Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 12:34 PM EDT

PDB ID	:	5VK2
Title	:	Structural basis for antibody-mediated neutralization of Lassa virus
Authors	:	Hastie, K.M.; Zandonatti, M.A.; Kleinfelter, L.M.; Rowland, M.L.; Rowland, M.M.; Chandra, K.; Branco, L.M.; Robinson, J.E.; Garry, R.F.; Saphire, E.O.
Deposited on	:	2017-04-20
Resolution	:	3.20 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:

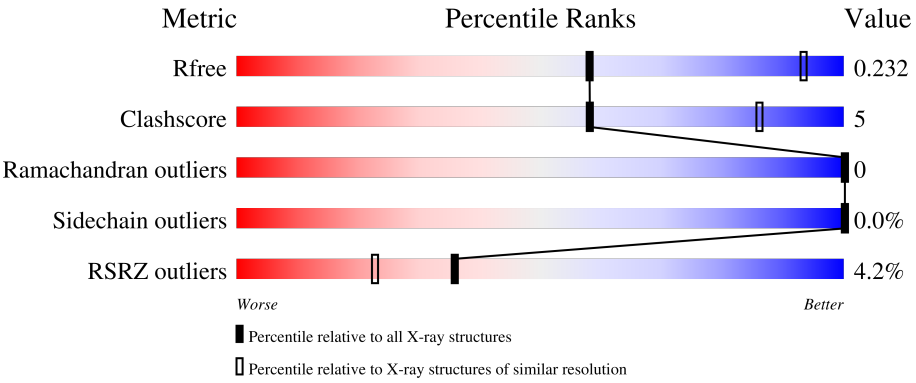
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	259	3% 64% 8% 28%
1	B	259	9% 63% 8% 29%
1	C	259	5% 62% 10% 29%
2	a	164	6% 95% 5%
2	b	164	5% 96%

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Mol	Chain	Length	Quality of chain
2	c	164	8% 96%
3	D	229	83% 12% 5%
3	F	229	% 81% 14% 5%
3	H	229	% 83% 12% 5%
4	E	217	4% 87% 10%
4	G	217	% 90% 7%
4	L	217	% 91% 7%
5	I	3	100%
5	V	3	33% 67%
5	Z	3	67% 33%
6	J	2	100%
6	K	2	50% 50%
6	M	2	100%
6	O	2	100%
6	Q	2	100%
6	R	2	100%
6	S	2	50% 50%
6	W	2	100%
6	X	2	50% 50%
6	Y	2	100%
6	e	2	100%
7	N	4	75% 25%
7	T	4	50% 50%
7	d	4	75% 25%
8	P	3	67% 33%

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Mol	Chain	Length	Quality of chain
8	U	3	67% 33%
8	f	3	67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	M	2	-	-	-	X
6	NAG	R	2	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 18672 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 Pre-glycoprotein polyprotein GP complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1466	923	245	282	16			
1	B	185	Total	C	N	O	S	0	0	0
			1456	917	242	281	16			
1	C	185	Total	C	N	O	S	0	0	0
			1456	917	242	281	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	CYS	ARG	engineered mutation	UNP P08669
A	258	ARG	LEU	engineered mutation	UNP P08669
A	259	ARG	LEU	engineered mutation	UNP P08669
B	207	CYS	ARG	engineered mutation	UNP P08669
B	258	ARG	LEU	engineered mutation	UNP P08669
B	259	ARG	LEU	engineered mutation	UNP P08669
C	207	CYS	ARG	engineered mutation	UNP P08669
C	258	ARG	LEU	engineered mutation	UNP P08669
C	259	ARG	LEU	engineered mutation	UNP P08669

- Molecule 2 is a protein called Pre-glycoprotein polyprotein GP complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	155	Total	C	N	O	S	0	0	0
			1255	790	212	240	13			
2	b	159	Total	C	N	O	S	0	0	0
			1285	809	217	246	13			
2	c	157	Total	C	N	O	S	0	0	0
			1273	801	215	244	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	329	PRO	GLU	engineered mutation	UNP P08669
a	332	THR	MET	engineered mutation	UNP P08669
a	360	CYS	GLY	engineered mutation	UNP P08669
b	329	PRO	GLU	engineered mutation	UNP P08669
b	332	THR	MET	engineered mutation	UNP P08669
b	360	CYS	GLY	engineered mutation	UNP P08669
c	329	PRO	GLU	engineered mutation	UNP P08669
c	332	THR	MET	engineered mutation	UNP P08669
c	360	CYS	GLY	engineered mutation	UNP P08669

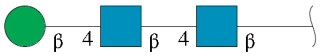
- Molecule 3 is a protein called Fab 37.7H heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	218	Total	C	N	O	S	0	0	0
			1636	1028	285	317	6			
3	F	217	Total	C	N	O	S	0	0	0
			1628	1024	284	314	6			
3	H	217	Total	C	N	O	S	0	0	0
			1625	1021	283	315	6			

- Molecule 4 is a protein called Fab 37.7H light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	211	Total	C	N	O	S	0	0	0
			1580	993	265	318	4			
4	G	211	Total	C	N	O	S	0	0	0
			1580	993	265	318	4			
4	L	212	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			

- Molecule 5 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
5	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	V	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

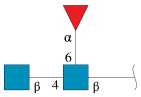
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	e	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

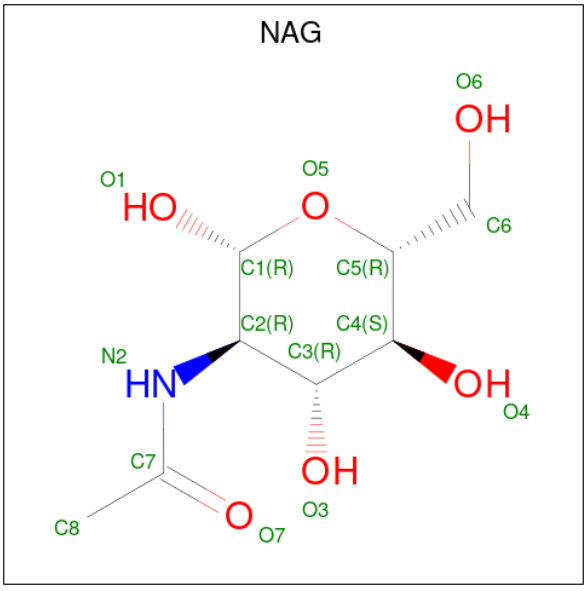
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	N	4	Total C N O 50 28 2 20	0	0	0
7	T	4	Total C N O 50 28 2 20	0	0	0
7	d	4	Total C N O 50 28 2 20	0	0	0

- Molecule 8 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
8	P	3	Total C N O 38 22 2 14	0	0	0
8	U	3	Total C N O 38 22 2 14	0	0	0
8	f	3	Total C N O 38 22 2 14	0	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



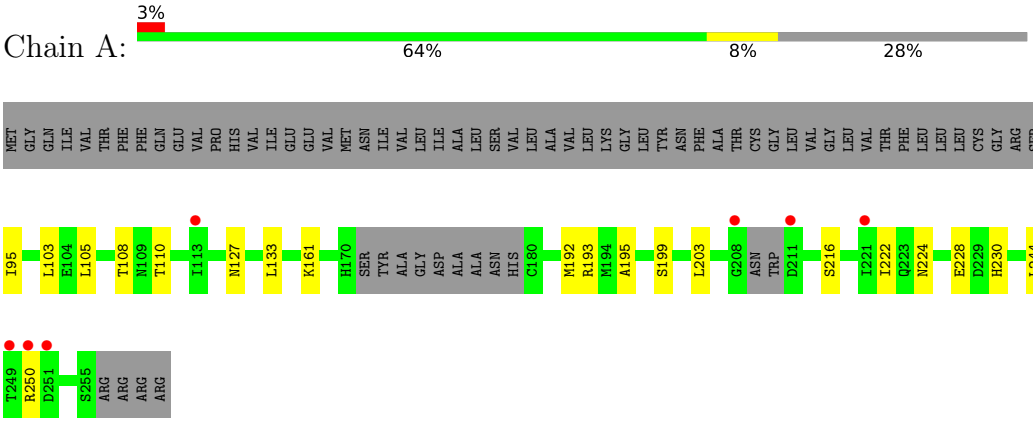
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	a	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	b	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	c	1	Total	C	N	O	0	0
			14	8	1	5		

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.

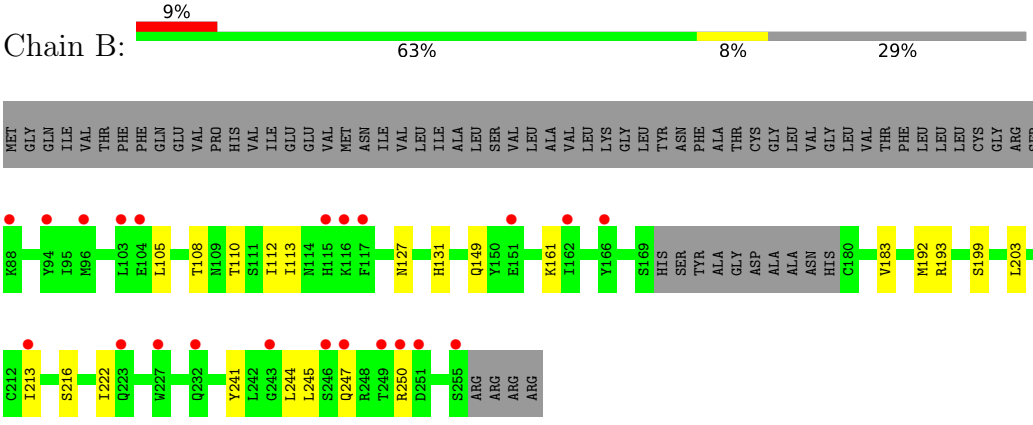
• Molecule 1: Pre-glycoprotein polyprotein GP complex

Chain A:



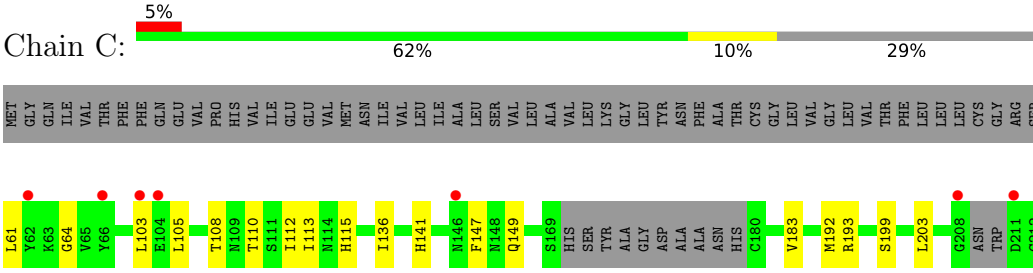
• Molecule 1: Pre-glycoprotein polyprotein GP complex

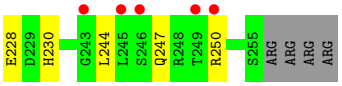
Chain B:



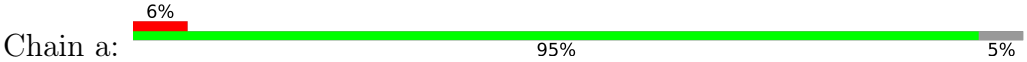
• Molecule 1: Pre-glycoprotein polyprotein GP complex

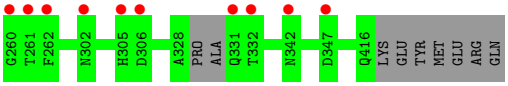
Chain C:



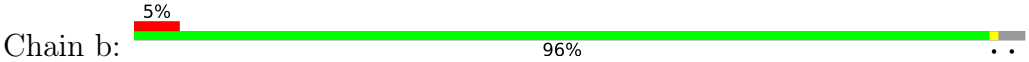


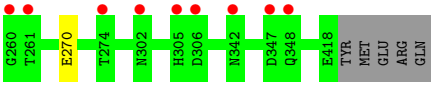
• Molecule 2: Pre-glycoprotein polyprotein GP complex



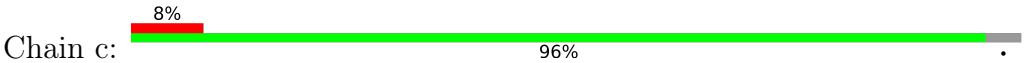


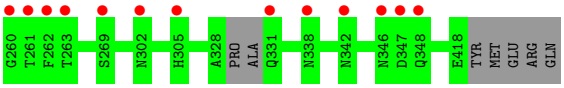
• Molecule 2: Pre-glycoprotein polyprotein GP complex



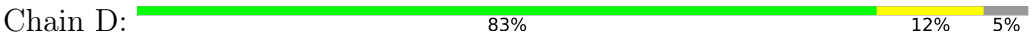


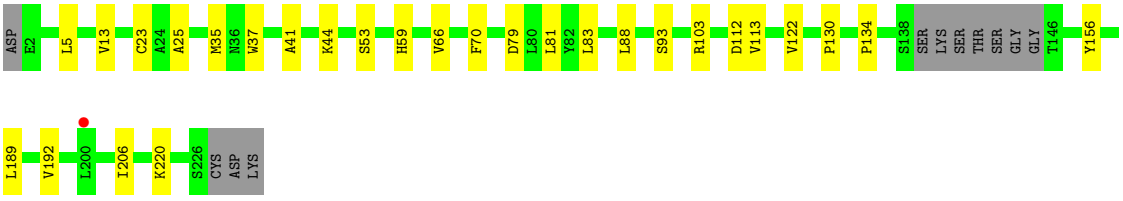
• Molecule 2: Pre-glycoprotein polyprotein GP complex



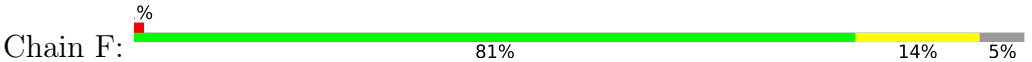


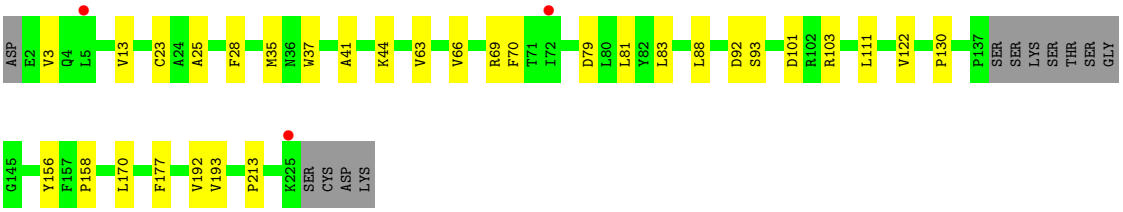
• Molecule 3: Fab 37.7H heavy chain



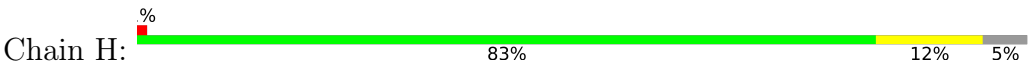


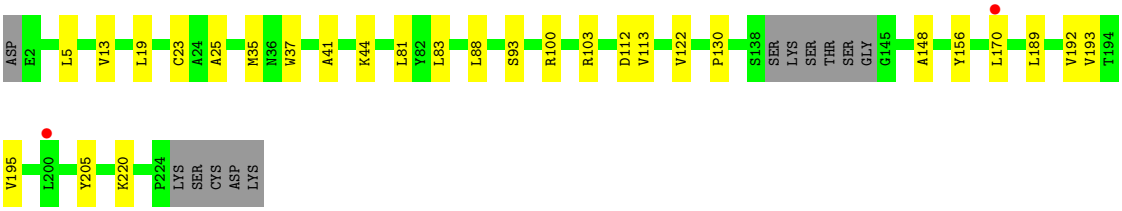
• Molecule 3: Fab 37.7H heavy chain



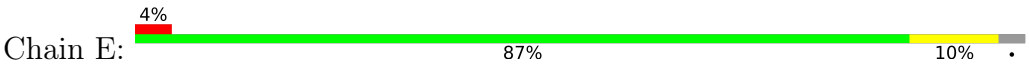


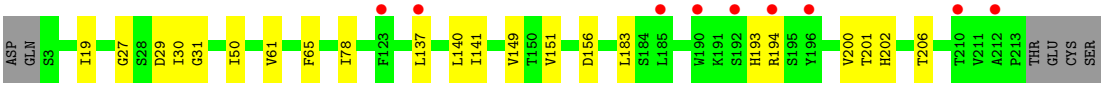
• Molecule 3: Fab 37.7H heavy chain





• Molecule 4: Fab 37.7H light chain





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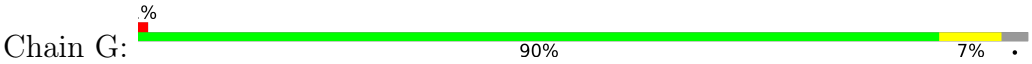
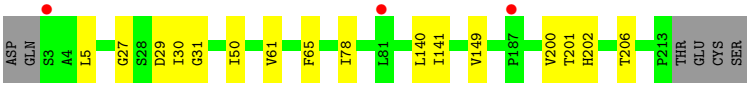
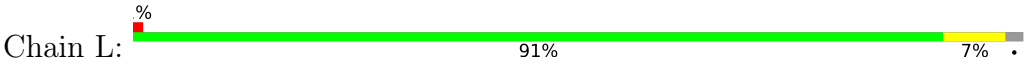
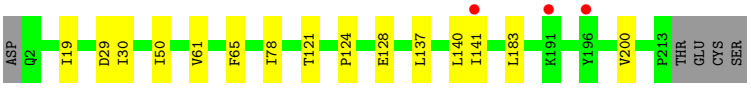




• Molecule 4: Fab 37.7H light chain





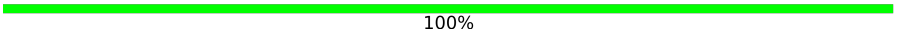
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

Chain J:

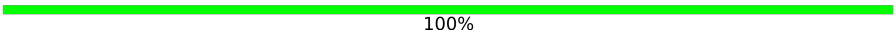


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

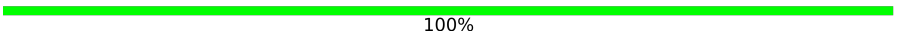
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



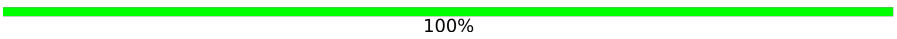
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



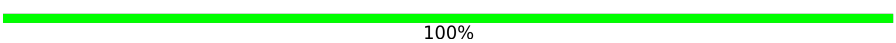
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



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

Chain R:

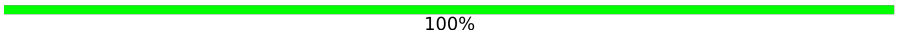


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

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

Chain W:

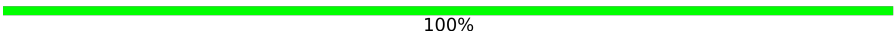


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

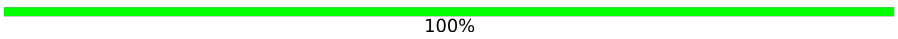
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



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

Chain e:



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

Chain N:

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

Chain T:

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

Chain d:

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

Chain P:

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

Chain U:

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

Chain f:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	152.70Å 152.70Å 456.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.60 – 3.20 49.60 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.60-3.20) 86.0 (49.60-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.189 , 0.231 0.189 , 0.232	Depositor DCC
R_{free} test set	2296 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	100.5	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 81.6	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	0.93	EDS
Total number of atoms	18672	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC, BMA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/1496	0.45	0/2024
1	B	0.25	0/1485	0.44	0/2009
1	C	0.25	0/1485	0.46	0/2009
2	a	0.25	0/1280	0.42	0/1729
2	b	0.26	0/1312	0.43	0/1774
2	c	0.25	0/1298	0.42	0/1752
3	D	0.26	0/1672	0.49	0/2275
3	F	0.26	0/1664	0.50	0/2264
3	H	0.26	0/1661	0.50	0/2261
4	E	0.26	0/1620	0.45	0/2210
4	G	0.26	0/1620	0.45	0/2210
4	L	0.26	0/1629	0.46	0/2222
All	All	0.26	0/18222	0.46	0/24739

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	1466	0	1400	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1456	0	1394	17	0
1	C	1456	0	1393	15	0
2	a	1255	0	1203	0	0
2	b	1285	0	1236	0	0
2	c	1273	0	1222	0	0
3	D	1636	0	1618	18	0
3	F	1628	0	1611	19	0
3	H	1625	0	1603	19	0
4	E	1580	0	1533	13	0
4	G	1580	0	1533	9	0
4	L	1589	0	1541	10	0
5	I	39	0	34	0	0
5	V	39	0	34	0	0
5	Z	39	0	34	0	0
6	J	28	0	25	0	0
6	K	28	0	25	1	0
6	M	28	0	25	0	0
6	O	28	0	25	0	0
6	Q	28	0	25	0	0
6	R	28	0	25	0	0
6	S	28	0	25	1	0
6	W	28	0	25	0	0
6	X	28	0	25	1	0
6	Y	28	0	25	0	0
6	e	28	0	25	0	0
7	N	50	0	43	0	0
7	T	50	0	43	0	0
7	d	50	0	43	0	0
8	P	38	0	34	0	0
8	U	38	0	34	0	0
8	f	38	0	34	0	0
9	A	42	0	39	1	0
9	B	42	0	39	1	0
9	C	28	0	26	0	0
9	a	14	0	13	0	0
9	b	14	0	13	0	0
9	c	14	0	13	0	0
All	All	18672	0	18038	130	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 5.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:SER:HB2	6:K:1:NAG:H3	1.65	0.78
1:B:105:LEU:HD23	1:B:222:ILE:HG12	1.74	0.69
1:A:108:THR:HG22	1:A:110:THR:H	1.58	0.68
1:C:61:LEU:HD13	1:C:64:GLY:HA2	1.76	0.67
1:B:216:SER:HB2	6:S:1:NAG:H3	1.78	0.65
1:C:108:THR:HG22	1:C:110:THR:H	1.61	0.65
1:B:108:THR:HG22	1:B:110:THR:H	1.62	0.64
4:E:29:ASP:OD2	4:E:30:ILE:N	2.29	0.63
3:D:192:VAL:HG11	4:E:140:LEU:HD13	1.81	0.62
1:B:127:ASN:HD21	1:B:131:HIS:HE1	1.47	0.62
1:A:161:LYS:HG2	9:A:512:NAG:H5	1.82	0.61
1:B:161:LYS:HG2	9:B:509:NAG:H5	1.83	0.61
4:G:29:ASP:OD1	4:G:30:ILE:N	2.30	0.59
3:F:192:VAL:HG11	4:G:140:LEU:HD13	1.84	0.58
1:A:193:ARG:HB3	1:A:244:LEU:HD11	1.85	0.58
3:H:100:ARG:HG2	3:H:113:VAL:HB	1.86	0.57
3:H:130:PRO:HB3	3:H:156:TYR:HB3	1.86	0.57
1:C:216:SER:HB2	6:X:1:NAG:H3	1.87	0.57
3:H:35:MET:HB3	3:H:81:LEU:HD22	1.86	0.57
1:A:247:GLN:HA	1:A:250:ARG:HG3	1.86	0.56
4:G:201:THR:HG23	4:G:206:THR:HG22	1.86	0.56
1:B:193:ARG:HB3	1:B:244:LEU:HD11	1.87	0.56
3:D:130:PRO:HB3	3:D:156:TYR:HB3	1.88	0.56
4:E:201:THR:HG23	4:E:206:THR:HG22	1.86	0.55
3:H:192:VAL:HG11	4:L:140:LEU:HD13	1.88	0.55
1:C:149:GLN:HB2	1:C:183:VAL:HG21	1.87	0.55
3:H:13:VAL:HG11	3:H:88:LEU:HD13	1.89	0.54
3:D:5:LEU:HD23	3:D:25:ALA:HA	1.90	0.53
3:D:35:MET:HB3	3:D:81:LEU:HD22	1.90	0.53
3:F:37:TRP:CD2	3:F:83:LEU:HD12	2.44	0.53
4:L:50:ILE:HG23	4:L:61:VAL:HG11	1.90	0.53
3:H:5:LEU:HD23	3:H:25:ALA:HA	1.92	0.52
4:L:29:ASP:OD1	4:L:30:ILE:N	2.38	0.52
4:L:19:ILE:HD11	4:L:78:ILE:HD12	1.91	0.52
3:D:37:TRP:CG	3:D:83:LEU:HD12	2.44	0.52
3:H:37:TRP:CG	3:H:83:LEU:HD12	2.45	0.52
3:F:93:SER:HB3	3:F:122:VAL:H	1.75	0.52
3:F:35:MET:HB3	3:F:81:LEU:HD22	1.90	0.51
3:D:93:SER:HB3	3:D:122:VAL:H	1.76	0.51
3:F:63:VAL:O	3:F:66:VAL:HG12	2.11	0.51
1:C:103:LEU:HD13	1:C:136:ILE:HD11	1.93	0.50
3:F:25:ALA:HB3	3:F:79:ASP:HB3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:LEU:HD22	1:C:213:ILE:HG21	1.94	0.50
1:A:103:LEU:HD13	1:A:133:LEU:HD12	1.92	0.50
3:D:53:SER:OG	3:D:59:HIS:HB3	2.12	0.49
1:A:103:LEU:HD12	1:A:224:ASN:HA	1.93	0.49
4:E:50:ILE:HG23	4:E:61:VAL:HG11	1.95	0.49
1:B:127:ASN:HD21	1:B:131:HIS:CE1	2.29	0.49
3:H:103:ARG:HA	3:H:103:ARG:HD2	1.65	0.48
4:L:141:ILE:HG12	4:L:200:VAL:HG21	1.93	0.48
4:G:27:GLY:HA2	4:G:31:GLY:HA3	1.95	0.48
1:A:127:ASN:O	1:A:127:ASN:ND2	2.45	0.48
3:D:41:ALA:HB3	3:D:44:LYS:HB2	1.94	0.48
1:A:95:ILE:HD11	1:A:105:LEU:HD11	1.96	0.48
4:E:137:LEU:HD12	4:E:183:LEU:HD23	1.95	0.48
1:B:241:TYR:CZ	1:B:245:LEU:HD21	2.48	0.48
1:C:193:ARG:HB3	1:C:244:LEU:HD11	1.95	0.48
4:G:149:VAL:HG12	4:G:202:HIS:HB2	1.95	0.47
1:B:127:ASN:ND2	1:B:131:HIS:HE1	2.09	0.47
3:H:195:VAL:HG11	3:H:205:TYR:CE1	2.50	0.47
4:E:156:ASP:OD1	4:E:194:ARG:HB3	2.14	0.47
3:F:37:TRP:CG	3:F:83:LEU:HD12	2.49	0.47
4:E:151:VAL:HG12	4:E:200:VAL:HG22	1.96	0.47
1:B:203:LEU:HD22	1:B:213:ILE:HG21	1.96	0.47
3:H:93:SER:HB3	3:H:122:VAL:H	1.79	0.46
3:H:220:LYS:NZ	4:L:128:GLU:OE1	2.45	0.46
3:F:70:PHE:CD2	3:F:83:LEU:HD21	2.51	0.46
3:H:41:ALA:HB3	3:H:44:LYS:HB2	1.97	0.46
3:D:66:VAL:HG13	3:D:70:PHE:CG	2.51	0.46
4:E:27:GLY:HA2	4:E:31:GLY:HA3	1.97	0.46
1:C:112:ILE:HG23	1:C:113:ILE:HG13	1.97	0.46
1:B:192:MET:HA	1:B:199:SER:OG	2.16	0.45
3:F:170:LEU:HD21	3:F:193:VAL:HG21	1.99	0.45
3:D:112:ASP:OD1	3:D:113:VAL:N	2.50	0.45
1:B:149:GLN:HB2	1:B:183:VAL:HG21	1.99	0.45
1:C:113:ILE:HG23	1:C:115:HIS:CE1	2.52	0.45
4:G:141:ILE:HG12	4:G:200:VAL:HG21	1.99	0.45
3:F:41:ALA:HB3	3:F:44:LYS:HB2	1.99	0.44
3:F:23:CYS:HB3	3:F:81:LEU:HB3	1.98	0.44
1:B:112:ILE:HG23	1:B:113:ILE:HG13	2.00	0.44
3:H:156:TYR:OH	3:H:189:LEU:HD23	2.18	0.44
1:A:192:MET:HA	1:A:199:SER:OG	2.18	0.44
1:B:199:SER:O	1:B:203:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:65:PHE:CD2	4:E:78:ILE:HG12	2.53	0.44
4:E:141:ILE:HG12	4:E:200:VAL:HG21	1.99	0.44
4:L:137:LEU:HD12	4:L:183:LEU:HD23	1.98	0.44
3:D:37:TRP:CD2	3:D:83:LEU:HD12	2.52	0.44
3:D:134:PRO:HD3	3:D:220:LYS:HZ3	1.83	0.44
3:D:25:ALA:HB3	3:D:79:ASP:HB3	1.99	0.43
1:C:141:HIS:HE1	1:C:147:PHE:CE2	2.36	0.43
4:E:156:ASP:HB2	4:E:193:HIS:ND1	2.34	0.43
3:H:13:VAL:HB	3:H:19:LEU:HD21	2.00	0.43
1:A:247:GLN:HG2	1:A:250:ARG:HB2	2.00	0.43
1:B:247:GLN:HA	1:B:250:ARG:HG3	2.00	0.43
3:D:23:CYS:HB3	3:D:81:LEU:HB3	2.00	0.43
3:F:101:ASP:HB3	3:F:111:LEU:HD23	2.00	0.43
3:D:206:ILE:O	3:D:206:ILE:HG13	2.18	0.43
4:E:19:ILE:HD11	4:E:78:ILE:HD12	2.01	0.43
4:G:50:ILE:HG23	4:G:61:VAL:HG11	2.01	0.43
3:F:103:ARG:HD3	3:F:103:ARG:HA	1.76	0.43
4:E:149:VAL:HG12	4:E:202:HIS:HB2	2.01	0.42
3:F:3:VAL:HG23	3:F:28:PHE:CD1	2.54	0.42
3:H:23:CYS:HB3	3:H:81:LEU:HB3	2.01	0.42
3:F:177:PHE:HE1	3:F:192:VAL:HG22	1.82	0.42
1:A:105:LEU:HD23	1:A:222:ILE:HG12	2.02	0.42
1:B:127:ASN:ND2	1:B:127:ASN:O	2.52	0.42
1:A:228:GLU:HB2	1:A:230:HIS:NE2	2.35	0.42
1:C:199:SER:O	1:C:203:LEU:HG	2.20	0.42
3:D:103:ARG:HD3	3:D:103:ARG:HA	1.78	0.42
3:D:13:VAL:HG11	3:D:88:LEU:HD13	2.01	0.42
1:C:247:GLN:HA	1:C:250:ARG:HG3	2.02	0.42
3:F:13:VAL:HG11	3:F:88:LEU:HD13	2.02	0.42
3:F:130:PRO:HB3	3:F:156:TYR:HB3	2.01	0.42
1:A:195:ALA:O	1:A:199:SER:HB2	2.20	0.42
4:G:65:PHE:CD2	4:G:78:ILE:HG12	2.55	0.41
3:H:37:TRP:CD2	3:H:83:LEU:HD12	2.55	0.41
1:C:105:LEU:H	1:C:105:LEU:HD23	1.85	0.41
1:C:228:GLU:HB2	1:C:230:HIS:NE2	2.35	0.41
3:F:158:PRO:HD2	3:F:213:PRO:HB2	2.02	0.41
3:D:156:TYR:OH	3:D:189:LEU:HD23	2.21	0.41
4:G:5:LEU:HD23	4:G:30:ILE:HD11	2.03	0.41
3:H:170:LEU:HD21	3:H:193:VAL:HG21	2.02	0.41
3:H:112:ASP:OD1	3:H:113:VAL:N	2.53	0.41
4:L:124:PRO:HA	4:L:137:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:69:ARG:NH2	3:F:92:ASP:OD2	2.54	0.40
1:C:192:MET:HA	1:C:199:SER:OG	2.20	0.40
4:L:65:PHE:CD1	4:L:78:ILE:HG12	2.56	0.40
1:A:199:SER:O	1:A:203:LEU:HG	2.20	0.40
1:B:241:TYR:O	1:B:245:LEU:HD23	2.22	0.40
3:H:148:ALA:HB3	4:L:121:THR:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/259 (70%)	169 (94%)	11 (6%)	0	100	100
1	B	179/259 (69%)	172 (96%)	7 (4%)	0	100	100
1	C	179/259 (69%)	169 (94%)	10 (6%)	0	100	100
2	a	151/164 (92%)	145 (96%)	6 (4%)	0	100	100
2	b	157/164 (96%)	152 (97%)	5 (3%)	0	100	100
2	c	153/164 (93%)	149 (97%)	4 (3%)	0	100	100
3	D	214/229 (93%)	206 (96%)	8 (4%)	0	100	100
3	F	213/229 (93%)	205 (96%)	8 (4%)	0	100	100
3	H	213/229 (93%)	204 (96%)	9 (4%)	0	100	100
4	E	209/217 (96%)	202 (97%)	7 (3%)	0	100	100
4	G	209/217 (96%)	203 (97%)	6 (3%)	0	100	100
4	L	210/217 (97%)	202 (96%)	8 (4%)	0	100	100
All	All	2267/2607 (87%)	2178 (96%)	89 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	167/228 (73%)	167 (100%)	0	100	100
1	B	166/228 (73%)	166 (100%)	0	100	100
1	C	166/228 (73%)	166 (100%)	0	100	100
2	a	140/148 (95%)	140 (100%)	0	100	100
2	b	143/148 (97%)	142 (99%)	1 (1%)	84	94
2	c	142/148 (96%)	142 (100%)	0	100	100
3	D	185/194 (95%)	185 (100%)	0	100	100
3	F	183/194 (94%)	183 (100%)	0	100	100
3	H	183/194 (94%)	183 (100%)	0	100	100
4	E	176/182 (97%)	176 (100%)	0	100	100
4	G	176/182 (97%)	176 (100%)	0	100	100
4	L	177/182 (97%)	177 (100%)	0	100	100
All	All	2004/2256 (89%)	2003 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	270	GLU

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

Mol	Chain	Res	Type
1	A	148	ASN
1	B	131	HIS
2	c	321	GLN
3	F	211	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

52 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	$\#\|Z\| > 2$
5	NAG	I	1	5,1	14,14,15	0.47	0	17,19,21	0.50	0
5	NAG	I	2	5	14,14,15	0.30	0	17,19,21	0.54	0
5	BMA	I	3	5	11,11,12	0.56	0	15,15,17	0.80	0
6	NAG	J	1	6,1	14,14,15	0.30	0	17,19,21	0.45	0
6	NAG	J	2	6	14,14,15	0.19	0	17,19,21	0.52	0
6	NAG	K	1	6,1	14,14,15	0.35	0	17,19,21	0.41	0
6	NAG	K	2	6	14,14,15	0.28	0	17,19,21	0.46	0
6	NAG	M	1	6,1	14,14,15	0.19	0	17,19,21	0.54	0
6	NAG	M	2	6	14,14,15	0.16	0	17,19,21	0.49	0
7	NAG	N	1	7,2	14,14,15	0.30	0	17,19,21	0.50	0
7	NAG	N	2	7	14,14,15	0.26	0	17,19,21	0.49	0
7	BMA	N	3	7	11,11,12	0.79	0	15,15,17	0.91	0
7	MAN	N	4	7	11,11,12	0.77	0	15,15,17	1.02	2 (13%)
6	NAG	O	1	6,2	14,14,15	0.37	0	17,19,21	0.51	0
6	NAG	O	2	6	14,14,15	0.32	0	17,19,21	0.38	0
8	NAG	P	1	2,8	14,14,15	0.55	0	17,19,21	0.56	0
8	NAG	P	2	8	14,14,15	0.31	0	17,19,21	0.38	0
8	FUC	P	3	8	10,10,11	1.02	1 (10%)	14,14,16	0.67	0
6	NAG	Q	1	6,1	14,14,15	0.51	0	17,19,21	0.48	0
6	NAG	Q	2	6	14,14,15	0.27	0	17,19,21	0.50	0
6	NAG	R	1	6,1	14,14,15	0.30	0	17,19,21	0.41	0
6	NAG	R	2	6	14,14,15	0.18	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	S	1	6,1	14,14,15	0.32	0	17,19,21	0.46	0
6	NAG	S	2	6	14,14,15	0.26	0	17,19,21	0.41	0
7	NAG	T	1	7,2	14,14,15	0.35	0	17,19,21	0.52	0
7	NAG	T	2	7	14,14,15	0.35	0	17,19,21	0.49	0
7	BMA	T	3	7	11,11,12	0.91	0	15,15,17	1.11	1 (6%)
7	MAN	T	4	7	11,11,12	1.13	1 (9%)	15,15,17	1.34	3 (20%)
8	NAG	U	1	2,8	14,14,15	0.57	0	17,19,21	0.48	0
8	NAG	U	2	8	14,14,15	0.26	0	17,19,21	0.44	0
8	FUC	U	3	8	10,10,11	1.04	1 (10%)	14,14,16	0.68	0
5	NAG	V	1	5,1	14,14,15	0.44	0	17,19,21	0.47	0
5	NAG	V	2	5	14,14,15	0.32	0	17,19,21	0.63	1 (5%)
5	BMA	V	3	5	11,11,12	0.59	0	15,15,17	0.80	1 (6%)
6	NAG	W	1	6,1	14,14,15	0.27	0	17,19,21	0.40	0
6	NAG	W	2	6	14,14,15	0.26	0	17,19,21	0.50	0
6	NAG	X	1	6,1	14,14,15	0.34	0	17,19,21	0.42	0
6	NAG	X	2	6	14,14,15	0.26	0	17,19,21	0.44	0
6	NAG	Y	1	6,1	14,14,15	0.22	0	17,19,21	0.51	0
6	NAG	Y	2	6	14,14,15	0.22	0	17,19,21	0.49	0
5	NAG	Z	1	5,1	14,14,15	0.28	0	17,19,21	0.39	0
5	NAG	Z	2	5	14,14,15	0.29	0	17,19,21	0.46	0
5	BMA	Z	3	5	11,11,12	0.63	0	15,15,17	0.96	1 (6%)
7	NAG	d	1	7,2	14,14,15	0.35	0	17,19,21	0.51	0
7	NAG	d	2	7	14,14,15	0.31	0	17,19,21	0.53	0
7	BMA	d	3	7	11,11,12	0.87	0	15,15,17	0.94	0
7	MAN	d	4	7	11,11,12	0.81	1 (9%)	15,15,17	1.05	2 (13%)
6	NAG	e	1	6,2	14,14,15	0.35	0	17,19,21	0.43	0
6	NAG	e	2	6	14,14,15	0.33	0	17,19,21	0.41	0
8	NAG	f	1	2,8	14,14,15	0.41	0	17,19,21	0.52	0
8	NAG	f	2	8	14,14,15	0.29	0	17,19,21	0.41	0
8	FUC	f	3	8	10,10,11	0.97	1 (10%)	14,14,16	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	Z	3	5	-	0/2/19/22	0/1/1/1
7	NAG	d	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
7	BMA	d	3	7	-	1/2/19/22	0/1/1/1
7	MAN	d	4	7	-	0/2/19/22	0/1/1/1
6	NAG	e	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	e	2	6	-	2/6/23/26	0/1/1/1
8	NAG	f	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
8	FUC	f	3	8	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	3	FUC	O5-C1	-2.67	1.39	1.43
8	U	3	FUC	O5-C1	-2.55	1.39	1.43
7	T	4	MAN	C1-C2	2.51	1.57	1.52
8	f	3	FUC	O5-C1	-2.32	1.40	1.43
7	d	4	MAN	C1-C2	2.06	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	3	BMA	C1-C2-C3	2.55	112.80	109.67
7	d	4	MAN	C1-O5-C5	2.48	115.55	112.19
7	T	4	MAN	C1-C2-C3	2.43	112.66	109.67
7	N	4	MAN	C1-O5-C5	2.42	115.47	112.19
7	T	4	MAN	C1-O5-C5	2.31	115.32	112.19
7	T	4	MAN	O2-C2-C3	-2.24	105.65	110.14
7	N	4	MAN	O2-C2-C3	-2.19	105.75	110.14
7	d	4	MAN	O2-C2-C3	-2.17	105.79	110.14
5	V	2	NAG	C1-O5-C5	2.07	115.00	112.19
5	V	3	BMA	O2-C2-C3	-2.02	106.08	110.14
5	Z	3	BMA	C1-O5-C5	2.02	114.92	112.19

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	N	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	I	1	NAG	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
7	N	3	BMA	C4-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
6	Q	1	NAG	O5-C5-C6-O6
6	e	1	NAG	O5-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6
6	e	1	NAG	C4-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
6	Q	1	NAG	C4-C5-C6-O6
5	Z	1	NAG	C4-C5-C6-O6
8	P	1	NAG	O5-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
8	f	1	NAG	O5-C5-C6-O6
8	P	1	NAG	C4-C5-C6-O6
6	e	2	NAG	O5-C5-C6-O6
8	f	1	NAG	C4-C5-C6-O6
6	e	2	NAG	C4-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	Y	1	NAG	C4-C5-C6-O6
7	d	3	BMA	O5-C5-C6-O6
8	U	1	NAG	O5-C5-C6-O6
8	U	1	NAG	C4-C5-C6-O6
6	Y	1	NAG	O5-C5-C6-O6
6	W	1	NAG	C4-C5-C6-O6
7	N	4	MAN	C4-C5-C6-O6
7	N	4	MAN	O5-C5-C6-O6
6	W	1	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
8	f	2	NAG	C4-C5-C6-O6
7	T	3	BMA	O5-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
8	f	2	NAG	O5-C5-C6-O6

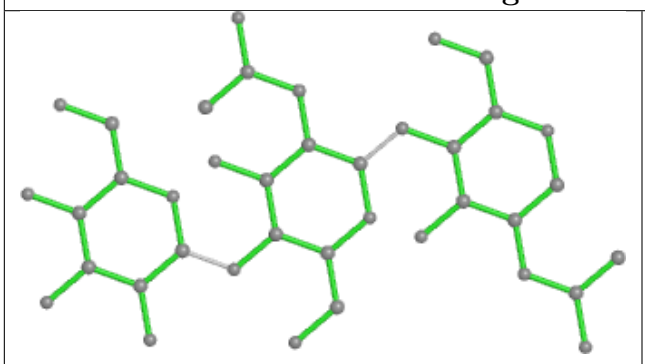
There are no ring outliers.

3 monomers are involved in 3 short contacts:

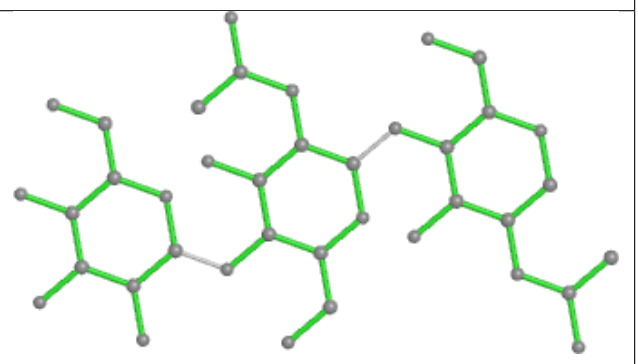
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	X	1	NAG	1	0
6	K	1	NAG	1	0
6	S	1	NAG	1	0

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

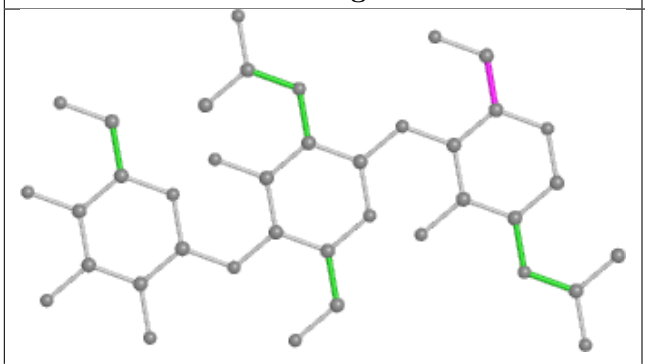
Oligosaccharide Chain I



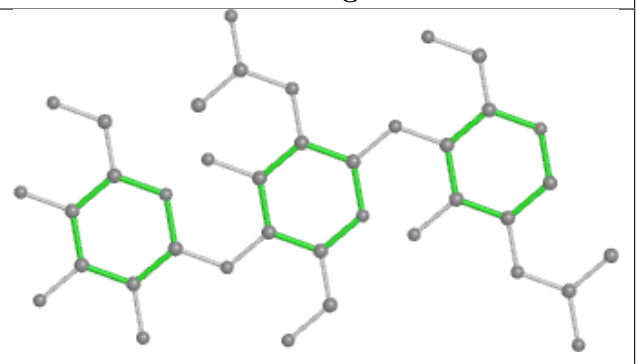
Bond lengths



Bond angles

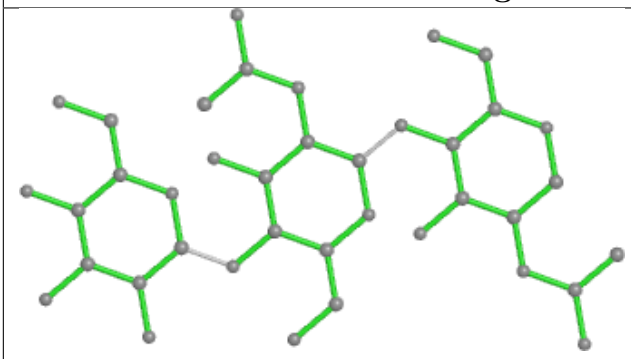


Torsions

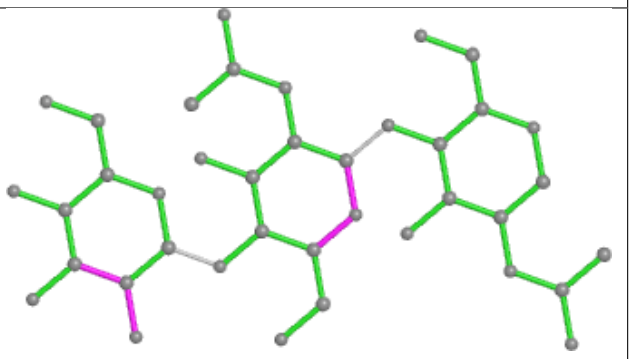


Rings

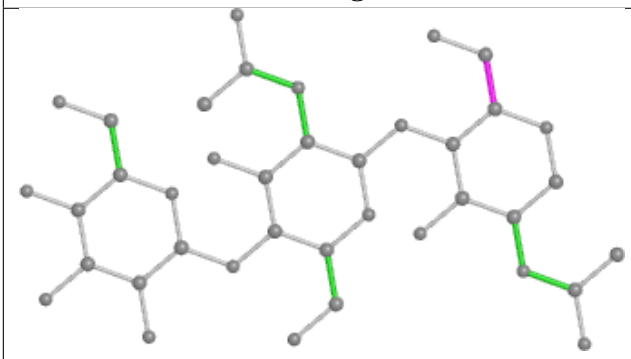
Oligosaccharide Chain V



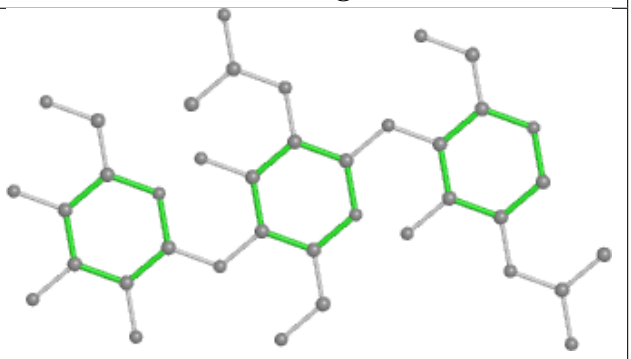
Bond lengths



Bond angles

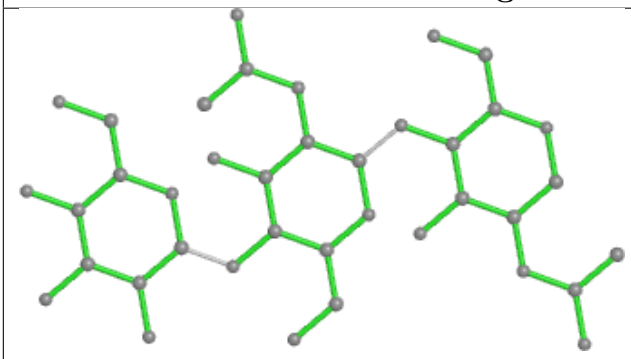


Torsions

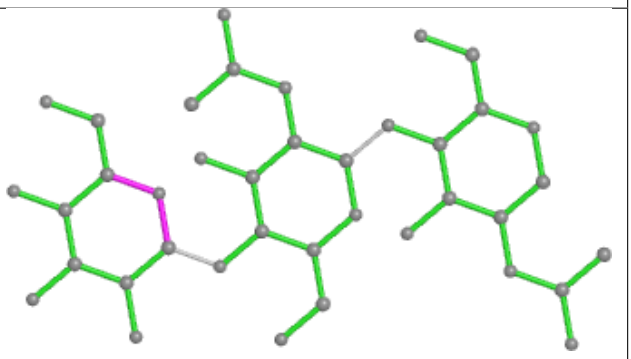


Rings

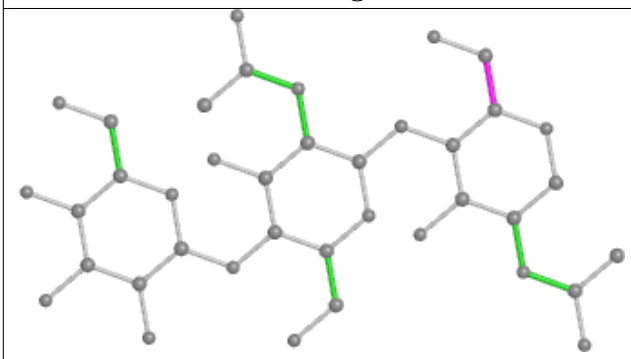
Oligosaccharide Chain Z



Bond lengths



Bond angles



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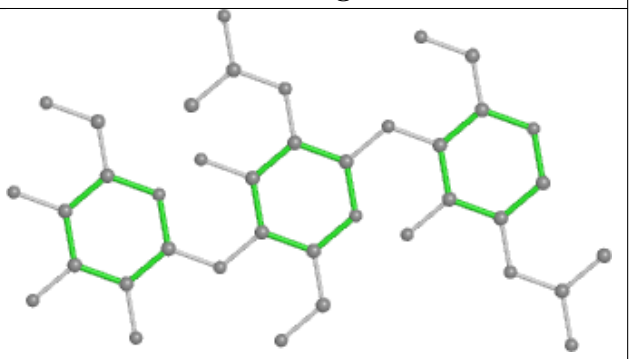
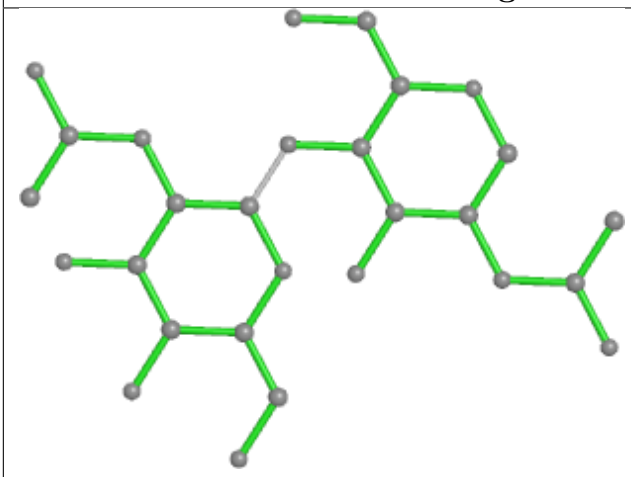


Rings

Oligosaccharide Chain J



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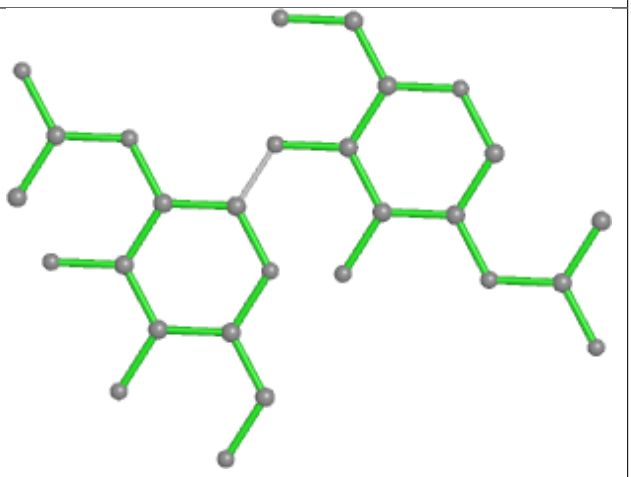
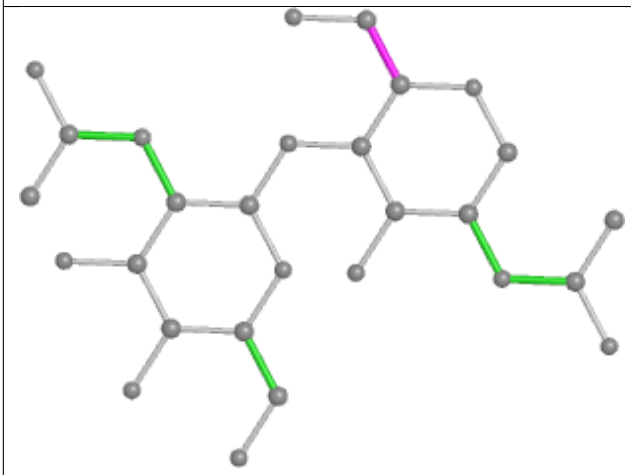


Bond angles



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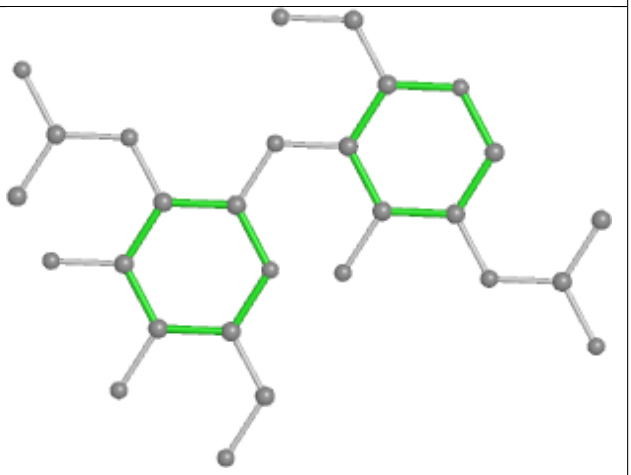
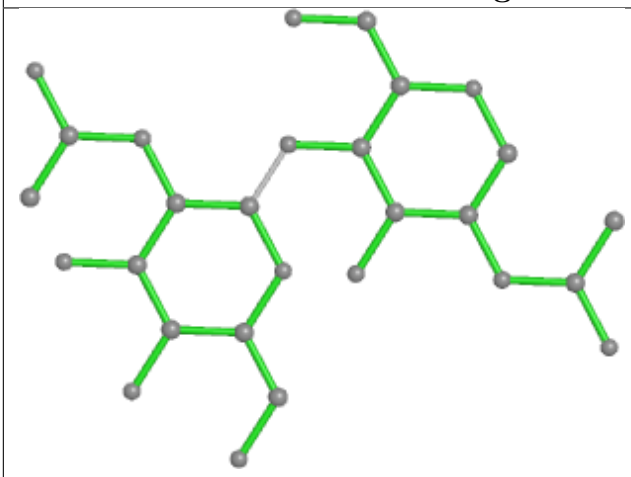


Rings

Oligosaccharide Chain K



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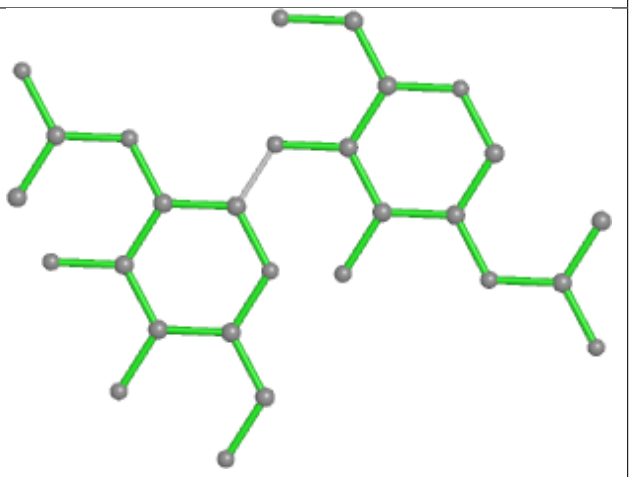
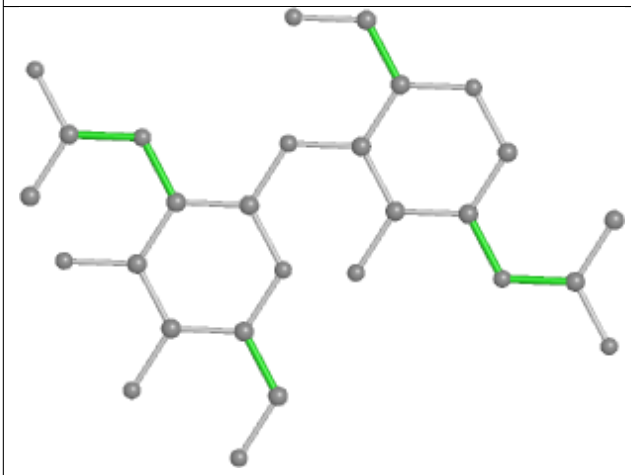


Bond angles



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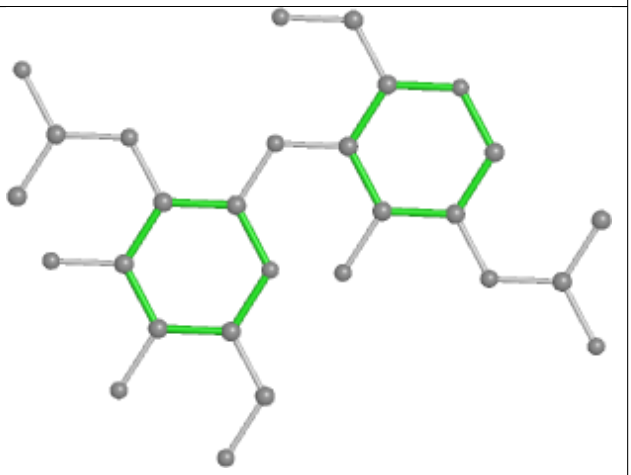
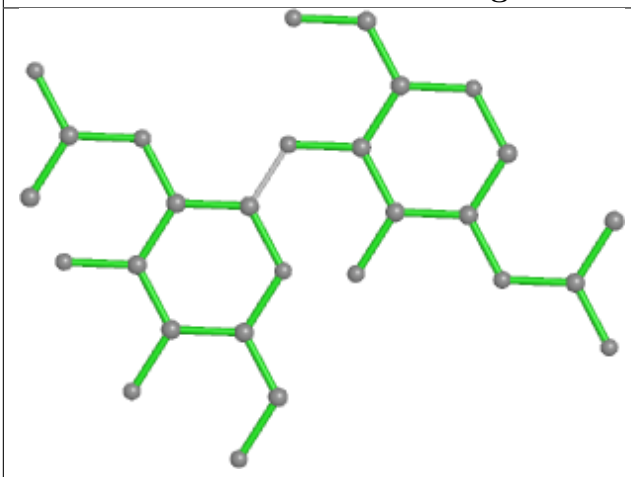


Rings

Oligosaccharide Chain M



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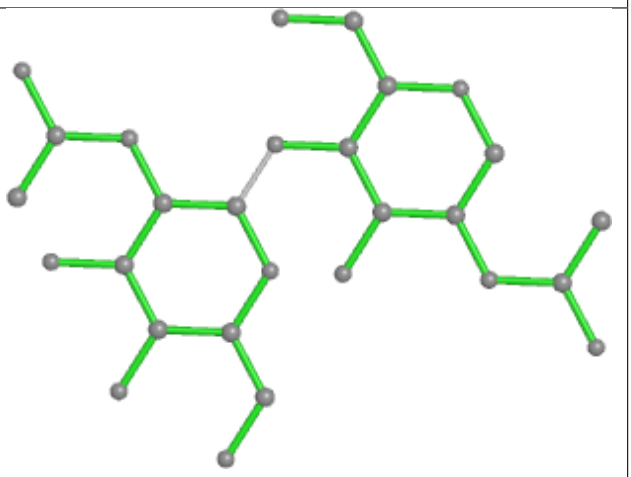
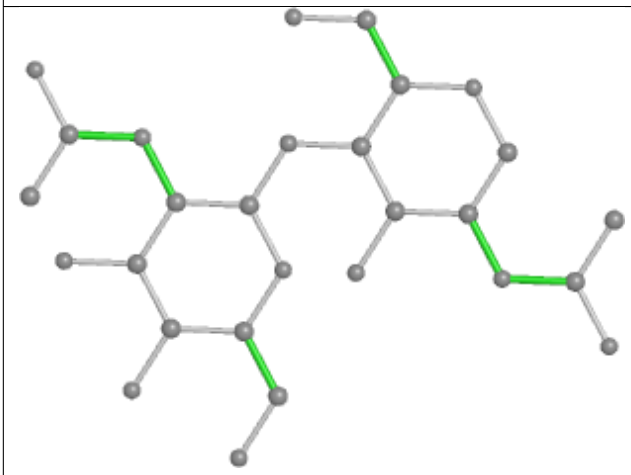


Bond angles



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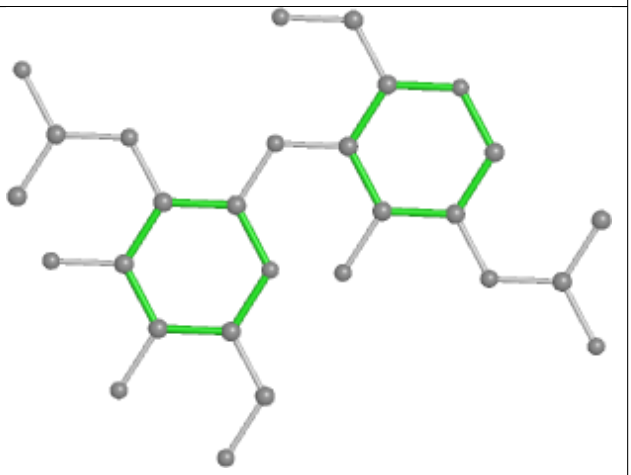
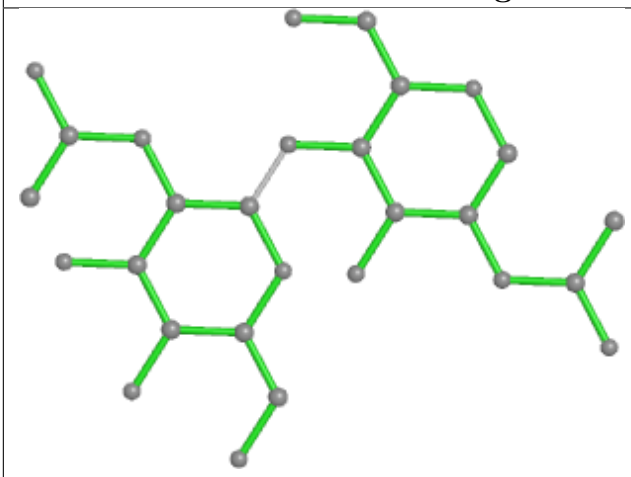


Rings

Oligosaccharide Chain O



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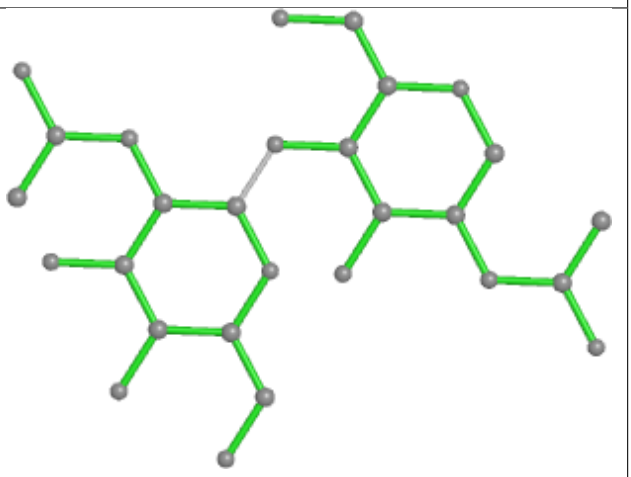

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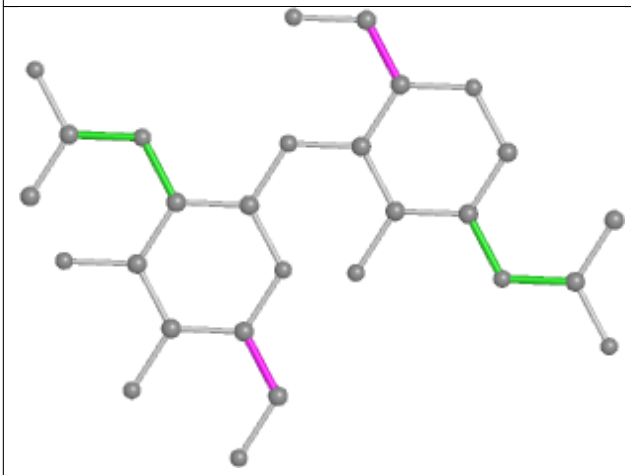

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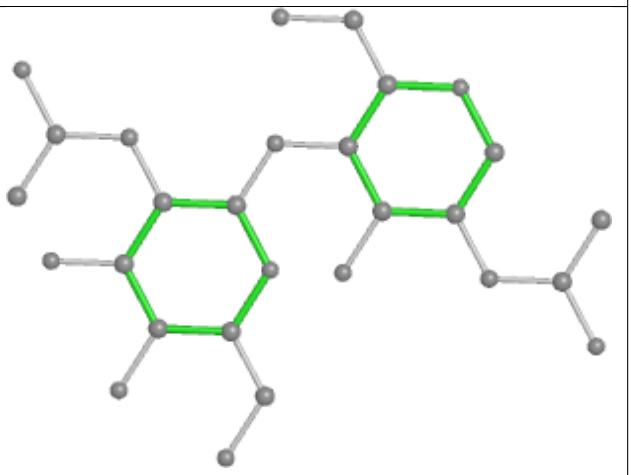
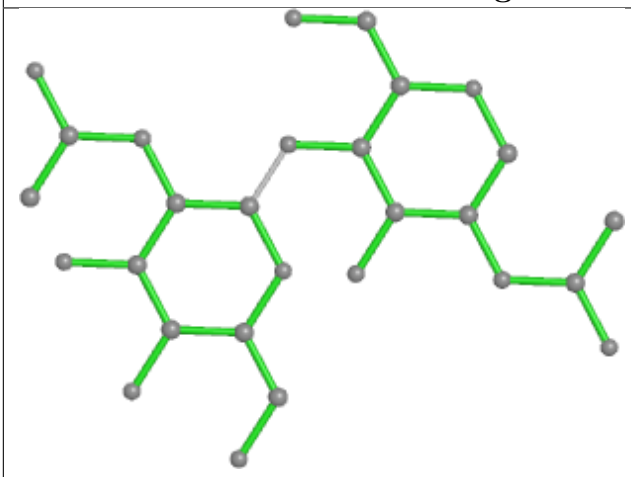


Rings

Oligosaccharide Chain Q



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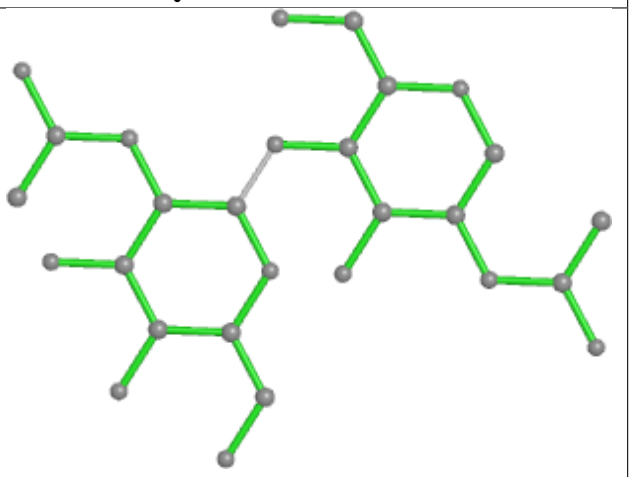

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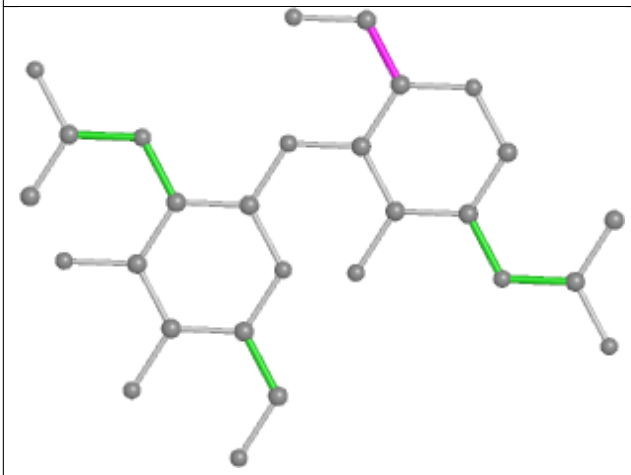

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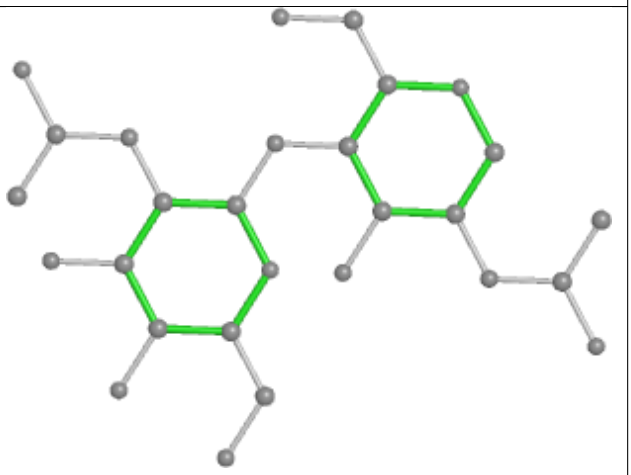
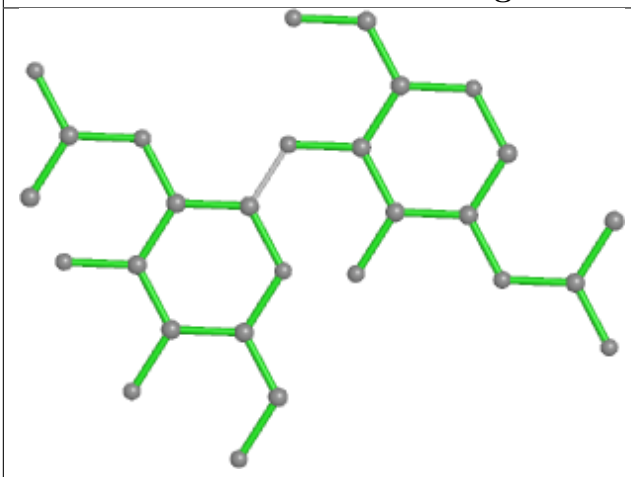


Rings

Oligosaccharide Chain R



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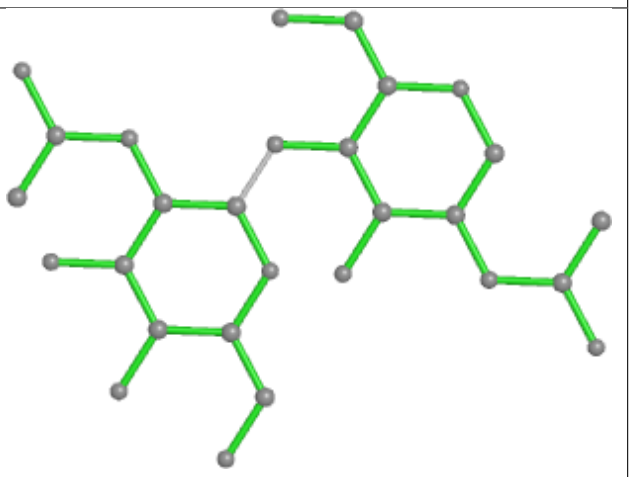
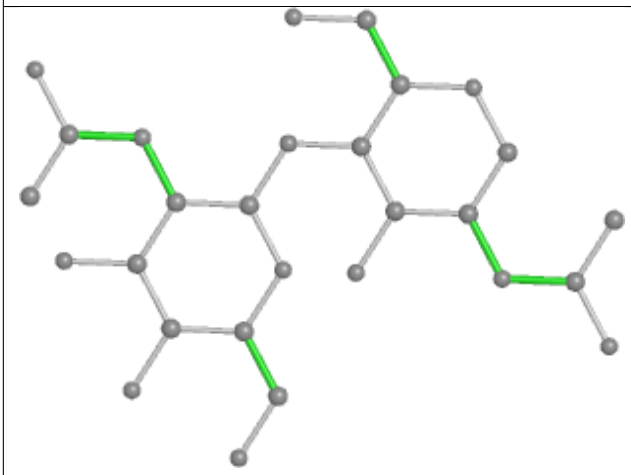


Bond angles



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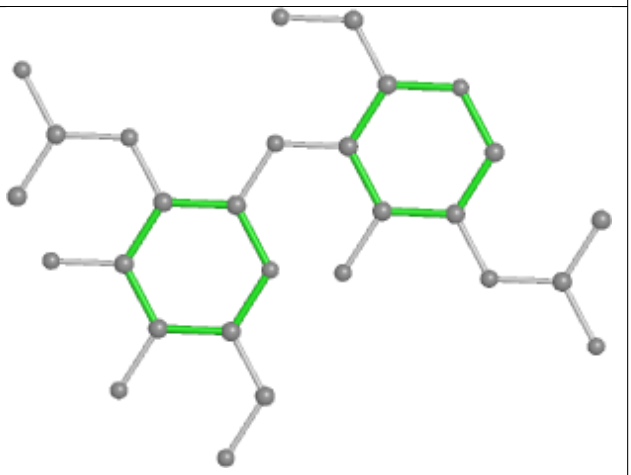
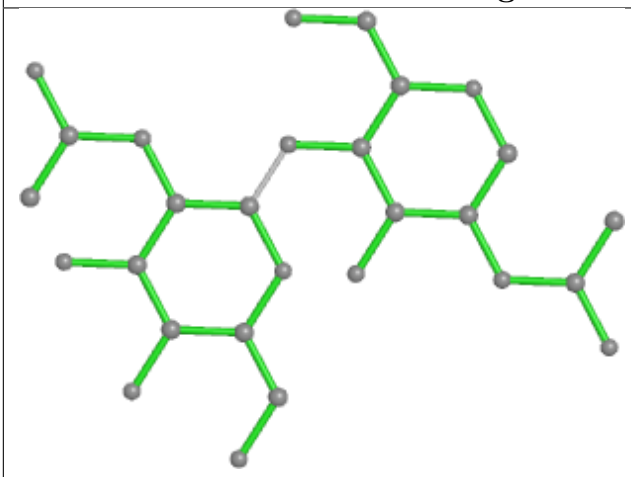


Rings

Oligosaccharide Chain S



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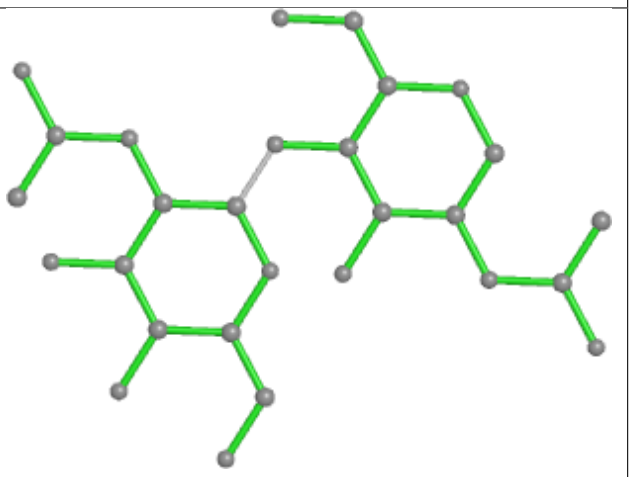
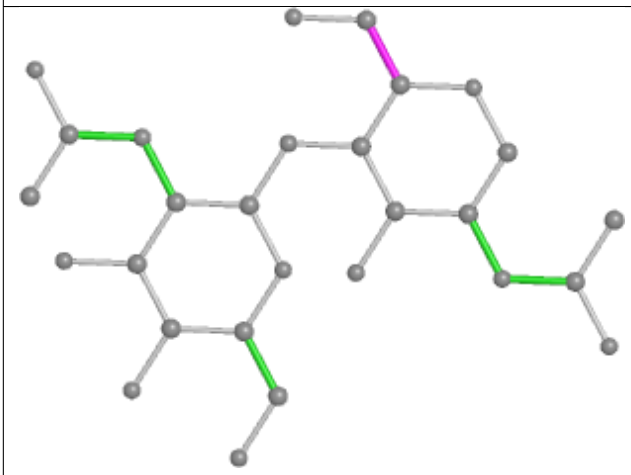


Bond angles



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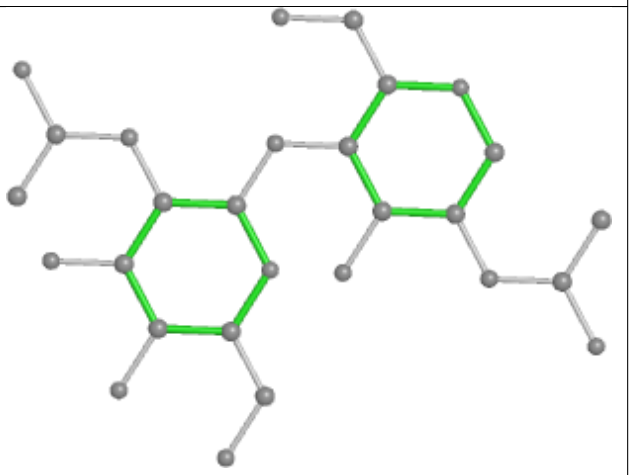
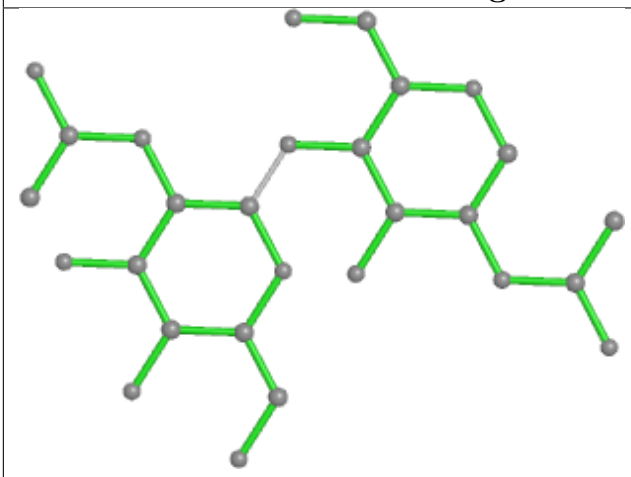


Rings

Oligosaccharide Chain W



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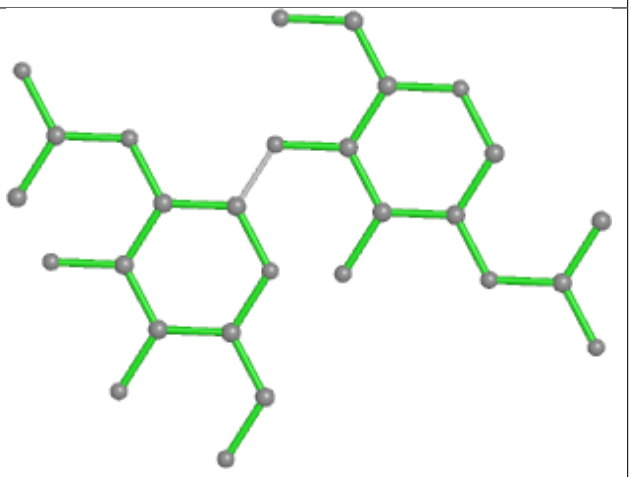
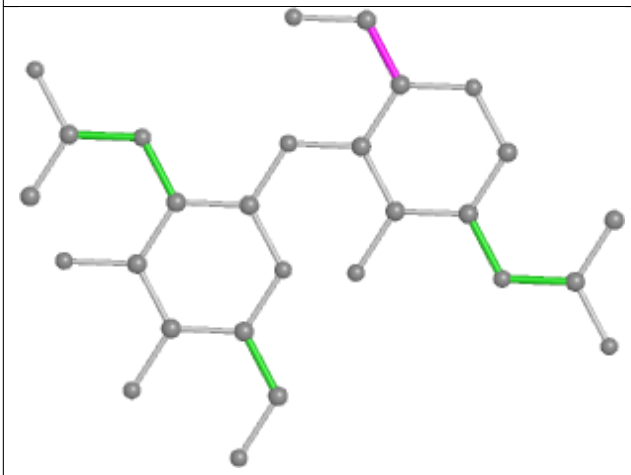


Bond angles



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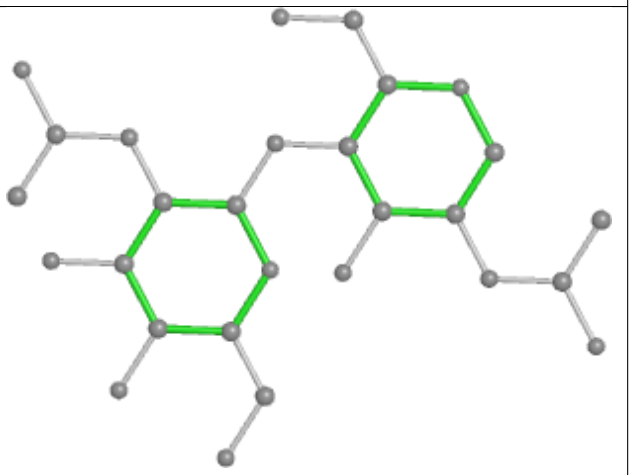
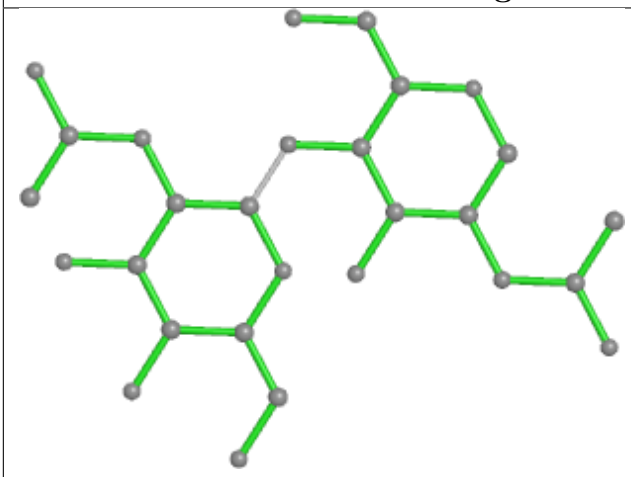


Rings

Oligosaccharide Chain X



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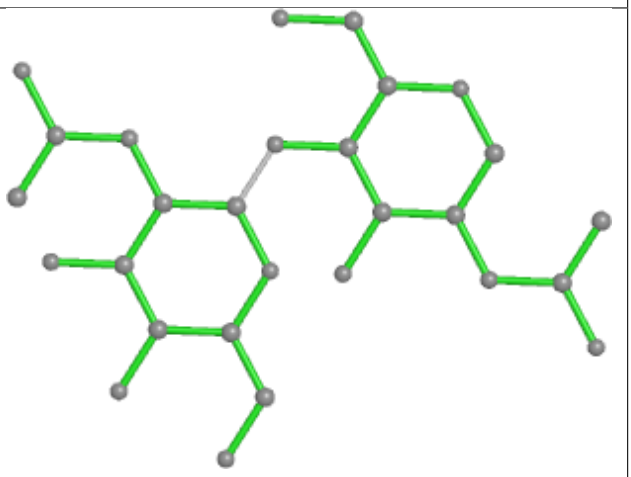

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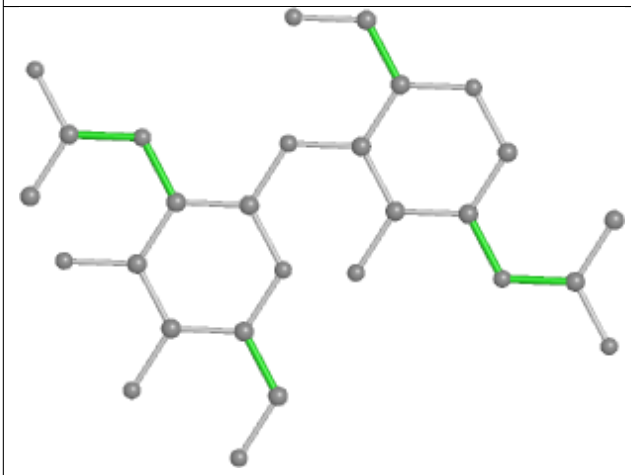

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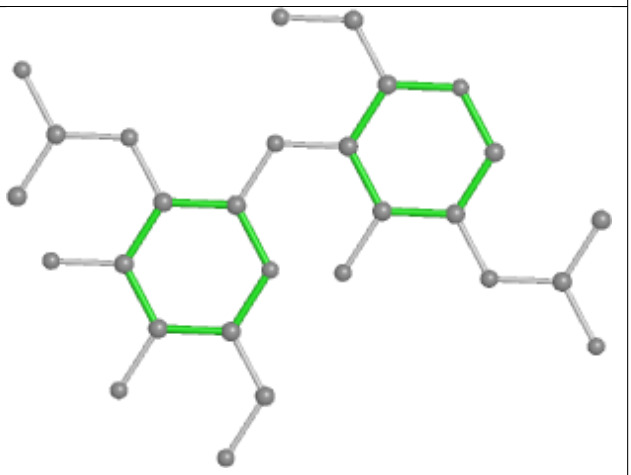
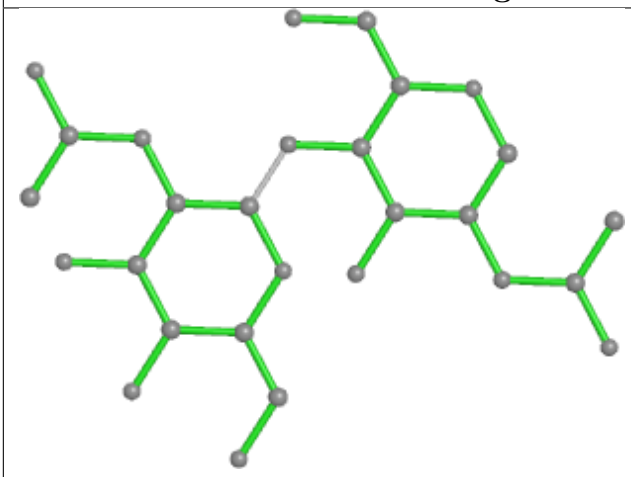


Rings

Oligosaccharide Chain Y



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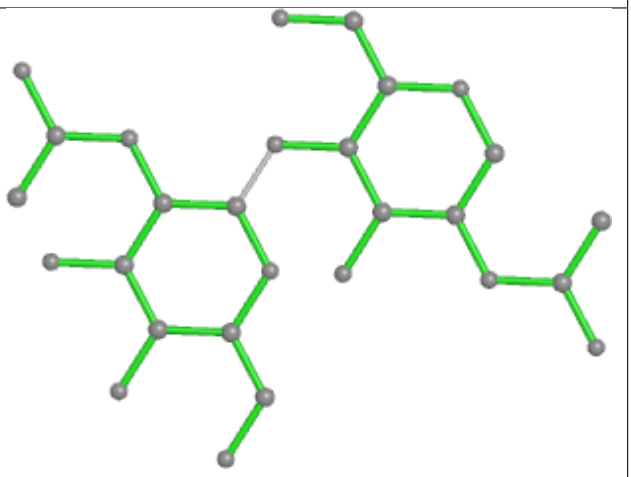

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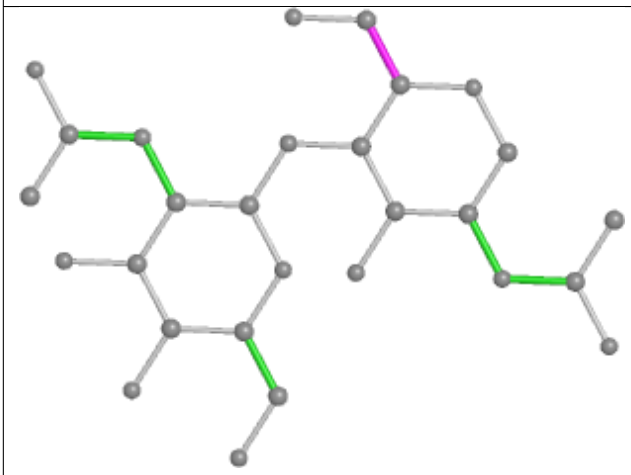

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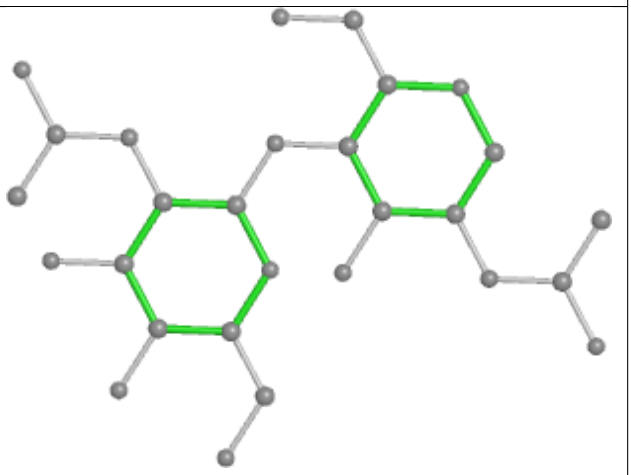
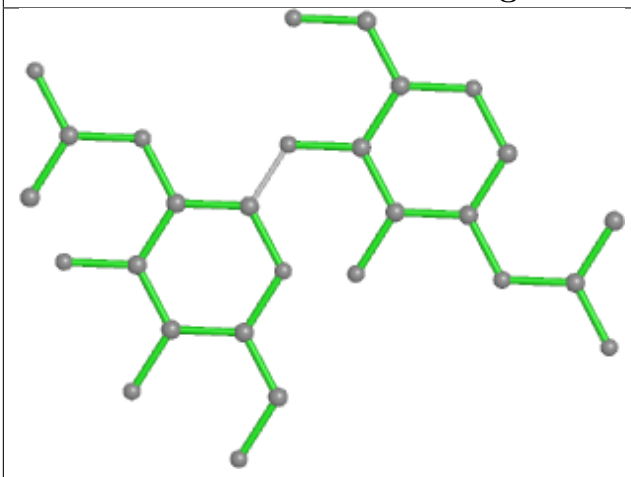


Rings

Oligosaccharide Chain e



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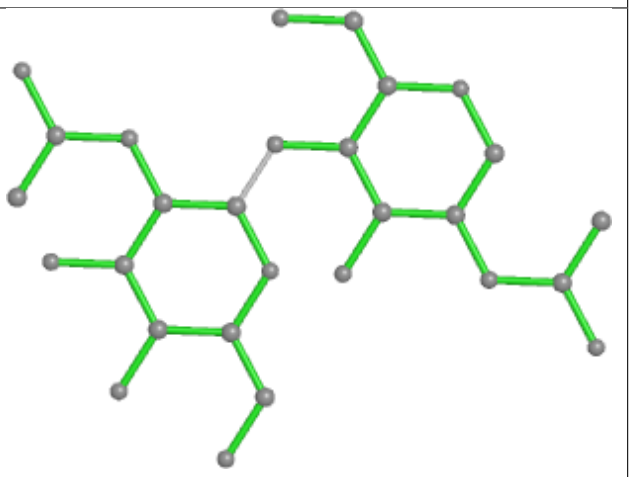
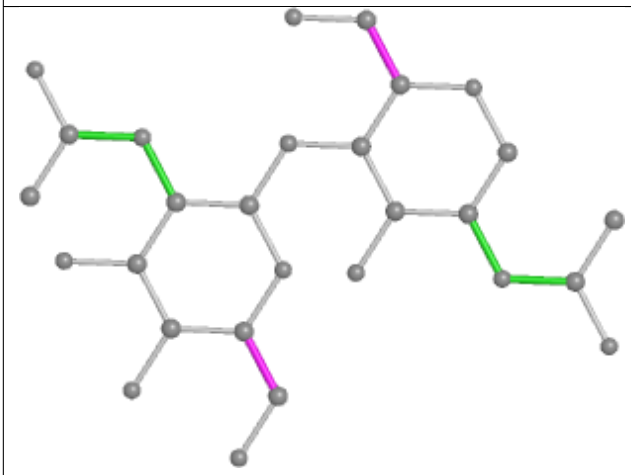


Bond angles



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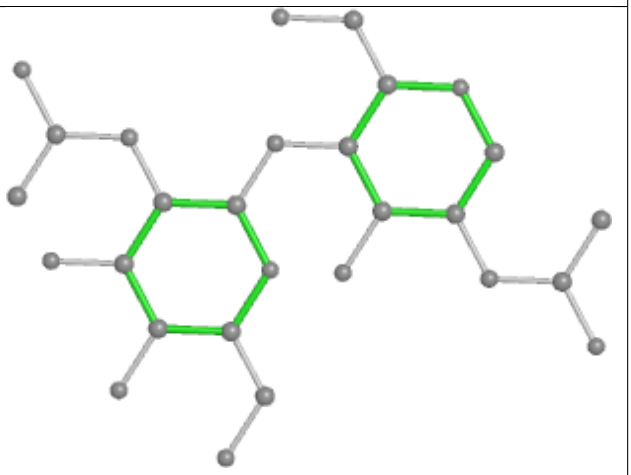
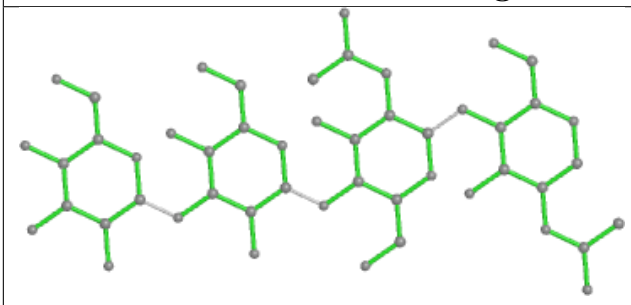


Rings

Oligosaccharide Chain N



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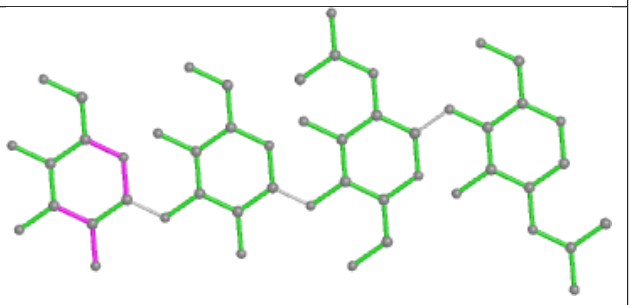
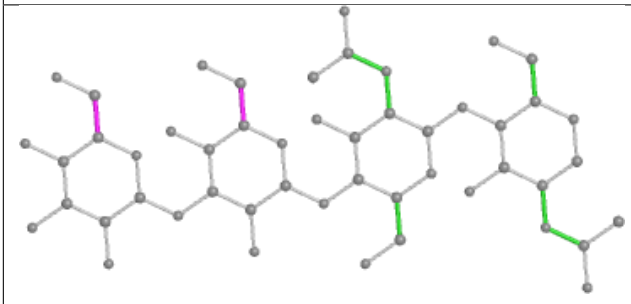


Bond angles



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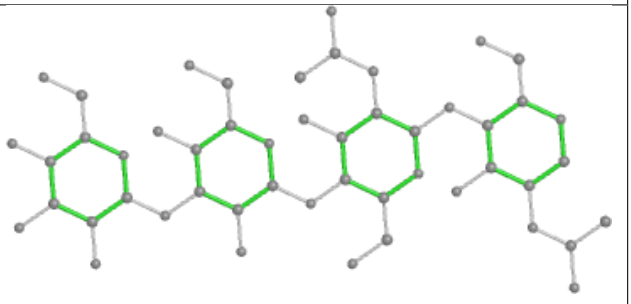
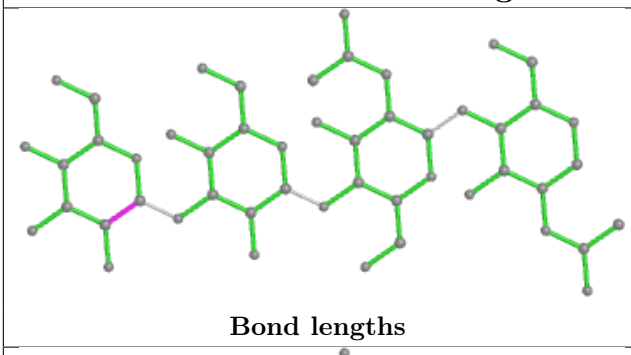
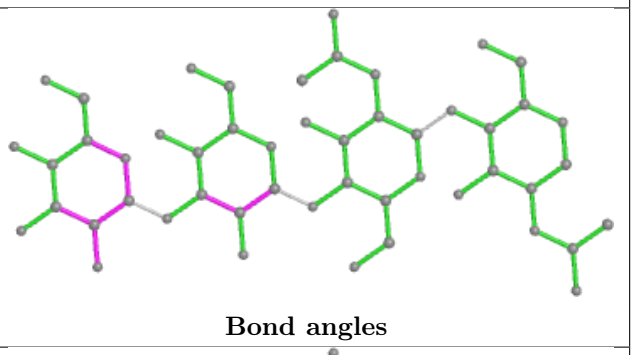


Rings

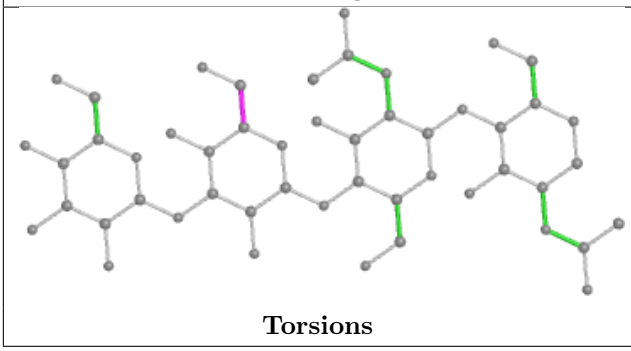
Oligosaccharide Chain T



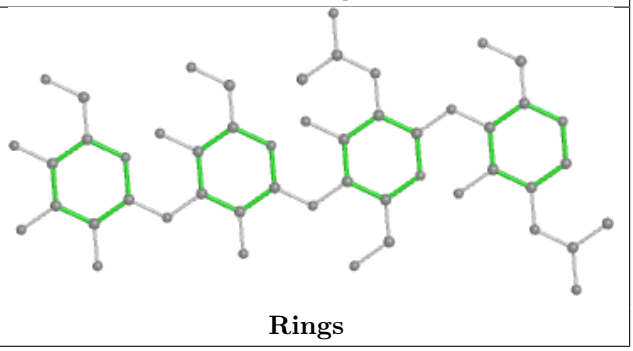
Bond lengths



Bond angles

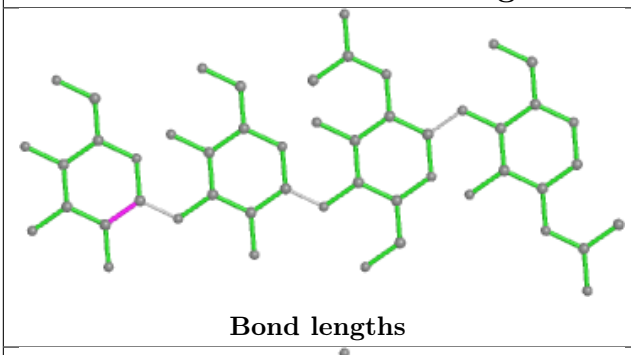


Torsions

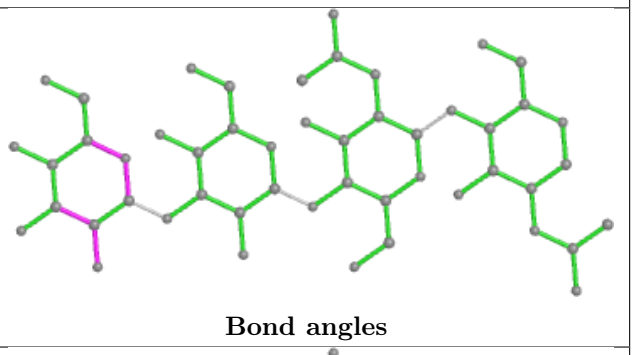


Rings

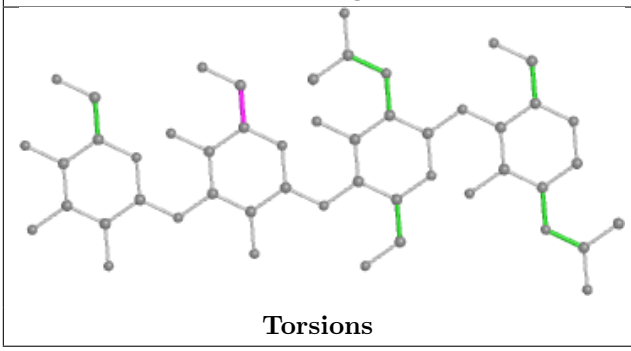
Oligosaccharide Chain d



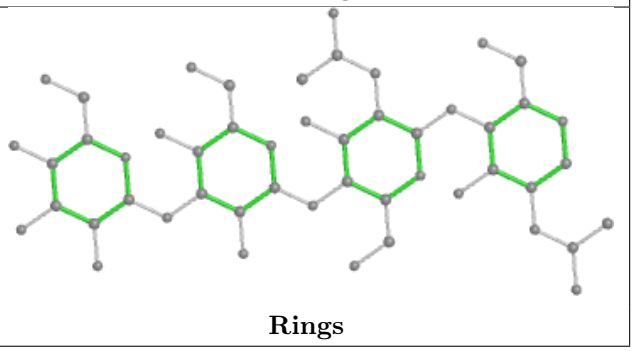
Bond lengths



Bond angles

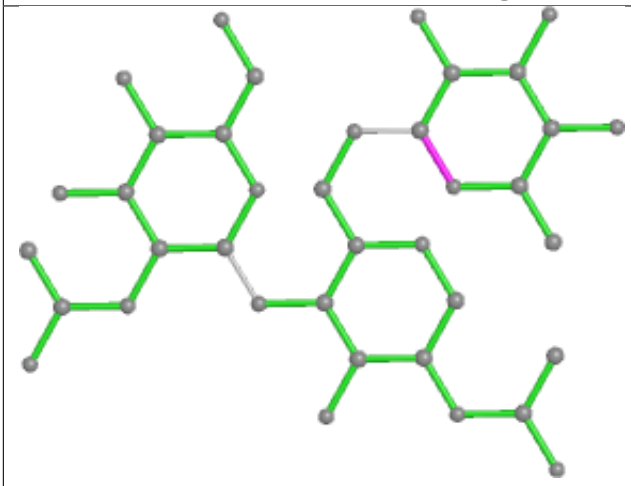


Torsions

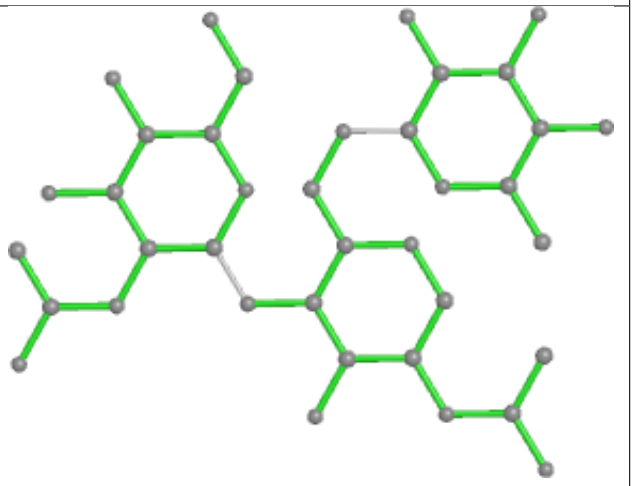


Rings

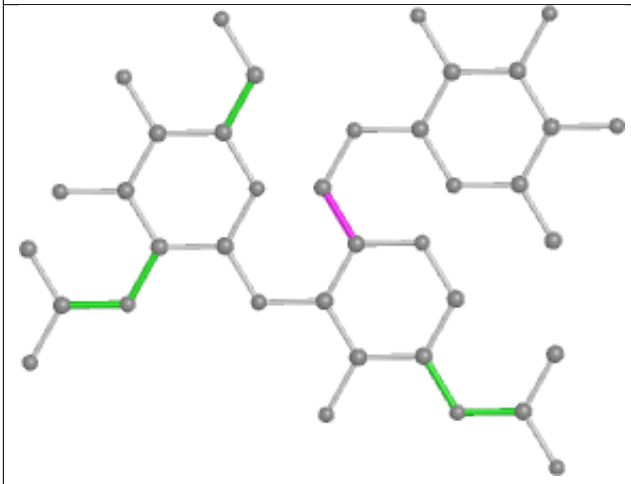
Oligosaccharide Chain P



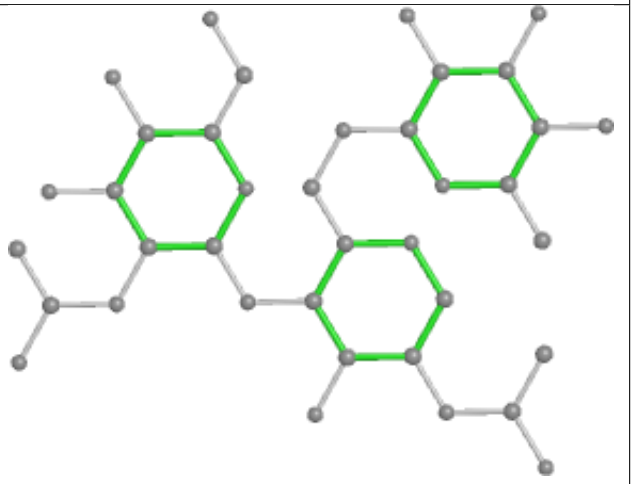
Bond lengths



Bond angles

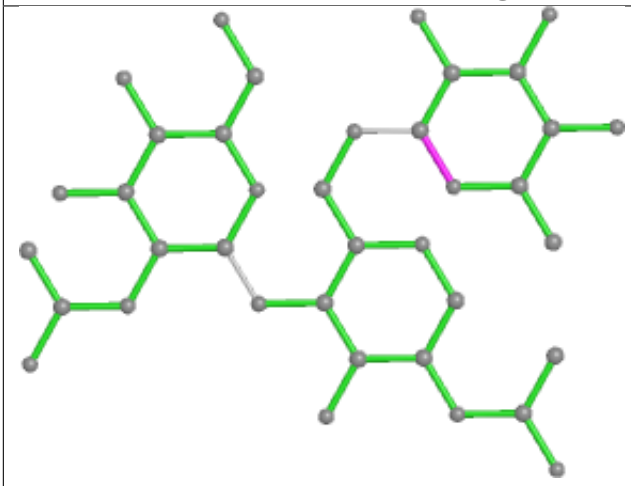


Torsions

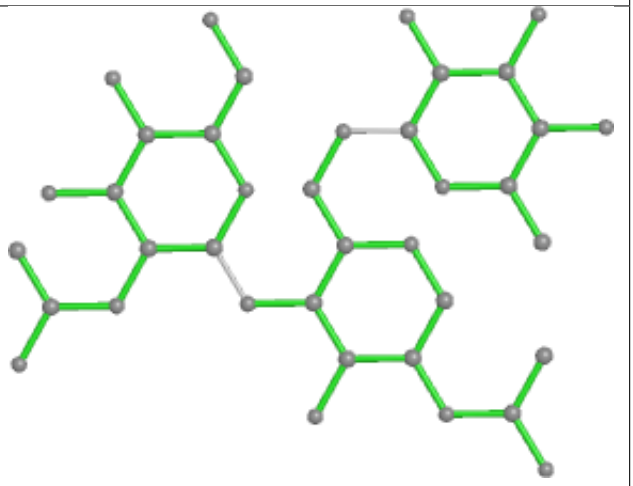


Rings

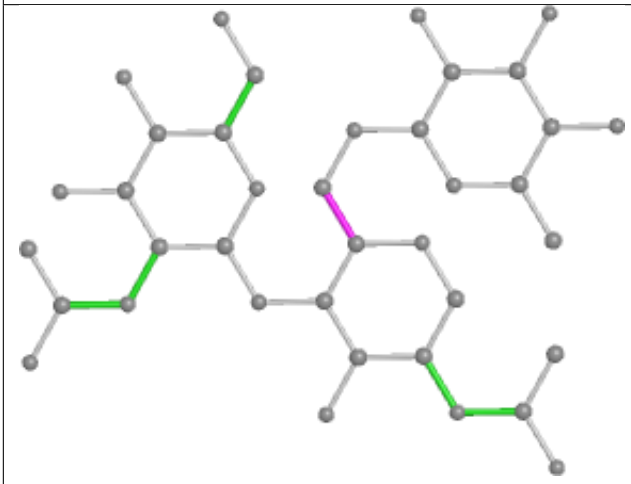
Oligosaccharide Chain U



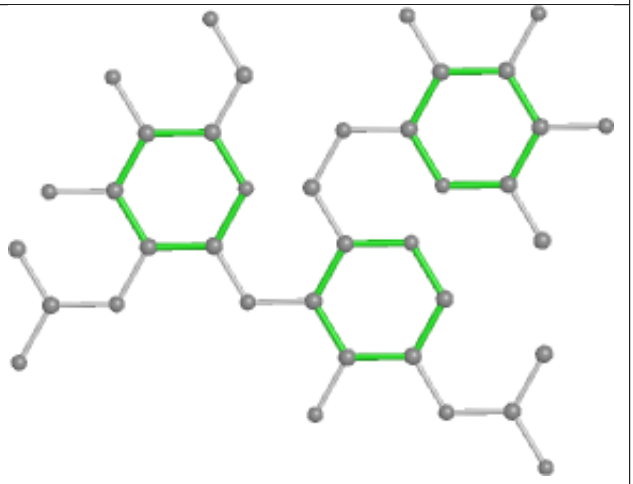
Bond lengths



Bond angles

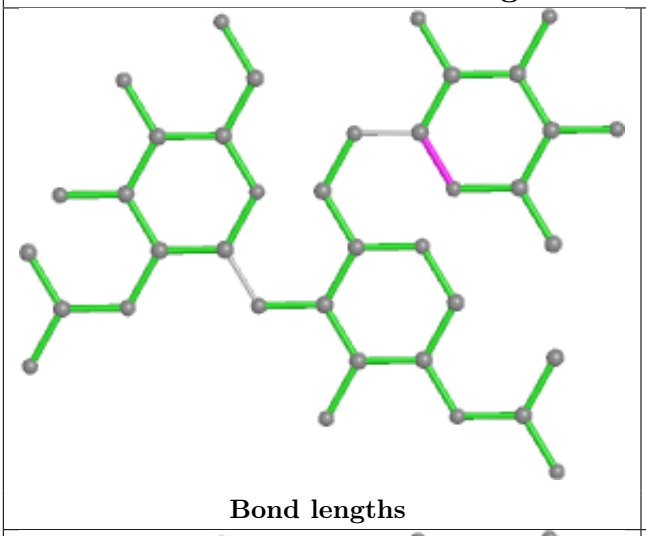


Torsions

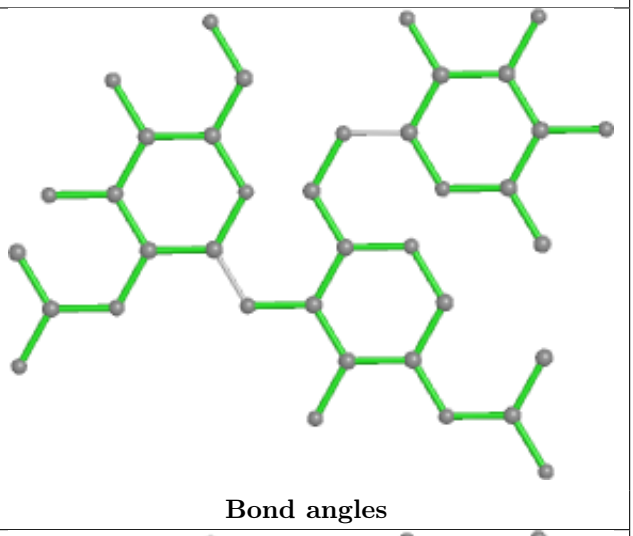


Rings

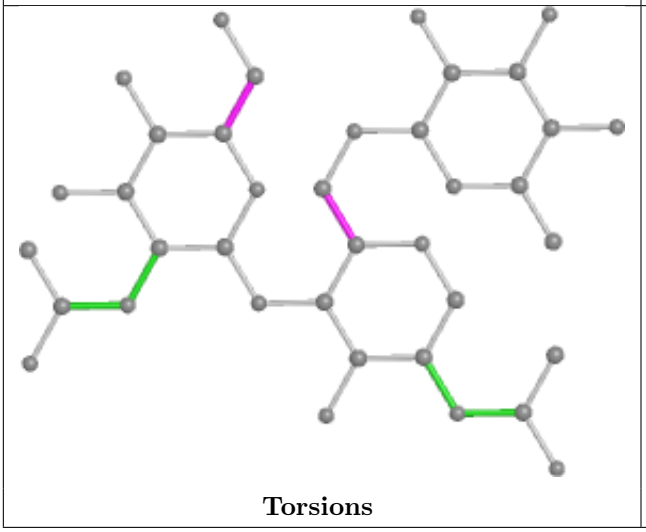
Oligosaccharide Chain f



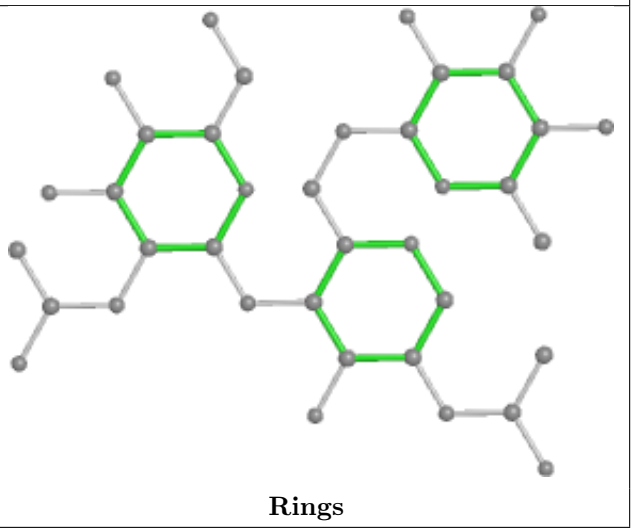
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
9	NAG	C	506	1	14,14,15	0.23	0	17,19,21	0.37	0
9	NAG	a	507	2	14,14,15	0.34	0	17,19,21	0.49	0
9	NAG	A	506	1	14,14,15	0.31	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	B	505	1	14,14,15	0.31	0	17,19,21	0.35	0
9	NAG	A	511	1	14,14,15	0.29	0	17,19,21	0.43	0
9	NAG	B	509	1	14,14,15	0.42	0	17,19,21	0.55	0
9	NAG	c	507	2	14,14,15	0.36	0	17,19,21	0.53	0
9	NAG	b	505	2	14,14,15	0.33	0	17,19,21	0.51	0
9	NAG	A	512	1	14,14,15	0.39	0	17,19,21	0.53	0
9	NAG	C	514	1	14,14,15	0.37	0	17,19,21	0.55	0
9	NAG	B	508	1	14,14,15	0.31	0	17,19,21	0.39	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
9	NAG	C	506	1	-	2/6/23/26	0/1/1/1
9	NAG	a	507	2	-	2/6/23/26	0/1/1/1
9	NAG	A	506	1	-	2/6/23/26	0/1/1/1
9	NAG	B	505	1	-	2/6/23/26	0/1/1/1
9	NAG	A	511	1	-	2/6/23/26	0/1/1/1
9	NAG	B	509	1	-	0/6/23/26	0/1/1/1
9	NAG	c	507	2	-	2/6/23/26	0/1/1/1
9	NAG	b	505	2	-	2/6/23/26	0/1/1/1
9	NAG	A	512	1	-	2/6/23/26	0/1/1/1
9	NAG	C	514	1	-	2/6/23/26	0/1/1/1
9	NAG	B	508	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	511	NAG	O5-C5-C6-O6
9	C	506	NAG	O5-C5-C6-O6
9	A	511	NAG	C4-C5-C6-O6
9	a	507	NAG	O5-C5-C6-O6
9	B	508	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	C	506	NAG	C4-C5-C6-O6
9	A	506	NAG	O5-C5-C6-O6
9	a	507	NAG	C4-C5-C6-O6
9	A	506	NAG	C4-C5-C6-O6
9	B	508	NAG	C4-C5-C6-O6
9	c	507	NAG	O5-C5-C6-O6
9	c	507	NAG	C4-C5-C6-O6
9	B	505	NAG	C4-C5-C6-O6
9	B	505	NAG	O5-C5-C6-O6
9	b	505	NAG	C4-C5-C6-O6
9	b	505	NAG	O5-C5-C6-O6
9	C	514	NAG	C4-C5-C6-O6
9	C	514	NAG	O5-C5-C6-O6
9	A	512	NAG	C4-C5-C6-O6
9	A	512	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	509	NAG	1	0
9	A	512	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	186/259 (71%)	0.43	9 (4%) 30 18	57, 108, 158, 192	0
1	B	185/259 (71%)	0.78	23 (12%) 4 2	70, 127, 172, 235	0
1	C	185/259 (71%)	0.53	12 (6%) 18 11	72, 124, 174, 213	0
2	a	155/164 (94%)	0.39	10 (6%) 18 11	50, 84, 167, 199	0
2	b	159/164 (96%)	0.42	9 (5%) 23 13	68, 100, 165, 233	0
2	c	157/164 (95%)	0.56	13 (8%) 11 6	63, 100, 172, 215	0
3	D	218/229 (95%)	0.06	1 (0%) 91 86	60, 104, 155, 185	0
3	F	217/229 (94%)	0.12	3 (1%) 75 63	67, 100, 137, 201	0
3	H	217/229 (94%)	-0.01	2 (0%) 84 75	57, 87, 132, 174	0
4	E	211/217 (97%)	0.12	9 (4%) 35 22	55, 95, 154, 217	0
4	G	211/217 (97%)	-0.03	3 (1%) 75 63	64, 94, 128, 170	0
4	L	212/217 (97%)	0.09	3 (1%) 75 63	22, 85, 126, 159	0
All	All	2313/2607 (88%)	0.26	97 (4%) 36 23	22, 99, 159, 235	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	c	260	GLY	12.3
2	a	260	GLY	11.3
2	b	260	GLY	8.9
2	c	342	ASN	5.3
1	C	246	SER	5.3
1	A	246	SER	5.2
1	B	255	SER	5.0
1	B	246	SER	4.7
1	B	250	ARG	4.5
1	A	211	ASP	4.5
1	B	88	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	249	THR	4.0
2	a	261	THR	3.7
1	B	227	TRP	3.7
2	b	261	THR	3.7
1	A	250	ARG	3.6
2	b	342	ASN	3.6
1	C	250	ARG	3.5
2	c	347	ASP	3.5
4	G	3	SER	3.4
2	b	302	ASN	3.4
1	A	249	THR	3.4
1	C	103	LEU	3.3
2	c	261	THR	3.3
2	a	342	ASN	3.3
1	A	208	GLY	3.2
1	B	94	TYR	3.2
2	b	305	HIS	3.2
1	C	243	GLY	3.1
2	a	305	HIS	3.1
4	E	212	ALA	3.1
1	B	103	LEU	3.1
3	F	5	LEU	3.1
1	B	223	GLN	3.0
2	c	331	GLN	3.0
1	B	251	ASP	2.9
2	c	305	HIS	2.9
2	c	346	ASN	2.9
1	C	208	GLY	2.8
1	B	115	HIS	2.8
2	c	348	GLN	2.8
1	A	247	GLN	2.8
2	a	347	ASP	2.8
1	C	249	THR	2.7
2	a	332	THR	2.7
2	b	306	ASP	2.7
1	A	113	ILE	2.7
4	G	187	PRO	2.6
4	G	81	LEU	2.6
4	E	192	SER	2.6
4	L	196	TYR	2.6
2	a	331	GLN	2.5
1	C	146	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	247	GLN	2.5
4	E	194	ARG	2.5
3	F	225	LYS	2.5
1	B	162	ILE	2.5
2	a	262	PHE	2.5
1	C	66	TYR	2.5
1	C	211	ASP	2.4
2	a	306	ASP	2.4
1	B	117	PHE	2.4
1	C	104	GLU	2.4
1	B	104	GLU	2.4
1	B	151	GLU	2.4
2	b	348	GLN	2.4
2	c	302	ASN	2.4
4	E	185	LEU	2.3
3	H	200	LEU	2.3
2	c	269	SER	2.3
2	c	338	ASN	2.3
3	D	200	LEU	2.3
1	B	166	TYR	2.3
1	B	243	GLY	2.3
4	E	196	TYR	2.3
1	B	116	LYS	2.2
1	B	208	GLY	2.2
1	B	213	ILE	2.2
1	A	251	ASP	2.2
1	B	96	MET	2.2
2	c	263	THR	2.2
1	B	232	GLN	2.2
4	E	190	TRP	2.1
2	c	262	PHE	2.1
2	a	302	ASN	2.1
4	L	141	ILE	2.1
2	b	274	THR	2.1
4	L	191	LYS	2.1
1	C	245	LEU	2.1
3	H	170	LEU	2.1
1	A	221	ILE	2.1
2	b	347	ASP	2.1
4	E	123	PHE	2.0
4	E	210	THR	2.0
1	C	62	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
3	F	72	ILE	2.0
4	E	137	LEU	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	NAG	J	2	14/15	0.71	0.29	122,147,156,159	0
8	NAG	U	2	14/15	0.71	0.34	131,172,187,190	0
6	NAG	M	1	14/15	0.72	0.38	153,159,183,186	0
5	BMA	I	3	11/12	0.72	0.32	164,172,175,175	0
7	MAN	N	4	11/12	0.73	0.29	149,155,158,162	0
7	MAN	T	4	11/12	0.74	0.19	140,154,155,156	0
6	NAG	e	2	14/15	0.74	0.21	125,150,155,157	0
5	BMA	Z	3	11/12	0.75	0.36	176,188,193,193	0
6	NAG	R	2	14/15	0.78	0.43	167,176,182,184	0
6	NAG	O	2	14/15	0.79	0.26	124,142,153,154	0
6	NAG	M	2	14/15	0.79	0.46	166,187,198,207	0
5	BMA	V	3	11/12	0.80	0.17	146,149,161,161	0
6	NAG	Y	2	14/15	0.81	0.24	163,179,180,181	0
5	NAG	Z	2	14/15	0.82	0.24	157,170,184,186	0
6	NAG	X	2	14/15	0.82	0.28	164,169,178,182	0
7	BMA	N	3	11/12	0.82	0.22	137,146,161,169	0
6	NAG	Q	2	14/15	0.84	0.21	155,162,173,177	0
7	MAN	d	4	11/12	0.85	0.24	162,167,173,173	0
7	BMA	d	3	11/12	0.85	0.30	153,160,166,171	0
6	NAG	W	2	14/15	0.86	0.29	161,167,175,178	0
8	NAG	P	2	14/15	0.86	0.27	116,133,143,148	0
6	NAG	Y	1	14/15	0.86	0.17	136,148,159,168	0
8	FUC	U	3	10/11	0.86	0.20	141,145,156,158	0
6	NAG	X	1	14/15	0.88	0.18	112,131,146,160	0
7	BMA	T	3	11/12	0.88	0.19	143,151,157,159	0
5	NAG	I	2	14/15	0.88	0.36	138,149,159,165	0

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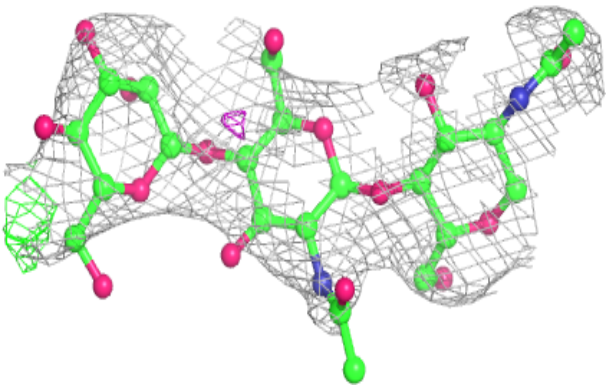
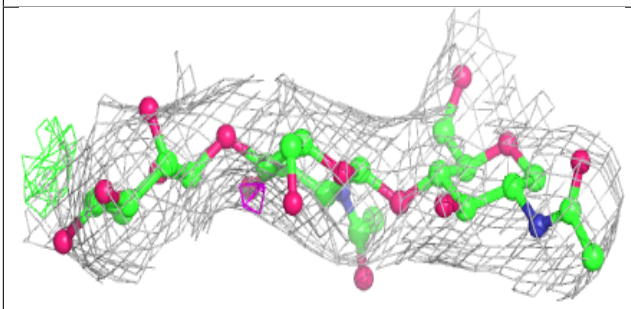
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	K	2	14/15	0.88	0.21	152,163,171,173	0
6	NAG	R	1	14/15	0.89	0.23	102,121,137,154	0
8	NAG	f	2	14/15	0.89	0.28	131,140,153,154	0
8	NAG	U	1	14/15	0.90	0.16	102,121,145,167	0
7	NAG	T	1	14/15	0.90	0.29	95,110,126,127	0
5	NAG	V	2	14/15	0.90	0.17	134,145,154,156	0
8	FUC	P	3	10/11	0.90	0.18	119,125,129,130	0
7	NAG	N	2	14/15	0.91	0.26	97,107,115,126	0
6	NAG	S	2	14/15	0.91	0.15	147,156,162,164	0
8	FUC	f	3	10/11	0.91	0.31	125,128,134,135	0
7	NAG	T	2	14/15	0.92	0.33	125,138,143,145	0
8	NAG	f	1	14/15	0.92	0.17	78,101,122,134	0
6	NAG	K	1	14/15	0.92	0.14	99,115,139,140	0
6	NAG	W	1	14/15	0.92	0.27	114,131,151,153	0
6	NAG	J	1	14/15	0.93	0.24	96,116,134,136	0
5	NAG	Z	1	14/15	0.93	0.14	115,135,152,157	0
6	NAG	S	1	14/15	0.93	0.14	100,120,127,131	0
7	NAG	d	1	14/15	0.93	0.28	102,115,128,134	0
7	NAG	d	2	14/15	0.93	0.18	126,136,150,153	0
6	NAG	Q	1	14/15	0.94	0.19	83,109,128,142	0
5	NAG	I	1	14/15	0.94	0.18	72,92,105,124	0
6	NAG	O	1	14/15	0.94	0.14	66,83,103,120	0
5	NAG	V	1	14/15	0.94	0.17	81,110,124,124	0
6	NAG	e	1	14/15	0.94	0.16	93,110,134,137	0
7	NAG	N	1	14/15	0.95	0.27	72,83,98,99	0
8	NAG	P	1	14/15	0.95	0.14	69,96,112,125	0

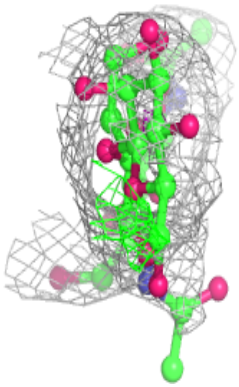
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

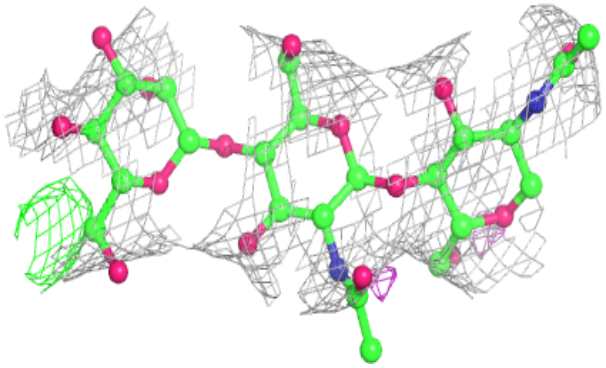


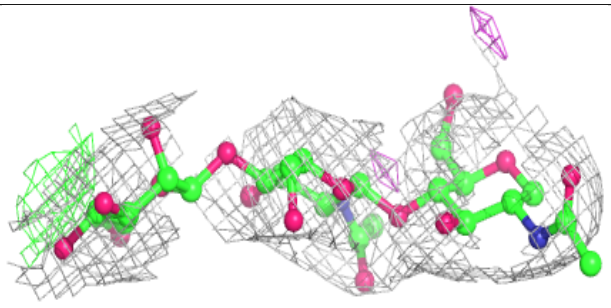


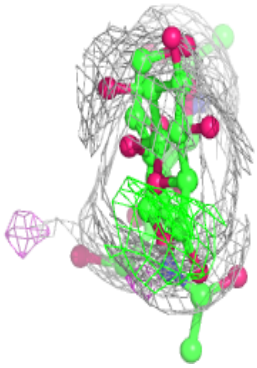


Electron density around Chain V:

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

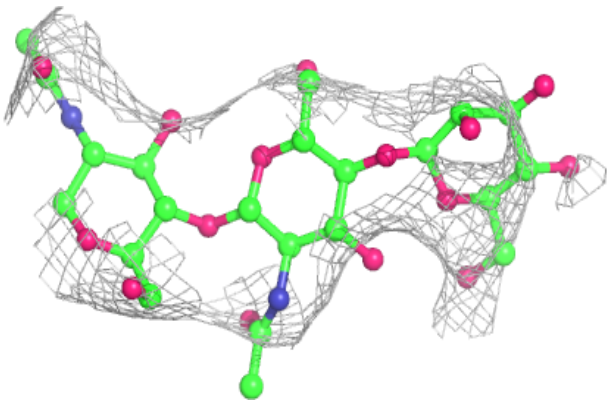


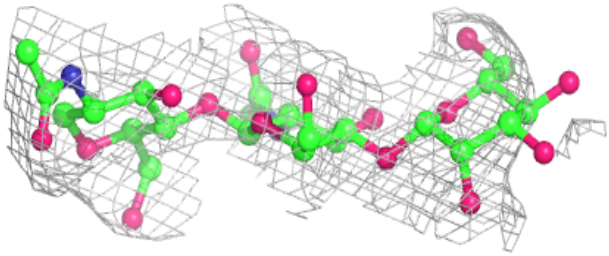


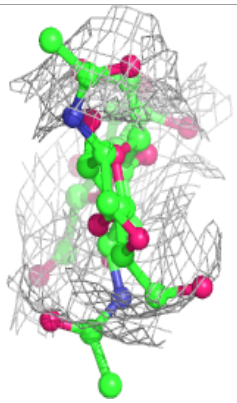


Electron density around Chain Z:

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

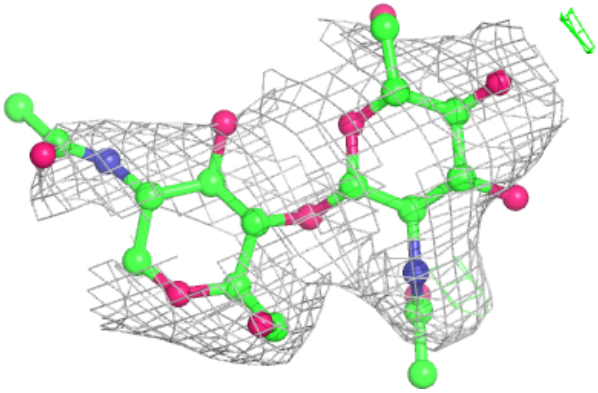


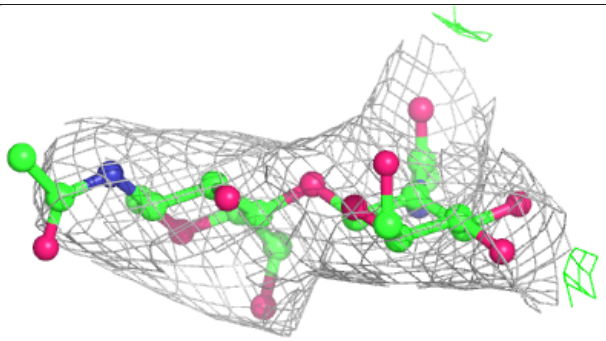


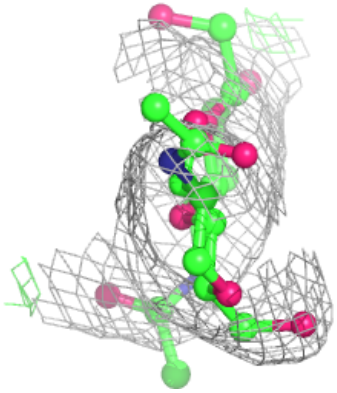


Electron density around Chain J:

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

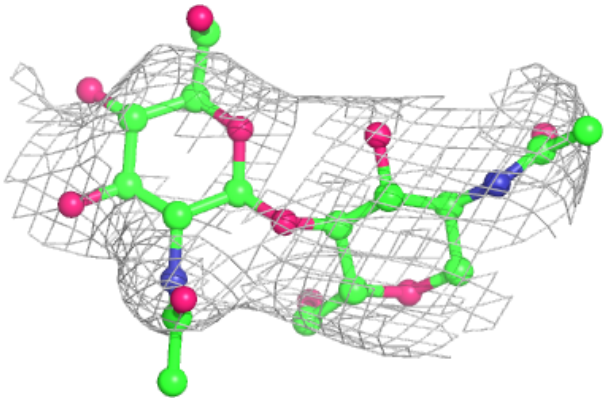


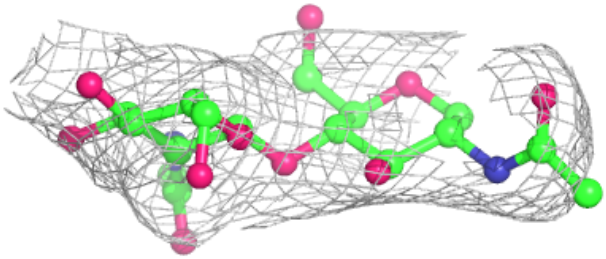


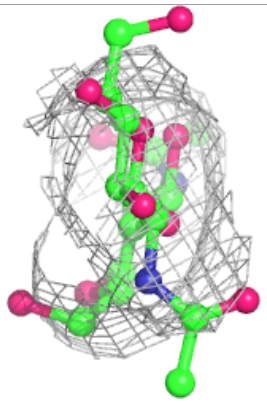


Electron density around Chain K:

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

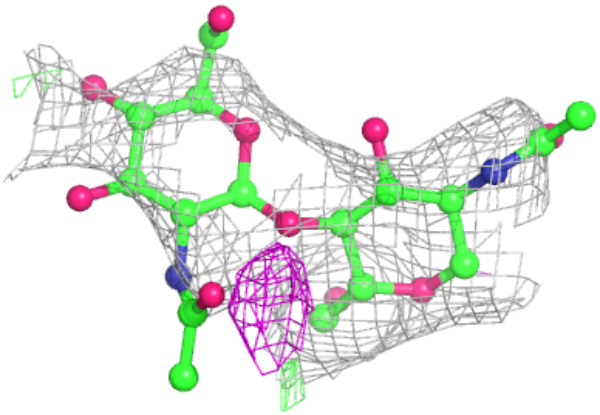


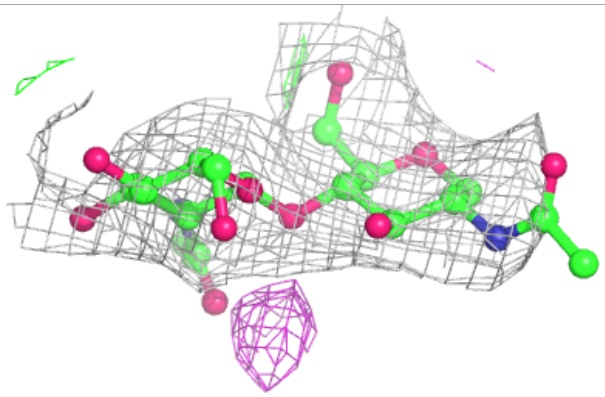


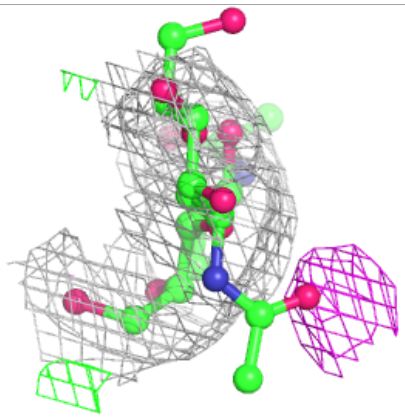


Electron density around Chain M:

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

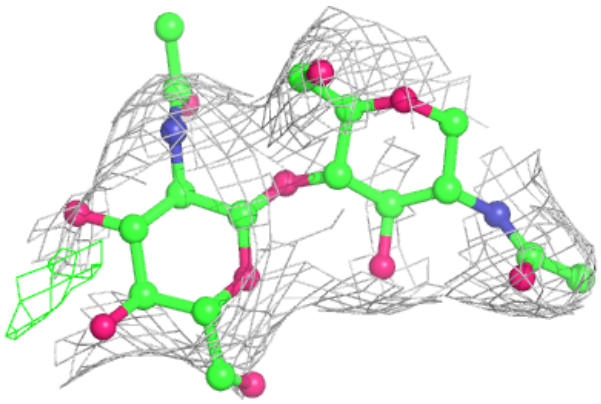


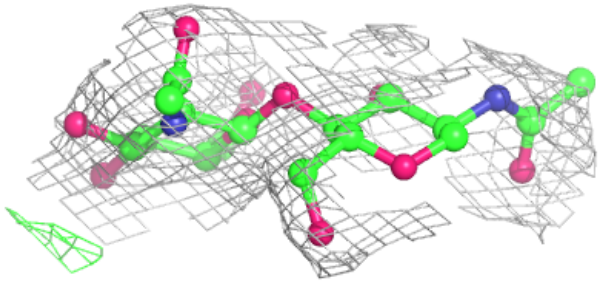


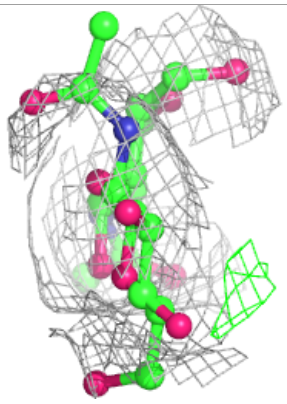


Electron density around Chain O:

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

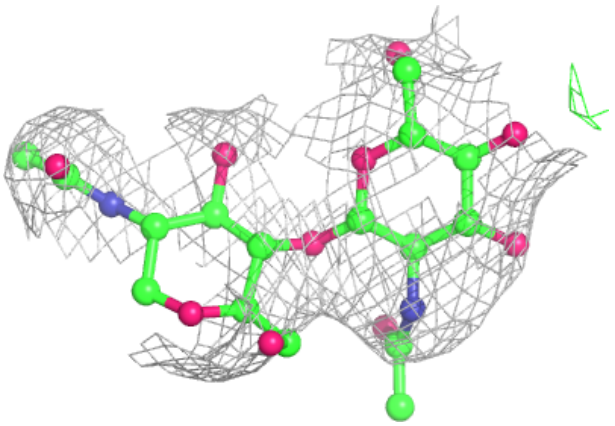


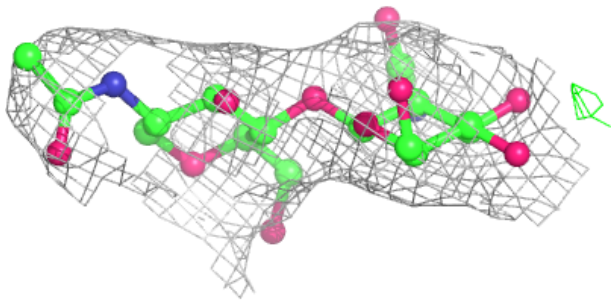


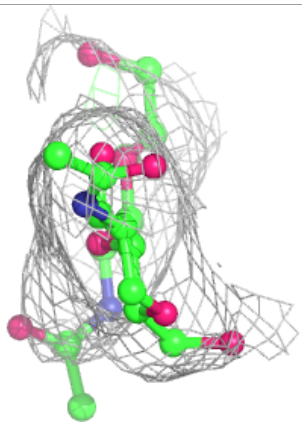


Electron density around Chain Q:

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

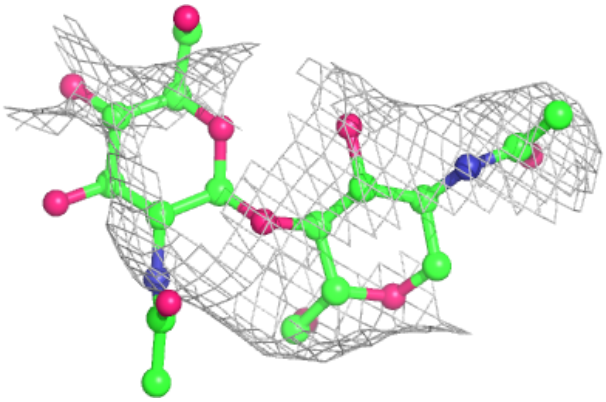


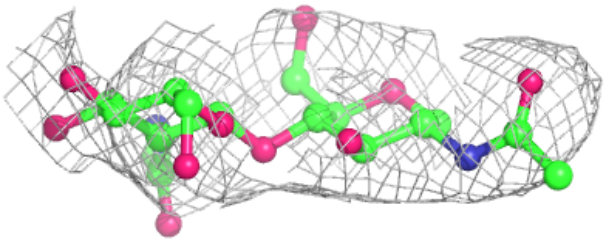


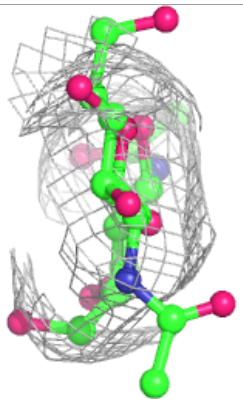


Electron density around Chain R:

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

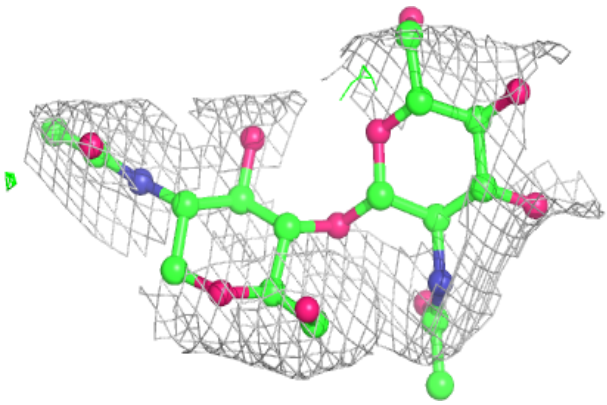


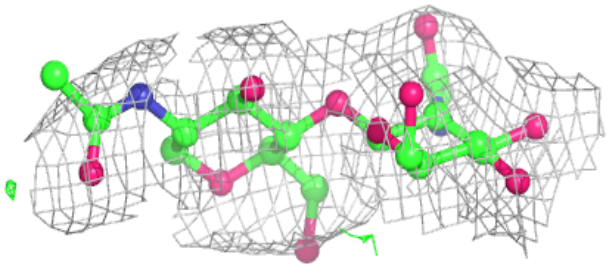


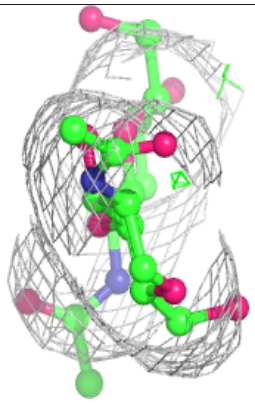


Electron density around Chain S:

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

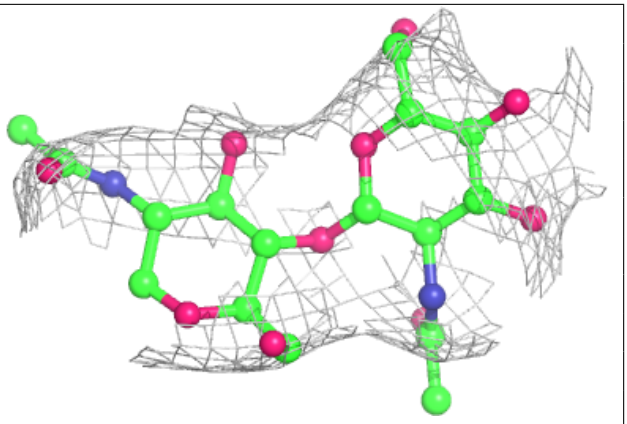


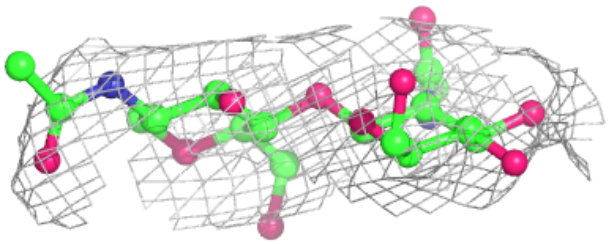


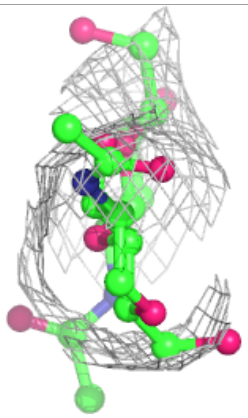


Electron density around Chain W:

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

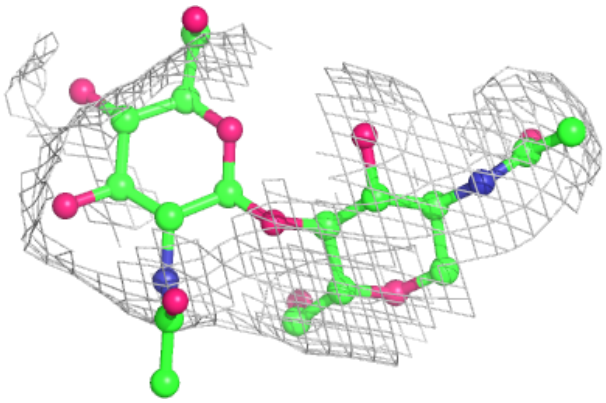


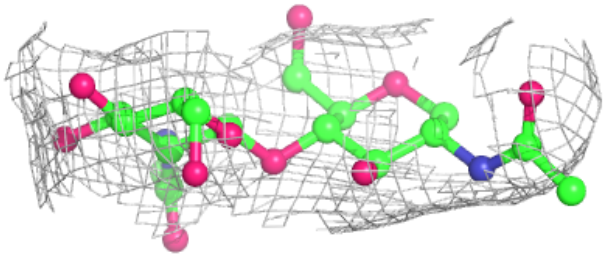


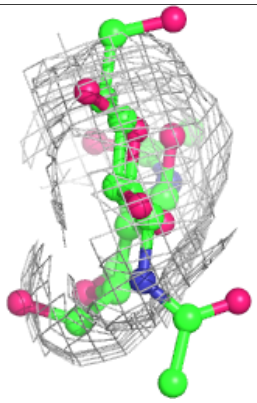


Electron density around Chain X:

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

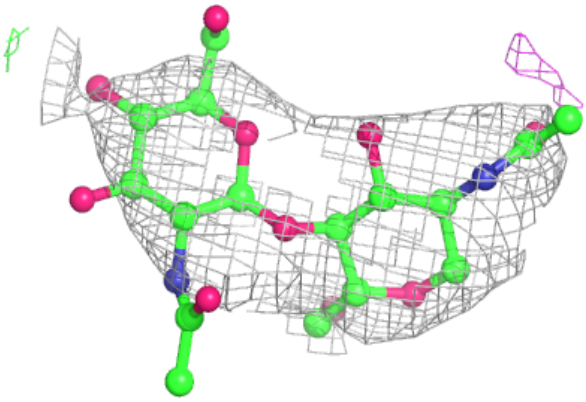


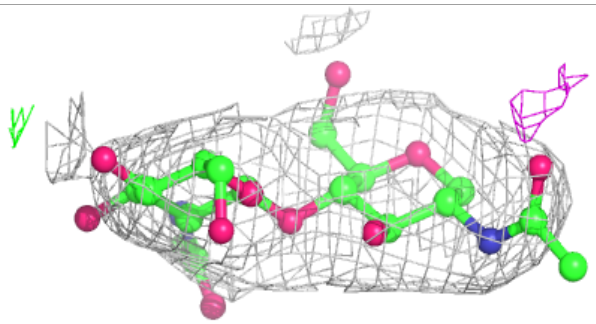


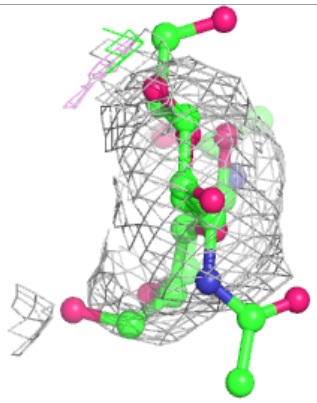


Electron density around Chain Y:

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

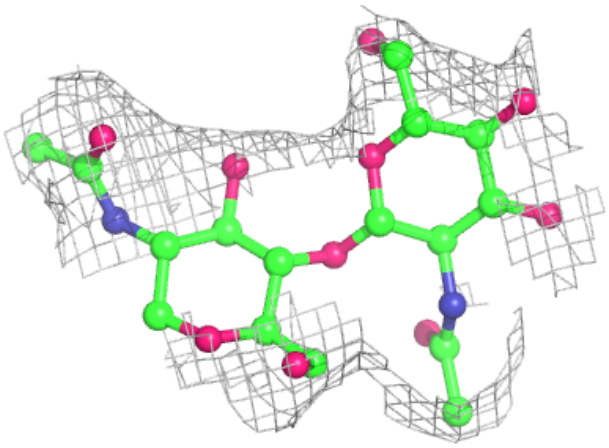


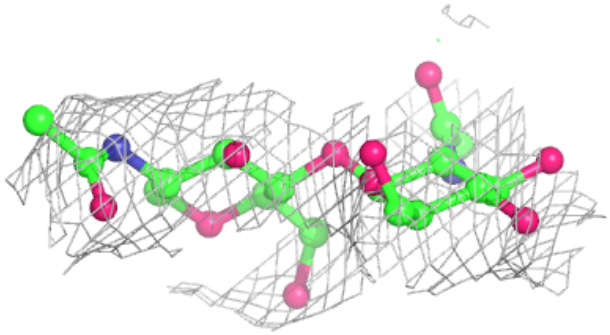


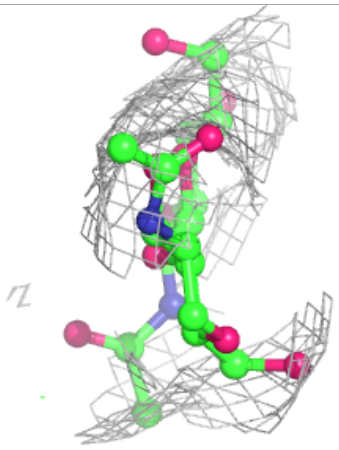


Electron density around Chain e:

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

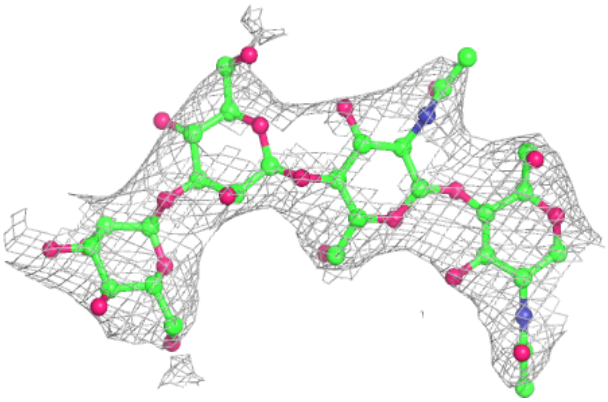


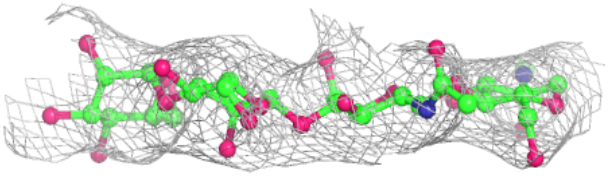


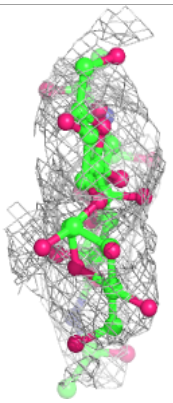


Electron density around Chain N:

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

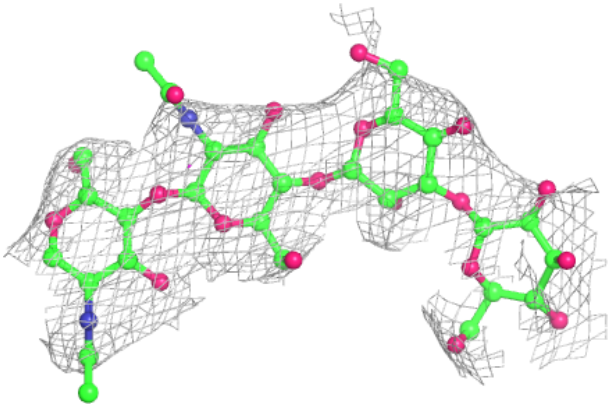


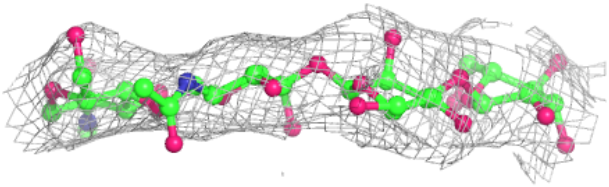


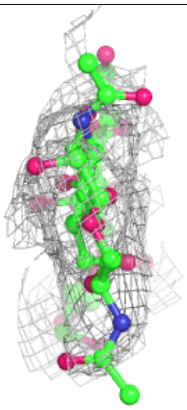


Electron density around Chain T:

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

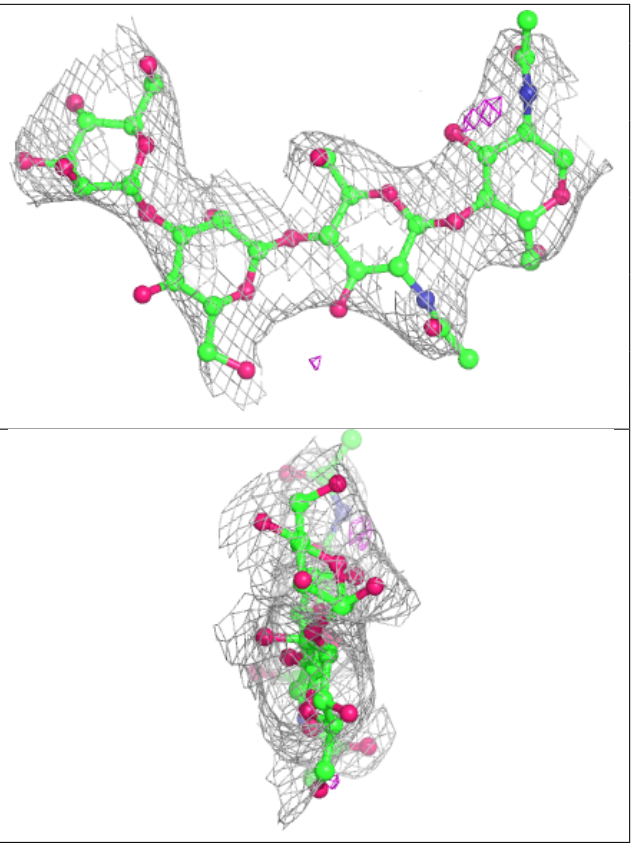


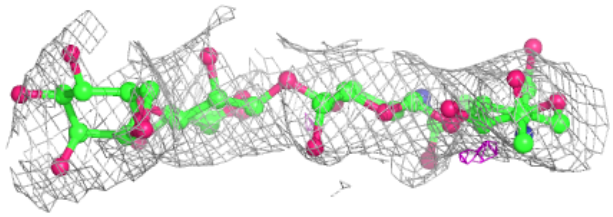




Electron density around Chain d:

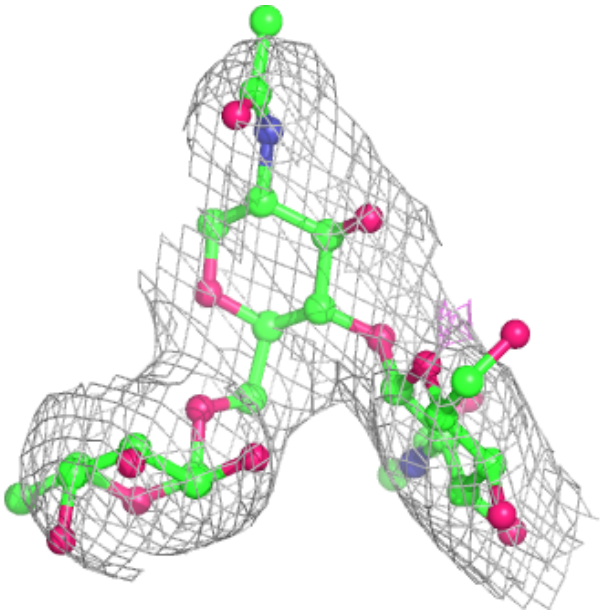
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

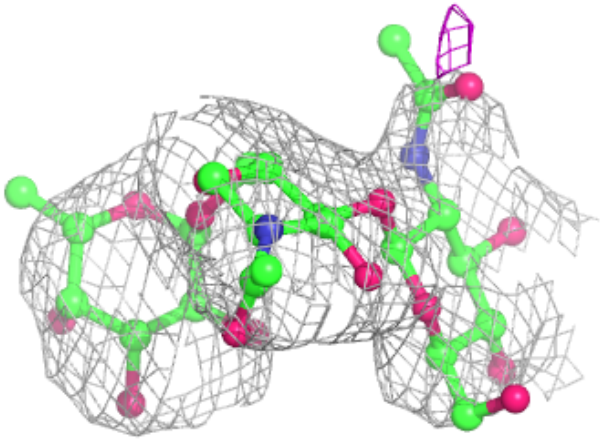


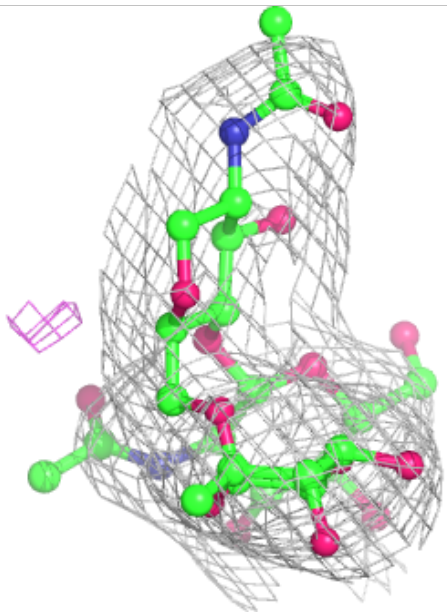


Electron density around Chain P:

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

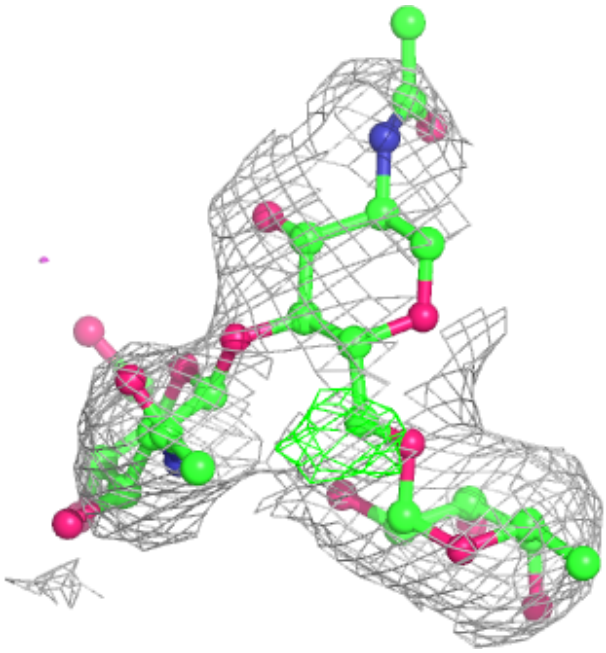


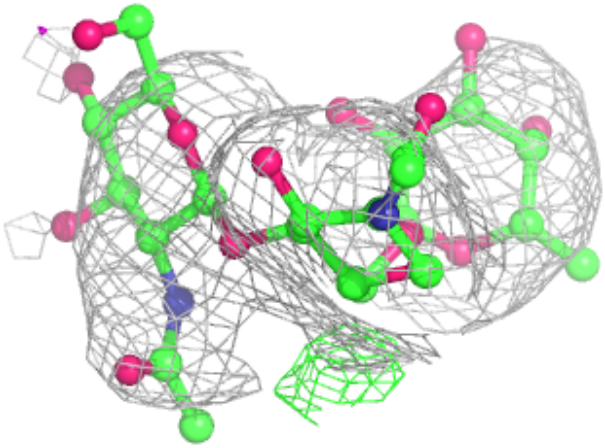


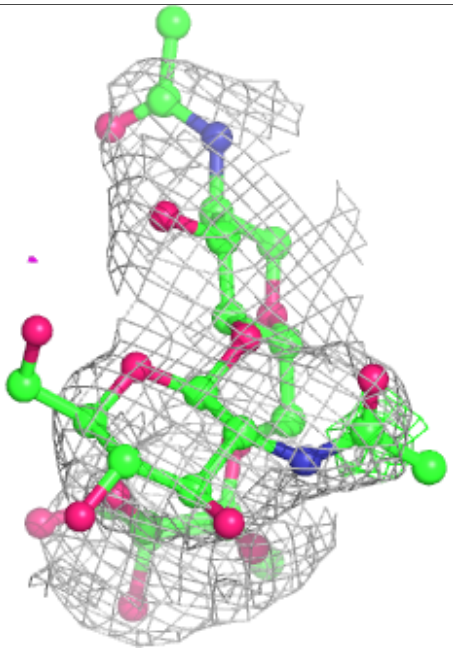


Electron density around Chain U:

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

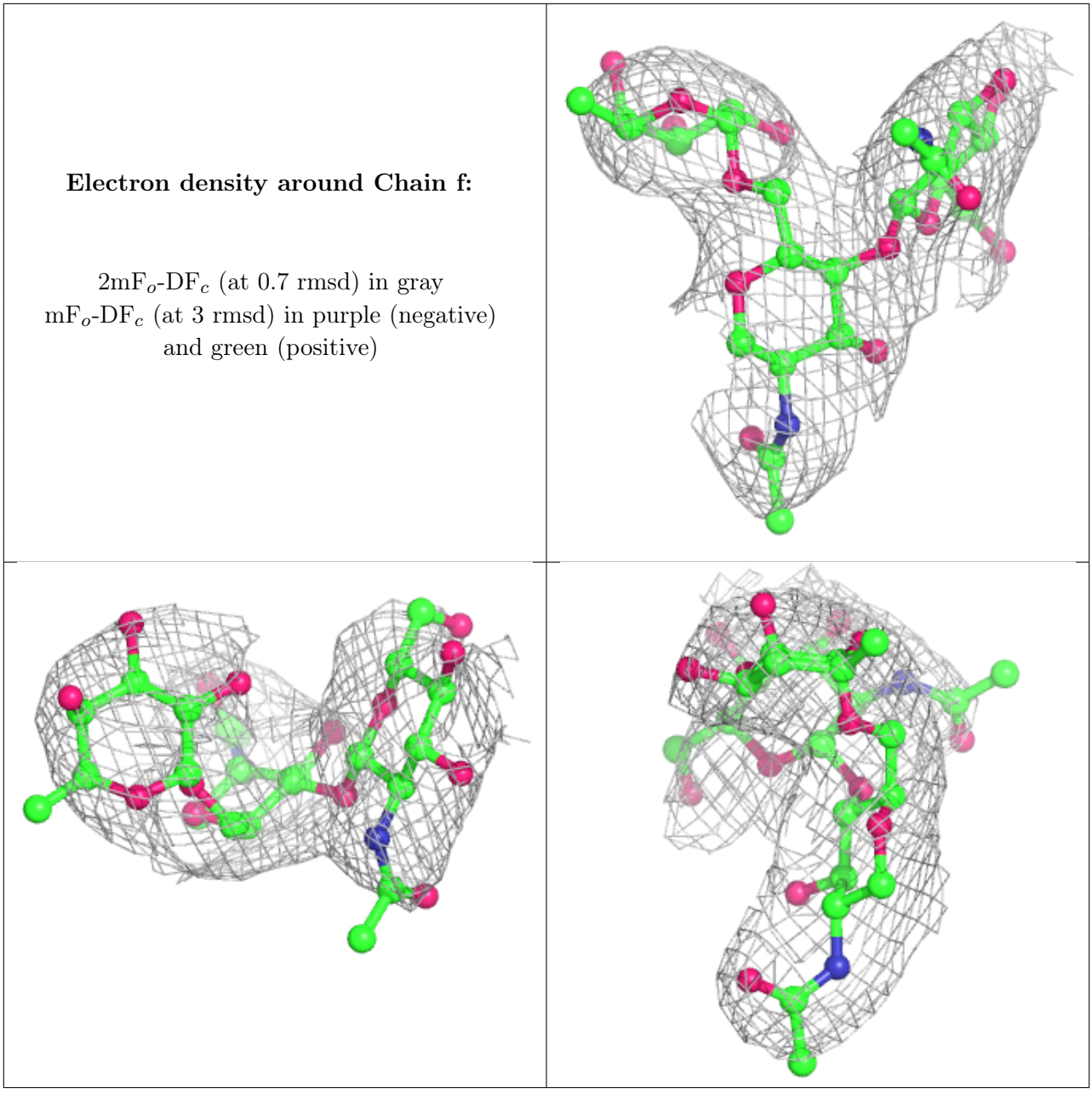






Electron density around Chain f:

$2mF_o$-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
9	NAG	B	505	14/15	0.75	0.28	139,155,171,172	0
9	NAG	a	507	14/15	0.79	0.30	136,155,166,166	0
9	NAG	B	508	14/15	0.80	0.28	115,130,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	A	511	14/15	0.81	0.28	122,133,138,141	0
9	NAG	C	506	14/15	0.82	0.33	137,155,163,164	0
9	NAG	c	507	14/15	0.82	0.23	150,164,172,174	0
9	NAG	b	505	14/15	0.86	0.21	112,128,139,140	0
9	NAG	B	509	14/15	0.88	0.16	85,110,114,123	0
9	NAG	C	514	14/15	0.89	0.22	108,122,131,133	0
9	NAG	A	506	14/15	0.90	0.22	130,145,153,154	0
9	NAG	A	512	14/15	0.90	0.23	92,110,121,125	0

6.5 Other polymers (i)

There are no such residues in this entry.