wwPDB EM Validation Summary Report (i)

Mar 10, 2022 – 02:04 am GMT

PDB ID	:	7PC2
EMDB ID	:	EMD-13316
Title	:	HIV-1 Env (BG505 SOSIP.664) in complex with the IgA bNAb 7-269 and the antibody 3BNC117.
Authors	:	Fernandez, I.; Bontems, F.; Pehau-Arnaudet, G.; Rey, F.
Deposited on	:	2021-08-03
Resolution	:	2.80 Å(reported)
Based on initial model	:	5V8M

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

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

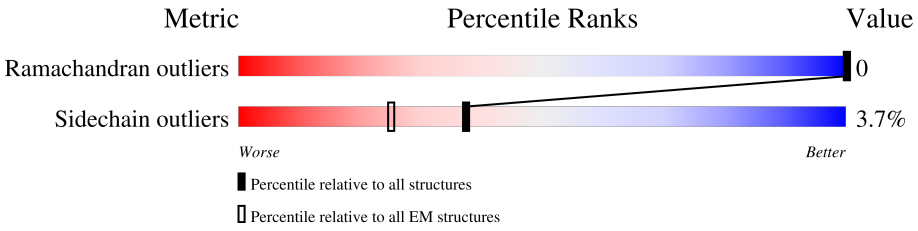
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	M	240	48% 51% · 46%
1	O	240	36% 52% · 46%
1	Q	240	41% 50% · 46%
2	N	215	37% 47% · 50%
2	P	215	33% 47% · 50%
2	R	215	40% 48% · 50%
3	A	481	65% 91% · 7%
3	B	481	62% 90% · 7%
3	C	481	62% 91% · 7%

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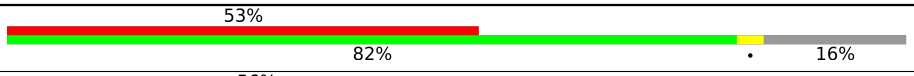
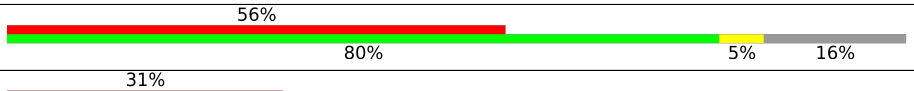
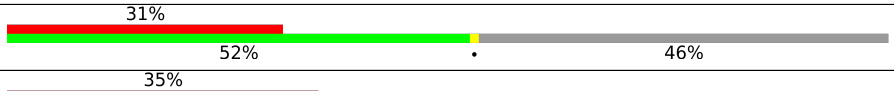
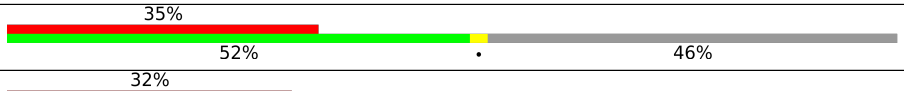
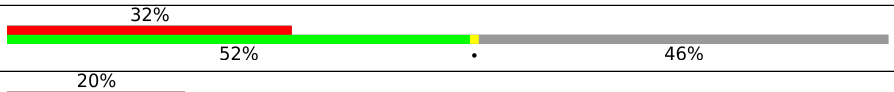
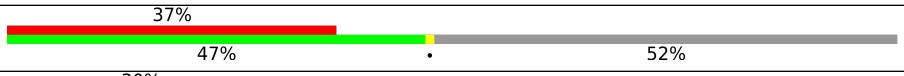
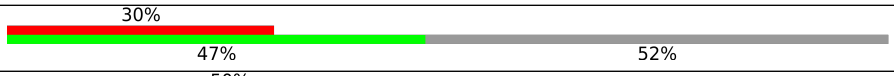
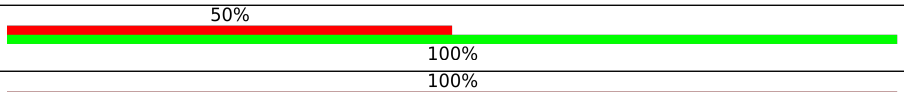
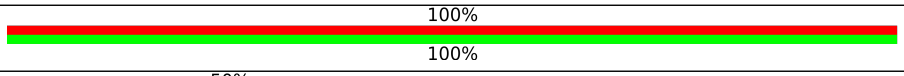
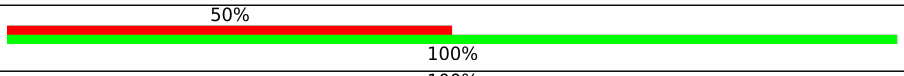
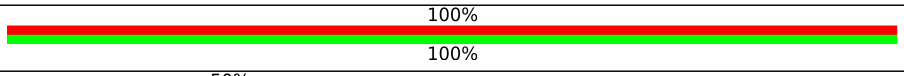
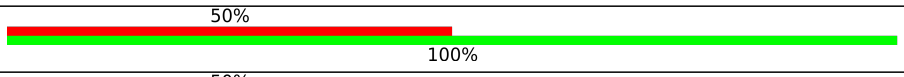
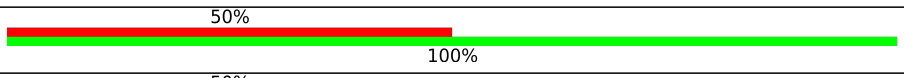
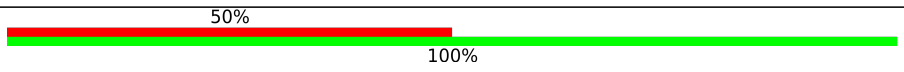
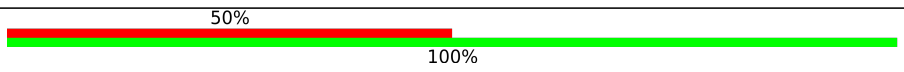
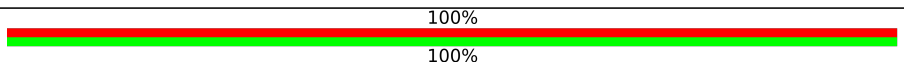
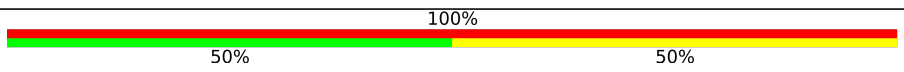
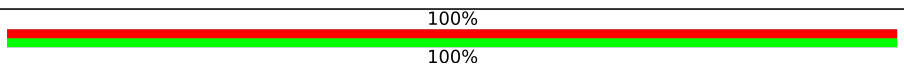
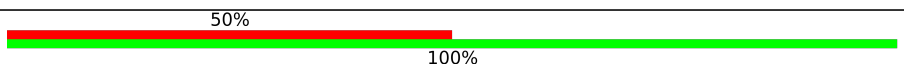
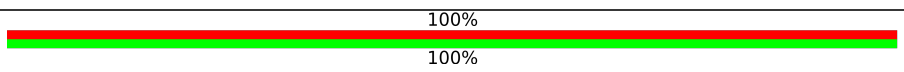
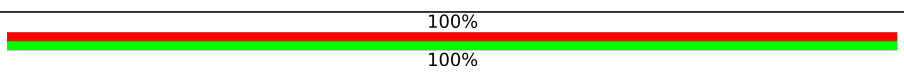
Mol	Chain	Length	Quality of chain
4	D	153	
4	E	153	
4	F	153	
5	G	226	
5	I	226	
5	K	226	
6	H	206	
6	J	206	
6	L	206	
7	4	2	
7	7	2	
7	8	2	
7	9	2	
7	S	2	
7	T	2	
7	U	2	
7	V	2	
7	Z	2	
7	d	2	
7	g	2	
7	h	2	
7	i	2	
7	j	2	
7	k	2	
7	p	2	

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Mol	Chain	Length	Quality of chain
7	v	2	100% 100%
7	w	2	50% 100%
7	x	2	100% 100%
8	W	9	78% 22% 78%
8	s	9	89% 22% 78%
8	y	9	89% 33% 67%
9	X	8	100% 25% 75%
9	l	8	100% 38% 62%
9	z	8	75% 38% 62%
10	0	3	100% 100%
10	2	3	67% 67% 33%
10	3	3	100% 100%
10	Y	3	67% 100%
10	c	3	100% 67% 33%
10	f	3	100% 100%
10	m	3	100% 100%
10	o	3	67% 100%
10	t	3	67% 100%
10	u	3	100% 67% 33%
11	6	11	82% 18% 82%
11	a	11	82% 18% 82%
11	r	11	64% 18% 82%
12	b	7	71% 43% 57%
13	1	5	100% 60% 40%
13	e	5	40% 60% 40%

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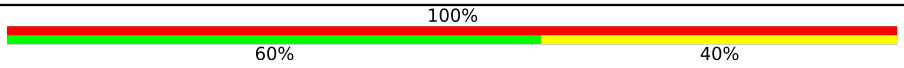
Mol	Chain	Length	Quality of chain
13	n	5	
14	5	8	
14	q	8	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 27063 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 7-269 IgA Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	130	Total	C	N	O	S	0	0
			1031	646	181	195	9		
1	M	130	Total	C	N	O	S	0	0
			1031	646	181	195	9		
1	Q	130	Total	C	N	O	S	0	0
			1031	646	181	195	9		

- Molecule 2 is a protein called 7-269 IgA Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	108	Total	C	N	O	S	0	0
			821	515	140	163	3		
2	N	108	Total	C	N	O	S	0	0
			821	515	140	163	3		
2	R	108	Total	C	N	O	S	0	0
			821	515	140	163	3		

- Molecule 3 is a protein called gp120, BG505 SOSIP.664 T332N.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	445	Total	C	N	O	S	0	0
			3499	2195	618	658	28		
3	B	445	Total	C	N	O	S	0	0
			3499	2195	618	658	28		
3	C	445	Total	C	N	O	S	0	0
			3499	2195	618	658	28		

- Molecule 4 is a protein called gp41 BG505 T332N SOSIP.664.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		
4	F	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		

- Molecule 5 is a protein called 3BNC IgG Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
5	G	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
5	I	121	Total	C	N	O	S	0	0
			985	626	177	179	3		

- Molecule 6 is a protein called 3BNC117 IgG Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
6	H	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
6	J	98	Total	C	N	O	S	0	0
			783	493	137	150	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		

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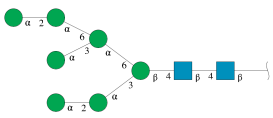
Mol	Chain	Residues	Atoms				AltConf	Trace
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	d	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	h	2	Total	C	N	O	0	0
			28	16	2	10		
7	i	2	Total	C	N	O	0	0
			28	16	2	10		
7	j	2	Total	C	N	O	0	0
			28	16	2	10		
7	k	2	Total	C	N	O	0	0
			28	16	2	10		
7	p	2	Total	C	N	O	0	0
			28	16	2	10		
7	v	2	Total	C	N	O	0	0
			28	16	2	10		
7	w	2	Total	C	N	O	0	0
			28	16	2	10		
7	x	2	Total	C	N	O	0	0
			28	16	2	10		
7	4	2	Total	C	N	O	0	0
			28	16	2	10		
7	7	2	Total	C	N	O	0	0
			28	16	2	10		
7	8	2	Total	C	N	O	0	0
			28	16	2	10		
7	9	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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				AltConf	Trace
8	W	9	Total	C	N	O	0	0
			105	58	2	45		

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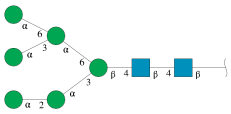
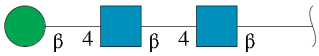
Mol	Chain	Residues	Atoms				AltConf	Trace
8	s	9	Total 105	C 58	N 2	O 45	0	0
8	y	9	Total 105	C 58	N 2	O 45	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	8	Total 94	C 52	N 2	O 40	0	0
9	l	8	Total 94	C 52	N 2	O 40	0	0
9	z	8	Total 94	C 52	N 2	O 40	0	0

- Molecule 10 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				AltConf	Trace
10	Y	3	Total 39	C 22	N 2	O 15	0	0
10	c	3	Total 39	C 22	N 2	O 15	0	0
10	f	3	Total 39	C 22	N 2	O 15	0	0
10	m	3	Total 39	C 22	N 2	O 15	0	0
10	o	3	Total 39	C 22	N 2	O 15	0	0
10	t	3	Total 39	C 22	N 2	O 15	0	0

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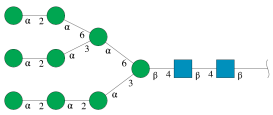
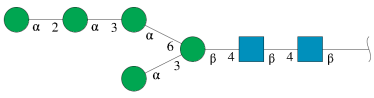
Mol	Chain	Residues	Atoms				AltConf	Trace
10	u	3	Total	C	N	O	0	0
			39	22	2	15		
10	0	3	Total	C	N	O	0	0
			39	22	2	15		
10	2	3	Total	C	N	O	0	0
			39	22	2	15		
10	3	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
11	a	11	Total	C	N	O	0	0
			127	70	2	55		
11	r	11	Total	C	N	O	0	0
			127	70	2	55		
11	6	11	Total	C	N	O	0	0
			127	70	2	55		

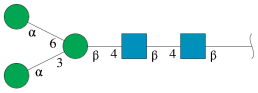
- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

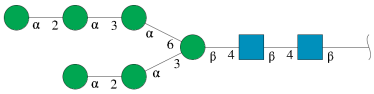
- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-

acetamido-2-deoxy-beta-D-glucopyranose.



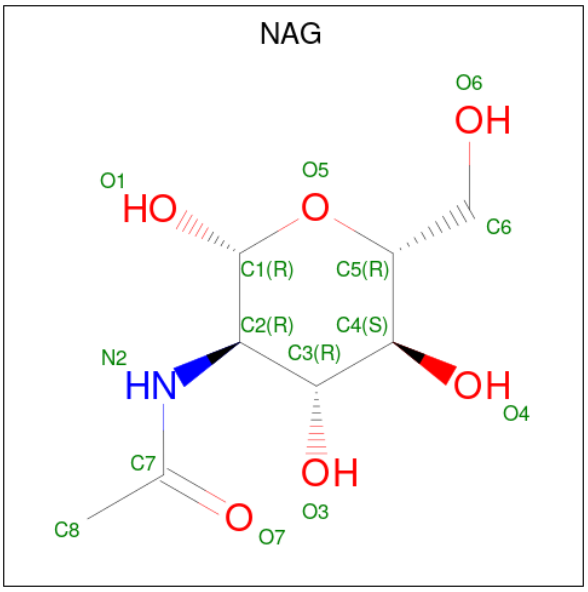
Mol	Chain	Residues	Atoms				AltConf	Trace
13	e	5	Total	C	N	O	0	0
			61	34	2	25		
13	n	5	Total	C	N	O	0	0
			61	34	2	25		
13	1	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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				AltConf	Trace
14	q	8	Total	C	N	O	0	0
			94	52	2	40		
14	5	8	Total	C	N	O	0	0
			94	52	2	40		

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



Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total	C	N	O	0
			70	40	5	25	
15	A	1	Total	C	N	O	0
			70	40	5	25	
15	A	1	Total	C	N	O	0
			70	40	5	25	
15	A	1	Total	C	N	O	0
			70	40	5	25	
15	A	1	Total	C	N	O	0
			70	40	5	25	
15	B	1	Total	C	N	O	0
			70	40	5	25	
15	B	1	Total	C	N	O	0
			70	40	5	25	
15	B	1	Total	C	N	O	0
			70	40	5	25	
15	B	1	Total	C	N	O	0
			70	40	5	25	
15	B	1	Total	C	N	O	0
			70	40	5	25	
15	C	1	Total	C	N	O	0
			56	32	4	20	
15	C	1	Total	C	N	O	0
			56	32	4	20	
15	C	1	Total	C	N	O	0
			56	32	4	20	
15	C	1	Total	C	N	O	0
			56	32	4	20	

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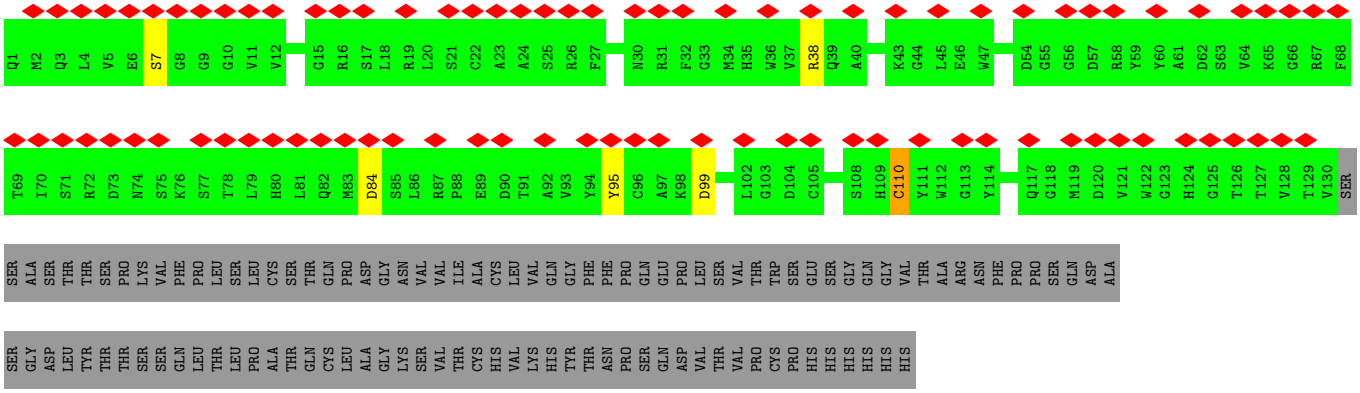
Mol	Chain	Residues	Atoms				AltConf
15	D	1	Total	C	N	O	0
			28	16	2	10	
15	D	1	Total	C	N	O	0
			28	16	2	10	
15	E	1	Total	C	N	O	0
			28	16	2	10	
15	E	1	Total	C	N	O	0
			28	16	2	10	
15	F	1	Total	C	N	O	0
			28	16	2	10	
15	F	1	Total	C	N	O	0
			28	16	2	10	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

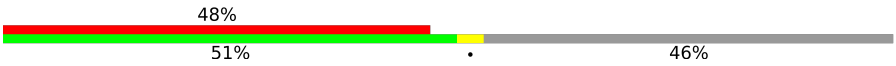
- Molecule 1: 7-269 IgA Fab heavy chain

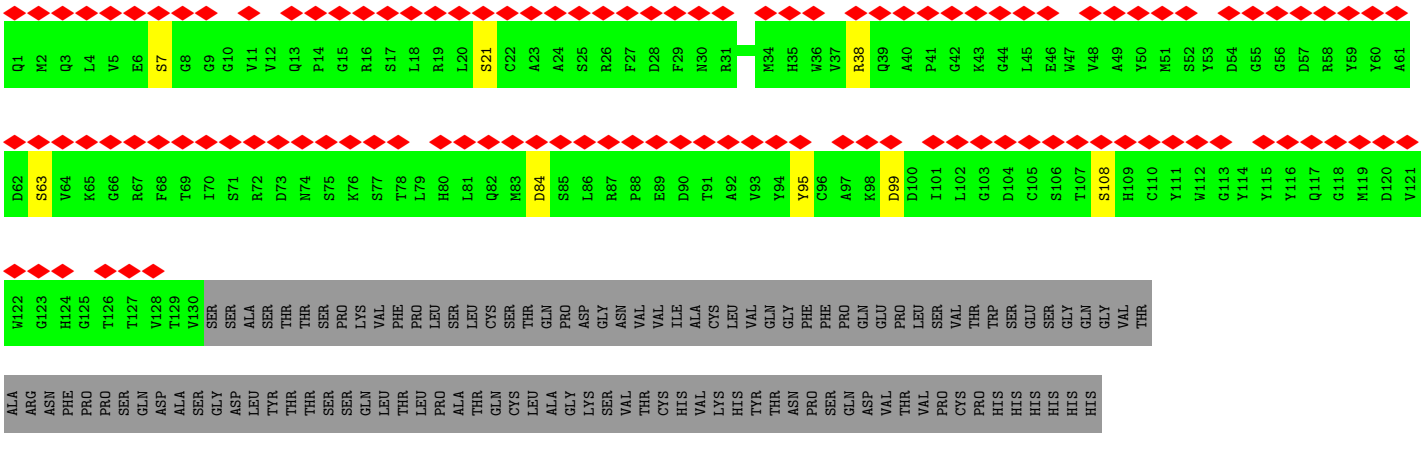
Chain O:



- Molecule 1: 7-269 IgA Fab heavy chain

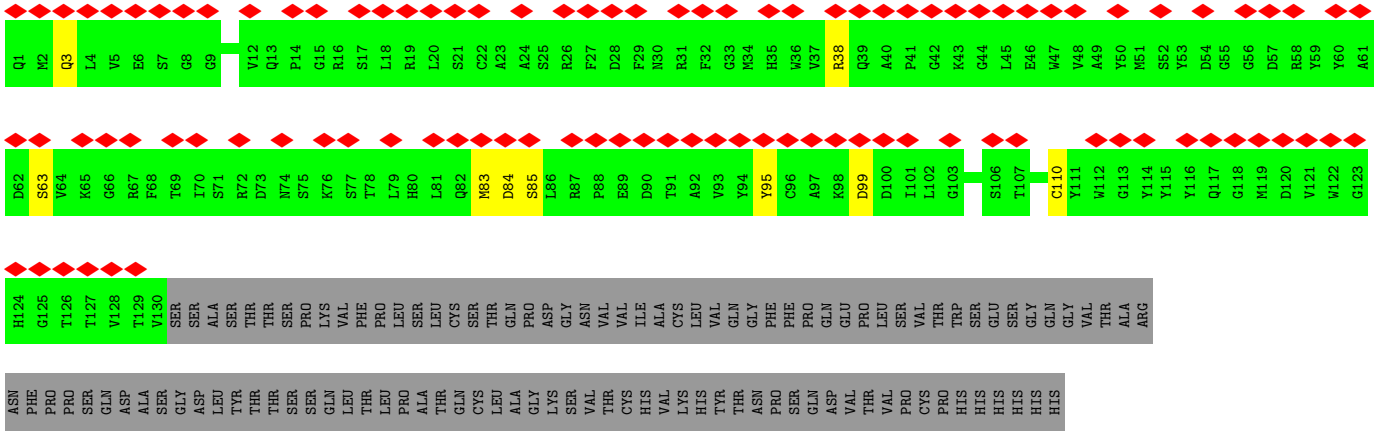
Chain M:





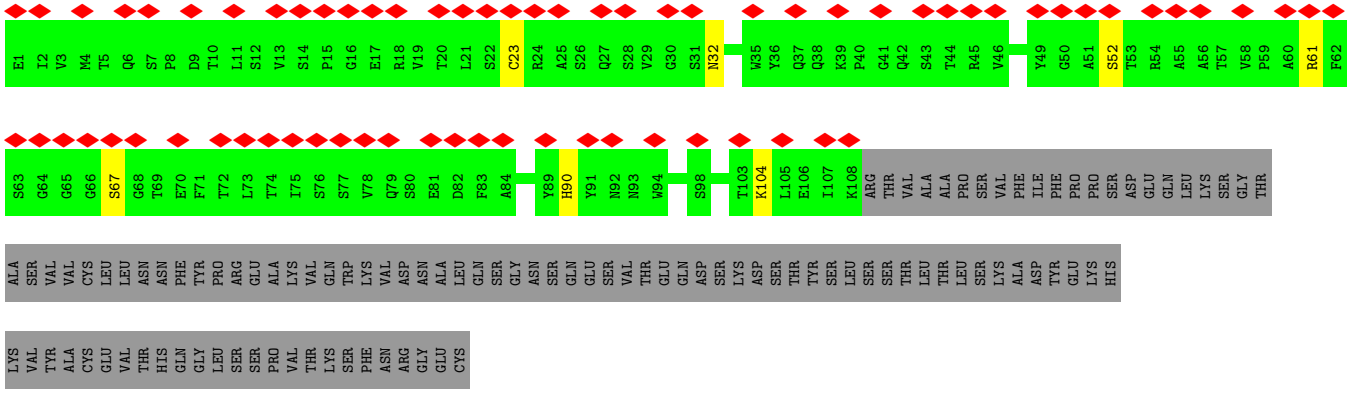
- Molecule 1: 7-269 IgA Fab heavy chain

Chain Q:



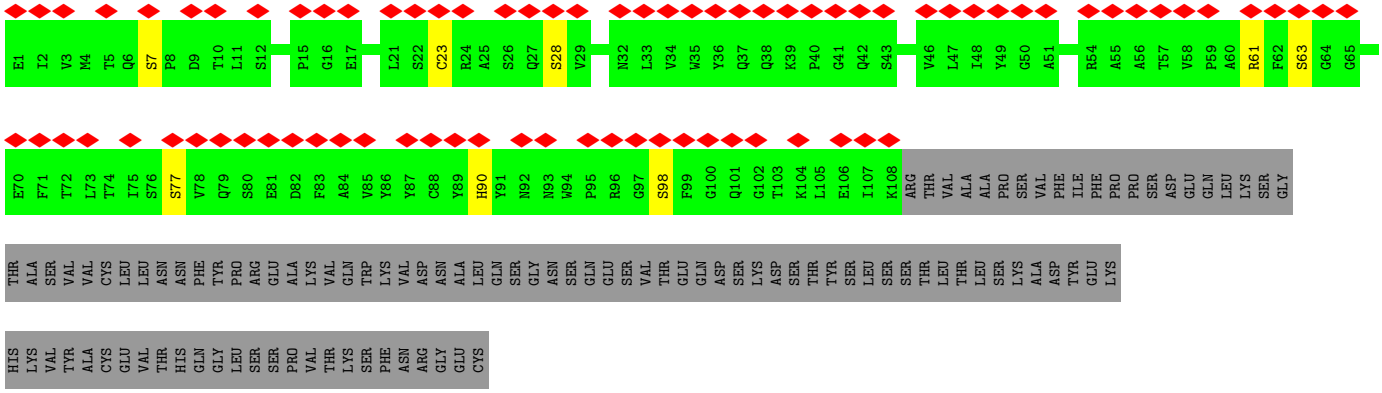
• Molecule 2: 7-269 IgA Fab light chain

Chain P:



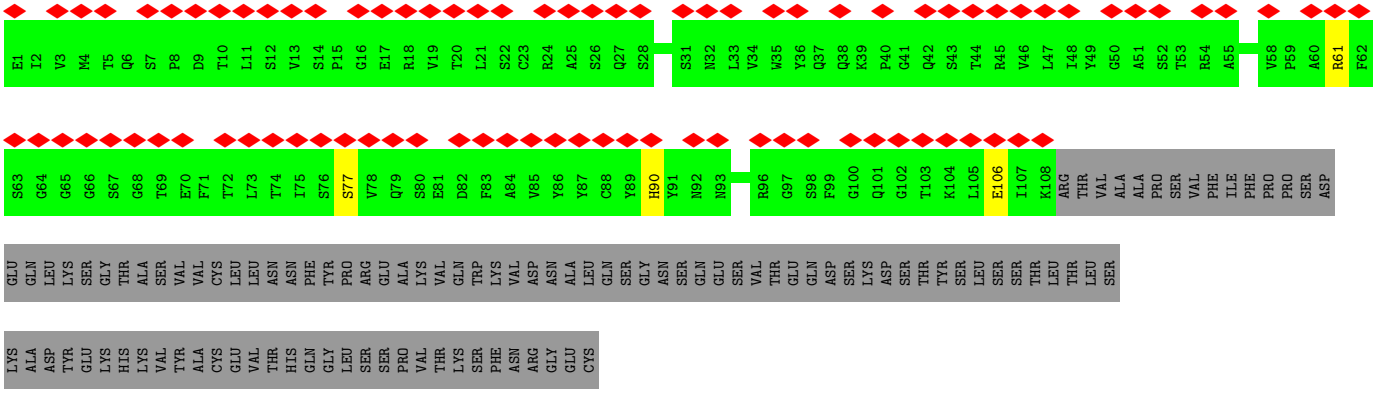
• Molecule 2: 7-269 IgA Fab light chain

Chain N:



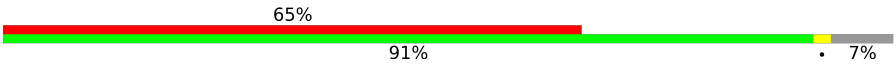
• Molecule 2: 7-269 IgA Fab light chain

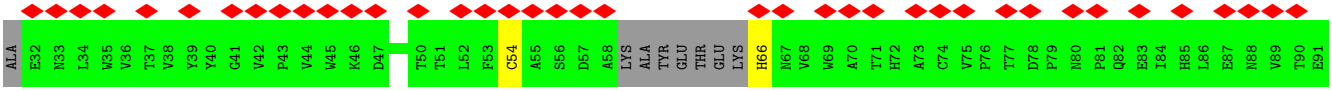
Chain R:

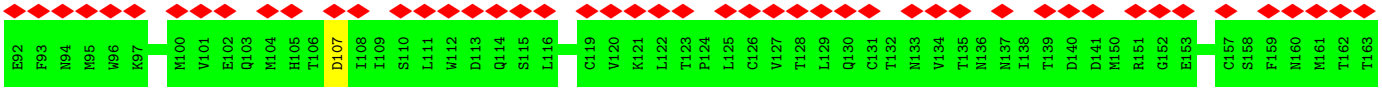


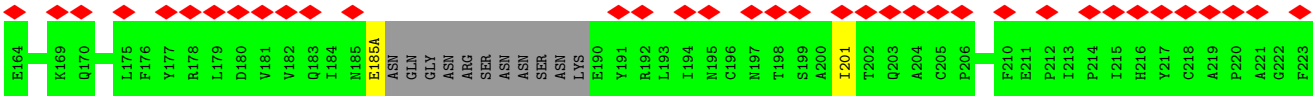
• Molecule 3: gp120, BG505 SOSIP.664 T332N

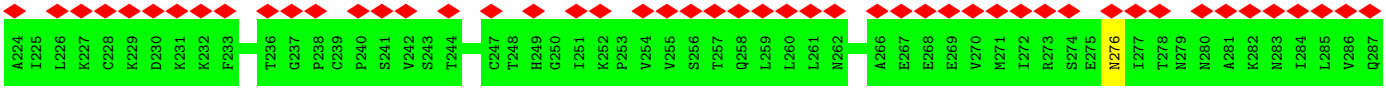
Chain A:

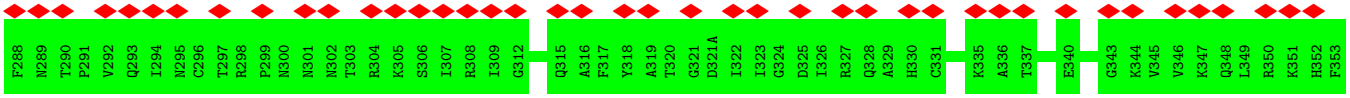


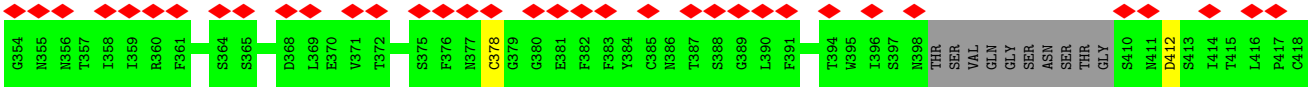


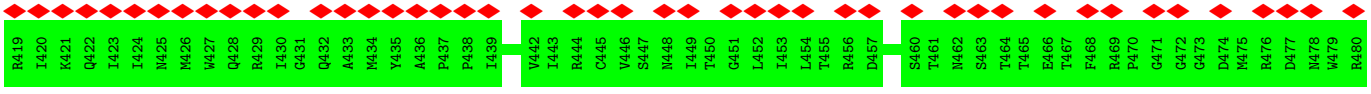


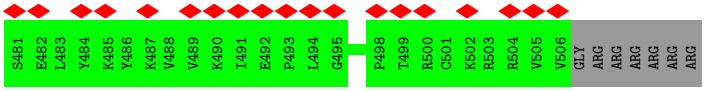






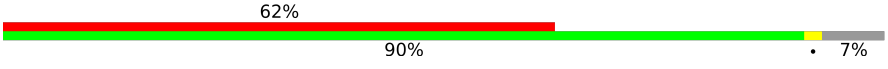


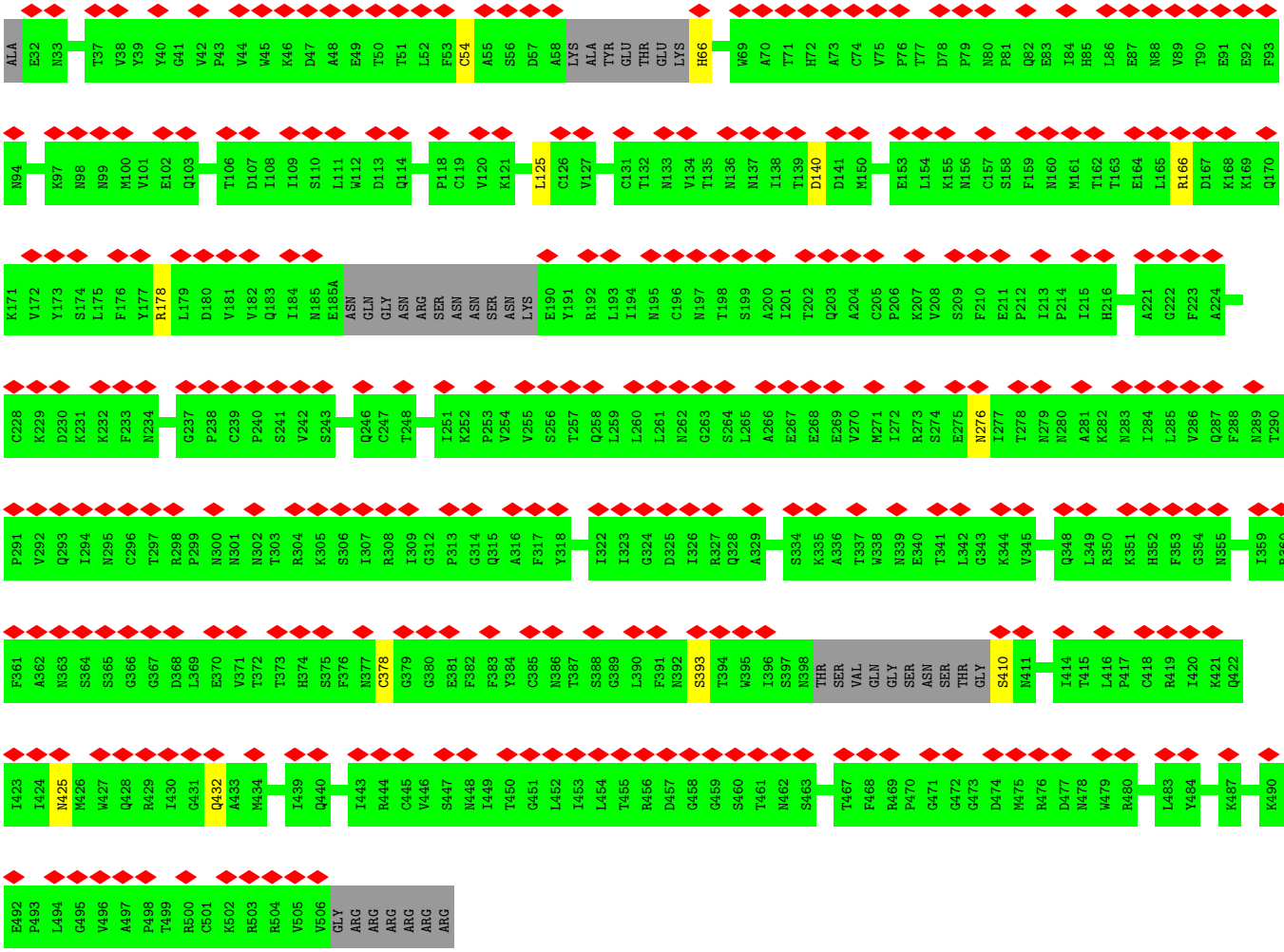




• Molecule 3: gp120, BG505 SOSIP.664 T332N

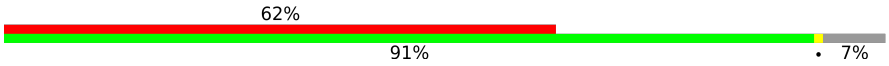
Chain B:

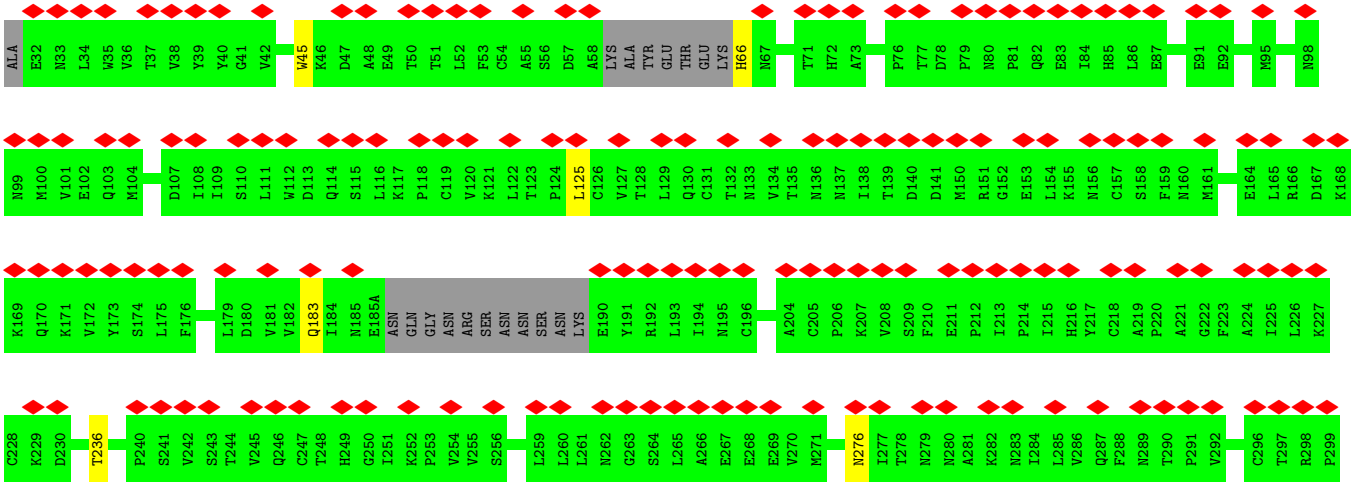


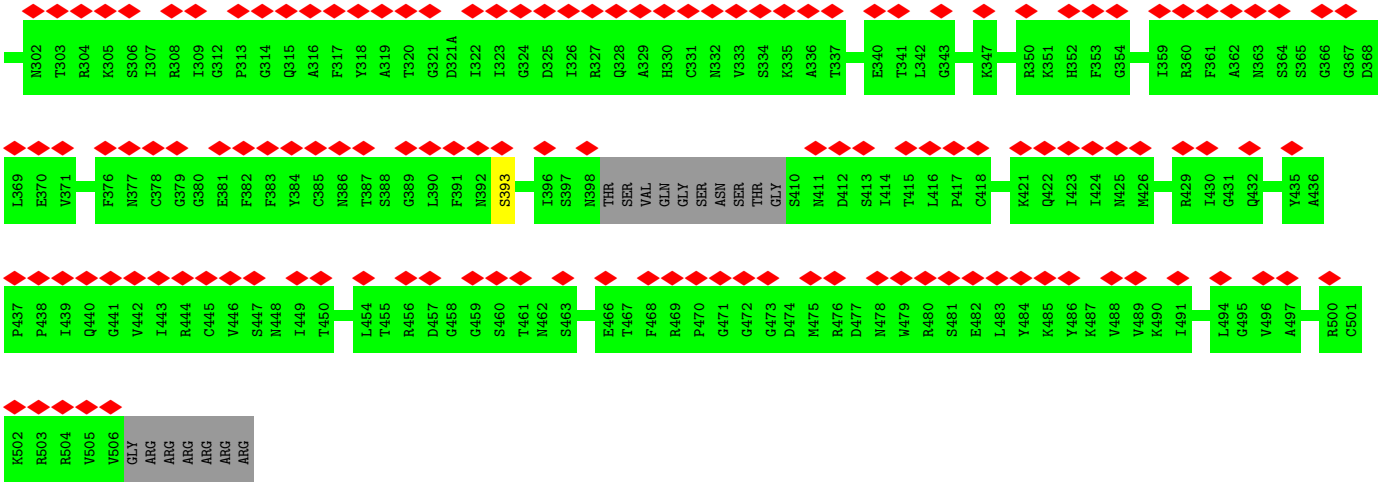


• Molecule 3: gp120, BG505 SOSIP.664 T332N

Chain C:

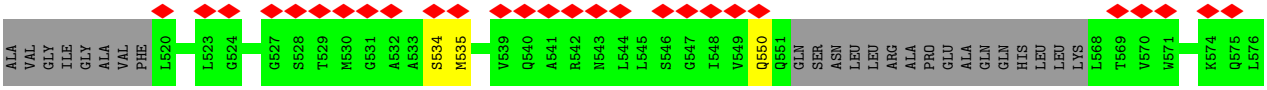


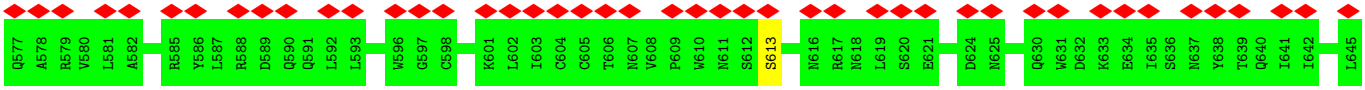


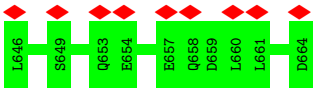


• Molecule 4: gp41 BG505 T332N SOSIP.664

Chain D:

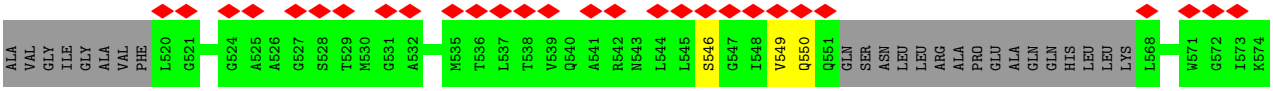


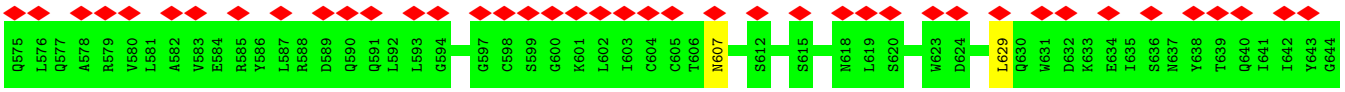


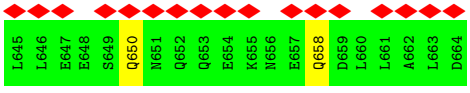


• Molecule 4: gp41 BG505 T332N SOSIP.664

Chain E:

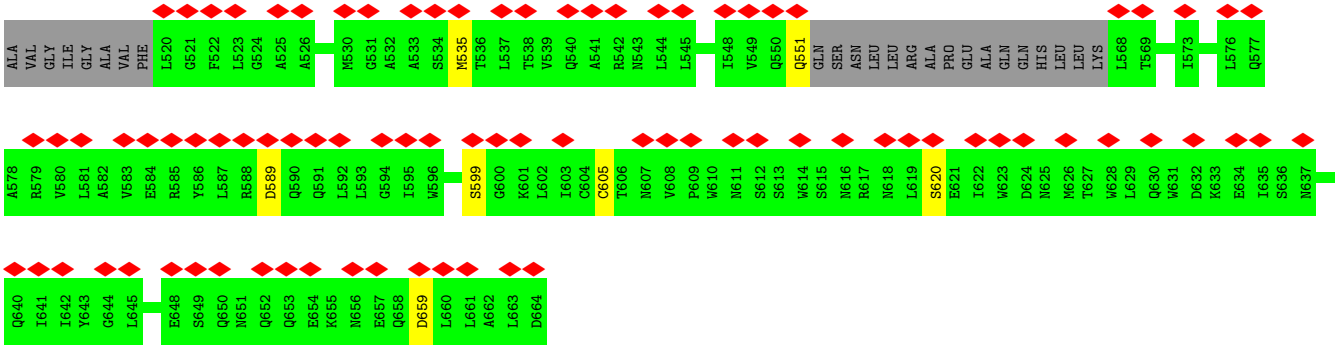






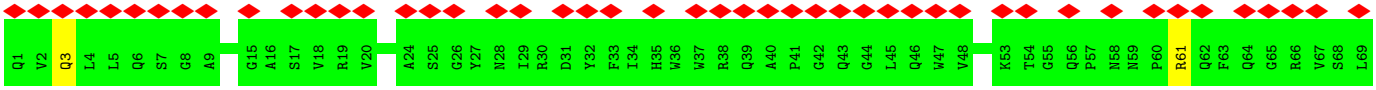
• Molecule 4: gp41 BG505 T332N SOSIP.664

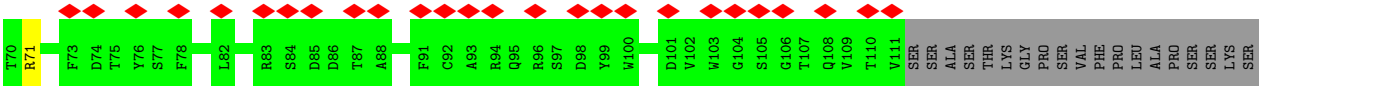
Chain F:

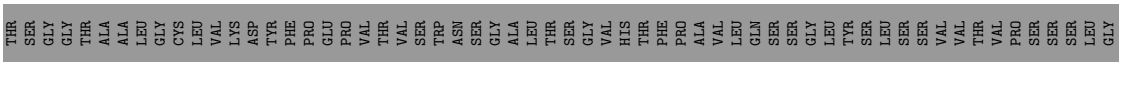


• Molecule 5: 3BNC IgG Fab heavy chain

Chain K:

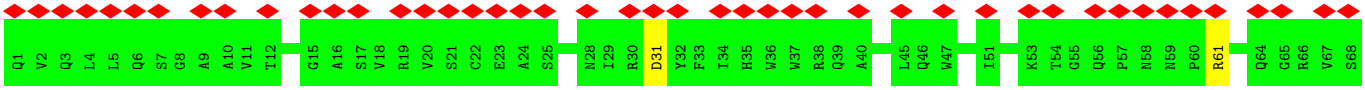


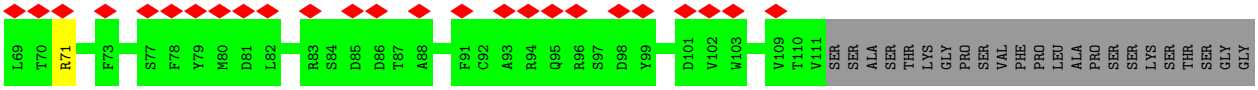


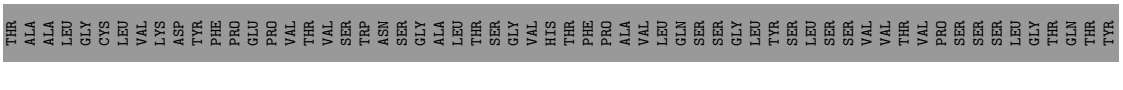


• Molecule 5: 3BNC IgG Fab heavy chain

Chain G:

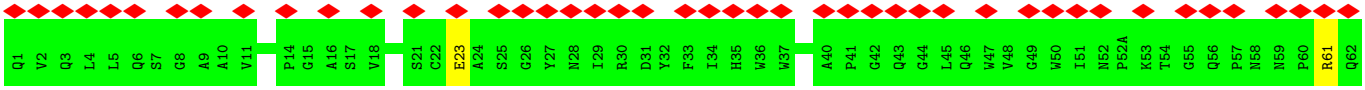


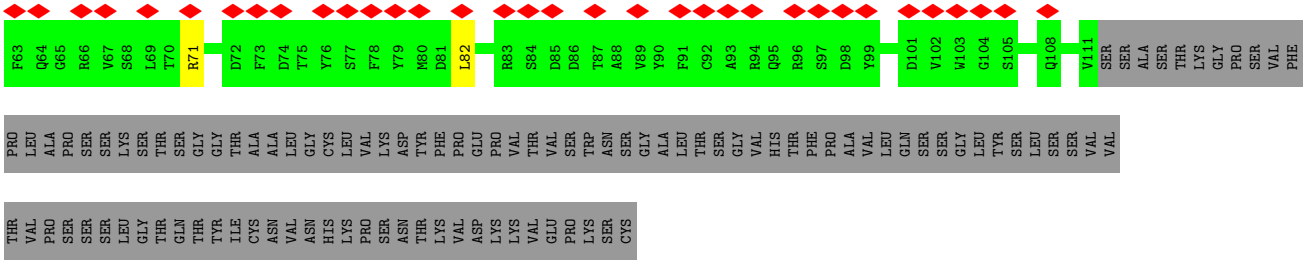




• Molecule 5: 3BNC IgG Fab heavy chain

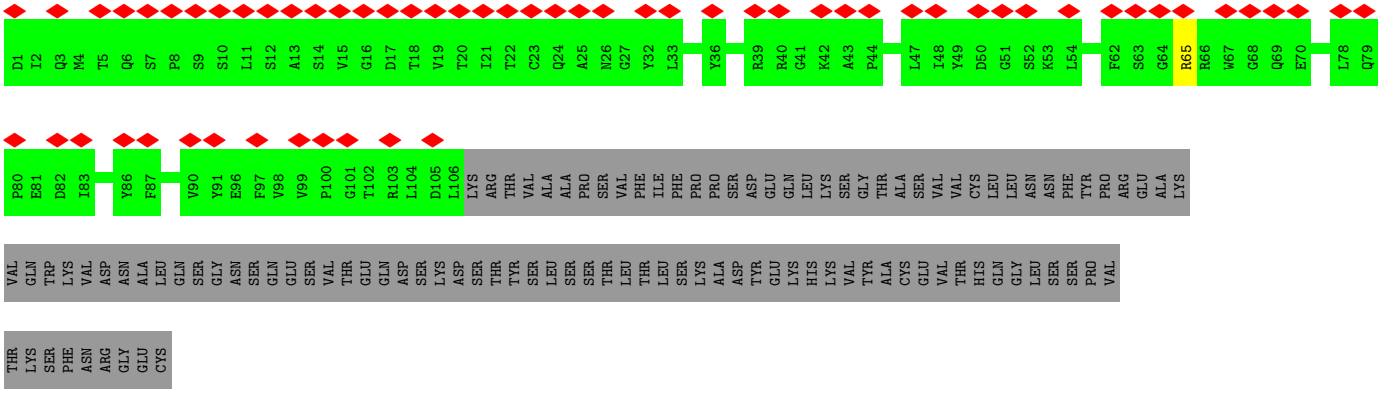
Chain I:





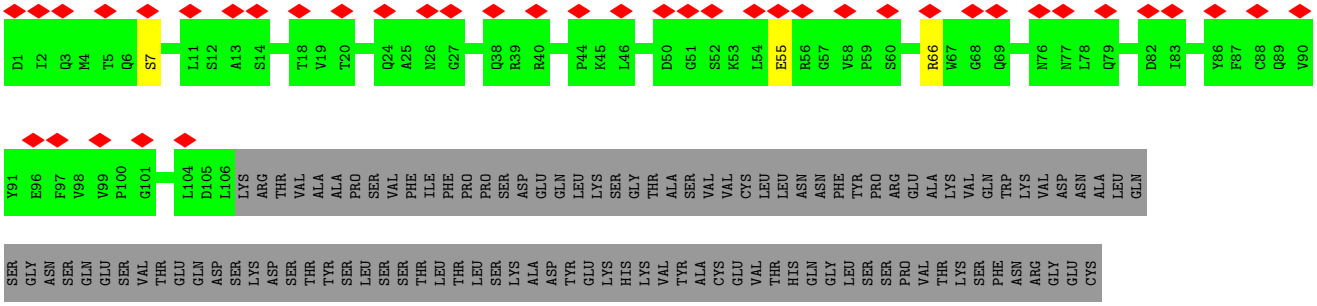
• Molecule 6: 3BNC117 IgG Fab light chain

Chain L:



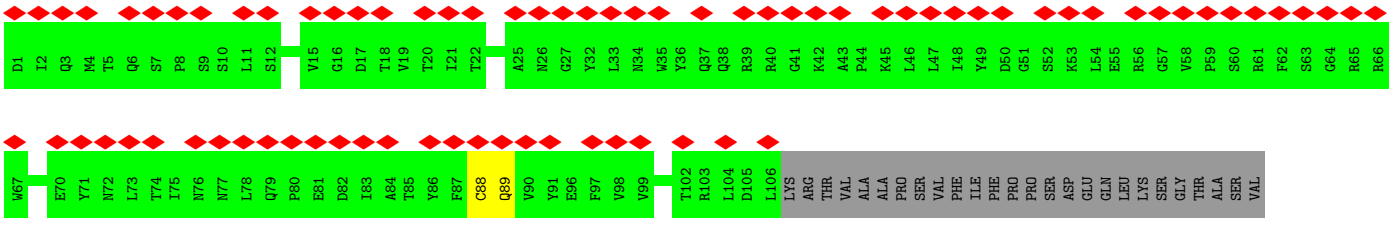
• Molecule 6: 3BNC117 IgG Fab light chain

Chain H:



• Molecule 6: 3BNC117 IgG Fab light chain

Chain J:



VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP SER LYS ASP SER THR TYR SER LEU SER SER THR LEU THR LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR

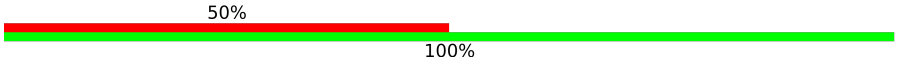
ALA CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

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

Chain S:

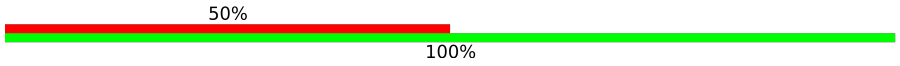
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



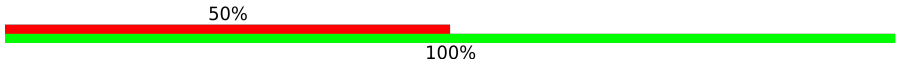
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



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

Chain V:

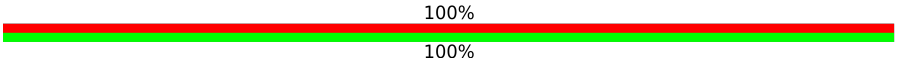


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

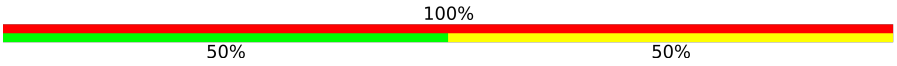
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



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

Chain g:

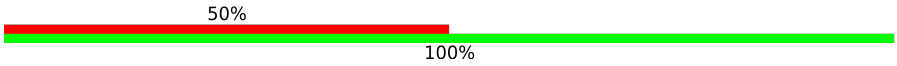


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

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

Chain i:



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

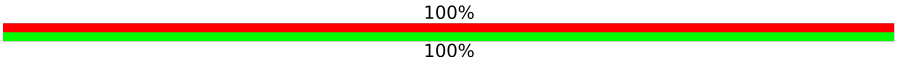
Chain j:

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

Chain k:

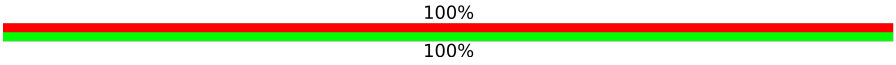
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:



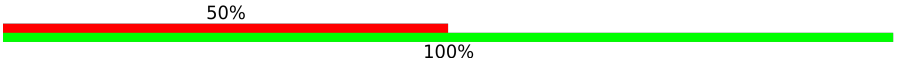
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:



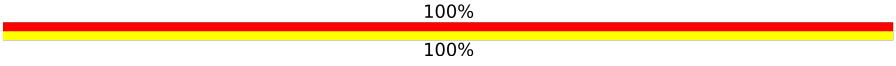
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:



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

Chain x:

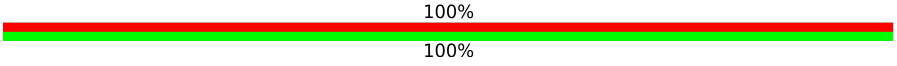


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:

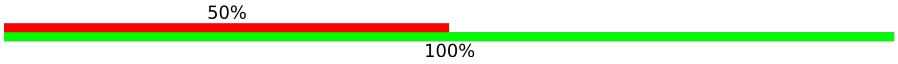
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:



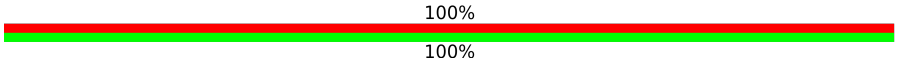
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8:



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

Chain 9:



• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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

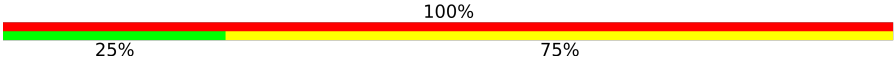
Chain s:

• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 y:

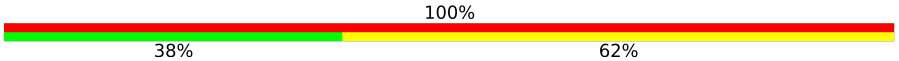
• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

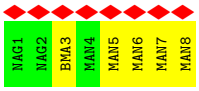
Chain X:



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

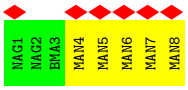
Chain l:





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

Chain z:



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

Chain Y:

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

Chain c:

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

Chain f:

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

Chain m:

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

Chain o:

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

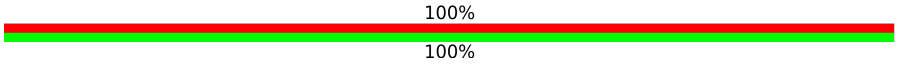
Chain t:

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

Chain u:

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

Chain 0:



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

Chain 2:

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

Chain 3:

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

Chain a:

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

Chain r:

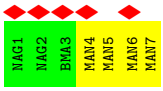
• Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1

-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos
e

Chain 6:

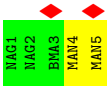
• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyra
nose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta
-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



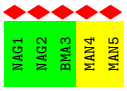
• Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyran
ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra
nose

Chain e:



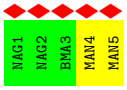
• Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyran
ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra
nose

Chain n:



• Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyran
ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra
nose

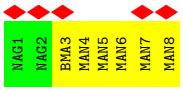
Chain 1:



• Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyra
nose-(1-6)-[alpha-D-mannopyranose-(1-2)-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-glucopyranos
e

Chain q:



• Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyra
nose-(1-6)-[alpha-D-mannopyranose-(1-2)-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-glucopyranos
e

Chain 5:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	115394	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.634	Depositor
Minimum map value	-0.659	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.29	Depositor
Map size (Å)	357.0, 357.0, 357.0	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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

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	M	0.51	0/1059	0.63	2/1432 (0.1%)
1	O	0.31	0/1059	0.50	1/1432 (0.1%)
1	Q	0.31	0/1059	0.50	1/1432 (0.1%)
2	N	0.30	0/840	0.47	0/1142
2	P	0.30	0/840	0.47	0/1142
2	R	0.29	0/840	0.47	0/1142
3	A	0.44	0/3569	0.52	0/4844
3	B	0.54	0/3569	0.54	0/4844
3	C	0.48	0/3569	0.53	0/4844
4	D	0.31	0/1041	0.44	0/1412
4	E	0.31	0/1041	0.45	0/1412
4	F	0.31	0/1041	0.46	0/1412
5	G	0.37	0/1017	0.48	0/1386
5	I	0.36	0/1017	0.48	0/1386
5	K	0.36	0/1017	0.48	0/1386
6	H	0.33	0/798	0.79	2/1080 (0.2%)
6	J	0.31	0/798	0.46	0/1080
6	L	0.30	0/798	0.45	0/1080
All	All	0.41	0/24972	0.52	6/33888 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	7	SER	CB-CA-C	-15.52	80.62	110.10
6	H	7	SER	N-CA-C	13.66	147.88	111.00
1	M	108	SER	CB-CA-C	-7.99	94.93	110.10
1	M	108	SER	N-CA-C	7.81	132.09	111.00
1	Q	110	CYS	CA-CB-SG	5.30	123.54	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 PDB entries followed by that with respect to all EM entries.

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	M	128/240 (53%)	114 (89%)	14 (11%)	0	100	100
1	O	128/240 (53%)	115 (90%)	13 (10%)	0	100	100
1	Q	128/240 (53%)	117 (91%)	11 (9%)	0	100	100
2	N	106/215 (49%)	96 (91%)	10 (9%)	0	100	100
2	P	106/215 (49%)	97 (92%)	9 (8%)	0	100	100
2	R	106/215 (49%)	98 (92%)	8 (8%)	0	100	100
3	A	433/481 (90%)	398 (92%)	35 (8%)	0	100	100
3	B	433/481 (90%)	405 (94%)	28 (6%)	0	100	100
3	C	433/481 (90%)	405 (94%)	28 (6%)	0	100	100
4	D	125/153 (82%)	113 (90%)	12 (10%)	0	100	100
4	E	125/153 (82%)	114 (91%)	11 (9%)	0	100	100
4	F	125/153 (82%)	111 (89%)	14 (11%)	0	100	100
5	G	119/226 (53%)	112 (94%)	7 (6%)	0	100	100
5	I	119/226 (53%)	111 (93%)	8 (7%)	0	100	100
5	K	119/226 (53%)	112 (94%)	7 (6%)	0	100	100
6	H	92/206 (45%)	83 (90%)	9 (10%)	0	100	100
6	J	92/206 (45%)	86 (94%)	6 (6%)	0	100	100
6	L	92/206 (45%)	86 (94%)	6 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3009/4563 (66%)	2773 (92%)	236 (8%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	M	108/206 (52%)	101 (94%)	7 (6%)	17 44
1	O	108/206 (52%)	102 (94%)	6 (6%)	21 51
1	Q	108/206 (52%)	100 (93%)	8 (7%)	13 37
2	N	90/187 (48%)	82 (91%)	8 (9%)	9 28
2	P	90/187 (48%)	83 (92%)	7 (8%)	12 35
2	R	90/187 (48%)	86 (96%)	4 (4%)	28 61
3	A	398/428 (93%)	390 (98%)	8 (2%)	55 84
3	B	398/428 (93%)	386 (97%)	12 (3%)	41 75
3	C	398/428 (93%)	391 (98%)	7 (2%)	59 86
4	D	111/129 (86%)	107 (96%)	4 (4%)	35 69
4	E	111/129 (86%)	104 (94%)	7 (6%)	18 46
4	F	111/129 (86%)	104 (94%)	7 (6%)	18 46
5	G	102/193 (53%)	99 (97%)	3 (3%)	42 76
5	I	102/193 (53%)	98 (96%)	4 (4%)	32 66
5	K	102/193 (53%)	99 (97%)	3 (3%)	42 76
6	H	86/183 (47%)	84 (98%)	2 (2%)	50 82
6	J	86/183 (47%)	84 (98%)	2 (2%)	50 82
6	L	86/183 (47%)	85 (99%)	1 (1%)	71 92
All	All	2685/3978 (68%)	2585 (96%)	100 (4%)	37 68

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	410	SER
4	E	546	SER
6	J	89	GLN
3	B	432	GLN
3	C	276	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	432	GLN
3	C	355	ASN
3	C	33	ASN
3	C	203	GLN
4	F	540	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

190 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	$\#\|Z\| > 2$
10	NAG	0	1	3,10	14,14,15	0.22	0	17,19,21	0.47	0
10	NAG	0	2	10	14,14,15	0.21	0	17,19,21	0.46	0
10	BMA	0	3	10	11,11,12	0.50	0	15,15,17	0.75	0
13	NAG	1	1	3,13	14,14,15	0.40	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	NAG	1	2	13	14,14,15	0.31	0	17,19,21	0.45	0
13	BMA	1	3	13	11,11,12	0.58	0	15,15,17	0.73	0
13	MAN	1	4	13	11,11,12	0.63	0	15,15,17	1.11	2 (13%)
13	MAN	1	5	13	11,11,12	0.65	0	15,15,17	1.00	2 (13%)
10	NAG	2	1	3,10	14,14,15	0.30	0	17,19,21	0.66	1 (5%)
10	NAG	2	2	10	14,14,15	0.22	0	17,19,21	0.40	0
10	BMA	2	3	10	11,11,12	0.51	0	15,15,17	0.75	0
10	NAG	3	1	3,10	14,14,15	0.25	0	17,19,21	0.44	0
10	NAG	3	2	10	14,14,15	0.17	0	17,19,21	0.41	0
10	BMA	3	3	10	11,11,12	0.60	0	15,15,17	0.91	0
7	NAG	4	1	3,7	14,14,15	0.20	0	17,19,21	0.59	0
7	NAG	4	2	7	14,14,15	0.26	0	17,19,21	0.43	0
14	NAG	5	1	3,14	14,14,15	0.40	0	17,19,21	1.30	2 (11%)
14	NAG	5	2	14	14,14,15	0.34	0	17,19,21	0.53	0
14	BMA	5	3	14	11,11,12	0.72	0	15,15,17	0.96	1 (6%)
14	MAN	5	4	14	11,11,12	0.62	0	15,15,17	0.96	1 (6%)
14	MAN	5	5	14	11,11,12	0.63	0	15,15,17	1.15	2 (13%)
14	MAN	5	6	14	11,11,12	0.71	0	15,15,17	1.11	1 (6%)
14	MAN	5	7	14	11,11,12	0.87	1 (9%)	15,15,17	1.20	1 (6%)
14	MAN	5	8	14	11,11,12	0.71	0	15,15,17	0.99	1 (6%)
11	NAG	6	1	11,3	14,14,15	0.50	0	17,19,21	0.41	0
11	MAN	6	10	11	11,11,12	0.75	0	15,15,17	1.24	2 (13%)
11	MAN	6	11	11	11,11,12	0.76	1 (9%)	15,15,17	0.93	1 (6%)
11	NAG	6	2	11	14,14,15	0.32	0	17,19,21	0.49	0
11	BMA	6	3	11	11,11,12	0.59	0	15,15,17	0.96	1 (6%)
11	MAN	6	4	11	11,11,12	0.76	0	15,15,17	1.25	2 (13%)
11	MAN	6	5	11	11,11,12	0.69	0	15,15,17	0.93	1 (6%)
11	MAN	6	6	11	11,11,12	0.55	0	15,15,17	1.12	2 (13%)
11	MAN	6	7	11	11,11,12	0.67	0	15,15,17	1.23	2 (13%)
11	MAN	6	8	11	11,11,12	0.59	0	15,15,17	1.19	2 (13%)
11	MAN	6	9	11	11,11,12	0.59	0	15,15,17	0.99	1 (6%)
7	NAG	7	1	7,6	14,14,15	0.22	0	17,19,21	0.38	0
7	NAG	7	2	7	14,14,15	0.20	0	17,19,21	0.41	0
7	NAG	8	1	7,6	14,14,15	0.24	0	17,19,21	0.37	0
7	NAG	8	2	7	14,14,15	0.19	0	17,19,21	0.41	0
7	NAG	9	1	7,6	14,14,15	0.23	0	17,19,21	0.37	0
7	NAG	9	2	7	14,14,15	0.20	0	17,19,21	0.37	0
7	NAG	S	1	3,7	14,14,15	0.24	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	S	2	7	14,14,15	0.40	0	17,19,21	1.25	1 (5%)
7	NAG	T	1	3,7	14,14,15	0.22	0	17,19,21	0.47	0
7	NAG	T	2	7	14,14,15	0.20	0	17,19,21	0.40	0
7	NAG	U	1	3,7	14,14,15	0.36	0	17,19,21	0.41	0
7	NAG	U	2	7	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	V	1	3,7	14,14,15	0.44	0	17,19,21	0.46	0
7	NAG	V	2	7	14,14,15	0.23	0	17,19,21	0.41	0
8	NAG	W	1	3,8	14,14,15	0.30	0	17,19,21	0.52	0
8	NAG	W	2	8	14,14,15	0.32	0	17,19,21	0.51	0
8	BMA	W	3	8	11,11,12	0.84	0	15,15,17	0.99	1 (6%)
8	MAN	W	4	8	11,11,12	0.55	0	15,15,17	1.18	2 (13%)
8	MAN	W	5	8	11,11,12	0.58	0	15,15,17	1.09	2 (13%)
8	MAN	W	6	8	11,11,12	0.65	0	15,15,17	0.91	1 (6%)
8	MAN	W	7	8	11,11,12	0.66	0	15,15,17	1.43	2 (13%)
8	MAN	W	8	8	11,11,12	0.67	0	15,15,17	1.30	2 (13%)
8	MAN	W	9	8	11,11,12	0.53	0	15,15,17	1.15	2 (13%)
9	NAG	X	1	3,9	14,14,15	0.39	0	17,19,21	0.43	0
9	NAG	X	2	9	14,14,15	0.18	0	17,19,21	0.42	0
9	BMA	X	3	9	11,11,12	0.58	0	15,15,17	0.71	1 (6%)
9	MAN	X	4	9	11,11,12	0.68	0	15,15,17	1.24	2 (13%)
9	MAN	X	5	9	11,11,12	0.71	0	15,15,17	0.88	1 (6%)
9	MAN	X	6	9	11,11,12	0.61	0	15,15,17	1.06	2 (13%)
9	MAN	X	7	9	11,11,12	0.60	0	15,15,17	1.06	2 (13%)
9	MAN	X	8	9	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
10	NAG	Y	1	3,10	14,14,15	0.24	0	17,19,21	0.46	0
10	NAG	Y	2	10	14,14,15	0.20	0	17,19,21	0.45	0
10	BMA	Y	3	10	11,11,12	0.54	0	15,15,17	0.75	0
7	NAG	Z	1	3,7	14,14,15	0.21	0	17,19,21	0.57	0
7	NAG	Z	2	7	14,14,15	0.26	0	17,19,21	0.43	0
11	NAG	a	1	11,3	14,14,15	0.53	0	17,19,21	0.40	0
11	MAN	a	10	11	11,11,12	0.86	0	15,15,17	1.51	2 (13%)
11	MAN	a	11	11	11,11,12	0.62	0	15,15,17	1.65	2 (13%)
11	NAG	a	2	11	14,14,15	0.34	0	17,19,21	0.48	0
11	BMA	a	3	11	11,11,12	0.59	0	15,15,17	0.97	1 (6%)
11	MAN	a	4	11	11,11,12	0.78	0	15,15,17	1.25	2 (13%)
11	MAN	a	5	11	11,11,12	0.69	0	15,15,17	0.93	1 (6%)
11	MAN	a	6	11	11,11,12	0.56	0	15,15,17	1.20	2 (13%)
11	MAN	a	7	11	11,11,12	0.69	0	15,15,17	1.23	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	MAN	a	8	11	11,11,12	0.56	0	15,15,17	1.19	2 (13%)
11	MAN	a	9	11	11,11,12	0.54	0	15,15,17	1.01	2 (13%)
12	NAG	b	1	12,3	14,14,15	0.60	0	17,19,21	0.46	0
12	NAG	b	2	12	14,14,15	0.24	0	17,19,21	0.56	0
12	BMA	b	3	12	11,11,12	0.73	0	15,15,17	0.96	0
12	MAN	b	4	12	11,11,12	0.55	0	15,15,17	1.02	2 (13%)
12	MAN	b	5	12	11,11,12	0.61	0	15,15,17	1.08	2 (13%)
12	MAN	b	6	12	11,11,12	0.67	0	15,15,17	1.12	2 (13%)
12	MAN	b	7	12	11,11,12	0.68	0	15,15,17	0.93	1 (6%)
10	NAG	c	1	3,10	14,14,15	0.41	0	17,19,21	1.30	2 (11%)
10	NAG	c	2	10	14,14,15	0.20	0	17,19,21	0.43	0
10	BMA	c	3	10	11,11,12	0.60	0	15,15,17	0.70	0
7	NAG	d	1	3,7	14,14,15	0.31	0	17,19,21	0.47	0
7	NAG	d	2	7	14,14,15	0.23	0	17,19,21	0.39	0
13	NAG	e	1	3,13	14,14,15	0.42	0	17,19,21	0.40	0
13	NAG	e	2	13	14,14,15	0.27	0	17,19,21	0.50	0
13	BMA	e	3	13	11,11,12	0.62	0	15,15,17	0.75	0
13	MAN	e	4	13	11,11,12	0.65	0	15,15,17	0.95	1 (6%)
13	MAN	e	5	13	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
10	NAG	f	1	3,10	14,14,15	0.29	0	17,19,21	0.65	0
10	NAG	f	2	10	14,14,15	0.22	0	17,19,21	0.44	0
10	BMA	f	3	10	11,11,12	0.54	0	15,15,17	0.75	0
7	NAG	g	1	3,7	14,14,15	0.26	0	17,19,21	0.47	0
7	NAG	g	2	7	14,14,15	0.41	0	17,19,21	1.24	2 (11%)
7	NAG	h	1	3,7	14,14,15	0.17	0	17,19,21	0.49	0
7	NAG	h	2	7	14,14,15	0.18	0	17,19,21	0.41	0
7	NAG	i	1	3,7	14,14,15	0.34	0	17,19,21	0.41	0
7	NAG	i	2	7	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	j	1	3,7	14,14,15	0.41	0	17,19,21	0.46	0
7	NAG	j	2	7	14,14,15	0.25	0	17,19,21	0.38	0
7	NAG	k	1	3,7	14,14,15	0.41	0	17,19,21	1.33	2 (11%)
7	NAG	k	2	7	14,14,15	0.23	0	17,19,21	0.37	0
9	NAG	l	1	3,9	14,14,15	0.49	0	17,19,21	0.40	0
9	NAG	l	2	9	14,14,15	0.19	0	17,19,21	0.44	0
9	BMA	l	3	9	11,11,12	0.55	0	15,15,17	0.71	1 (6%)
9	MAN	l	4	9	11,11,12	0.70	0	15,15,17	1.06	0
9	MAN	l	5	9	11,11,12	0.78	0	15,15,17	1.15	2 (13%)
9	MAN	l	6	9	11,11,12	0.72	0	15,15,17	1.07	1 (6%)
9	MAN	l	7	9	11,11,12	0.63	0	15,15,17	1.24	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	MAN	l	8	9	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
10	NAG	m	1	3,10	14,14,15	0.23	0	17,19,21	0.46	0
10	NAG	m	2	10	14,14,15	0.21	0	17,19,21	0.43	0
10	BMA	m	3	10	11,11,12	0.51	0	15,15,17	0.73	0
13	NAG	n	1	3,13	14,14,15	0.42	0	17,19,21	0.40	0
13	NAG	n	2	13	14,14,15	0.30	0	17,19,21	0.46	0
13	BMA	n	3	13	11,11,12	0.62	0	15,15,17	0.86	0
13	MAN	n	4	13	11,11,12	0.72	0	15,15,17	1.39	2 (13%)
13	MAN	n	5	13	11,11,12	0.74	0	15,15,17	1.27	2 (13%)
10	NAG	o	1	3,10	14,14,15	0.32	0	17,19,21	0.63	0
10	NAG	o	2	10	14,14,15	0.23	0	17,19,21	0.39	0
10	BMA	o	3	10	11,11,12	0.54	0	15,15,17	0.75	0
7	NAG	p	1	3,7	14,14,15	0.21	0	17,19,21	0.57	0
7	NAG	p	2	7	14,14,15	0.24	0	17,19,21	0.44	0
14	NAG	q	1	3,14	14,14,15	0.50	0	17,19,21	0.48	0
14	NAG	q	2	14	14,14,15	0.28	0	17,19,21	0.52	0
14	BMA	q	3	14	11,11,12	0.64	0	15,15,17	0.96	1 (6%)
14	MAN	q	4	14	11,11,12	0.60	0	15,15,17	0.95	1 (6%)
14	MAN	q	5	14	11,11,12	0.62	0	15,15,17	1.13	2 (13%)
14	MAN	q	6	14	11,11,12	0.71	0	15,15,17	1.12	1 (6%)
14	MAN	q	7	14	11,11,12	0.61	0	15,15,17	1.10	2 (13%)
14	MAN	q	8	14	11,11,12	0.66	0	15,15,17	0.94	1 (6%)
11	NAG	r	1	11,3	14,14,15	0.52	0	17,19,21	0.40	0
11	MAN	r	10	11	11,11,12	0.71	0	15,15,17	1.20	2 (13%)
11	MAN	r	11	11	11,11,12	0.73	1 (9%)	15,15,17	0.92	1 (6%)
11	NAG	r	2	11	14,14,15	0.35	0	17,19,21	0.54	0
11	BMA	r	3	11	11,11,12	0.64	0	15,15,17	0.98	1 (6%)
11	MAN	r	4	11	11,11,12	0.75	0	15,15,17	1.24	2 (13%)
11	MAN	r	5	11	11,11,12	0.67	0	15,15,17	0.98	1 (6%)
11	MAN	r	6	11	11,11,12	0.54	0	15,15,17	1.16	2 (13%)
11	MAN	r	7	11	11,11,12	0.68	0	15,15,17	1.21	2 (13%)
11	MAN	r	8	11	11,11,12	0.57	0	15,15,17	1.16	2 (13%)
11	MAN	r	9	11	11,11,12	0.52	0	15,15,17	1.03	2 (13%)
8	NAG	s	1	3,8	14,14,15	0.29	0	17,19,21	0.51	0
8	NAG	s	2	8	14,14,15	0.33	0	17,19,21	0.52	0
8	BMA	s	3	8	11,11,12	0.89	0	15,15,17	1.02	2 (13%)
8	MAN	s	4	8	11,11,12	0.61	0	15,15,17	1.19	2 (13%)
8	MAN	s	5	8	11,11,12	0.61	0	15,15,17	1.11	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	MAN	s	6	8	11,11,12	0.65	0	15,15,17	0.94	1 (6%)
8	MAN	s	7	8	11,11,12	0.63	0	15,15,17	0.89	1 (6%)
8	MAN	s	8	8	11,11,12	0.87	1 (9%)	15,15,17	1.38	3 (20%)
8	MAN	s	9	8	11,11,12	0.76	1 (9%)	15,15,17	0.91	1 (6%)
10	NAG	t	1	3,10	14,14,15	0.28	0	17,19,21	0.43	0
10	NAG	t	2	10	14,14,15	0.19	0	17,19,21	0.39	0
10	BMA	t	3	10	11,11,12	0.56	0	15,15,17	0.73	0
10	NAG	u	1	3,10	14,14,15	0.26	0	17,19,21	0.43	0
10	NAG	u	2	10	14,14,15	0.39	0	17,19,21	1.25	1 (5%)
10	BMA	u	3	10	11,11,12	0.54	0	15,15,17	0.78	0
7	NAG	v	1	3,7	14,14,15	0.36	0	17,19,21	0.41	0
7	NAG	v	2	7	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	w	1	3,7	14,14,15	0.38	0	17,19,21	0.46	0
7	NAG	w	2	7	14,14,15	0.22	0	17,19,21	0.40	0
7	NAG	x	1	3,7	14,14,15	0.46	0	17,19,21	0.72	1 (5%)
7	NAG	x	2	7	14,14,15	0.40	0	17,19,21	0.74	1 (5%)
8	NAG	y	1	3,8	14,14,15	0.29	0	17,19,21	0.52	0
8	NAG	y	2	8	14,14,15	0.33	0	17,19,21	0.56	0
8	BMA	y	3	8	11,11,12	0.80	0	15,15,17	0.94	0
8	MAN	y	4	8	11,11,12	0.64	0	15,15,17	1.16	2 (13%)
8	MAN	y	5	8	11,11,12	0.56	0	15,15,17	1.10	2 (13%)
8	MAN	y	6	8	11,11,12	0.65	0	15,15,17	0.94	1 (6%)
8	MAN	y	7	8	11,11,12	0.63	0	15,15,17	0.91	1 (6%)
8	MAN	y	8	8	11,11,12	0.67	0	15,15,17	1.26	2 (13%)
8	MAN	y	9	8	11,11,12	0.68	0	15,15,17	1.32	2 (13%)
9	NAG	z	1	3,9	14,14,15	0.51	0	17,19,21	0.38	0
9	NAG	z	2	9	14,14,15	0.18	0	17,19,21	0.44	0
9	BMA	z	3	9	11,11,12	0.51	0	15,15,17	0.73	0
9	MAN	z	4	9	11,11,12	0.76	1 (9%)	15,15,17	1.09	1 (6%)
9	MAN	z	5	9	11,11,12	0.81	1 (9%)	15,15,17	1.13	2 (13%)
9	MAN	z	6	9	11,11,12	0.68	0	15,15,17	0.92	1 (6%)
9	MAN	z	7	9	11,11,12	0.53	0	15,15,17	1.15	2 (13%)
9	MAN	z	8	9	11,11,12	0.60	0	15,15,17	0.99	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	0	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	0	2	10	-	2/6/23/26	0/1/1/1
10	BMA	0	3	10	-	0/2/19/22	0/1/1/1
13	NAG	1	1	3,13	-	0/6/23/26	0/1/1/1
13	NAG	1	2	13	-	0/6/23/26	0/1/1/1
13	BMA	1	3	13	-	1/2/19/22	0/1/1/1
13	MAN	1	4	13	-	2/2/19/22	1/1/1/1
13	MAN	1	5	13	-	2/2/19/22	0/1/1/1
10	NAG	2	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	2	2	10	-	0/6/23/26	0/1/1/1
10	BMA	2	3	10	-	0/2/19/22	0/1/1/1
10	NAG	3	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	3	2	10	-	0/6/23/26	0/1/1/1
10	BMA	3	3	10	-	2/2/19/22	0/1/1/1
7	NAG	4	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	4	2	7	-	1/6/23/26	0/1/1/1
14	NAG	5	1	3,14	-	5/6/23/26	0/1/1/1
14	NAG	5	2	14	-	2/6/23/26	0/1/1/1
14	BMA	5	3	14	-	0/2/19/22	0/1/1/1
14	MAN	5	4	14	-	2/2/19/22	0/1/1/1
14	MAN	5	5	14	-	2/2/19/22	0/1/1/1
14	MAN	5	6	14	-	0/2/19/22	0/1/1/1
14	MAN	5	7	14	-	2/2/19/22	0/1/1/1
14	MAN	5	8	14	-	2/2/19/22	0/1/1/1
11	NAG	6	1	11,3	-	2/6/23/26	0/1/1/1
11	MAN	6	10	11	-	2/2/19/22	0/1/1/1
11	MAN	6	11	11	-	2/2/19/22	0/1/1/1
11	NAG	6	2	11	-	0/6/23/26	0/1/1/1
11	BMA	6	3	11	-	2/2/19/22	0/1/1/1
11	MAN	6	4	11	-	0/2/19/22	0/1/1/1
11	MAN	6	5	11	-	2/2/19/22	0/1/1/1
11	MAN	6	6	11	-	2/2/19/22	0/1/1/1
11	MAN	6	7	11	-	1/2/19/22	1/1/1/1
11	MAN	6	8	11	-	0/2/19/22	0/1/1/1
11	MAN	6	9	11	-	0/2/19/22	0/1/1/1
7	NAG	7	1	7,6	-	1/6/23/26	0/1/1/1
7	NAG	7	2	7	-	2/6/23/26	0/1/1/1
7	NAG	8	1	7,6	-	0/6/23/26	0/1/1/1
7	NAG	8	2	7	-	1/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	a	5	11	-	0/2/19/22	0/1/1/1
11	MAN	a	6	11	-	2/2/19/22	0/1/1/1
11	MAN	a	7	11	-	0/2/19/22	1/1/1/1
11	MAN	a	8	11	-	0/2/19/22	0/1/1/1
11	MAN	a	9	11	-	0/2/19/22	0/1/1/1
12	NAG	b	1	12,3	-	2/6/23/26	0/1/1/1
12	NAG	b	2	12	-	2/6/23/26	0/1/1/1
12	BMA	b	3	12	-	0/2/19/22	0/1/1/1
12	MAN	b	4	12	-	2/2/19/22	0/1/1/1
12	MAN	b	5	12	-	2/2/19/22	0/1/1/1
12	MAN	b	6	12	-	0/2/19/22	0/1/1/1
12	MAN	b	7	12	-	1/2/19/22	0/1/1/1
10	NAG	c	1	3,10	-	3/6/23/26	0/1/1/1
10	NAG	c	2	10	-	0/6/23/26	0/1/1/1
10	BMA	c	3	10	-	1/2/19/22	0/1/1/1
7	NAG	d	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	d	2	7	-	2/6/23/26	0/1/1/1
13	NAG	e	1	3,13	-	2/6/23/26	0/1/1/1
13	NAG	e	2	13	-	0/6/23/26	0/1/1/1
13	BMA	e	3	13	-	0/2/19/22	0/1/1/1
13	MAN	e	4	13	-	2/2/19/22	0/1/1/1
13	MAN	e	5	13	-	0/2/19/22	0/1/1/1
10	NAG	f	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	f	2	10	-	0/6/23/26	0/1/1/1
10	BMA	f	3	10	-	1/2/19/22	0/1/1/1
7	NAG	g	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	g	2	7	-	3/6/23/26	0/1/1/1
7	NAG	h	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	h	2	7	-	0/6/23/26	0/1/1/1
7	NAG	i	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	i	2	7	-	1/6/23/26	0/1/1/1
7	NAG	j	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	j	2	7	-	2/6/23/26	0/1/1/1
7	NAG	k	1	3,7	-	3/6/23/26	0/1/1/1
7	NAG	k	2	7	-	2/6/23/26	0/1/1/1
9	NAG	l	1	3,9	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	l	4	9	-	2/2/19/22	0/1/1/1
9	MAN	l	5	9	-	1/2/19/22	1/1/1/1
9	MAN	l	6	9	-	2/2/19/22	0/1/1/1
9	MAN	l	7	9	-	2/2/19/22	1/1/1/1
9	MAN	l	8	9	-	0/2/19/22	0/1/1/1
10	NAG	m	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	m	2	10	-	0/6/23/26	0/1/1/1
10	BMA	m	3	10	-	0/2/19/22	0/1/1/1
13	NAG	n	1	3,13	-	2/6/23/26	0/1/1/1
13	NAG	n	2	13	-	0/6/23/26	0/1/1/1
13	BMA	n	3	13	-	2/2/19/22	0/1/1/1
13	MAN	n	4	13	-	2/2/19/22	0/1/1/1
13	MAN	n	5	13	-	1/2/19/22	1/1/1/1
10	NAG	o	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	o	2	10	-	0/6/23/26	0/1/1/1
10	BMA	o	3	10	-	1/2/19/22	0/1/1/1
7	NAG	p	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	p	2	7	-	2/6/23/26	0/1/1/1
14	NAG	q	1	3,14	-	2/6/23/26	0/1/1/1
14	NAG	q	2	14	-	2/6/23/26	0/1/1/1
14	BMA	q	3	14	-	0/2/19/22	0/1/1/1
14	MAN	q	4	14	-	0/2/19/22	0/1/1/1
14	MAN	q	5	14	-	2/2/19/22	0/1/1/1
14	MAN	q	6	14	-	1/2/19/22	0/1/1/1
14	MAN	q	7	14	-	0/2/19/22	0/1/1/1
14	MAN	q	8	14	-	1/2/19/22	0/1/1/1
11	NAG	r	1	11,3	-	1/6/23/26	0/1/1/1
11	MAN	r	10	11	-	2/2/19/22	0/1/1/1
11	MAN	r	11	11	-	2/2/19/22	0/1/1/1
11	NAG	r	2	11	-	2/6/23/26	0/1/1/1
11	BMA	r	3	11	-	2/2/19/22	0/1/1/1
11	MAN	r	4	11	-	2/2/19/22	0/1/1/1
11	MAN	r	5	11	-	1/2/19/22	0/1/1/1
11	MAN	r	6	11	-	2/2/19/22	0/1/1/1
11	MAN	r	7	11	-	0/2/19/22	1/1/1/1
11	MAN	r	8	11	-	1/2/19/22	0/1/1/1
11	MAN	r	9	11	-	2/2/19/22	0/1/1/1
8	NAG	s	1	3,8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	s	2	8	-	0/6/23/26	0/1/1/1
8	BMA	s	3	8	-	0/2/19/22	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	0/1/1/1
8	MAN	s	6	8	-	2/2/19/22	0/1/1/1
8	MAN	s	7	8	-	0/2/19/22	0/1/1/1
8	MAN	s	8	8	-	0/2/19/22	0/1/1/1
8	MAN	s	9	8	-	2/2/19/22	0/1/1/1
10	NAG	t	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	t	2	10	-	2/6/23/26	0/1/1/1
10	BMA	t	3	10	-	0/2/19/22	0/1/1/1
10	NAG	u	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	u	2	10	-	3/6/23/26	0/1/1/1
10	BMA	u	3	10	-	0/2/19/22	0/1/1/1
7	NAG	v	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	v	2	7	-	1/6/23/26	0/1/1/1
7	NAG	w	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	w	2	7	-	2/6/23/26	0/1/1/1
7	NAG	x	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	x	2	7	-	3/6/23/26	0/1/1/1
8	NAG	y	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	y	3	8	-	0/2/19/22	0/1/1/1
8	MAN	y	4	8	-	0/2/19/22	0/1/1/1
8	MAN	y	5	8	-	1/2/19/22	0/1/1/1
8	MAN	y	6	8	-	0/2/19/22	0/1/1/1
8	MAN	y	7	8	-	0/2/19/22	0/1/1/1
8	MAN	y	8	8	-	0/2/19/22	0/1/1/1
8	MAN	y	9	8	-	1/2/19/22	1/1/1/1
9	NAG	z	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	z	2	9	-	2/6/23/26	0/1/1/1
9	BMA	z	3	9	-	0/2/19/22	0/1/1/1
9	MAN	z	4	9	-	2/2/19/22	0/1/1/1
9	MAN	z	5	9	-	1/2/19/22	0/1/1/1
9	MAN	z	6	9	-	0/2/19/22	0/1/1/1
9	MAN	z	7	9	-	0/2/19/22	0/1/1/1
9	MAN	z	8	9	-	1/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	z	5	MAN	C1-C2	2.34	1.57	1.52
14	5	7	MAN	O5-C1	-2.19	1.40	1.43
11	6	11	MAN	O5-C1	-2.17	1.40	1.43
8	s	8	MAN	O5-C1	-2.17	1.40	1.43
11	r	11	MAN	O5-C1	-2.15	1.40	1.43

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	11	MAN	C1-O5-C5	5.19	119.22	112.19
10	c	1	NAG	C2-N2-C7	4.37	129.13	122.90
14	5	1	NAG	C2-N2-C7	4.36	129.11	122.90
11	a	10	MAN	O2-C2-C3	-4.29	101.55	110.14
13	n	4	MAN	C1-O5-C5	4.29	118.00	112.19

There are no chirality outliers.

5 of 199 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	k	2	NAG	C4-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
12	b	1	NAG	C4-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
9	l	7	MAN	O5-C5-C6-O6

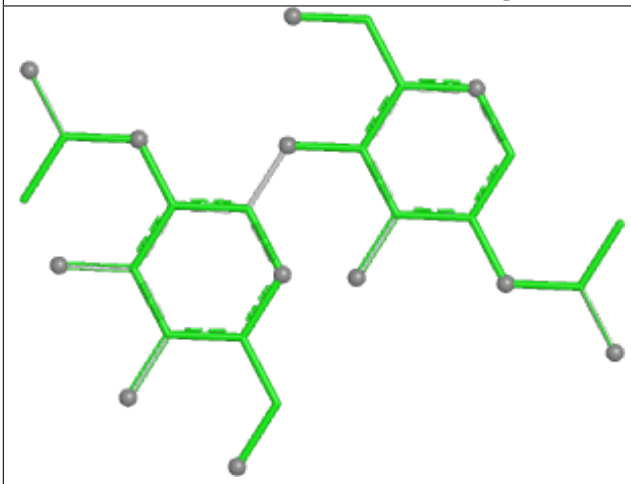
5 of 10 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	l	7	MAN	C1-C2-C3-C4-C5-O5
8	y	9	MAN	C1-C2-C3-C4-C5-O5
11	a	11	MAN	C1-C2-C3-C4-C5-O5
9	X	7	MAN	C1-C2-C3-C4-C5-O5
9	l	5	MAN	C1-C2-C3-C4-C5-O5

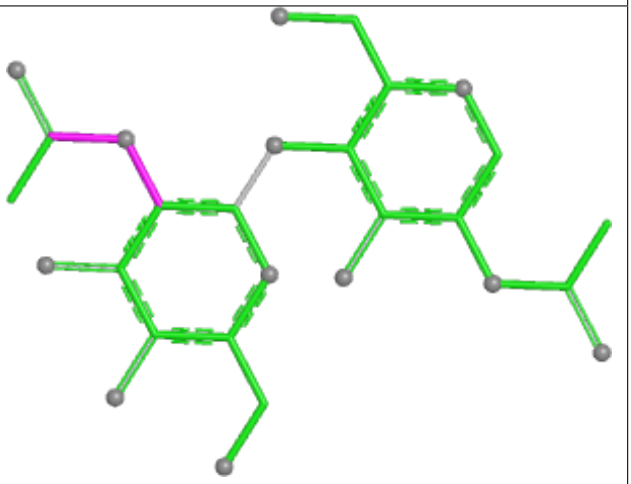
No monomer is involved in short contacts.

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

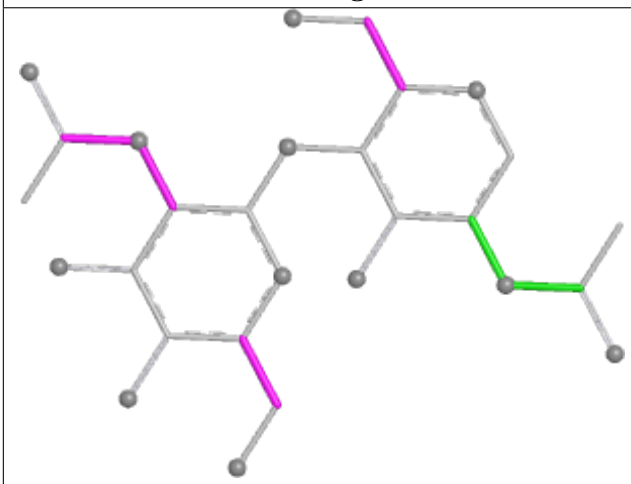
Oligosaccharide Chain S



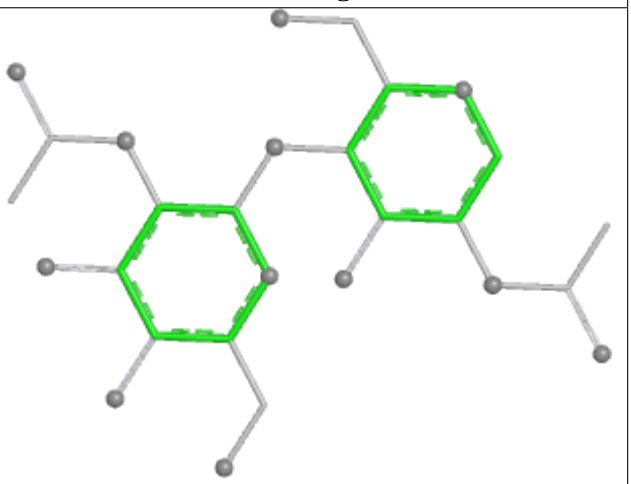
Bond lengths



Bond angles

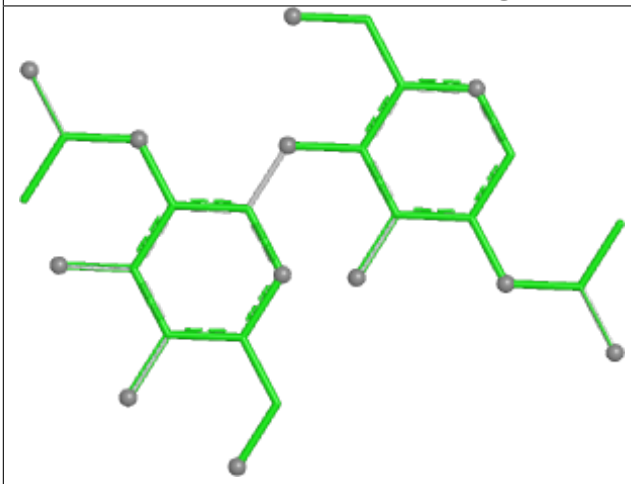


Torsions

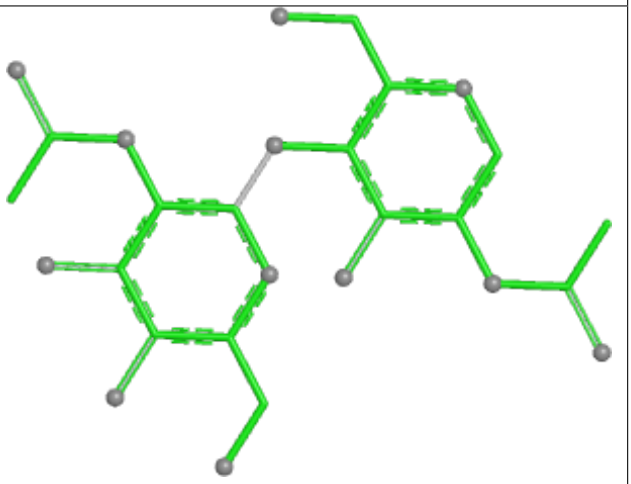


Rings

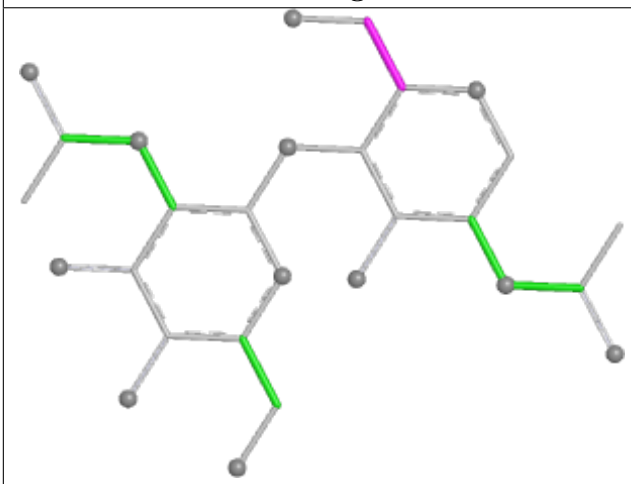
Oligosaccharide Chain T



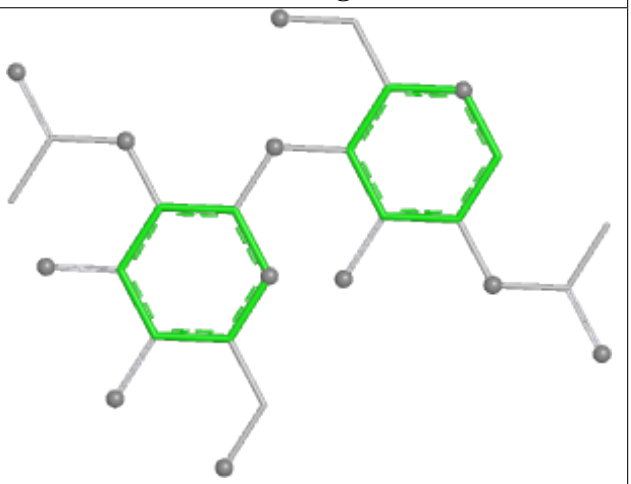
Bond lengths



Bond angles

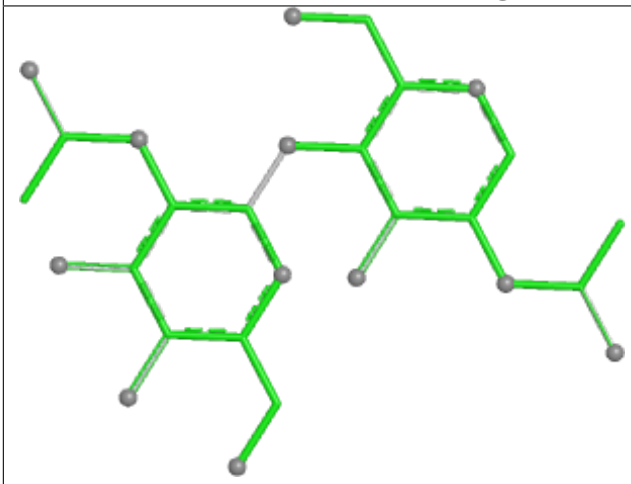


Torsions

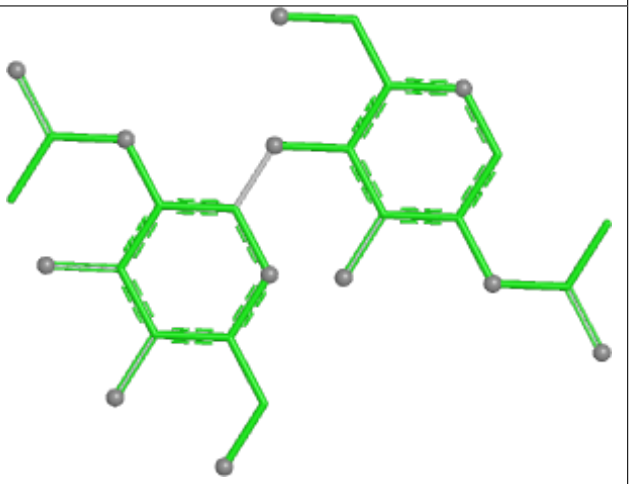


Rings

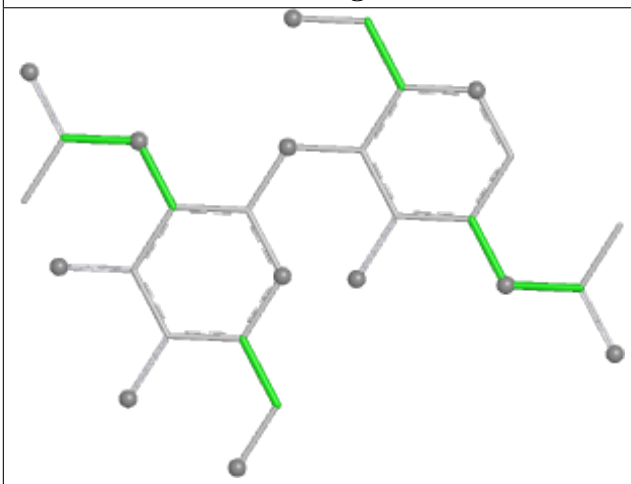
Oligosaccharide Chain U



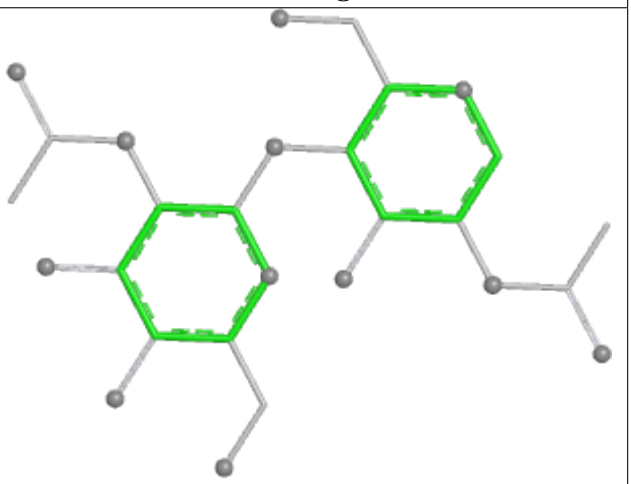
Bond lengths



Bond angles

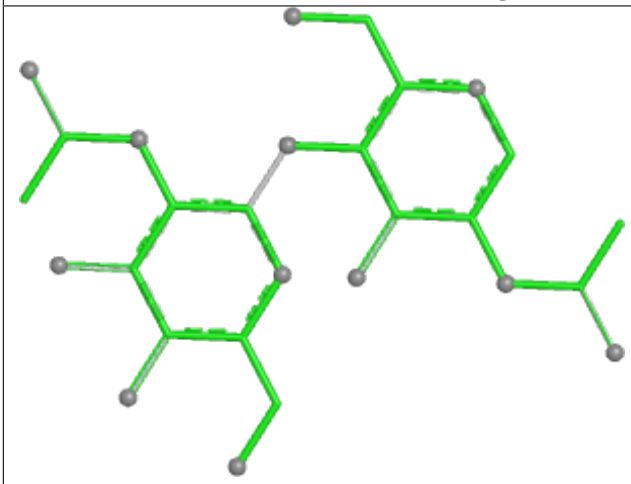


Torsions



Rings

Oligosaccharide Chain V



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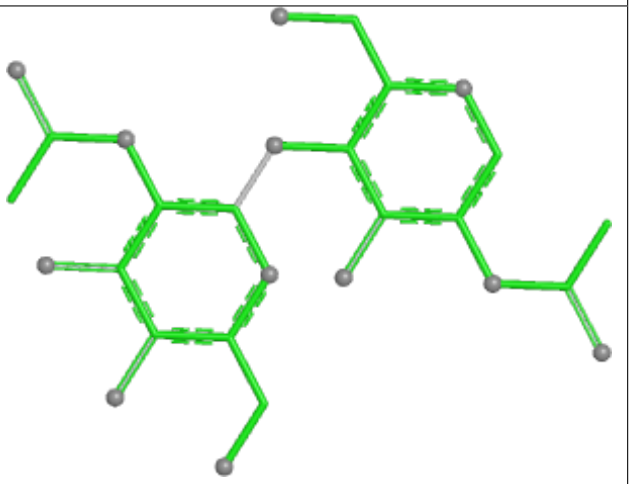
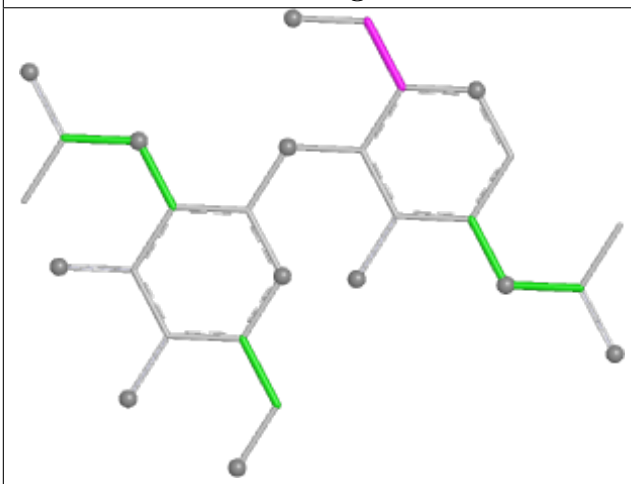
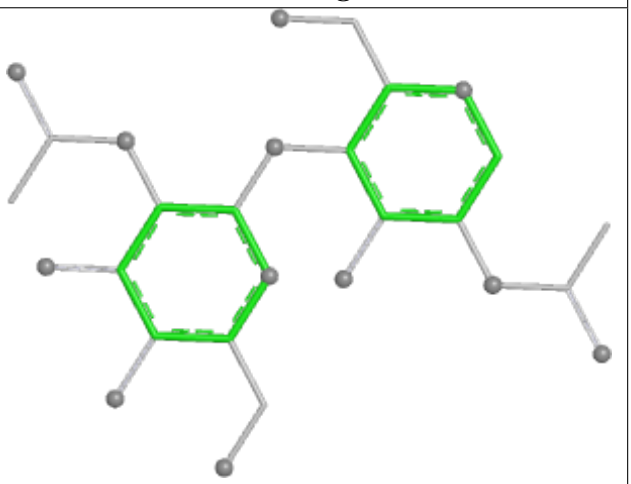


Bond angles

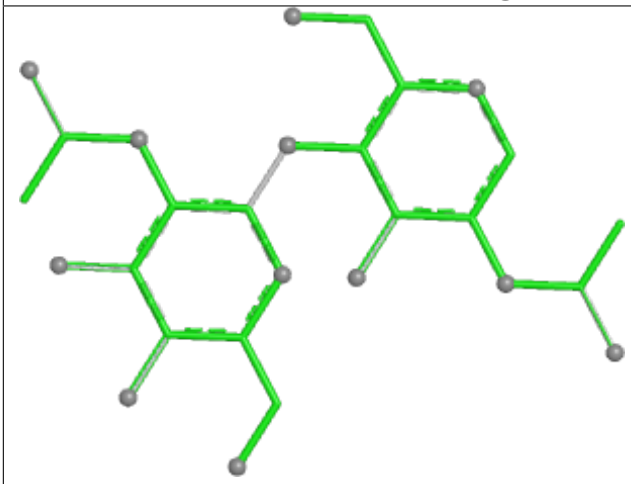


Torsions



Rings

Oligosaccharide Chain Z



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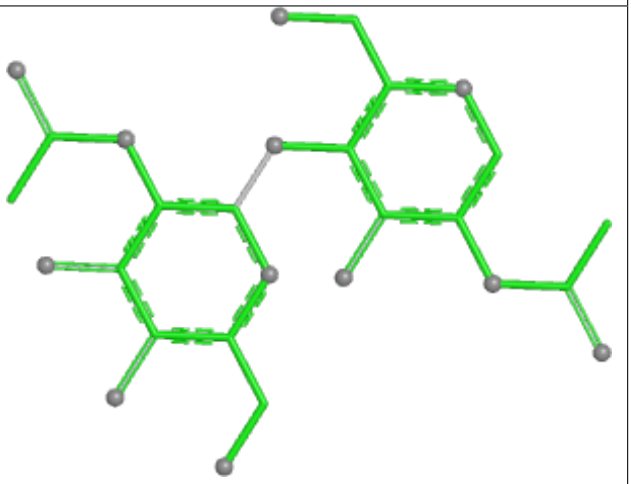
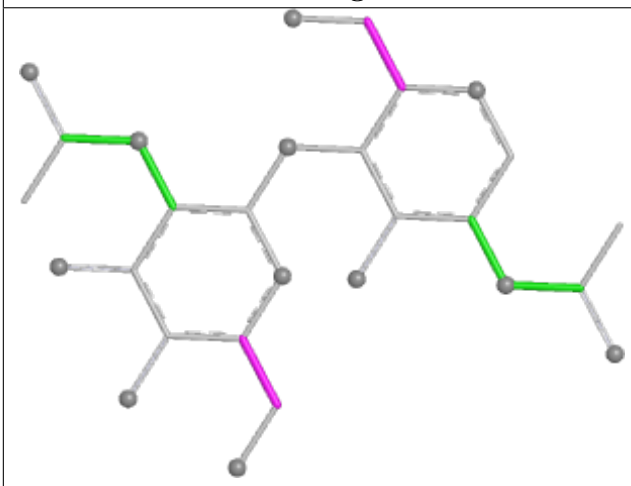
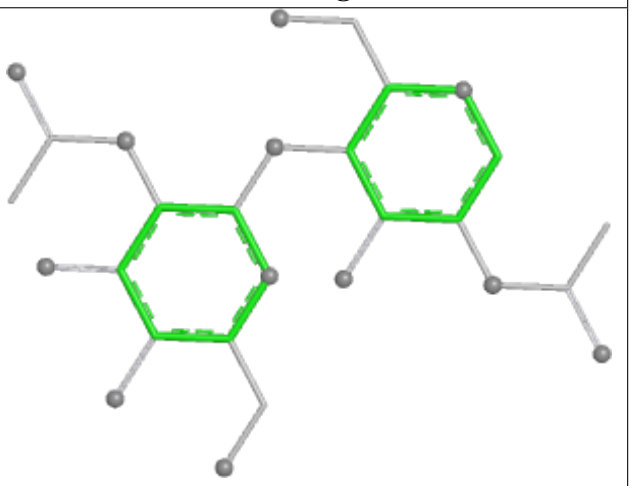


Bond angles

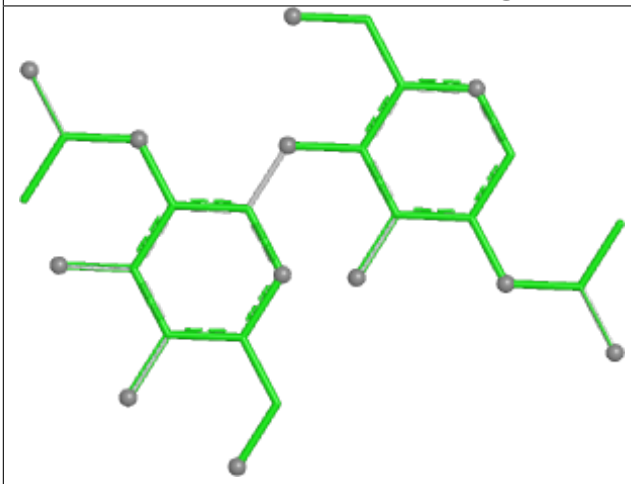


Torsions



Rings

Oligosaccharide Chain d



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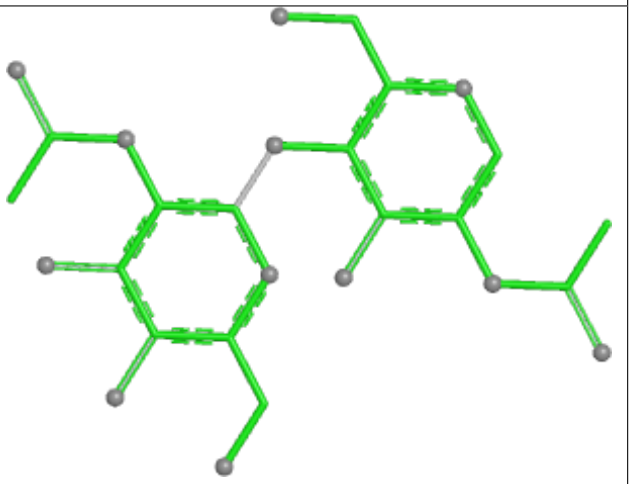
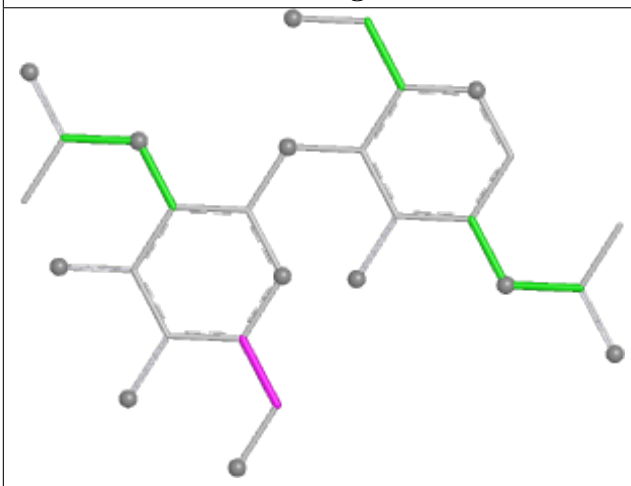
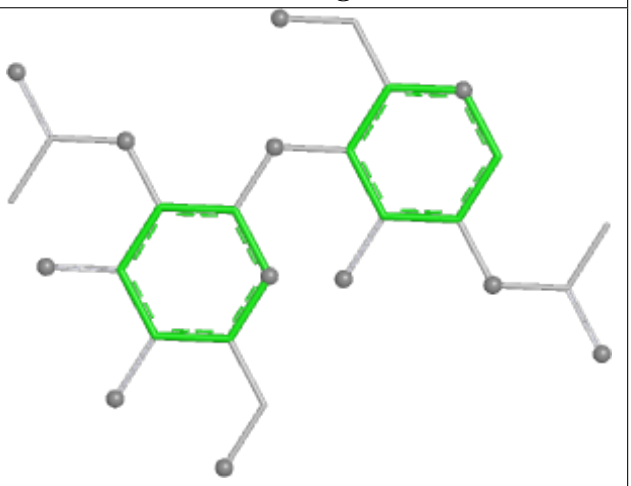


Bond angles

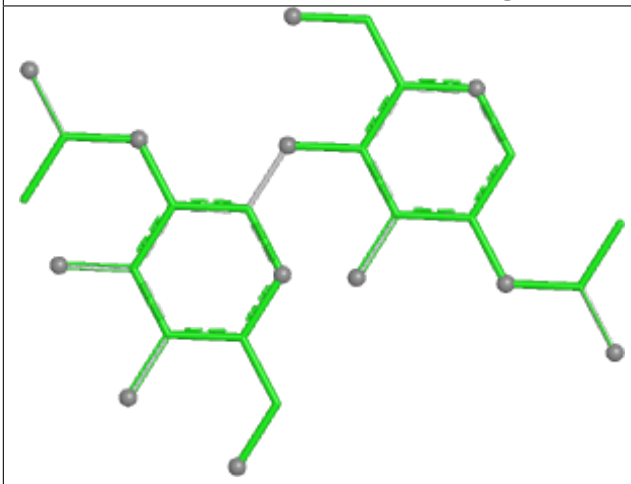


Torsions

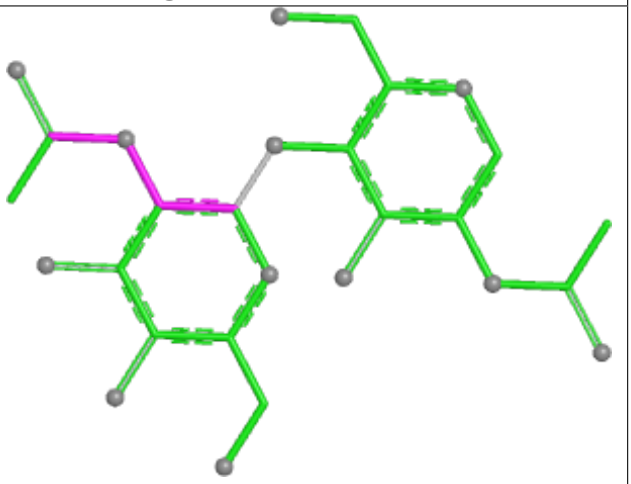


Rings

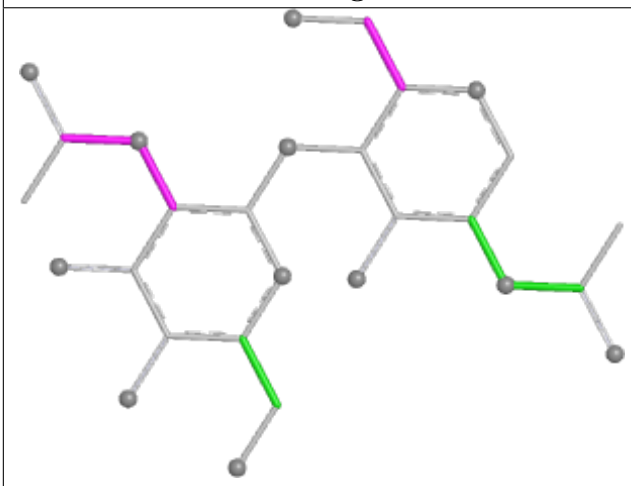
Oligosaccharide Chain g



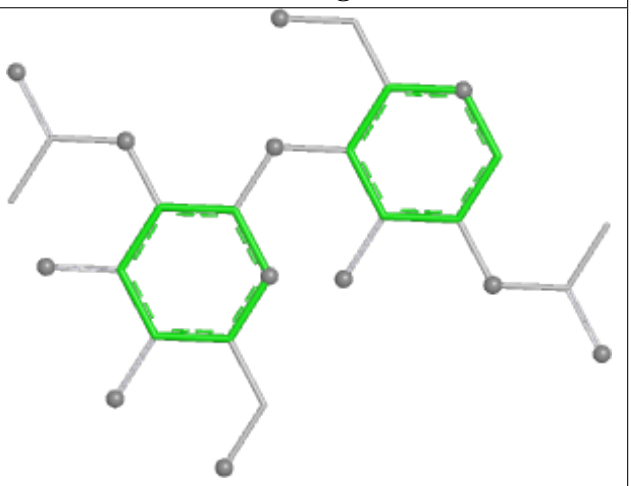
Bond lengths



Bond angles

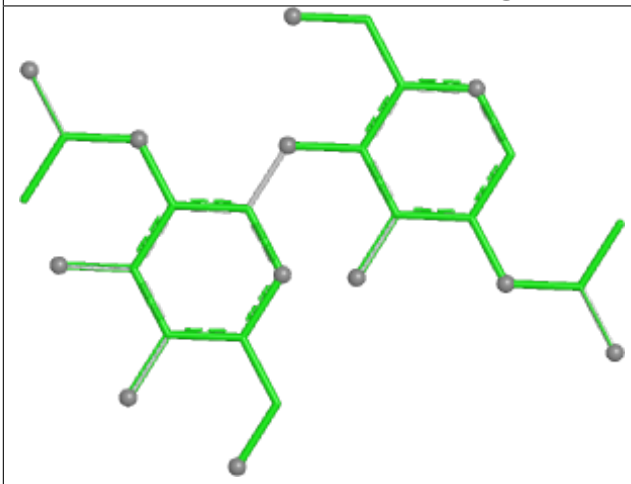


Torsions

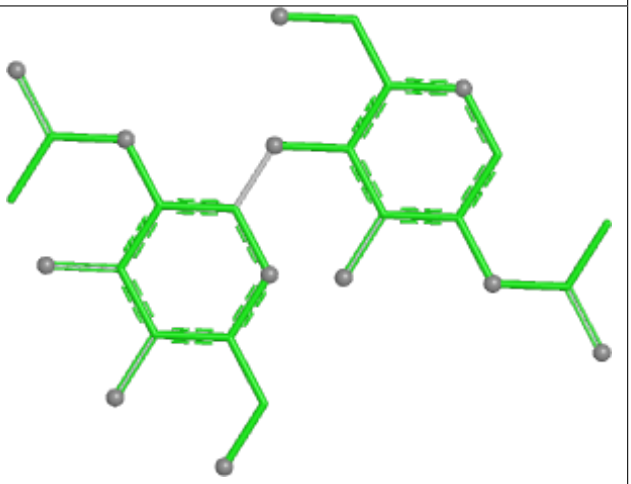


Rings

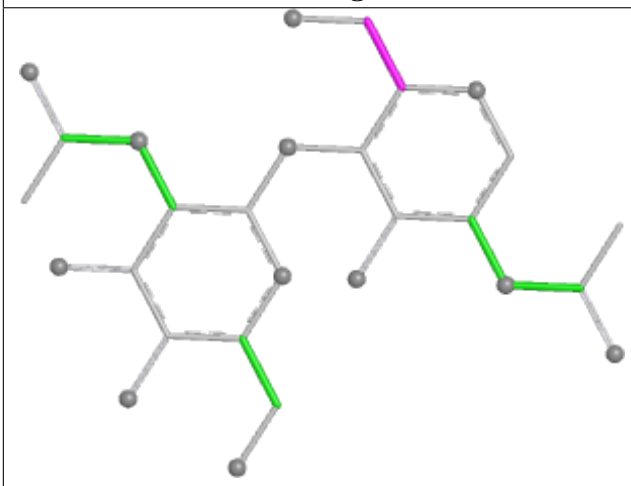
Oligosaccharide Chain h



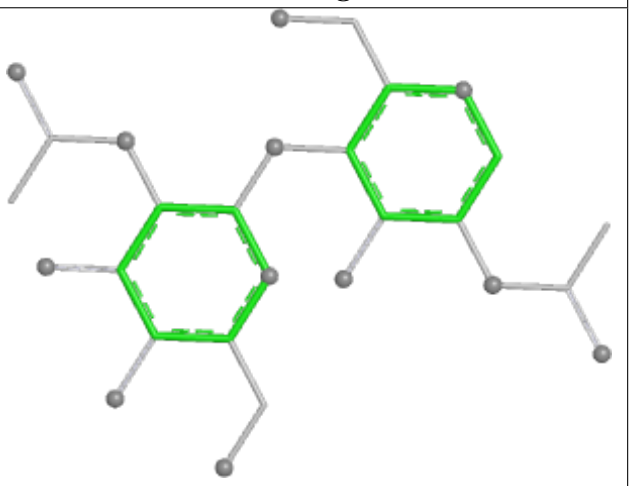
Bond lengths



Bond angles

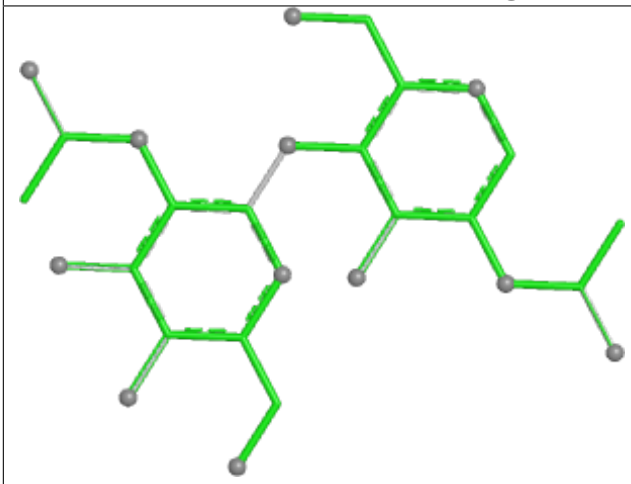


Torsions



Rings

Oligosaccharide Chain i



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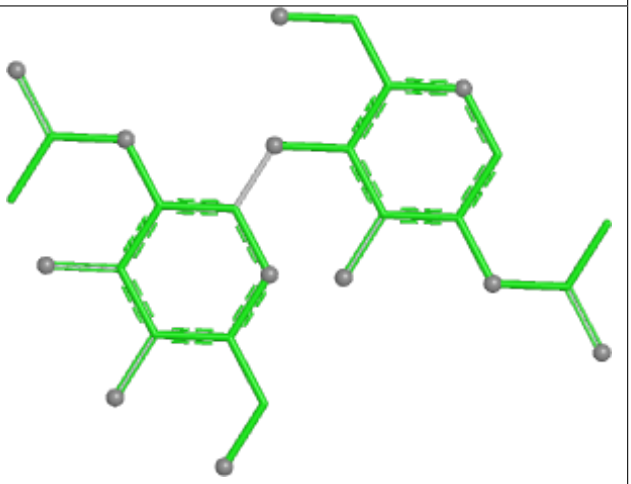
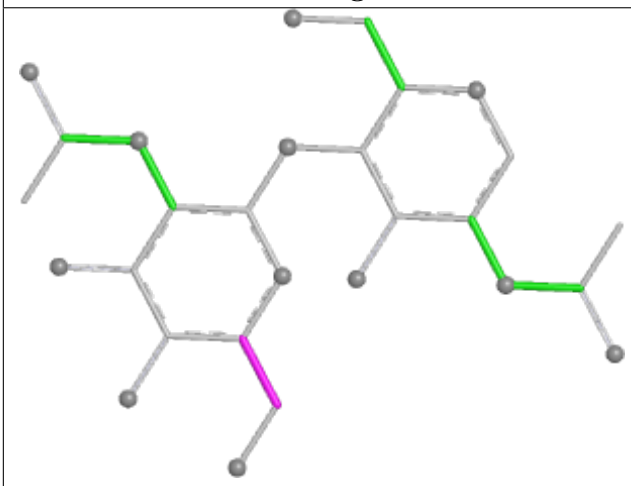


Bond angles



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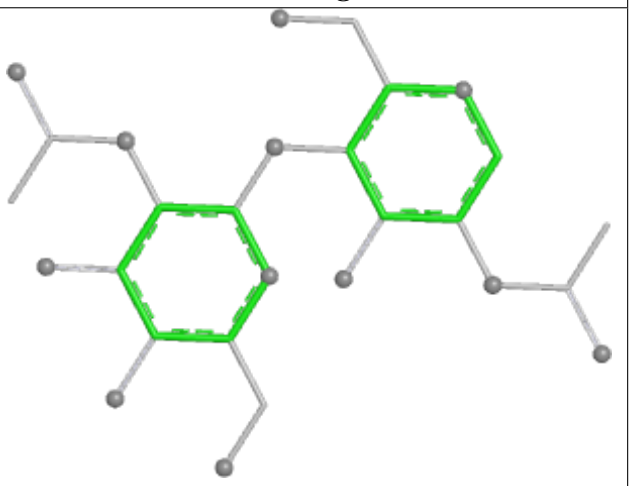
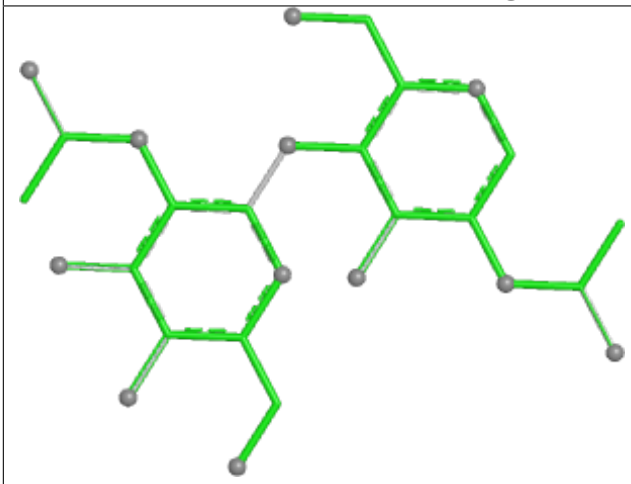


Rings

Oligosaccharide Chain j



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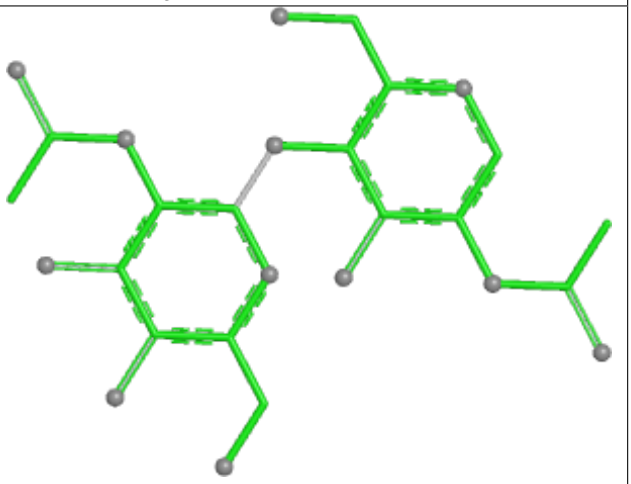
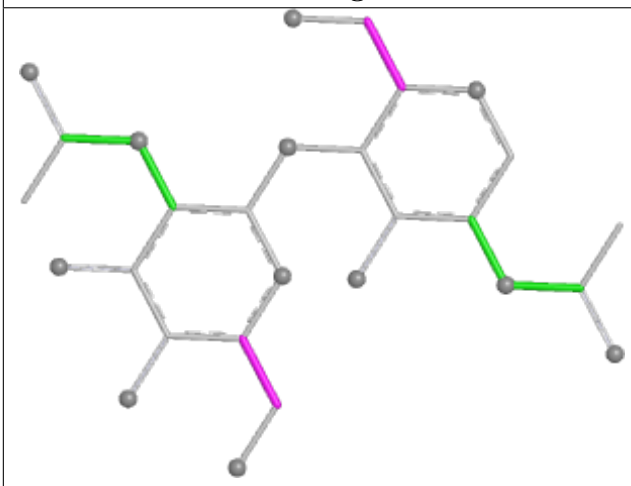
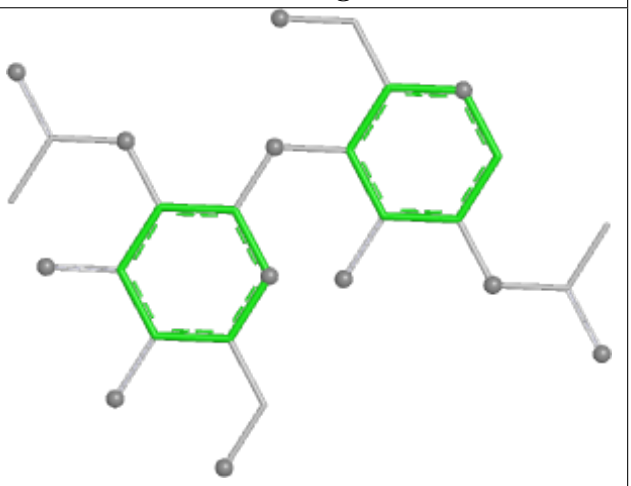


Bond angles

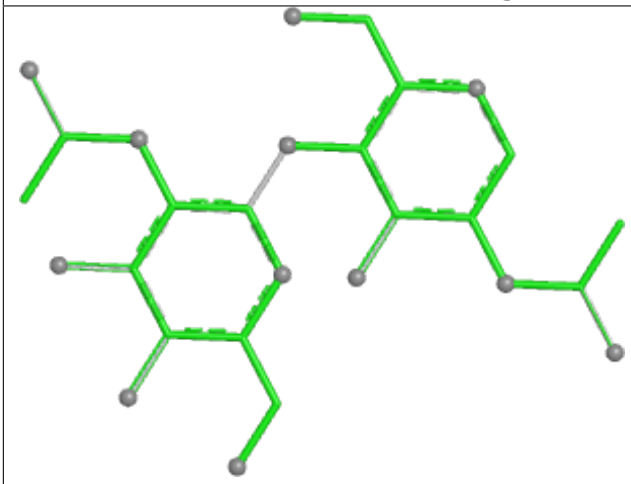


Torsions

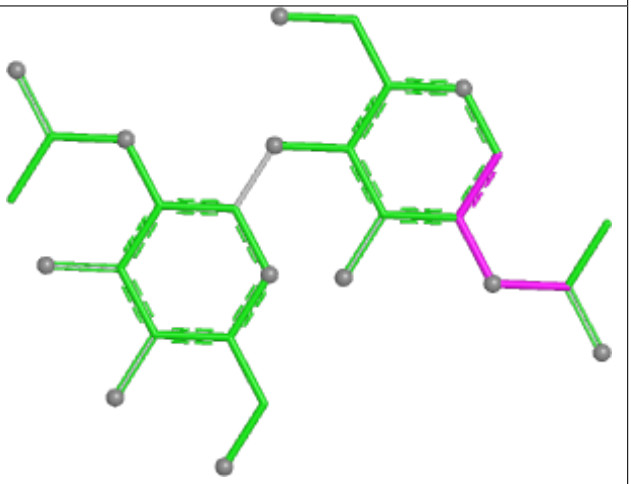


Rings

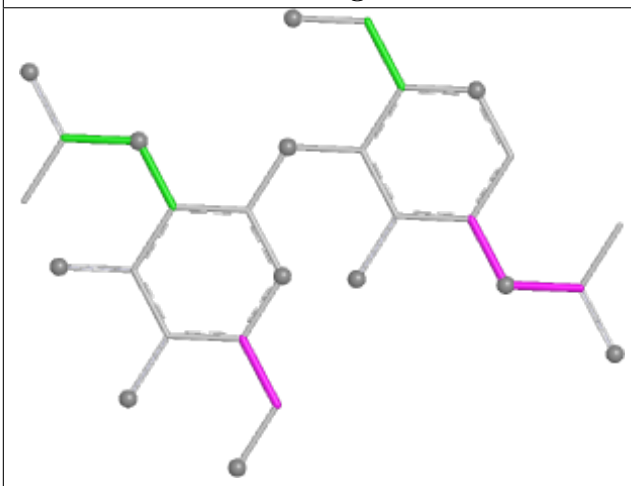
Oligosaccharide Chain k



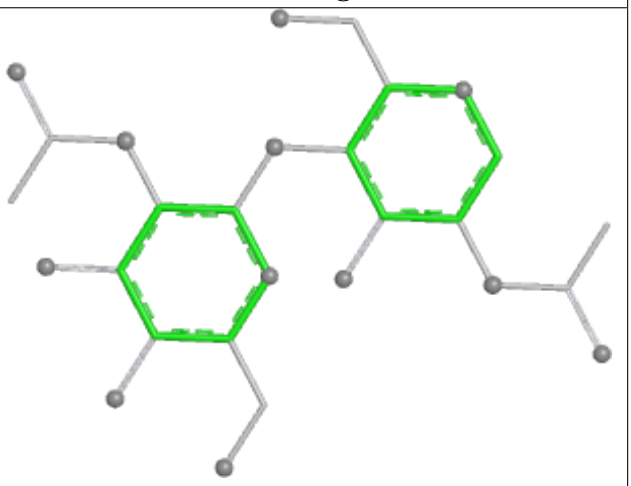
Bond lengths



Bond angles

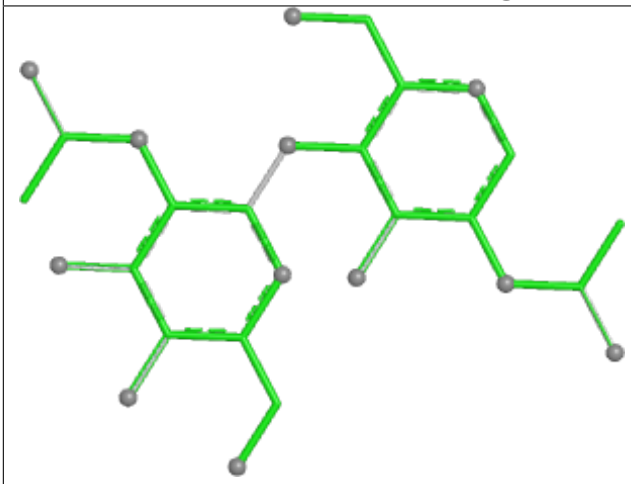


Torsions



Rings

Oligosaccharide Chain p



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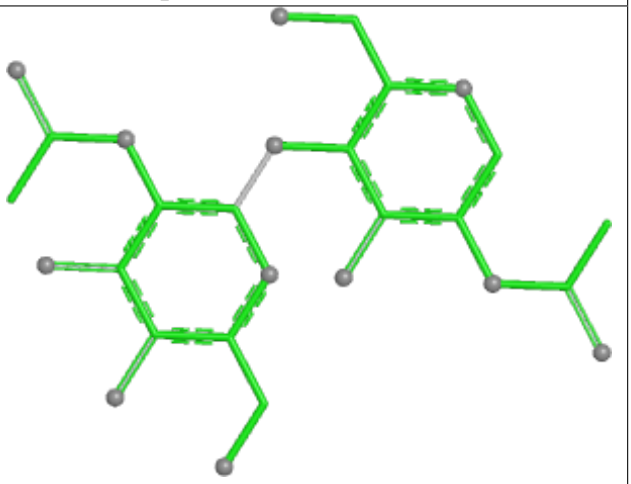
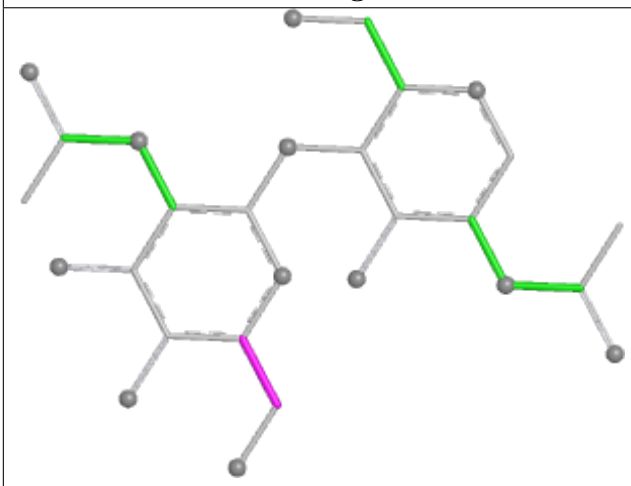
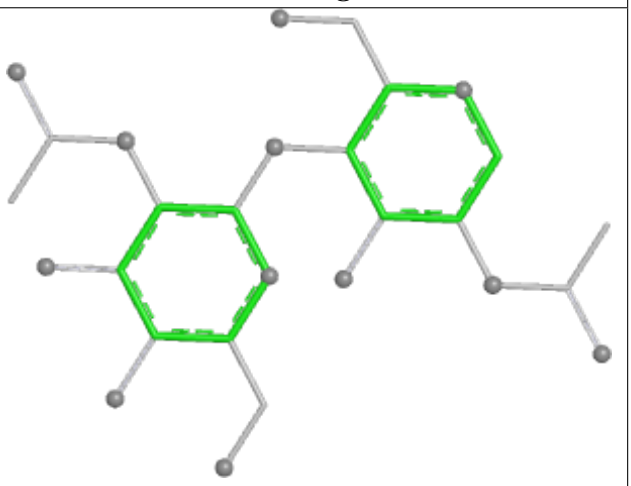


Bond angles

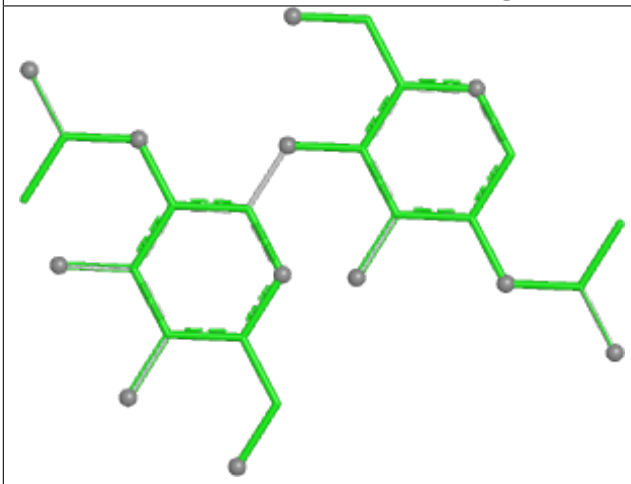


Torsions



Rings

Oligosaccharide Chain v



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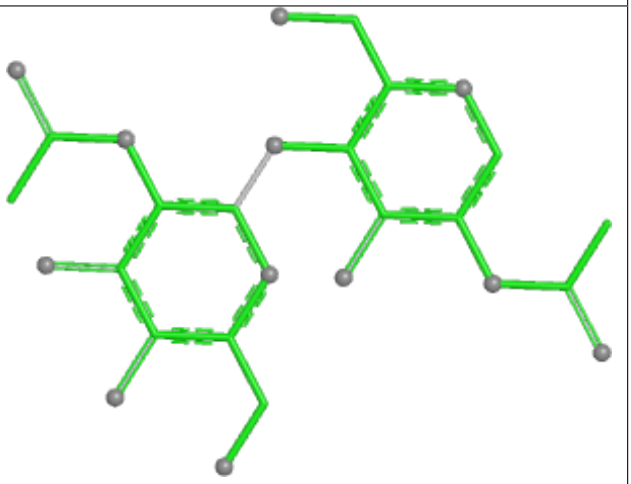
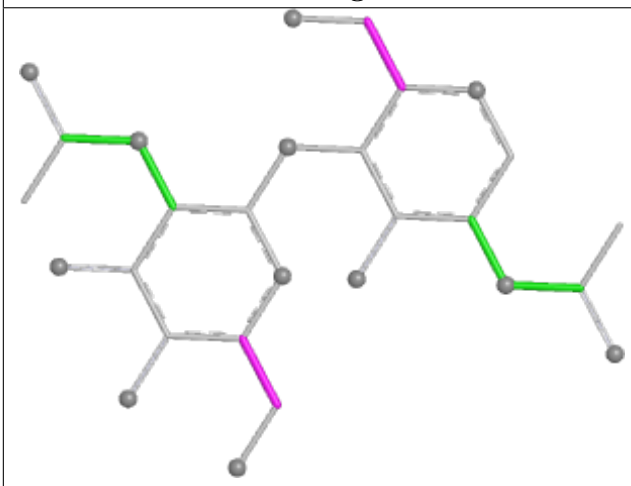
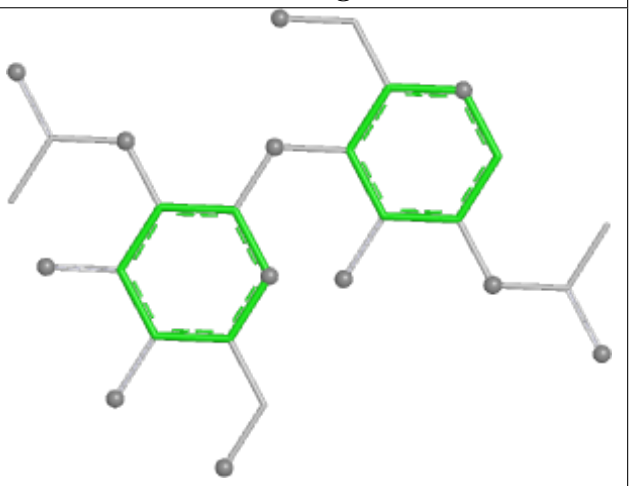


Bond angles

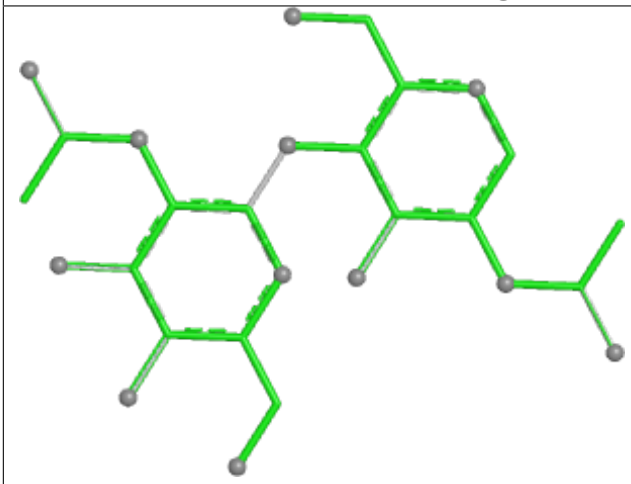


Torsions

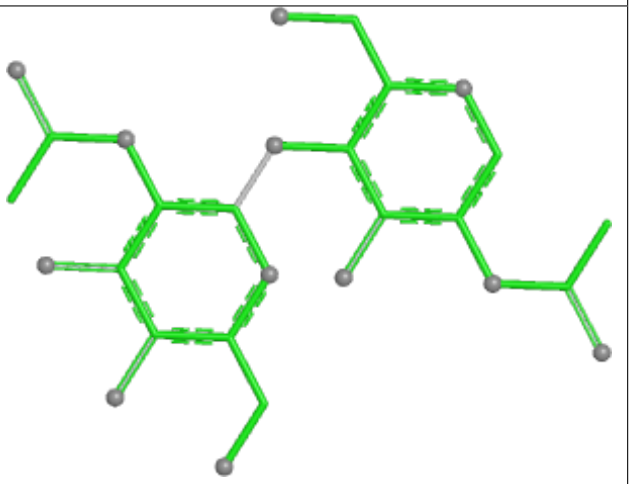


Rings

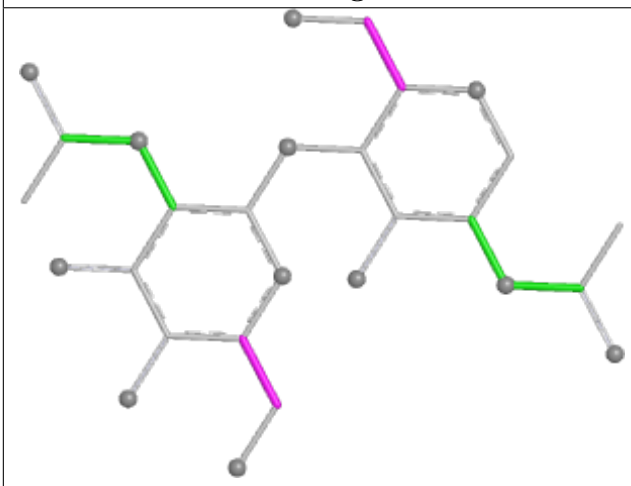
Oligosaccharide Chain w



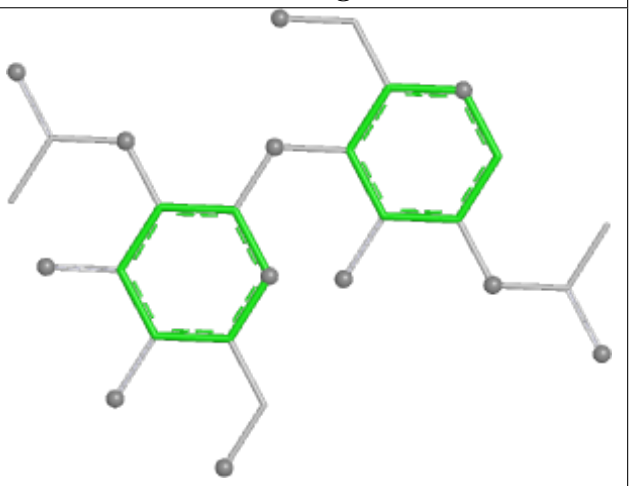
Bond lengths



Bond angles

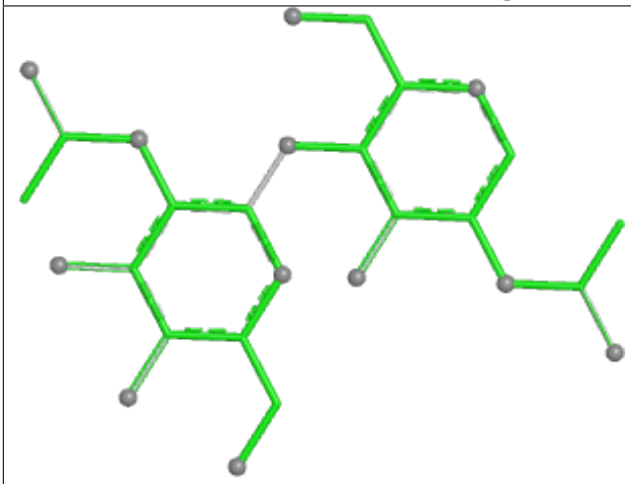


Torsions

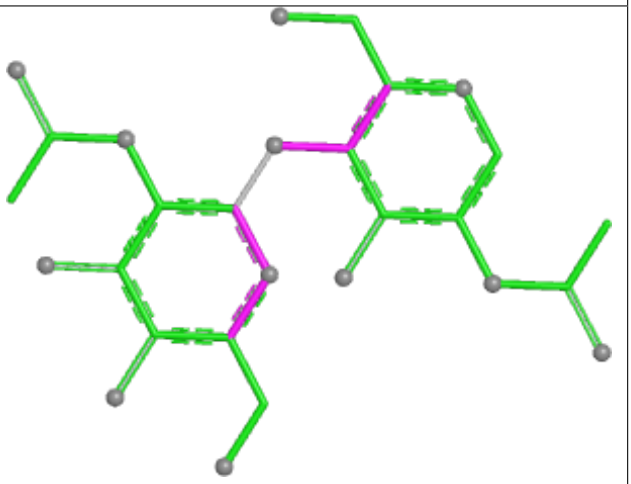


Rings

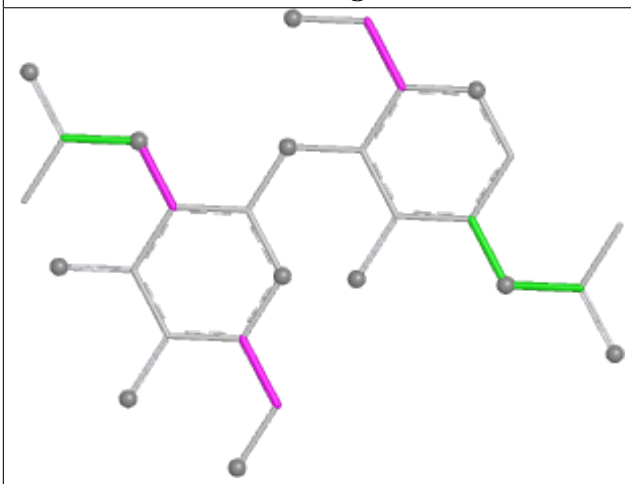
Oligosaccharide Chain x



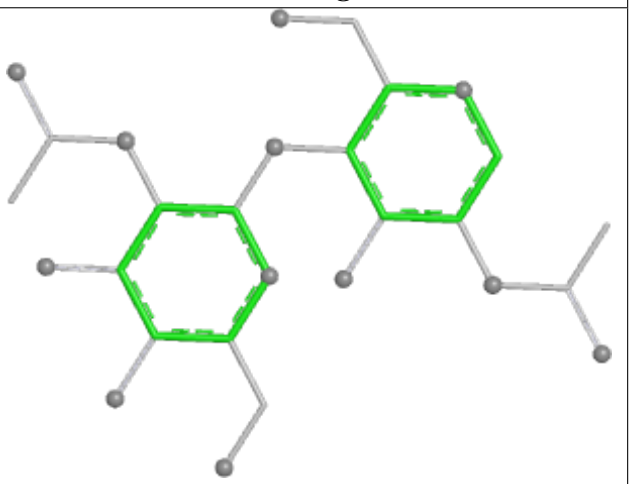
Bond lengths



Bond angles

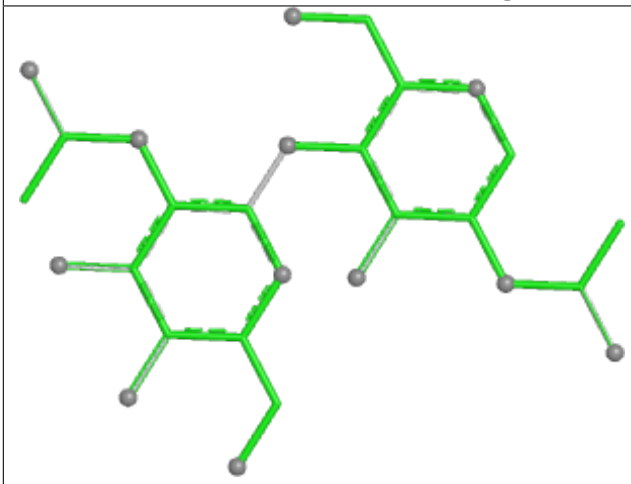


Torsions

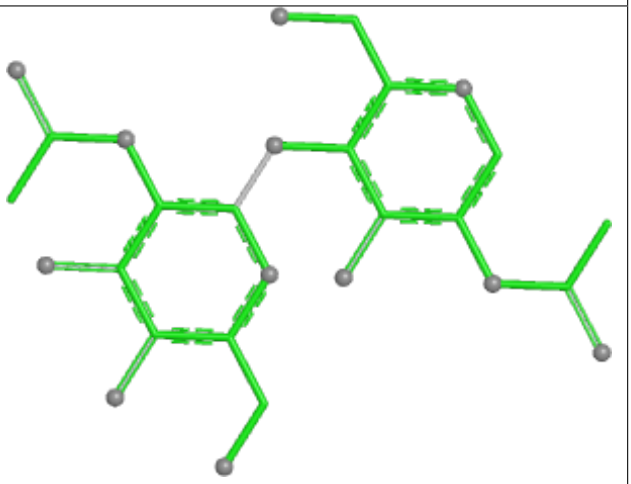


Rings

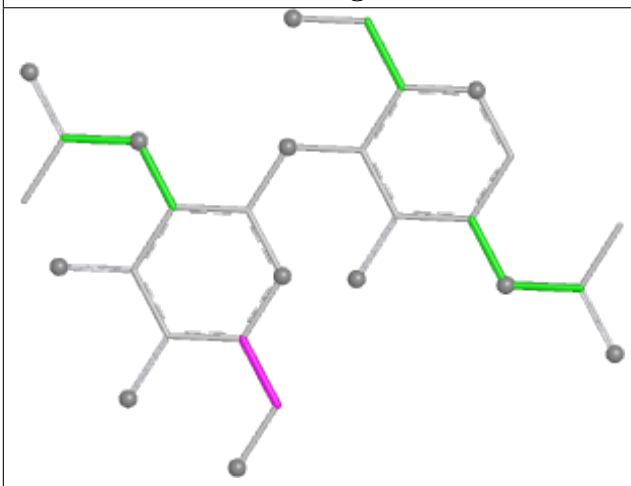
Oligosaccharide Chain 4



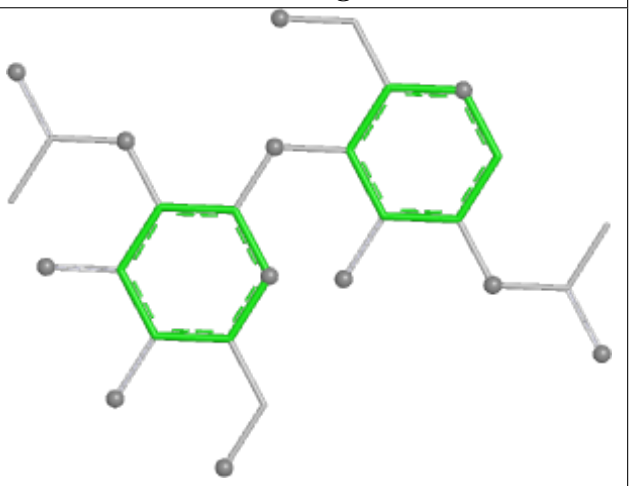
Bond lengths



Bond angles

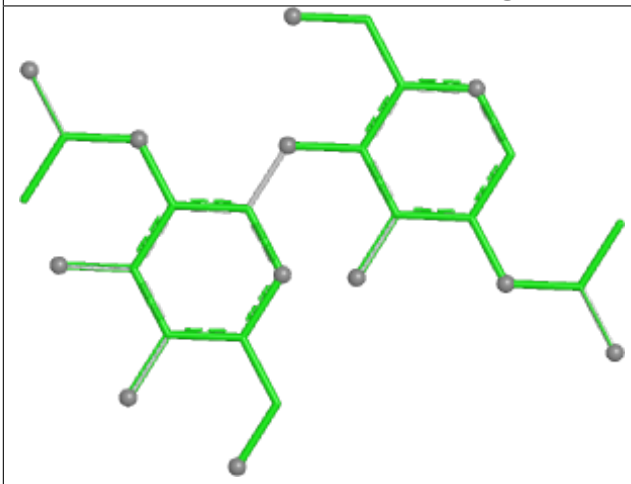


Torsions

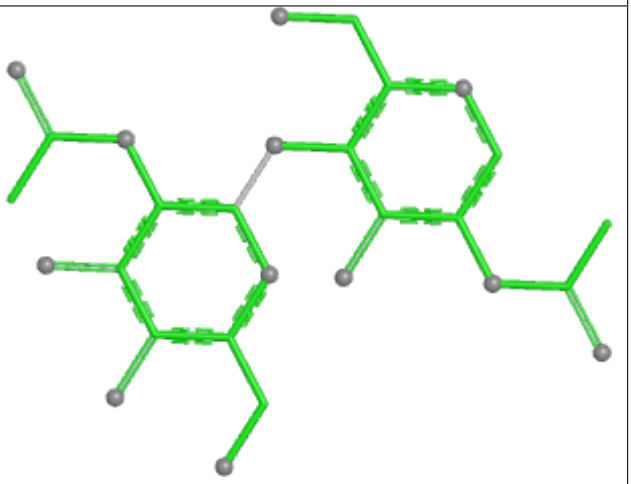


Rings

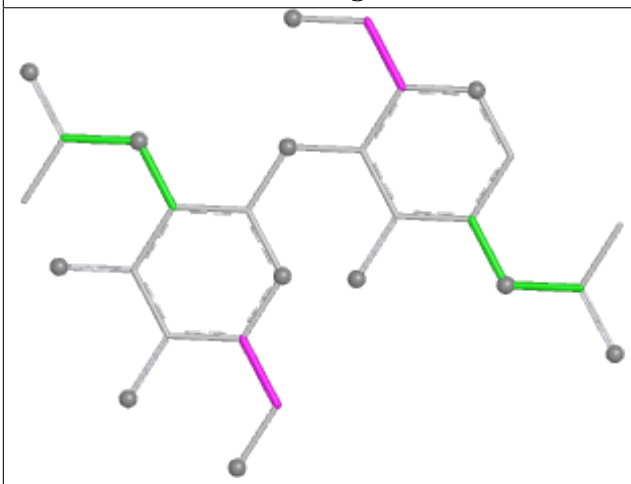
Oligosaccharide Chain 7



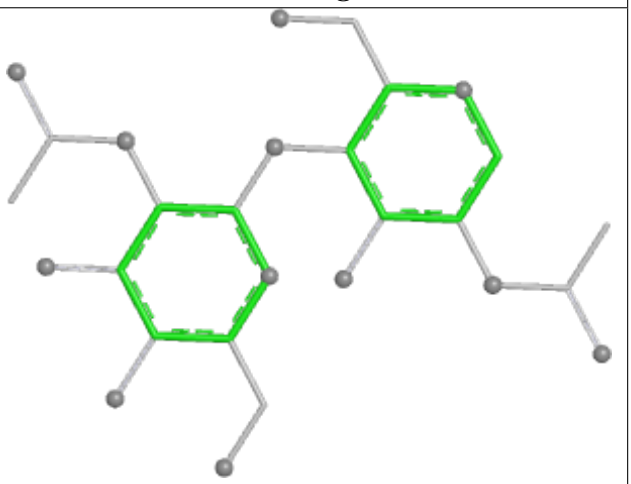
Bond lengths



Bond angles

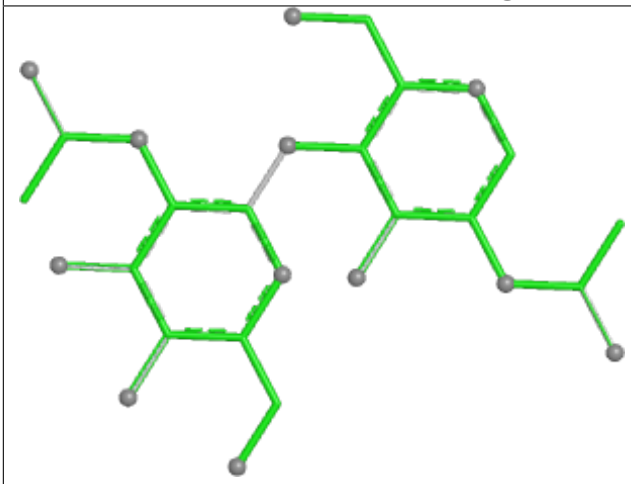


Torsions

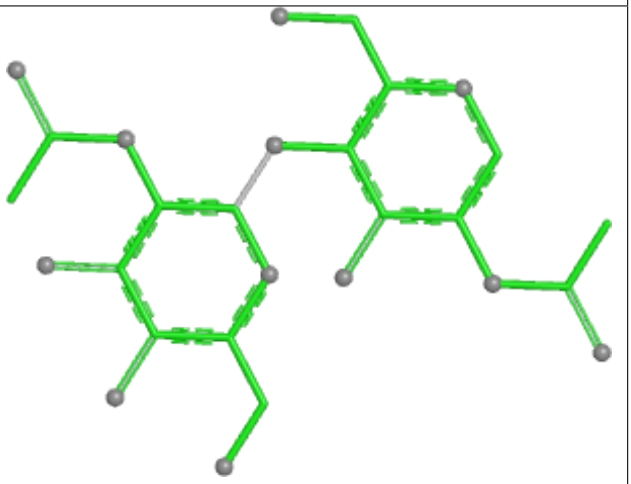


Rings

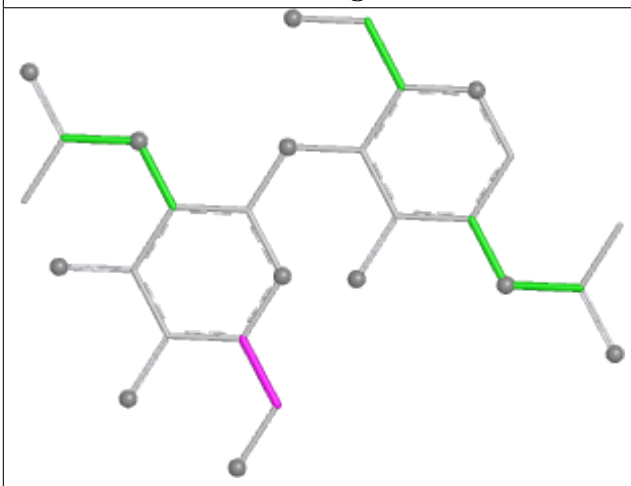
Oligosaccharide Chain 8



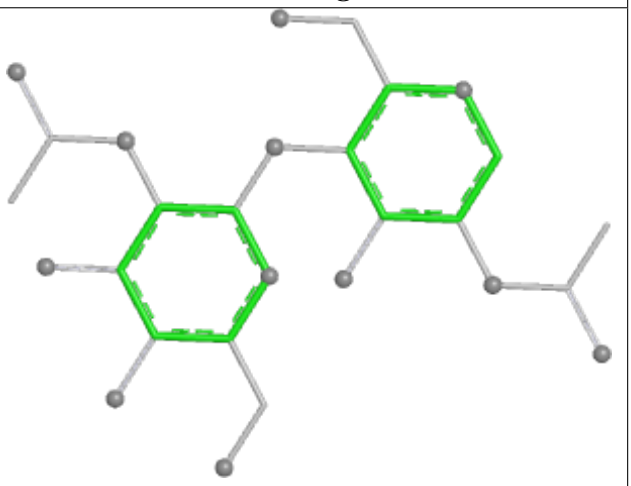
Bond lengths



Bond angles

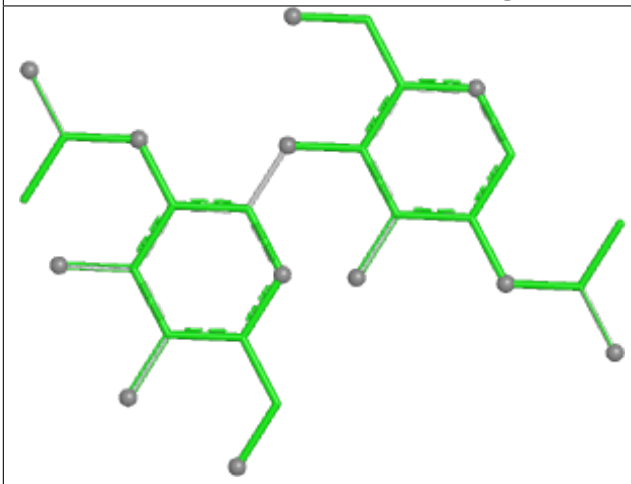


Torsions



Rings

Oligosaccharide Chain 9



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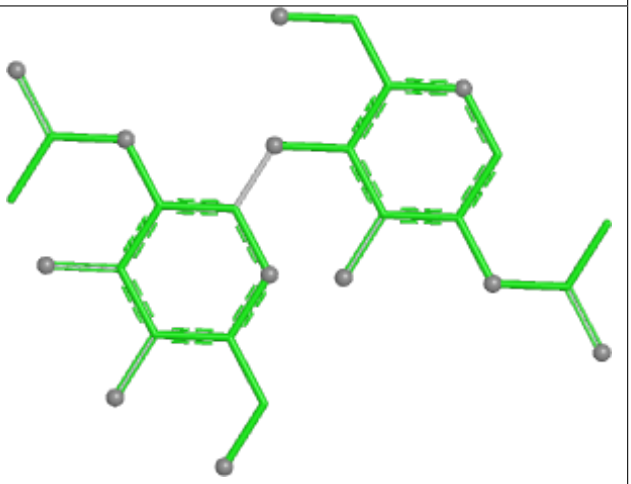
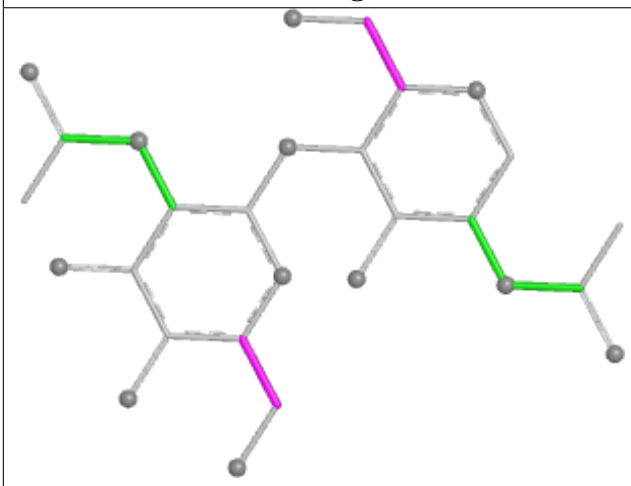
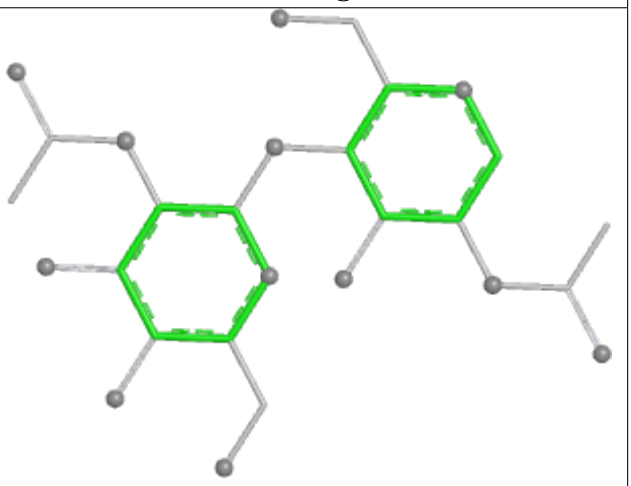


Bond angles

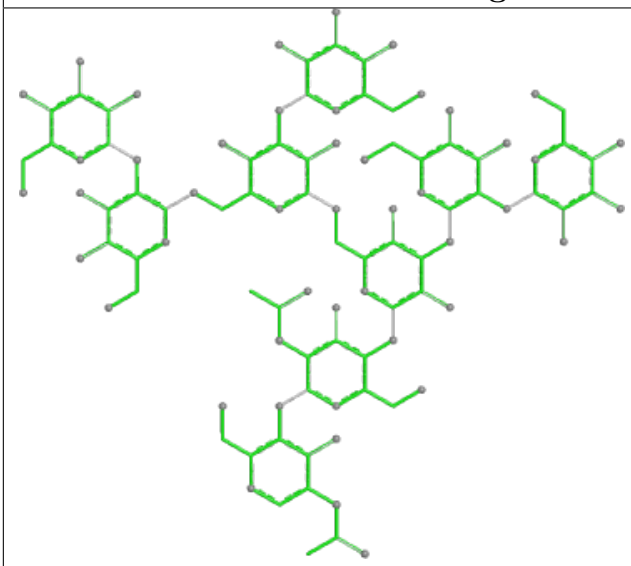


Torsions

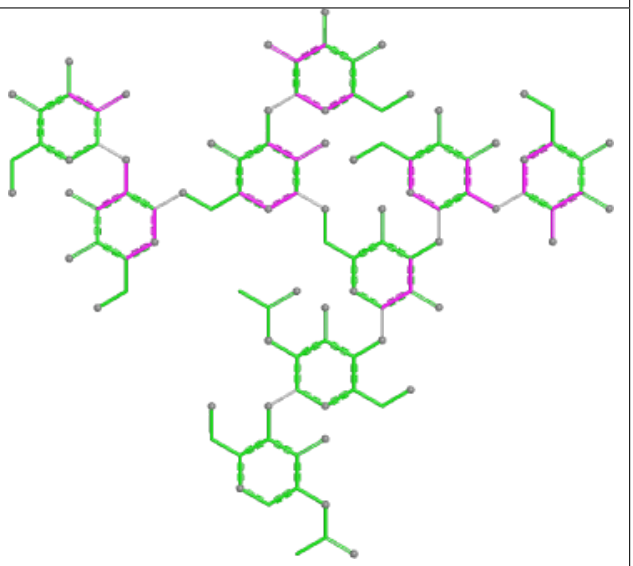


Rings

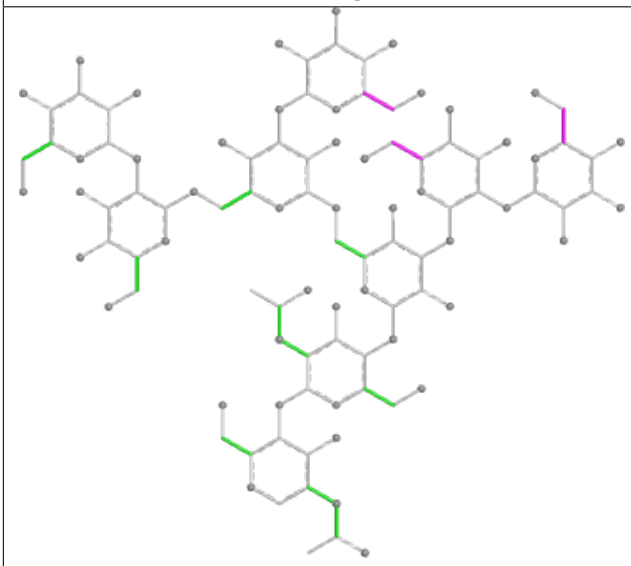
Oligosaccharide Chain W



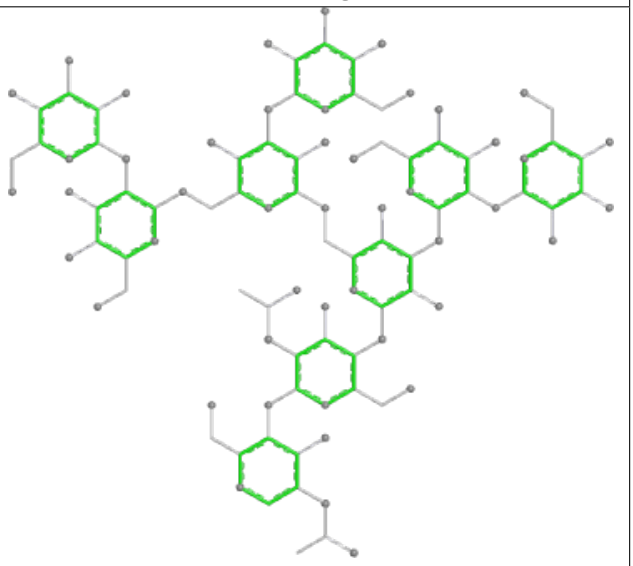
Bond lengths



Bond angles

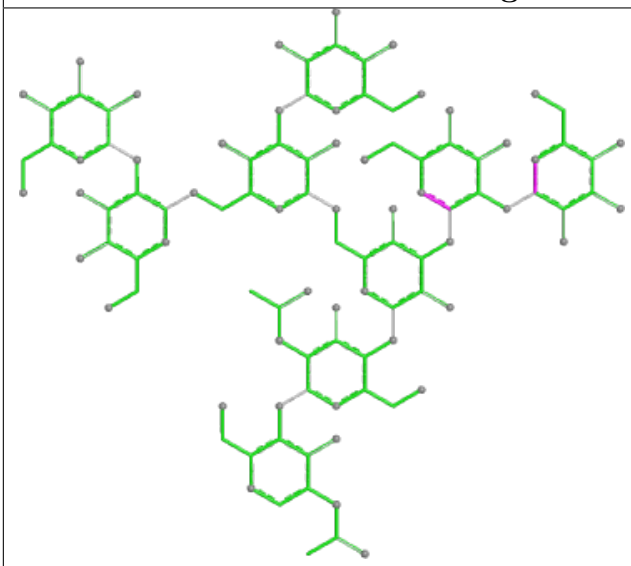


Torsions

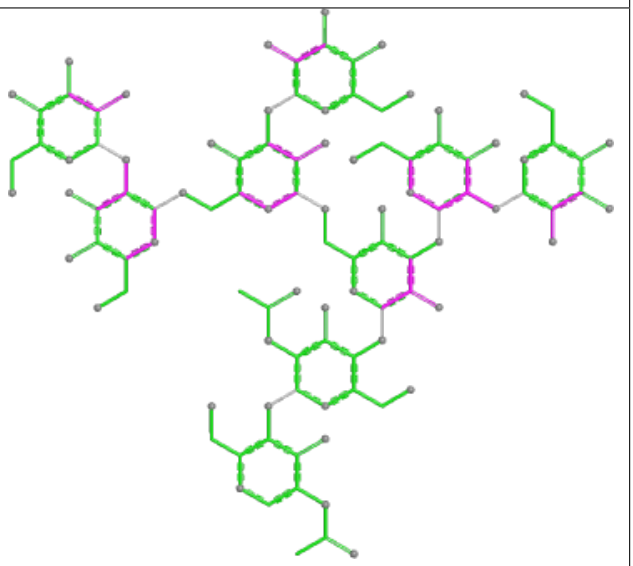


Rings

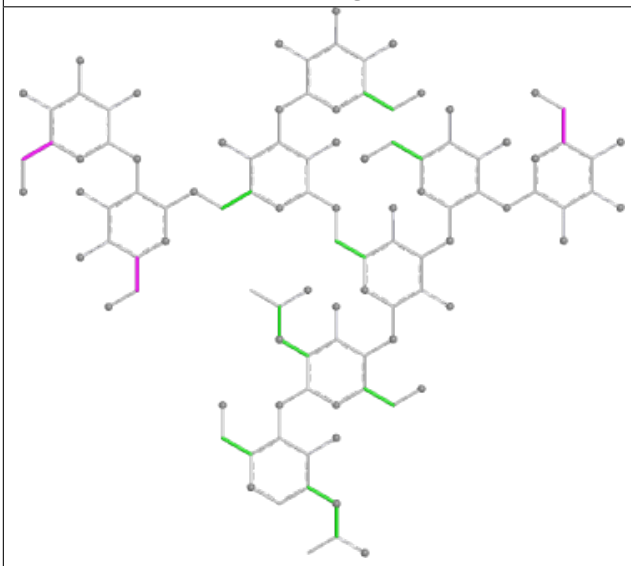
Oligosaccharide Chain s



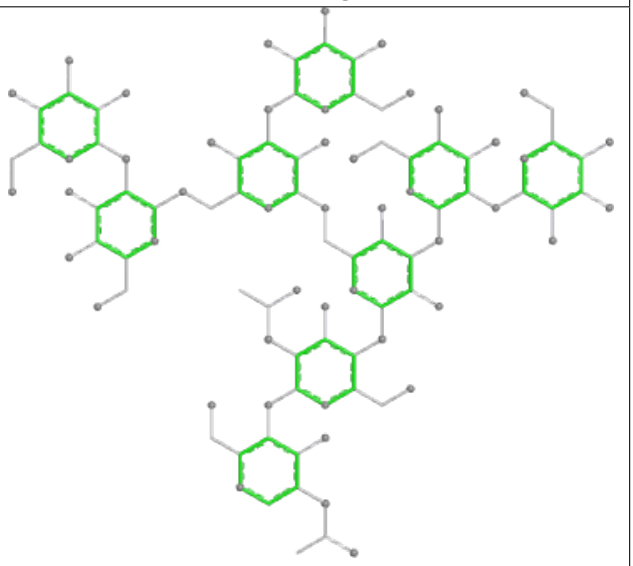
Bond lengths



Bond angles

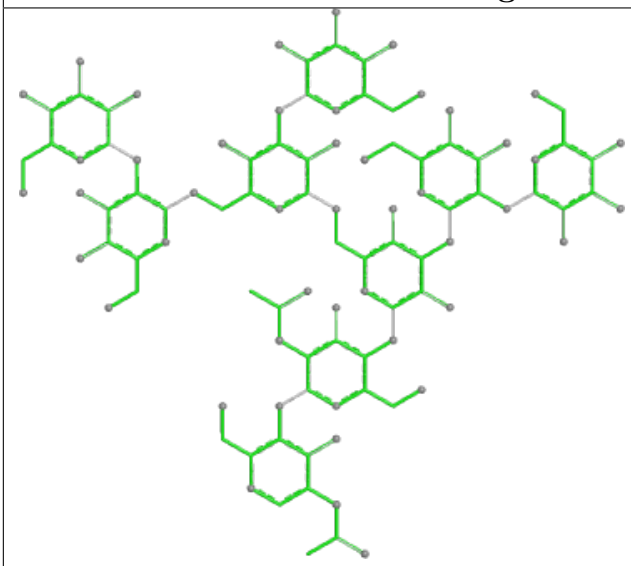


Torsions

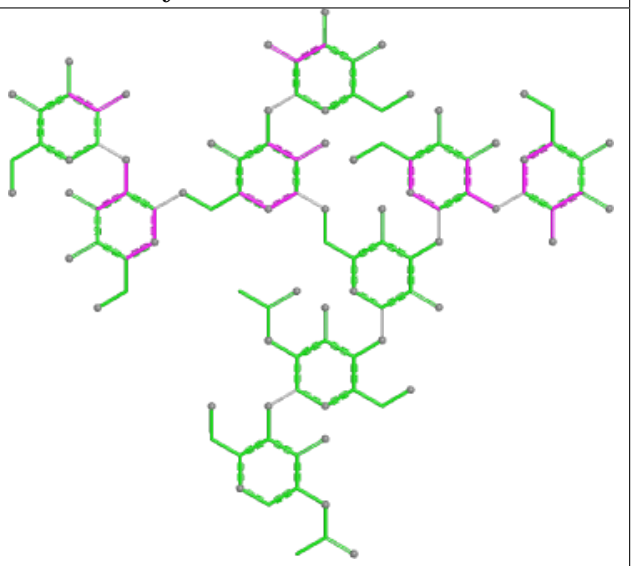


Rings

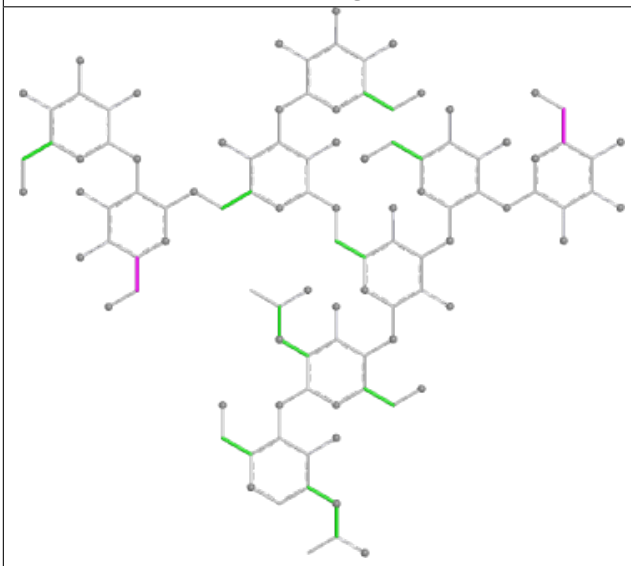
Oligosaccharide Chain y



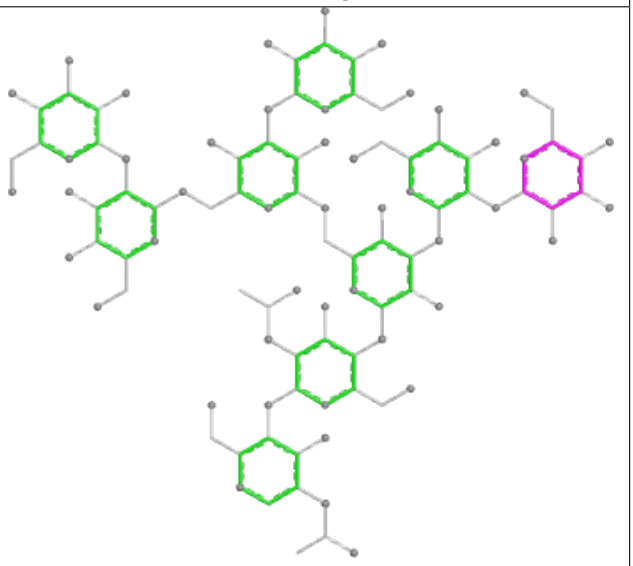
Bond lengths



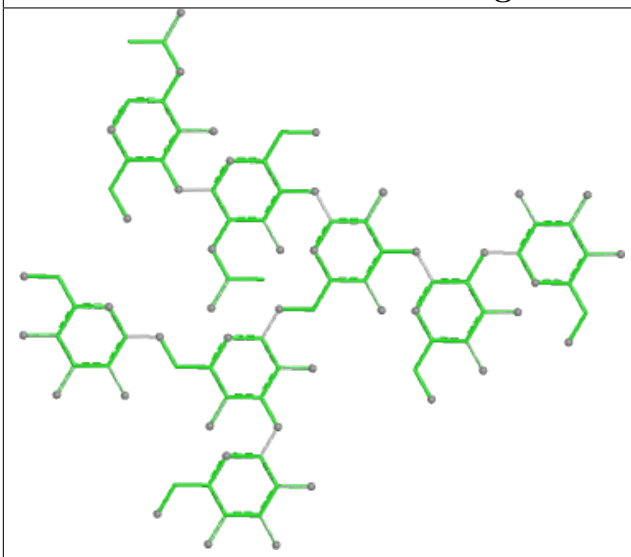
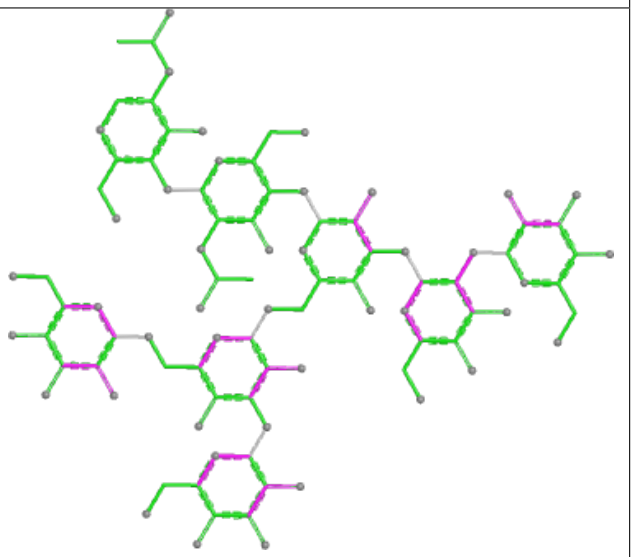
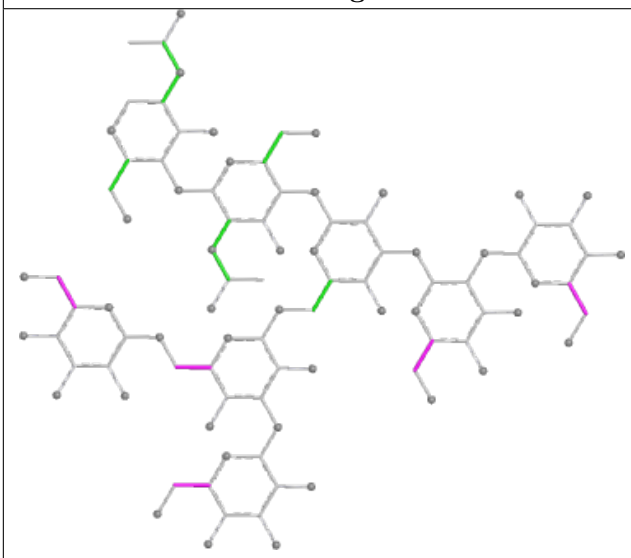
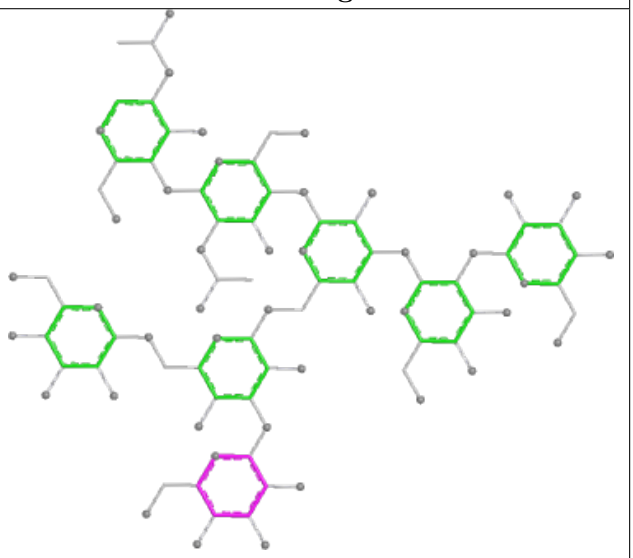
Bond angles

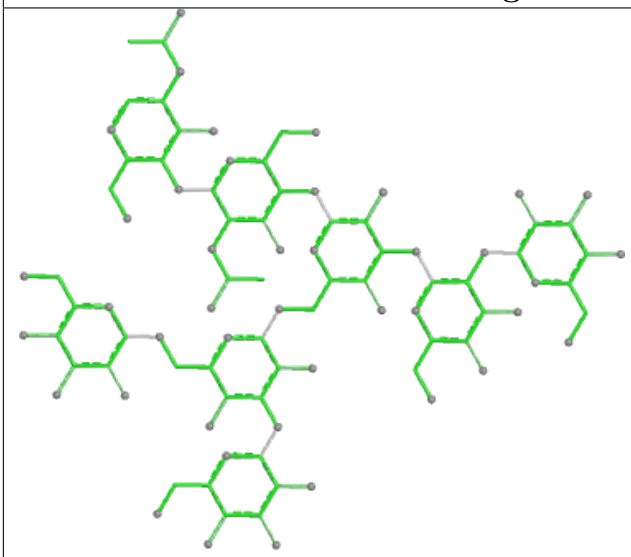
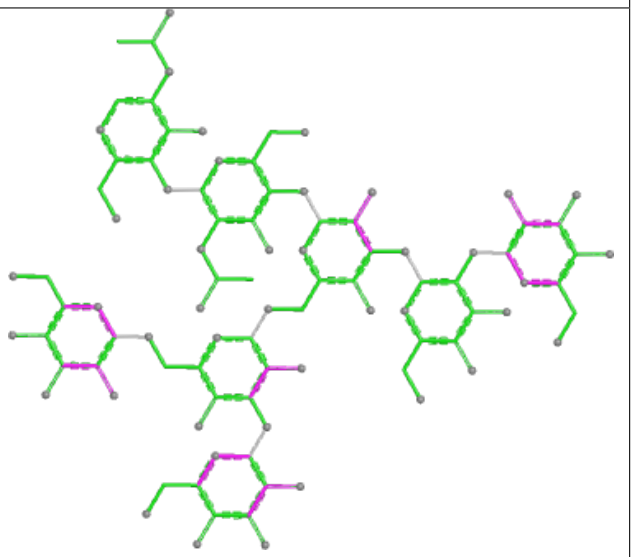
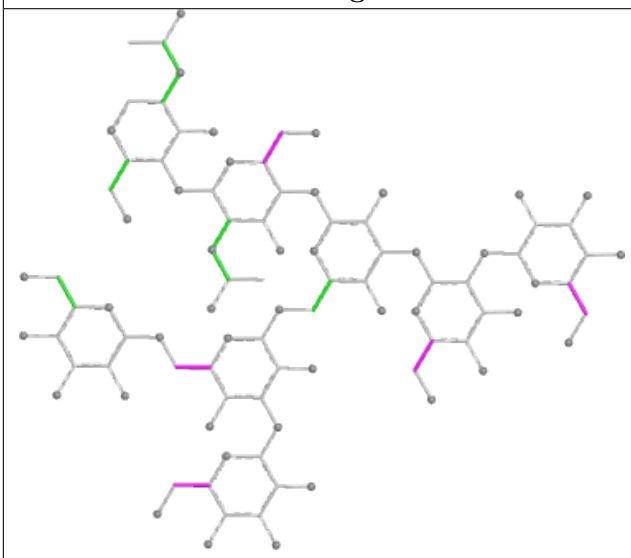
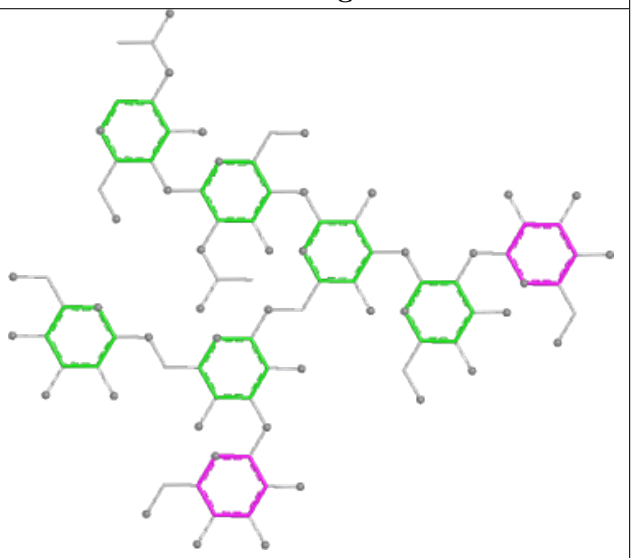


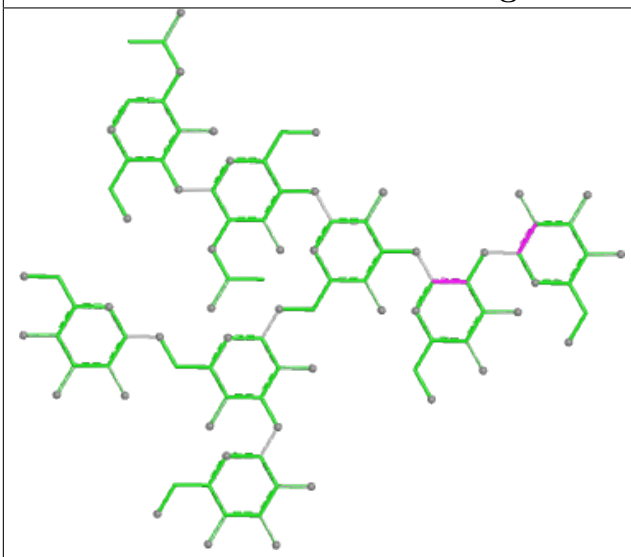
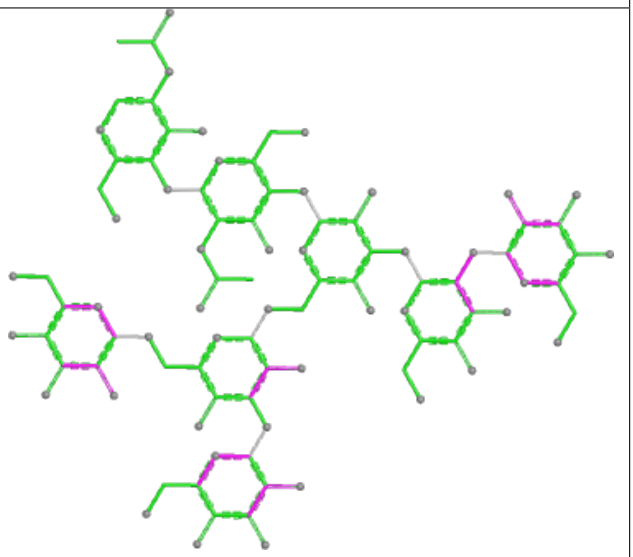
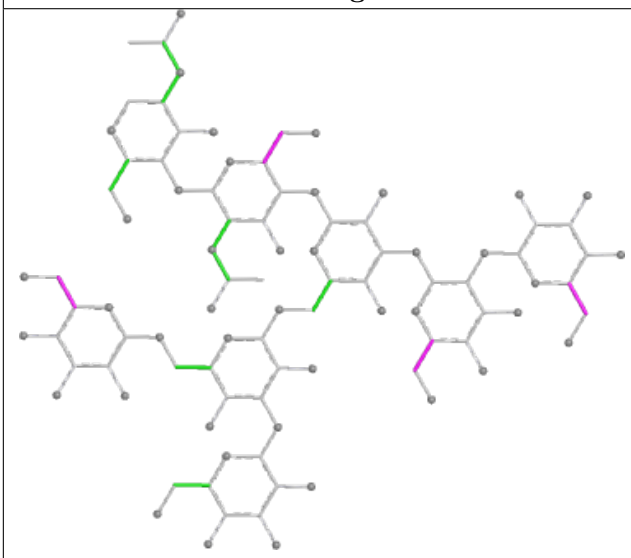
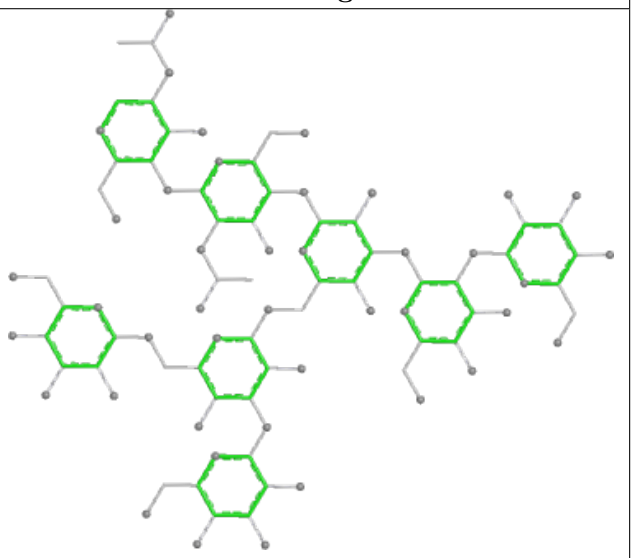
Torsions

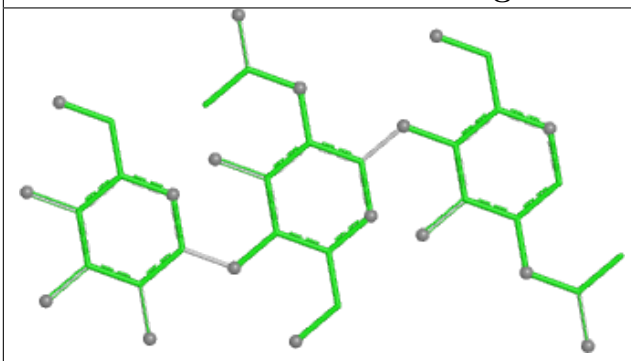
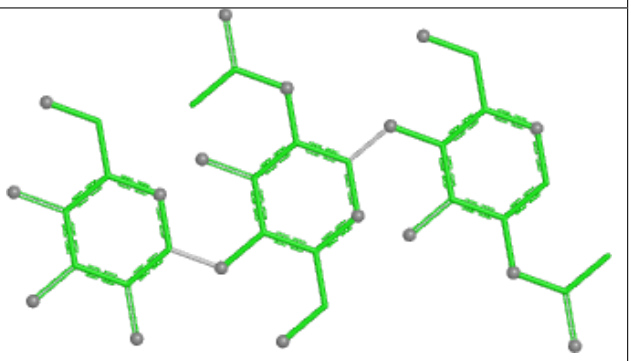
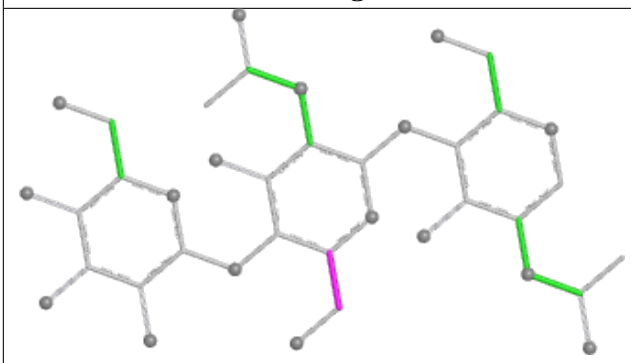
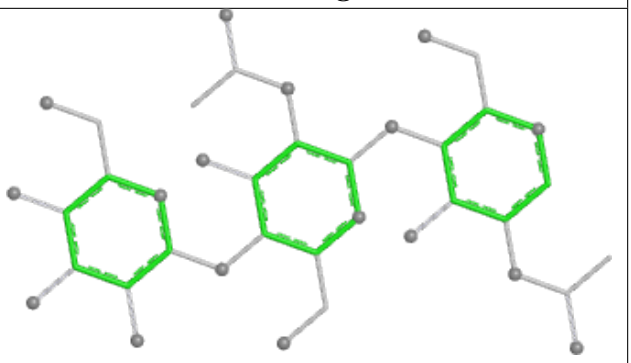


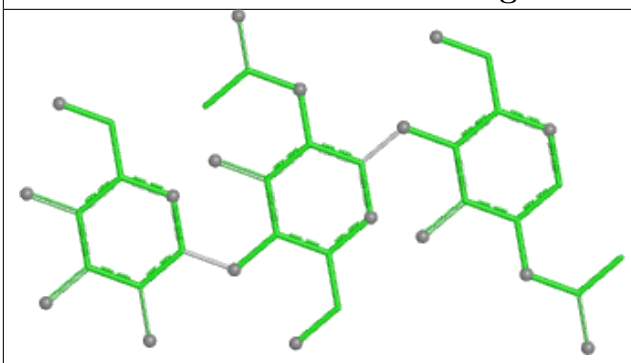
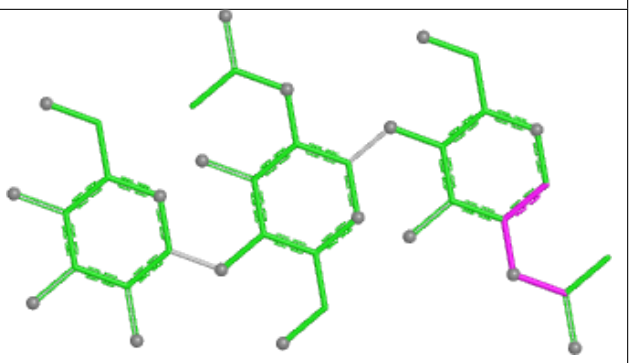
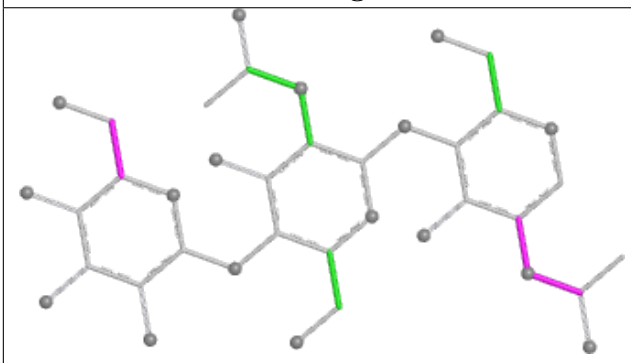
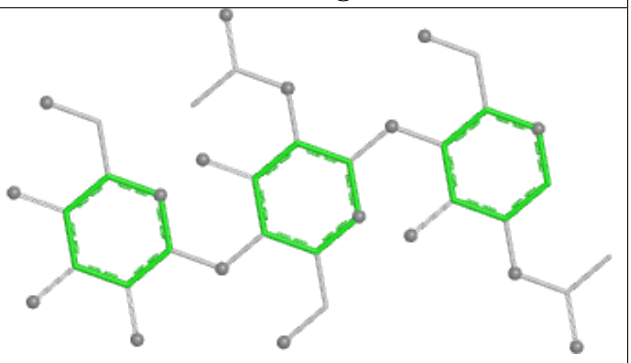
Rings

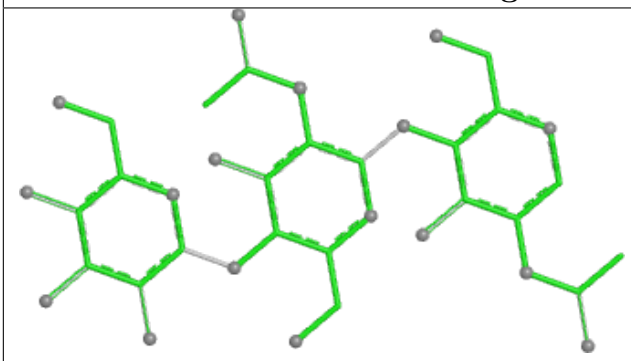
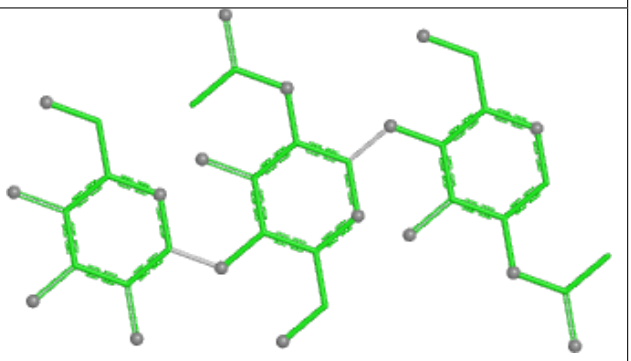
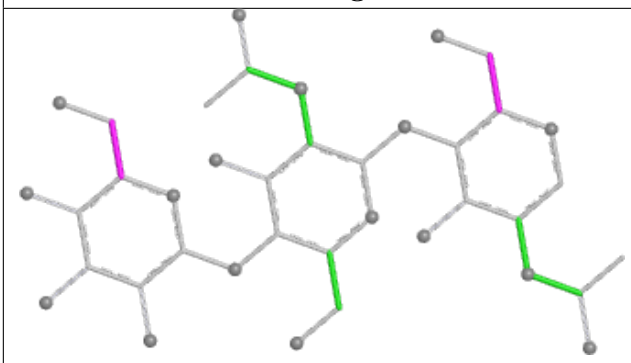
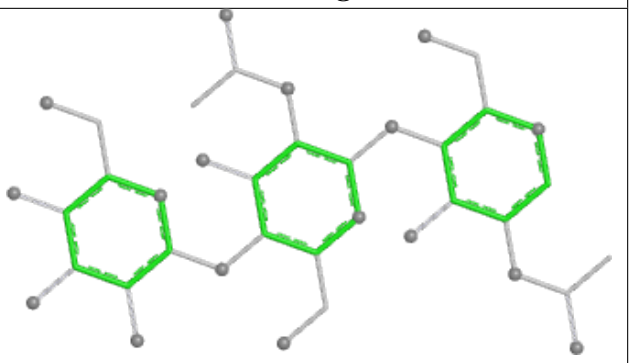
Oligosaccharide Chain X	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

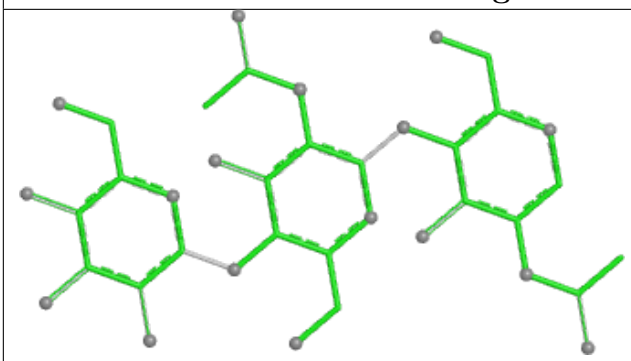
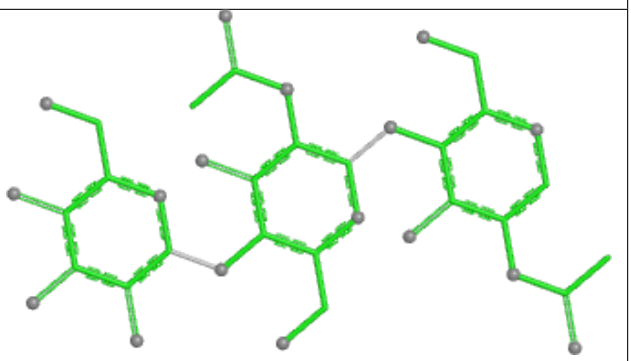
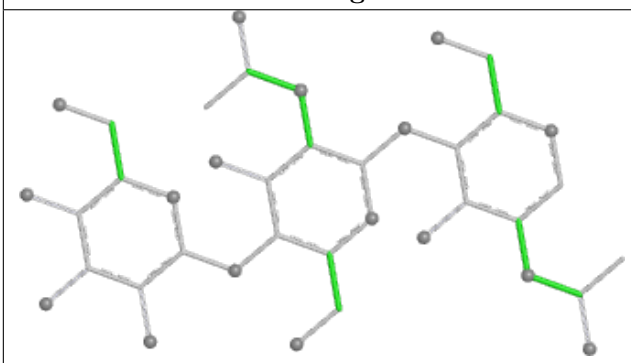
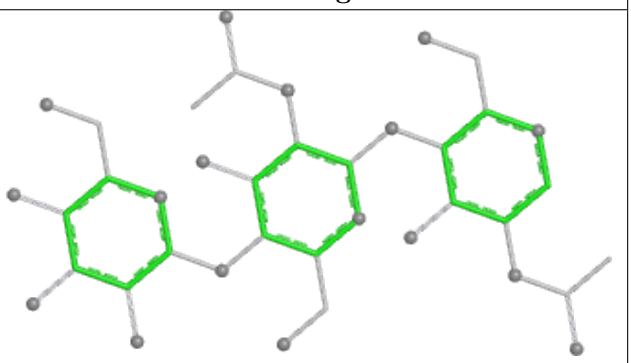
Oligosaccharide Chain l	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain z	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

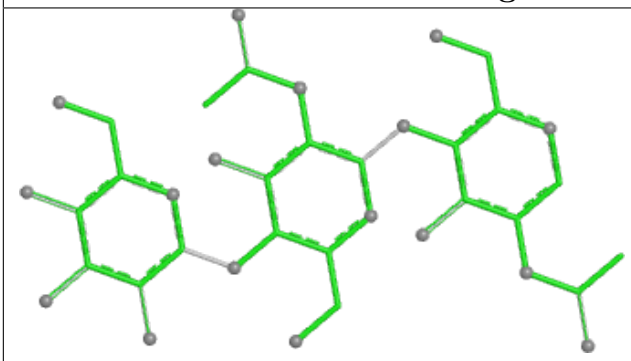
Oligosaccharide Chain Y	
	
Bond lengths	Bond angles
	
Torsions	Rings

Oligosaccharide Chain c	
	
Bond lengths	Bond angles
	
Torsions	Rings

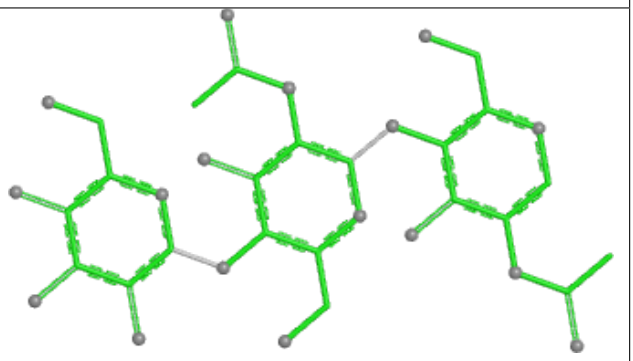
Oligosaccharide Chain f	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain m	
 Bond lengths	 Bond angles
 Torsions	 Rings

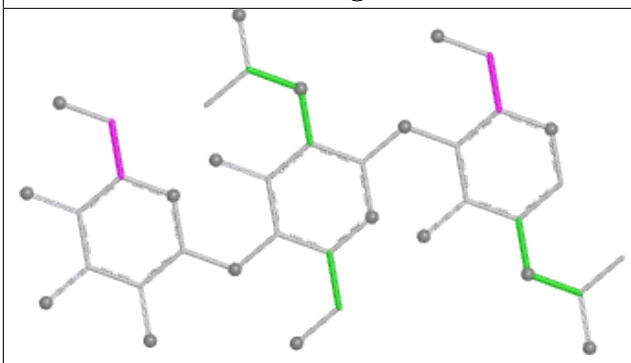
Oligosaccharide Chain o



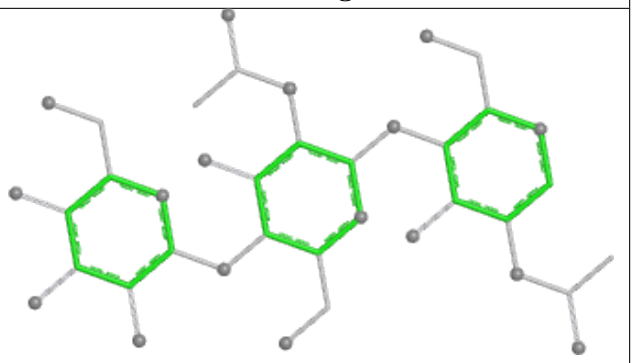
Bond lengths



Bond angles

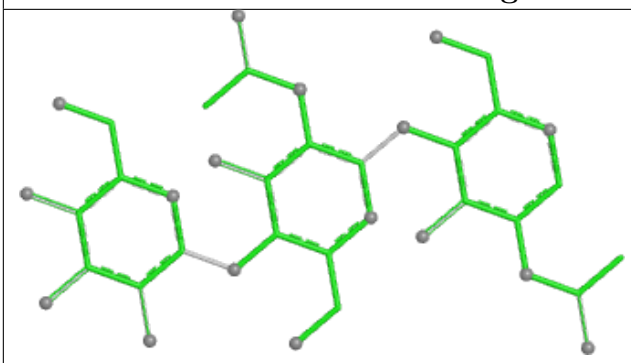


Torsions

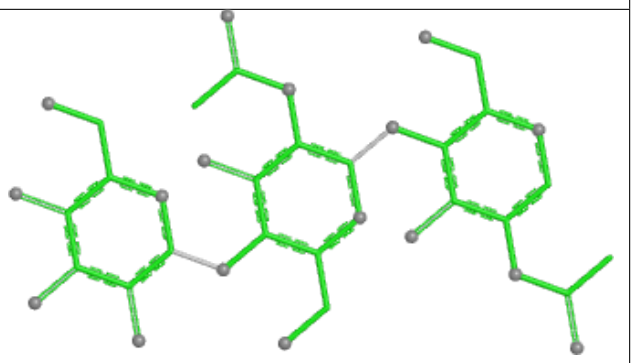


Rings

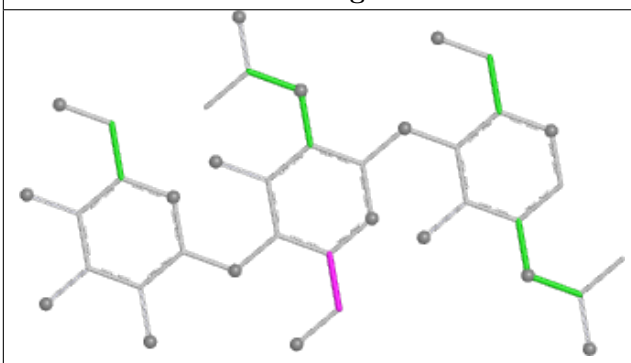
Oligosaccharide Chain t



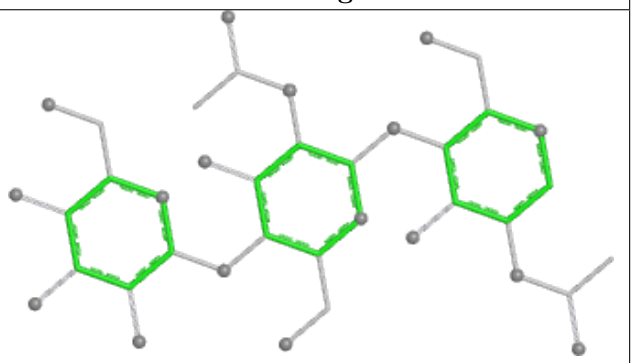
Bond lengths



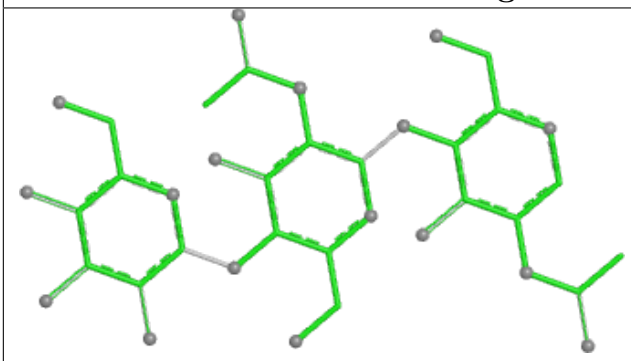
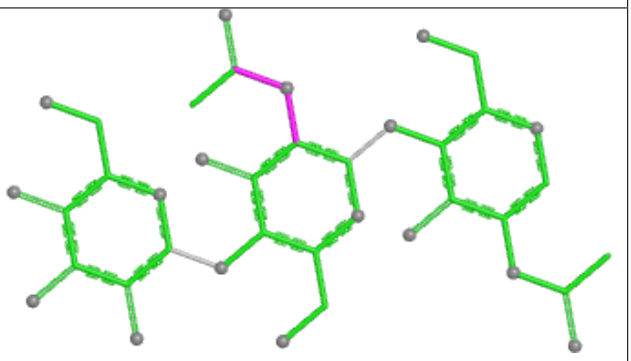
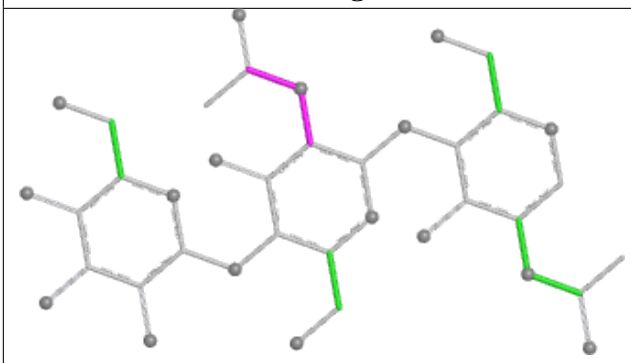
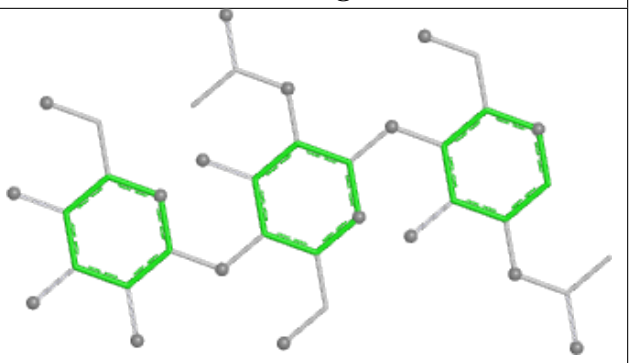
Bond angles

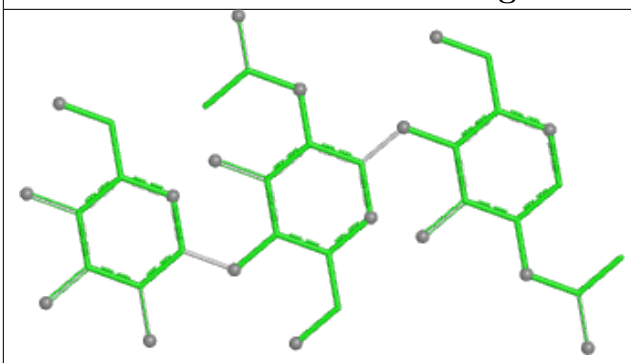
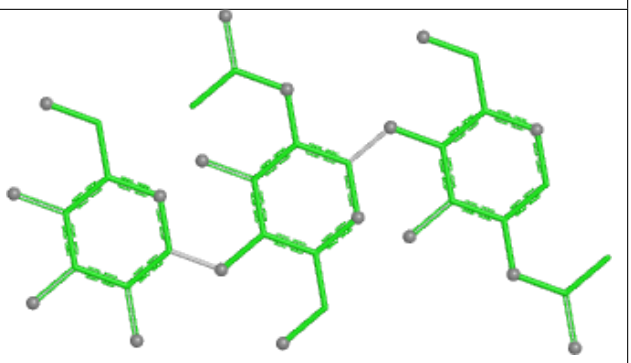
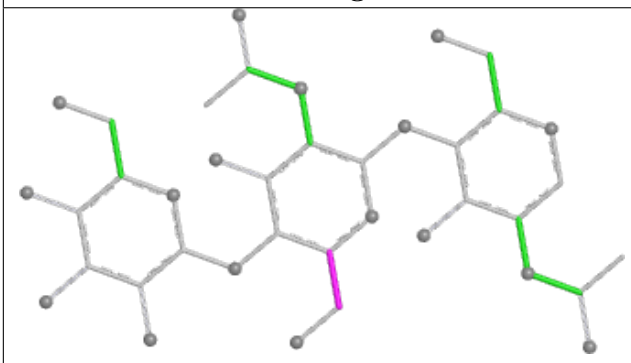
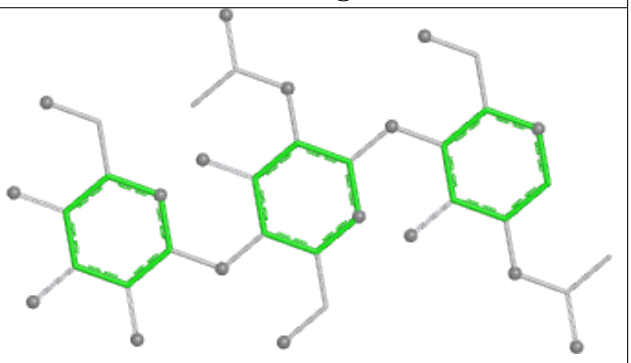


Torsions



Rings

Oligosaccharide Chain u	
	
Bond lengths	Bond angles
	
Torsions	Rings

Oligosaccharide Chain 0	
	
Bond lengths	Bond angles
	
Torsions	Rings

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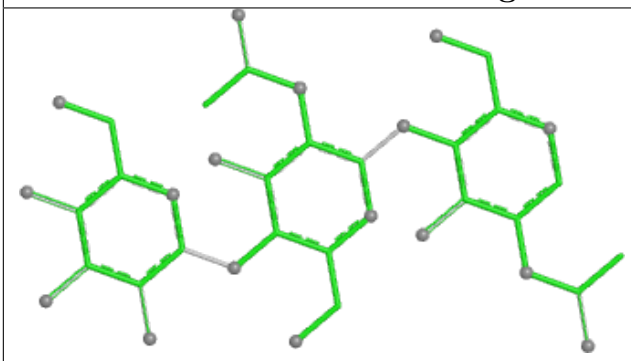
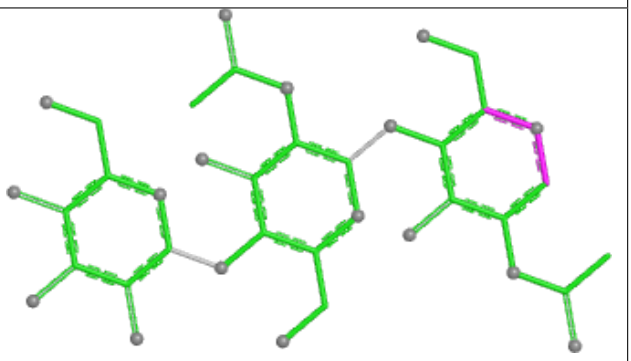
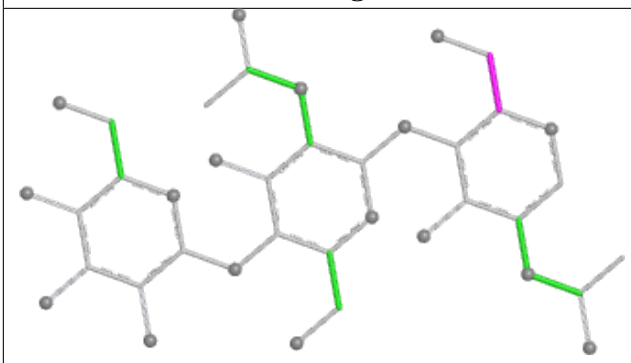
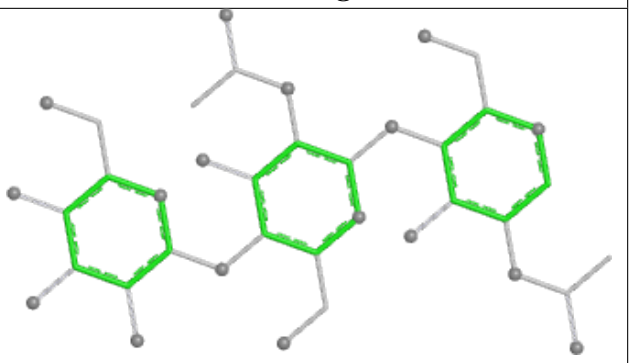
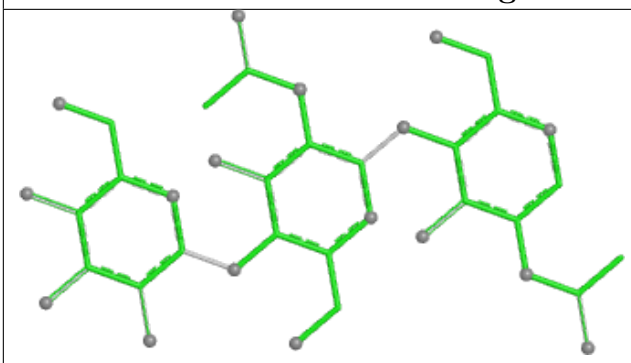
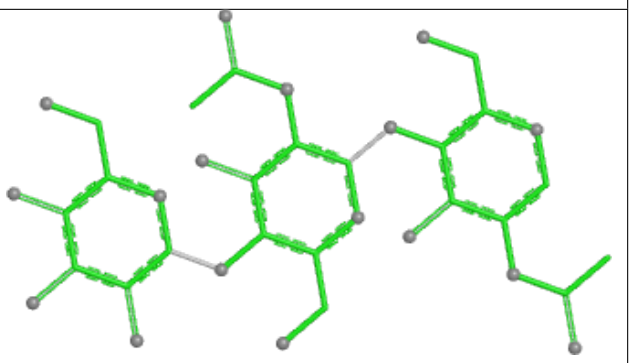
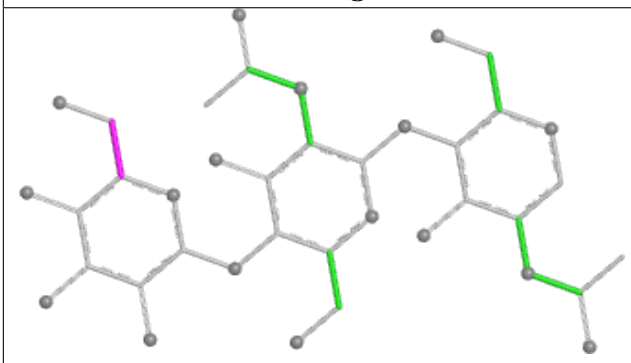
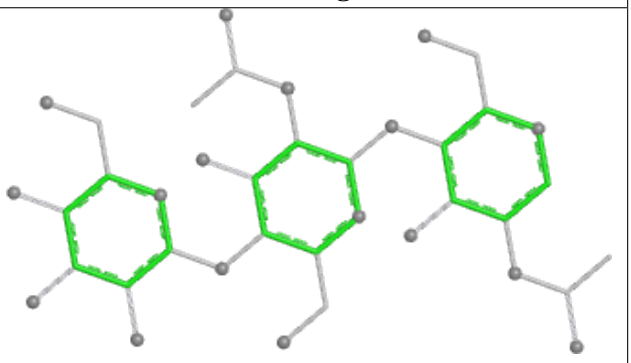
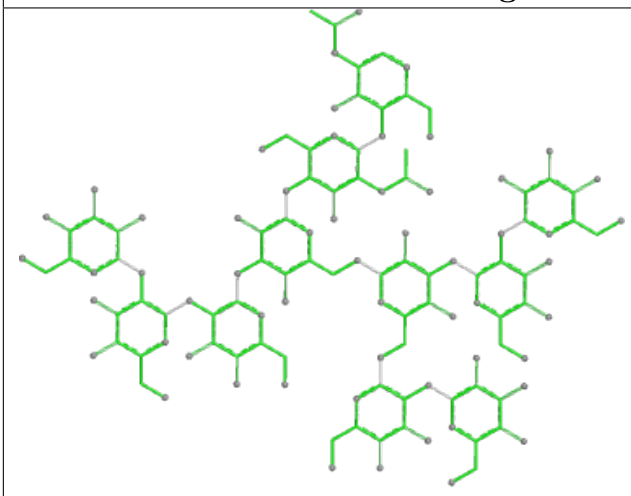
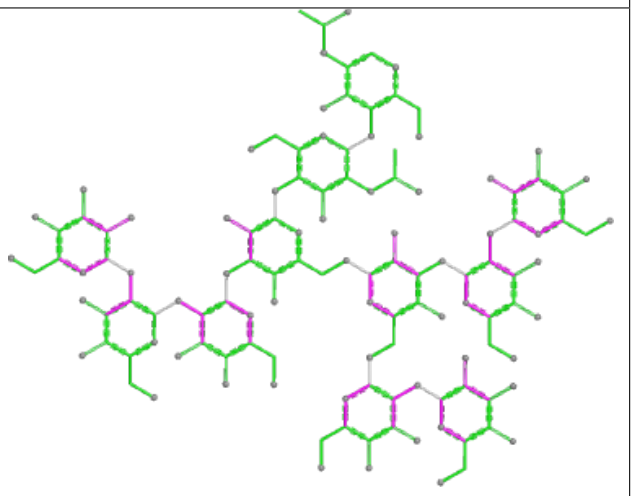
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 3	
 Bond lengths	 Bond angles
 Torsions	 Rings

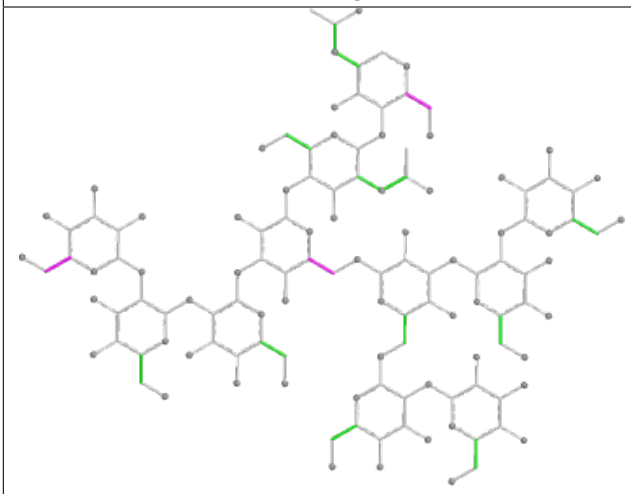
Oligosaccharide Chain a



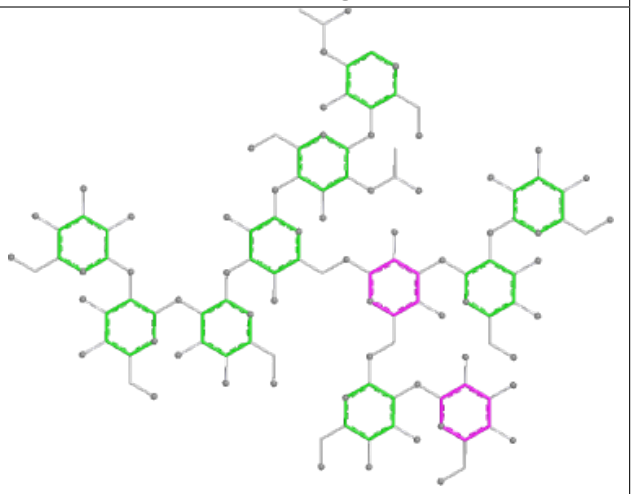
Bond lengths



Bond angles

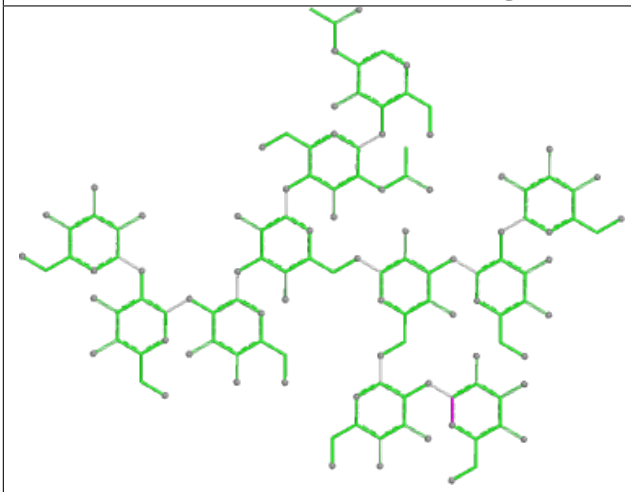


Torsions

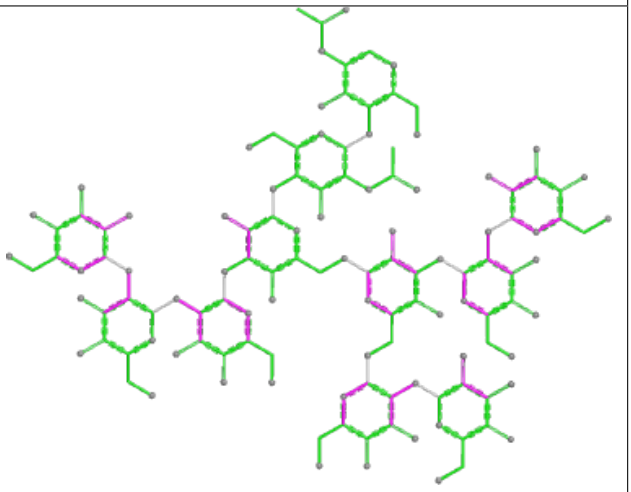


Rings

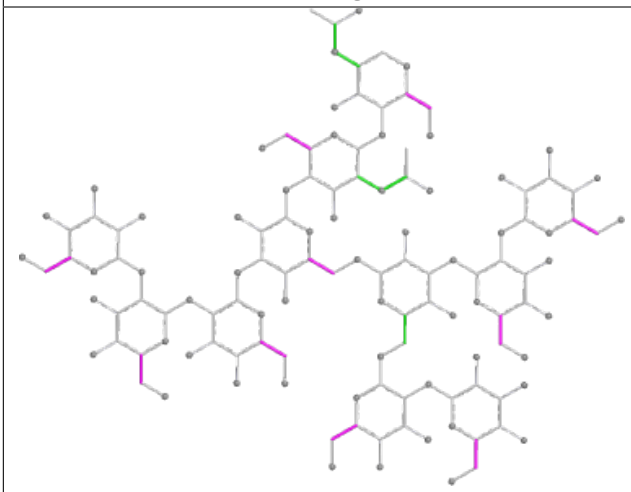
Oligosaccharide Chain r



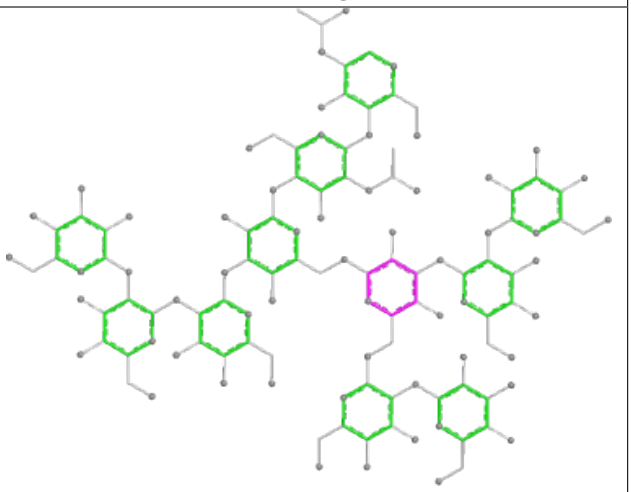
Bond lengths



Bond angles

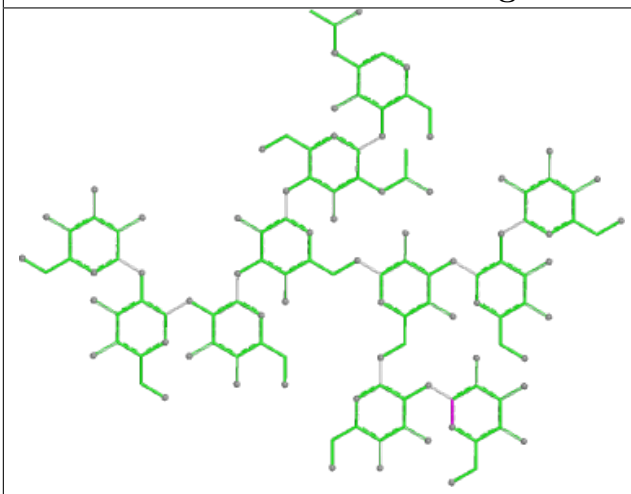


Torsions

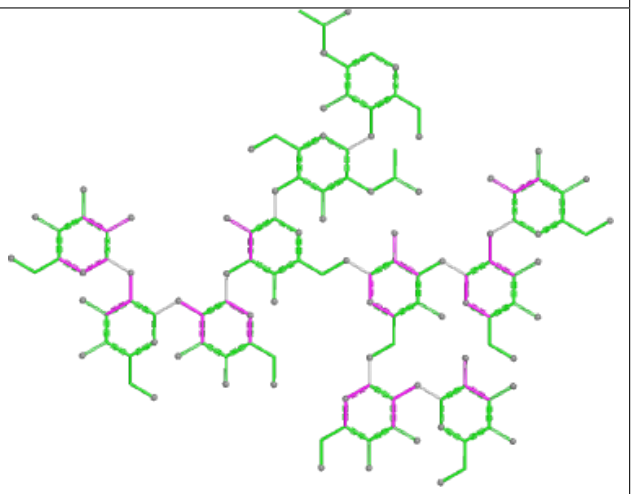


Rings

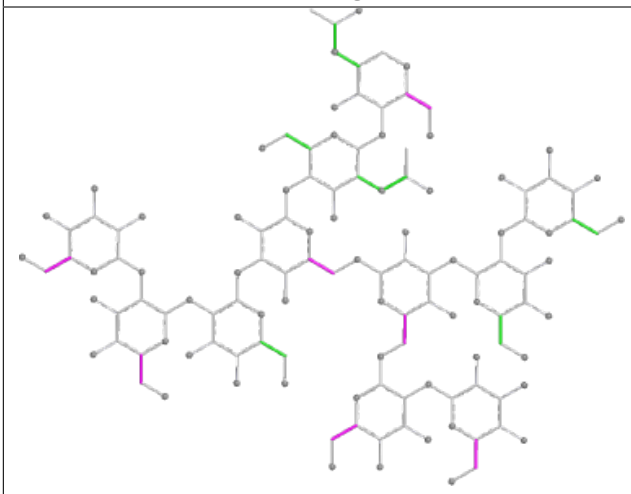
Oligosaccharide Chain 6



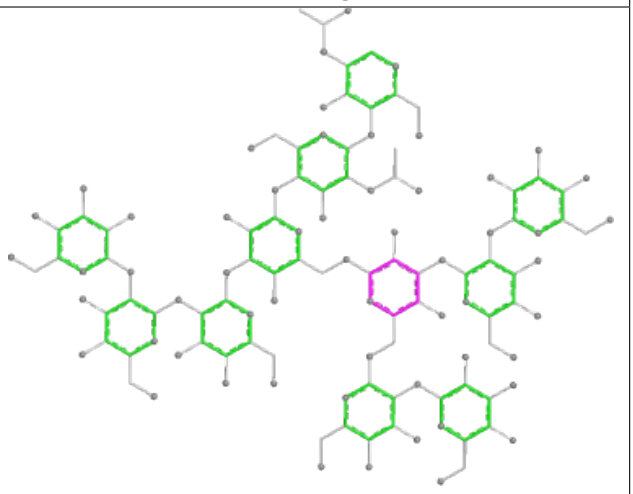
Bond lengths



Bond angles

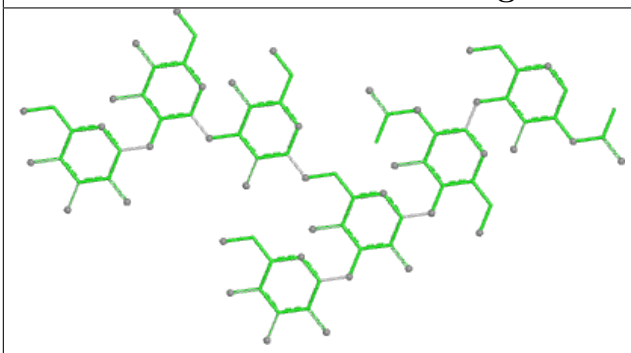


Torsions

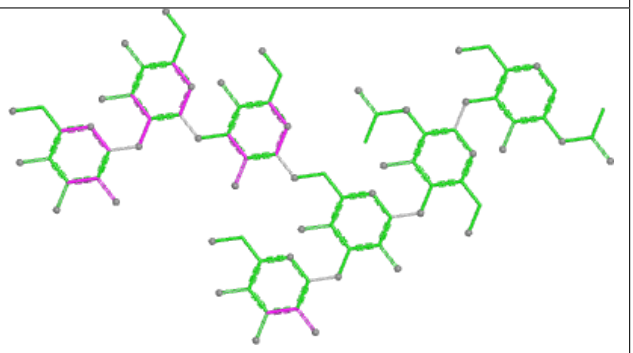


Rings

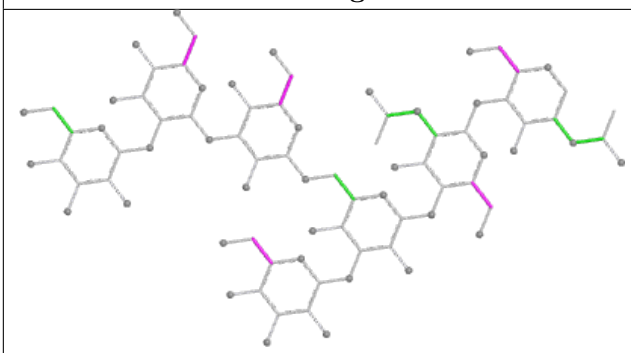
Oligosaccharide Chain b



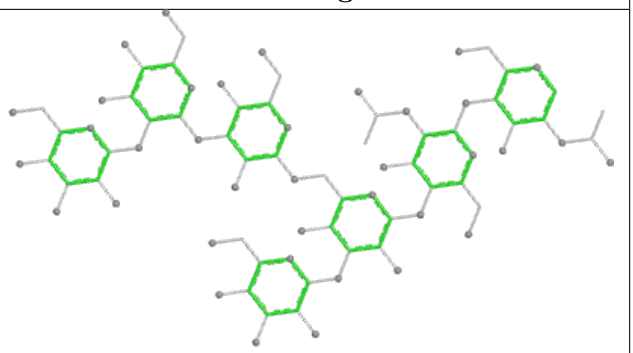
Bond lengths



Bond angles

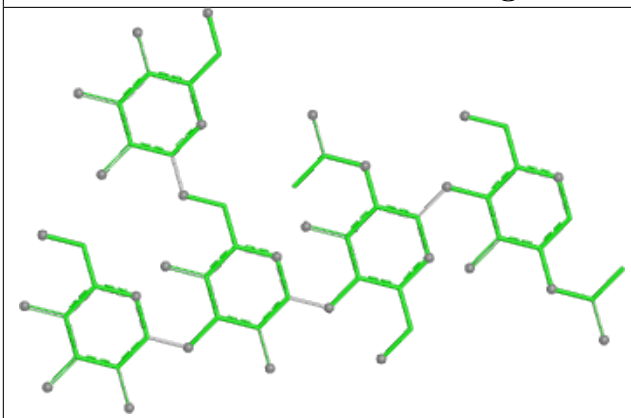


Torsions

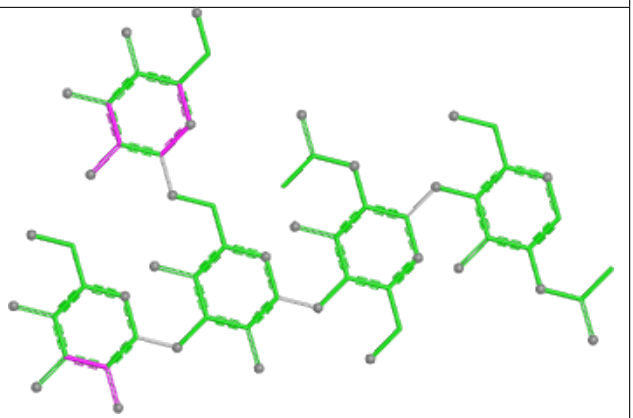


Rings

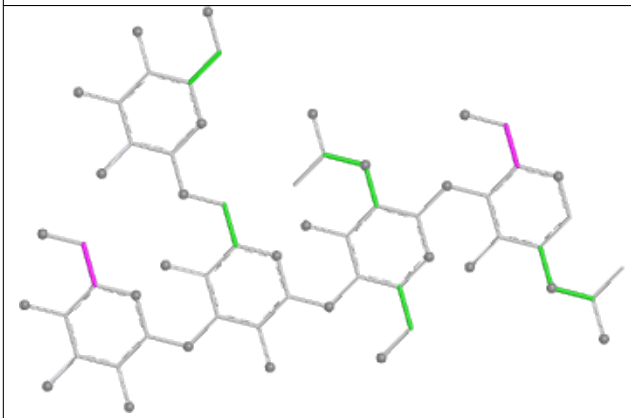
Oligosaccharide Chain e



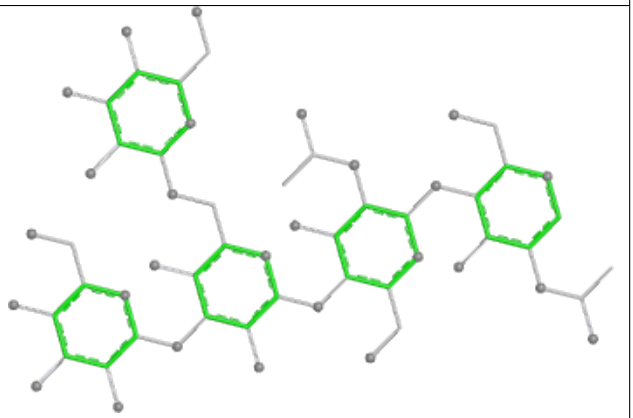
Bond lengths



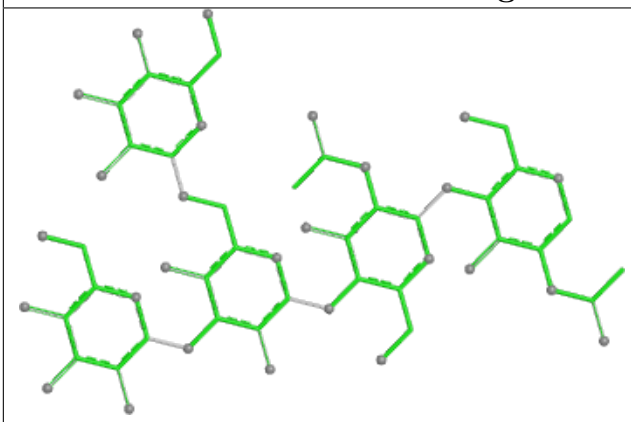
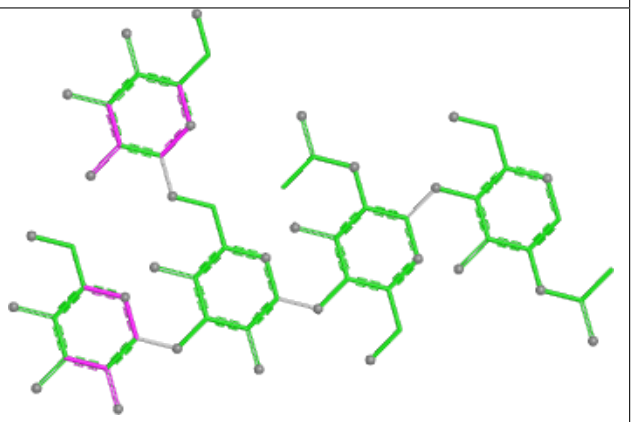
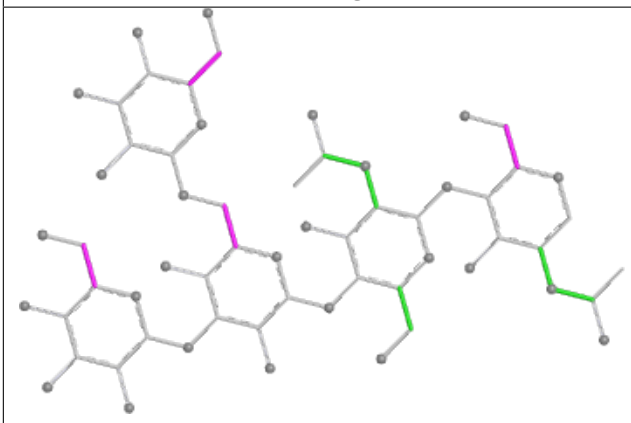
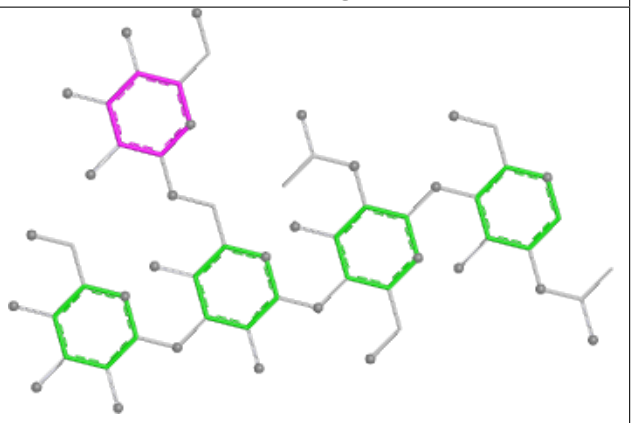
Bond angles

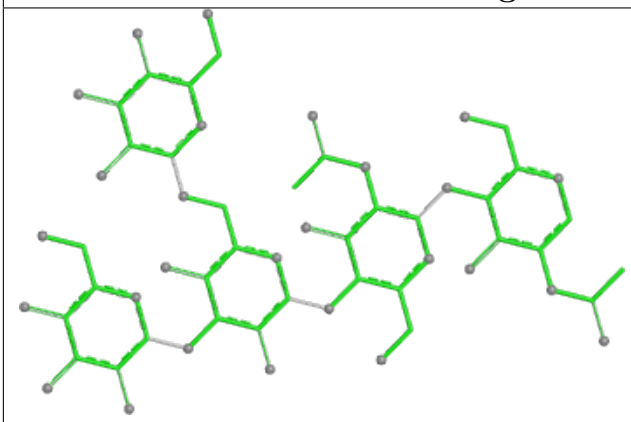
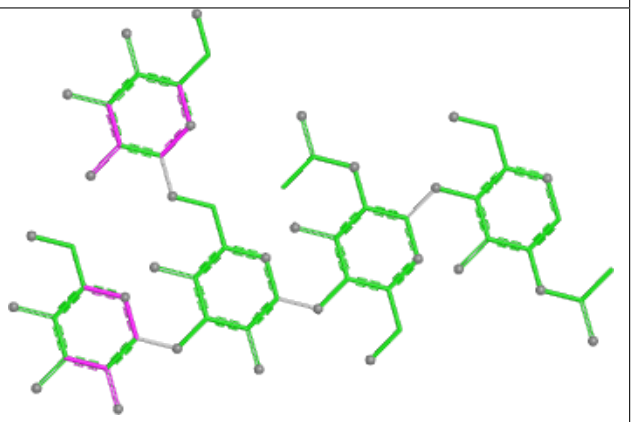
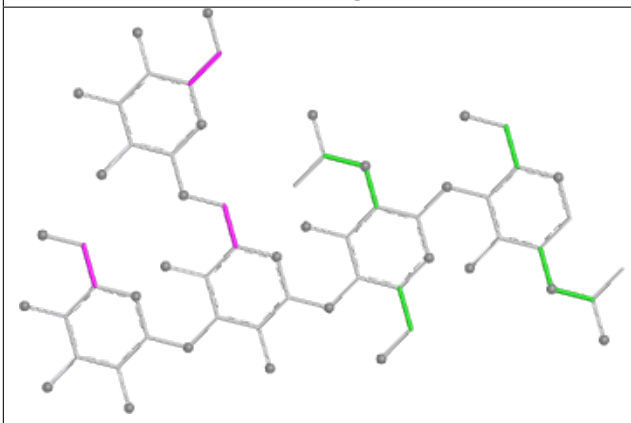
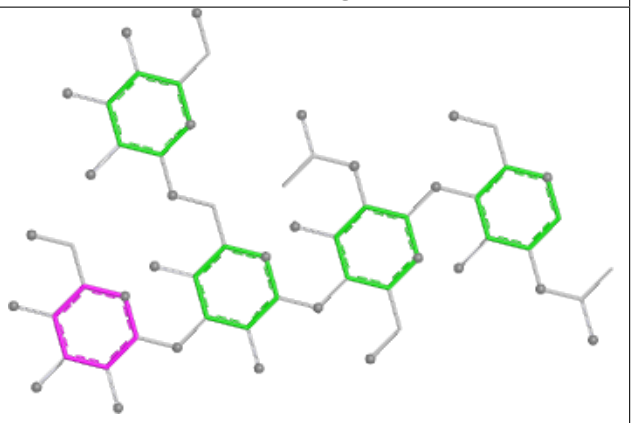


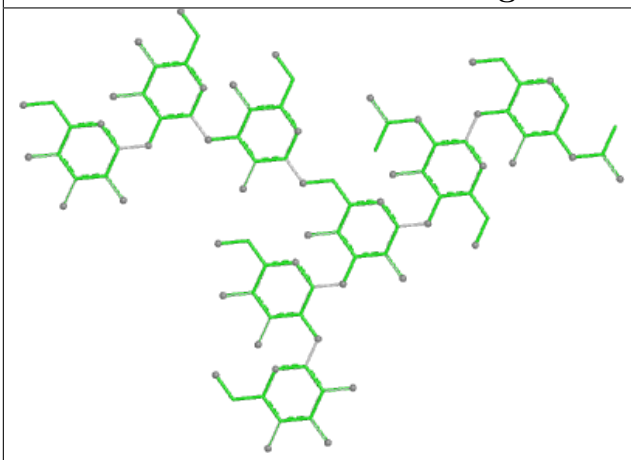
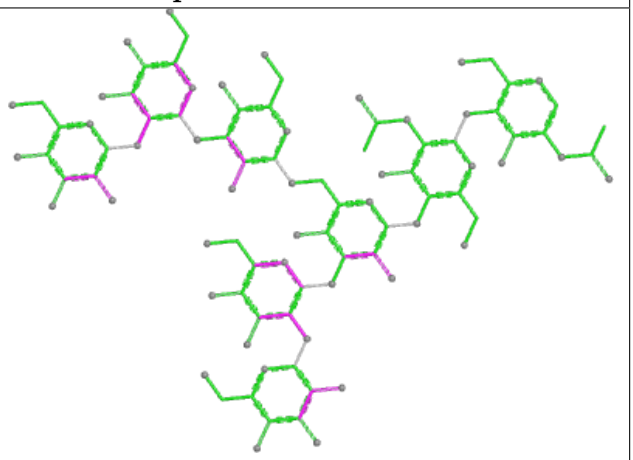
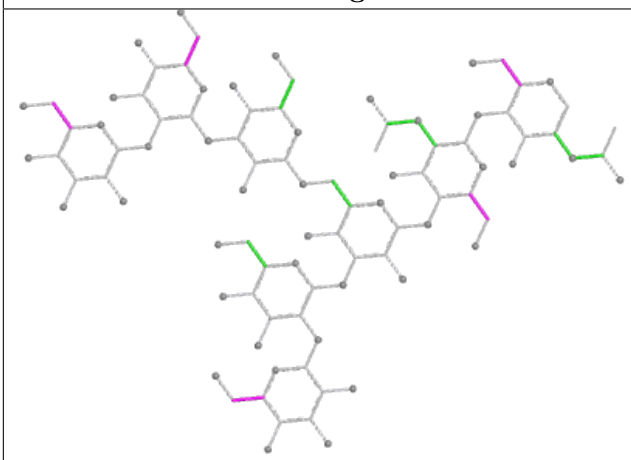
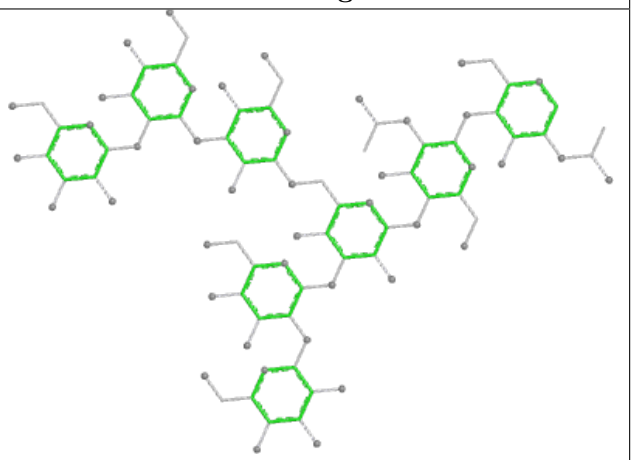
Torsions



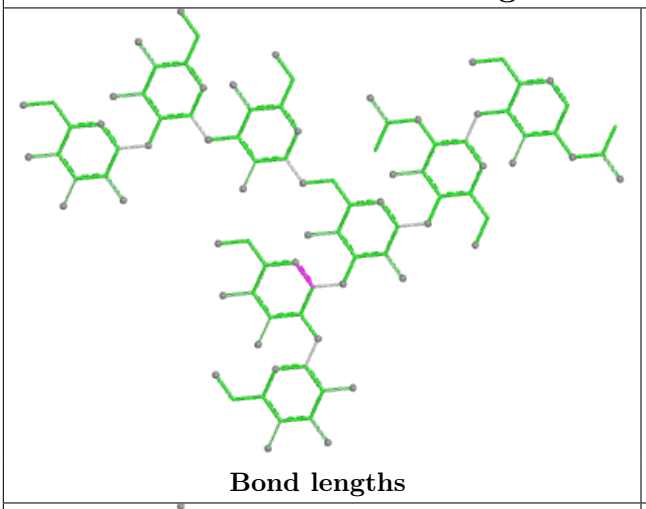
Rings

Oligosaccharide Chain n	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

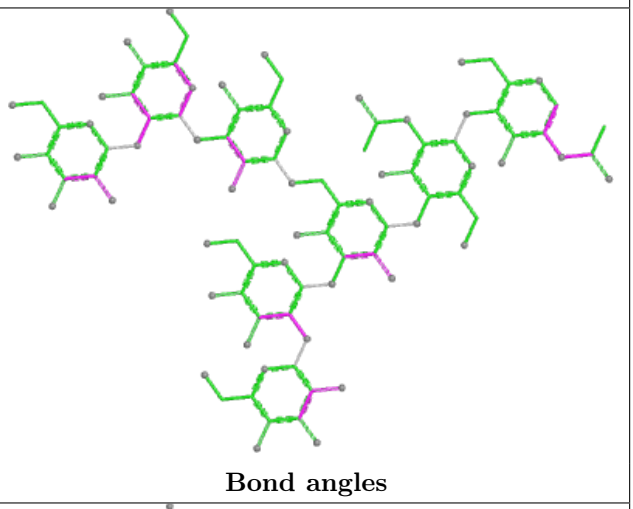
Oligosaccharide Chain 1	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain q	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

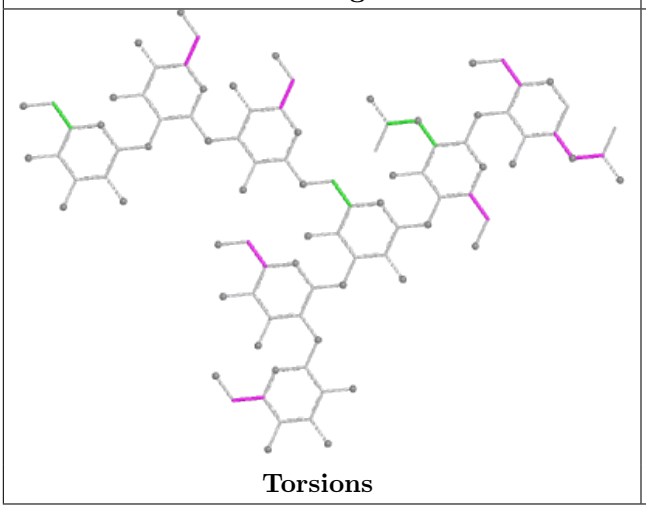
Oligosaccharide Chain 5



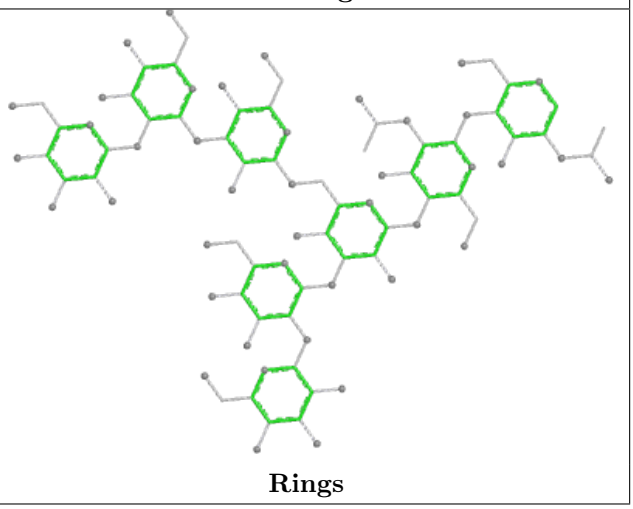
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

20 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	$\#\|Z\| > 2$
15	NAG	C	602	3	14,14,15	0.21	0	17,19,21	0.49	0
15	NAG	B	605	3	14,14,15	0.27	0	17,19,21	0.43	0
15	NAG	B	603	3	14,14,15	0.26	0	17,19,21	0.38	0
15	NAG	C	603	3	14,14,15	0.28	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	NAG	C	604	3	14,14,15	0.21	0	17,19,21	0.45	0
15	NAG	A	601	3	14,14,15	0.25	0	17,19,21	0.39	0
15	NAG	F	701	4	14,14,15	0.20	0	17,19,21	0.43	0
15	NAG	B	604	3	14,14,15	0.19	0	17,19,21	0.45	0
15	NAG	B	602	3	14,14,15	0.19	0	17,19,21	0.39	0
15	NAG	D	701	4	14,14,15	0.22	0	17,19,21	0.46	0
15	NAG	E	702	4	14,14,15	0.20	0	17,19,21	0.42	0
15	NAG	D	702	4	14,14,15	0.22	0	17,19,21	0.41	0
15	NAG	A	605	3	14,14,15	0.22	0	17,19,21	0.47	0
15	NAG	A	602	3	14,14,15	0.17	0	17,19,21	0.42	0
15	NAG	B	601	3	14,14,15	0.22	0	17,19,21	0.47	0
15	NAG	C	601	3	14,14,15	0.27	0	17,19,21	0.46	0
15	NAG	A	603	3	14,14,15	0.19	0	17,19,21	0.44	0
15	NAG	A	604	3	14,14,15	0.29	0	17,19,21	0.39	0
15	NAG	F	702	4	14,14,15	0.21	0	17,19,21	0.41	0
15	NAG	E	701	4	14,14,15	0.19	0	17,19,21	0.45	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
15	NAG	C	602	3	-	2/6/23/26	0/1/1/1
15	NAG	B	605	3	-	4/6/23/26	0/1/1/1
15	NAG	B	603	3	-	0/6/23/26	0/1/1/1
15	NAG	C	603	3	-	0/6/23/26	0/1/1/1
15	NAG	C	604	3	-	1/6/23/26	0/1/1/1
15	NAG	A	601	3	-	0/6/23/26	0/1/1/1
15	NAG	F	701	4	-	0/6/23/26	0/1/1/1
15	NAG	B	604	3	-	2/6/23/26	0/1/1/1
15	NAG	B	602	3	-	2/6/23/26	0/1/1/1
15	NAG	D	701	4	-	2/6/23/26	0/1/1/1
15	NAG	E	702	4	-	0/6/23/26	0/1/1/1
15	NAG	D	702	4	-	2/6/23/26	0/1/1/1
15	NAG	A	605	3	-	2/6/23/26	0/1/1/1
15	NAG	A	602	3	-	2/6/23/26	0/1/1/1
15	NAG	B	601	3	-	2/6/23/26	0/1/1/1
15	NAG	C	601	3	-	2/6/23/26	0/1/1/1
15	NAG	A	603	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	A	604	3	-	1/6/23/26	0/1/1/1
15	NAG	F	702	4	-	2/6/23/26	0/1/1/1
15	NAG	E	701	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	603	NAG	C4-C5-C6-O6
15	A	602	NAG	C4-C5-C6-O6
15	B	602	NAG	C4-C5-C6-O6
15	B	604	NAG	C4-C5-C6-O6
15	A	605	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	B	2
6	H	2
6	J	2
3	A	2
3	C	2
6	L	2

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	141:ASP	C	150:MET	N	3.05

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	27:GLY	C	32:TYR	N	2.98
1	J	91:TYR	C	96:GLU	N	2.97
1	A	141:ASP	C	150:MET	N	2.96
1	B	309:ILE	C	312:GLY	N	2.95

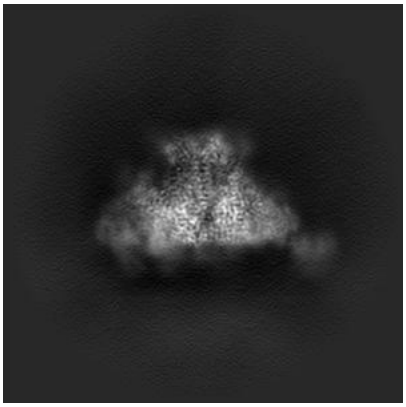
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13316. These allow visual inspection of the internal detail of the map and identification of artifacts.

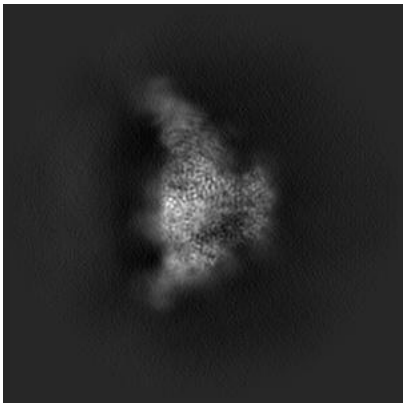
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

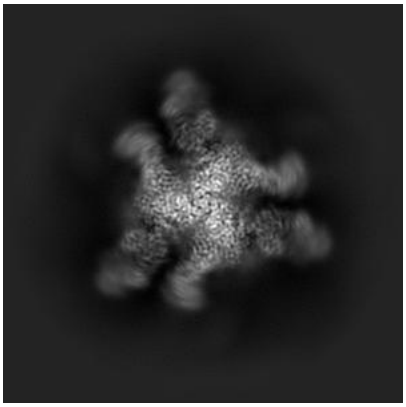
6.1.1 Primary map



X



Y

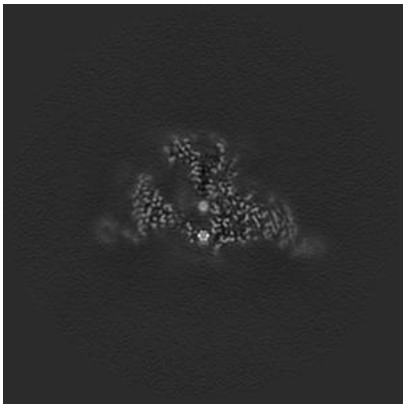


Z

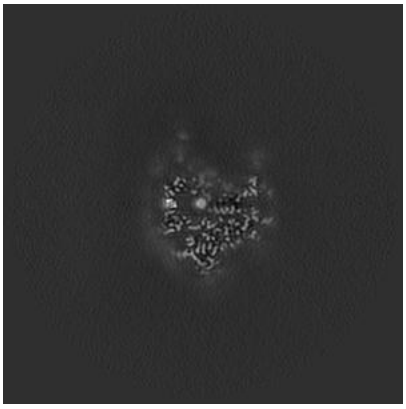
The images above show the map projected in three orthogonal directions.

6.2 Central slices

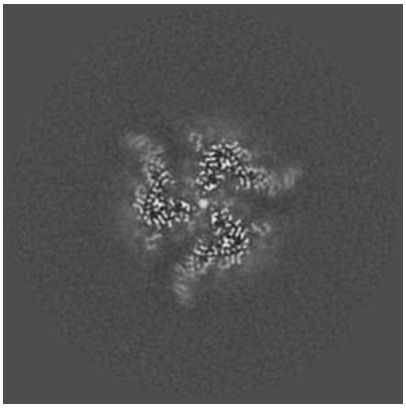
6.2.1 Primary map



X Index: 210



Y Index: 210

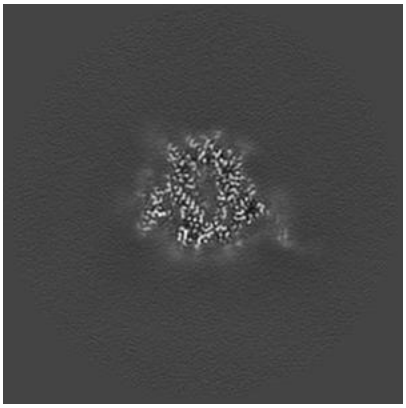


Z Index: 210

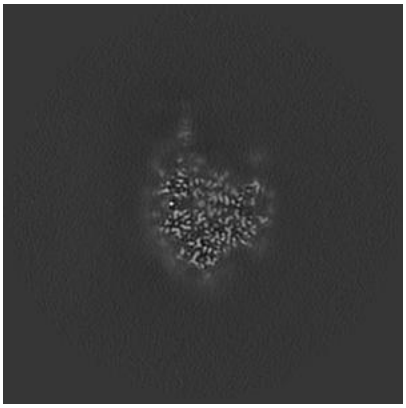
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

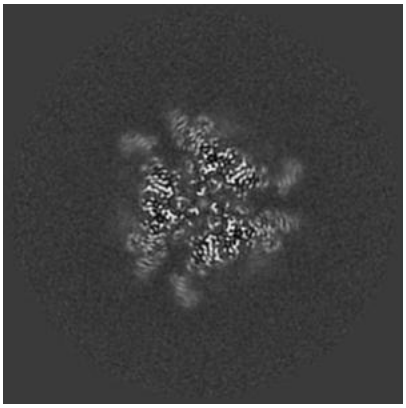
6.3.1 Primary map



X Index: 223



Y Index: 205

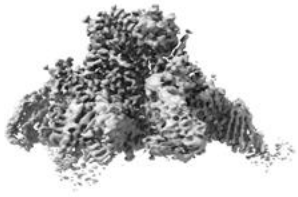


Z Index: 201

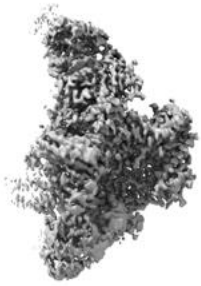
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

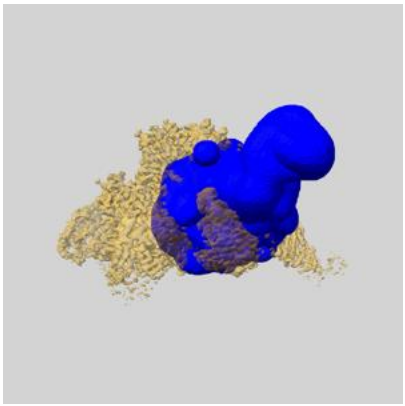
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

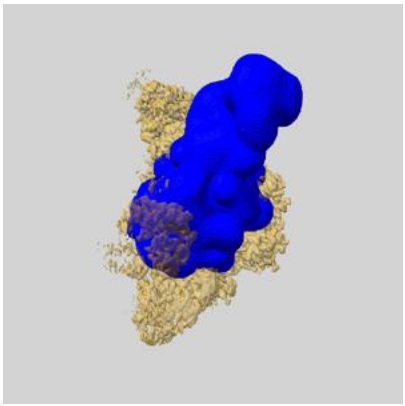
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

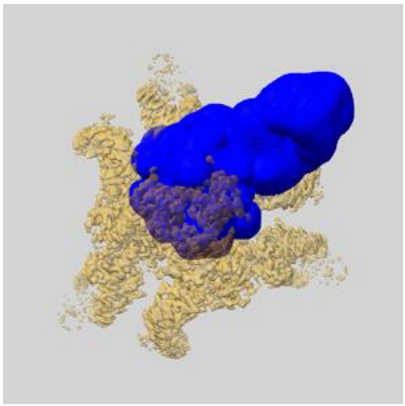
6.5.1 emd_13316_msk_1.map (i)



X



Y

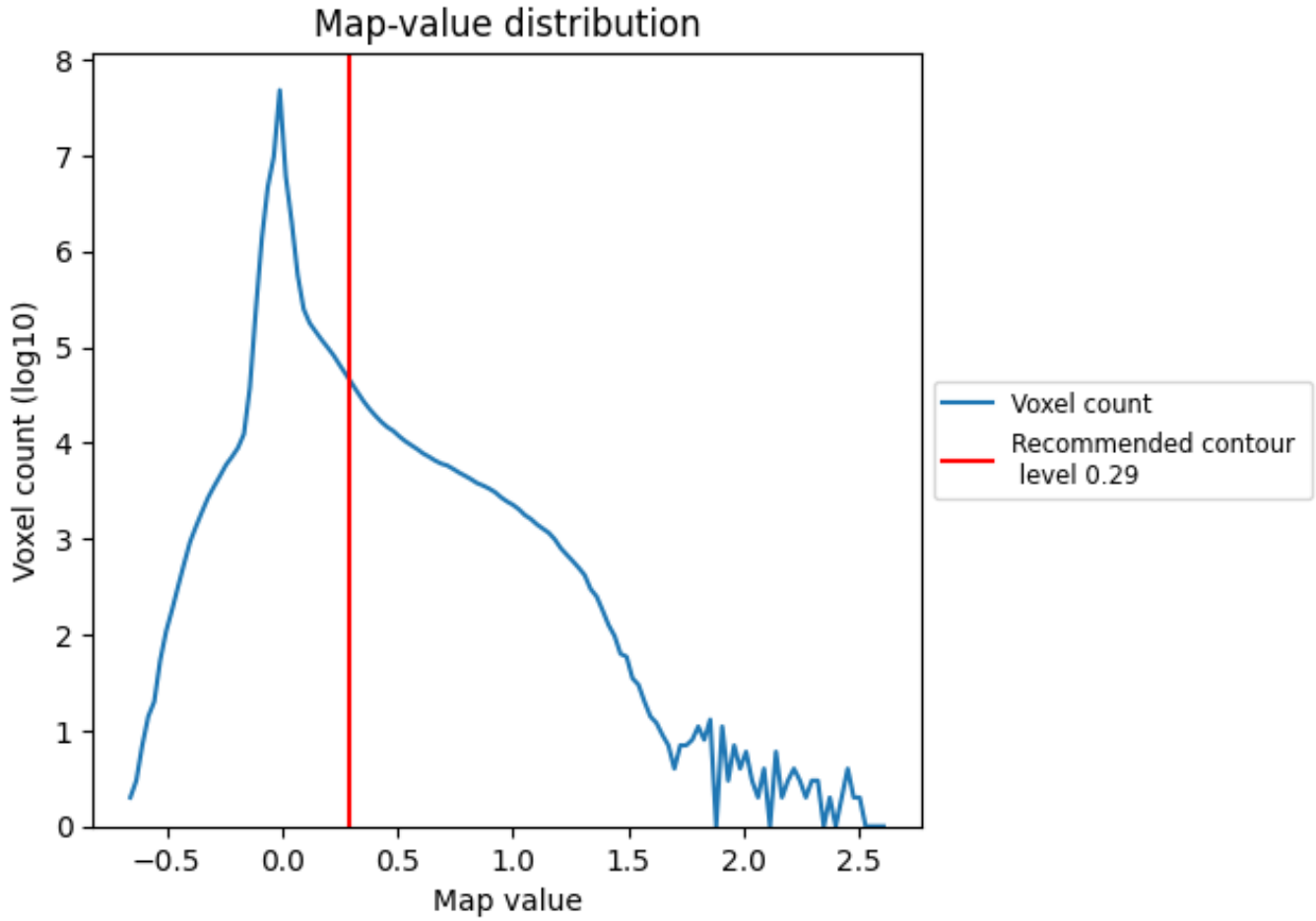


Z

7 Map analysis

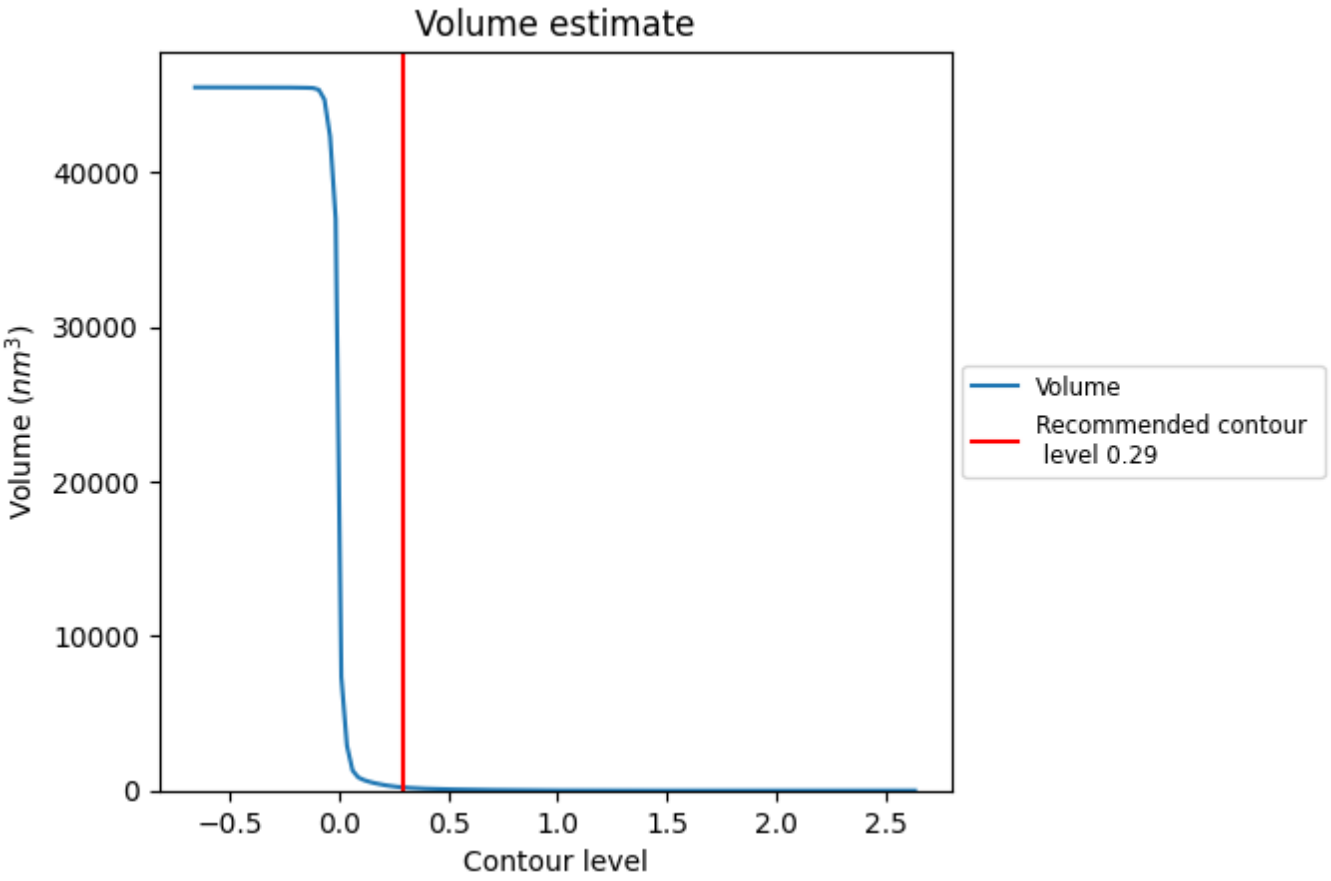
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

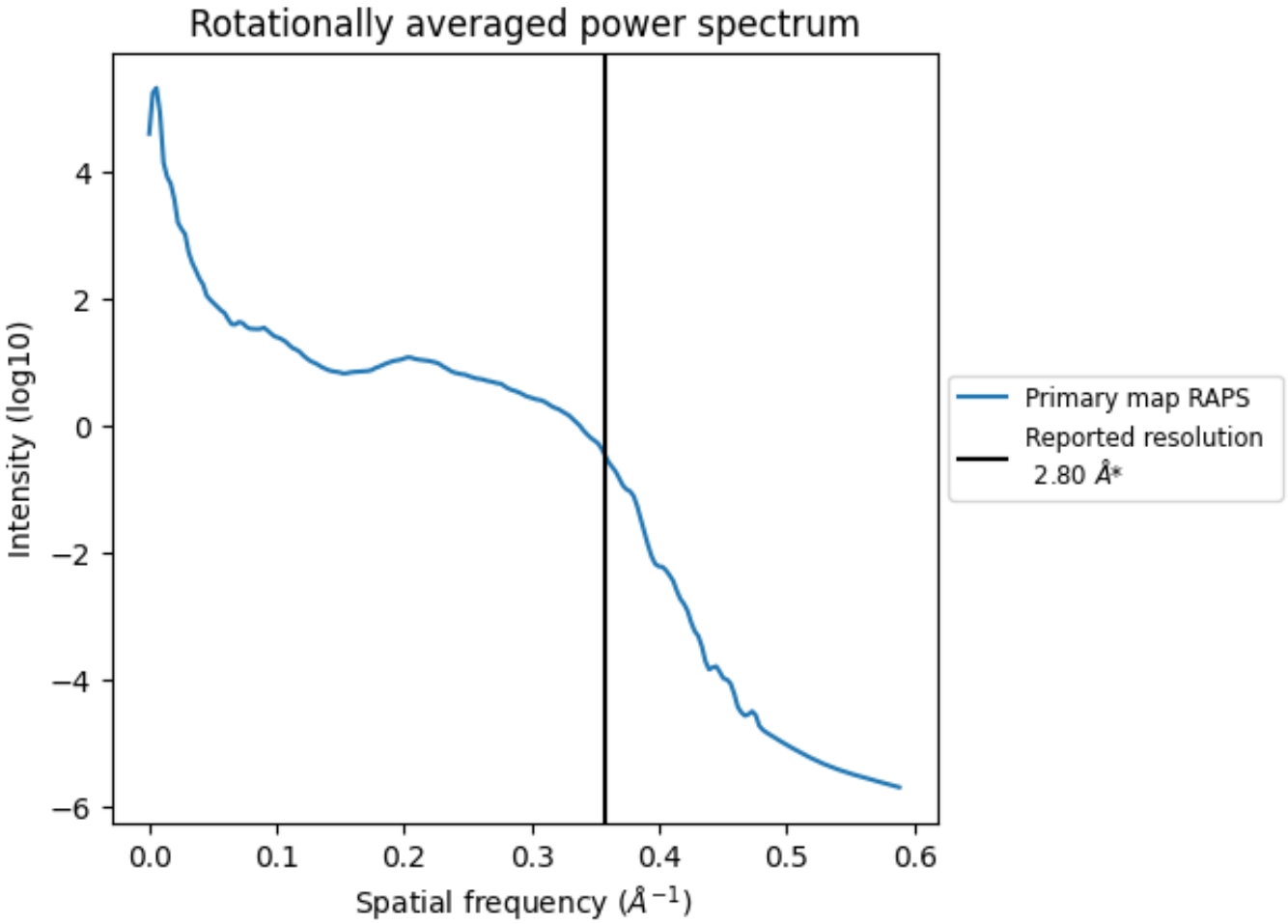
7.2 Volume estimate (i)



The volume at the recommended contour level is 208 nm^3; this corresponds to an approximate mass of 188 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

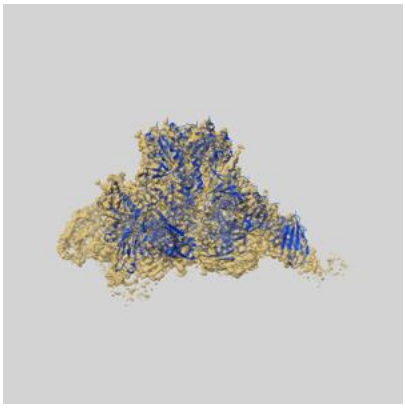
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

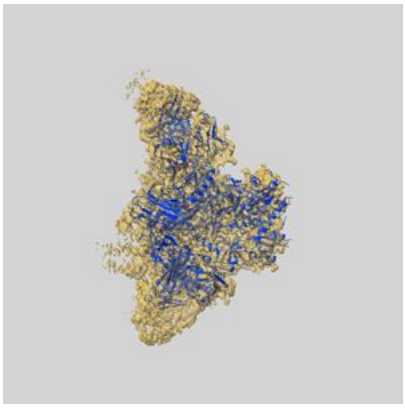
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13316 and PDB model 7PC2. Per-residue inclusion information can be found in section 3 on page 14.

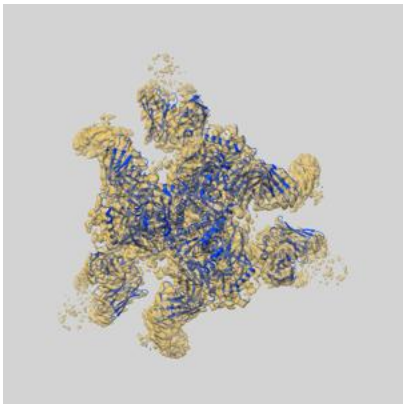
9.1 Map-model overlay



X



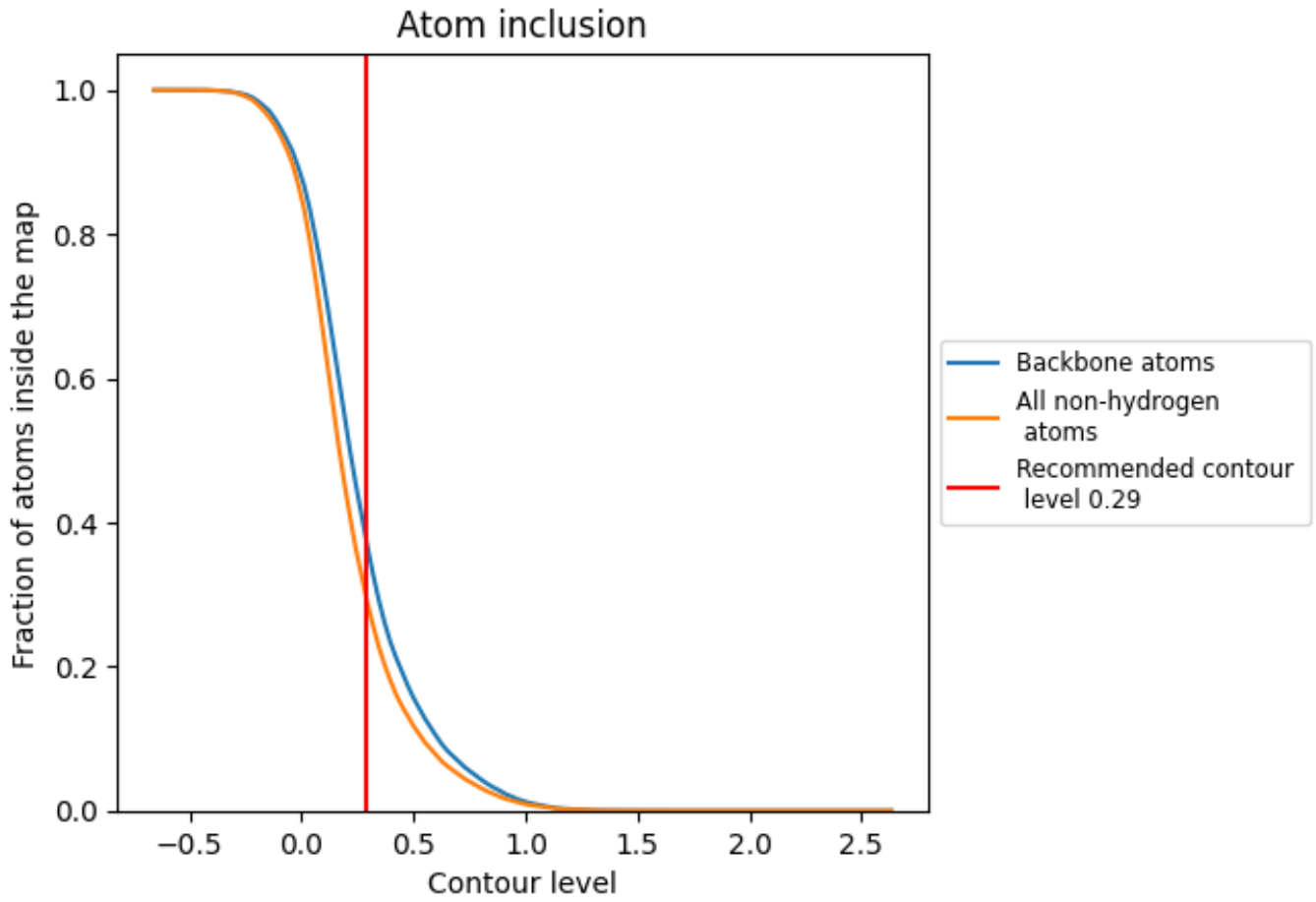
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 37% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.