Full wwPDB EM Validation Report

Jun 3, 2025 – 03:45 PM EDT

PDB ID	:	9BTJ / pdb_00009btj
EMDB ID	:	EMD-44892
Title	:	Rhesus Fab 6561-a.01 in complex with HIV-1 Ce1176.A3 RnS SOSIP Env
Authors	:	Gorman, J.; Kwong, P.D.
Deposited on	:	2024-05-15
Resolution	:	4.22 Å(reported)
Based on initial model	:	6VTT

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

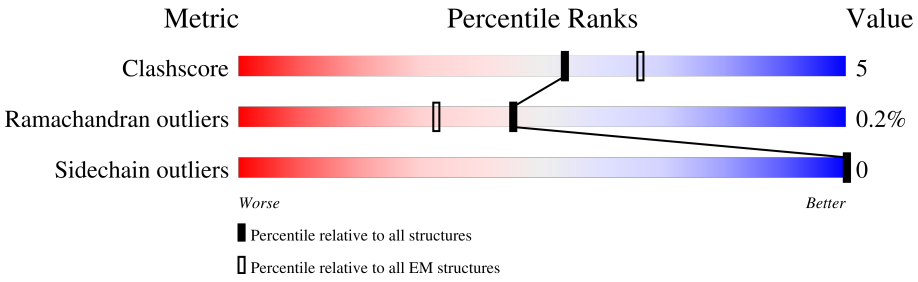
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 4.22 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	L	217	12% 45% 5% 50%
2	H	246	5% 42% 12% • 46%
3	A	477	• 84% 13% •
3	D	477	• 84% 13% •
3	G	477	• 81% 17% •
4	B	153	6% 76% 7% 17%
4	C	153	5% 76% 6% 18%
4	E	153	5% 73% 9% 18%

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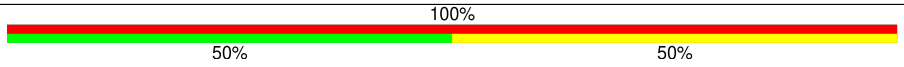
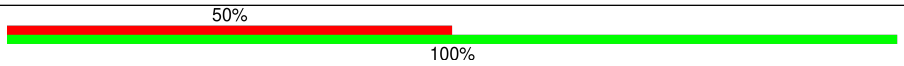
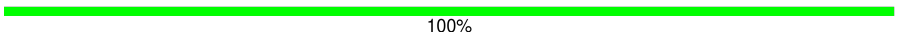
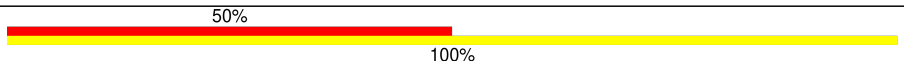
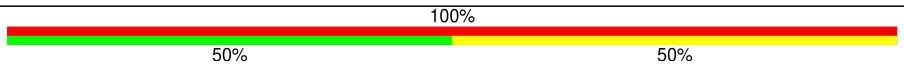
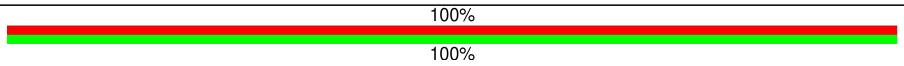
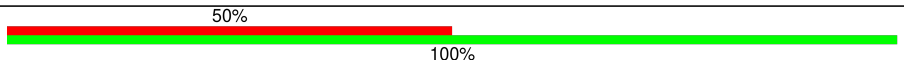
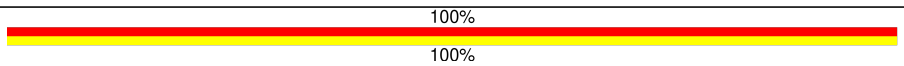
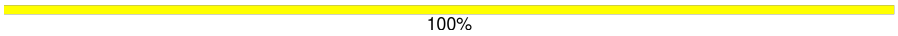
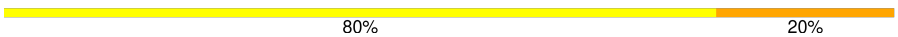
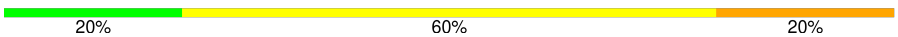
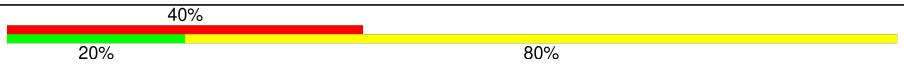
Mol	Chain	Length	Quality of chain
5	F	2	
5	K	2	
5	M	2	
5	Q	2	
5	R	2	
5	S	2	
5	V	2	
5	W	2	
5	Y	2	
5	Z	2	
5	a	2	
5	b	2	
5	c	2	
5	g	2	
5	h	2	
5	i	2	
5	j	2	
5	k	2	
5	l	2	
5	o	2	
6	I	5	
6	N	5	
6	T	5	
6	d	5	
6	n	5	

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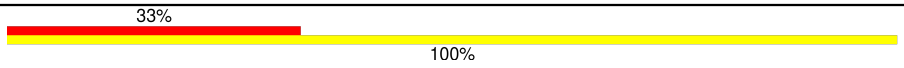
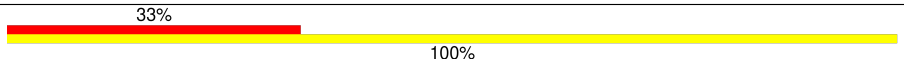
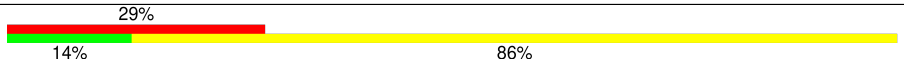
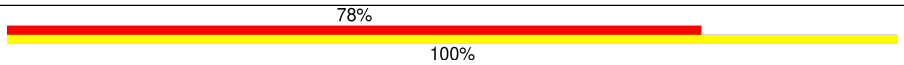
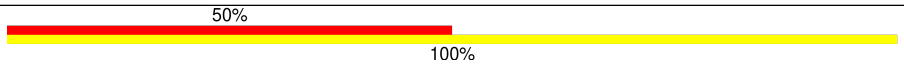
Mol	Chain	Length	Quality of chain
7	J	3	
7	X	3	
7	m	3	
8	O	7	
9	P	8	
10	U	9	
11	e	4	
12	f	6	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 17952 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 Fab 6561-a.01 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	108	Total	C	N	O	S	0	0
			806	497	144	162	3		

- Molecule 2 is a protein called Fab 6561-a.01 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	134	Total	C	N	O	S	0	0
			1106	700	185	217	4		

- Molecule 3 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	464	Total	C	N	O	S	0	0
			3642	2282	640	690	30		
3	A	462	Total	C	N	O	S	0	0
			3630	2276	637	687	30		
3	D	464	Total	C	N	O	S	0	0
			3642	2282	640	690	30		

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	29	GLY	-	expression tag	UNP C6G0D7
G	30	PRO	-	expression tag	UNP C6G0D7
G	31	ALA	-	expression tag	UNP C6G0D7
G	32	GLU	-	expression tag	UNP C6G0D7
G	130	ASN	THR	conflict	UNP C6G0D7
G	201	CYS	ILE	conflict	UNP C6G0D7
G	202	THR	ALA	conflict	UNP C6G0D7
G	204	ILE	ALA	conflict	UNP C6G0D7
G	286	VAL	ILE	conflict	UNP C6G0D7
G	288	LEU	PHE	conflict	UNP C6G0D7
G	302	MET	ASN	conflict	UNP C6G0D7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	320	LEU	THR	conflict	UNP C6G0D7
G	329	PRO	ALA	conflict	UNP C6G0D7
G	333	ILE	VAL	conflict	UNP C6G0D7
G	433	CYS	ALA	conflict	UNP C6G0D7
G	448	ASN	THR	conflict	UNP C6G0D7
G	481	SER	ASN	conflict	UNP C6G0D7
G	501	CYS	ALA	conflict	UNP C6G0D7
G	509	ARG	-	expression tag	UNP C6G0D7
G	510	ARG	-	expression tag	UNP C6G0D7
G	511	ARG	-	expression tag	UNP C6G0D7
G	512	ARG	-	expression tag	UNP C6G0D7
G	513	ARG	-	expression tag	UNP C6G0D7
A	29	GLY	-	expression tag	UNP C6G0D7
A	30	PRO	-	expression tag	UNP C6G0D7
A	31	ALA	-	expression tag	UNP C6G0D7
A	32	GLU	-	expression tag	UNP C6G0D7
A	130	ASN	THR	conflict	UNP C6G0D7
A	201	CYS	ILE	conflict	UNP C6G0D7
A	202	THR	ALA	conflict	UNP C6G0D7
A	204	ILE	ALA	conflict	UNP C6G0D7
A	286	VAL	ILE	conflict	UNP C6G0D7
A	288	LEU	PHE	conflict	UNP C6G0D7
A	302	MET	ASN	conflict	UNP C6G0D7
A	320	LEU	THR	conflict	UNP C6G0D7
A	329	PRO	ALA	conflict	UNP C6G0D7
A	333	ILE	VAL	conflict	UNP C6G0D7
A	433	CYS	ALA	conflict	UNP C6G0D7
A	448	ASN	THR	conflict	UNP C6G0D7
A	481	SER	ASN	conflict	UNP C6G0D7
A	501	CYS	ALA	conflict	UNP C6G0D7
A	509	ARG	-	expression tag	UNP C6G0D7
A	510	ARG	-	expression tag	UNP C6G0D7
A	511	ARG	-	expression tag	UNP C6G0D7
A	512	ARG	-	expression tag	UNP C6G0D7
A	513	ARG	-	expression tag	UNP C6G0D7
D	29	GLY	-	expression tag	UNP C6G0D7
D	30	PRO	-	expression tag	UNP C6G0D7
D	31	ALA	-	expression tag	UNP C6G0D7
D	32	GLU	-	expression tag	UNP C6G0D7
D	130	ASN	THR	conflict	UNP C6G0D7
D	201	CYS	ILE	conflict	UNP C6G0D7
D	202	THR	ALA	conflict	UNP C6G0D7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	204	ILE	ALA	conflict	UNP C6G0D7
D	286	VAL	ILE	conflict	UNP C6G0D7
D	288	LEU	PHE	conflict	UNP C6G0D7
D	302	MET	ASN	conflict	UNP C6G0D7
D	320	LEU	THR	conflict	UNP C6G0D7
D	329	PRO	ALA	conflict	UNP C6G0D7
D	333	ILE	VAL	conflict	UNP C6G0D7
D	433	CYS	ALA	conflict	UNP C6G0D7
D	448	ASN	THR	conflict	UNP C6G0D7
D	481	SER	ASN	conflict	UNP C6G0D7
D	501	CYS	ALA	conflict	UNP C6G0D7
D	509	ARG	-	expression tag	UNP C6G0D7
D	510	ARG	-	expression tag	UNP C6G0D7
D	511	ARG	-	expression tag	UNP C6G0D7
D	512	ARG	-	expression tag	UNP C6G0D7
D	513	ARG	-	expression tag	UNP C6G0D7

- Molecule 4 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	127	Total	C	N	O	S	0	0
			1013	644	172	191	6		
4	C	126	Total	C	N	O	S	0	0
			1009	642	171	190	6		
4	E	125	Total	C	N	O	S	0	0
			1004	639	170	189	6		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	535	ASN	ILE	conflict	UNP C6G0E7
B	559	PRO	ILE	conflict	UNP C6G0E7
B	569	GLY	THR	conflict	UNP C6G0E7
B	573	PHE	ILE	conflict	UNP C6G0E7
B	588	GLU	LYS	conflict	UNP C6G0E7
B	589	VAL	ASP	conflict	UNP C6G0E7
B	605	CYS	THR	conflict	UNP C6G0E7
B	613	THR	SER	conflict	UNP C6G0E7
B	618	THR	SER	conflict	UNP C6G0E7
B	636	GLY	ASP	conflict	UNP C6G0E7
B	651	PHE	ILE	conflict	UNP C6G0E7
B	655	ILE	LYS	conflict	UNP C6G0E7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	535	ASN	ILE	conflict	UNP C6G0E7
C	559	PRO	ILE	conflict	UNP C6G0E7
C	569	GLY	THR	conflict	UNP C6G0E7
C	573	PHE	ILE	conflict	UNP C6G0E7
C	588	GLU	LYS	conflict	UNP C6G0E7
C	589	VAL	ASP	conflict	UNP C6G0E7
C	605	CYS	THR	conflict	UNP C6G0E7
C	613	THR	SER	conflict	UNP C6G0E7
C	618	THR	SER	conflict	UNP C6G0E7
C	636	GLY	ASP	conflict	UNP C6G0E7
C	651	PHE	ILE	conflict	UNP C6G0E7
C	655	ILE	LYS	conflict	UNP C6G0E7
E	535	ASN	ILE	conflict	UNP C6G0E7
E	559	PRO	ILE	conflict	UNP C6G0E7
E	569	GLY	THR	conflict	UNP C6G0E7
E	573	PHE	ILE	conflict	UNP C6G0E7
E	588	GLU	LYS	conflict	UNP C6G0E7
E	589	VAL	ASP	conflict	UNP C6G0E7
E	605	CYS	THR	conflict	UNP C6G0E7
E	613	THR	SER	conflict	UNP C6G0E7
E	618	THR	SER	conflict	UNP C6G0E7
E	636	GLY	ASP	conflict	UNP C6G0E7
E	651	PHE	ILE	conflict	UNP C6G0E7
E	655	ILE	LYS	conflict	UNP C6G0E7

- Molecule 5 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
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		

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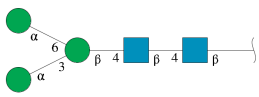
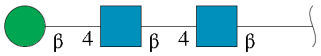
Mol	Chain	Residues	Atoms				AltConf	Trace
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	a	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	g	2	Total	C	N	O	0	0
			28	16	2	10		
5	h	2	Total	C	N	O	0	0
			28	16	2	10		
5	i	2	Total	C	N	O	0	0
			28	16	2	10		
5	j	2	Total	C	N	O	0	0
			28	16	2	10		
5	k	2	Total	C	N	O	0	0
			28	16	2	10		
5	l	2	Total	C	N	O	0	0
			28	16	2	10		
5	o	2	Total	C	N	O	0	0
			28	16	2	10		

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



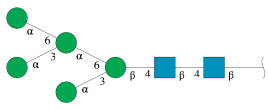
Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	5	Total	C	N	O	0	0
			61	34	2	25		
6	N	5	Total	C	N	O	0	0
			61	34	2	25		
6	T	5	Total	C	N	O	0	0
			61	34	2	25		
6	d	5	Total	C	N	O	0	0
			61	34	2	25		
6	n	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 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.



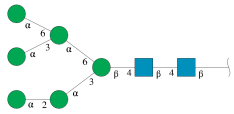
Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	3	Total	C	N	O	0	0
			39	22	2	15		
7	X	3	Total	C	N	O	0	0
			39	22	2	15		
7	m	3	Total	C	N	O	0	0
			39	22	2	15		

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



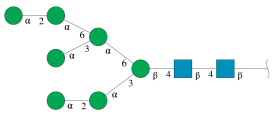
Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	7	Total	C	N	O	0	0
			83	46	2	35		

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



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

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

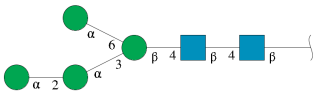


Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 11 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.

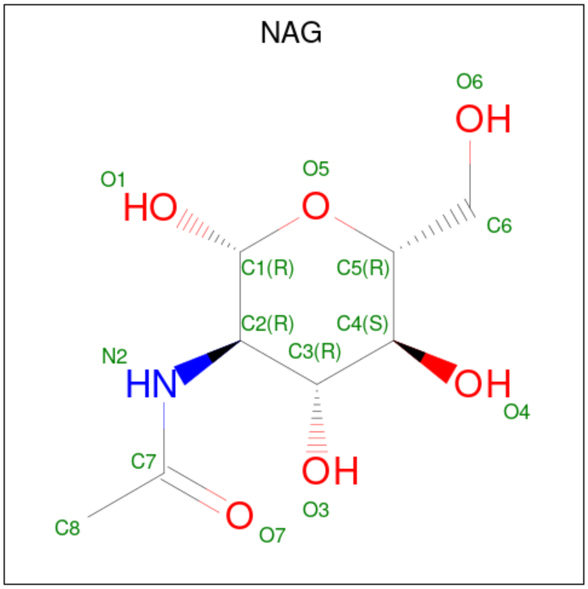
Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 12 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
12	f	6	Total 72	C 40	N 2	O 30	0	0

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



Mol	Chain	Residues	Atoms				AltConf
13	G	1	Total 14	C 8	N 1	O 5	0
13	G	1	Total 14	C 8	N 1	O 5	0
13	G	1	Total 14	C 8	N 1	O 5	0
13	G	1	Total 14	C 8	N 1	O 5	0
13	G	1	Total 14	C 8	N 1	O 5	0
13	G	1	Total 14	C 8	N 1	O 5	0
13	G	1	Total 14	C 8	N 1	O 5	0
13	G	1	Total 14	C 8	N 1	O 5	0
13	G	1	Total 14	C 8	N 1	O 5	0
13	G	1	Total 14	C 8	N 1	O 5	0

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

Continued on next page...

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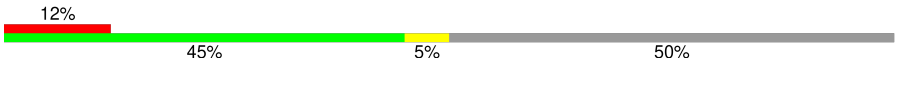
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total 14	C 8	N 1	O 5	0
13	A	1	Total 14	C 8	N 1	O 5	0
13	A	1	Total 14	C 8	N 1	O 5	0
13	C	1	Total 14	C 8	N 1	O 5	0
13	C	1	Total 14	C 8	N 1	O 5	0
13	C	1	Total 14	C 8	N 1	O 5	0
13	D	1	Total 14	C 8	N 1	O 5	0
13	D	1	Total 14	C 8	N 1	O 5	0
13	D	1	Total 14	C 8	N 1	O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

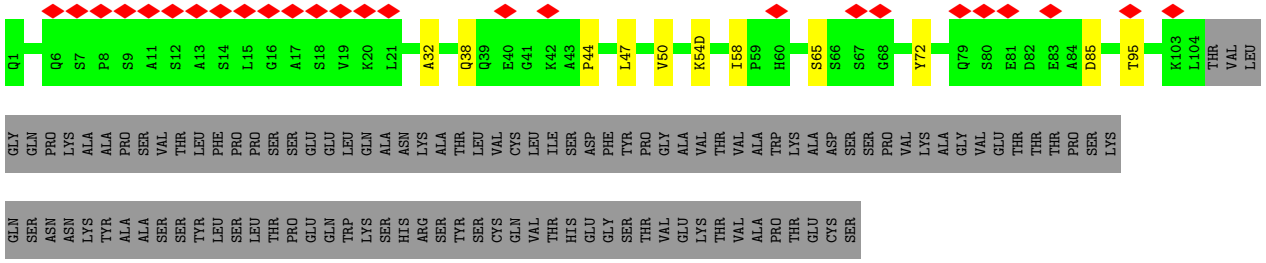
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Fab 6561-a.01 light chain

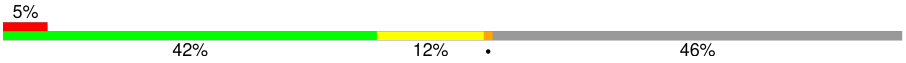
Chain L:

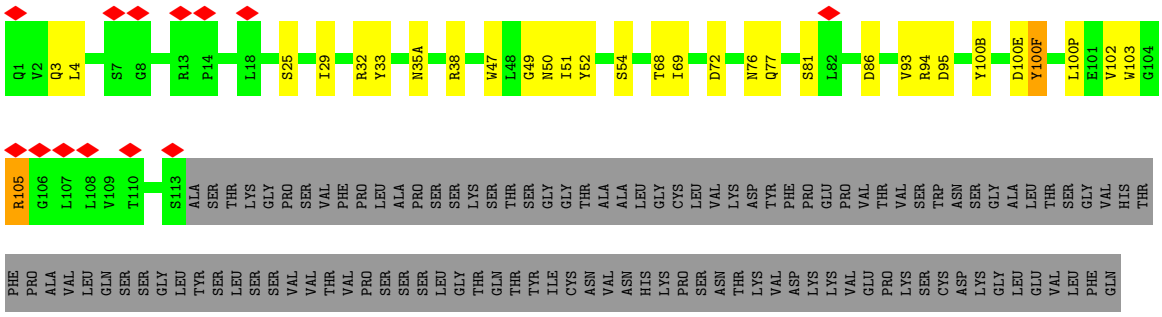




• Molecule 2: Fab 6561-a.01 heavy chain

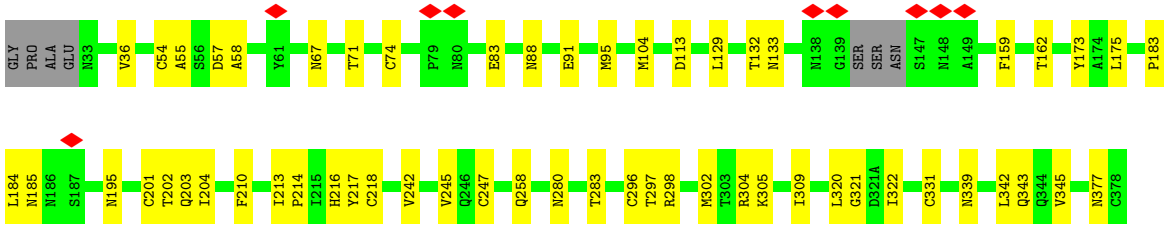
Chain H:

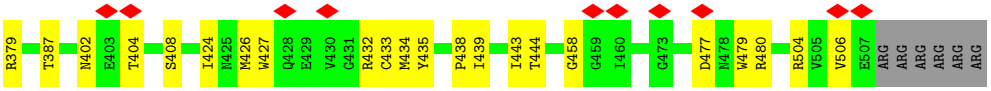




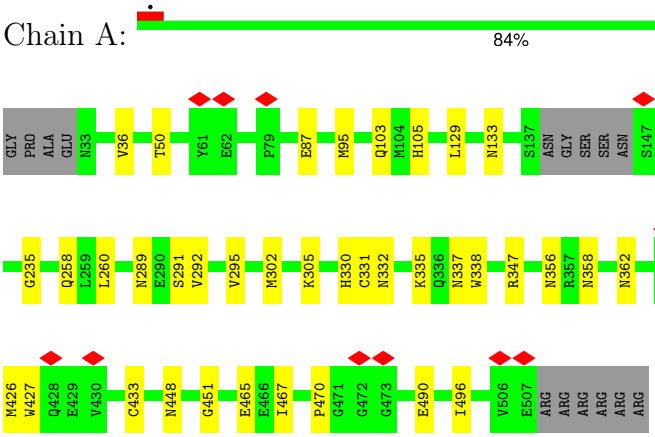
• Molecule 3: Envelope glycoprotein gp120

Chain G:

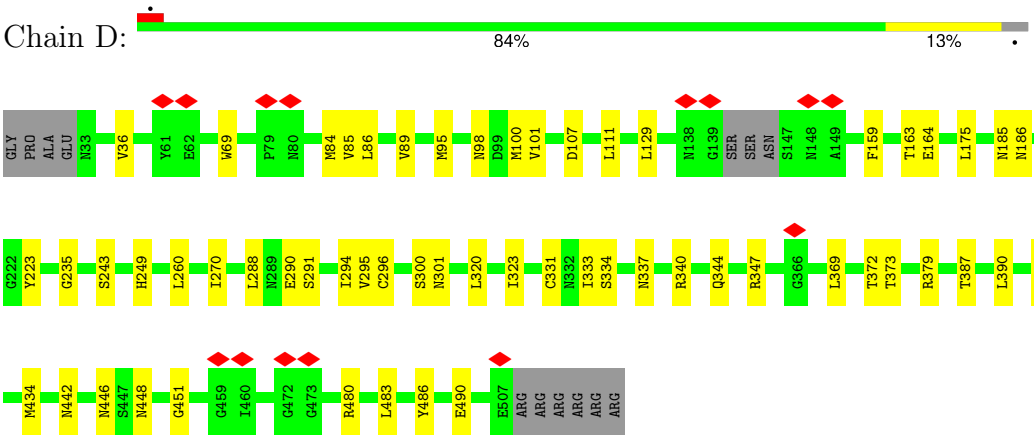




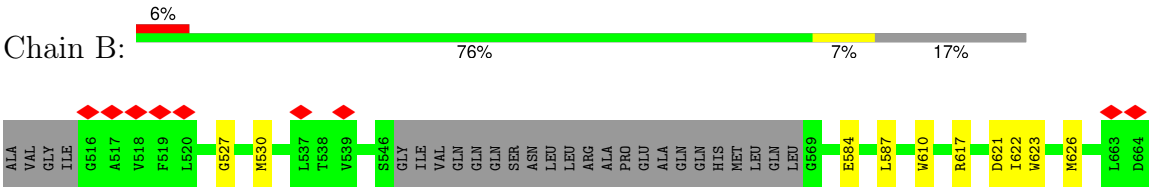
• Molecule 3: Envelope glycoprotein gp120



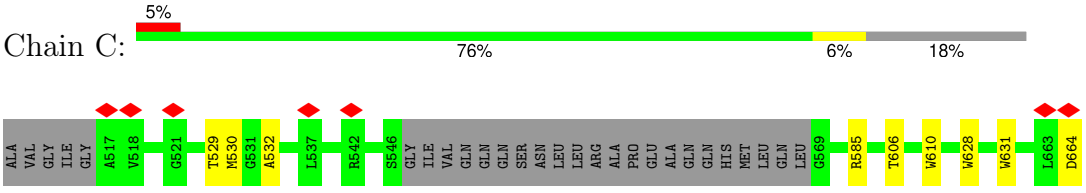
• Molecule 3: Envelope glycoprotein gp120



• Molecule 4: Envelope glycoprotein gp41

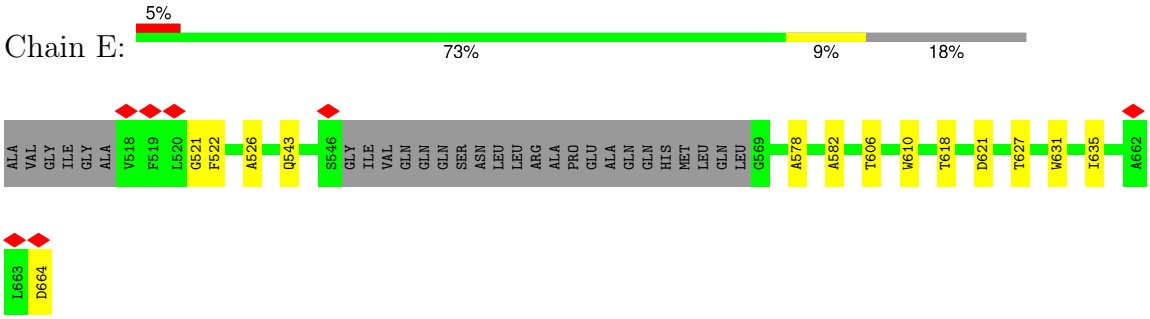


• Molecule 4: Envelope glycoprotein gp41



• Molecule 4: Envelope glycoprotein gp41

Chain E:



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

Chain F:

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

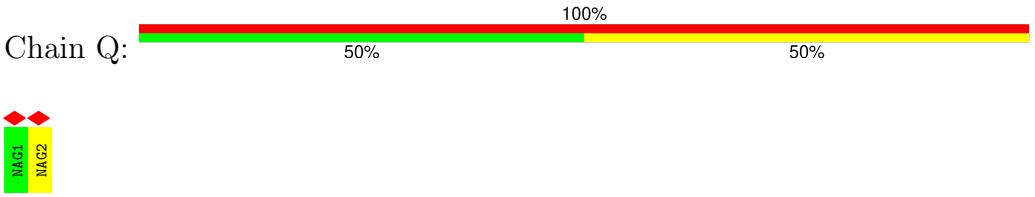
Chain K:

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

Chain M:

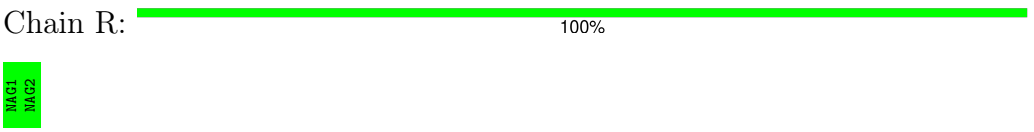
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



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

Chain R:



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

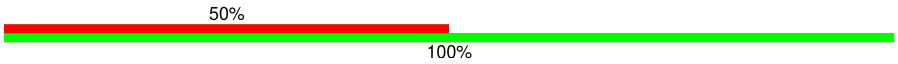
Chain S:

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

Chain V:

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

Chain W:



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

Chain Y:

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

Chain Z:

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

Chain a:

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

Chain b:

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

Chain c:

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

Chain g:

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

Chain h:

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

Chain i:

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

Chain j:

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

Chain k:

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

Chain l:

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

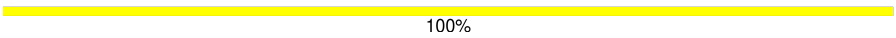
Chain o:

• Molecule 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:

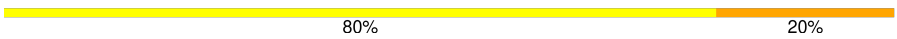
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

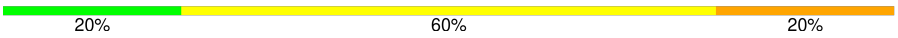
Chain T:



• Molecule 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-glucopyra

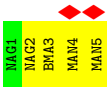
nose

Chain d:



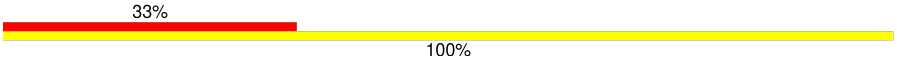
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:



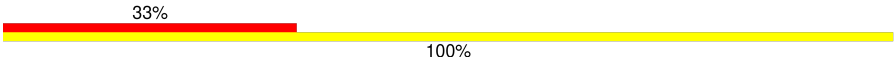
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



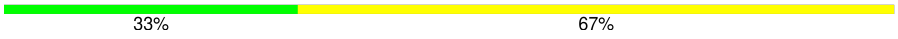
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



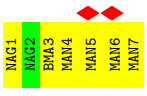
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



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

Chain O:



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

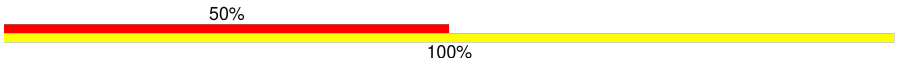
Chain P:

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

Chain U:

• Molecule 11: 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 e:



• Molecule 12: 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 f:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	150641	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 ($e^-/Å^2$)	69.48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.295	Depositor
Minimum map value	-0.228	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	309.1104, 309.1104, 309.1104	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0733, 1.0733, 1.0733	Depositor

5 Model quality

5.1 Standard geometry

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

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	L	0.10	0/824	0.29	0/1116
2	H	0.13	0/1100	0.45	1/1493 (0.1%)
3	A	0.12	0/3708	0.34	0/5038
3	D	0.13	0/3720	0.34	0/5054
3	G	0.13	0/3720	0.36	0/5054
4	B	0.10	0/1034	0.29	0/1403
4	C	0.11	0/1030	0.32	0/1398
4	E	0.08	0/1025	0.24	0/1391
All	All	0.12	0/16161	0.34	1/21947 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	33	TYR	CB-CA-C	-5.68	110.04	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	806	0	766	9	0
2	H	1106	0	1045	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3630	0	3541	42	0
3	D	3642	0	3552	41	0
3	G	3642	0	3551	52	0
4	B	1013	0	972	7	0
4	C	1009	0	969	7	0
4	E	1004	0	964	10	0
5	F	28	0	25	0	0
5	K	28	0	25	0	0
5	M	28	0	25	0	0
5	Q	28	0	25	0	0
5	R	28	0	25	0	0
5	S	28	0	25	0	0
5	V	28	0	25	1	0
5	W	28	0	25	0	0
5	Y	28	0	25	0	0
5	Z	28	0	25	0	0
5	a	28	0	25	0	0
5	b	28	0	25	0	0
5	c	28	0	25	0	0
5	g	28	0	25	0	0
5	h	28	0	25	0	0
5	i	28	0	25	0	0
5	j	28	0	25	0	0
5	k	28	0	25	0	0
5	l	28	0	25	0	0
5	o	28	0	25	0	0
6	I	61	0	52	2	0
6	N	61	0	52	0	0
6	T	61	0	52	1	0
6	d	61	0	52	3	0
6	n	61	0	52	0	0
7	J	39	0	34	0	0
7	X	39	0	34	0	0
7	m	39	0	34	0	0
8	O	83	0	70	0	0
9	P	94	0	79	1	0
10	U	105	0	88	0	0
11	e	50	0	43	0	0
12	f	72	0	61	0	0
13	A	210	0	195	3	0
13	B	42	0	39	0	0
13	C	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D	154	0	143	0	0
13	E	42	0	39	0	0
13	G	224	0	208	3	0
All	All	17952	0	17226	176	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (176) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100(E):ASP:OD1	2:H:100(F):TYS:N	2.13	0.80
3:D:84:MET:HE1	4:E:521:GLY:HA3	1.70	0.73
2:H:32:ARG:HB3	2:H:94:ARG:HH21	1.57	0.70
3:A:347:ARG:O	3:A:347:ARG:NH1	2.24	0.70
3:D:101:VAL:HG21	3:D:480:ARG:HD3	1.75	0.68
3:D:100:MET:HG3	3:D:483:LEU:HD13	1.76	0.68
3:D:296:CYS:HB3	3:D:331:CYS:HA	1.76	0.67
3:G:104:MET:HG2	3:G:217:TYR:HE2	1.59	0.67
3:G:339:ASN:HA	3:G:342:LEU:HB2	1.78	0.65
3:D:95:MET:HA	3:D:98:ASN:HB2	1.79	0.65
4:B:584:GLU:HA	4:B:587:LEU:HB2	1.78	0.64
3:G:402:ASN:ND2	3:G:404:THR:OG1	2.31	0.64
3:A:402:ASN:ND2	3:A:404:THR:OG1	2.31	0.64
4:B:530:MET:HB2	4:B:623:TRP:HA	1.80	0.63
3:G:201:CYS:HB2	3:G:433:CYS:H	1.62	0.63
3:D:69:TRP:HA	3:D:111:LEU:HD23	1.82	0.62
2:H:35(A):ASN:HB2	2:H:93:VAL:HB	1.82	0.62
3:D:291:SER:HB2	3:D:448:ASN:HB3	1.82	0.62
3:A:179:LEU:HD11	3:A:419:ARG:HD3	1.82	0.61
3:A:170:LYS:NZ	3:A:172:GLU:OE2	2.28	0.61
2:H:47:TRP:HZ2	2:H:50:ASN:HB2	1.66	0.60
3:D:379:ARG:HH12	6:d:3:BMA:H3	1.66	0.60
2:H:38:ARG:NH2	2:H:86:ASP:O	2.35	0.60
3:G:204:ILE:HD11	3:G:434:MET:HB3	1.83	0.60
3:D:340:ARG:HG2	3:D:344:GLN:HE22	1.67	0.59
3:A:295:VAL:HB	3:A:332:ASN:HB2	1.83	0.59
3:D:379:ARG:NH2	6:d:3:BMA:O4	2.31	0.58
3:A:133:ASN:HB2	13:A:612:NAG:N2	2.18	0.58
3:D:270:ILE:HG12	3:D:288:LEU:HA	1.85	0.58
3:D:295:VAL:HG12	3:D:446:ASN:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:95:MET:HE1	3:D:235:GLY:HA2	1.86	0.57
3:D:290:GLU:OE2	3:D:340:ARG:NH2	2.38	0.56
3:G:55:ALA:HB3	3:G:216:HIS:HB2	1.88	0.56
3:G:113:ASP:OD1	3:G:432:ARG:NH1	2.39	0.55
3:A:291:SER:HB2	3:A:448:ASN:HB3	1.89	0.55
3:G:36:VAL:HG22	4:B:610:TRP:HE3	1.69	0.55
3:A:335:LYS:HD3	3:A:414:ILE:HD11	1.87	0.55
3:G:297:THR:OG1	3:G:443:ILE:O	2.14	0.55
3:A:50:THR:O	3:A:103:GLN:NE2	2.39	0.55
3:G:280:ASN:HD22	3:G:458:GLY:HA3	1.72	0.55
2:H:47:TRP:NE1	2:H:49:GLY:O	2.37	0.54
3:A:195:ASN:ND2	3:A:433:CYS:SG	2.77	0.54
1:L:44:PRO:HB2	2:H:103:TRP:CZ3	2.43	0.53
3:A:362:ASN:HD22	3:A:467:ILE:HG23	1.74	0.53
3:G:195:ASN:ND2	3:G:201:CYS:SG	2.77	0.53
2:H:100(P):LEU:HD23	2:H:103:TRP:HE1	1.74	0.53
3:G:296:CYS:HB3	3:G:331:CYS:HA	1.91	0.52
3:G:302:MET:HE2	3:G:322:ILE:HG12	1.90	0.52
3:D:344:GLN:HA	3:D:347:ARG:HG2	1.91	0.52
3:G:83:GLU:HG3	3:G:245:VAL:HG23	1.92	0.52
3:G:91:GLU:HB3	3:G:242:VAL:HG21	1.90	0.52
2:H:51:ILE:HB	2:H:69:ILE:HG21	1.90	0.52
3:G:213:ILE:HD12	3:G:214:PRO:HD2	1.92	0.52
1:L:38:GLN:HA	1:L:44:PRO:HB3	1.92	0.52
3:G:210:PHE:HE2	3:G:377:ASN:HD21	1.58	0.52
3:A:496:ILE:O	4:C:631:TRP:NE1	2.42	0.52
3:G:95:MET:HE1	3:G:480:ARG:HB3	1.92	0.51
3:A:192:ARG:NH1	3:A:193:LEU:O	2.40	0.51
3:G:104:MET:HG2	3:G:217:TYR:CE2	2.42	0.51
3:G:304:ARG:NH2	3:G:438:PRO:O	2.33	0.51
3:D:36:VAL:HG22	4:E:610:TRP:HE3	1.75	0.51
3:G:504:ARG:HH12	3:G:506:VAL:HA	1.75	0.51
3:G:88:ASN:OD1	13:G:611:NAG:N2	2.44	0.50
3:G:305:LYS:HE2	3:G:321:GLY:HA2	1.93	0.50
2:H:29:ILE:HG22	2:H:76:ASN:HA	1.93	0.50
3:G:183:PRO:O	3:G:185:ASN:N	2.45	0.50
3:A:183:PRO:O	3:A:185:ASN:N	2.45	0.50
2:H:3:GLN:HB2	2:H:25:SER:HB3	1.94	0.50
3:A:368:ASP:N	3:A:368:ASP:OD1	2.45	0.50
3:D:379:ARG:HH22	6:d:3:BMA:HO4	1.56	0.50
2:H:52:TYR:HD2	2:H:54:SER:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:88:ASN:HB2	4:B:527:GLY:HA3	1.94	0.49
3:A:36:VAL:HG22	4:C:610:TRP:HE3	1.77	0.49
2:H:68:THR:OG1	2:H:81:SER:OG	2.26	0.49
3:G:379:ARG:NH2	6:I:3:BMA:O4	2.46	0.49
4:C:530:MET:HG2	4:C:628:TRP:CD1	2.48	0.49
3:G:55:ALA:N	3:G:216:HIS:O	2.46	0.48
3:G:439:ILE:HD13	3:G:443:ILE:HG12	1.94	0.48
3:A:490:GLU:OE2	4:C:585:ARG:NH1	2.46	0.48
4:E:522:PHE:HB2	4:E:543:GLN:HG3	1.94	0.48
3:D:294:ILE:HD12	3:D:333:ILE:HD11	1.95	0.48
3:G:133:ASN:OD1	13:G:612:NAG:N2	2.47	0.47
3:G:203:GLN:HG3	3:G:435:TYR:HD2	1.79	0.47
3:A:379:ARG:NH2	6:T:3:BMA:O4	2.42	0.47
3:G:175:LEU:HB2	3:G:320:LEU:HB2	1.95	0.47
3:A:292:VAL:HG12	3:A:337:ASN:HB3	1.96	0.47
3:A:129:LEU:HD13	3:A:192:ARG:HA	1.97	0.47
3:A:332:ASN:HD22	3:A:413:THR:HG21	1.79	0.47
2:H:102:VAL:HG23	2:H:103:TRP:H	1.80	0.47
3:G:283:THR:OG1	3:G:477:ASP:OD2	2.31	0.47
3:G:298:ARG:NH2	3:G:302:MET:SD	2.83	0.47
3:G:173:TYR:O	3:G:305:LYS:NZ	2.37	0.47
3:G:218:CYS:HA	3:G:247:CYS:HB2	1.96	0.47
3:A:358:ASN:HB2	3:A:465:GLU:HA	1.95	0.47
3:G:424:ILE:HG22	3:G:426:MET:HE3	1.98	0.46
1:L:38:GLN:N	1:L:85:ASP:O	2.44	0.46
1:L:54(D):LYS:HB3	1:L:58:ILE:HB	1.98	0.46
3:G:408:SER:HB3	13:G:613:NAG:H82	1.97	0.46
3:A:105:HIS:HE2	3:A:427:TRP:CD1	2.33	0.46
3:A:385:CYS:HA	3:A:418:CYS:CB	2.46	0.46
3:D:129:LEU:HD23	3:D:159:PHE:HB3	1.98	0.46
3:A:347:ARG:HH11	3:A:347:ARG:C	2.19	0.45
3:D:185:ASN:OD1	3:D:186:ASN:ND2	2.49	0.45
3:D:426:MET:HG2	3:D:427:TRP:CE2	2.50	0.45
1:L:44:PRO:HB2	2:H:103:TRP:HZ3	1.82	0.45
3:G:54:CYS:SG	3:G:55:ALA:N	2.89	0.45
3:A:260:LEU:HB2	3:A:451:GLY:H	1.82	0.45
3:G:379:ARG:HH21	6:I:3:BMA:H3	1.82	0.45
3:G:258:GLN:NE2	3:G:387:THR:OG1	2.38	0.45
3:A:258:GLN:NE2	3:A:372:THR:O	2.50	0.45
4:E:631:TRP:O	4:E:635:ILE:HG12	2.17	0.45
3:G:162:THR:OG1	3:G:309:ILE:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:ASN:OD1	2:H:51:ILE:N	2.50	0.44
4:B:584:GLU:OE1	4:B:584:GLU:N	2.34	0.44
3:D:220:PRO:HG3	4:E:578:ALA:HB1	1.99	0.44
2:H:93:VAL:HG21	2:H:100(P):LEU:HD23	1.99	0.44
3:D:163:THR:OG1	3:D:164:GLU:N	2.51	0.44
3:G:129:LEU:HD23	3:G:159:PHE:HB3	1.99	0.44
3:A:163:THR:HG23	3:A:165:ILE:H	1.82	0.44
3:A:173:TYR:O	3:A:305:LYS:NZ	2.50	0.44
3:D:175:LEU:HB2	3:D:320:LEU:HB2	1.99	0.44
4:E:618:THR:HG23	4:E:621:ASP:H	1.83	0.44
3:D:300:SER:H	3:D:442:ASN:HB3	1.84	0.43
3:G:297:THR:HB	3:G:444:THR:HG23	2.00	0.43
3:A:87:GLU:N	3:A:87:GLU:OE2	2.51	0.43
3:A:330:HIS:HB2	3:A:415:THR:HG23	2.01	0.43
1:L:95:THR:H	2:H:47:TRP:HZ3	1.66	0.43
4:B:622:ILE:HA	4:B:626:MET:HE3	2.00	0.43
3:A:260:LEU:HD12	3:A:451:GLY:HA3	2.01	0.43
3:A:332:ASN:OD1	13:A:607:NAG:N2	2.52	0.43
4:C:529:THR:HG23	4:C:532:ALA:H	1.84	0.43
3:D:36:VAL:O	4:E:606:THR:OG1	2.35	0.42
1:L:47:LEU:HD13	1:L:58:ILE:HD12	2.00	0.42
3:A:356:ASN:HB2	5:V:2:NAG:H62	2.02	0.42
3:D:372:THR:HG23	3:D:373:THR:HG23	2.01	0.42
3:D:387:THR:HG23	3:D:390:LEU:HD12	2.02	0.42
3:A:426:MET:HG3	3:A:427:TRP:CE3	2.54	0.42
3:G:104:MET:HE1	3:G:479:TRP:CD2	2.54	0.42
3:A:154:MET:HE1	3:A:302:MET:HE1	2.00	0.42
3:D:260:LEU:HD12	3:D:451:GLY:HA3	2.00	0.42
4:C:664:ASP:N	4:C:664:ASP:OD1	2.53	0.42
1:L:65:SER:O	1:L:72:TYR:N	2.52	0.42
3:G:339:ASN:O	3:G:343:GLN:N	2.45	0.42
4:B:617:ARG:NH2	4:B:621:ASP:OD2	2.52	0.42
3:D:204:ILE:HD11	3:D:434:MET:HB3	2.02	0.42
4:E:526:ALA:O	4:E:627:THR:OG1	2.36	0.42
3:A:391:PHE:HE1	3:A:470:PRO:HB3	1.84	0.41
9:P:3:BMA:H61	9:P:6:MAN:H2	1.74	0.41
2:H:94:ARG:NH1	2:H:95:ASP:O	2.53	0.41
3:D:86:LEU:HB3	3:D:89:VAL:HG11	2.01	0.41
3:G:71:THR:HA	3:G:74:CYS:SG	2.61	0.41
3:D:221:ALA:HB3	4:E:582:ALA:HB1	2.02	0.41
3:G:57:ASP:OD1	3:G:58:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:ASP:HB3	2:H:77:GLN:O	2.20	0.41
3:A:289:ASN:ND2	13:A:605:NAG:O7	2.53	0.41
3:D:369:LEU:HA	3:D:372:THR:HG22	2.03	0.41
3:D:426:MET:HG2	3:D:427:TRP:CD2	2.55	0.41
4:E:664:ASP:N	4:E:664:ASP:OD1	2.53	0.41
2:H:4:LEU:O	2:H:105:ARG:NH1	2.53	0.41
3:G:426:MET:HG2	3:G:427:TRP:CE3	2.56	0.41
3:G:67:ASN:HD21	3:G:213:ILE:HG21	1.85	0.41
3:G:202:THR:OG1	3:G:203:GLN:N	2.54	0.41
3:A:36:VAL:O	4:C:606:THR:OG1	2.34	0.41
3:A:95:MET:HE2	3:A:235:GLY:HA3	2.03	0.41
3:D:334:SER:HB3	3:D:337:ASN:HB2	2.03	0.41
1:L:32:ALA:HB1	1:L:50:VAL:O	2.21	0.40
3:G:132:THR:OG1	3:G:133:ASN:N	2.54	0.40
3:D:85:VAL:HA	3:D:243:SER:HB2	2.02	0.40
3:D:163:THR:OG1	3:D:164:GLU:OE1	2.38	0.40
3:G:342:LEU:HA	3:G:345:VAL:HG12	2.03	0.40
3:D:107:ASP:OD2	3:D:217:TYR:OH	2.28	0.40
3:D:301:ASN:OD1	3:D:323:ILE:HB	2.22	0.40
3:A:331:CYS:HB2	3:A:416:LEU:HB2	2.04	0.40
3:D:249:HIS:ND1	3:D:486:TYR:OH	2.42	0.40
3:A:338:TRP:HZ2	3:A:391:PHE:HE2	1.69	0.40
3:D:223:TYR:CE1	3:D:490:GLU:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	L	106/217 (49%)	100 (94%)	6 (6%)	0	100	100
2	H	130/246 (53%)	115 (88%)	14 (11%)	1 (1%)	16	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	458/477 (96%)	433 (94%)	24 (5%)	1 (0%)	44 77
3	D	460/477 (96%)	442 (96%)	18 (4%)	0	100 100
3	G	460/477 (96%)	435 (95%)	24 (5%)	1 (0%)	44 77
4	B	123/153 (80%)	121 (98%)	2 (2%)	0	100 100
4	C	122/153 (80%)	117 (96%)	5 (4%)	0	100 100
4	E	121/153 (79%)	120 (99%)	1 (1%)	0	100 100
All	All	1980/2353 (84%)	1883 (95%)	94 (5%)	3 (0%)	45 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	184	LEU
3	A	184	LEU
2	H	105	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	L	87/181 (48%)	87 (100%)	0	100 100
2	H	119/216 (55%)	119 (100%)	0	100 100
3	A	412/424 (97%)	412 (100%)	0	100 100
3	D	413/424 (97%)	413 (100%)	0	100 100
3	G	413/424 (97%)	413 (100%)	0	100 100
4	B	107/128 (84%)	107 (100%)	0	100 100
4	C	107/128 (84%)	107 (100%)	0	100 100
4	E	107/128 (84%)	107 (100%)	0	100 100
All	All	1765/2053 (86%)	1765 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	36	HIS
1	L	38	GLN
2	H	5	GLN
2	H	59	HIS
3	G	105	HIS
3	G	216	HIS
3	G	258	GLN
3	G	315	GLN
3	G	374	HIS
3	G	402	ASN
3	G	448	ASN
3	G	462	GLN
3	G	478	ASN
3	A	356	ASN
3	A	362	ASN
3	A	402	ASN
3	A	422	GLN
4	C	590	GLN
4	C	619	GLN
3	D	114	GLN
3	D	186	ASN
3	D	246	GLN
3	D	374	HIS
4	E	619	GLN
4	E	652	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
2	TYS	H	100(B)	2	15,16,17	1.60	2 (13%)	15,22,24	0.87	0
2	TYS	H	100(F)	2	15,16,17	1.60	2 (13%)	15,22,24	0.84	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
2	TYS	H	100(B)	2	-	3/10/11/13	0/1/1/1
2	TYS	H	100(F)	2	-	2/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	100(F)	TYS	OH-S	5.08	1.68	1.58
2	H	100(B)	TYS	OH-S	5.03	1.68	1.58
2	H	100(B)	TYS	OH-CZ	-3.24	1.37	1.42
2	H	100(F)	TYS	OH-CZ	-3.18	1.37	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	100(F)	TYS	C-CA-CB-CG
2	H	100(B)	TYS	N-CA-CB-CG
2	H	100(F)	TYS	N-CA-CB-CG
2	H	100(B)	TYS	C-CA-CB-CG
2	H	100(B)	TYS	CZ-OH-S-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	100(F)	TYS	1	0

5.5 Carbohydrates (i)

108 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	F	1	5	14,14,15	0.71	0	17,19,21	0.78	0
5	NAG	F	2	5	14,14,15	0.69	0	17,19,21	1.31	1 (5%)
6	NAG	I	1	6,3	14,14,15	0.73	0	17,19,21	1.03	0
6	NAG	I	2	6	14,14,15	0.72	0	17,19,21	0.85	0
6	BMA	I	3	6	11,11,12	0.86	0	15,15,17	2.29	6 (40%)
6	MAN	I	4	6	11,11,12	0.65	0	15,15,17	1.41	1 (6%)
6	MAN	I	5	6	11,11,12	0.68	0	15,15,17	1.15	1 (6%)
7	NAG	J	1	7,3	14,14,15	0.81	0	17,19,21	2.62	4 (23%)
7	NAG	J	2	7	14,14,15	0.69	0	17,19,21	1.46	2 (11%)
7	BMA	J	3	7	11,11,12	0.86	0	15,15,17	2.44	3 (20%)
5	NAG	K	1	5,3	14,14,15	0.78	0	17,19,21	1.54	3 (17%)
5	NAG	K	2	5	14,14,15	0.70	0	17,19,21	0.85	0
5	NAG	M	1	5,3	14,14,15	0.70	0	17,19,21	1.16	3 (17%)
5	NAG	M	2	5	14,14,15	0.76	0	17,19,21	0.90	0
6	NAG	N	1	6,3	14,14,15	0.82	0	17,19,21	1.56	4 (23%)
6	NAG	N	2	6	14,14,15	0.71	0	17,19,21	1.27	3 (17%)
6	BMA	N	3	6	11,11,12	0.83	0	15,15,17	2.22	7 (46%)
6	MAN	N	4	6	11,11,12	0.59	0	15,15,17	1.85	1 (6%)
6	MAN	N	5	6	11,11,12	0.70	0	15,15,17	1.13	1 (6%)
8	NAG	O	1	8,3	14,14,15	0.68	0	17,19,21	1.44	1 (5%)
8	NAG	O	2	8	14,14,15	0.76	0	17,19,21	0.95	0
8	BMA	O	3	8	11,11,12	0.82	0	15,15,17	2.63	7 (46%)
8	MAN	O	4	8	11,11,12	0.72	0	15,15,17	1.14	1 (6%)
8	MAN	O	5	8	11,11,12	0.71	0	15,15,17	1.15	1 (6%)
8	MAN	O	6	8	11,11,12	0.66	0	15,15,17	1.34	1 (6%)
8	MAN	O	7	8	11,11,12	0.65	0	15,15,17	1.57	1 (6%)
9	NAG	P	1	3,9	14,14,15	0.93	1 (7%)	17,19,21	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	P	2	9	14,14,15	0.73	0	17,19,21	0.92	1 (5%)
9	BMA	P	3	9	11,11,12	0.86	0	15,15,17	2.39	4 (26%)
9	MAN	P	4	9	11,11,12	0.63	0	15,15,17	1.38	1 (6%)
9	MAN	P	5	9	11,11,12	0.67	0	15,15,17	1.30	1 (6%)
9	MAN	P	6	9	11,11,12	0.75	0	15,15,17	1.12	1 (6%)
9	MAN	P	7	9	11,11,12	0.56	0	15,15,17	1.85	1 (6%)
9	MAN	P	8	9	11,11,12	0.72	0	15,15,17	1.10	1 (6%)
5	NAG	Q	1	4,5	14,14,15	0.74	0	17,19,21	0.96	0
5	NAG	Q	2	5	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
5	NAG	R	1	5,3	14,14,15	0.69	0	17,19,21	0.82	0
5	NAG	R	2	5	14,14,15	0.72	0	17,19,21	0.82	0
5	NAG	S	1	5,3	14,14,15	0.72	0	17,19,21	0.79	0
5	NAG	S	2	5	14,14,15	0.73	0	17,19,21	1.28	1 (5%)
6	NAG	T	1	6,3	14,14,15	0.73	0	17,19,21	0.95	1 (5%)
6	NAG	T	2	6	14,14,15	0.70	0	17,19,21	1.39	2 (11%)
6	BMA	T	3	6	11,11,12	0.87	0	15,15,17	2.39	5 (33%)
6	MAN	T	4	6	11,11,12	0.65	0	15,15,17	1.35	1 (6%)
6	MAN	T	5	6	11,11,12	0.71	0	15,15,17	1.09	1 (6%)
10	NAG	U	1	10,3	14,14,15	0.84	0	17,19,21	2.65	4 (23%)
10	NAG	U	2	10	14,14,15	0.69	0	17,19,21	1.38	2 (11%)
10	BMA	U	3	10	11,11,12	0.82	0	15,15,17	2.77	5 (33%)
10	MAN	U	4	10	11,11,12	0.75	0	15,15,17	0.94	1 (6%)
10	MAN	U	5	10	11,11,12	0.66	0	15,15,17	1.32	1 (6%)
10	MAN	U	6	10	11,11,12	0.71	0	15,15,17	1.05	1 (6%)
10	MAN	U	7	10	11,11,12	0.71	0	15,15,17	1.10	1 (6%)
10	MAN	U	8	10	11,11,12	0.60	0	15,15,17	1.55	1 (6%)
10	MAN	U	9	10	11,11,12	0.68	0	15,15,17	1.18	1 (6%)
5	NAG	V	1	5	14,14,15	0.71	0	17,19,21	0.85	0
5	NAG	V	2	5	14,14,15	0.71	0	17,19,21	0.85	0
5	NAG	W	1	5	14,14,15	0.73	0	17,19,21	0.84	0
5	NAG	W	2	5	14,14,15	0.70	0	17,19,21	0.80	0
7	NAG	X	1	7,3	14,14,15	0.71	0	17,19,21	0.90	1 (5%)
7	NAG	X	2	7	14,14,15	0.69	0	17,19,21	1.43	2 (11%)
7	BMA	X	3	7	11,11,12	0.87	0	15,15,17	2.01	3 (20%)
5	NAG	Y	1	5	14,14,15	0.72	0	17,19,21	0.75	0
5	NAG	Y	2	5	14,14,15	0.70	0	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	Z	1	5,3	14,14,15	0.68	0	17,19,21	1.04	1 (5%)
5	NAG	Z	2	5	14,14,15	0.72	0	17,19,21	0.85	0
5	NAG	a	1	4,5	14,14,15	0.77	0	17,19,21	1.17	2 (11%)
5	NAG	a	2	5	14,14,15	0.71	0	17,19,21	1.07	1 (5%)
5	NAG	b	1	5,3	14,14,15	0.70	0	17,19,21	0.80	0
5	NAG	b	2	5	14,14,15	0.71	0	17,19,21	0.82	0
5	NAG	c	1	5	14,14,15	0.70	0	17,19,21	0.77	0
5	NAG	c	2	5	14,14,15	0.70	0	17,19,21	1.31	1 (5%)
6	NAG	d	1	6,3	14,14,15	0.70	0	17,19,21	0.86	0
6	NAG	d	2	6	14,14,15	0.70	0	17,19,21	1.42	2 (11%)
6	BMA	d	3	6	11,11,12	0.85	0	15,15,17	2.35	6 (40%)
6	MAN	d	4	6	11,11,12	0.67	0	15,15,17	1.32	1 (6%)
6	MAN	d	5	6	11,11,12	0.71	0	15,15,17	1.07	1 (6%)
11	NAG	e	1	11,3	14,14,15	0.81	0	17,19,21	2.65	4 (23%)
11	NAG	e	2	11	14,14,15	0.69	0	17,19,21	1.46	2 (11%)
11	BMA	e	3	11	11,11,12	0.84	0	15,15,17	2.53	4 (26%)
11	MAN	e	4	11	11,11,12	0.65	0	15,15,17	1.35	1 (6%)
12	NAG	f	1	12,3	14,14,15	0.70	0	17,19,21	0.93	0
12	NAG	f	2	12	14,14,15	0.71	0	17,19,21	1.02	1 (5%)
12	BMA	f	3	12	11,11,12	0.84	0	15,15,17	2.37	4 (26%)
12	MAN	f	4	12	11,11,12	0.65	0	15,15,17	1.21	1 (6%)
12	MAN	f	5	12	11,11,12	0.65	0	15,15,17	1.49	1 (6%)
12	MAN	f	6	12	11,11,12	0.70	0	15,15,17	1.21	1 (6%)
5	NAG	g	1	5,3	14,14,15	0.76	0	17,19,21	1.64	2 (11%)
5	NAG	g	2	5	14,14,15	0.74	0	17,19,21	0.95	1 (5%)
5	NAG	h	1	5	14,14,15	0.69	0	17,19,21	0.91	0
5	NAG	h	2	5	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
5	NAG	i	1	5	14,14,15	0.71	0	17,19,21	0.86	0
5	NAG	i	2	5	14,14,15	0.70	0	17,19,21	0.81	0
5	NAG	j	1	5,3	14,14,15	0.78	0	17,19,21	0.84	0
5	NAG	j	2	5	14,14,15	0.71	0	17,19,21	0.87	1 (5%)
5	NAG	k	1	5	14,14,15	0.69	0	17,19,21	1.32	1 (5%)
5	NAG	k	2	5	14,14,15	0.71	0	17,19,21	0.82	0
5	NAG	l	1	5	14,14,15	0.72	0	17,19,21	0.86	0
5	NAG	l	2	5	14,14,15	0.70	0	17,19,21	0.81	0
7	NAG	m	1	7,3	14,14,15	0.72	0	17,19,21	0.92	0
7	NAG	m	2	7	14,14,15	0.68	0	17,19,21	1.44	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BMA	m	3	7	11,11,12	0.88	0	15,15,17	2.04	3 (20%)
6	NAG	n	1	6	14,14,15	0.73	0	17,19,21	0.84	0
6	NAG	n	2	6	14,14,15	0.67	0	17,19,21	1.20	1 (5%)
6	BMA	n	3	6	11,11,12	0.84	0	15,15,17	2.00	5 (33%)
6	MAN	n	4	6	11,11,12	0.66	0	15,15,17	1.31	1 (6%)
6	MAN	n	5	6	11,11,12	0.69	0	15,15,17	1.12	1 (6%)
5	NAG	o	1	4,5	14,14,15	0.73	0	17,19,21	0.98	1 (5%)
5	NAG	o	2	5	14,14,15	0.72	0	17,19,21	0.92	1 (5%)

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	F	1	5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	3/6/23/26	0/1/1/1
6	NAG	I	1	6,3	-	1/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
6	MAN	I	4	6	-	1/2/19/22	0/1/1/1
6	MAN	I	5	6	-	0/2/19/22	0/1/1/1
7	NAG	J	1	7,3	-	4/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
7	BMA	J	3	7	-	1/2/19/22	0/1/1/1
5	NAG	K	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	NAG	M	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
6	NAG	N	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	3/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
6	MAN	N	4	6	-	1/2/19/22	0/1/1/1
6	MAN	N	5	6	-	0/2/19/22	0/1/1/1
8	NAG	O	1	8,3	-	3/6/23/26	0/1/1/1
8	NAG	O	2	8	-	0/6/23/26	0/1/1/1
8	BMA	O	3	8	-	0/2/19/22	0/1/1/1
8	MAN	O	4	8	-	0/2/19/22	0/1/1/1
8	MAN	O	5	8	-	0/2/19/22	0/1/1/1

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

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	P	1	NAG	C1-C2	2.34	1.55	1.52

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	1	NAG	C2-N2-C7	9.39	135.48	122.90
11	e	1	NAG	C2-N2-C7	9.37	135.46	122.90
7	J	1	NAG	C2-N2-C7	9.33	135.40	122.90
10	U	3	BMA	C1-O5-C5	8.75	123.91	112.19
11	e	3	BMA	C1-O5-C5	7.97	122.87	112.19
7	J	3	BMA	C1-O5-C5	7.81	122.65	112.19
8	O	3	BMA	C1-O5-C5	7.49	122.23	112.19
6	d	3	BMA	C1-O5-C5	7.19	121.82	112.19
9	P	3	BMA	C1-O5-C5	7.10	121.70	112.19
12	f	3	BMA	C1-O5-C5	7.00	121.56	112.19
9	P	7	MAN	C1-O5-C5	6.55	120.97	112.19
6	T	3	BMA	C1-O5-C5	6.54	120.95	112.19
6	N	4	MAN	C1-O5-C5	6.34	120.68	112.19
6	I	3	BMA	C1-O5-C5	6.11	120.37	112.19
7	m	3	BMA	C1-O5-C5	5.74	119.88	112.19
7	X	3	BMA	C1-O5-C5	5.60	119.69	112.19
10	U	8	MAN	C1-O5-C5	5.17	119.11	112.19
8	O	7	MAN	C1-O5-C5	5.02	118.92	112.19
12	f	5	MAN	C1-O5-C5	4.67	118.44	112.19
6	I	4	MAN	C1-O5-C5	4.41	118.09	112.19
6	T	4	MAN	C1-O5-C5	4.18	117.79	112.19
9	P	5	MAN	C1-O5-C5	4.18	117.78	112.19
10	U	5	MAN	C1-O5-C5	4.18	117.78	112.19
11	e	4	MAN	C1-O5-C5	4.15	117.74	112.19
9	P	4	MAN	C1-O5-C5	4.13	117.72	112.19
8	O	6	MAN	C1-O5-C5	4.10	117.67	112.19
6	n	4	MAN	C1-O5-C5	4.07	117.63	112.19
6	d	4	MAN	C1-O5-C5	4.04	117.61	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	g	1	NAG	C2-N2-C7	4.01	128.27	122.90
6	N	3	BMA	C1-C2-C3	-3.95	103.89	109.64
5	K	1	NAG	C2-N2-C7	3.95	128.19	122.90
11	e	2	NAG	C2-N2-C7	3.92	128.16	122.90
7	J	2	NAG	C2-N2-C7	3.91	128.14	122.90
5	k	1	NAG	C2-N2-C7	3.89	128.12	122.90
10	U	2	NAG	C2-N2-C7	3.86	128.07	122.90
6	T	2	NAG	C2-N2-C7	3.84	128.05	122.90
6	d	2	NAG	C2-N2-C7	3.83	128.04	122.90
5	S	2	NAG	C2-N2-C7	3.81	128.01	122.90
5	F	2	NAG	C2-N2-C7	3.81	128.00	122.90
5	c	2	NAG	C2-N2-C7	3.79	127.98	122.90
7	m	2	NAG	C2-N2-C7	3.77	127.95	122.90
12	f	4	MAN	C1-O5-C5	3.73	117.19	112.19
8	O	1	NAG	C2-N2-C7	3.73	127.89	122.90
7	X	2	NAG	C2-N2-C7	3.68	127.83	122.90
12	f	6	MAN	C1-O5-C5	3.64	117.07	112.19
6	n	3	BMA	C3-C4-C5	3.64	116.83	110.23
10	U	9	MAN	C1-O5-C5	3.62	117.04	112.19
6	T	3	BMA	C3-C4-C5	3.56	116.68	110.23
6	n	3	BMA	C1-O5-C5	3.56	116.95	112.19
8	O	3	BMA	C3-C4-C5	3.52	116.61	110.23
6	N	3	BMA	C3-C4-C5	3.49	116.55	110.23
5	g	1	NAG	O5-C1-C2	-3.44	105.97	111.29
6	n	5	MAN	C1-O5-C5	3.37	116.70	112.19
8	O	5	MAN	C1-O5-C5	3.37	116.70	112.19
6	I	3	BMA	C3-C4-C5	3.36	116.32	110.23
6	N	5	MAN	C1-O5-C5	3.36	116.69	112.19
6	N	1	NAG	O5-C1-C2	-3.29	106.20	111.29
6	I	5	MAN	C1-O5-C5	3.25	116.54	112.19
10	U	3	BMA	C3-C4-C5	3.25	116.13	110.23
12	f	3	BMA	C3-C4-C5	3.22	116.08	110.23
6	N	3	BMA	C1-O5-C5	3.22	116.50	112.19
7	J	1	NAG	C8-C7-N2	3.19	121.41	116.12
11	e	1	NAG	C8-C7-N2	3.17	121.37	116.12
9	P	8	MAN	C1-O5-C5	3.16	116.42	112.19
10	U	1	NAG	C8-C7-N2	3.15	121.34	116.12
10	U	7	MAN	C1-O5-C5	3.13	116.39	112.19
6	N	2	NAG	O5-C1-C2	-3.12	106.47	111.29
9	P	3	BMA	C3-C4-C5	3.04	115.75	110.23
10	U	6	MAN	C1-O5-C5	3.02	116.23	112.19
8	O	4	MAN	C1-O5-C5	3.01	116.23	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	5	MAN	C1-O5-C5	3.01	116.22	112.19
6	d	5	MAN	C1-O5-C5	2.94	116.12	112.19
11	e	3	BMA	C3-C4-C5	2.90	115.49	110.23
5	a	1	NAG	O5-C1-C2	-2.90	106.81	111.29
6	d	2	NAG	O5-C1-C2	-2.69	107.13	111.29
6	N	1	NAG	C2-N2-C7	2.68	126.49	122.90
6	T	3	BMA	C2-C3-C4	2.67	115.55	110.86
6	I	3	BMA	O4-C4-C3	-2.67	104.09	110.38
6	N	1	NAG	C1-O5-C5	2.65	115.74	112.19
7	m	3	BMA	C2-C3-C4	2.65	115.52	110.86
7	X	3	BMA	C2-C3-C4	2.64	115.50	110.86
11	e	2	NAG	O5-C1-C2	-2.64	107.21	111.29
6	n	3	BMA	C2-C3-C4	2.64	115.50	110.86
7	J	3	BMA	C2-C3-C4	2.64	115.50	110.86
7	J	2	NAG	O5-C1-C2	-2.61	107.25	111.29
5	M	1	NAG	O3-C3-C2	-2.60	104.00	109.40
8	O	3	BMA	O4-C4-C3	-2.59	104.28	110.38
6	I	3	BMA	C2-C3-C4	2.58	115.41	110.86
11	e	3	BMA	C2-C3-C4	2.56	115.36	110.86
7	m	3	BMA	C3-C4-C5	2.54	114.84	110.23
6	T	3	BMA	O4-C4-C3	-2.54	104.40	110.38
7	X	3	BMA	C3-C4-C5	2.50	114.76	110.23
5	g	2	NAG	C1-O5-C5	2.48	115.51	112.19
9	P	3	BMA	C2-C3-C4	2.47	115.21	110.86
10	U	3	BMA	O4-C4-C3	-2.46	104.58	110.38
6	N	3	BMA	O4-C4-C3	-2.46	104.58	110.38
6	N	2	NAG	O4-C4-C3	-2.46	104.59	110.38
6	d	3	BMA	O4-C4-C3	-2.44	104.62	110.38
5	Z	1	NAG	O5-C1-C2	-2.44	107.52	111.29
5	a	1	NAG	C1-O5-C5	2.43	115.44	112.19
5	K	1	NAG	C1-O5-C5	2.42	115.43	112.19
6	n	3	BMA	O4-C4-C3	-2.42	104.68	110.38
8	O	3	BMA	O3-C3-C4	2.41	116.06	110.38
6	d	3	BMA	C3-C4-C5	2.39	114.56	110.23
6	T	2	NAG	O5-C1-C2	-2.38	107.61	111.29
5	a	2	NAG	C2-N2-C7	2.37	126.07	122.90
6	N	3	BMA	O5-C1-C2	-2.37	105.14	110.79
8	O	3	BMA	C1-C2-C3	-2.35	106.22	109.64
10	U	3	BMA	C2-C3-C4	2.35	115.00	110.86
5	h	2	NAG	C2-N2-C7	2.35	126.04	122.90
10	U	4	MAN	C1-O5-C5	2.33	115.31	112.19
7	J	3	BMA	C3-C4-C5	2.33	114.46	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	e	1	NAG	C1-C2-N2	2.33	114.11	110.43
6	N	3	BMA	C2-C3-C4	2.33	114.96	110.86
6	T	3	BMA	O5-C5-C4	2.30	116.41	110.83
12	f	3	BMA	O4-C4-C3	-2.29	104.98	110.38
9	P	3	BMA	O4-C4-C3	-2.27	105.02	110.38
6	I	3	BMA	O5-C5-C4	2.26	116.33	110.83
6	N	1	NAG	C1-C2-N2	2.26	113.99	110.43
8	O	3	BMA	O5-C5-C4	2.26	116.32	110.83
6	n	2	NAG	C2-N2-C7	2.26	125.92	122.90
5	M	1	NAG	O3-C3-C4	2.24	115.67	110.38
11	e	3	BMA	O4-C4-C3	-2.24	105.10	110.38
12	f	2	NAG	C2-N2-C7	2.23	125.89	122.90
6	N	2	NAG	C2-N2-C7	2.23	125.89	122.90
6	N	3	BMA	O3-C3-C4	2.22	115.62	110.38
12	f	3	BMA	C2-C3-C4	2.22	114.77	110.86
5	j	2	NAG	O5-C1-C2	-2.22	107.86	111.29
10	U	1	NAG	C1-C2-N2	2.21	113.91	110.43
6	d	3	BMA	O3-C3-C4	2.20	115.56	110.38
10	U	2	NAG	O5-C1-C2	-2.16	107.94	111.29
7	J	1	NAG	O7-C7-C8	-2.16	118.21	122.05
7	J	1	NAG	C1-C2-N2	2.15	113.83	110.43
6	n	3	BMA	O3-C3-C2	-2.13	105.70	110.05
10	U	1	NAG	O7-C7-C8	-2.13	118.26	122.05
7	X	2	NAG	O4-C4-C3	-2.13	105.35	110.38
6	d	3	BMA	O5-C5-C4	2.13	116.01	110.83
5	M	1	NAG	O5-C1-C2	-2.13	108.00	111.29
5	Q	2	NAG	C2-N2-C7	2.12	125.75	122.90
7	X	1	NAG	C1-O5-C5	2.12	115.03	112.19
6	d	3	BMA	C2-C3-C4	2.12	114.58	110.86
8	O	3	BMA	O2-C2-C3	2.10	114.50	110.15
6	I	3	BMA	O3-C3-C4	2.09	115.31	110.38
11	e	1	NAG	O7-C7-C8	-2.09	118.34	122.05
10	U	3	BMA	O5-C5-C4	2.08	115.90	110.83
5	o	2	NAG	C2-N2-C7	2.08	125.69	122.90
6	T	1	NAG	O5-C1-C2	-2.04	108.13	111.29
9	P	2	NAG	O5-C1-C2	-2.04	108.14	111.29
5	o	1	NAG	C1-O5-C5	2.04	114.92	112.19
7	m	2	NAG	O4-C4-C3	-2.02	105.61	110.38
9	P	6	MAN	C1-O5-C5	2.02	114.89	112.19
5	Y	2	NAG	C2-N2-C7	2.01	125.59	122.90
5	K	1	NAG	O7-C7-N2	2.01	125.53	121.98

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	n	1	NAG	O5-C5-C6-O6
6	N	3	BMA	O5-C5-C6-O6
7	X	3	BMA	O5-C5-C6-O6
7	m	3	BMA	O5-C5-C6-O6
6	n	1	NAG	C4-C5-C6-O6
5	Q	2	NAG	C8-C7-N2-C2
5	Q	2	NAG	O7-C7-N2-C2
5	Y	2	NAG	C8-C7-N2-C2
5	Y	2	NAG	O7-C7-N2-C2
5	a	2	NAG	C8-C7-N2-C2
5	a	2	NAG	O7-C7-N2-C2
5	h	2	NAG	C8-C7-N2-C2
5	h	2	NAG	O7-C7-N2-C2
5	i	1	NAG	C8-C7-N2-C2
5	i	1	NAG	O7-C7-N2-C2
5	o	2	NAG	C8-C7-N2-C2
5	o	2	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
6	n	2	NAG	C8-C7-N2-C2
6	n	2	NAG	O7-C7-N2-C2
7	J	1	NAG	C8-C7-N2-C2
7	J	1	NAG	O7-C7-N2-C2
10	U	1	NAG	C8-C7-N2-C2
10	U	1	NAG	O7-C7-N2-C2
11	e	1	NAG	C8-C7-N2-C2
11	e	1	NAG	O7-C7-N2-C2
12	f	2	NAG	C8-C7-N2-C2
12	f	2	NAG	O7-C7-N2-C2
10	U	5	MAN	O5-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	j	2	NAG	O5-C5-C6-O6
8	O	7	MAN	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
6	n	2	NAG	O5-C5-C6-O6
6	d	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	R	1	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
6	I	4	MAN	O5-C5-C6-O6
6	T	4	MAN	O5-C5-C6-O6
6	n	4	MAN	O5-C5-C6-O6
8	O	1	NAG	O5-C5-C6-O6
5	i	1	NAG	O5-C5-C6-O6
6	N	4	MAN	O5-C5-C6-O6
12	f	5	MAN	O5-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
6	d	1	NAG	O5-C5-C6-O6
9	P	3	BMA	O5-C5-C6-O6
6	n	3	BMA	O5-C5-C6-O6
12	f	3	BMA	O5-C5-C6-O6
5	F	2	NAG	C1-C2-N2-C7
5	S	2	NAG	C1-C2-N2-C7
5	c	2	NAG	C1-C2-N2-C7
5	g	1	NAG	C1-C2-N2-C7
6	T	2	NAG	C1-C2-N2-C7
6	d	2	NAG	C1-C2-N2-C7
7	X	2	NAG	C1-C2-N2-C7
7	m	2	NAG	C1-C2-N2-C7
5	a	1	NAG	O5-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
9	P	7	MAN	O5-C5-C6-O6
10	U	3	BMA	O5-C5-C6-O6
7	m	3	BMA	C4-C5-C6-O6
7	X	3	BMA	C4-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6
5	K	1	NAG	C3-C2-N2-C7
5	g	1	NAG	C3-C2-N2-C7
5	k	1	NAG	C3-C2-N2-C7
6	T	2	NAG	C3-C2-N2-C7
6	d	2	NAG	C3-C2-N2-C7
7	J	2	NAG	C3-C2-N2-C7
8	O	1	NAG	C3-C2-N2-C7
10	U	2	NAG	C3-C2-N2-C7
11	e	2	NAG	C3-C2-N2-C7
7	J	3	BMA	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
11	e	3	BMA	O5-C5-C6-O6
5	K	1	NAG	C1-C2-N2-C7

Continued on next page...

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Mol	Chain	Res	Type	Atoms
5	k	1	NAG	C1-C2-N2-C7
7	J	1	NAG	C1-C2-N2-C7
7	J	2	NAG	C1-C2-N2-C7
8	O	1	NAG	C1-C2-N2-C7
10	U	1	NAG	C1-C2-N2-C7
10	U	2	NAG	C1-C2-N2-C7
11	e	1	NAG	C1-C2-N2-C7
11	e	2	NAG	C1-C2-N2-C7
5	F	2	NAG	C3-C2-N2-C7
5	S	2	NAG	C3-C2-N2-C7
5	c	2	NAG	C3-C2-N2-C7
7	J	1	NAG	C3-C2-N2-C7
7	X	2	NAG	C3-C2-N2-C7
7	m	2	NAG	C3-C2-N2-C7
10	U	1	NAG	C3-C2-N2-C7
11	e	1	NAG	C3-C2-N2-C7
5	a	2	NAG	O5-C5-C6-O6

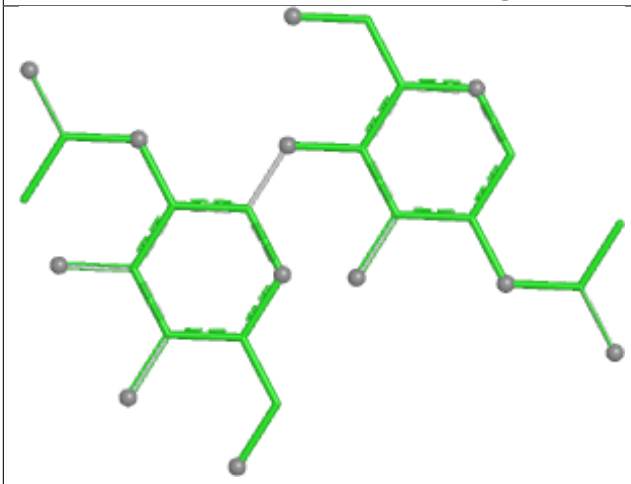
There are no ring outliers.

6 monomers are involved in 8 short contacts:

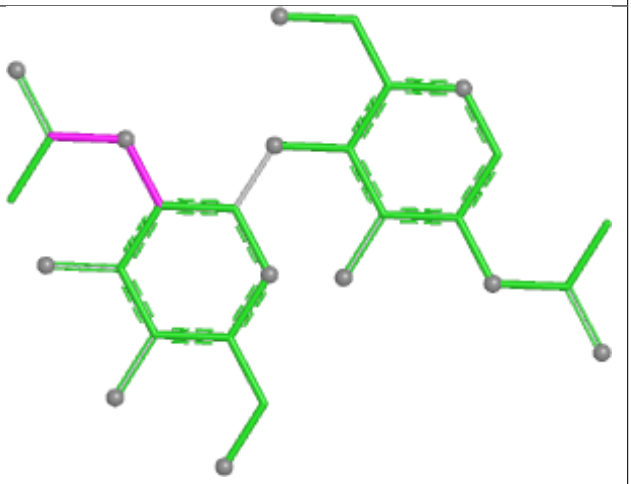
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	V	2	NAG	1	0
9	P	3	BMA	1	0
6	T	3	BMA	1	0
6	d	3	BMA	3	0
6	I	3	BMA	2	0
9	P	6	MAN	1	0

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

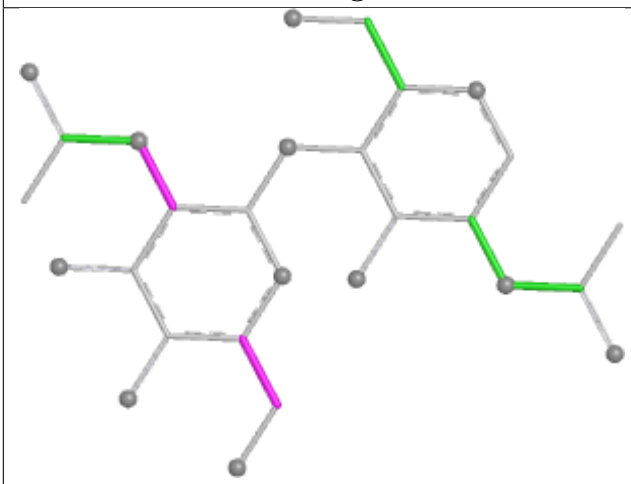
Oligosaccharide Chain F



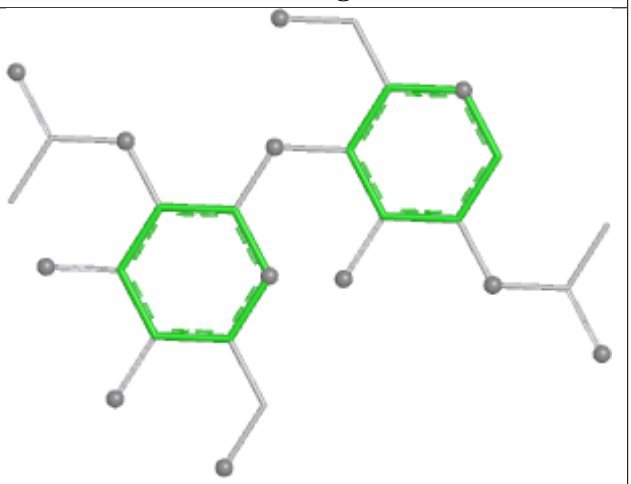
Bond lengths



Bond angles

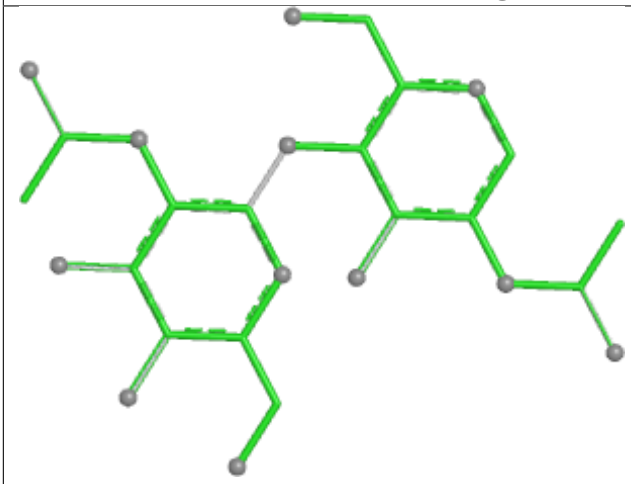


Torsions

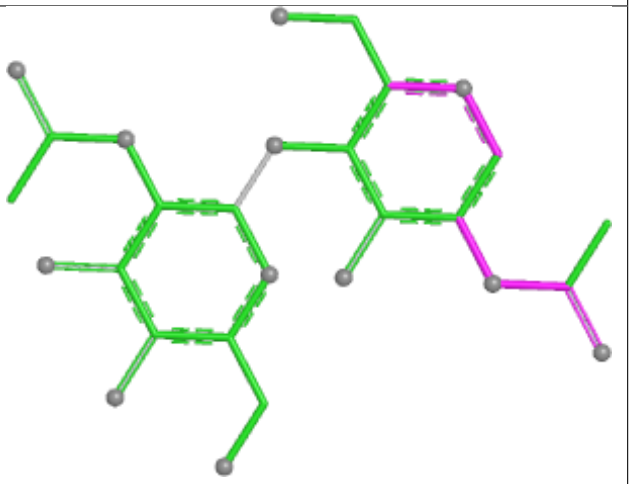


Rings

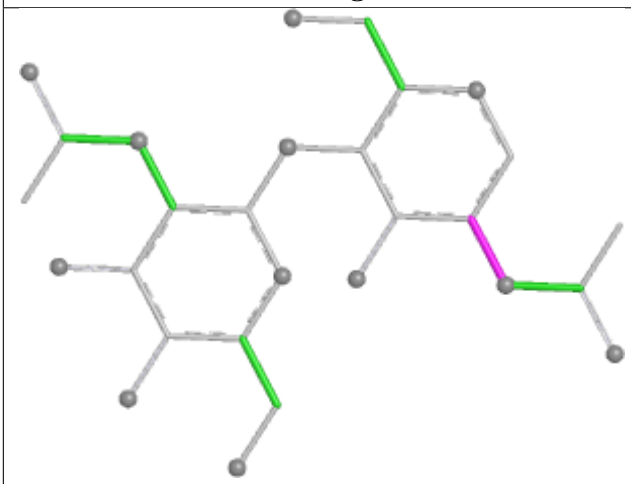
Oligosaccharide Chain K



Bond lengths



Bond angles



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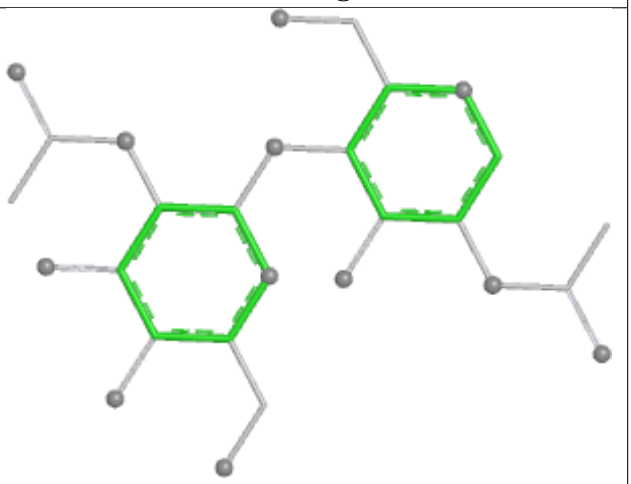
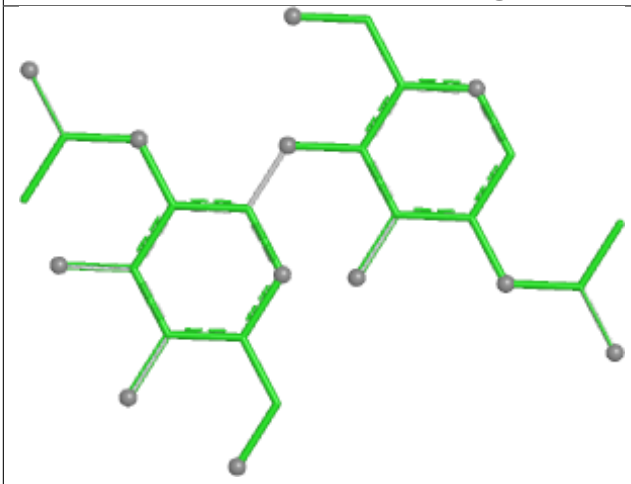
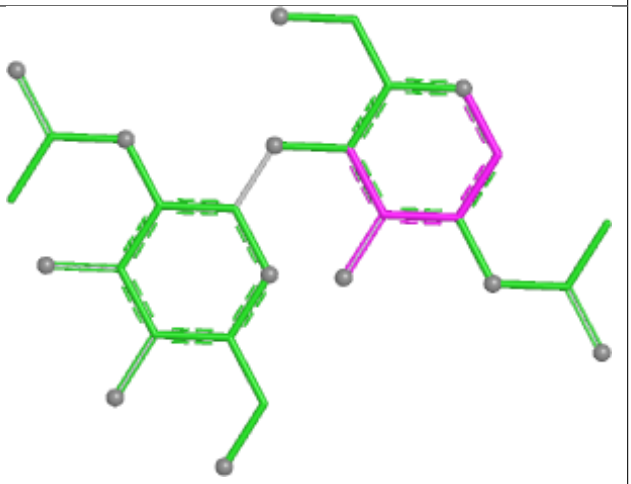


Rings

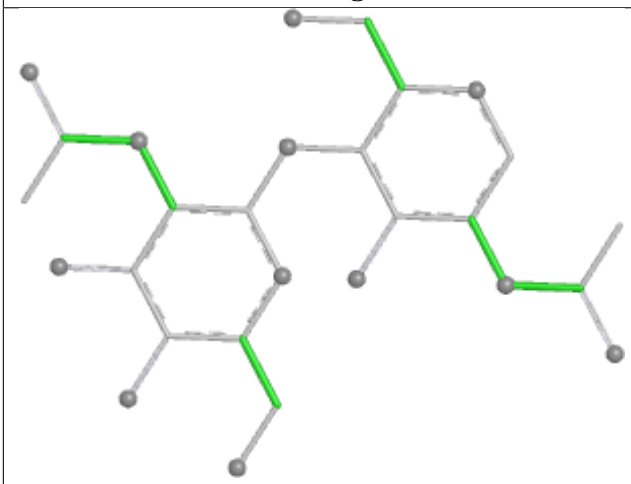
Oligosaccharide Chain M



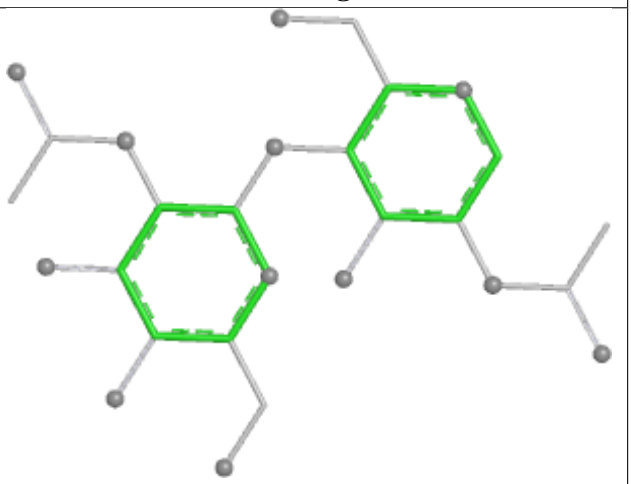
Bond lengths



Bond angles

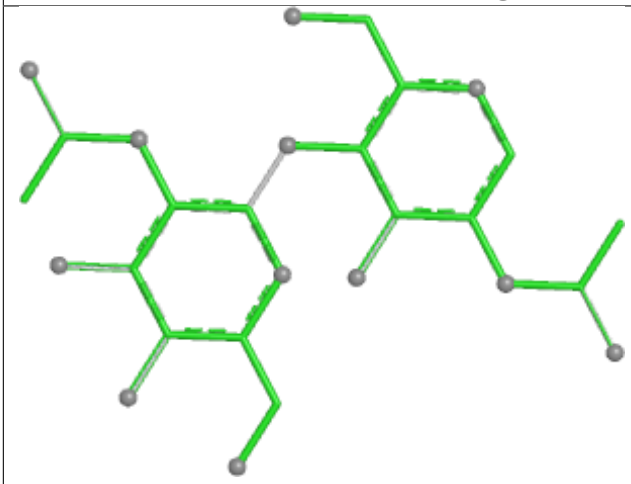


Torsions

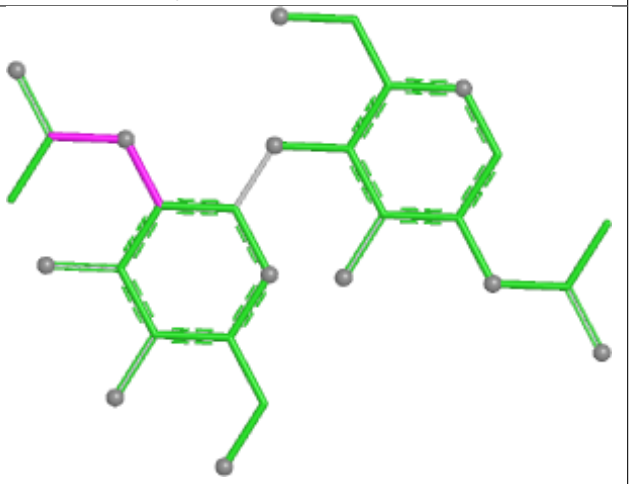


Rings

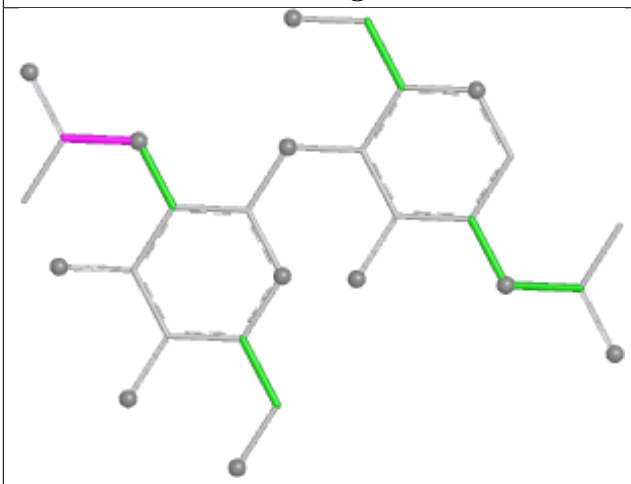
Oligosaccharide Chain Q



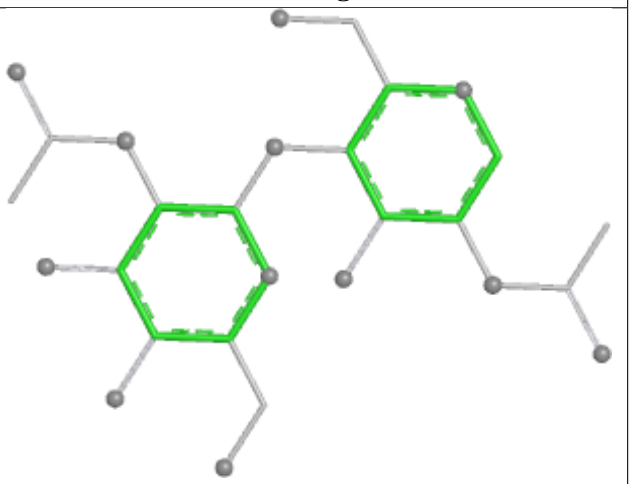
Bond lengths



Bond angles

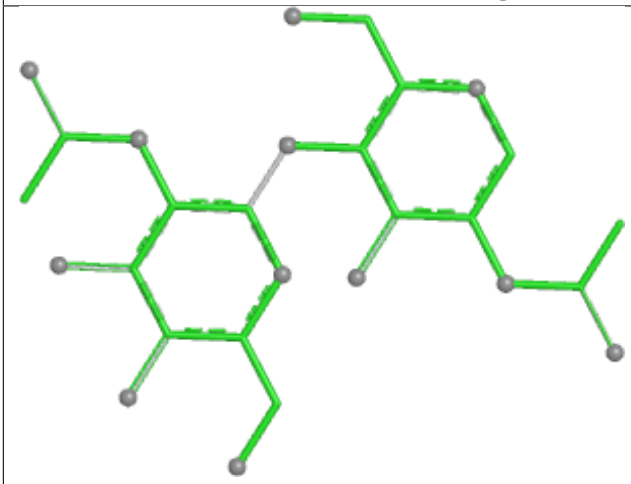


Torsions

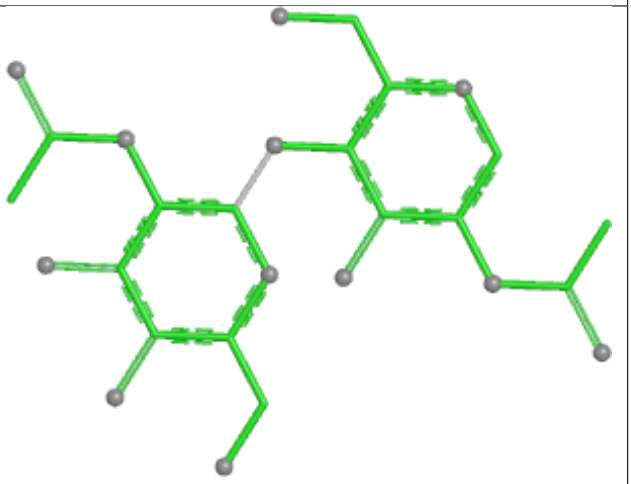


Rings

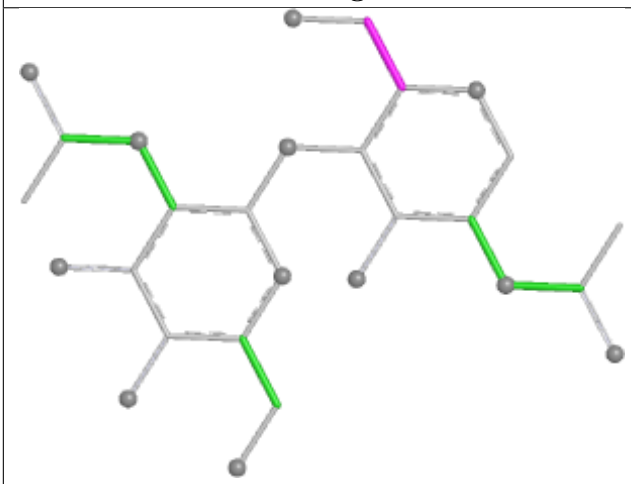
Oligosaccharide Chain R



Bond lengths



Bond angles



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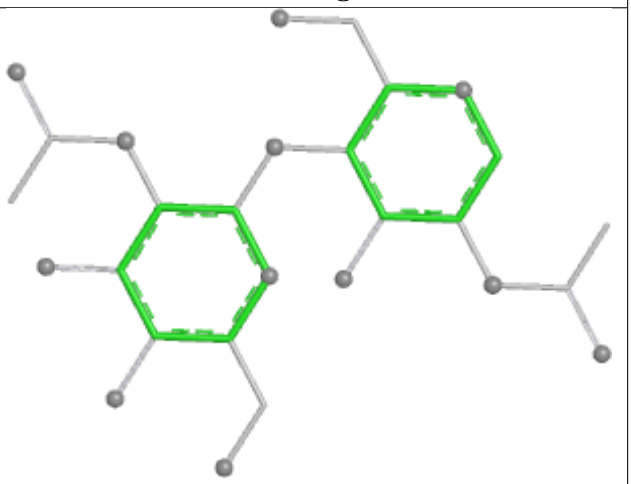
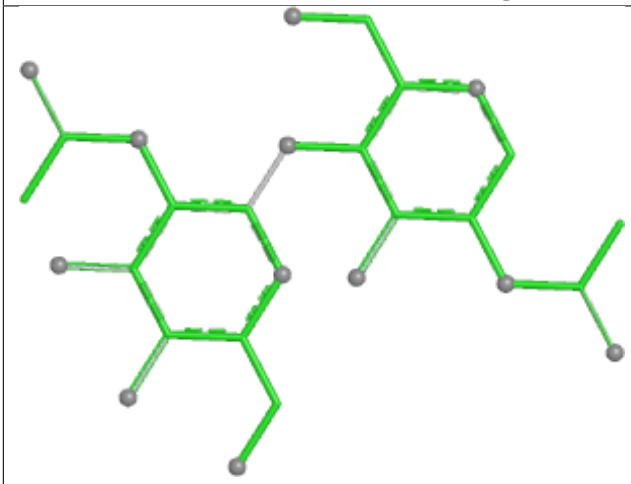


Rings

Oligosaccharide Chain S



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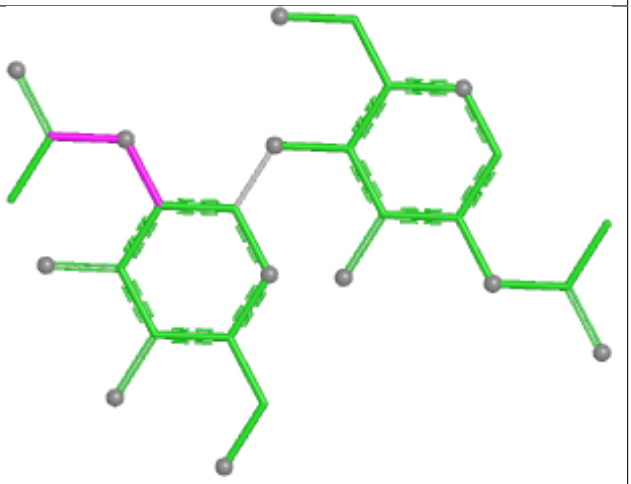
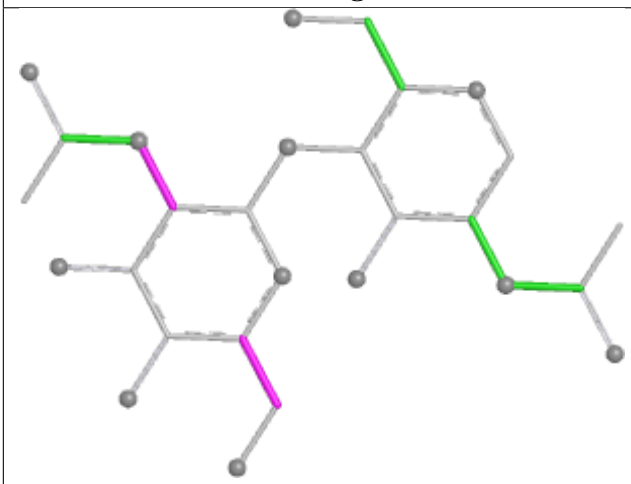


Bond angles



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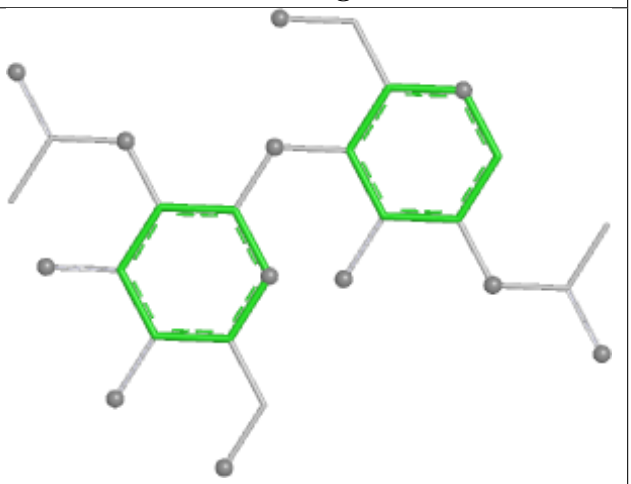
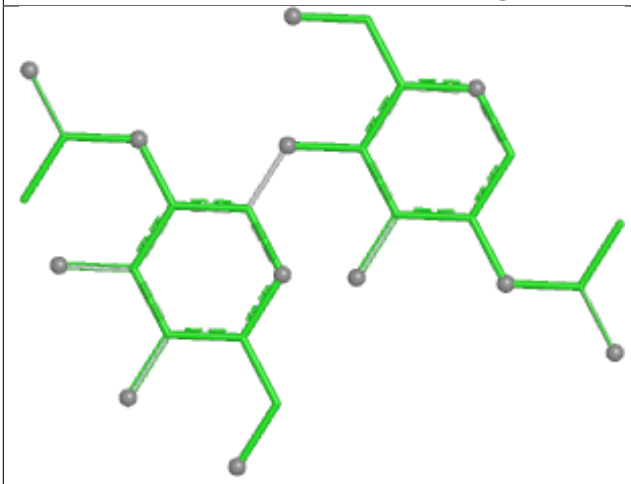


Rings

Oligosaccharide Chain V



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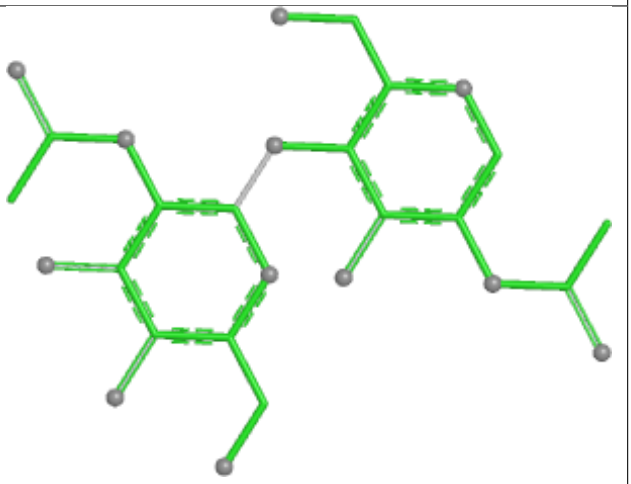
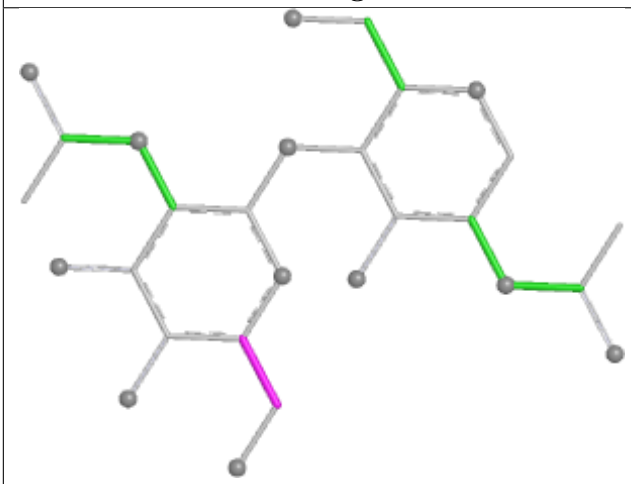


Bond angles



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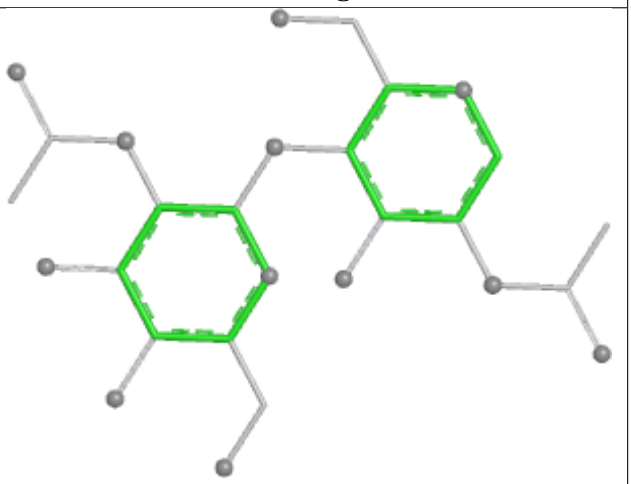
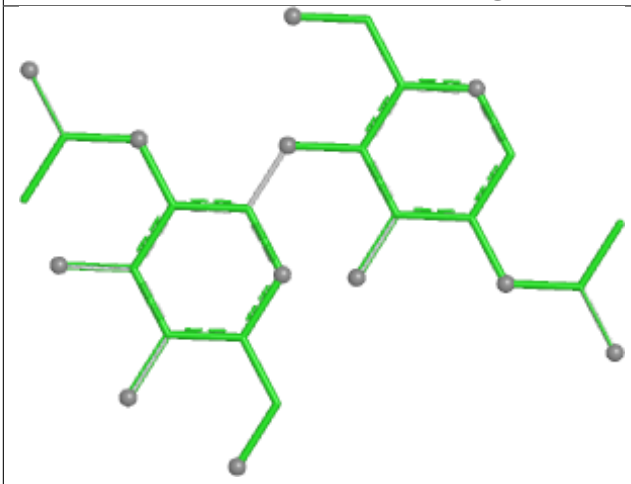
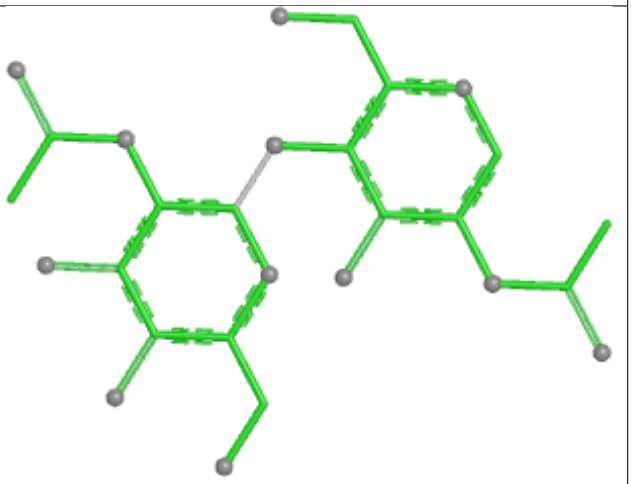


Rings

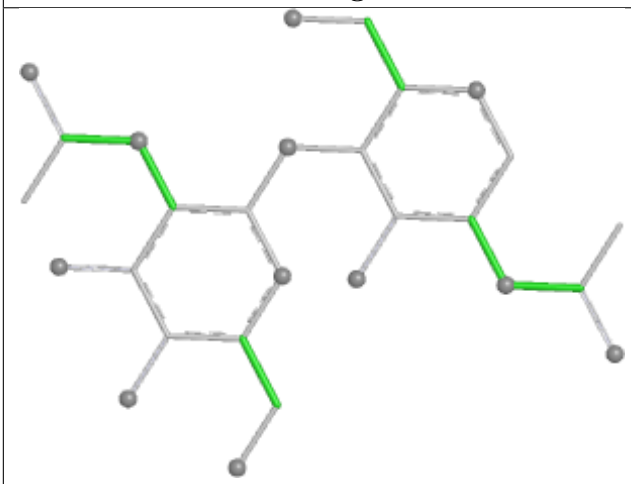
Oligosaccharide Chain W



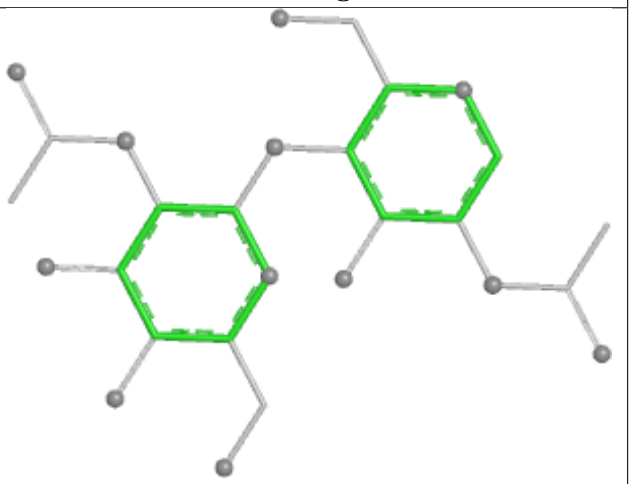
Bond lengths



Bond angles

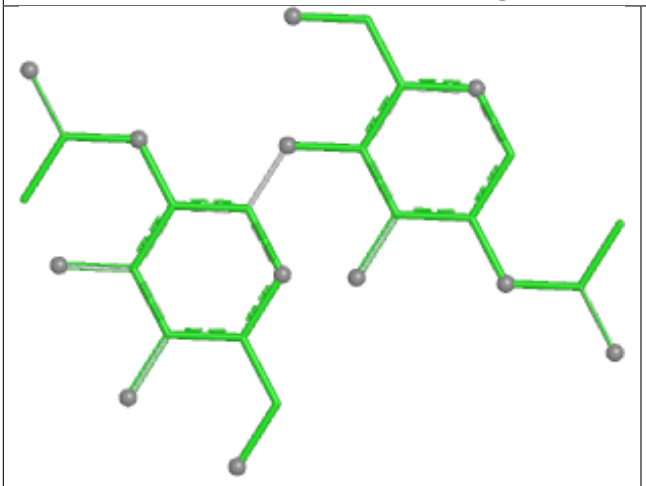


Torsions



Rings

Oligosaccharide Chain Y



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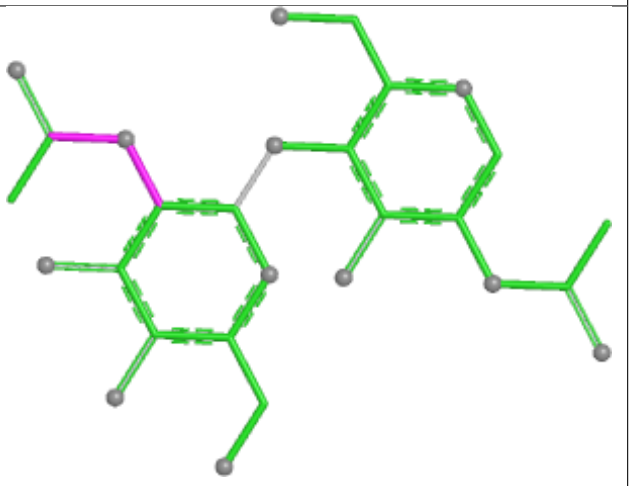
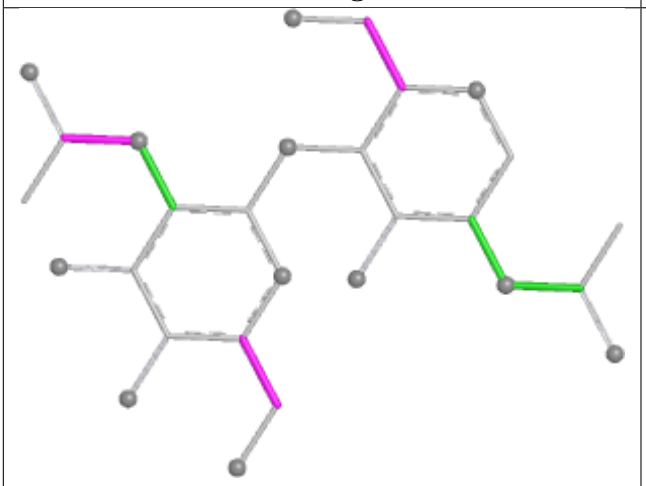


Bond angles



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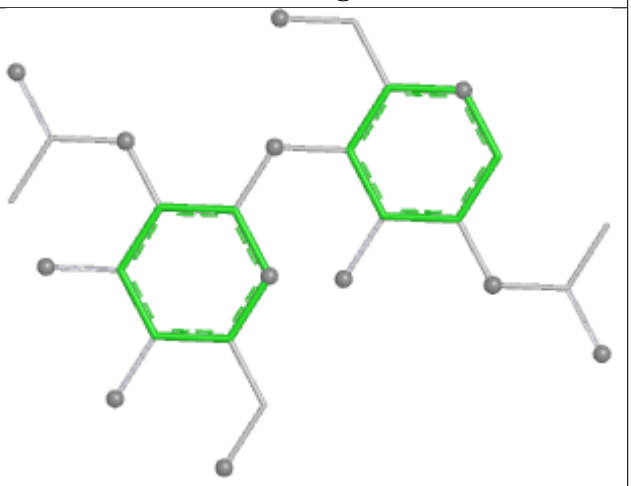
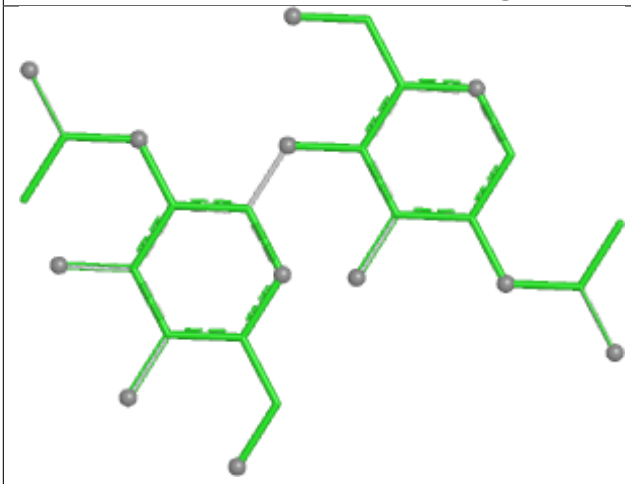


Rings

Oligosaccharide Chain Z



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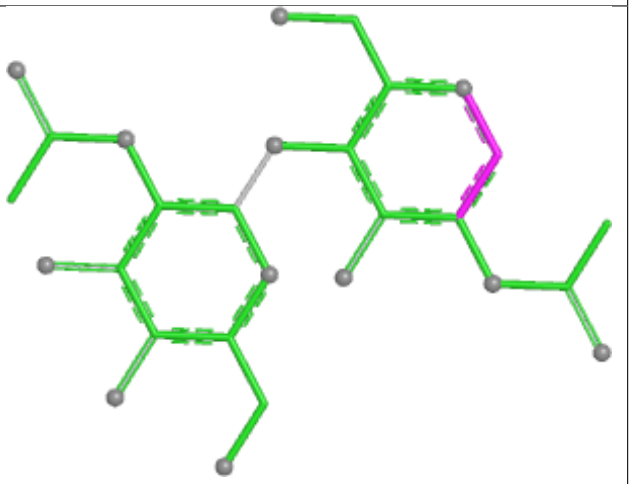

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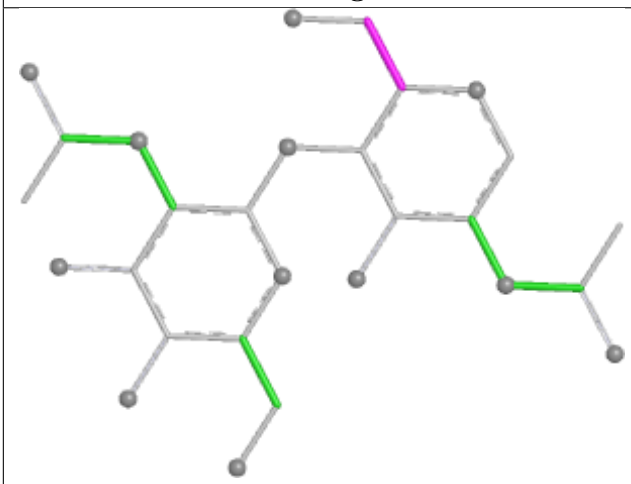
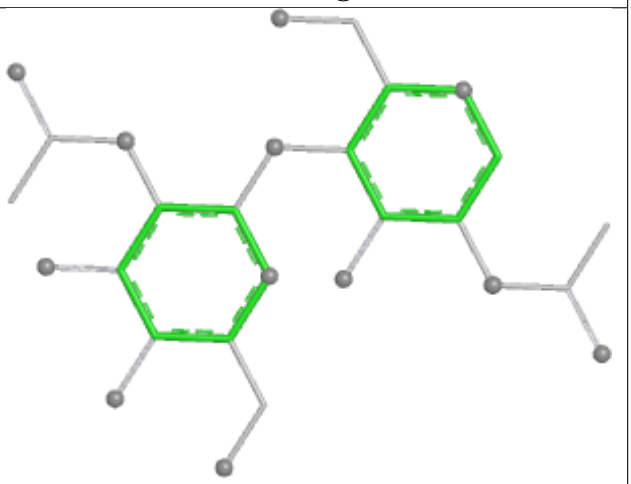
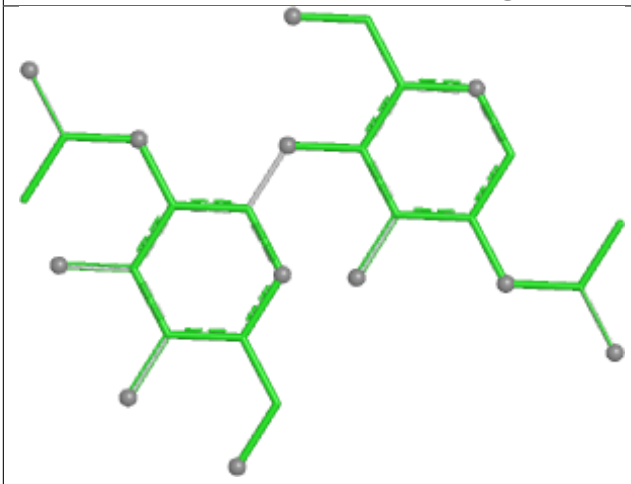


Torsions

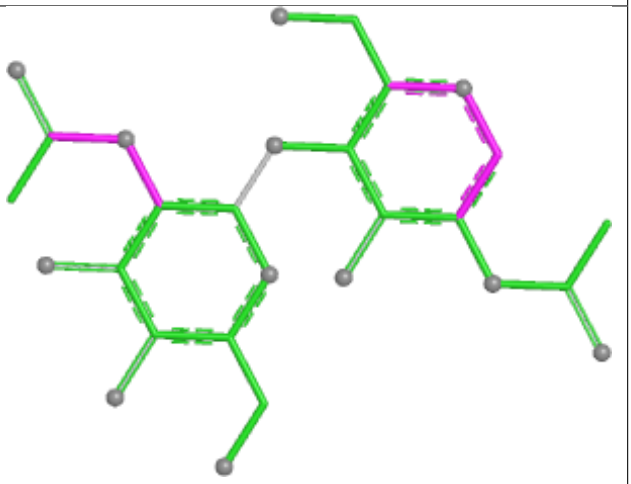


Rings

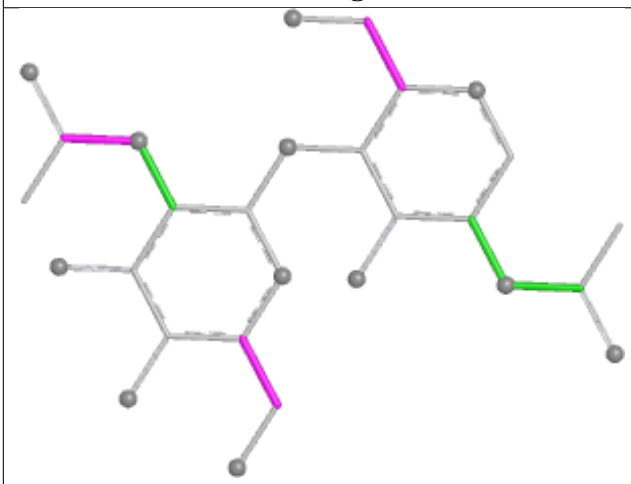
Oligosaccharide Chain a



Bond lengths



Bond angles



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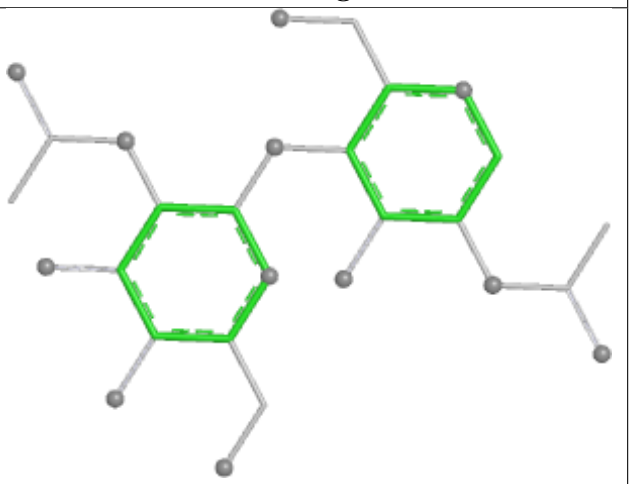
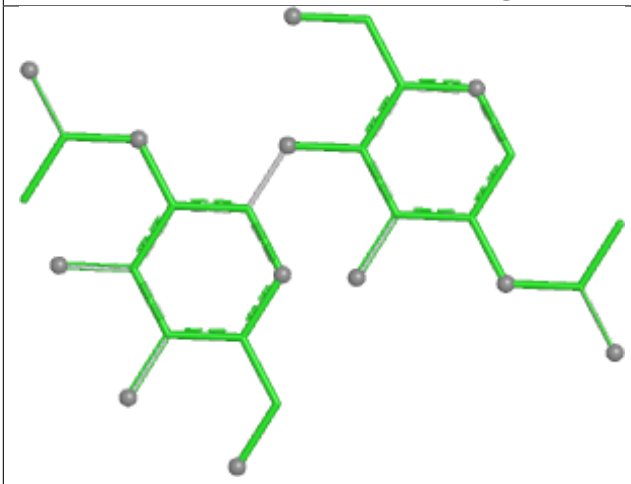
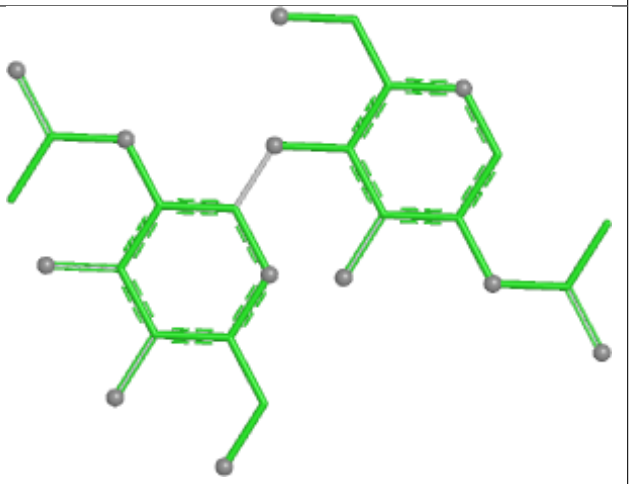


Rings

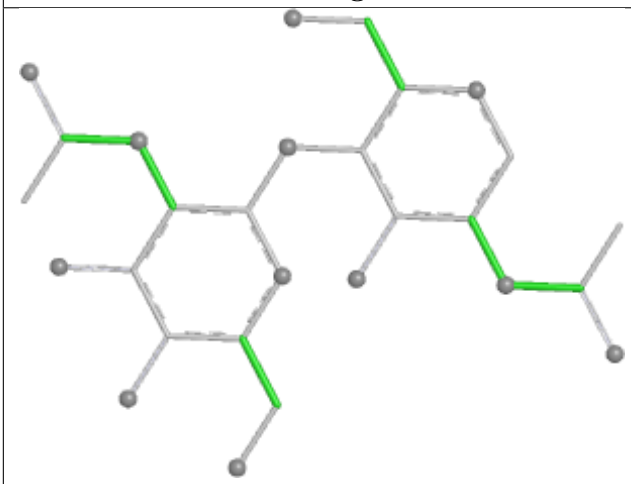
Oligosaccharide Chain b



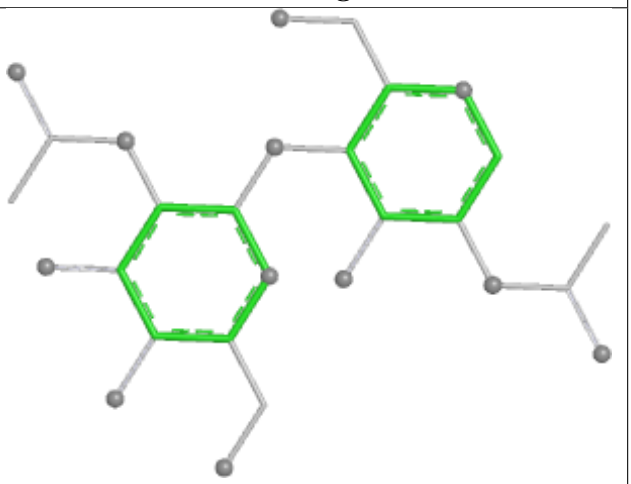
Bond lengths



Bond angles

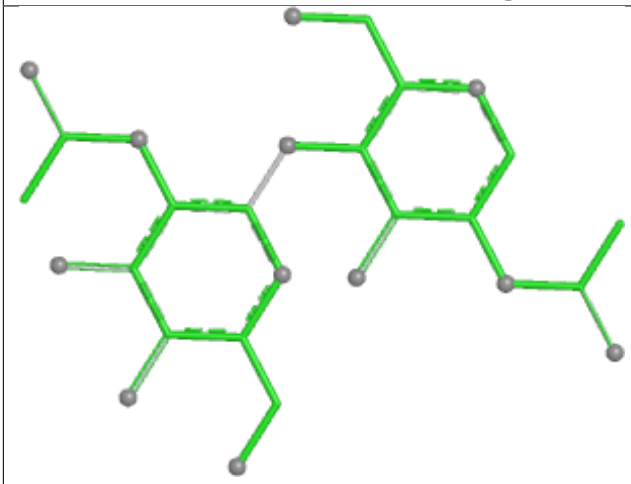


Torsions

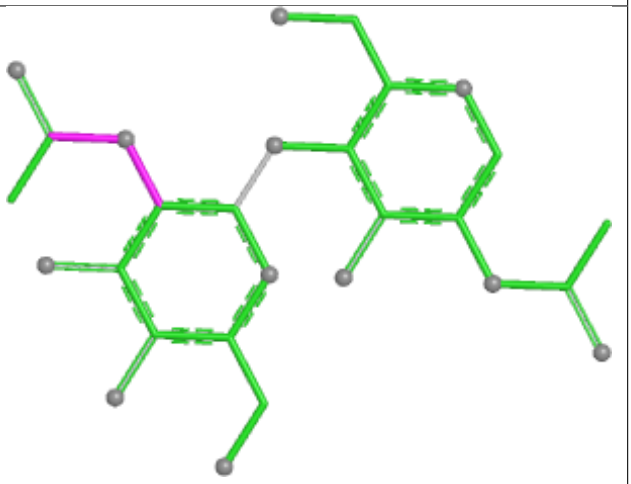


Rings

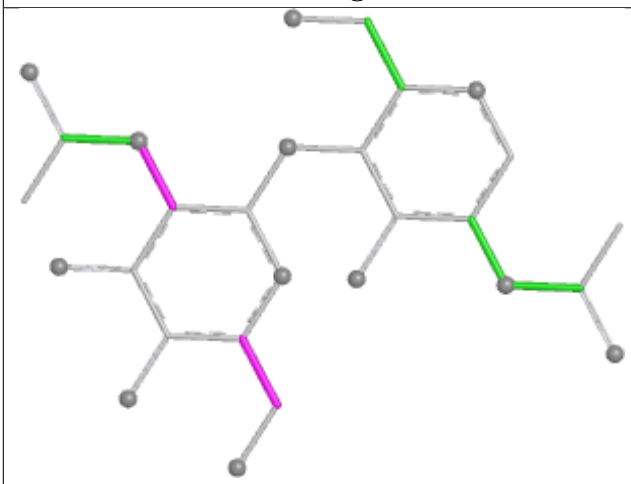
Oligosaccharide Chain c



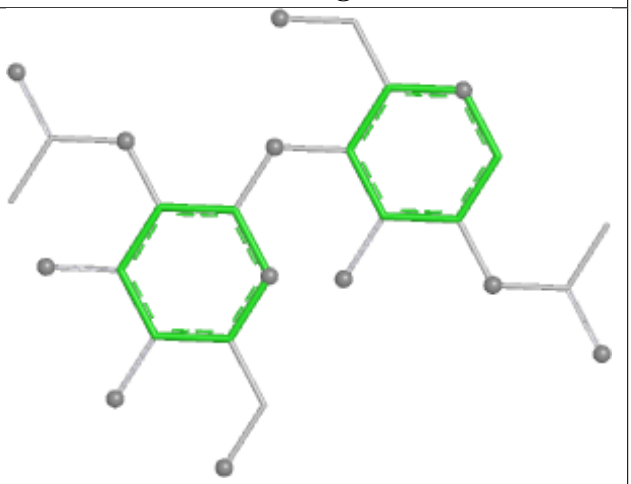
Bond lengths



Bond angles

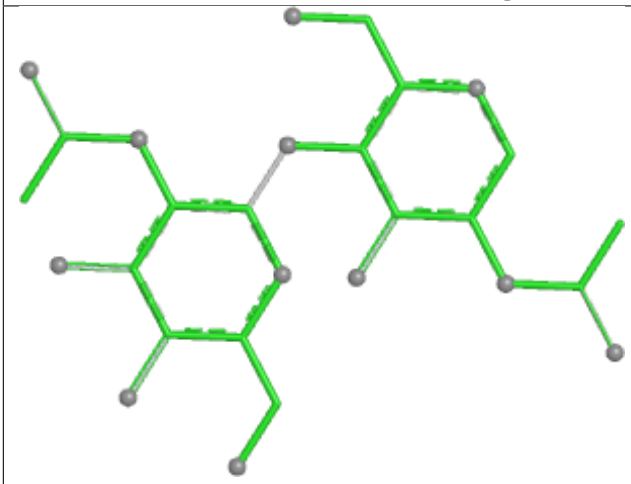


Torsions



Rings

Oligosaccharide Chain g



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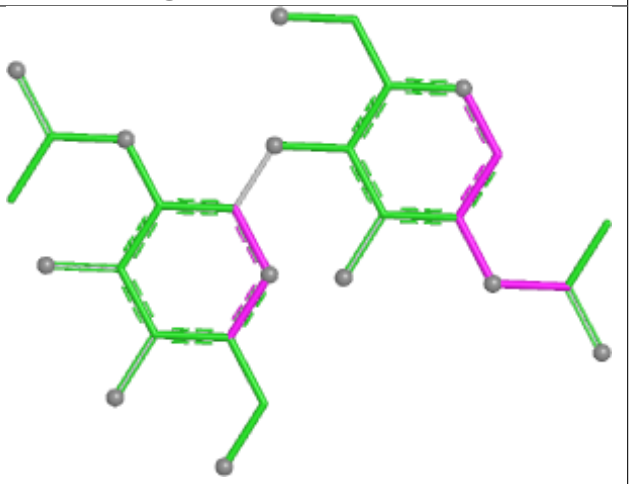
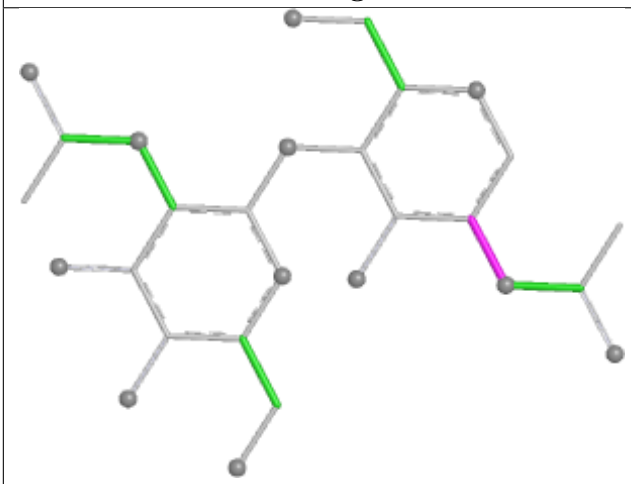


Bond angles



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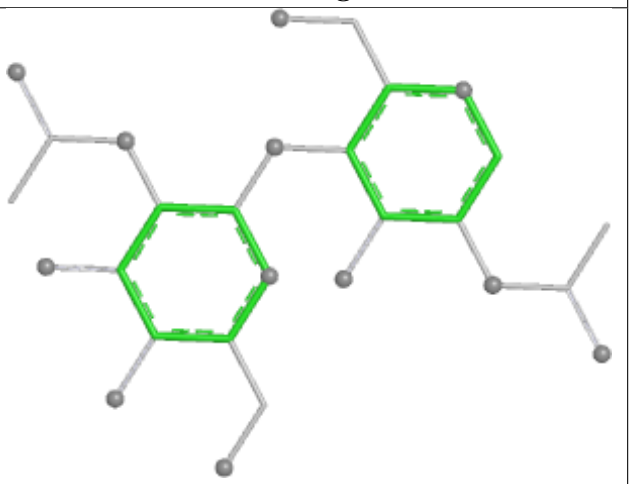
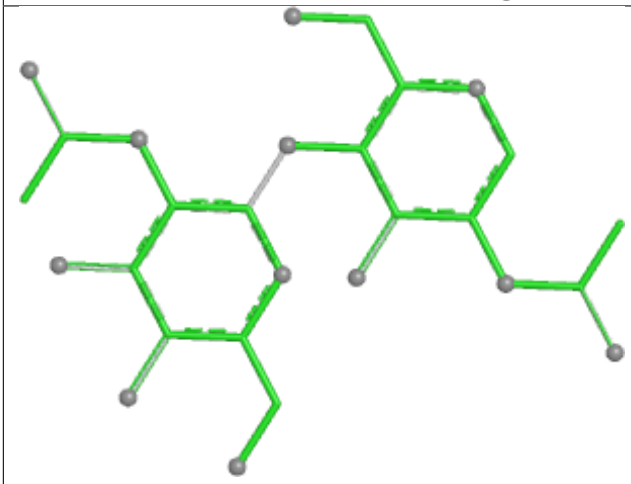


Rings

Oligosaccharide Chain h



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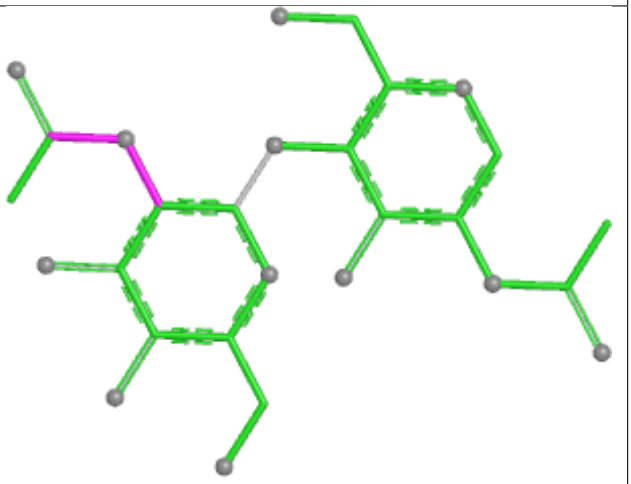
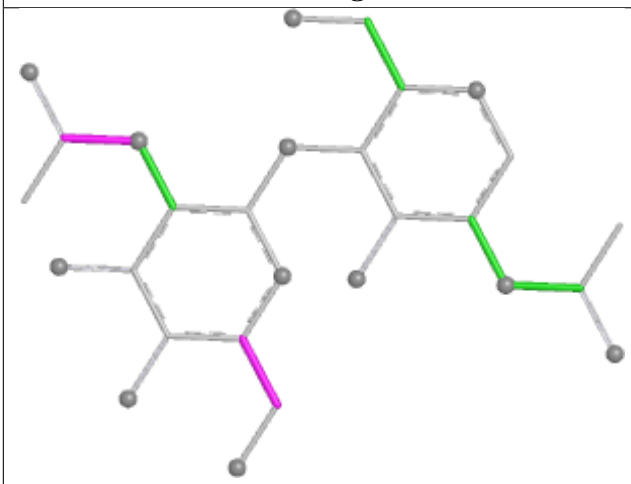


Bond angles



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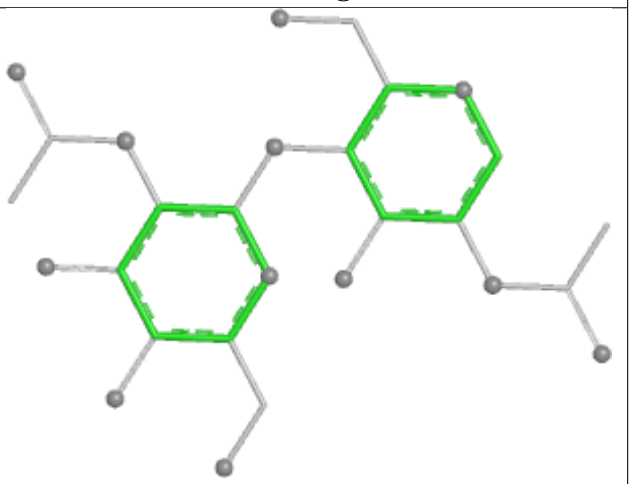
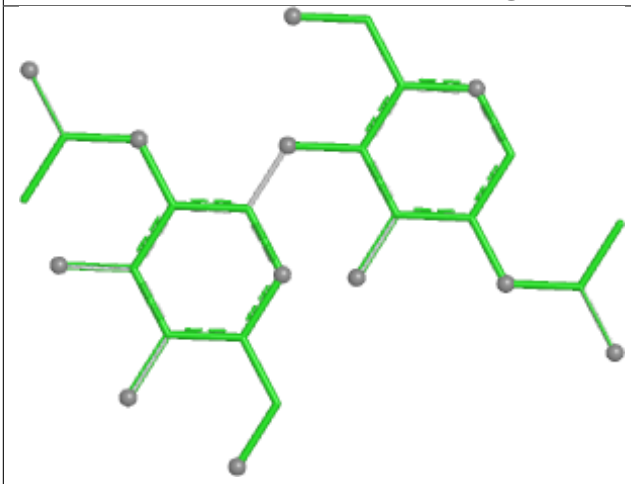


Rings

Oligosaccharide Chain i



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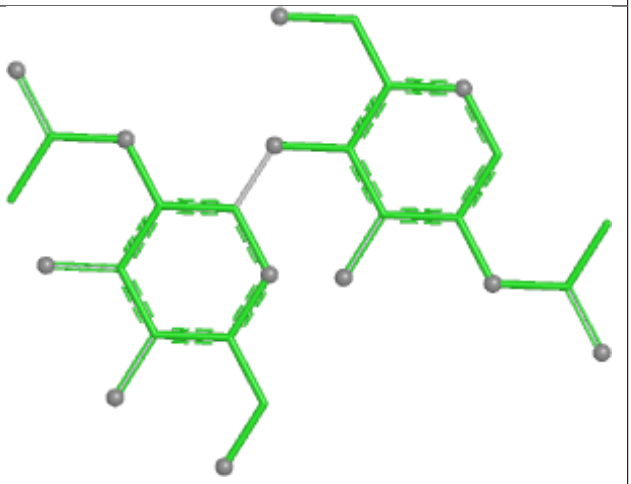

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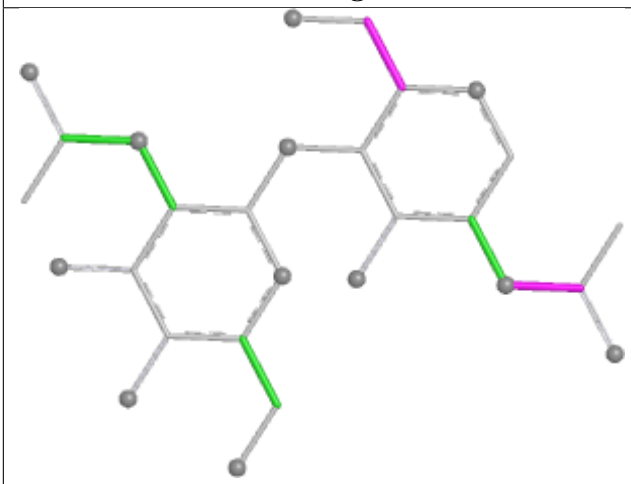

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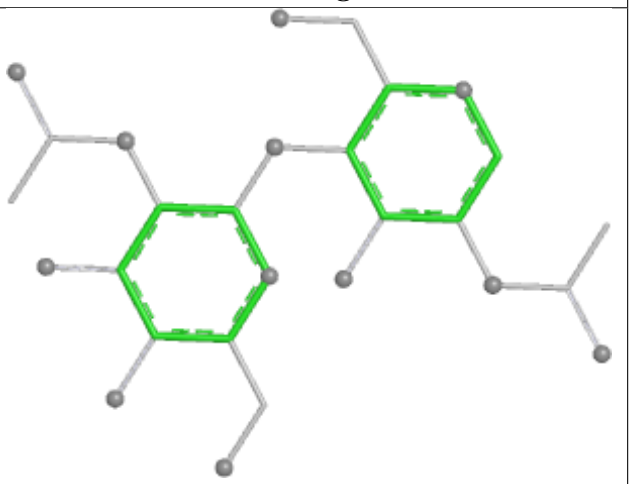
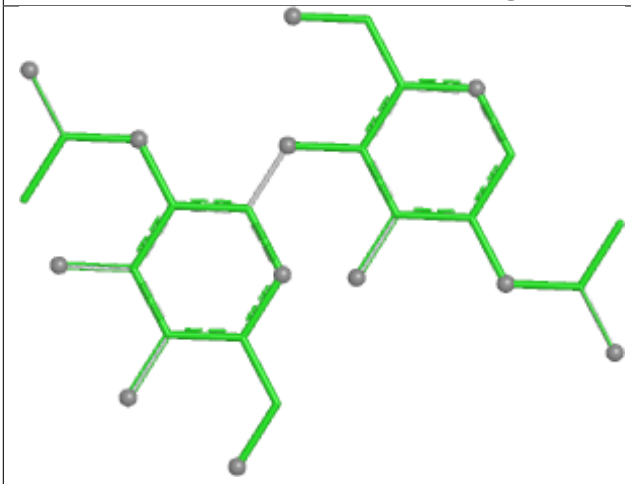


Rings

Oligosaccharide Chain j



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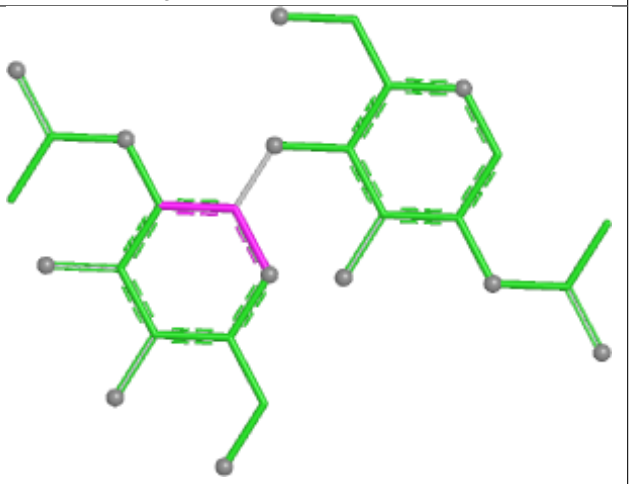
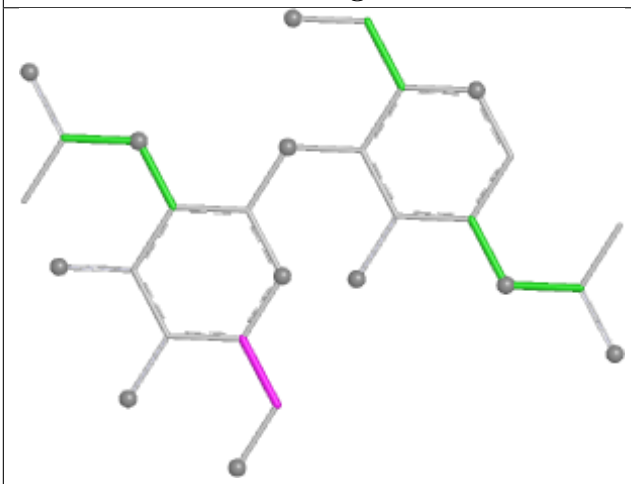


Bond angles



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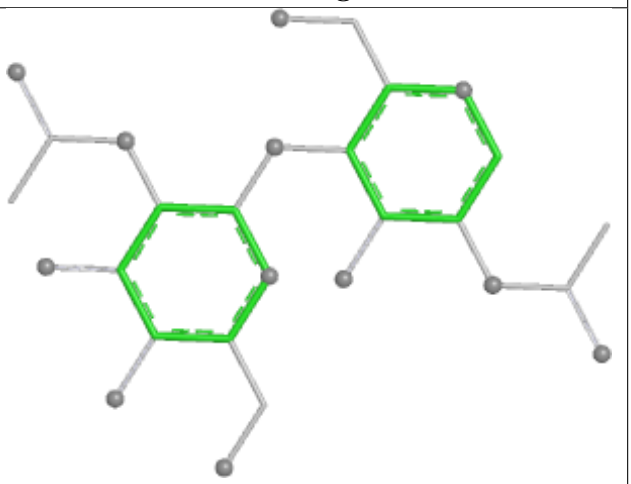
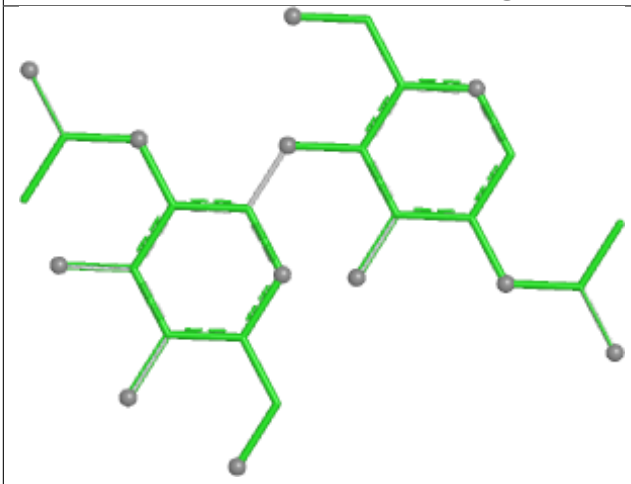


Rings

Oligosaccharide Chain k



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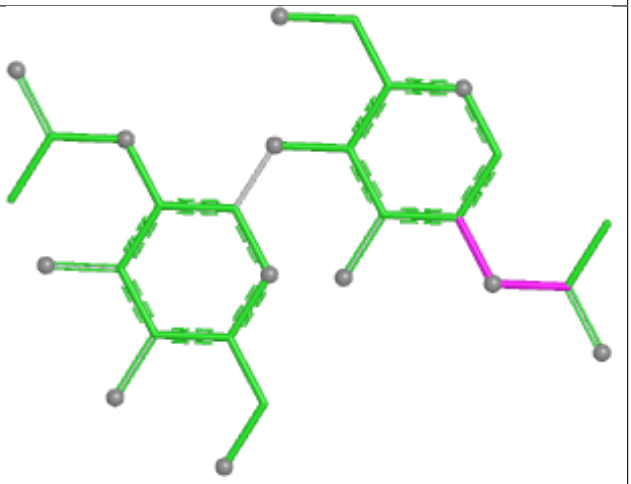
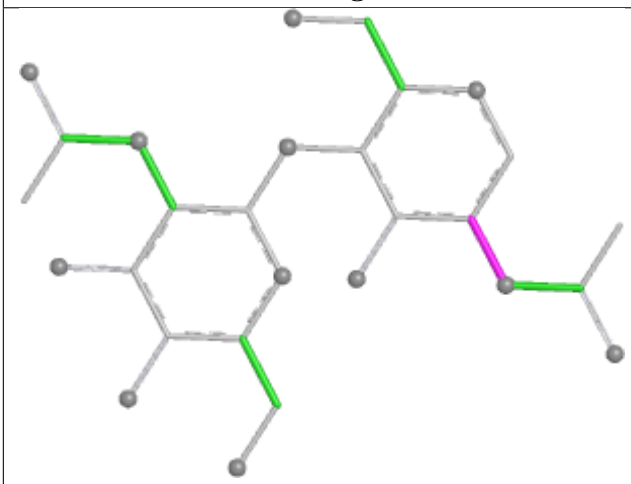


Bond angles



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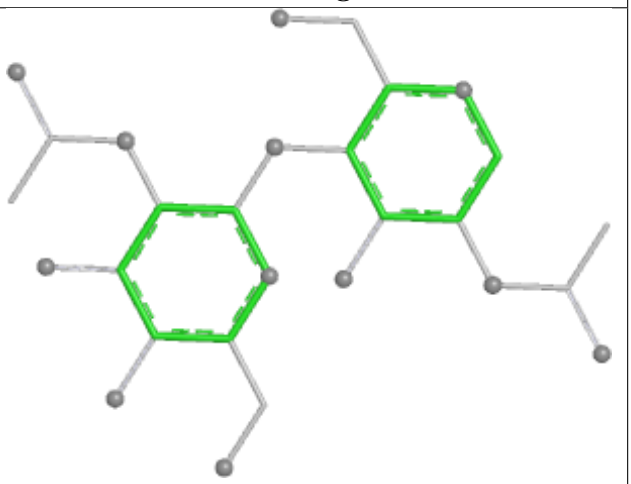
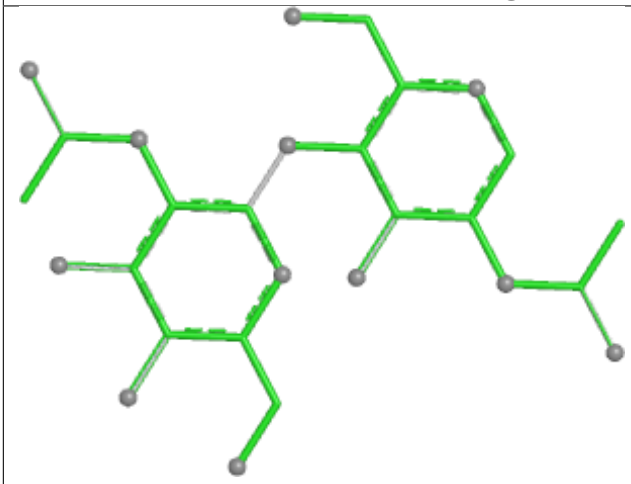


Rings

Oligosaccharide Chain l



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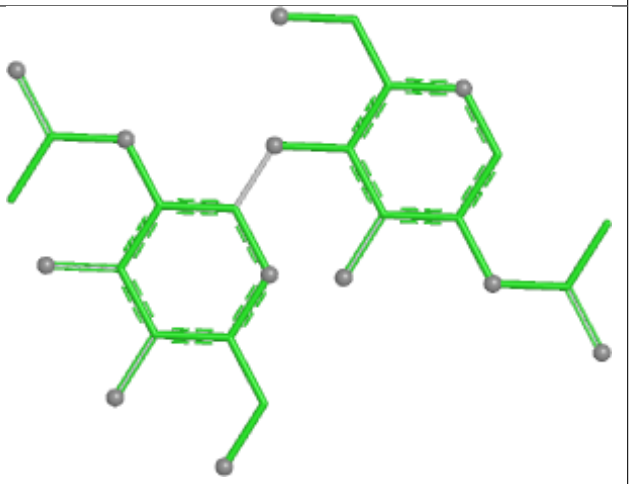
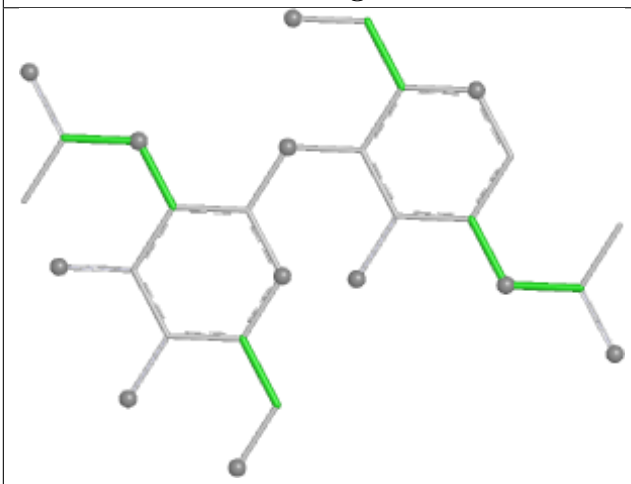


Bond angles



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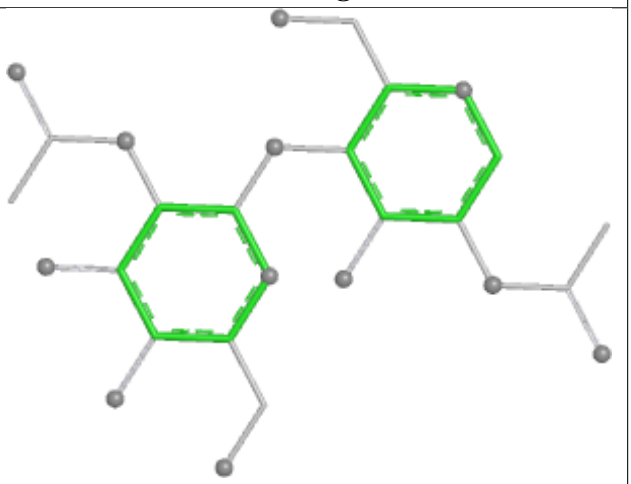
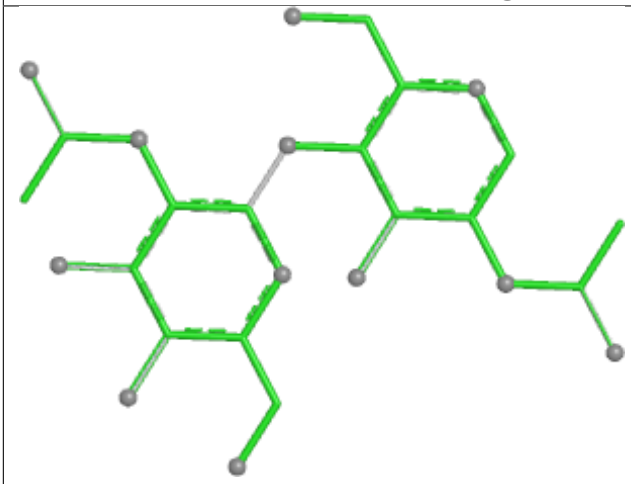


Rings

Oligosaccharide Chain o



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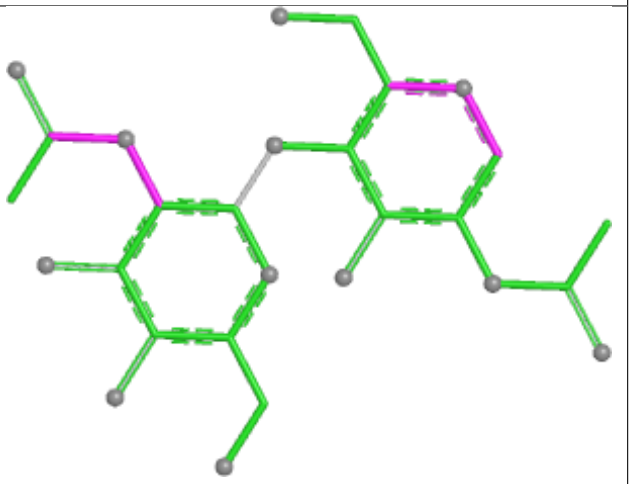
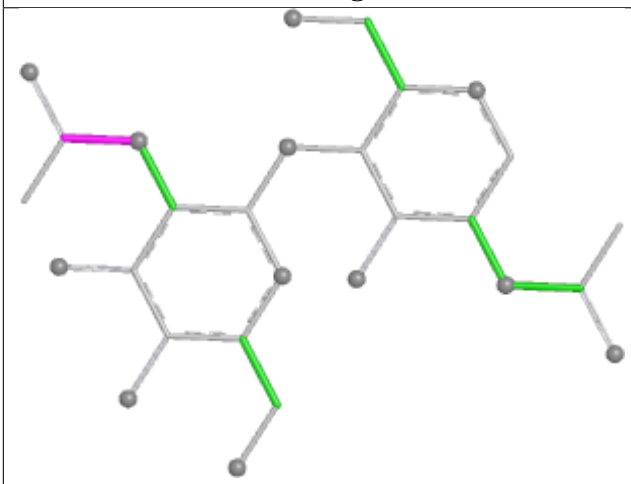


Bond angles



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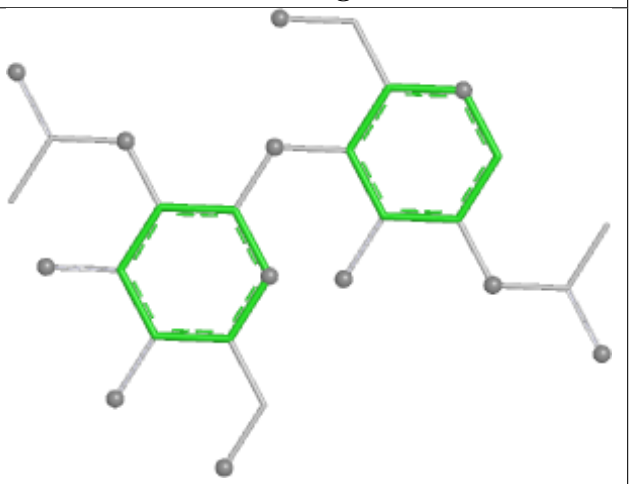
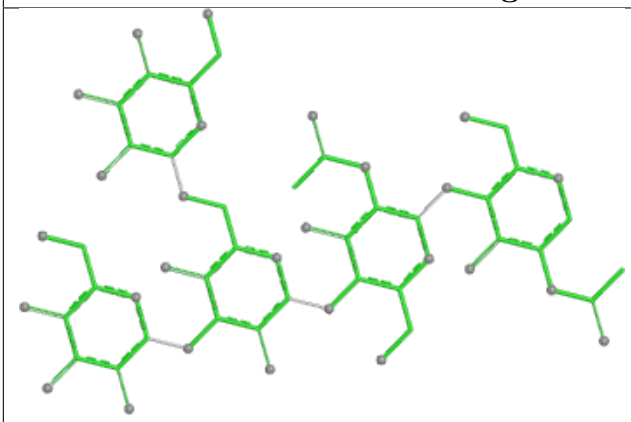


Rings

Oligosaccharide Chain I



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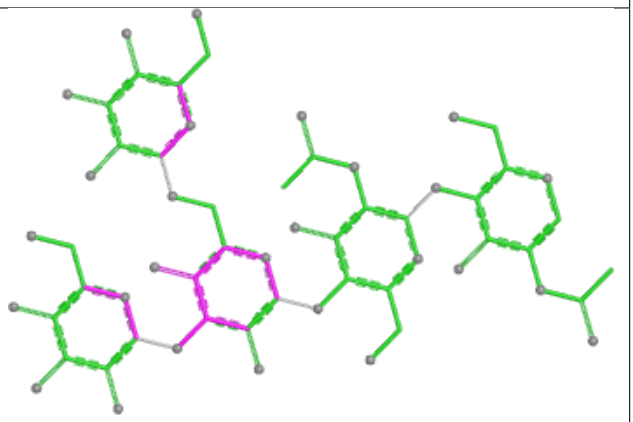

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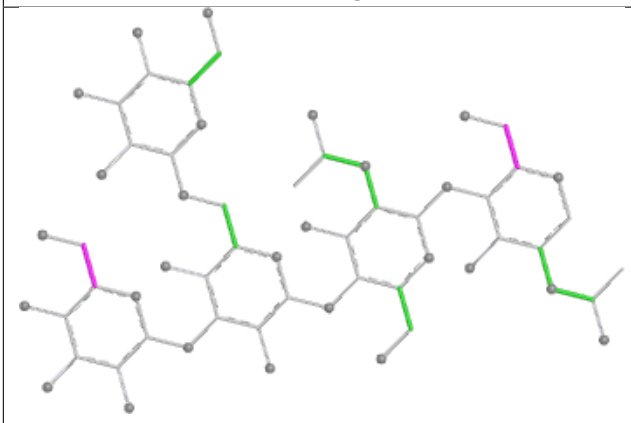

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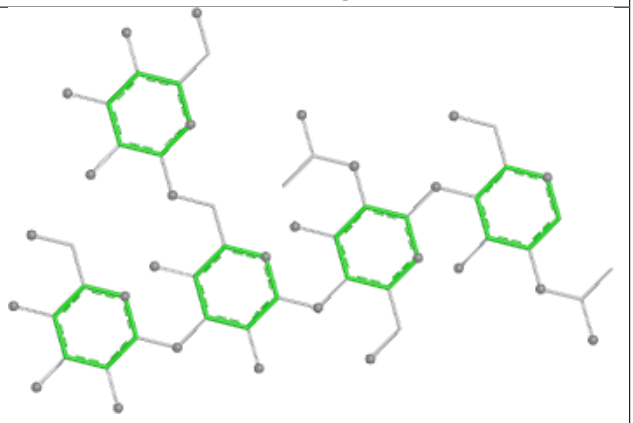
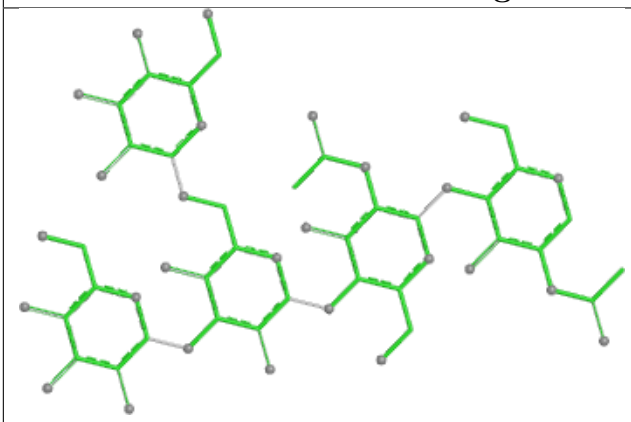


Rings

Oligosaccharide Chain N



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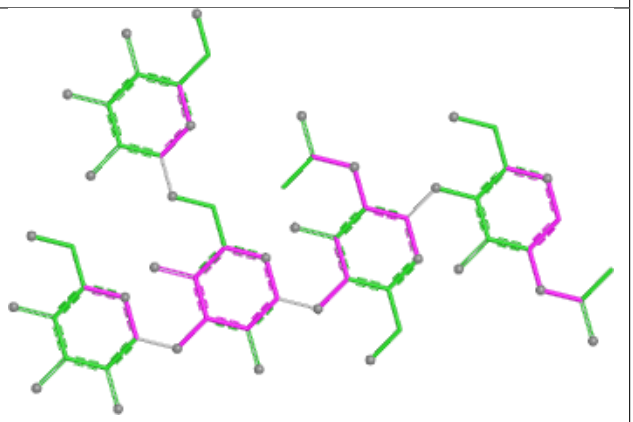
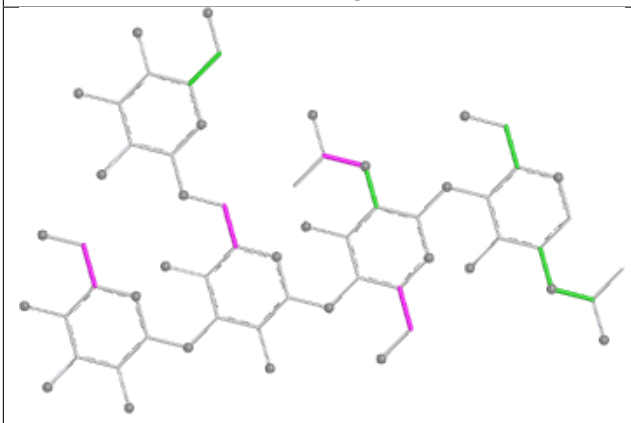


Bond angles



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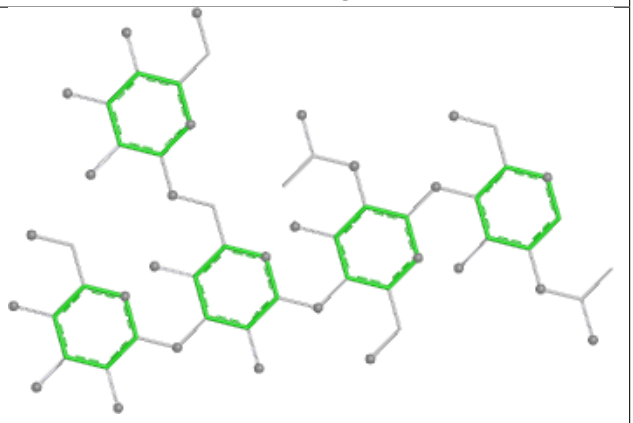
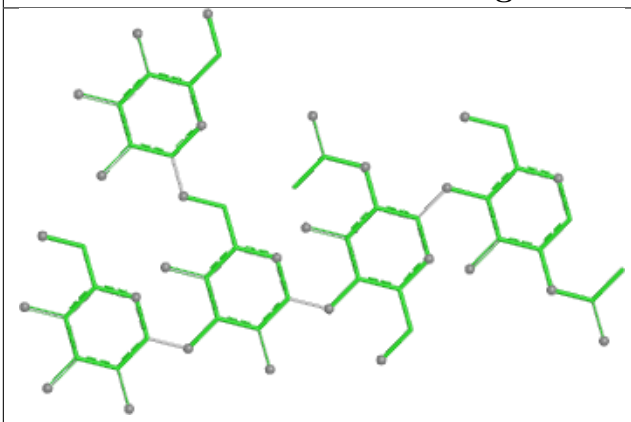


Rings

Oligosaccharide Chain T



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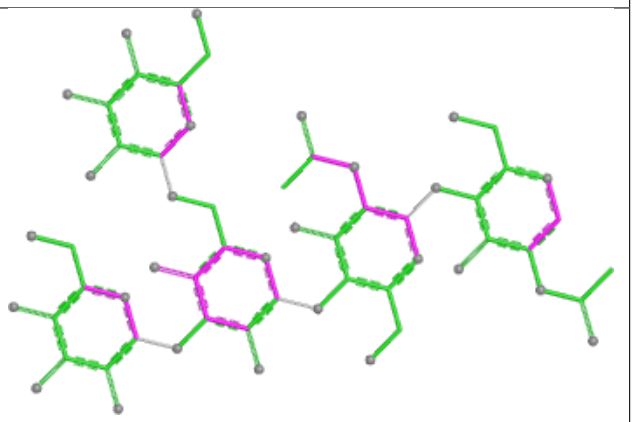
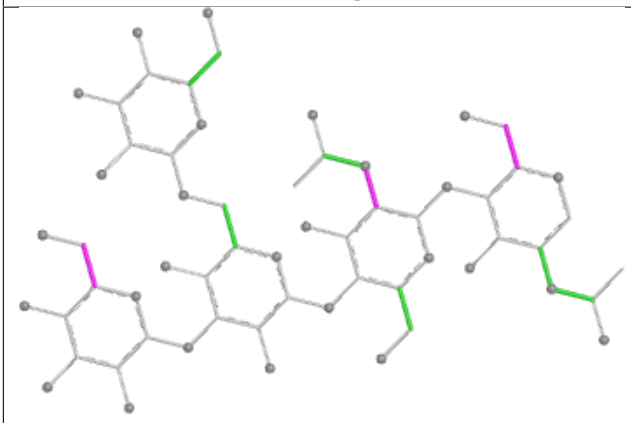


Bond angles



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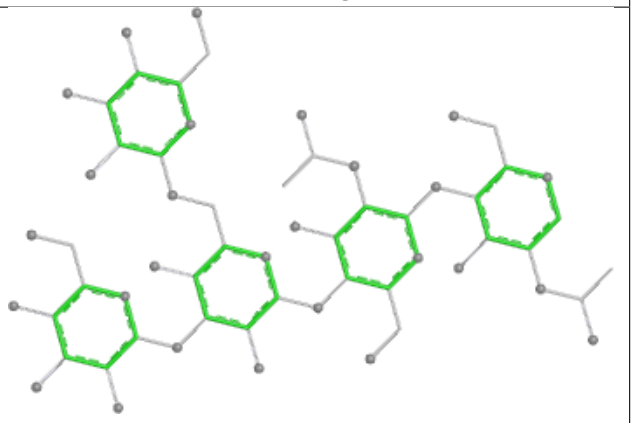
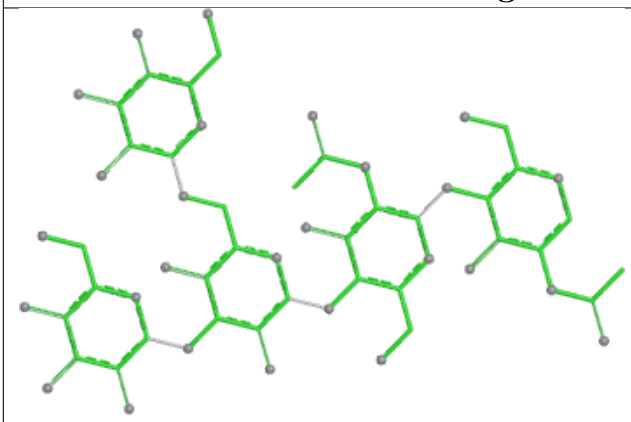


Rings

Oligosaccharide Chain d



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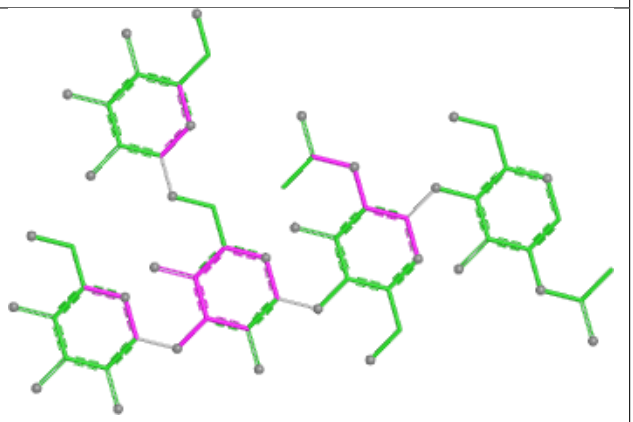
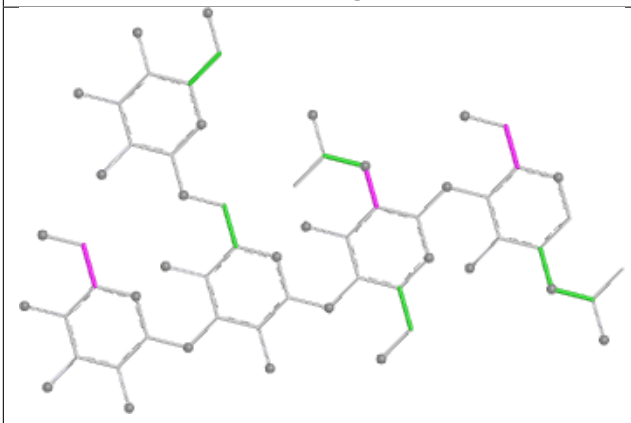


Bond angles



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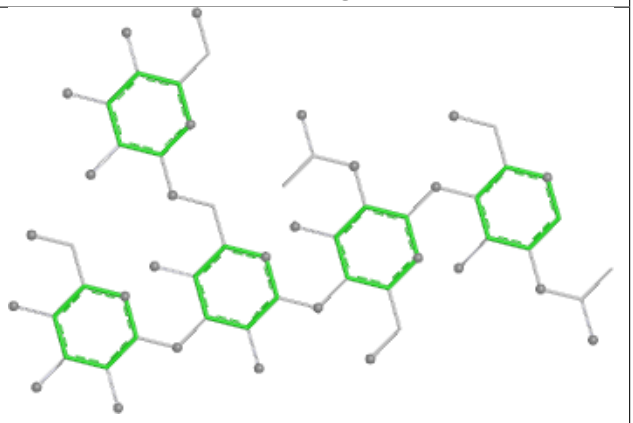
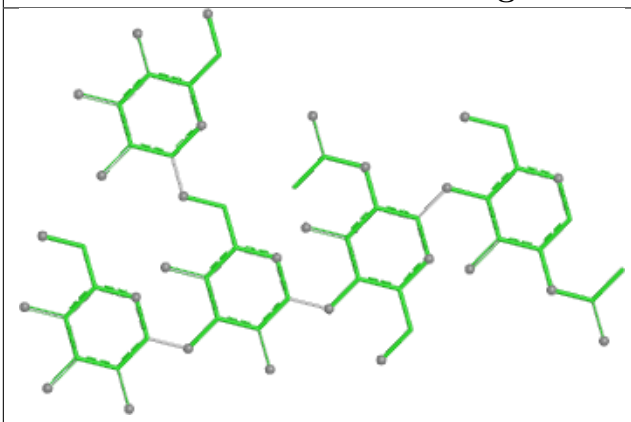


Rings

Oligosaccharide Chain n



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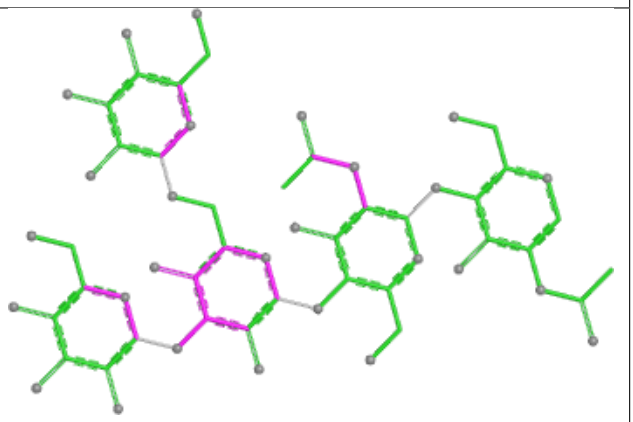
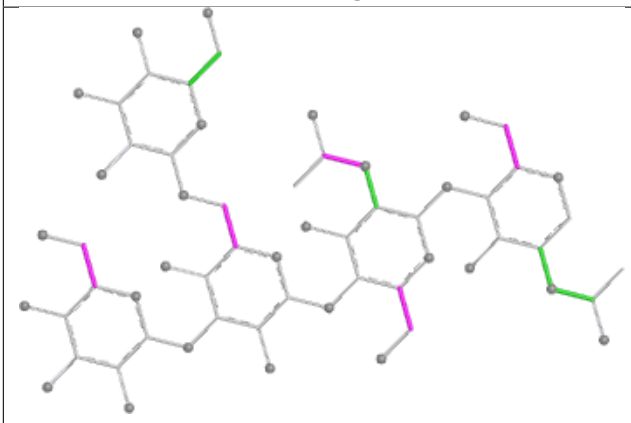


Bond angles



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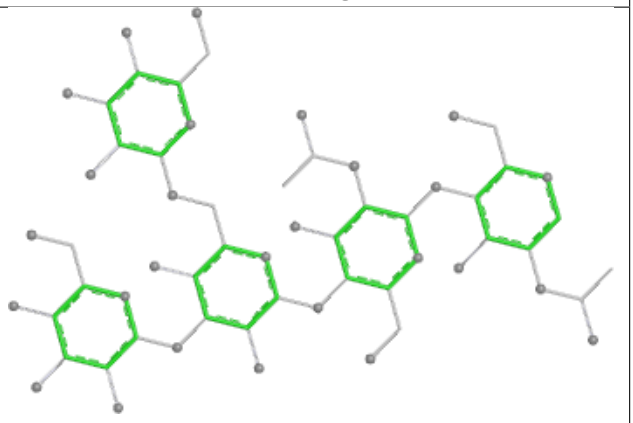
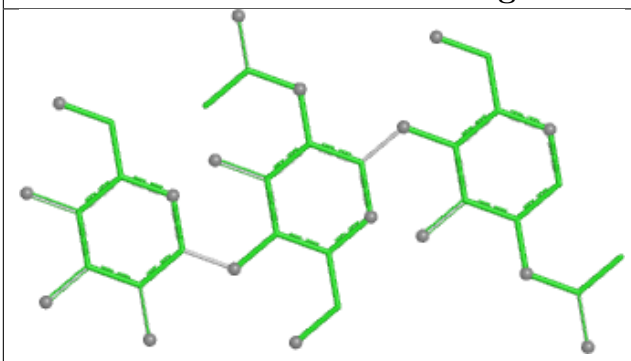


Rings

Oligosaccharide Chain J



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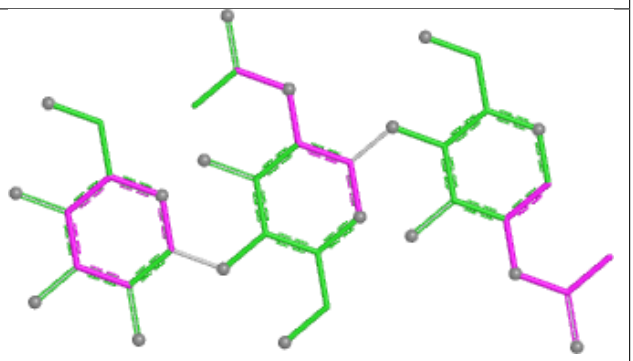
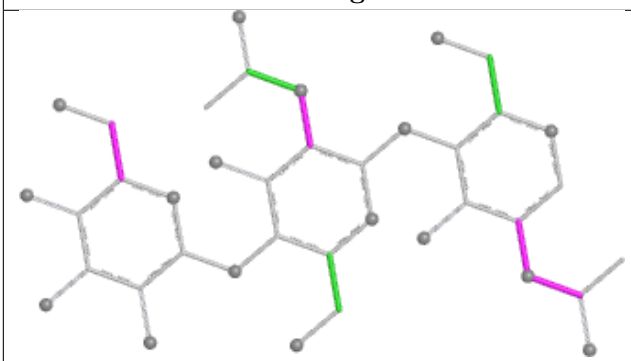


Bond angles



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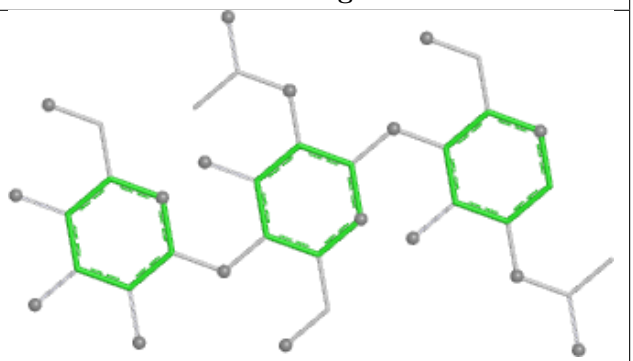
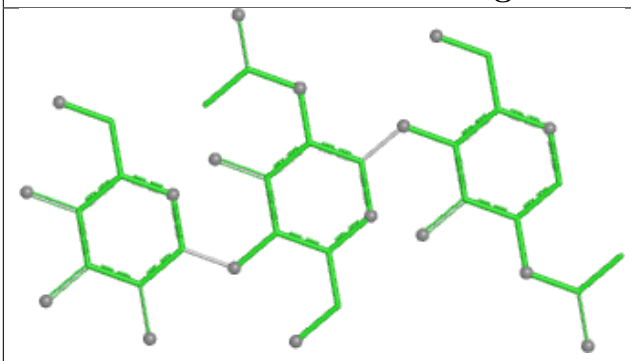


Rings

Oligosaccharide Chain X



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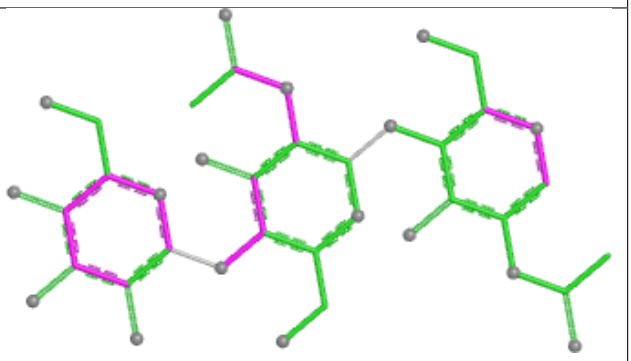
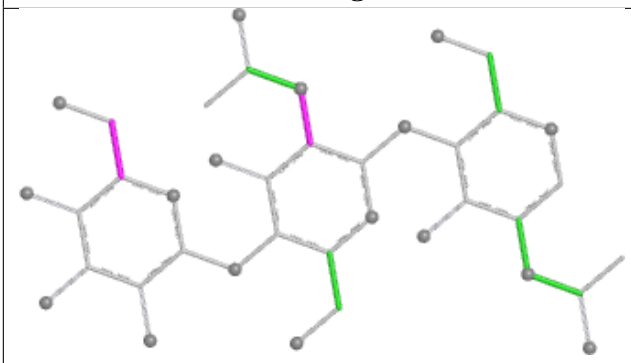


Bond angles



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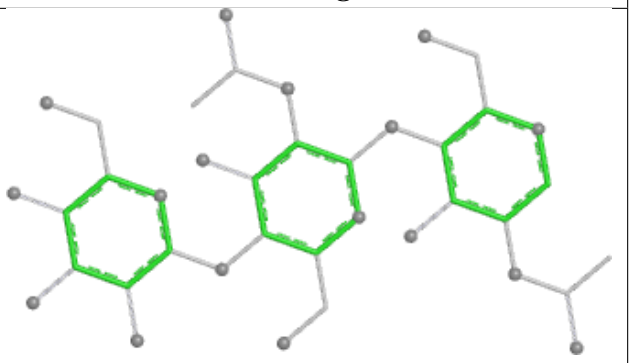
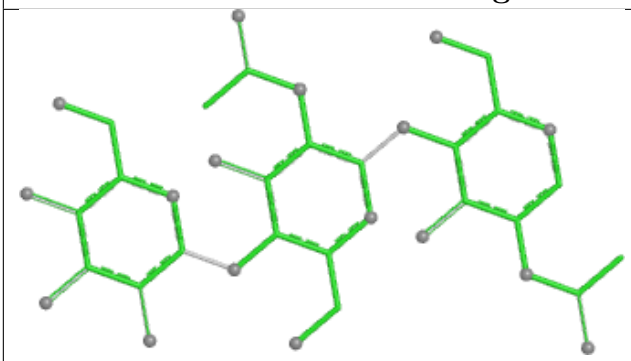
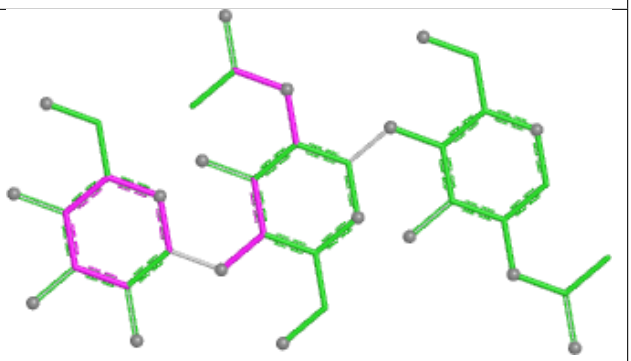


Rings

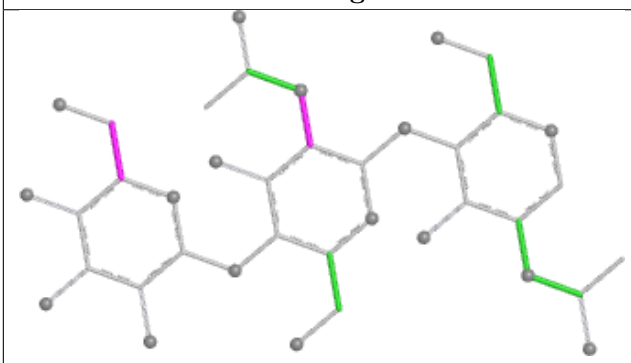
Oligosaccharide Chain m



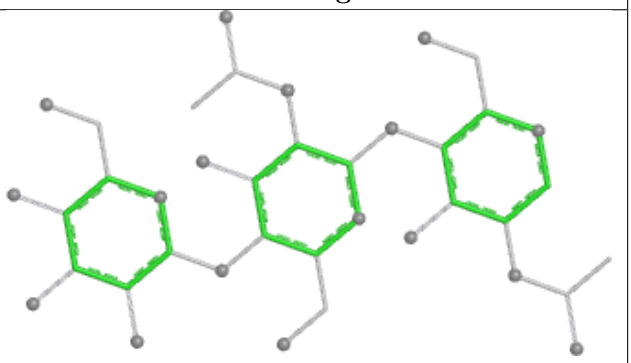
Bond lengths



Bond angles

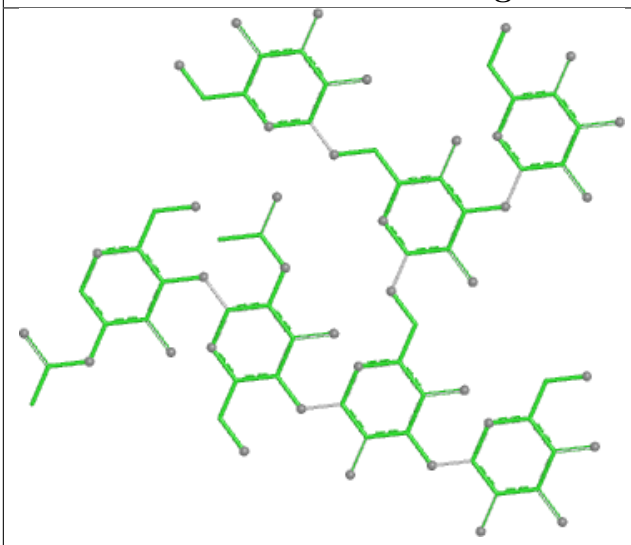


Torsions

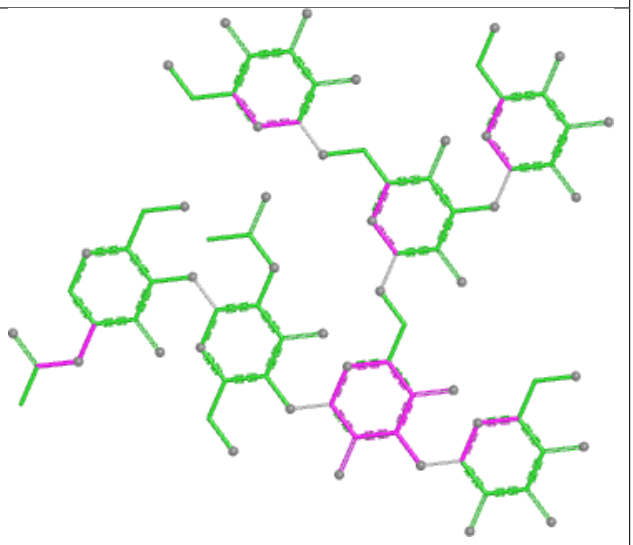


Rings

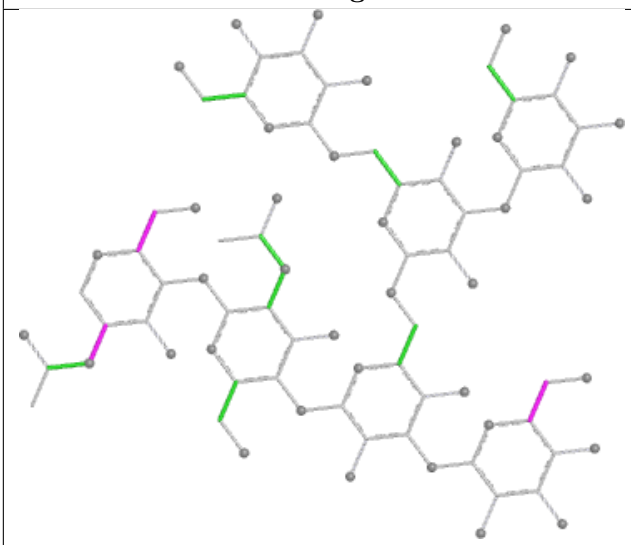
Oligosaccharide Chain O



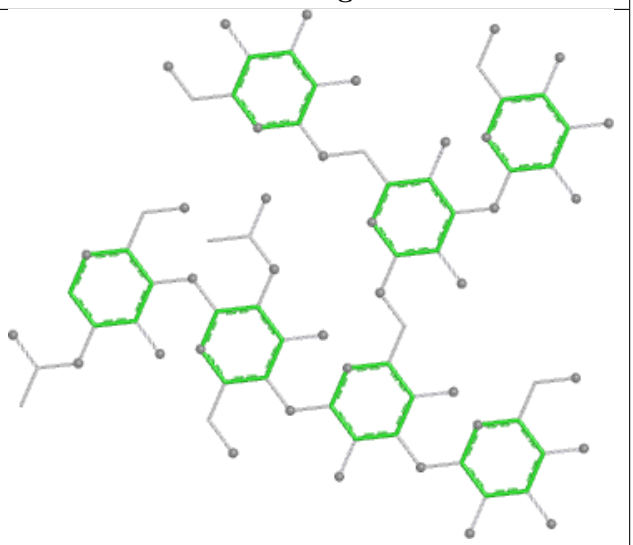
Bond lengths



Bond angles

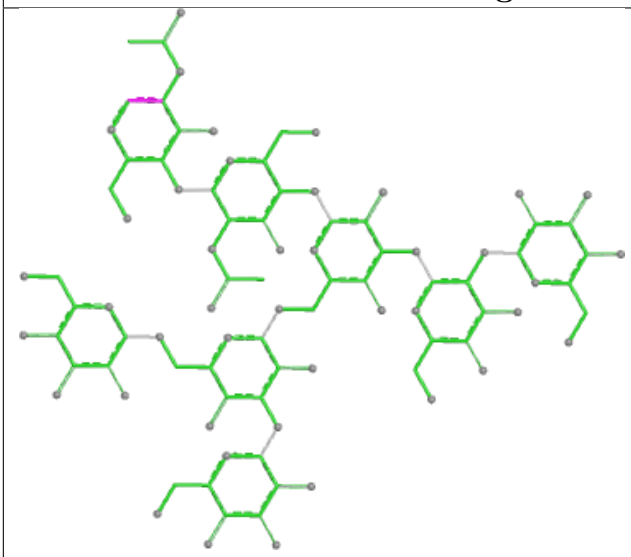


Torsions

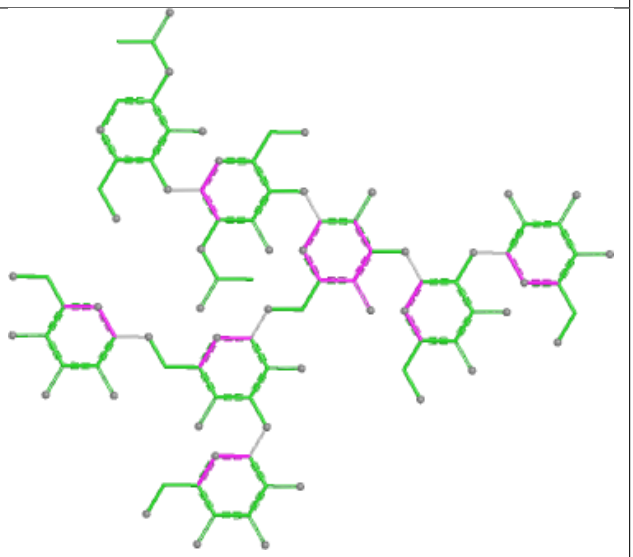


Rings

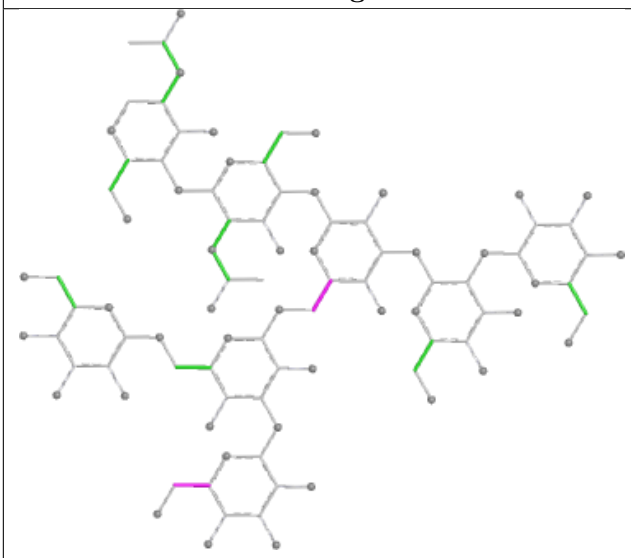
Oligosaccharide Chain P



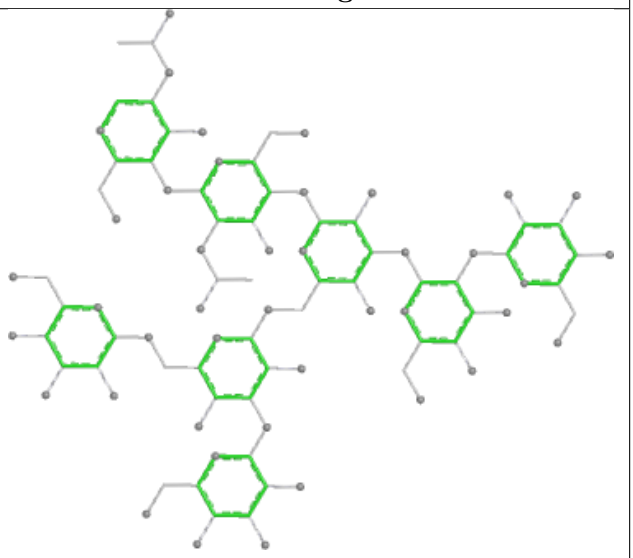
Bond lengths



Bond angles

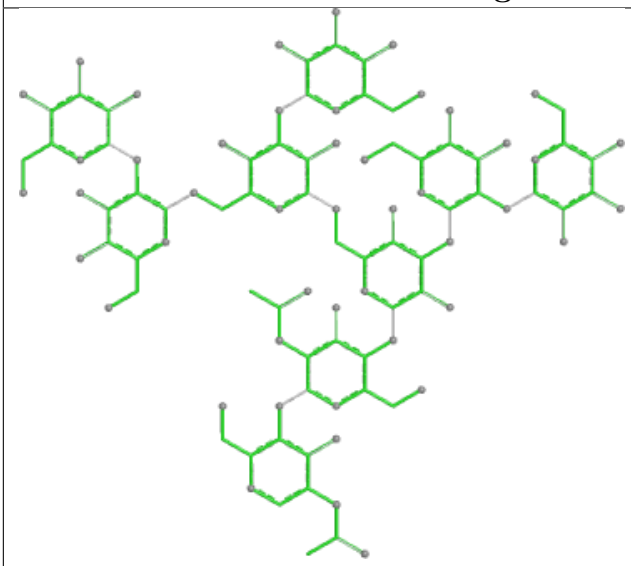


Torsions

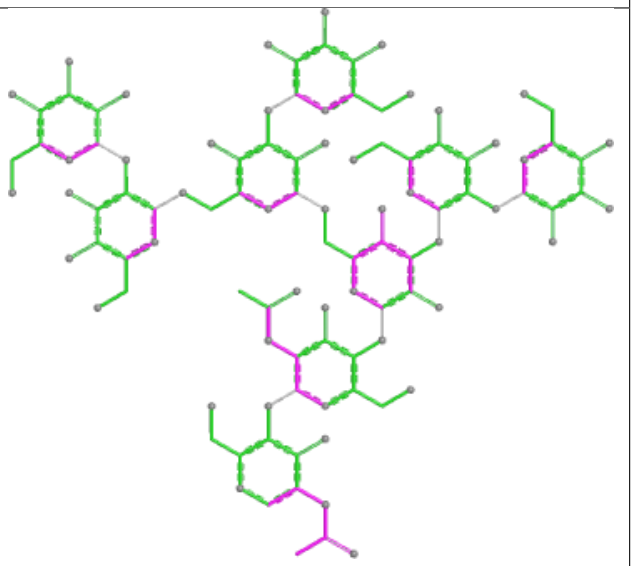


Rings

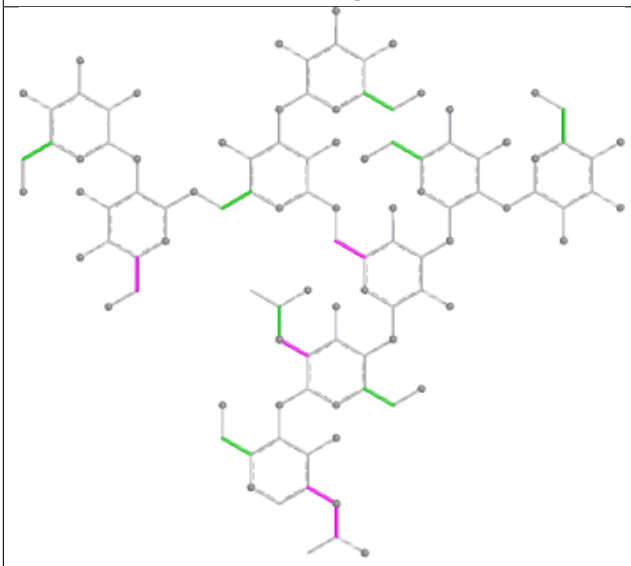
Oligosaccharide Chain U



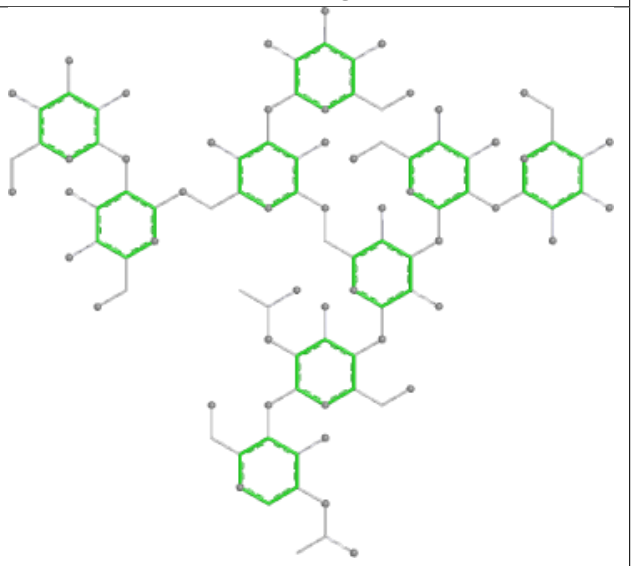
Bond lengths



Bond angles

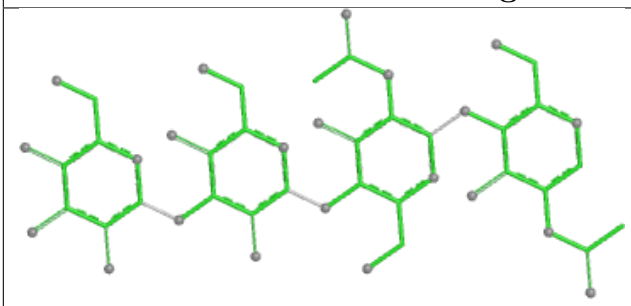


Torsions

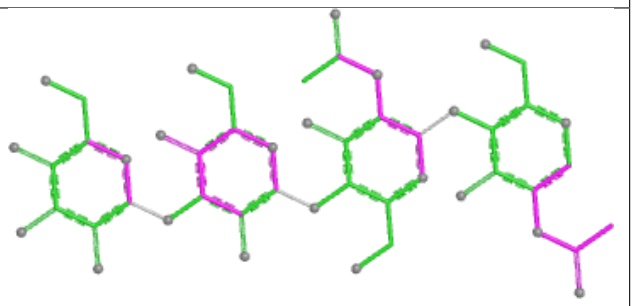


Rings

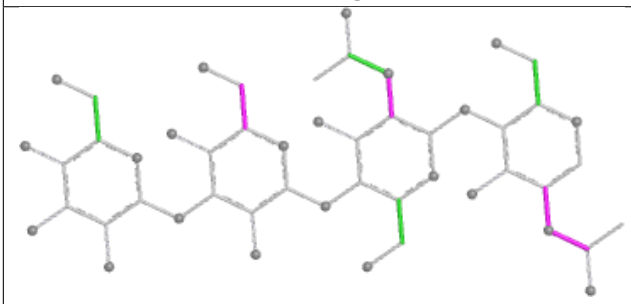
Oligosaccharide Chain e



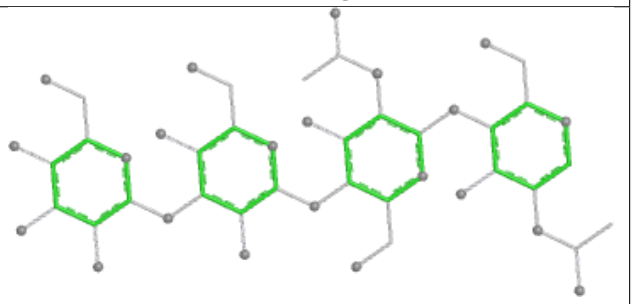
Bond lengths



Bond angles

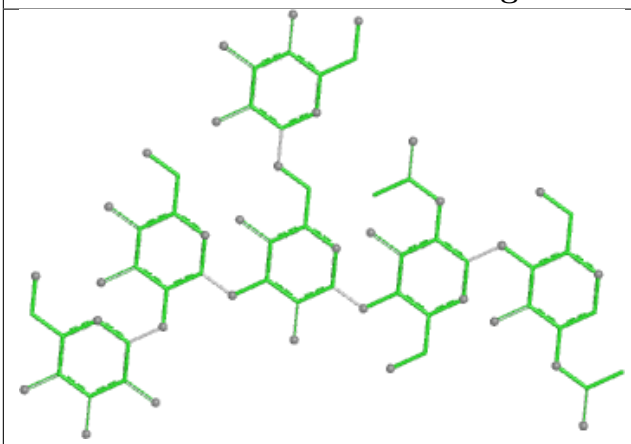


Torsions

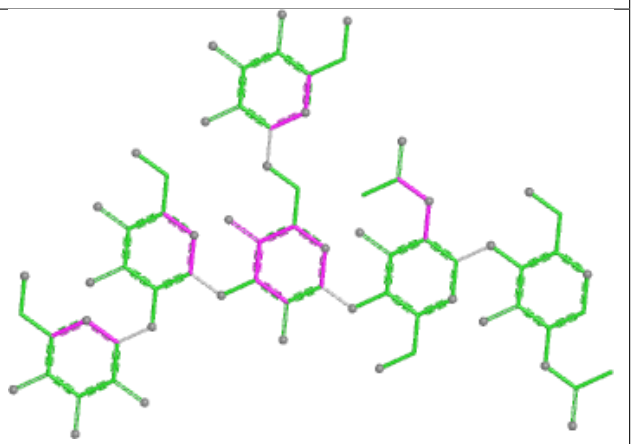


Rings

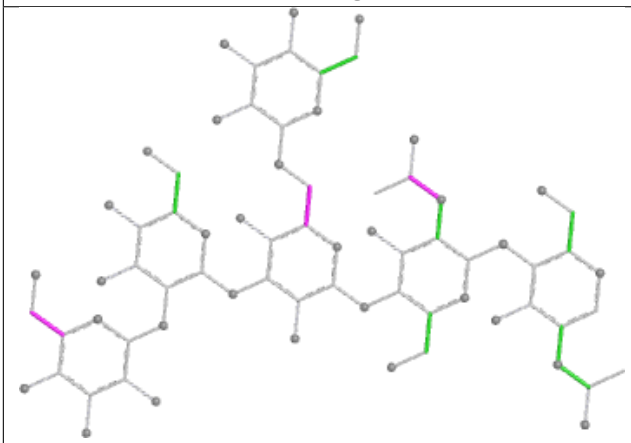
Oligosaccharide Chain f



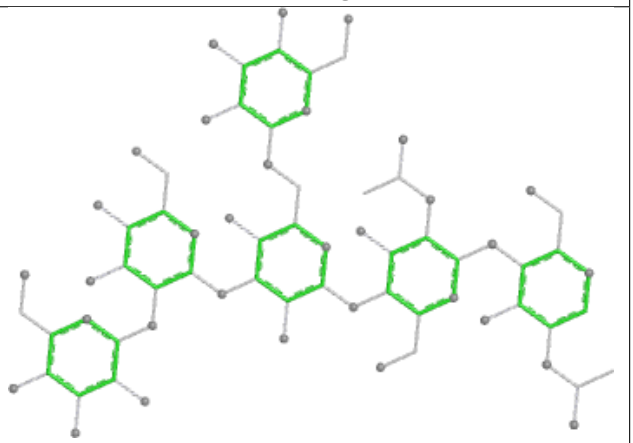
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

51 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	NAG	A	611	3	14,14,15	0.74	0	17,19,21	0.89	0
13	NAG	B	703	4	14,14,15	0.72	0	17,19,21	0.88	1 (5%)
13	NAG	B	702	4	14,14,15	0.71	0	17,19,21	0.80	0
13	NAG	G	610	-	14,14,15	0.71	0	17,19,21	0.75	0
13	NAG	A	605	-	14,14,15	0.71	0	17,19,21	0.76	0
13	NAG	A	607	3	14,14,15	0.78	1 (7%)	17,19,21	1.28	2 (11%)
13	NAG	A	610	3	14,14,15	0.71	0	17,19,21	1.07	1 (5%)
13	NAG	G	607	3	14,14,15	0.76	0	17,19,21	0.95	1 (5%)
13	NAG	D	608	3	14,14,15	0.72	0	17,19,21	0.84	0
13	NAG	G	613	-	14,14,15	0.71	0	17,19,21	0.78	0
13	NAG	A	612	3	14,14,15	0.88	1 (7%)	17,19,21	1.59	2 (11%)
13	NAG	E	701	4	14,14,15	0.70	0	17,19,21	0.81	0
13	NAG	G	612	3	14,14,15	0.78	0	17,19,21	1.10	2 (11%)
13	NAG	E	702	4	14,14,15	0.70	0	17,19,21	0.86	1 (5%)
13	NAG	A	603	-	14,14,15	0.69	0	17,19,21	1.26	1 (5%)
13	NAG	A	613	-	14,14,15	0.71	0	17,19,21	0.76	0
13	NAG	A	601	3	14,14,15	0.72	0	17,19,21	0.78	0
13	NAG	G	615	3	14,14,15	0.70	0	17,19,21	0.76	0
13	NAG	D	606	3	14,14,15	0.74	0	17,19,21	1.13	1 (5%)
13	NAG	G	609	-	14,14,15	0.70	0	17,19,21	1.29	1 (5%)
13	NAG	G	611	3	14,14,15	0.80	0	17,19,21	1.08	2 (11%)
13	NAG	A	606	3	14,14,15	0.71	0	17,19,21	0.79	0
13	NAG	G	605	-	14,14,15	0.71	0	17,19,21	0.76	0
13	NAG	E	703	4	14,14,15	0.72	0	17,19,21	0.73	0
13	NAG	C	702	4	14,14,15	0.71	0	17,19,21	0.84	0
13	NAG	D	603	-	14,14,15	0.71	0	17,19,21	1.27	1 (5%)
13	NAG	D	601	3	14,14,15	0.72	0	17,19,21	0.78	0
13	NAG	D	609	-	14,14,15	0.70	0	17,19,21	1.28	1 (5%)
13	NAG	D	611	3	14,14,15	0.74	0	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	NAG	G	606	3	14,14,15	0.70	0	17,19,21	1.31	1 (5%)
13	NAG	G	616	-	14,14,15	0.69	0	17,19,21	0.77	0
13	NAG	G	602	3	14,14,15	0.70	0	17,19,21	1.00	1 (5%)
13	NAG	G	603	-	14,14,15	0.70	0	17,19,21	1.29	1 (5%)
13	NAG	G	614	-	14,14,15	0.71	0	17,19,21	0.86	1 (5%)
13	NAG	A	604	3	14,14,15	0.72	0	17,19,21	0.88	1 (5%)
13	NAG	D	605	-	14,14,15	0.72	0	17,19,21	0.76	0
13	NAG	A	615	3	14,14,15	0.76	0	17,19,21	1.47	2 (11%)
13	NAG	G	601	3	14,14,15	0.71	0	17,19,21	0.77	0
13	NAG	B	701	4	14,14,15	0.71	0	17,19,21	0.79	0
13	NAG	A	614	-	14,14,15	0.71	0	17,19,21	0.87	1 (5%)
13	NAG	A	609	3	14,14,15	0.69	0	17,19,21	1.28	1 (5%)
13	NAG	D	604	3	14,14,15	0.70	0	17,19,21	0.90	1 (5%)
13	NAG	A	608	3	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
13	NAG	D	610	3	14,14,15	0.76	0	17,19,21	0.81	0
13	NAG	D	602	3	14,14,15	0.71	0	17,19,21	1.00	2 (11%)
13	NAG	G	608	3	14,14,15	0.77	0	17,19,21	1.00	1 (5%)
13	NAG	D	607	3	14,14,15	0.70	0	17,19,21	1.02	1 (5%)
13	NAG	A	602	3	14,14,15	0.71	0	17,19,21	0.93	1 (5%)
13	NAG	C	701	4	14,14,15	0.71	0	17,19,21	0.78	0
13	NAG	G	604	3	14,14,15	0.70	0	17,19,21	0.88	1 (5%)
13	NAG	C	703	4	14,14,15	0.73	0	17,19,21	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	A	611	3	-	1/6/23/26	0/1/1/1
13	NAG	B	703	4	-	0/6/23/26	0/1/1/1
13	NAG	B	702	4	-	1/6/23/26	0/1/1/1
13	NAG	G	610	-	-	0/6/23/26	0/1/1/1
13	NAG	A	605	-	-	1/6/23/26	0/1/1/1
13	NAG	A	607	3	-	3/6/23/26	0/1/1/1
13	NAG	A	610	3	-	0/6/23/26	0/1/1/1
13	NAG	G	607	3	-	3/6/23/26	0/1/1/1
13	NAG	D	608	3	-	1/6/23/26	0/1/1/1
13	NAG	G	613	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	A	612	3	-	1/6/23/26	0/1/1/1
13	NAG	E	701	4	-	2/6/23/26	0/1/1/1
13	NAG	G	612	3	-	1/6/23/26	0/1/1/1
13	NAG	E	702	4	-	1/6/23/26	0/1/1/1
13	NAG	A	603	-	-	2/6/23/26	0/1/1/1
13	NAG	A	613	-	-	0/6/23/26	0/1/1/1
13	NAG	A	601	3	-	1/6/23/26	0/1/1/1
13	NAG	G	615	3	-	1/6/23/26	0/1/1/1
13	NAG	D	606	3	-	0/6/23/26	0/1/1/1
13	NAG	G	609	-	-	4/6/23/26	0/1/1/1
13	NAG	G	611	3	-	2/6/23/26	0/1/1/1
13	NAG	A	606	3	-	0/6/23/26	0/1/1/1
13	NAG	G	605	-	-	1/6/23/26	0/1/1/1
13	NAG	E	703	4	-	0/6/23/26	0/1/1/1
13	NAG	C	702	4	-	1/6/23/26	0/1/1/1
13	NAG	D	603	-	-	2/6/23/26	0/1/1/1
13	NAG	D	601	3	-	1/6/23/26	0/1/1/1
13	NAG	D	609	-	-	2/6/23/26	0/1/1/1
13	NAG	D	611	3	-	1/6/23/26	0/1/1/1
13	NAG	G	606	3	-	2/6/23/26	0/1/1/1
13	NAG	G	616	-	-	0/6/23/26	0/1/1/1
13	NAG	G	602	3	-	3/6/23/26	0/1/1/1
13	NAG	G	603	-	-	2/6/23/26	0/1/1/1
13	NAG	G	614	-	-	3/6/23/26	0/1/1/1
13	NAG	A	604	3	-	3/6/23/26	0/1/1/1
13	NAG	D	605	-	-	1/6/23/26	0/1/1/1
13	NAG	A	615	3	-	2/6/23/26	0/1/1/1
13	NAG	G	601	3	-	1/6/23/26	0/1/1/1
13	NAG	B	701	4	-	1/6/23/26	0/1/1/1
13	NAG	A	614	-	-	3/6/23/26	0/1/1/1
13	NAG	A	609	3	-	4/6/23/26	0/1/1/1
13	NAG	D	604	3	-	3/6/23/26	0/1/1/1
13	NAG	A	608	3	-	1/6/23/26	0/1/1/1
13	NAG	D	610	3	-	0/6/23/26	0/1/1/1
13	NAG	D	602	3	-	4/6/23/26	0/1/1/1
13	NAG	G	608	3	-	0/6/23/26	0/1/1/1
13	NAG	D	607	3	-	3/6/23/26	0/1/1/1
13	NAG	A	602	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	C	701	4	-	0/6/23/26	0/1/1/1
13	NAG	G	604	3	-	3/6/23/26	0/1/1/1
13	NAG	C	703	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	612	NAG	C1-C2	2.45	1.55	1.52
13	A	607	NAG	C1-C2	2.01	1.55	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	612	NAG	C1-O5-C5	5.14	119.07	112.19
13	G	603	NAG	C2-N2-C7	3.88	128.11	122.90
13	D	603	NAG	C2-N2-C7	3.87	128.09	122.90
13	D	609	NAG	C2-N2-C7	3.81	128.01	122.90
13	A	609	NAG	C2-N2-C7	3.79	127.98	122.90
13	A	603	NAG	C2-N2-C7	3.78	127.97	122.90
13	G	609	NAG	C2-N2-C7	3.77	127.96	122.90
13	G	606	NAG	C2-N2-C7	3.69	127.84	122.90
13	A	615	NAG	C2-N2-C7	3.68	127.83	122.90
13	A	610	NAG	C1-O5-C5	3.30	116.61	112.19
13	D	606	NAG	C1-O5-C5	3.14	116.39	112.19
13	A	607	NAG	C1-O5-C5	3.04	116.26	112.19
13	A	615	NAG	C1-O5-C5	2.91	116.08	112.19
13	A	607	NAG	C2-N2-C7	2.84	126.71	122.90
13	G	612	NAG	C1-O5-C5	2.69	115.79	112.19
13	D	611	NAG	C1-O5-C5	2.61	115.68	112.19
13	D	607	NAG	O5-C1-C2	-2.57	107.31	111.29
13	G	611	NAG	C1-O5-C5	2.45	115.47	112.19
13	G	607	NAG	C2-N2-C7	2.41	126.14	122.90
13	G	602	NAG	C1-O5-C5	2.39	115.39	112.19
13	D	602	NAG	C1-O5-C5	2.37	115.37	112.19
13	G	608	NAG	C1-O5-C5	2.21	115.15	112.19
13	G	614	NAG	C2-N2-C7	2.20	125.84	122.90
13	G	611	NAG	O5-C1-C2	-2.18	107.91	111.29
13	A	604	NAG	C2-N2-C7	2.17	125.81	122.90
13	A	614	NAG	C2-N2-C7	2.16	125.79	122.90
13	G	604	NAG	C2-N2-C7	2.14	125.77	122.90
13	D	604	NAG	C2-N2-C7	2.11	125.73	122.90
13	G	612	NAG	C2-N2-C7	2.07	125.68	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	702	NAG	C1-O5-C5	2.05	114.93	112.19
13	D	602	NAG	C2-N2-C7	2.03	125.63	122.90
13	A	612	NAG	C2-N2-C7	2.03	125.62	122.90
13	A	608	NAG	O5-C1-C2	-2.02	108.17	111.29
13	A	602	NAG	C2-N2-C7	2.01	125.59	122.90
13	B	703	NAG	O5-C1-C2	-2.00	108.20	111.29

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	602	NAG	C4-C5-C6-O6
13	G	609	NAG	O5-C5-C6-O6
13	A	602	NAG	O5-C5-C6-O6
13	G	609	NAG	C4-C5-C6-O6
13	A	609	NAG	O5-C5-C6-O6
13	A	609	NAG	C4-C5-C6-O6
13	G	602	NAG	C8-C7-N2-C2
13	G	602	NAG	O7-C7-N2-C2
13	G	604	NAG	C8-C7-N2-C2
13	G	604	NAG	O7-C7-N2-C2
13	G	607	NAG	C8-C7-N2-C2
13	G	607	NAG	O7-C7-N2-C2
13	G	614	NAG	C8-C7-N2-C2
13	G	614	NAG	O7-C7-N2-C2
13	A	602	NAG	C8-C7-N2-C2
13	A	602	NAG	O7-C7-N2-C2
13	A	604	NAG	C8-C7-N2-C2
13	A	604	NAG	O7-C7-N2-C2
13	A	607	NAG	C8-C7-N2-C2
13	A	607	NAG	O7-C7-N2-C2
13	A	614	NAG	C8-C7-N2-C2
13	A	614	NAG	O7-C7-N2-C2
13	D	602	NAG	C8-C7-N2-C2
13	D	602	NAG	O7-C7-N2-C2
13	D	604	NAG	C8-C7-N2-C2
13	D	604	NAG	O7-C7-N2-C2
13	D	607	NAG	C8-C7-N2-C2
13	D	607	NAG	O7-C7-N2-C2
13	E	701	NAG	O5-C5-C6-O6
13	D	602	NAG	O5-C5-C6-O6
13	G	611	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	G	612	NAG	O5-C5-C6-O6
13	C	702	NAG	O5-C5-C6-O6
13	E	702	NAG	O5-C5-C6-O6
13	A	612	NAG	O5-C5-C6-O6
13	G	601	NAG	O5-C5-C6-O6
13	D	605	NAG	O5-C5-C6-O6
13	D	611	NAG	O5-C5-C6-O6
13	G	605	NAG	O5-C5-C6-O6
13	G	615	NAG	O5-C5-C6-O6
13	B	702	NAG	O5-C5-C6-O6
13	A	601	NAG	O5-C5-C6-O6
13	A	608	NAG	O5-C5-C6-O6
13	G	607	NAG	O5-C5-C6-O6
13	A	614	NAG	O5-C5-C6-O6
13	D	604	NAG	O5-C5-C6-O6
13	G	614	NAG	O5-C5-C6-O6
13	A	604	NAG	O5-C5-C6-O6
13	A	605	NAG	O5-C5-C6-O6
13	D	601	NAG	O5-C5-C6-O6
13	G	604	NAG	O5-C5-C6-O6
13	D	607	NAG	O5-C5-C6-O6
13	E	701	NAG	C4-C5-C6-O6
13	G	602	NAG	O5-C5-C6-O6
13	A	607	NAG	O5-C5-C6-O6
13	G	603	NAG	C1-C2-N2-C7
13	G	609	NAG	C1-C2-N2-C7
13	A	603	NAG	C1-C2-N2-C7
13	A	609	NAG	C1-C2-N2-C7
13	D	603	NAG	C1-C2-N2-C7
13	D	609	NAG	C1-C2-N2-C7
13	G	606	NAG	C3-C2-N2-C7
13	A	609	NAG	C3-C2-N2-C7
13	A	615	NAG	C3-C2-N2-C7
13	G	611	NAG	C4-C5-C6-O6
13	G	606	NAG	C1-C2-N2-C7
13	A	615	NAG	C1-C2-N2-C7
13	G	603	NAG	C3-C2-N2-C7
13	G	609	NAG	C3-C2-N2-C7
13	A	603	NAG	C3-C2-N2-C7
13	D	603	NAG	C3-C2-N2-C7
13	D	609	NAG	C3-C2-N2-C7
13	A	611	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	D	608	NAG	O5-C5-C6-O6
13	D	602	NAG	C4-C5-C6-O6
13	B	701	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	605	NAG	1	0
13	A	607	NAG	1	0
13	G	613	NAG	1	0
13	A	612	NAG	1	0
13	G	612	NAG	1	0
13	G	611	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

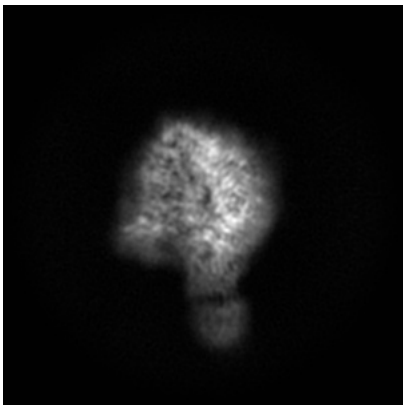
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44892. These allow visual inspection of the internal detail of the map and identification of artifacts.

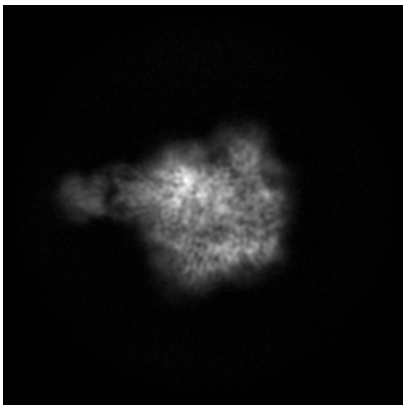
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

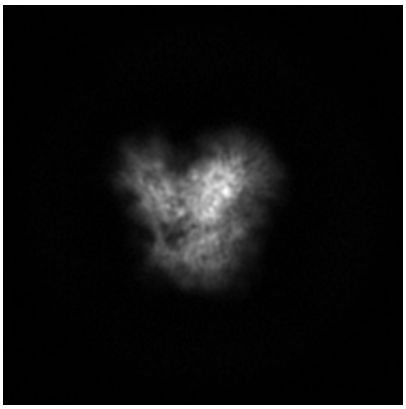
6.1.1 Primary map



X

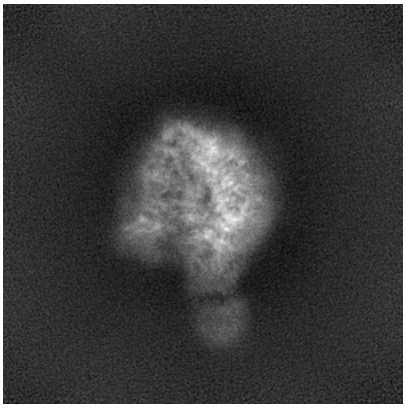


Y

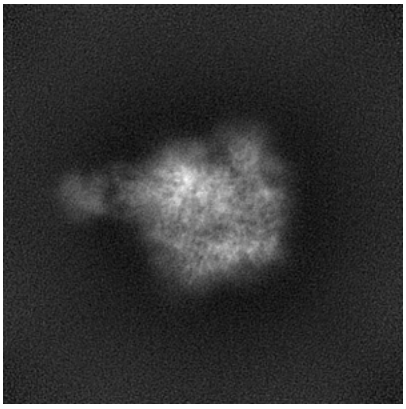


Z

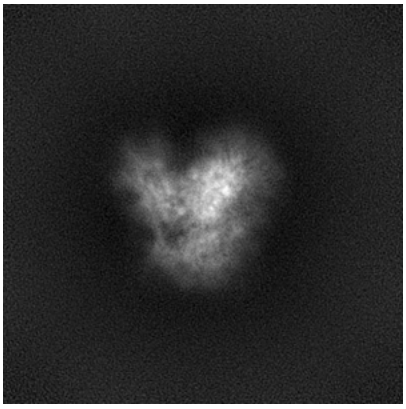
6.1.2 Raw map



X



Y

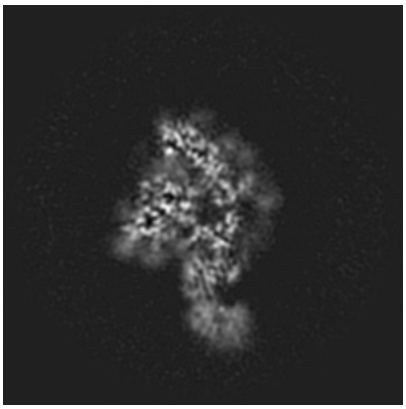


Z

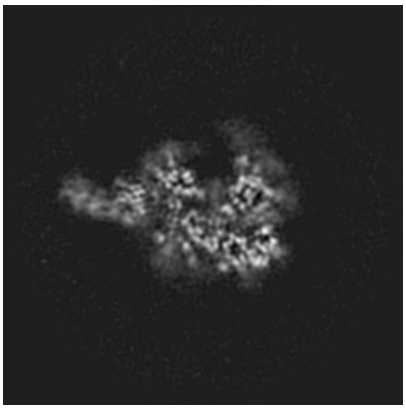
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

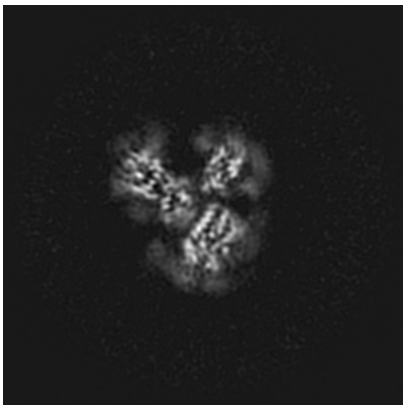
6.2.1 Primary map



X Index: 144

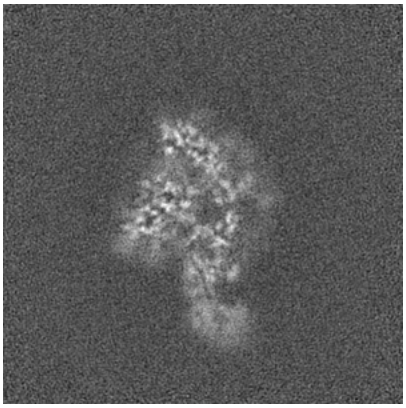


Y Index: 144

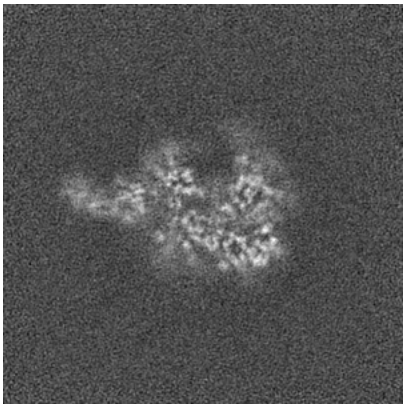


Z Index: 144

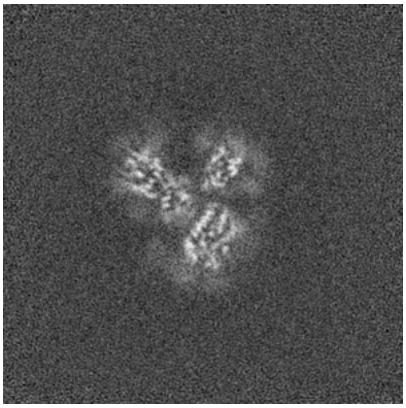
6.2.2 Raw map



X Index: 144



Y Index: 144

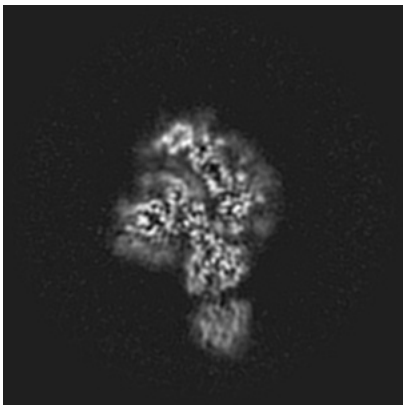


Z Index: 144

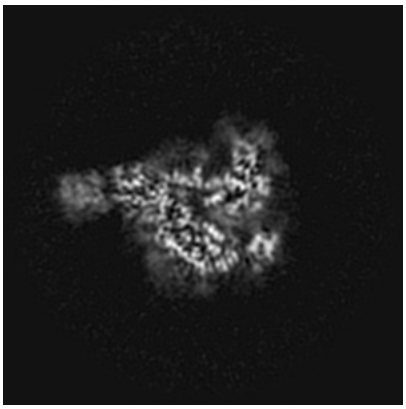
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

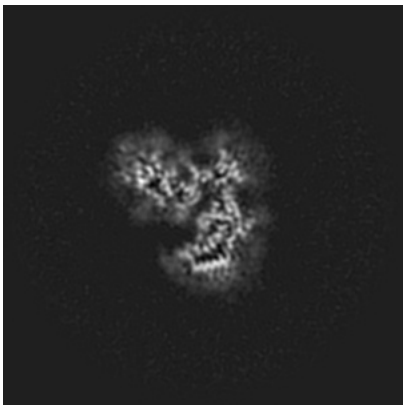
6.3.1 Primary map



X Index: 151

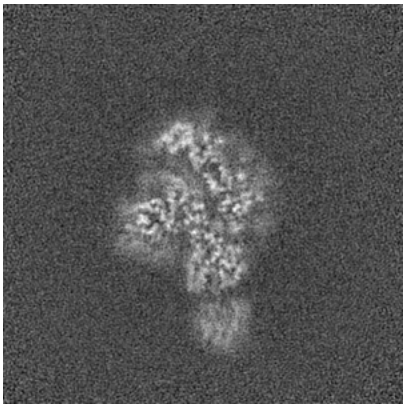


Y Index: 153

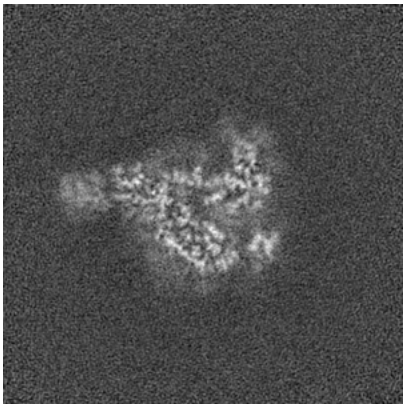


Z Index: 133

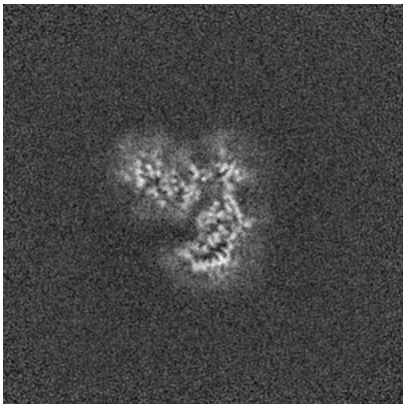
6.3.2 Raw map



X Index: 151



Y Index: 153

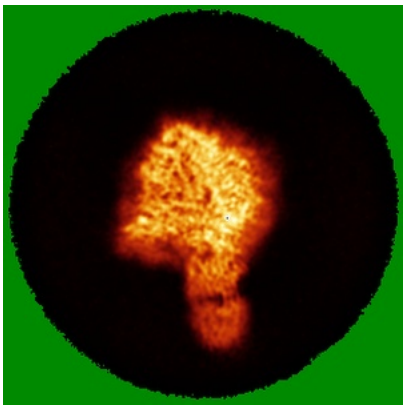


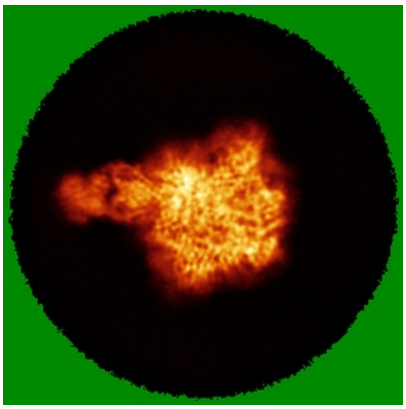
Z Index: 132

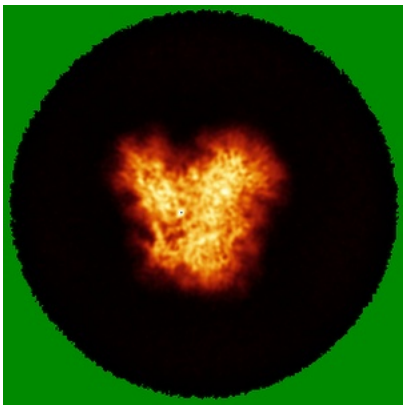
The images above show the largest variance slices of the map in three orthogonal directions.

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

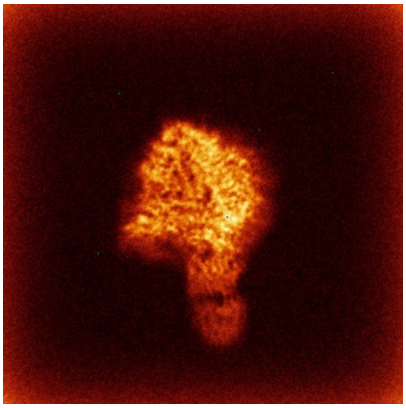
6.4.1 Primary map

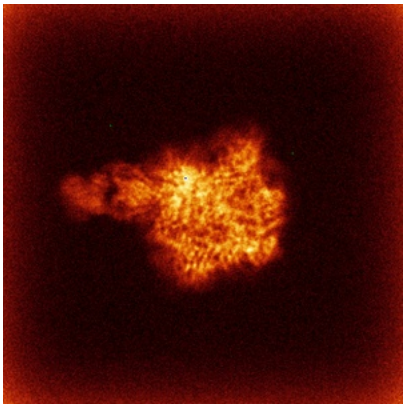

X

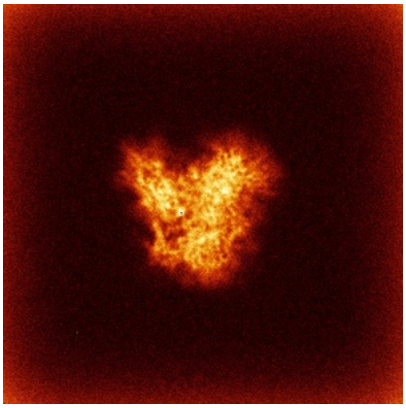

Y


Z

6.4.2 Raw map


X

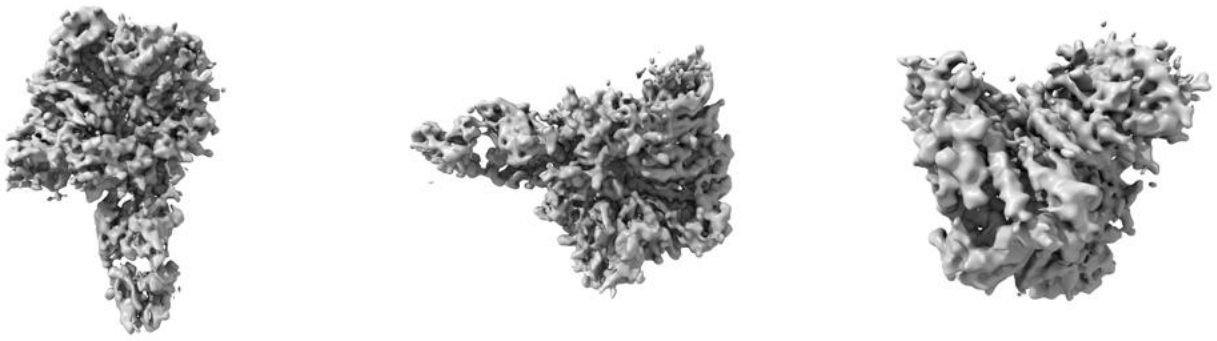

Y


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 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

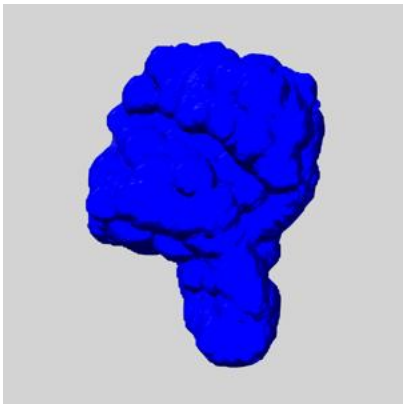
6.6 Mask visualisation

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

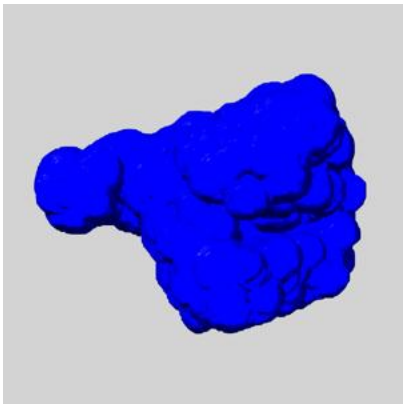
A mask typically either:

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

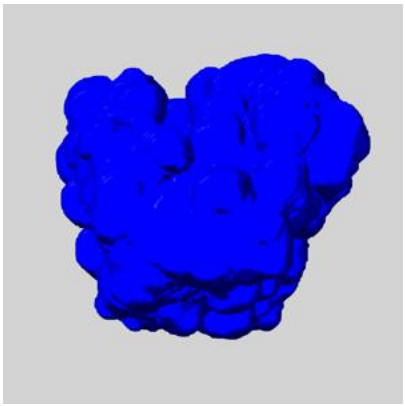
6.6.1 emd_44892_msk_1.map



X



Y

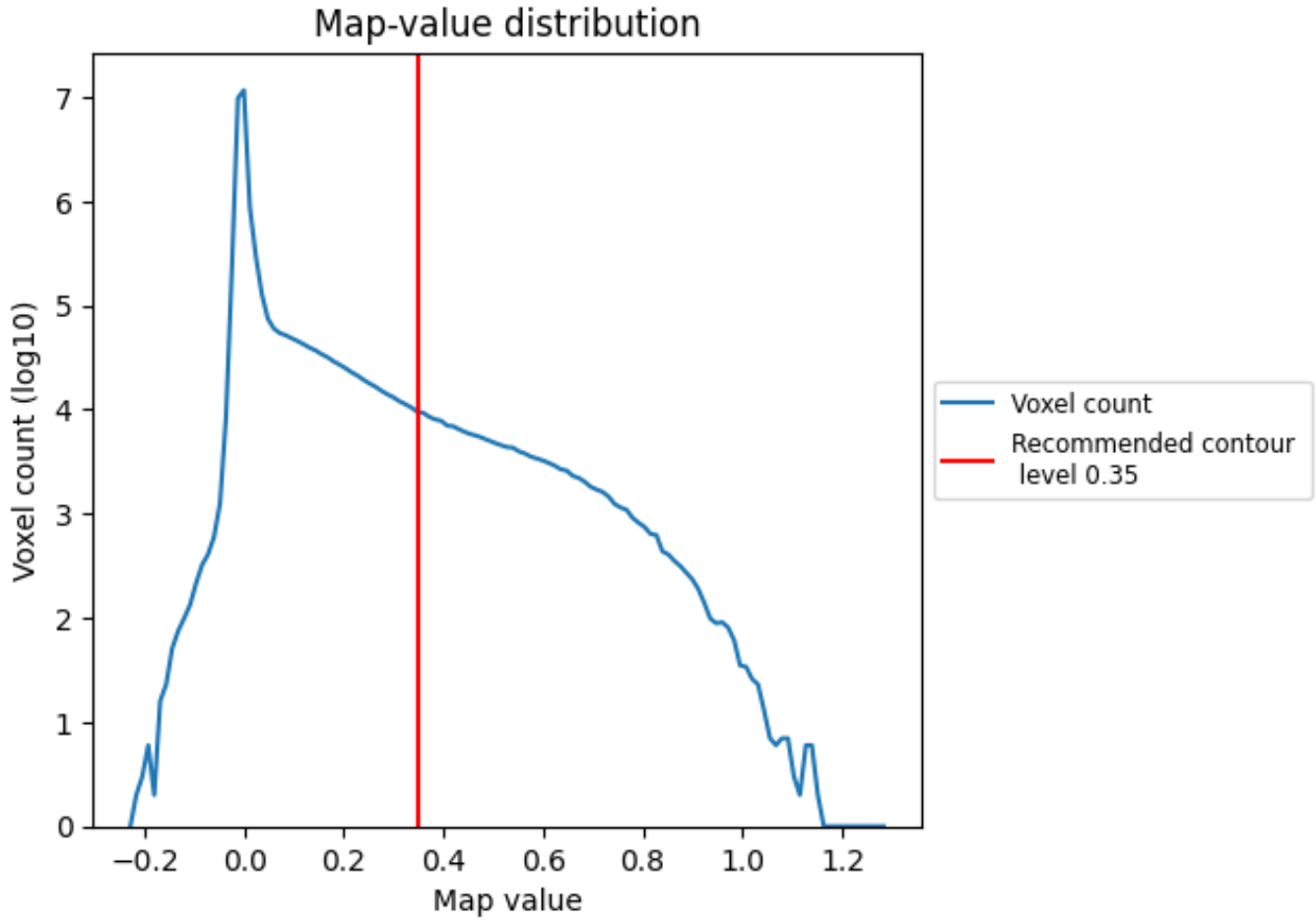


Z

7 Map analysis

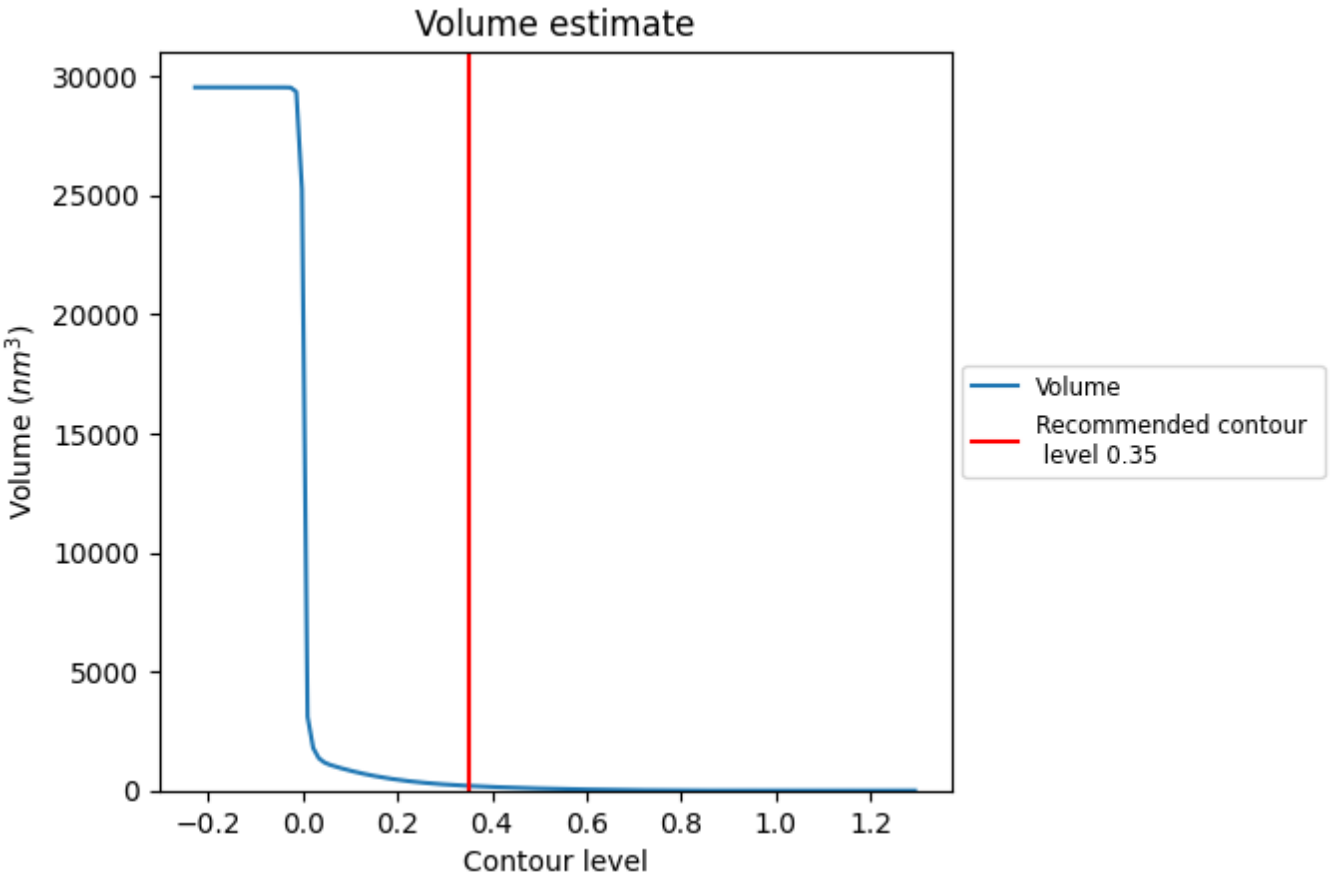
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

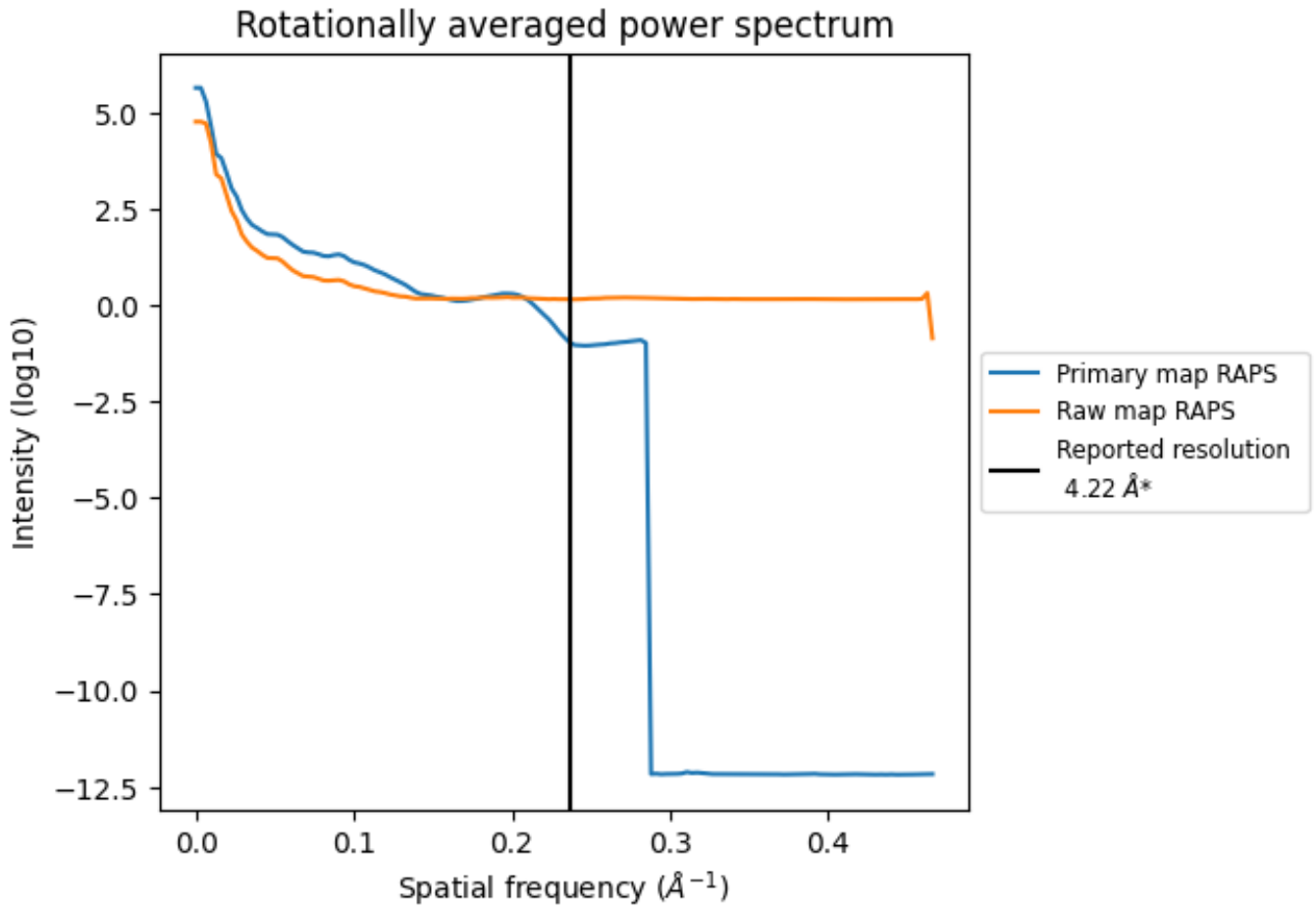
7.2 Volume estimate



The volume at the recommended contour level is 198 nm^3; this corresponds to an approximate mass of 179 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)

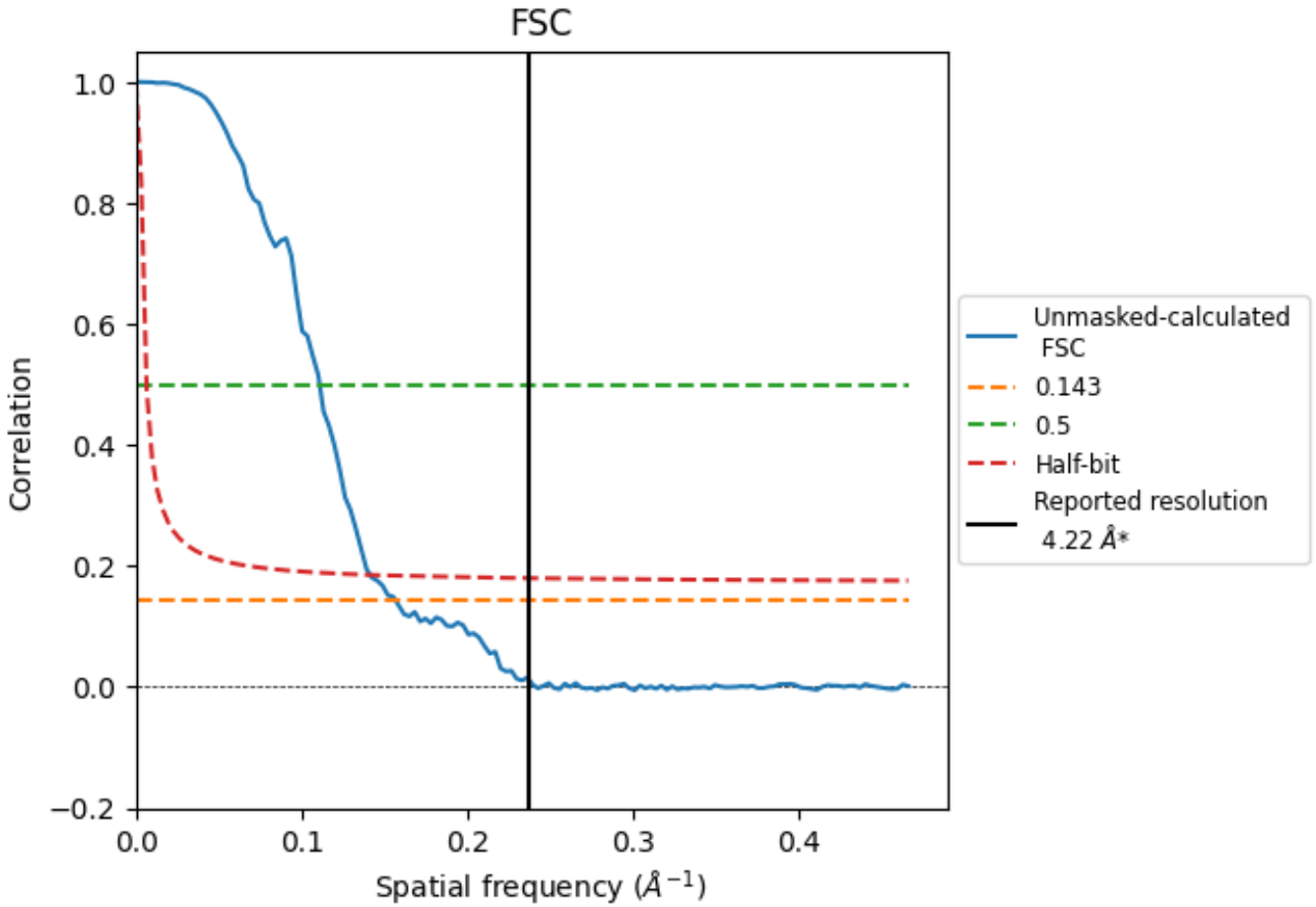


*Reported resolution corresponds to spatial frequency of 0.237 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.237 Å^{-1}

8.2 Resolution estimates (i)

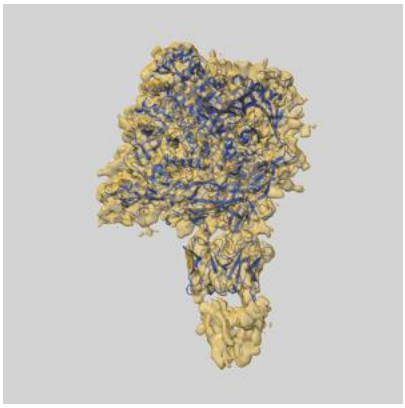
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.22	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.39	9.03	7.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.39 differs from the reported value 4.22 by more than 10 %

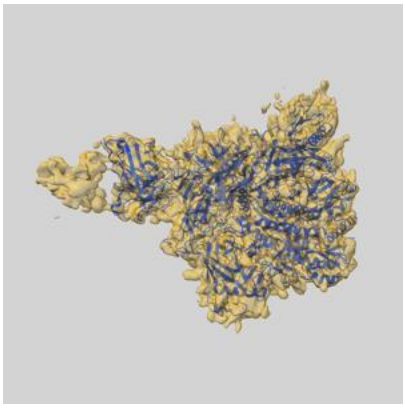
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44892 and PDB model 9BTJ. Per-residue inclusion information can be found in section 3 on page 15.

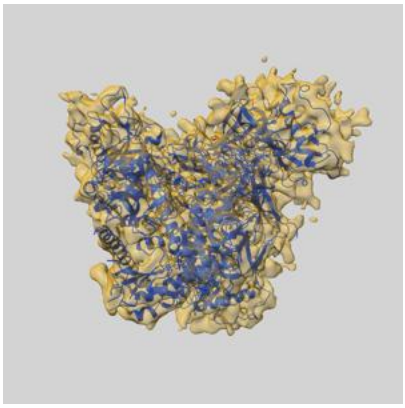
9.1 Map-model overlay



X



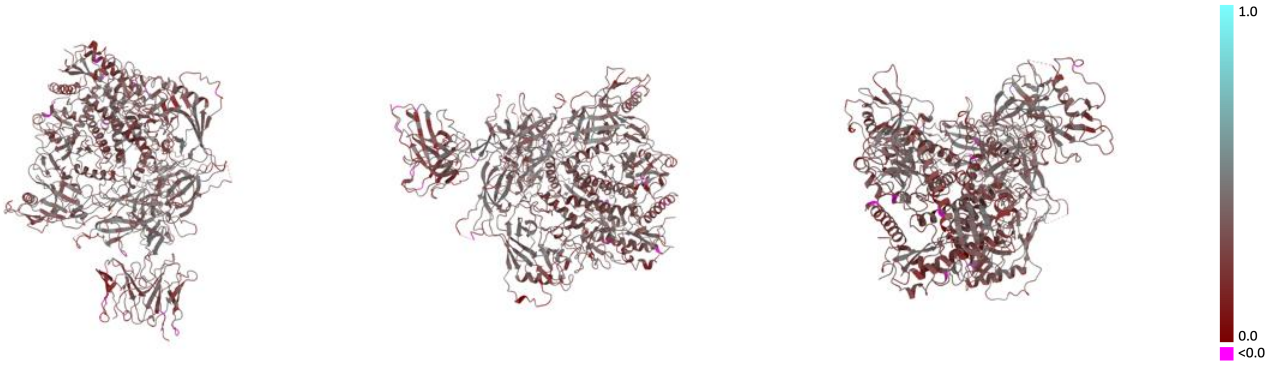
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

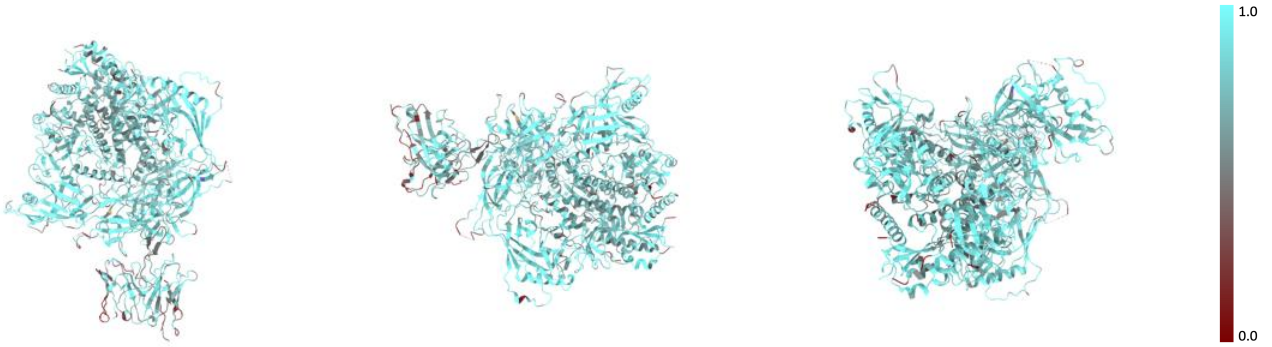
9.2 Q-score mapped to coordinate model (i)



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.

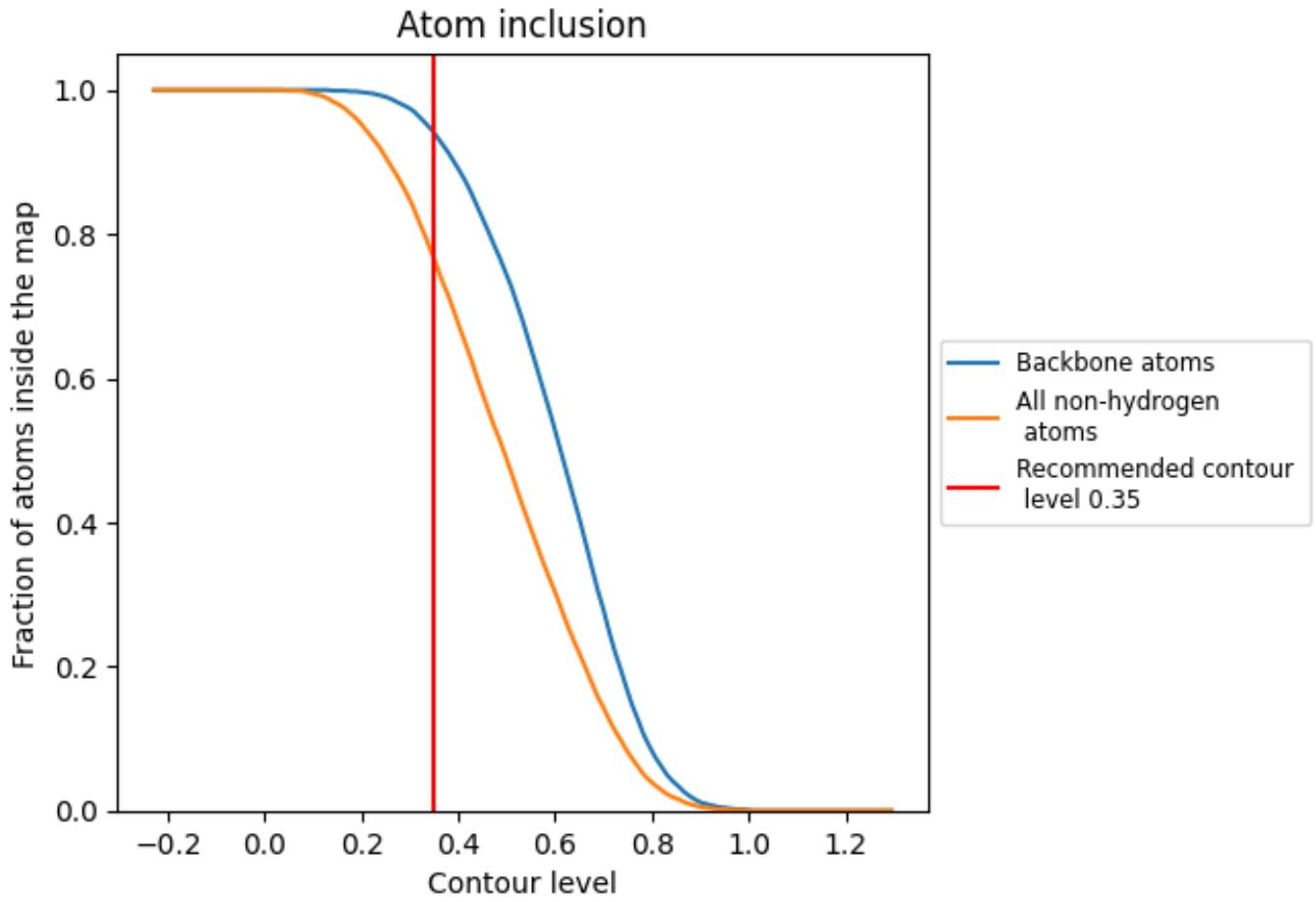
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 77% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7660	0.3280
A	0.8050	0.3470
B	0.7650	0.2890
C	0.7470	0.2730
D	0.8200	0.3500
E	0.7620	0.2870
F	0.6070	0.3040
G	0.8070	0.3470
H	0.7060	0.3150
I	0.8200	0.4320
J	0.4870	0.3180
K	0.8570	0.3600
L	0.6320	0.2620
M	0.6790	0.3770
N	0.7870	0.3870
O	0.5780	0.3890
P	0.5850	0.3440
Q	0.1430	0.2280
R	0.7500	0.3440
S	0.6790	0.3840
T	0.8690	0.4110
U	0.1520	0.1190
V	0.5710	0.1920
W	0.5000	0.1840
X	0.6150	0.3140
Y	0.7500	0.2250
Z	0.6790	0.3720
a	0.0710	0.2460
b	0.8210	0.3840
c	0.6430	0.2940
d	0.8530	0.3970
e	0.4400	0.2840
f	0.1110	0.3160
g	0.6070	0.3350
h	0.0000	0.2490

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Chain	Atom inclusion	Q-score
i	0.1070	0.1190
j	0.6430	0.1800
k	0.8210	0.2440
l	0.6430	0.2360
m	0.6670	0.3300
n	0.6390	0.2640
o	0.1430	0.2810