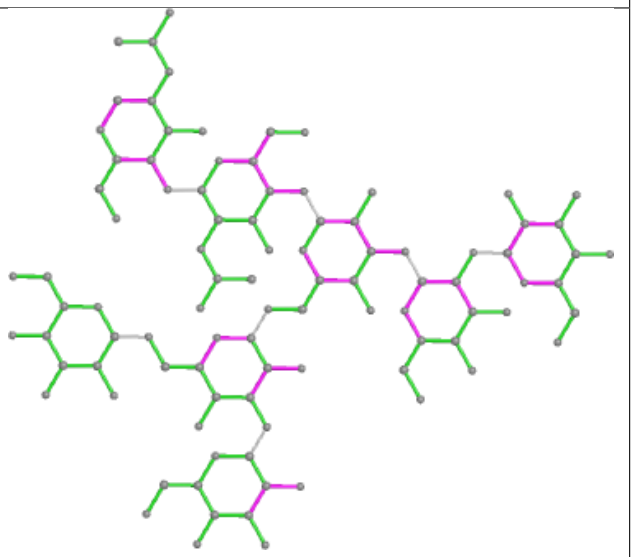


Rings

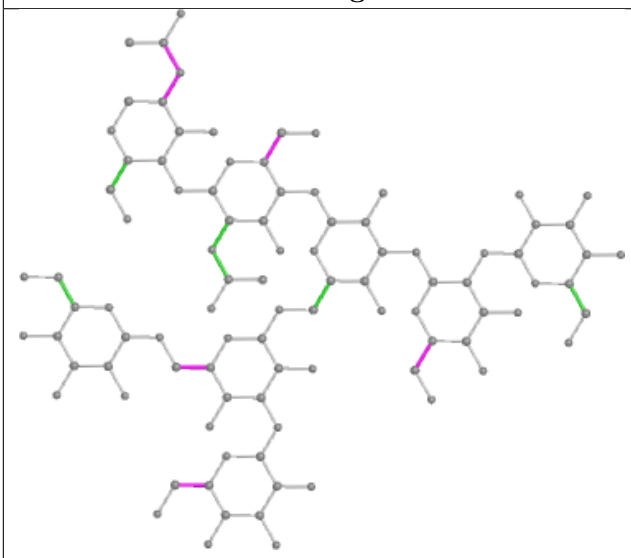
Oligosaccharide Chain P



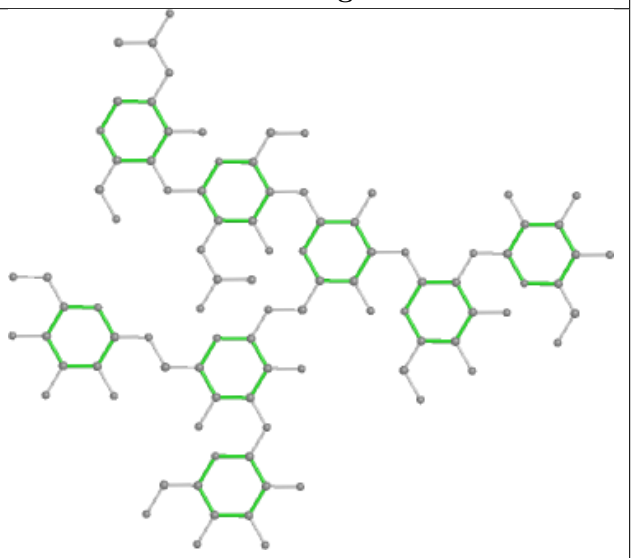
Bond lengths



Bond angles

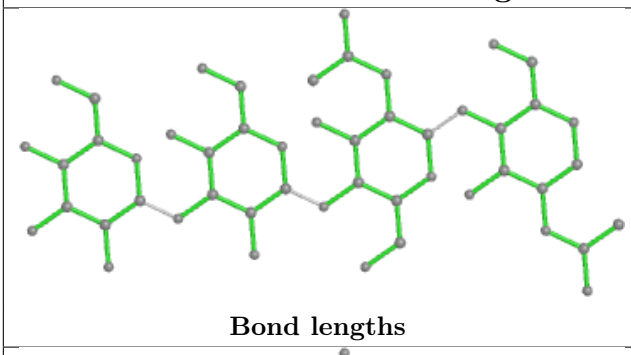


Torsions

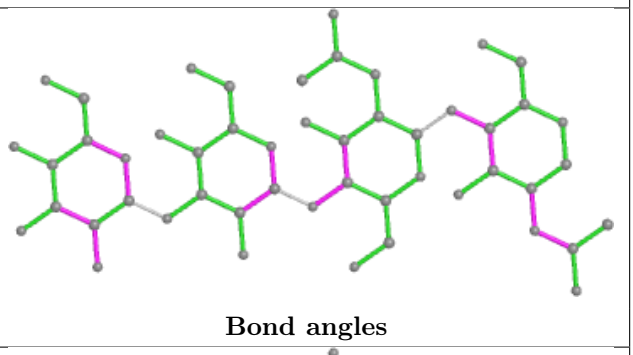


Rings

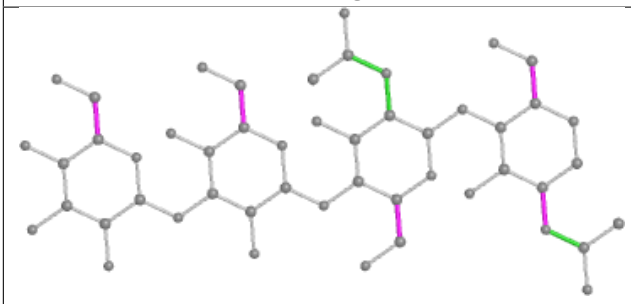
Oligosaccharide Chain R



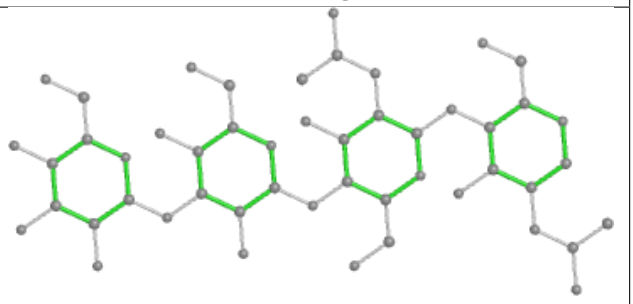
Bond lengths



Bond angles

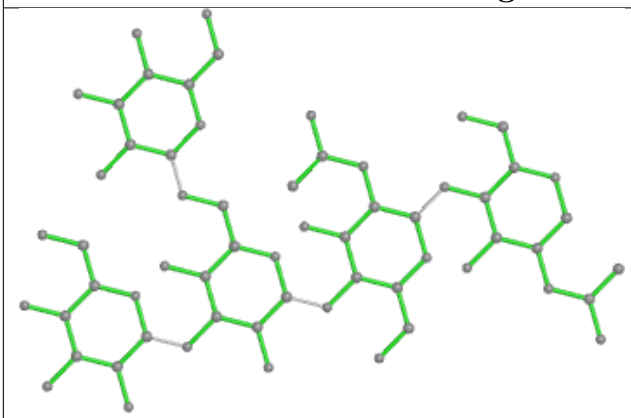


Torsions

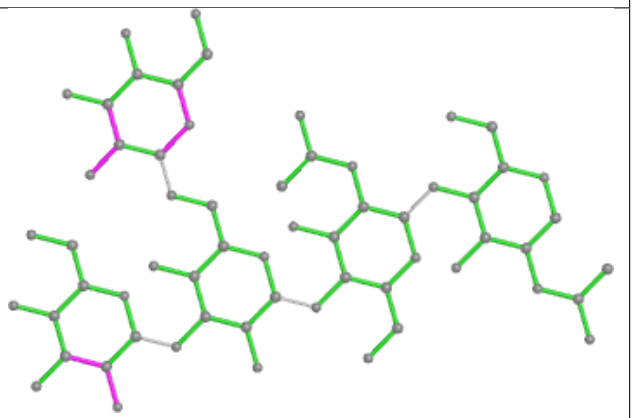


Rings

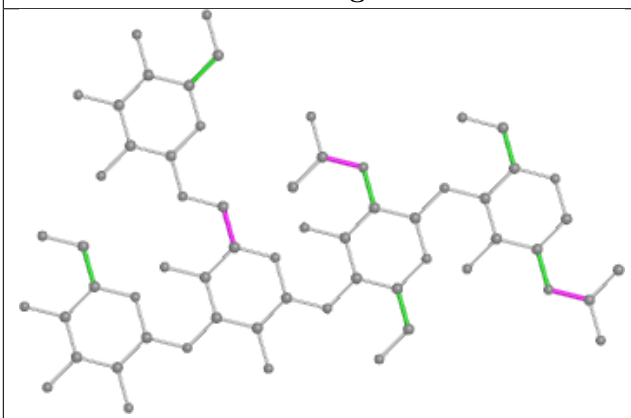
Oligosaccharide Chain S



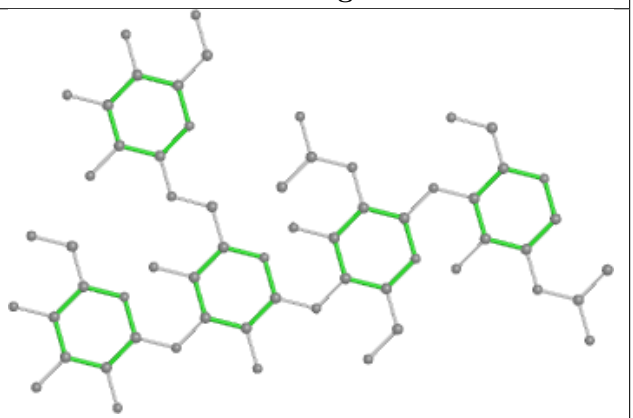
Bond lengths



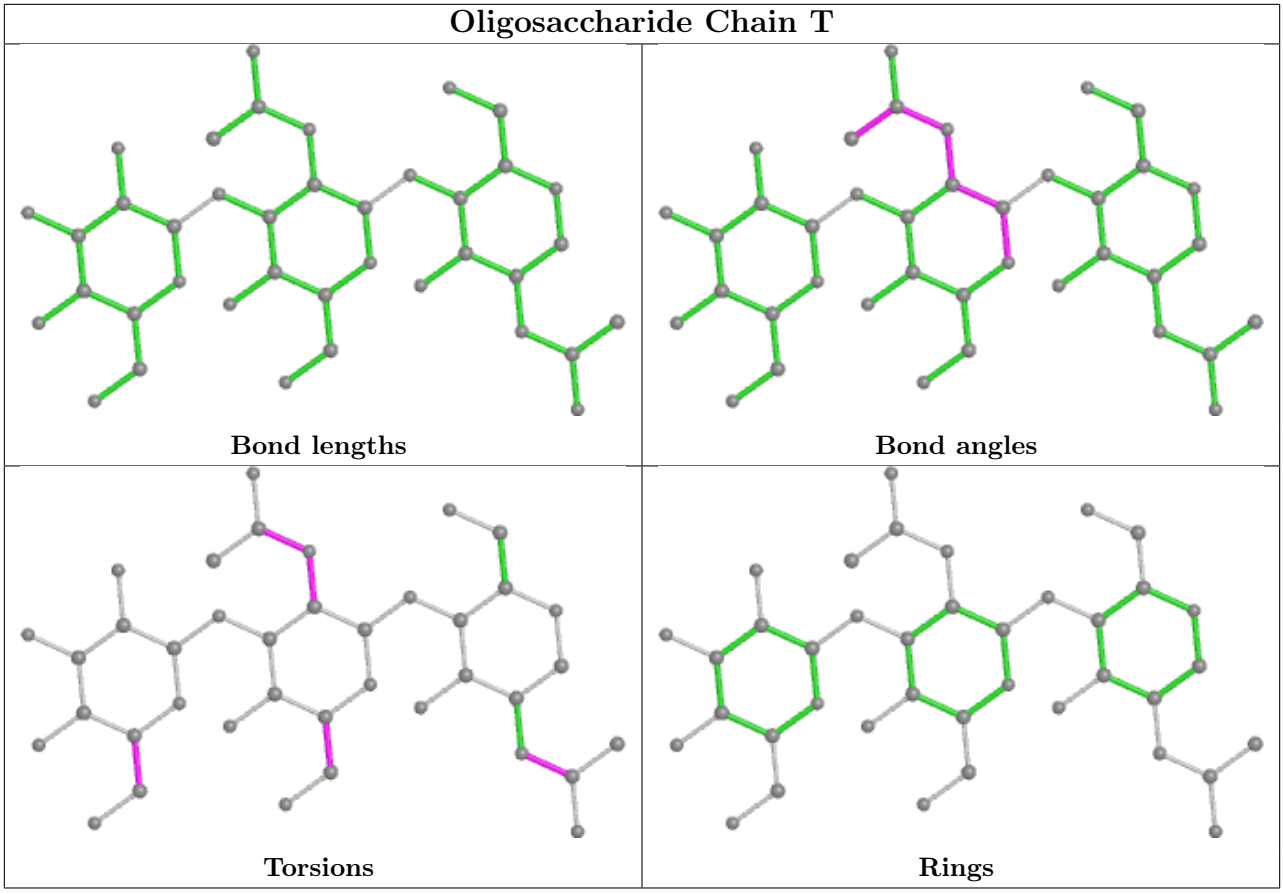
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
16	NAG	B	708	1	14,14,15	0.27	0	17,19,21	0.62	0
16	NAG	G	616	4	14,14,15	0.27	0	17,19,21	0.57	0
16	NAG	G	603	4	14,14,15	0.28	0	17,19,21	0.73	0
16	NAG	G	631	4	14,14,15	0.29	0	17,19,21	0.66	0
16	NAG	G	643	4	14,14,15	0.27	0	17,19,21	0.63	0
16	NAG	G	650	4	14,14,15	0.49	0	17,19,21	1.94	3 (17%)
16	NAG	G	604	4	14,14,15	0.30	0	17,19,21	0.74	0
16	NAG	B	701	1	14,14,15	0.26	0	17,19,21	0.84	1 (5%)

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
16	NAG	B	708	1	-	1/6/23/26	0/1/1/1
16	NAG	G	616	4	-	0/6/23/26	0/1/1/1
16	NAG	G	603	4	-	2/6/23/26	0/1/1/1
16	NAG	G	631	4	-	0/6/23/26	0/1/1/1
16	NAG	G	643	4	-	0/6/23/26	0/1/1/1
16	NAG	G	650	4	-	3/6/23/26	0/1/1/1
16	NAG	G	604	4	-	0/6/23/26	0/1/1/1
16	NAG	B	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	650	NAG	C2-N2-C7	6.18	131.70	122.90
16	G	650	NAG	C8-C7-N2	3.11	121.36	116.10
16	G	650	NAG	C1-O5-C5	2.21	115.19	112.19
16	B	701	NAG	O5-C5-C6	2.03	110.38	107.20

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	G	603	NAG	C8-C7-N2-C2
16	G	650	NAG	C8-C7-N2-C2
16	G	650	NAG	O7-C7-N2-C2
16	G	603	NAG	O7-C7-N2-C2
16	B	708	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	603	NAG	1	0
16	G	631	NAG	2	0
16	G	650	NAG	1	0
16	G	604	NAG	1	0
16	B	701	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	133/153 (86%)	0.30	5 (3%) 40 30	46, 76, 144, 167	0
2	D	240/243 (98%)	0.63	35 (14%) 2 2	46, 98, 243, 277	0
3	E	213/216 (98%)	0.26	10 (4%) 31 23	45, 113, 181, 199	0
4	G	456/482 (94%)	0.19	20 (4%) 34 25	44, 105, 174, 218	0
5	H	231/236 (97%)	0.86	33 (14%) 2 2	64, 161, 217, 255	0
6	L	211/214 (98%)	0.70	24 (11%) 5 5	62, 156, 210, 224	0
All	All	1484/1544 (96%)	0.46	127 (8%) 10 9	44, 119, 206, 277	0

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	222	VAL	11.8
1	B	536	ALA	8.5
5	H	131	GLY	6.9
2	D	218	LYS	6.6
4	G	140	ASN	6.3

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
13	MAN	R	4	11/12	0.46	0.35	138,138,138,138	0
10	BMA	M	3	11/12	0.51	0.27	179,179,179,179	0
12	MAN	P	8	11/12	0.55	0.54	138,138,138,138	0
8	NAG	C	1	14/15	0.56	0.40	138,138,138,138	0
7	MAN	A	5	11/12	0.57	0.45	90,90,90,90	0
12	MAN	P	6	11/12	0.60	0.24	138,138,138,138	0
8	NAG	C	2	14/15	0.61	0.64	138,138,138,138	0
10	MAN	J	4	11/12	0.62	0.22	138,138,138,138	0
11	BMA	U	3	11/12	0.63	0.21	179,179,179,179	0
14	BMA	S	3	11/12	0.63	0.22	179,179,179,179	0
14	MAN	S	4	11/12	0.63	0.29	179,179,179,179	0
8	NAG	Q	2	14/15	0.65	0.41	179,179,179,179	0
15	NAG	T	2	14/15	0.65	0.29	179,179,179,179	0
11	NAG	U	2	14/15	0.68	0.17	179,179,179,179	0
8	NAG	I	2	14/15	0.68	0.27	179,179,179,179	0
9	NAG	F	2	14/15	0.69	0.59	179,179,179,179	0
15	BMA	T	3	11/12	0.69	0.17	179,179,179,179	0
11	BMA	O	3	11/12	0.70	0.23	138,138,138,138	0
7	MAN	A	4	11/12	0.70	0.54	138,138,138,138	0
13	BMA	R	3	11/12	0.70	0.33	138,138,138,138	0
11	BMA	N	3	11/12	0.70	0.20	179,179,179,179	0
10	MAN	M	4	11/12	0.71	0.30	138,138,138,138	0
11	NAG	N	1	14/15	0.73	0.26	179,179,179,179	0
7	BMA	A	3	11/12	0.74	0.25	179,179,179,179	0
12	MAN	P	7	11/12	0.74	0.23	138,138,138,138	0
8	NAG	Q	1	14/15	0.74	0.28	179,179,179,179	0
10	BMA	J	3	11/12	0.75	0.32	138,138,138,138	0
7	MAN	A	6	11/12	0.75	0.33	138,138,138,138	0
11	NAG	U	1	14/15	0.76	0.28	179,179,179,179	0
13	NAG	R	1	14/15	0.76	0.26	179,179,179,179	0
12	MAN	P	5	11/12	0.77	0.20	138,138,138,138	0
10	NAG	J	2	14/15	0.78	0.21	138,138,138,138	0
9	MAN	F	6	11/12	0.78	0.55	179,179,179,179	0
11	NAG	O	2	14/15	0.79	0.25	138,138,138,138	0
14	MAN	S	5	11/12	0.79	0.28	179,179,179,179	0
15	NAG	T	1	14/15	0.81	0.20	179,179,179,179	0
9	MAN	F	5	11/12	0.81	0.51	179,179,179,179	0
9	MAN	F	4	11/12	0.81	0.52	179,179,179,179	0
7	NAG	A	1	14/15	0.82	0.34	179,179,179,179	0
10	NAG	M	2	14/15	0.83	0.23	179,179,179,179	0
14	NAG	S	2	14/15	0.83	0.27	179,179,179,179	0
13	NAG	R	2	14/15	0.83	0.22	179,179,179,179	0
7	NAG	A	2	14/15	0.83	0.21	179,179,179,179	0

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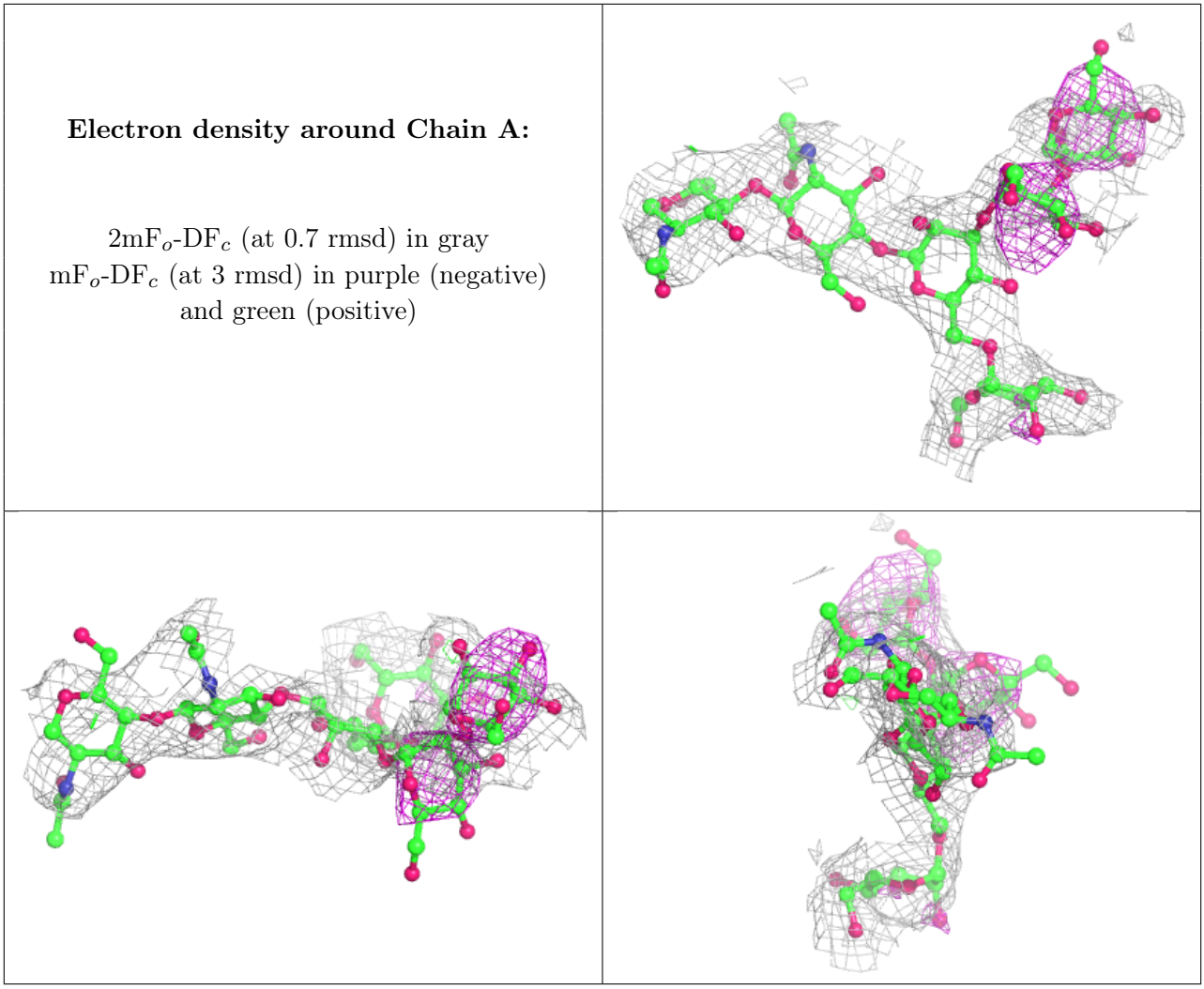
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	BMA	K	3	11/12	0.84	0.32	41,41,41,41	0
10	NAG	J	1	14/15	0.85	0.22	179,179,179,179	0
9	BMA	F	3	11/12	0.86	0.54	179,179,179,179	0
11	NAG	K	1	14/15	0.86	0.25	179,179,179,179	0
12	NAG	P	1	14/15	0.86	0.29	179,179,179,179	0
12	BMA	P	3	11/12	0.87	0.18	138,138,138,138	0
11	NAG	K	2	14/15	0.87	0.22	41,41,41,41	0
11	NAG	N	2	14/15	0.88	0.22	179,179,179,179	0
14	NAG	S	1	14/15	0.88	0.29	179,179,179,179	0
9	NAG	F	1	14/15	0.88	0.48	179,179,179,179	0
8	NAG	I	1	14/15	0.89	0.18	179,179,179,179	0
12	MAN	P	4	11/12	0.89	0.17	138,138,138,138	0
11	NAG	O	1	14/15	0.89	0.27	179,179,179,179	0
12	NAG	P	2	14/15	0.91	0.21	179,179,179,179	0
10	NAG	M	1	14/15	0.93	0.31	179,179,179,179	0
9	MAN	F	7	11/12	0.94	0.49	179,179,179,179	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.

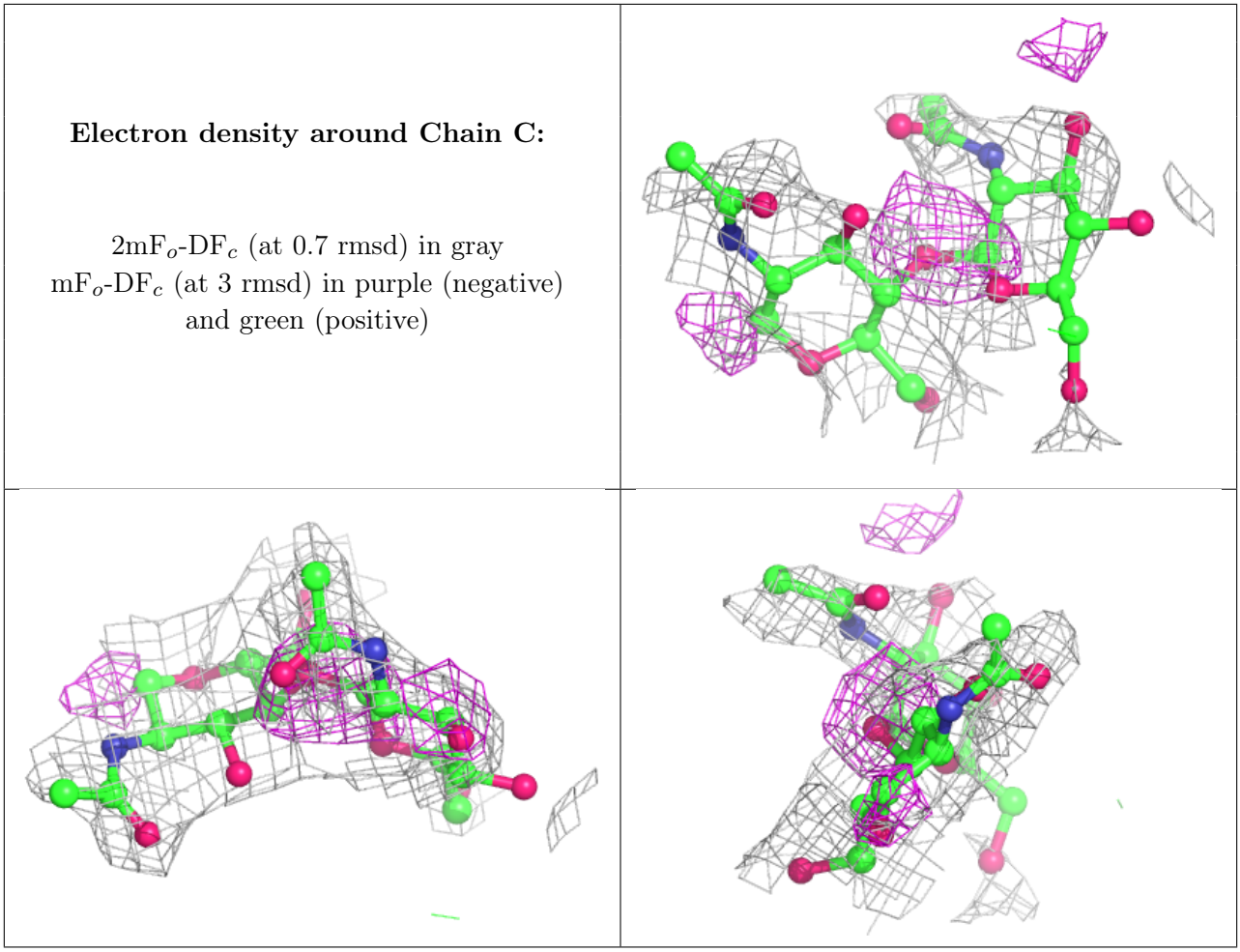
Electron density around Chain A:

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



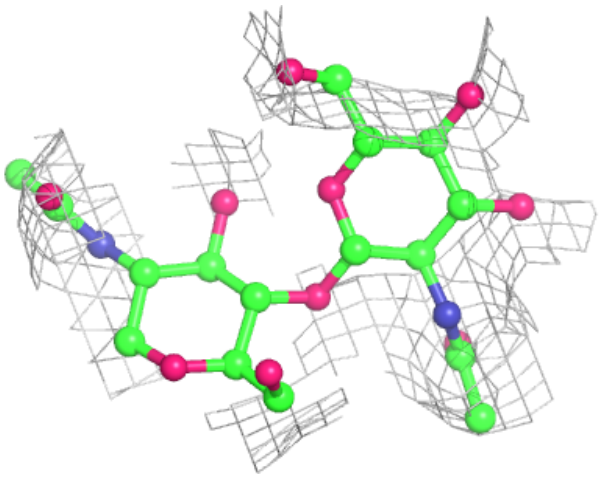
Electron density around Chain C:

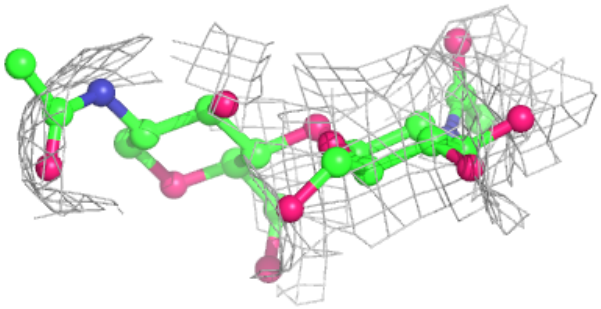
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

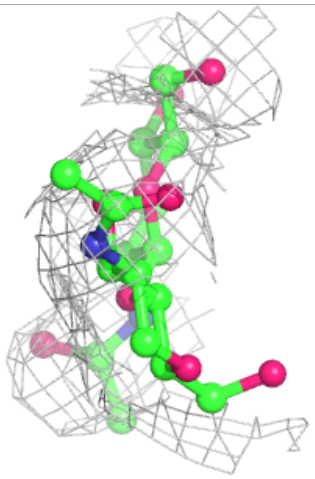


Electron density around Chain I:

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

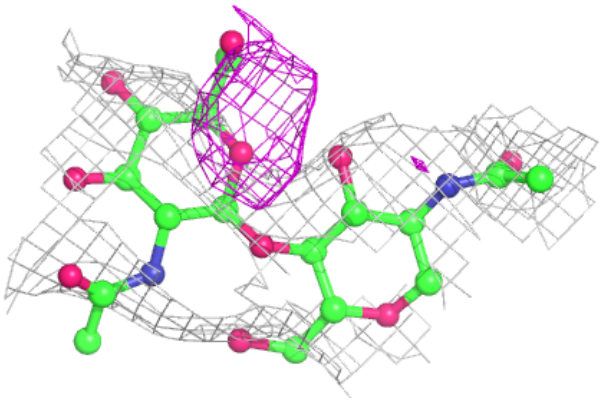


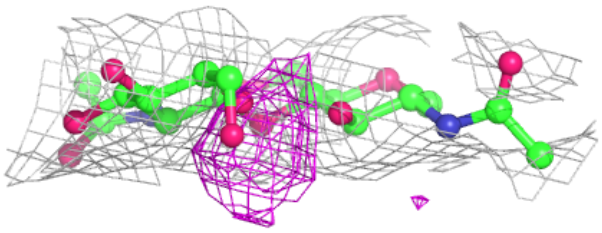


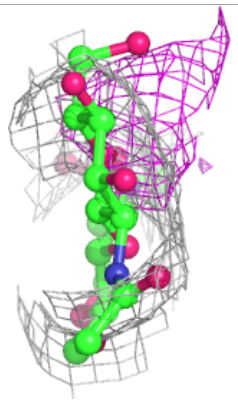


Electron density around Chain Q:

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

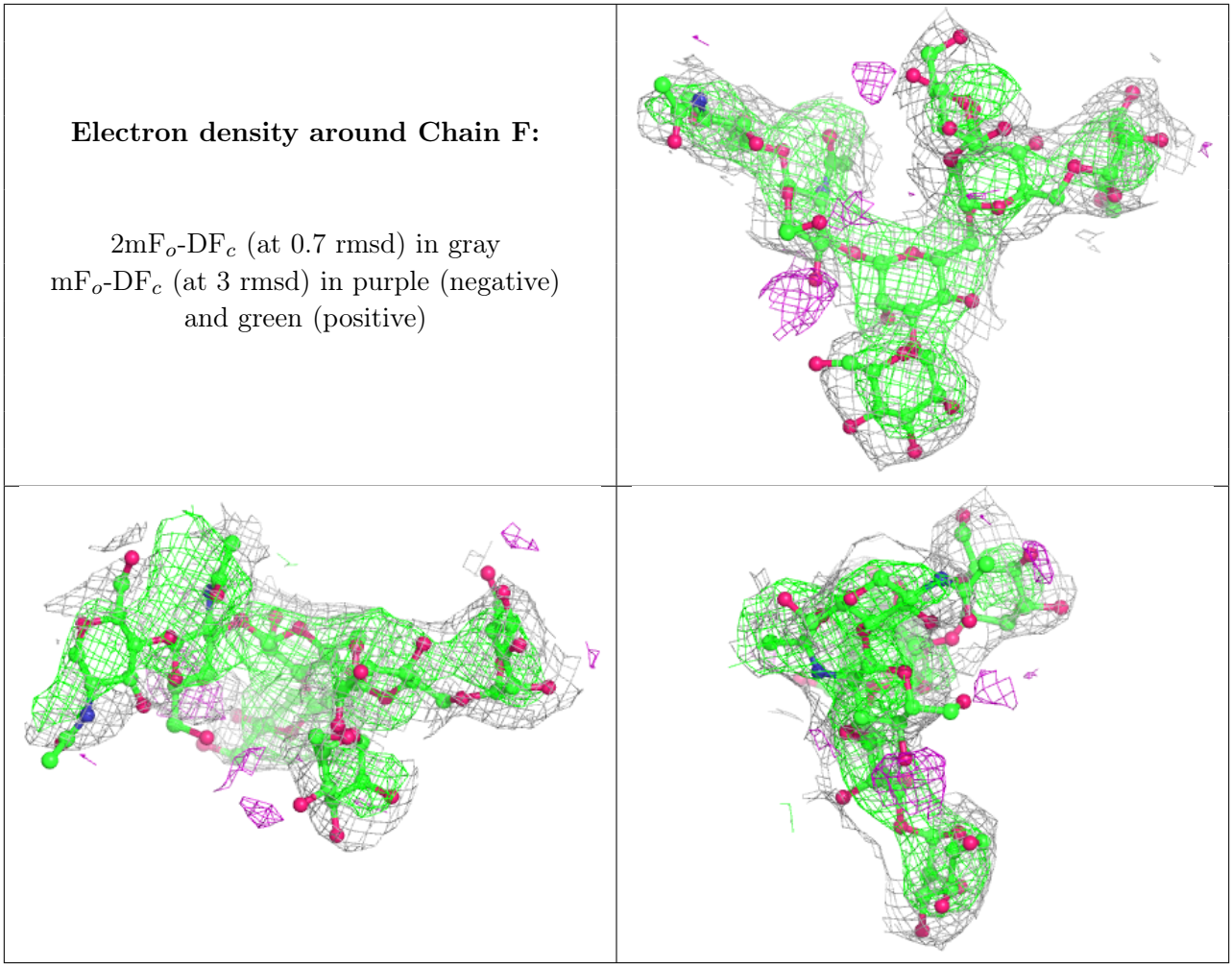






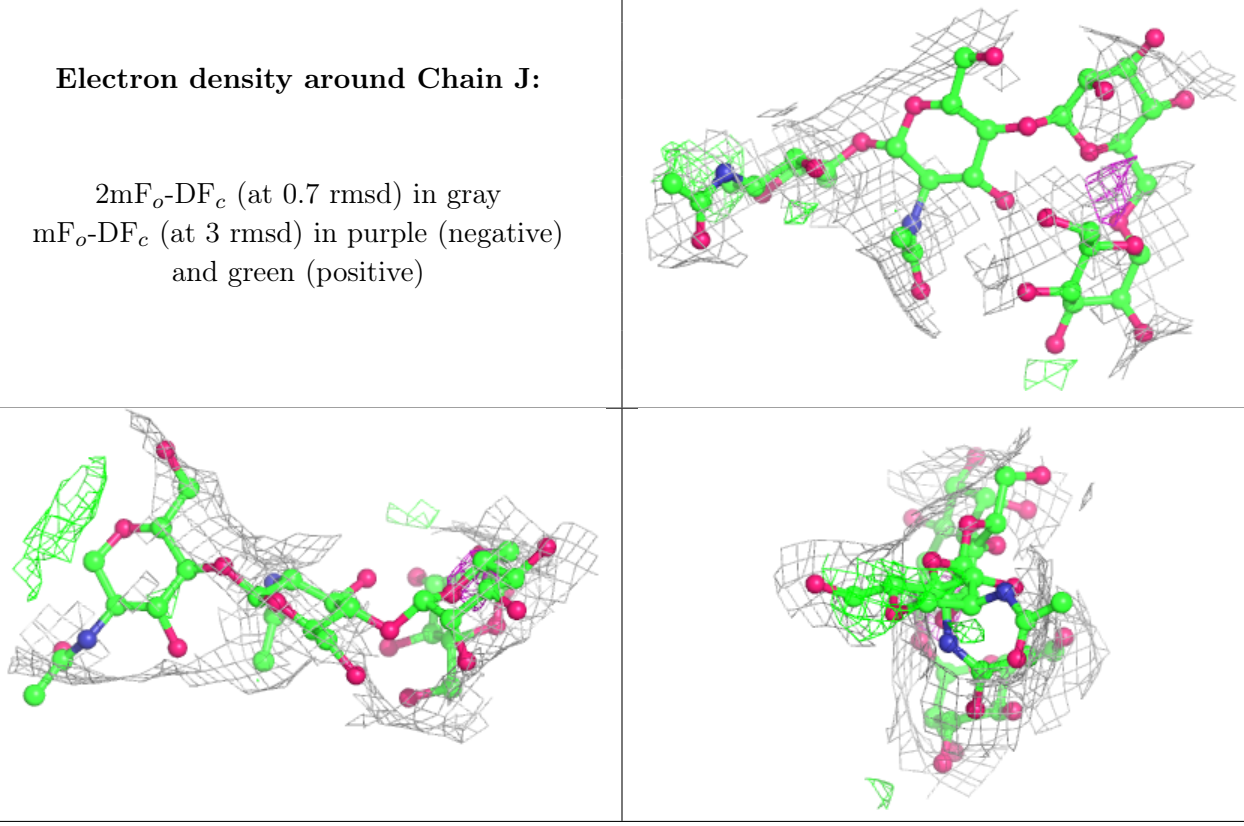
Electron density around Chain F:

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



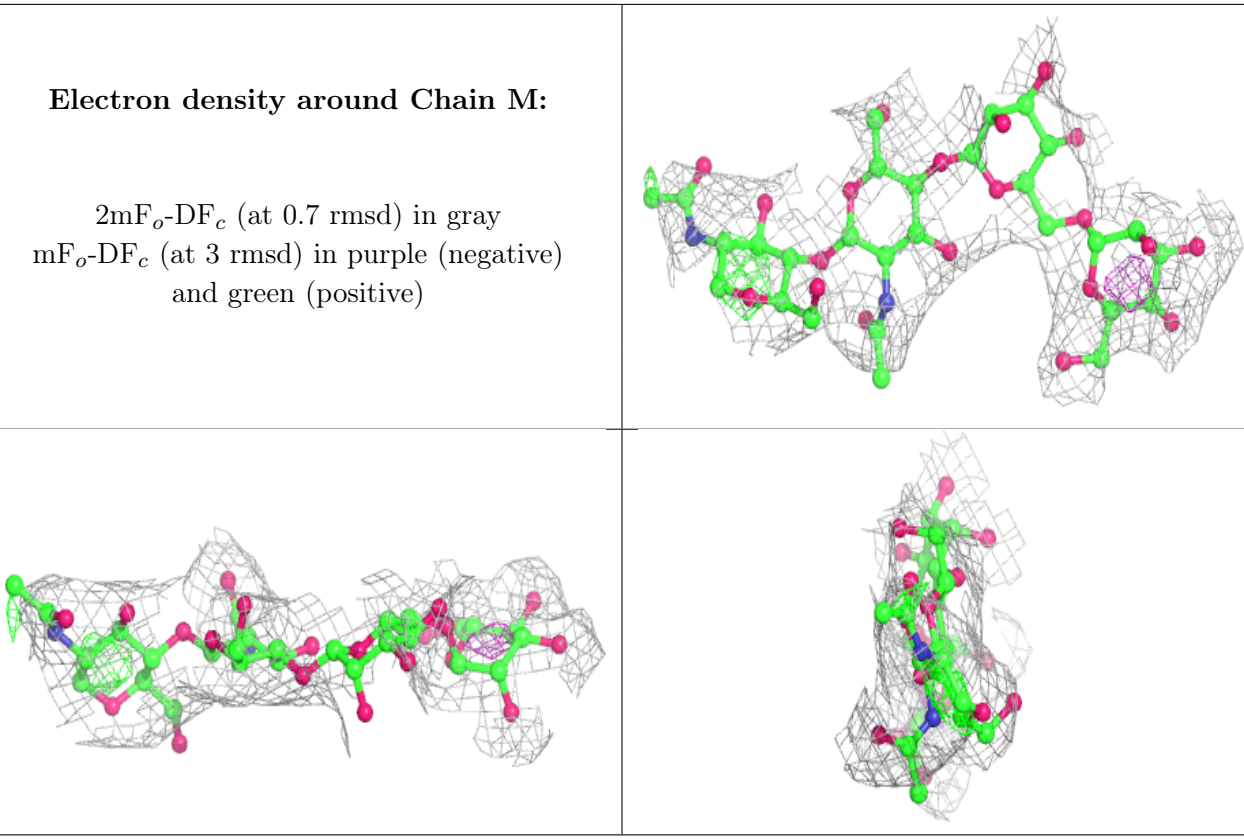
Electron density around Chain J:

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



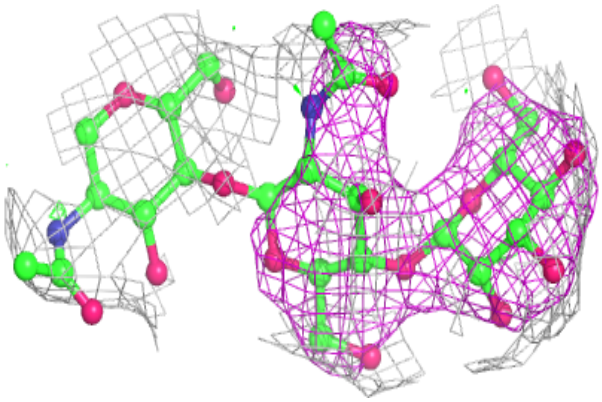
Electron density around Chain M:

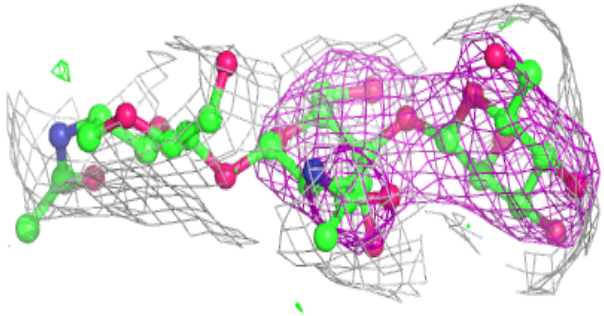
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

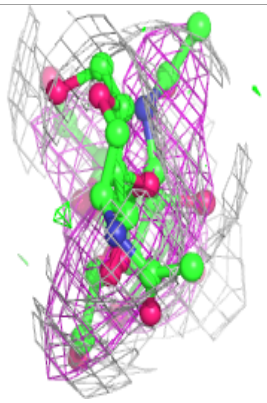


Electron density around Chain K:

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

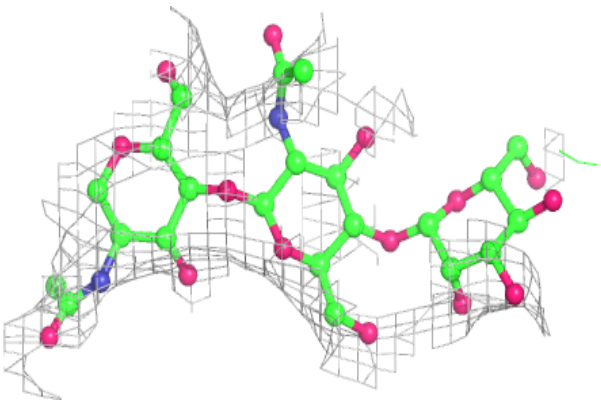


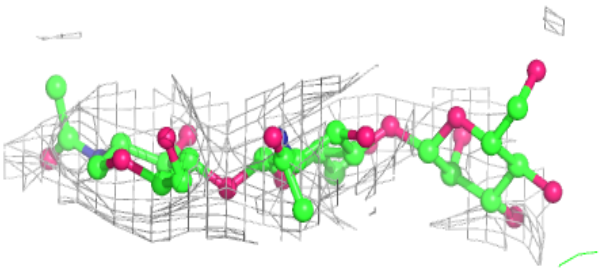


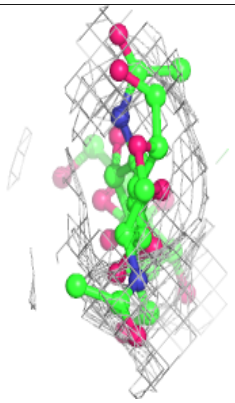


Electron density around Chain N:

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

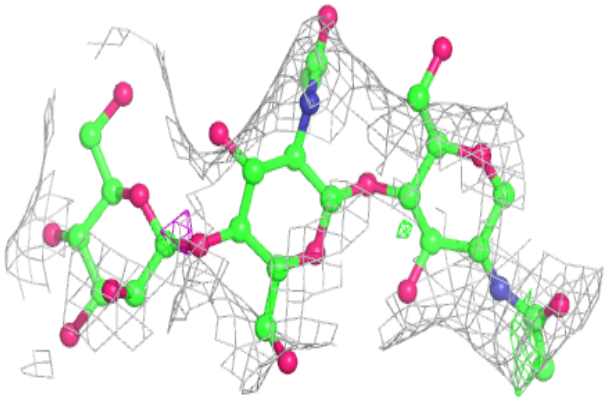


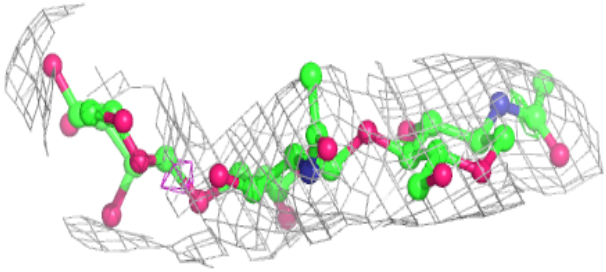


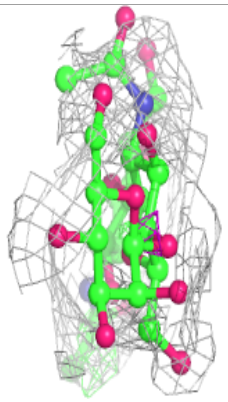


Electron density around Chain O:

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

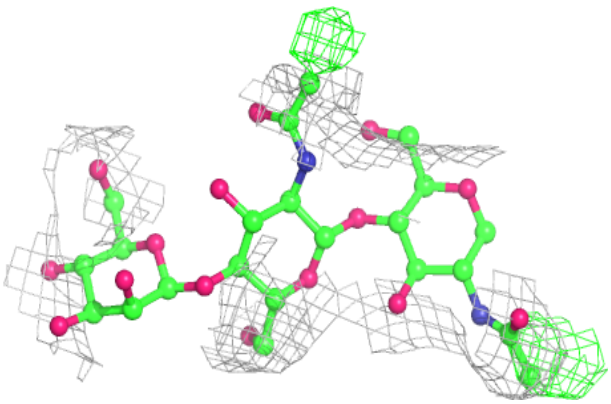


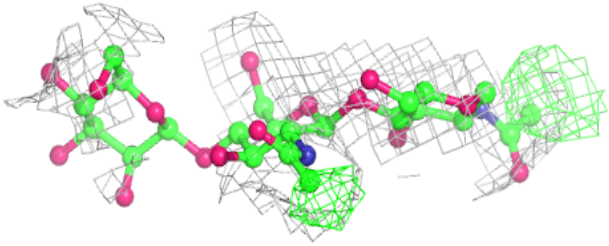


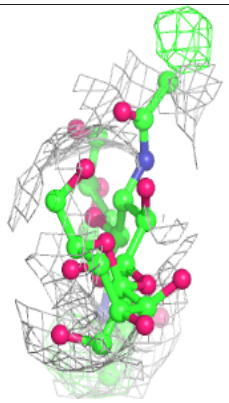


Electron density around Chain U:

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

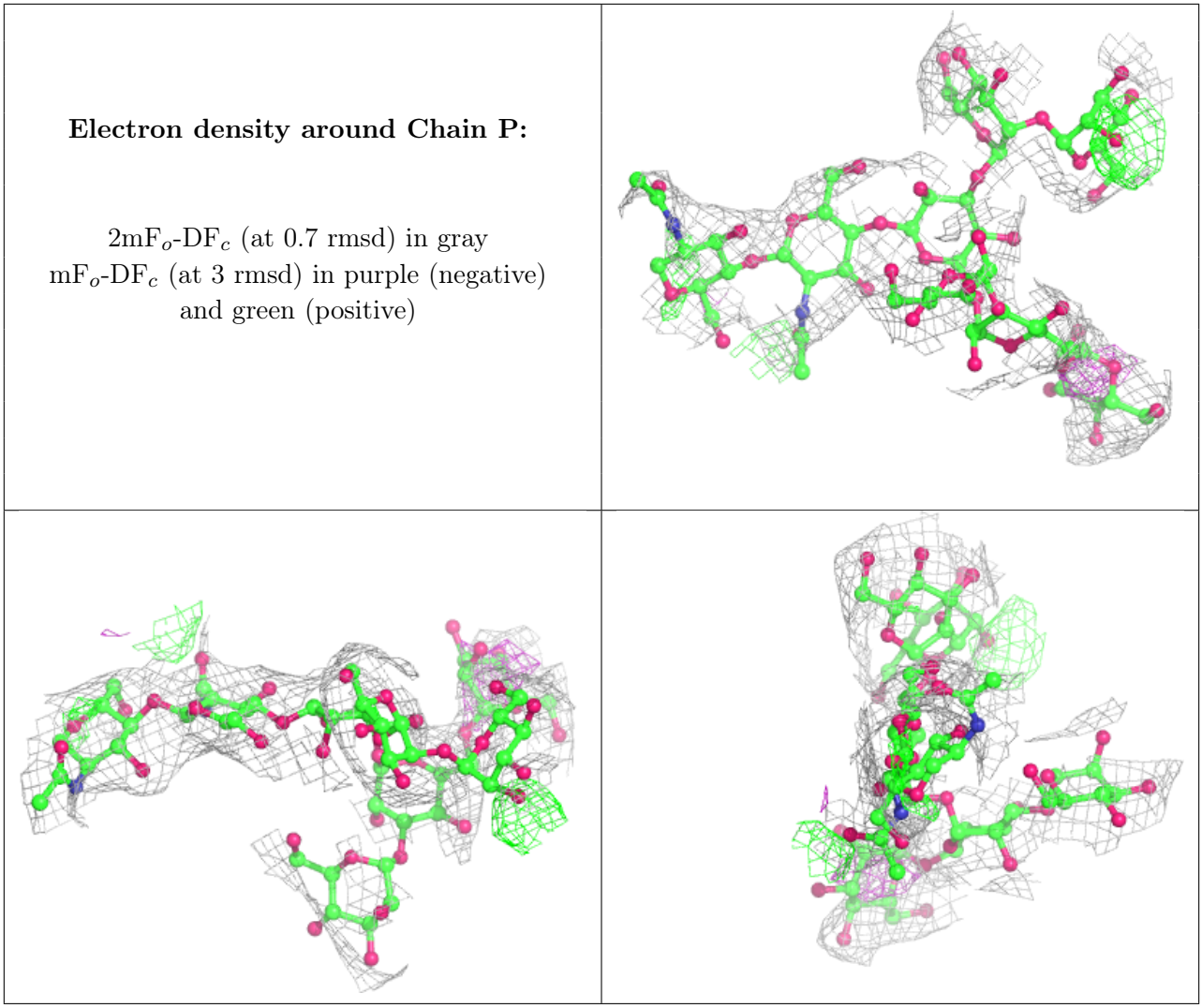






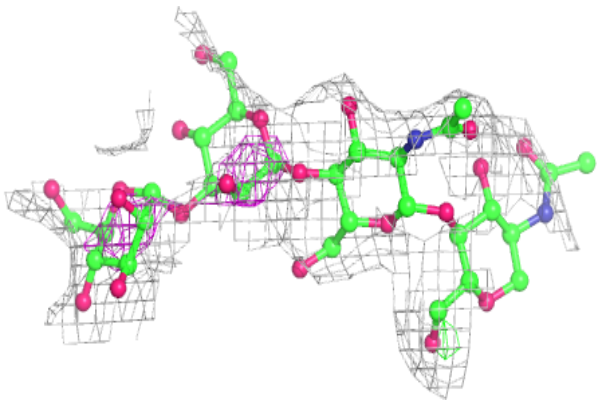
Electron density around Chain P:

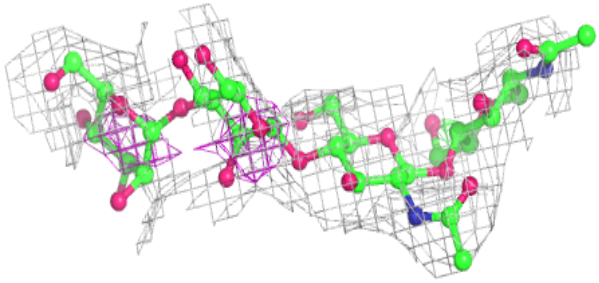
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

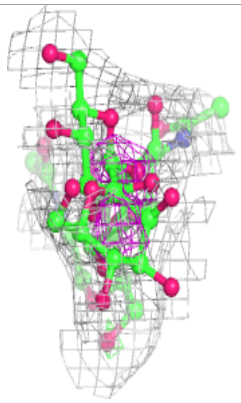


Electron density around Chain R:

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

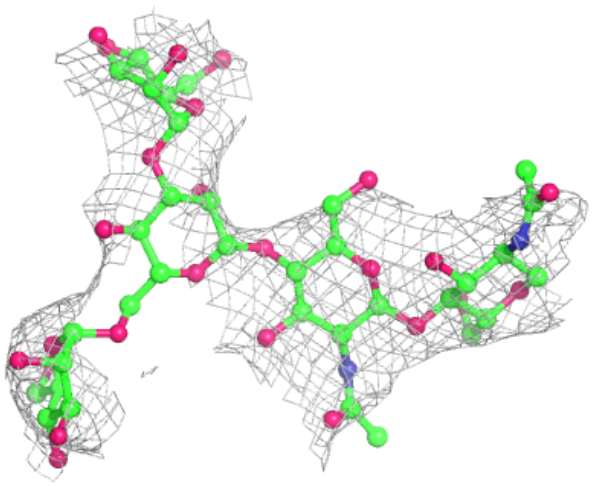


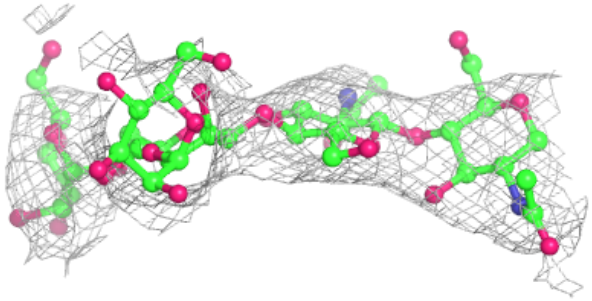


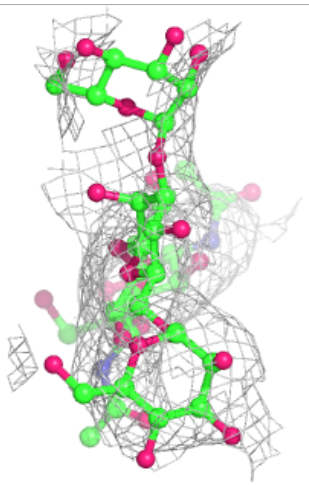


Electron density around Chain S:

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

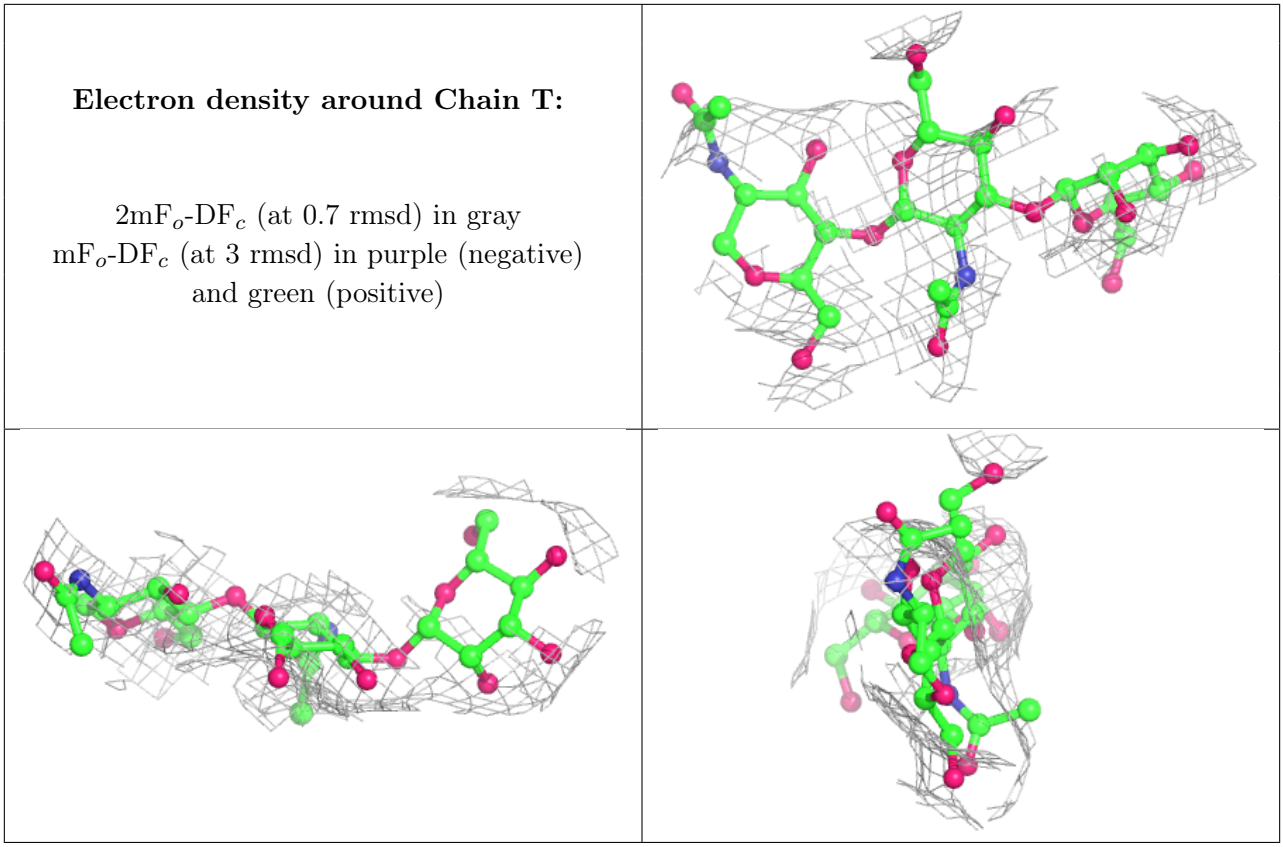






Electron density around Chain T:

$2mF_o$-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
16	NAG	G	604	14/15	0.67	0.27	179,179,179,179	0
16	NAG	G	603	14/15	0.69	0.31	179,179,179,179	0
16	NAG	G	650	14/15	0.69	0.62	179,179,179,179	0
16	NAG	G	631	14/15	0.74	0.33	179,179,179,179	0
16	NAG	B	701	14/15	0.78	0.27	179,179,179,179	0
16	NAG	B	708	14/15	0.79	0.36	179,179,179,179	0
16	NAG	G	616	14/15	0.82	0.40	179,179,179,179	0
16	NAG	G	643	14/15	0.84	0.26	179,179,179,179	0

6.5 Other polymers

There are no such residues in this entry.