Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 02:38 AM EDT

PDB ID	:	3WO3
Title	:	Crystal structure of IL-18 in complex with IL-18 receptor alpha
Authors	:	Tsutsumi, N.; Kimura, T.; Arita, K.; Ariyoshi, M.; Ohnishi, H.; Kondo, N.; Shirakawa, M.; Kato, Z.; Tochio, H.
Deposited on	:	2013-12-19
Resolution	:	3.10 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:

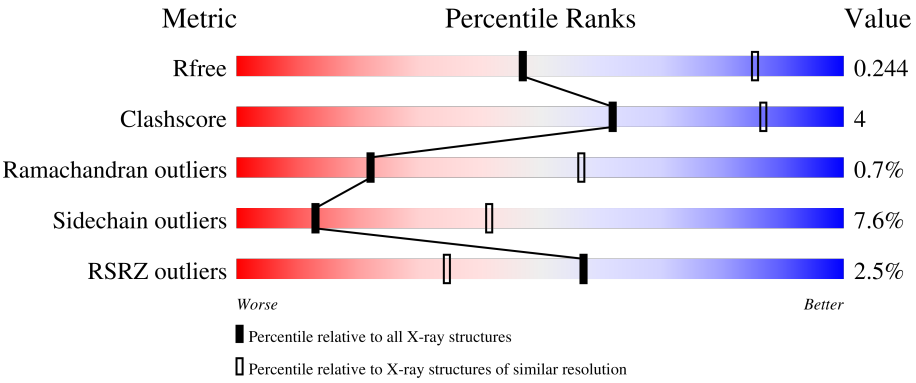
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	157	82% 17%
1	C	157	85% 13%
1	E	157	85% 15%
1	G	157	83% 15%
1	I	157	83% 14%

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Mol	Chain	Length	Quality of chain
1	K	157	83% 14%
2	B	312	2% 76% 17% 6%
2	D	312	% 75% 17% 7%
2	F	312	2% 75% 16% 8%
2	H	312	2% 76% 15% 8%
2	J	312	6% 72% 13% 13%
2	L	312	8% 67% 14% 18%
3	M	3	100%
3	Q	3	67% 33%
3	h	3	67% 33%
4	N	6	17% 67% 17%
4	W	6	33% 67%
5	O	2	100%
5	b	2	50% 50%
5	g	2	100%
5	j	2	50% 50%
5	k	2	100%
6	P	3	33% 67%
6	T	3	33% 67%
6	U	3	100%
6	X	3	67% 33%
6	c	3	67% 33%
6	e	3	100%
6	f	3	100%
6	i	3	33% 67%

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Mol	Chain	Length	Quality of chain
7	R	2	100%
8	S	5	100%
8	a	5	100%
9	V	4	50% 50%
9	d	4	25% 75%
9	l	4	75% 25%
10	Y	4	100%
11	Z	5	40% 60%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MAN	Y	4	-	-	-	X
11	MAN	Z	4	-	-	-	X
12	SO4	F	824	-	-	-	X
13	NAG	B	901	-	-	-	X
13	NAG	F	901	-	-	-	X
13	NAG	F	903	-	-	-	X
13	NAG	J	903	-	-	-	X
3	NAG	M	2	-	-	-	X
4	MAN	N	4	-	-	-	X
4	MAN	W	5	-	-	-	X
9	BMA	l	3	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 22047 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 Interleukin-18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1245	783	207	245	10			
1	C	156	Total	C	N	O	S	0	0	0
			1258	791	209	248	10			
1	E	157	Total	C	N	O	S	0	1	0
			1255	787	208	250	10			
1	G	156	Total	C	N	O	S	0	0	0
			1240	782	208	240	10			
1	I	156	Total	C	N	O	S	0	0	0
			1179	739	195	235	10			
1	K	156	Total	C	N	O	S	0	0	0
			1180	737	197	236	10			

- Molecule 2 is a protein called Interleukin-18 receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	294	Total	C	N	O	S	0	1	0
			2336	1477	403	442	14			
2	D	290	Total	C	N	O	S	0	0	0
			2316	1470	395	437	14			
2	F	288	Total	C	N	O	S	0	1	0
			2280	1445	392	429	14			
2	H	288	Total	C	N	O	S	0	0	0
			2284	1445	391	434	14			
2	J	272	Total	C	N	O	S	0	0	0
			2037	1286	341	397	13			
2	L	255	Total	C	N	O	S	0	0	0
			1923	1213	327	370	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q13478

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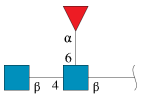
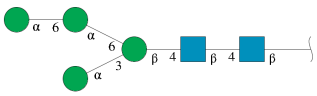
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	PRO	-	expression tag	UNP Q13478
D	-2	GLY	-	expression tag	UNP Q13478
D	-1	PRO	-	expression tag	UNP Q13478
F	-2	GLY	-	expression tag	UNP Q13478
F	-1	PRO	-	expression tag	UNP Q13478
H	-2	GLY	-	expression tag	UNP Q13478
H	-1	PRO	-	expression tag	UNP Q13478
J	-2	GLY	-	expression tag	UNP Q13478
J	-1	PRO	-	expression tag	UNP Q13478
L	-2	GLY	-	expression tag	UNP Q13478
L	-1	PRO	-	expression tag	UNP Q13478

- Molecule 3 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
3	M	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	Q	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	h	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



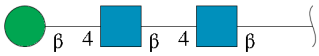
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	6	Total	C	N	O	0	0	0
			72	40	2	30			
4	W	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	O	2	Total C N O 28 16 2 10	0	0	0
5	b	2	Total C N O 28 16 2 10	0	0	0
5	g	2	Total C N O 28 16 2 10	0	0	0
5	j	2	Total C N O 28 16 2 10	0	0	0
5	k	2	Total C N O 28 16 2 10	0	0	0

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



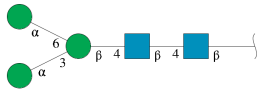
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	P	3	Total C N O 39 22 2 15	0	0	0
6	T	3	Total C N O 39 22 2 15	0	0	0
6	U	3	Total C N O 39 22 2 15	0	0	0
6	X	3	Total C N O 39 22 2 15	0	0	0
6	c	3	Total C N O 39 22 2 15	0	0	0
6	e	3	Total C N O 39 22 2 15	0	0	0
6	f	3	Total C N O 39 22 2 15	0	0	0
6	i	3	Total C N O 39 22 2 15	0	0	0

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet

a-D-glucopyranose.

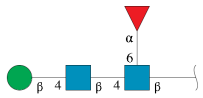
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	R	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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

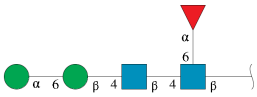


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	V	4	Total	C	N	O	0	0	0
			49	28	2	19			
9	d	4	Total	C	N	O	0	0	0
			49	28	2	19			
9	l	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

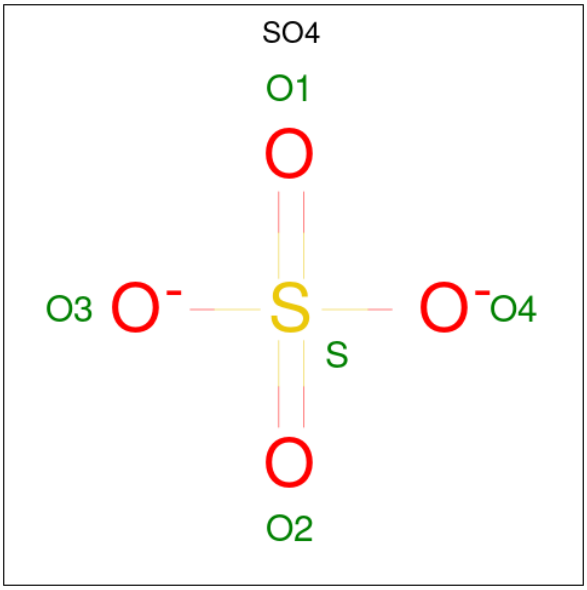
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	Y	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	Z	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	O	S	0	0
			5	4	1		
12	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total O S 5 4 1	0	0
12	B	1	Total O S 5 4 1	0	0
12	B	1	Total O S 5 4 1	0	0
12	B	1	Total O S 5 4 1	0	0
12	B	1	Total O S 5 4 1	0	0
12	C	1	Total O S 5 4 1	0	0
12	C	1	Total O S 5 4 1	0	0
12	C	1	Total O S 5 4 1	0	0
12	C	1	Total O S 5 4 1	0	0
12	C	1	Total O S 5 4 1	0	0
12	D	1	Total O S 5 4 1	0	0
12	D	1	Total O S 5 4 1	0	0
12	D	1	Total O S 5 4 1	0	0
12	D	1	Total O S 5 4 1	0	0
12	D	1	Total O S 5 4 1	0	0
12	D	1	Total O S 5 4 1	0	0
12	D	1	Total O S 5 4 1	0	0
12	E	1	Total O S 5 4 1	0	0
12	E	1	Total O S 5 4 1	0	0
12	E	1	Total O S 5 4 1	0	0
12	F	1	Total O S 5 4 1	0	0

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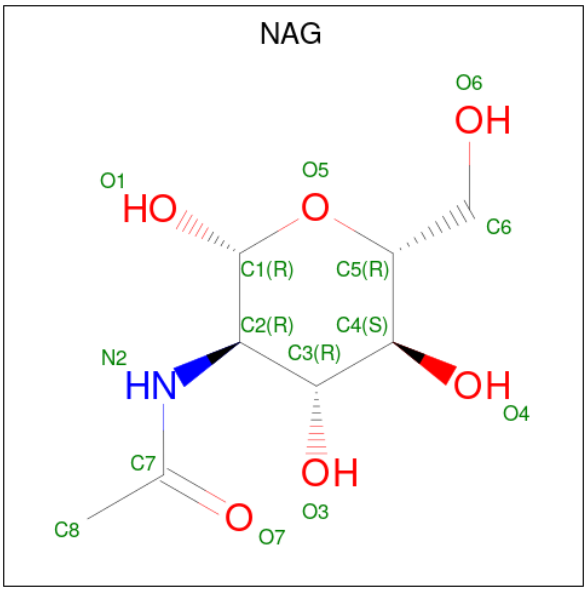
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	F	1	Total O S 5 4 1	0	0
12	F	1	Total O S 5 4 1	0	0
12	F	1	Total O S 5 4 1	0	0
12	F	1	Total O S 5 4 1	0	0
12	G	1	Total O S 5 4 1	0	0
12	G	1	Total O S 5 4 1	0	0
12	H	1	Total O S 5 4 1	0	0
12	H	1	Total O S 5 4 1	0	0
12	H	1	Total O S 5 4 1	0	0
12	H	1	Total O S 5 4 1	0	0
12	H	1	Total O S 5 4 1	0	0
12	I	1	Total O S 5 4 1	0	0
12	J	1	Total O S 5 4 1	0	0
12	K	1	Total O S 5 4 1	0	0
12	L	1	Total O S 5 4 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C N O 14 8 1 5	0	0
13	B	1	Total C N O 14 8 1 5	0	0
13	D	1	Total C N O 14 8 1 5	0	0
13	F	1	Total C N O 14 8 1 5	0	0
13	F	1	Total C N O 14 8 1 5	0	0
13	H	1	Total C N O 14 8 1 5	0	0
13	H	1	Total C N O 14 8 1 5	0	0
13	J	1	Total C N O 14 8 1 5	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	15	Total O 15 15	0	0
14	B	10	Total O 10 10	0	0
14	C	9	Total O 9 9	0	0
14	D	18	Total O 18 18	0	0

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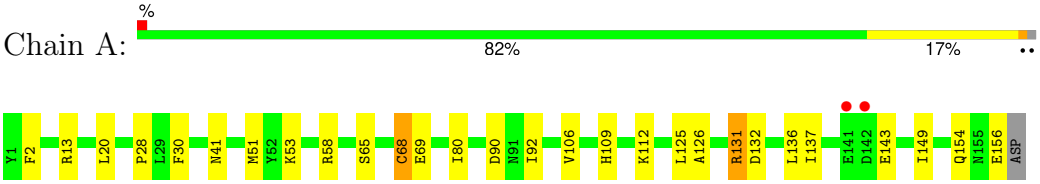
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	E	5	Total O 5 5	0	0
14	F	12	Total O 12 12	0	0
14	G	3	Total O 3 3	0	0
14	H	11	Total O 11 11	0	0
14	I	6	Total O 6 6	0	0
14	J	3	Total O 3 3	0	0
14	K	1	Total O 1 1	0	0
14	L	6	Total O 6 6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

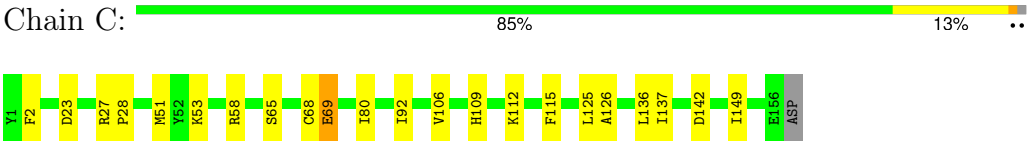
• Molecule 1: Interleukin-18

Chain A:



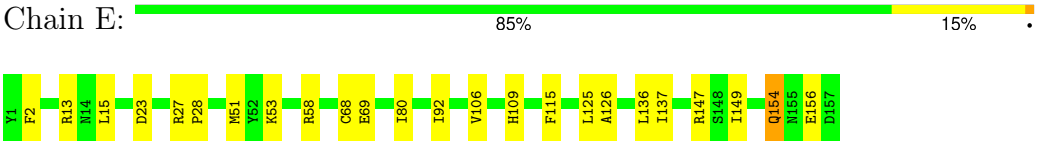
• Molecule 1: Interleukin-18

Chain C:



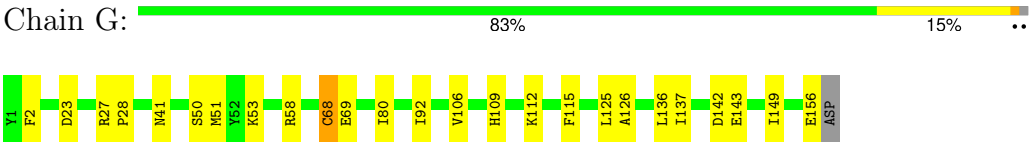
• Molecule 1: Interleukin-18

Chain E:



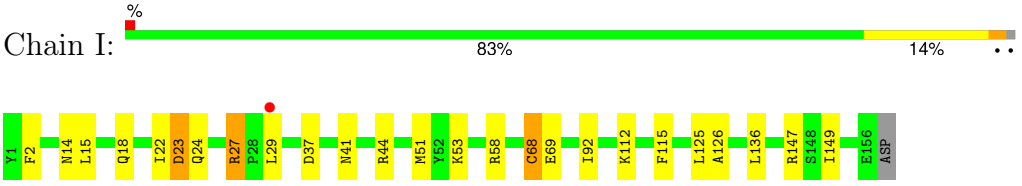
• Molecule 1: Interleukin-18

Chain G:



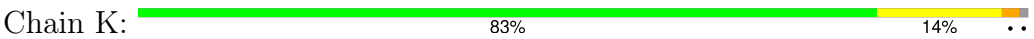
• Molecule 1: Interleukin-18

Chain I:



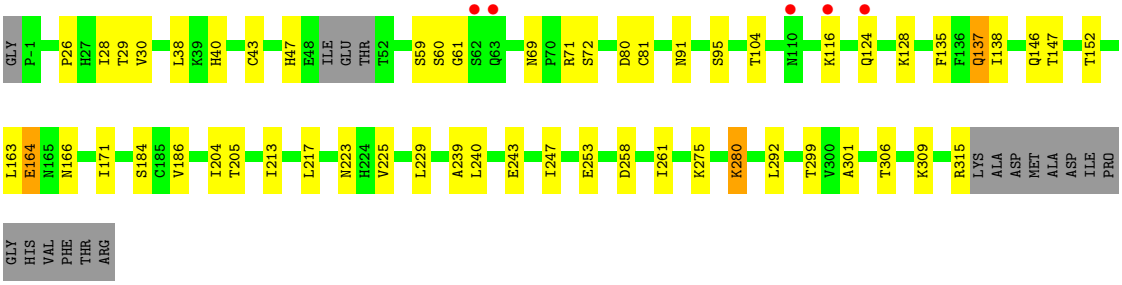
• Molecule 1: Interleukin-18

Chain K:



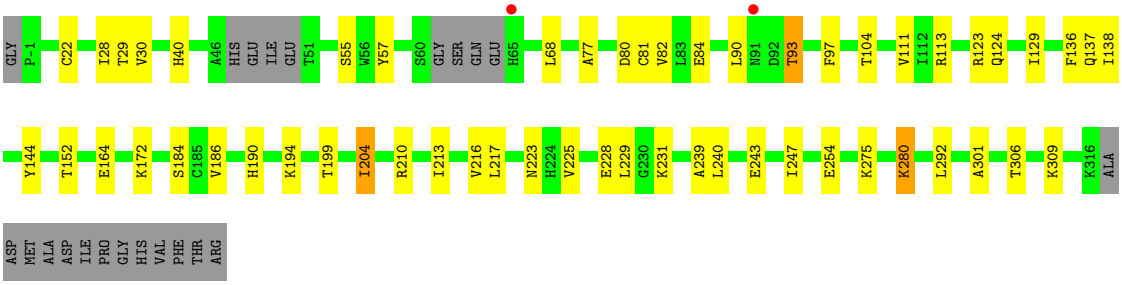
• Molecule 2: Interleukin-18 receptor 1

Chain B:



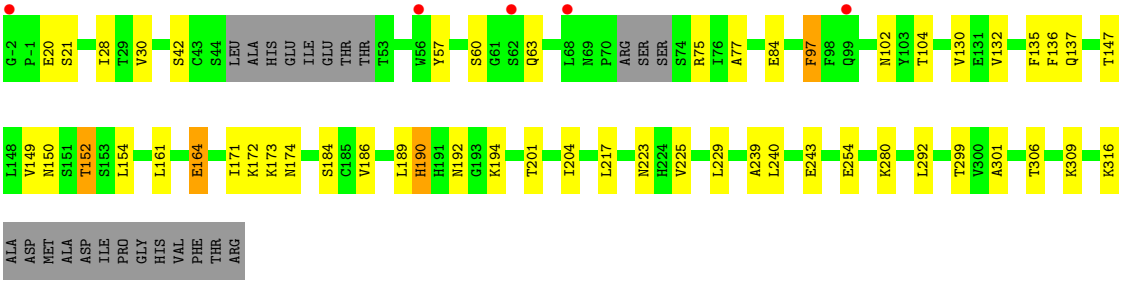
• Molecule 2: Interleukin-18 receptor 1

Chain D:



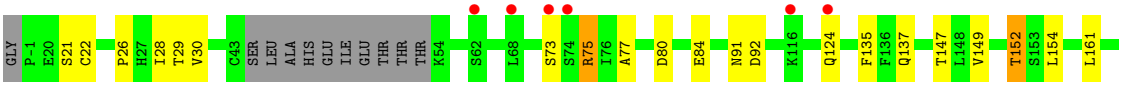
• Molecule 2: Interleukin-18 receptor 1

Chain F:

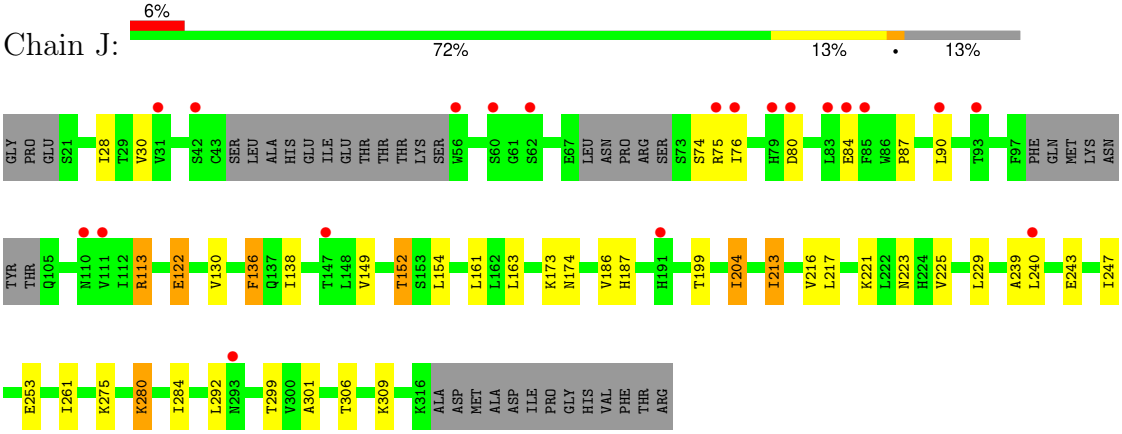


• Molecule 2: Interleukin-18 receptor 1

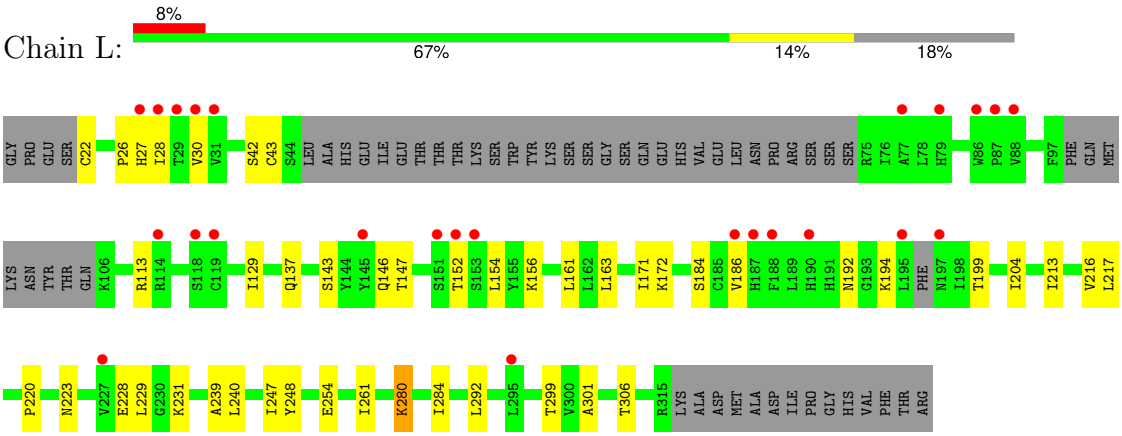
Chain H:



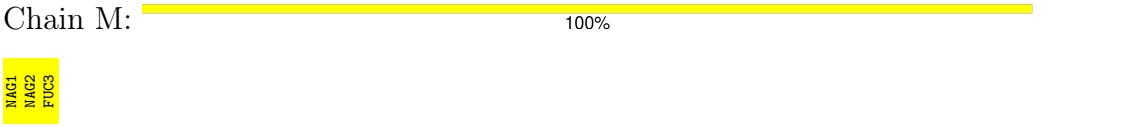
• Molecule 2: Interleukin-18 receptor 1



• Molecule 2: Interleukin-18 receptor 1



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



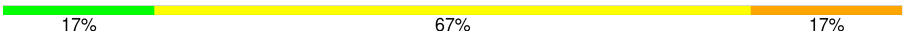
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

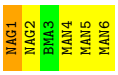
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

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

Chain N:



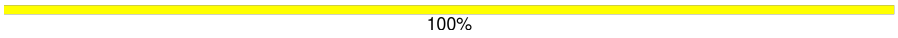


• Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

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

Chain O:

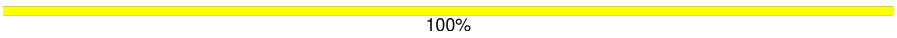


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

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

Chain g:

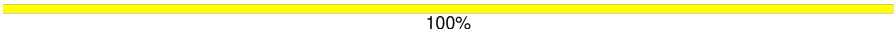


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:

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

Chain k:



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

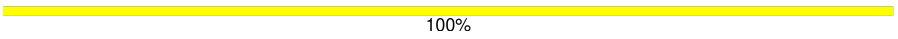
Chain P:

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

Chain T:

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

Chain U:



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

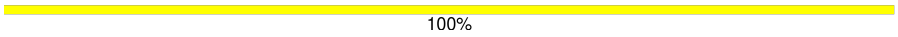
Chain X:

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

Chain c:

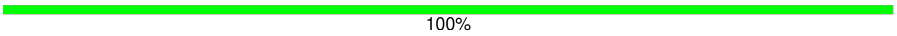
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



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

Chain f:

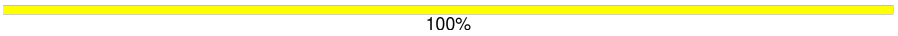


• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

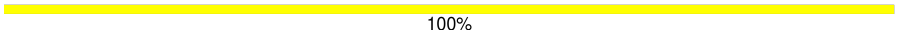
• Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



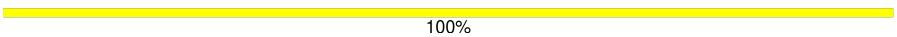
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



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

Chain a:



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

Chain V:

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

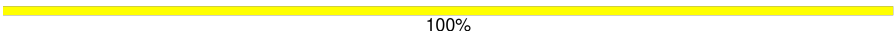
Chain d:

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

Chain l:

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

Chain Y:



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

Chain Z:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	135.49Å 174.81Å 183.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.25 – 3.10 43.85 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (31.25-3.10) 99.4 (43.85-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.191 , 0.222 0.210 , 0.244	Depositor DCC
R_{free} test set	3974 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	69.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 84.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22047	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: FUC, SO4, NAG, 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	0.49	0/1266	0.65	0/1701
1	C	0.50	0/1279	0.68	0/1717
1	E	0.46	0/1279	0.66	0/1719
1	G	0.52	0/1261	0.66	0/1695
1	I	0.43	0/1200	0.64	0/1625
1	K	0.44	0/1200	0.63	0/1622
2	B	0.46	0/2390	0.68	0/3244
2	D	0.47	0/2368	0.69	0/3209
2	F	0.45	0/2335	0.69	0/3166
2	H	0.46	0/2337	0.67	0/3174
2	J	0.43	0/2077	0.69	0/2830
2	L	0.42	0/1964	0.65	0/2677
All	All	0.46	0/20956	0.67	0/28379

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	1245	0	1207	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1258	0	1233	11	0
1	E	1255	0	1206	11	0
1	G	1240	0	1210	13	0
1	I	1179	0	1066	13	0
1	K	1180	0	1074	13	0
2	B	2336	0	2208	18	0
2	D	2316	0	2233	22	0
2	F	2280	0	2166	16	0
2	H	2284	0	2154	21	0
2	J	2037	0	1832	18	0
2	L	1923	0	1715	15	0
3	M	38	0	34	0	0
3	Q	38	0	34	0	0
3	h	38	0	34	0	0
4	N	72	0	61	1	0
4	W	72	0	61	3	0
5	O	28	0	25	0	0
5	b	28	0	25	0	0
5	g	28	0	25	0	0
5	j	28	0	25	0	0
5	k	28	0	25	0	0
6	P	39	0	34	0	0
6	T	39	0	34	0	0
6	U	39	0	34	0	0
6	X	39	0	34	0	0
6	c	39	0	34	0	0
6	e	39	0	34	0	0
6	f	39	0	34	0	0
6	i	39	0	34	0	0
7	R	24	0	22	1	0
8	S	61	0	52	0	0
8	a	61	0	52	0	0
9	V	49	0	43	0	0
9	d	49	0	43	0	0
9	l	49	0	43	0	0
10	Y	50	0	43	0	0
11	Z	60	0	52	1	0
12	A	10	0	0	0	0
12	B	25	0	0	0	0
12	C	25	0	0	0	0
12	D	35	0	0	0	0
12	E	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	F	25	0	0	1	0
12	G	10	0	0	0	0
12	H	25	0	0	1	0
12	I	5	0	0	0	0
12	J	5	0	0	0	0
12	K	5	0	0	0	0
12	L	5	0	0	0	0
13	B	28	0	26	0	0
13	D	14	0	13	0	0
13	F	28	0	26	0	0
13	H	28	0	26	0	0
13	J	14	0	13	0	0
14	A	15	0	0	1	0
14	B	10	0	0	0	0
14	C	9	0	0	0	0
14	D	18	0	0	0	0
14	E	5	0	0	0	0
14	F	12	0	0	0	0
14	G	3	0	0	0	0
14	H	11	0	0	0	0
14	I	6	0	0	0	0
14	J	3	0	0	0	0
14	K	1	0	0	0	0
14	L	6	0	0	0	0
All	All	22047	0	20379	179	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (179) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:221:LYS:HG2	11:Z:2:NAG:H83	1.73	0.70
2:D:90:LEU:O	2:D:93:THR:HG23	1.92	0.70
1:G:106:VAL:HG22	1:G:109:HIS:HB2	1.74	0.69
1:E:106:VAL:HG22	1:E:109:HIS:HB2	1.76	0.68
1:K:41:ASN:HD21	2:L:27:HIS:H	1.41	0.67
2:J:149:VAL:HG11	2:J:152:THR:HG22	1.77	0.65
1:C:106:VAL:HG22	1:C:109:HIS:HB2	1.78	0.65
1:A:41:ASN:OD1	2:B:26:PRO:HD2	1.98	0.63
1:A:106:VAL:HG22	1:A:109:HIS:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:93:THR:HG22	2:D:111:VAL:HB	1.82	0.62
2:D:129:ILE:HD13	2:D:210:ARG:HH22	1.66	0.59
2:F:150:ASN:HB2	2:F:190:HIS:CE1	2.38	0.59
1:G:142:ASP:CG	1:G:143:GLU:H	2.07	0.58
2:J:152:THR:HB	2:J:187:HIS:HA	1.83	0.58
2:B:40:HIS:CE1	2:B:81:CYS:HA	2.39	0.57
2:J:261:ILE:HG12	2:J:284:ILE:HG12	1.87	0.56
2:H:252:GLY:O	2:H:257:SER:HA	2.05	0.56
1:K:41:ASN:ND2	2:L:26:PRO:HD2	2.23	0.54
2:B:29:THR:HG22	2:B:124:GLN:HE22	1.71	0.54
2:D:93:THR:HG22	2:D:111:VAL:H	1.72	0.54
1:I:37:ASP:O	1:I:41:ASN:HB2	2.08	0.53
1:A:90:ASP:HB3	14:A:315:HOH:O	2.07	0.53
1:K:106:VAL:HG22	1:K:109:HIS:HB2	1.91	0.53
1:K:15:LEU:HD11	1:K:112:LYS:HG3	1.91	0.52
1:E:13:ARG:NH2	1:E:154:GLN:HE21	2.08	0.52
2:J:74:SER:HB2	2:J:87:PRO:HD2	1.91	0.52
2:B:137:GLN:HA	2:B:171:ILE:O	2.10	0.52
1:I:125:LEU:HG	1:I:136:LEU:HD11	1.93	0.51
2:B:138:ILE:HD11	2:B:204:ILE:HD13	1.92	0.51
1:A:13:ARG:NH2	1:A:154:GLN:OE1	2.43	0.51
1:E:15:LEU:HD23	1:E:147[B]:ARG:NE	2.25	0.51
1:K:125:LEU:HG	1:K:136:LEU:HD11	1.92	0.51
2:D:29:THR:HG22	2:D:124:GLN:HE22	1.74	0.51
2:B:217:LEU:HD23	2:B:239:ALA:HB2	1.93	0.51
1:C:28:PRO:HB2	1:C:136:LEU:HB3	1.92	0.50
2:H:29:THR:HG22	2:H:124:GLN:HE22	1.75	0.50
2:B:223:ASN:HD21	2:B:309:LYS:HE3	1.77	0.50
2:D:190:HIS:CE1	7:R:2:FUC:H5	2.47	0.50
2:D:217:LEU:HD23	2:D:239:ALA:HB2	1.94	0.49
2:L:228:GLU:HG3	2:L:231:LYS:HG3	1.95	0.49
2:L:217:LEU:HD23	2:L:239:ALA:HB2	1.94	0.49
2:L:229:LEU:HD11	2:L:292:LEU:HD11	1.94	0.49
1:G:126:ALA:HB2	1:G:149:ILE:HG22	1.95	0.49
1:A:125:LEU:HG	1:A:136:LEU:HD11	1.95	0.49
1:A:28:PRO:HB2	1:A:136:LEU:HB3	1.94	0.49
2:B:69:ASN:H	2:B:72:SER:HB2	1.78	0.49
2:D:223:ASN:HD21	2:D:309:LYS:HE3	1.77	0.49
2:D:57:TYR:HB2	2:D:97:PHE:HB2	1.95	0.49
1:I:2:PHE:HA	1:I:53:LYS:O	2.13	0.49
1:C:109:HIS:HB3	1:C:112:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:LEU:HD11	2:D:113:ARG:HG2	1.95	0.48
2:J:217:LEU:HD23	2:J:239:ALA:HB2	1.95	0.48
2:H:137:GLN:HG3	2:H:172:LYS:HG2	1.95	0.48
2:D:137:GLN:HG3	2:D:172:LYS:HG2	1.94	0.48
1:G:23:ASP:OD1	1:G:27:ARG:HG2	2.13	0.48
1:E:28:PRO:HB2	1:E:136:LEU:HB3	1.96	0.48
2:F:137:GLN:HG3	2:F:172:LYS:HG2	1.95	0.48
1:E:23:ASP:OD1	1:E:27:ARG:HG2	2.14	0.47
1:K:117:SER:HB2	1:K:138:LEU:HD11	1.95	0.47
2:F:217:LEU:HD23	2:F:239:ALA:HB2	1.95	0.47
1:E:2:PHE:HA	1:E:53:LYS:O	2.14	0.47
2:H:229:LEU:HD11	2:H:292:LEU:HD11	1.96	0.47
2:H:223:ASN:HD21	2:H:309:LYS:HE3	1.78	0.47
2:F:223:ASN:HD21	2:F:309:LYS:HE3	1.80	0.47
1:A:2:PHE:HA	1:A:53:LYS:O	2.15	0.47
2:B:116:LYS:HE2	4:W:5:MAN:H62	1.96	0.47
1:G:125:LEU:HG	1:G:136:LEU:HD11	1.95	0.46
1:I:68:CYS:HB3	1:I:69:GLU:H	1.63	0.46
2:J:229:LEU:HD11	2:J:292:LEU:HD11	1.97	0.46
1:C:126:ALA:HB2	1:C:149:ILE:HG22	1.96	0.46
1:E:69:GLU:HA	2:H:289:GLU:HB2	1.97	0.46
1:A:20:LEU:HB2	1:A:30:PHE:CE1	2.51	0.46
1:G:2:PHE:HA	1:G:53:LYS:O	2.15	0.46
2:J:223:ASN:HD21	2:J:309:LYS:HE3	1.80	0.46
2:H:154:LEU:HG	2:H:161:LEU:HD12	1.98	0.46
1:G:28:PRO:HB2	1:G:136:LEU:HB3	1.98	0.46
1:A:109:HIS:HB3	1:A:112:LYS:HD2	1.98	0.46
2:B:247:ILE:HG23	2:B:280:LYS:HG3	1.97	0.46
2:D:93:THR:HG22	2:D:111:VAL:CB	2.44	0.46
2:D:229:LEU:HD11	2:D:292:LEU:HD11	1.96	0.46
1:E:125:LEU:HG	1:E:136:LEU:HD11	1.96	0.46
1:E:126:ALA:HB2	1:E:149:ILE:HG22	1.98	0.46
2:B:213:ILE:HG12	2:B:275:LYS:HG2	1.96	0.46
2:L:161:LEU:HD13	2:L:171:ILE:HD11	1.98	0.46
1:C:2:PHE:HA	1:C:53:LYS:O	2.15	0.46
1:C:68:CYS:HB3	1:C:69:GLU:H	1.66	0.46
2:L:186:VAL:HG22	2:L:199:THR:HG23	1.97	0.46
1:K:23:ASP:OD1	1:K:27:ARG:HG2	2.16	0.45
2:H:149:VAL:HG11	2:H:152:THR:HG22	1.98	0.45
1:G:115:PHE:HB2	1:G:125:LEU:HB2	1.98	0.45
1:I:14:ASN:ND2	1:I:18:GLN:HB2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:28:PRO:HB2	1:K:136:LEU:HB3	1.97	0.45
1:K:115:PHE:HB2	1:K:125:LEU:HB2	1.99	0.45
2:B:258:ASP:HB3	2:B:261:ILE:HG13	1.98	0.45
1:C:125:LEU:HG	1:C:136:LEU:HD11	1.99	0.45
1:I:15:LEU:HD23	1:I:147:ARG:HD2	1.98	0.45
1:G:2:PHE:HB2	1:G:92:ILE:HB	1.99	0.45
2:J:130:VAL:HG11	2:J:136:PHE:HB2	1.98	0.45
2:B:229:LEU:HD11	2:B:292:LEU:HD11	1.98	0.45
2:F:77:ALA:HB3	2:F:84:GLU:HB2	1.99	0.45
1:I:2:PHE:HB2	1:I:92:ILE:HB	1.99	0.45
1:E:2:PHE:HB2	1:E:92:ILE:HB	1.99	0.45
1:A:2:PHE:HB2	1:A:92:ILE:HB	1.99	0.44
2:D:247:ILE:HG23	2:D:280:LYS:HG3	1.98	0.44
1:K:126:ALA:HB2	1:K:149:ILE:HG22	1.98	0.44
1:K:68:CYS:HB3	1:K:69:GLU:H	1.62	0.44
2:H:135:PHE:CE2	2:H:137:GLN:HB2	2.52	0.44
2:H:235:LEU:HD22	2:H:284:ILE:HD11	1.98	0.44
1:C:23:ASP:OD1	1:C:27:ARG:HG2	2.17	0.44
1:I:115:PHE:HB2	1:I:125:LEU:HB2	2.00	0.44
2:D:77:ALA:HB3	2:D:84:GLU:HB2	1.99	0.44
2:F:149:VAL:HG11	2:F:152:THR:HG22	1.99	0.44
1:I:126:ALA:HB2	1:I:149:ILE:HG22	1.99	0.44
1:C:2:PHE:HB2	1:C:92:ILE:HB	2.00	0.44
2:H:217:LEU:HD23	2:H:239:ALA:HB2	1.99	0.44
1:A:126:ALA:HB2	1:A:149:ILE:HG22	1.98	0.44
1:G:68:CYS:HB3	1:G:69:GLU:H	1.60	0.43
2:H:77:ALA:HB3	2:H:84:GLU:HB2	2.00	0.43
2:J:213:ILE:HG12	2:J:275:LYS:HG2	2.00	0.43
1:K:53:LYS:HB2	2:L:248:TYR:CE1	2.53	0.43
2:H:213:ILE:HG12	2:H:275:LYS:HG2	2.00	0.43
2:L:220:PRO:O	2:L:223:ASN:ND2	2.51	0.43
1:I:23:ASP:HB3	1:I:29:LEU:HD12	2.00	0.43
2:F:154:LEU:HG	2:F:161:LEU:HD12	1.99	0.43
2:F:301:ALA:HA	2:F:306:THR:HG22	2.00	0.43
1:K:2:PHE:HA	1:K:53:LYS:O	2.19	0.43
2:F:229:LEU:HD11	2:F:292:LEU:HD11	2.00	0.43
2:D:228:GLU:HG3	2:D:231:LYS:HG3	2.01	0.43
2:J:186:VAL:HG22	2:J:199:THR:HG23	2.01	0.42
1:C:115:PHE:HB2	1:C:125:LEU:HB2	2.01	0.42
2:D:82:VAL:HG21	2:D:144:TYR:OH	2.19	0.42
2:J:301:ALA:HA	2:J:306:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301:ALA:HA	2:D:306:THR:HG22	2.00	0.42
1:I:22:ILE:HG23	1:I:44:ARG:HG2	2.01	0.42
2:J:90:LEU:HD12	2:J:90:LEU:H	1.85	0.42
2:B:186:VAL:HG11	4:N:1:NAG:H82	2.01	0.42
2:L:154:LEU:HG	2:L:161:LEU:HD12	2.00	0.42
1:E:115:PHE:HB2	1:E:125:LEU:HB2	2.02	0.42
2:F:135:PHE:CE2	2:F:137:GLN:HB2	2.54	0.42
2:H:301:ALA:HA	2:H:306:THR:HG22	2.02	0.42
2:L:137:GLN:HG3	2:L:172:LYS:HG2	2.02	0.42
2:L:261:ILE:HG12	2:L:284:ILE:HG23	2.02	0.42
1:A:131:ARG:HB3	1:A:132:ASP:H	1.71	0.42
2:B:138:ILE:HD11	2:B:204:ILE:CD1	2.49	0.42
2:H:189:LEU:HD21	2:H:198:ILE:HD12	2.02	0.42
2:J:247:ILE:HG23	2:J:280:LYS:HG3	2.02	0.42
2:H:253:GLU:HB3	2:H:257:SER:HB3	2.01	0.42
1:G:106:VAL:CG2	1:G:109:HIS:HB2	2.47	0.42
2:J:113:ARG:HE	2:J:113:ARG:H	1.66	0.42
1:C:106:VAL:CG2	1:C:109:HIS:HB2	2.48	0.41
2:F:186:VAL:HG11	4:W:1:NAG:H82	2.02	0.41
2:B:59:SER:OG	2:B:95:SER:HB2	2.20	0.41
2:B:135:PHE:CE2	2:B:137:GLN:HB3	2.56	0.41
4:W:3:BMA:H3	4:W:6:MAN:H2	1.77	0.41
2:J:154:LEU:HG	2:J:161:LEU:HD12	2.01	0.41
2:D:138:ILE:HD11	2:D:204:ILE:HD13	2.03	0.41
2:D:213:ILE:HG12	2:D:275:LYS:HG2	2.02	0.41
2:H:247:ILE:HG23	2:H:280:LYS:HG3	2.02	0.41
2:B:301:ALA:HA	2:B:306:THR:HG22	2.03	0.41
2:D:186:VAL:HG22	2:D:199:THR:HG23	2.02	0.41
2:H:252:GLY:HA2	12:H:817:SO4:S	2.61	0.41
2:J:138:ILE:HD11	2:J:204:ILE:HD13	2.03	0.41
1:A:68:CYS:HB3	1:A:69:GLU:H	1.65	0.41
2:L:301:ALA:HA	2:L:306:THR:HG22	2.01	0.41
2:F:130:VAL:HG11	2:F:136:PHE:HB2	2.03	0.41
2:F:161:LEU:HD13	2:F:171:ILE:HD11	2.03	0.41
2:H:228:GLU:HG3	2:H:231:LYS:HG3	2.03	0.41
2:D:40:HIS:CD2	2:D:81:CYS:HA	2.56	0.40
2:F:57:TYR:HB2	2:F:97:PHE:HD1	1.85	0.40
2:F:254:GLU:HB2	12:F:821:SO4:O4	2.21	0.40
1:I:24:GLN:HA	1:I:44:ARG:HH21	1.85	0.40
1:G:106:VAL:HG13	1:G:112:LYS:O	2.21	0.40
2:H:75:ARG:NH2	2:H:92:ASP:OD2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:173:LYS:HE2	2:F:174:ASN:O	2.22	0.40
1:G:41:ASN:OD1	2:H:26:PRO:HD2	2.19	0.40
1:I:23:ASP:OD1	1:I:27:ARG:HB2	2.22	0.40
2:J:173:LYS:HE2	2:J:174:ASN:O	2.21	0.40
2:L:156:LYS:HB2	2:L:161:LEU:HD11	2.02	0.40
2:L:247:ILE:HG23	2:L:280:LYS:HG3	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	154/157 (98%)	145 (94%)	9 (6%)	0	100	100
1	C	154/157 (98%)	145 (94%)	8 (5%)	1 (1%)	25	59
1	E	156/157 (99%)	148 (95%)	8 (5%)	0	100	100
1	G	154/157 (98%)	144 (94%)	10 (6%)	0	100	100
1	I	154/157 (98%)	143 (93%)	11 (7%)	0	100	100
1	K	154/157 (98%)	143 (93%)	11 (7%)	0	100	100
2	B	291/312 (93%)	278 (96%)	10 (3%)	3 (1%)	15	49
2	D	284/312 (91%)	274 (96%)	9 (3%)	1 (0%)	34	69
2	F	283/312 (91%)	266 (94%)	13 (5%)	4 (1%)	11	40
2	H	284/312 (91%)	270 (95%)	12 (4%)	2 (1%)	22	57
2	J	264/312 (85%)	240 (91%)	21 (8%)	3 (1%)	14	46
2	L	247/312 (79%)	237 (96%)	6 (2%)	4 (2%)	9	37
All	All	2579/2814 (92%)	2433 (94%)	128 (5%)	18 (1%)	22	57

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	61	GLY
2	B	164	GLU
2	F	42	SER
1	C	142	ASP
2	F	20	GLU
2	H	164	GLU
2	J	75	ARG
2	L	192	ASN
2	D	254	GLU
2	F	164	GLU
2	L	42	SER
2	L	43	CYS
2	B	47	HIS
2	H	73	SER
2	L	194	LYS
2	F	63	GLN
2	J	80	ASP
2	J	122	GLU

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	141/148 (95%)	132 (94%)	9 (6%)	17 48
1	C	145/148 (98%)	139 (96%)	6 (4%)	30 64
1	E	142/148 (96%)	135 (95%)	7 (5%)	25 57
1	G	140/148 (95%)	133 (95%)	7 (5%)	24 57
1	I	124/148 (84%)	118 (95%)	6 (5%)	25 58
1	K	125/148 (84%)	116 (93%)	9 (7%)	14 44
2	B	259/288 (90%)	233 (90%)	26 (10%)	7 28
2	D	262/288 (91%)	242 (92%)	20 (8%)	13 41
2	F	253/288 (88%)	228 (90%)	25 (10%)	8 29
2	H	254/288 (88%)	234 (92%)	20 (8%)	12 40
2	J	212/288 (74%)	194 (92%)	18 (8%)	10 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	199/288 (69%)	181 (91%)	18 (9%)	9 34
All	All	2256/2616 (86%)	2085 (92%)	171 (8%)	13 41

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	MET
1	A	58	ARG
1	A	65	SER
1	A	68	CYS
1	A	80	ILE
1	A	131	ARG
1	A	137	ILE
1	A	143	GLU
1	A	156	GLU
2	B	28	ILE
2	B	30	VAL
2	B	38	LEU
2	B	43	CYS
2	B	60	SER
2	B	71	ARG
2	B	80	ASP
2	B	91	ASN
2	B	104	THR
2	B	128	LYS
2	B	137	GLN
2	B	146	GLN
2	B	147	THR
2	B	152	THR
2	B	163	LEU
2	B	164	GLU
2	B	166	ASN
2	B	184	SER
2	B	205	THR
2	B	225	VAL
2	B	240	LEU
2	B	243	GLU
2	B	253	GLU
2	B	280	LYS
2	B	299	THR
2	B	315	ARG
1	C	51	MET

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Mol	Chain	Res	Type
1	C	58	ARG
1	C	65	SER
1	C	69	GLU
1	C	80	ILE
1	C	137	ILE
2	D	22	CYS
2	D	28	ILE
2	D	30	VAL
2	D	55	SER
2	D	68	LEU
2	D	80	ASP
2	D	93	THR
2	D	104	THR
2	D	123	ARG
2	D	136	PHE
2	D	152	THR
2	D	164	GLU
2	D	184	SER
2	D	194	LYS
2	D	204	ILE
2	D	216	VAL
2	D	225	VAL
2	D	240	LEU
2	D	243	GLU
2	D	280	LYS
1	E	51	MET
1	E	58	ARG
1	E	68	CYS
1	E	80	ILE
1	E	137	ILE
1	E	154	GLN
1	E	156	GLU
2	F	21	SER
2	F	28	ILE
2	F	30	VAL
2	F	60	SER
2	F	75	ARG
2	F	97	PHE
2	F	102	ASN
2	F	104	THR
2	F	132	VAL
2	F	147	THR

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Mol	Chain	Res	Type
2	F	152	THR
2	F	164	GLU
2	F	184	SER
2	F	189	LEU
2	F	190	HIS
2	F	192	ASN
2	F	194	LYS
2	F	201	THR
2	F	204	ILE
2	F	225	VAL
2	F	240	LEU
2	F	243	GLU
2	F	280	LYS
2	F	299	THR
2	F	316	LYS
1	G	50	SER
1	G	51	MET
1	G	58	ARG
1	G	68	CYS
1	G	80	ILE
1	G	137	ILE
1	G	156	GLU
2	H	21	SER
2	H	22	CYS
2	H	28	ILE
2	H	30	VAL
2	H	75	ARG
2	H	80	ASP
2	H	91	ASN
2	H	147	THR
2	H	152	THR
2	H	184	SER
2	H	189	LEU
2	H	190	HIS
2	H	213	ILE
2	H	216	VAL
2	H	225	VAL
2	H	240	LEU
2	H	243	GLU
2	H	253	GLU
2	H	280	LYS
2	H	315	ARG

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Mol	Chain	Res	Type
1	I	23	ASP
1	I	27	ARG
1	I	51	MET
1	I	58	ARG
1	I	68	CYS
1	I	112	LYS
2	J	28	ILE
2	J	30	VAL
2	J	76	ILE
2	J	84	GLU
2	J	113	ARG
2	J	122	GLU
2	J	136	PHE
2	J	152	THR
2	J	163	LEU
2	J	204	ILE
2	J	213	ILE
2	J	216	VAL
2	J	225	VAL
2	J	240	LEU
2	J	243	GLU
2	J	253	GLU
2	J	280	LYS
2	J	299	THR
1	K	51	MET
1	K	58	ARG
1	K	68	CYS
1	K	91	ASN
1	K	94	ASP
1	K	105	SER
1	K	106	VAL
1	K	112	LYS
1	K	133	LEU
2	L	22	CYS
2	L	28	ILE
2	L	30	VAL
2	L	113	ARG
2	L	129	ILE
2	L	143	SER
2	L	146	GLN
2	L	147	THR
2	L	152	THR

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Mol	Chain	Res	Type
2	L	163	LEU
2	L	184	SER
2	L	204	ILE
2	L	213	ILE
2	L	216	VAL
2	L	240	LEU
2	L	254	GLU
2	L	280	LYS
2	L	299	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	40	HIS
2	B	124	GLN
2	B	137	GLN
2	B	286	ASN
1	C	114	GLN
2	D	124	GLN
2	D	190	HIS
2	D	223	ASN
1	E	154	GLN
2	F	190	HIS
2	F	192	ASN
2	H	79	HIS
2	H	124	GLN
1	I	114	GLN
1	I	154	GLN
1	K	41	ASN
2	L	223	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

88 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	M	1	3,2	14,14,15	0.32	0	17,19,21	0.71	1 (5%)
3	NAG	M	2	3	14,14,15	0.35	0	17,19,21	1.18	2 (11%)
3	FUC	M	3	3	10,10,11	0.46	0	14,14,16	0.78	1 (7%)
4	NAG	N	1	2,4	14,14,15	0.28	0	17,19,21	0.86	1 (5%)
4	NAG	N	2	4	14,14,15	0.27	0	17,19,21	1.05	2 (11%)
4	BMA	N	3	4	11,11,12	0.34	0	15,15,17	0.56	0
4	MAN	N	4	4	11,11,12	0.45	0	15,15,17	1.01	1 (6%)
4	MAN	N	5	4	11,11,12	0.37	0	15,15,17	0.84	1 (6%)
4	MAN	N	6	4	11,11,12	0.45	0	15,15,17	0.85	1 (6%)
5	NAG	O	1	5,2	14,14,15	0.27	0	17,19,21	0.77	1 (5%)
5	NAG	O	2	5	14,14,15	0.30	0	17,19,21	0.76	1 (5%)
6	NAG	P	1	6,2	14,14,15	0.34	0	17,19,21	0.74	0
6	NAG	P	2	6	14,14,15	0.32	0	17,19,21	1.34	2 (11%)
6	BMA	P	3	6	11,11,12	0.49	0	15,15,17	1.06	2 (13%)
3	NAG	Q	1	3,2	14,14,15	0.29	0	17,19,21	0.90	1 (5%)
3	NAG	Q	2	3	14,14,15	0.29	0	17,19,21	0.57	0
3	FUC	Q	3	3	10,10,11	0.43	0	14,14,16	0.59	0
7	NAG	R	1	7,2	14,14,15	0.31	0	17,19,21	0.72	1 (5%)
7	FUC	R	2	7	10,10,11	0.43	0	14,14,16	0.67	0
8	NAG	S	1	8,2	14,14,15	0.23	0	17,19,21	0.91	1 (5%)
8	NAG	S	2	8	14,14,15	0.25	0	17,19,21	1.05	2 (11%)
8	BMA	S	3	8	11,11,12	0.32	0	15,15,17	0.76	1 (6%)
8	MAN	S	4	8	11,11,12	0.40	0	15,15,17	0.86	1 (6%)
8	MAN	S	5	8	11,11,12	0.42	0	15,15,17	0.87	1 (6%)
6	NAG	T	1	6,2	14,14,15	0.28	0	17,19,21	0.76	1 (5%)
6	NAG	T	2	6	14,14,15	0.31	0	17,19,21	0.70	0
6	BMA	T	3	6	11,11,12	0.36	0	15,15,17	0.60	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	U	1	6,2	14,14,15	0.32	0	17,19,21	0.92	1 (5%)
6	NAG	U	2	6	14,14,15	0.29	0	17,19,21	1.46	2 (11%)
6	BMA	U	3	6	11,11,12	0.39	0	15,15,17	0.90	1 (6%)
9	NAG	V	1	2,9	14,14,15	0.32	0	17,19,21	1.03	1 (5%)
9	NAG	V	2	9	14,14,15	0.33	0	17,19,21	0.57	0
9	BMA	V	3	9	11,11,12	0.37	0	15,15,17	0.72	1 (6%)
9	FUC	V	4	9	10,10,11	0.43	0	14,14,16	0.52	0
4	NAG	W	1	2,4	14,14,15	0.26	0	17,19,21	0.86	1 (5%)
4	NAG	W	2	4	14,14,15	0.28	0	17,19,21	1.06	2 (11%)
4	BMA	W	3	4	11,11,12	0.33	0	15,15,17	0.83	1 (6%)
4	MAN	W	4	4	11,11,12	0.32	0	15,15,17	0.87	1 (6%)
4	MAN	W	5	4	11,11,12	0.41	0	15,15,17	0.84	1 (6%)
4	MAN	W	6	4	11,11,12	0.51	0	15,15,17	1.21	1 (6%)
6	NAG	X	1	6,2	14,14,15	0.22	0	17,19,21	0.73	1 (5%)
6	NAG	X	2	6	14,14,15	0.28	0	17,19,21	0.69	0
6	BMA	X	3	6	11,11,12	0.32	0	15,15,17	0.48	0
10	NAG	Y	1	2,10	14,14,15	0.31	0	17,19,21	0.95	1 (5%)
10	NAG	Y	2	10	14,14,15	0.28	0	17,19,21	1.13	2 (11%)
10	BMA	Y	3	10	11,11,12	0.40	0	15,15,17	0.83	1 (6%)
10	MAN	Y	4	10	11,11,12	0.38	0	15,15,17	0.95	1 (6%)
11	NAG	Z	1	11,2	14,14,15	0.29	0	17,19,21	1.02	1 (5%)
11	NAG	Z	2	11	14,14,15	0.33	0	17,19,21	0.55	0
11	BMA	Z	3	11	11,11,12	0.42	0	15,15,17	0.77	1 (6%)
11	MAN	Z	4	11	11,11,12	0.51	0	15,15,17	0.78	0
11	FUC	Z	5	11	10,10,11	0.38	0	14,14,16	0.57	0
8	NAG	a	1	8,2	14,14,15	0.27	0	17,19,21	0.86	1 (5%)
8	NAG	a	2	8	14,14,15	0.25	0	17,19,21	1.03	2 (11%)
8	BMA	a	3	8	11,11,12	0.28	0	15,15,17	0.95	1 (6%)
8	MAN	a	4	8	11,11,12	0.42	0	15,15,17	0.87	1 (6%)
8	MAN	a	5	8	11,11,12	0.41	0	15,15,17	0.92	1 (6%)
5	NAG	b	1	5,2	14,14,15	0.27	0	17,19,21	0.66	0
5	NAG	b	2	5	14,14,15	0.30	0	17,19,21	0.72	1 (5%)
6	NAG	c	1	6,2	14,14,15	0.36	0	17,19,21	0.86	0
6	NAG	c	2	6	14,14,15	0.35	0	17,19,21	1.33	1 (5%)
6	BMA	c	3	6	11,11,12	0.47	0	15,15,17	0.77	0
9	NAG	d	1	2,9	14,14,15	0.32	0	17,19,21	1.05	1 (5%)
9	NAG	d	2	9	14,14,15	0.31	0	17,19,21	0.67	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BMA	d	3	9	11,11,12	0.47	0	15,15,17	0.90	1 (6%)
9	FUC	d	4	9	10,10,11	0.40	0	14,14,16	0.55	0
6	NAG	e	1	6,2	14,14,15	0.27	0	17,19,21	0.77	1 (5%)
6	NAG	e	2	6	14,14,15	0.32	0	17,19,21	2.01	4 (23%)
6	BMA	e	3	6	11,11,12	0.32	0	15,15,17	0.77	1 (6%)
6	NAG	f	1	6,2	14,14,15	0.27	0	17,19,21	0.54	0
6	NAG	f	2	6	14,14,15	0.29	0	17,19,21	0.72	0
6	BMA	f	3	6	11,11,12	0.35	0	15,15,17	0.53	0
5	NAG	g	1	5,2	14,14,15	0.32	0	17,19,21	0.86	1 (5%)
5	NAG	g	2	5	14,14,15	0.29	0	17,19,21	1.28	2 (11%)
3	NAG	h	1	3,2	14,14,15	0.29	0	17,19,21	0.99	2 (11%)
3	NAG	h	2	3	14,14,15	0.31	0	17,19,21	0.55	0
3	FUC	h	3	3	10,10,11	0.41	0	14,14,16	0.54	0
6	NAG	i	1	6,2	14,14,15	0.27	0	17,19,21	0.79	1 (5%)
6	NAG	i	2	6	14,14,15	0.26	0	17,19,21	1.07	2 (11%)
6	BMA	i	3	6	11,11,12	0.33	0	15,15,17	0.51	0
5	NAG	j	1	5,2	14,14,15	0.30	0	17,19,21	0.79	1 (5%)
5	NAG	j	2	5	14,14,15	0.29	0	17,19,21	0.61	0
5	NAG	k	1	5,2	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
5	NAG	k	2	5	14,14,15	0.30	0	17,19,21	0.97	1 (5%)
9	NAG	l	1	2,9	14,14,15	0.31	0	17,19,21	0.94	1 (5%)
9	NAG	l	2	9	14,14,15	0.35	0	17,19,21	0.66	0
9	BMA	l	3	9	11,11,12	0.36	0	15,15,17	0.57	0
9	FUC	l	4	9	10,10,11	0.38	0	14,14,16	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	FUC	M	3	3	-	-	0/1/1/1
4	NAG	N	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	1/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1
4	MAN	N	4	4	-	1/2/19/22	0/1/1/1
4	MAN	N	5	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	N	6	4	-	0/2/19/22	0/1/1/1
5	NAG	O	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
6	NAG	P	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	1/6/23/26	0/1/1/1
6	BMA	P	3	6	-	2/2/19/22	0/1/1/1
3	NAG	Q	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	FUC	Q	3	3	-	-	0/1/1/1
7	NAG	R	1	7,2	-	0/6/23/26	0/1/1/1
7	FUC	R	2	7	-	-	0/1/1/1
8	NAG	S	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	S	2	8	-	1/6/23/26	0/1/1/1
8	BMA	S	3	8	-	2/2/19/22	0/1/1/1
8	MAN	S	4	8	-	0/2/19/22	0/1/1/1
8	MAN	S	5	8	-	1/2/19/22	1/1/1/1
6	NAG	T	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	BMA	T	3	6	-	0/2/19/22	0/1/1/1
6	NAG	U	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	1/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
9	NAG	V	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	2/6/23/26	0/1/1/1
9	BMA	V	3	9	-	0/2/19/22	0/1/1/1
9	FUC	V	4	9	-	-	0/1/1/1
4	NAG	W	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	1/6/23/26	0/1/1/1
4	BMA	W	3	4	-	0/2/19/22	0/1/1/1
4	MAN	W	4	4	-	2/2/19/22	0/1/1/1
4	MAN	W	5	4	-	0/2/19/22	0/1/1/1
4	MAN	W	6	4	-	0/2/19/22	1/1/1/1
6	NAG	X	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	0/6/23/26	0/1/1/1
6	BMA	X	3	6	-	0/2/19/22	0/1/1/1
10	NAG	Y	1	2,10	-	1/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	0/6/23/26	0/1/1/1
10	BMA	Y	3	10	-	2/2/19/22	0/1/1/1
10	MAN	Y	4	10	-	2/2/19/22	0/1/1/1
11	NAG	Z	1	11,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	Z	2	11	-	2/6/23/26	0/1/1/1
11	BMA	Z	3	11	-	0/2/19/22	0/1/1/1
11	MAN	Z	4	11	-	0/2/19/22	0/1/1/1
11	FUC	Z	5	11	-	-	0/1/1/1
8	NAG	a	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	1/6/23/26	0/1/1/1
8	BMA	a	3	8	-	2/2/19/22	0/1/1/1
8	MAN	a	4	8	-	0/2/19/22	0/1/1/1
8	MAN	a	5	8	-	0/2/19/22	0/1/1/1
5	NAG	b	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
6	NAG	c	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	c	2	6	-	1/6/23/26	0/1/1/1
6	BMA	c	3	6	-	0/2/19/22	0/1/1/1
9	NAG	d	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	d	2	9	-	2/6/23/26	0/1/1/1
9	BMA	d	3	9	-	0/2/19/22	0/1/1/1
9	FUC	d	4	9	-	-	0/1/1/1
6	NAG	e	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	e	2	6	-	2/6/23/26	0/1/1/1
6	BMA	e	3	6	-	0/2/19/22	0/1/1/1
6	NAG	f	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	f	2	6	-	0/6/23/26	0/1/1/1
6	BMA	f	3	6	-	2/2/19/22	0/1/1/1
5	NAG	g	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	g	2	5	-	0/6/23/26	0/1/1/1
3	NAG	h	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	FUC	h	3	3	-	-	0/1/1/1
6	NAG	i	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	i	2	6	-	0/6/23/26	0/1/1/1
6	BMA	i	3	6	-	0/2/19/22	0/1/1/1
5	NAG	j	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	j	2	5	-	0/6/23/26	0/1/1/1
5	NAG	k	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	k	2	5	-	0/6/23/26	0/1/1/1
9	NAG	l	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	l	2	9	-	2/6/23/26	0/1/1/1
9	BMA	l	3	9	-	0/2/19/22	0/1/1/1
9	FUC	l	4	9	-	-	0/1/1/1

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	e	2	NAG	C1-C2-N2	6.02	119.92	110.43
6	P	2	NAG	O5-C1-C2	-4.51	104.31	111.29
5	g	2	NAG	O5-C1-C2	-4.39	104.50	111.29
4	W	6	MAN	C1-O5-C5	4.38	118.06	112.19
6	c	2	NAG	O5-C1-C2	-4.37	104.53	111.29
6	e	2	NAG	O5-C1-C2	-4.09	104.96	111.29
6	U	2	NAG	O5-C1-C2	-3.98	105.13	111.29
10	Y	2	NAG	O5-C1-C2	-3.55	105.79	111.29
6	U	2	NAG	C1-O5-C5	3.53	116.92	112.19
6	i	2	NAG	O5-C1-C2	-3.35	106.11	111.29
3	M	2	NAG	O5-C1-C2	3.34	116.45	111.29
8	S	1	NAG	C1-O5-C5	3.27	116.57	112.19
8	S	2	NAG	C1-O5-C5	3.19	116.46	112.19
8	a	5	MAN	C1-O5-C5	3.11	116.35	112.19
4	N	2	NAG	C1-O5-C5	3.09	116.33	112.19
4	N	4	MAN	C1-O5-C5	3.07	116.31	112.19
5	k	2	NAG	O5-C1-C2	-3.05	106.57	111.29
8	a	1	NAG	C1-O5-C5	3.04	116.26	112.19
8	a	3	BMA	O3-C3-C4	3.02	117.51	110.38
6	e	2	NAG	C2-N2-C7	3.01	126.94	122.90
4	W	1	NAG	C1-O5-C5	3.01	116.22	112.19
6	P	3	BMA	C1-O5-C5	3.01	116.22	112.19
4	W	4	MAN	C1-O5-C5	3.00	116.21	112.19
4	N	1	NAG	C1-O5-C5	3.00	116.20	112.19
8	S	5	MAN	C1-O5-C5	2.95	116.15	112.19
9	d	1	NAG	C1-C2-N2	-2.95	105.78	110.43
4	W	2	NAG	O5-C1-C2	-2.95	106.73	111.29
8	a	2	NAG	O5-C1-C2	-2.91	106.79	111.29
10	Y	4	MAN	C1-O5-C5	2.86	116.02	112.19
6	U	1	NAG	O5-C1-C2	-2.84	106.90	111.29
9	V	1	NAG	C1-C2-N2	-2.83	105.97	110.43
4	W	2	NAG	C1-O5-C5	2.82	115.97	112.19
6	e	3	BMA	C1-O5-C5	2.70	115.80	112.19
6	T	1	NAG	C1-O5-C5	2.67	115.77	112.19
6	U	3	BMA	C1-O5-C5	2.67	115.76	112.19
8	a	2	NAG	C1-O5-C5	2.67	115.76	112.19
4	N	2	NAG	O5-C1-C2	-2.60	107.27	111.29
6	i	1	NAG	C1-O5-C5	2.59	115.66	112.19
3	M	2	NAG	C1-O5-C5	2.59	115.66	112.19
4	N	5	MAN	C1-O5-C5	2.58	115.65	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	k	1	NAG	O5-C1-C2	-2.52	107.39	111.29
11	Z	1	NAG	C1-C2-N2	-2.51	106.47	110.43
8	S	2	NAG	O5-C1-C2	-2.50	107.42	111.29
9	l	1	NAG	C1-C2-N2	-2.50	106.50	110.43
4	W	5	MAN	C1-O5-C5	2.50	115.53	112.19
8	S	4	MAN	C1-O5-C5	2.49	115.52	112.19
5	j	1	NAG	C1-O5-C5	2.47	115.50	112.19
7	R	1	NAG	C1-O5-C5	2.45	115.47	112.19
4	W	3	BMA	C1-O5-C5	2.45	115.46	112.19
5	O	1	NAG	C1-O5-C5	2.43	115.45	112.19
5	g	2	NAG	C1-O5-C5	2.39	115.39	112.19
6	P	2	NAG	C1-O5-C5	2.36	115.36	112.19
6	e	1	NAG	C1-O5-C5	2.36	115.35	112.19
3	M	1	NAG	C1-O5-C5	2.32	115.30	112.19
6	i	2	NAG	C1-O5-C5	2.31	115.28	112.19
5	O	2	NAG	C1-O5-C5	2.30	115.27	112.19
9	d	3	BMA	C1-C2-C3	2.30	112.99	109.64
11	Z	3	BMA	C1-O5-C5	2.28	115.24	112.19
10	Y	3	BMA	C1-O5-C5	2.26	115.21	112.19
3	M	3	FUC	C1-O5-C5	2.25	118.27	112.97
10	Y	2	NAG	C1-O5-C5	2.25	115.20	112.19
6	e	2	NAG	C1-O5-C5	2.23	115.17	112.19
8	a	4	MAN	C1-O5-C5	2.22	115.17	112.19
6	X	1	NAG	C1-O5-C5	2.19	115.12	112.19
5	b	2	NAG	O5-C1-C2	-2.19	107.91	111.29
8	S	3	BMA	O3-C3-C4	2.16	115.46	110.38
3	h	1	NAG	O5-C1-C2	2.14	114.60	111.29
3	Q	1	NAG	O5-C1-C2	2.11	114.56	111.29
4	N	6	MAN	C1-C2-C3	2.09	112.68	109.64
10	Y	1	NAG	O4-C4-C3	-2.08	105.47	110.38
9	V	3	BMA	C1-O5-C5	2.04	114.92	112.19
6	P	3	BMA	C1-C2-C3	2.04	112.61	109.64
3	h	1	NAG	C1-C2-N2	-2.03	107.23	110.43
9	d	2	NAG	C1-O5-C5	2.02	114.89	112.19
5	g	1	NAG	O5-C1-C2	-2.02	108.17	111.29
6	T	3	BMA	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	e	2	NAG	C1-C2-N2-C7

Continued on next page...

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Mol	Chain	Res	Type	Atoms
4	W	4	MAN	O5-C5-C6-O6
6	f	3	BMA	C4-C5-C6-O6
4	W	4	MAN	C4-C5-C6-O6
6	f	3	BMA	O5-C5-C6-O6
6	P	3	BMA	O5-C5-C6-O6
8	a	3	BMA	C4-C5-C6-O6
4	N	3	BMA	C4-C5-C6-O6
8	a	3	BMA	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
8	S	3	BMA	C4-C5-C6-O6
10	Y	4	MAN	O5-C5-C6-O6
8	S	3	BMA	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
4	N	4	MAN	O5-C5-C6-O6
8	S	5	MAN	O5-C5-C6-O6
11	Z	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
6	P	3	BMA	C4-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
6	c	2	NAG	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
9	V	2	NAG	C4-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
8	S	2	NAG	O5-C5-C6-O6
11	Z	2	NAG	O5-C5-C6-O6
9	l	2	NAG	C4-C5-C6-O6
9	d	2	NAG	C4-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
10	Y	3	BMA	C4-C5-C6-O6
10	Y	1	NAG	C4-C5-C6-O6
9	l	2	NAG	O5-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
3	M	2	NAG	C1-C2-N2-C7
6	e	2	NAG	O5-C5-C6-O6
8	a	2	NAG	O5-C5-C6-O6
6	U	3	BMA	C4-C5-C6-O6
10	Y	3	BMA	O5-C5-C6-O6
10	Y	4	MAN	C4-C5-C6-O6

All (2) ring outliers are listed below:

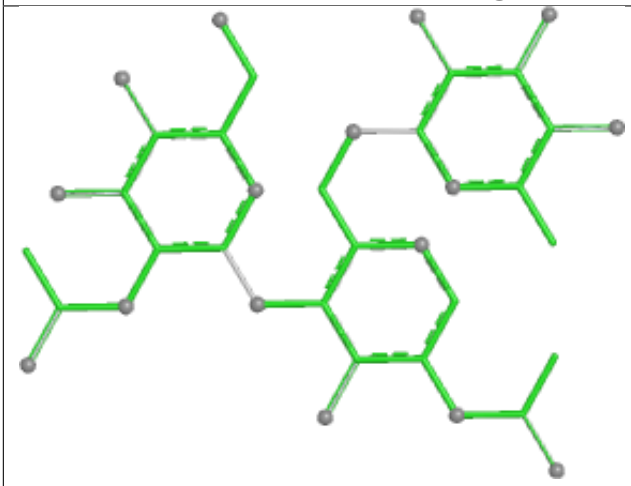
Mol	Chain	Res	Type	Atoms
8	S	5	MAN	C1-C2-C3-C4-C5-O5
4	W	6	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 6 short contacts:

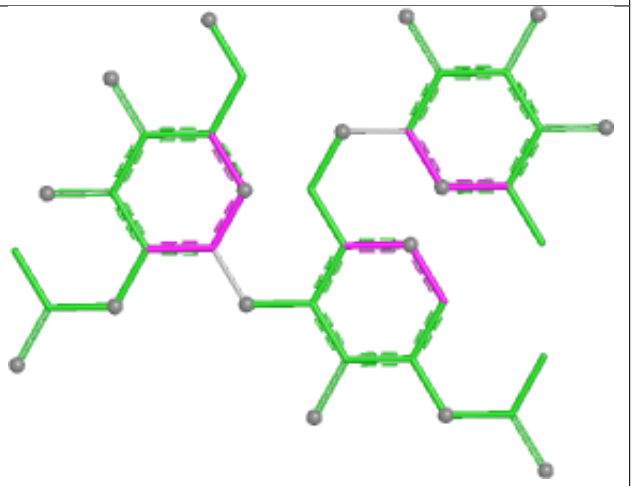
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	W	5	MAN	1	0
7	R	2	FUC	1	0
4	W	3	BMA	1	0
4	W	6	MAN	1	0
11	Z	2	NAG	1	0
4	N	1	NAG	1	0
4	W	1	NAG	1	0

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

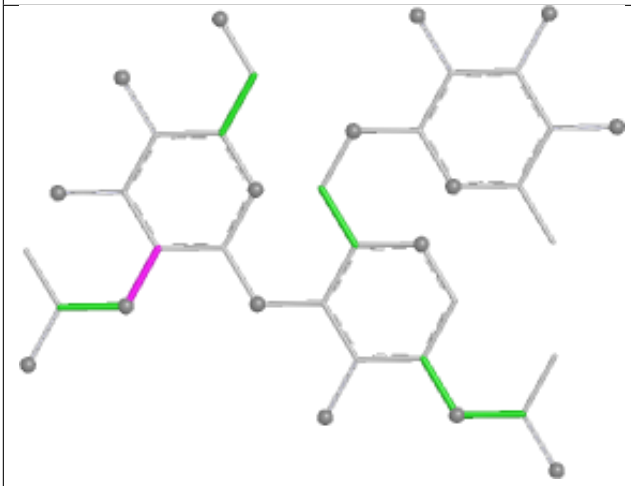
Oligosaccharide Chain M



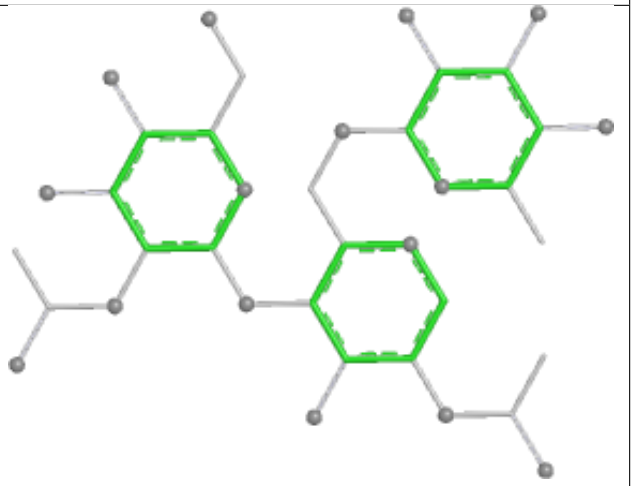
Bond lengths



Bond angles

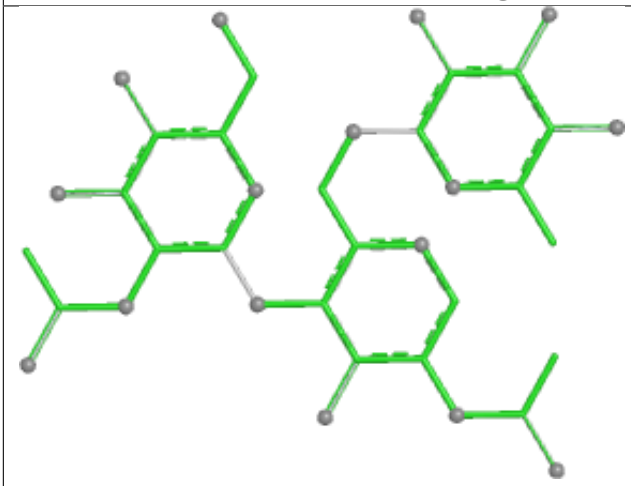


Torsions

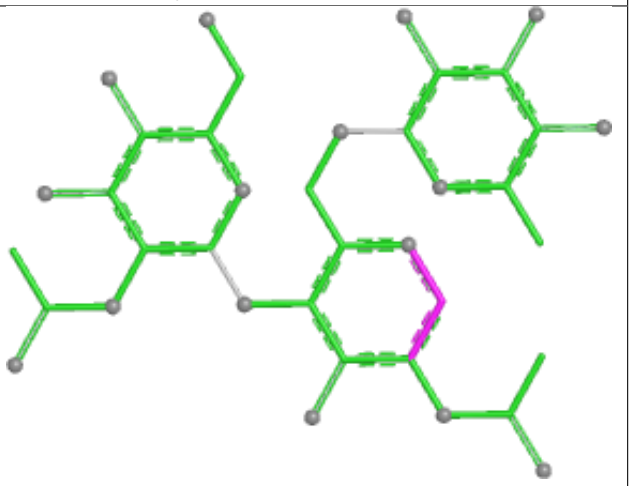


Rings

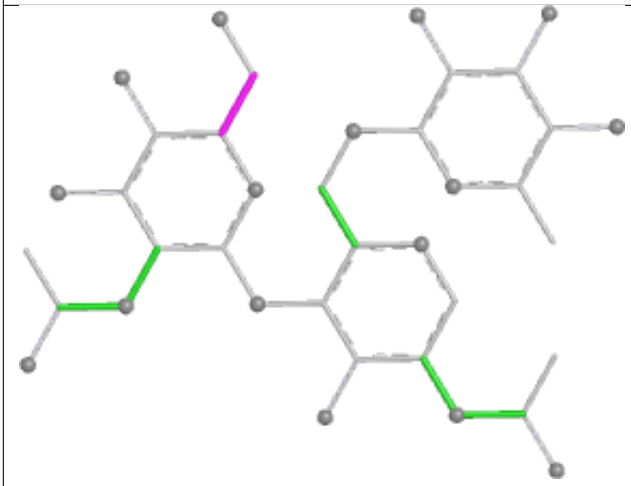
Oligosaccharide Chain Q



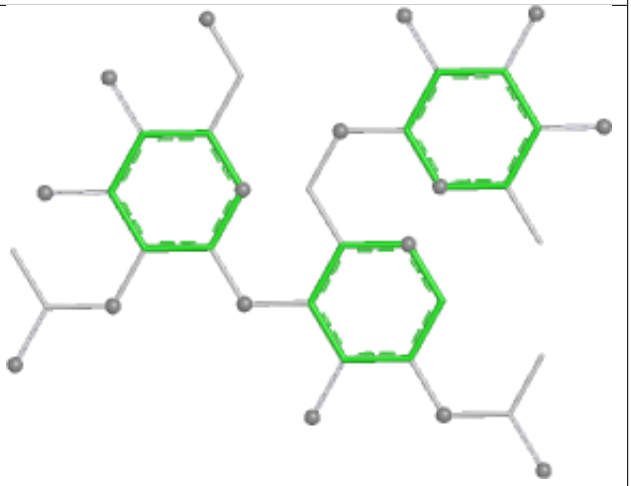
Bond lengths



Bond angles

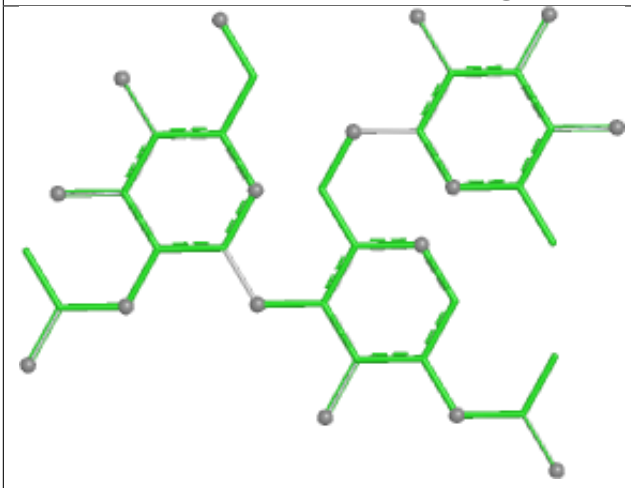


Torsions

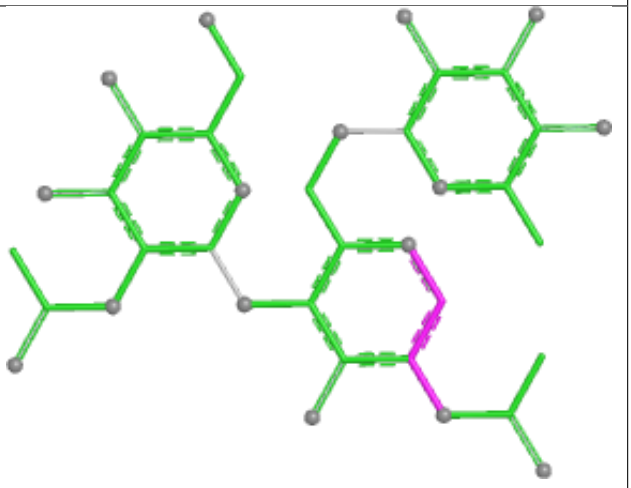


Rings

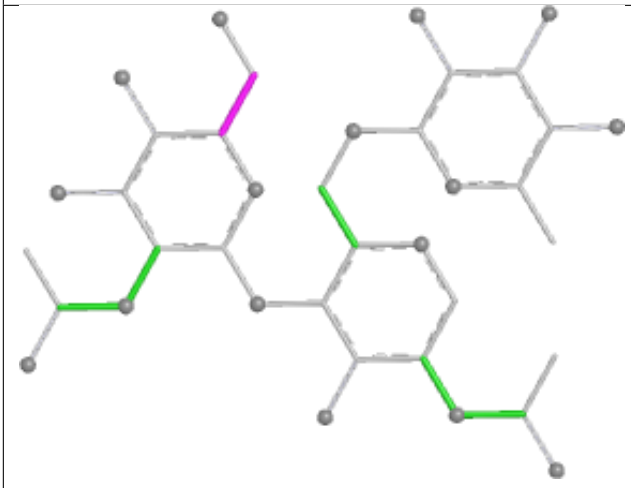
Oligosaccharide Chain h



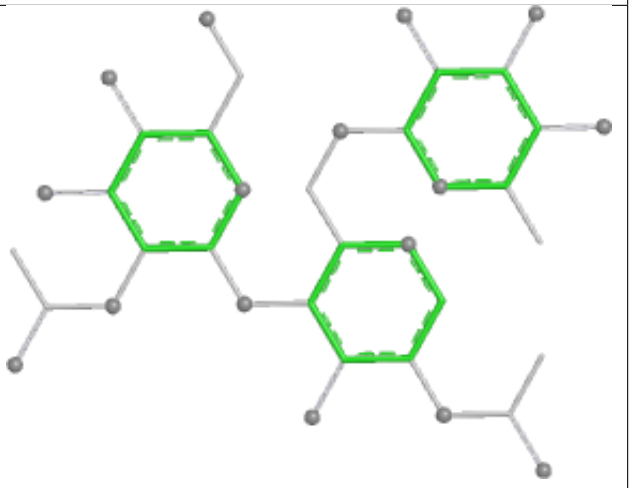
Bond lengths



Bond angles

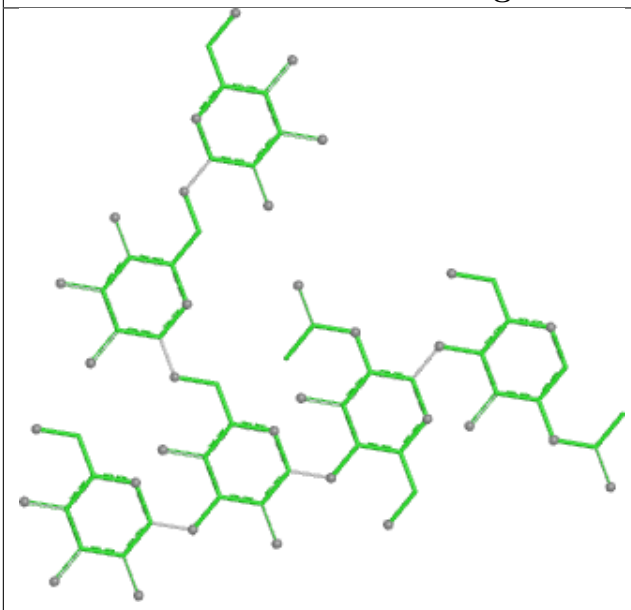


Torsions

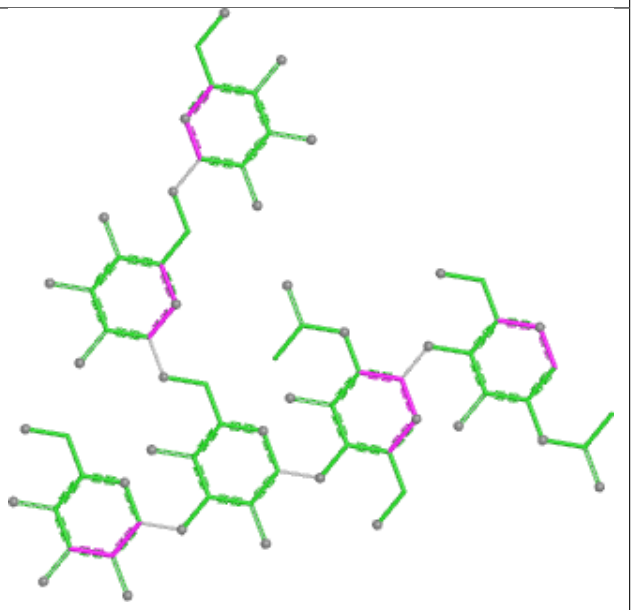


Rings

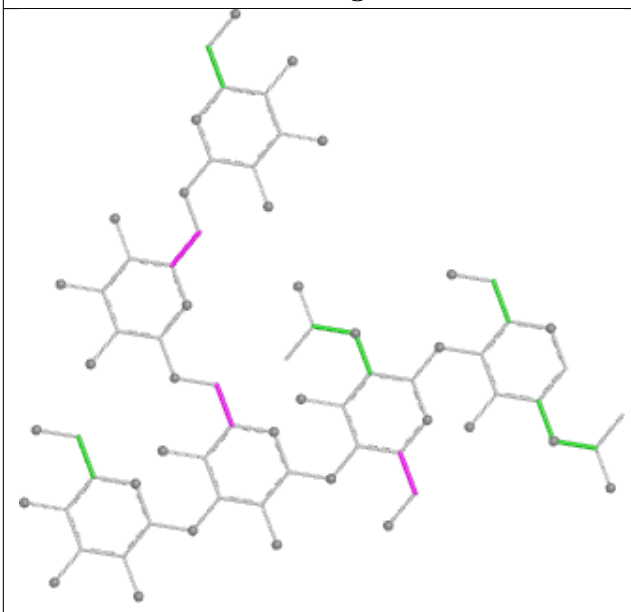
Oligosaccharide Chain N



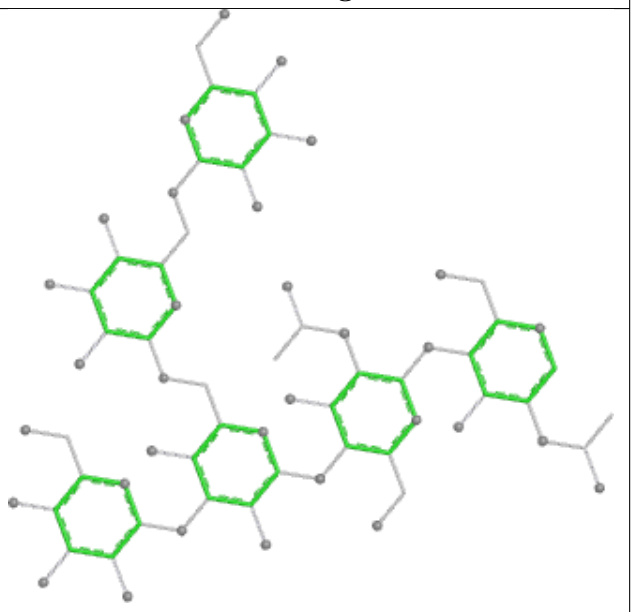
Bond lengths



Bond angles

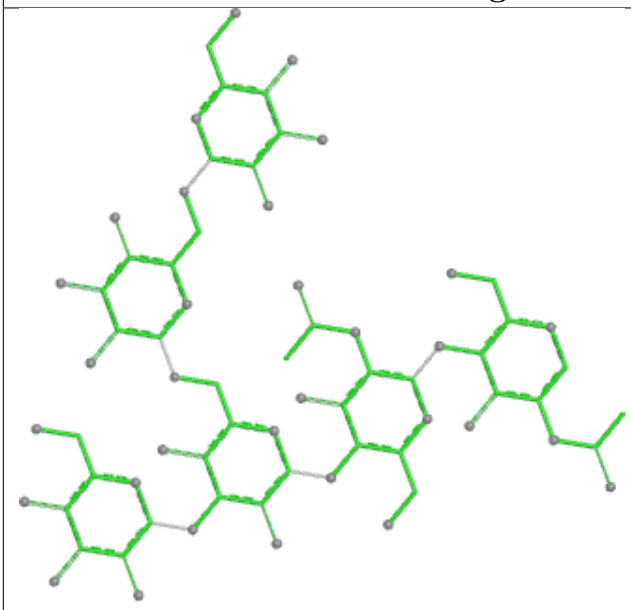


Torsions

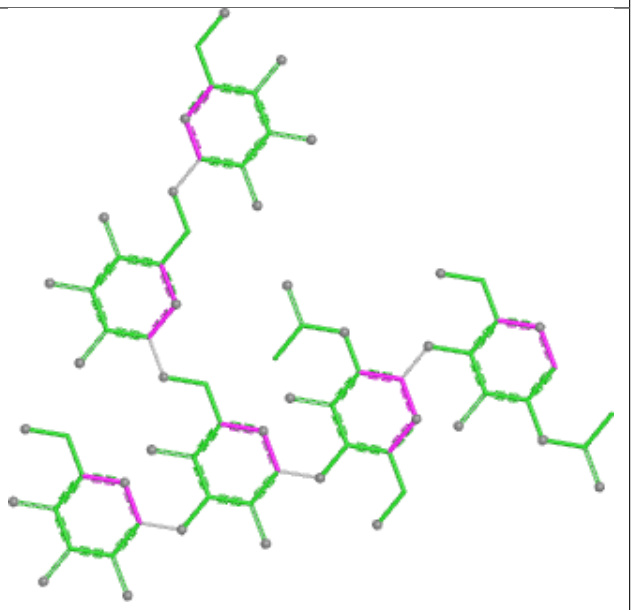


Rings

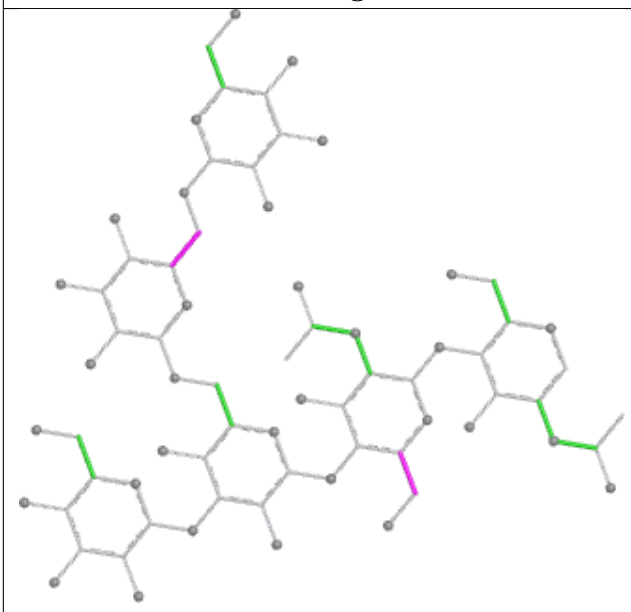
Oligosaccharide Chain W



Bond lengths



Bond angles



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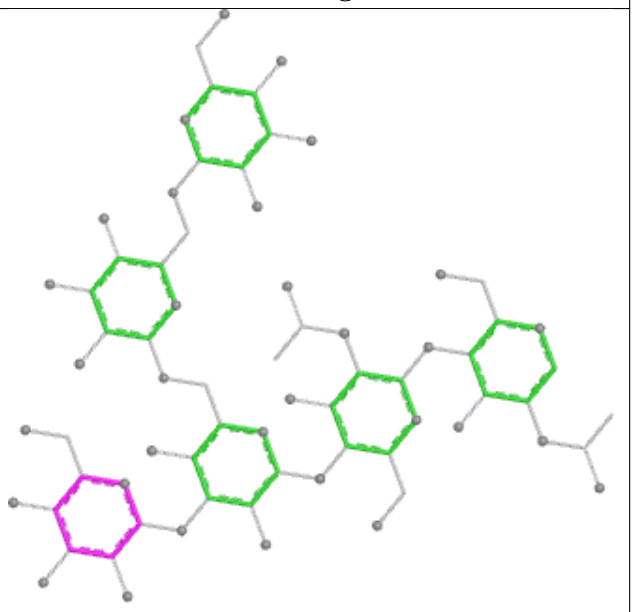
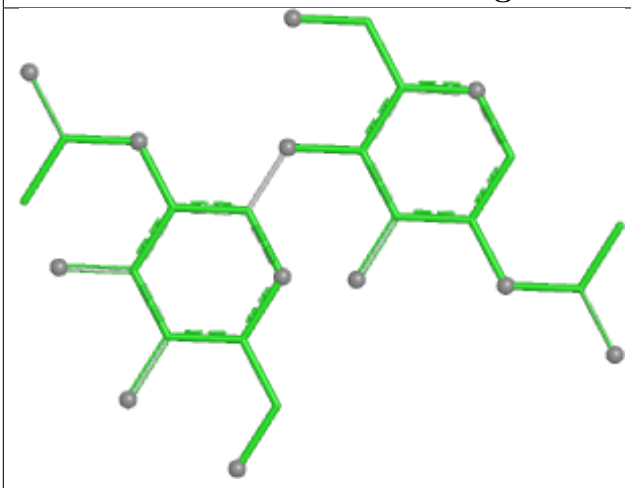
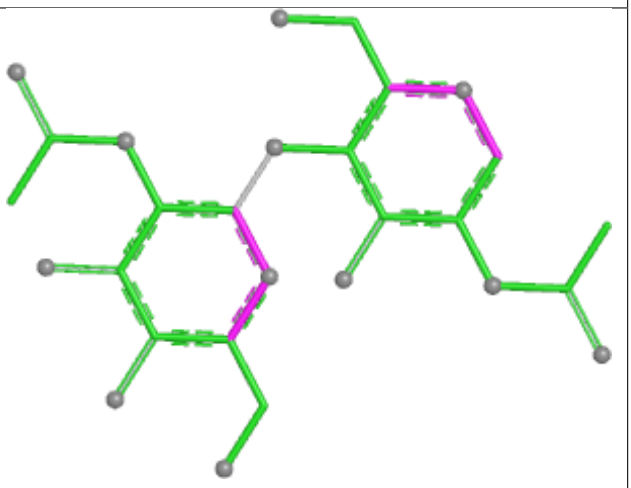


Rings

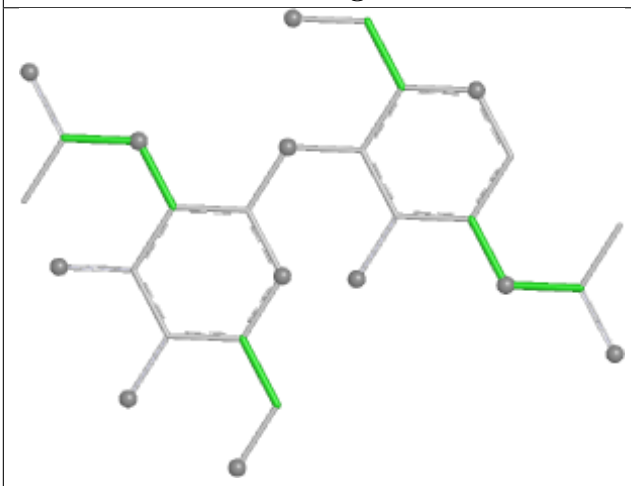
Oligosaccharide Chain O



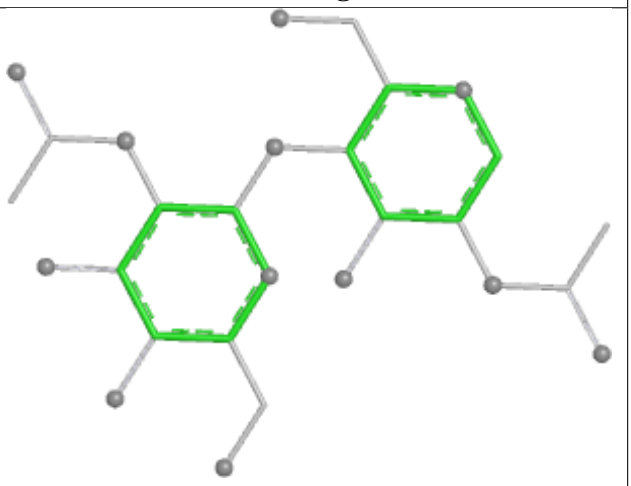
Bond lengths



Bond angles

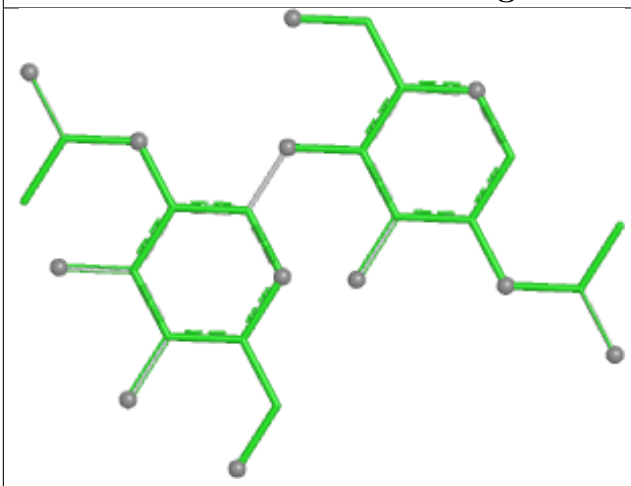


Torsions

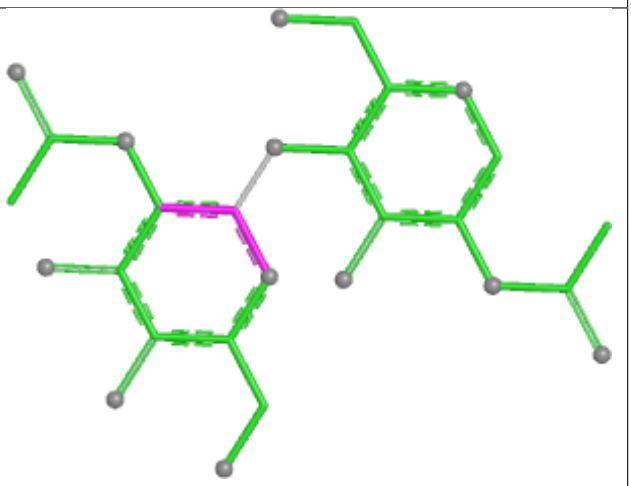


Rings

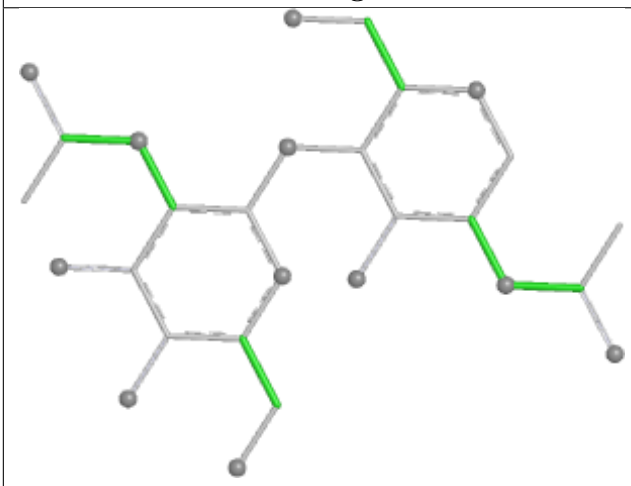
Oligosaccharide Chain b



Bond lengths



Bond angles



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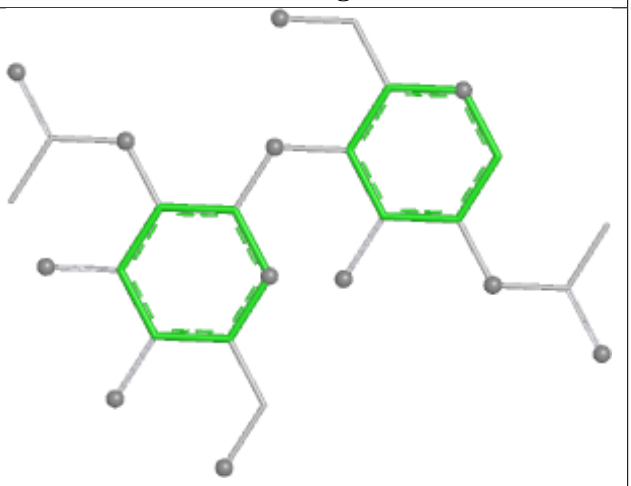
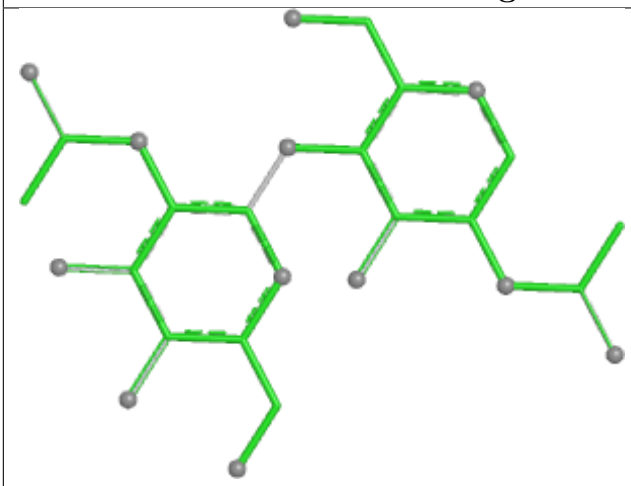
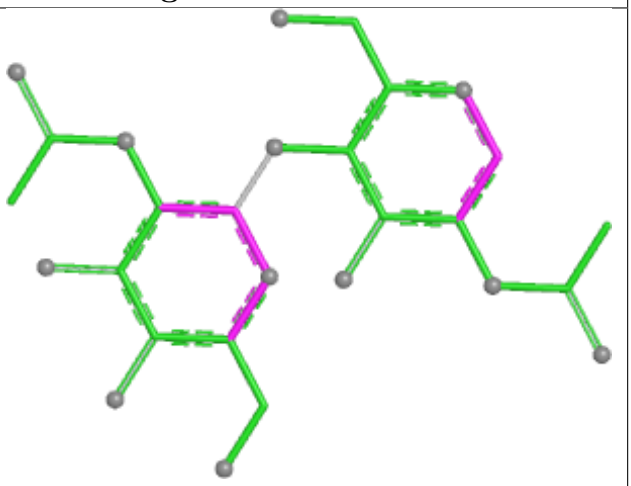


Rings

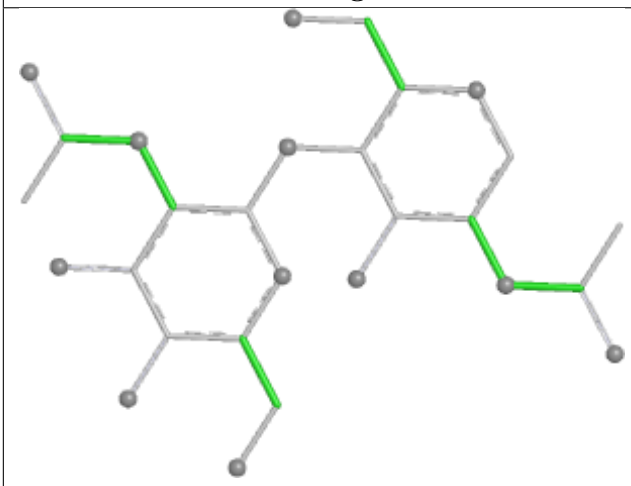
Oligosaccharide Chain g



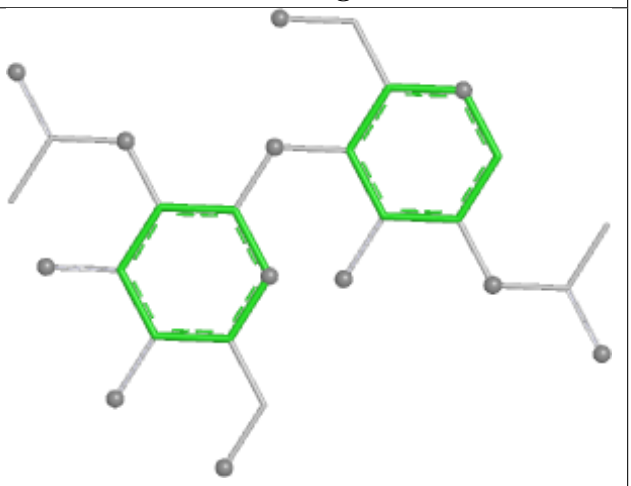
Bond lengths



Bond angles

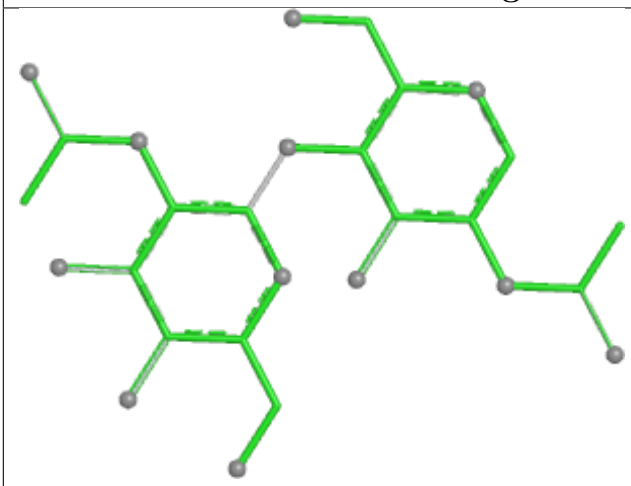


Torsions

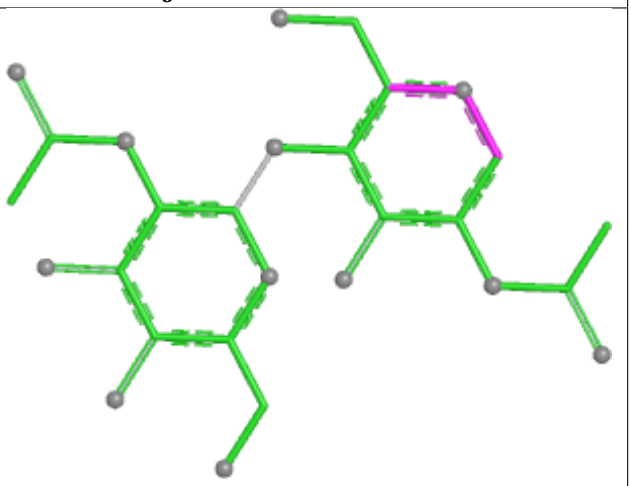


Rings

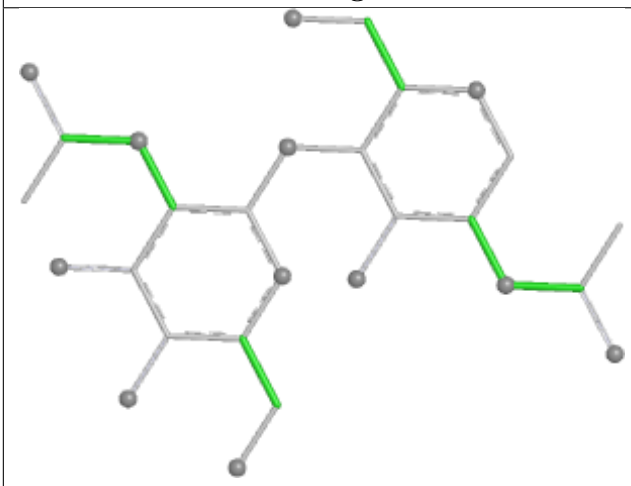
Oligosaccharide Chain j



Bond lengths



Bond angles



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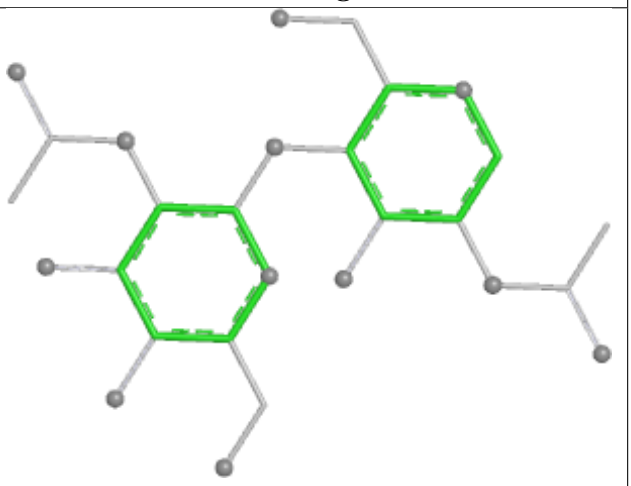
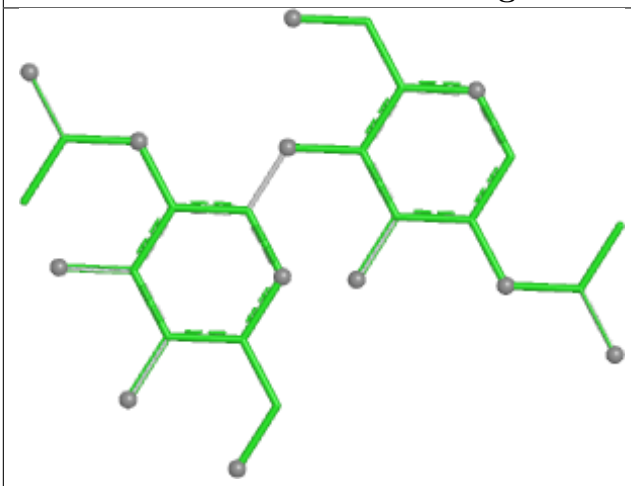
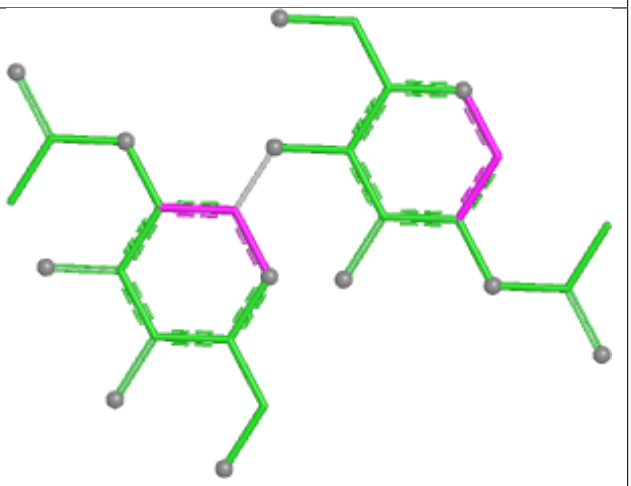


Rings

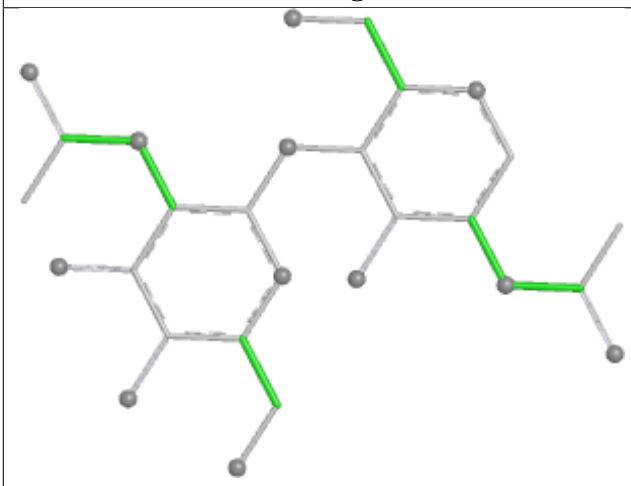
Oligosaccharide Chain k



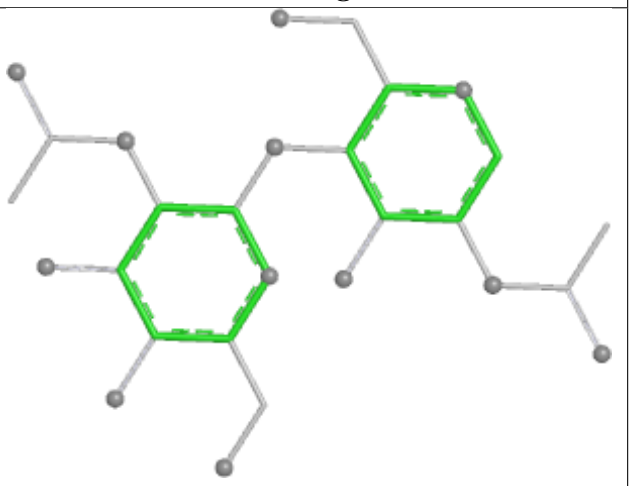
Bond lengths



Bond angles

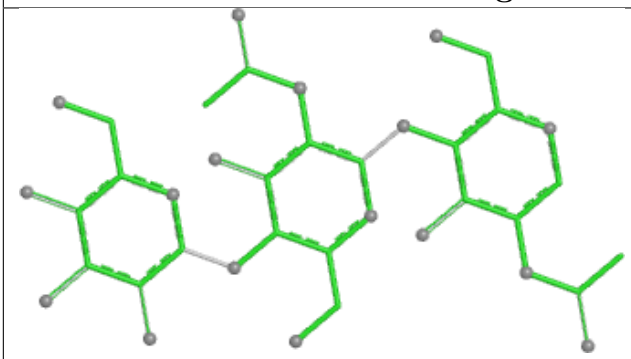


Torsions

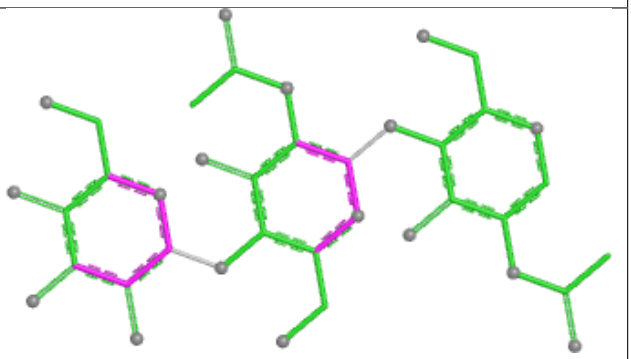


Rings

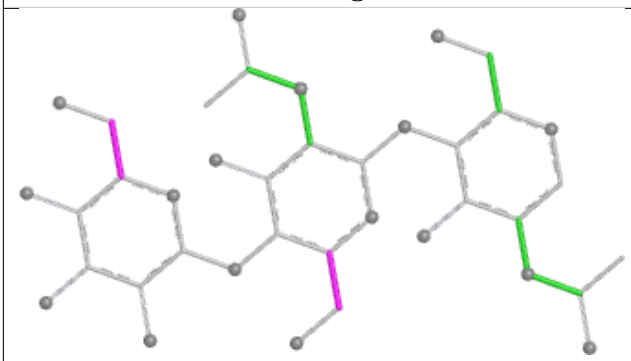
Oligosaccharide Chain P



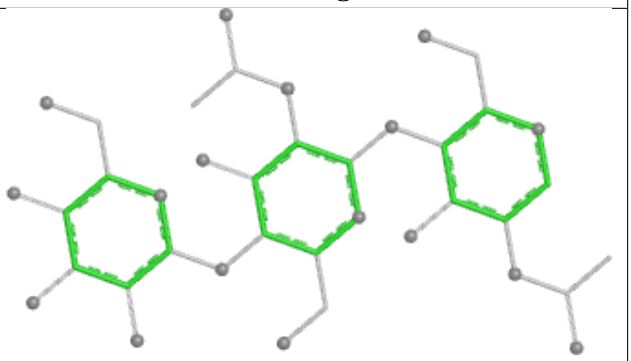
Bond lengths



Bond angles

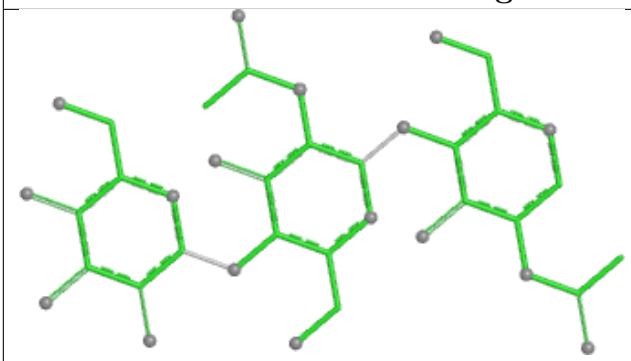


Torsions

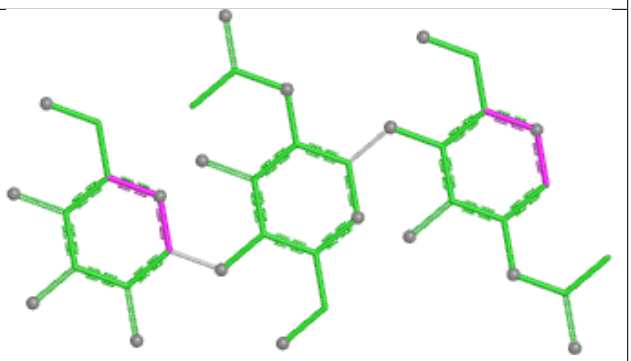


Rings

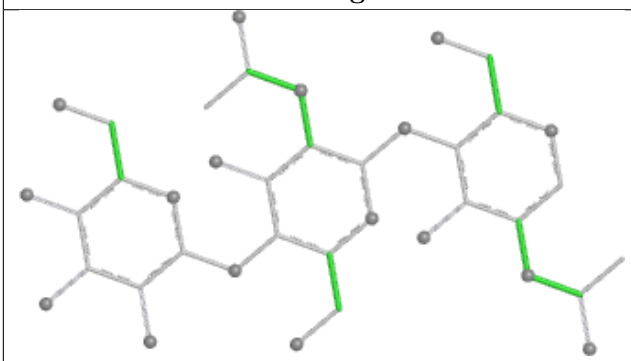
Oligosaccharide Chain T



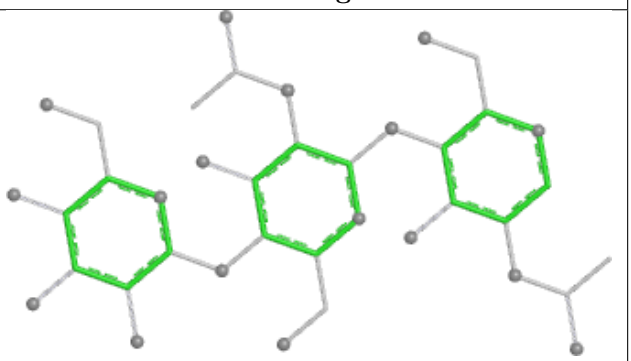
Bond lengths



Bond angles

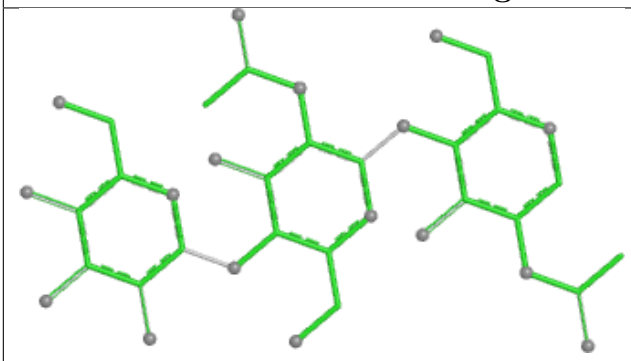


Torsions

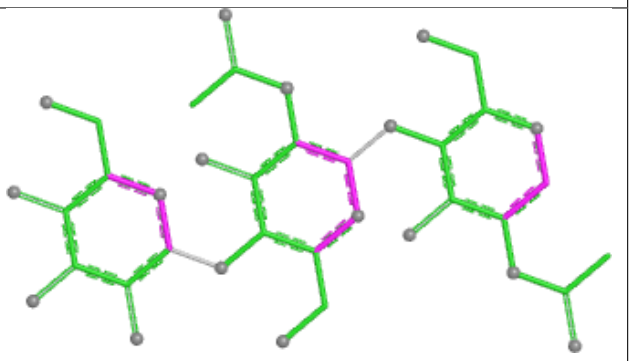


Rings

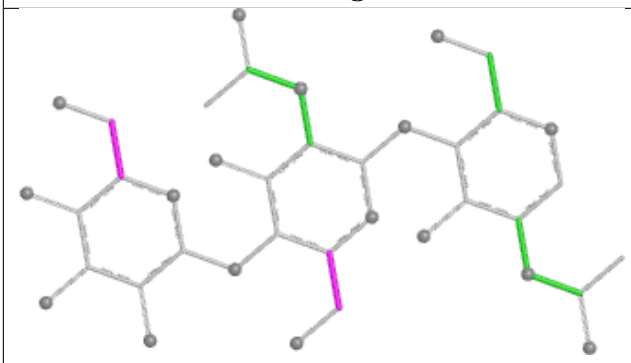
Oligosaccharide Chain U



Bond lengths



Bond angles



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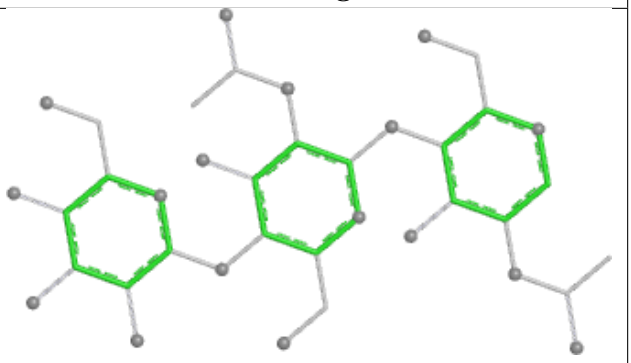
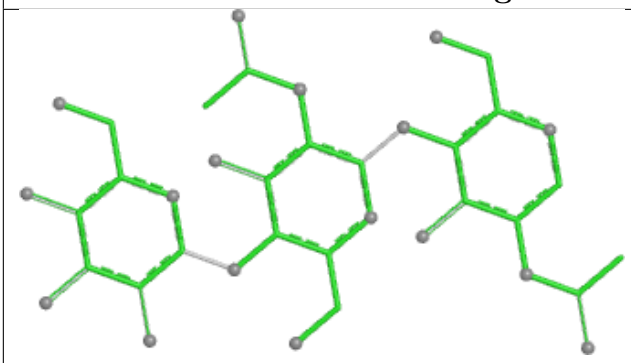


Rings

Oligosaccharide Chain X



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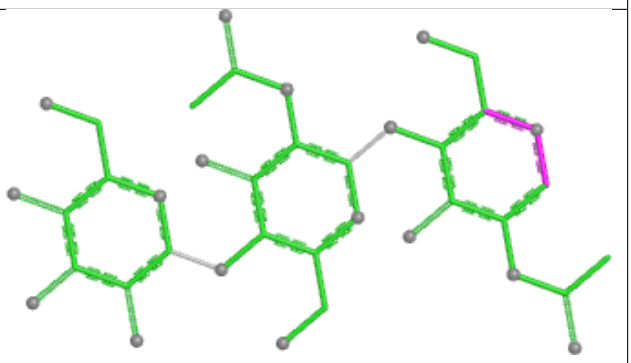
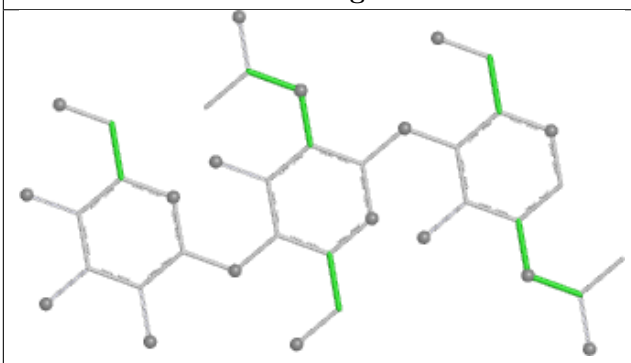


Bond angles



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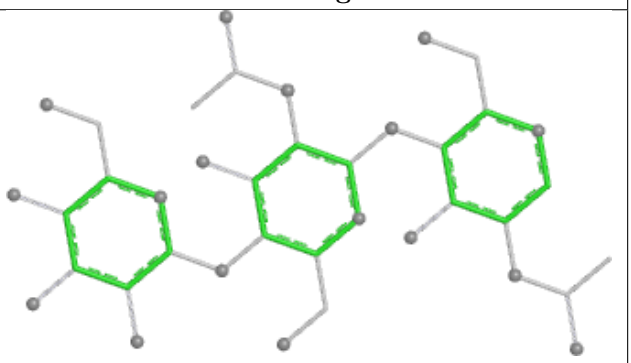
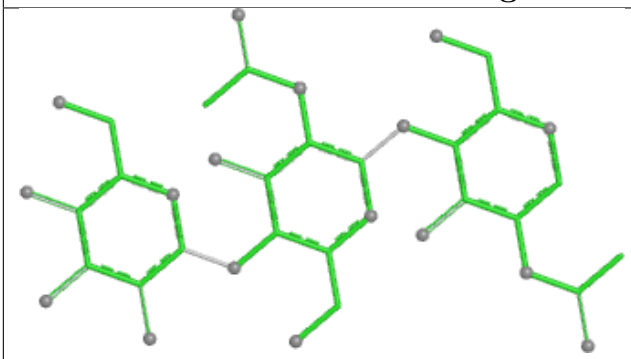


Rings

Oligosaccharide Chain c



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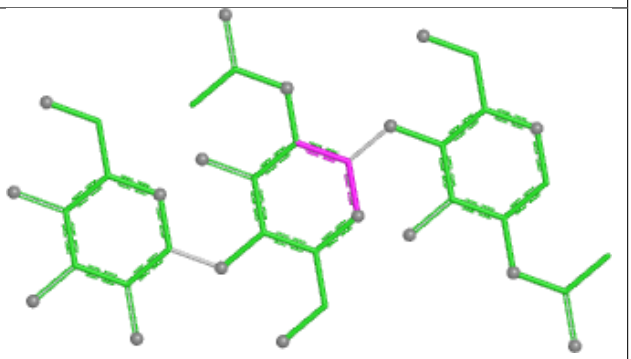
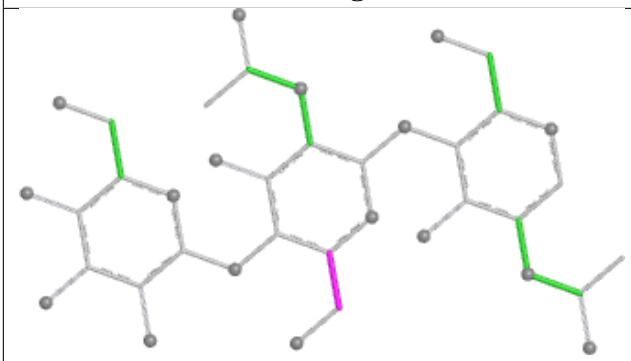


Bond angles



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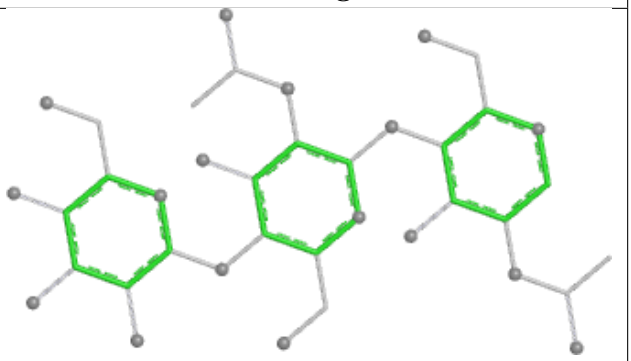
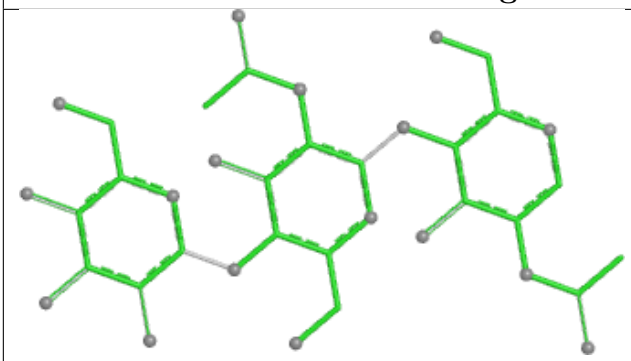
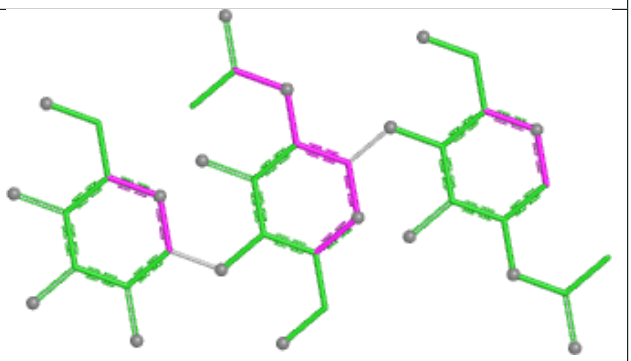


Rings

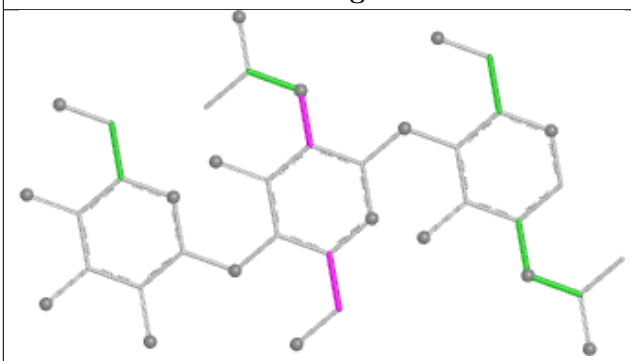
Oligosaccharide Chain e



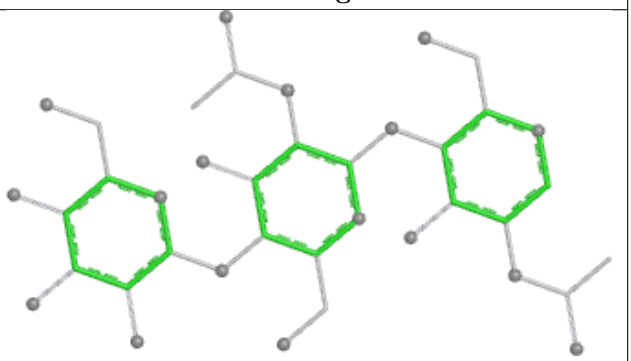
Bond lengths



Bond angles

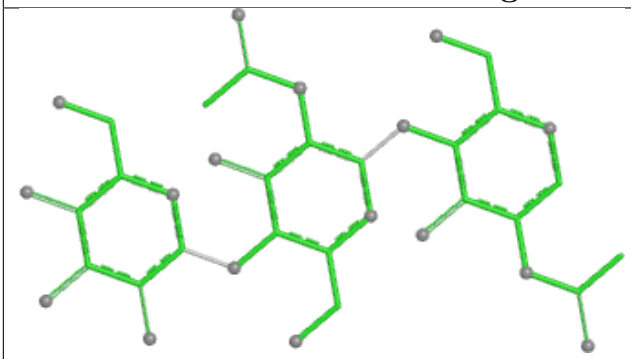


Torsions

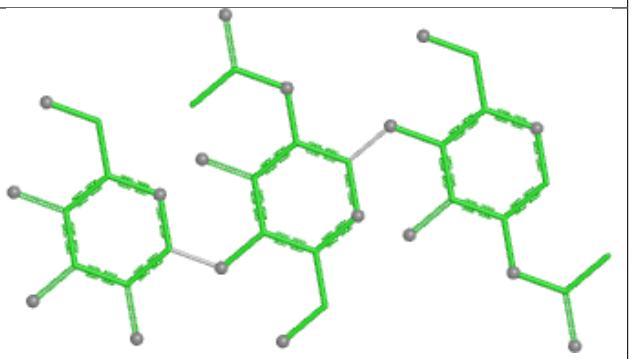


Rings

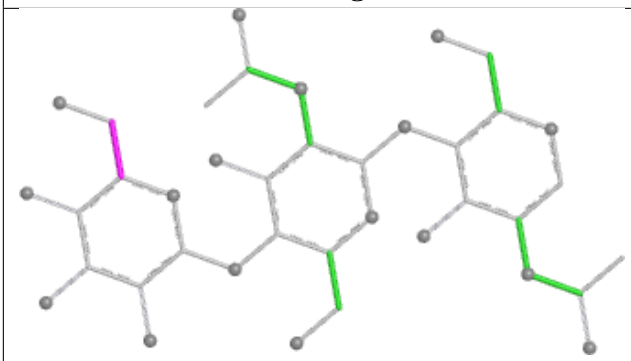
Oligosaccharide Chain f



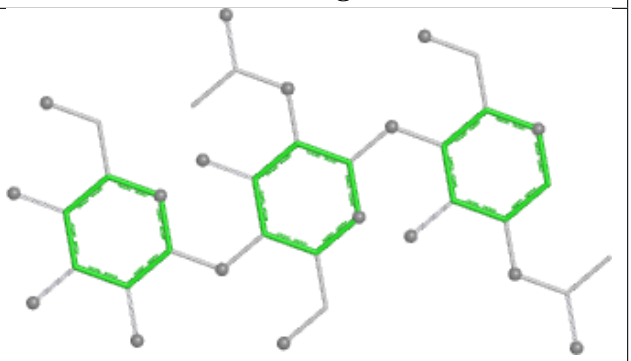
Bond lengths



Bond angles

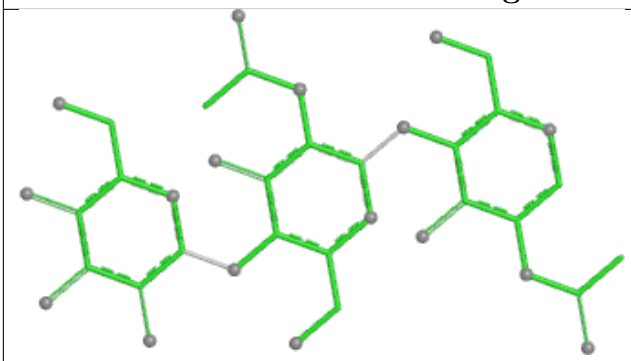


Torsions

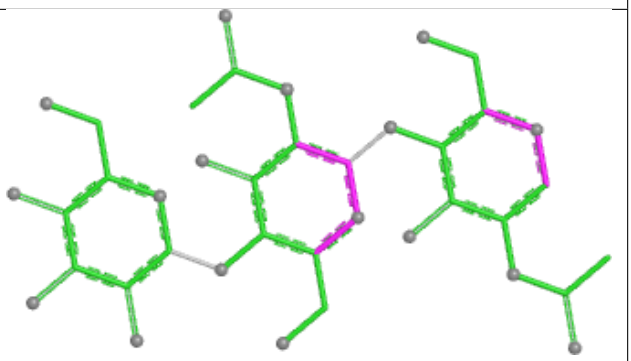


Rings

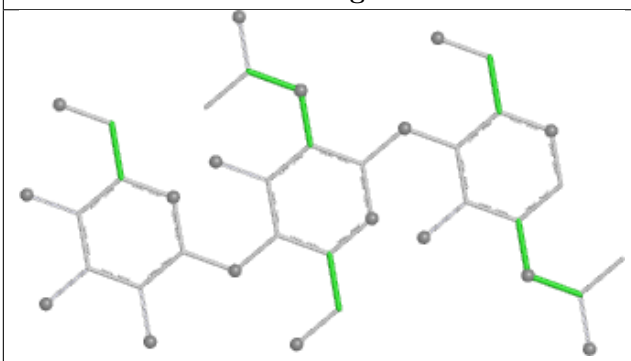
Oligosaccharide Chain i



Bond lengths



Bond angles



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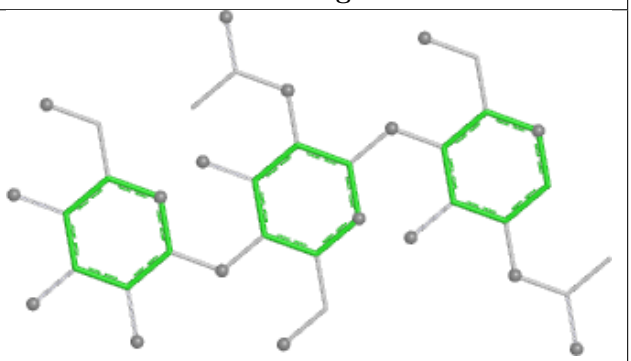
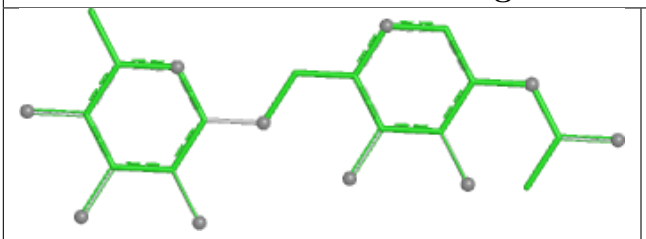
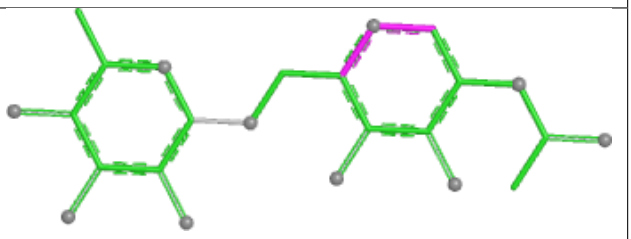


Rings

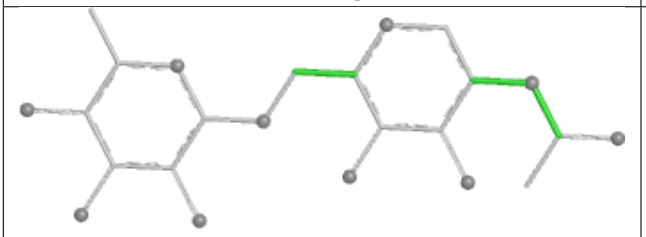
Oligosaccharide Chain R



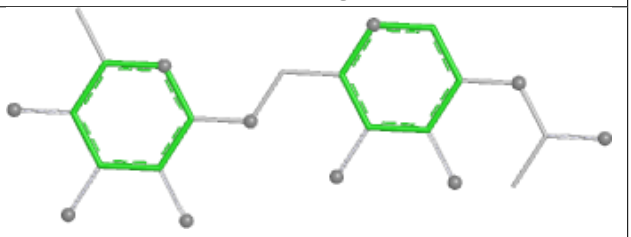
Bond lengths



Bond angles

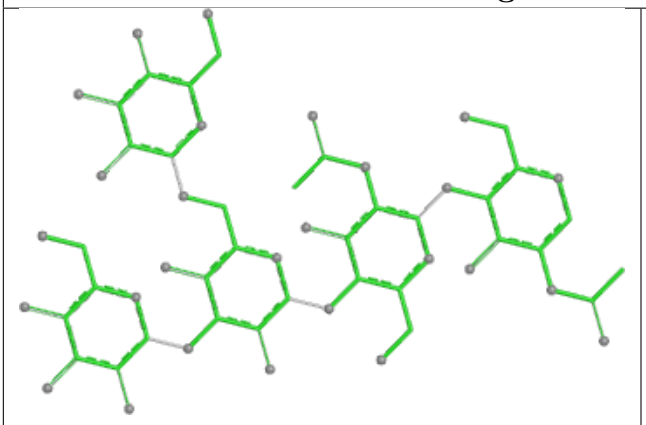


Torsions

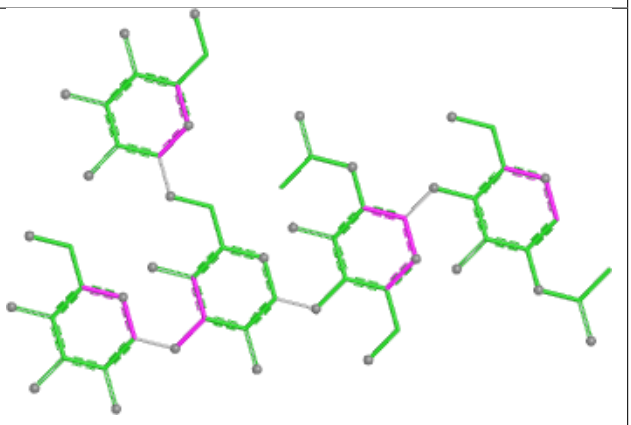


Rings

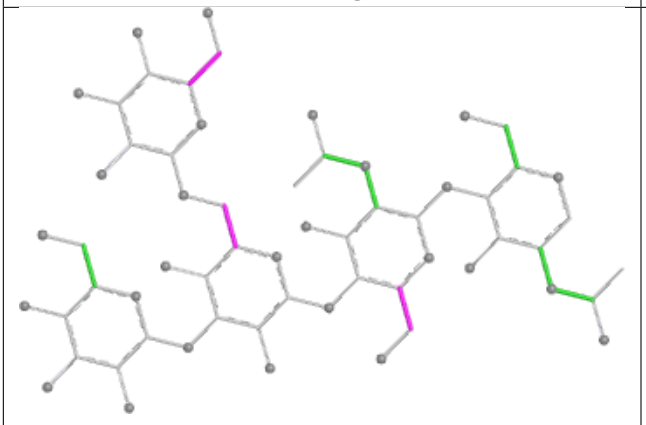
Oligosaccharide Chain S



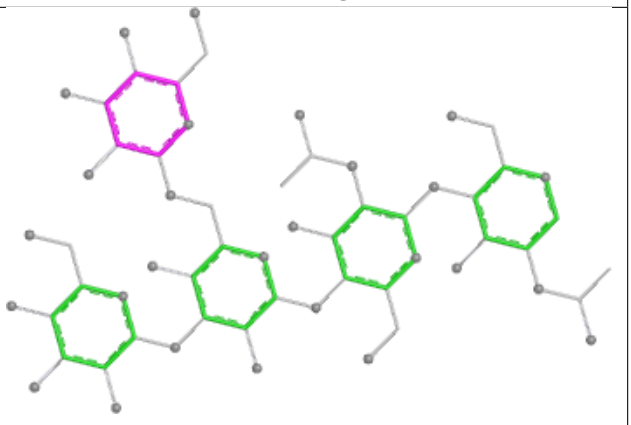
Bond lengths



Bond angles

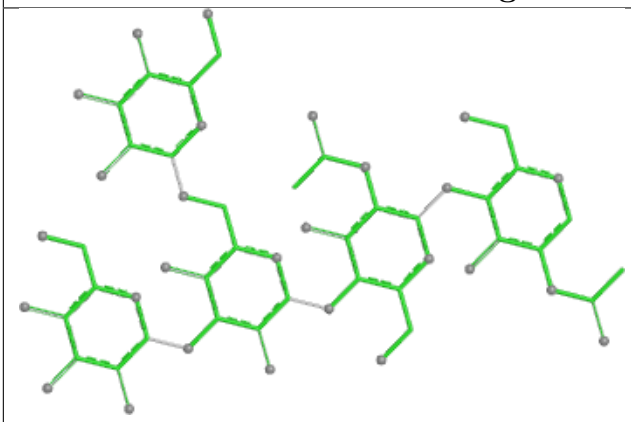


Torsions

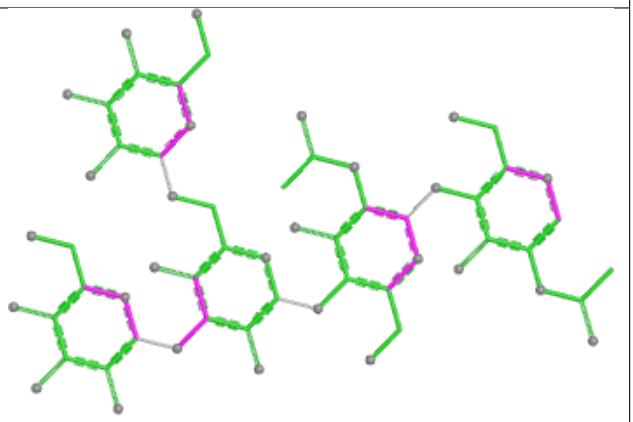


Rings

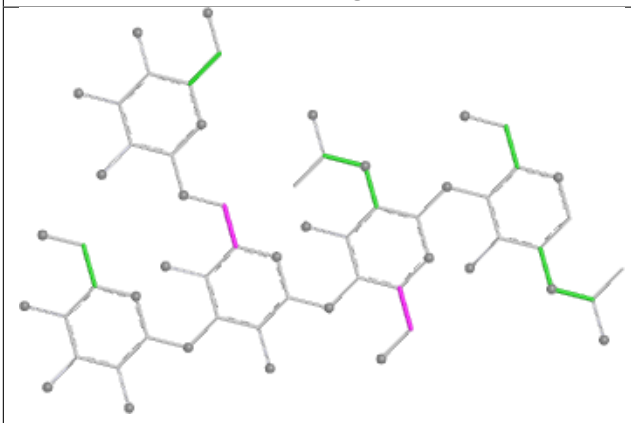
Oligosaccharide Chain a



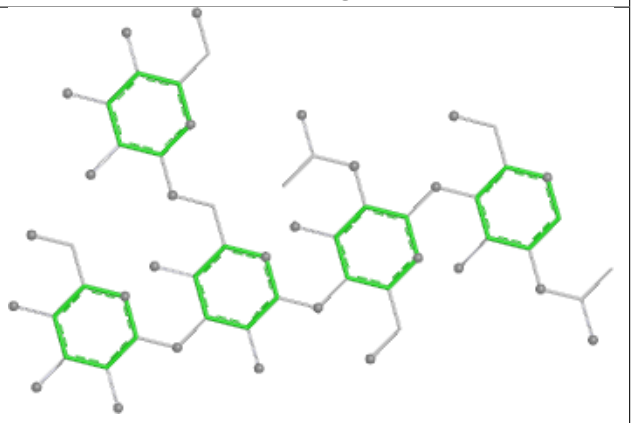
Bond lengths



Bond angles

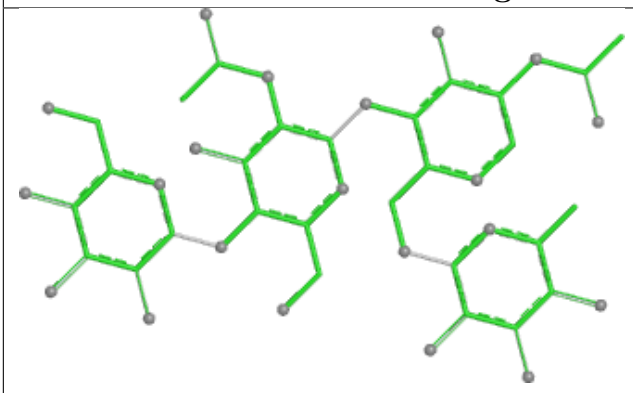


Torsions

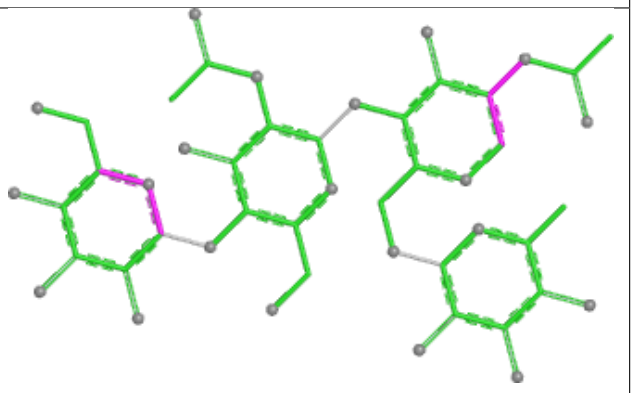


Rings

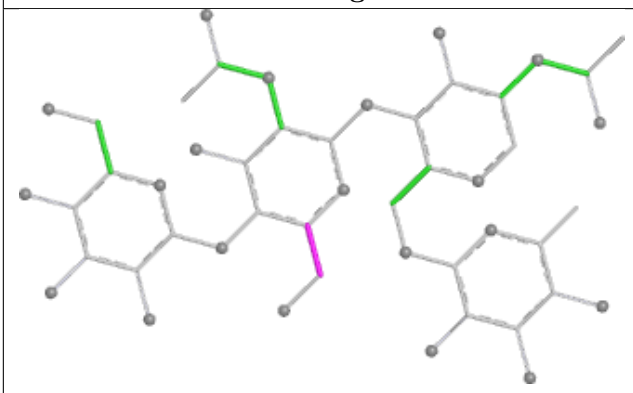
Oligosaccharide Chain V



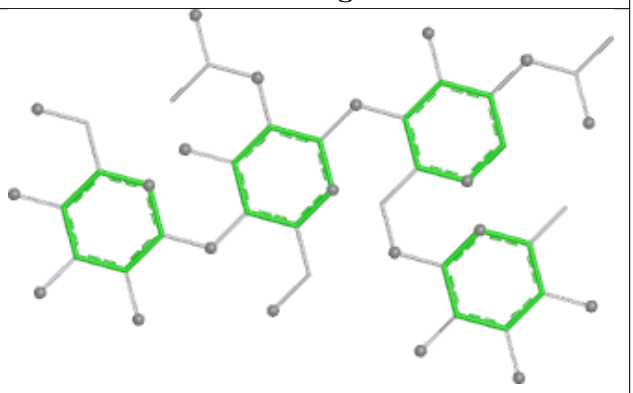
Bond lengths



Bond angles

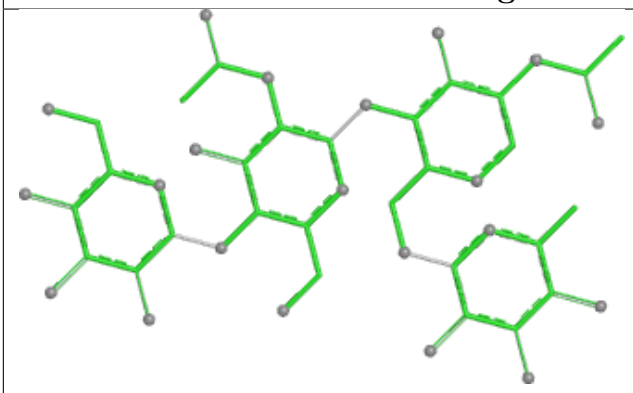


Torsions

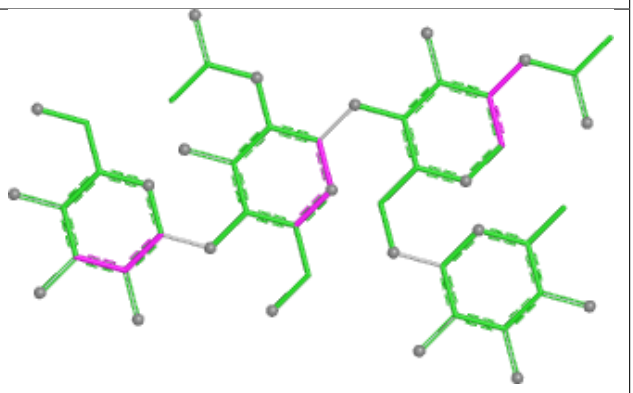


Rings

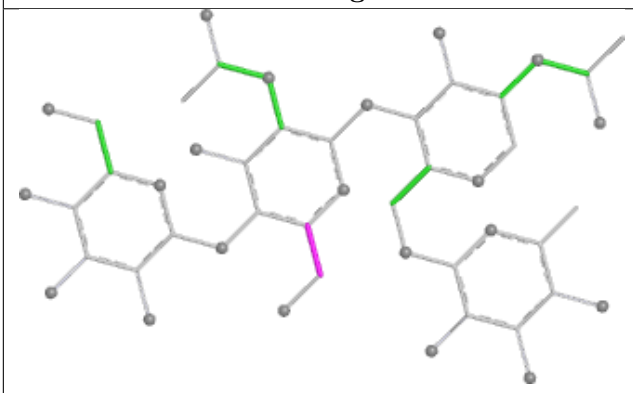
Oligosaccharide Chain d



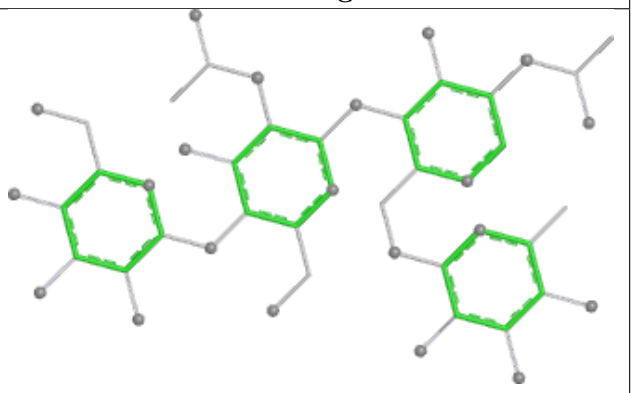
Bond lengths



Bond angles

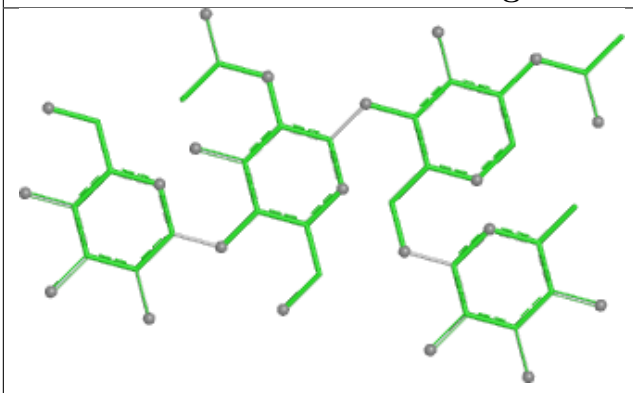


Torsions

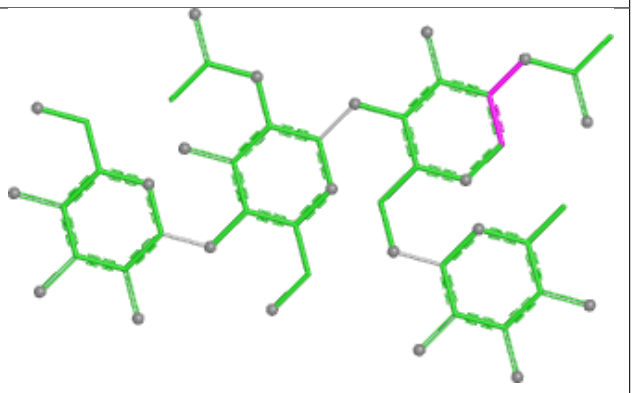


Rings

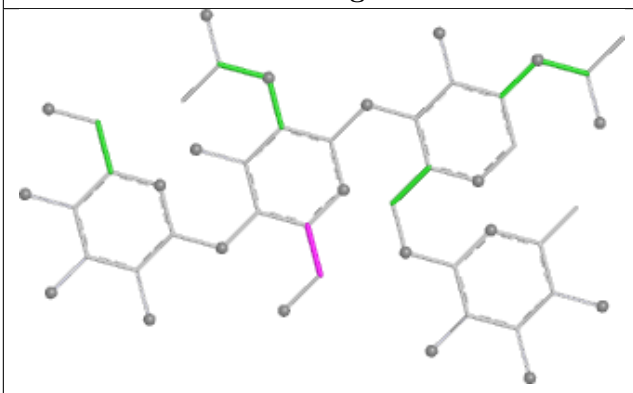
Oligosaccharide Chain l



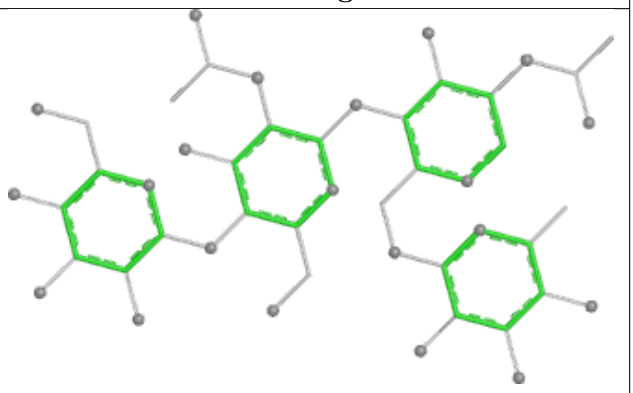
Bond lengths



Bond angles

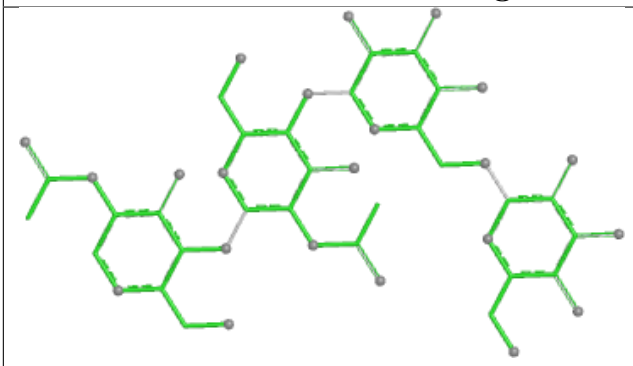


Torsions

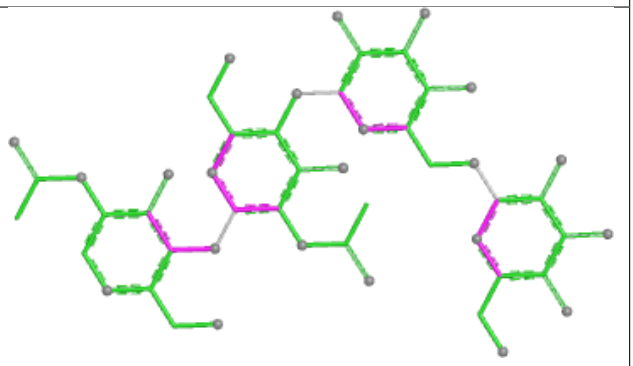


Rings

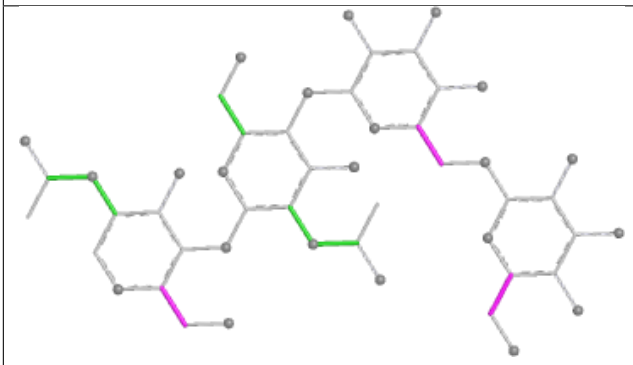
Oligosaccharide Chain Y



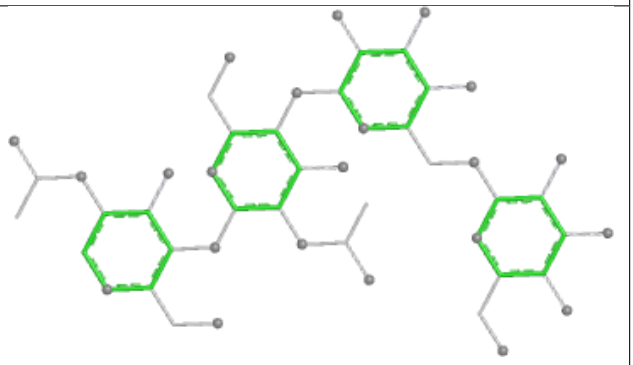
Bond lengths



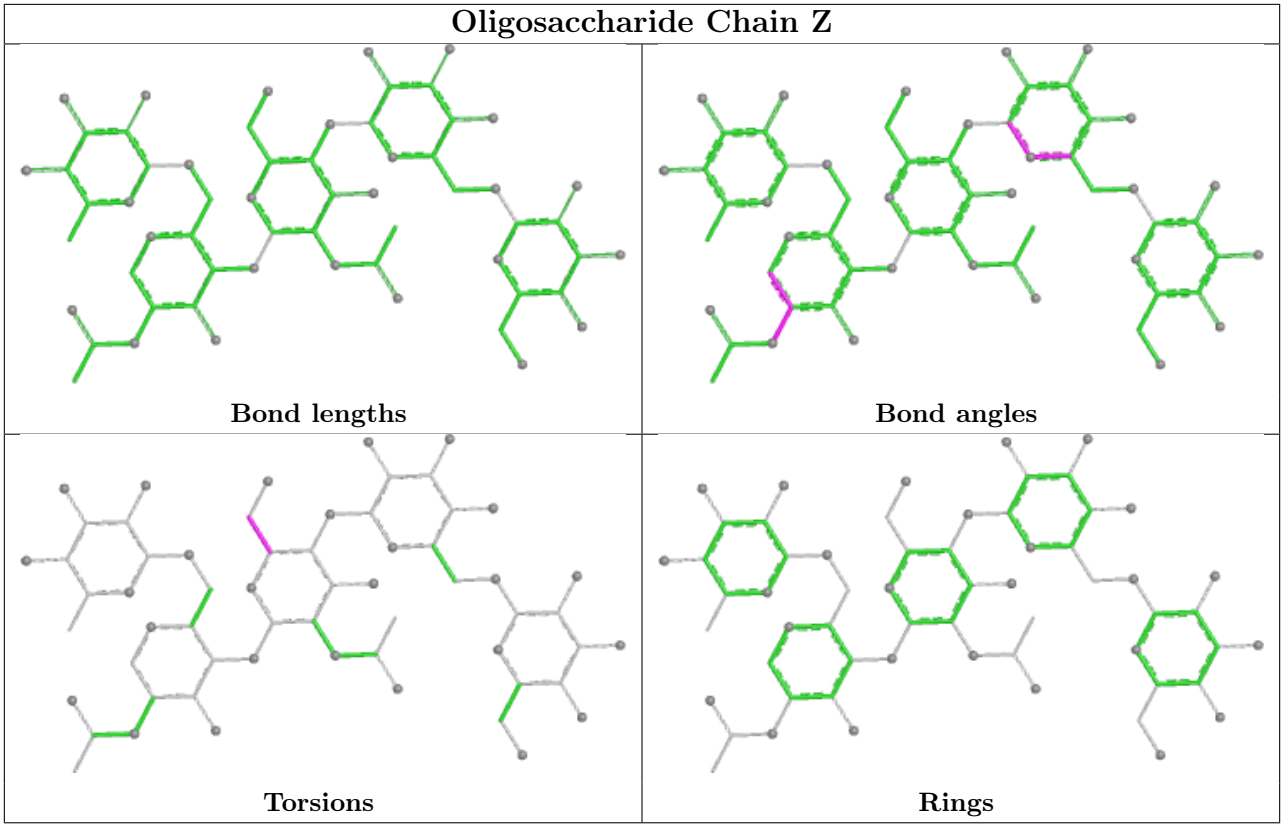
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

46 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	NAG	F	901	2	14,14,15	0.29	0	17,19,21	0.76	0
13	NAG	F	903	2	14,14,15	0.33	0	17,19,21	0.76	1 (5%)
12	SO4	H	817	-	4,4,4	0.30	0	6,6,6	0.10	0
12	SO4	E	202	-	4,4,4	0.32	0	6,6,6	0.12	0
12	SO4	F	822	-	4,4,4	0.28	0	6,6,6	0.10	0
13	NAG	B	902	2	14,14,15	0.32	0	17,19,21	0.88	1 (5%)
12	SO4	C	203	-	4,4,4	0.29	0	6,6,6	0.08	0
12	SO4	D	420	-	4,4,4	0.26	0	6,6,6	0.12	0
12	SO4	A	202	-	4,4,4	0.26	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	SO4	F	823	-	4,4,4	0.26	0	6,6,6	0.29	0
12	SO4	D	424	-	4,4,4	0.23	0	6,6,6	0.16	0
12	SO4	H	821	-	4,4,4	0.21	0	6,6,6	0.25	0
12	SO4	D	421	-	4,4,4	0.25	0	6,6,6	0.21	0
13	NAG	J	903	2	14,14,15	0.30	0	17,19,21	0.52	0
13	NAG	D	902	2	14,14,15	0.41	0	17,19,21	0.91	1 (5%)
12	SO4	B	824	-	4,4,4	0.25	0	6,6,6	0.15	0
12	SO4	F	825	-	4,4,4	0.34	0	6,6,6	0.10	0
12	SO4	H	818	-	4,4,4	0.21	0	6,6,6	0.26	0
12	SO4	C	201	-	4,4,4	0.26	0	6,6,6	0.13	0
12	SO4	D	419	-	4,4,4	0.24	0	6,6,6	0.24	0
12	SO4	C	202	-	4,4,4	0.25	0	6,6,6	0.13	0
12	SO4	D	423	-	4,4,4	0.31	0	6,6,6	0.08	0
12	SO4	K	201	-	4,4,4	0.28	0	6,6,6	0.11	0
12	SO4	G	201	-	4,4,4	0.24	0	6,6,6	0.27	0
12	SO4	H	819	-	4,4,4	0.19	0	6,6,6	0.16	0
12	SO4	D	422	-	4,4,4	0.29	0	6,6,6	0.09	0
12	SO4	F	821	-	4,4,4	0.31	0	6,6,6	0.14	0
12	SO4	I	201	-	4,4,4	0.23	0	6,6,6	0.16	0
12	SO4	H	820	-	4,4,4	0.34	0	6,6,6	0.15	0
13	NAG	B	901	2	14,14,15	0.29	0	17,19,21	0.68	1 (5%)
12	SO4	E	203	-	4,4,4	0.35	0	6,6,6	0.20	0
12	SO4	C	204	-	4,4,4	0.27	0	6,6,6	0.30	0
12	SO4	D	425	-	4,4,4	0.30	0	6,6,6	0.20	0
12	SO4	G	202	-	4,4,4	0.37	0	6,6,6	0.15	0
12	SO4	C	205	-	4,4,4	0.29	0	6,6,6	0.13	0
13	NAG	H	901	2	14,14,15	0.30	0	17,19,21	0.91	2 (11%)
12	SO4	B	822	-	4,4,4	0.21	0	6,6,6	0.14	0
13	NAG	H	903	2	14,14,15	0.28	0	17,19,21	0.74	1 (5%)
12	SO4	L	412	-	4,4,4	0.23	0	6,6,6	0.10	0
12	SO4	E	201	-	4,4,4	0.23	0	6,6,6	0.19	0
12	SO4	B	821	-	4,4,4	0.34	0	6,6,6	0.16	0
12	SO4	J	413	-	4,4,4	0.26	0	6,6,6	0.25	0
12	SO4	F	824	-	4,4,4	0.27	0	6,6,6	0.10	0
12	SO4	B	820	-	4,4,4	0.24	0	6,6,6	0.11	0
12	SO4	B	823	-	4,4,4	0.22	0	6,6,6	0.21	0
12	SO4	A	201	-	4,4,4	0.32	0	6,6,6	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	F	901	2	-	0/6/23/26	0/1/1/1
13	NAG	F	903	2	-	0/6/23/26	0/1/1/1
13	NAG	J	903	2	-	0/6/23/26	0/1/1/1
13	NAG	D	902	2	-	0/6/23/26	0/1/1/1
13	NAG	B	902	2	-	0/6/23/26	0/1/1/1
13	NAG	B	901	2	-	0/6/23/26	0/1/1/1
13	NAG	H	901	2	-	1/6/23/26	0/1/1/1
13	NAG	H	903	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	902	NAG	C1-O5-C5	3.20	116.48	112.19
13	F	903	NAG	C1-O5-C5	2.84	116.00	112.19
13	H	903	NAG	C1-O5-C5	2.72	115.83	112.19
13	H	901	NAG	C1-O5-C5	2.58	115.64	112.19
13	B	901	NAG	C1-O5-C5	2.18	115.11	112.19
13	D	902	NAG	O5-C1-C2	2.12	114.56	111.29
13	H	901	NAG	O5-C1-C2	-2.03	108.14	111.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	H	901	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
12	H	817	SO4	1	0
12	F	821	SO4	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	156/157 (99%)	-0.26	2 (1%) 77 59	38, 57, 90, 110	0
1	C	156/157 (99%)	-0.29	0 100 100	32, 58, 85, 109	0
1	E	157/157 (100%)	-0.22	0 100 100	35, 64, 92, 129	0
1	G	156/157 (99%)	-0.32	0 100 100	34, 53, 80, 95	0
1	I	156/157 (99%)	-0.12	1 (0%) 89 78	75, 99, 132, 145	0
1	K	156/157 (99%)	-0.06	0 100 100	71, 96, 121, 130	0
2	B	294/312 (94%)	0.07	5 (1%) 70 49	32, 68, 111, 139	0
2	D	290/312 (92%)	-0.00	2 (0%) 87 75	36, 67, 102, 136	0
2	F	288/312 (92%)	0.04	5 (1%) 70 49	36, 72, 129, 152	0
2	H	288/312 (92%)	0.07	6 (2%) 63 43	35, 68, 121, 161	0
2	J	272/312 (87%)	0.52	20 (7%) 14 5	54, 94, 165, 191	0
2	L	255/312 (81%)	0.59	25 (9%) 7 2	69, 101, 137, 163	0
All	All	2624/2814 (93%)	0.06	66 (2%) 57 34	32, 76, 128, 191	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	63	GLN	4.6
2	B	62	SER	4.5
2	L	151	SER	4.0
2	L	88	VAL	3.8
2	L	227	VAL	3.7
1	A	141	GLU	3.7
2	J	62	SER	3.6
2	J	76	ILE	3.5
2	J	56	TRP	3.4
2	F	68	LEU	3.3
2	L	87	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	J	111	VAL	3.2
2	L	29	THR	3.0
2	J	79	HIS	3.0
2	L	30	VAL	2.9
2	L	79	HIS	2.9
1	I	29	LEU	2.9
1	A	142	ASP	2.9
2	H	73	SER	2.8
2	J	191	HIS	2.8
2	J	293	ASN	2.8
2	F	-2	GLY	2.7
2	J	75	ARG	2.7
2	L	190	HIS	2.7
2	L	31	VAL	2.7
2	J	80	ASP	2.7
2	D	91	ASN	2.7
2	L	187	HIS	2.6
2	J	83	LEU	2.6
2	H	62	SER	2.6
2	L	197	ASN	2.6
2	J	31	VAL	2.5
2	J	84	GLU	2.5
2	J	42	SER	2.5
2	L	119	CYS	2.5
2	J	93	THR	2.5
2	L	86	TRP	2.4
2	L	152	THR	2.4
2	L	145	TYR	2.4
2	L	195	LEU	2.3
2	L	28	ILE	2.3
2	J	147	THR	2.3
2	L	118	SER	2.3
2	D	65	HIS	2.3
2	H	74	SER	2.3
2	F	56	TRP	2.3
2	J	90	LEU	2.3
2	L	188	PHE	2.3
2	L	77	ALA	2.2
2	B	110	ASN	2.2
2	J	60	SER	2.2
2	J	240	LEU	2.1
2	L	295	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	27	HIS	2.1
2	L	186	VAL	2.1
2	H	116	LYS	2.1
2	B	116	LYS	2.1
2	F	62	SER	2.1
2	L	153	SER	2.1
2	B	124	GLN	2.1
2	H	68	LEU	2.1
2	J	85	PHE	2.0
2	F	99	GLN	2.0
2	L	114	ARG	2.0
2	J	110	ASN	2.0
2	H	124	GLN	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
3	NAG	M	2	14/15	0.45	0.62	164,166,172,174	0
10	MAN	Y	4	11/12	0.51	0.48	160,163,165,166	0
4	MAN	N	6	11/12	0.53	0.37	146,151,153,154	0
11	MAN	Z	4	11/12	0.57	0.44	138,143,148,152	0
6	BMA	f	3	11/12	0.58	0.38	158,159,163,163	0
4	MAN	N	4	11/12	0.60	0.42	149,151,159,161	0
4	MAN	W	5	11/12	0.60	0.51	155,162,169,172	0
6	BMA	X	3	11/12	0.60	0.35	138,145,147,150	0
6	BMA	T	3	11/12	0.61	0.34	121,125,128,131	0
11	BMA	Z	3	11/12	0.63	0.28	122,130,137,138	0
9	BMA	d	3	11/12	0.64	0.33	123,127,131,135	0
10	BMA	Y	3	11/12	0.65	0.27	140,148,154,157	0
9	BMA	l	3	11/12	0.71	0.43	161,165,170,171	0
5	NAG	b	2	14/15	0.72	0.37	120,125,132,133	0
9	BMA	V	3	11/12	0.72	0.36	127,130,132,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	N	5	11/12	0.74	0.38	163,166,172,174	0
5	NAG	j	2	14/15	0.74	0.30	126,128,129,130	0
6	NAG	f	2	14/15	0.75	0.37	133,142,147,153	0
4	MAN	W	6	11/12	0.75	0.32	150,151,157,157	0
6	BMA	c	3	11/12	0.75	0.32	119,125,132,135	0
8	MAN	a	5	11/12	0.76	0.25	157,159,161,163	0
6	BMA	U	3	11/12	0.76	0.28	123,130,134,134	0
7	NAG	R	1	14/15	0.78	0.28	124,128,137,138	0
6	NAG	c	2	14/15	0.79	0.26	92,101,110,118	0
8	MAN	S	4	11/12	0.79	0.30	137,142,144,144	0
5	NAG	k	2	14/15	0.81	0.24	116,125,132,133	0
6	NAG	P	2	14/15	0.81	0.22	93,100,104,110	0
6	BMA	P	3	11/12	0.81	0.26	108,114,117,118	0
8	MAN	a	4	11/12	0.81	0.38	158,163,168,169	0
3	NAG	h	2	14/15	0.82	0.27	120,125,130,133	0
5	NAG	g	2	14/15	0.82	0.24	113,121,124,126	0
6	BMA	e	3	11/12	0.82	0.34	132,135,138,139	0
5	NAG	O	2	14/15	0.82	0.29	119,125,131,131	0
6	BMA	i	3	11/12	0.83	0.43	165,169,171,172	0
8	MAN	S	5	11/12	0.84	0.33	138,140,143,143	0
3	NAG	M	1	14/15	0.84	0.39	149,154,157,161	0
3	FUC	M	3	10/11	0.84	0.35	152,154,157,158	0
6	NAG	X	2	14/15	0.84	0.23	106,115,124,131	0
4	MAN	W	4	11/12	0.84	0.33	139,144,155,159	0
4	BMA	N	3	11/12	0.85	0.24	129,136,144,145	0
3	NAG	Q	2	14/15	0.87	0.34	96,104,111,111	0
10	NAG	Y	2	14/15	0.87	0.23	111,118,125,133	0
8	BMA	a	3	11/12	0.87	0.34	145,152,156,156	0
6	NAG	i	1	14/15	0.88	0.35	142,147,151,152	0
6	NAG	T	2	14/15	0.88	0.18	93,98,109,114	0
6	NAG	U	2	14/15	0.88	0.14	91,96,105,114	0
9	NAG	l	2	14/15	0.88	0.36	150,155,161,164	0
8	BMA	S	3	11/12	0.88	0.30	122,130,136,137	0
9	NAG	d	2	14/15	0.89	0.43	92,100,111,118	0
6	NAG	e	2	14/15	0.89	0.38	116,125,130,132	0
5	NAG	j	1	14/15	0.89	0.18	110,113,119,124	0
6	NAG	i	2	14/15	0.90	0.35	149,155,161,163	0
7	FUC	R	2	10/11	0.90	0.27	126,129,131,131	0
6	NAG	f	1	14/15	0.90	0.20	109,114,121,129	0
9	NAG	V	2	14/15	0.91	0.26	105,111,124,125	0
4	BMA	W	3	11/12	0.91	0.39	131,137,143,148	0
9	FUC	V	4	10/11	0.91	0.26	96,99,102,105	0

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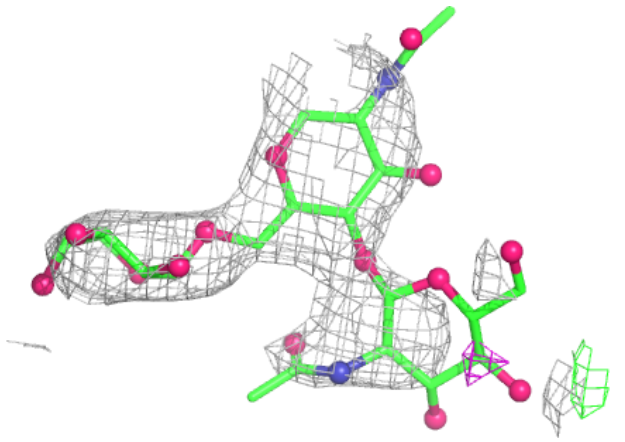
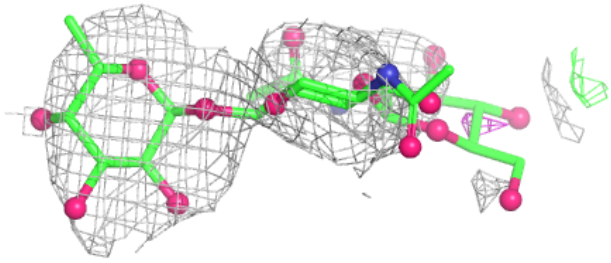
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	W	2	14/15	0.91	0.33	109,111,120,127	0
6	NAG	X	1	14/15	0.92	0.27	87,90,96,104	0
5	NAG	b	1	14/15	0.92	0.20	69,83,99,111	0
6	NAG	e	1	14/15	0.92	0.25	107,109,115,116	0
11	NAG	Z	2	14/15	0.92	0.23	83,94,108,114	0
3	NAG	h	1	14/15	0.92	0.23	99,105,109,115	0
8	NAG	a	2	14/15	0.92	0.31	121,126,133,139	0
4	NAG	N	2	14/15	0.93	0.25	104,107,117,123	0
6	NAG	T	1	14/15	0.93	0.18	62,71,77,86	0
9	FUC	d	4	10/11	0.93	0.30	79,82,85,85	0
9	NAG	l	1	14/15	0.93	0.30	120,128,136,145	0
6	NAG	P	1	14/15	0.93	0.22	67,73,79,84	0
5	NAG	k	1	14/15	0.93	0.25	100,104,110,115	0
5	NAG	O	1	14/15	0.94	0.18	81,88,99,110	0
6	NAG	c	1	14/15	0.94	0.21	68,76,81,88	0
6	NAG	U	1	14/15	0.94	0.16	63,67,74,81	0
8	NAG	S	2	14/15	0.94	0.25	94,98,107,116	0
9	FUC	l	4	10/11	0.94	0.36	130,135,140,143	0
10	NAG	Y	1	14/15	0.94	0.18	74,84,91,100	0
11	FUC	Z	5	10/11	0.94	0.20	81,87,93,97	0
3	FUC	h	3	10/11	0.95	0.22	106,111,114,115	0
3	NAG	Q	1	14/15	0.95	0.17	68,76,84,94	0
11	NAG	Z	1	14/15	0.95	0.16	55,66,81,82	0
9	NAG	d	1	14/15	0.95	0.23	65,70,80,91	0
3	FUC	Q	3	10/11	0.95	0.33	74,80,83,89	0
9	NAG	V	1	14/15	0.95	0.24	78,82,96,101	0
5	NAG	g	1	14/15	0.95	0.20	86,90,96,103	0
8	NAG	S	1	14/15	0.96	0.20	64,74,85,89	0
4	NAG	W	1	14/15	0.96	0.22	88,94,105,105	0
8	NAG	a	1	14/15	0.97	0.18	96,105,111,116	0
4	NAG	N	1	14/15	0.97	0.26	91,97,102,103	0

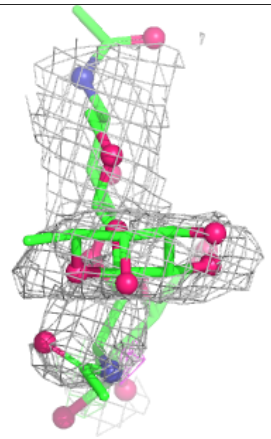
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

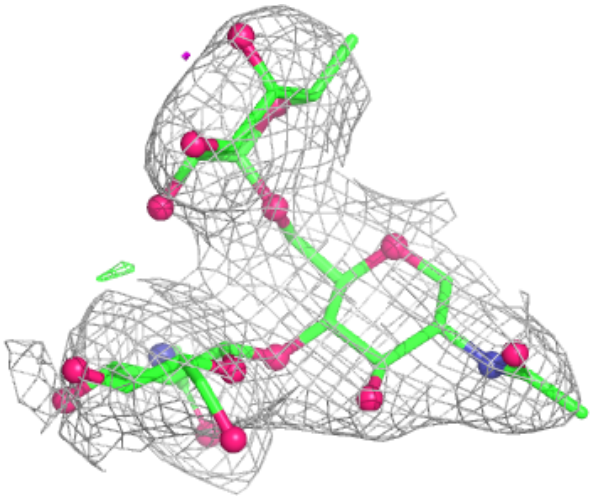


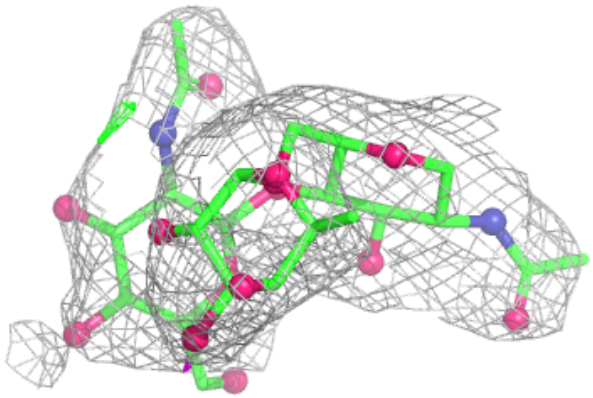


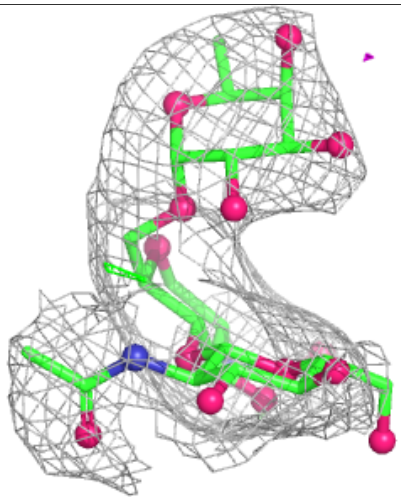


Electron density around Chain Q:

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

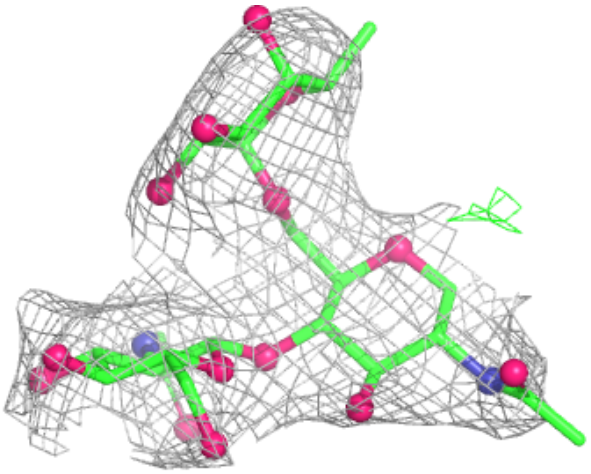


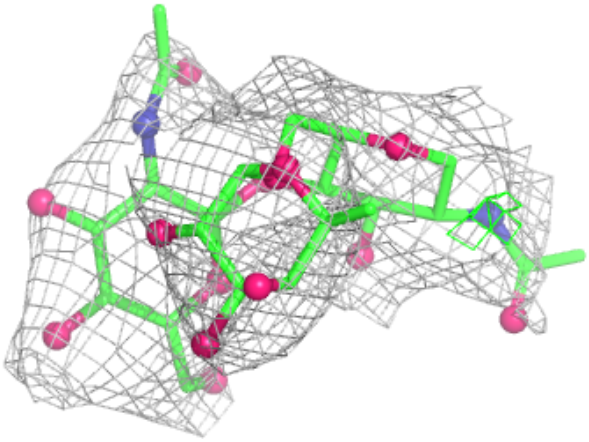


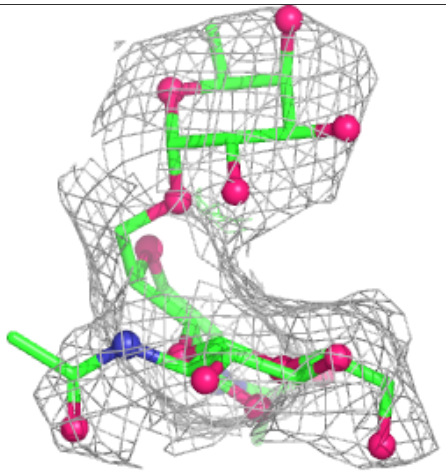


Electron density around Chain h:

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

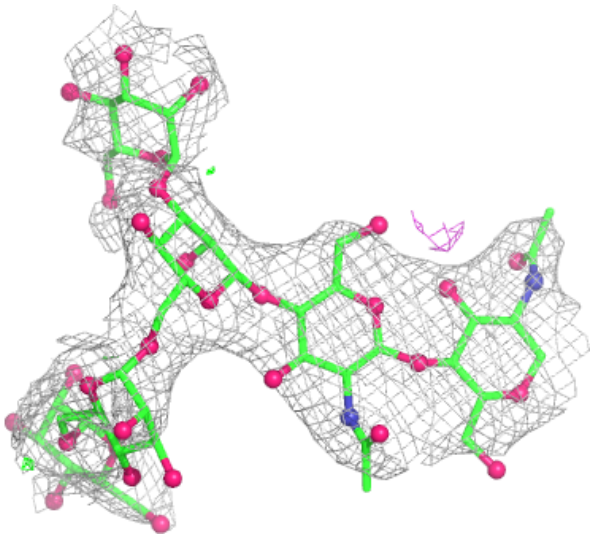


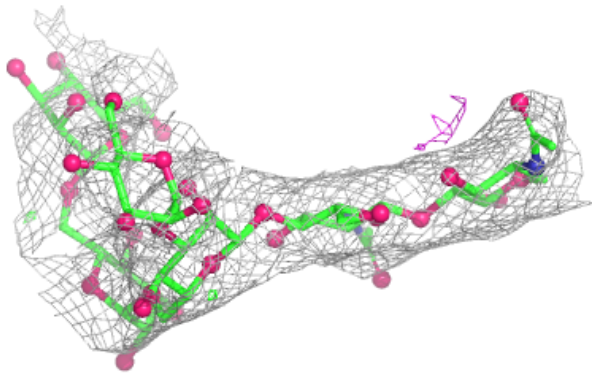


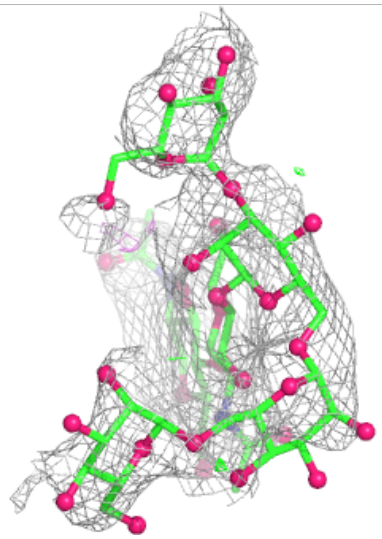


Electron density around Chain N:

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

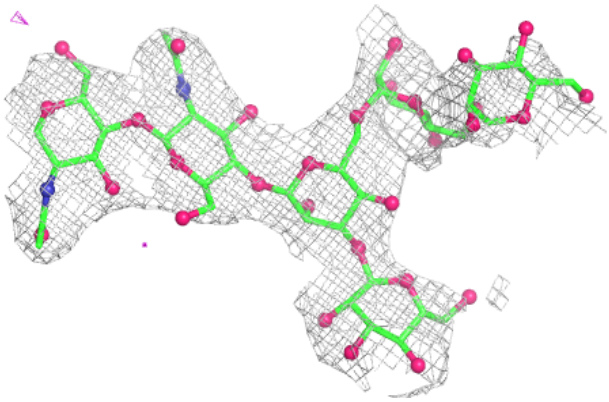


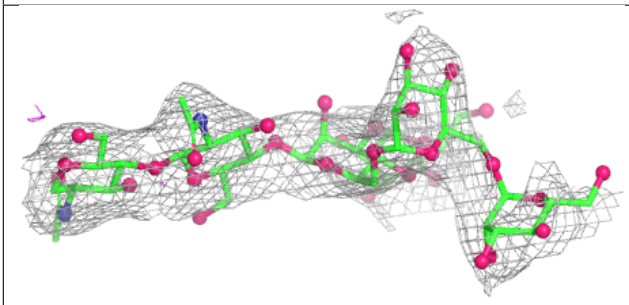


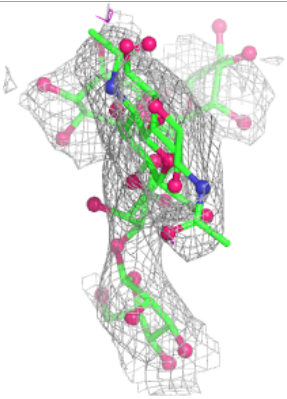


Electron density around Chain W:

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

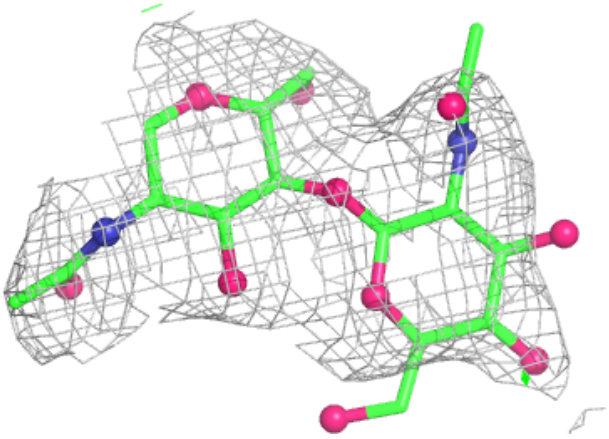


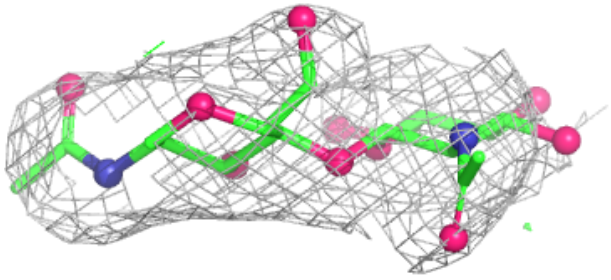


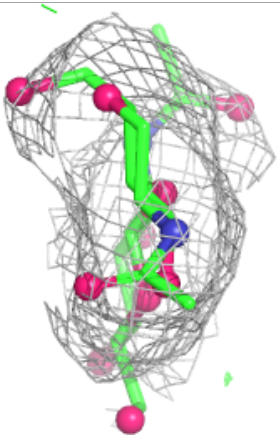


Electron density around Chain O:

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

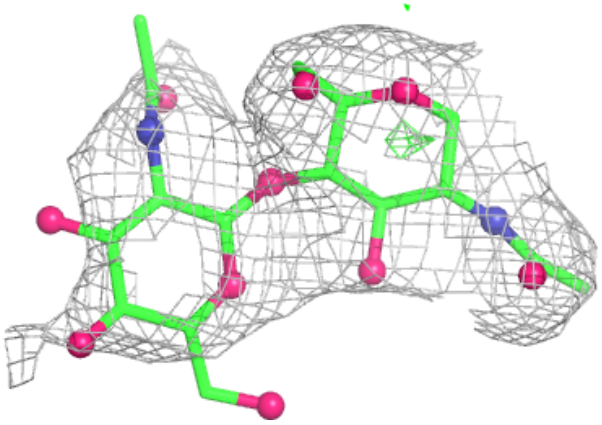


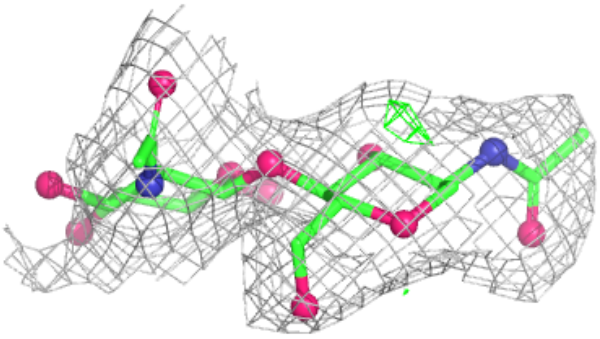


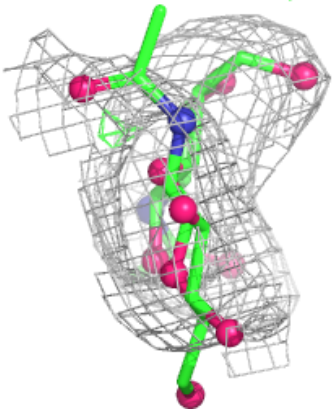


Electron density around Chain b:

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

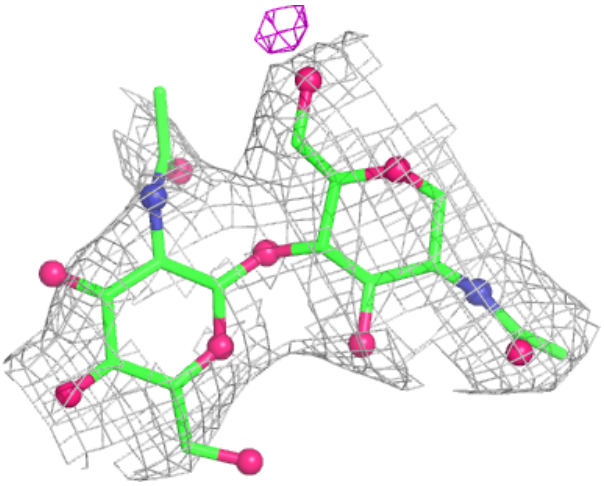


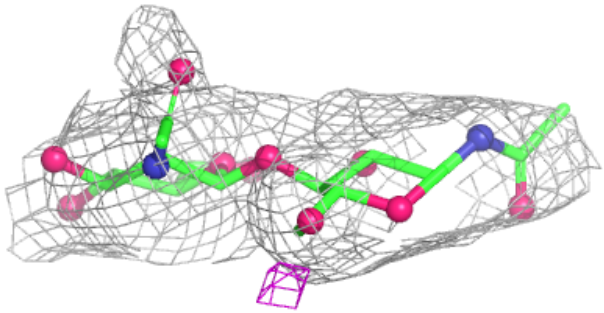


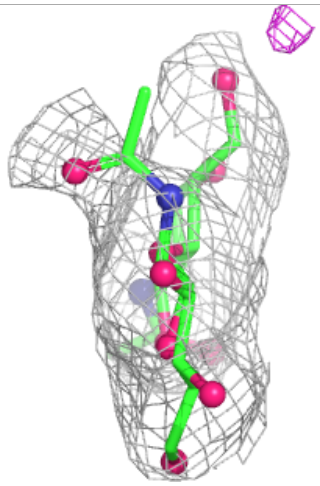


Electron density around Chain g:

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

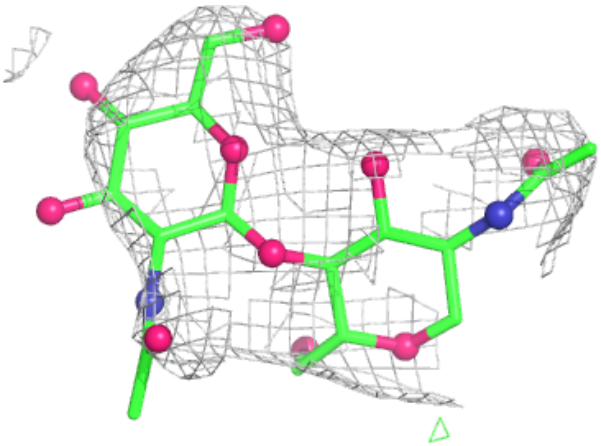


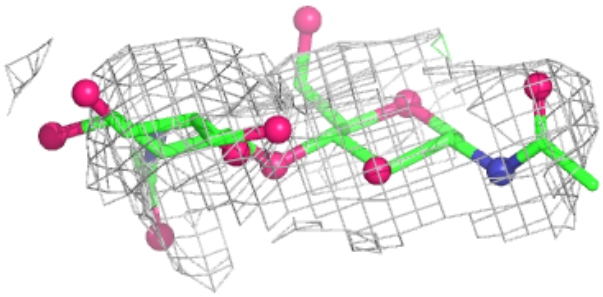


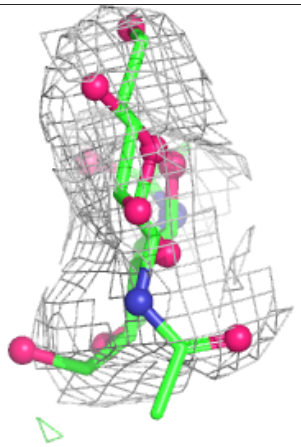


Electron density around Chain j:

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

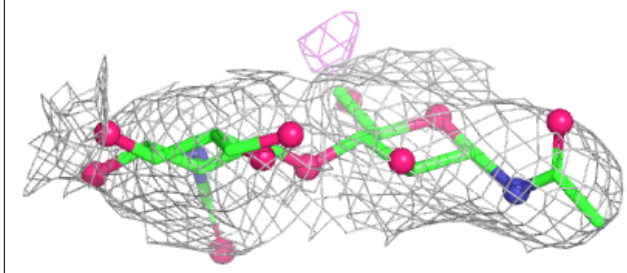


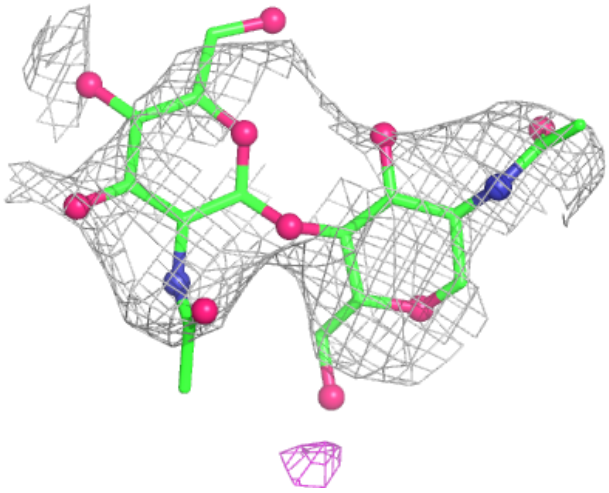


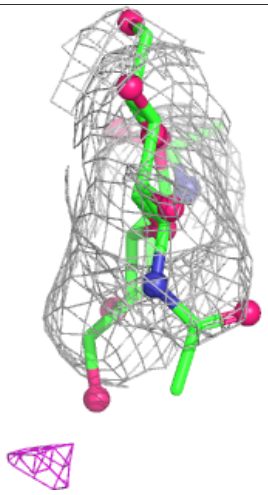


Electron density around Chain k:

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

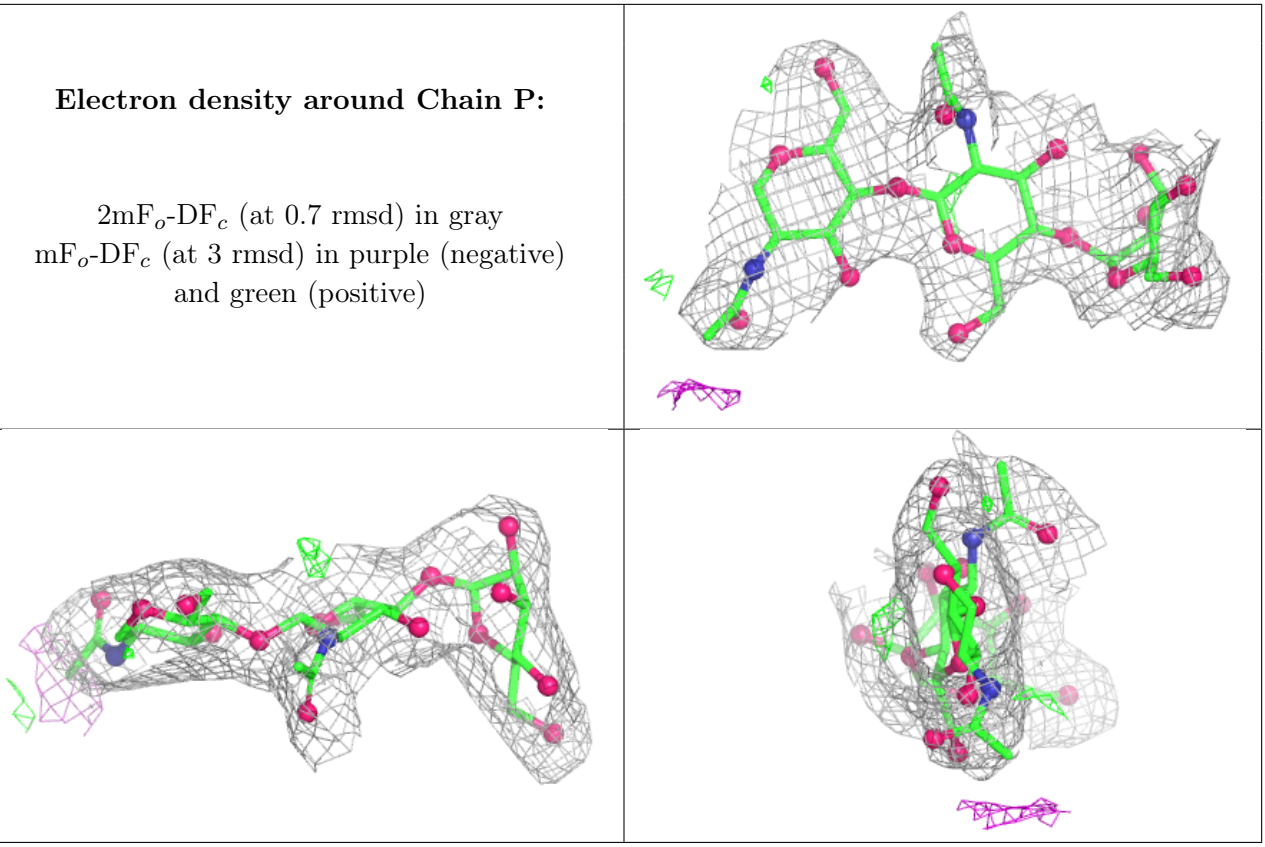






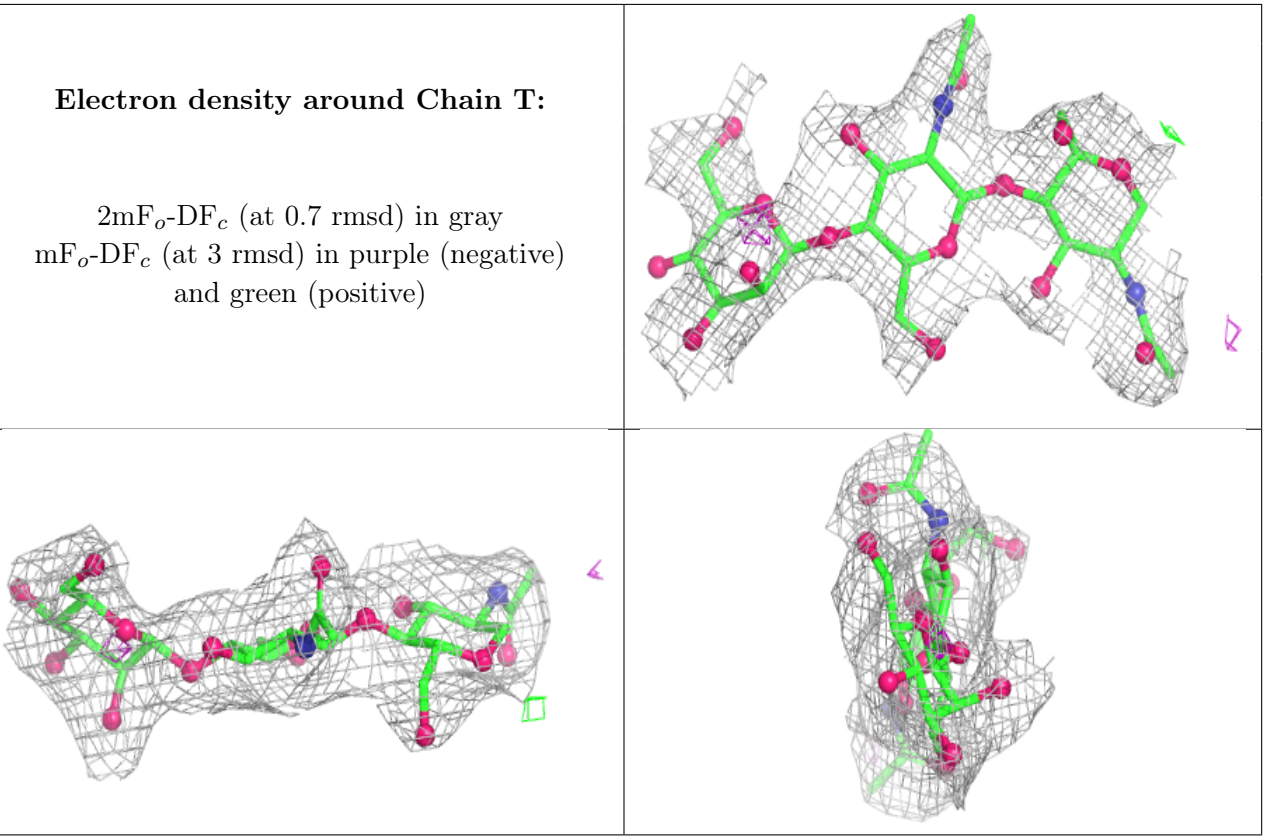
Electron density around Chain P:

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



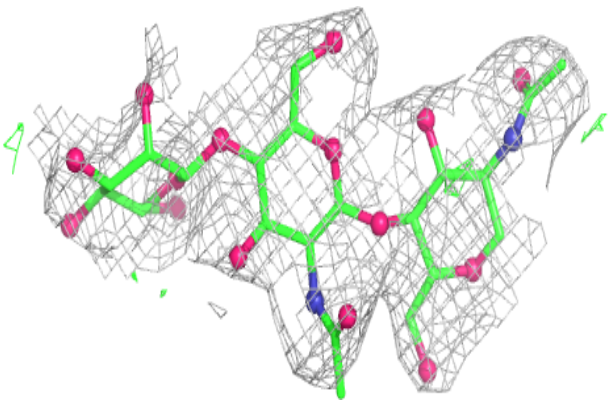
Electron density around Chain T:

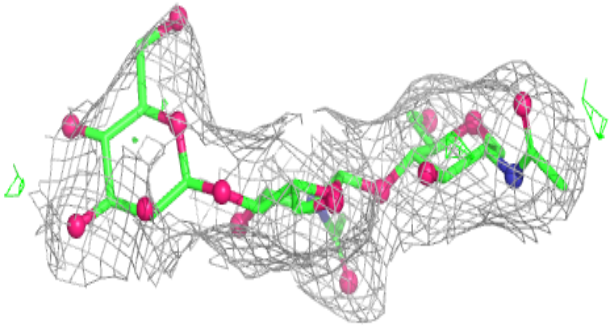
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

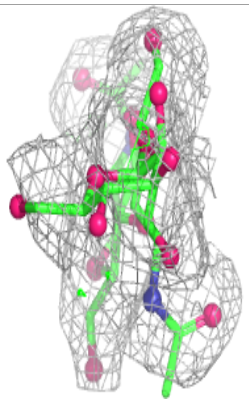


Electron density around Chain U:

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

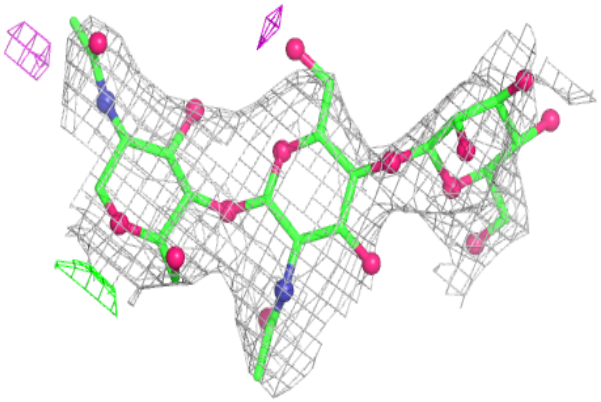


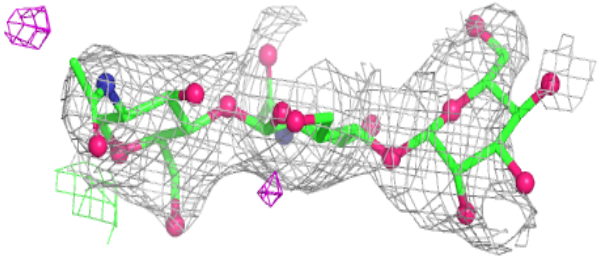


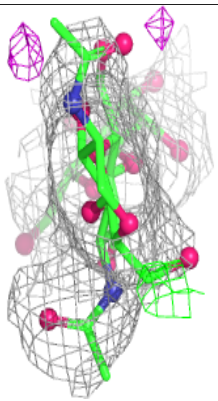


Electron density around Chain X:

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

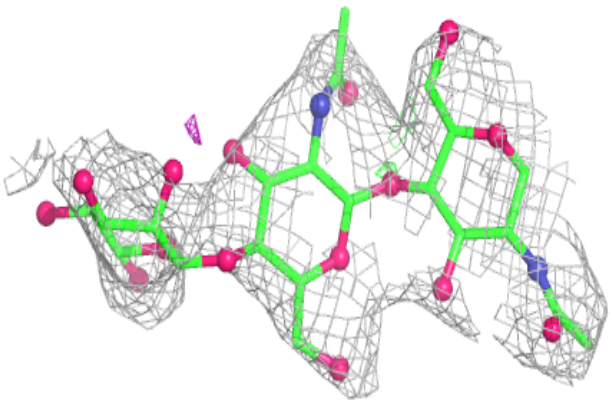


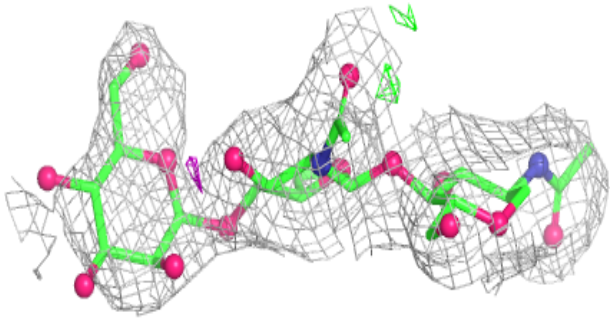


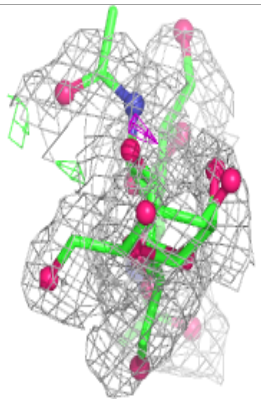


Electron density around Chain c:

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

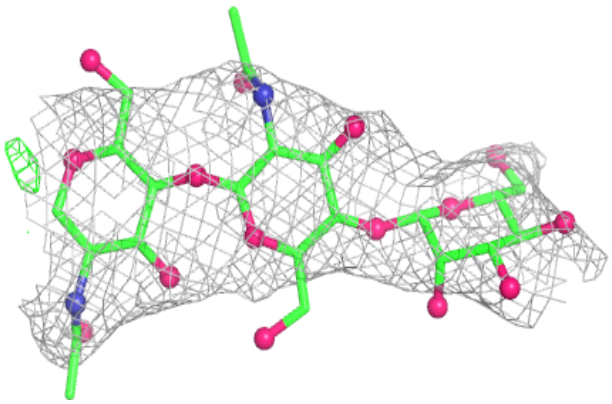


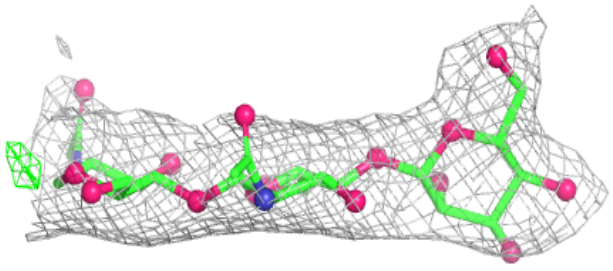


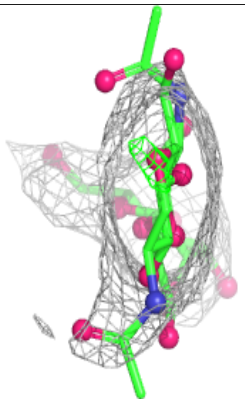


Electron density around Chain e:

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

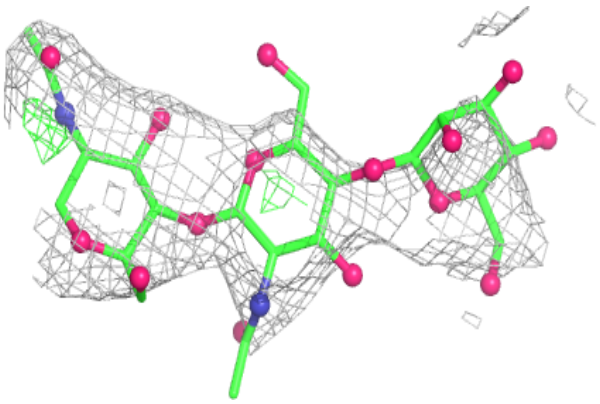


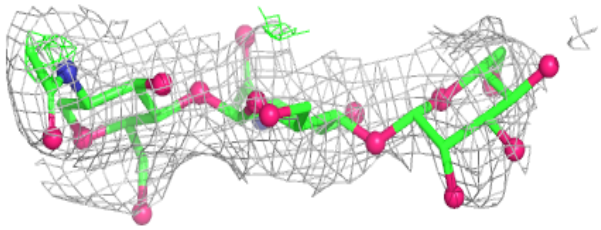


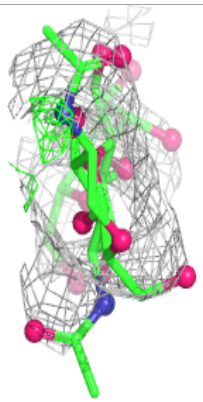


Electron density around Chain f:

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

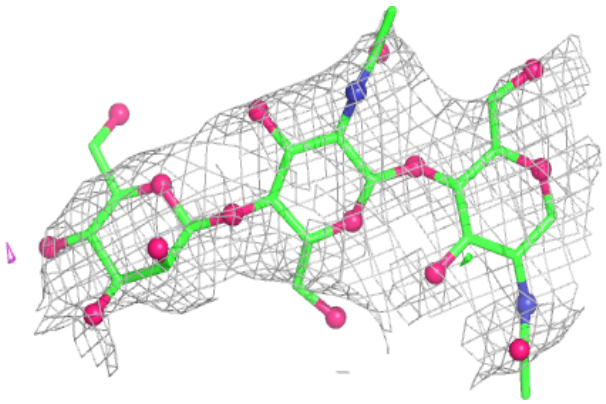


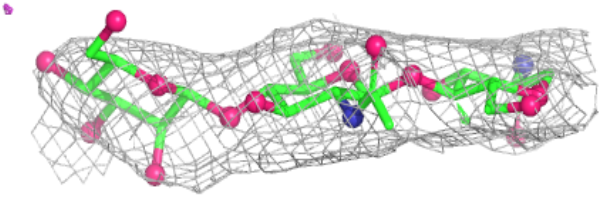


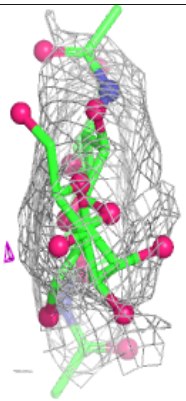


Electron density around Chain i:

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

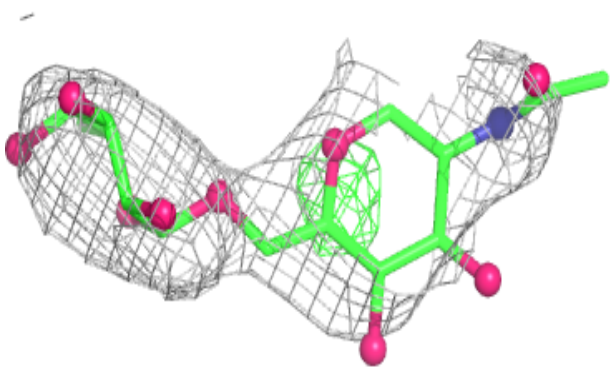


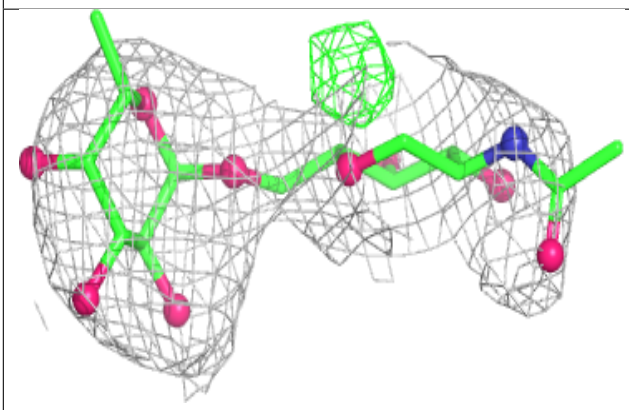


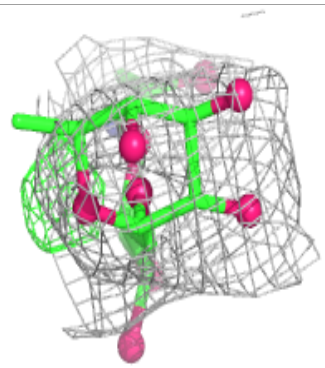


Electron density around Chain R:

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

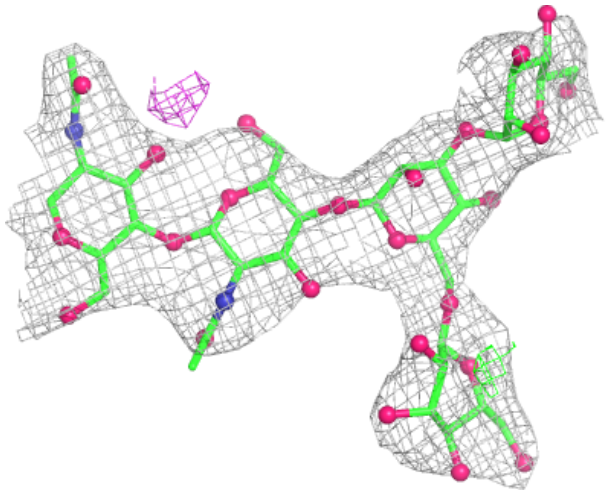


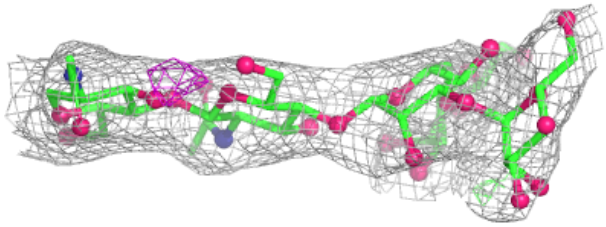


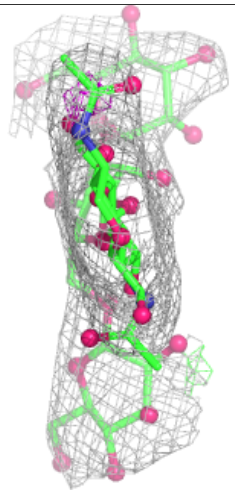


Electron density around Chain S:

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

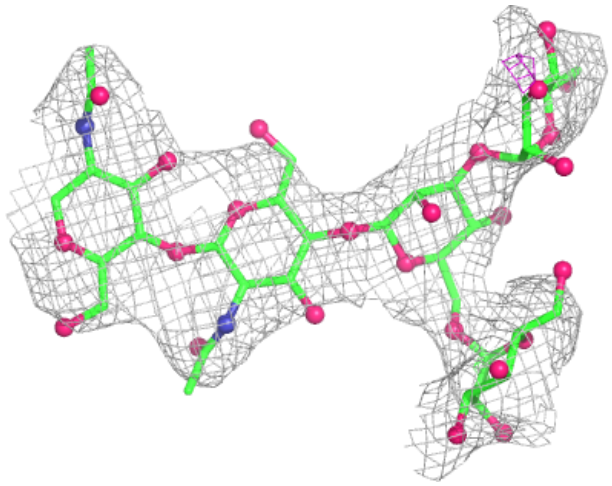


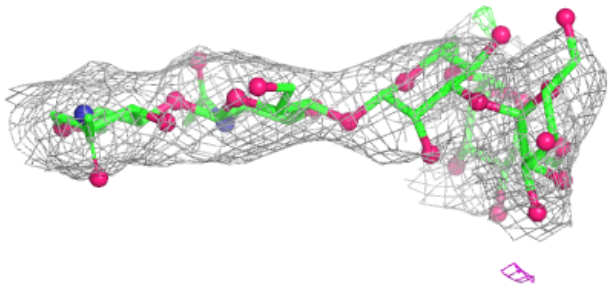


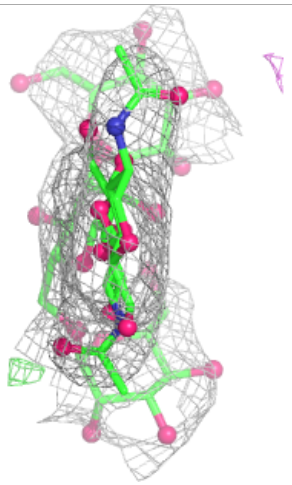


Electron density around Chain a:

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

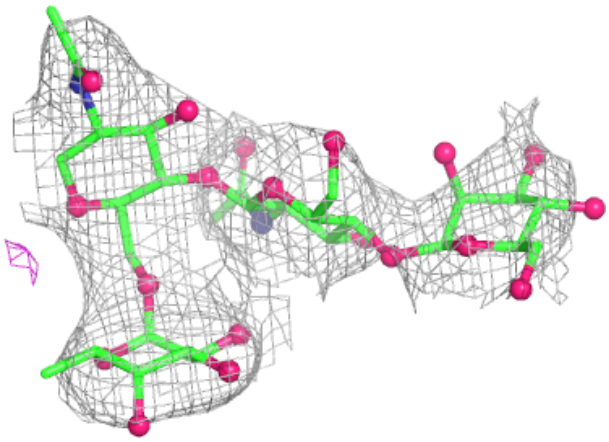


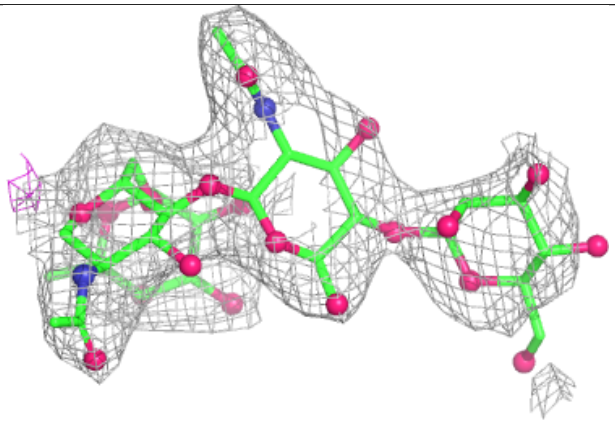


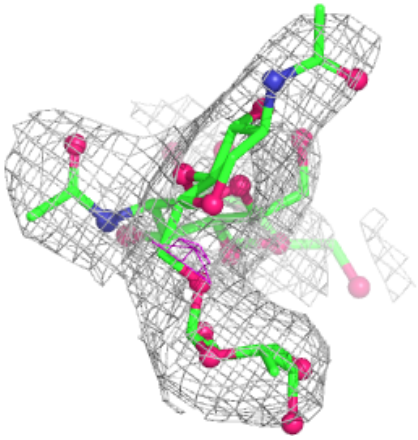


Electron density around Chain V:

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

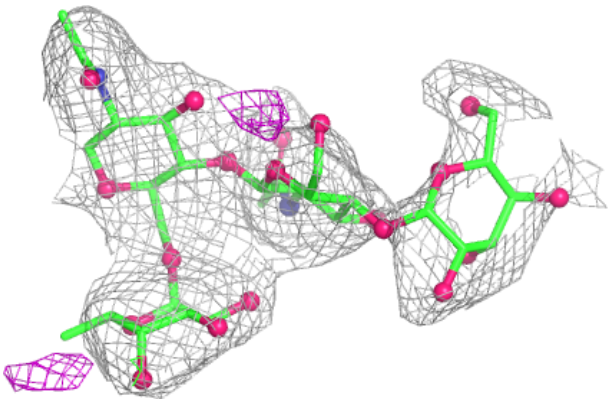


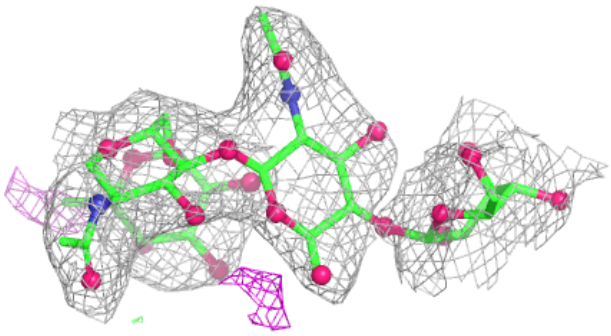


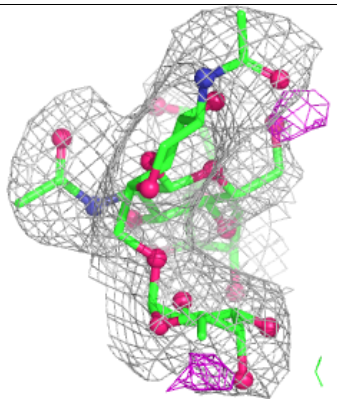


Electron density around Chain d:

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

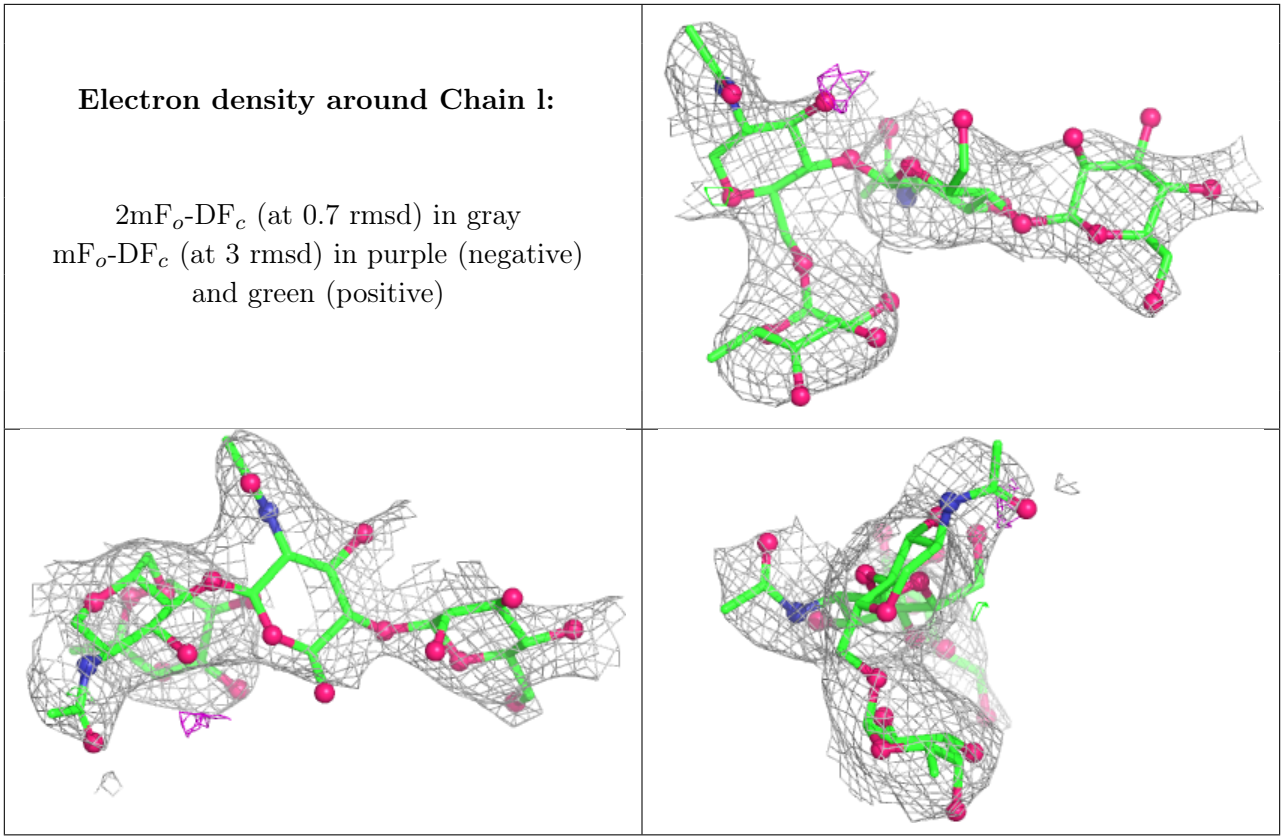






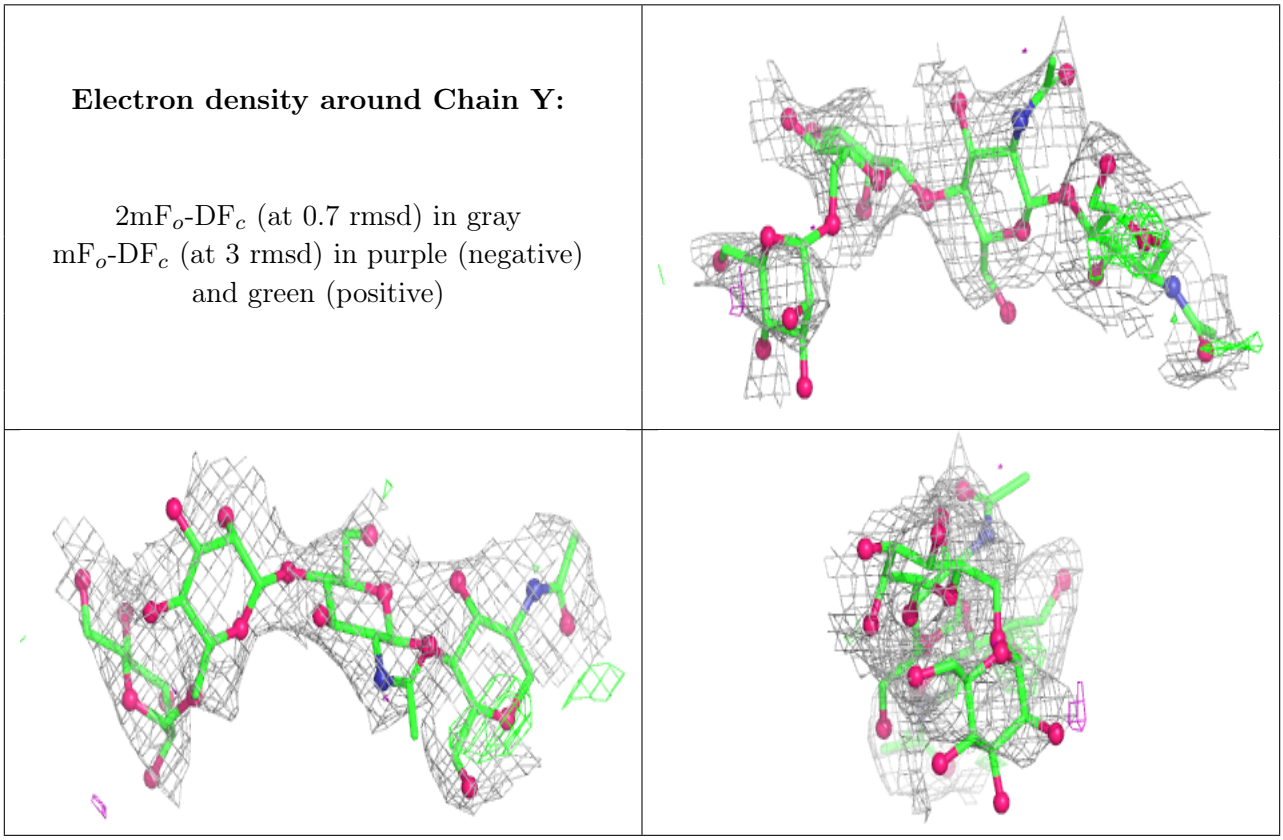
Electron density around Chain l:

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



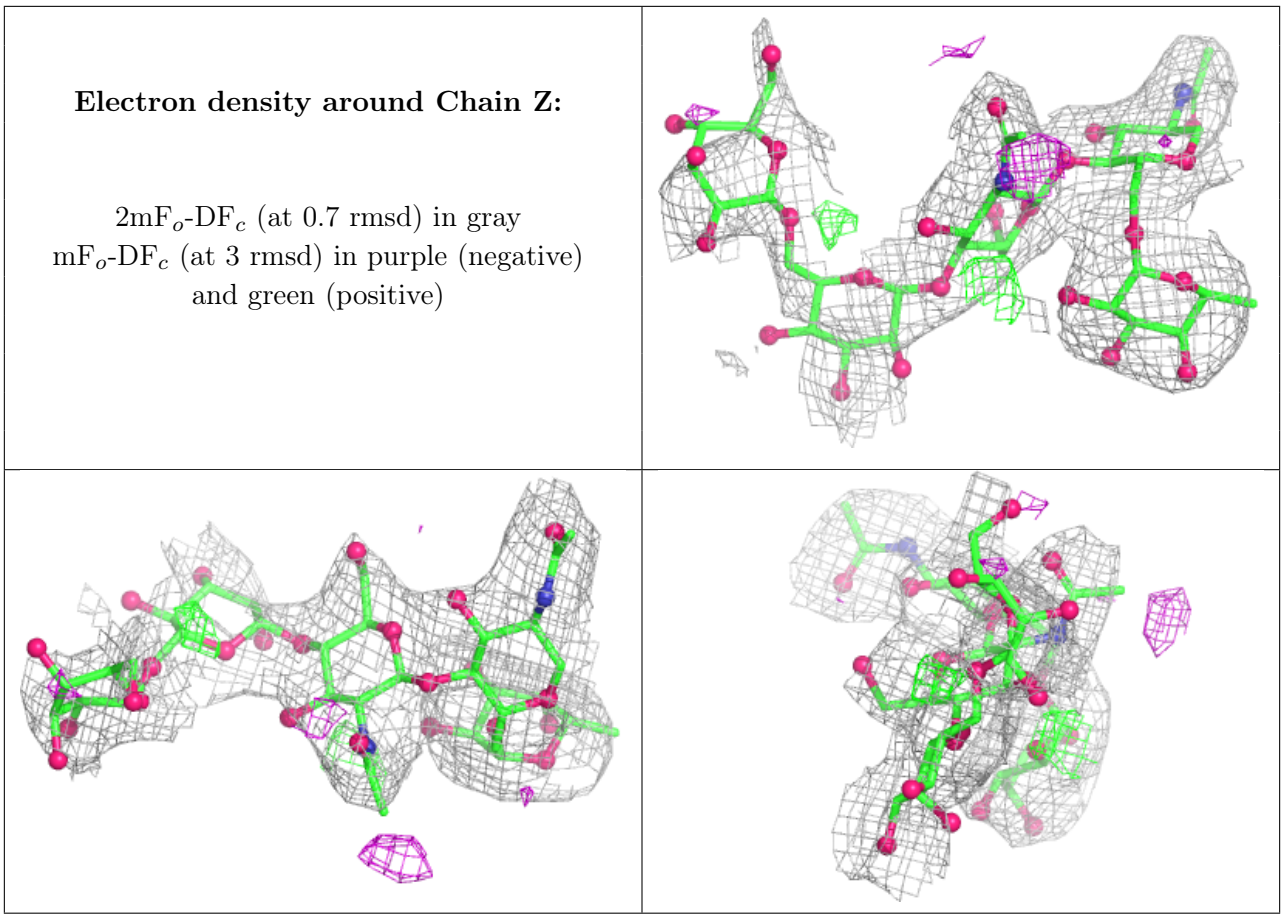
Electron density around Chain Y:

$2mF_o$-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 Z:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	NAG	F	903	14/15	0.53	0.48	123,127,133,137	0
12	SO4	E	202	5/5	0.54	0.39	185,186,186,187	0
13	NAG	J	903	14/15	0.55	0.47	144,150,154,156	0
12	SO4	C	205	5/5	0.63	0.30	191,191,192,192	0
12	SO4	C	203	5/5	0.69	0.34	174,175,176,176	0
13	NAG	F	901	14/15	0.69	0.43	151,155,162,163	0
13	NAG	B	901	14/15	0.70	0.44	145,152,156,156	0
13	NAG	H	903	14/15	0.70	0.34	127,135,140,144	0
12	SO4	D	423	5/5	0.70	0.23	158,159,159,159	0
12	SO4	G	202	5/5	0.73	0.29	160,160,160,160	0
12	SO4	D	422	5/5	0.73	0.20	171,172,173,174	0
12	SO4	F	824	5/5	0.76	0.47	163,163,163,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	NAG	B	902	14/15	0.76	0.25	128,137,143,144	0
13	NAG	D	902	14/15	0.77	0.27	119,125,137,138	0
12	SO4	F	825	5/5	0.79	0.17	158,159,161,161	0
12	SO4	A	202	5/5	0.80	0.31	147,148,148,150	0
12	SO4	H	821	5/5	0.81	0.25	166,169,169,171	0
12	SO4	J	413	5/5	0.81	0.19	125,126,126,127	0
12	SO4	H	820	5/5	0.81	0.50	142,143,144,147	0
12	SO4	D	420	5/5	0.82	0.22	146,147,147,148	0
12	SO4	E	203	5/5	0.83	0.25	121,121,122,123	0
13	NAG	H	901	14/15	0.83	0.30	124,131,134,135	0
12	SO4	H	817	5/5	0.85	0.57	142,143,143,144	0
12	SO4	D	425	5/5	0.85	0.14	144,146,147,147	0
12	SO4	D	424	5/5	0.85	0.18	130,130,132,133	0
12	SO4	B	824	5/5	0.86	0.26	155,155,156,156	0
12	SO4	B	821	5/5	0.86	0.32	144,145,145,147	0
12	SO4	D	421	5/5	0.86	0.40	129,129,132,133	0
12	SO4	H	818	5/5	0.87	0.34	147,148,148,149	0
12	SO4	C	204	5/5	0.87	0.30	126,129,129,131	0
12	SO4	B	822	5/5	0.87	0.17	162,163,163,163	0
12	SO4	H	819	5/5	0.88	0.17	159,159,159,160	0
12	SO4	B	820	5/5	0.88	0.29	126,127,129,129	0
12	SO4	D	419	5/5	0.88	0.45	144,145,146,146	0
12	SO4	C	202	5/5	0.88	0.22	142,143,143,144	0
12	SO4	L	412	5/5	0.89	0.18	157,159,159,160	0
12	SO4	B	823	5/5	0.90	0.15	155,157,159,160	0
12	SO4	F	822	5/5	0.91	0.21	119,120,121,121	0
12	SO4	F	821	5/5	0.92	0.34	112,114,115,116	0
12	SO4	F	823	5/5	0.94	0.19	121,122,123,123	0
12	SO4	I	201	5/5	0.94	0.11	124,125,125,126	0
12	SO4	K	201	5/5	0.96	0.16	123,124,124,125	0
12	SO4	C	201	5/5	0.97	0.14	118,118,119,119	0
12	SO4	E	201	5/5	0.98	0.12	81,82,82,83	0
12	SO4	A	201	5/5	0.98	0.18	76,77,78,78	0
12	SO4	G	201	5/5	0.99	0.13	63,68,68,70	0

6.5 Other polymers (i)

There are no such residues in this entry.