wwPDB X-ray Structure Validation Summary Report (i)

Nov 25, 2024 – 07:15 PM EST

PDB ID	:	5I8H
Title	:	Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer in Complex with V3 Loop-targeting Antibody PGT122 Fab and Fusion Peptide-targeting Antibody VRC34.01 Fab
Authors	:	Xu, K.; Zhou, T.; Kwong, P.D.
Deposited on	:	2016-02-18
Resolution	:	4.30 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

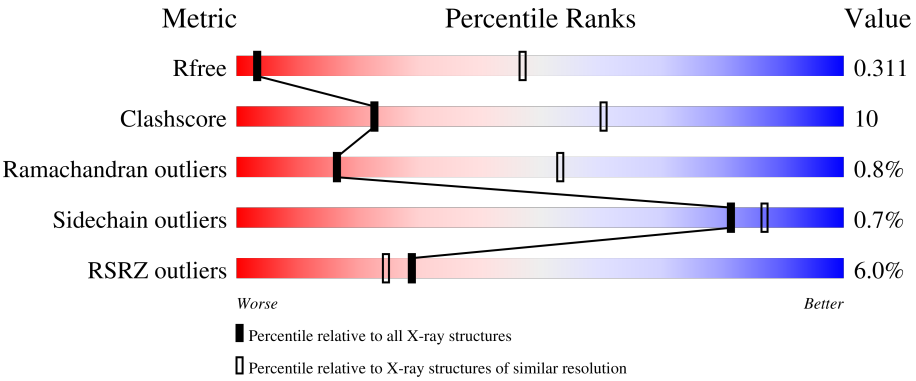
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1028 (4.72-3.86)
Clashscore	180529	1030 (4.70-3.90)
Ramachandran outliers	177936	1014 (4.76-3.84)
Sidechain outliers	177891	1022 (4.76-3.82)
RSRZ outliers	164620	1026 (4.72-3.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	481	6% 71% 22% • 5%
1	C	481	6% 68% 25% • 6%
2	B	153	3% 58% 29% 14%
2	D	153	6% 59% 26% • 14%
3	J	210	7% 70% 28% •
3	L	210	3% 69% 31%

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Mol	Chain	Length	Quality of chain
4	E	223	5% 91% 9%
4	G	223	7% 90% 10%
5	F	212	4% 97%
5	H	212	5% 96%
6	I	235	3% 65% 30%
6	K	235	11% 65% 30%
7	M	7	14% 57% 29%
7	Z	7	86% 14%
8	N	5	60% 40%
8	a	5	60% 40%
9	O	2	50% 50%
9	P	2	100%
9	Q	2	100%
9	T	2	100%
9	V	2	100%
9	W	2	100%
9	X	2	100%
9	b	2	50% 50%
9	c	2	100%
9	d	2	100%
9	f	2	100%
9	g	2	100%
9	i	2	100%
9	j	2	100%
10	R	6	50% 33% 17%

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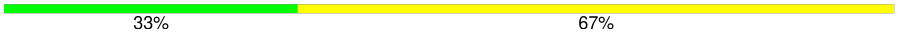
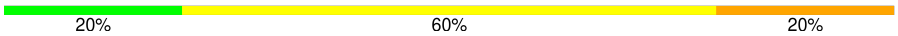
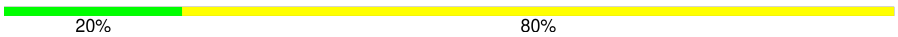
Mol	Chain	Length	Quality of chain
10	e	6	
11	S	3	
11	Y	3	
11	k	3	
11	l	3	
12	U	10	
12	h	10	
13	m	4	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 23938 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BG505 SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3576	2243	632	673	28			
1	C	450	Total	C	N	O	S	0	0	0
			3542	2223	625	666	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	GLU	conflict	UNP Q2N0S6
A	510	ARG	LYS	conflict	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	509	ARG	GLU	conflict	UNP Q2N0S6
C	510	ARG	LYS	conflict	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1034	654	178	196	6			
2	D	132	Total	C	N	O	S	0	0	0
			1034	654	178	196	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP Q2N0S6
D	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called PGT122 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			
3	J	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			

- Molecule 4 is a protein called VRC34.01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	223	Total	C	N	O	S	0	0	0
			1674	1054	285	329	6			
4	G	223	Total	C	N	O	S	0	0	0
			1674	1054	285	329	6			

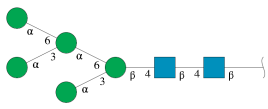
- Molecule 5 is a protein called VRC34.01 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	212	Total	C	N	O	S	0	0	0
			1628	1024	274	325	5			
5	H	212	Total	C	N	O	S	0	0	0
			1628	1024	274	325	5			

- Molecule 6 is a protein called PGT122 Fab heavy chain.

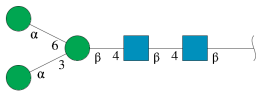
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			
6	K	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



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

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	O	2	Total C N O 28 16 2 10	0	0	0
9	P	2	Total C N O 28 16 2 10	0	0	0
9	Q	2	Total C N O 28 16 2 10	0	0	0
9	T	2	Total C N O 28 16 2 10	0	0	0
9	V	2	Total C N O 28 16 2 10	0	0	0
9	W	2	Total C N O 28 16 2 10	0	0	0
9	X	2	Total C N O 28 16 2 10	0	0	0
9	b	2	Total C N O 28 16 2 10	0	0	0

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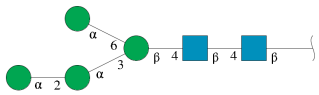
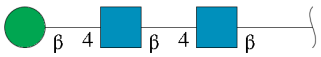
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	c	2	Total C N O 28 16 2 10	0	0	0
9	d	2	Total C N O 28 16 2 10	0	0	0
9	f	2	Total C N O 28 16 2 10	0	0	0
9	g	2	Total C N O 28 16 2 10	0	0	0
9	i	2	Total C N O 28 16 2 10	0	0	0
9	j	2	Total C N O 28 16 2 10	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	R	6	Total C N O 72 40 2 30	0	0	0
10	e	6	Total C N O 72 40 2 30	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	S	3	Total C N O 39 22 2 15	0	0	0
11	Y	3	Total C N O 39 22 2 15	0	0	0
11	k	3	Total C N O 39 22 2 15	0	0	0

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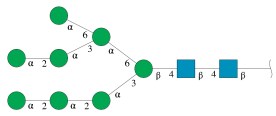
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	l	3	Total C N O 39 22 2 15	0	0	0

- Molecule 12 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-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

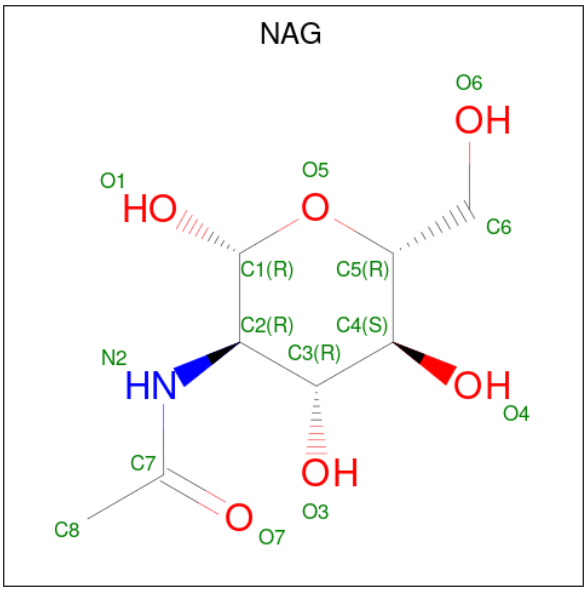


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	U	10	Total C N O 116 64 2 50	0	0	0
12	h	10	Total C N O 116 64 2 50	0	0	0

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

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

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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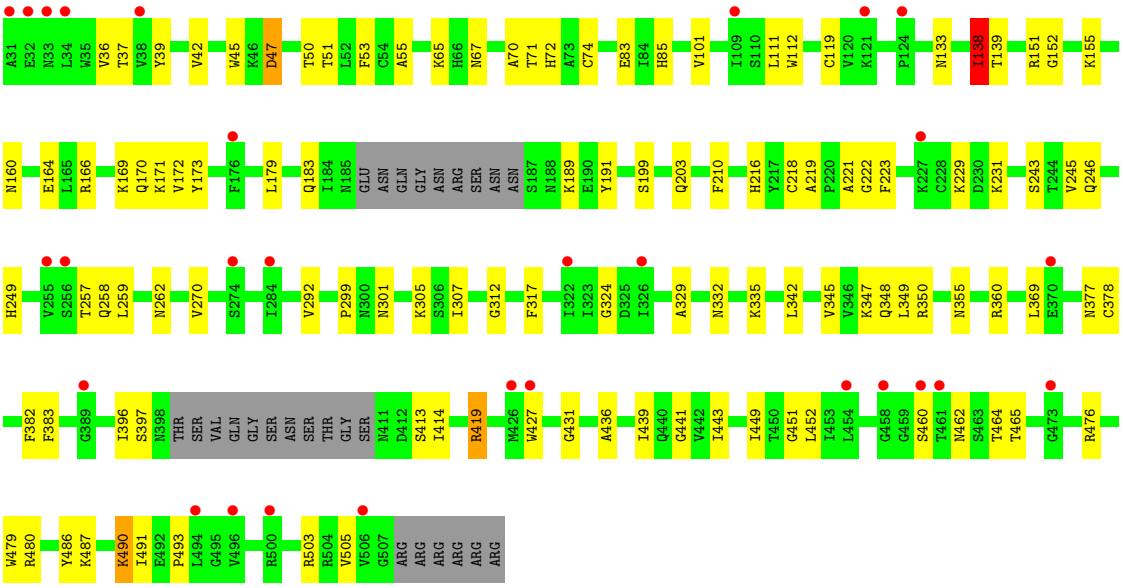
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	I	1	Total	C	N	O	0	0
			14	8	1	5		
14	K	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

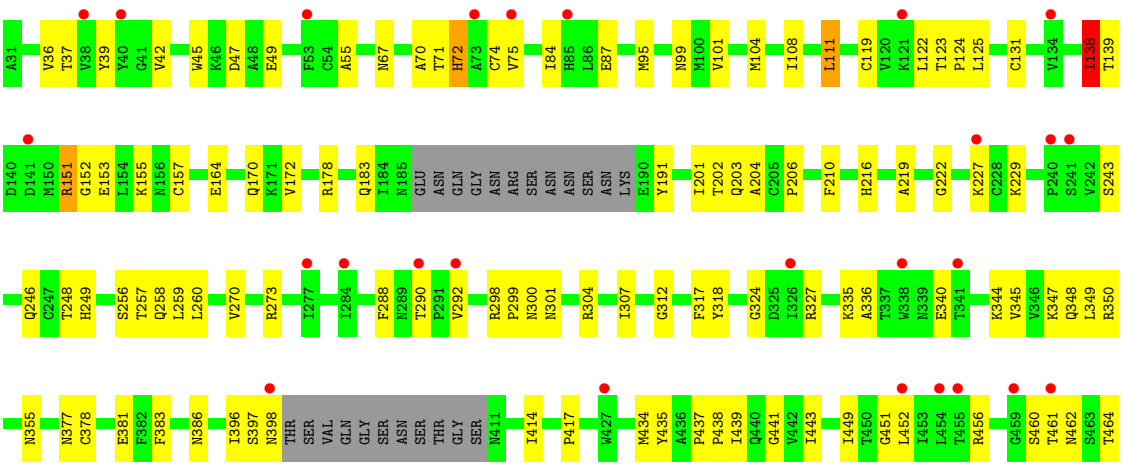
• Molecule 1: BG505 SOSIP.664 gp120

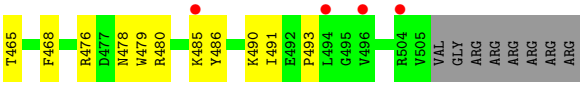
Chain A:



• Molecule 1: BG505 SOSIP.664 gp120

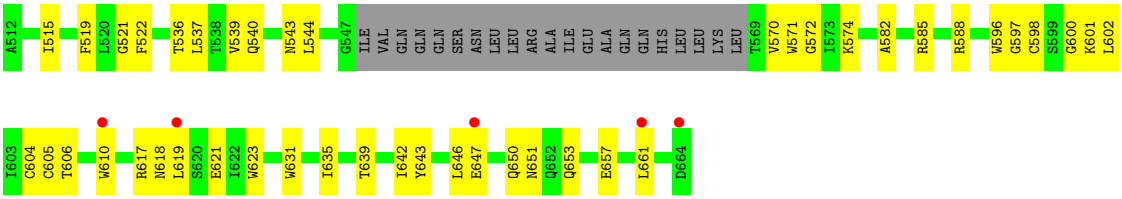
Chain C:





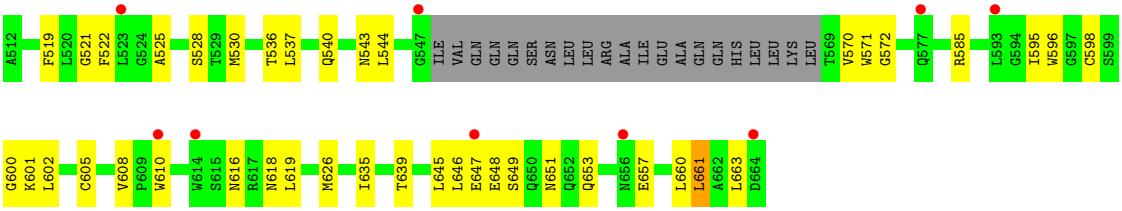
• Molecule 2: BG505 SOSIP.664 gp41

Chain B:



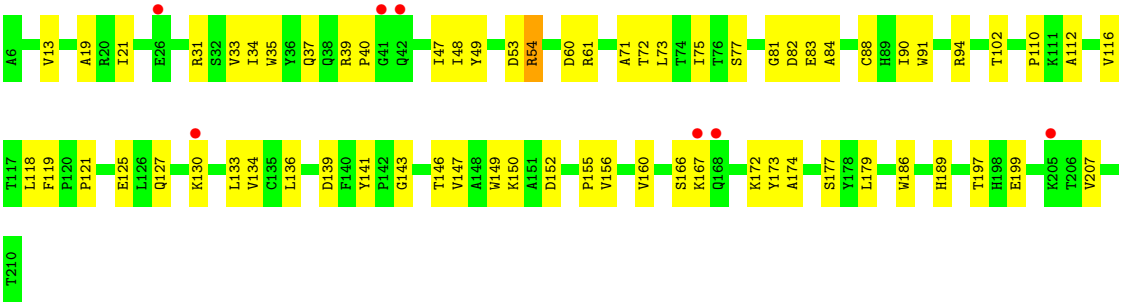
• Molecule 2: BG505 SOSIP.664 gp41

Chain D:



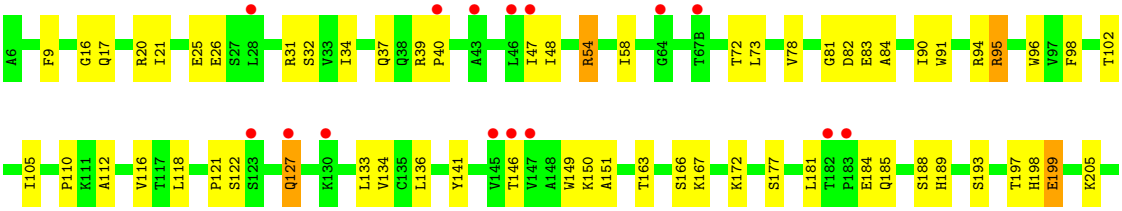
• Molecule 3: PGT122 Fab light chain

Chain L:



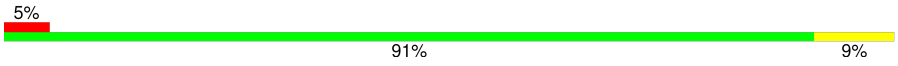
• Molecule 3: PGT122 Fab light chain

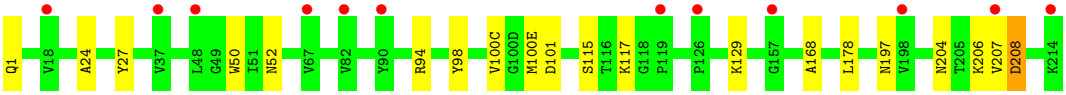
Chain J:



• Molecule 4: VRC34.01 Fab heavy chain

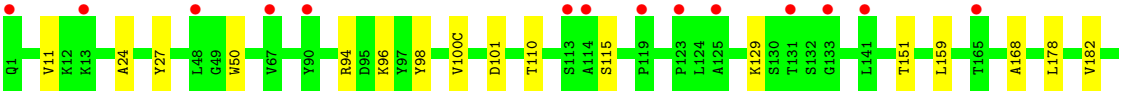
Chain E:

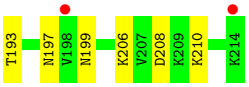




• Molecule 4: VRC34.01 Fab heavy chain

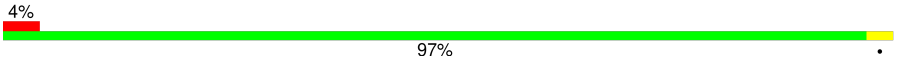
Chain G:





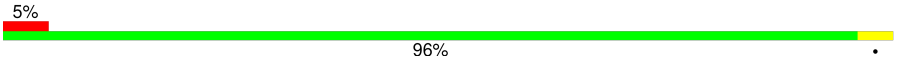
• Molecule 5: VRC34.01 Fab light chain

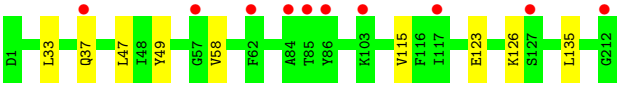
Chain F:



• Molecule 5: VRC34.01 Fab light chain

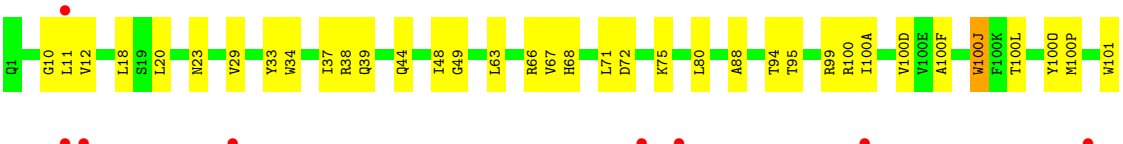
Chain H:

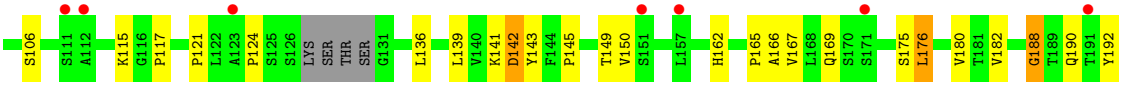




• Molecule 6: PGT122 Fab heavy chain

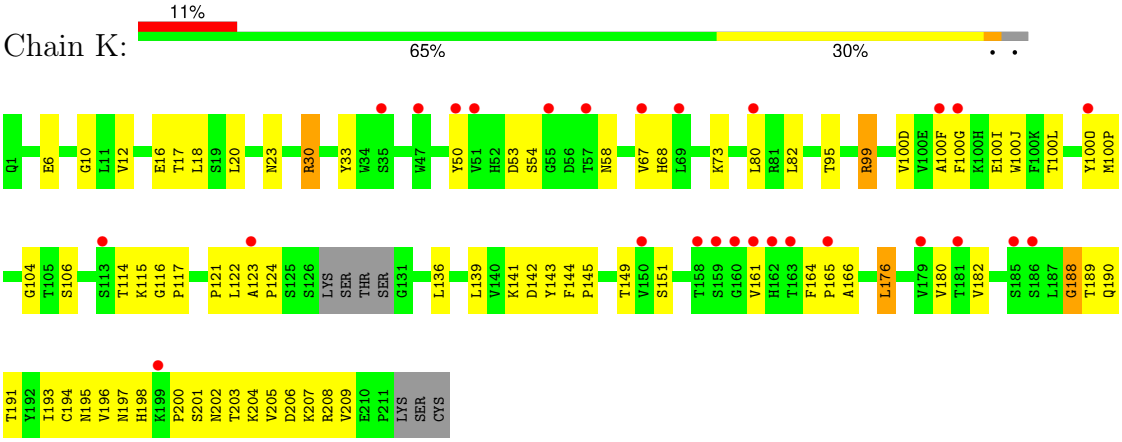
Chain I:





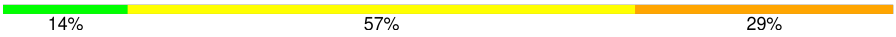
• Molecule 6: PGT122 Fab heavy chain

Chain K:



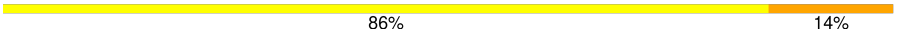
• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain Z:



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

Chain N:

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

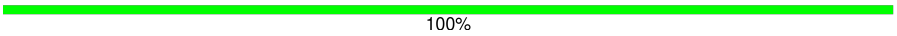
Chain a:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

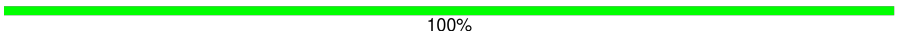
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



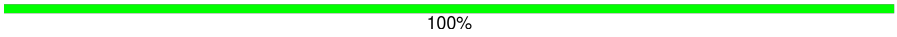
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



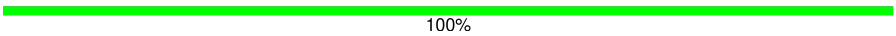
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



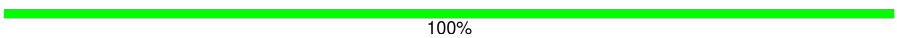
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



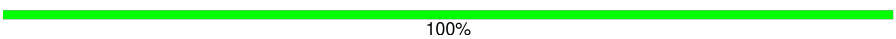
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

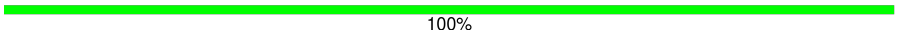


• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

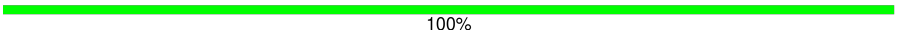
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



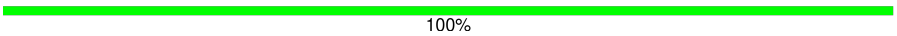
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



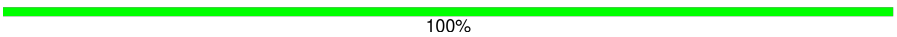
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



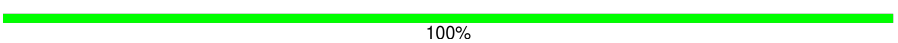
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



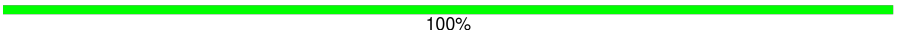
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



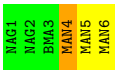
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



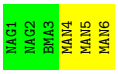
• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



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

Chain S:

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

Chain Y:

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

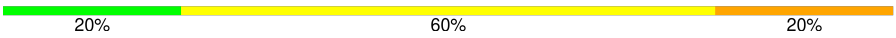
Chain k:

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

Chain l:

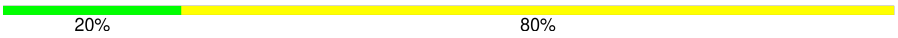
• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



• Molecule 12: 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-(1-6)]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 h:



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

Chain m:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	252.30Å 252.30Å 561.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.34 – 4.30 48.34 – 4.30	Depositor EDS
% Data completeness (in resolution range)	54.9 (48.34-4.30) 55.0 (48.34-4.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.74 (at 4.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.281 , 0.309 0.282 , 0.311	Depositor DCC
R_{free} test set	1319 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	127.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 181.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	23938	wwPDB-VP
Average B, all atoms (Å^2)	215.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8659e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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	A	0.34	0/3650	0.66	3/4956 (0.1%)
1	C	0.34	0/3616	0.63	2/4911 (0.0%)
2	B	0.33	0/1052	0.59	0/1427
2	D	0.31	0/1052	0.61	1/1427 (0.1%)
3	J	0.36	0/1632	0.64	1/2236 (0.0%)
3	L	0.57	4/1632 (0.2%)	0.62	1/2236 (0.0%)
4	E	0.31	0/1715	0.56	0/2337
4	G	0.28	0/1715	0.50	0/2337
5	F	0.28	0/1665	0.52	0/2262
5	H	0.26	0/1665	0.50	0/2262
6	I	0.32	0/1789	0.65	3/2443 (0.1%)
6	K	0.33	0/1789	0.66	4/2443 (0.2%)
All	All	0.34	4/22972 (0.0%)	0.61	15/31277 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	54	ARG	CZ-NH1	-11.18	1.18	1.33
3	L	54	ARG	NE-CZ	-9.07	1.21	1.33
3	L	54	ARG	CZ-NH2	-7.11	1.23	1.33
3	L	54	ARG	CD-NE	-7.05	1.34	1.46

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	176	LEU	CA-CB-CG	9.21	136.48	115.30
1	A	138	ILE	CG1-CB-CG2	-9.11	91.35	111.40
6	K	176	LEU	CA-CB-CG	8.41	134.65	115.30
1	C	138	ILE	CG1-CB-CG2	-8.06	93.68	111.40
1	A	490	LYS	CA-CB-CG	6.53	127.77	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	208	ASP	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3576	0	3509	88	0
1	C	3542	0	3471	90	0
2	B	1034	0	1011	42	0
2	D	1034	0	1012	31	0
3	J	1589	0	1530	55	0
3	L	1589	0	1529	54	0
4	E	1674	0	1638	25	0
4	G	1674	0	1638	20	0
5	F	1628	0	1588	12	0
5	H	1628	0	1588	8	0
6	I	1742	0	1713	59	0
6	K	1742	0	1715	66	0
7	M	83	0	69	3	0
7	Z	83	0	70	2	0
8	N	61	0	52	0	0
8	a	61	0	52	0	0
9	O	28	0	25	4	0
9	P	28	0	25	0	0
9	Q	28	0	25	0	0
9	T	28	0	25	0	0
9	V	28	0	25	0	0
9	W	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	X	28	0	25	0	0
9	b	28	0	25	0	0
9	c	28	0	25	0	0
9	d	28	0	25	0	0
9	f	28	0	25	0	0
9	g	28	0	25	0	0
9	i	28	0	25	0	0
9	j	28	0	25	0	0
10	R	72	0	61	2	0
10	e	72	0	61	0	0
11	S	39	0	34	0	0
11	Y	39	0	34	1	0
11	k	39	0	34	0	0
11	l	39	0	34	0	0
12	U	116	0	97	1	0
12	h	116	0	97	0	0
13	m	50	0	42	0	0
14	A	56	0	52	3	0
14	B	42	0	39	0	0
14	C	70	0	65	1	0
14	D	28	0	26	0	0
14	I	14	0	13	0	0
14	K	14	0	13	0	0
All	All	23938	0	23237	479	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 479 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:39:ARG:HD3	3:L:84:ALA:HB2	1.35	1.09
1:C:138:ILE:HG22	1:C:139:THR:HA	1.40	1.04
1:A:490:LYS:HG2	2:B:585:ARG:HH12	1.25	0.95
1:A:138:ILE:HG22	1:A:139:THR:HA	1.48	0.94
1:A:350:ARG:NH2	1:A:396:ILE:O	2.04	0.90

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/481 (93%)	405 (90%)	38 (8%)	6 (1%)	10	42
1	C	444/481 (92%)	402 (90%)	37 (8%)	5 (1%)	12	46
2	B	128/153 (84%)	113 (88%)	13 (10%)	2 (2%)	8	37
2	D	128/153 (84%)	113 (88%)	13 (10%)	2 (2%)	8	37
3	J	208/210 (99%)	194 (93%)	12 (6%)	2 (1%)	13	48
3	L	208/210 (99%)	194 (93%)	12 (6%)	2 (1%)	13	48
4	E	221/223 (99%)	218 (99%)	3 (1%)	0	100	100
4	G	221/223 (99%)	218 (99%)	3 (1%)	0	100	100
5	F	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
5	H	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
6	I	224/235 (95%)	213 (95%)	9 (4%)	2 (1%)	14	50
6	K	224/235 (95%)	212 (95%)	10 (4%)	2 (1%)	14	50
All	All	2875/3028 (95%)	2691 (94%)	161 (6%)	23 (1%)	16	53

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ILE
1	C	138	ILE
3	L	110	PRO
3	J	110	PRO
1	A	71	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	405/428 (95%)	401 (99%)	4 (1%)	73	82
1	C	401/428 (94%)	399 (100%)	2 (0%)	86	90
2	B	110/129 (85%)	108 (98%)	2 (2%)	54	72
2	D	110/129 (85%)	109 (99%)	1 (1%)	75	83
3	J	178/178 (100%)	176 (99%)	2 (1%)	70	80
3	L	178/178 (100%)	178 (100%)	0	100	100
4	E	187/187 (100%)	186 (100%)	1 (0%)	86	90
4	G	187/187 (100%)	186 (100%)	1 (0%)	86	90
5	F	185/185 (100%)	185 (100%)	0	100	100
5	H	185/185 (100%)	184 (100%)	1 (0%)	86	90
6	I	198/205 (97%)	195 (98%)	3 (2%)	60	75
6	K	198/205 (97%)	197 (100%)	1 (0%)	86	90
All	All	2522/2624 (96%)	2504 (99%)	18 (1%)	81	87

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	I	207	LYS
6	K	100(J)	TRP
3	J	95	ARG
4	E	50	TRP
6	I	175	SER

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

Mol	Chain	Res	Type
2	B	650	GLN
2	B	651	ASN
1	C	195	ASN
6	I	202	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

100 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	M	1	7,1	14,14,15	0.35	0	17,19,21	0.48	0
7	NAG	M	2	7	14,14,15	0.53	0	17,19,21	1.43	2 (11%)
7	BMA	M	3	7	11,11,12	0.64	0	15,15,17	0.86	1 (6%)
7	MAN	M	4	7	11,11,12	0.83	0	15,15,17	1.41	2 (13%)
7	MAN	M	5	7	11,11,12	1.22	1 (9%)	15,15,17	1.02	1 (6%)
7	MAN	M	6	7	11,11,12	4.17	8 (72%)	15,15,17	2.66	5 (33%)
7	MAN	M	7	7	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
8	NAG	N	1	8,1	14,14,15	0.21	0	17,19,21	0.44	0
8	NAG	N	2	8	14,14,15	0.25	0	17,19,21	0.42	0
8	BMA	N	3	8	11,11,12	0.68	0	15,15,17	0.72	0
8	MAN	N	4	8	11,11,12	0.69	0	15,15,17	0.98	2 (13%)
8	MAN	N	5	8	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
9	NAG	O	1	1,9	14,14,15	0.24	0	17,19,21	0.48	0
9	NAG	O	2	9	14,14,15	0.50	0	17,19,21	1.34	2 (11%)
9	NAG	P	1	1,9	14,14,15	0.20	0	17,19,21	0.44	0
9	NAG	P	2	9	14,14,15	0.32	0	17,19,21	0.44	0
9	NAG	Q	1	1,9	14,14,15	0.23	0	17,19,21	0.43	0
9	NAG	Q	2	9	14,14,15	0.29	0	17,19,21	0.40	0
10	NAG	R	1	10	14,14,15	0.19	0	17,19,21	0.55	0
10	NAG	R	2	10	14,14,15	0.30	0	17,19,21	0.54	0
10	BMA	R	3	10	11,11,12	0.56	0	15,15,17	0.64	0
10	MAN	R	4	10	11,11,12	0.52	0	15,15,17	1.03	2 (13%)
10	MAN	R	5	10	11,11,12	0.85	0	15,15,17	1.17	2 (13%)
10	MAN	R	6	10	11,11,12	0.66	0	15,15,17	1.01	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	NAG	S	1	11,1	14,14,15	0.44	0	17,19,21	0.55	0
11	NAG	S	2	11	14,14,15	0.44	0	17,19,21	0.67	1 (5%)
11	BMA	S	3	11	11,11,12	1.23	1 (9%)	15,15,17	0.97	1 (6%)
9	NAG	T	1	1,9	14,14,15	0.26	0	17,19,21	0.40	0
9	NAG	T	2	9	14,14,15	0.31	0	17,19,21	0.45	0
12	NAG	U	1	1,12	14,14,15	0.17	0	17,19,21	0.46	0
12	MAN	U	10	12	11,11,12	0.68	0	15,15,17	0.94	2 (13%)
12	NAG	U	2	12	14,14,15	0.22	0	17,19,21	0.55	0
12	BMA	U	3	12	11,11,12	0.78	0	15,15,17	1.20	1 (6%)
12	MAN	U	4	12	11,11,12	0.60	0	15,15,17	1.04	1 (6%)
12	MAN	U	5	12	11,11,12	0.77	0	15,15,17	0.96	1 (6%)
12	MAN	U	6	12	11,11,12	0.77	1 (9%)	15,15,17	1.32	1 (6%)
12	MAN	U	7	12	11,11,12	0.57	0	15,15,17	0.89	1 (6%)
12	MAN	U	8	12	11,11,12	0.72	0	15,15,17	0.97	2 (13%)
12	MAN	U	9	12	11,11,12	0.87	1 (9%)	15,15,17	1.13	1 (6%)
9	NAG	V	1	9	14,14,15	0.28	0	17,19,21	0.39	0
9	NAG	V	2	9	14,14,15	0.25	0	17,19,21	0.43	0
9	NAG	W	1	1,9	14,14,15	0.27	0	17,19,21	0.65	0
9	NAG	W	2	9	14,14,15	0.30	0	17,19,21	0.45	0
9	NAG	X	1	1,9	14,14,15	0.20	0	17,19,21	0.45	0
9	NAG	X	2	9	14,14,15	0.27	0	17,19,21	0.45	0
11	NAG	Y	1	11,1	14,14,15	0.74	1 (7%)	17,19,21	0.56	0
11	NAG	Y	2	11	14,14,15	0.27	0	17,19,21	0.44	0
11	BMA	Y	3	11	11,11,12	0.61	0	15,15,17	0.75	0
7	NAG	Z	1	7,1	14,14,15	0.42	0	17,19,21	0.58	0
7	NAG	Z	2	7	14,14,15	0.65	0	17,19,21	1.65	3 (17%)
7	BMA	Z	3	7	11,11,12	1.46	1 (9%)	15,15,17	1.54	2 (13%)
7	MAN	Z	4	7	11,11,12	1.63	2 (18%)	15,15,17	1.15	1 (6%)
7	MAN	Z	5	7	11,11,12	2.47	4 (36%)	15,15,17	2.46	8 (53%)
7	MAN	Z	6	7	11,11,12	1.70	1 (9%)	15,15,17	1.23	1 (6%)
7	MAN	Z	7	7	11,11,12	1.16	2 (18%)	15,15,17	1.22	2 (13%)
8	NAG	a	1	8,1	14,14,15	0.32	0	17,19,21	0.42	0
8	NAG	a	2	8	14,14,15	0.24	0	17,19,21	0.41	0
8	BMA	a	3	8	11,11,12	0.77	0	15,15,17	0.71	0
8	MAN	a	4	8	11,11,12	0.66	0	15,15,17	0.97	1 (6%)
8	MAN	a	5	8	11,11,12	0.71	0	15,15,17	1.02	2 (13%)
9	NAG	b	1	1,9	14,14,15	0.27	0	17,19,21	0.46	0
9	NAG	b	2	9	14,14,15	0.57	0	17,19,21	1.36	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	c	1	1,9	14,14,15	0.22	0	17,19,21	0.45	0
9	NAG	c	2	9	14,14,15	0.31	0	17,19,21	0.44	0
9	NAG	d	1	1,9	14,14,15	0.27	0	17,19,21	0.42	0
9	NAG	d	2	9	14,14,15	0.31	0	17,19,21	0.41	0
10	NAG	e	1	10,1	14,14,15	0.45	0	17,19,21	0.58	0
10	NAG	e	2	10	14,14,15	0.26	0	17,19,21	0.48	0
10	BMA	e	3	10	11,11,12	0.67	0	15,15,17	0.73	0
10	MAN	e	4	10	11,11,12	0.70	0	15,15,17	1.04	2 (13%)
10	MAN	e	5	10	11,11,12	0.81	0	15,15,17	1.14	2 (13%)
10	MAN	e	6	10	11,11,12	0.57	0	15,15,17	1.00	2 (13%)
9	NAG	f	1	1,9	14,14,15	0.53	0	17,19,21	0.54	0
9	NAG	f	2	9	14,14,15	0.33	0	17,19,21	0.39	0
9	NAG	g	1	1,9	14,14,15	0.23	0	17,19,21	0.39	0
9	NAG	g	2	9	14,14,15	0.30	0	17,19,21	0.46	0
12	NAG	h	1	1,12	14,14,15	0.20	0	17,19,21	0.48	0
12	MAN	h	10	12	11,11,12	0.70	0	15,15,17	0.99	2 (13%)
12	NAG	h	2	12	14,14,15	0.22	0	17,19,21	0.58	0
12	BMA	h	3	12	11,11,12	0.65	0	15,15,17	1.18	1 (6%)
12	MAN	h	4	12	11,11,12	0.79	0	15,15,17	1.01	1 (6%)
12	MAN	h	5	12	11,11,12	0.85	0	15,15,17	1.02	1 (6%)
12	MAN	h	6	12	11,11,12	0.86	1 (9%)	15,15,17	1.32	1 (6%)
12	MAN	h	7	12	11,11,12	0.65	0	15,15,17	0.89	2 (13%)
12	MAN	h	8	12	11,11,12	0.68	0	15,15,17	0.95	1 (6%)
12	MAN	h	9	12	11,11,12	0.85	0	15,15,17	1.23	2 (13%)
9	NAG	i	1	1,9	14,14,15	0.39	0	17,19,21	0.55	0
9	NAG	i	2	9	14,14,15	0.27	0	17,19,21	0.48	0
9	NAG	j	1	1,9	14,14,15	0.44	0	17,19,21	0.69	0
9	NAG	j	2	9	14,14,15	0.35	0	17,19,21	0.45	0
11	NAG	k	1	11,1	14,14,15	0.40	0	17,19,21	0.58	0
11	NAG	k	2	11	14,14,15	0.37	0	17,19,21	0.75	0
11	BMA	k	3	11	11,11,12	0.72	0	15,15,17	0.86	1 (6%)
11	NAG	l	1	11,1	14,14,15	0.36	0	17,19,21	0.62	0
11	NAG	l	2	11	14,14,15	0.31	0	17,19,21	0.37	0
11	BMA	l	3	11	11,11,12	0.55	0	15,15,17	0.78	0
13	NAG	m	1	1,13	14,14,15	0.42	0	17,19,21	0.55	0
13	NAG	m	2	13	14,14,15	0.37	0	17,19,21	0.39	0
13	BMA	m	3	13	11,11,12	0.59	0	15,15,17	0.73	0
13	MAN	m	4	6,13	11,11,12	0.93	1 (9%)	15,15,17	1.15	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	U	7	12	-	2/2/19/22	0/1/1/1
12	MAN	U	8	12	-	0/2/19/22	0/1/1/1
12	MAN	U	9	12	-	0/2/19/22	1/1/1/1
9	NAG	V	1	9	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	2/6/23/26	0/1/1/1
9	NAG	W	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	W	2	9	-	0/6/23/26	0/1/1/1
9	NAG	X	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
11	NAG	Y	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	Y	2	11	-	2/6/23/26	0/1/1/1
11	BMA	Y	3	11	-	1/2/19/22	0/1/1/1
7	NAG	Z	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	4/6/23/26	0/1/1/1
7	BMA	Z	3	7	-	2/2/19/22	0/1/1/1
7	MAN	Z	4	7	-	0/2/19/22	1/1/1/1
7	MAN	Z	5	7	-	1/2/19/22	1/1/1/1
7	MAN	Z	6	7	-	0/2/19/22	0/1/1/1
7	MAN	Z	7	7	-	0/2/19/22	0/1/1/1
8	NAG	a	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	a	2	8	-	2/6/23/26	0/1/1/1
8	BMA	a	3	8	-	2/2/19/22	0/1/1/1
8	MAN	a	4	8	-	1/2/19/22	0/1/1/1
8	MAN	a	5	8	-	0/2/19/22	0/1/1/1
9	NAG	b	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	b	2	9	-	6/6/23/26	0/1/1/1
9	NAG	c	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	c	2	9	-	2/6/23/26	0/1/1/1
9	NAG	d	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	d	2	9	-	1/6/23/26	0/1/1/1
10	NAG	e	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	e	2	10	-	0/6/23/26	0/1/1/1
10	BMA	e	3	10	-	0/2/19/22	0/1/1/1
10	MAN	e	4	10	-	2/2/19/22	0/1/1/1
10	MAN	e	5	10	-	0/2/19/22	1/1/1/1
10	MAN	e	6	10	-	0/2/19/22	0/1/1/1
9	NAG	f	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	f	2	9	-	1/6/23/26	0/1/1/1

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

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	6	MAN	O5-C5	7.43	1.57	1.43
7	M	6	MAN	O2-C2	5.61	1.55	1.43
7	M	6	MAN	C4-C5	5.37	1.64	1.53
7	M	6	MAN	C2-C3	5.20	1.60	1.52
7	Z	5	MAN	C1-C2	4.55	1.63	1.52

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	6	MAN	O3-C3-C2	6.02	122.33	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Z	5	MAN	C1-C2-C3	5.10	117.07	109.64
7	M	6	MAN	C3-C4-C5	-5.07	101.05	110.23
7	Z	2	NAG	C2-N2-C7	4.83	129.37	122.90
9	O	2	NAG	C2-N2-C7	4.72	129.22	122.90

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	N	3	BMA	C4-C5-C6-O6
8	a	3	BMA	C4-C5-C6-O6
12	U	2	NAG	O5-C5-C6-O6
7	Z	3	BMA	C4-C5-C6-O6
9	T	2	NAG	O5-C5-C6-O6

5 of 8 ring outliers are listed below:

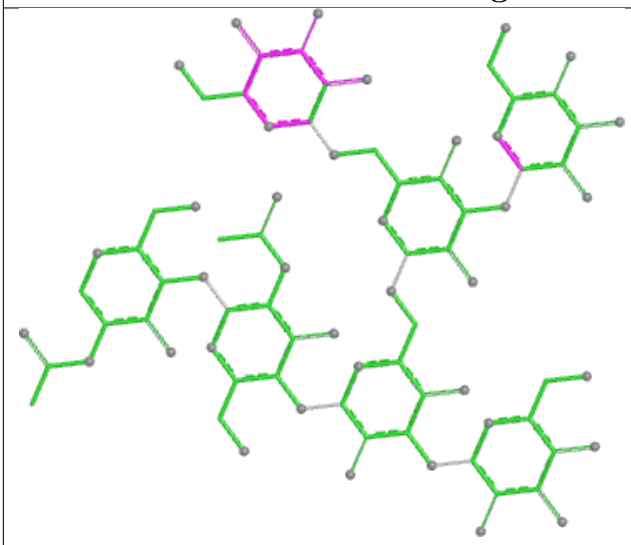
Mol	Chain	Res	Type	Atoms
7	M	4	MAN	C1-C2-C3-C4-C5-O5
7	Z	5	MAN	C1-C2-C3-C4-C5-O5
7	Z	4	MAN	C1-C2-C3-C4-C5-O5
12	U	9	MAN	C1-C2-C3-C4-C5-O5
12	h	9	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 13 short contacts:

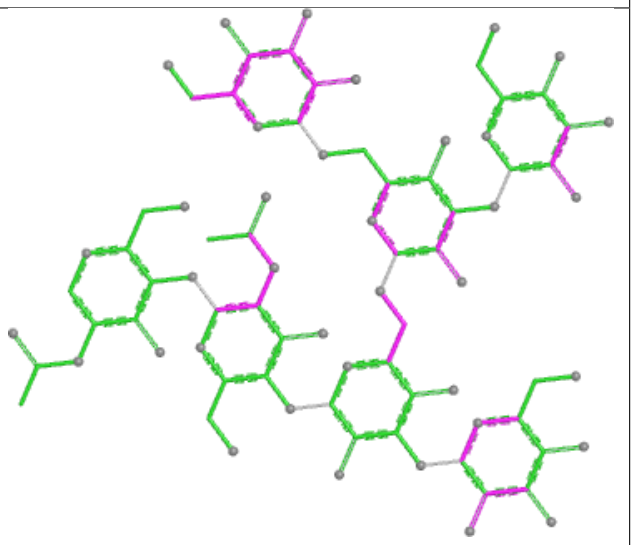
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Z	2	NAG	1	0
7	M	2	NAG	1	0
11	Y	1	NAG	1	0
10	R	4	MAN	2	0
9	O	2	NAG	2	0
9	O	1	NAG	3	0
12	U	8	MAN	1	0
7	M	4	MAN	2	0
12	U	9	MAN	1	0
7	Z	1	NAG	1	0

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

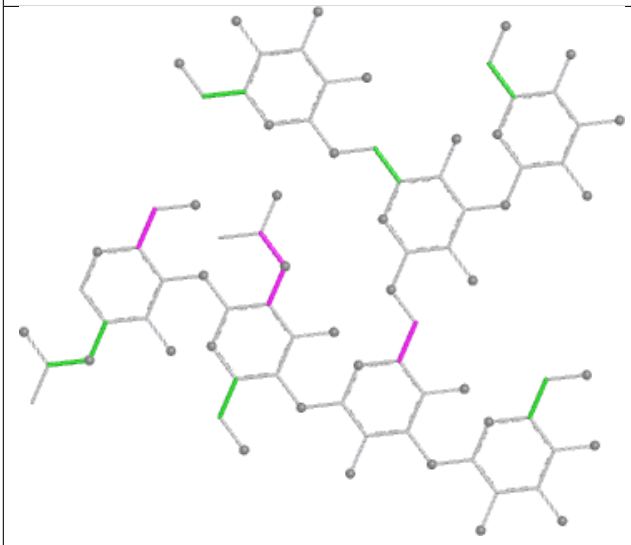
Oligosaccharide Chain M



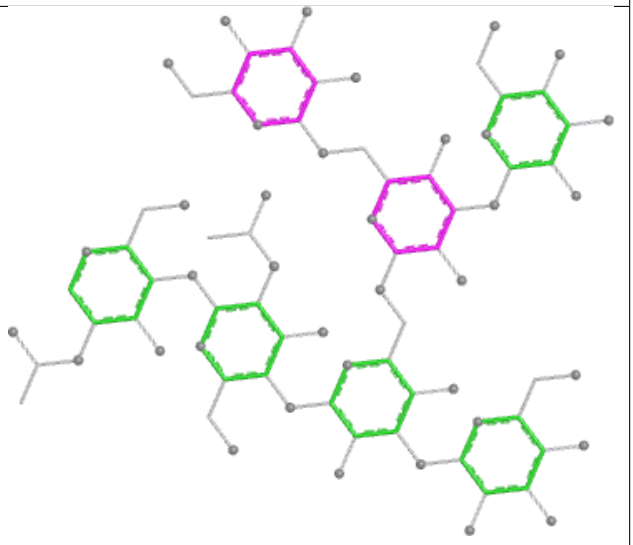
Bond lengths



Bond angles

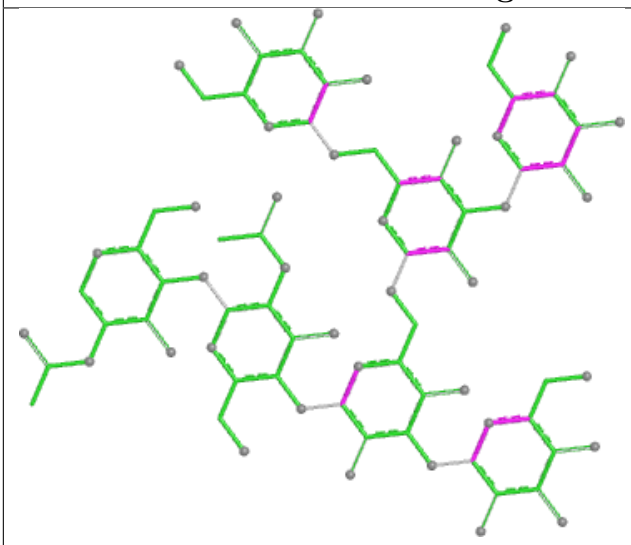


Torsions

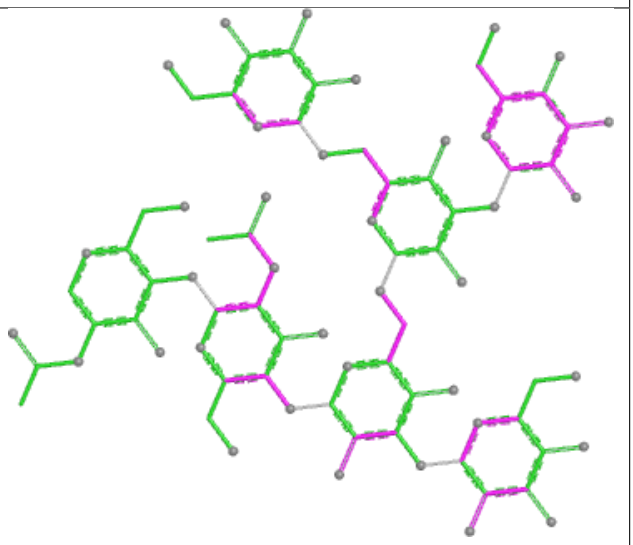


Rings

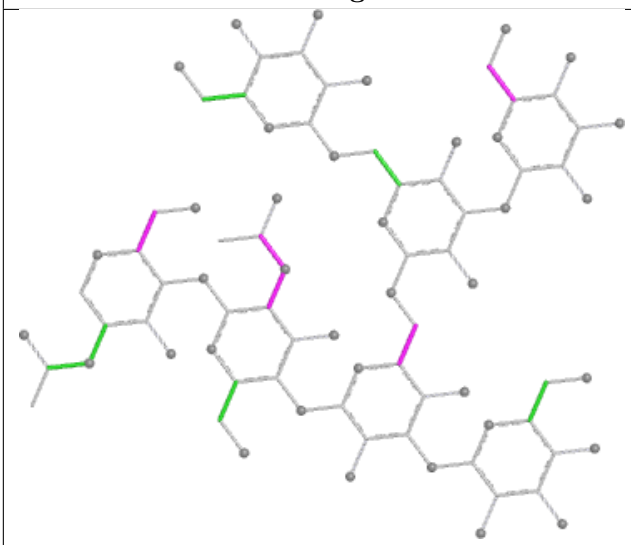
Oligosaccharide Chain Z



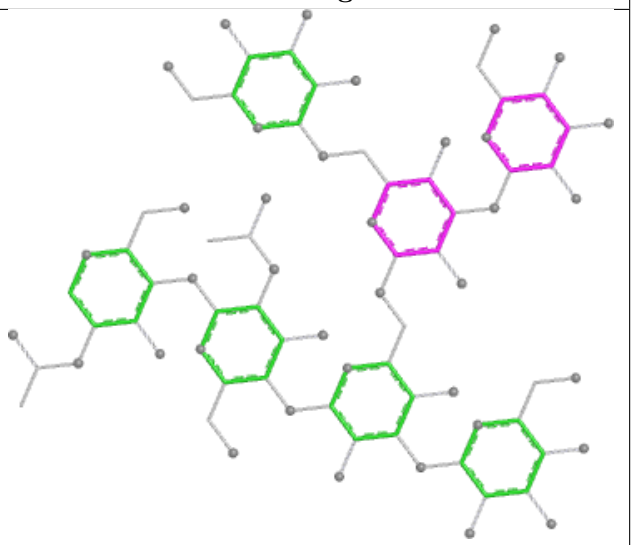
Bond lengths



Bond angles

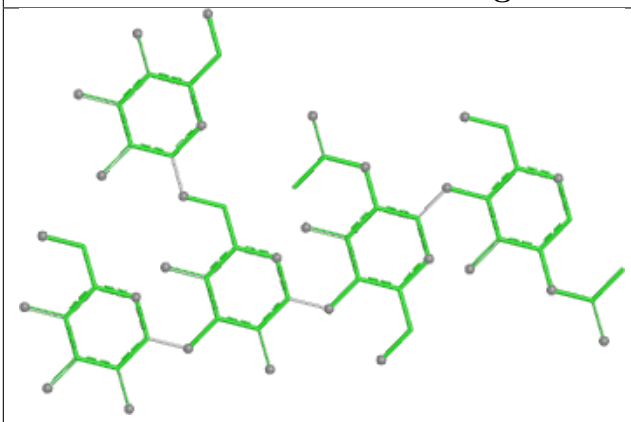


Torsions

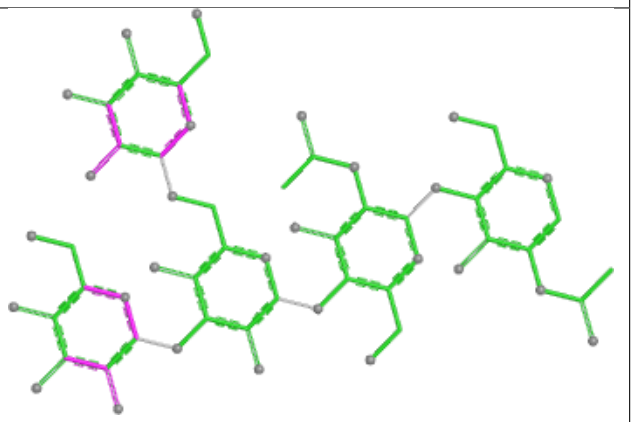


Rings

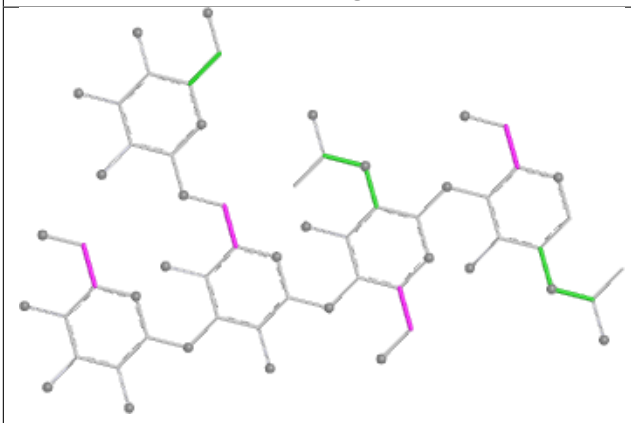
Oligosaccharide Chain N



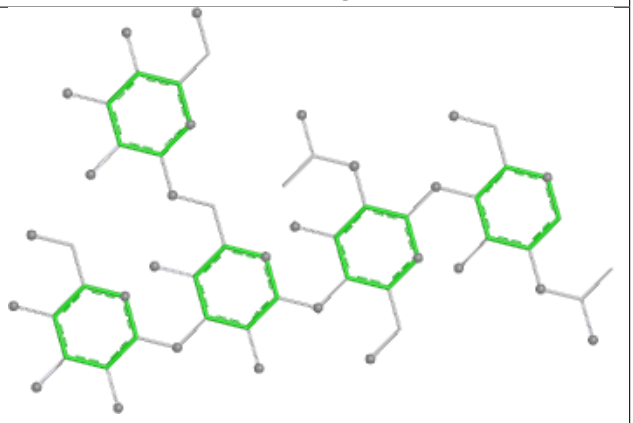
Bond lengths



Bond angles

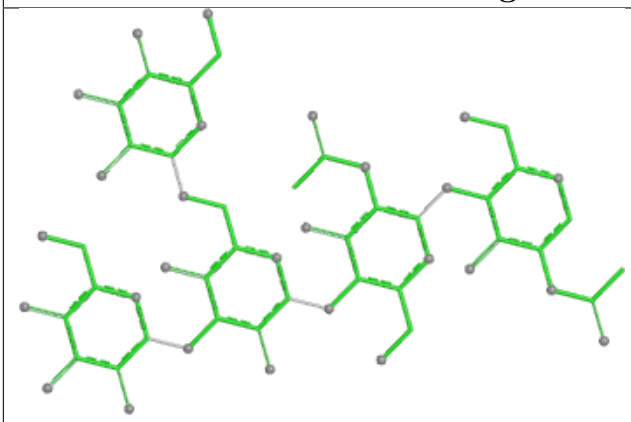


Torsions

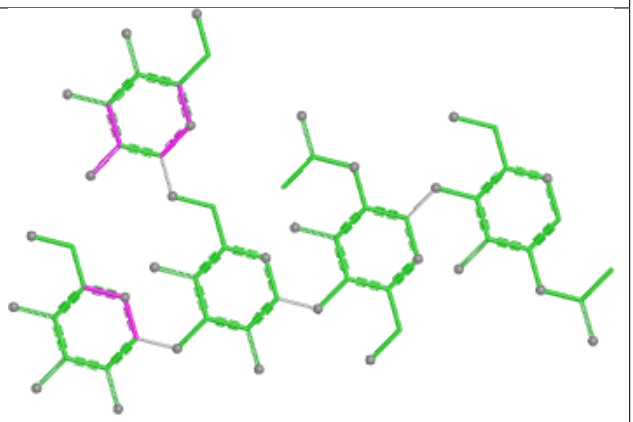


Rings

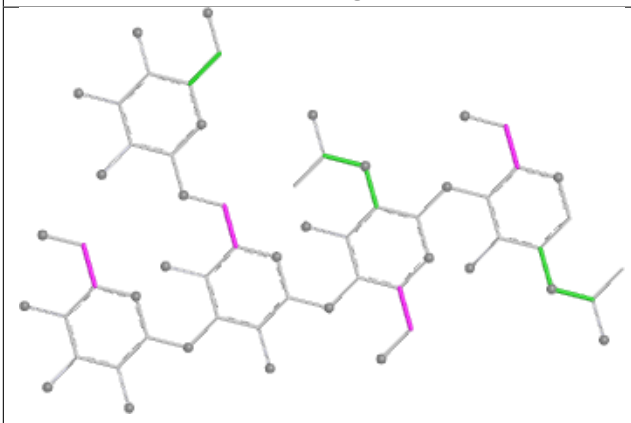
Oligosaccharide Chain a



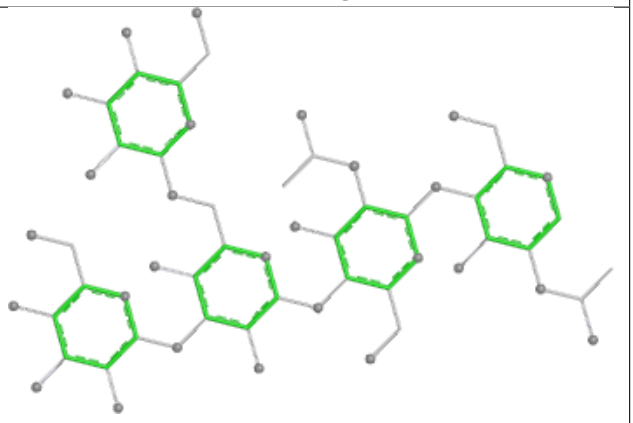
Bond lengths



Bond angles

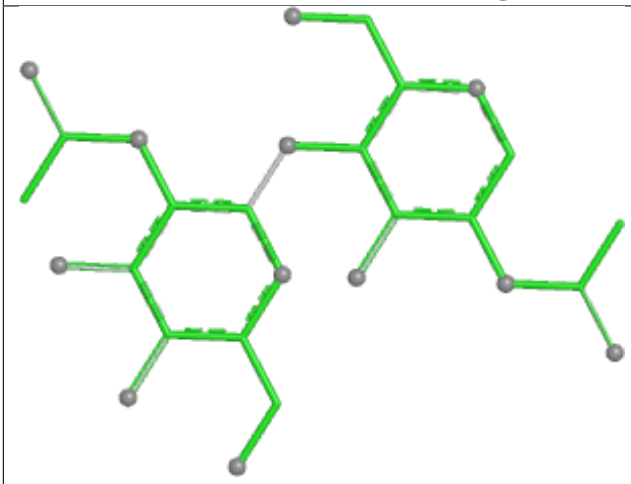


Torsions

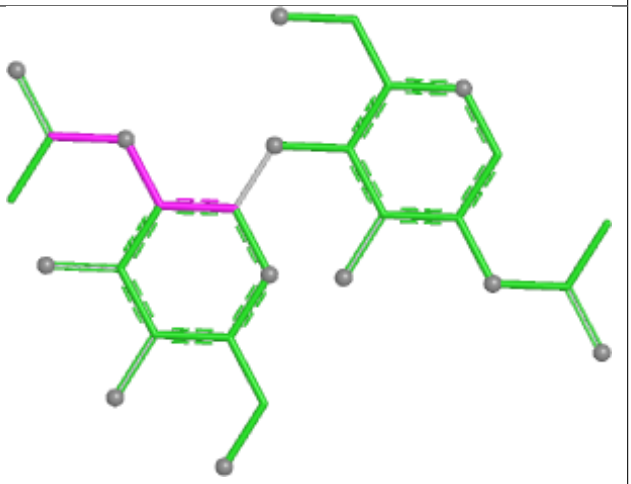


Rings

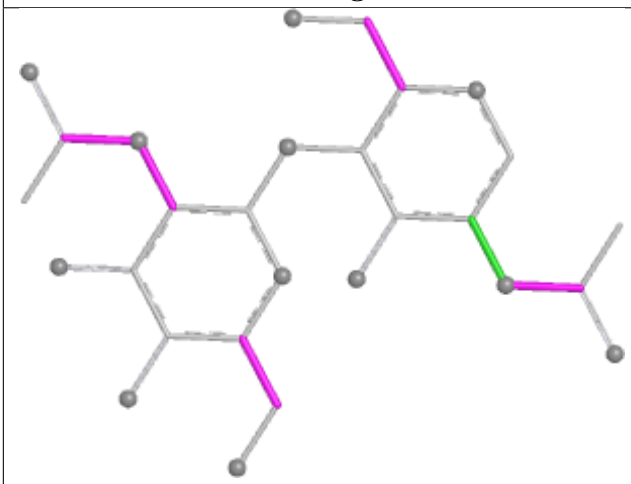
Oligosaccharide Chain O



Bond lengths



Bond angles



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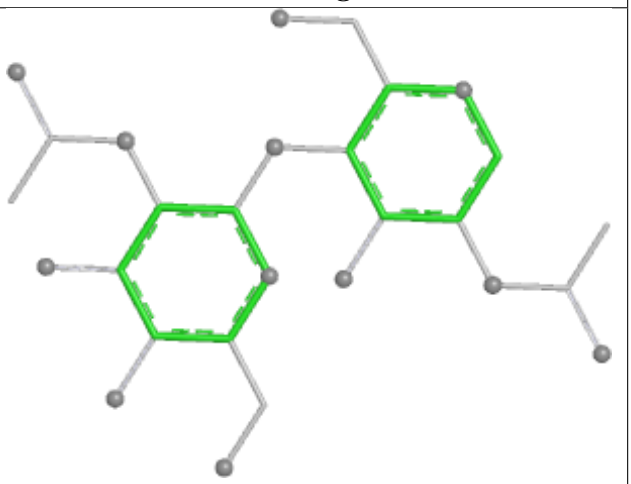
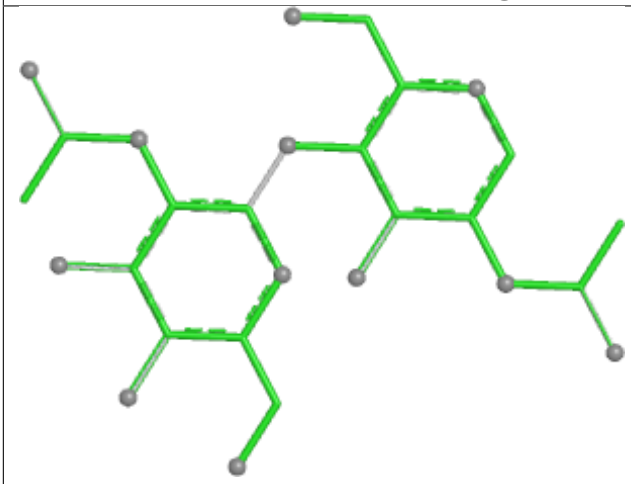


Rings

Oligosaccharide Chain P



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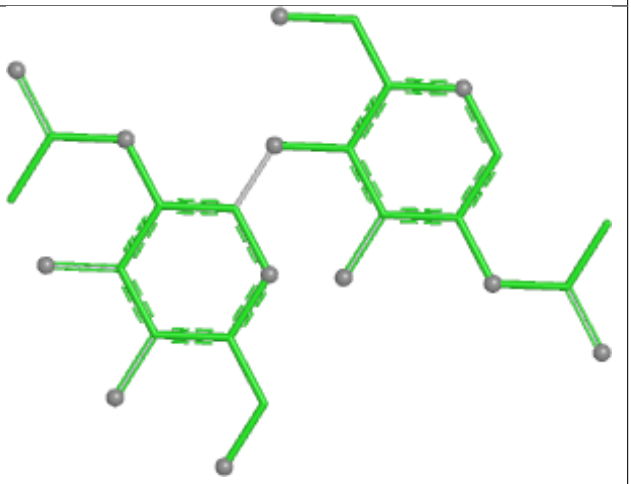
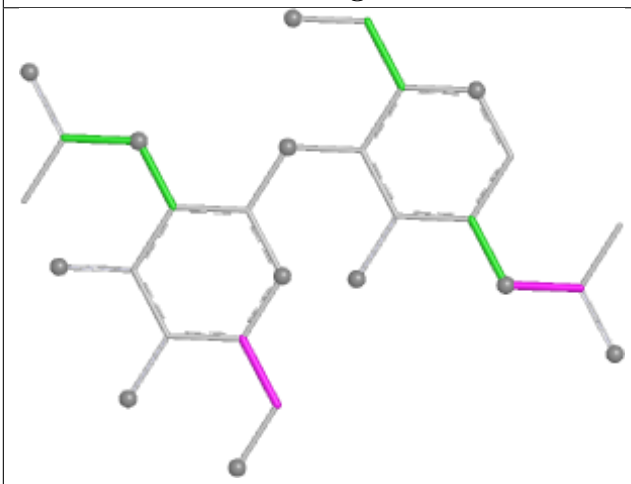


Bond angles



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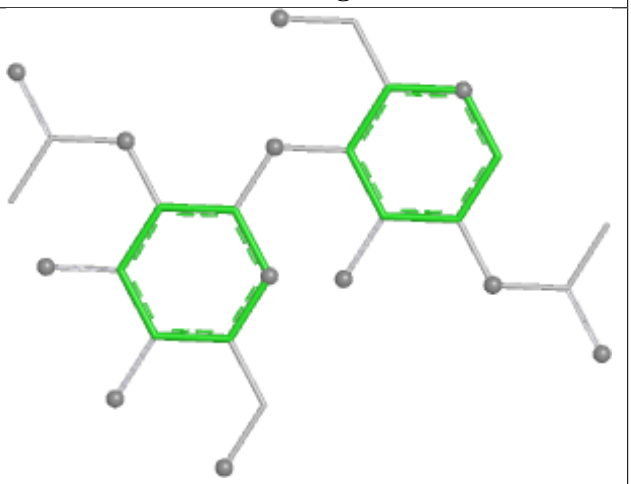
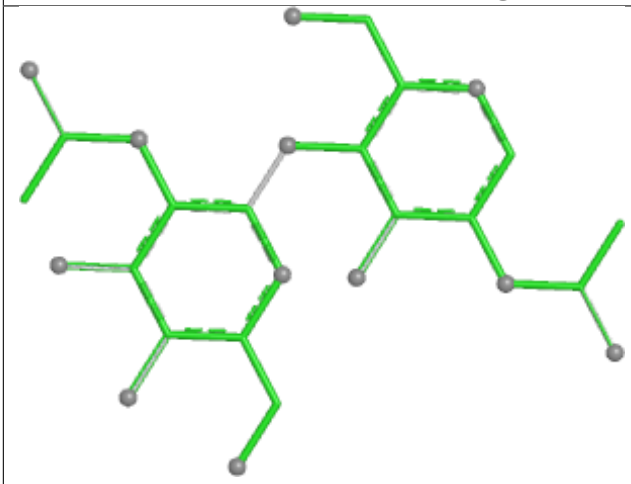
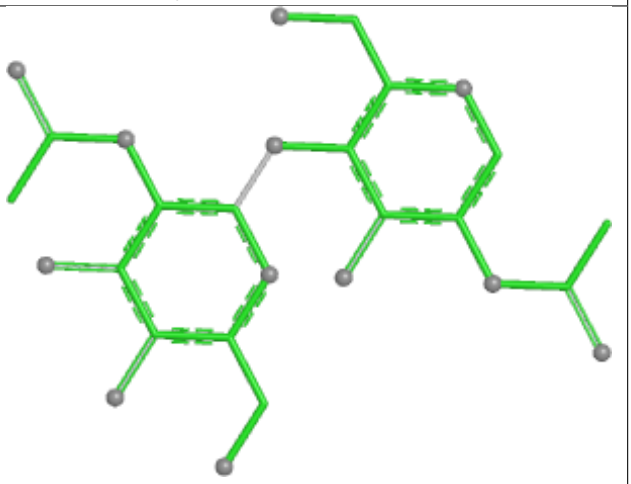


Rings

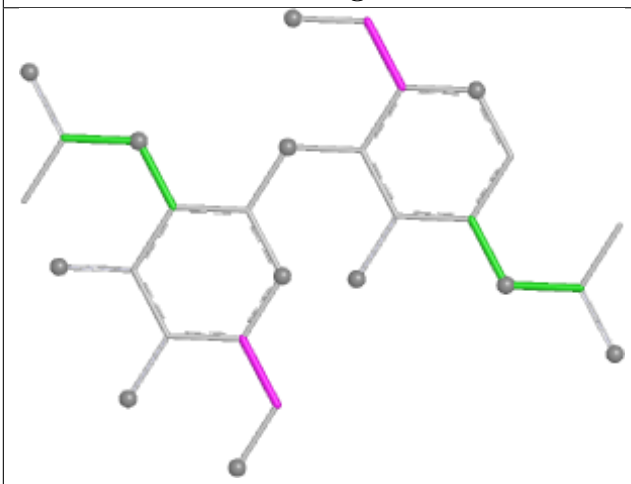
Oligosaccharide Chain Q



Bond lengths



Bond angles



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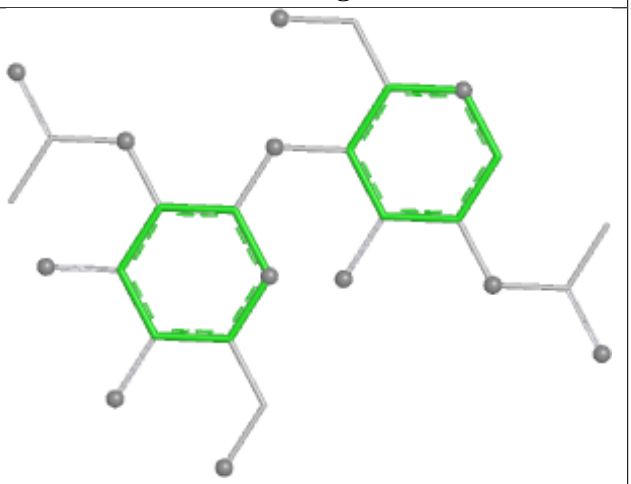
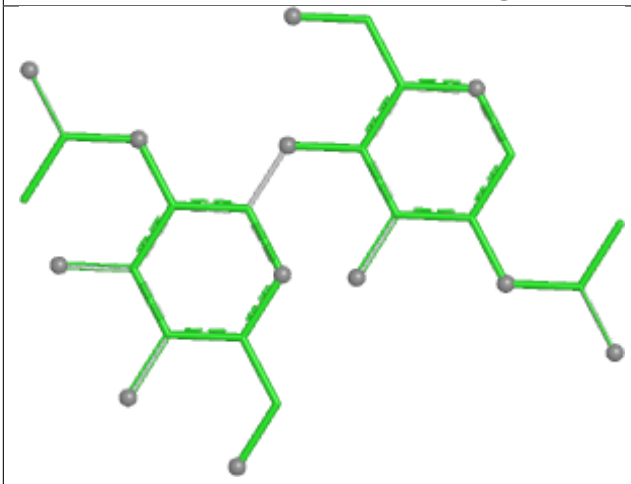
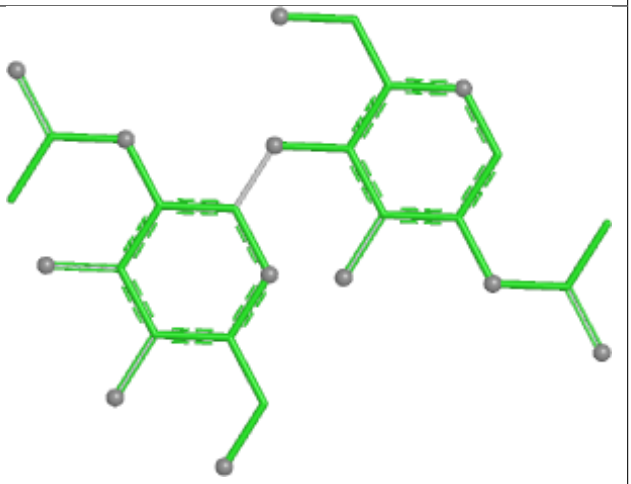


Rings

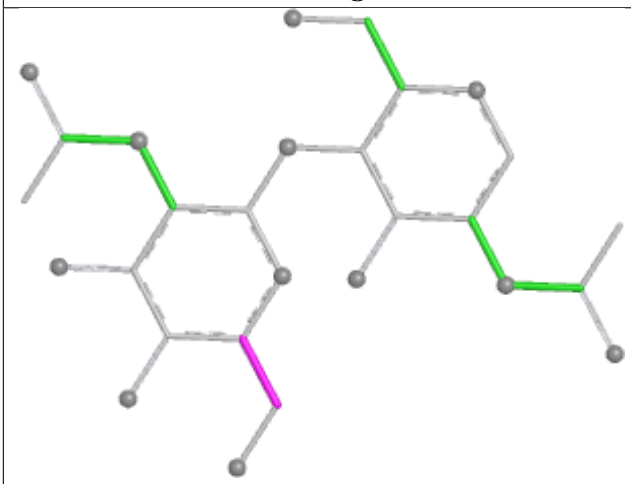
Oligosaccharide Chain T



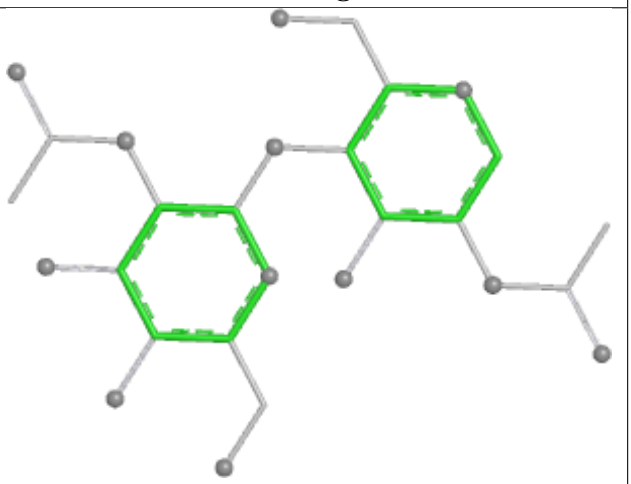
Bond lengths



Bond angles

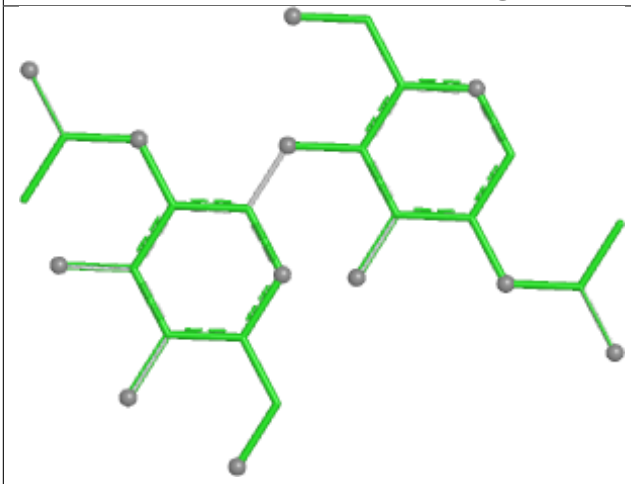


Torsions



Rings

Oligosaccharide Chain V



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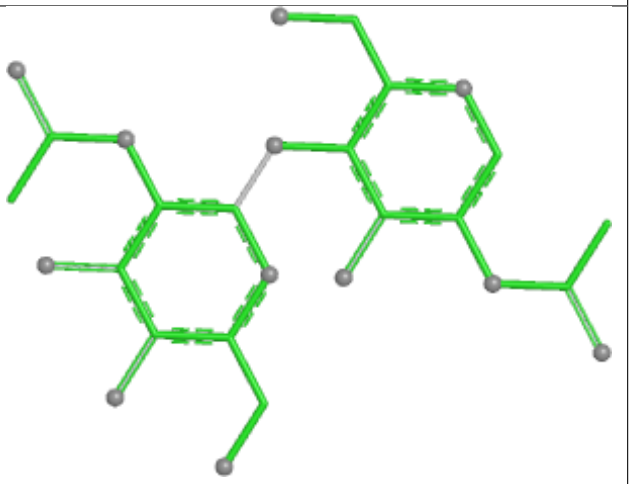
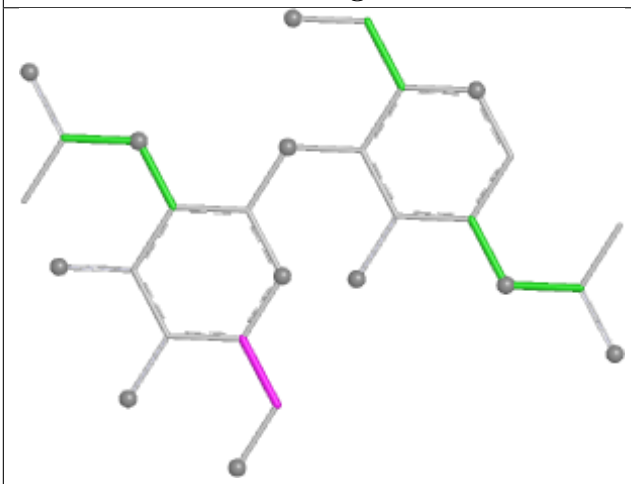


Bond angles



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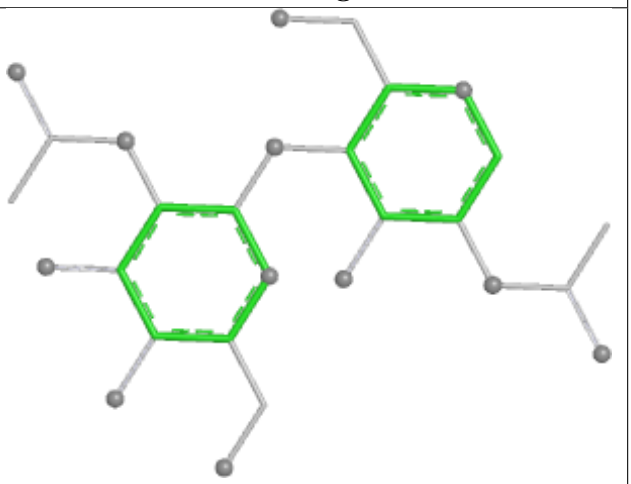
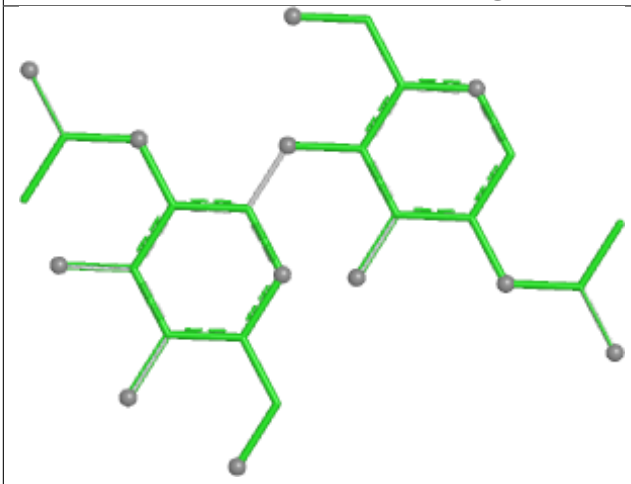
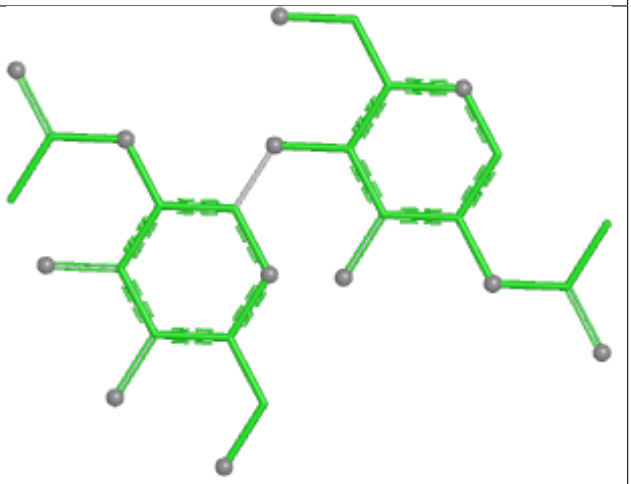


Rings

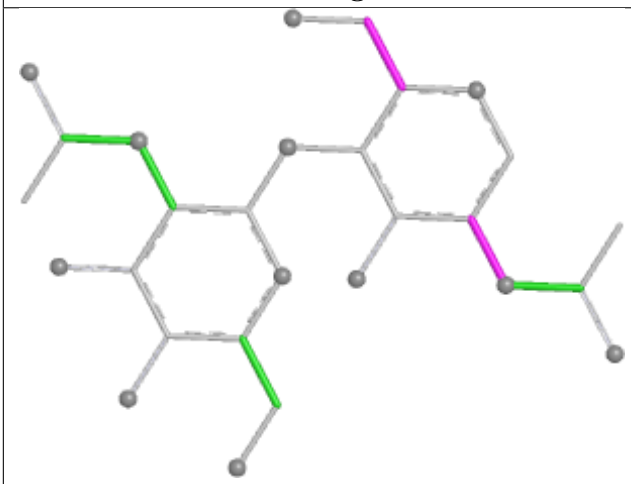
Oligosaccharide Chain W



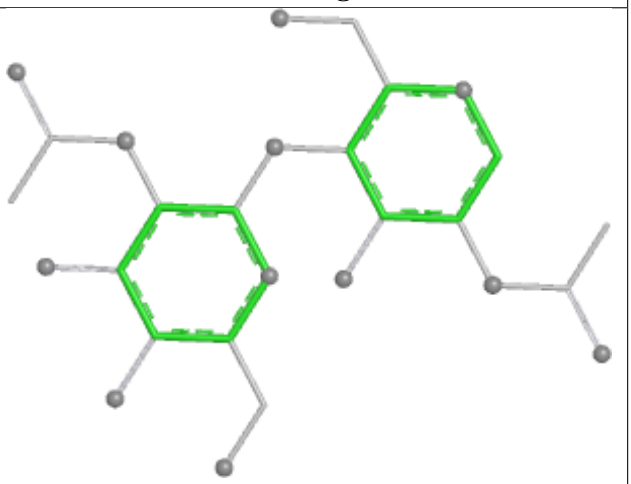
Bond lengths



Bond angles

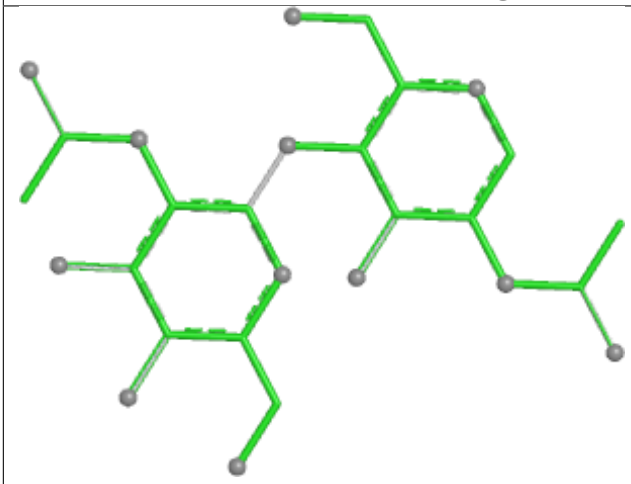


Torsions

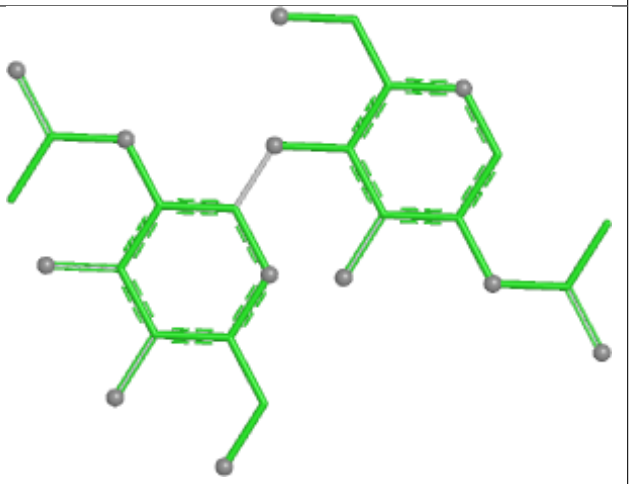


Rings

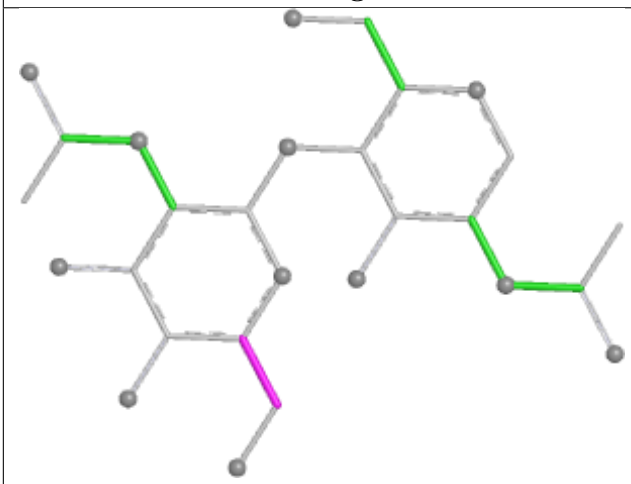
Oligosaccharide Chain X



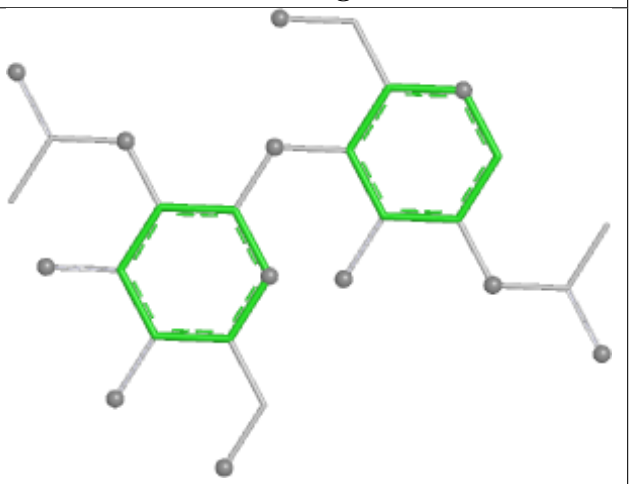
Bond lengths



Bond angles

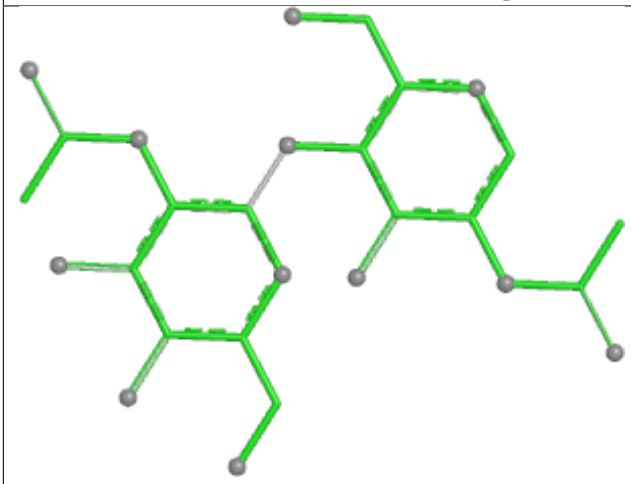


Torsions

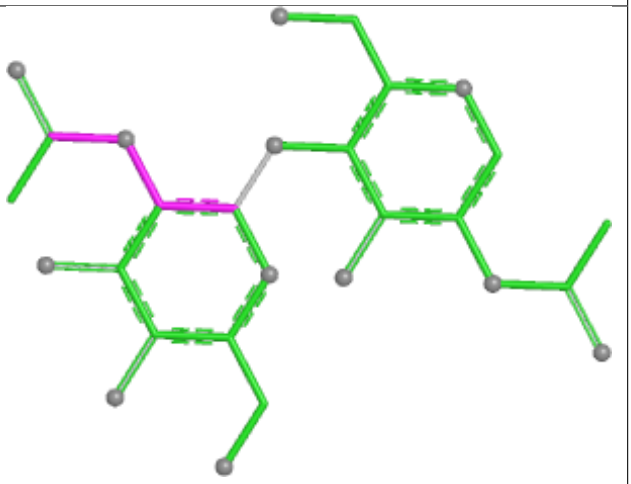


Rings

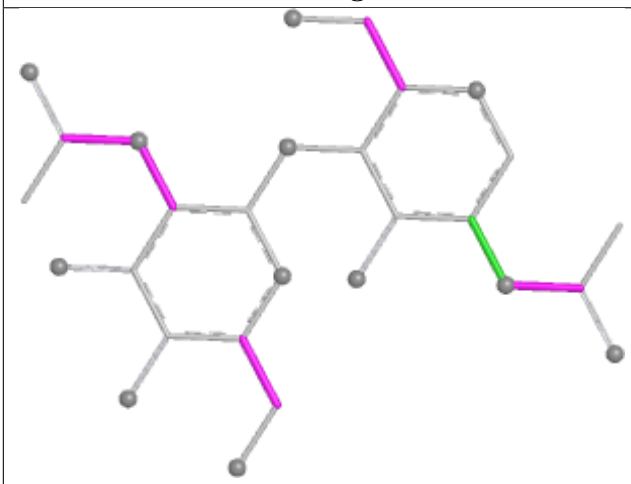
Oligosaccharide Chain b



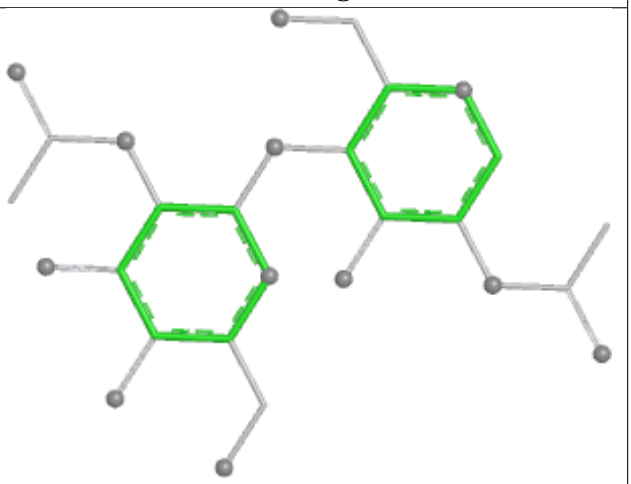
Bond lengths



Bond angles

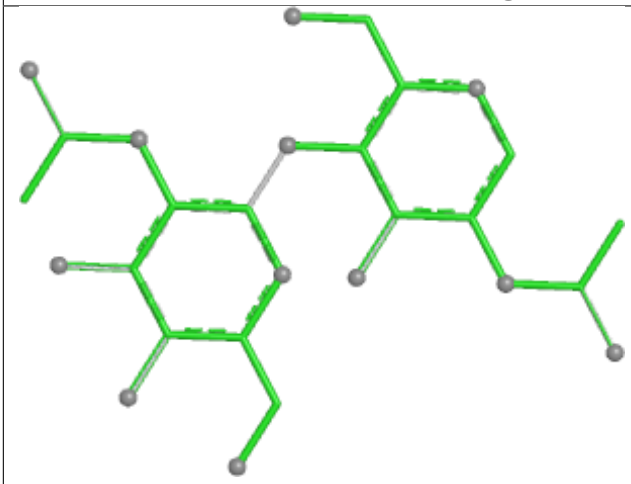


Torsions

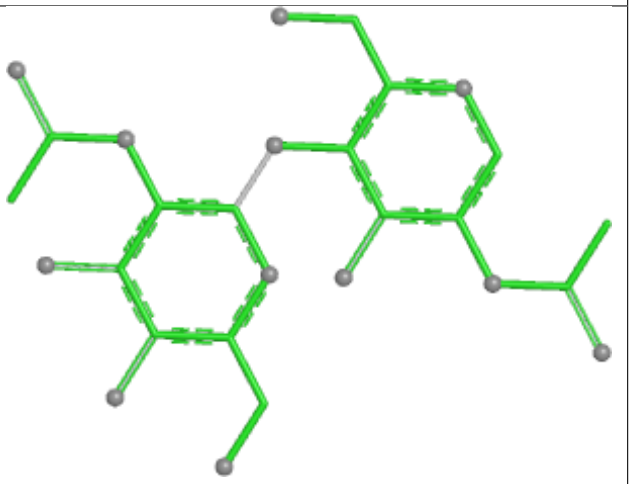


Rings

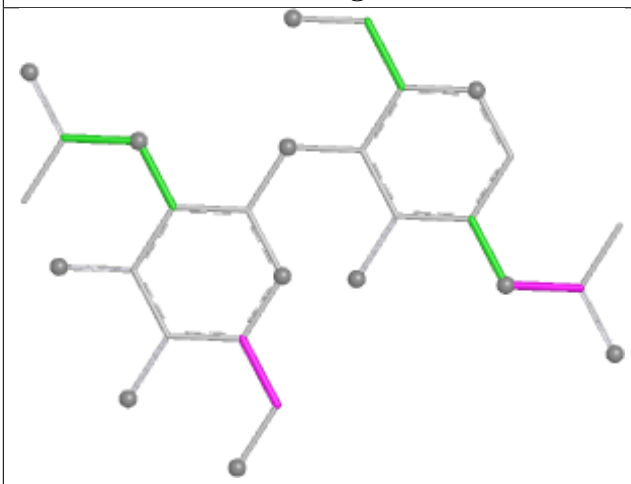
Oligosaccharide Chain c



Bond lengths



Bond angles



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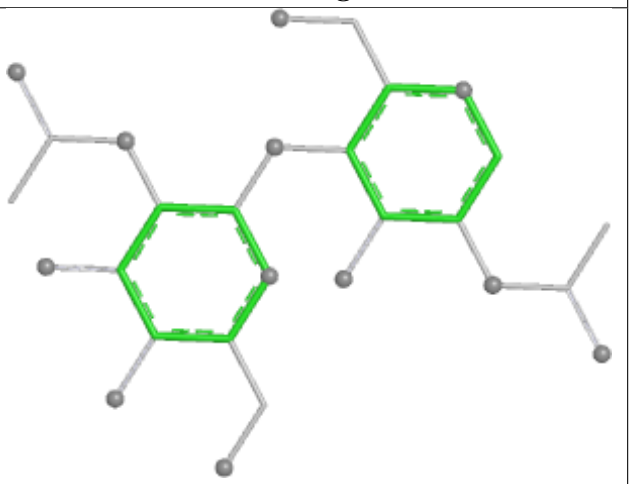
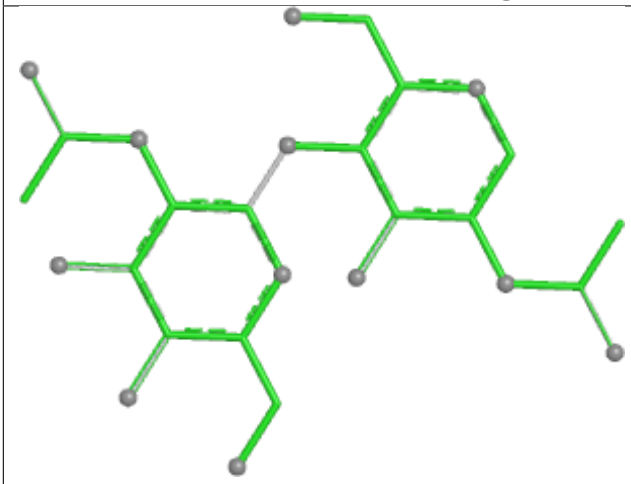
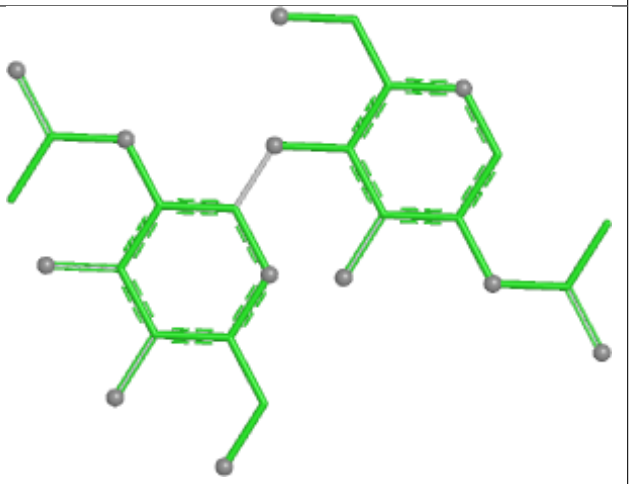


Rings

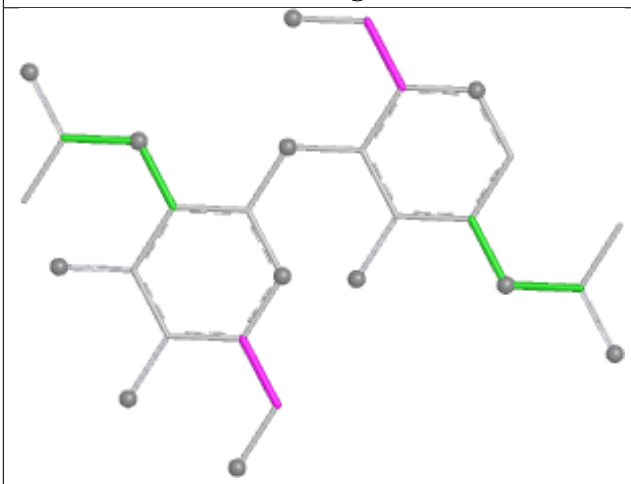
Oligosaccharide Chain d



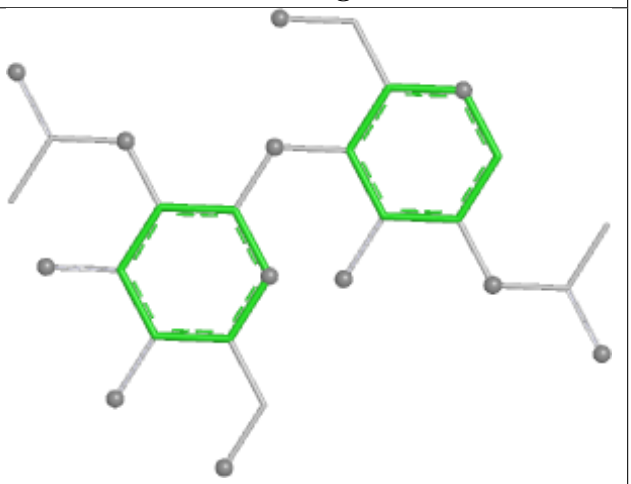
Bond lengths



Bond angles

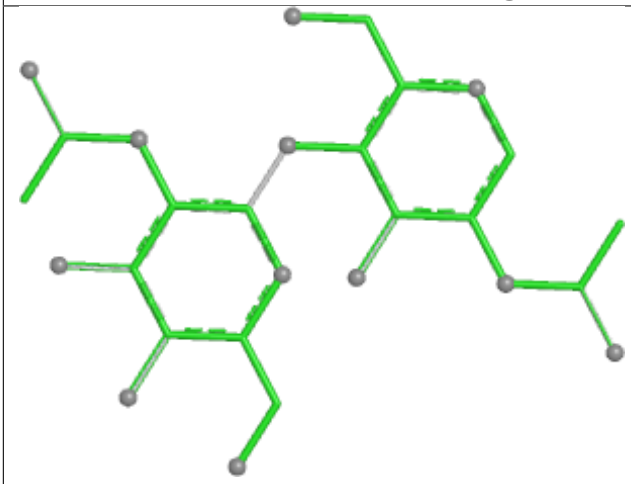


Torsions



Rings

Oligosaccharide Chain f



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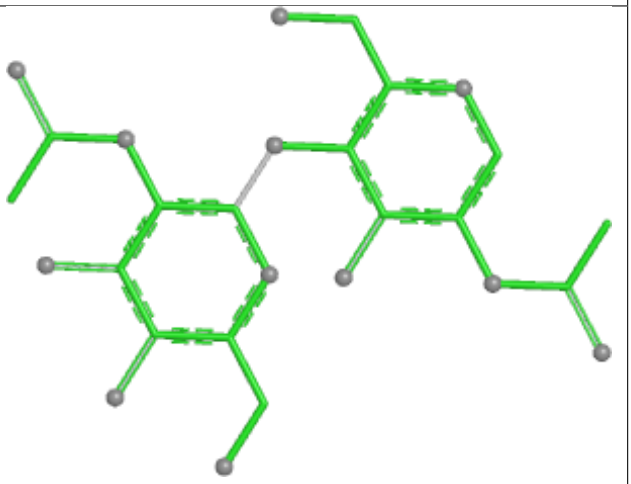
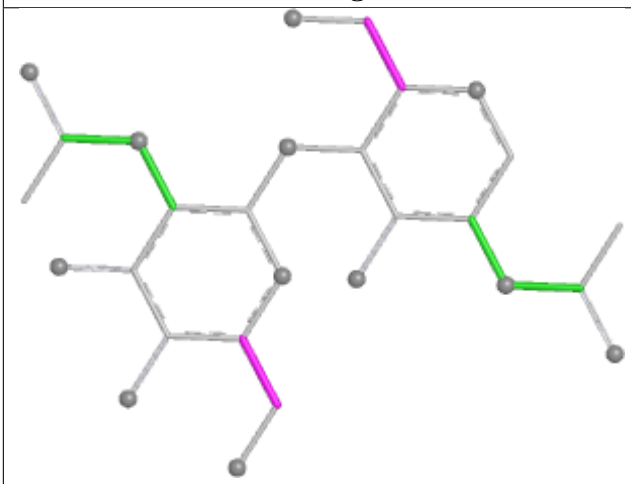


Bond angles



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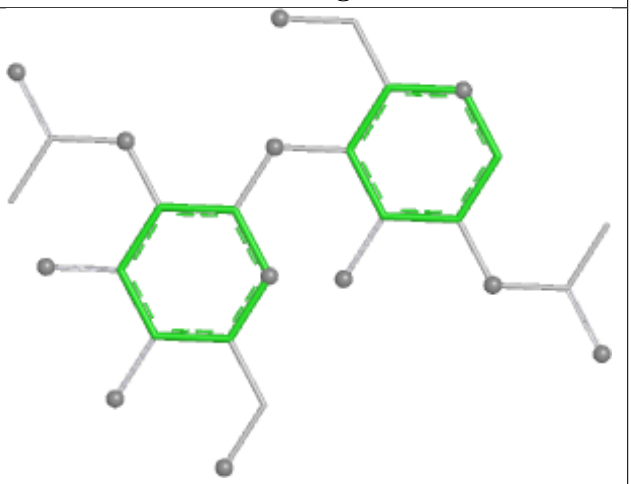
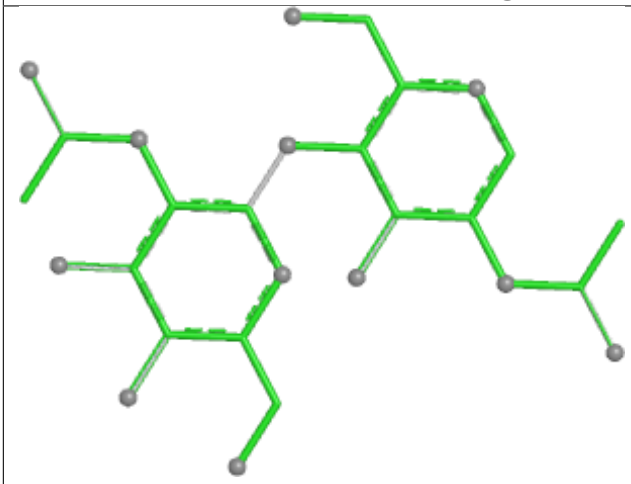


Rings

Oligosaccharide Chain g



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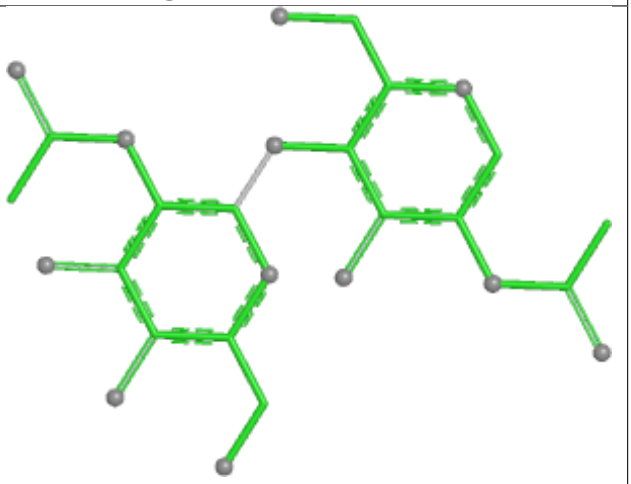
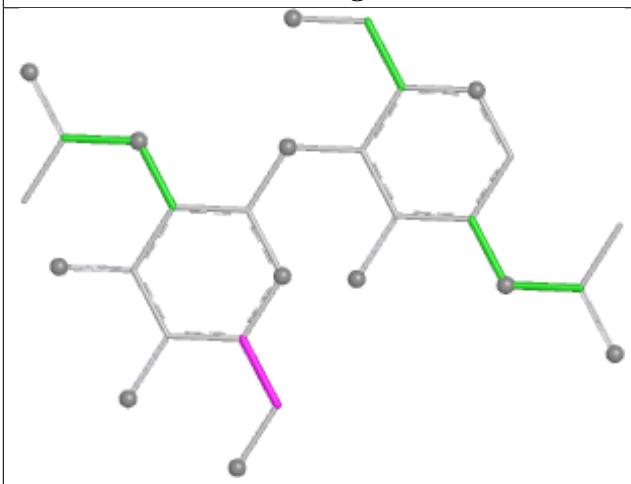


Bond angles



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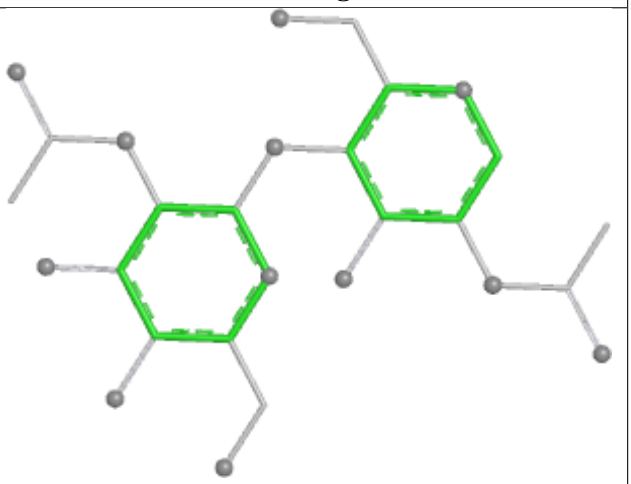
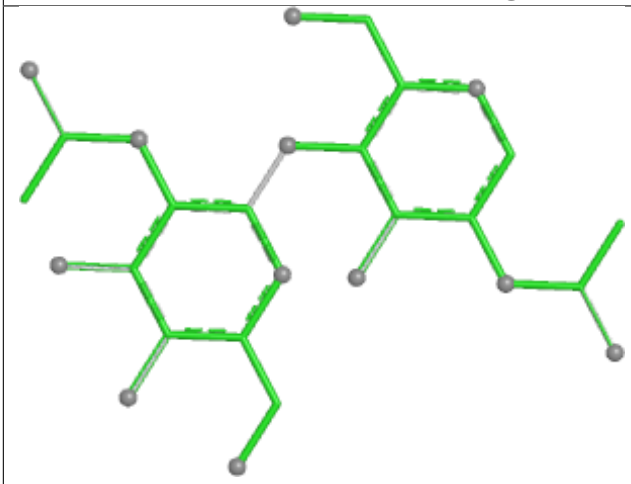


Rings

Oligosaccharide Chain i



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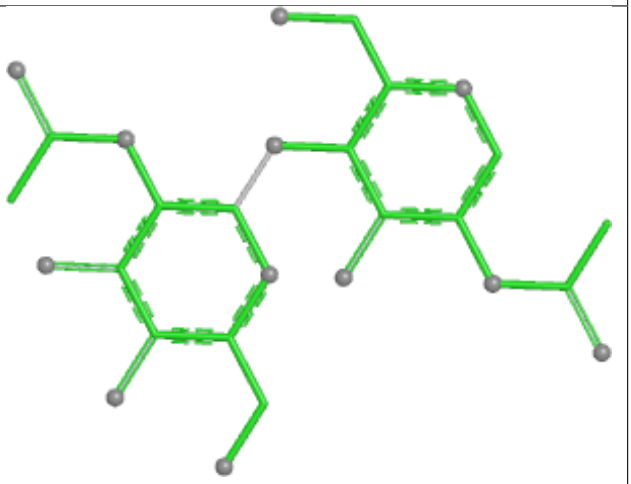

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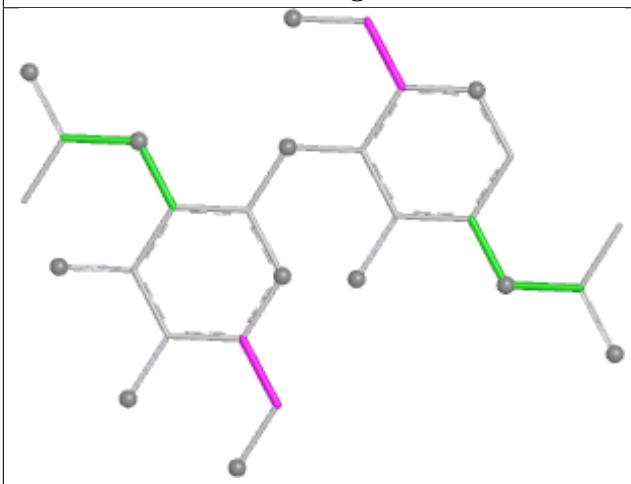
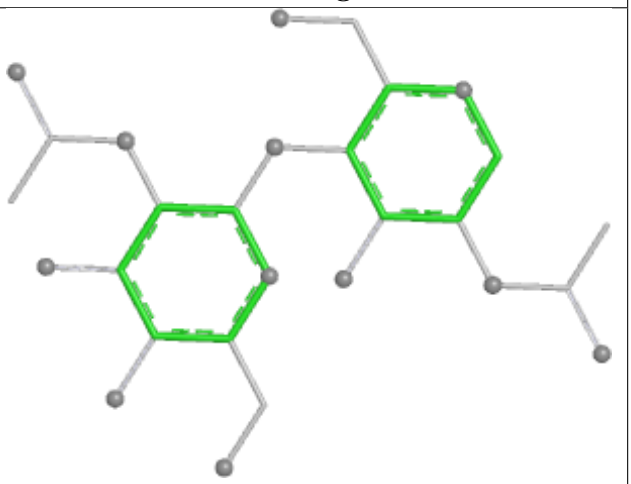
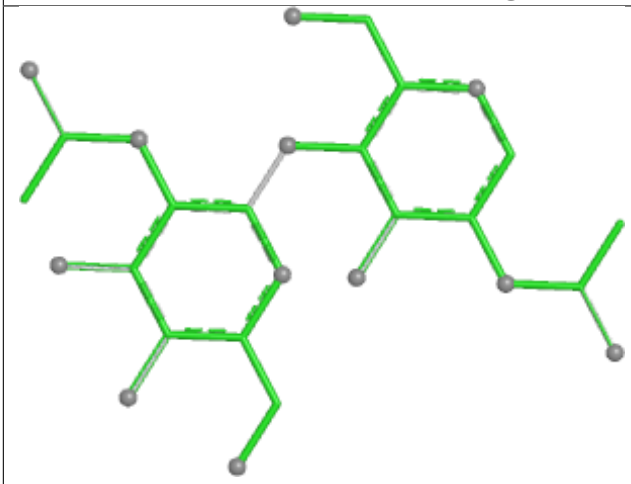


Torsions

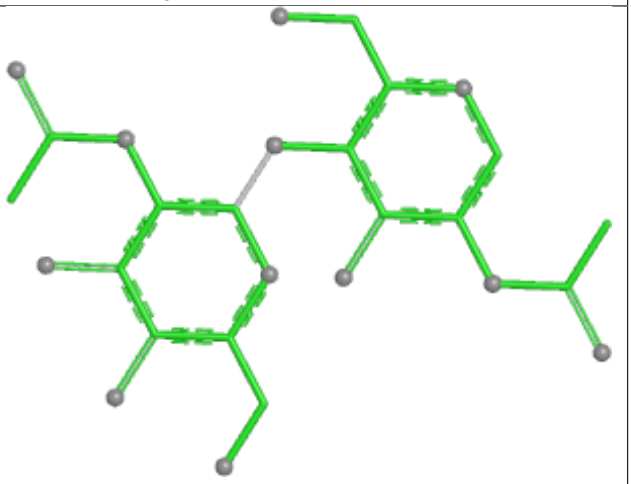


Rings

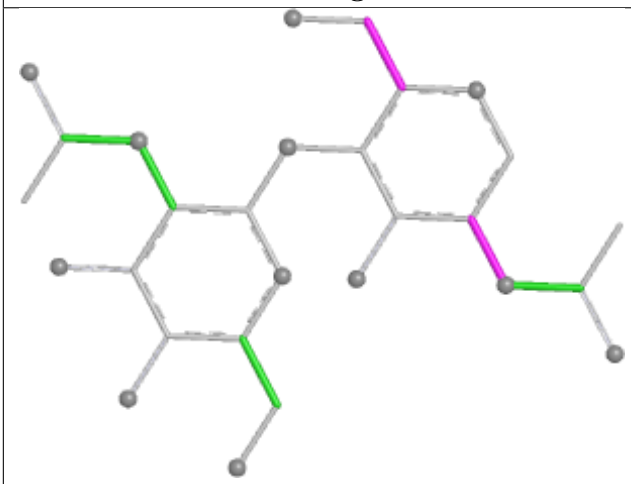
Oligosaccharide Chain j



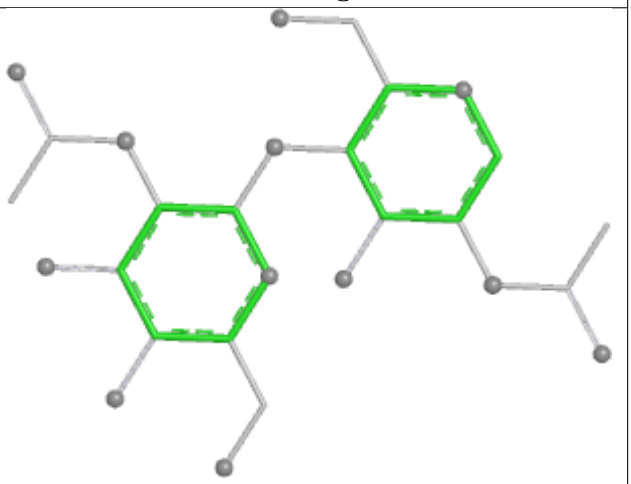
Bond lengths



Bond angles

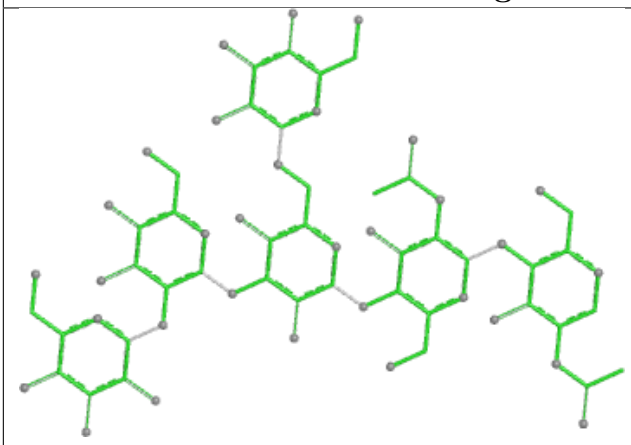


Torsions

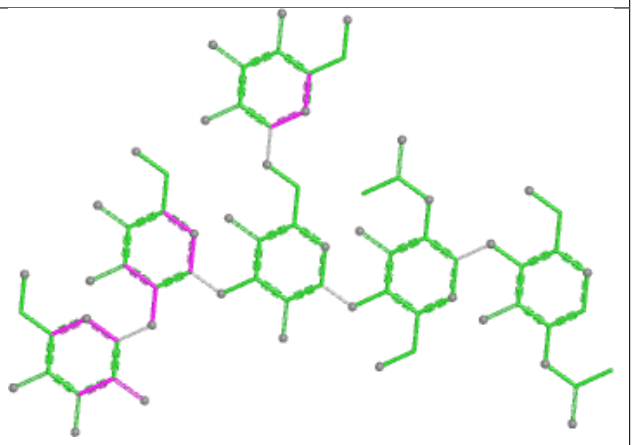


Rings

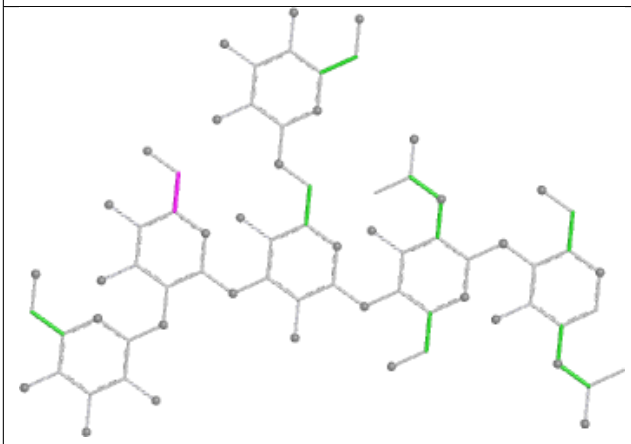
Oligosaccharide Chain R



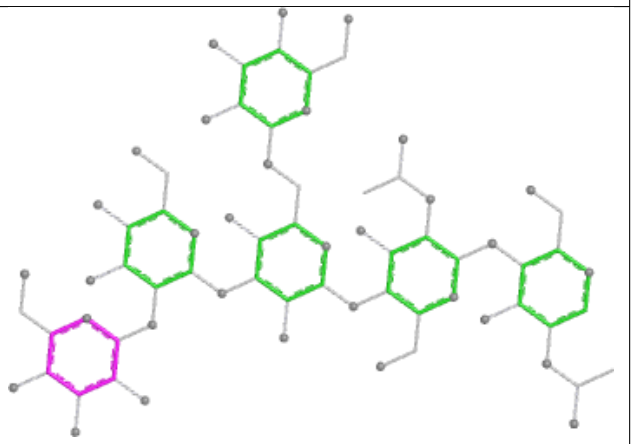
Bond lengths



Bond angles

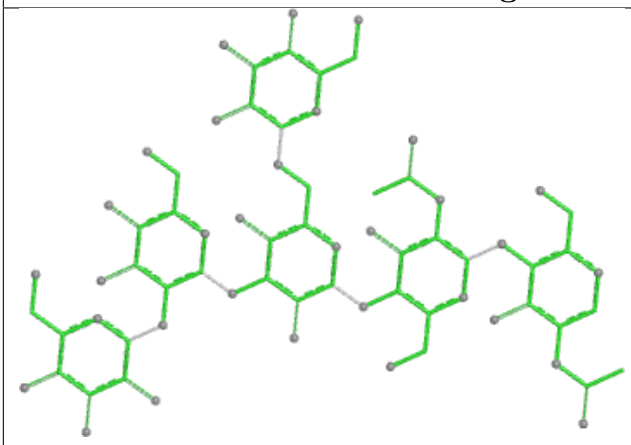


Torsions

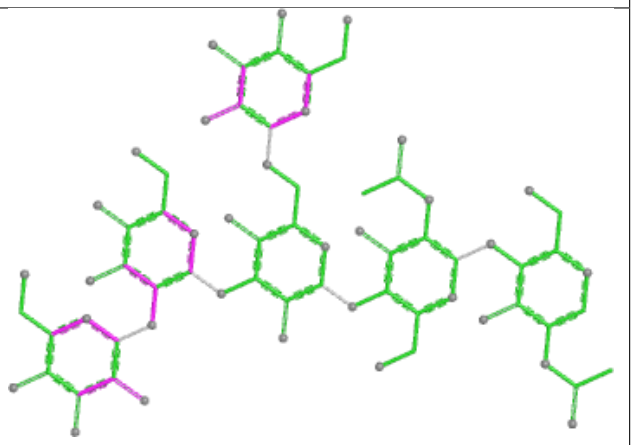


Rings

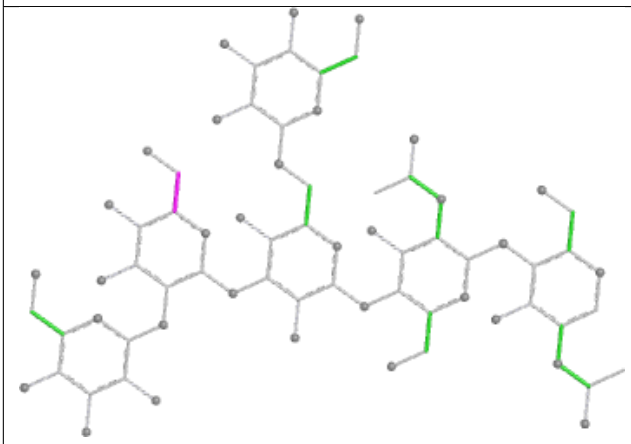
Oligosaccharide Chain e



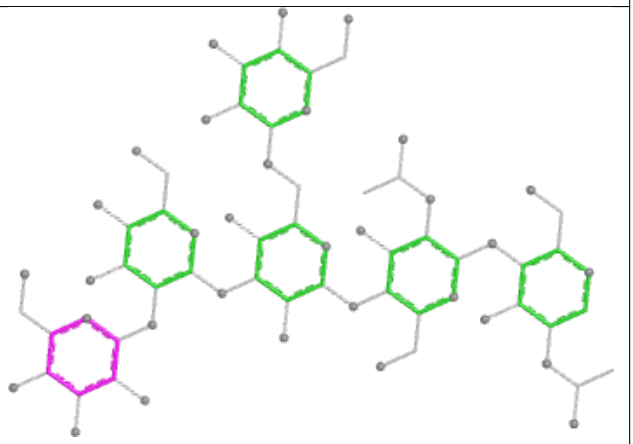
Bond lengths



Bond angles

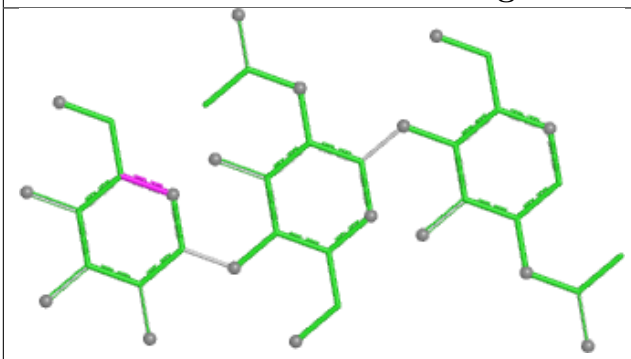


Torsions

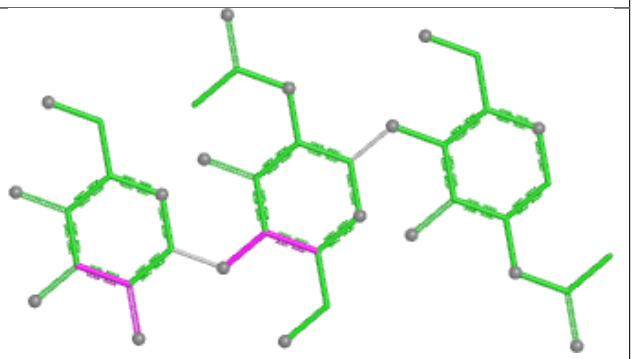


Rings

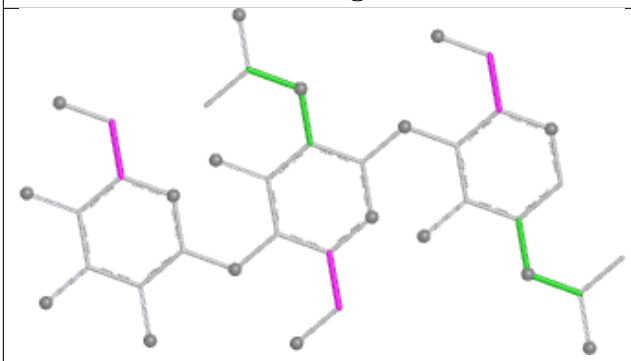
Oligosaccharide Chain S



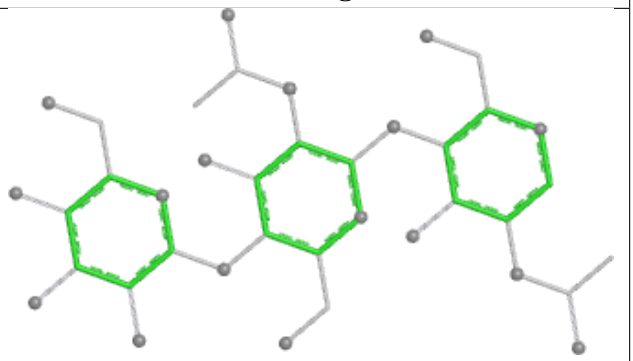
Bond lengths



Bond angles

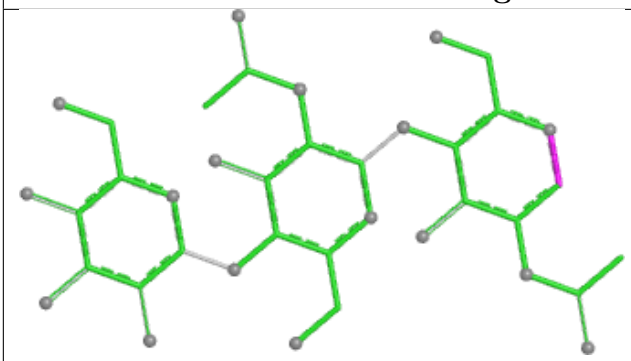


Torsions

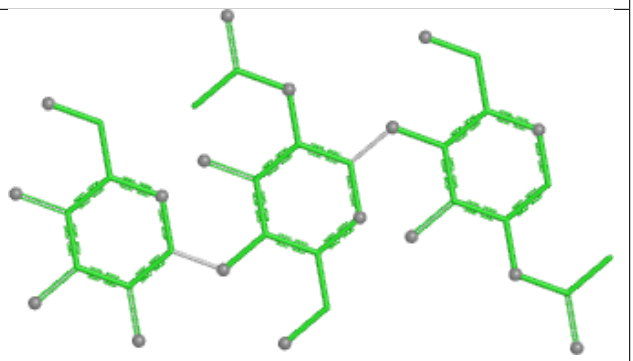


Rings

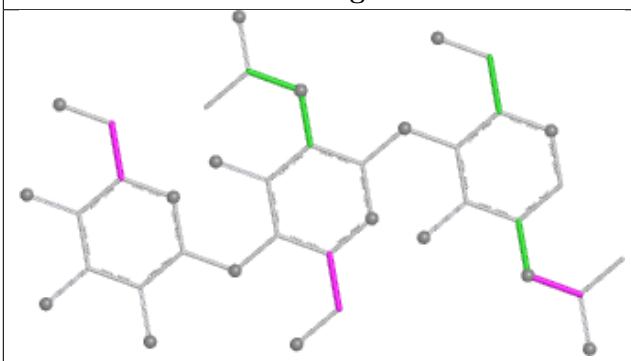
Oligosaccharide Chain Y



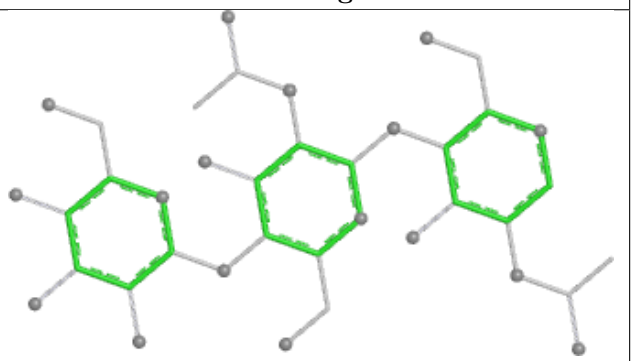
Bond lengths



Bond angles

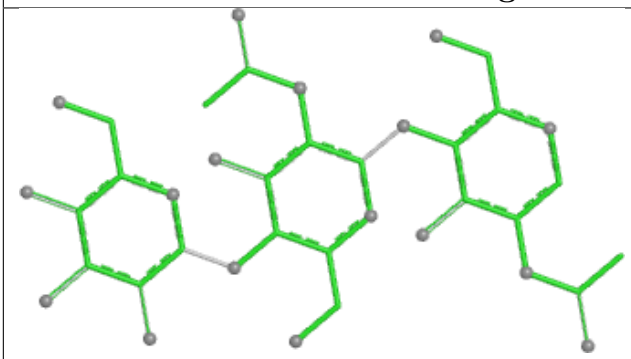


Torsions

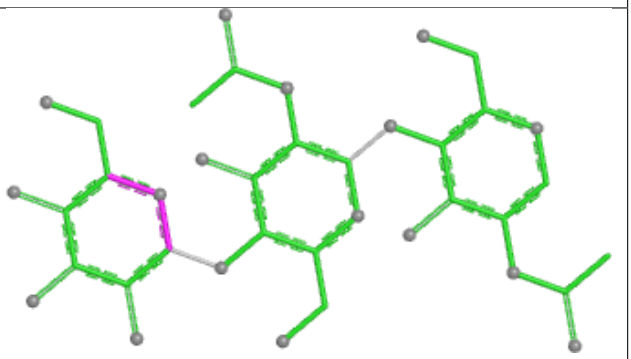


Rings

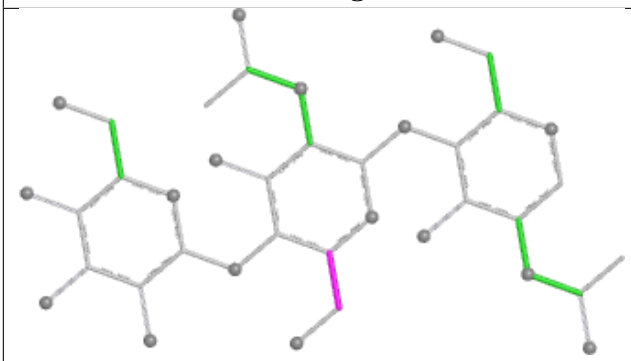
Oligosaccharide Chain k



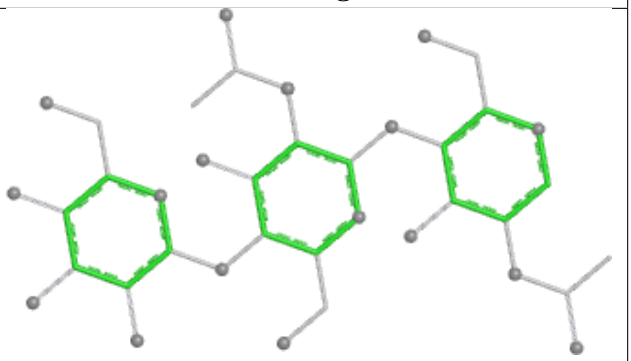
Bond lengths



Bond angles

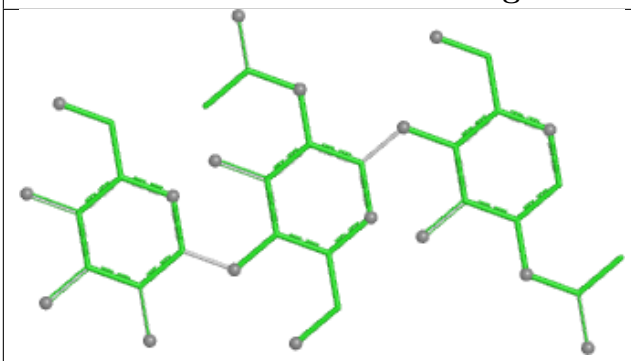


Torsions

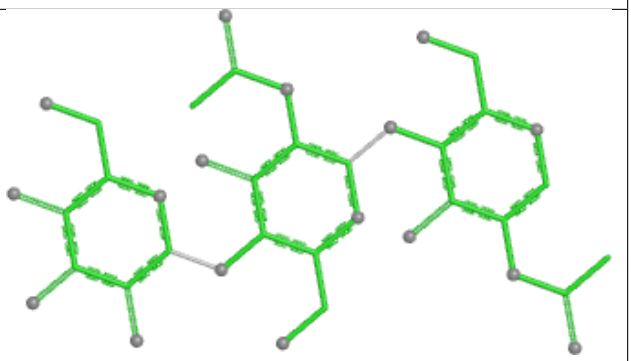


Rings

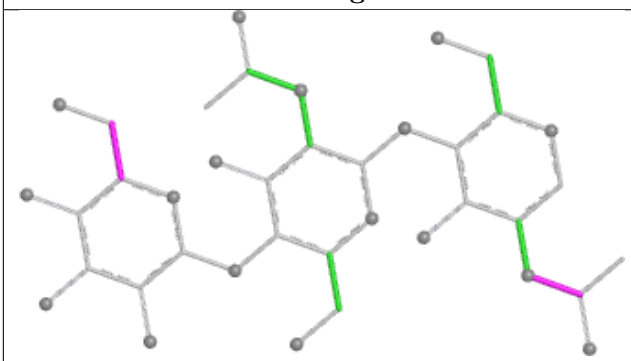
Oligosaccharide Chain l



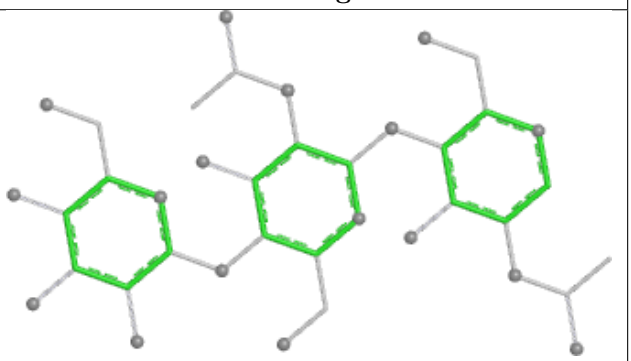
Bond lengths



Bond angles

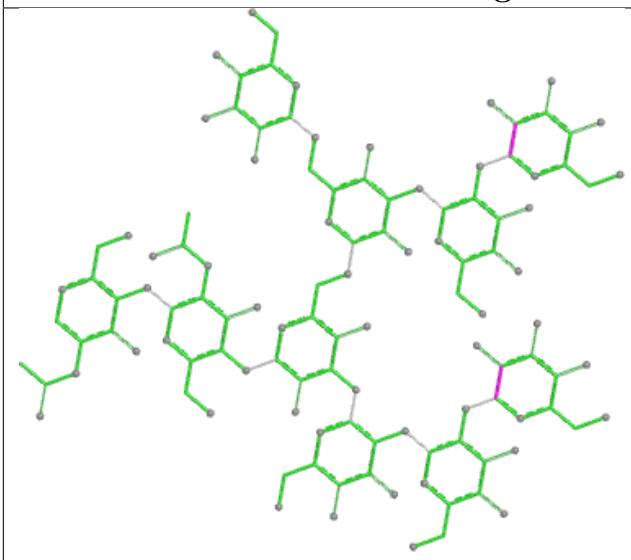


Torsions

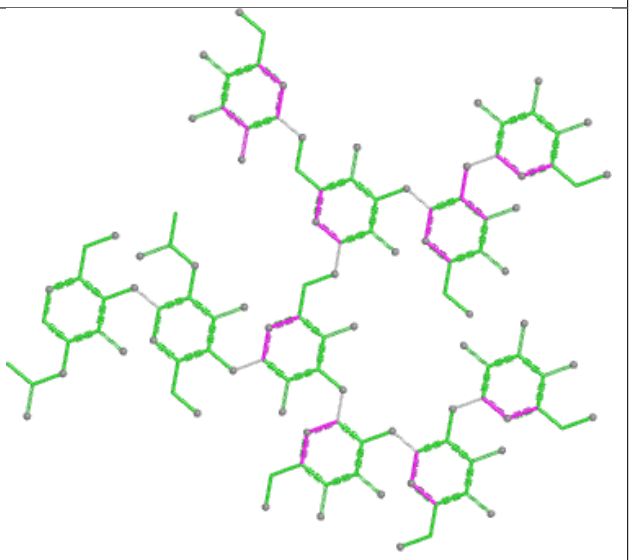


Rings

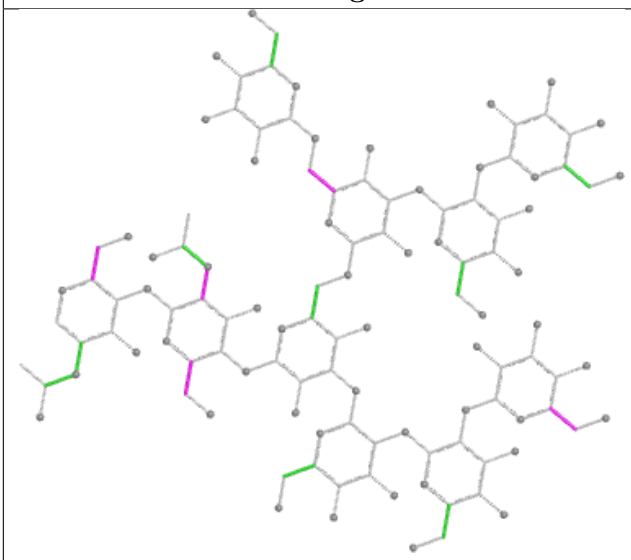
Oligosaccharide Chain U



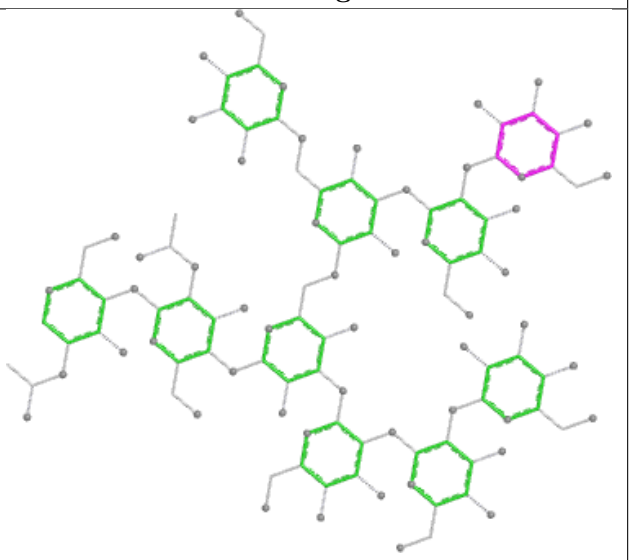
Bond lengths



Bond angles

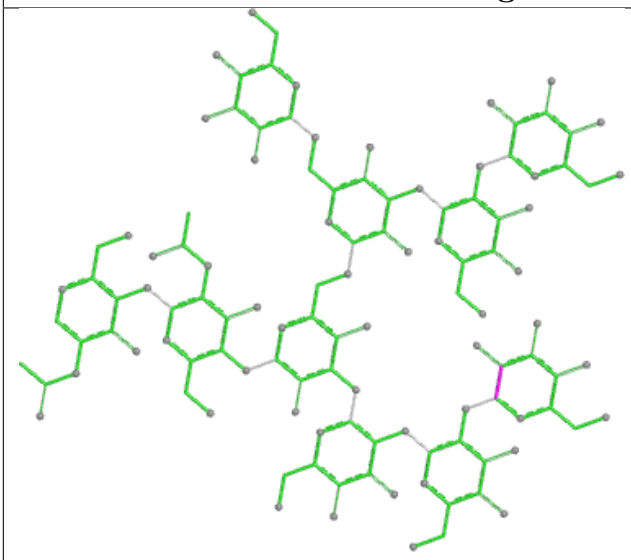


Torsions

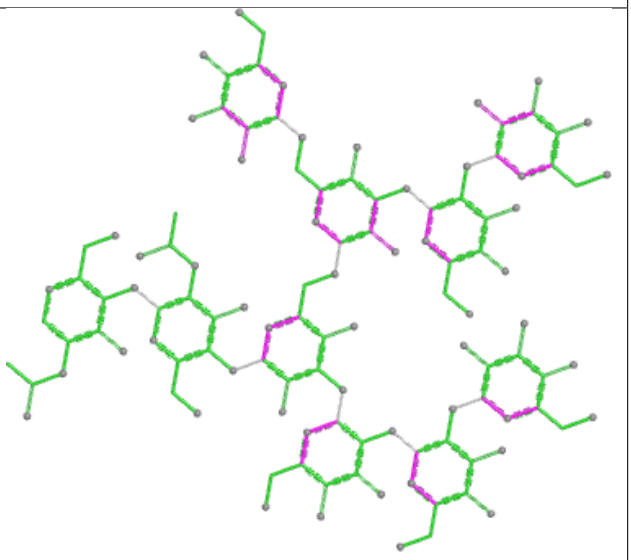


Rings

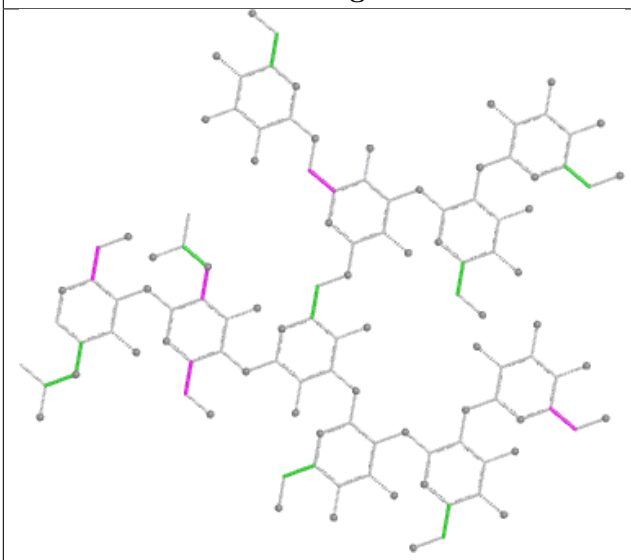
Oligosaccharide Chain h



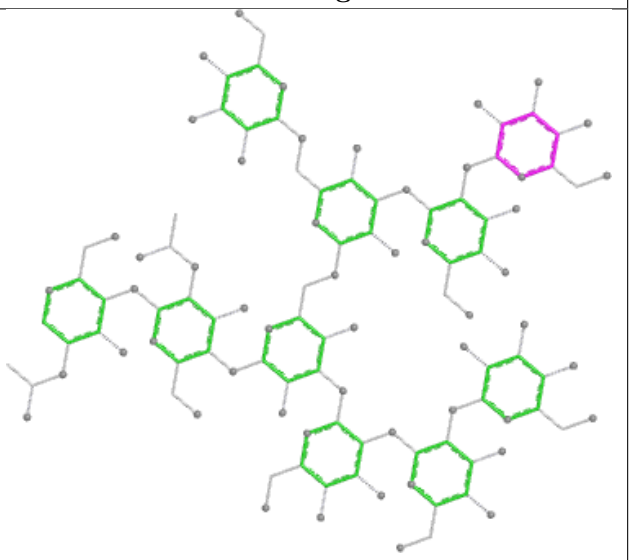
Bond lengths



Bond angles

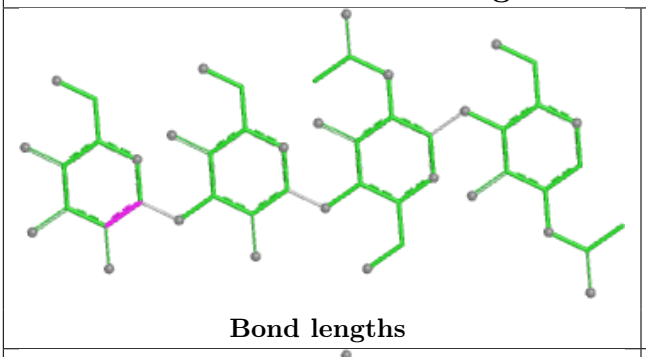


Torsions

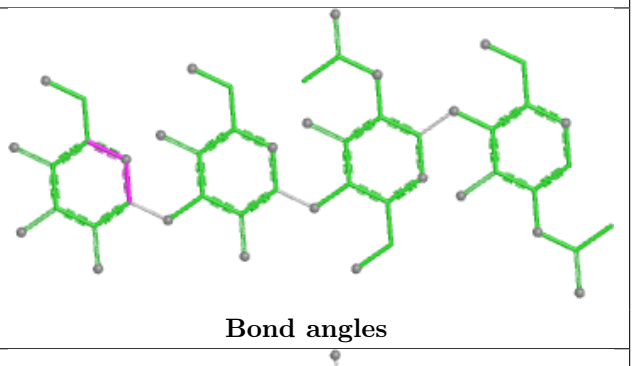


Rings

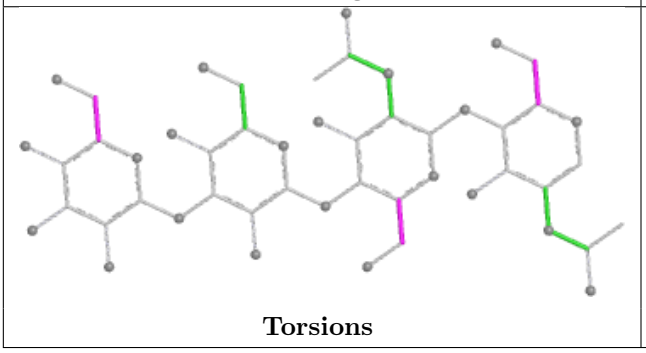
Oligosaccharide Chain m



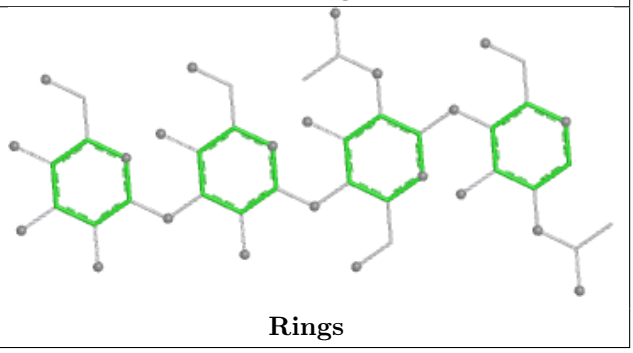
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
14	NAG	B	903	2	14,14,15	0.34	0	17,19,21	0.41	0
14	NAG	D	902	2	14,14,15	0.34	0	17,19,21	0.40	0
14	NAG	D	901	2	14,14,15	0.41	0	17,19,21	0.61	0
14	NAG	C	942	1	14,14,15	0.29	0	17,19,21	0.76	0
14	NAG	A	952	1	14,14,15	0.67	1 (7%)	17,19,21	0.49	0
14	NAG	A	942	1	14,14,15	0.19	0	17,19,21	0.37	0
14	NAG	B	901	2	14,14,15	0.33	0	17,19,21	0.59	0
14	NAG	I	305	6	14,14,15	2.07	2 (14%)	17,19,21	0.89	0
14	NAG	C	909	1	14,14,15	0.33	0	17,19,21	0.52	0
14	NAG	C	927	1	14,14,15	0.48	0	17,19,21	1.34	2 (11%)
14	NAG	A	926	1	14,14,15	0.47	0	17,19,21	1.34	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	NAG	A	908	1	14,14,15	0.20	0	17,19,21	0.46	0
14	NAG	B	902	2	14,14,15	0.16	0	17,19,21	0.49	0
14	NAG	C	908	1	14,14,15	0.29	0	17,19,21	0.43	0
14	NAG	C	953	1	14,14,15	0.27	0	17,19,21	0.45	0
14	NAG	K	301	6	14,14,15	1.98	2 (14%)	17,19,21	0.91	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
14	NAG	B	903	2	-	2/6/23/26	0/1/1/1
14	NAG	D	902	2	-	2/6/23/26	0/1/1/1
14	NAG	D	901	2	-	2/6/23/26	0/1/1/1
14	NAG	C	942	1	-	4/6/23/26	0/1/1/1
14	NAG	A	952	1	-	0/6/23/26	0/1/1/1
14	NAG	A	942	1	-	2/6/23/26	0/1/1/1
14	NAG	B	901	2	-	1/6/23/26	0/1/1/1
14	NAG	I	305	6	-	1/6/23/26	0/1/1/1
14	NAG	C	909	1	-	2/6/23/26	0/1/1/1
14	NAG	C	927	1	-	6/6/23/26	0/1/1/1
14	NAG	A	926	1	-	6/6/23/26	0/1/1/1
14	NAG	A	908	1	-	1/6/23/26	0/1/1/1
14	NAG	B	902	2	-	2/6/23/26	0/1/1/1
14	NAG	C	908	1	-	1/6/23/26	0/1/1/1
14	NAG	C	953	1	-	2/6/23/26	0/1/1/1
14	NAG	K	301	6	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	I	305	NAG	O5-C1	7.06	1.55	1.43
14	K	301	NAG	O5-C1	6.81	1.55	1.43
14	I	305	NAG	C1-C2	-2.77	1.48	1.52
14	K	301	NAG	C1-C2	-2.52	1.48	1.52
14	A	952	NAG	O5-C1	-2.31	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	926	NAG	C2-N2-C7	4.61	129.07	122.90
14	C	927	NAG	C2-N2-C7	4.60	129.06	122.90
14	A	926	NAG	C1-C2-N2	2.16	113.84	110.43
14	C	927	NAG	C1-C2-N2	2.13	113.80	110.43

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	926	NAG	O5-C5-C6-O6
14	C	927	NAG	O5-C5-C6-O6
14	C	942	NAG	O5-C5-C6-O6
14	B	902	NAG	O5-C5-C6-O6
14	C	927	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	927	NAG	1	0
14	A	926	NAG	1	0
14	A	908	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Warning: The R factor obtained from EDS is 0.3314, which does not match the depositor's R factor of 0.2811. Please interpret the results in this section carefully.

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	455/481 (94%)	0.47	29 (6%)	27	24	118, 169, 241, 272	0
1	C	450/481 (93%)	0.46	30 (6%)	25	22	125, 167, 239, 284	0
2	B	132/153 (86%)	0.48	5 (3%)	44	34	115, 171, 238, 256	0
2	D	132/153 (86%)	0.62	9 (6%)	25	22	122, 177, 233, 246	0
3	J	210/210 (100%)	0.50	15 (7%)	23	22	190, 267, 327, 375	0
3	L	210/210 (100%)	0.55	7 (3%)	49	38	188, 278, 318, 331	0
4	E	223/223 (100%)	0.39	12 (5%)	32	26	136, 205, 293, 332	0
4	G	223/223 (100%)	0.34	16 (7%)	23	21	141, 192, 284, 320	0
5	F	212/212 (100%)	0.44	8 (3%)	44	34	171, 266, 317, 340	0
5	H	212/212 (100%)	0.38	10 (4%)	37	31	157, 244, 296, 314	0
6	I	228/235 (97%)	0.30	8 (3%)	47	36	187, 251, 285, 313	0
6	K	228/235 (97%)	0.56	27 (11%)	10	11	188, 249, 281, 302	0
All	All	2915/3028 (96%)	0.45	176 (6%)	29	24	115, 214, 301, 375	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	ALA	10.4
5	F	2	ILE	5.7
1	C	454	LEU	5.2
4	G	114	ALA	5.1
4	E	67	VAL	5.1

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

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

6.3 Carbohydrates (i)

SUGAR-RSR INFOmissingINFO

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	NAG	A	942	14/15	0.15	0.18	246,259,268,272	0
14	NAG	K	301	14/15	0.28	0.19	255,274,293,293	0
14	NAG	I	305	14/15	0.29	0.15	262,282,291,294	0
14	NAG	B	902	14/15	0.44	0.16	260,274,299,300	0
14	NAG	A	926	14/15	0.54	0.17	210,217,221,223	0
14	NAG	C	908	14/15	0.56	0.21	232,249,265,272	0
14	NAG	C	942	14/15	0.58	0.13	230,246,255,260	0
14	NAG	D	902	14/15	0.60	0.13	225,248,271,272	0
14	NAG	C	953	14/15	0.62	0.17	212,234,244,246	0
14	NAG	B	903	14/15	0.66	0.12	230,262,292,295	0
14	NAG	A	908	14/15	0.72	0.19	217,234,248,253	0
14	NAG	A	952	14/15	0.72	0.15	233,255,262,265	0
14	NAG	C	927	14/15	0.74	0.13	218,225,232,234	0
14	NAG	C	909	14/15	0.74	0.26	197,225,250,254	0
14	NAG	D	901	14/15	0.77	0.14	265,277,303,319	0
14	NAG	B	901	14/15	0.84	0.10	239,260,288,303	0

6.5 Other polymers (i)

There are no such residues in this entry.