Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 05:04 pm GMT

PDB ID	:	4UO0
Title	:	Structure of the A_Equine_Richmond_07 H3 haemagglutinin
Authors	:	Vachieri, S.G.; Collins, P.J.; Haire, L.F.; Ogrodowicz, R.W.; Martin, S.R.; Walker, P.A.; Xiong, X.; Gamblin, S.J.; Skehel, J.J.
Deposited on	:	2014-05-31
Resolution	:	1.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

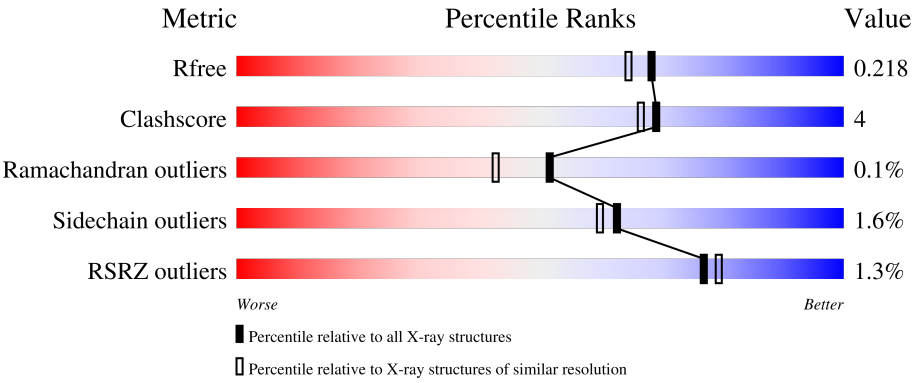
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	A	329	2% 91% 7%
1	C	329	92% 5%
1	E	329	91% 7%
2	B	172	92% 8%
2	D	172	2% 88% 9%

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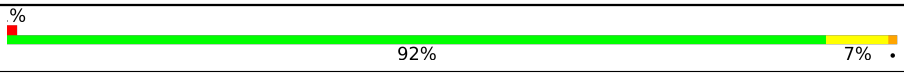
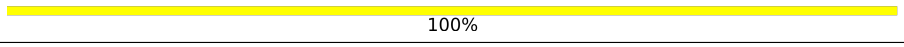
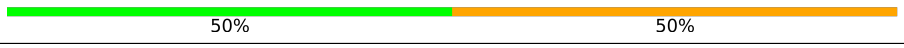
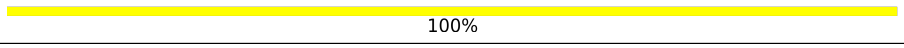
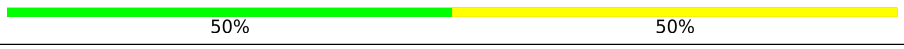
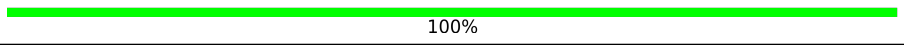
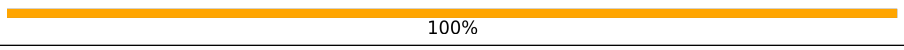
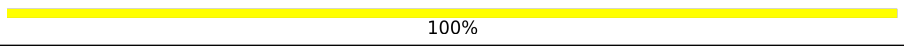
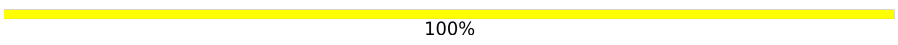
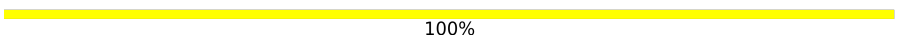
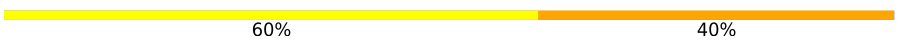
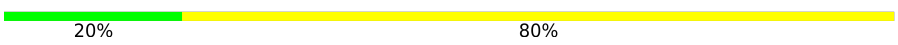
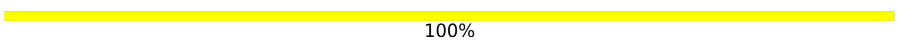
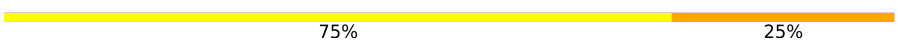
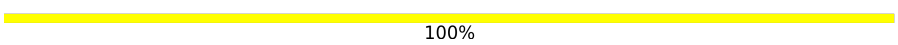
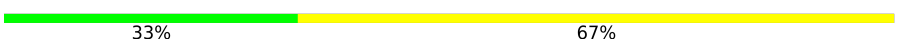
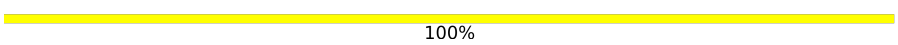
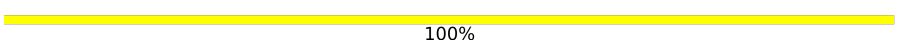
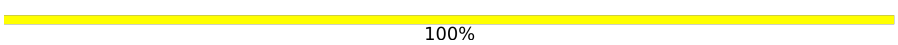
Mol	Chain	Length	Quality of chain
2	F	172	
3	G	2	
3	H	2	
3	J	2	
3	L	2	
3	R	2	
3	V	2	
3	W	2	
3	Y	2	
3	a	2	
4	I	5	
4	P	5	
4	Q	5	
4	X	5	
5	K	4	
6	M	3	
6	O	3	
6	T	3	
7	N	2	
8	S	6	
9	U	3	
9	Z	3	
9	b	3	

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
10	BMA	A	604	-	-	-	X
12	NAG	C	601	-	-	-	X
12	NAG	E	621	-	-	-	X
3	NAG	G	2	-	-	-	X
3	NAG	H	2	-	-	-	X
3	NAG	L	1	X	-	-	-
3	NAG	W	2	-	-	-	X
3	NAG	Y	2	-	-	-	X
4	MAN	P	4	-	-	-	X
4	MAN	P	5	-	-	-	X
5	FUC	K	4	X	-	-	-
7	FUC	N	2	X	-	-	-
8	FUC	S	6	X	-	-	-
9	FUC	U	3	X	-	-	-
9	FUC	Z	3	X	-	-	-
9	FUC	b	3	X	-	-	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 14213 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 HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	8	0
			2573	1612	454	492	15			
1	C	320	Total	C	N	O	S	0	1	0
			2496	1560	441	480	15			
1	E	325	Total	C	N	O	S	0	4	0
			2548	1593	449	491	15			

- Molecule 2 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	6	0
			1428	896	242	283	7			
2	D	172	Total	C	N	O	S	0	4	0
			1421	890	245	279	7			
2	F	172	Total	C	N	O	S	0	7	0
			1437	903	245	281	8			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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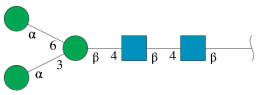
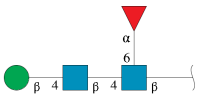
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	L	2	Total C N O 28 16 2 10	0	0	0
3	R	2	Total C N O 28 16 2 10	0	0	0
3	V	2	Total C N O 28 16 2 10	0	0	0
3	W	2	Total C N O 28 16 2 10	0	0	0
3	Y	2	Total C N O 28 16 2 10	0	0	0
3	a	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 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.



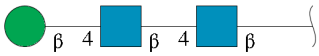
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	I	5	Total C N O 61 34 2 25	0	0	0
4	P	5	Total C N O 61 34 2 25	0	0	0
4	Q	5	Total C N O 61 34 2 25	0	0	0
4	X	5	Total C N O 61 34 2 25	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	K	4	Total C N O 49 28 2 19	0	0	0

- Molecule 6 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.

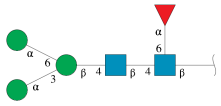


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	T	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

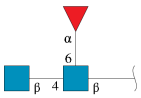
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	N	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 8 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



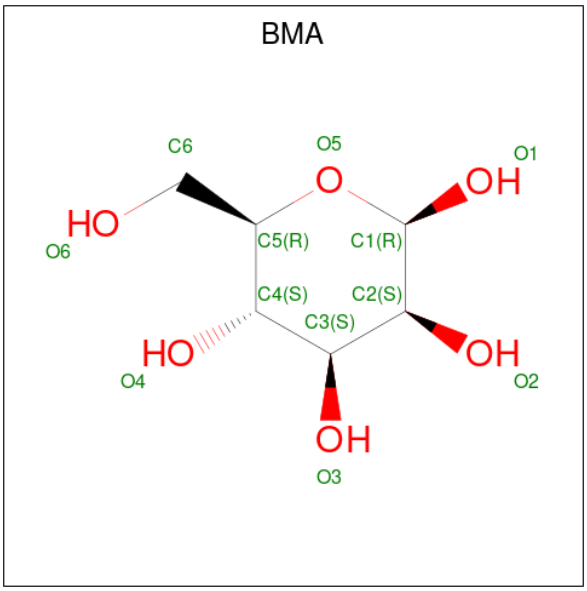
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	S	6	Total	C	N	O	0	0	0
			71	40	2	29			

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



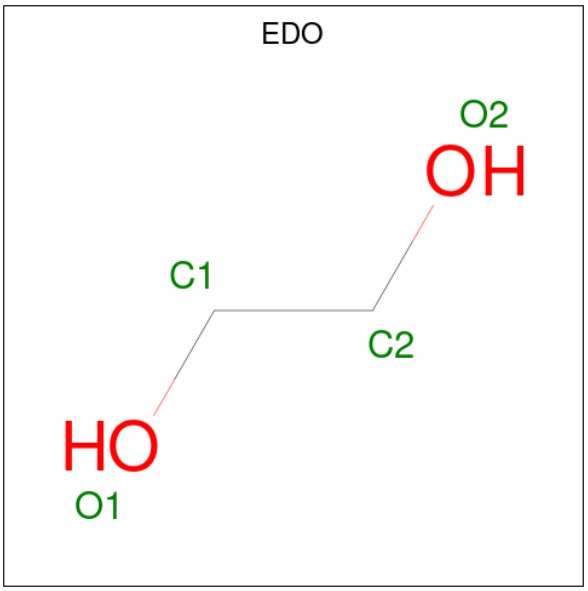
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	U	3	Total C N O 38 22 2 14	0	0	0
9	Z	3	Total C N O 38 22 2 14	0	0	0
9	b	3	Total C N O 38 22 2 14	0	0	0

- Molecule 10 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



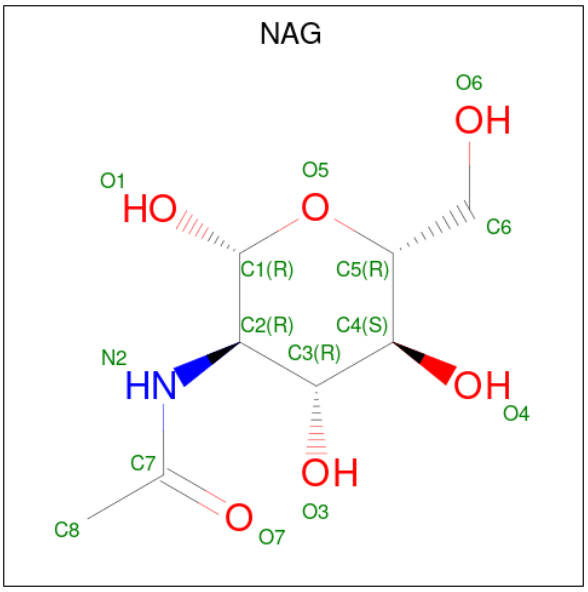
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 11 6 5	0	0

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	E	1	Total C O 4 2 2	0	0
11	E	1	Total C O 4 2 2	0	0
11	F	1	Total C O 4 2 2	0	0
11	F	1	Total C O 4 2 2	0	0
11	F	1	Total C O 4 2 2	0	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 13 is water.

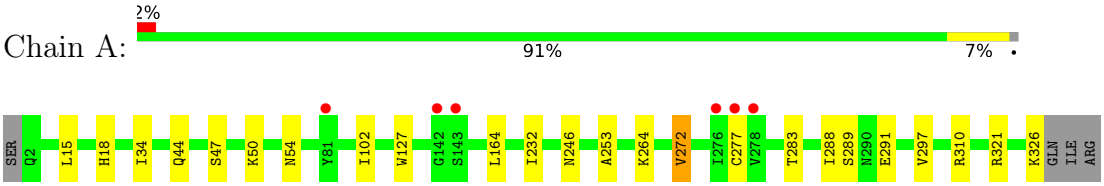
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	314	Total O 314 314	0	0
13	B	191	Total O 191 191	0	0
13	C	283	Total O 283 283	0	0
13	D	174	Total O 174 174	0	0
13	E	256	Total O 256 256	0	0
13	F	134	Total O 134 134	0	0

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.

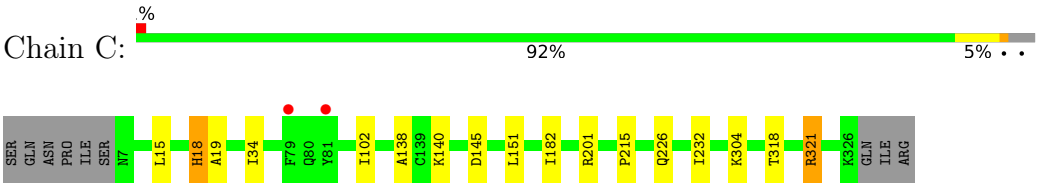
• Molecule 1: HEMAGGLUTININ

Chain A:



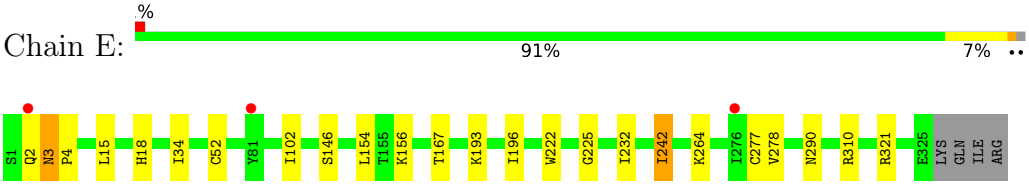
• Molecule 1: HEMAGGLUTININ

Chain C:



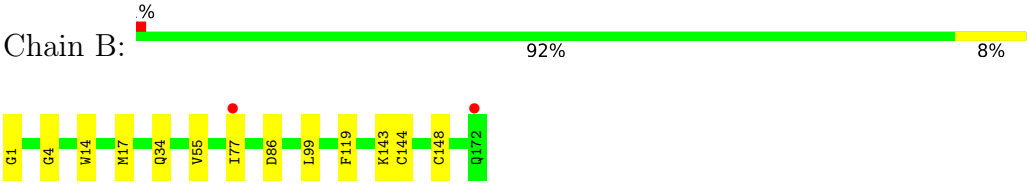
• Molecule 1: HEMAGGLUTININ

Chain E:



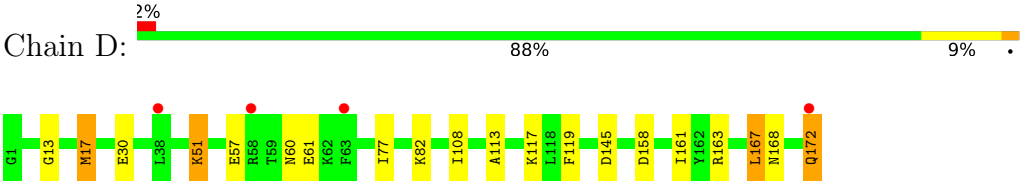
• Molecule 2: HEMAGGLUTININ

Chain B:



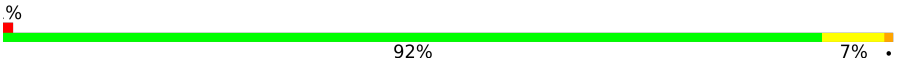
• Molecule 2: HEMAGGLUTININ

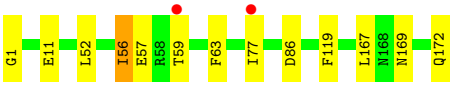
Chain D:



• Molecule 2: HEMAGGLUTININ

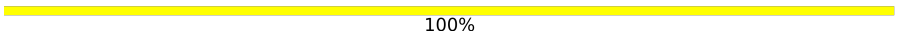
Chain F:





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

Chain G:

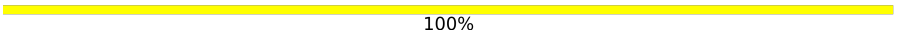


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

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

Chain J:

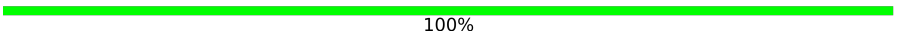


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

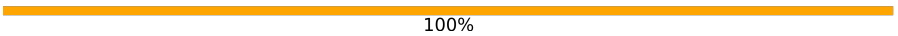
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



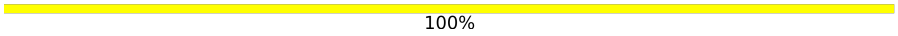
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



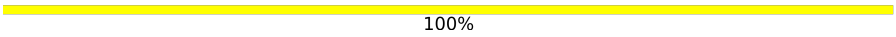
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



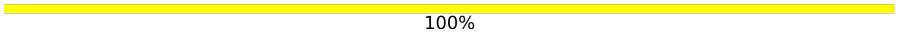
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



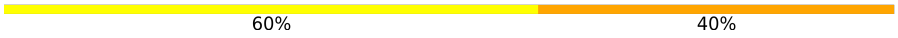
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 4: 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 I:



• Molecule 4: 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

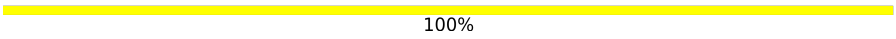
Chain P:

• Molecule 4: 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 Q:

• Molecule 4: 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 X:

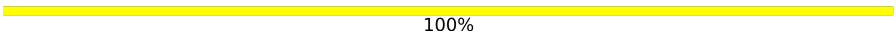


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

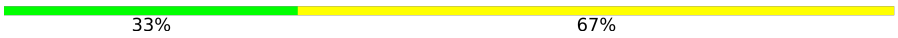
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

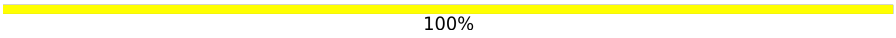


• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

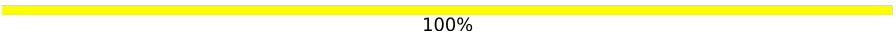
• Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



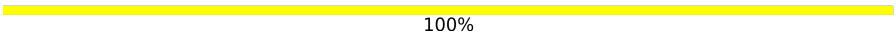
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



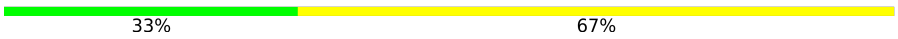
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



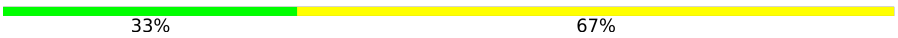
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



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

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.41Å 129.33Å 192.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.37 – 1.90 46.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (107.37-1.90) 97.3 (46.58-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.191 , 0.218 0.191 , 0.218	Depositor DCC
R_{free} test set	7614 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14213	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: EDO, NAG, MAN, FUC, 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	A	0.39	0/2651	0.56	0/3598
1	C	0.41	0/2552	0.58	0/3464
1	E	0.39	0/2614	0.57	0/3551
2	B	0.44	0/1471	0.57	0/1978
2	D	0.42	0/1458	0.59	0/1960
2	F	0.44	0/1483	0.61	0/1994
All	All	0.41	0/12229	0.58	0/16545

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2573	0	2547	16	0
1	C	2496	0	2440	14	0
1	E	2548	0	2499	16	0
2	B	1428	0	1363	25	0
2	D	1421	0	1360	19	0
2	F	1437	0	1386	19	0
3	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	28	0	25	1	0
3	J	28	0	25	0	0
3	L	28	0	25	0	0
3	R	28	0	25	0	0
3	V	28	0	25	1	0
3	W	28	0	25	0	0
3	Y	28	0	25	0	0
3	a	28	0	25	0	0
4	I	61	0	52	2	0
4	P	61	0	52	4	0
4	Q	61	0	52	1	0
4	X	61	0	52	0	0
5	K	49	0	43	2	0
6	M	39	0	34	0	0
6	O	39	0	34	0	0
6	T	39	0	34	1	0
7	N	24	0	22	0	0
8	S	71	0	61	0	0
9	U	38	0	34	0	0
9	Z	38	0	34	0	0
9	b	38	0	34	0	0
10	A	11	0	10	0	0
11	A	8	0	12	1	0
11	B	8	0	12	0	0
11	C	8	0	12	0	0
11	D	4	0	6	0	0
11	E	8	0	12	1	0
11	F	12	0	18	0	0
12	C	14	0	13	0	0
12	E	14	0	13	0	0
13	A	314	0	0	4	0
13	B	191	0	0	2	0
13	C	283	0	0	0	0
13	D	174	0	0	2	0
13	E	256	0	0	1	0
13	F	134	0	0	2	0
All	All	14213	0	12466	93	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 4.

All (93) 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)
2:B:77[A]:ILE:HD12	2:F:77[A]:ILE:CD1	2.03	0.88
2:B:77[A]:ILE:HD12	2:F:77[A]:ILE:HD11	1.58	0.83
2:B:77[A]:ILE:CD1	2:F:77[A]:ILE:CD1	2.57	0.82
1:E:167:THR:OG1	1:E:242:ILE:HD11	1.80	0.81
4:I:3:BMA:H62	4:I:5:MAN:H5	1.68	0.76
1:C:102:ILE:HG12	1:C:232:ILE:HB	1.67	0.74
1:E:156:LYS:HE3	1:E:193:LYS:O	1.88	0.74
2:B:77[A]:ILE:HD11	2:F:77[A]:ILE:HD13	1.73	0.71
1:C:15:LEU:CD2	2:D:119:PHE:HA	2.21	0.71
1:C:304:LYS:HG3	2:D:61:GLU:HG3	1.74	0.69
2:B:77[B]:ILE:HD11	2:D:77[B]:ILE:HD12	1.76	0.68
13:B:2079:HOH:O	2:F:86[B]:ASP:OD2	2.12	0.67
2:B:77[B]:ILE:HD13	2:D:77[B]:ILE:HD11	1.77	0.65
2:B:77[A]:ILE:CD1	2:F:77[A]:ILE:HD11	2.26	0.64
1:A:44:GLN:HG2	1:A:288[B]:ILE:HG23	1.78	0.63
1:E:34:ILE:HD11	1:E:321:ARG:HD2	1.80	0.63
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.83	0.60
2:B:77[A]:ILE:CD1	2:F:77[A]:ILE:HD13	2.29	0.60
1:E:15[B]:LEU:HD13	2:F:119:PHE:HA	1.83	0.60
1:E:156:LYS:HD3	1:E:196:ILE:HD11	1.83	0.60
1:A:44:GLN:HG2	1:A:288[B]:ILE:CG2	2.32	0.59
1:C:304:LYS:CG	2:D:61:GLU:HG3	2.33	0.58
1:C:138:ALA:HB2	1:C:226:GLN:HG2	1.85	0.58
2:B:143:LYS:HD2	5:K:4:FUC:H62	1.86	0.57
3:V:1:NAG:H3	3:V:2:NAG:H61	1.86	0.57
2:B:77[B]:ILE:CD1	2:D:77[B]:ILE:HD12	2.33	0.57
1:C:18:HIS:HD2	13:D:2020:HOH:O	1.87	0.57
2:D:168:ASN:O	2:D:172:GLN:HB3	2.05	0.56
1:C:34:ILE:HD11	1:C:321:ARG:HD2	1.87	0.56
2:B:14:TRP:HE3	2:B:17[B]:MET:HE2	1.72	0.55
1:A:288[B]:ILE:HD11	1:A:297:VAL:HG11	1.88	0.55
2:B:77[B]:ILE:CD1	2:D:77[B]:ILE:CD1	2.85	0.55
1:C:15:LEU:HD22	2:D:119:PHE:HA	1.89	0.54
1:E:15[A]:LEU:HD22	2:F:119:PHE:HA	1.89	0.54
4:P:2:NAG:H62	4:P:3:BMA:H2	1.89	0.54
2:B:77[B]:ILE:HD13	2:D:77[B]:ILE:CD1	2.38	0.53
13:A:2075:HOH:O	3:H:1:NAG:H82	2.09	0.52
2:B:144:CYS:HG	2:B:148:CYS:HG	1.57	0.52
1:A:289[A]:SER:OG	1:A:291:GLU:HG2	2.10	0.52
1:E:310:ARG:NH2	2:F:86[B]:ASP:OD1	2.44	0.51
1:E:290:ASN:HB2	2:F:59:THR:HG21	1.92	0.50
1:A:283:THR:CG2	1:A:288[B]:ILE:HD13	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:SER:HA	1:A:288[A]:ILE:HG22	1.94	0.50
2:D:30:GLU:OE2	2:D:145:ASP:HB2	2.12	0.49
1:A:47:SER:HA	1:A:288[B]:ILE:HG13	1.94	0.49
13:E:2012:HOH:O	2:F:169:ASN:ND2	2.40	0.49
1:A:102:ILE:HG12	1:A:232:ILE:HB	1.95	0.49
2:F:52:LEU:HD13	2:F:56[A]:ILE:HD11	1.96	0.48
1:E:167:THR:HG1	1:E:242:ILE:HD11	1.79	0.48
1:C:19:ALA:HB2	2:D:13:GLY:HA3	1.95	0.48
2:B:4:GLY:HA3	2:D:117:LYS:HD2	1.95	0.47
2:B:17[A]:MET:HE3	2:B:34:GLN:CG	2.44	0.47
1:C:182:ILE:HD11	1:C:215:PRO:HG3	1.96	0.47
4:P:2:NAG:H5	4:P:3:BMA:O2	2.14	0.47
2:B:77[A]:ILE:HD11	2:F:77[A]:ILE:CD1	2.33	0.47
2:D:158:ASP:HB3	2:D:161:ILE:HD12	1.98	0.46
1:E:102:ILE:HG12	1:E:232:ILE:HB	1.97	0.46
2:D:17[A]:MET:HE3	2:D:17[A]:MET:HA	1.97	0.46
2:D:82:LYS:NZ	13:D:2108:HOH:O	2.43	0.46
4:I:3:BMA:H62	4:I:5:MAN:C5	2.42	0.46
2:D:113:ALA:O	2:D:117:LYS:HG3	2.16	0.46
1:A:54:ASN:HB2	1:A:277:CYS:O	2.16	0.46
1:A:164:LEU:O	1:A:246:ASN:HA	2.16	0.45
2:B:17[A]:MET:CE	2:B:34:GLN:HG2	2.45	0.45
13:A:2228:HOH:O	4:Q:1:NAG:H82	2.17	0.45
1:C:318:THR:HG21	6:T:1:NAG:H61	1.97	0.45
1:E:264:LYS:HB3	2:F:63:PHE:CD2	2.52	0.45
1:C:321:ARG:HH11	1:C:321:ARG:HG3	1.82	0.44
11:A:1328:EDO:H11	13:A:2207:HOH:O	2.18	0.44
2:F:169:ASN:HA	2:F:172:GLN:HE21	1.83	0.44
1:E:222:TRP:CZ2	1:E:225:GLY:HA2	2.52	0.44
2:B:17[A]:MET:HE2	2:B:34:GLN:HG2	2.00	0.43
1:E:52:CYS:HB3	1:E:277:CYS:O	2.20	0.42
2:B:17[A]:MET:CE	2:B:34:GLN:CG	2.97	0.42
1:E:264:LYS:HE3	2:F:63:PHE:CE2	2.54	0.42
1:A:50:LYS:HA	1:A:272:VAL:HG13	2.02	0.42
2:B:143:LYS:HD2	5:K:4:FUC:C6	2.50	0.42
1:E:146:SER:OG	11:E:1327:EDO:H11	2.20	0.42
1:C:140:LYS:NZ	1:C:145:ASP:OD1	2.52	0.42
2:D:163:ARG:HG2	2:D:167:LEU:HD22	2.01	0.41
4:P:2:NAG:C6	4:P:3:BMA:H2	2.50	0.41
4:P:3:BMA:H3	4:P:4:MAN:H2	1.65	0.41
1:A:34:ILE:HD11	1:A:321:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:2196:HOH:O	1:C:201:ARG:NE	2.53	0.41
1:E:3[B]:ASN:HA	1:E:4:PRO:HD2	1.86	0.41
2:F:1:GLY:HA3	13:F:2003:HOH:O	2.19	0.41
2:B:1:GLY:HA3	13:B:2003:HOH:O	2.21	0.41
2:B:55:VAL:HG21	2:B:99:LEU:HD11	2.03	0.41
1:A:127:TRP:CZ2	1:A:253:ALA:HB1	2.56	0.40
2:D:51:LYS:HB2	2:D:51:LYS:HE2	1.96	0.40
2:F:11:GLU:HG3	13:F:2007:HOH:O	2.22	0.40
1:A:310:ARG:NH2	2:B:86[B]:ASP:OD1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	331/329 (101%)	323 (98%)	8 (2%)	0	100 100
1	C	319/329 (97%)	309 (97%)	10 (3%)	0	100 100
1	E	327/329 (99%)	314 (96%)	10 (3%)	3 (1%)	17 7
2	B	176/172 (102%)	167 (95%)	9 (5%)	0	100 100
2	D	174/172 (101%)	166 (95%)	8 (5%)	0	100 100
2	F	177/172 (103%)	169 (96%)	8 (4%)	0	100 100
All	All	1504/1503 (100%)	1448 (96%)	53 (4%)	3 (0%)	51 38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	GLN
1	E	3[A]	ASN
1	E	3[B]	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/292 (101%)	292 (99%)	4 (1%)	67	65
1	C	283/292 (97%)	280 (99%)	3 (1%)	73	73
1	E	291/292 (100%)	287 (99%)	4 (1%)	67	65
2	B	151/146 (103%)	151 (100%)	0	100	100
2	D	150/146 (103%)	142 (95%)	8 (5%)	22	13
2	F	153/146 (105%)	149 (97%)	4 (3%)	46	39
All	All	1324/1314 (101%)	1301 (98%)	23 (2%)	62	57

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	264	LYS
1	A	272	VAL
1	A	326	LYS
1	C	18	HIS
1	C	151	LEU
1	C	321	ARG
2	D	17[A]	MET
2	D	17[B]	MET
2	D	51	LYS
2	D	57	GLU
2	D	60	ASN
2	D	108	ILE
2	D	167	LEU
2	D	172	GLN
1	E	18	HIS
1	E	154	LEU
1	E	242	ILE
1	E	278	VAL
2	F	56[A]	ILE
2	F	56[B]	ILE
2	F	57	GLU

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Mol	Chain	Res	Type
2	F	167	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	188	ASN
1	C	18	HIS
1	C	296	ASN
2	F	172	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)

68 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	G	1	1,3	14,14,15	0.54	0	17,19,21	1.48	2 (11%)
3	NAG	G	2	3	14,14,15	0.53	0	17,19,21	1.03	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.62	0	17,19,21	1.21	1 (5%)
3	NAG	H	2	3	14,14,15	0.55	0	17,19,21	0.84	0
4	NAG	I	1	1,4	14,14,15	0.66	0	17,19,21	1.05	1 (5%)
4	NAG	I	2	4	14,14,15	0.59	0	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BMA	I	3	4	11,11,12	0.63	0	15,15,17	2.75	5 (33%)
4	MAN	I	4	4	11,11,12	0.52	0	15,15,17	0.91	1 (6%)
4	MAN	I	5	4	11,11,12	0.60	0	15,15,17	1.40	2 (13%)
3	NAG	J	1	1,3	14,14,15	0.62	0	17,19,21	0.90	1 (5%)
3	NAG	J	2	3	14,14,15	0.67	0	17,19,21	1.66	3 (17%)
5	NAG	K	1	1,5	14,14,15	0.67	0	17,19,21	1.07	2 (11%)
5	NAG	K	2	5	14,14,15	0.59	0	17,19,21	1.25	3 (17%)
5	BMA	K	3	5	11,11,12	0.43	0	15,15,17	1.34	3 (20%)
5	FUC	K	4	5	10,10,11	0.65	0	14,14,16	1.00	1 (7%)
3	NAG	L	1	1,3	14,14,15	0.62	0	17,19,21	1.08	0
3	NAG	L	2	3	14,14,15	0.59	0	17,19,21	1.39	2 (11%)
6	NAG	M	1	6,1	14,14,15	0.46	0	17,19,21	1.10	2 (11%)
6	NAG	M	2	6	14,14,15	0.52	0	17,19,21	1.07	1 (5%)
6	BMA	M	3	6	11,11,12	0.42	0	15,15,17	0.94	1 (6%)
7	NAG	N	1	2,7	14,14,15	0.55	0	17,19,21	1.73	2 (11%)
7	FUC	N	2	7	10,10,11	0.65	0	14,14,16	1.06	2 (14%)
6	NAG	O	1	6,1	14,14,15	0.60	0	17,19,21	0.93	0
6	NAG	O	2	6	14,14,15	0.61	0	17,19,21	1.32	3 (17%)
6	BMA	O	3	6	11,11,12	0.67	0	15,15,17	2.41	4 (26%)
4	NAG	P	1	1,4	14,14,15	0.62	0	17,19,21	1.72	3 (17%)
4	NAG	P	2	4	14,14,15	0.75	0	17,19,21	1.20	1 (5%)
4	BMA	P	3	4	11,11,12	0.50	0	15,15,17	0.98	1 (6%)
4	MAN	P	4	4	11,11,12	0.81	0	15,15,17	1.68	2 (13%)
4	MAN	P	5	4	11,11,12	0.52	0	15,15,17	1.59	2 (13%)
4	NAG	Q	1	1,4	14,14,15	0.60	0	17,19,21	0.90	0
4	NAG	Q	2	4	14,14,15	0.52	0	17,19,21	1.42	3 (17%)
4	BMA	Q	3	4	11,11,12	0.38	0	15,15,17	0.84	0
4	MAN	Q	4	4	11,11,12	0.59	0	15,15,17	0.90	1 (6%)
4	MAN	Q	5	4	11,11,12	0.61	0	15,15,17	1.29	2 (13%)
3	NAG	R	1	1,3	14,14,15	0.62	0	17,19,21	1.04	0
3	NAG	R	2	3	14,14,15	0.49	0	17,19,21	0.74	0
8	NAG	S	1	8,1	14,14,15	0.61	0	17,19,21	1.12	2 (11%)
8	NAG	S	2	8	14,14,15	0.56	0	17,19,21	0.95	1 (5%)
8	BMA	S	3	8	11,11,12	0.56	0	15,15,17	1.36	3 (20%)
8	MAN	S	4	8	11,11,12	0.53	0	15,15,17	1.02	1 (6%)
8	MAN	S	5	8	11,11,12	0.59	0	15,15,17	2.35	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	FUC	S	6	8	10,10,11	0.76	0	14,14,16	2.78	5 (35%)
6	NAG	T	1	6,1	14,14,15	0.64	0	17,19,21	1.42	3 (17%)
6	NAG	T	2	6	14,14,15	0.61	0	17,19,21	0.99	1 (5%)
6	BMA	T	3	6	11,11,12	0.38	0	15,15,17	1.01	2 (13%)
9	NAG	U	1	2,9	14,14,15	0.55	0	17,19,21	1.30	3 (17%)
9	NAG	U	2	9	14,14,15	0.53	0	17,19,21	1.05	1 (5%)
9	FUC	U	3	9	10,10,11	0.78	0	14,14,16	1.41	2 (14%)
3	NAG	V	1	1,3	14,14,15	0.73	0	17,19,21	2.47	6 (35%)
3	NAG	V	2	3	14,14,15	0.46	0	17,19,21	1.96	2 (11%)
3	NAG	W	1	1,3	14,14,15	0.66	0	17,19,21	1.67	3 (17%)
3	NAG	W	2	3	14,14,15	0.53	0	17,19,21	0.91	1 (5%)
4	NAG	X	1	1,4	14,14,15	0.63	0	17,19,21	0.94	1 (5%)
4	NAG	X	2	4	14,14,15	0.65	0	17,19,21	0.91	1 (5%)
4	BMA	X	3	4	11,11,12	0.37	0	15,15,17	1.22	1 (6%)
4	MAN	X	4	4	11,11,12	0.60	0	15,15,17	0.95	1 (6%)
4	MAN	X	5	4	11,11,12	0.62	0	15,15,17	1.16	1 (6%)
3	NAG	Y	1	1,3	14,14,15	0.62	0	17,19,21	1.80	4 (23%)
3	NAG	Y	2	3	14,14,15	0.62	0	17,19,21	2.15	4 (23%)
9	NAG	Z	1	1,9	14,14,15	0.51	0	17,19,21	1.14	1 (5%)
9	NAG	Z	2	9	14,14,15	0.64	0	17,19,21	0.93	0
9	FUC	Z	3	9	10,10,11	0.81	0	14,14,16	1.73	3 (21%)
3	NAG	a	1	1,3	14,14,15	0.64	0	17,19,21	1.35	3 (17%)
3	NAG	a	2	3	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
9	NAG	b	1	2,9	14,14,15	0.56	0	17,19,21	1.61	3 (17%)
9	NAG	b	2	9	14,14,15	0.42	0	17,19,21	1.04	1 (5%)
9	FUC	b	3	9	10,10,11	0.73	0	14,14,16	0.80	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
3	NAG	G	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
4	MAN	I	4	4	-	2/2/19/22	0/1/1/1
4	MAN	I	5	4	-	2/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1
5	BMA	K	3	5	-	2/2/19/22	0/1/1/1
5	FUC	K	4	5	1/1/4/5	-	0/1/1/1
3	NAG	L	1	1,3	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
6	NAG	M	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
6	BMA	M	3	6	-	2/2/19/22	0/1/1/1
7	NAG	N	1	2,7	-	2/6/23/26	0/1/1/1
7	FUC	N	2	7	1/1/4/5	-	0/1/1/1
6	NAG	O	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	2/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	BMA	P	3	4	-	2/2/19/22	0/1/1/1
4	MAN	P	4	4	-	2/2/19/22	0/1/1/1
4	MAN	P	5	4	-	2/2/19/22	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	0/2/19/22	0/1/1/1
4	MAN	Q	4	4	-	0/2/19/22	1/1/1/1
4	MAN	Q	5	4	-	2/2/19/22	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
8	NAG	S	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	S	2	8	-	0/6/23/26	0/1/1/1
8	BMA	S	3	8	-	2/2/19/22	0/1/1/1
8	MAN	S	4	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	S	5	8	-	1/2/19/22	0/1/1/1
8	FUC	S	6	8	1/1/4/5	-	0/1/1/1
6	NAG	T	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	BMA	T	3	6	-	2/2/19/22	0/1/1/1
9	NAG	U	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	U	2	9	-	0/6/23/26	0/1/1/1
9	FUC	U	3	9	1/1/4/5	-	0/1/1/1
3	NAG	V	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
4	NAG	X	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	BMA	X	3	4	-	0/2/19/22	0/1/1/1
4	MAN	X	4	4	-	2/2/19/22	0/1/1/1
4	MAN	X	5	4	-	2/2/19/22	0/1/1/1
3	NAG	Y	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	6/6/23/26	0/1/1/1
9	NAG	Z	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	0/6/23/26	0/1/1/1
9	FUC	Z	3	9	1/1/4/5	-	0/1/1/1
3	NAG	a	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
9	NAG	b	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	b	2	9	-	2/6/23/26	0/1/1/1
9	FUC	b	3	9	1/1/4/5	-	0/1/1/1

There are no bond length outliers.

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	6	FUC	C1-C2-C3	-8.04	99.78	109.67
3	V	2	NAG	C1-O5-C5	7.02	121.71	112.19
3	Y	2	NAG	C2-N2-C7	6.60	132.30	122.90
3	V	1	NAG	C1-O5-C5	6.38	120.84	112.19
4	I	3	BMA	C1-C2-C3	6.32	117.43	109.67
8	S	5	MAN	C1-O5-C5	5.54	119.69	112.19
6	O	3	BMA	C1-C2-C3	5.21	116.07	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	1	NAG	C1-O5-C5	5.17	119.19	112.19
3	V	1	NAG	C4-C3-C2	5.10	118.49	111.02
6	O	3	BMA	C1-O5-C5	5.06	119.05	112.19
4	P	4	MAN	C1-C2-C3	4.96	115.77	109.67
4	P	5	MAN	C1-O5-C5	4.89	118.82	112.19
4	P	1	NAG	C1-O5-C5	4.84	118.74	112.19
3	W	1	NAG	C4-C3-C2	4.83	118.10	111.02
4	I	3	BMA	C1-O5-C5	4.80	118.69	112.19
8	S	5	MAN	C1-C2-C3	4.80	115.56	109.67
6	O	3	BMA	O5-C1-C2	4.71	118.04	110.77
8	S	5	MAN	O5-C1-C2	4.69	118.01	110.77
9	b	1	NAG	O5-C5-C6	4.25	113.86	107.20
9	Z	1	NAG	C1-O5-C5	4.07	117.71	112.19
3	Y	1	NAG	C4-C3-C2	4.05	116.95	111.02
4	I	5	MAN	C1-O5-C5	3.96	117.56	112.19
4	I	3	BMA	C2-C3-C4	3.95	117.72	110.89
3	J	2	NAG	C2-N2-C7	3.94	128.51	122.90
3	L	2	NAG	C2-N2-C7	3.93	128.51	122.90
9	Z	3	FUC	C1-C2-C3	3.76	114.29	109.67
4	P	2	NAG	O4-C4-C5	3.75	118.62	109.30
3	a	1	NAG	C4-C3-C2	3.74	116.50	111.02
4	I	3	BMA	C3-C4-C5	3.61	116.68	110.24
3	J	2	NAG	C4-C3-C2	3.57	116.26	111.02
3	Y	2	NAG	C8-C7-N2	3.50	122.03	116.10
9	Z	3	FUC	C3-C4-C5	3.48	115.19	109.77
3	G	1	NAG	C2-N2-C7	3.43	127.79	122.90
8	S	3	BMA	C1-O5-C5	3.42	116.82	112.19
4	I	3	BMA	O5-C5-C6	-3.41	101.86	107.20
3	H	1	NAG	C4-C3-C2	3.40	116.00	111.02
6	T	1	NAG	C1-O5-C5	3.34	116.71	112.19
3	Y	1	NAG	C2-N2-C7	3.28	127.58	122.90
8	S	6	FUC	C1-O5-C5	-3.27	105.37	112.78
8	S	6	FUC	O5-C1-C2	-3.26	105.74	110.77
3	W	1	NAG	C3-C4-C5	3.21	115.97	110.24
9	Z	3	FUC	C2-C3-C4	3.18	116.39	110.89
4	Q	2	NAG	C1-O5-C5	3.12	116.42	112.19
4	Q	5	MAN	C3-C4-C5	3.08	115.74	110.24
3	G	1	NAG	C1-C2-N2	3.05	115.70	110.49
7	N	1	NAG	C1-C2-N2	3.05	115.70	110.49
6	M	1	NAG	C1-O5-C5	3.05	116.32	112.19
3	V	1	NAG	O5-C5-C6	3.00	111.91	107.20
6	O	2	NAG	O5-C5-C6	2.90	111.76	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	4	MAN	C2-C3-C4	2.89	115.90	110.89
9	U	3	FUC	C3-C4-C5	2.88	114.26	109.77
9	b	1	NAG	C4-C3-C2	2.84	115.17	111.02
4	X	2	NAG	C1-O5-C5	2.83	116.03	112.19
3	J	2	NAG	C3-C4-C5	2.80	115.23	110.24
5	K	3	BMA	C2-C3-C4	2.77	115.68	110.89
4	I	2	NAG	C1-O5-C5	2.76	115.94	112.19
4	P	1	NAG	C4-C3-C2	2.73	115.03	111.02
8	S	4	MAN	C1-O5-C5	2.73	115.89	112.19
5	K	2	NAG	C2-N2-C7	-2.68	119.08	122.90
8	S	2	NAG	C1-O5-C5	2.67	115.81	112.19
8	S	1	NAG	C2-N2-C7	-2.62	119.17	122.90
4	I	5	MAN	C1-C2-C3	2.58	112.84	109.67
5	K	3	BMA	C1-C2-C3	2.55	112.81	109.67
6	M	2	NAG	C4-C3-C2	2.53	114.72	111.02
4	X	3	BMA	C1-C2-C3	2.49	112.72	109.67
3	V	1	NAG	C2-N2-C7	2.48	126.43	122.90
3	V	2	NAG	O5-C5-C6	2.46	111.06	107.20
9	U	1	NAG	C1-O5-C5	2.41	115.46	112.19
3	Y	1	NAG	C8-C7-N2	2.41	120.17	116.10
3	V	1	NAG	C3-C4-C5	2.40	114.51	110.24
3	Y	1	NAG	O3-C3-C2	-2.39	104.52	109.47
4	P	5	MAN	C1-C2-C3	2.39	112.60	109.67
6	O	2	NAG	C4-C3-C2	2.38	114.50	111.02
6	T	3	BMA	O5-C5-C6	2.37	110.92	107.20
9	U	1	NAG	C2-N2-C7	2.37	126.27	122.90
4	P	1	NAG	C3-C4-C5	2.36	114.45	110.24
5	K	2	NAG	C1-O5-C5	2.34	115.37	112.19
4	I	1	NAG	C1-O5-C5	2.34	115.36	112.19
4	Q	5	MAN	C2-C3-C4	2.33	114.93	110.89
3	Y	2	NAG	O7-C7-C8	-2.33	117.73	122.06
6	M	3	BMA	C3-C4-C5	2.32	114.38	110.24
4	X	1	NAG	C2-N2-C7	-2.31	119.61	122.90
4	X	4	MAN	C1-C2-C3	2.30	112.49	109.67
3	Y	2	NAG	C1-C2-N2	2.29	114.40	110.49
4	Q	2	NAG	C1-C2-N2	2.29	114.40	110.49
4	Q	4	MAN	C1-O5-C5	2.28	115.28	112.19
8	S	3	BMA	C1-C2-C3	2.27	112.46	109.67
6	T	2	NAG	C1-O5-C5	2.27	115.26	112.19
3	W	1	NAG	C1-C2-N2	-2.24	106.66	110.49
3	a	1	NAG	C1-O5-C5	2.24	115.23	112.19
9	U	2	NAG	C1-O5-C5	2.23	115.22	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	1	NAG	O5-C1-C2	2.23	114.81	111.29
9	b	2	NAG	C1-O5-C5	2.23	115.21	112.19
4	X	5	MAN	C2-C3-C4	2.22	114.74	110.89
8	S	6	FUC	O2-C2-C3	2.22	114.58	110.14
4	Q	2	NAG	C6-C5-C4	-2.20	107.84	113.00
4	P	3	BMA	O5-C5-C6	2.19	110.64	107.20
8	S	3	BMA	C3-C4-C5	2.18	114.13	110.24
3	a	2	NAG	C4-C3-C2	2.17	114.20	111.02
9	b	1	NAG	O6-C6-C5	2.17	118.75	111.29
6	O	2	NAG	O5-C1-C2	2.14	114.67	111.29
3	L	2	NAG	C1-C2-N2	2.14	114.14	110.49
9	U	1	NAG	O6-C6-C5	2.13	118.58	111.29
3	W	2	NAG	O5-C5-C6	2.12	110.53	107.20
5	K	2	NAG	O5-C1-C2	-2.11	107.96	111.29
6	T	1	NAG	O6-C6-C5	-2.10	104.07	111.29
3	J	1	NAG	C8-C7-N2	2.10	119.66	116.10
5	K	1	NAG	C6-C5-C4	2.10	117.91	113.00
6	T	3	BMA	C1-C2-C3	2.08	112.22	109.67
9	U	3	FUC	O5-C1-C2	-2.07	107.57	110.77
5	K	3	BMA	C3-C4-C5	2.07	113.93	110.24
6	O	3	BMA	O5-C5-C6	2.07	110.44	107.20
5	K	4	FUC	C1-C2-C3	-2.05	107.14	109.67
8	S	1	NAG	O5-C1-C2	-2.05	108.05	111.29
4	I	4	MAN	C1-C2-C3	-2.05	107.15	109.67
6	M	1	NAG	C4-C3-C2	2.04	114.01	111.02
7	N	2	FUC	O5-C1-C2	-2.02	107.66	110.77
8	S	6	FUC	O2-C2-C1	2.02	113.28	109.15
5	K	1	NAG	O6-C6-C5	2.01	118.20	111.29
3	a	1	NAG	O4-C4-C3	-2.01	105.70	110.35
3	G	2	NAG	C2-N2-C7	2.01	125.76	122.90
6	T	1	NAG	O5-C5-C6	-2.01	104.06	107.20
7	N	2	FUC	C3-C4-C5	2.00	112.89	109.77

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	L	1	NAG	C1
5	K	4	FUC	C1
7	N	2	FUC	C1
8	S	6	FUC	C1
9	U	3	FUC	C1
9	Z	3	FUC	C1

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Mol	Chain	Res	Type	Atom
9	b	3	FUC	C1

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	T	3	BMA	O5-C5-C6-O6
4	X	5	MAN	O5-C5-C6-O6
8	S	1	NAG	C4-C5-C6-O6
6	O	3	BMA	O5-C5-C6-O6
9	b	1	NAG	O5-C5-C6-O6
6	M	3	BMA	C4-C5-C6-O6
7	N	1	NAG	C4-C5-C6-O6
4	P	4	MAN	O5-C5-C6-O6
4	Q	5	MAN	C4-C5-C6-O6
4	P	5	MAN	O5-C5-C6-O6
4	P	5	MAN	C4-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
4	Q	5	MAN	O5-C5-C6-O6
6	M	3	BMA	O5-C5-C6-O6
9	b	2	NAG	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
4	P	4	MAN	C4-C5-C6-O6
5	K	3	BMA	C4-C5-C6-O6
4	X	4	MAN	O5-C5-C6-O6
6	T	3	BMA	C4-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
8	S	3	BMA	O5-C5-C6-O6
4	I	4	MAN	C4-C5-C6-O6
6	O	3	BMA	C4-C5-C6-O6
4	I	5	MAN	C4-C5-C6-O6
9	b	1	NAG	C4-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	X	5	MAN	C4-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
9	b	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
3	R	1	NAG	C8-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
3	Y	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2
3	Y	2	NAG	C8-C7-N2-C2
3	Y	2	NAG	O7-C7-N2-C2
8	S	3	BMA	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
7	N	1	NAG	O5-C5-C6-O6
8	S	1	NAG	O5-C5-C6-O6
4	I	3	BMA	C4-C5-C6-O6
4	P	3	BMA	C4-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
4	I	4	MAN	O5-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
9	U	1	NAG	C4-C5-C6-O6
4	I	5	MAN	O5-C5-C6-O6
4	P	3	BMA	O5-C5-C6-O6
9	U	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
4	X	4	MAN	C4-C5-C6-O6
3	G	1	NAG	C1-C2-N2-C7
3	L	1	NAG	C4-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C3-C2-N2-C7
3	G	1	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
9	Z	1	NAG	C4-C5-C6-O6
3	V	1	NAG	C3-C2-N2-C7
3	a	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	L	2	NAG	C1-C2-N2-C7
3	Y	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
8	S	5	MAN	C4-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7
3	Y	2	NAG	C3-C2-N2-C7
9	Z	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C1-C2-N2-C7
3	Y	2	NAG	C1-C2-N2-C7
6	O	1	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

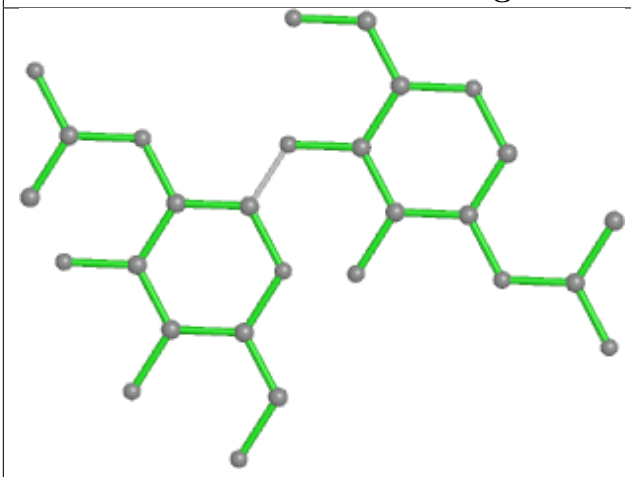
Mol	Chain	Res	Type	Atoms
4	Q	4	MAN	C1-C2-C3-C4-C5-O5

11 monomers are involved in 12 short contacts:

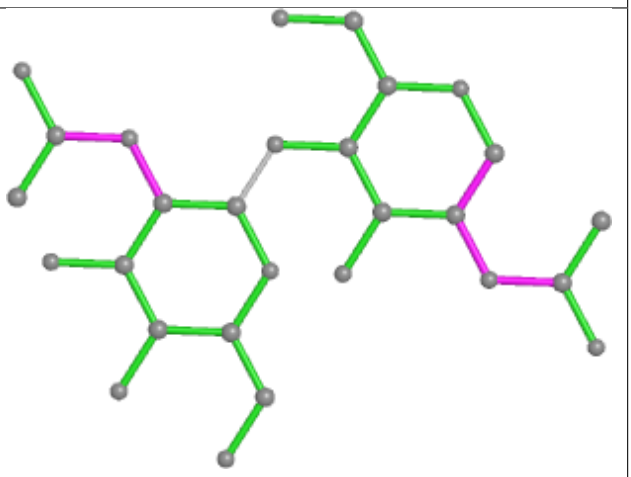
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
3	V	2	NAG	1	0
4	I	5	MAN	2	0
6	T	1	NAG	1	0
4	I	3	BMA	2	0
5	K	4	FUC	2	0
3	V	1	NAG	1	0
4	P	4	MAN	1	0
4	Q	1	NAG	1	0
4	P	3	BMA	4	0
4	P	2	NAG	3	0

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

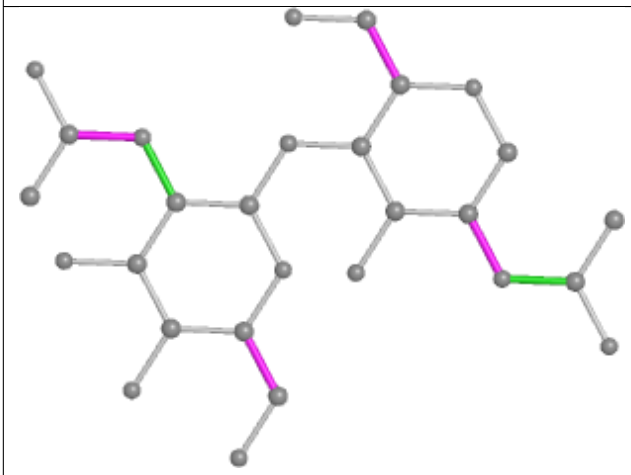
Oligosaccharide Chain G



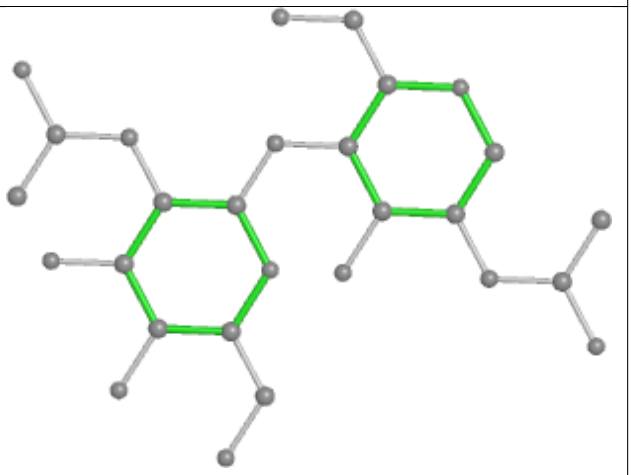
Bond lengths



Bond angles

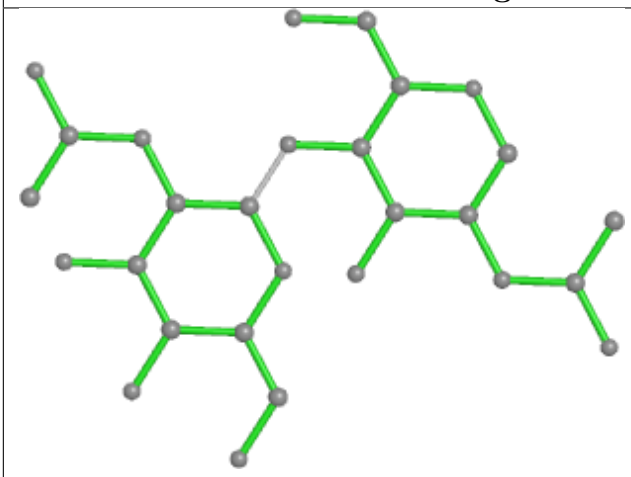


Torsions

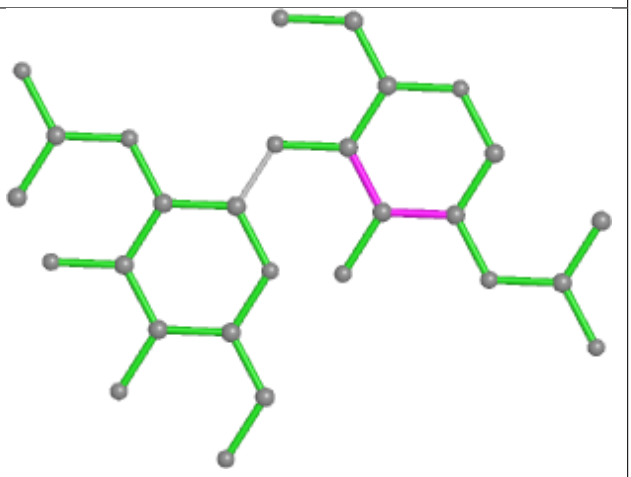


Rings

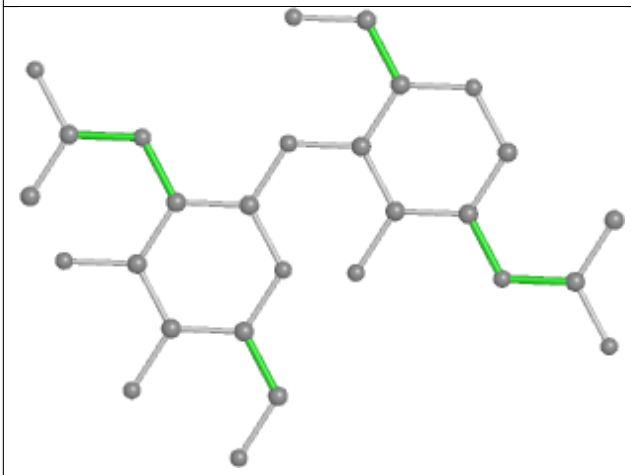
Oligosaccharide Chain H



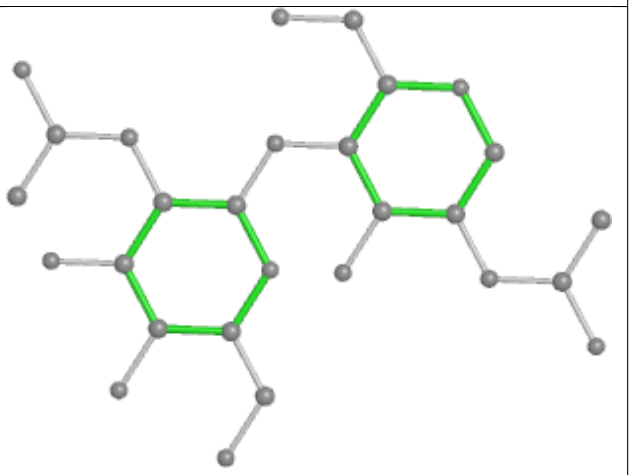
Bond lengths



Bond angles

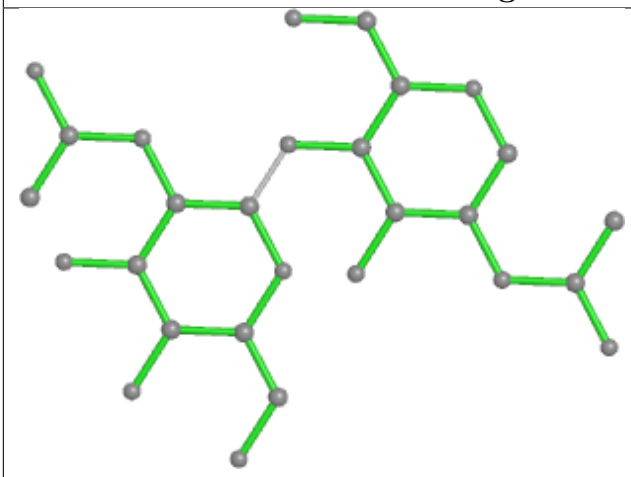


Torsions

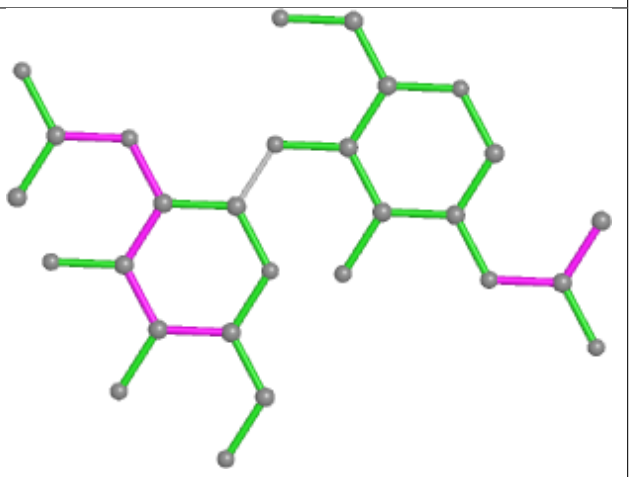


Rings

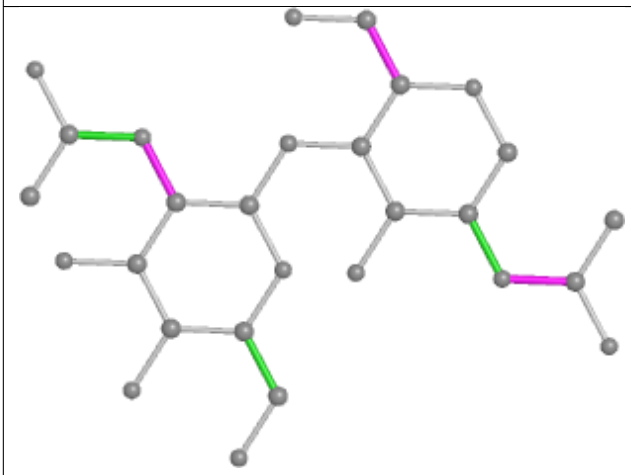
Oligosaccharide Chain J



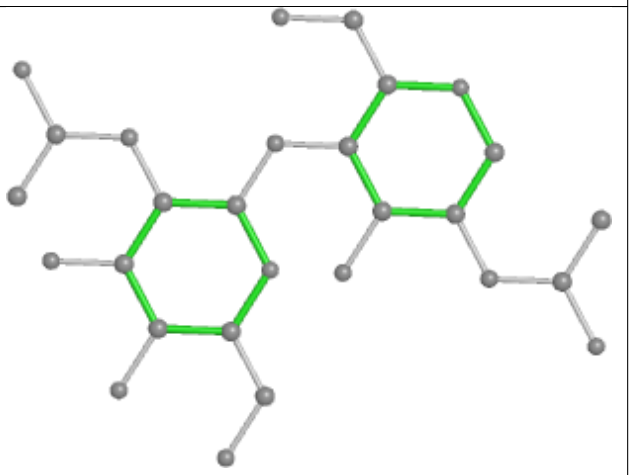
Bond lengths



Bond angles

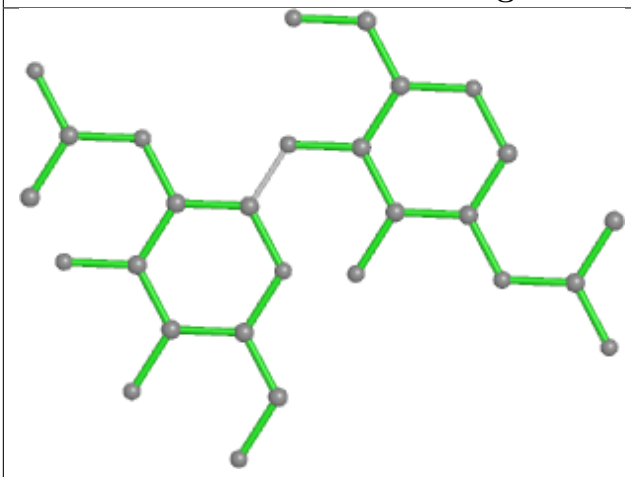


Torsions

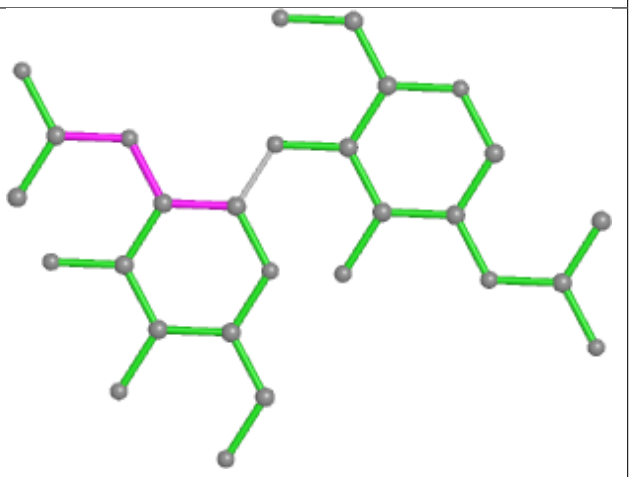


Rings

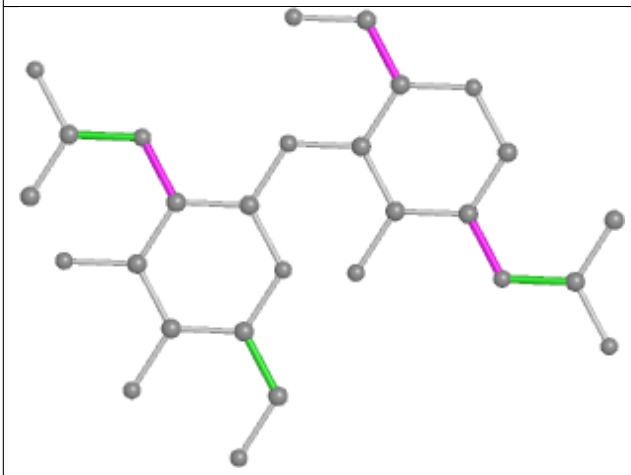
Oligosaccharide Chain L



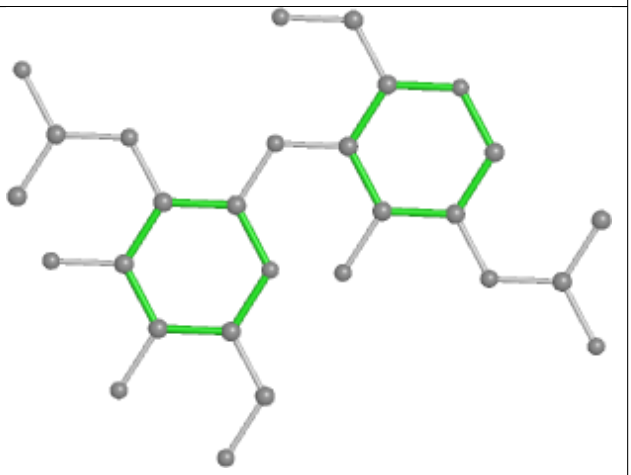
Bond lengths



Bond angles

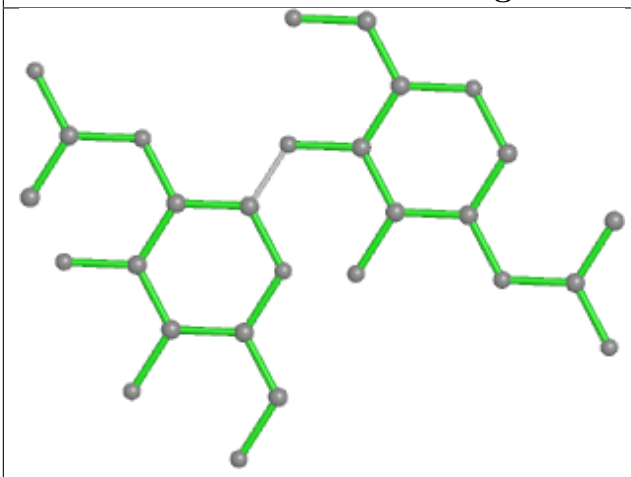


Torsions



Rings

Oligosaccharide Chain R



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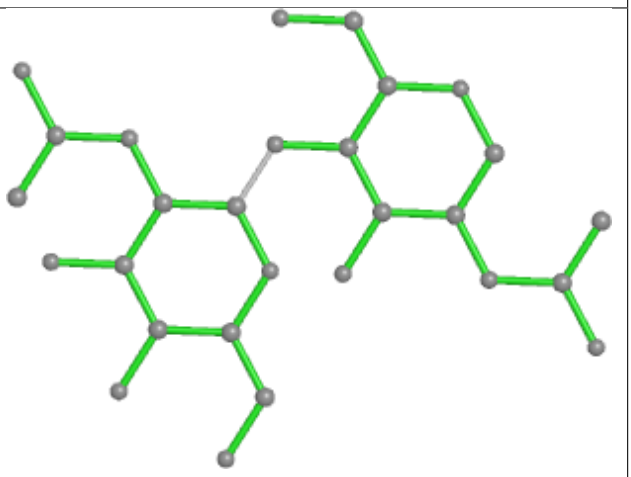
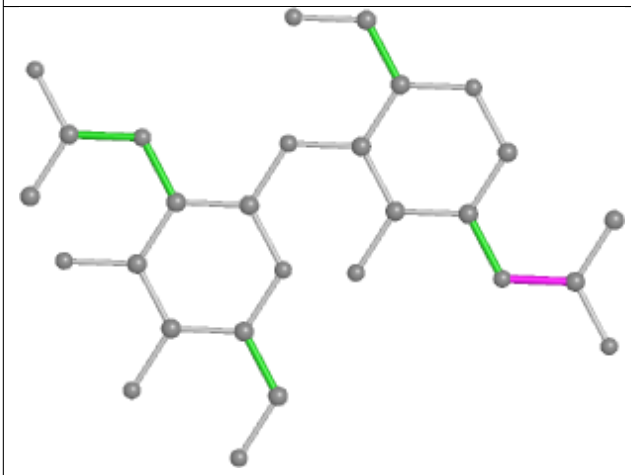


Bond angles



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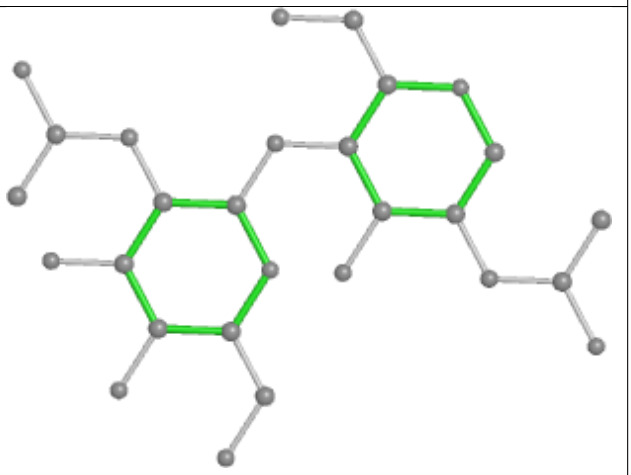
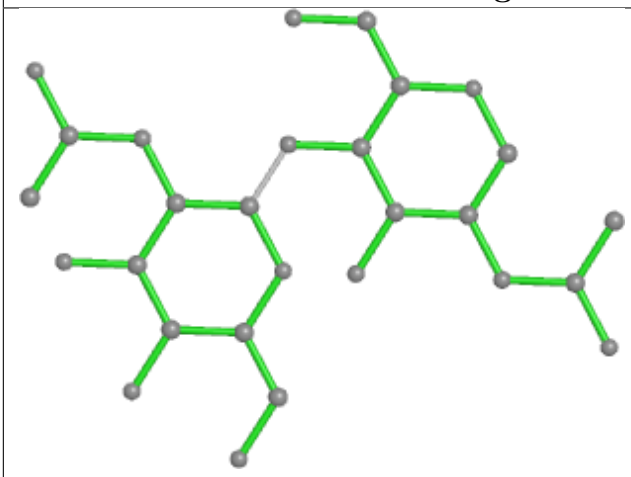


Rings

Oligosaccharide Chain V



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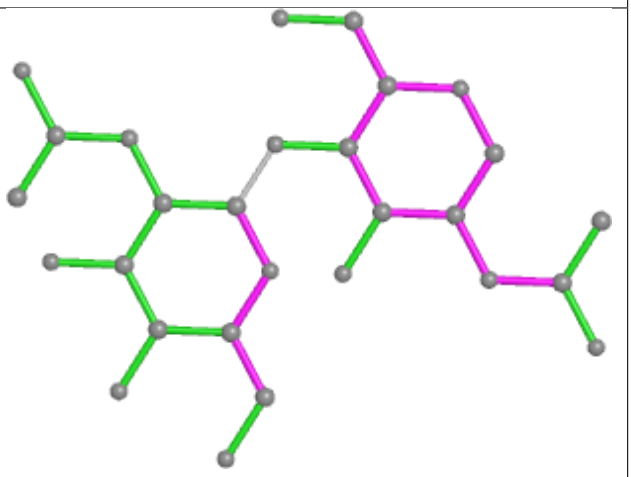
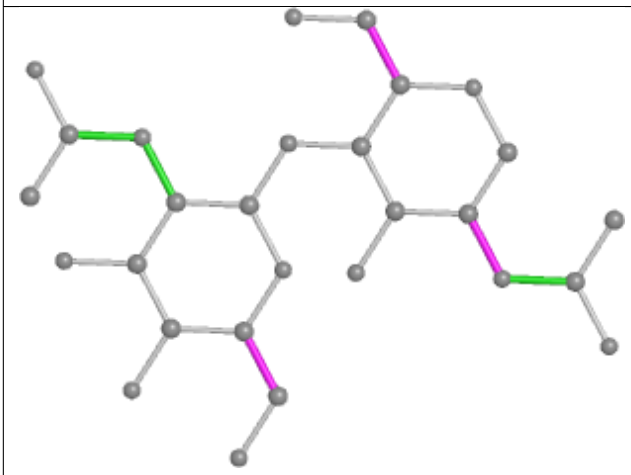


Bond angles



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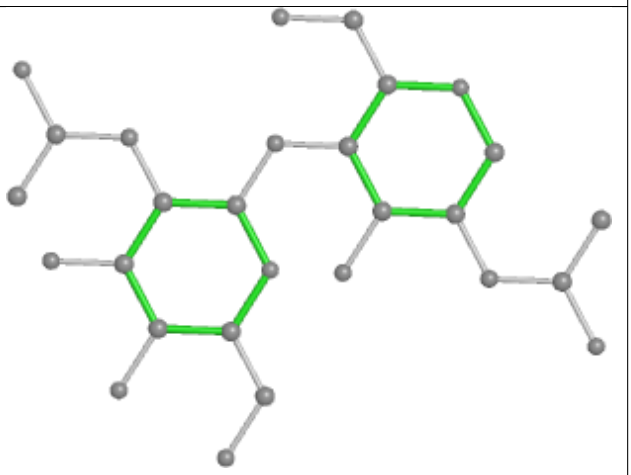
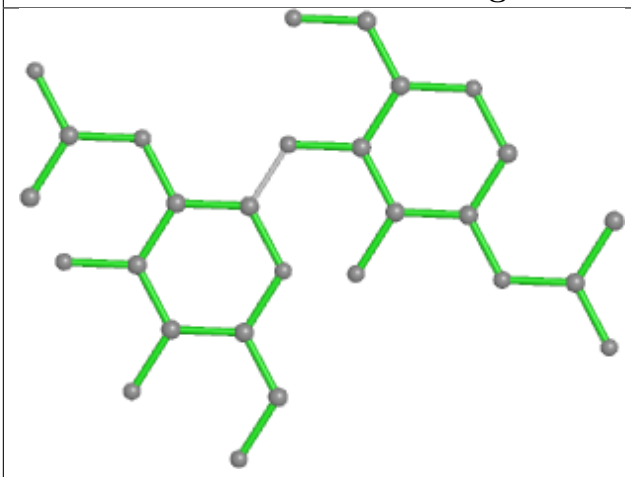


Rings

Oligosaccharide Chain W



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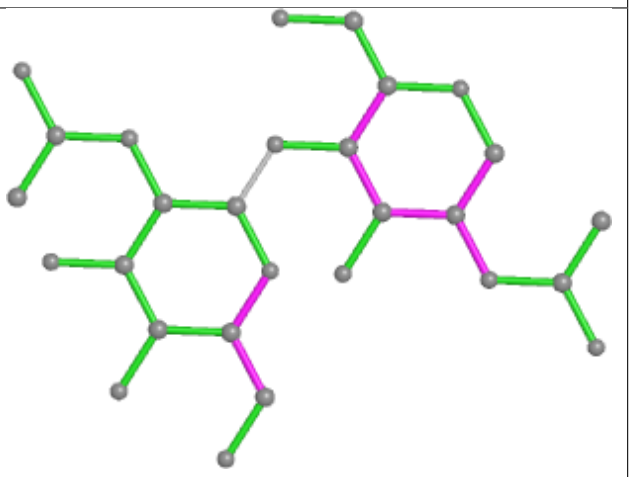
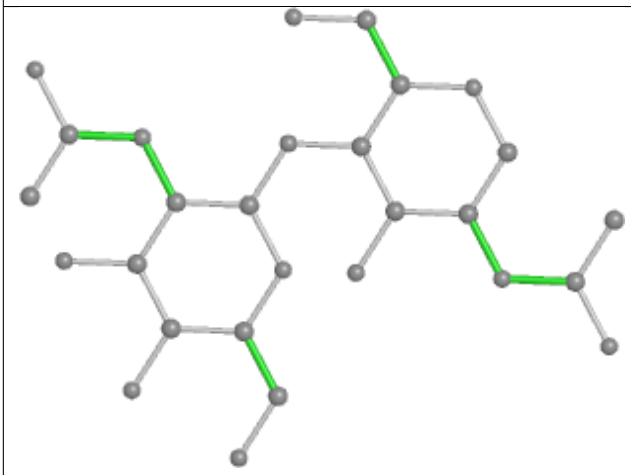


Bond angles



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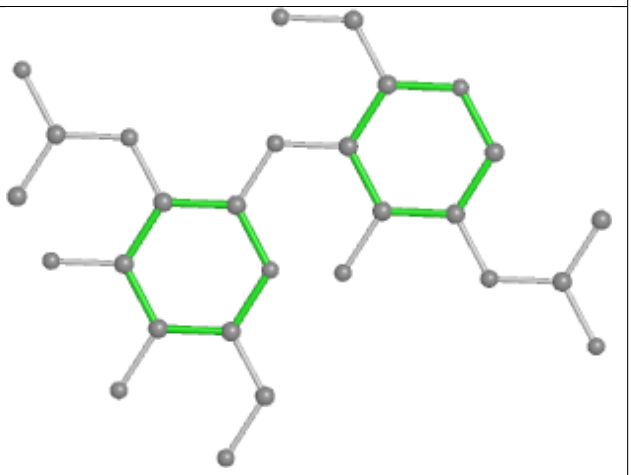
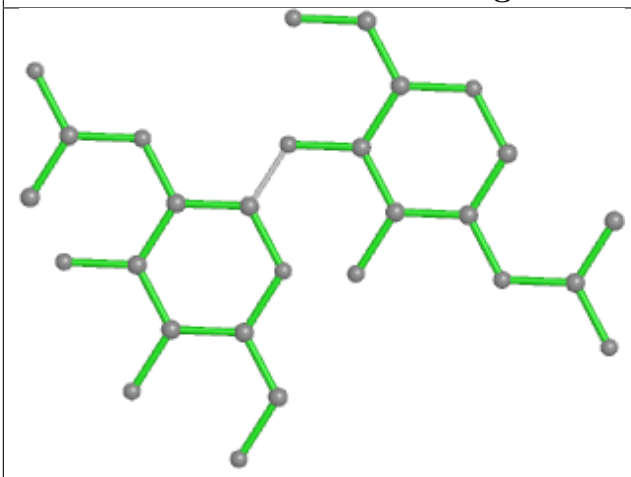


Rings

Oligosaccharide Chain Y



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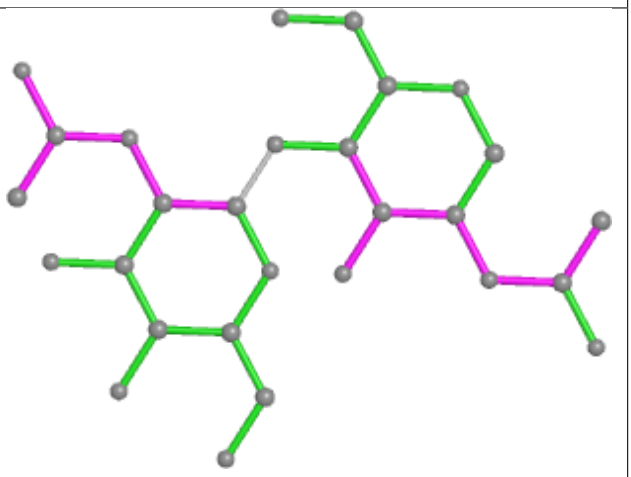
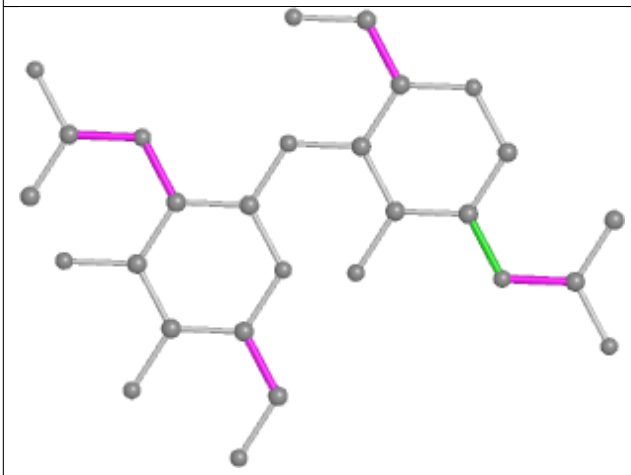
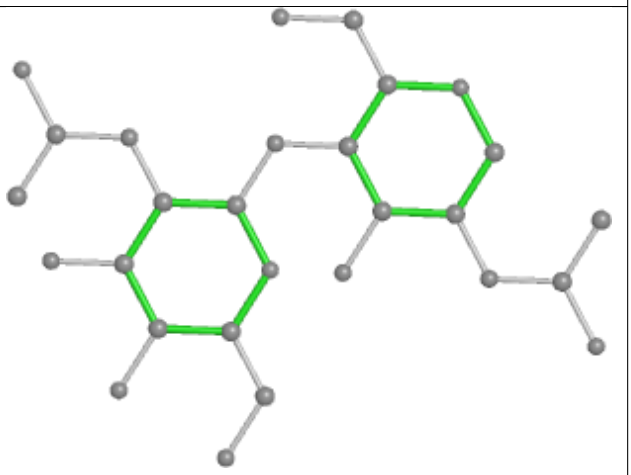


Bond angles

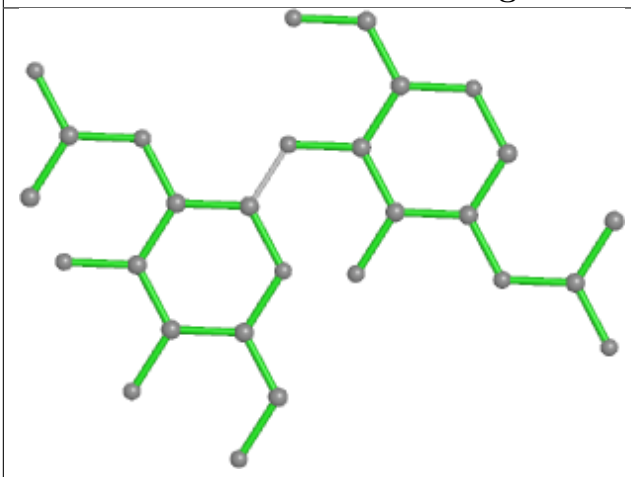


Torsions



Rings

Oligosaccharide Chain a



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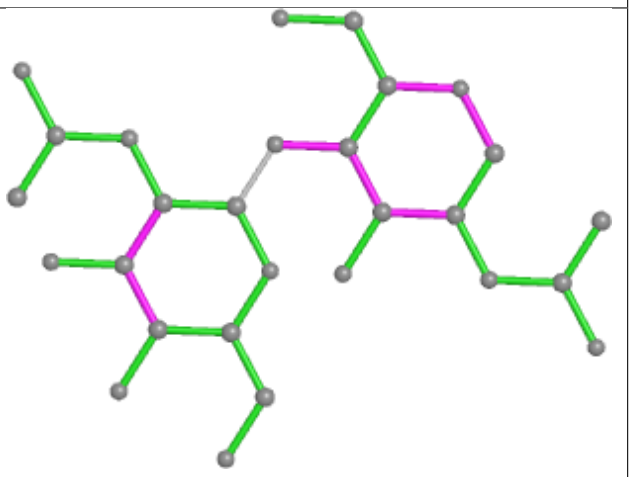
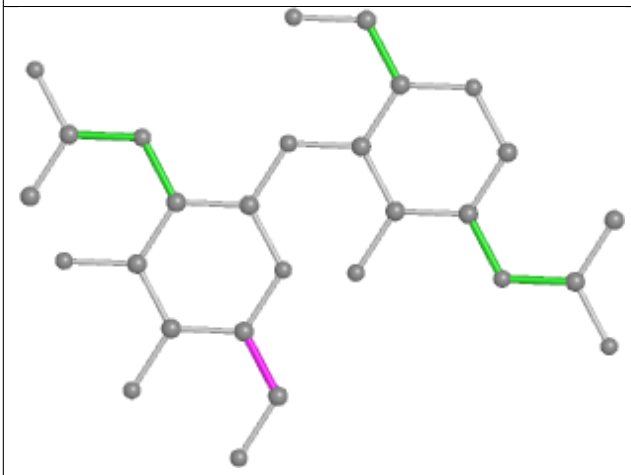


Bond angles



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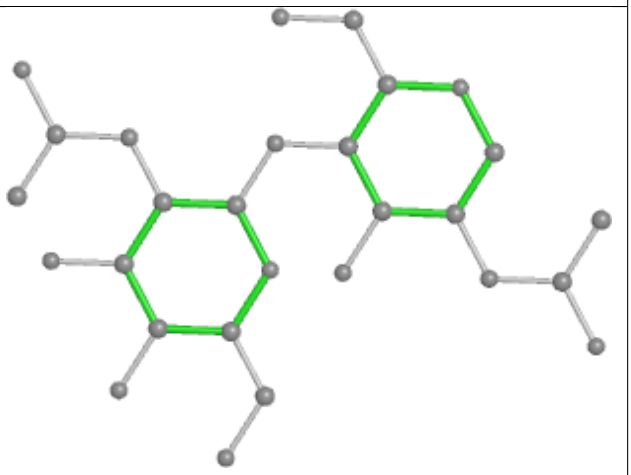
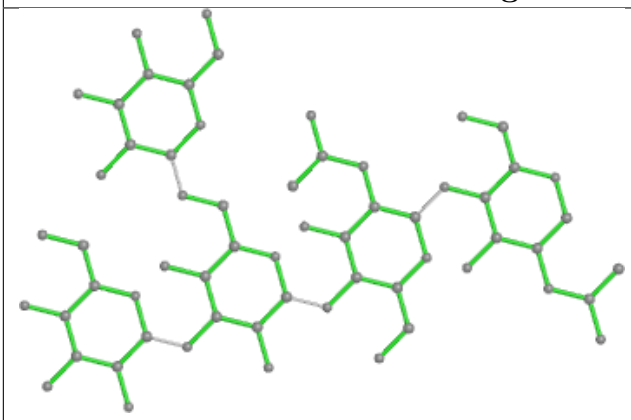


Rings

Oligosaccharide Chain I



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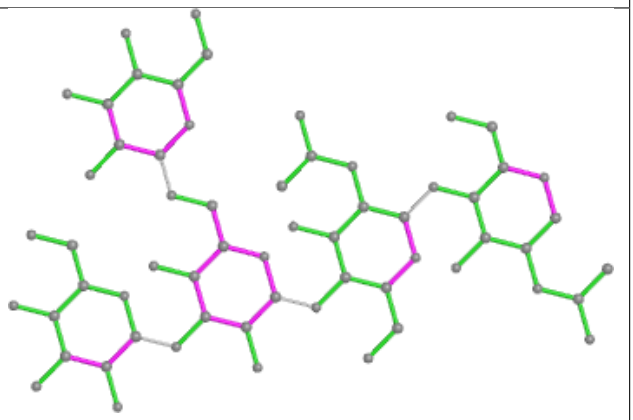
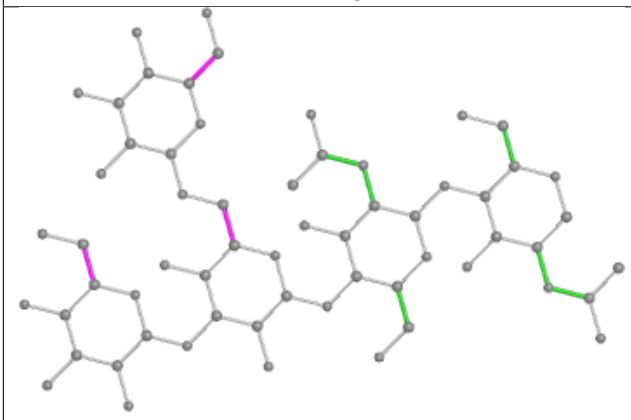


Bond angles



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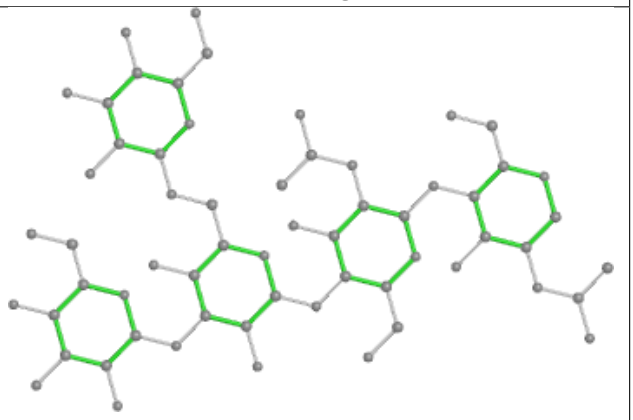
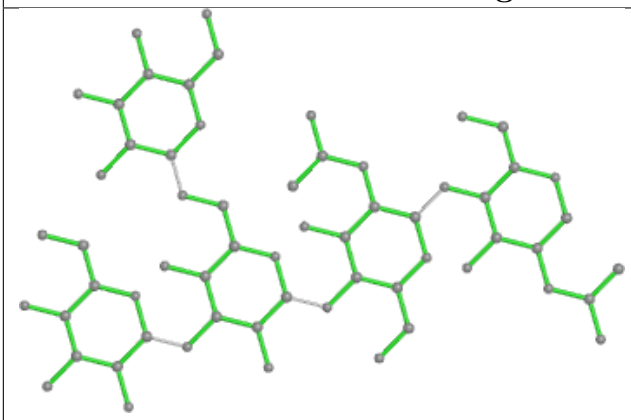


Rings

Oligosaccharide Chain P



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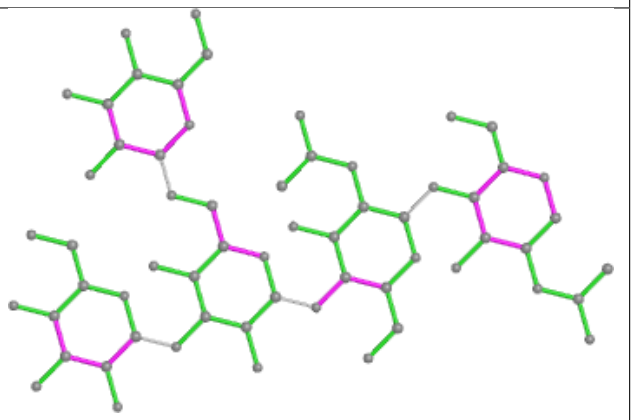

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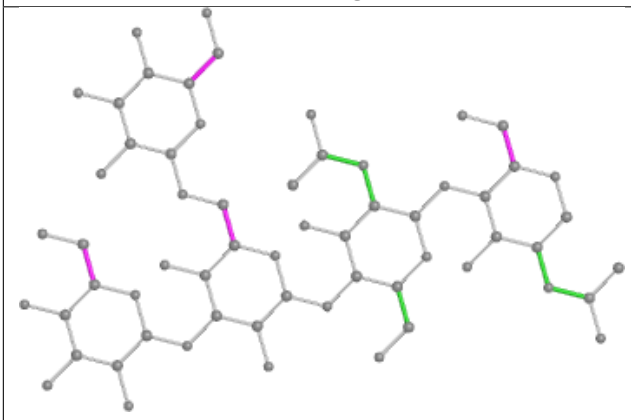

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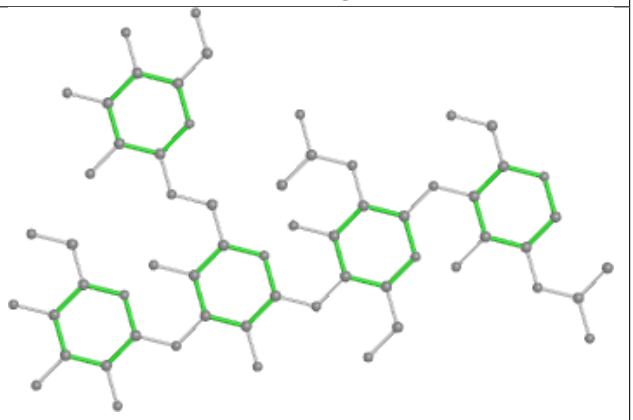
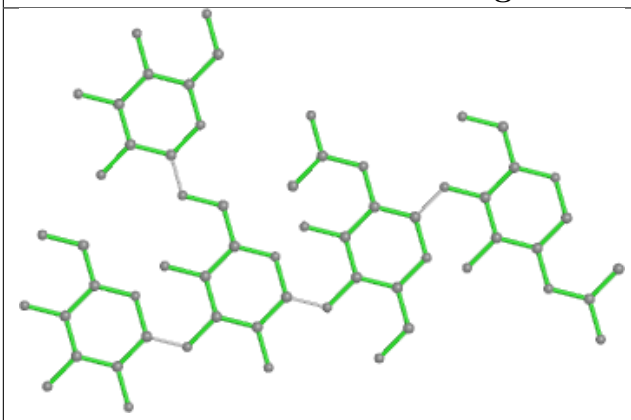


Rings

Oligosaccharide Chain Q



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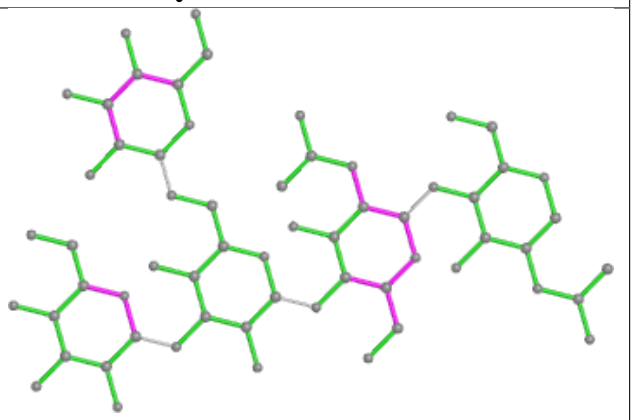
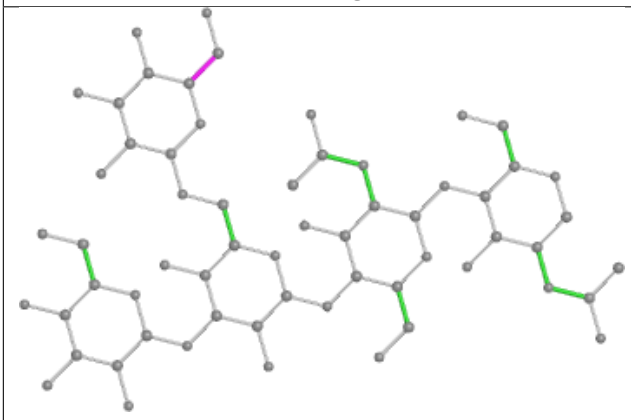


Bond angles



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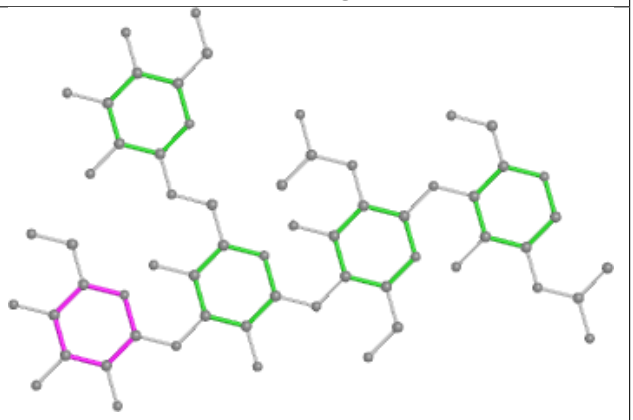
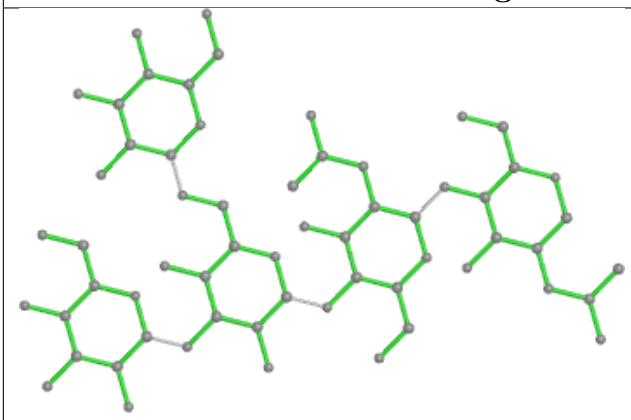


Rings

Oligosaccharide Chain X



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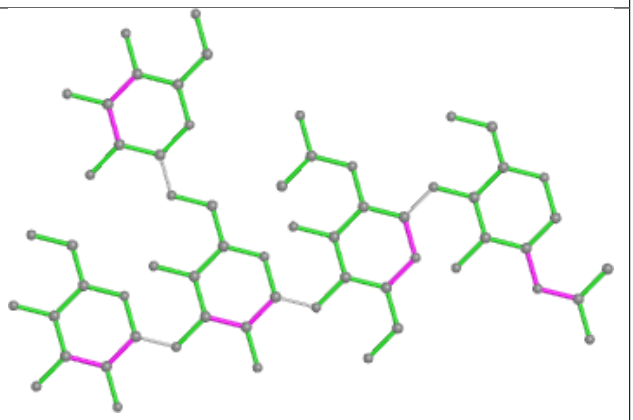
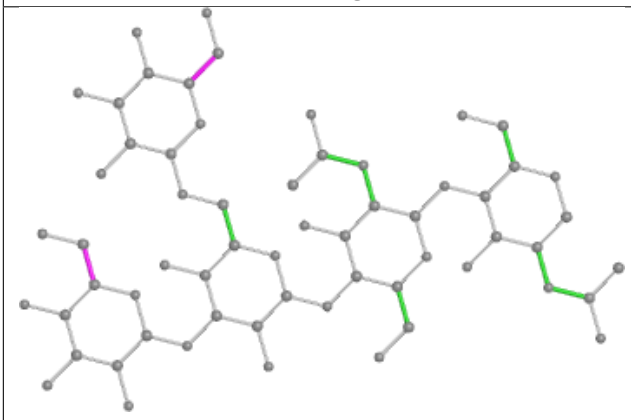


Bond angles



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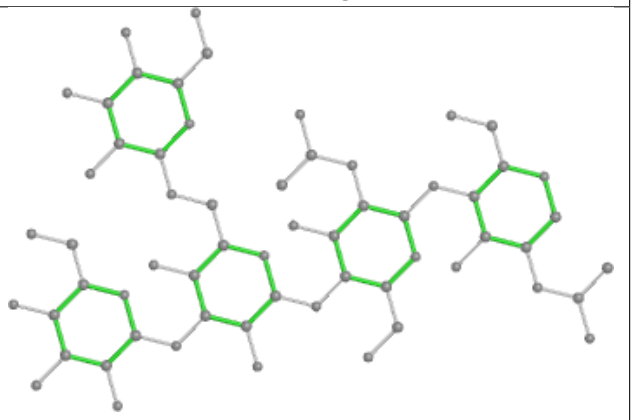
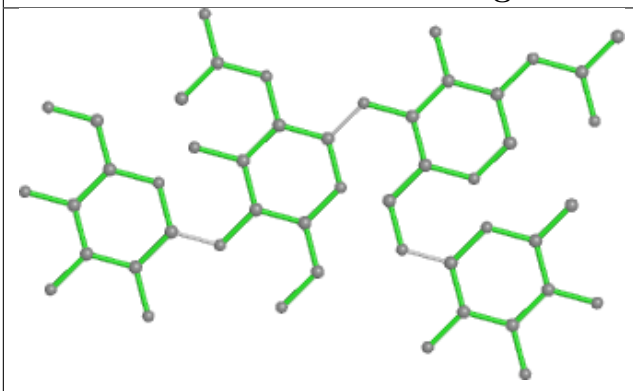
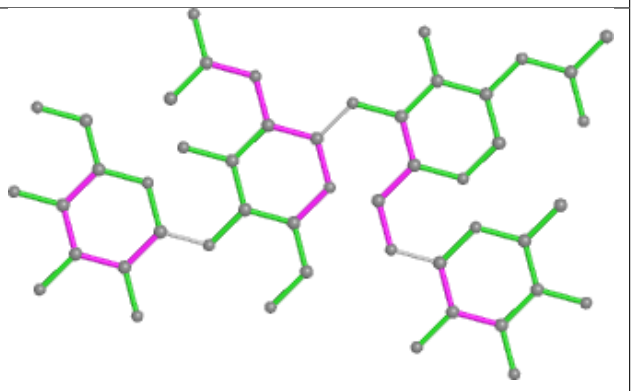


Rings

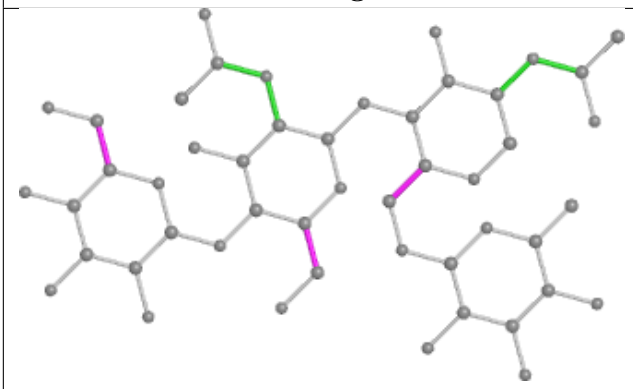
Oligosaccharide Chain K



Bond lengths



Bond angles



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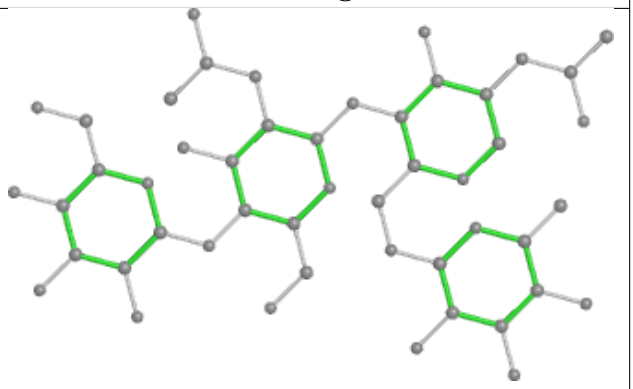
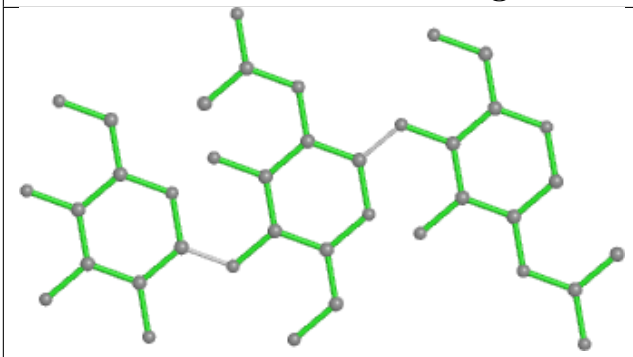


Rings

Oligosaccharide Chain M



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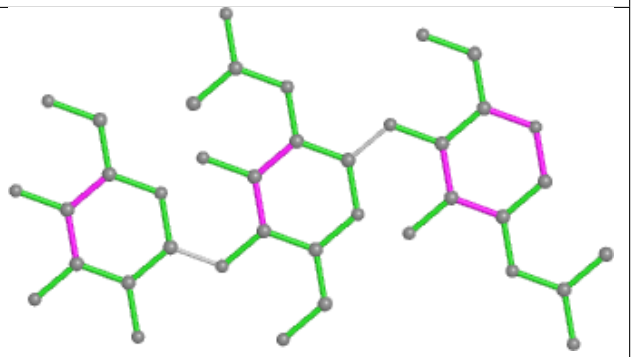
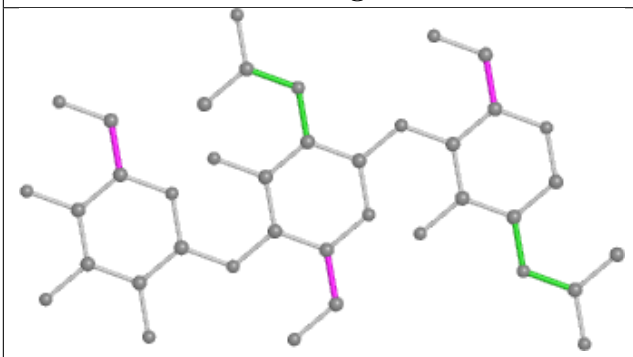


Bond angles



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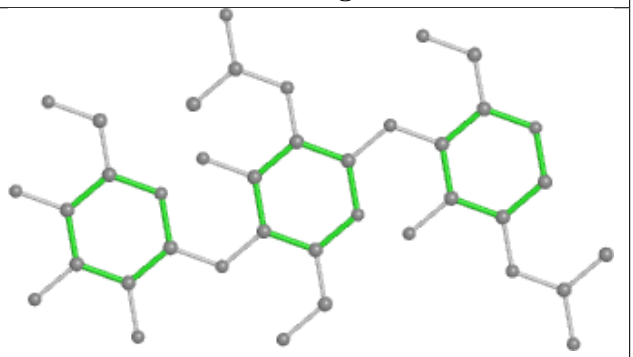
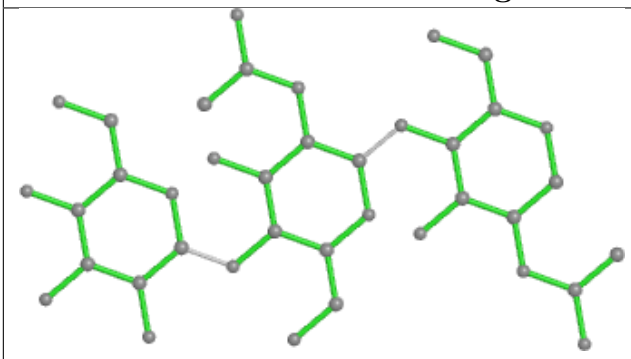


Rings

Oligosaccharide Chain O



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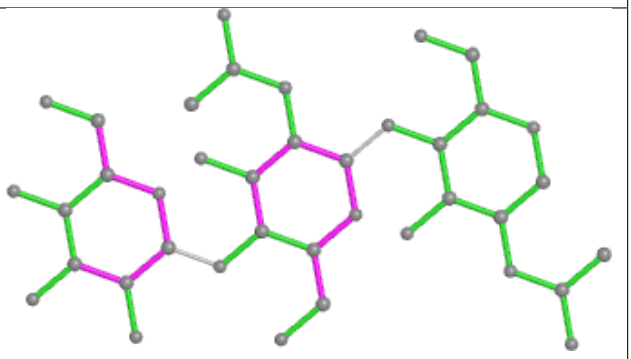
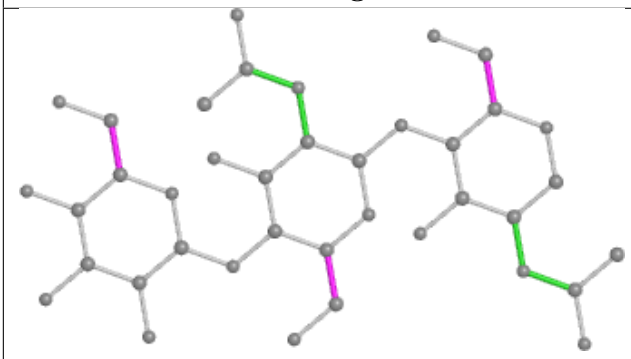


Bond angles



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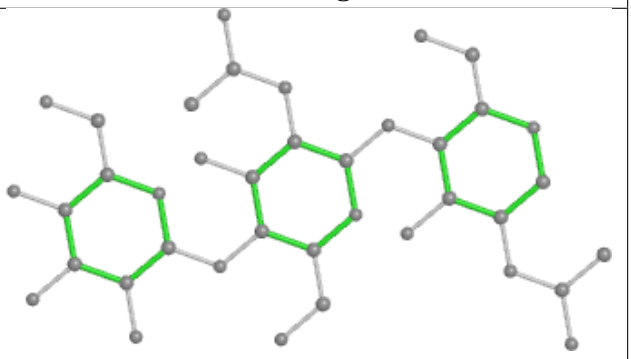
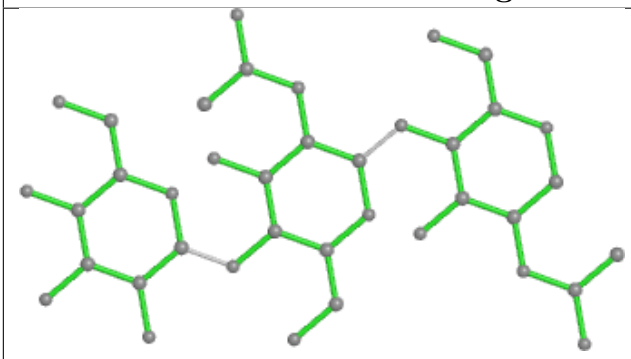
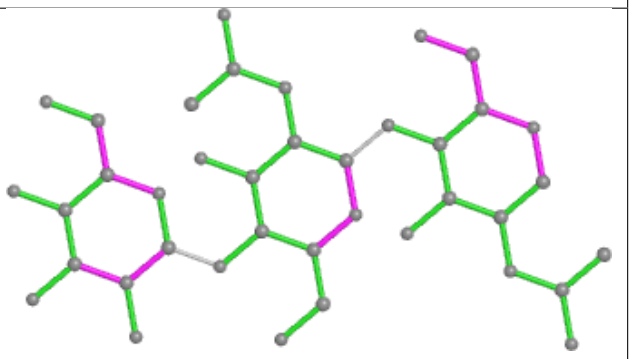


Rings

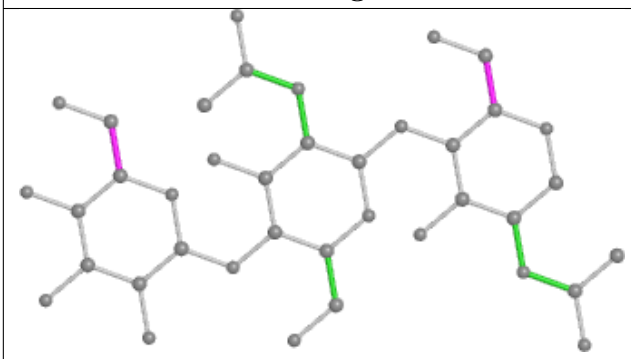
Oligosaccharide Chain T



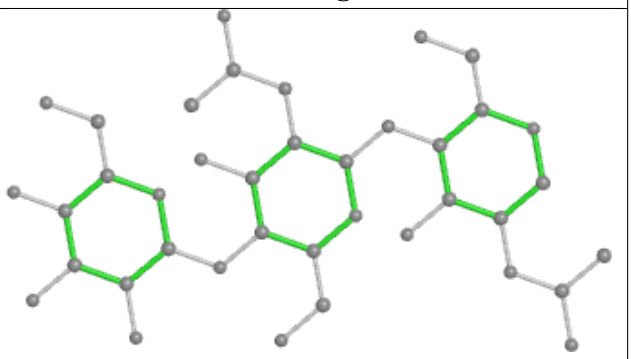
Bond lengths



Bond angles

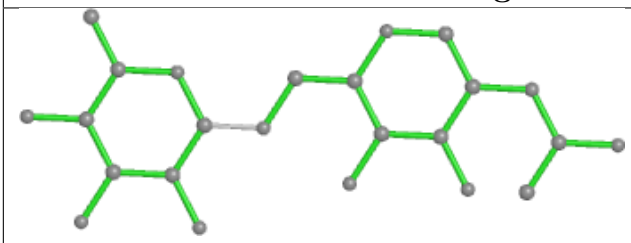


Torsions

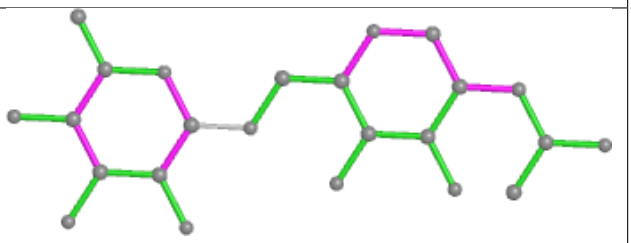


Rings

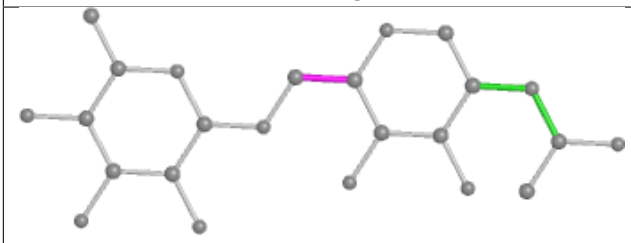
Oligosaccharide Chain N



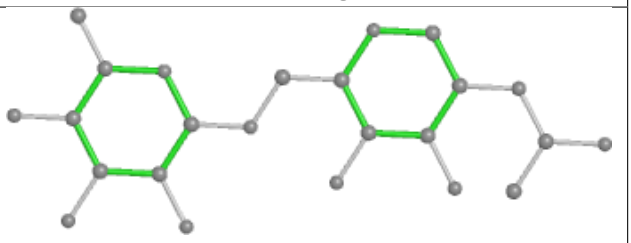
Bond lengths



Bond angles

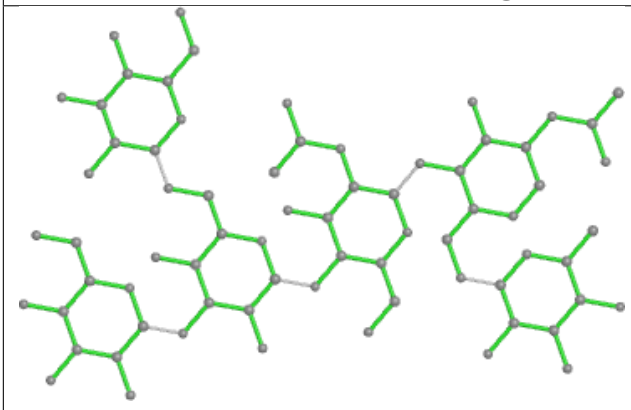


Torsions

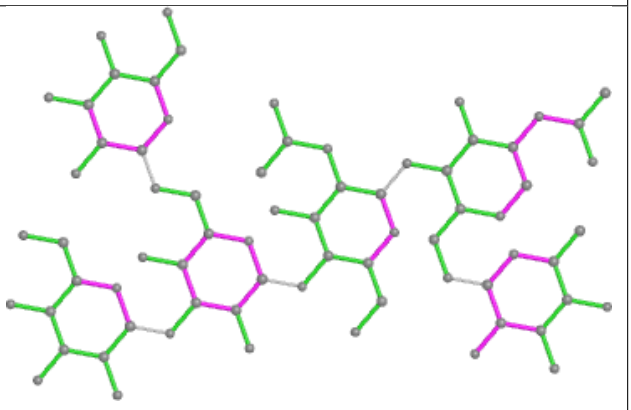


Rings

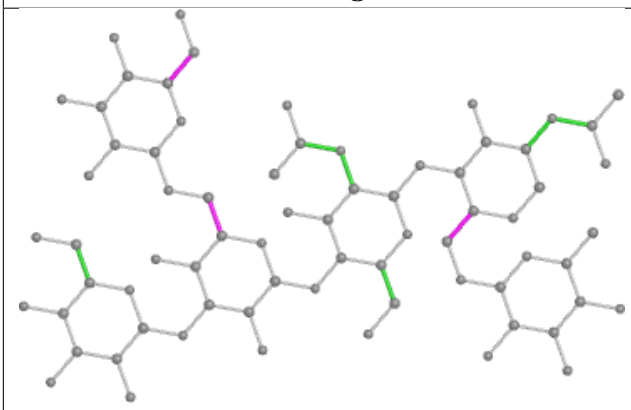
Oligosaccharide Chain S



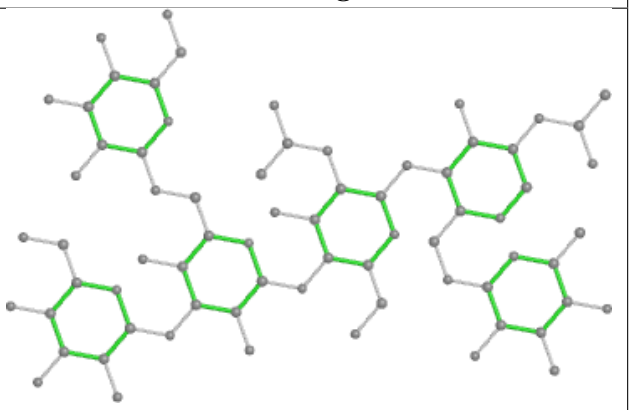
Bond lengths



Bond angles

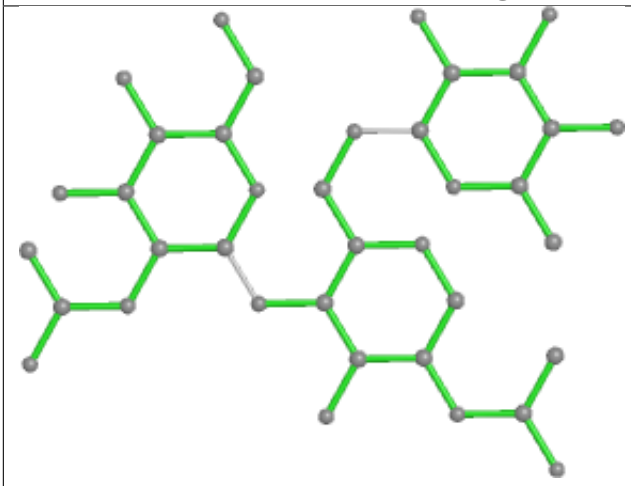


Torsions

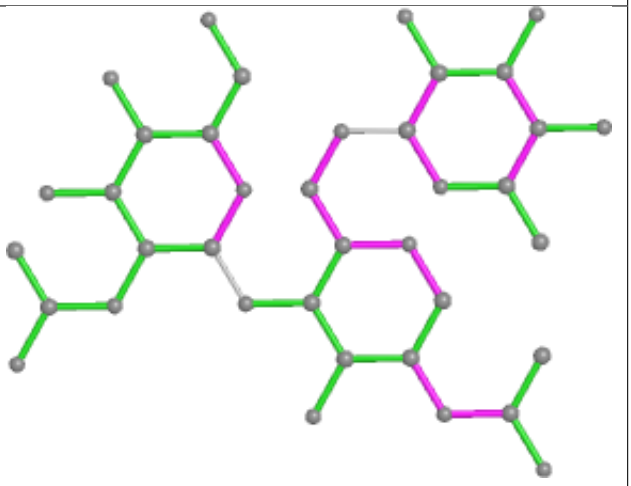


Rings

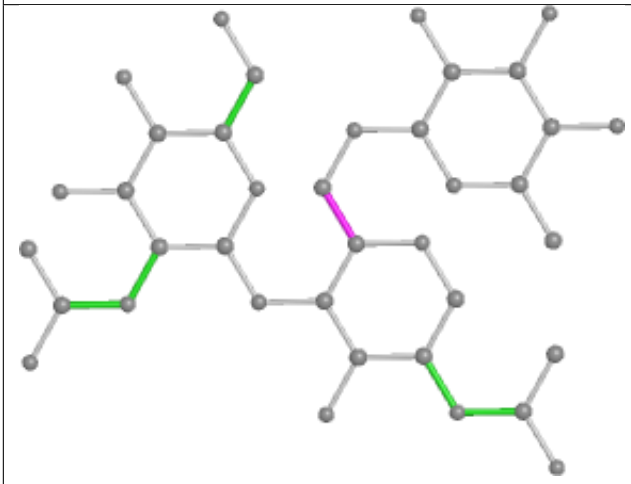
Oligosaccharide Chain U



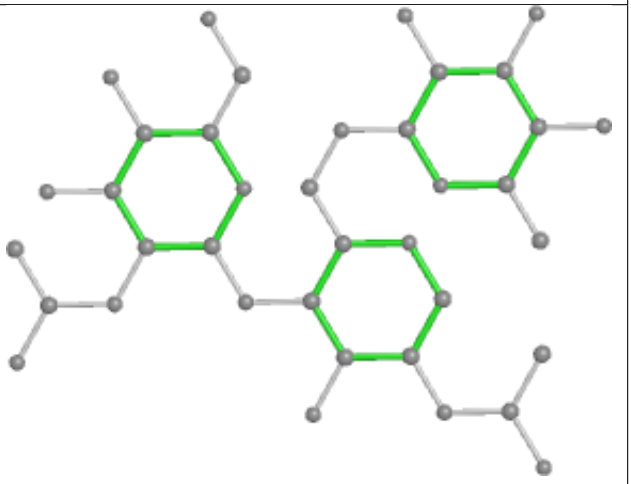
Bond lengths



Bond angles

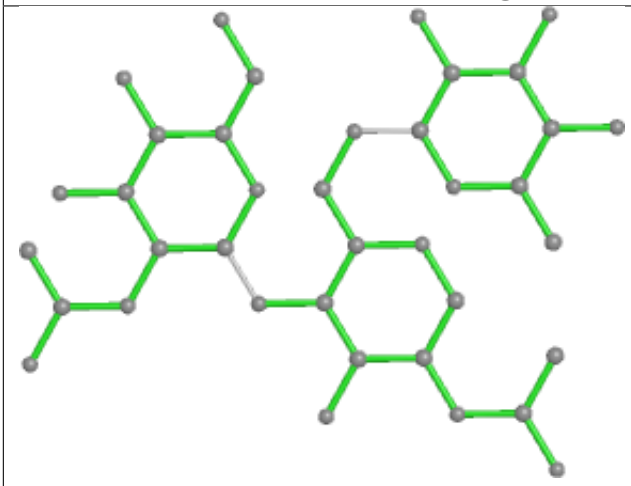


Torsions

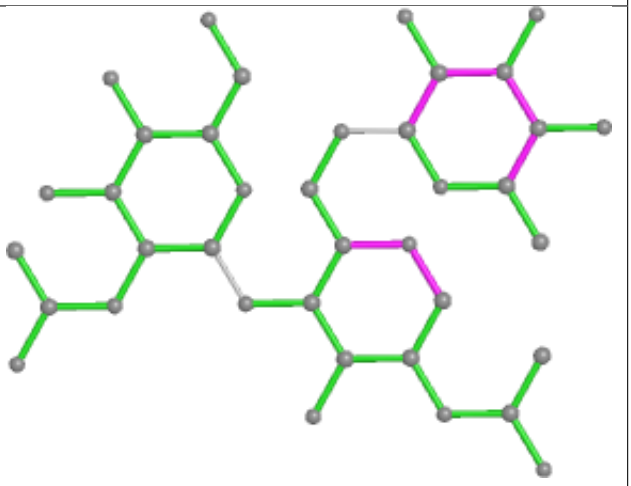


Rings

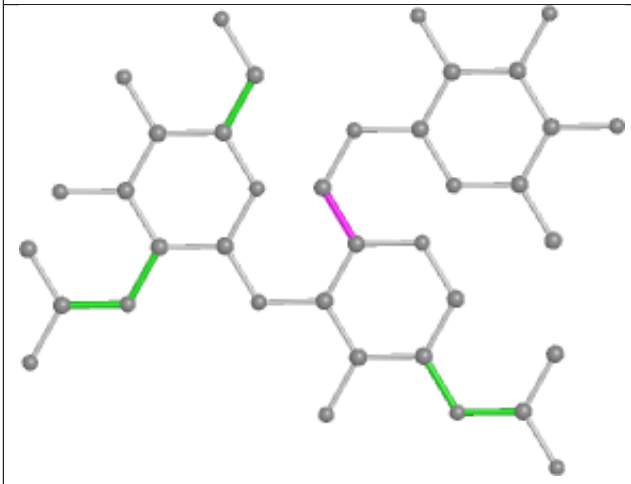
Oligosaccharide Chain Z



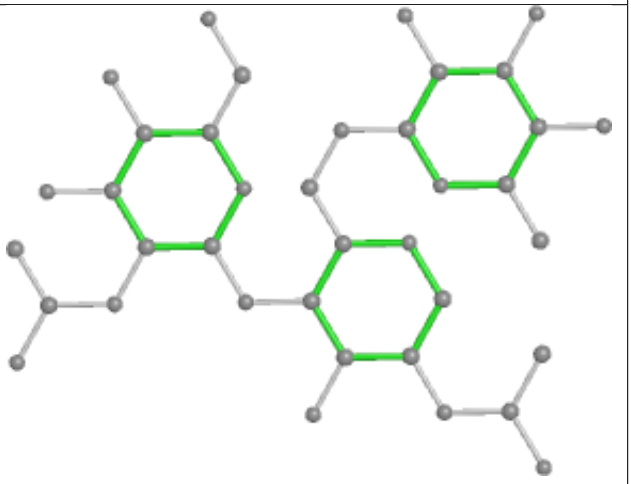
Bond lengths



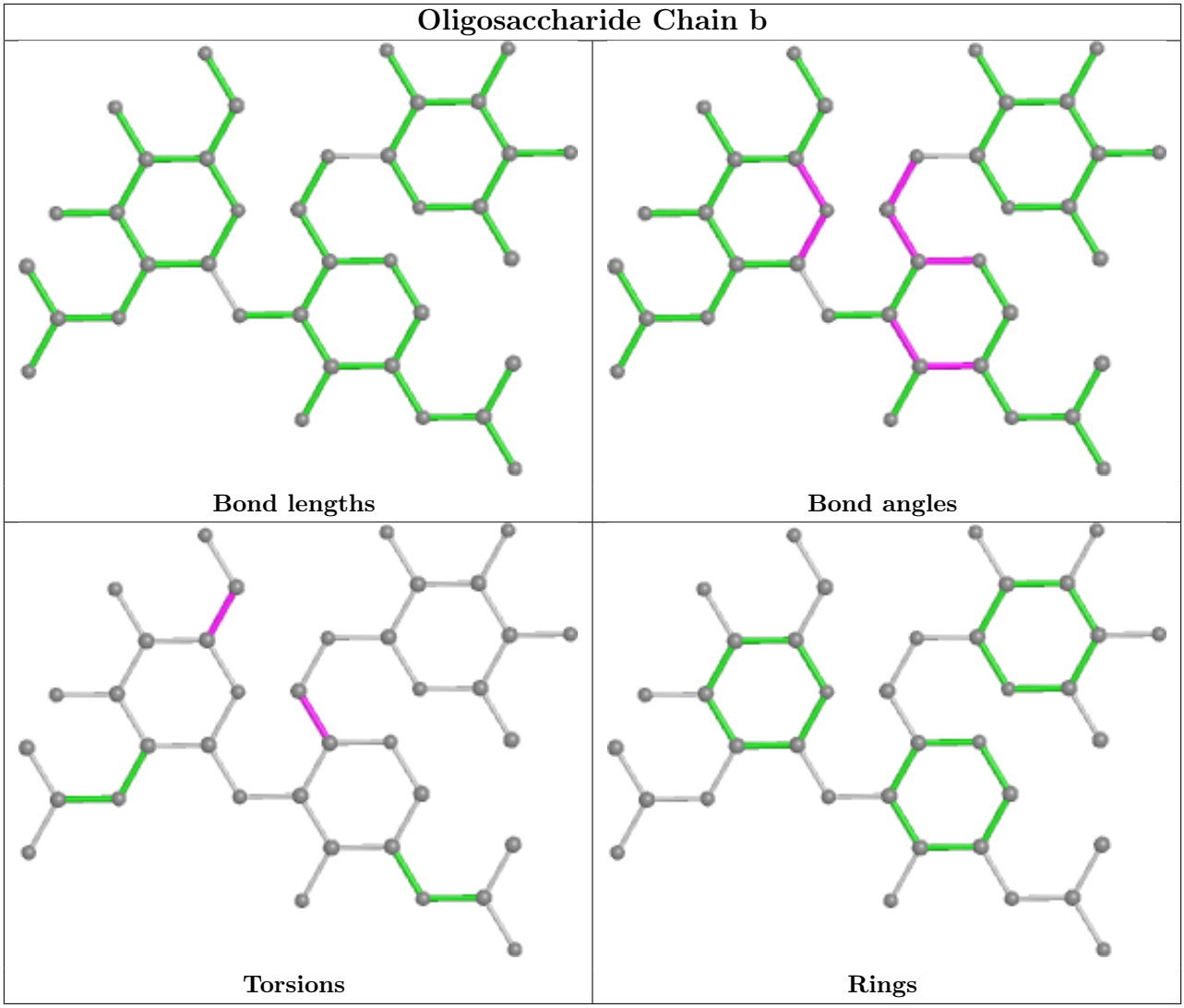
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	EDO	A	1327	-	3,3,3	0.35	0	2,2,2	0.62	0
11	EDO	C	1327	-	3,3,3	0.48	0	2,2,2	0.37	0
11	EDO	E	1326	-	3,3,3	0.45	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	EDO	A	1328	-	3,3,3	0.47	0	2,2,2	0.37	0
10	BMA	A	604	-	11,11,12	0.38	0	15,15,17	0.72	0
11	EDO	C	1328	-	3,3,3	0.47	0	2,2,2	0.45	0
11	EDO	D	1173	-	3,3,3	0.46	0	2,2,2	0.37	0
11	EDO	F	1175	-	3,3,3	0.46	0	2,2,2	0.38	0
11	EDO	B	1174	-	3,3,3	0.46	0	2,2,2	0.36	0
11	EDO	B	1173	-	3,3,3	0.38	0	2,2,2	0.50	0
11	EDO	F	1173	-	3,3,3	0.46	0	2,2,2	0.41	0
11	EDO	F	1174	-	3,3,3	0.51	0	2,2,2	0.15	0
12	NAG	C	601	1	14,14,15	0.54	0	17,19,21	1.01	1 (5%)
11	EDO	E	1327	-	3,3,3	0.47	0	2,2,2	0.38	0
12	NAG	E	621	1	14,14,15	0.65	0	17,19,21	1.11	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
11	EDO	A	1327	-	-	1/1/1/1	-
11	EDO	C	1327	-	-	0/1/1/1	-
11	EDO	E	1326	-	-	1/1/1/1	-
11	EDO	A	1328	-	-	1/1/1/1	-
10	BMA	A	604	-	-	2/2/19/22	0/1/1/1
11	EDO	C	1328	-	-	0/1/1/1	-
11	EDO	D	1173	-	-	1/1/1/1	-
11	EDO	F	1175	-	-	1/1/1/1	-
11	EDO	B	1174	-	-	0/1/1/1	-
11	EDO	B	1173	-	-	0/1/1/1	-
11	EDO	F	1173	-	-	1/1/1/1	-
11	EDO	F	1174	-	-	1/1/1/1	-
12	NAG	C	601	1	-	4/6/23/26	0/1/1/1
11	EDO	E	1327	-	-	1/1/1/1	-
12	NAG	E	621	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	E	621	NAG	C4-C3-C2	3.60	116.29	111.02
12	C	601	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	601	NAG	O5-C5-C6-O6
12	E	621	NAG	C4-C5-C6-O6
12	C	601	NAG	C8-C7-N2-C2
12	C	601	NAG	O7-C7-N2-C2
12	E	621	NAG	O5-C5-C6-O6
11	F	1175	EDO	O1-C1-C2-O2
12	C	601	NAG	C4-C5-C6-O6
11	A	1328	EDO	O1-C1-C2-O2
11	D	1173	EDO	O1-C1-C2-O2
10	A	604	BMA	C4-C5-C6-O6
11	F	1174	EDO	O1-C1-C2-O2
10	A	604	BMA	O5-C5-C6-O6
11	A	1327	EDO	O1-C1-C2-O2
11	E	1326	EDO	O1-C1-C2-O2
11	E	1327	EDO	O1-C1-C2-O2
11	F	1173	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1328	EDO	1	0
11	E	1327	EDO	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	A	325/329 (98%)	-0.04	6 (1%)	68	71	19, 29, 48, 64	0
1	C	320/329 (97%)	-0.03	2 (0%)	89	90	17, 29, 48, 71	0
1	E	325/329 (98%)	-0.07	3 (0%)	84	85	18, 30, 47, 66	0
2	B	172/172 (100%)	0.03	2 (1%)	79	81	15, 26, 42, 59	0
2	D	172/172 (100%)	0.10	4 (2%)	60	63	15, 27, 44, 63	0
2	F	172/172 (100%)	0.17	2 (1%)	79	81	16, 24, 41, 61	0
All	All	1486/1503 (98%)	0.00	19 (1%)	77	79	15, 28, 47, 71	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	81	TYR	4.7
1	A	276	ILE	4.2
1	A	142	GLY	3.7
1	A	278	VAL	3.3
2	D	58	ARG	3.2
1	A	81	TYR	3.2
1	A	143	SER	3.2
2	F	77[A]	ILE	2.8
2	D	172	GLN	2.7
1	E	276	ILE	2.7
2	B	77[A]	ILE	2.5
2	D	38[A]	LEU	2.5
1	A	277	CYS	2.4
2	D	63	PHE	2.4
2	B	172	GLN	2.3
1	E	2	GLN	2.2
2	F	59	THR	2.2
1	C	79	PHE	2.2
1	E	81	TYR	2.1

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	P	5	11/12	0.50	0.56	94,100,104,107	0
3	NAG	L	1	14/15	0.55	0.34	66,72,76,82	0
3	NAG	W	2	14/15	0.56	0.40	85,89,96,97	0
6	BMA	O	3	11/12	0.56	0.30	90,95,101,101	0
3	NAG	J	2	14/15	0.58	0.36	71,79,82,84	0
3	NAG	V	2	14/15	0.59	0.39	95,99,101,101	0
6	BMA	M	3	11/12	0.59	0.28	84,87,91,93	0
3	NAG	Y	2	14/15	0.59	0.47	81,84,87,90	0
3	NAG	G	2	14/15	0.63	0.49	94,100,105,105	0
3	NAG	H	2	14/15	0.65	0.50	84,88,94,95	0
4	MAN	I	4	11/12	0.66	0.22	79,86,93,95	0
4	MAN	P	4	11/12	0.68	0.47	84,87,90,90	0
3	NAG	R	2	14/15	0.69	0.31	72,77,80,80	0
9	NAG	U	2	14/15	0.69	0.35	74,80,85,85	0
9	NAG	b	2	14/15	0.69	0.34	82,87,91,93	0
9	NAG	Z	2	14/15	0.71	0.19	70,72,77,78	0
4	MAN	Q	5	11/12	0.71	0.27	79,80,84,85	0
3	NAG	W	1	14/15	0.73	0.30	61,69,74,80	0
6	NAG	O	2	14/15	0.73	0.35	82,85,89,89	0
3	NAG	J	1	14/15	0.74	0.20	51,62,66,71	0
3	NAG	L	2	14/15	0.74	0.39	83,89,93,94	0
9	FUC	Z	3	10/11	0.74	0.28	71,76,79,79	0
3	NAG	R	1	14/15	0.74	0.24	52,61,65,68	0
6	NAG	M	2	14/15	0.75	0.26	70,75,80,84	0
4	MAN	Q	4	11/12	0.75	0.27	70,75,81,83	0
4	BMA	I	3	11/12	0.76	0.12	64,71,78,78	0
4	BMA	P	3	11/12	0.77	0.34	84,86,91,97	0
5	BMA	K	3	11/12	0.77	0.36	80,86,89,92	0
9	FUC	U	3	10/11	0.78	0.26	62,68,71,72	0
6	NAG	O	1	14/15	0.78	0.30	65,69,74,78	0
9	NAG	b	1	14/15	0.79	0.21	54,62,68,76	0
8	MAN	S	5	11/12	0.79	0.40	72,74,81,85	0

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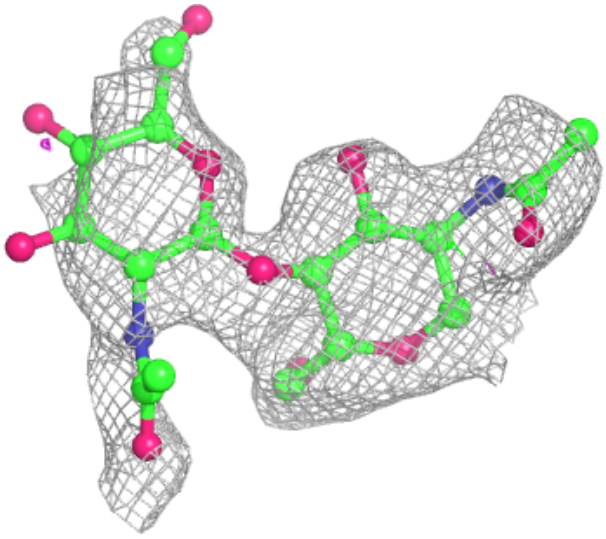
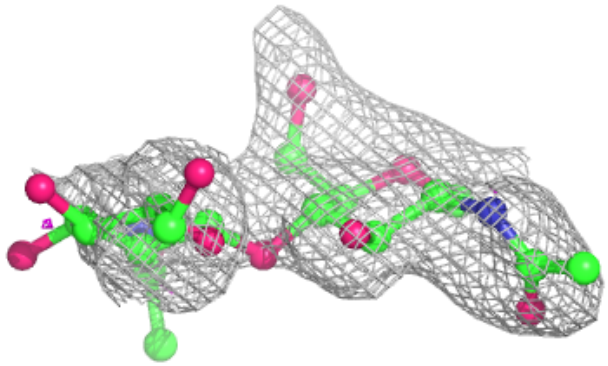
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	X	4	11/12	0.80	0.25	78,81,84,87	0
3	NAG	V	1	14/15	0.80	0.35	76,82,88,90	0
9	FUC	b	3	10/11	0.80	0.38	74,78,80,82	0
4	BMA	Q	3	11/12	0.81	0.15	62,69,74,74	0
4	MAN	X	5	11/12	0.81	0.20	77,80,84,85	0
5	NAG	K	2	14/15	0.82	0.26	58,63,71,75	0
4	NAG	P	2	14/15	0.83	0.24	65,69,73,79	0
6	BMA	T	3	11/12	0.84	0.14	51,54,57,60	0
8	BMA	S	3	11/12	0.84	0.19	49,51,62,68	0
6	NAG	M	1	14/15	0.84	0.20	48,57,61,65	0
3	NAG	Y	1	14/15	0.84	0.23	52,60,68,72	0
5	FUC	K	4	10/11	0.84	0.30	59,64,68,68	0
9	NAG	U	1	14/15	0.85	0.20	56,64,69,69	0
7	NAG	N	1	14/15	0.85	0.23	54,61,65,68	0
3	NAG	a	2	14/15	0.85	0.28	61,67,69,69	0
3	NAG	H	1	14/15	0.85	0.20	62,67,74,79	0
4	MAN	I	5	11/12	0.86	0.20	82,85,90,91	0
7	FUC	N	2	10/11	0.86	0.35	72,76,79,81	0
9	NAG	Z	1	14/15	0.87	0.18	56,60,68,72	0
4	BMA	X	3	11/12	0.87	0.12	61,67,73,75	0
3	NAG	G	1	14/15	0.87	0.24	71,75,81,89	0
5	NAG	K	1	14/15	0.88	0.15	43,45,55,58	0
8	FUC	S	6	10/11	0.89	0.16	49,52,54,56	0
8	MAN	S	4	11/12	0.90	0.12	44,49,53,54	0
4	NAG	P	1	14/15	0.90	0.24	51,57,60,62	0
6	NAG	T	2	14/15	0.90	0.12	38,42,44,48	0
3	NAG	a	1	14/15	0.90	0.13	41,48,52,54	0
4	NAG	I	2	14/15	0.91	0.11	43,48,54,59	0
8	NAG	S	2	14/15	0.91	0.11	39,45,48,49	0
4	NAG	X	2	14/15	0.91	0.12	41,47,53,57	0
4	NAG	Q	1	14/15	0.92	0.12	38,41,42,43	0
6	NAG	T	1	14/15	0.92	0.13	28,32,35,36	0
4	NAG	Q	2	14/15	0.93	0.11	43,48,52,57	0
8	NAG	S	1	14/15	0.93	0.09	30,35,41,45	0
4	NAG	I	1	14/15	0.93	0.10	37,40,42,43	0
4	NAG	X	1	14/15	0.93	0.12	39,42,44,44	0

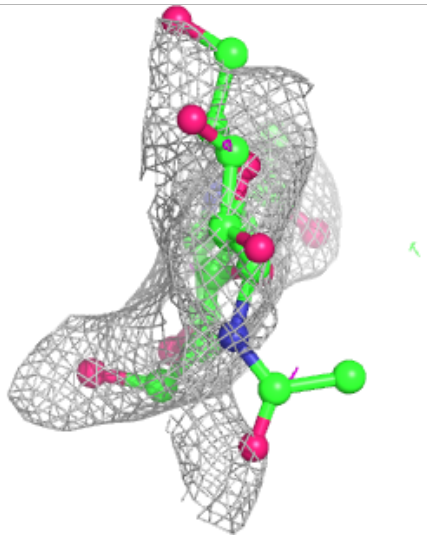
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

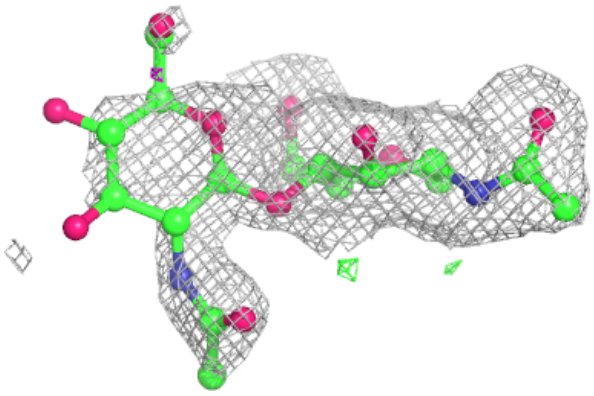


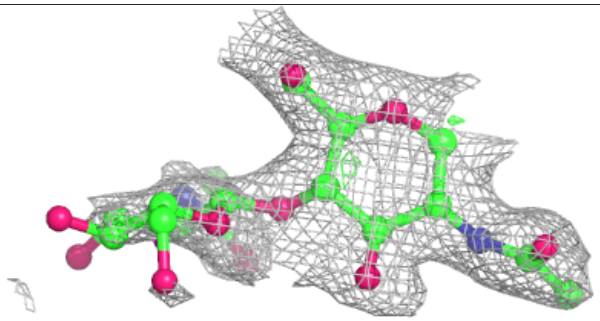


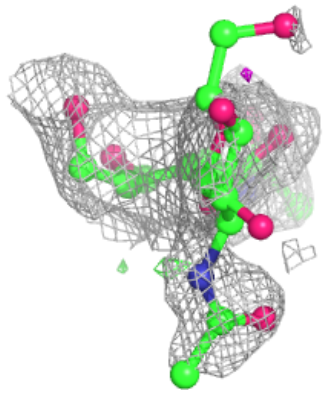


Electron density around Chain H:

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

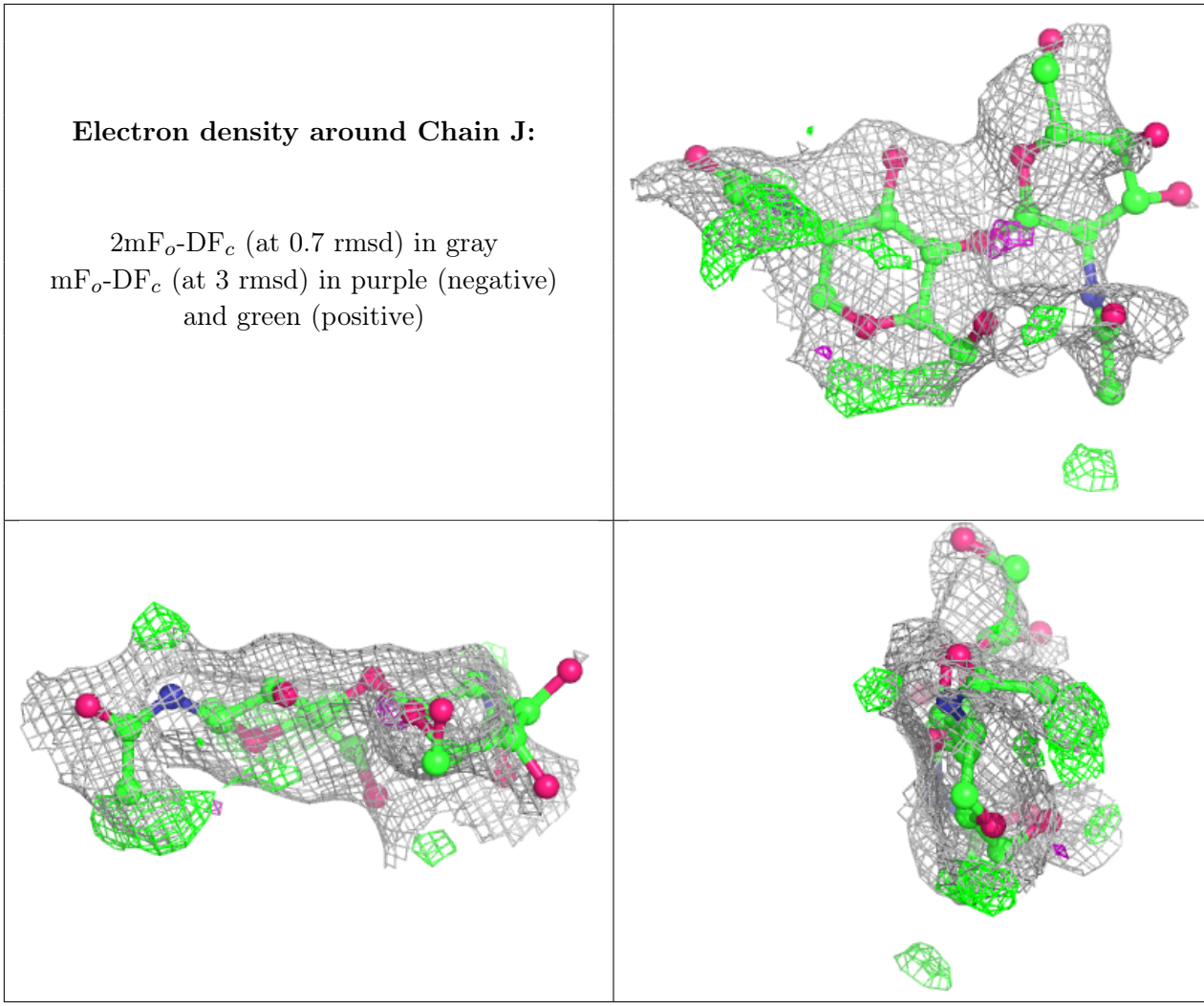






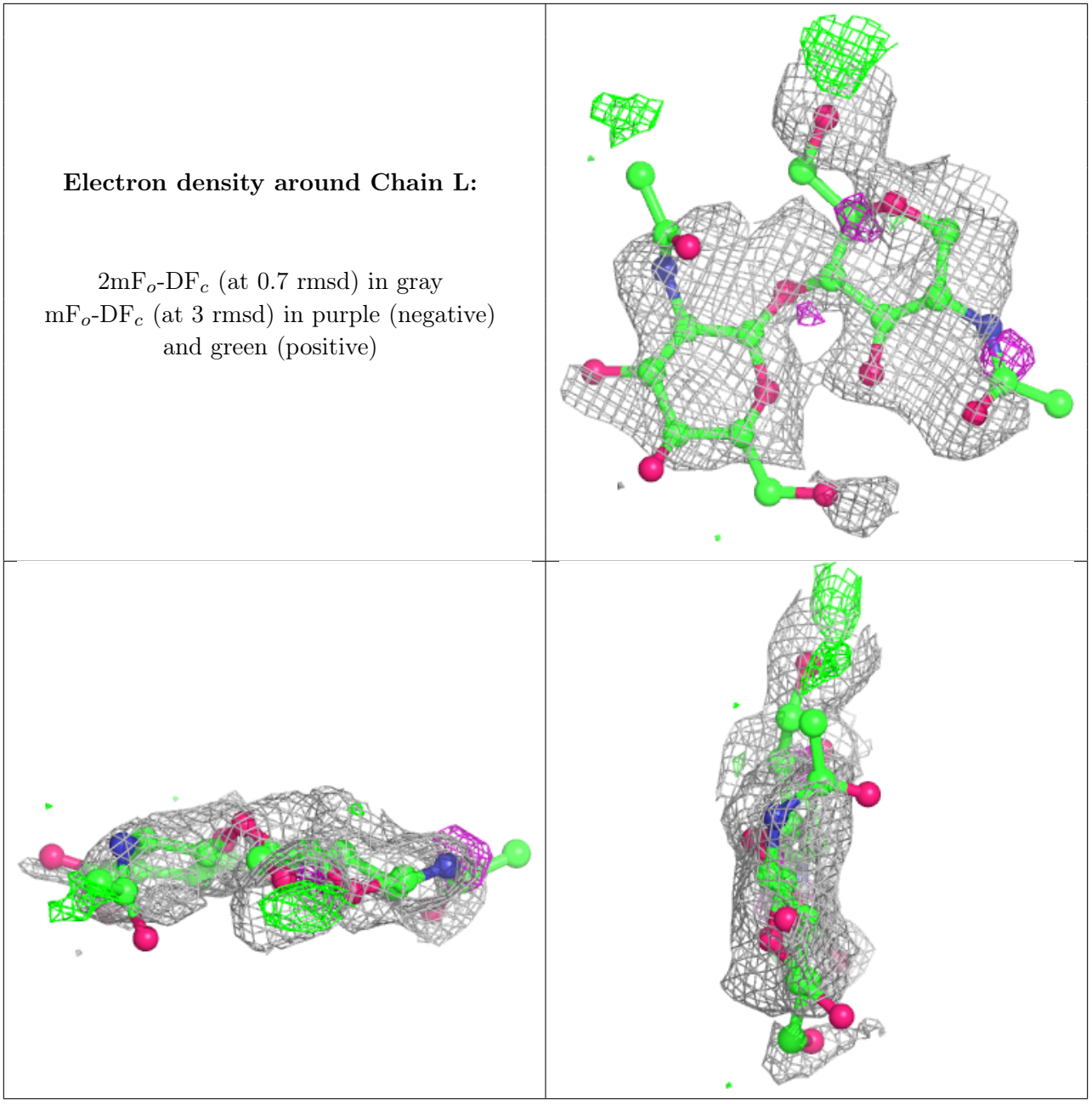
Electron density around Chain J:

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



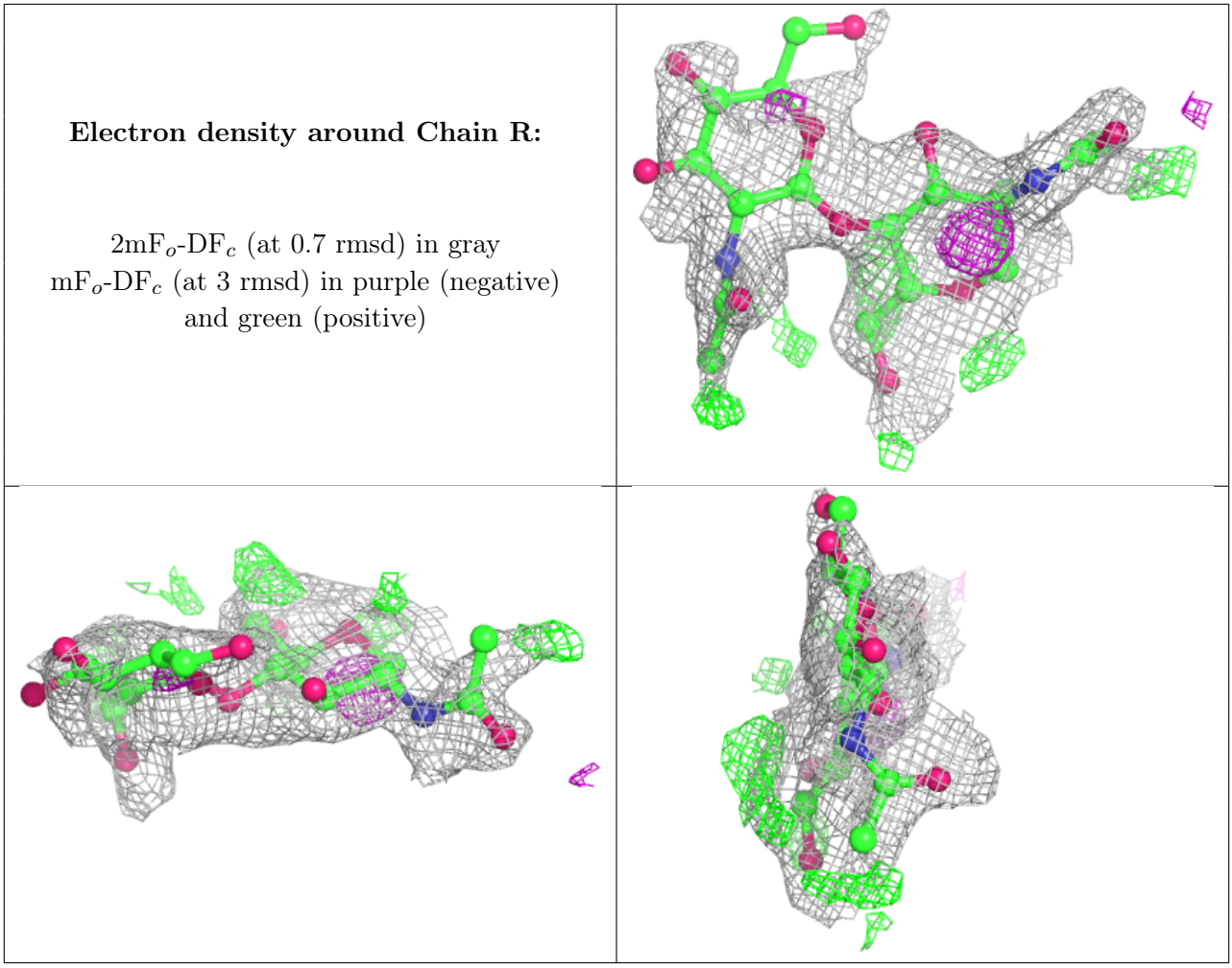
Electron density around Chain L:

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



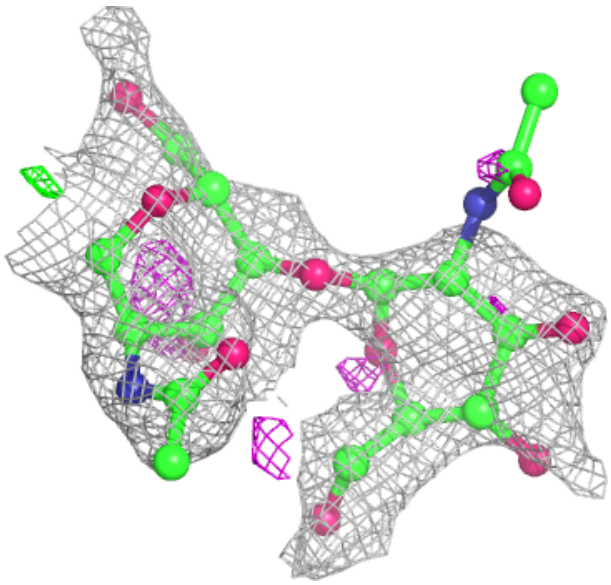
Electron density around Chain R:

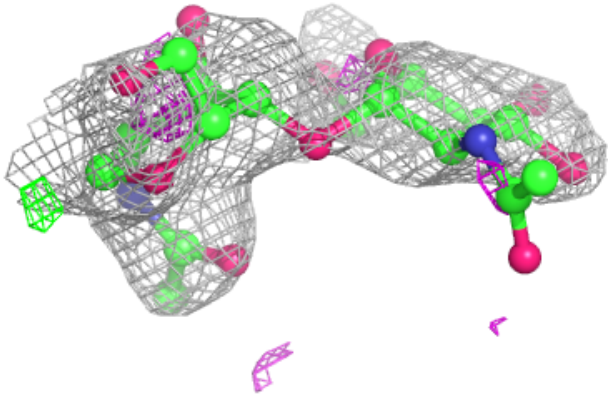
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

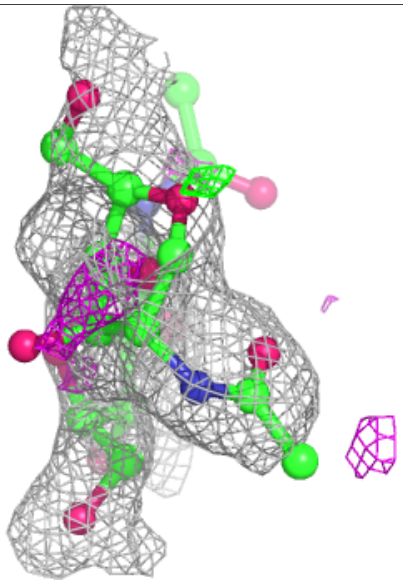


Electron density around Chain V:

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

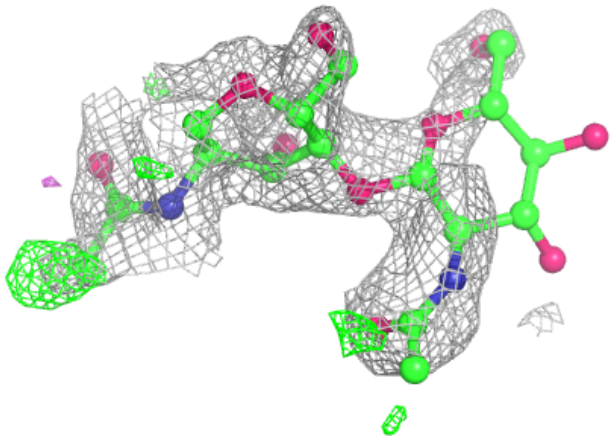


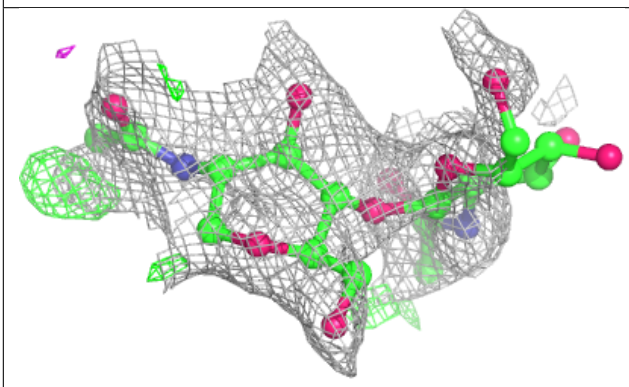


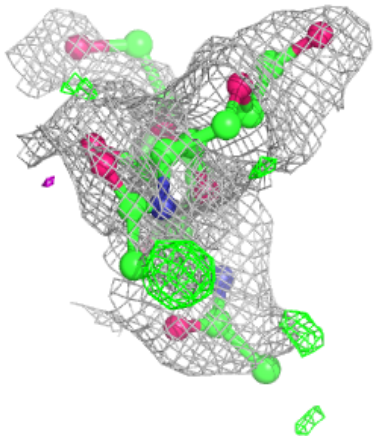


Electron density around Chain W:

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

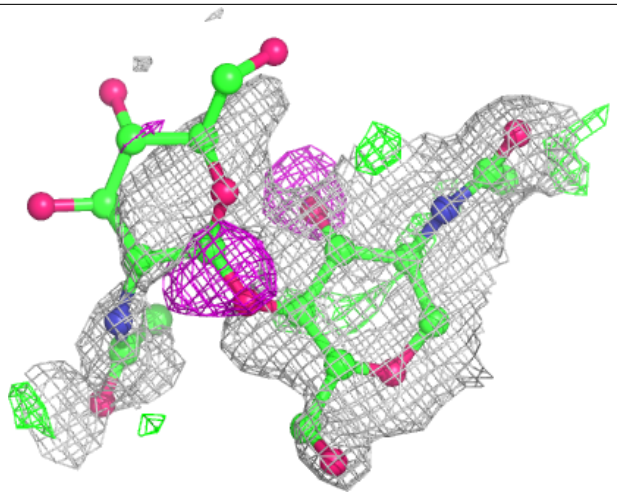


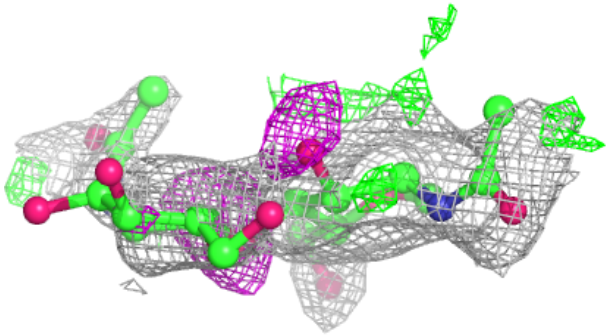


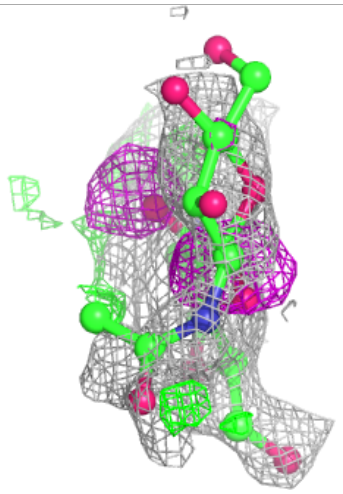


Electron density around Chain Y:

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

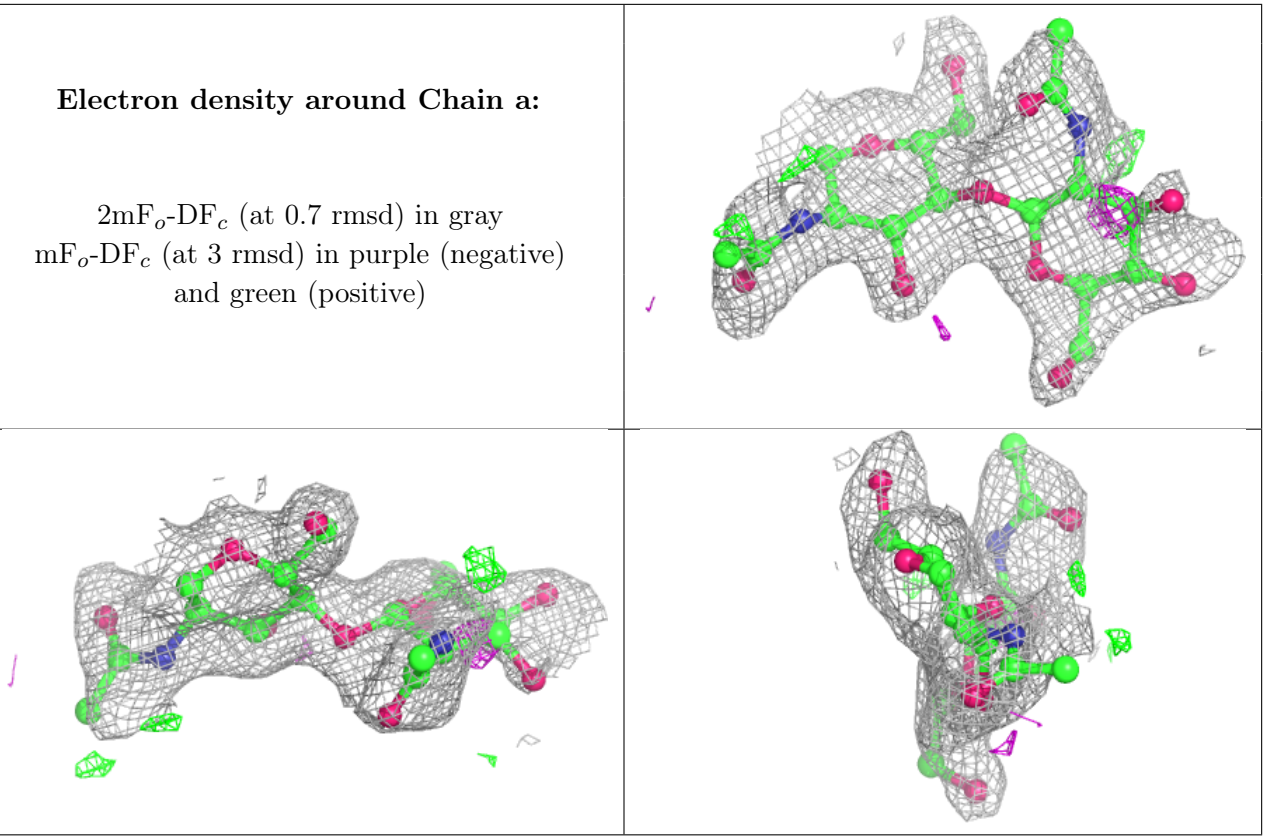






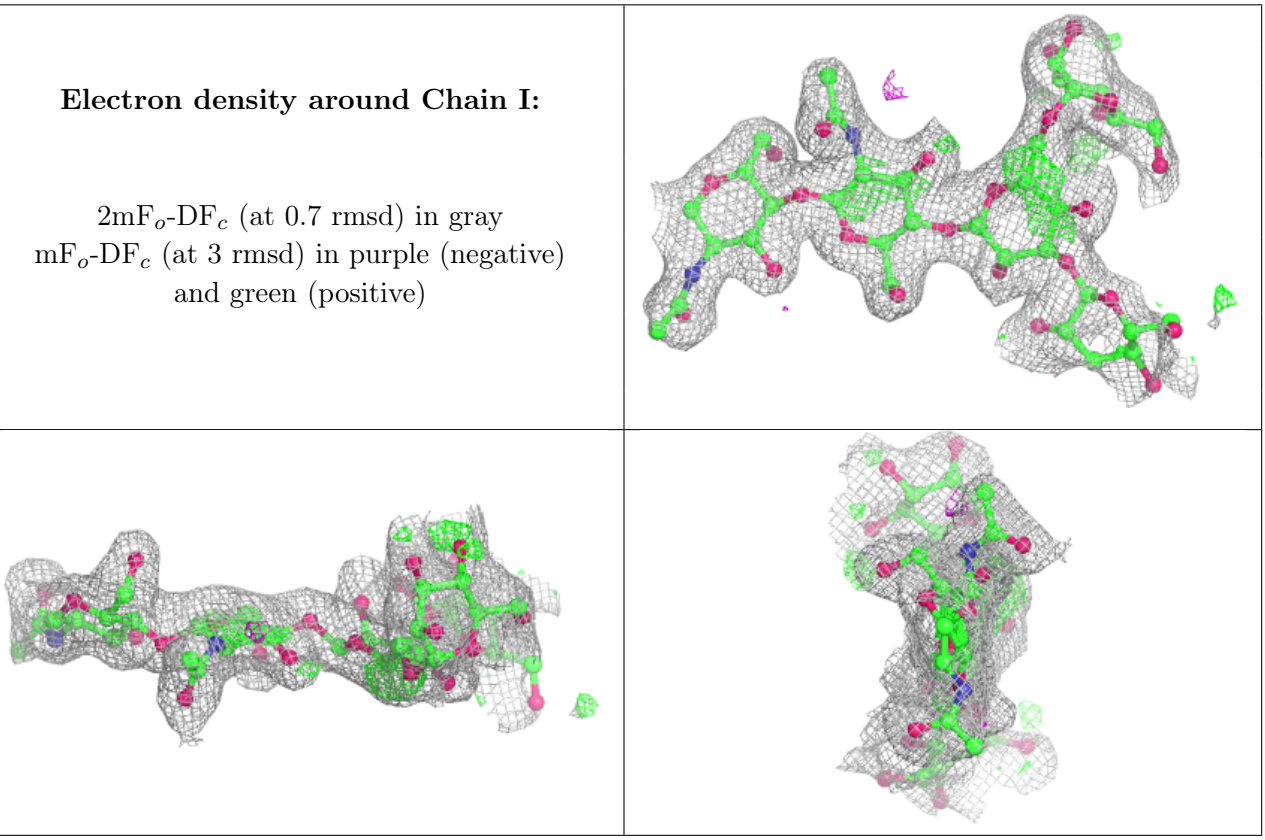
Electron density around Chain a:

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



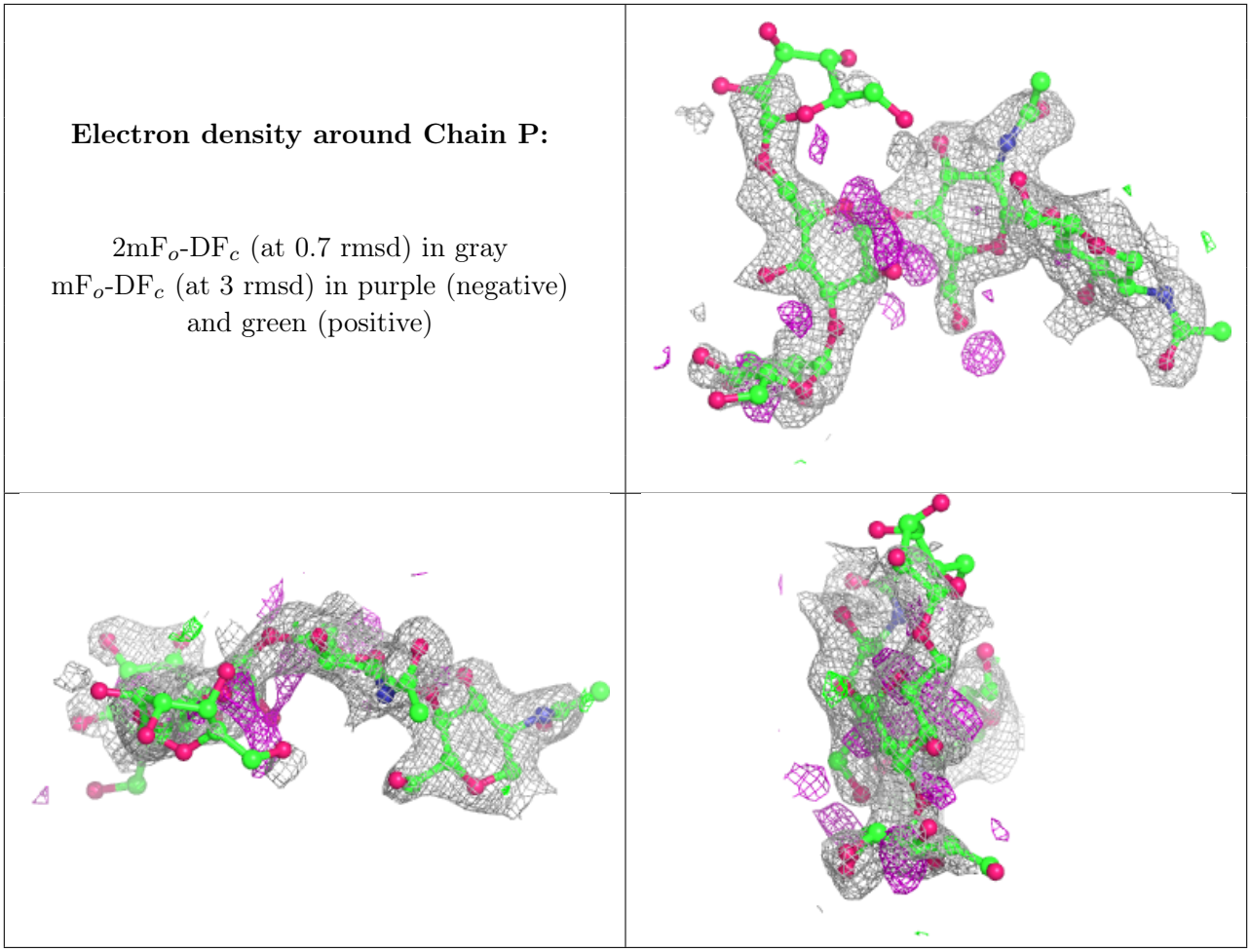
Electron density around Chain I:

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



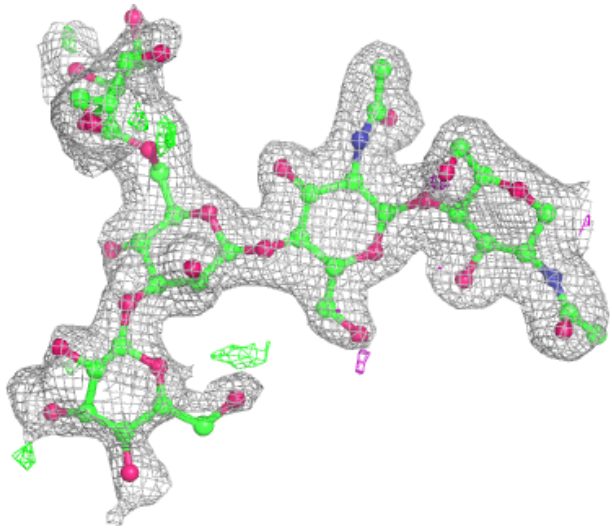
Electron density around Chain P:

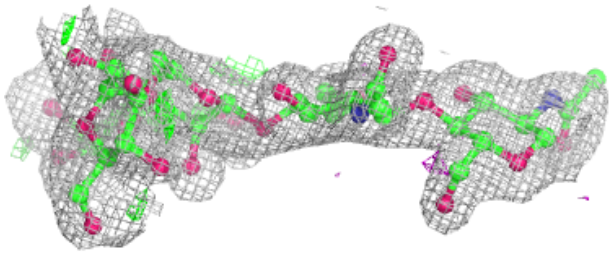
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

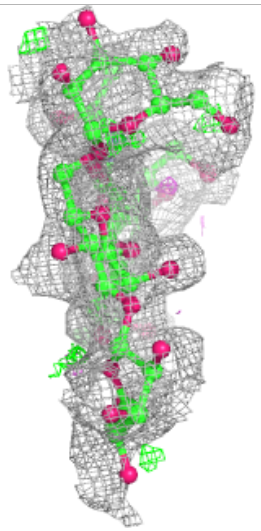


Electron density around Chain Q:

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

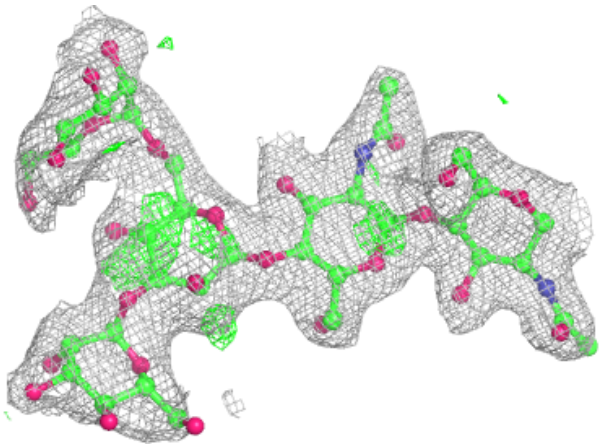


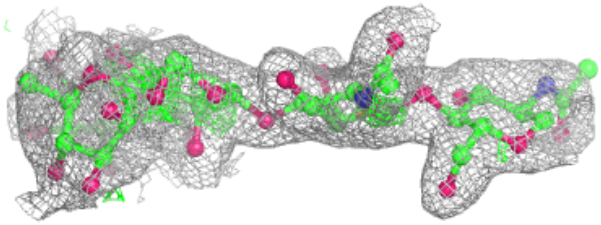


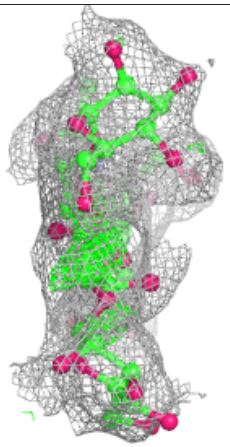


Electron density around Chain X:

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

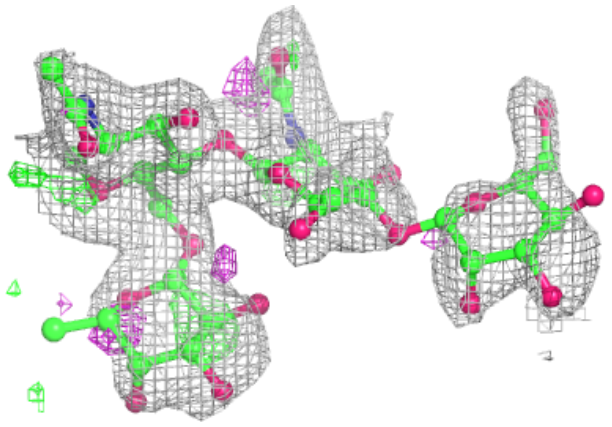


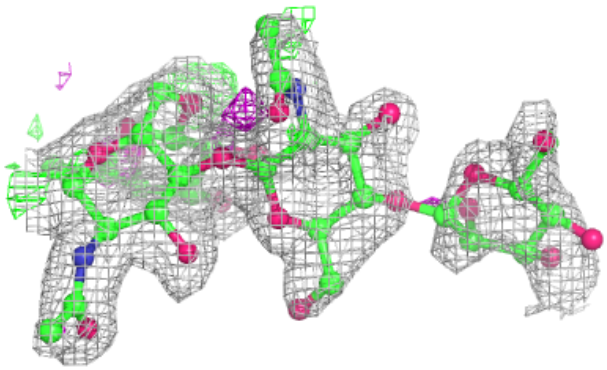


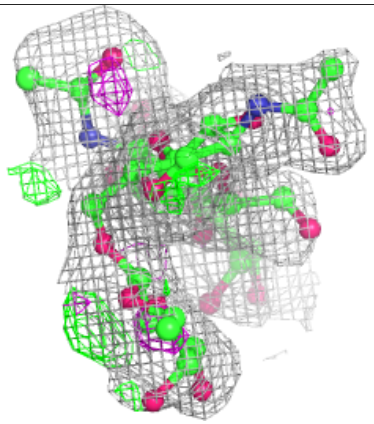


Electron density around Chain K:

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

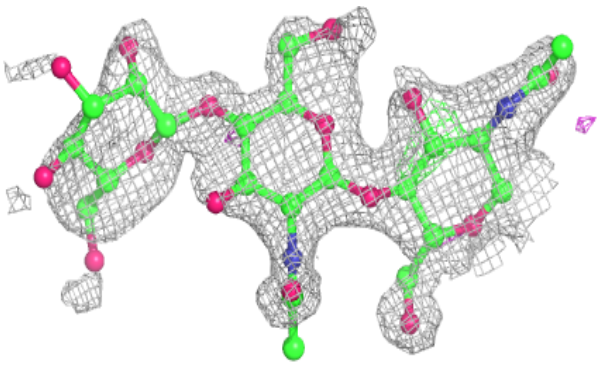


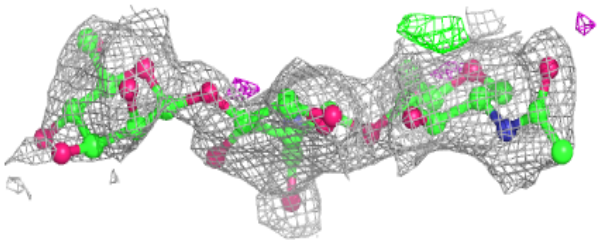


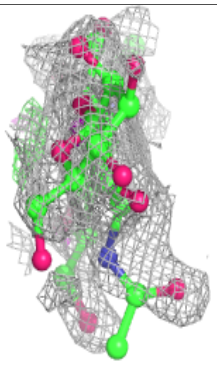


Electron density around Chain M:

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

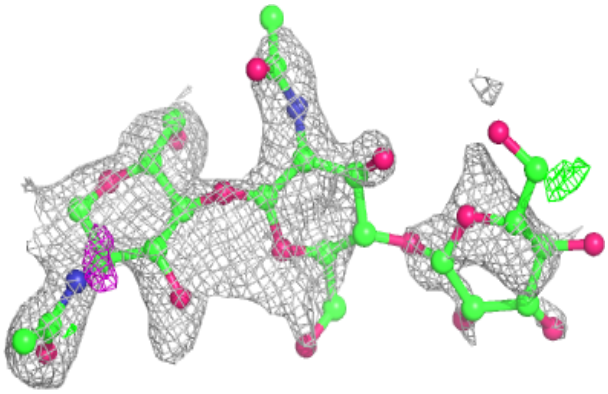


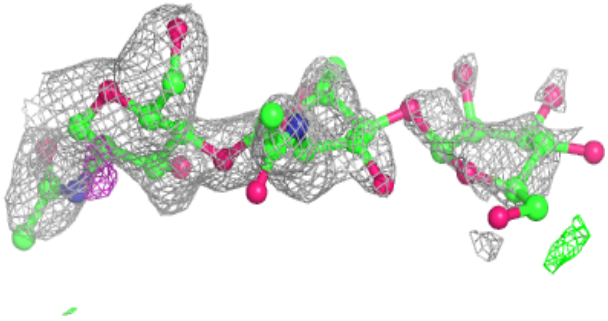


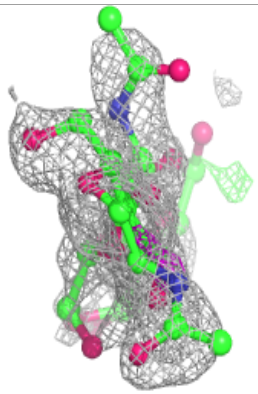


Electron density around Chain O:

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

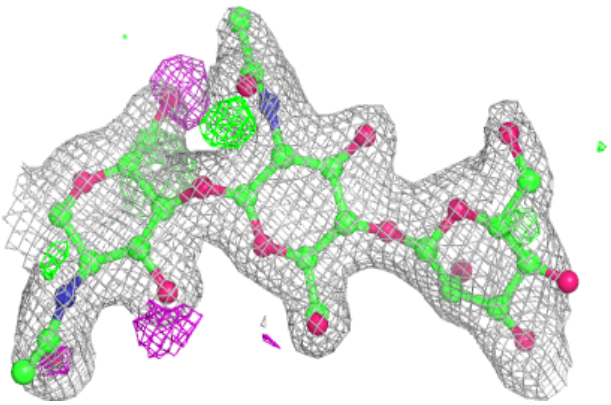


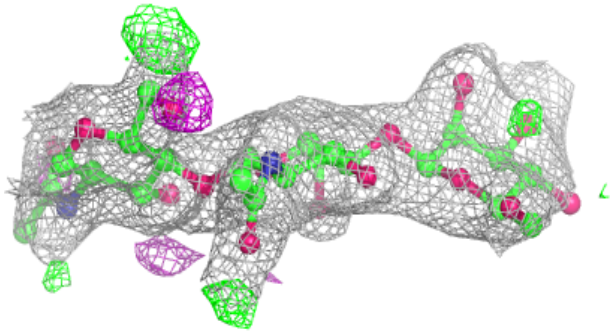


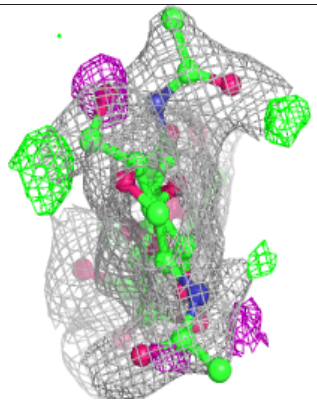


Electron density around Chain T:

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

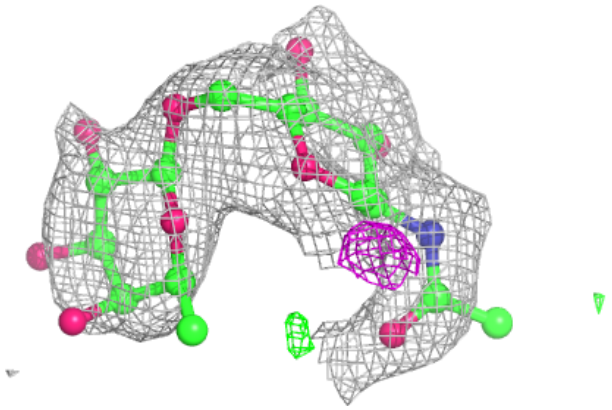


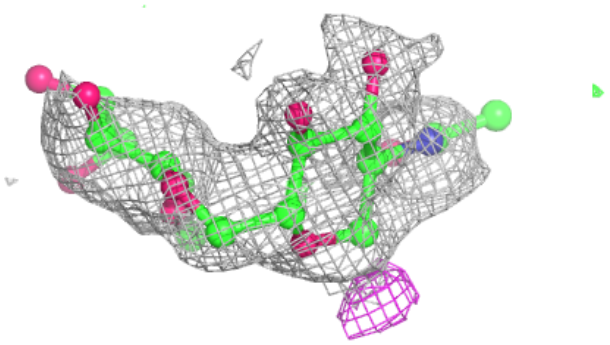


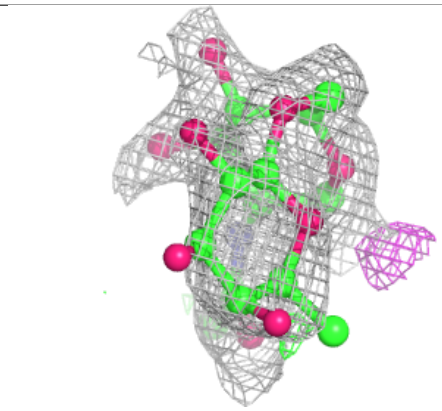


Electron density around Chain N:

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

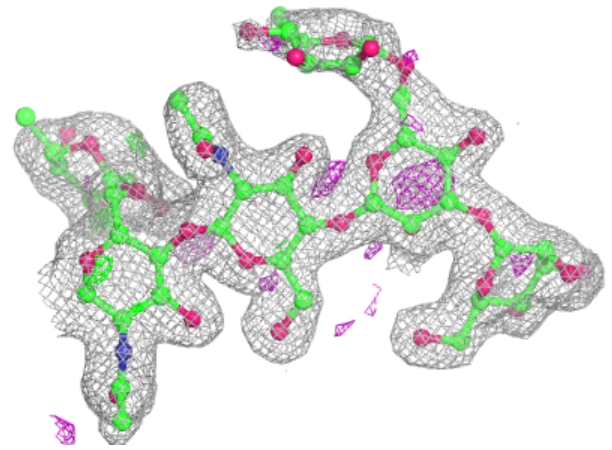


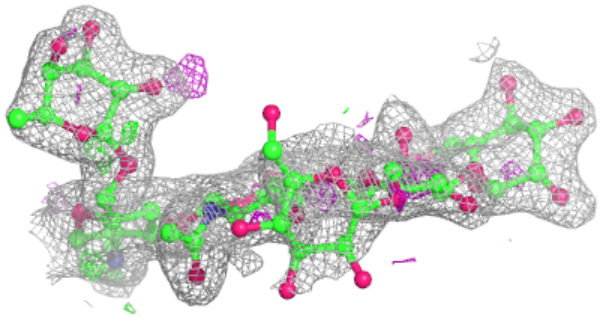


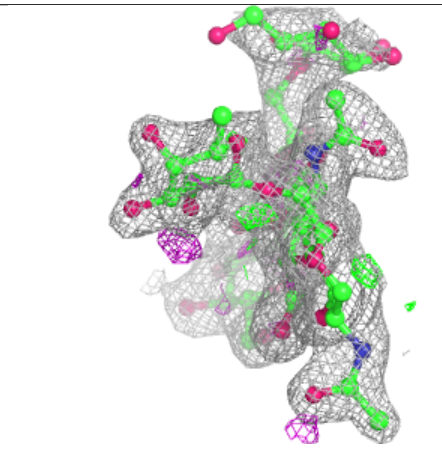


Electron density around Chain S:

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

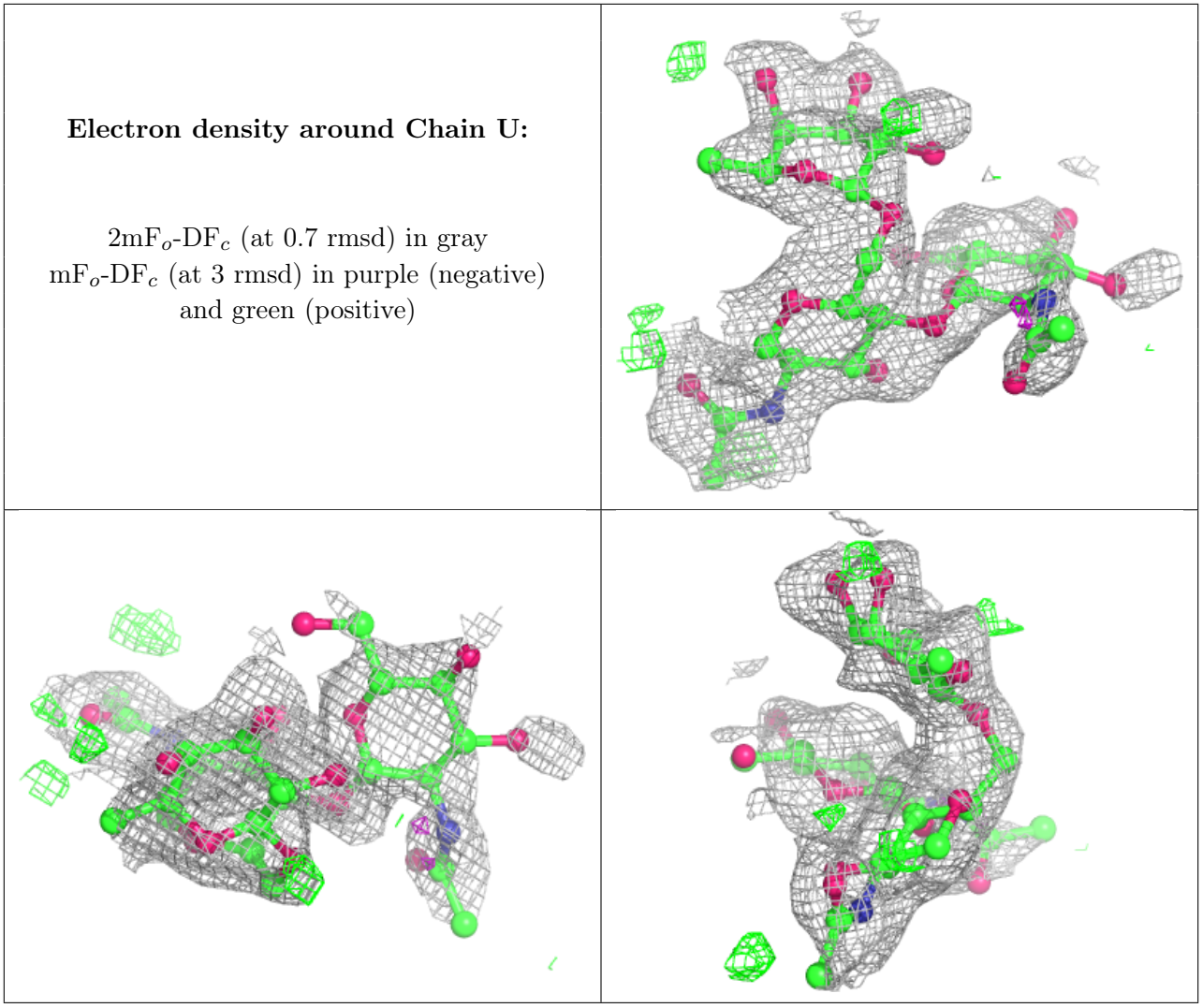






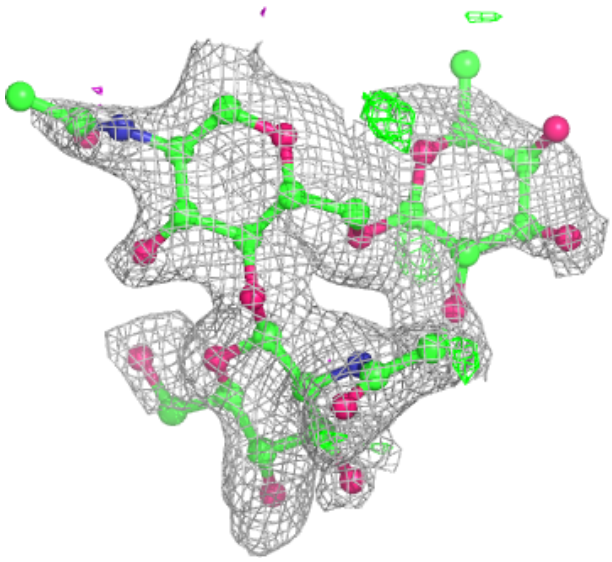
Electron density around Chain U:

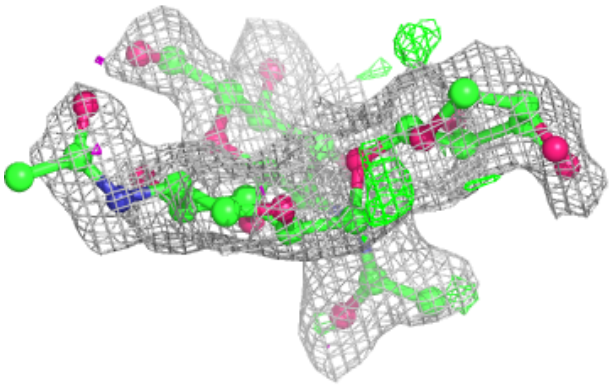
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

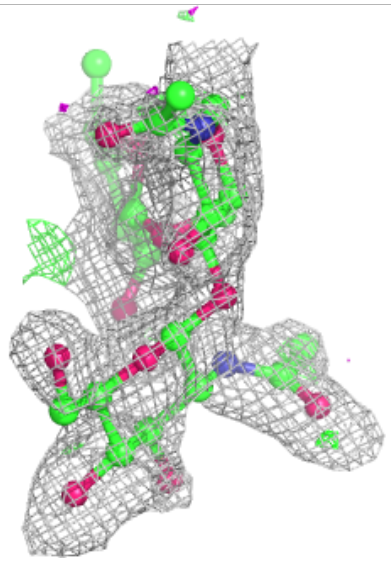


Electron density around Chain Z:

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

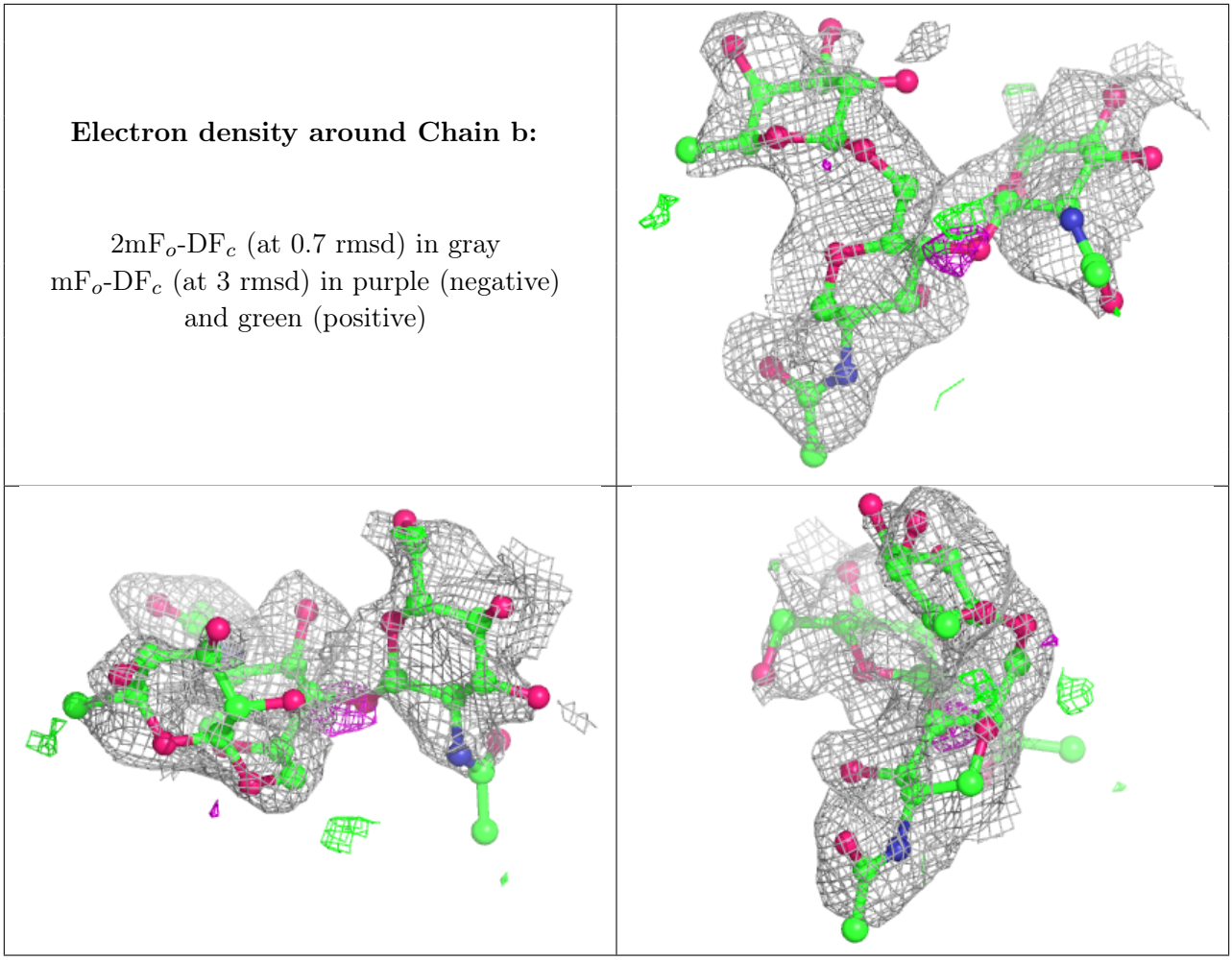






Electron density around Chain b:

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



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
10	BMA	A	604	11/12	0.60	0.52	126,134,137,137	0
12	NAG	C	601	14/15	0.61	0.44	90,93,98,100	0
11	EDO	C	1327	4/4	0.62	0.19	65,65,67,67	0
12	NAG	E	621	14/15	0.71	0.51	68,76,80,81	0
11	EDO	A	1328	4/4	0.77	0.28	61,63,64,65	0
11	EDO	C	1328	4/4	0.81	0.25	35,38,42,43	0
11	EDO	E	1327	4/4	0.82	0.14	48,50,52,53	0
11	EDO	F	1173	4/4	0.85	0.19	58,59,60,61	0
11	EDO	E	1326	4/4	0.86	0.18	54,55,57,61	0
11	EDO	F	1174	4/4	0.86	0.16	53,53,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	EDO	F	1175	4/4	0.88	0.12	48,51,52,52	0
11	EDO	A	1327	4/4	0.88	0.14	37,37,39,40	0
11	EDO	D	1173	4/4	0.88	0.29	51,52,52,53	0
11	EDO	B	1173	4/4	0.90	0.22	40,40,42,45	0
11	EDO	B	1174	4/4	0.93	0.16	44,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.