wwPDB EM Validation Summary Report

Oct 5, 2024 – 09:25 PM EDT

PDB ID	:	6NQD
EMDB ID	:	EMD-0485
Title	:	Cryo-EM structure of T/F100 SOSIP.664 HIV-1 Env trimer in complex with 8ANC195 Fab
Authors	:	Fang, Q.; Rossmann, M.G.
Deposited on	:	2019-01-21
Resolution	:	3.90 Å(reported)

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 ⓘ symbol.

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

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

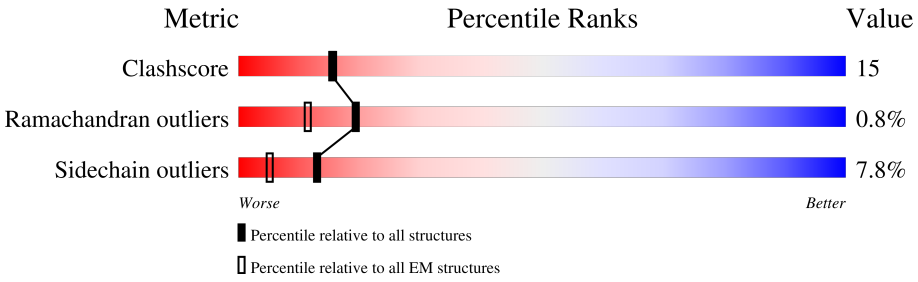
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	486	7% 58% 30% • 10%
1	E	486	7% 59% 28% • 10%
1	I	486	7% 59% 28% • 10%
2	B	184	8% 51% 16% • 33%
2	F	184	7% 52% 15% • 33%
2	J	184	8% 49% 18% • 33%
3	C	244	5% 35% 16% • 47%
3	G	244	7% 36% 16% • 47%

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Mol	Chain	Length	Quality of chain
3	K	244	7% 35% 16% 47%
4	D	215	7% 38% 12% 50%
4	H	215	10% 37% 13% 50%
4	L	215	9% 37% 12% 50%
5	M	10	20% 80%
5	X	10	20% 80%
5	i	10	20% 80%
6	N	6	33% 50% 50%
6	Y	6	33% 50% 50%
6	j	6	33% 50% 50%
7	O	2	100%
7	P	2	50% 50% 50%
7	Q	2	50% 50% 50%
7	R	2	50% 50%
7	S	2	50% 100%
7	T	2	50% 50% 50%
7	U	2	100%
7	Z	2	100%
7	a	2	50% 50% 50%
7	b	2	50% 50%
7	c	2	50% 50% 50%
7	d	2	50% 100%
7	e	2	50% 50%
7	f	2	100%
7	k	2	100%

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Mol	Chain	Length	Quality of chain
7	l	2	50% 50% 50%
7	m	2	50% 50%
7	n	2	50% 50%
7	o	2	50% 100%
7	p	2	50% 50% 50%
7	q	2	100%
8	V	3	67% 33%
8	g	3	67% 33%
8	r	3	67% 33%
9	W	4	50% 50% 50%
9	h	4	50% 50% 50%
9	s	4	50% 50% 50%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 20175 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 T/F100 Env gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	439	Total	C	N	O	S	0	0
			3399	2151	595	626	27		
1	E	439	Total	C	N	O	S	0	0
			3399	2151	595	626	27		
1	I	439	Total	C	N	O	S	0	0
			3399	2151	595	626	27		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	CYS	ALA	conflict	UNP A0A140EMT3
A	508	ARG	-	expression tag	UNP A0A140EMT3
A	509	ARG	-	expression tag	UNP A0A140EMT3
A	510	ARG	-	expression tag	UNP A0A140EMT3
A	511	ARG	-	expression tag	UNP A0A140EMT3
A	512	ARG	-	expression tag	UNP A0A140EMT3
A	513	ARG	-	expression tag	UNP A0A140EMT3
E	501	CYS	ALA	conflict	UNP A0A140EMT3
E	508	ARG	-	expression tag	UNP A0A140EMT3
E	509	ARG	-	expression tag	UNP A0A140EMT3
E	510	ARG	-	expression tag	UNP A0A140EMT3
E	511	ARG	-	expression tag	UNP A0A140EMT3
E	512	ARG	-	expression tag	UNP A0A140EMT3
E	513	ARG	-	expression tag	UNP A0A140EMT3
I	501	CYS	ALA	conflict	UNP A0A140EMT3
I	508	ARG	-	expression tag	UNP A0A140EMT3
I	509	ARG	-	expression tag	UNP A0A140EMT3
I	510	ARG	-	expression tag	UNP A0A140EMT3
I	511	ARG	-	expression tag	UNP A0A140EMT3
I	512	ARG	-	expression tag	UNP A0A140EMT3
I	513	ARG	-	expression tag	UNP A0A140EMT3

- Molecule 2 is a protein called T/F100 Env gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	124	Total	C	N	O	S	0	0
			944	599	158	182	5		
2	F	124	Total	C	N	O	S	0	0
			944	599	158	182	5		
2	J	124	Total	C	N	O	S	0	0
			944	599	158	182	5		

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP A0A140EMT3
B	605	CYS	THR	conflict	UNP A0A140EMT3
B	665	ALA	-	expression tag	UNP A0A140EMT3
B	666	ALA	-	expression tag	UNP A0A140EMT3
B	667	ALA	-	expression tag	UNP A0A140EMT3
B	668	TRP	-	expression tag	UNP A0A140EMT3
B	669	SER	-	expression tag	UNP A0A140EMT3
B	670	HIS	-	expression tag	UNP A0A140EMT3
B	671	PRO	-	expression tag	UNP A0A140EMT3
B	672	GLN	-	expression tag	UNP A0A140EMT3
B	673	PHE	-	expression tag	UNP A0A140EMT3
B	674	GLU	-	expression tag	UNP A0A140EMT3
B	675	LYS	-	expression tag	UNP A0A140EMT3
B	676	GLY	-	expression tag	UNP A0A140EMT3
B	677	GLY	-	expression tag	UNP A0A140EMT3
B	678	GLY	-	expression tag	UNP A0A140EMT3
B	679	SER	-	expression tag	UNP A0A140EMT3
B	680	GLY	-	expression tag	UNP A0A140EMT3
B	681	GLY	-	expression tag	UNP A0A140EMT3
B	682	GLY	-	expression tag	UNP A0A140EMT3
B	683	SER	-	expression tag	UNP A0A140EMT3
B	684	GLY	-	expression tag	UNP A0A140EMT3
B	685	GLY	-	expression tag	UNP A0A140EMT3
B	686	SER	-	expression tag	UNP A0A140EMT3
B	687	ALA	-	expression tag	UNP A0A140EMT3
B	688	TRP	-	expression tag	UNP A0A140EMT3
B	689	SER	-	expression tag	UNP A0A140EMT3
B	690	HIS	-	expression tag	UNP A0A140EMT3
B	691	PRO	-	expression tag	UNP A0A140EMT3
B	692	GLN	-	expression tag	UNP A0A140EMT3
B	693	PHE	-	expression tag	UNP A0A140EMT3
B	694	GLU	-	expression tag	UNP A0A140EMT3
B	695	LYS	-	expression tag	UNP A0A140EMT3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	559	PRO	ILE	conflict	UNP A0A140EMT3
F	605	CYS	THR	conflict	UNP A0A140EMT3
F	665	ALA	-	expression tag	UNP A0A140EMT3
F	666	ALA	-	expression tag	UNP A0A140EMT3
F	667	ALA	-	expression tag	UNP A0A140EMT3
F	668	TRP	-	expression tag	UNP A0A140EMT3
F	669	SER	-	expression tag	UNP A0A140EMT3
F	670	HIS	-	expression tag	UNP A0A140EMT3
F	671	PRO	-	expression tag	UNP A0A140EMT3
F	672	GLN	-	expression tag	UNP A0A140EMT3
F	673	PHE	-	expression tag	UNP A0A140EMT3
F	674	GLU	-	expression tag	UNP A0A140EMT3
F	675	LYS	-	expression tag	UNP A0A140EMT3
F	676	GLY	-	expression tag	UNP A0A140EMT3
F	677	GLY	-	expression tag	UNP A0A140EMT3
F	678	GLY	-	expression tag	UNP A0A140EMT3
F	679	SER	-	expression tag	UNP A0A140EMT3
F	680	GLY	-	expression tag	UNP A0A140EMT3
F	681	GLY	-	expression tag	UNP A0A140EMT3
F	682	GLY	-	expression tag	UNP A0A140EMT3
F	683	SER	-	expression tag	UNP A0A140EMT3
F	684	GLY	-	expression tag	UNP A0A140EMT3
F	685	GLY	-	expression tag	UNP A0A140EMT3
F	686	SER	-	expression tag	UNP A0A140EMT3
F	687	ALA	-	expression tag	UNP A0A140EMT3
F	688	TRP	-	expression tag	UNP A0A140EMT3
F	689	SER	-	expression tag	UNP A0A140EMT3
F	690	HIS	-	expression tag	UNP A0A140EMT3
F	691	PRO	-	expression tag	UNP A0A140EMT3
F	692	GLN	-	expression tag	UNP A0A140EMT3
F	693	PHE	-	expression tag	UNP A0A140EMT3
F	694	GLU	-	expression tag	UNP A0A140EMT3
F	695	LYS	-	expression tag	UNP A0A140EMT3
J	559	PRO	ILE	conflict	UNP A0A140EMT3
J	605	CYS	THR	conflict	UNP A0A140EMT3
J	665	ALA	-	expression tag	UNP A0A140EMT3
J	666	ALA	-	expression tag	UNP A0A140EMT3
J	667	ALA	-	expression tag	UNP A0A140EMT3
J	668	TRP	-	expression tag	UNP A0A140EMT3
J	669	SER	-	expression tag	UNP A0A140EMT3
J	670	HIS	-	expression tag	UNP A0A140EMT3
J	671	PRO	-	expression tag	UNP A0A140EMT3

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Chain	Residue	Modelled	Actual	Comment	Reference
J	672	GLN	-	expression tag	UNP A0A140EMT3
J	673	PHE	-	expression tag	UNP A0A140EMT3
J	674	GLU	-	expression tag	UNP A0A140EMT3
J	675	LYS	-	expression tag	UNP A0A140EMT3
J	676	GLY	-	expression tag	UNP A0A140EMT3
J	677	GLY	-	expression tag	UNP A0A140EMT3
J	678	GLY	-	expression tag	UNP A0A140EMT3
J	679	SER	-	expression tag	UNP A0A140EMT3
J	680	GLY	-	expression tag	UNP A0A140EMT3
J	681	GLY	-	expression tag	UNP A0A140EMT3
J	682	GLY	-	expression tag	UNP A0A140EMT3
J	683	SER	-	expression tag	UNP A0A140EMT3
J	684	GLY	-	expression tag	UNP A0A140EMT3
J	685	GLY	-	expression tag	UNP A0A140EMT3
J	686	SER	-	expression tag	UNP A0A140EMT3
J	687	ALA	-	expression tag	UNP A0A140EMT3
J	688	TRP	-	expression tag	UNP A0A140EMT3
J	689	SER	-	expression tag	UNP A0A140EMT3
J	690	HIS	-	expression tag	UNP A0A140EMT3
J	691	PRO	-	expression tag	UNP A0A140EMT3
J	692	GLN	-	expression tag	UNP A0A140EMT3
J	693	PHE	-	expression tag	UNP A0A140EMT3
J	694	GLU	-	expression tag	UNP A0A140EMT3
J	695	LYS	-	expression tag	UNP A0A140EMT3

- Molecule 3 is a protein called 8ANC195 G52K5 heavy chain, IG gamma-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	130	Total	C	N	O	S	0	0
			976	619	167	187	3		
3	G	130	Total	C	N	O	S	0	0
			976	619	167	187	3		
3	K	130	Total	C	N	O	S	0	0
			976	619	167	187	3		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	221	HIS	-	expression tag	UNP S6B2A6
C	222	HIS	-	expression tag	UNP S6B2A6
C	223	HIS	-	expression tag	UNP S6B2A6
C	224	HIS	-	expression tag	UNP S6B2A6

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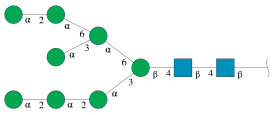
Chain	Residue	Modelled	Actual	Comment	Reference
C	225	HIS	-	expression tag	UNP S6B2A6
G	221	HIS	-	expression tag	UNP S6B2A6
G	222	HIS	-	expression tag	UNP S6B2A6
G	223	HIS	-	expression tag	UNP S6B2A6
G	224	HIS	-	expression tag	UNP S6B2A6
G	225	HIS	-	expression tag	UNP S6B2A6
K	221	HIS	-	expression tag	UNP S6B2A6
K	222	HIS	-	expression tag	UNP S6B2A6
K	223	HIS	-	expression tag	UNP S6B2A6
K	224	HIS	-	expression tag	UNP S6B2A6
K	225	HIS	-	expression tag	UNP S6B2A6

- Molecule 4 is a protein called 8ANC195 G52K5 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	108	Total	C	N	O	S	0	0
			793	500	139	151	3		
4	H	108	Total	C	N	O	S	0	0
			793	500	139	151	3		
4	L	108	Total	C	N	O	S	0	0
			793	500	139	151	3		

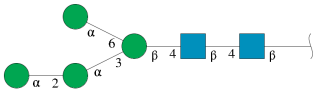
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	10	Total	C	N	O	0	0
			116	64	2	50		
5	X	10	Total	C	N	O	0	0
			116	64	2	50		
5	i	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 6 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				AltConf	Trace
6	N	6	Total	C	N	O	0	0
			72	40	2	30		
6	Y	6	Total	C	N	O	0	0
			72	40	2	30		
6	j	6	Total	C	N	O	0	0
			72	40	2	30		

- 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	O	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	Q	2	Total	C	N	O	0	0
			28	16	2	10		
7	R	2	Total	C	N	O	0	0
			28	16	2	10		
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	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	a	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		
7	c	2	Total	C	N	O	0	0
			28	16	2	10		

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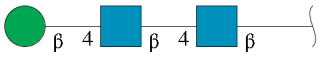
Mol	Chain	Residues	Atoms				AltConf	Trace
7	d	2	Total	C	N	O	0	0
			28	16	2	10		
7	e	2	Total	C	N	O	0	0
			28	16	2	10		
7	f	2	Total	C	N	O	0	0
			28	16	2	10		
7	k	2	Total	C	N	O	0	0
			28	16	2	10		
7	l	2	Total	C	N	O	0	0
			28	16	2	10		
7	m	2	Total	C	N	O	0	0
			28	16	2	10		
7	n	2	Total	C	N	O	0	0
			28	16	2	10		
7	o	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	q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 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.

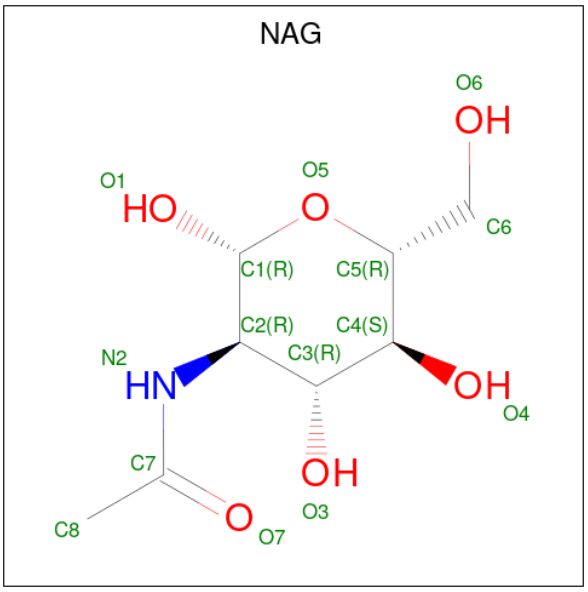


Mol	Chain	Residues	Atoms				AltConf	Trace
8	V	3	Total	C	N	O	0	0
			39	22	2	15		
8	g	3	Total	C	N	O	0	0
			39	22	2	15		
8	r	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 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	AltConf	Trace
9	W	4	Total C N O 50 28 2 20	0	0
9	h	4	Total C N O 50 28 2 20	0	0
9	s	4	Total C N O 50 28 2 20	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C N O 14 8 1 5	0
10	A	1	Total C N O 14 8 1 5	0
10	A	1	Total C N O 14 8 1 5	0
10	A	1	Total C N O 14 8 1 5	0
10	A	1	Total C N O 14 8 1 5	0
10	A	1	Total C N O 14 8 1 5	0

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Mol	Chain	Residues	Atoms				AltConf
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	F	1	Total	C	N	O	0
			14	8	1	5	
10	F	1	Total	C	N	O	0
			14	8	1	5	
10	F	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	I	1	Total	C	N	O	0
			14	8	1	5	
10	I	1	Total	C	N	O	0
			14	8	1	5	
10	I	1	Total	C	N	O	0
			14	8	1	5	
10	I	1	Total	C	N	O	0
			14	8	1	5	
10	I	1	Total	C	N	O	0
			14	8	1	5	
10	I	1	Total	C	N	O	0
			14	8	1	5	
10	J	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

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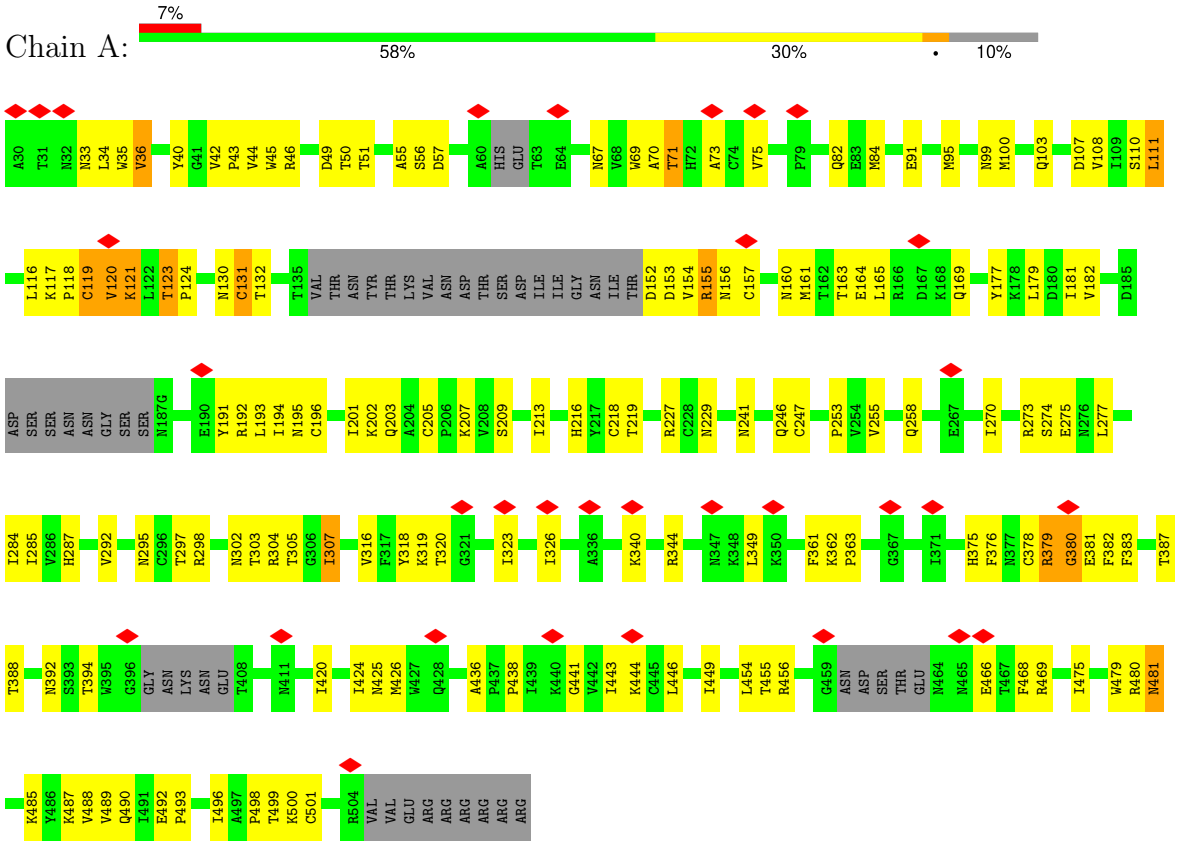
Mol	Chain	Residues	Atoms				AltConf
10	J	1	Total	C	N	O	0
			14	8	1	5	
10	J	1	Total	C	N	O	0
			14	8	1	5	
10	K	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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

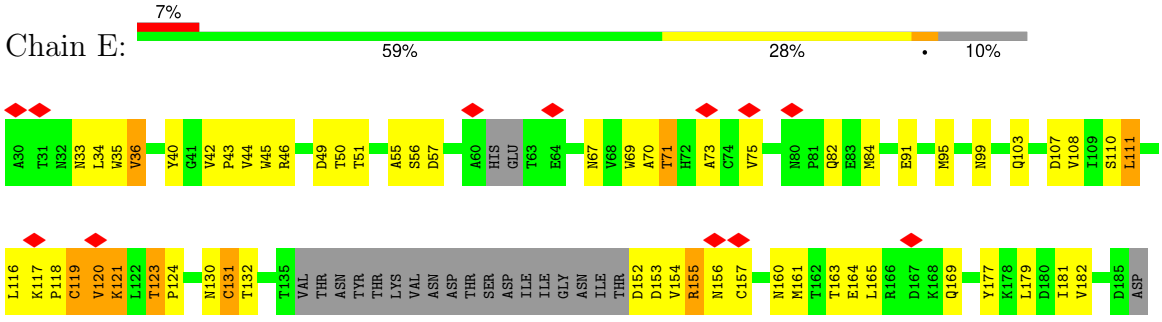
• Molecule 1: T/F100 Env gp120

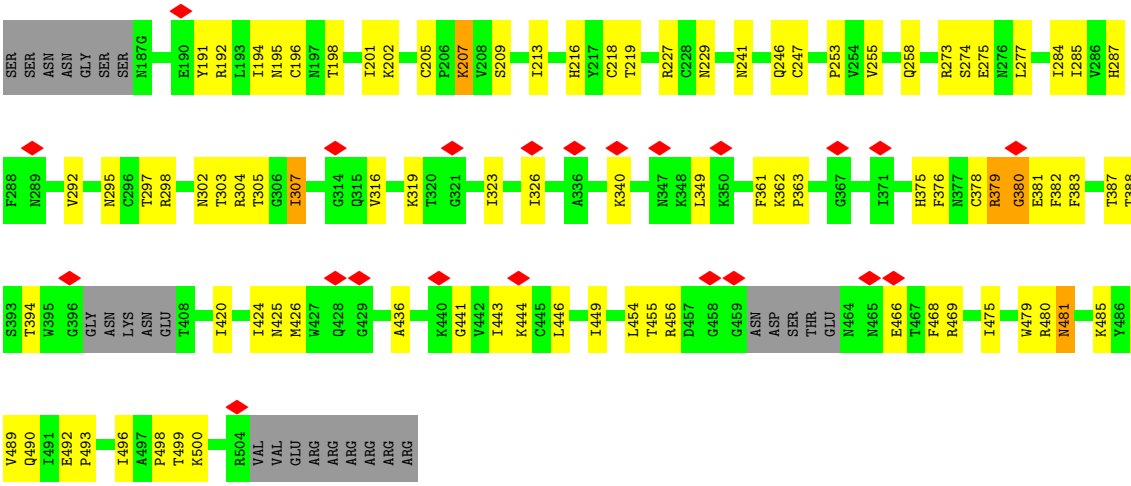
Chain A:



• Molecule 1: T/F100 Env gp120

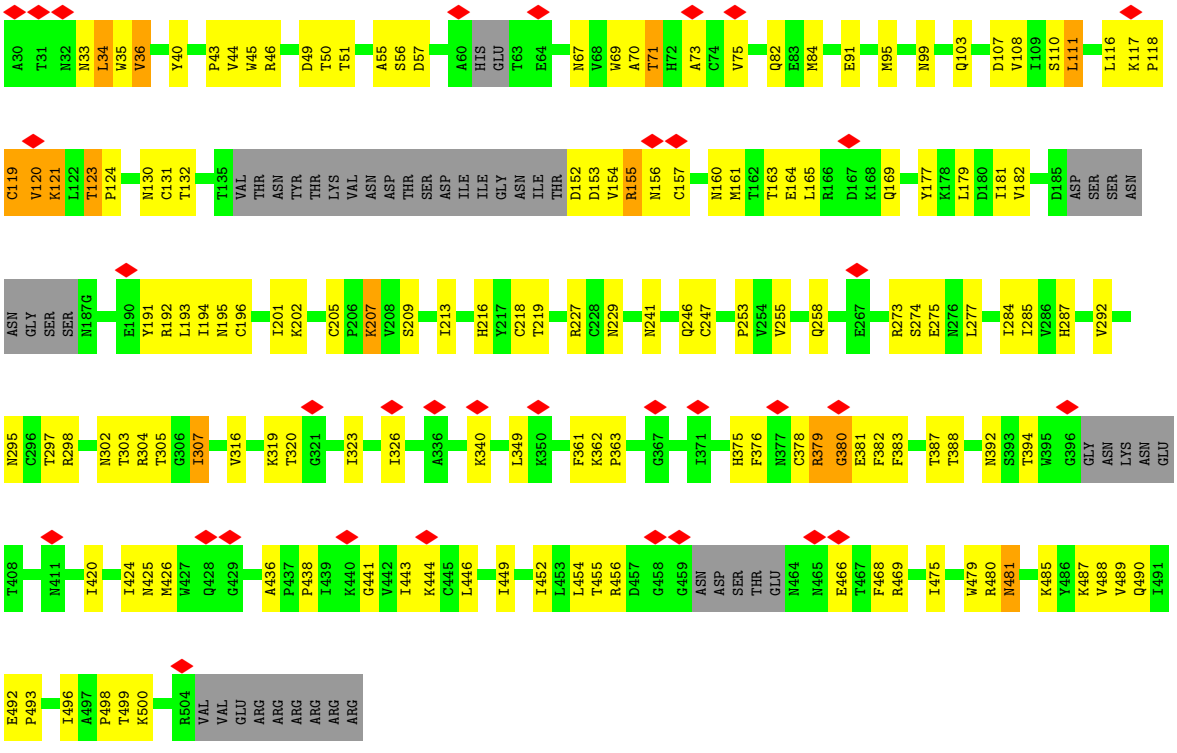
Chain E:





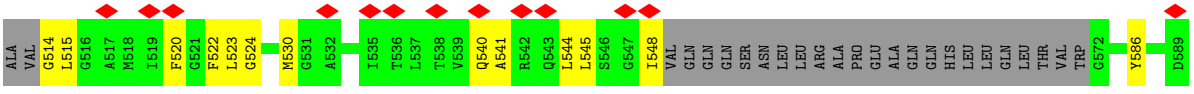
• Molecule 1: T/F100 Env gp120

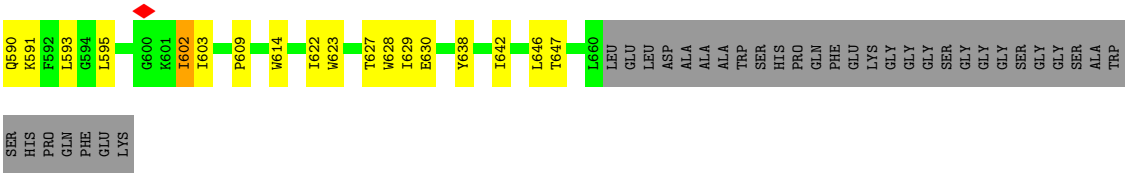
Chain I:



• Molecule 2: T/F100 Env gp41

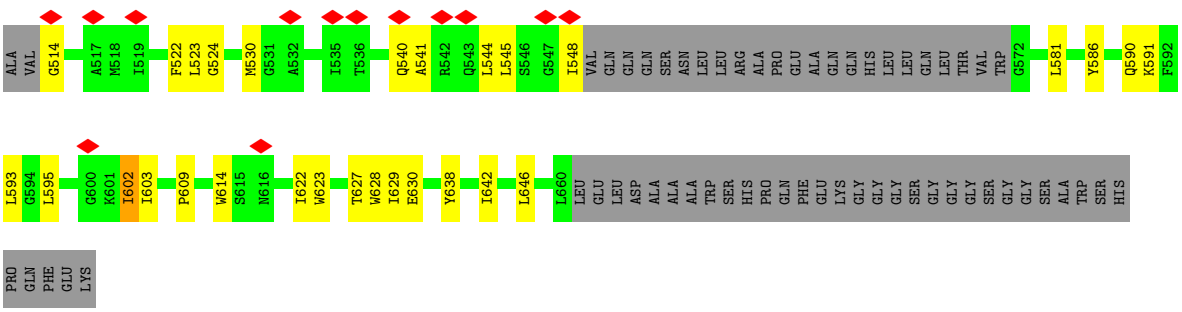
Chain B:





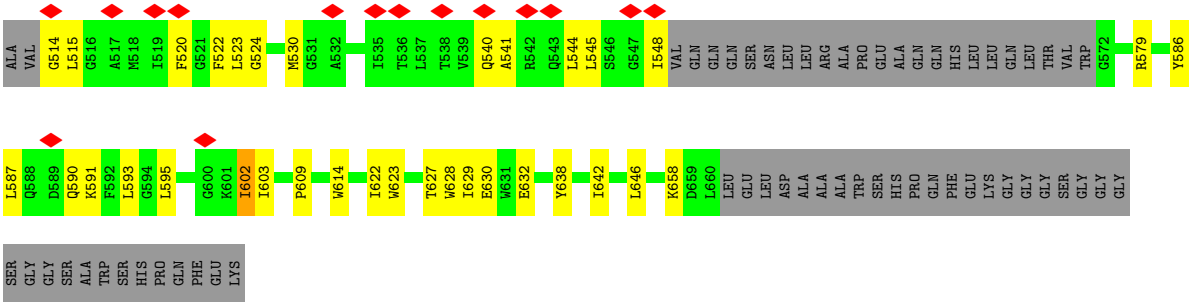
• Molecule 2: T/F100 Env gp41

Chain F:



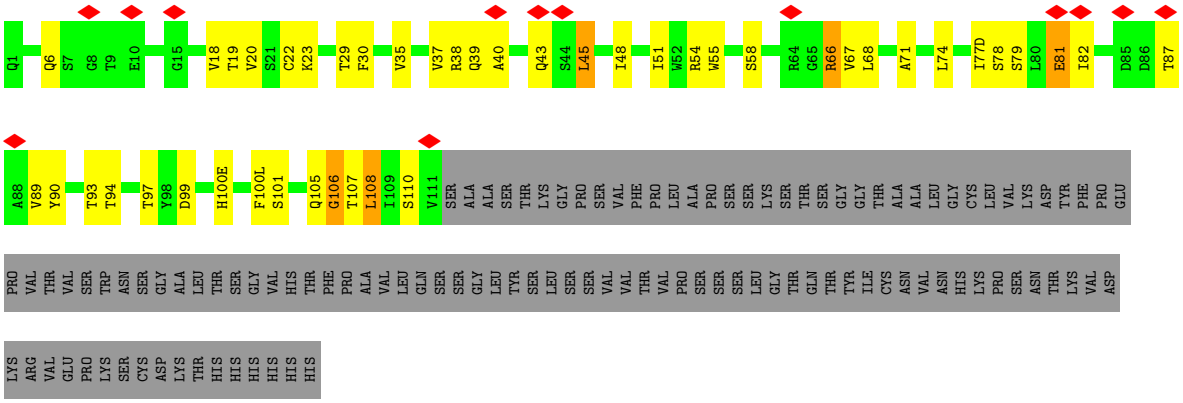
• Molecule 2: T/F100 Env gp41

Chain J:



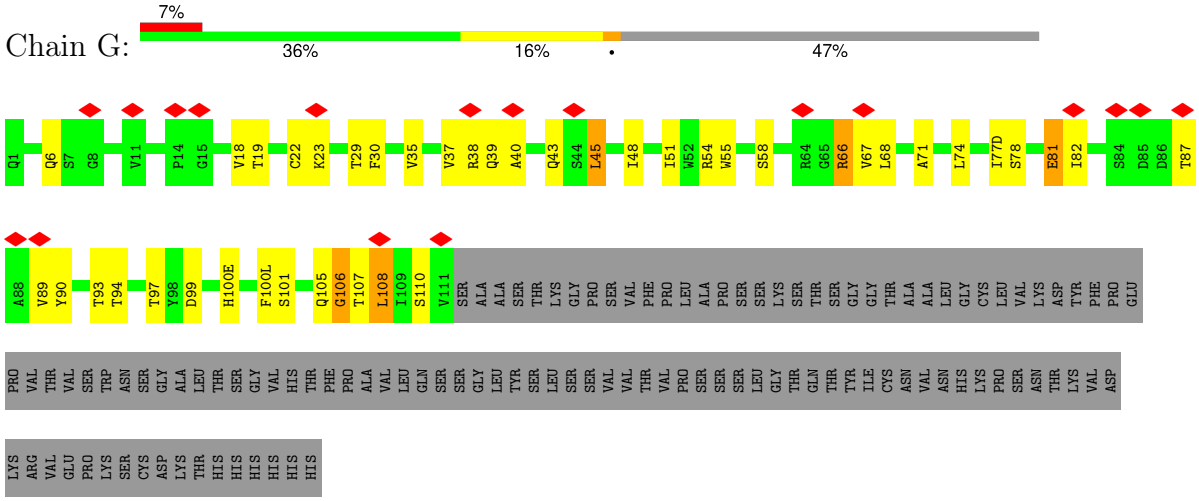
• Molecule 3: 8ANC195 G52K5 heavy chain, IG gamma-1 chain

Chain C:



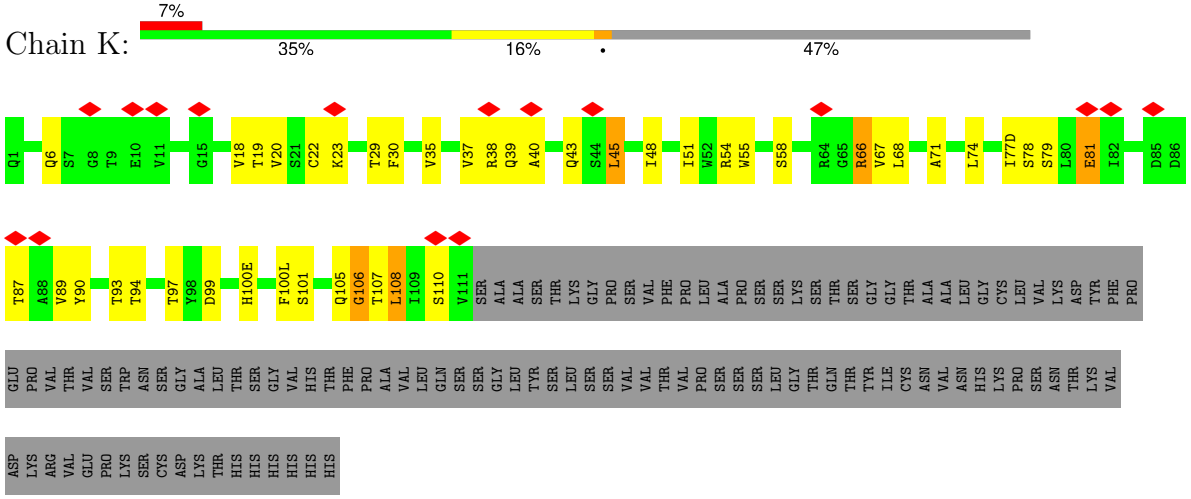
• Molecule 3: 8ANC195 G52K5 heavy chain, IG gamma-1 chain

Chain G:



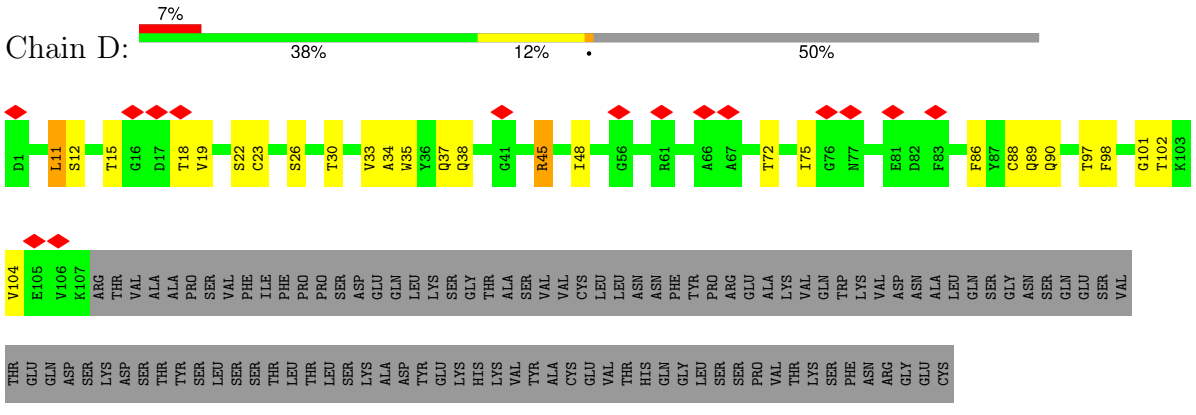
• Molecule 3: 8ANC195 G52K5 heavy chain, IG gamma-1 chain

Chain K:



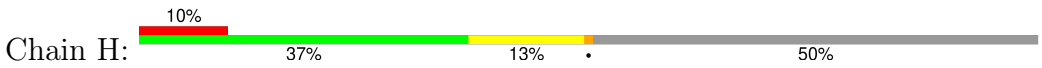
• Molecule 4: 8ANC195 G52K5 light chain

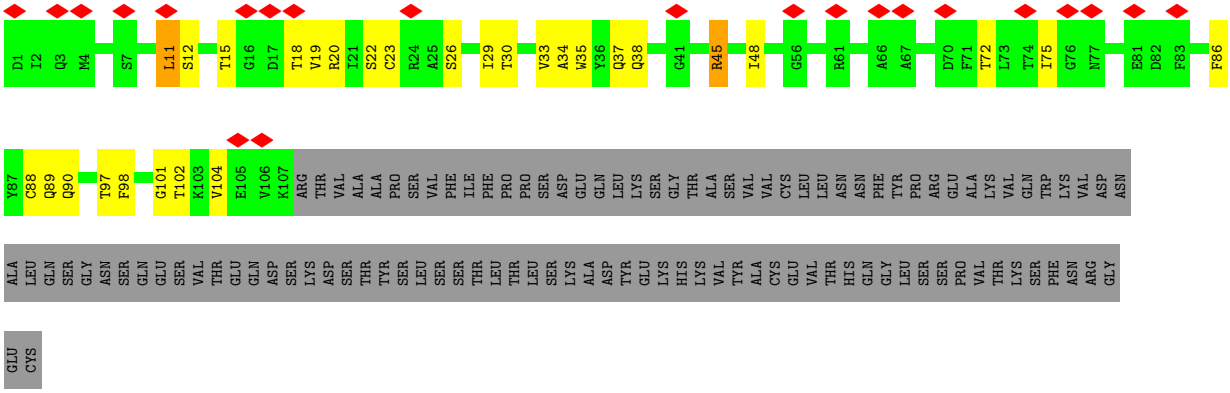
Chain D:



• Molecule 4: 8ANC195 G52K5 light chain

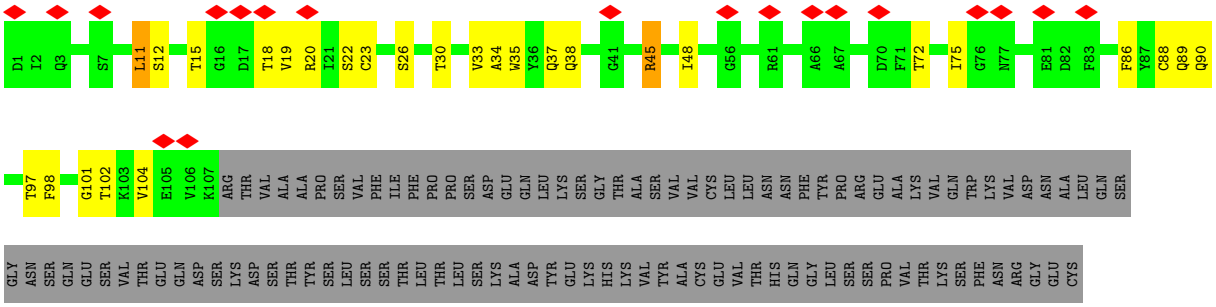
Chain H:





• Molecule 4: 8ANC195 G52K5 light chain

Chain L:



• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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

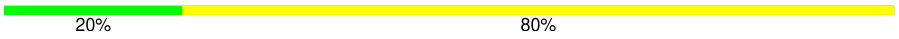
Chain M:

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

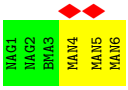
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



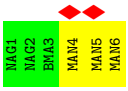
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



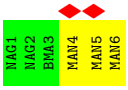
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



• Molecule 6: 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 j:



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

Chain O:

• 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

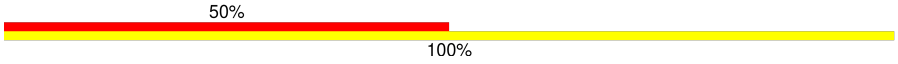
Chain Q:

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

Chain R:

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

Chain S:

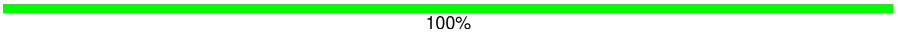


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

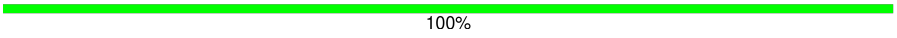
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



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

Chain Z:



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

Chain a:

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

Chain b:

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

Chain c:

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

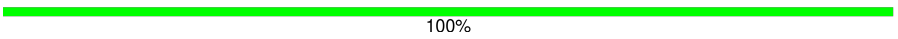
Chain d:

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

Chain e:

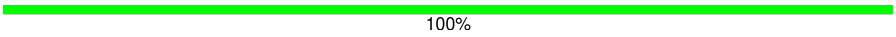
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



• 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 l:

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

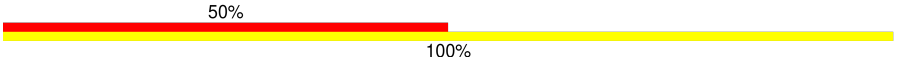
Chain m:

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

Chain n:

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

Chain o:

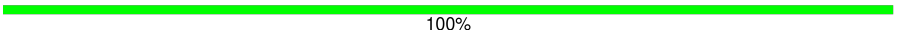


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

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

Chain q:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:

• Molecule 9: 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 9: 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 h:

• Molecule 9: 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:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170716	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 ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.052	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	300.0, 300.0, 300.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.57	0/3473	0.71	2/4720 (0.0%)
1	E	0.57	0/3473	0.71	2/4720 (0.0%)
1	I	0.57	0/3473	0.71	1/4720 (0.0%)
2	B	0.62	0/961	0.80	0/1304
2	F	0.62	0/961	0.80	0/1304
2	J	0.62	0/961	0.80	0/1304
3	C	0.54	0/1003	0.67	0/1372
3	G	0.54	0/1003	0.67	0/1372
3	K	0.54	0/1003	0.67	0/1372
4	D	0.49	0/811	0.70	0/1106
4	H	0.48	0/811	0.70	0/1106
4	L	0.48	0/811	0.70	0/1106
All	All	0.56	0/18744	0.72	5/25506 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	CYS	CA-CB-SG	5.97	124.74	114.00
1	E	205	CYS	CA-CB-SG	5.97	124.74	114.00
1	I	205	CYS	CA-CB-SG	5.97	124.74	114.00
1	A	131	CYS	CA-CB-SG	5.01	123.03	114.00
1	E	131	CYS	CA-CB-SG	5.01	123.02	114.00

There are no chirality outliers.

There are no planarity outliers.

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	3399	0	3303	113	0
1	E	3399	0	3303	107	0
1	I	3399	0	3303	108	0
2	B	944	0	894	40	0
2	F	944	0	894	41	0
2	J	944	0	894	42	0
3	C	976	0	914	40	0
3	G	976	0	914	39	0
3	K	976	0	914	37	0
4	D	793	0	748	28	0
4	H	793	0	748	31	0
4	L	793	0	748	28	0
5	M	116	0	97	0	0
5	X	116	0	97	0	0
5	i	116	0	97	0	0
6	N	72	0	61	0	0
6	Y	72	0	61	0	0
6	j	72	0	61	0	0
7	O	28	0	25	0	0
7	P	28	0	25	2	0
7	Q	28	0	25	0	0
7	R	28	0	25	0	0
7	S	28	0	25	0	0
7	T	28	0	25	0	0
7	U	28	0	25	0	0
7	Z	28	0	25	0	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
7	d	28	0	25	0	0
7	e	28	0	25	0	0
7	f	28	0	25	0	0
7	k	28	0	25	0	0
7	l	28	0	25	0	0
7	m	28	0	25	0	0
7	n	28	0	25	0	0
7	o	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	p	28	0	25	0	0
7	q	28	0	25	0	0
8	V	39	0	34	0	0
8	g	39	0	34	0	0
8	r	39	0	34	0	0
9	W	50	0	43	0	0
9	h	50	0	43	0	0
9	s	50	0	43	0	0
10	A	84	0	78	0	0
10	B	42	0	39	0	0
10	C	14	0	13	0	0
10	E	84	0	78	0	0
10	F	42	0	39	0	0
10	G	14	0	13	0	0
10	I	84	0	78	0	0
10	J	42	0	39	0	0
10	K	14	0	13	0	0
All	All	20175	0	19197	568	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 15.

The worst 5 of 568 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:C:45:LEU:HD11	4:D:98:PHE:CE2	1.57	1.40
3:K:45:LEU:HD11	4:L:98:PHE:CE2	1.57	1.39
3:G:45:LEU:HD11	4:H:98:PHE:CE2	1.57	1.36
2:B:541:ALA:HA	2:B:544:LEU:CD2	1.83	1.09
2:F:541:ALA:HA	2:F:544:LEU:CD2	1.83	1.08

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 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	A	427/486 (88%)	368 (86%)	54 (13%)	5 (1%)	11	43
1	E	427/486 (88%)	368 (86%)	54 (13%)	5 (1%)	11	43
1	I	427/486 (88%)	368 (86%)	54 (13%)	5 (1%)	11	43
2	B	120/184 (65%)	112 (93%)	8 (7%)	0	100	100
2	F	120/184 (65%)	112 (93%)	8 (7%)	0	100	100
2	J	120/184 (65%)	112 (93%)	8 (7%)	0	100	100
3	C	128/244 (52%)	114 (89%)	13 (10%)	1 (1%)	16	51
3	G	128/244 (52%)	114 (89%)	13 (10%)	1 (1%)	16	51
3	K	128/244 (52%)	114 (89%)	13 (10%)	1 (1%)	16	51
4	D	106/215 (49%)	96 (91%)	10 (9%)	0	100	100
4	H	106/215 (49%)	96 (91%)	10 (9%)	0	100	100
4	L	106/215 (49%)	96 (91%)	10 (9%)	0	100	100
All	All	2343/3387 (69%)	2070 (88%)	255 (11%)	18 (1%)	19	51

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	LYS
1	A	155	ARG
1	A	380	GLY
1	E	121	LYS
1	E	155	ARG

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	A	376/434 (87%)	346 (92%)	30 (8%)	10	33
1	E	376/434 (87%)	346 (92%)	30 (8%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	376/434 (87%)	346 (92%)	30 (8%)	10	33
2	B	96/149 (64%)	93 (97%)	3 (3%)	35	56
2	F	96/149 (64%)	93 (97%)	3 (3%)	35	56
2	J	96/149 (64%)	93 (97%)	3 (3%)	35	56
3	C	104/210 (50%)	95 (91%)	9 (9%)	8	30
3	G	104/210 (50%)	95 (91%)	9 (9%)	8	30
3	K	104/210 (50%)	95 (91%)	9 (9%)	8	30
4	D	78/182 (43%)	69 (88%)	9 (12%)	4	20
4	H	78/182 (43%)	69 (88%)	9 (12%)	4	20
4	L	78/182 (43%)	69 (88%)	9 (12%)	4	20
All	All	1962/2925 (67%)	1809 (92%)	153 (8%)	13	33

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	218	CYS
3	K	108	LEU
1	I	304	ARG
1	I	489	VAL
4	L	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	354	ASN
2	J	590	GLN
1	E	481	ASN
4	L	90	GLN
1	I	375	HIS

5.3.3 RNA

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)

111 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	M	1	5,1	14,14,15	0.22	0	17,19,21	0.54	0
5	MAN	M	10	5	11,11,12	1.10	1 (9%)	15,15,17	1.04	1 (6%)
5	NAG	M	2	5	14,14,15	0.31	0	17,19,21	1.03	1 (5%)
5	BMA	M	3	5	11,11,12	1.05	1 (9%)	15,15,17	0.88	1 (6%)
5	MAN	M	4	5	11,11,12	0.83	0	15,15,17	0.88	0
5	MAN	M	5	5	11,11,12	0.78	0	15,15,17	1.59	2 (13%)
5	MAN	M	6	5	11,11,12	0.71	0	15,15,17	1.40	1 (6%)
5	MAN	M	7	5	11,11,12	0.86	1 (9%)	15,15,17	1.35	2 (13%)
5	MAN	M	8	5	11,11,12	0.75	0	15,15,17	1.02	2 (13%)
5	MAN	M	9	5	11,11,12	0.58	0	15,15,17	1.24	2 (13%)
6	NAG	N	1	6,1	14,14,15	0.43	0	17,19,21	0.45	0
6	NAG	N	2	6	14,14,15	0.42	0	17,19,21	0.56	0
6	BMA	N	3	6	11,11,12	0.63	0	15,15,17	0.78	0
6	MAN	N	4	6	11,11,12	1.05	1 (9%)	15,15,17	0.97	1 (6%)
6	MAN	N	5	6	11,11,12	1.23	2 (18%)	15,15,17	1.32	2 (13%)
6	MAN	N	6	6	11,11,12	0.77	0	15,15,17	1.01	1 (6%)
7	NAG	O	1	7,1	14,14,15	0.43	0	17,19,21	0.51	0
7	NAG	O	2	7	14,14,15	0.24	0	17,19,21	0.52	0
7	NAG	P	1	7,1	14,14,15	0.73	1 (7%)	17,19,21	0.80	0
7	NAG	P	2	7	14,14,15	0.24	0	17,19,21	0.60	0
7	NAG	Q	1	7,1	14,14,15	0.60	0	17,19,21	0.72	0
7	NAG	Q	2	7	14,14,15	0.38	0	17,19,21	1.05	1 (5%)
7	NAG	R	1	7,1	14,14,15	0.38	0	17,19,21	1.34	3 (17%)
7	NAG	R	2	7	14,14,15	0.27	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	S	1	7,1	14,14,15	1.13	1 (7%)	17,19,21	2.31	2 (11%)
7	NAG	S	2	7	14,14,15	0.44	0	17,19,21	1.07	2 (11%)
7	NAG	T	1	7,1	14,14,15	1.13	1 (7%)	17,19,21	0.99	1 (5%)
7	NAG	T	2	7	14,14,15	0.34	0	17,19,21	0.55	0
7	NAG	U	1	7,1	14,14,15	0.48	0	17,19,21	0.61	0
7	NAG	U	2	7	14,14,15	0.32	0	17,19,21	0.45	0
8	NAG	V	1	8,1	14,14,15	0.53	0	17,19,21	0.49	0
8	NAG	V	2	8	14,14,15	0.35	0	17,19,21	0.54	0
8	BMA	V	3	8	11,11,12	0.89	0	15,15,17	0.88	1 (6%)
9	NAG	W	1	2,9	14,14,15	0.62	0	17,19,21	0.83	1 (5%)
9	NAG	W	2	9	14,14,15	0.24	0	17,19,21	0.64	0
9	BMA	W	3	9	11,11,12	0.81	0	15,15,17	0.77	0
9	MAN	W	4	9	11,11,12	0.65	0	15,15,17	1.05	2 (13%)
5	NAG	X	1	5,1	14,14,15	0.22	0	17,19,21	0.54	0
5	MAN	X	10	5	11,11,12	1.10	1 (9%)	15,15,17	1.04	1 (6%)
5	NAG	X	2	5	14,14,15	0.31	0	17,19,21	1.04	1 (5%)
5	BMA	X	3	5	11,11,12	1.06	1 (9%)	15,15,17	0.88	1 (6%)
5	MAN	X	4	5	11,11,12	0.83	0	15,15,17	0.88	0
5	MAN	X	5	5	11,11,12	0.78	0	15,15,17	1.58	2 (13%)
5	MAN	X	6	5	11,11,12	0.71	0	15,15,17	1.40	1 (6%)
5	MAN	X	7	5	11,11,12	0.86	1 (9%)	15,15,17	1.36	2 (13%)
5	MAN	X	8	5	11,11,12	0.76	0	15,15,17	1.01	2 (13%)
5	MAN	X	9	5	11,11,12	0.59	0	15,15,17	1.25	2 (13%)
6	NAG	Y	1	6,1	14,14,15	0.43	0	17,19,21	0.45	0
6	NAG	Y	2	6	14,14,15	0.43	0	17,19,21	0.57	0
6	BMA	Y	3	6	11,11,12	0.63	0	15,15,17	0.78	0
6	MAN	Y	4	6	11,11,12	1.06	1 (9%)	15,15,17	0.97	1 (6%)
6	MAN	Y	5	6	11,11,12	1.23	2 (18%)	15,15,17	1.32	2 (13%)
6	MAN	Y	6	6	11,11,12	0.77	0	15,15,17	1.01	1 (6%)
7	NAG	Z	1	7,1	14,14,15	0.43	0	17,19,21	0.52	0
7	NAG	Z	2	7	14,14,15	0.23	0	17,19,21	0.53	0
7	NAG	a	1	7,1	14,14,15	0.74	1 (7%)	17,19,21	0.81	0
7	NAG	a	2	7	14,14,15	0.24	0	17,19,21	0.60	0
7	NAG	b	1	7,1	14,14,15	0.60	0	17,19,21	0.72	0
7	NAG	b	2	7	14,14,15	0.38	0	17,19,21	1.04	1 (5%)
7	NAG	c	1	7,1	14,14,15	0.38	0	17,19,21	1.34	3 (17%)
7	NAG	c	2	7	14,14,15	0.27	0	17,19,21	0.55	0
7	NAG	d	1	7,1	14,14,15	1.12	1 (7%)	17,19,21	2.31	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	d	2	7	14,14,15	0.44	0	17,19,21	1.08	2 (11%)
7	NAG	e	1	7,1	14,14,15	1.13	1 (7%)	17,19,21	0.99	1 (5%)
7	NAG	e	2	7	14,14,15	0.34	0	17,19,21	0.55	0
7	NAG	f	1	7,1	14,14,15	0.48	0	17,19,21	0.62	0
7	NAG	f	2	7	14,14,15	0.33	0	17,19,21	0.46	0
8	NAG	g	1	8,1	14,14,15	0.53	0	17,19,21	0.50	0
8	NAG	g	2	8	14,14,15	0.35	0	17,19,21	0.54	0
8	BMA	g	3	8	11,11,12	0.90	0	15,15,17	0.87	1 (6%)
9	NAG	h	1	2,9	14,14,15	0.62	0	17,19,21	0.83	1 (5%)
9	NAG	h	2	9	14,14,15	0.24	0	17,19,21	0.64	0
9	BMA	h	3	9	11,11,12	0.82	0	15,15,17	0.77	0
9	MAN	h	4	9	11,11,12	0.66	0	15,15,17	1.05	2 (13%)
5	NAG	i	1	5,1	14,14,15	0.22	0	17,19,21	0.54	0
5	MAN	i	10	5	11,11,12	1.10	1 (9%)	15,15,17	1.05	1 (6%)
5	NAG	i	2	5	14,14,15	0.31	0	17,19,21	1.03	1 (5%)
5	BMA	i	3	5	11,11,12	1.06	1 (9%)	15,15,17	0.89	1 (6%)
5	MAN	i	4	5	11,11,12	0.84	0	15,15,17	0.87	0
5	MAN	i	5	5	11,11,12	0.78	0	15,15,17	1.58	2 (13%)
5	MAN	i	6	5	11,11,12	0.71	0	15,15,17	1.40	1 (6%)
5	MAN	i	7	5	11,11,12	0.86	1 (9%)	15,15,17	1.36	2 (13%)
5	MAN	i	8	5	11,11,12	0.75	0	15,15,17	1.02	2 (13%)
5	MAN	i	9	5	11,11,12	0.57	0	15,15,17	1.24	2 (13%)
6	NAG	j	1	6,1	14,14,15	0.43	0	17,19,21	0.44	0
6	NAG	j	2	6	14,14,15	0.43	0	17,19,21	0.57	0
6	BMA	j	3	6	11,11,12	0.64	0	15,15,17	0.79	0
6	MAN	j	4	6	11,11,12	1.04	1 (9%)	15,15,17	0.96	1 (6%)
6	MAN	j	5	6	11,11,12	1.23	2 (18%)	15,15,17	1.32	2 (13%)
6	MAN	j	6	6	11,11,12	0.77	0	15,15,17	1.01	1 (6%)
7	NAG	k	1	7,1	14,14,15	0.44	0	17,19,21	0.51	0
7	NAG	k	2	7	14,14,15	0.24	0	17,19,21	0.52	0
7	NAG	l	1	7,1	14,14,15	0.74	1 (7%)	17,19,21	0.80	0
7	NAG	l	2	7	14,14,15	0.24	0	17,19,21	0.59	0
7	NAG	m	1	7,1	14,14,15	0.61	0	17,19,21	0.72	0
7	NAG	m	2	7	14,14,15	0.39	0	17,19,21	1.04	1 (5%)
7	NAG	n	1	7,1	14,14,15	0.39	0	17,19,21	1.35	3 (17%)
7	NAG	n	2	7	14,14,15	0.26	0	17,19,21	0.55	0
7	NAG	o	1	7,1	14,14,15	1.14	1 (7%)	17,19,21	2.31	2 (11%)
7	NAG	o	2	7	14,14,15	0.44	0	17,19,21	1.07	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	p	1	7,1	14,14,15	1.12	1 (7%)	17,19,21	0.99	1 (5%)
7	NAG	p	2	7	14,14,15	0.33	0	17,19,21	0.55	0
7	NAG	q	1	7,1	14,14,15	0.49	0	17,19,21	0.61	0
7	NAG	q	2	7	14,14,15	0.32	0	17,19,21	0.46	0
8	NAG	r	1	8,1	14,14,15	0.54	0	17,19,21	0.50	0
8	NAG	r	2	8	14,14,15	0.34	0	17,19,21	0.54	0
8	BMA	r	3	8	11,11,12	0.88	0	15,15,17	0.88	1 (6%)
9	NAG	s	1	2,9	14,14,15	0.61	0	17,19,21	0.83	1 (5%)
9	NAG	s	2	9	14,14,15	0.24	0	17,19,21	0.64	0
9	BMA	s	3	9	11,11,12	0.81	0	15,15,17	0.77	0
9	MAN	s	4	9	11,11,12	0.65	0	15,15,17	1.05	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
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	MAN	M	10	5	-	0/2/19/22	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	2/2/19/22	0/1/1/1
5	MAN	M	5	5	-	2/2/19/22	0/1/1/1
5	MAN	M	6	5	-	0/2/19/22	0/1/1/1
5	MAN	M	7	5	-	0/2/19/22	0/1/1/1
5	MAN	M	8	5	-	2/2/19/22	0/1/1/1
5	MAN	M	9	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
6	MAN	N	5	6	-	0/2/19/22	0/1/1/1
6	MAN	N	6	6	-	2/2/19/22	0/1/1/1
7	NAG	O	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1
7	NAG	P	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	NAG	Q	1	7,1	-	2/6/23/26	0/1/1/1

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

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

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

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	1	NAG	O5-C1	3.98	1.50	1.43
7	S	1	NAG	O5-C1	3.95	1.50	1.43
7	d	1	NAG	O5-C1	3.92	1.50	1.43
7	T	1	NAG	O5-C1	-3.55	1.37	1.43
7	e	1	NAG	O5-C1	-3.54	1.37	1.43

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	o	1	NAG	C1-O5-C5	8.94	124.17	112.19
7	d	1	NAG	C1-O5-C5	8.92	124.14	112.19
7	S	1	NAG	C1-O5-C5	8.91	124.13	112.19
5	M	5	MAN	C1-O5-C5	4.76	118.56	112.19
5	X	5	MAN	C1-O5-C5	4.75	118.55	112.19

There are no chirality outliers.

5 of 153 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	S	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	d	1	NAG	O5-C5-C6-O6
7	o	1	NAG	O5-C5-C6-O6
7	T	1	NAG	C4-C5-C6-O6
7	p	1	NAG	C4-C5-C6-O6

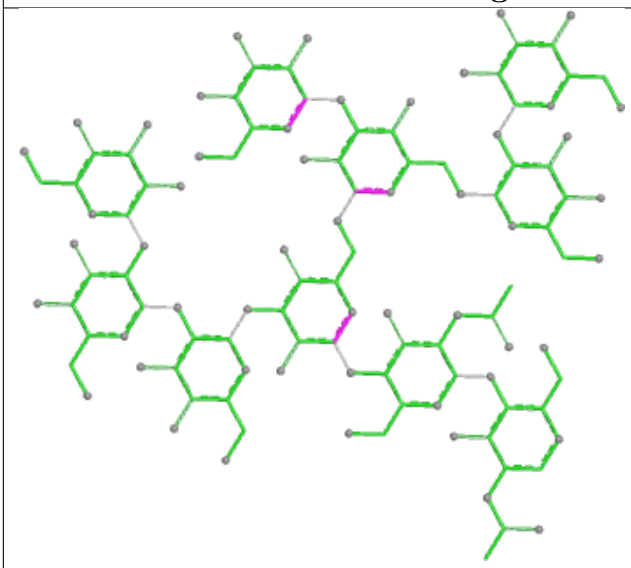
There are no ring outliers.

1 monomer is involved in 2 short contacts:

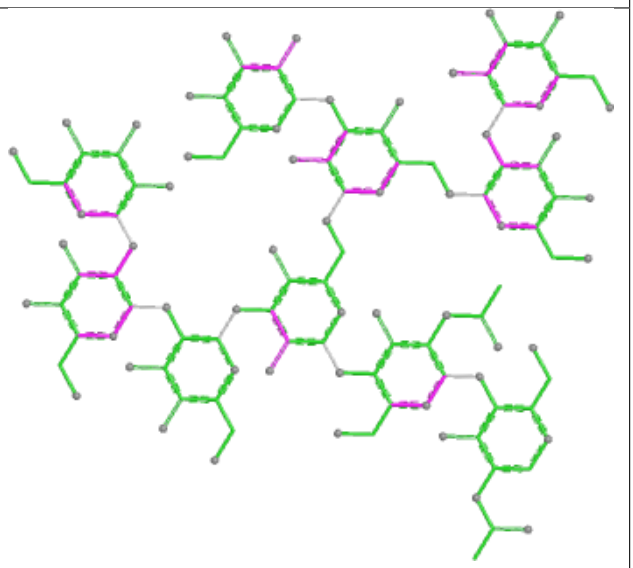
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	1	NAG	2	0

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

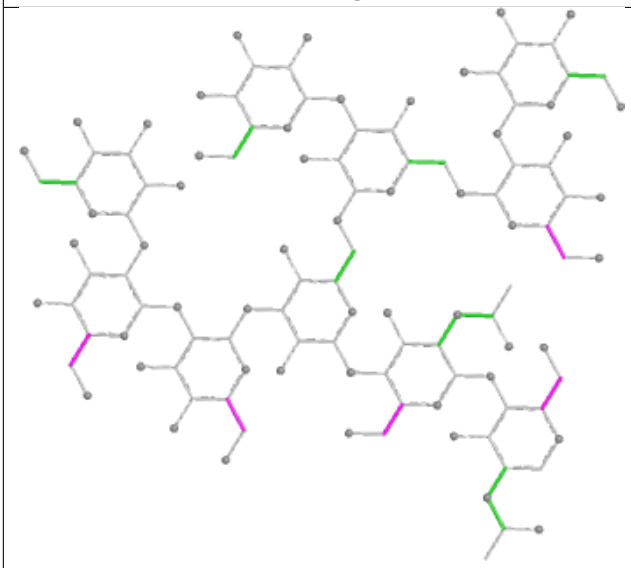
Oligosaccharide Chain M



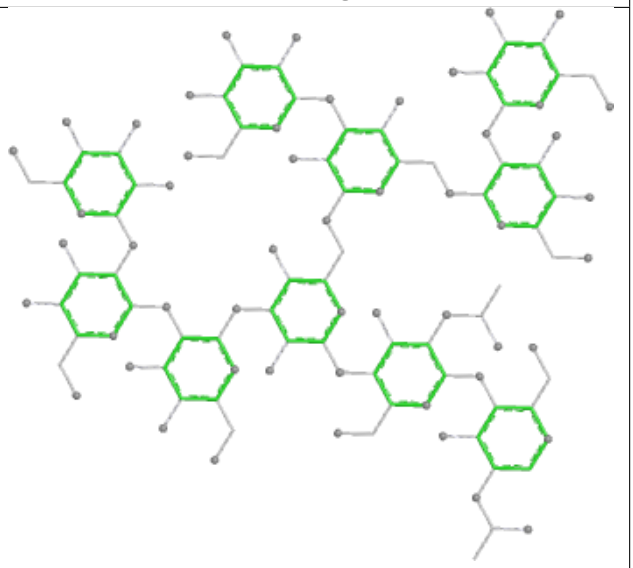
Bond lengths



Bond angles

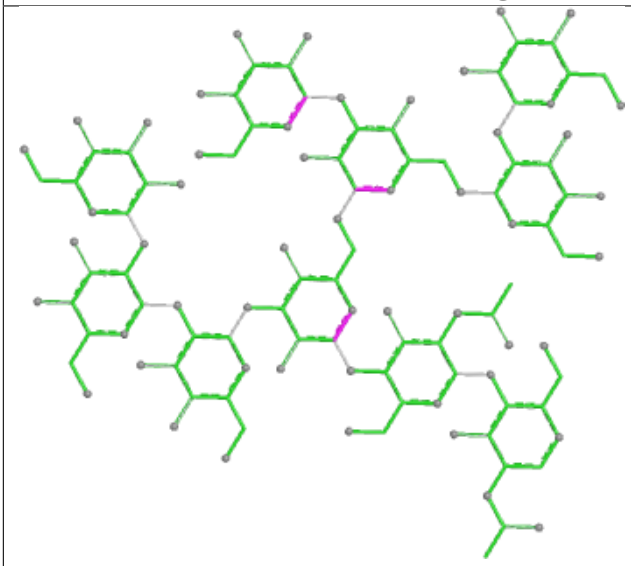


Torsions

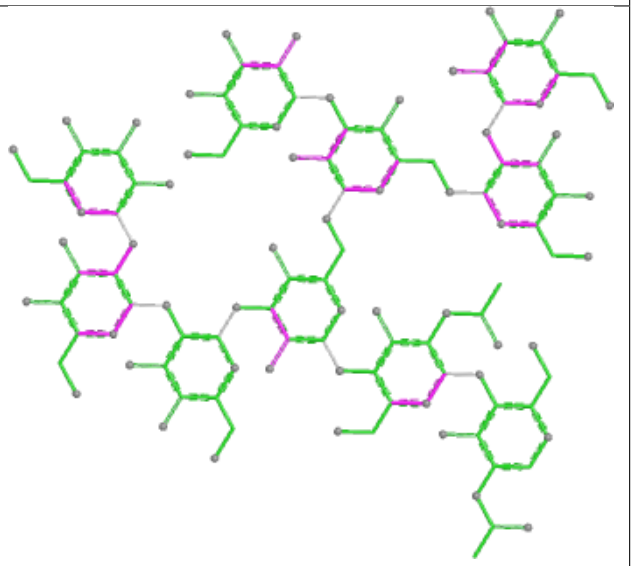


Rings

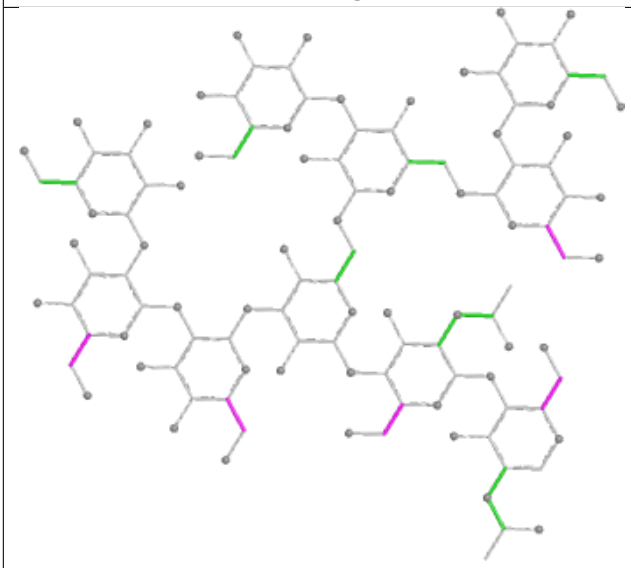
Oligosaccharide Chain X



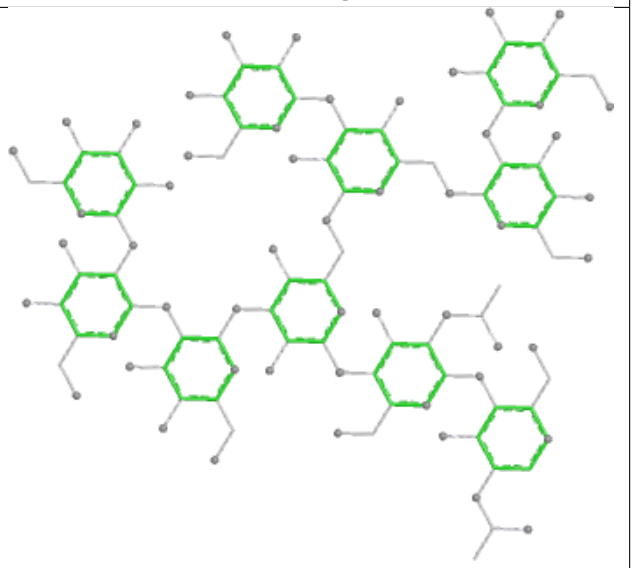
Bond lengths



Bond angles

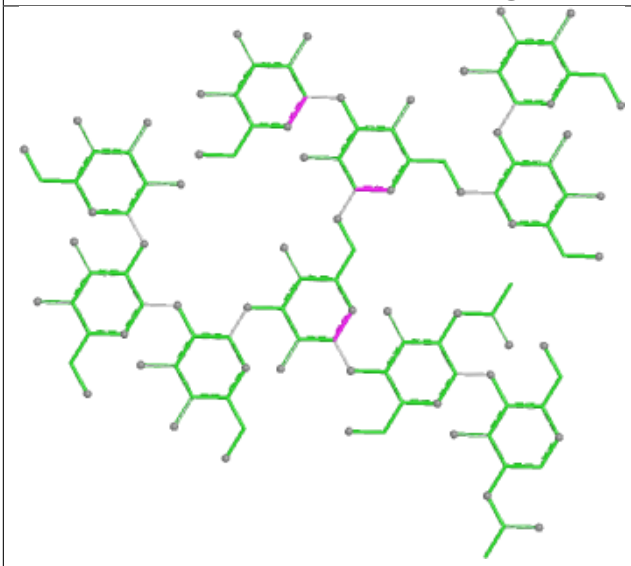


Torsions

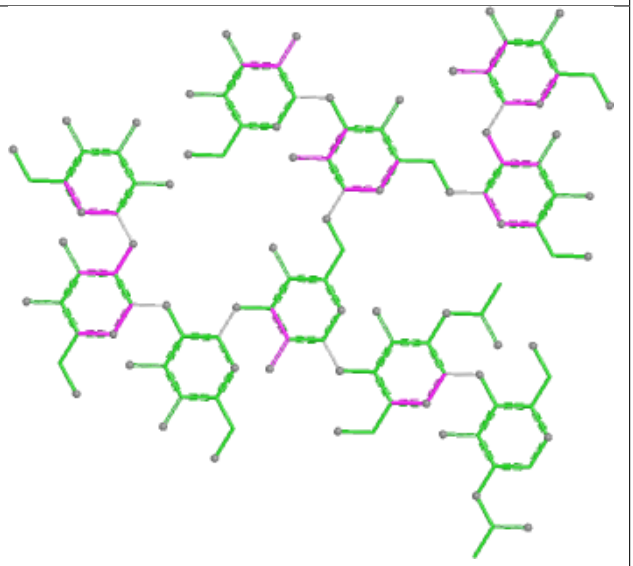


Rings

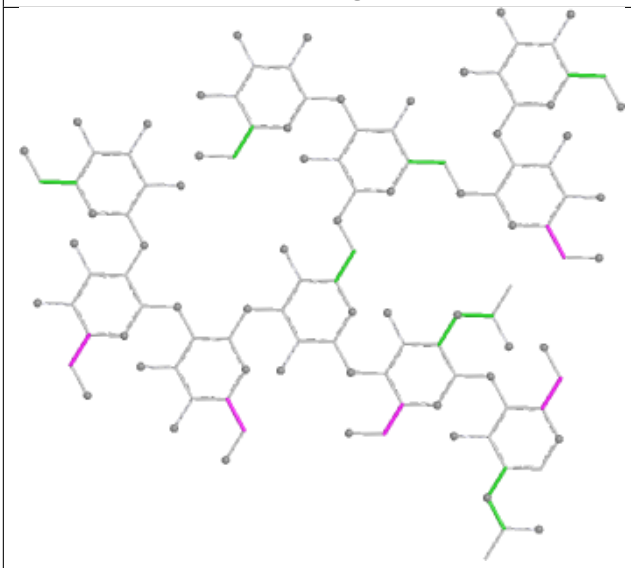
Oligosaccharide Chain i



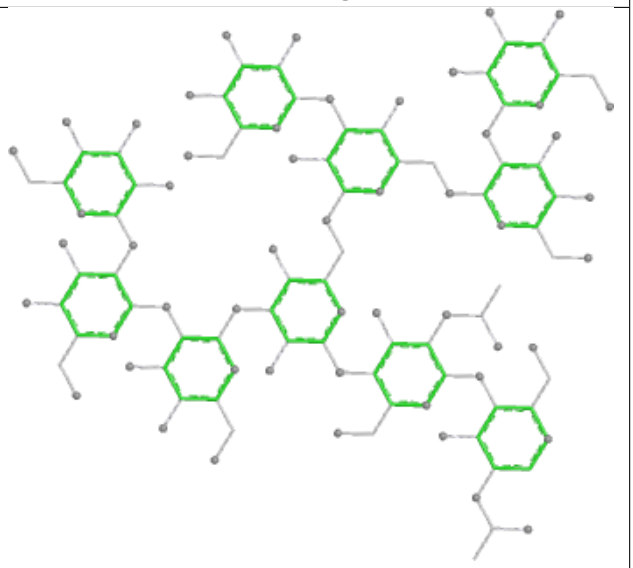
Bond lengths



Bond angles

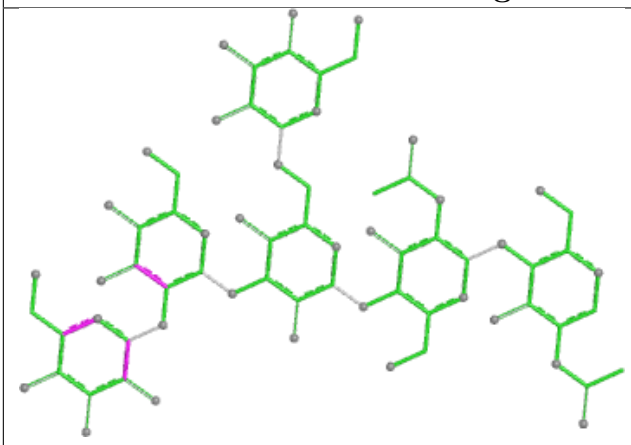


Torsions

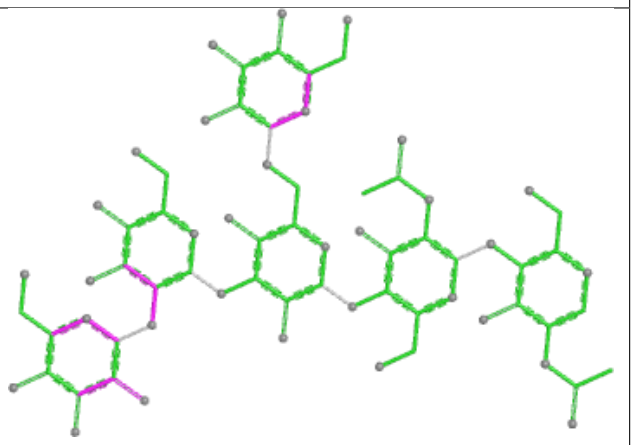


Rings

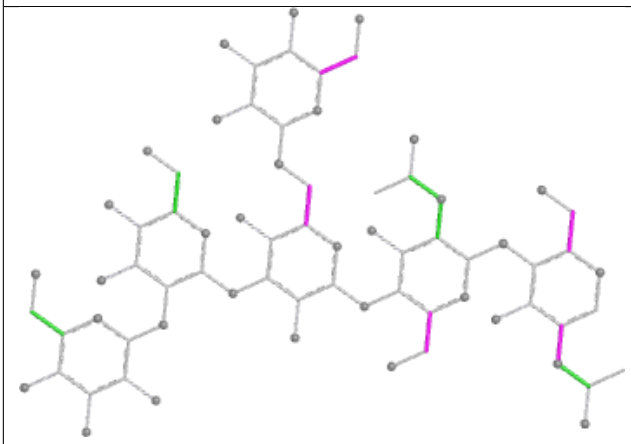
Oligosaccharide Chain N



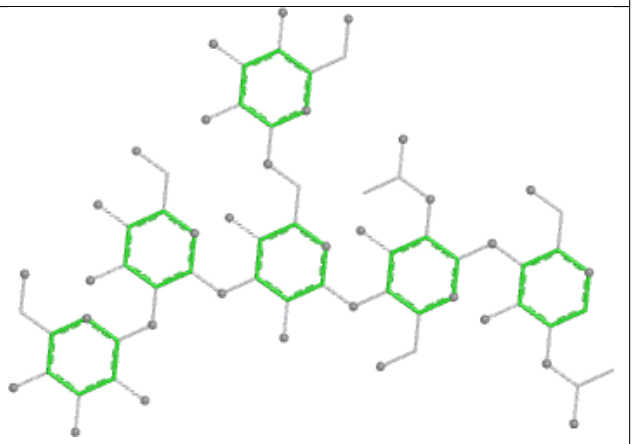
Bond lengths



Bond angles

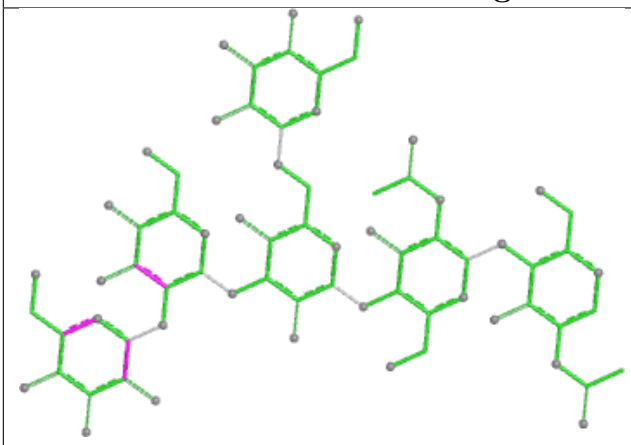


Torsions

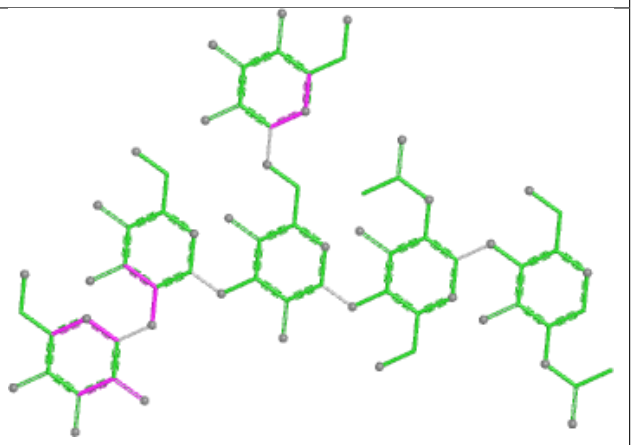


Rings

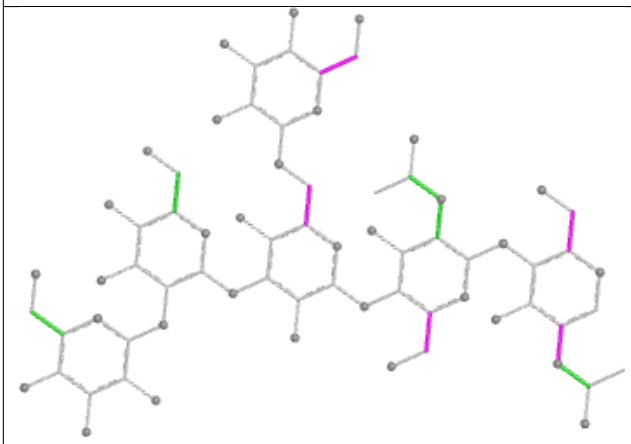
Oligosaccharide Chain Y



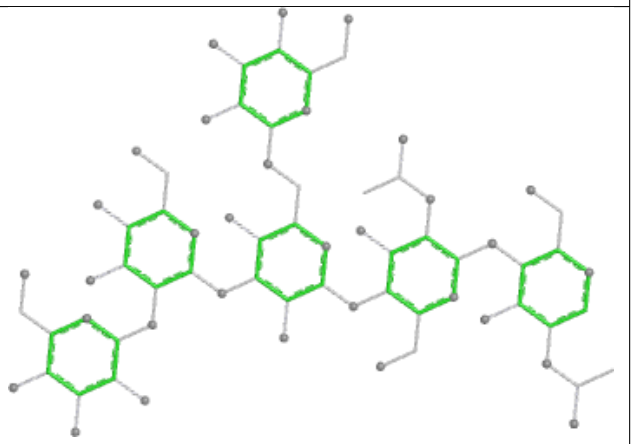
Bond lengths



Bond angles

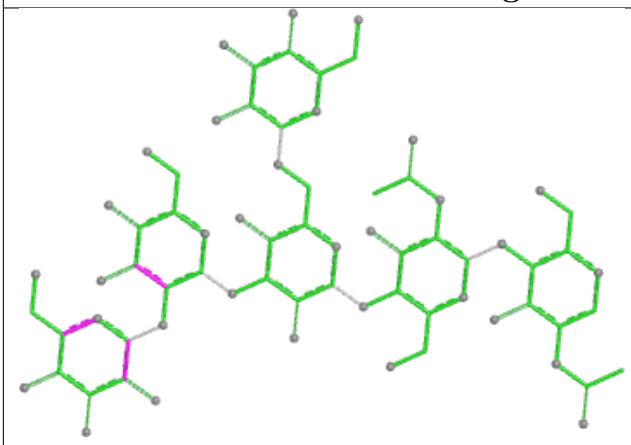


Torsions

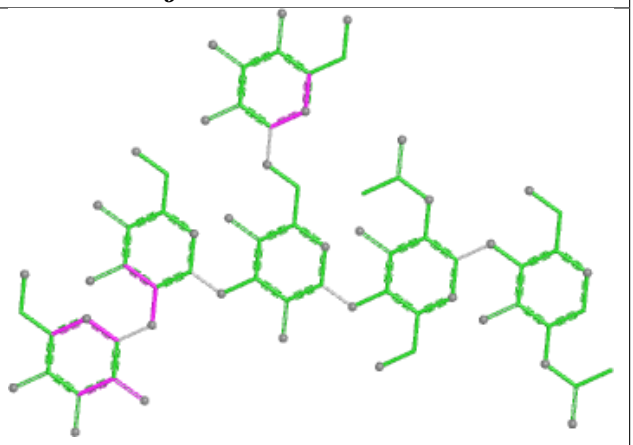


Rings

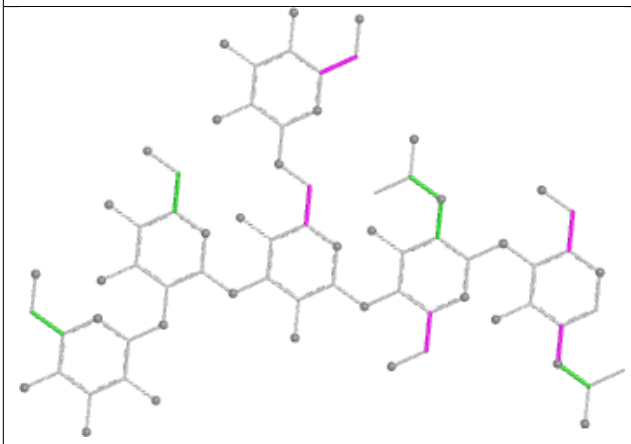
Oligosaccharide Chain j



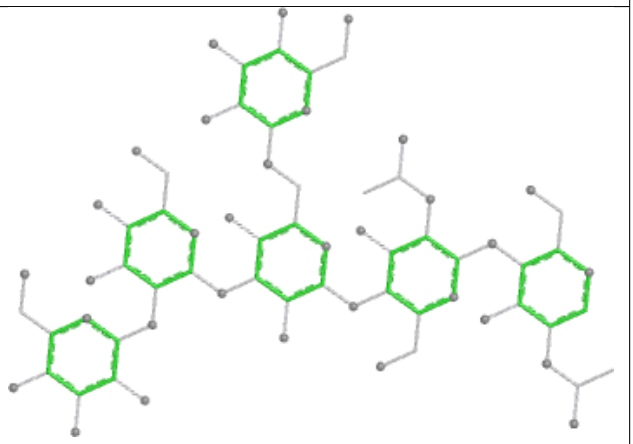
Bond lengths



Bond angles

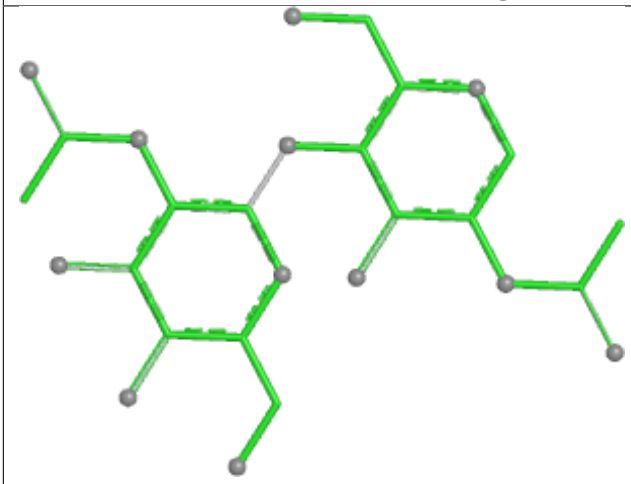


Torsions

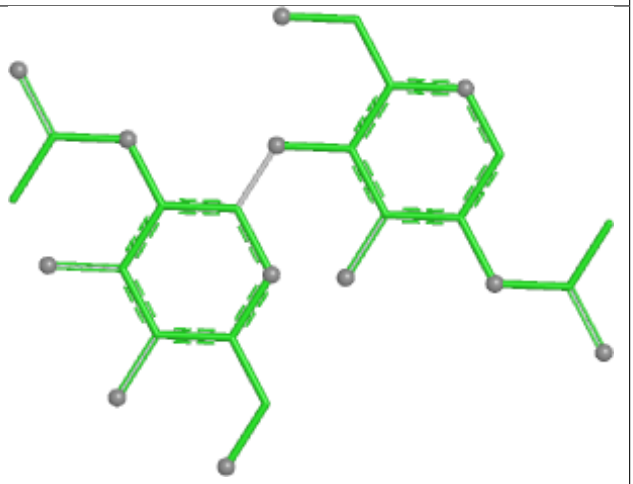


Rings

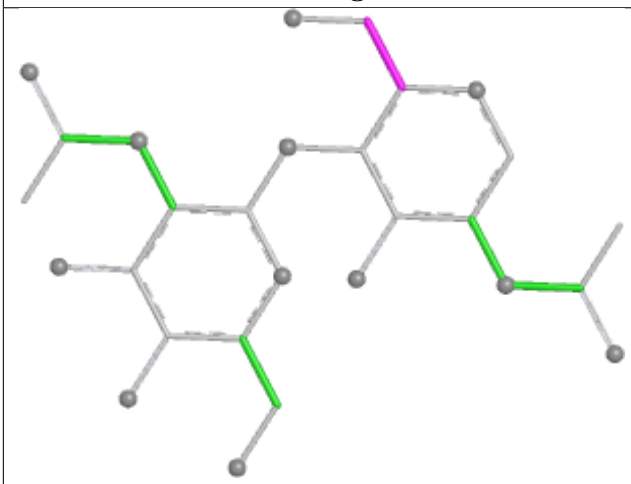
Oligosaccharide Chain O



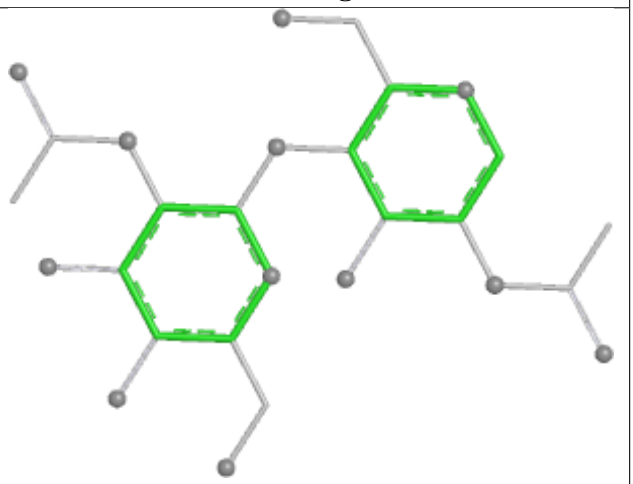
Bond lengths



Bond angles

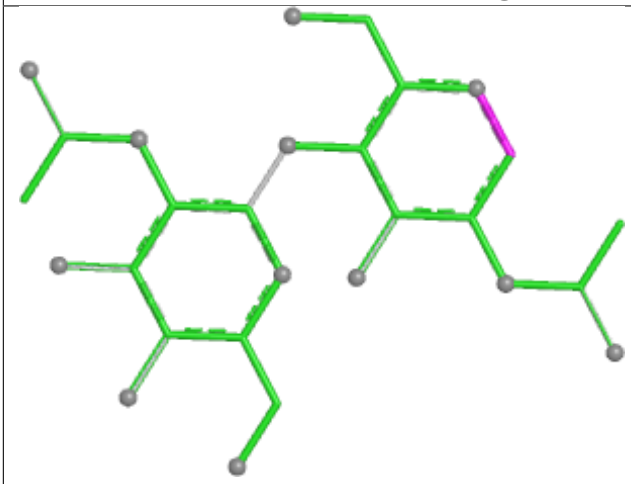


Torsions

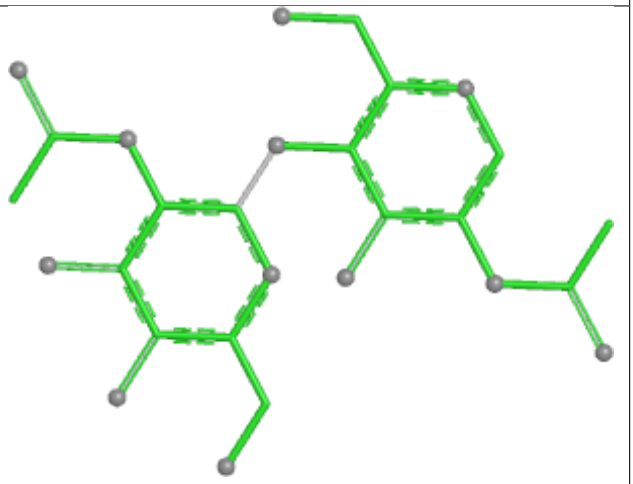


Rings

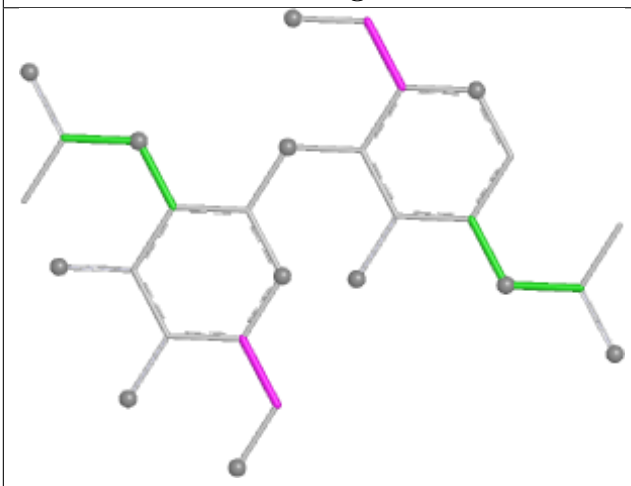
Oligosaccharide Chain P



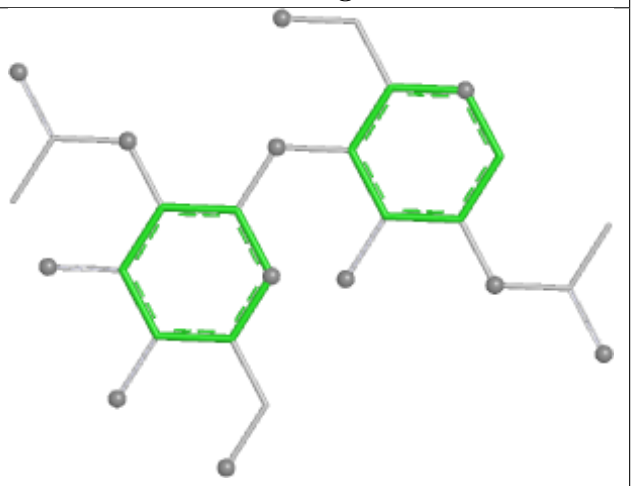
Bond lengths



Bond angles

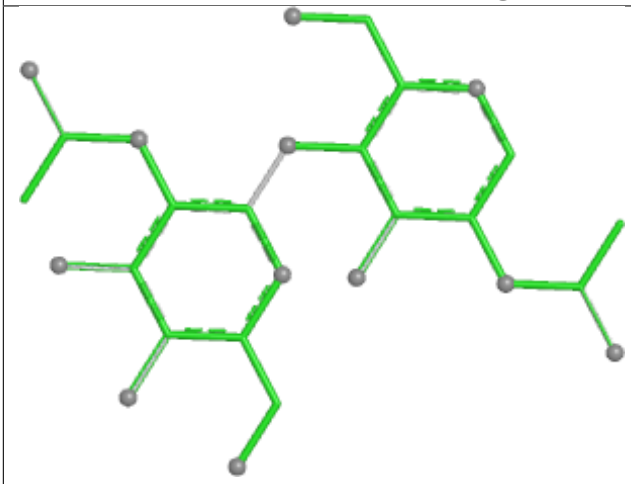


Torsions

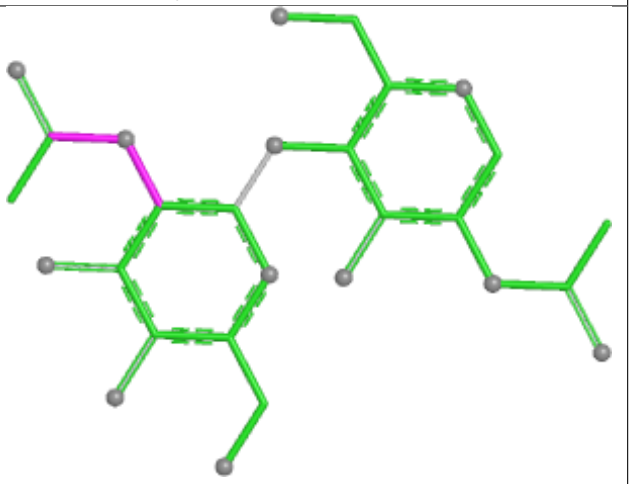


Rings

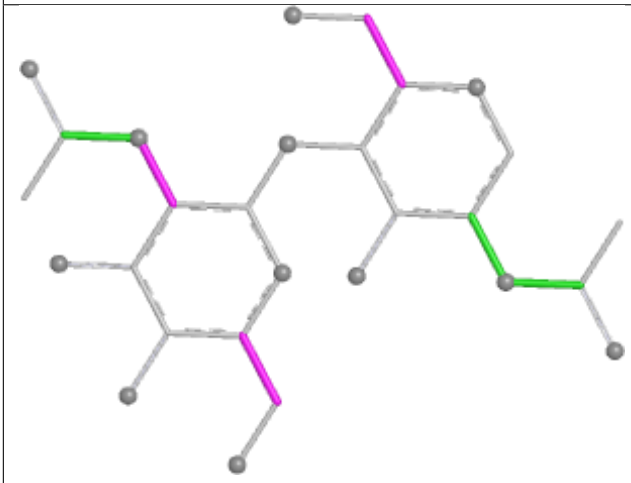
Oligosaccharide Chain Q



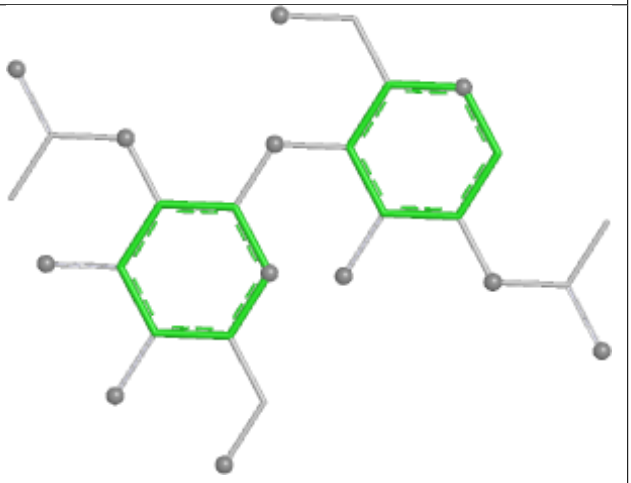
Bond lengths



Bond angles

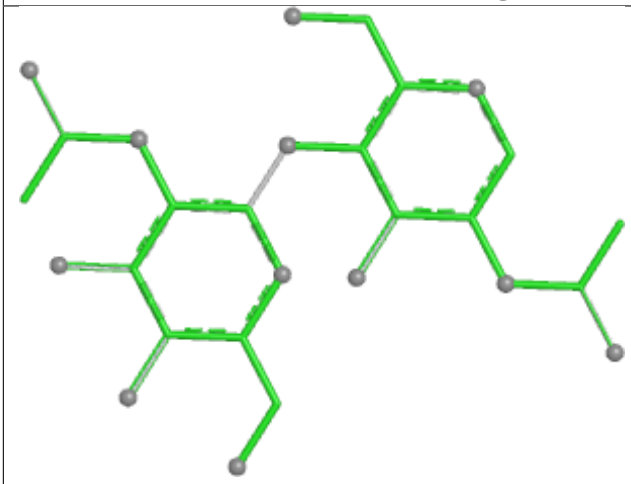


Torsions

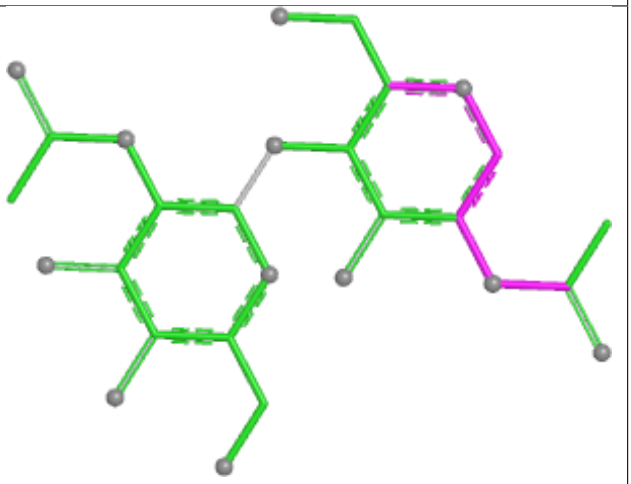


Rings

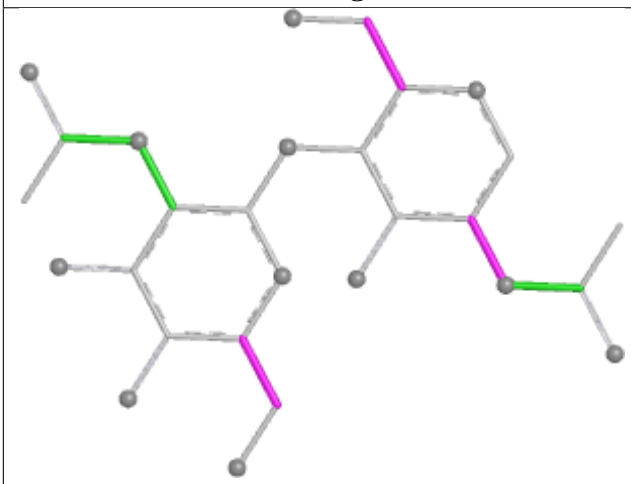
Oligosaccharide Chain R



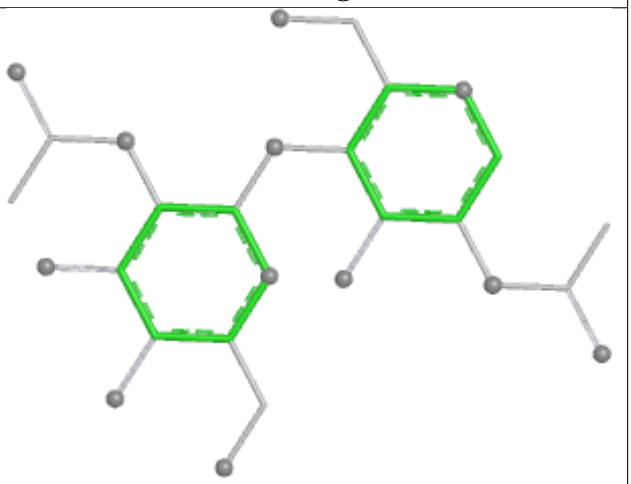
Bond lengths



Bond angles

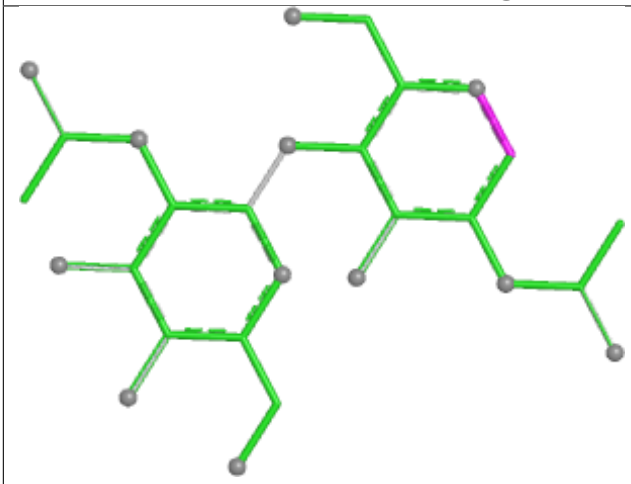


Torsions



Rings

Oligosaccharide Chain S



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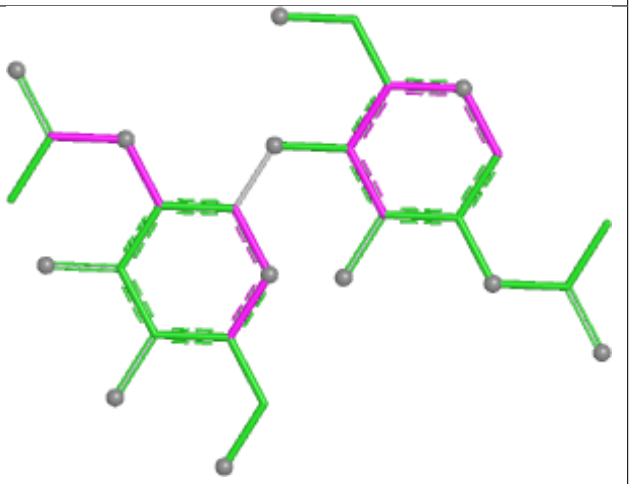

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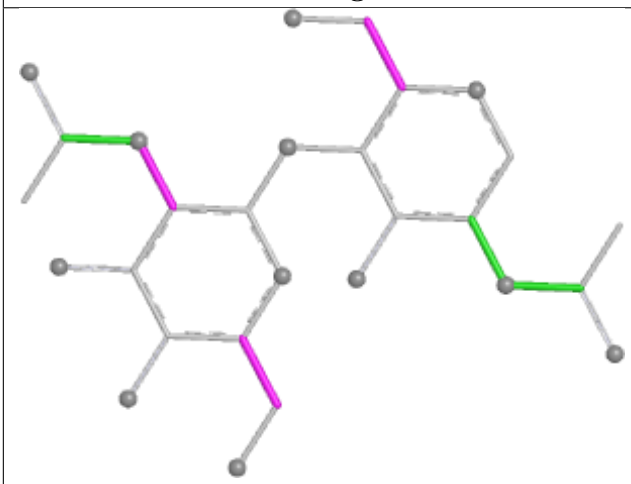

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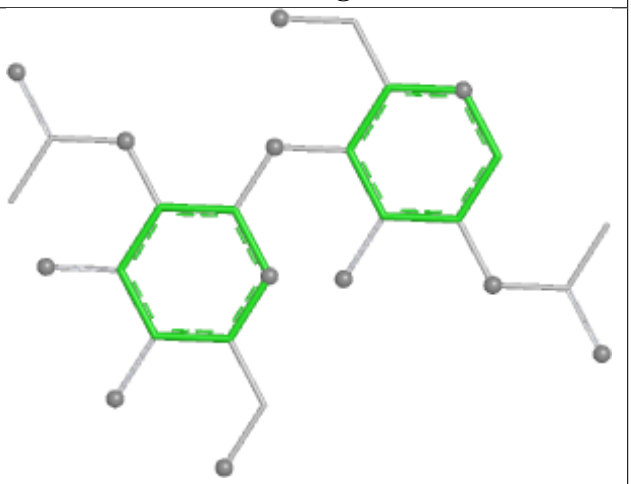
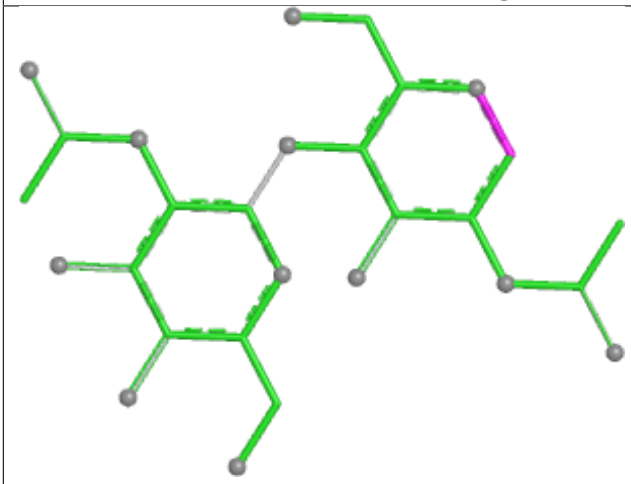


Rings

Oligosaccharide Chain T



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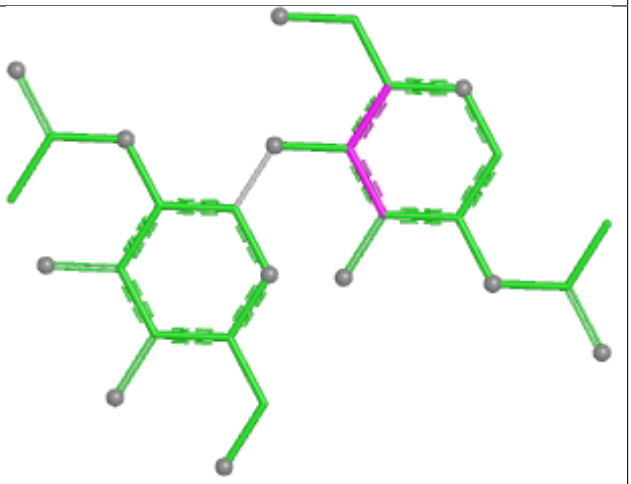
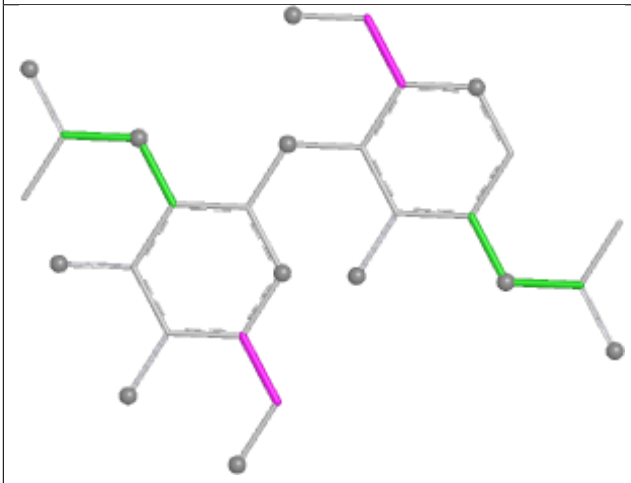


Bond angles



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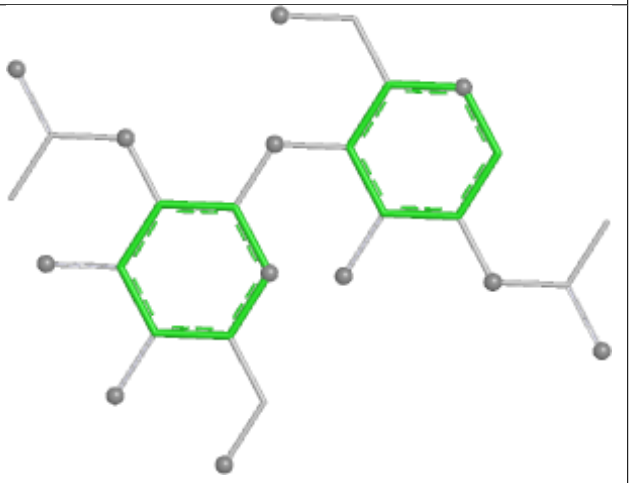
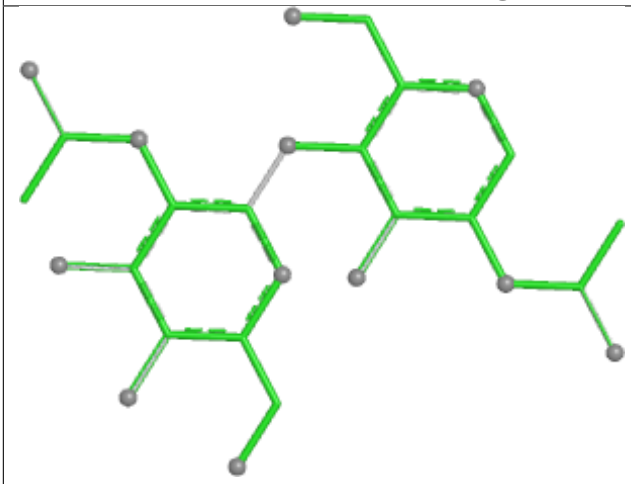


Rings

Oligosaccharide Chain U



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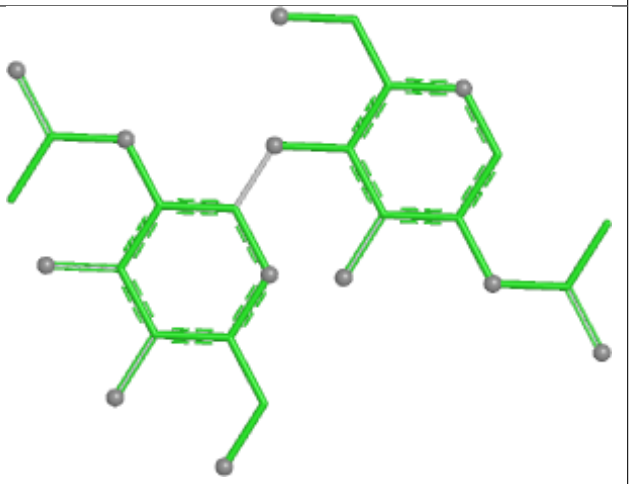
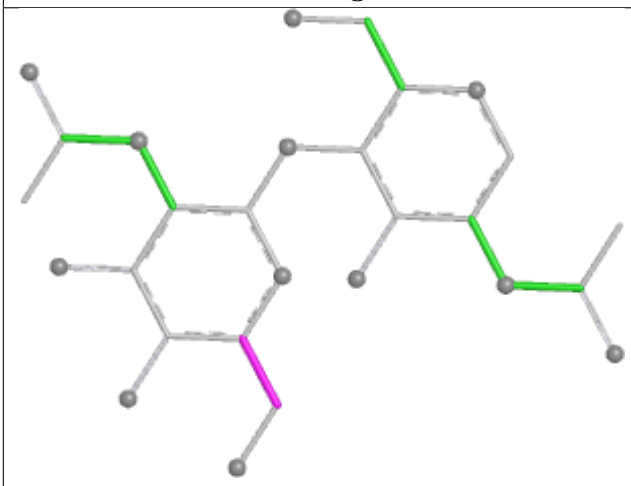


Bond angles



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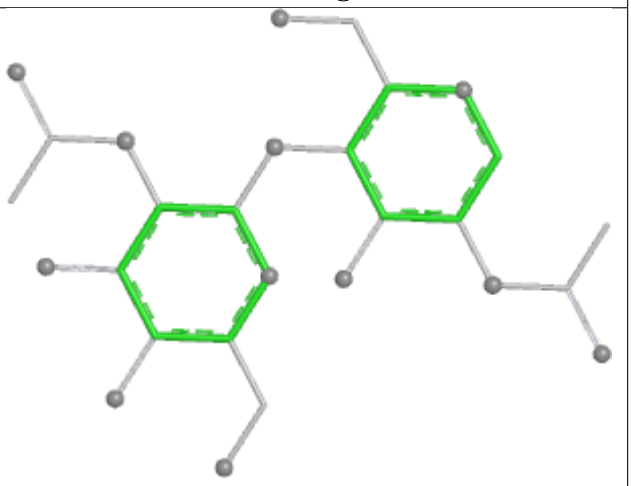
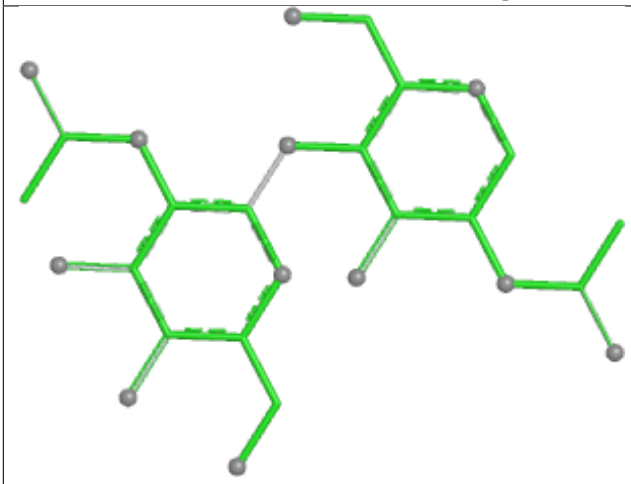


Rings

Oligosaccharide Chain Z



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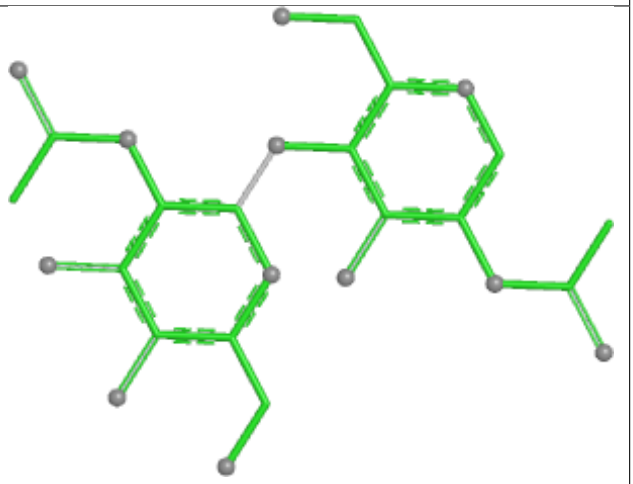

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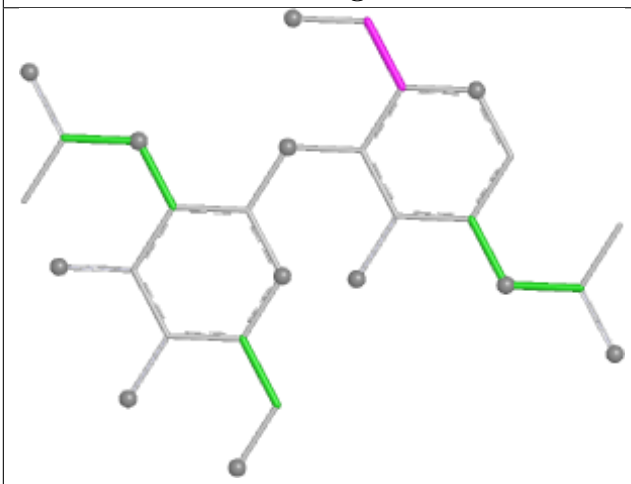

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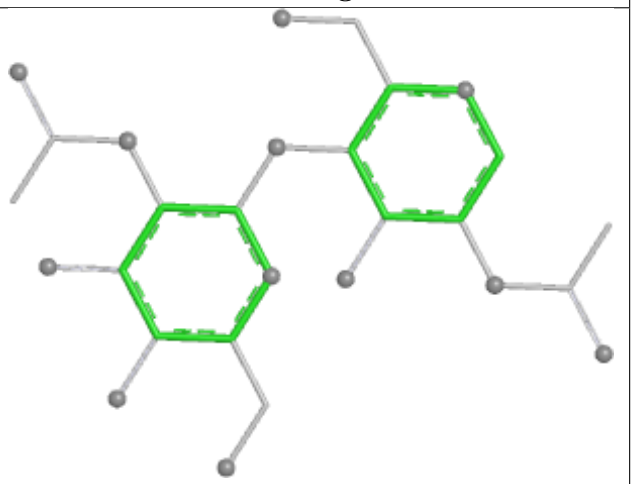
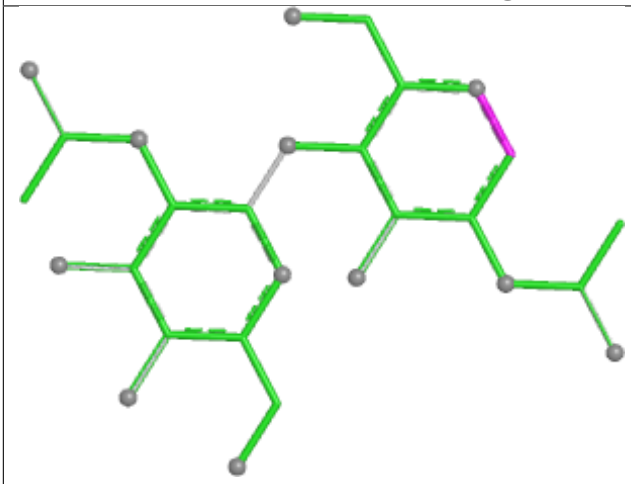


Rings

Oligosaccharide Chain a



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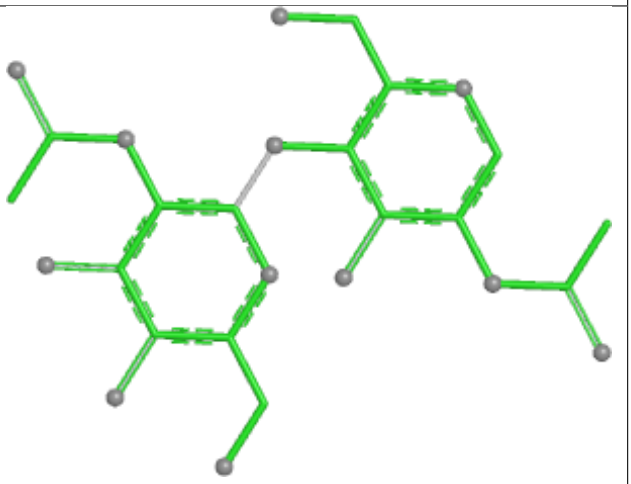

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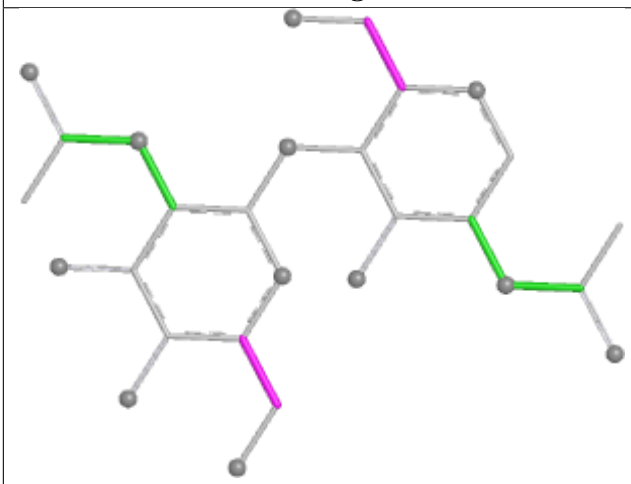

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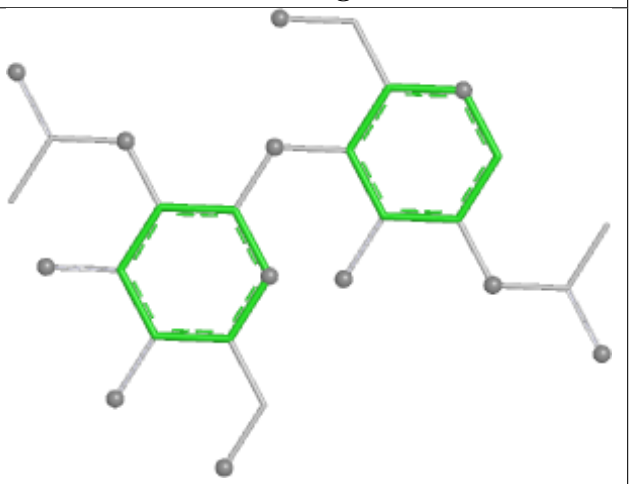
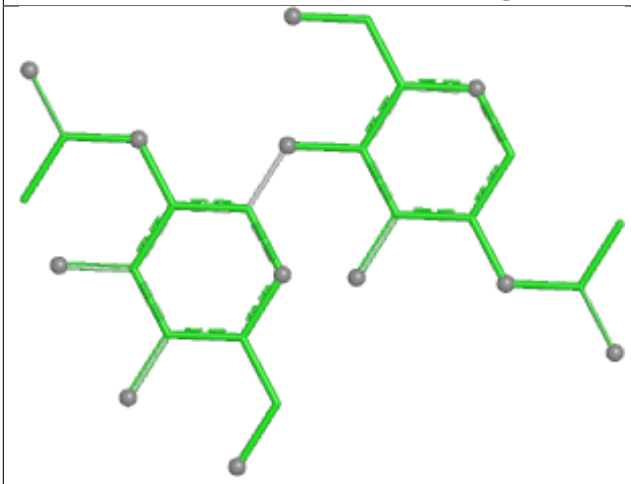


Rings

Oligosaccharide Chain b



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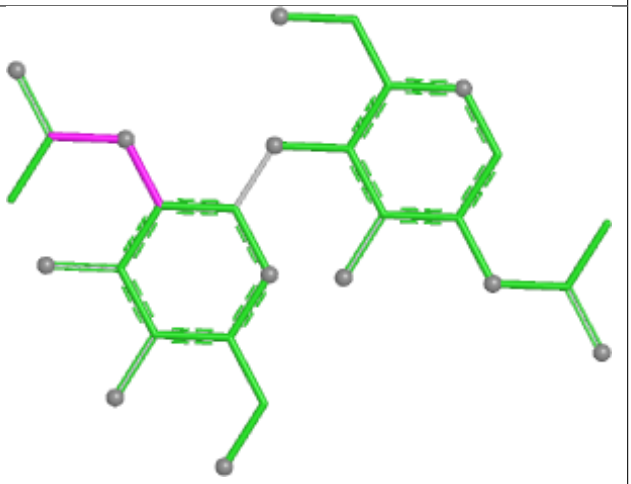

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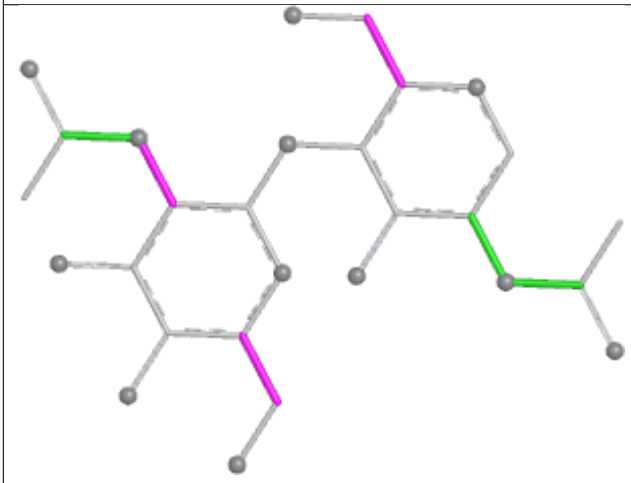

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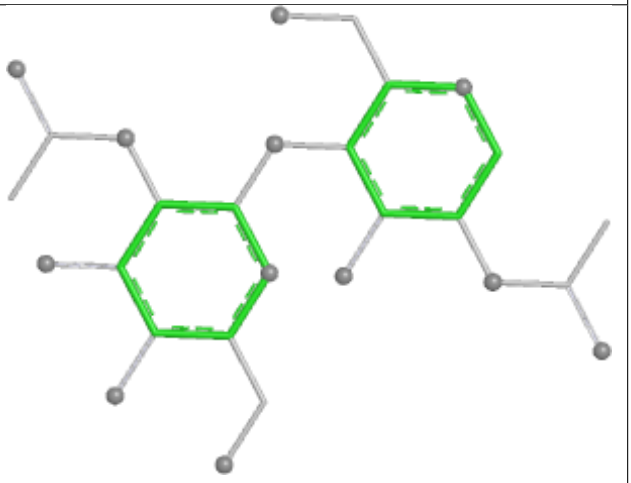
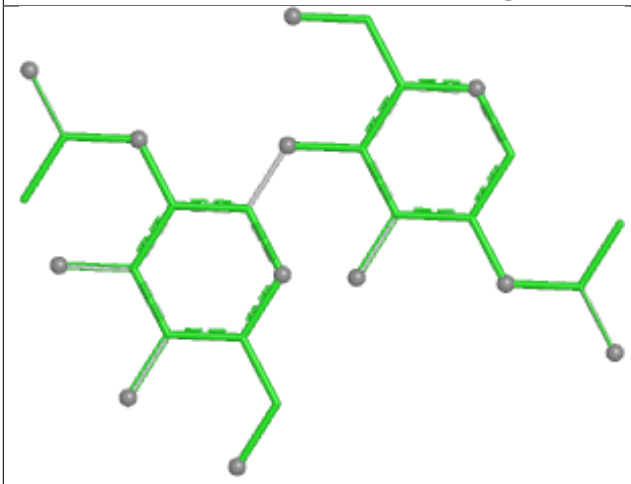


Rings

Oligosaccharide Chain c



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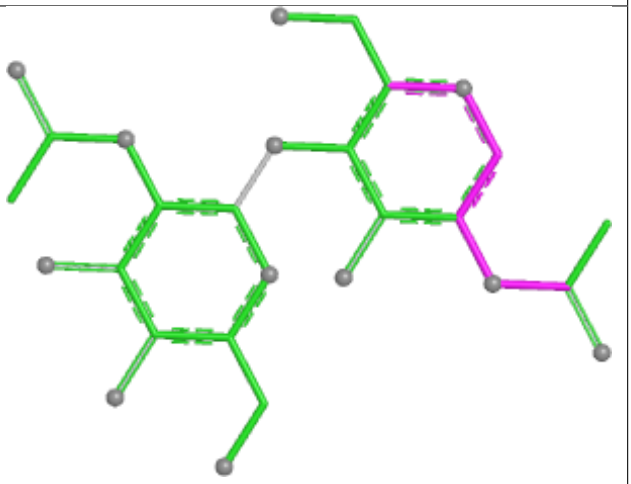
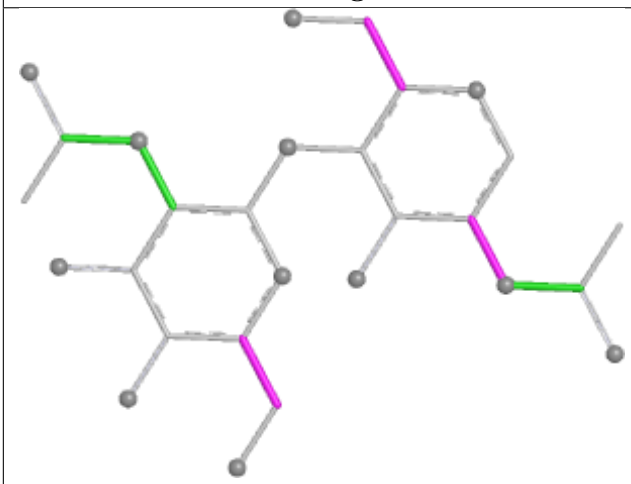


Bond angles



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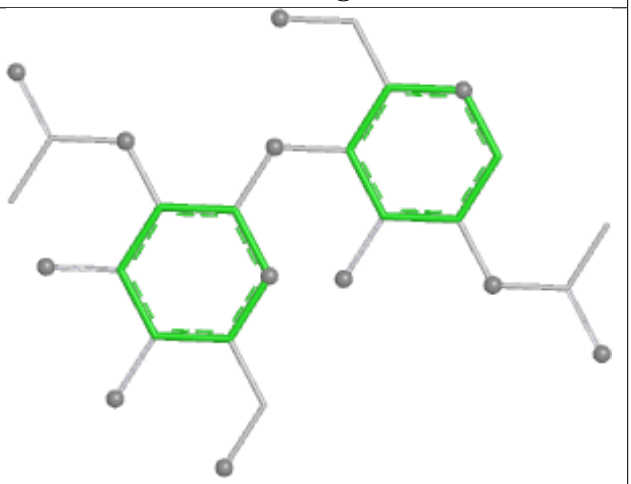
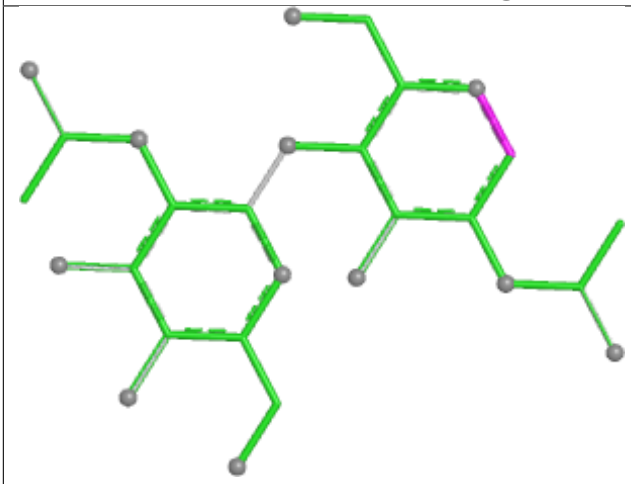


Rings

Oligosaccharide Chain d



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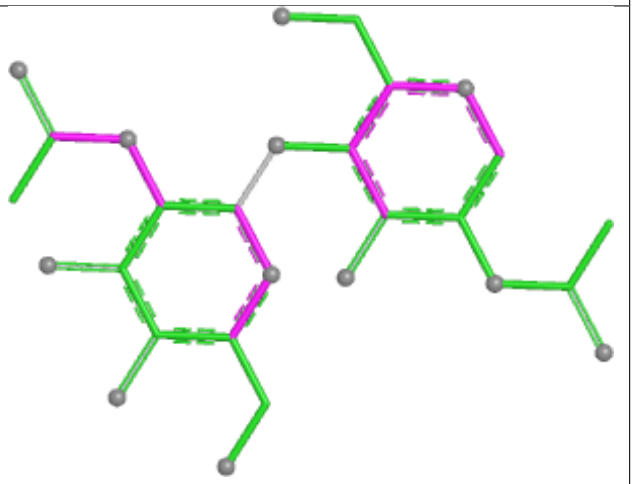
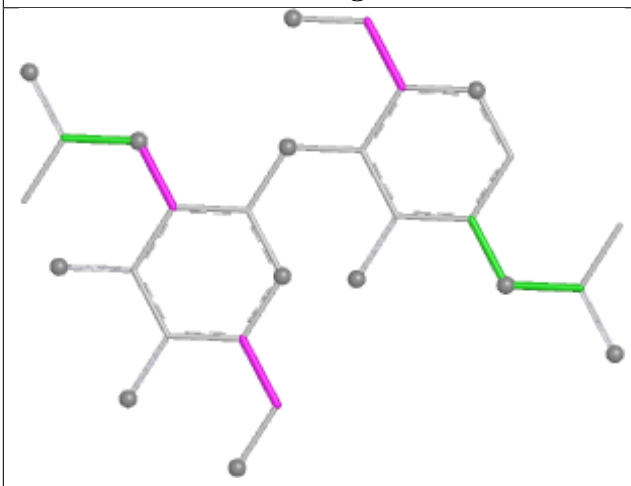


Bond angles



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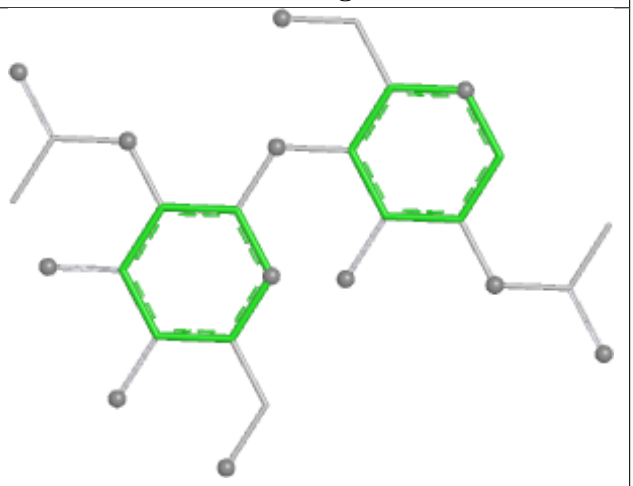
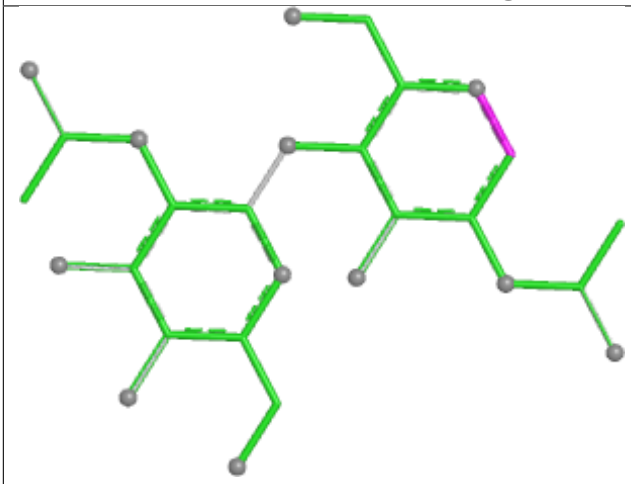


Rings

Oligosaccharide Chain e



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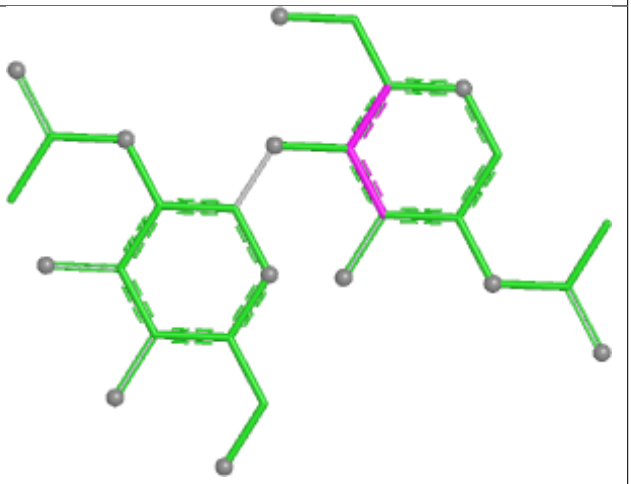
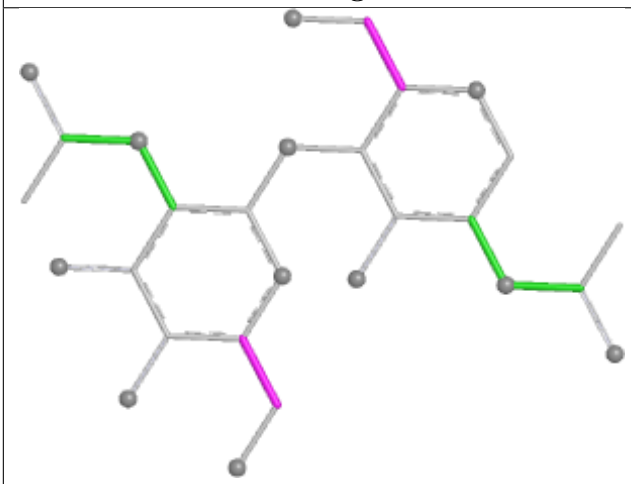


Bond angles



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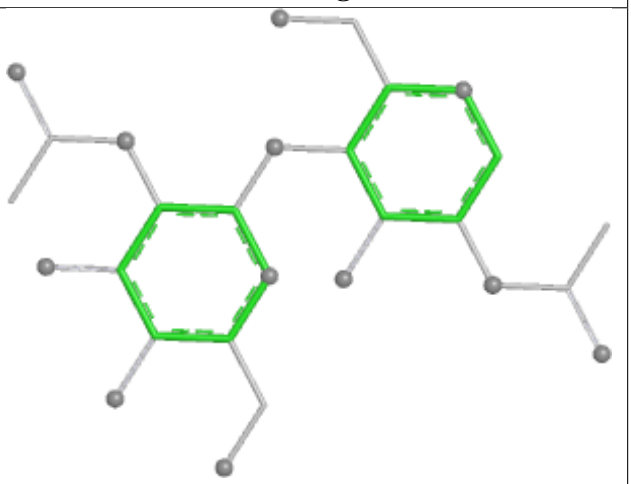
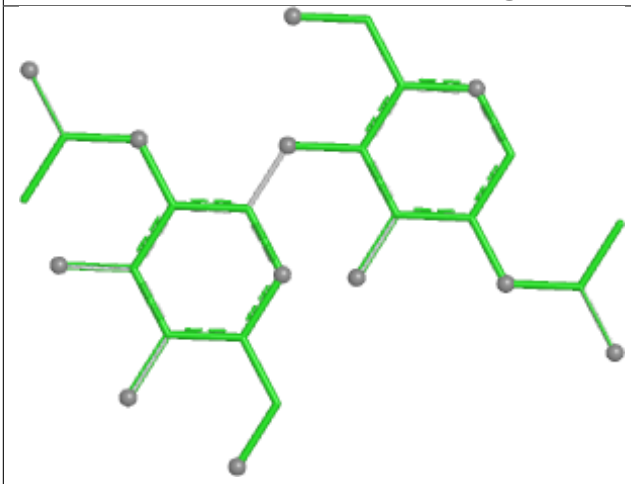


Rings

Oligosaccharide Chain f



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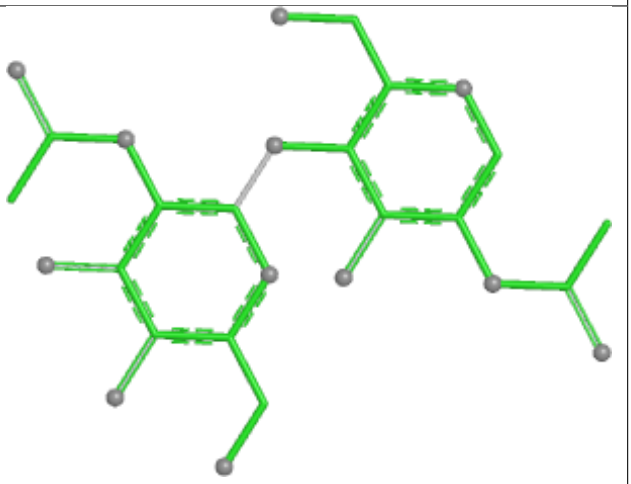
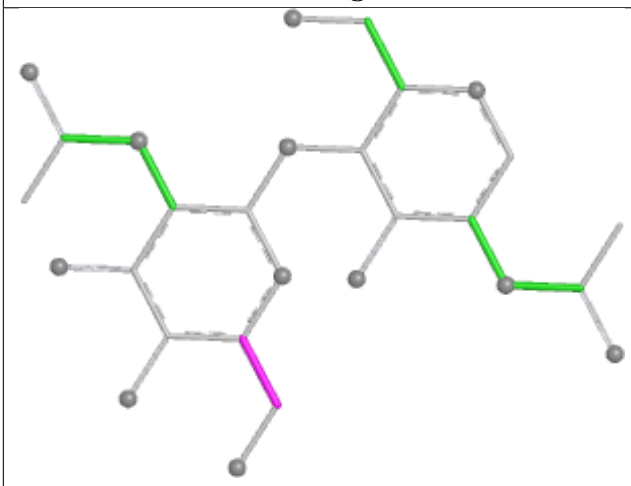


Bond angles



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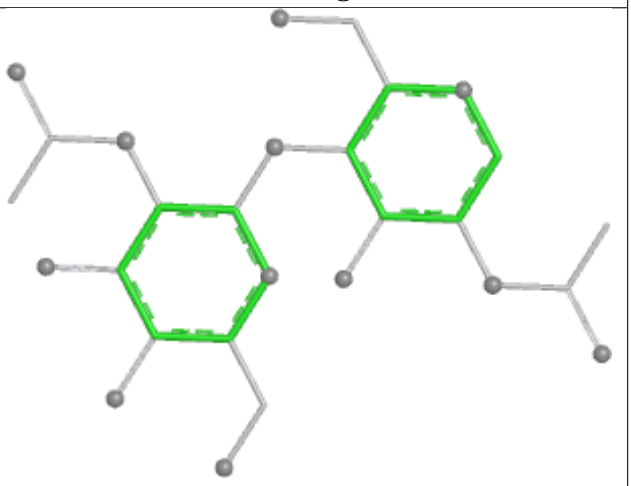
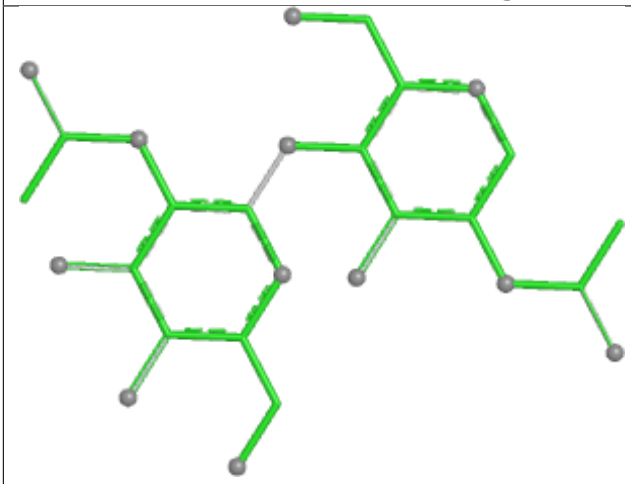


Rings

Oligosaccharide Chain k



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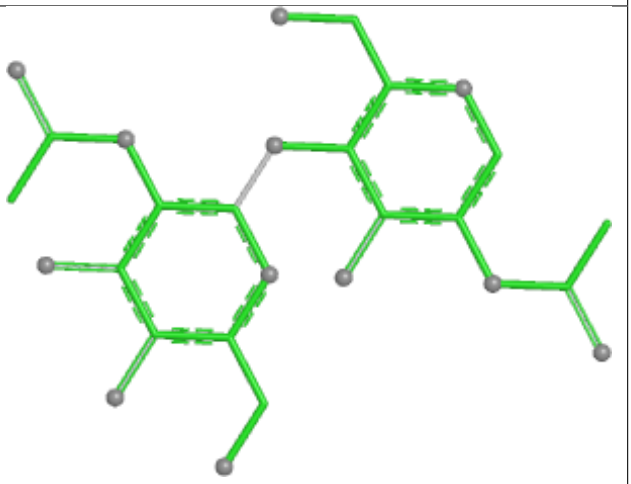
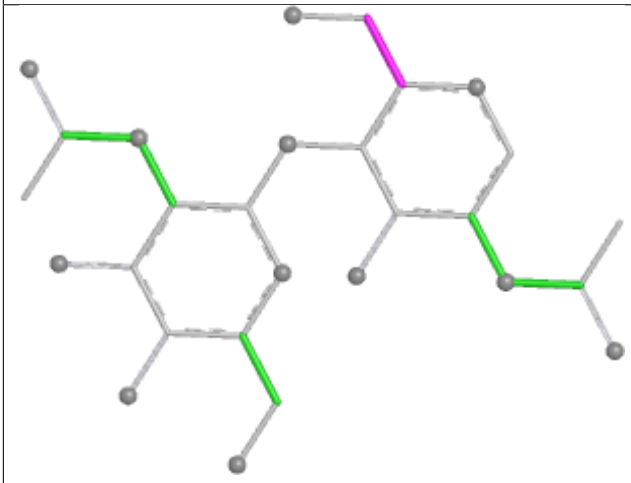


Bond angles



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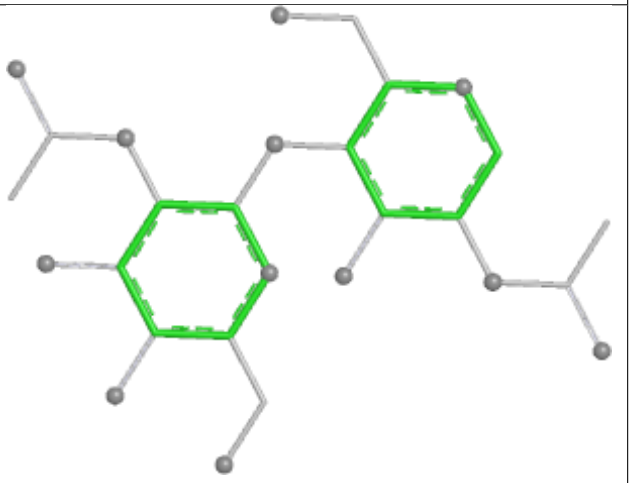
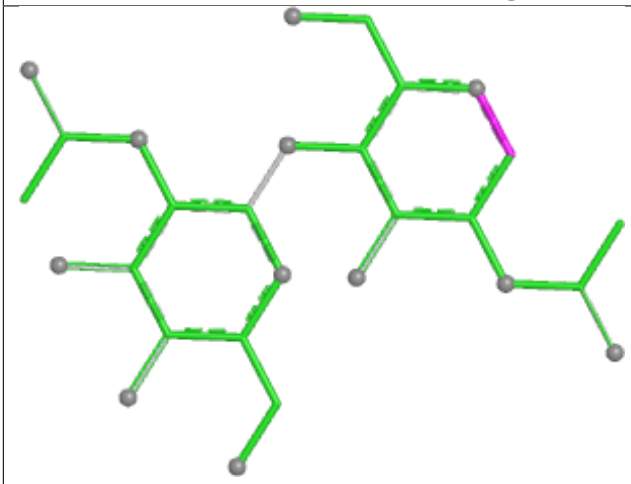


Rings

Oligosaccharide Chain l



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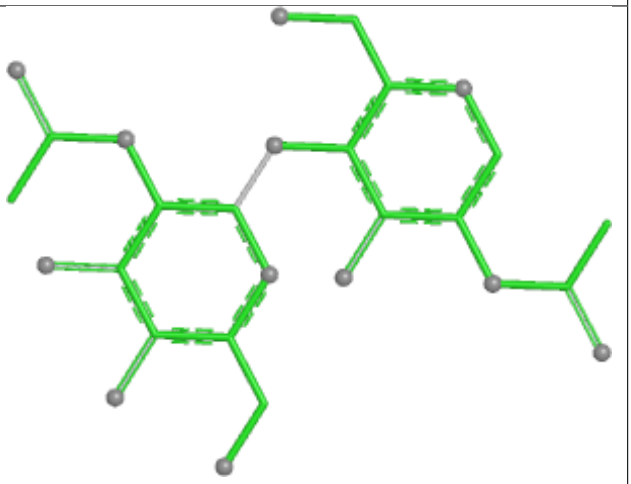
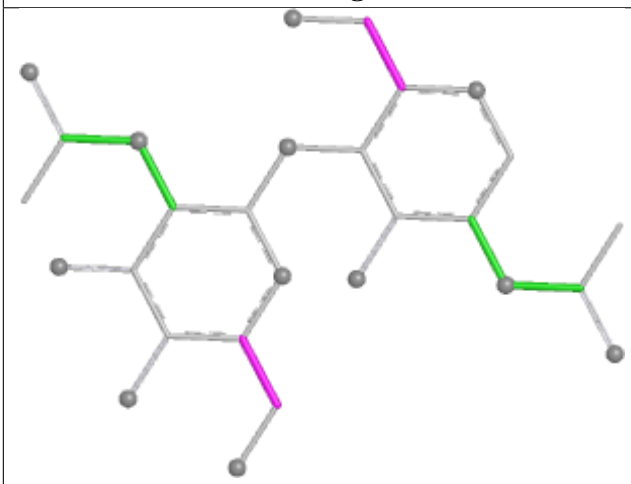


Bond angles



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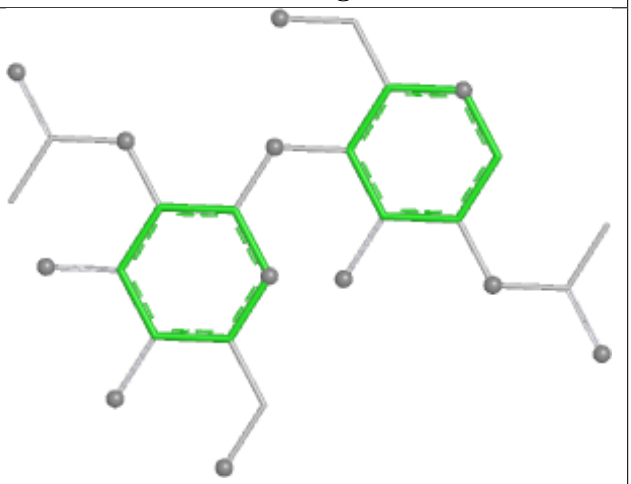
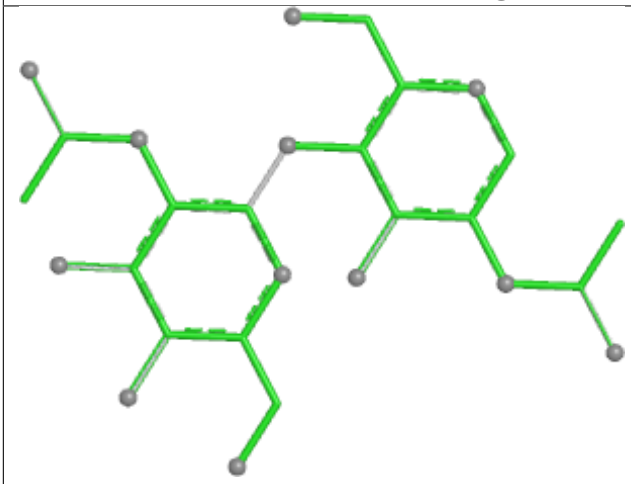


Rings

Oligosaccharide Chain m



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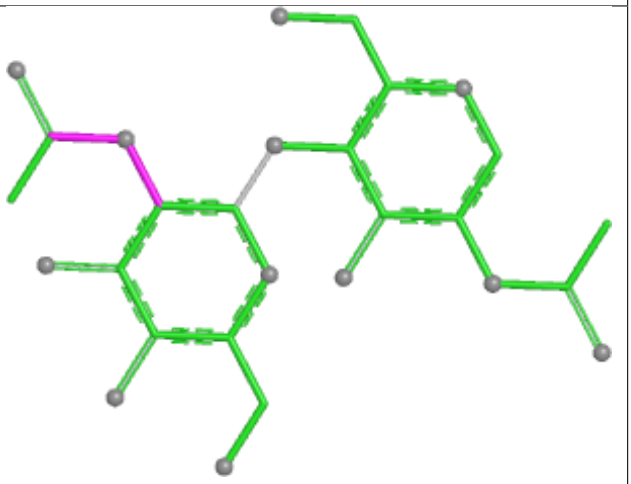
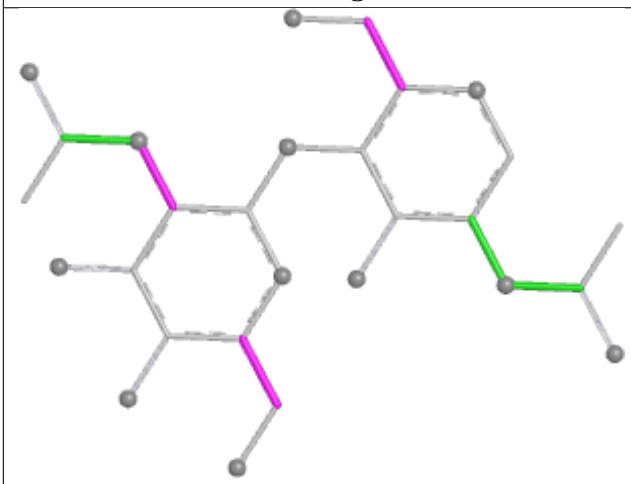


Bond angles



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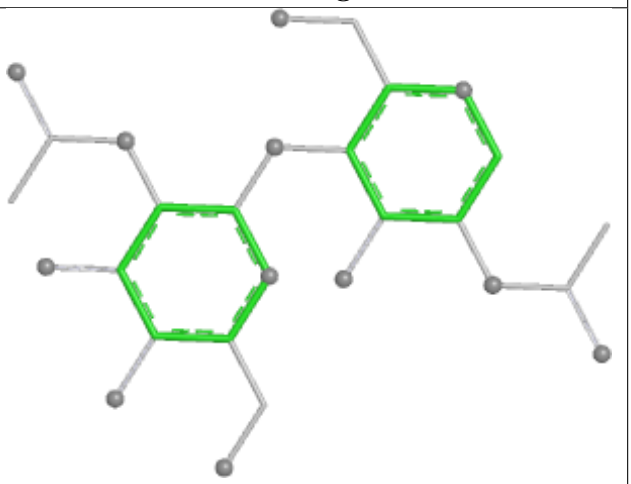
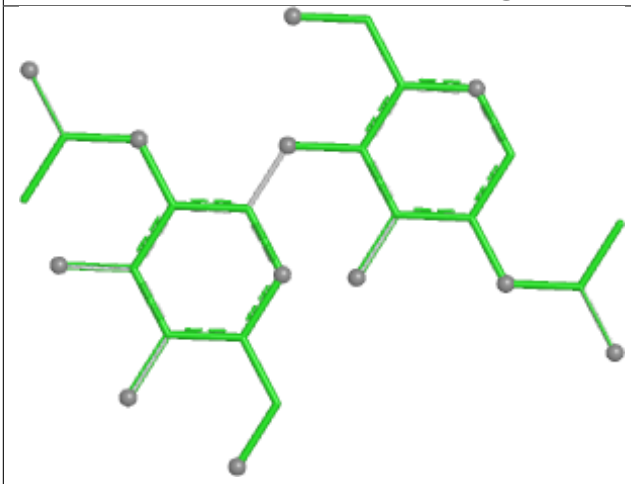


Rings

Oligosaccharide Chain n



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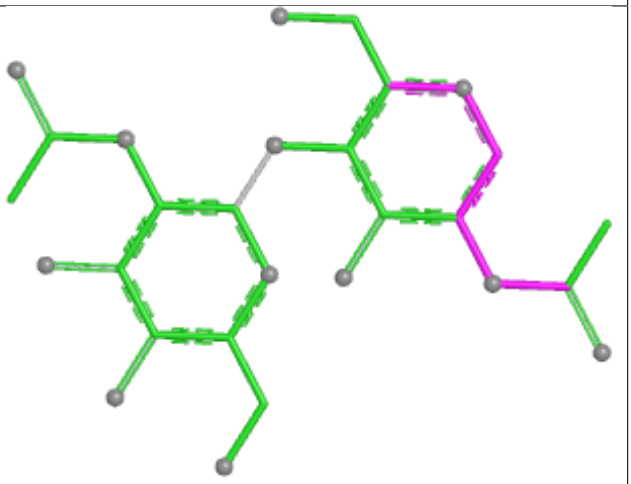
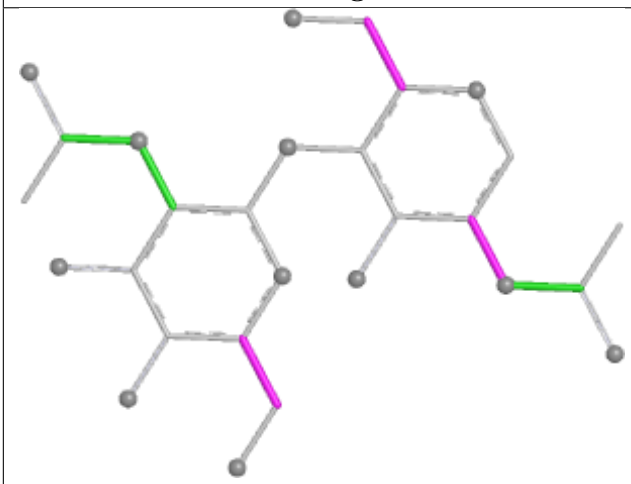


Bond angles



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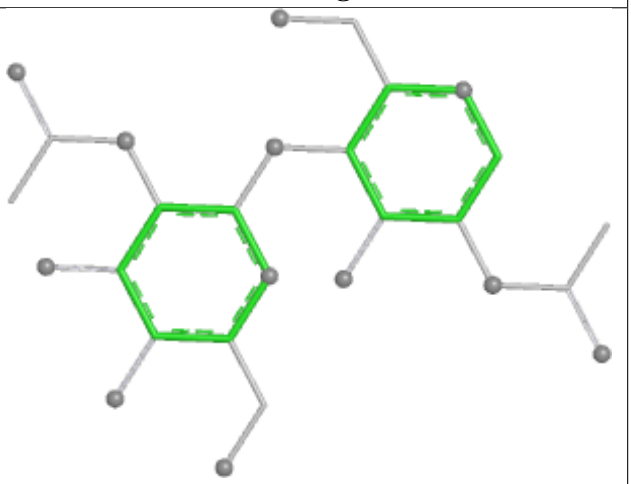
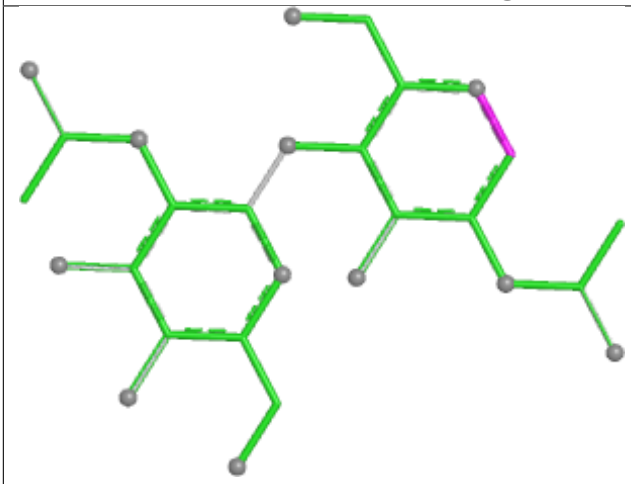
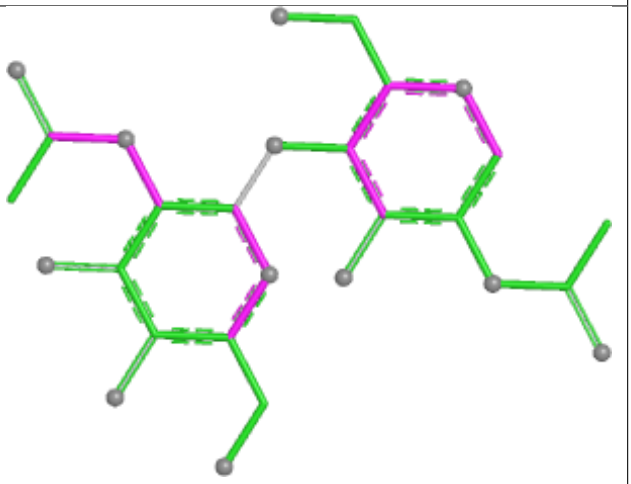


Rings

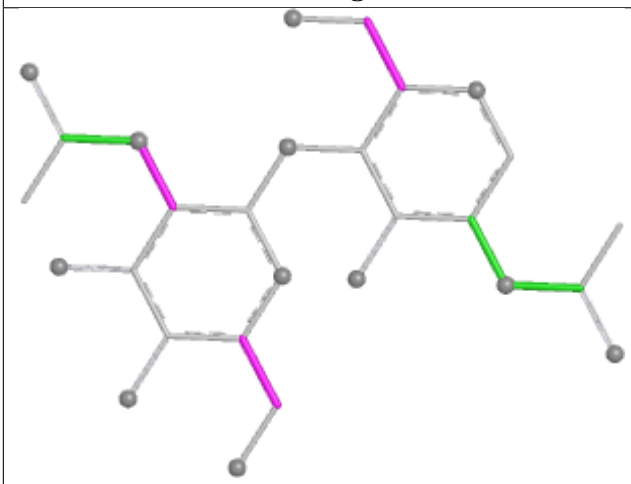
Oligosaccharide Chain o



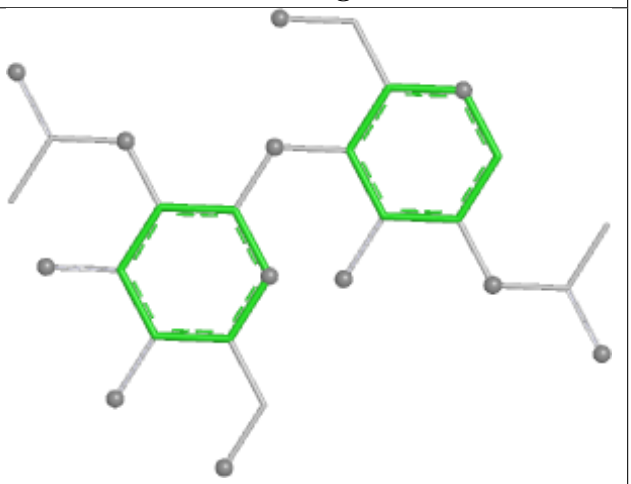
Bond lengths



Bond angles

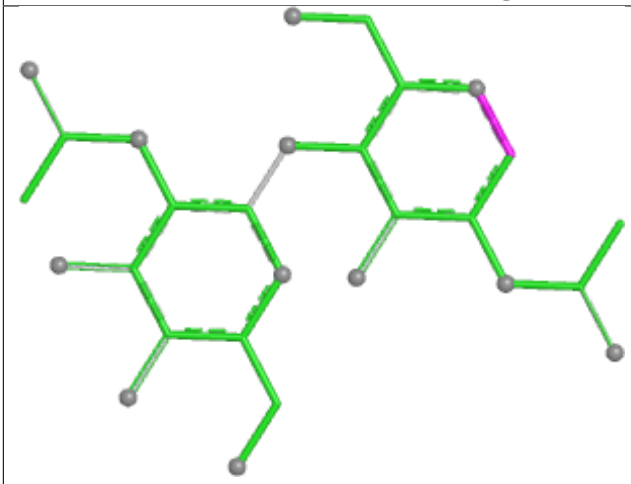


Torsions

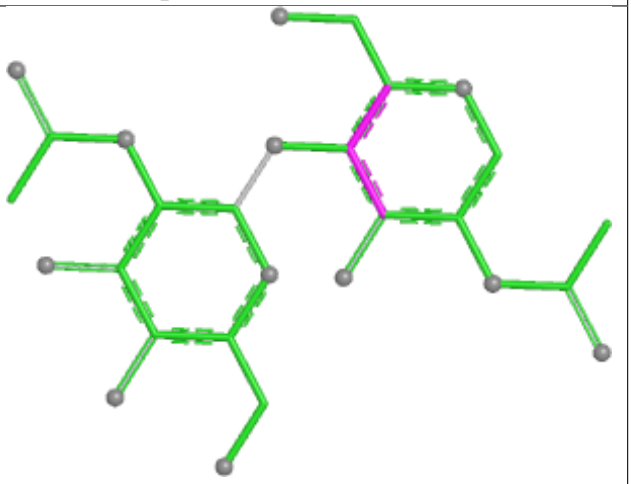


Rings

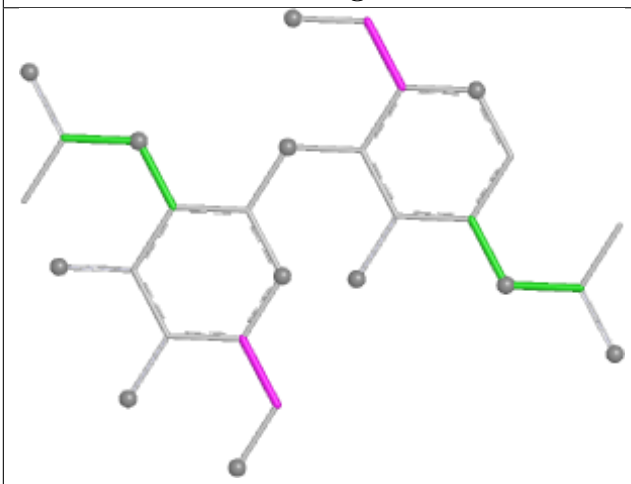
Oligosaccharide Chain p



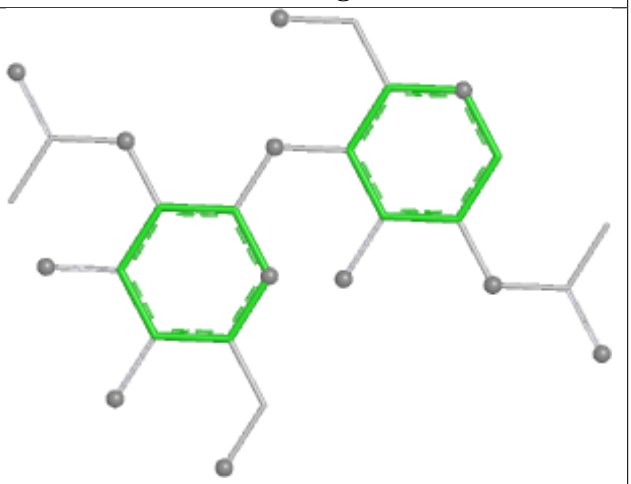
Bond lengths



Bond angles

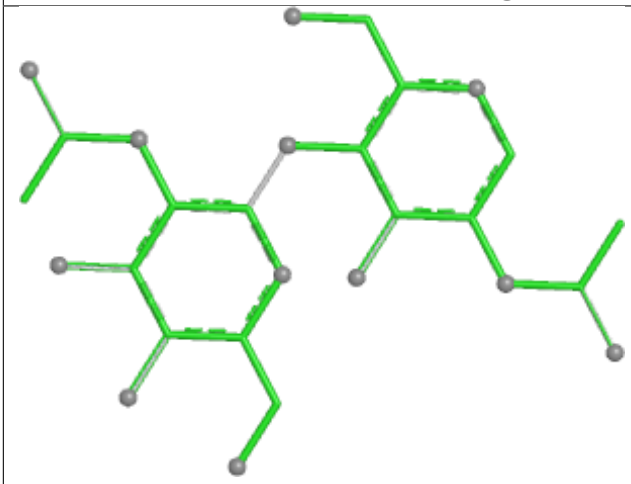


Torsions

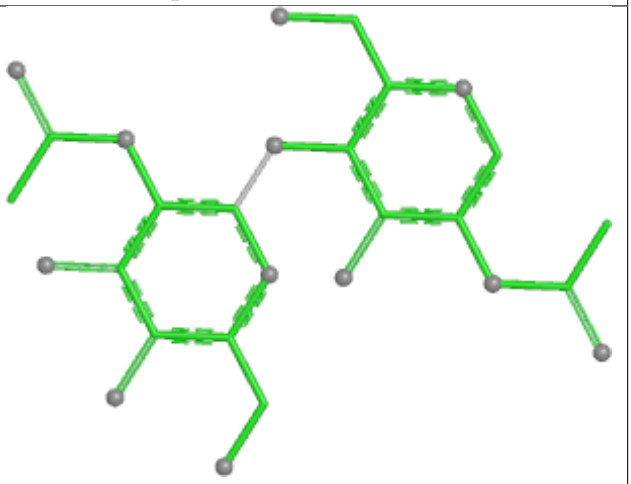


Rings

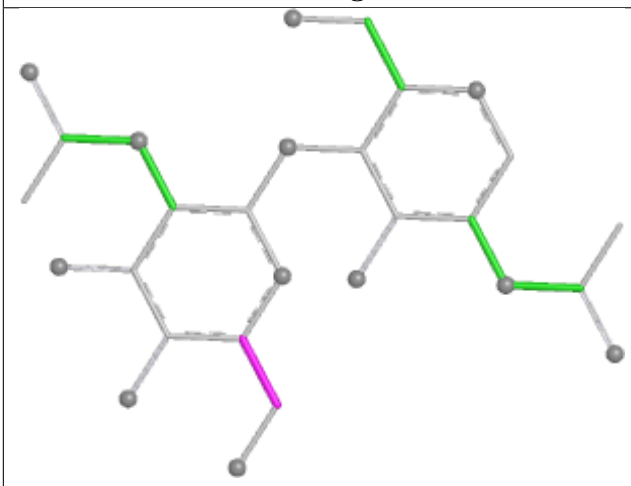
Oligosaccharide Chain q



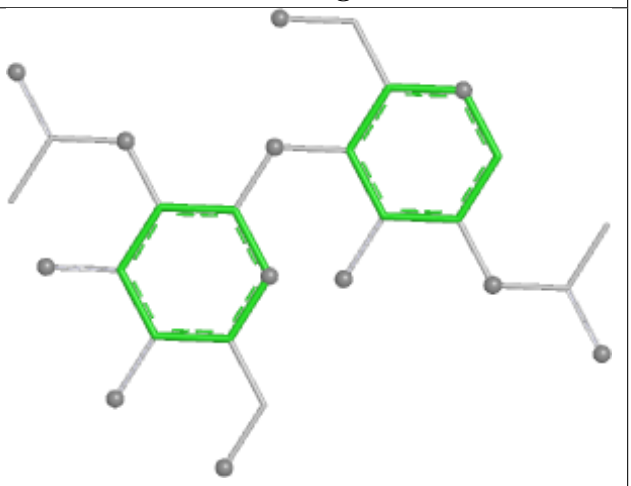
Bond lengths



Bond angles

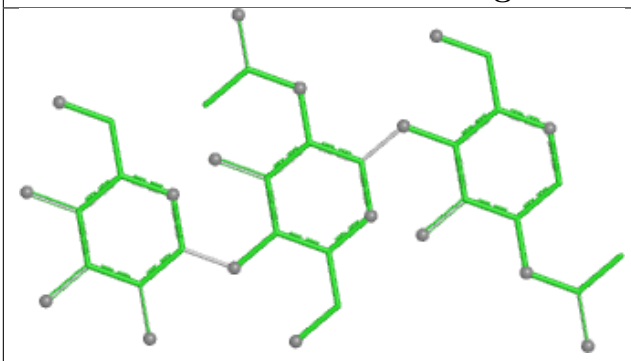


Torsions

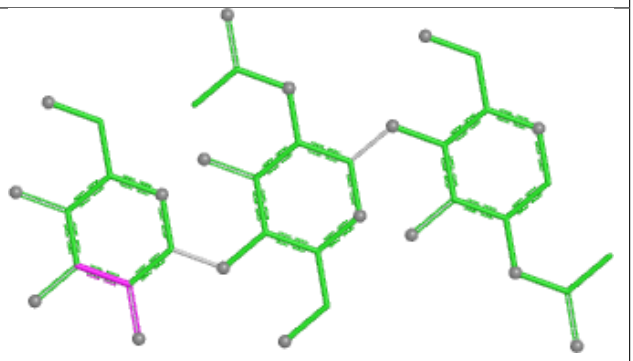


Rings

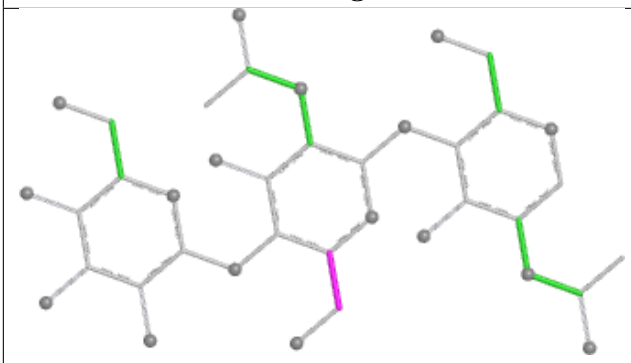
Oligosaccharide Chain V



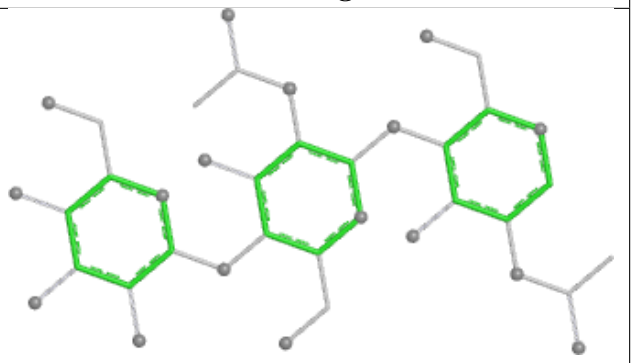
Bond lengths



Bond angles

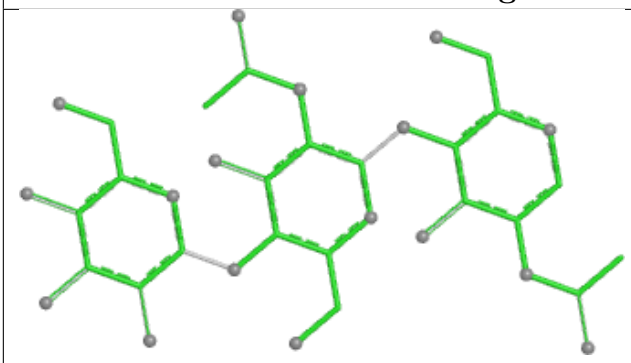


Torsions

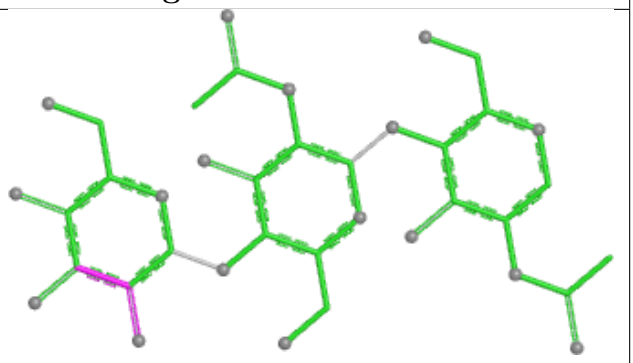


Rings

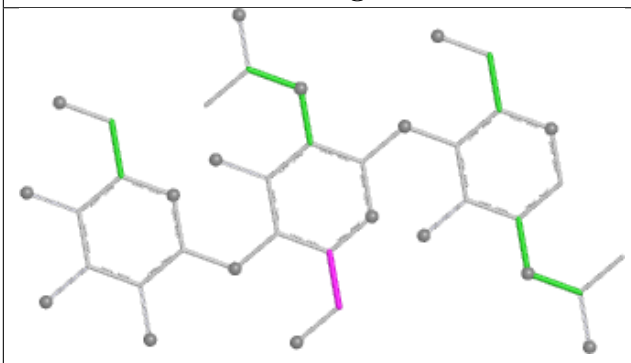
Oligosaccharide Chain g



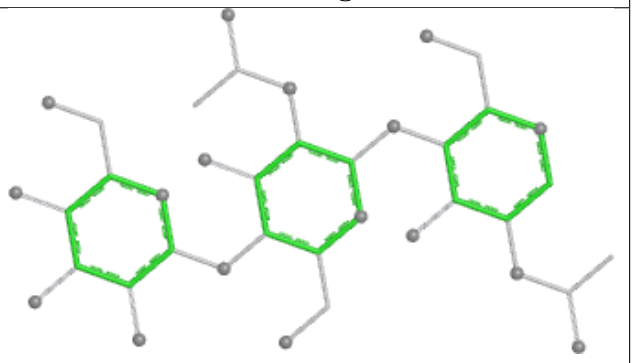
Bond lengths



Bond angles

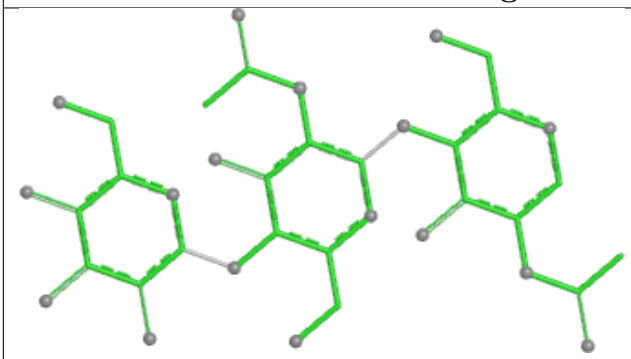


Torsions

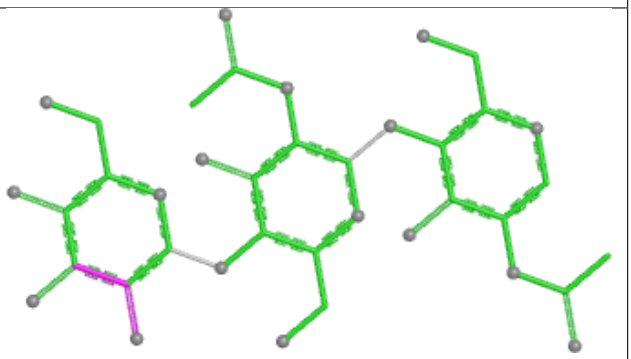


Rings

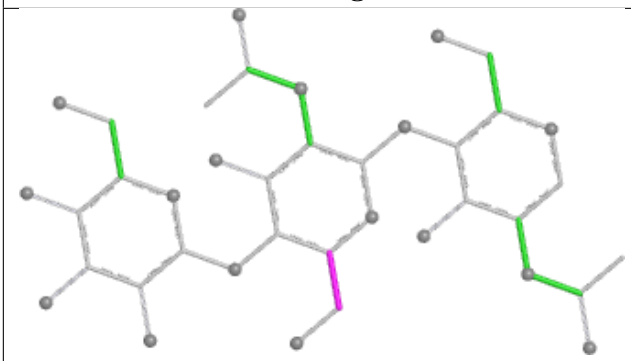
Oligosaccharide Chain r



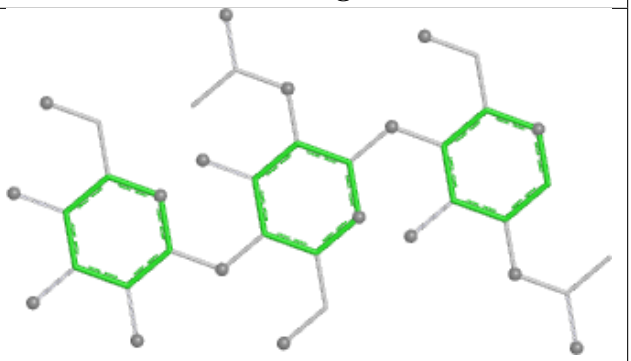
Bond lengths



Bond angles

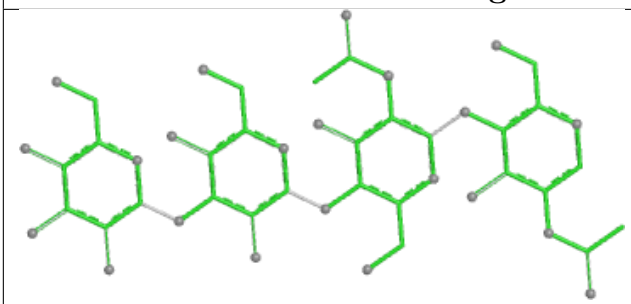


Torsions

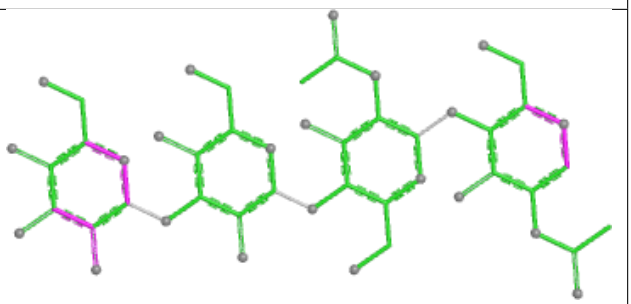


Rings

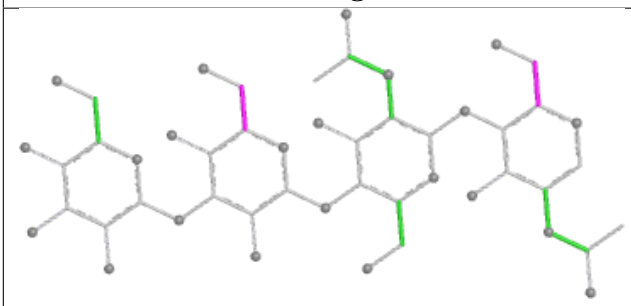
Oligosaccharide Chain W



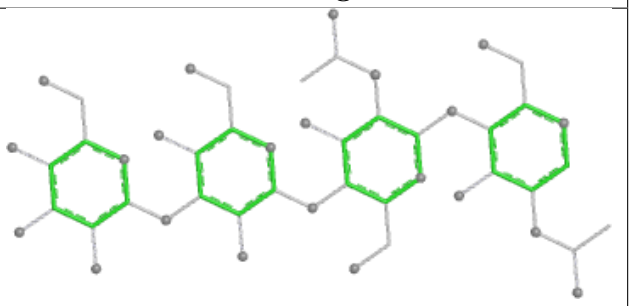
Bond lengths



Bond angles

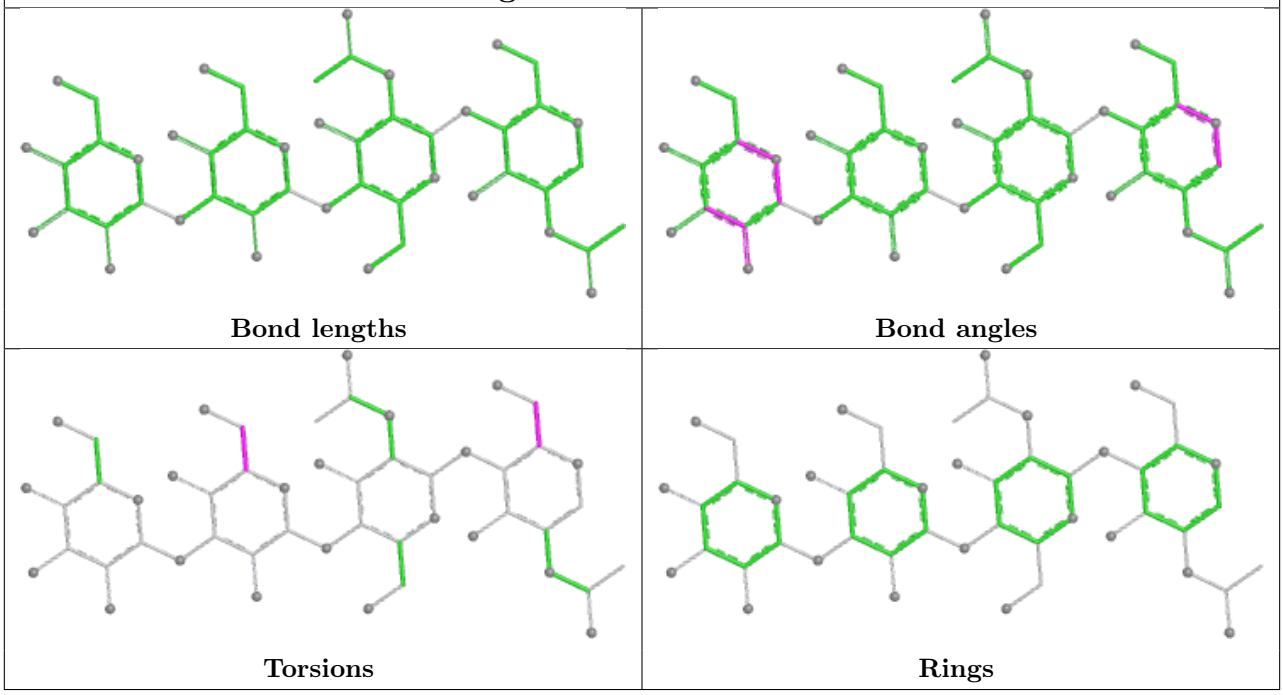


Torsions

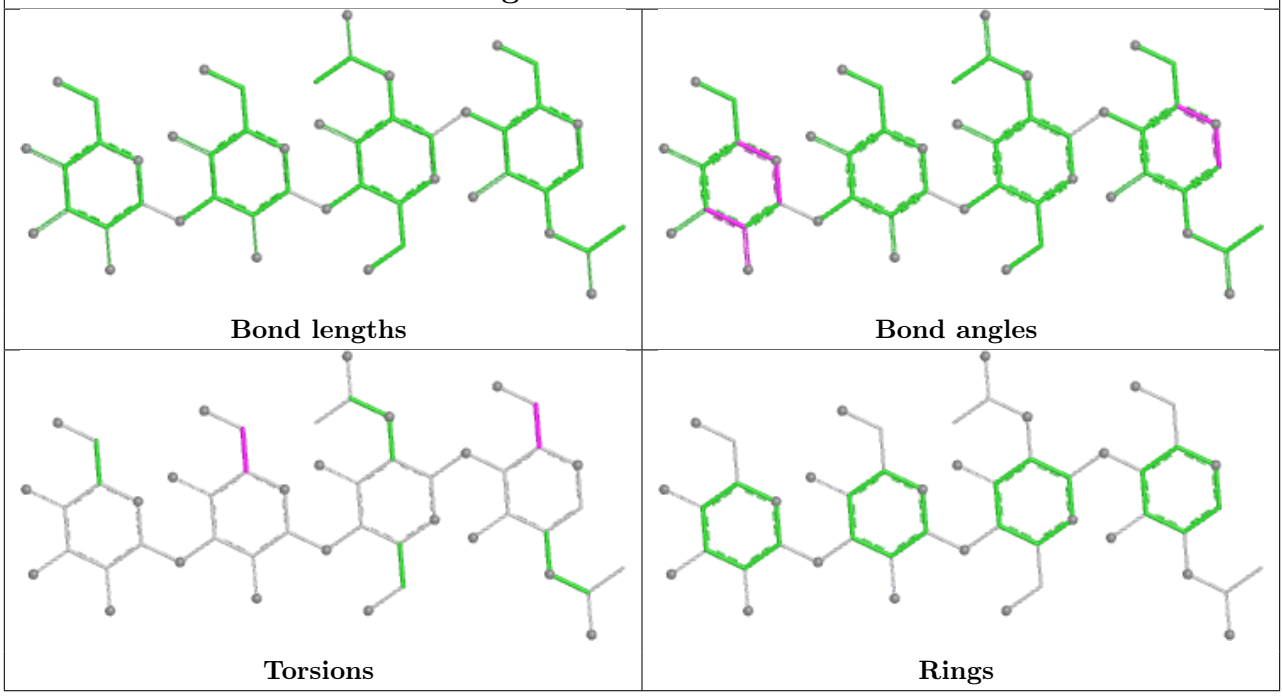


Rings

Oligosaccharide Chain h



Oligosaccharide Chain s



5.6 Ligand geometry (i)

30 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	$\#\|Z\| > 2$
10	NAG	A	623	1	14,14,15	0.35	0	17,19,21	0.49	0
10	NAG	I	620	1	14,14,15	0.34	0	17,19,21	0.63	1 (5%)
10	NAG	I	619	1	14,14,15	0.89	1 (7%)	17,19,21	0.52	0
10	NAG	F	705	2	14,14,15	0.33	0	17,19,21	0.79	1 (5%)
10	NAG	F	707	2	14,14,15	0.36	0	17,19,21	0.61	0
10	NAG	F	706	2	14,14,15	1.43	2 (14%)	17,19,21	1.41	1 (5%)
10	NAG	A	632	1	14,14,15	0.41	0	17,19,21	0.46	0
10	NAG	E	623	1	14,14,15	0.35	0	17,19,21	0.49	0
10	NAG	I	623	1	14,14,15	0.35	0	17,19,21	0.49	0
10	NAG	C	301	3	14,14,15	0.48	0	17,19,21	0.71	1 (5%)
10	NAG	G	301	3	14,14,15	0.48	0	17,19,21	0.71	1 (5%)
10	NAG	E	632	1	14,14,15	0.40	0	17,19,21	0.47	0
10	NAG	I	624	1	14,14,15	0.26	0	17,19,21	0.87	1 (5%)
10	NAG	E	620	1	14,14,15	0.36	0	17,19,21	0.63	1 (5%)
10	NAG	J	707	2	14,14,15	0.37	0	17,19,21	0.61	0
10	NAG	A	627	1	14,14,15	0.51	0	17,19,21	1.31	1 (5%)
10	NAG	B	706	2	14,14,15	1.43	2 (14%)	17,19,21	1.41	1 (5%)
10	NAG	K	301	3	14,14,15	0.48	0	17,19,21	0.72	1 (5%)
10	NAG	I	632	1	14,14,15	0.41	0	17,19,21	0.46	0
10	NAG	B	707	2	14,14,15	0.36	0	17,19,21	0.61	0
10	NAG	E	627	1	14,14,15	0.51	0	17,19,21	1.30	1 (5%)
10	NAG	J	705	2	14,14,15	0.33	0	17,19,21	0.78	1 (5%)
10	NAG	A	624	1	14,14,15	0.26	0	17,19,21	0.86	1 (5%)
10	NAG	B	705	2	14,14,15	0.33	0	17,19,21	0.78	1 (5%)
10	NAG	J	706	2	14,14,15	1.44	2 (14%)	17,19,21	1.41	1 (5%)
10	NAG	A	620	1	14,14,15	0.35	0	17,19,21	0.63	1 (5%)
10	NAG	I	627	1	14,14,15	0.51	0	17,19,21	1.31	1 (5%)
10	NAG	E	624	1	14,14,15	0.26	0	17,19,21	0.86	1 (5%)
10	NAG	E	619	1	14,14,15	0.89	1 (7%)	17,19,21	0.54	0
10	NAG	A	619	1	14,14,15	0.89	1 (7%)	17,19,21	0.53	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
10	NAG	A	623	1	-	2/6/23/26	0/1/1/1
10	NAG	I	620	1	-	2/6/23/26	0/1/1/1
10	NAG	I	619	1	-	2/6/23/26	0/1/1/1
10	NAG	F	705	2	-	2/6/23/26	0/1/1/1
10	NAG	F	707	2	-	2/6/23/26	0/1/1/1
10	NAG	F	706	2	-	2/6/23/26	0/1/1/1
10	NAG	A	632	1	-	2/6/23/26	0/1/1/1
10	NAG	E	623	1	-	2/6/23/26	0/1/1/1
10	NAG	I	623	1	-	2/6/23/26	0/1/1/1
10	NAG	C	301	3	-	2/6/23/26	0/1/1/1
10	NAG	G	301	3	-	2/6/23/26	0/1/1/1
10	NAG	E	632	1	-	2/6/23/26	0/1/1/1
10	NAG	I	624	1	-	2/6/23/26	0/1/1/1
10	NAG	E	620	1	-	2/6/23/26	0/1/1/1
10	NAG	J	707	2	-	2/6/23/26	0/1/1/1
10	NAG	A	627	1	-	2/6/23/26	0/1/1/1
10	NAG	B	706	2	-	2/6/23/26	0/1/1/1
10	NAG	K	301	3	-	2/6/23/26	0/1/1/1
10	NAG	I	632	1	-	2/6/23/26	0/1/1/1
10	NAG	B	707	2	-	2/6/23/26	0/1/1/1
10	NAG	E	627	1	-	2/6/23/26	0/1/1/1
10	NAG	J	705	2	-	2/6/23/26	0/1/1/1
10	NAG	A	624	1	-	2/6/23/26	0/1/1/1
10	NAG	B	705	2	-	2/6/23/26	0/1/1/1
10	NAG	J	706	2	-	2/6/23/26	0/1/1/1
10	NAG	A	620	1	-	2/6/23/26	0/1/1/1
10	NAG	I	627	1	-	2/6/23/26	0/1/1/1
10	NAG	E	624	1	-	2/6/23/26	0/1/1/1
10	NAG	E	619	1	-	2/6/23/26	0/1/1/1
10	NAG	A	619	1	-	2/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	706	NAG	O5-C1	3.85	1.50	1.43
10	F	706	NAG	O5-C1	3.84	1.50	1.43
10	B	706	NAG	O5-C1	3.83	1.50	1.43
10	J	706	NAG	C1-C2	3.72	1.57	1.52
10	B	706	NAG	C1-C2	3.67	1.57	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	706	NAG	C1-O5-C5	5.22	119.19	112.19
10	J	706	NAG	C1-O5-C5	5.20	119.16	112.19
10	B	706	NAG	C1-O5-C5	5.20	119.15	112.19
10	I	627	NAG	C1-O5-C5	4.99	118.87	112.19
10	A	627	NAG	C1-O5-C5	4.96	118.83	112.19

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	624	NAG	C4-C5-C6-O6
10	E	624	NAG	C4-C5-C6-O6
10	I	624	NAG	C4-C5-C6-O6
10	C	301	NAG	O5-C5-C6-O6
10	G	301	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)

There are no chain breaks in this entry.

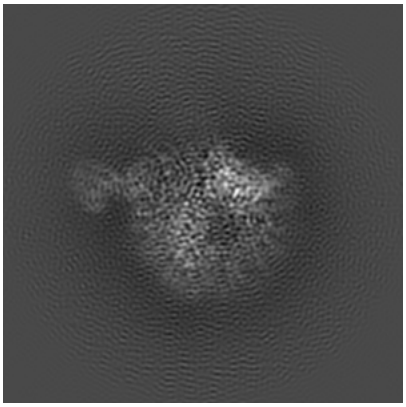
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0485. These allow visual inspection of the internal detail of the map and identification of artifacts.

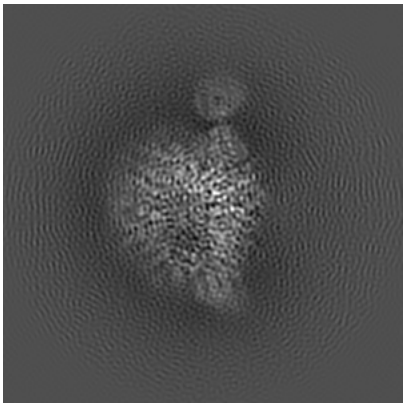
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

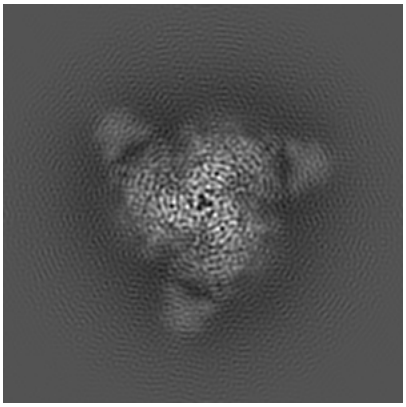
6.1.1 Primary map



X



Y

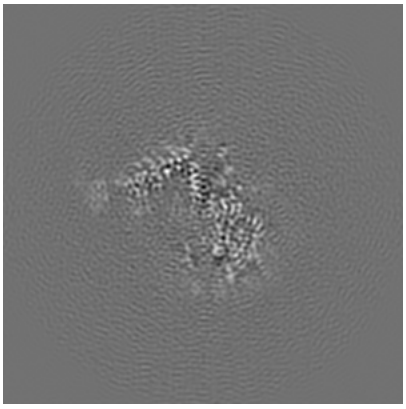


Z

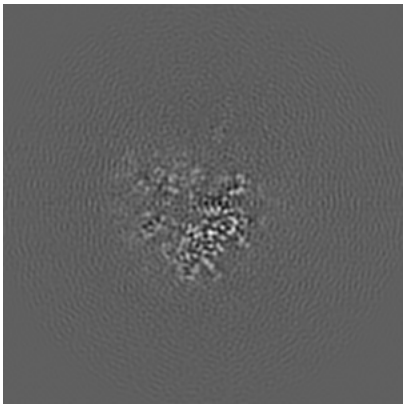
The images above show the map projected in three orthogonal directions.

6.2 Central slices

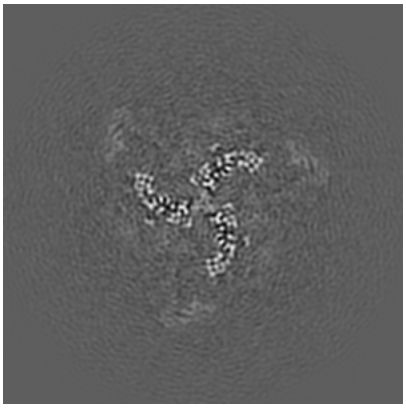
6.2.1 Primary map



X Index: 150



Y Index: 150

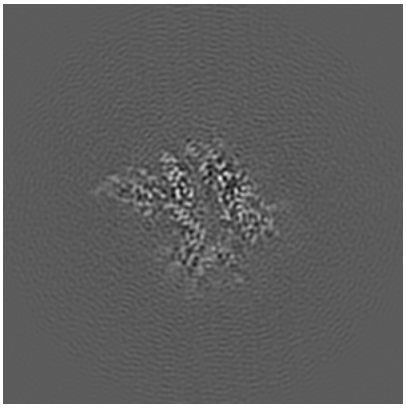


Z Index: 150

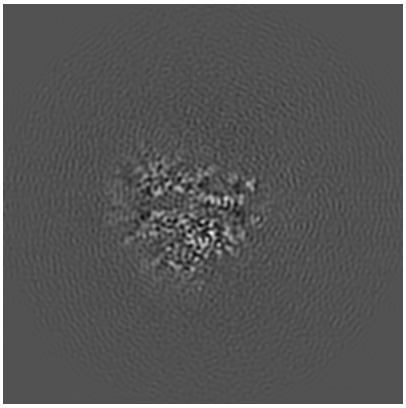
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

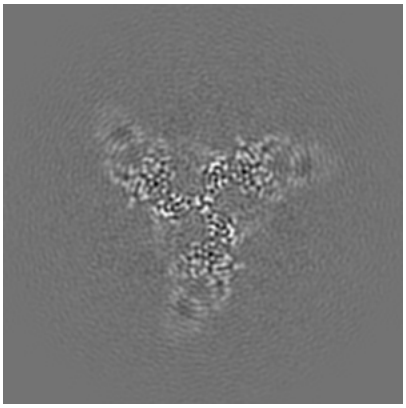
6.3.1 Primary map



X Index: 160



Y Index: 145

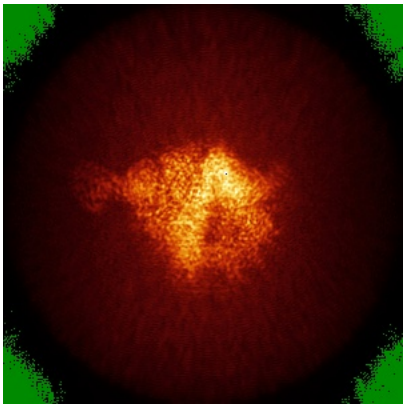


Z Index: 161

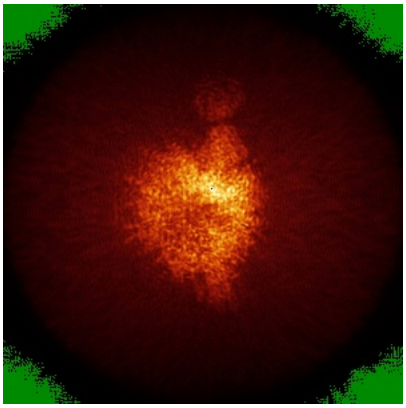
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

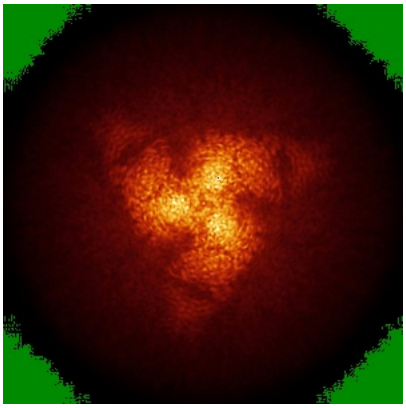
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

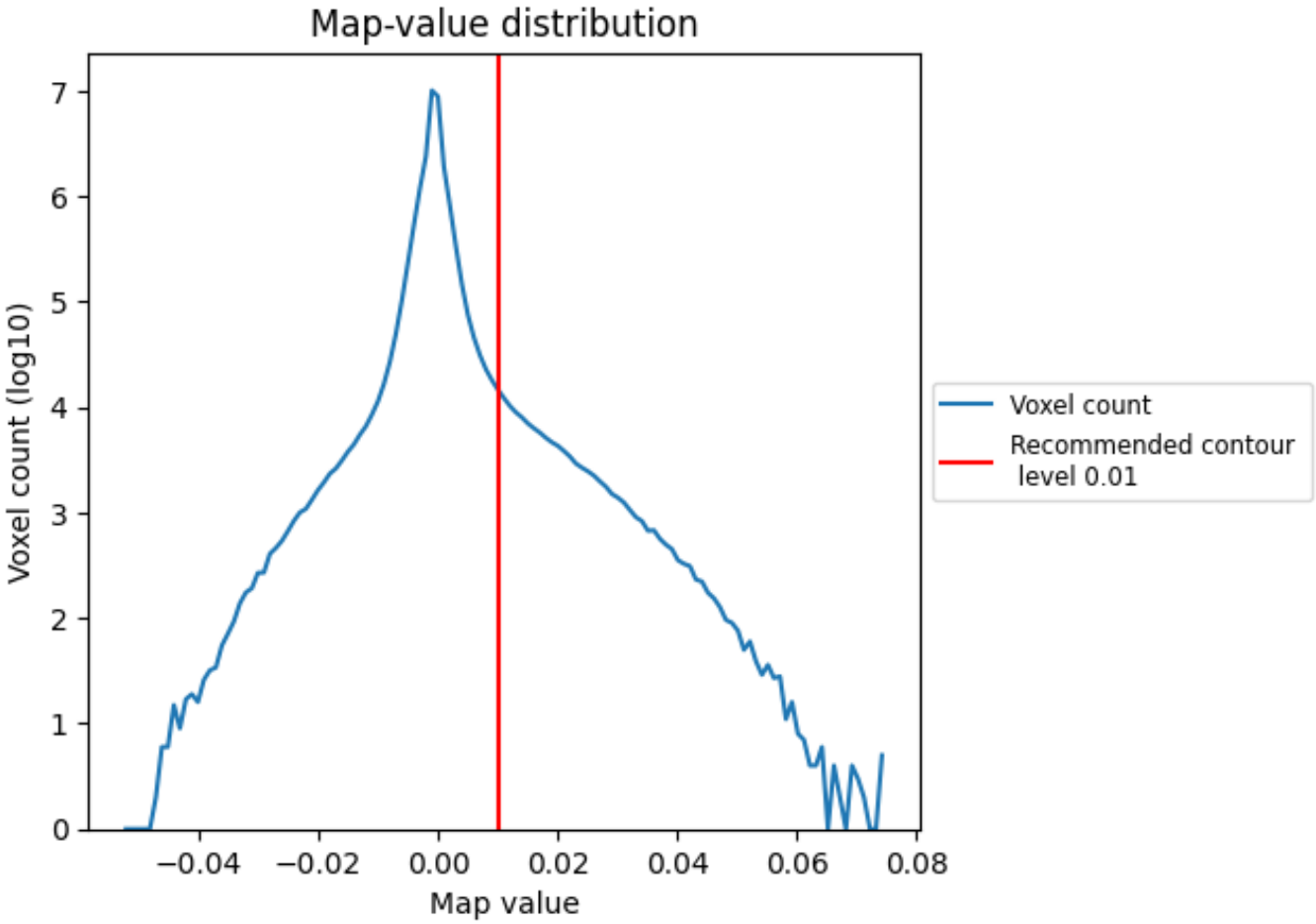
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

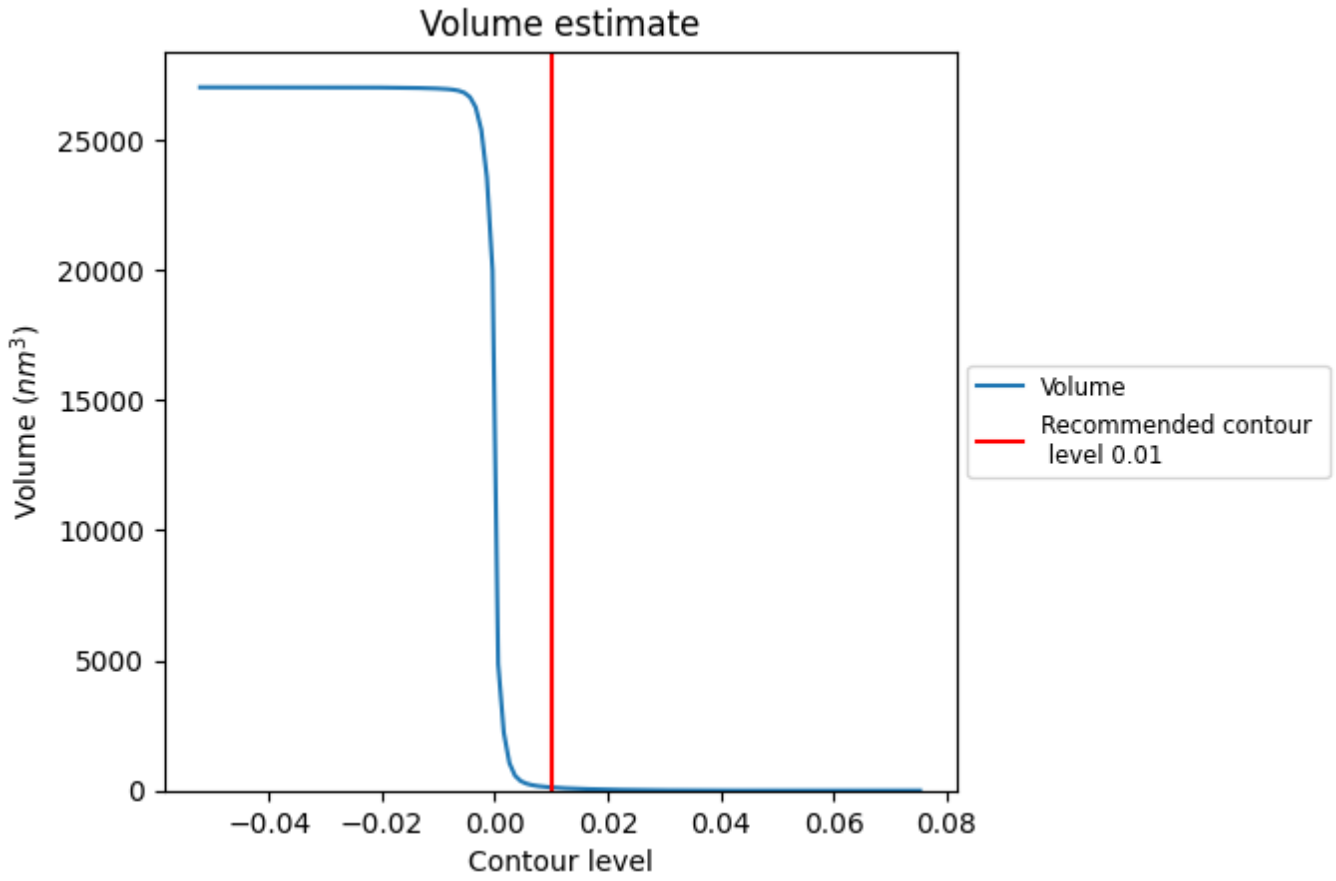
This section contains the results of statistical analysis of the map.

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.

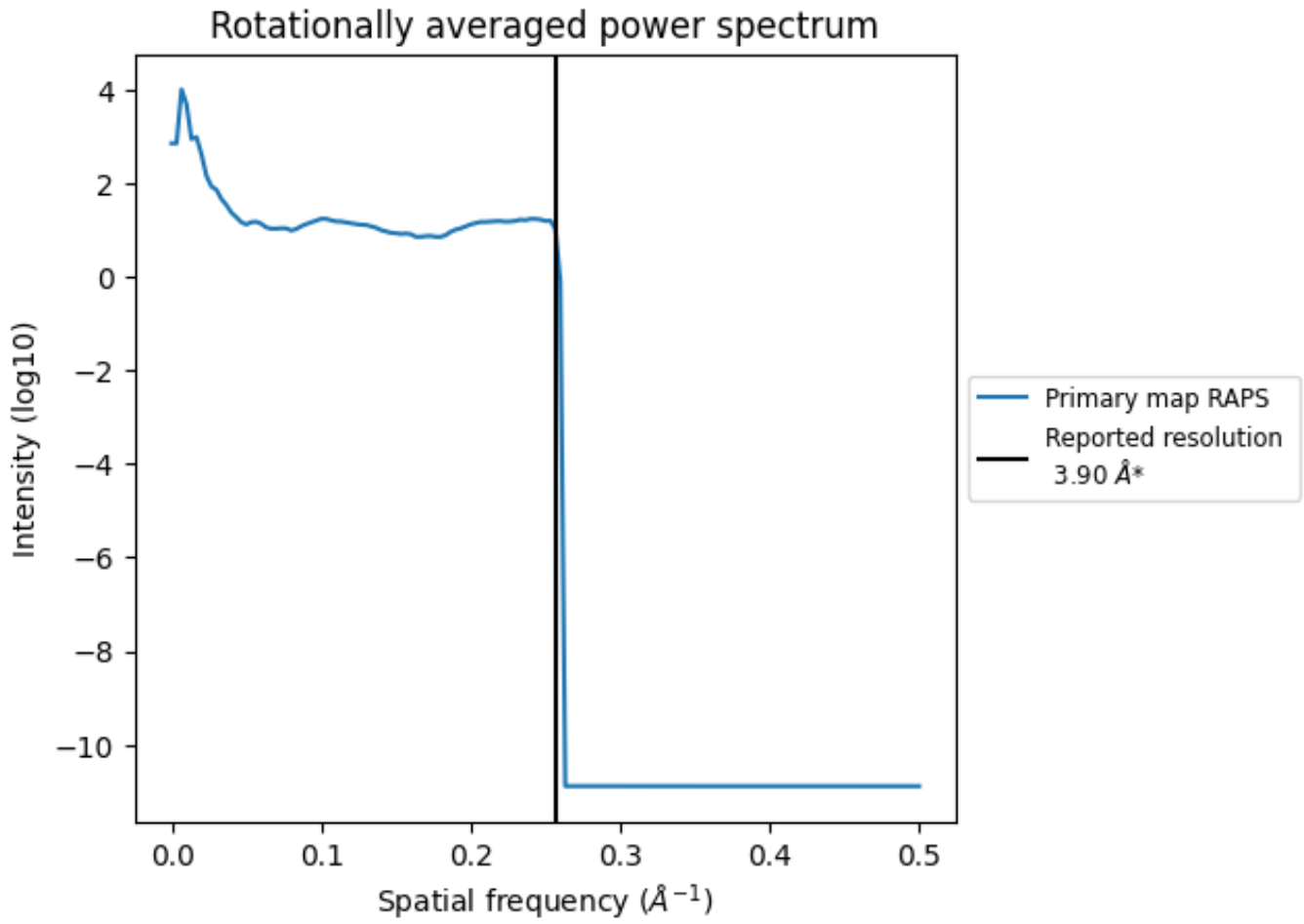
7.2 Volume estimate (i)



The volume at the recommended contour level is 122 nm^3; this corresponds to an approximate mass of 110 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 0.256 Å^{-1}

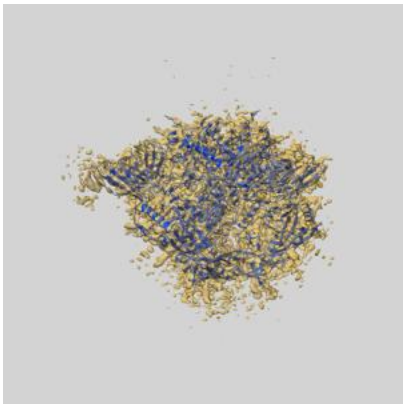
8 Fourier-Shell correlation (i)

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

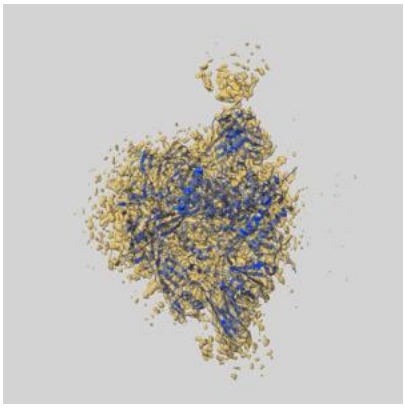
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0485 and PDB model 6NQD. Per-residue inclusion information can be found in section 3 on page 15.

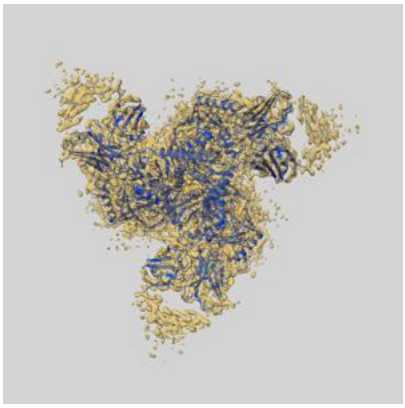
9.1 Map-model overlay



X



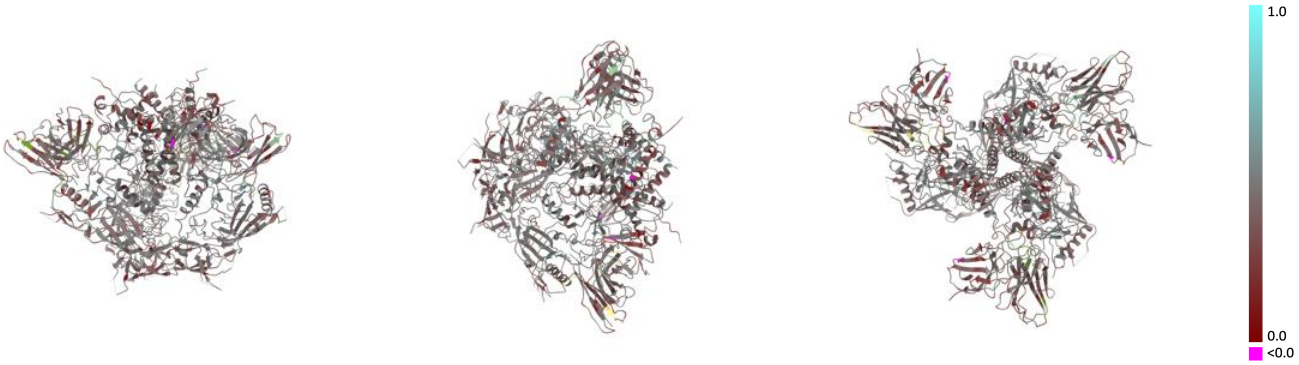
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

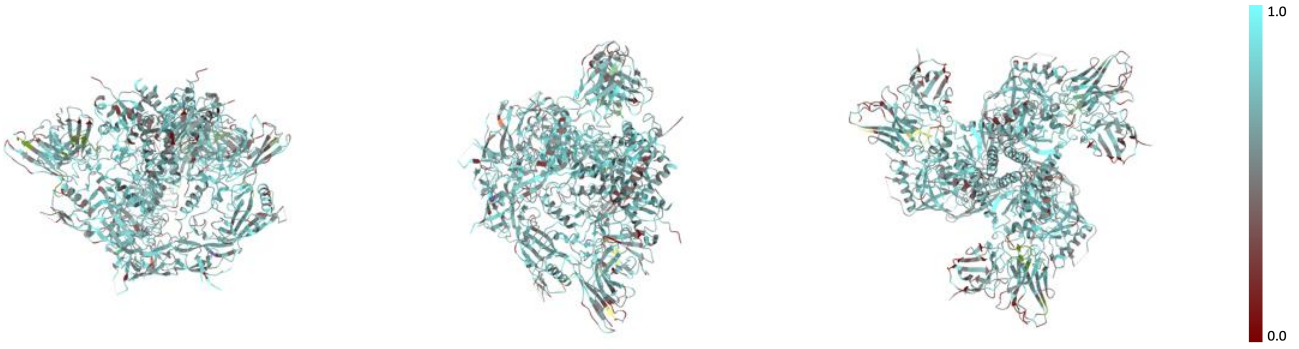
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

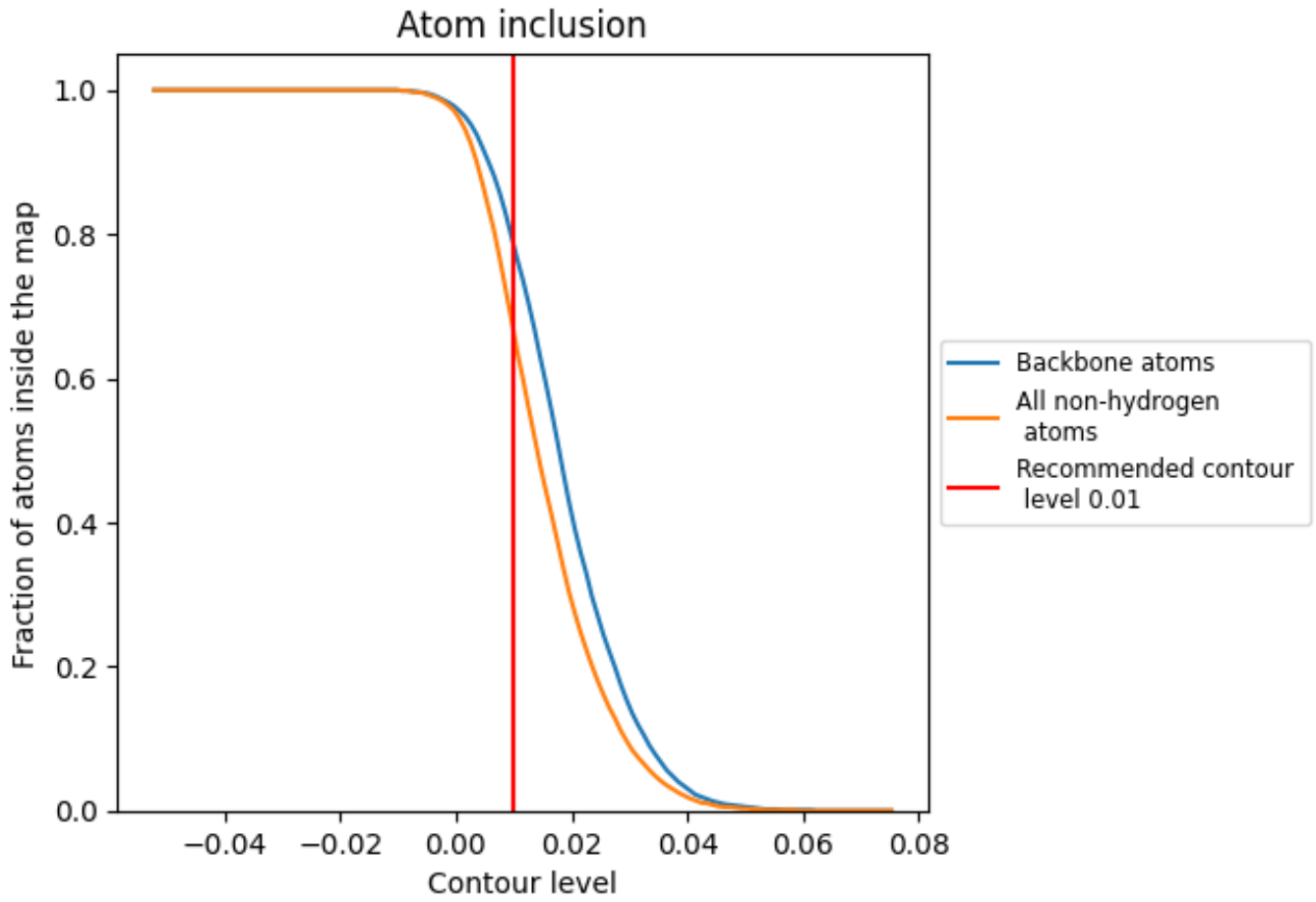
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6640	0.4230
A	0.6890	0.4420
B	0.6560	0.4060
C	0.6560	0.4210
D	0.6270	0.4100
E	0.6910	0.4370
F	0.6540	0.3990
G	0.6380	0.4020
H	0.6030	0.3840
I	0.6920	0.4430
J	0.6530	0.4030
K	0.6580	0.4140
L	0.6180	0.4030
M	0.7840	0.4640
N	0.5970	0.4090
O	0.5360	0.2910
P	0.4290	0.3570
Q	0.5360	0.4170
R	0.6070	0.3780
S	0.3210	0.3130
T	0.3930	0.3250
U	0.6430	0.4110
V	0.6410	0.4510
W	0.5200	0.3950
X	0.7500	0.4380
Y	0.5420	0.4010
Z	0.5000	0.2930
a	0.3930	0.3630
b	0.5360	0.4100
c	0.5710	0.3610
d	0.3210	0.2760
e	0.4290	0.3370
f	0.6430	0.4100
g	0.6410	0.4580
h	0.5000	0.3830

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Chain	Atom inclusion	Q-score
i	0.8020	0.4600
j	0.5830	0.4030
k	0.5360	0.3110
l	0.4290	0.3860
m	0.5710	0.4020
n	0.5710	0.3520
o	0.2860	0.3100
p	0.3930	0.3380
q	0.6430	0.4310
r	0.6410	0.4560
s	0.5400	0.3980