Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 10:44 AM EST

PDB ID	:	7N28
EMDB ID	:	EMD-24128
Title	:	Cryo-EM structure of broadly neutralizing V2-apex-targeting antibody J033 in complex with HIV-1 Env
Authors	:	Zhou, T.; Gao, F.
Deposited on	:	2021-05-28
Resolution	:	4.20 Å(reported)

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 (i) symbol.

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

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

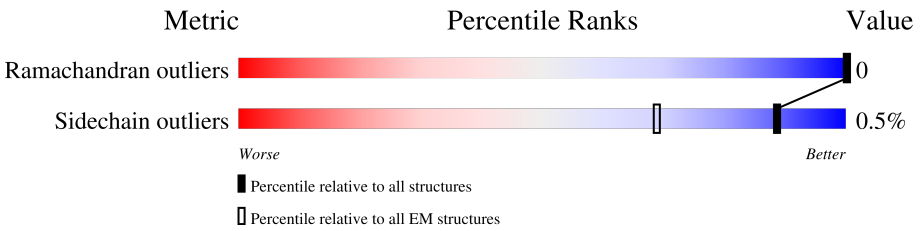
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	478	97%
1	F	478	99%
1	G	478	98%
2	C	226	95%
2	J	226	95%
2	S	226	95%
3	D	206	99%
3	K	206	99%
3	U	206	99%

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Mol	Chain	Length	Quality of chain
4	X	230	97%
5	Y	214	5%, 99%
6	B	170	80%, 20%
6	M	170	80%, 20%
6	N	170	80%, 20%
7	E	2	100%
7	H	2	100%
7	I	2	100%
7	P	2	50%, 50%
7	R	2	50%, 50%
7	T	2	100%
7	V	2	100%
7	W	2	100%
7	Z	2	100%
7	a	2	100%
7	b	2	100%
7	c	2	100%
7	f	2	100%
7	g	2	100%
7	h	2	100%
7	i	2	50%, 50%
7	j	2	100%
7	l	2	100%
7	o	2	50%, 50%
7	p	2	100%

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Mol	Chain	Length	Quality of chain
7	q	2	100%
7	r	2	50% 50%
7	s	2	100%
7	t	2	100%
7	u	2	100%
8	L	8	25% 75%
9	O	7	29% 71%
9	e	7	43% 57%
10	Q	3	67% 33%
11	d	4	75% 25%
12	k	6	50% 50%
13	m	6	50% 50%
14	n	4	25% 75%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 29461 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	472	3731	2352	642	708	29	0	0
1	F	472	3731	2352	642	708	29	0	0
1	G	472	3731	2352	642	708	29	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	SER	conflict	UNP I6NF57
A	32	GLU	ASP	conflict	UNP I6NF57
A	124	PRO	HIS	conflict	UNP I6NF57
A	179	LEU	THR	conflict	UNP I6NF57
A	201	CYS	ILE	conflict	UNP I6NF57
A	358	THR	LYS	conflict	UNP I6NF57
A	400	THR	GLY	conflict	UNP I6NF57
A	433	CYS	ALA	conflict	UNP I6NF57
A	501	CYS	ALA	conflict	UNP I6NF57
A	509	ARG	GLU	conflict	UNP I6NF57
A	510	ARG	LYS	conflict	UNP I6NF57
A	512	ARG	-	expression tag	UNP I6NF57
A	513	ARG	-	expression tag	UNP I6NF57
F	31	ALA	SER	conflict	UNP I6NF57
F	32	GLU	ASP	conflict	UNP I6NF57
F	124	PRO	HIS	conflict	UNP I6NF57
F	179	LEU	THR	conflict	UNP I6NF57
F	201	CYS	ILE	conflict	UNP I6NF57
F	358	THR	LYS	conflict	UNP I6NF57
F	400	THR	GLY	conflict	UNP I6NF57
F	433	CYS	ALA	conflict	UNP I6NF57
F	501	CYS	ALA	conflict	UNP I6NF57
F	509	ARG	GLU	conflict	UNP I6NF57
F	510	ARG	LYS	conflict	UNP I6NF57

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Chain	Residue	Modelled	Actual	Comment	Reference
F	512	ARG	-	expression tag	UNP I6NF57
F	513	ARG	-	expression tag	UNP I6NF57
G	31	ALA	SER	conflict	UNP I6NF57
G	32	GLU	ASP	conflict	UNP I6NF57
G	124	PRO	HIS	conflict	UNP I6NF57
G	179	LEU	THR	conflict	UNP I6NF57
G	201	CYS	ILE	conflict	UNP I6NF57
G	358	THR	LYS	conflict	UNP I6NF57
G	400	THR	GLY	conflict	UNP I6NF57
G	433	CYS	ALA	conflict	UNP I6NF57
G	501	CYS	ALA	conflict	UNP I6NF57
G	509	ARG	GLU	conflict	UNP I6NF57
G	510	ARG	LYS	conflict	UNP I6NF57
G	512	ARG	-	expression tag	UNP I6NF57
G	513	ARG	-	expression tag	UNP I6NF57

- Molecule 2 is a protein called 3BNC117 antibody heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	216	1676	1065	289	317	5	0	0
2	J	216	1676	1065	289	317	5	0	0
2	S	216	1676	1065	289	317	5	0	0

- Molecule 3 is a protein called 3BNC117 antibody light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	204	1603	1004	277	317	5	0	0
3	K	204	1603	1004	277	317	5	0	0
3	U	204	1603	1004	277	317	5	0	0

- Molecule 4 is a protein called J033 antibody heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	225	1684	1065	280	333	6	0	0

- Molecule 5 is a protein called J033 antibody light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Y	214	1637	1028	279	325	5	0	0

- Molecule 6 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	M	136	1090	699	183	203	5	0	0
6	B	136	1090	699	183	203	5	0	0
6	N	136	1090	699	183	203	5	0	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	535	ASN	ILE	conflict	UNP I6NF57
M	556	PRO	LEU	conflict	UNP I6NF57
M	559	PRO	ILE	conflict	UNP I6NF57
M	588	GLU	LYS	conflict	UNP I6NF57
M	589	VAL	ASP	conflict	UNP I6NF57
M	605	CYS	THR	conflict	UNP I6NF57
M	651	PHE	ASN	conflict	UNP I6NF57
M	655	ILE	ARG	conflict	UNP I6NF57
M	658	VAL	LYS	conflict	UNP I6NF57
M	665	GLY	-	expression tag	UNP I6NF57
M	666	SER	-	expression tag	UNP I6NF57
M	667	ALA	-	expression tag	UNP I6NF57
M	668	PRO	-	expression tag	UNP I6NF57
M	669	THR	-	expression tag	UNP I6NF57
M	670	LYS	-	expression tag	UNP I6NF57
M	671	ALA	-	expression tag	UNP I6NF57
M	672	LYS	-	expression tag	UNP I6NF57
M	673	ARG	-	expression tag	UNP I6NF57
M	674	ARG	-	expression tag	UNP I6NF57
M	675	VAL	-	expression tag	UNP I6NF57
M	676	VAL	-	expression tag	UNP I6NF57
M	677	GLN	-	expression tag	UNP I6NF57
M	678	ARG	-	expression tag	UNP I6NF57
M	679	GLU	-	expression tag	UNP I6NF57
M	680	LYS	-	expression tag	UNP I6NF57

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Chain	Residue	Modelled	Actual	Comment	Reference
M	681	ARG	-	expression tag	UNP I6NF57
B	535	ASN	ILE	conflict	UNP I6NF57
B	556	PRO	LEU	conflict	UNP I6NF57
B	559	PRO	ILE	conflict	UNP I6NF57
B	588	GLU	LYS	conflict	UNP I6NF57
B	589	VAL	ASP	conflict	UNP I6NF57
B	605	CYS	THR	conflict	UNP I6NF57
B	651	PHE	ASN	conflict	UNP I6NF57
B	655	ILE	ARG	conflict	UNP I6NF57
B	658	VAL	LYS	conflict	UNP I6NF57
B	665	GLY	-	expression tag	UNP I6NF57
B	666	SER	-	expression tag	UNP I6NF57
B	667	ALA	-	expression tag	UNP I6NF57
B	668	PRO	-	expression tag	UNP I6NF57
B	669	THR	-	expression tag	UNP I6NF57
B	670	LYS	-	expression tag	UNP I6NF57
B	671	ALA	-	expression tag	UNP I6NF57
B	672	LYS	-	expression tag	UNP I6NF57
B	673	ARG	-	expression tag	UNP I6NF57
B	674	ARG	-	expression tag	UNP I6NF57
B	675	VAL	-	expression tag	UNP I6NF57
B	676	VAL	-	expression tag	UNP I6NF57
B	677	GLN	-	expression tag	UNP I6NF57
B	678	ARG	-	expression tag	UNP I6NF57
B	679	GLU	-	expression tag	UNP I6NF57
B	680	LYS	-	expression tag	UNP I6NF57
B	681	ARG	-	expression tag	UNP I6NF57
N	535	ASN	ILE	conflict	UNP I6NF57
N	556	PRO	LEU	conflict	UNP I6NF57
N	559	PRO	ILE	conflict	UNP I6NF57
N	588	GLU	LYS	conflict	UNP I6NF57
N	589	VAL	ASP	conflict	UNP I6NF57
N	605	CYS	THR	conflict	UNP I6NF57
N	651	PHE	ASN	conflict	UNP I6NF57
N	655	ILE	ARG	conflict	UNP I6NF57
N	658	VAL	LYS	conflict	UNP I6NF57
N	665	GLY	-	expression tag	UNP I6NF57
N	666	SER	-	expression tag	UNP I6NF57
N	667	ALA	-	expression tag	UNP I6NF57
N	668	PRO	-	expression tag	UNP I6NF57
N	669	THR	-	expression tag	UNP I6NF57
N	670	LYS	-	expression tag	UNP I6NF57

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Chain	Residue	Modelled	Actual	Comment	Reference
N	671	ALA	-	expression tag	UNP I6NF57
N	672	LYS	-	expression tag	UNP I6NF57
N	673	ARG	-	expression tag	UNP I6NF57
N	674	ARG	-	expression tag	UNP I6NF57
N	675	VAL	-	expression tag	UNP I6NF57
N	676	VAL	-	expression tag	UNP I6NF57
N	677	GLN	-	expression tag	UNP I6NF57
N	678	ARG	-	expression tag	UNP I6NF57
N	679	GLU	-	expression tag	UNP I6NF57
N	680	LYS	-	expression tag	UNP I6NF57
N	681	ARG	-	expression tag	UNP I6NF57

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	E	2	28	16	2	10	0	0
7	H	2	28	16	2	10	0	0
7	I	2	28	16	2	10	0	0
7	P	2	28	16	2	10	0	0
7	R	2	28	16	2	10	0	0
7	T	2	28	16	2	10	0	0
7	V	2	28	16	2	10	0	0
7	W	2	28	16	2	10	0	0
7	Z	2	28	16	2	10	0	0
7	a	2	28	16	2	10	0	0
7	b	2	28	16	2	10	0	0

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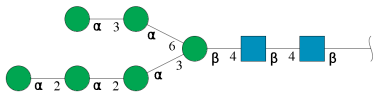
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	c	2	28	16	2	10	0	0
7	f	2	28	16	2	10	0	0
7	g	2	28	16	2	10	0	0
7	h	2	28	16	2	10	0	0
7	i	2	28	16	2	10	0	0
7	j	2	28	16	2	10	0	0
7	l	2	28	16	2	10	0	0
7	o	2	28	16	2	10	0	0
7	p	2	28	16	2	10	0	0
7	q	2	28	16	2	10	0	0
7	r	2	28	16	2	10	0	0
7	s	2	28	16	2	10	0	0
7	t	2	28	16	2	10	0	0
7	u	2	28	16	2	10	0	0

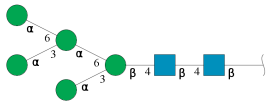
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

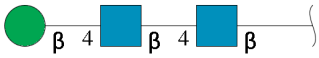
- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(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
			Total	C	N	O		
9	O	7	83	46	2	35	0	0
9	e	7	83	46	2	35	0	0

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

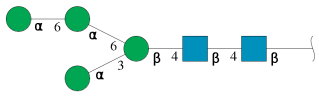


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	Q	3	39	22	2	15	0	0

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

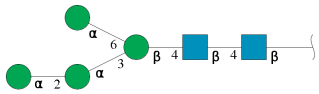
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	d	4	50	28	2	20	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	k	6	72	40	2	30	0	0

- Molecule 13 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.

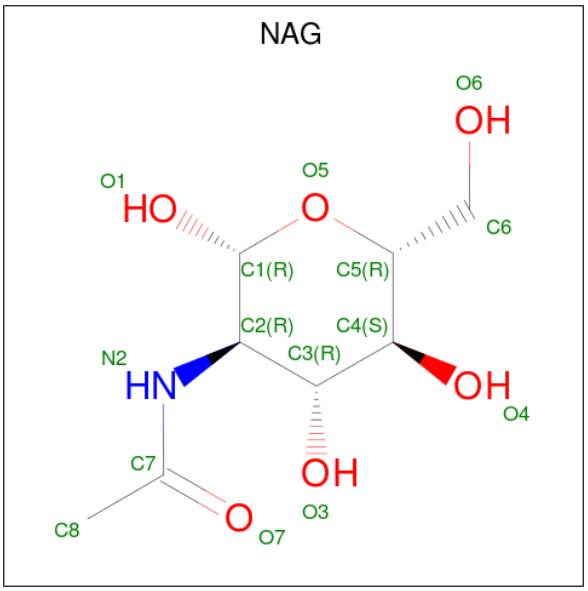


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	m	6	72	40	2	30	0	0

- Molecule 14 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
			Total	C	N	O		
14	n	4	50	28	2	20	0	0

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



Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total	C	N	O	0
			112	64	8	40	
15	A	1	Total	C	N	O	0
			112	64	8	40	
15	A	1	Total	C	N	O	0
			112	64	8	40	
15	A	1	Total	C	N	O	0
			112	64	8	40	
15	A	1	Total	C	N	O	0
			112	64	8	40	
15	A	1	Total	C	N	O	0
			112	64	8	40	
15	A	1	Total	C	N	O	0
			112	64	8	40	
15	A	1	Total	C	N	O	0
			112	64	8	40	
15	D	1	Total	C	N	O	0
			14	8	1	5	
15	F	1	Total	C	N	O	0
			140	80	10	50	
15	F	1	Total	C	N	O	0
			140	80	10	50	
15	F	1	Total	C	N	O	0
			140	80	10	50	
15	F	1	Total	C	N	O	0
			140	80	10	50	
15	F	1	Total	C	N	O	0
			140	80	10	50	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
15	F	1	140	80	10	50	0
15	F	1	140	80	10	50	0
15	F	1	140	80	10	50	0
15	F	1	140	80	10	50	0
15	F	1	140	80	10	50	0
15	G	1	126	72	9	45	0
15	G	1	126	72	9	45	0
15	G	1	126	72	9	45	0
15	G	1	126	72	9	45	0
15	G	1	126	72	9	45	0
15	G	1	126	72	9	45	0
15	G	1	126	72	9	45	0
15	G	1	126	72	9	45	0
15	G	1	126	72	9	45	0
15	K	1	14	8	1	5	0
15	U	1	14	8	1	5	0
15	M	1	42	24	3	15	0
15	M	1	42	24	3	15	0
15	M	1	42	24	3	15	0
15	B	1	56	32	4	20	0
15	B	1	56	32	4	20	0

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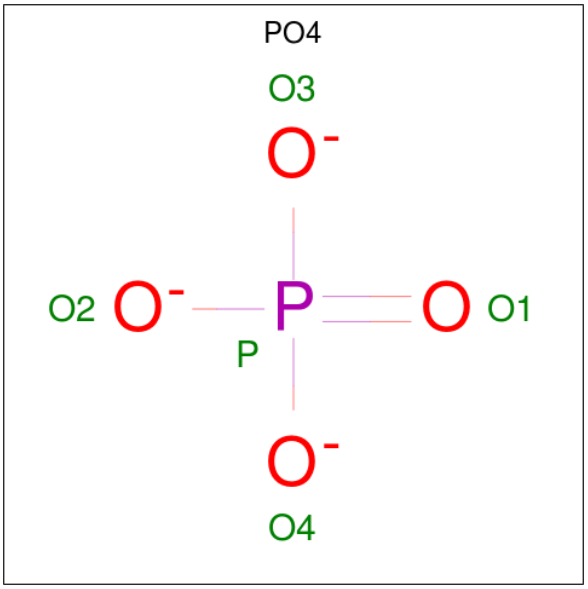
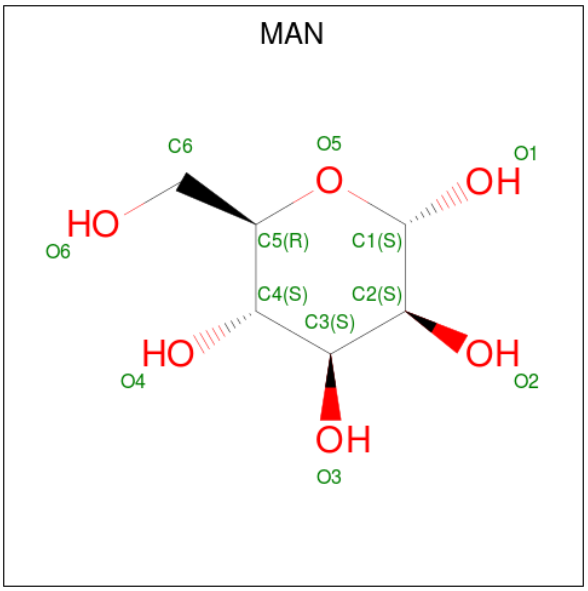
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
15	B	1	56	32	4	20	0
			Total	C	N	O	
15	B	1	56	32	4	20	0
			Total	C	N	O	
15	N	1	42	24	3	15	0
			Total	C	N	O	
15	N	1	42	24	3	15	0
			Total	C	N	O	
15	N	1	42	24	3	15	0

- Molecule 16 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
16	A	1	5	4	1	0
			Total	O	P	
16	F	1	10	8	2	0
			Total	O	P	
16	F	1	10	8	2	0

- Molecule 17 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



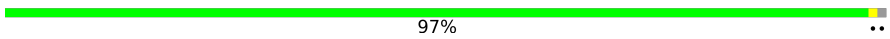
Mol	Chain	Residues	Atoms			AltConf
17	S	1	Total	C	O	0
			11	6	5	
17	X	1	Total	C	O	0
			11	6	5	

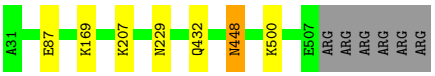
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Envelope glycoprotein gp120

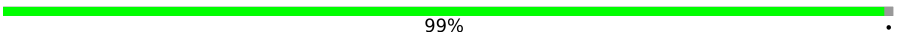
Chain A:

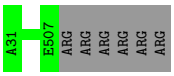




- Molecule 1: Envelope glycoprotein gp120

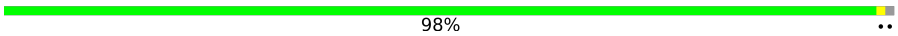
Chain F:

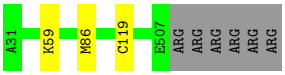




- Molecule 1: Envelope glycoprotein gp120

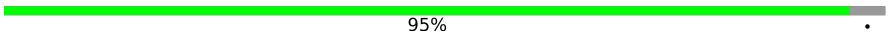
Chain G:





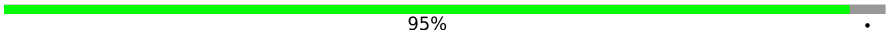
- Molecule 2: 3BNC117 antibody heavy chain

Chain C:



- Molecule 2: 3BNC117 antibody heavy chain

Chain J:

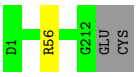


- Molecule 2: 3BNC117 antibody heavy chain

Chain S: 95%

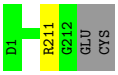
• Molecule 3: 3BNC117 antibody light chain

Chain D: 99%



• Molecule 3: 3BNC117 antibody light chain

Chain K: 99%

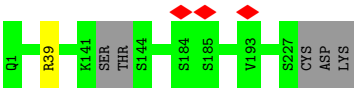


• Molecule 3: 3BNC117 antibody light chain

Chain U: 99%

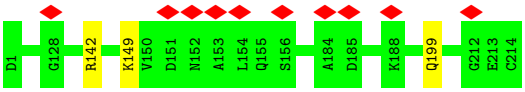
• Molecule 4: J033 antibody heavy chain

Chain X: 97%



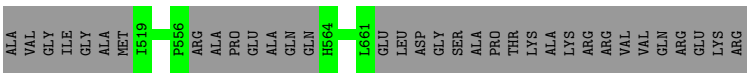
• Molecule 5: J033 antibody light chain

Chain Y: 5% 99%



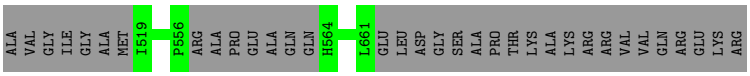
• Molecule 6: Envelope glycoprotein gp41

Chain M: 80% 20%



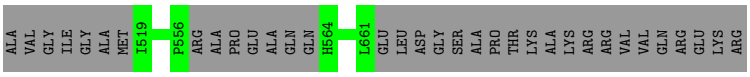
• Molecule 6: Envelope glycoprotein gp41

Chain B: 80% 20%



• Molecule 6: Envelope glycoprotein gp41

Chain N: 80% 20%



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

Chain E: 100%

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

Chain H: 100%

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

Chain I: 100%

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

Chain P: 50% 50%

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

Chain R: 50% 50%

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

Chain T: 100%

NAG1
NAG2

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

Chain V: 100%

NAG1
NAG2

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

Chain W: 100%

NAG1
NAG2

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

Chain Z: 100%

NAG1
NAG2

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

Chain a: 100%

NAG1
NAG2

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

Chain b: 100%

NAG1
NAG2

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

Chain c: 100%

NAG1
NAG2

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

Chain f: 100%

NAG1
NAG2

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

Chain g: 100%

NAG1
NAG2

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

Chain h: 100%

NAG1
NAG2

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

Chain i: 50% 50%

NAG1 NAG2

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

Chain j: 100%

NAG1
NAG2

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

Chain l: 100%

NAG1
NAG2

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

Chain o: 50% 50%

NAG1 NAG2

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

Chain p: 100%

NAG1 NAG2

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

Chain q: 100%

NAG1 NAG2

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

Chain r: 50% 50%

NAG1 NAG2

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

Chain s: 100%

NAG1 NAG2

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

Chain t: 100%

NAG1 NAG2

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

Chain u: 100%

NAG1 NAG2

• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 L: 25% 75%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7 MAN8

• Molecule 9: 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: 29% 71%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7

• Molecule 9: 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 e: 43% 57%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7

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

Chain Q: 67% 33%

NAG1 NAG2 BMA3

• Molecule 11: 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

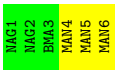
Chain d: 75% 25%

NAG1 NAG2 BMA3 MAN4

• Molecule 12: 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-aceta

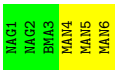
mido-2-deoxy-beta-D-glucopyranose

Chain k: 50% 50%



• Molecule 13: 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 m: 50% 50%



• Molecule 14: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n: 25% 75%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	383584	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	18000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0019	Depositor
Map size (Å)	489.59998, 489.59998, 489.59998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, PO4, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.27	0/3813	0.51	1/5188 (0.0%)
1	F	0.26	0/3813	0.49	0/5188
1	G	0.28	0/3813	0.51	0/5188
2	C	0.27	0/1726	0.53	0/2359
2	J	0.27	0/1726	0.50	0/2359
2	S	0.26	0/1726	0.51	0/2359
3	D	0.26	0/1637	0.53	0/2222
3	K	0.25	0/1637	0.52	0/2222
3	U	0.26	0/1637	0.52	0/2222
4	X	0.25	0/1726	0.54	0/2354
5	Y	0.25	0/1674	0.50	0/2273
6	B	0.27	0/1113	0.48	0/1513
6	M	0.26	0/1113	0.49	0/1513
6	N	0.27	0/1113	0.49	0/1513
All	All	0.26	0/28267	0.51	1/38473 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	G	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	ASN	CB-CA-C	5.50	121.41	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	448	ASN	Peptide
1	A	87	GLU	Peptide
1	G	119	CYS	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	470/478 (98%)	431 (92%)	39 (8%)	0	100	100
1	F	470/478 (98%)	436 (93%)	34 (7%)	0	100	100
1	G	470/478 (98%)	431 (92%)	39 (8%)	0	100	100
2	C	212/226 (94%)	196 (92%)	16 (8%)	0	100	100
2	J	212/226 (94%)	196 (92%)	16 (8%)	0	100	100
2	S	212/226 (94%)	198 (93%)	14 (7%)	0	100	100
3	D	202/206 (98%)	181 (90%)	21 (10%)	0	100	100
3	K	202/206 (98%)	185 (92%)	17 (8%)	0	100	100
3	U	202/206 (98%)	189 (94%)	13 (6%)	0	100	100
4	X	221/230 (96%)	197 (89%)	24 (11%)	0	100	100
5	Y	212/214 (99%)	193 (91%)	19 (9%)	0	100	100

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Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	B	132/170 (78%)	127 (96%)	5 (4%)	0	100	100
6	M	132/170 (78%)	124 (94%)	8 (6%)	0	100	100
6	N	132/170 (78%)	123 (93%)	9 (7%)	0	100	100
All	All	3481/3684 (94%)	3207 (92%)	274 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/432 (99%)	421 (99%)	5 (1%)	71	83
1	F	426/432 (99%)	426 (100%)	0	100	100
1	G	426/432 (99%)	424 (100%)	2 (0%)	88	93
2	C	185/193 (96%)	184 (100%)	1 (0%)	88	93
2	J	185/193 (96%)	184 (100%)	1 (0%)	88	93
2	S	185/193 (96%)	184 (100%)	1 (0%)	88	93
3	D	181/183 (99%)	180 (99%)	1 (1%)	86	92
3	K	181/183 (99%)	180 (99%)	1 (1%)	86	92
3	U	181/183 (99%)	181 (100%)	0	100	100
4	X	191/196 (97%)	190 (100%)	1 (0%)	88	93
5	Y	184/184 (100%)	181 (98%)	3 (2%)	62	79
6	B	119/144 (83%)	119 (100%)	0	100	100
6	M	119/144 (83%)	119 (100%)	0	100	100
6	N	119/144 (83%)	119 (100%)	0	100	100
All	All	3108/3236 (96%)	3092 (100%)	16 (0%)	89	93

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LYS
1	A	207	LYS
1	A	229	ASN
1	A	432	GLN
1	A	500	LYS
2	C	3	GLN
3	D	56	ARG
1	G	59	LYS
1	G	86	MET
2	J	3	GLN
3	K	211	ARG
2	S	3	GLN
4	X	39	ARG
5	Y	142	ARG
5	Y	149	LYS
5	Y	199	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	114	GLN
1	A	146	ASN
2	C	3	GLN
2	C	95	GLN
1	G	362	GLN
2	S	64	GLN
3	U	147	GLN
3	U	166	GLN
6	M	554	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

95 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	E	1	1,7	14,14,15	0.39	0	17,19,21	0.53	0
7	NAG	E	2	7	14,14,15	0.20	0	17,19,21	0.43	0
7	NAG	H	1	1,7	14,14,15	0.44	0	17,19,21	0.55	0
7	NAG	H	2	7	14,14,15	0.24	0	17,19,21	0.43	0
7	NAG	I	1	1,7	14,14,15	0.24	0	17,19,21	0.49	0
7	NAG	I	2	7	14,14,15	0.25	0	17,19,21	0.39	0
8	NAG	L	1	8,1	14,14,15	0.24	0	17,19,21	0.46	0
8	NAG	L	2	8	14,14,15	0.25	0	17,19,21	0.47	0
8	BMA	L	3	8	11,11,12	0.56	0	15,15,17	0.91	1 (6%)
8	MAN	L	4	8	11,11,12	0.55	0	15,15,17	0.96	2 (13%)
8	MAN	L	5	8	11,11,12	0.68	0	15,15,17	1.18	2 (13%)
8	MAN	L	6	8	11,11,12	0.73	0	15,15,17	0.87	1 (6%)
8	MAN	L	7	8	11,11,12	0.76	0	15,15,17	0.96	1 (6%)
8	MAN	L	8	8	11,11,12	0.71	0	15,15,17	1.28	2 (13%)
9	NAG	O	1	1,9	14,14,15	0.65	1 (7%)	17,19,21	0.69	0
9	NAG	O	2	9	14,14,15	0.30	0	17,19,21	0.53	0
9	BMA	O	3	9	11,11,12	0.55	0	15,15,17	0.74	0
9	MAN	O	4	9	11,11,12	0.59	0	15,15,17	1.04	2 (13%)
9	MAN	O	5	9	11,11,12	0.64	0	15,15,17	1.21	2 (13%)
9	MAN	O	6	9	11,11,12	0.60	0	15,15,17	1.04	2 (13%)
9	MAN	O	7	9	11,11,12	0.64	0	15,15,17	0.94	1 (6%)
7	NAG	P	1	1,7	14,14,15	0.34	0	17,19,21	0.61	1 (5%)
7	NAG	P	2	7	14,14,15	0.26	0	17,19,21	0.40	0
10	NAG	Q	1	10,1	14,14,15	0.37	0	17,19,21	0.37	0
10	NAG	Q	2	10	14,14,15	0.16	0	17,19,21	0.55	0
10	BMA	Q	3	10	11,11,12	0.84	1 (9%)	15,15,17	1.26	2 (13%)
7	NAG	R	1	1,7	14,14,15	0.97	1 (7%)	17,19,21	0.75	1 (5%)
7	NAG	R	2	7	14,14,15	0.40	0	17,19,21	0.56	0
7	NAG	T	1	1,7	14,14,15	0.37	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	T	2	7	14,14,15	0.32	0	17,19,21	0.58	0
7	NAG	V	1	1,7	14,14,15	0.22	0	17,19,21	0.38	0
7	NAG	V	2	7	14,14,15	0.22	0	17,19,21	0.42	0
7	NAG	W	1	1,7	14,14,15	0.29	0	17,19,21	0.41	0
7	NAG	W	2	7	14,14,15	0.25	0	17,19,21	0.50	0
7	NAG	Z	1	1,7	14,14,15	0.26	0	17,19,21	0.47	0
7	NAG	Z	2	7	14,14,15	0.25	0	17,19,21	0.45	0
7	NAG	a	1	6,7	14,14,15	0.44	0	17,19,21	0.42	0
7	NAG	a	2	7	14,14,15	0.22	0	17,19,21	0.51	0
7	NAG	b	1	1,7	14,14,15	0.24	0	17,19,21	0.57	0
7	NAG	b	2	7	14,14,15	0.29	0	17,19,21	0.41	0
7	NAG	c	1	1,7	14,14,15	0.20	0	17,19,21	0.46	0
7	NAG	c	2	7	14,14,15	0.26	0	17,19,21	0.38	0
11	NAG	d	1	11,1	14,14,15	0.43	0	17,19,21	0.48	0
11	NAG	d	2	11	14,14,15	0.18	0	17,19,21	0.40	0
11	BMA	d	3	11	11,11,12	0.54	0	15,15,17	0.84	0
11	MAN	d	4	11	11,11,12	0.72	0	15,15,17	0.90	1 (6%)
9	NAG	e	1	1,9	14,14,15	0.25	0	17,19,21	0.39	0
9	NAG	e	2	9	14,14,15	0.19	0	17,19,21	0.42	0
9	BMA	e	3	9	11,11,12	0.49	0	15,15,17	0.75	0
9	MAN	e	4	9	11,11,12	0.65	0	15,15,17	1.17	2 (13%)
9	MAN	e	5	9	11,11,12	0.78	1 (9%)	15,15,17	1.37	2 (13%)
9	MAN	e	6	9	11,11,12	0.66	0	15,15,17	0.89	1 (6%)
9	MAN	e	7	9	11,11,12	0.68	0	15,15,17	0.90	1 (6%)
7	NAG	f	1	1,7	14,14,15	0.22	0	17,19,21	0.46	0
7	NAG	f	2	7	14,14,15	0.22	0	17,19,21	0.42	0
7	NAG	g	1	1,7	14,14,15	0.28	0	17,19,21	0.51	0
7	NAG	g	2	7	14,14,15	0.27	0	17,19,21	0.56	0
7	NAG	h	1	1,7	14,14,15	0.24	0	17,19,21	0.42	0
7	NAG	h	2	7	14,14,15	0.19	0	17,19,21	0.40	0
7	NAG	i	1	1,7	14,14,15	0.89	1 (7%)	17,19,21	1.70	1 (5%)
7	NAG	i	2	7	14,14,15	0.22	0	17,19,21	0.45	0
7	NAG	j	1	1,7	14,14,15	0.18	0	17,19,21	0.50	0
7	NAG	j	2	7	14,14,15	0.25	0	17,19,21	0.48	0
12	NAG	k	1	12,1	14,14,15	0.23	0	17,19,21	0.57	0
12	NAG	k	2	12	14,14,15	0.26	0	17,19,21	0.38	0
12	BMA	k	3	12	11,11,12	0.50	0	15,15,17	0.97	0
12	MAN	k	4	12	11,11,12	0.78	1 (9%)	15,15,17	1.26	2 (13%)
12	MAN	k	5	12	11,11,12	0.67	0	15,15,17	0.91	2 (13%)
12	MAN	k	6	12	11,11,12	0.75	0	15,15,17	0.86	1 (6%)
7	NAG	l	1	1,7	14,14,15	0.18	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	l	2	7	14,14,15	0.24	0	17,19,21	0.53	0
13	NAG	m	1	13,1	14,14,15	0.57	0	17,19,21	0.67	0
13	NAG	m	2	13	14,14,15	0.23	0	17,19,21	0.36	0
13	BMA	m	3	13	11,11,12	0.54	0	15,15,17	0.82	0
13	MAN	m	4	13	11,11,12	0.63	0	15,15,17	1.08	2 (13%)
13	MAN	m	5	13	11,11,12	0.73	0	15,15,17	0.88	1 (6%)
13	MAN	m	6	13	11,11,12	0.69	0	15,15,17	0.95	1 (6%)
14	NAG	n	1	1,14	14,14,15	0.22	0	17,19,21	0.69	1 (5%)
14	NAG	n	2	14	14,14,15	0.46	0	17,19,21	1.27	1 (5%)
14	BMA	n	3	14	11,11,12	0.44	0	15,15,17	0.89	0
14	MAN	n	4	14	11,11,12	0.69	0	15,15,17	1.27	2 (13%)
7	NAG	o	1	1,7	14,14,15	0.24	0	17,19,21	0.65	1 (5%)
7	NAG	o	2	7	14,14,15	0.23	0	17,19,21	0.55	0
7	NAG	p	1	1,7	14,14,15	0.26	0	17,19,21	0.37	0
7	NAG	p	2	7	14,14,15	0.28	0	17,19,21	0.55	0
7	NAG	q	1	1,7	14,14,15	0.52	0	17,19,21	0.58	0
7	NAG	q	2	7	14,14,15	0.28	0	17,19,21	0.54	0
7	NAG	r	1	1,7	14,14,15	0.79	1 (7%)	17,19,21	0.71	0
7	NAG	r	2	7	14,14,15	0.17	0	17,19,21	0.45	0
7	NAG	s	1	1,7	14,14,15	0.33	0	17,19,21	0.47	0
7	NAG	s	2	7	14,14,15	0.20	0	17,19,21	0.63	0
7	NAG	t	1	1,7	14,14,15	0.37	0	17,19,21	0.50	0
7	NAG	t	2	7	14,14,15	0.32	0	17,19,21	0.58	0
7	NAG	u	1	1,7	14,14,15	0.29	0	17,19,21	0.47	0
7	NAG	u	2	7	14,14,15	0.22	0	17,19,21	0.39	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
7	NAG	E	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	E	2	7	-	4/6/23/26	0/1/1/1
7	NAG	H	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	NAG	I	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	2/6/23/26	0/1/1/1
8	NAG	L	1	8,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	L	2	8	-	2/6/23/26	0/1/1/1
8	BMA	L	3	8	-	1/2/19/22	0/1/1/1
8	MAN	L	4	8	-	0/2/19/22	0/1/1/1
8	MAN	L	5	8	-	0/2/19/22	0/1/1/1
8	MAN	L	6	8	-	0/2/19/22	0/1/1/1
8	MAN	L	7	8	-	1/2/19/22	0/1/1/1
8	MAN	L	8	8	-	1/2/19/22	1/1/1/1
9	NAG	O	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	O	2	9	-	2/6/23/26	0/1/1/1
9	BMA	O	3	9	-	0/2/19/22	0/1/1/1
9	MAN	O	4	9	-	0/2/19/22	0/1/1/1
9	MAN	O	5	9	-	0/2/19/22	0/1/1/1
9	MAN	O	6	9	-	0/2/19/22	0/1/1/1
9	MAN	O	7	9	-	1/2/19/22	0/1/1/1
7	NAG	P	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
10	NAG	Q	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	Q	2	10	-	3/6/23/26	0/1/1/1
10	BMA	Q	3	10	-	1/2/19/22	0/1/1/1
7	NAG	R	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	R	2	7	-	2/6/23/26	0/1/1/1
7	NAG	T	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	3/6/23/26	0/1/1/1
7	NAG	V	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	V	2	7	-	2/6/23/26	0/1/1/1
7	NAG	W	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	W	2	7	-	2/6/23/26	0/1/1/1
7	NAG	Z	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1
7	NAG	a	1	6,7	-	2/6/23/26	0/1/1/1
7	NAG	a	2	7	-	0/6/23/26	0/1/1/1
7	NAG	b	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	2/6/23/26	0/1/1/1
7	NAG	c	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
11	NAG	d	1	11,1	-	3/6/23/26	0/1/1/1
11	NAG	d	2	11	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BMA	d	3	11	-	2/2/19/22	0/1/1/1
11	MAN	d	4	11	-	0/2/19/22	0/1/1/1
9	NAG	e	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	e	2	9	-	1/6/23/26	0/1/1/1
9	BMA	e	3	9	-	0/2/19/22	0/1/1/1
9	MAN	e	4	9	-	2/2/19/22	0/1/1/1
9	MAN	e	5	9	-	0/2/19/22	0/1/1/1
9	MAN	e	6	9	-	0/2/19/22	0/1/1/1
9	MAN	e	7	9	-	2/2/19/22	0/1/1/1
7	NAG	f	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	f	2	7	-	2/6/23/26	0/1/1/1
7	NAG	g	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	g	2	7	-	3/6/23/26	0/1/1/1
7	NAG	h	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	h	2	7	-	2/6/23/26	0/1/1/1
7	NAG	i	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	i	2	7	-	2/6/23/26	0/1/1/1
7	NAG	j	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	j	2	7	-	2/6/23/26	0/1/1/1
12	NAG	k	1	12,1	-	4/6/23/26	0/1/1/1
12	NAG	k	2	12	-	3/6/23/26	0/1/1/1
12	BMA	k	3	12	-	2/2/19/22	0/1/1/1
12	MAN	k	4	12	-	2/2/19/22	0/1/1/1
12	MAN	k	5	12	-	1/2/19/22	0/1/1/1
12	MAN	k	6	12	-	0/2/19/22	0/1/1/1
7	NAG	l	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	l	2	7	-	3/6/23/26	0/1/1/1
13	NAG	m	1	13,1	-	2/6/23/26	0/1/1/1
13	NAG	m	2	13	-	2/6/23/26	0/1/1/1
13	BMA	m	3	13	-	2/2/19/22	0/1/1/1
13	MAN	m	4	13	-	1/2/19/22	0/1/1/1
13	MAN	m	5	13	-	0/2/19/22	0/1/1/1
13	MAN	m	6	13	-	0/2/19/22	0/1/1/1
14	NAG	n	1	1,14	-	2/6/23/26	0/1/1/1
14	NAG	n	2	14	-	5/6/23/26	0/1/1/1
14	BMA	n	3	14	-	1/2/19/22	0/1/1/1
14	MAN	n	4	14	-	1/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	o	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	o	2	7	-	3/6/23/26	0/1/1/1
7	NAG	p	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	p	2	7	-	3/6/23/26	0/1/1/1
7	NAG	q	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	q	2	7	-	2/6/23/26	0/1/1/1
7	NAG	r	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	r	2	7	-	0/6/23/26	0/1/1/1
7	NAG	s	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	s	2	7	-	3/6/23/26	0/1/1/1
7	NAG	t	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	t	2	7	-	1/6/23/26	0/1/1/1
7	NAG	u	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	u	2	7	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	i	1	NAG	O5-C1	3.16	1.48	1.43
7	R	1	NAG	O5-C1	-2.94	1.39	1.43
9	e	5	MAN	C1-C2	2.36	1.57	1.52
12	k	4	MAN	C1-C2	2.34	1.57	1.52
10	Q	3	BMA	C1-C2	2.33	1.57	1.52
7	r	1	NAG	C1-C2	2.29	1.55	1.52
9	O	1	NAG	O5-C1	-2.27	1.40	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	i	1	NAG	C1-O5-C5	6.60	121.13	112.19
14	n	2	NAG	C2-N2-C7	4.42	129.19	122.90
8	L	8	MAN	C1-O5-C5	3.89	117.46	112.19
9	e	5	MAN	C1-O5-C5	3.82	117.37	112.19
14	n	4	MAN	C1-O5-C5	3.44	116.86	112.19
9	O	5	MAN	C1-O5-C5	3.16	116.47	112.19
13	m	4	MAN	O2-C2-C3	-3.11	103.90	110.14
8	L	5	MAN	O2-C2-C3	-3.08	103.96	110.14
12	k	4	MAN	C1-O5-C5	2.71	115.87	112.19
9	O	6	MAN	C1-O5-C5	2.70	115.85	112.19
10	Q	3	BMA	C1-C2-C3	2.46	112.69	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	5	MAN	C1-O5-C5	2.46	115.53	112.19
8	L	4	MAN	O2-C2-C3	-2.46	105.22	110.14
9	O	7	MAN	O2-C2-C3	-2.36	105.40	110.14
9	O	5	MAN	O2-C2-C3	-2.34	105.45	110.14
9	O	6	MAN	O2-C2-C3	-2.32	105.49	110.14
12	k	4	MAN	O2-C2-C3	-2.32	105.49	110.14
9	e	6	MAN	O2-C2-C3	-2.31	105.50	110.14
9	e	5	MAN	O2-C2-C3	-2.31	105.52	110.14
8	L	6	MAN	O2-C2-C3	-2.30	105.53	110.14
9	e	4	MAN	C1-O5-C5	2.30	115.31	112.19
13	m	6	MAN	O2-C2-C3	-2.28	105.58	110.14
14	n	4	MAN	O2-C2-C3	-2.23	105.66	110.14
13	m	5	MAN	O2-C2-C3	-2.22	105.68	110.14
10	Q	3	BMA	C1-O5-C5	2.22	115.20	112.19
9	e	7	MAN	O2-C2-C3	-2.22	105.70	110.14
9	e	4	MAN	O2-C2-C3	-2.21	105.71	110.14
9	O	4	MAN	O2-C2-C3	-2.20	105.73	110.14
8	L	7	MAN	O2-C2-C3	-2.18	105.77	110.14
12	k	5	MAN	O2-C2-C3	-2.18	105.77	110.14
8	L	8	MAN	O2-C2-C3	-2.16	105.80	110.14
11	d	4	MAN	O2-C2-C3	-2.15	105.83	110.14
8	L	4	MAN	C1-O5-C5	2.14	115.09	112.19
12	k	6	MAN	O2-C2-C3	-2.12	105.90	110.14
7	o	1	NAG	C1-O5-C5	2.11	115.06	112.19
14	n	1	NAG	C1-O5-C5	2.11	115.05	112.19
12	k	5	MAN	C1-O5-C5	2.09	115.02	112.19
13	m	4	MAN	C1-O5-C5	2.08	115.02	112.19
7	P	1	NAG	C1-O5-C5	2.07	115.00	112.19
8	L	3	BMA	O5-C5-C6	2.04	110.40	107.20
7	R	1	NAG	C3-C4-C5	2.03	113.85	110.24
9	O	4	MAN	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	l	2	NAG	C4-C5-C6-O6
12	k	3	BMA	C4-C5-C6-O6
7	T	1	NAG	C4-C5-C6-O6
7	P	1	NAG	O5-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
7	c	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	H	2	NAG	C4-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
7	l	2	NAG	O5-C5-C6-O6
12	k	3	BMA	O5-C5-C6-O6
7	b	2	NAG	C4-C5-C6-O6
7	u	2	NAG	C4-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
14	n	2	NAG	O5-C5-C6-O6
7	i	1	NAG	C4-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6
7	T	2	NAG	O5-C5-C6-O6
7	j	2	NAG	O5-C5-C6-O6
7	o	1	NAG	O5-C5-C6-O6
7	r	1	NAG	O5-C5-C6-O6
13	m	2	NAG	O5-C5-C6-O6
13	m	3	BMA	O5-C5-C6-O6
7	j	1	NAG	C4-C5-C6-O6
7	p	2	NAG	O5-C5-C6-O6
7	t	1	NAG	O5-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
7	E	1	NAG	O5-C5-C6-O6
7	T	1	NAG	O5-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
7	t	1	NAG	C4-C5-C6-O6
11	d	2	NAG	C4-C5-C6-O6
14	n	2	NAG	C4-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6
7	H	2	NAG	O5-C5-C6-O6
7	j	1	NAG	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
7	u	2	NAG	O5-C5-C6-O6
11	d	3	BMA	O5-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
7	V	2	NAG	C4-C5-C6-O6
7	c	1	NAG	C4-C5-C6-O6
13	m	1	NAG	C1-C2-N2-C7
7	V	1	NAG	O5-C5-C6-O6
7	i	1	NAG	O5-C5-C6-O6
12	k	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	Z	1	NAG	C4-C5-C6-O6
7	r	1	NAG	C4-C5-C6-O6
7	E	1	NAG	C4-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
7	f	2	NAG	C4-C5-C6-O6
9	e	4	MAN	O5-C5-C6-O6
7	E	2	NAG	C4-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
7	E	2	NAG	C8-C7-N2-C2
7	E	2	NAG	O7-C7-N2-C2
7	b	1	NAG	C8-C7-N2-C2
7	b	1	NAG	O7-C7-N2-C2
12	k	1	NAG	C8-C7-N2-C2
12	k	1	NAG	O7-C7-N2-C2
12	k	2	NAG	C8-C7-N2-C2
12	k	2	NAG	O7-C7-N2-C2
14	n	1	NAG	C8-C7-N2-C2
14	n	1	NAG	O7-C7-N2-C2
14	n	2	NAG	C8-C7-N2-C2
14	n	2	NAG	O7-C7-N2-C2
7	s	2	NAG	O5-C5-C6-O6
7	j	2	NAG	C4-C5-C6-O6
9	O	2	NAG	O5-C5-C6-O6
10	Q	2	NAG	O5-C5-C6-O6
12	k	1	NAG	O5-C5-C6-O6
7	I	2	NAG	C4-C5-C6-O6
7	o	1	NAG	C4-C5-C6-O6
7	V	1	NAG	C4-C5-C6-O6
12	k	4	MAN	C4-C5-C6-O6
13	m	2	NAG	C4-C5-C6-O6
7	p	1	NAG	O5-C5-C6-O6
8	L	2	NAG	O5-C5-C6-O6
14	n	4	MAN	O5-C5-C6-O6
9	e	4	MAN	C4-C5-C6-O6
7	f	1	NAG	O5-C5-C6-O6
7	s	2	NAG	C4-C5-C6-O6
9	O	2	NAG	C4-C5-C6-O6
12	k	1	NAG	C4-C5-C6-O6
7	T	2	NAG	C4-C5-C6-O6
7	i	2	NAG	O5-C5-C6-O6
7	f	1	NAG	C4-C5-C6-O6
11	d	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	p	2	NAG	C4-C5-C6-O6
7	h	2	NAG	O5-C5-C6-O6
7	R	2	NAG	C4-C5-C6-O6
13	m	3	BMA	C4-C5-C6-O6
7	h	1	NAG	O5-C5-C6-O6
7	h	2	NAG	C4-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
7	f	2	NAG	O5-C5-C6-O6
7	E	2	NAG	O5-C5-C6-O6
7	q	1	NAG	C4-C5-C6-O6
7	H	1	NAG	C1-C2-N2-C7
7	W	2	NAG	O5-C5-C6-O6
8	L	8	MAN	O5-C5-C6-O6
13	m	4	MAN	O5-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
10	Q	2	NAG	C4-C5-C6-O6
9	O	7	MAN	O5-C5-C6-O6
8	L	3	BMA	O5-C5-C6-O6
7	q	2	NAG	O5-C5-C6-O6
10	Q	3	BMA	O5-C5-C6-O6
14	n	3	BMA	O5-C5-C6-O6
7	Z	2	NAG	C4-C5-C6-O6
7	o	2	NAG	C4-C5-C6-O6
7	i	2	NAG	C4-C5-C6-O6
7	o	2	NAG	O5-C5-C6-O6
7	Z	2	NAG	O5-C5-C6-O6
7	a	1	NAG	C4-C5-C6-O6
7	q	1	NAG	O5-C5-C6-O6
9	e	7	MAN	O5-C5-C6-O6
7	p	1	NAG	C4-C5-C6-O6
9	e	7	MAN	C4-C5-C6-O6
9	e	2	NAG	O5-C5-C6-O6
8	L	2	NAG	C4-C5-C6-O6
11	d	1	NAG	C1-C2-N2-C7
11	d	1	NAG	C4-C5-C6-O6
12	k	5	MAN	O5-C5-C6-O6
11	d	1	NAG	O5-C5-C6-O6
9	O	1	NAG	C4-C5-C6-O6
7	u	1	NAG	O5-C5-C6-O6
8	L	1	NAG	C4-C5-C6-O6
7	W	2	NAG	C3-C2-N2-C7
7	g	2	NAG	C3-C2-N2-C7

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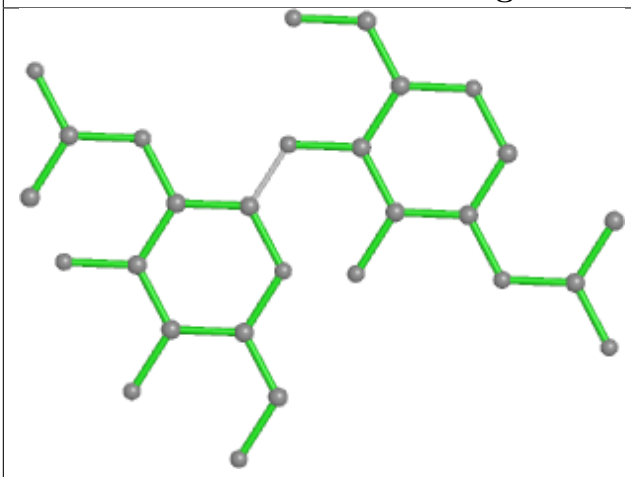
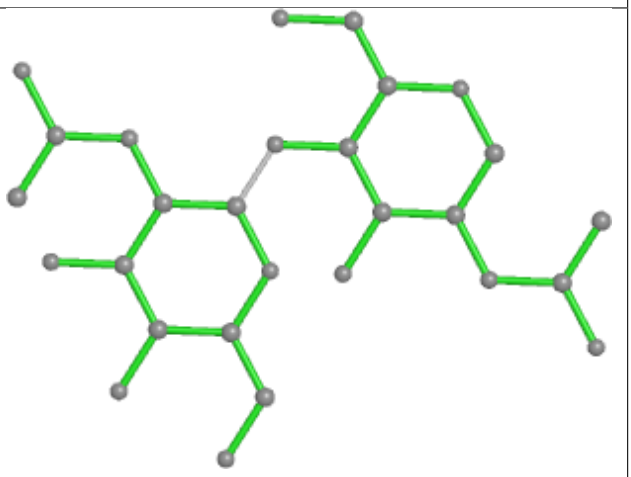
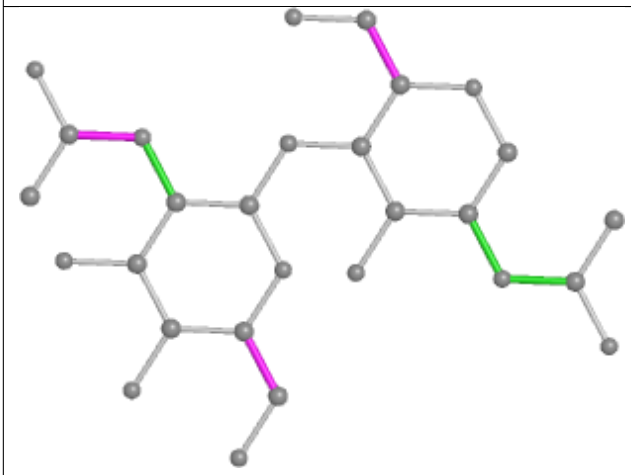
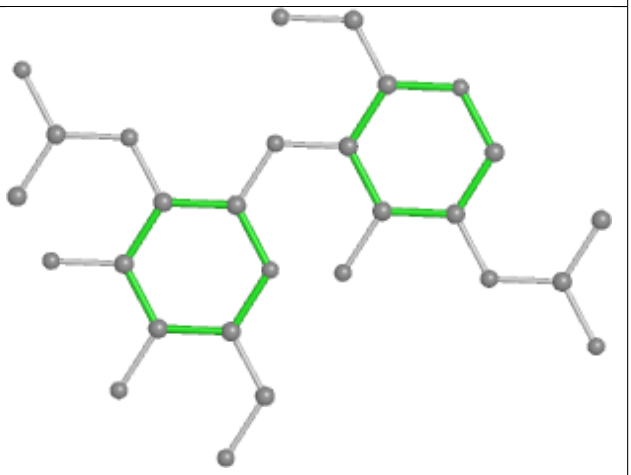
Mol	Chain	Res	Type	Atoms
7	l	2	NAG	C3-C2-N2-C7
7	o	2	NAG	C3-C2-N2-C7
7	p	2	NAG	C3-C2-N2-C7
7	q	2	NAG	C3-C2-N2-C7
7	s	2	NAG	C3-C2-N2-C7
7	t	1	NAG	C3-C2-N2-C7
7	t	2	NAG	C3-C2-N2-C7
10	Q	2	NAG	C3-C2-N2-C7
13	m	1	NAG	C3-C2-N2-C7
14	n	2	NAG	C3-C2-N2-C7
7	a	1	NAG	O5-C5-C6-O6
10	Q	1	NAG	C1-C2-N2-C7
8	L	7	MAN	C4-C5-C6-O6
11	d	3	BMA	C4-C5-C6-O6
7	R	1	NAG	C1-C2-N2-C7
7	r	1	NAG	C1-C2-N2-C7
7	s	1	NAG	O5-C5-C6-O6
12	k	2	NAG	C4-C5-C6-O6
7	H	1	NAG	C3-C2-N2-C7
7	T	2	NAG	C3-C2-N2-C7

All (2) ring outliers are listed below:

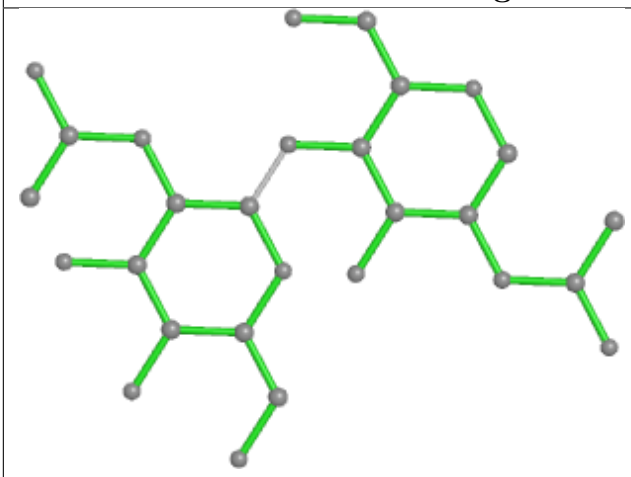
Mol	Chain	Res	Type	Atoms
14	n	4	MAN	C1-C2-C3-C4-C5-O5
8	L	8	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

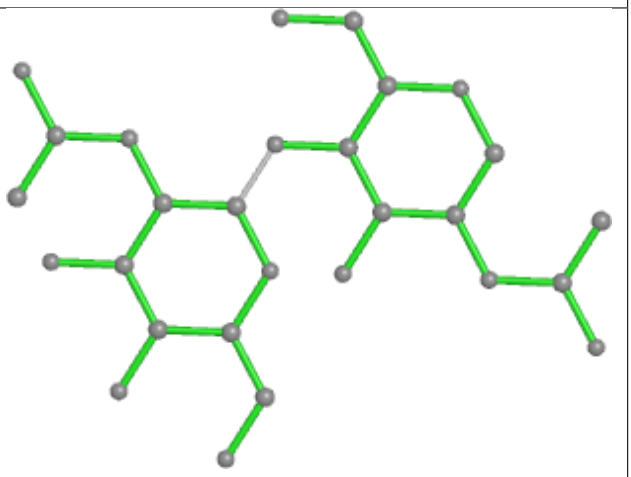
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E	
 Bond lengths	 Bond angles
 Torsions	 Rings

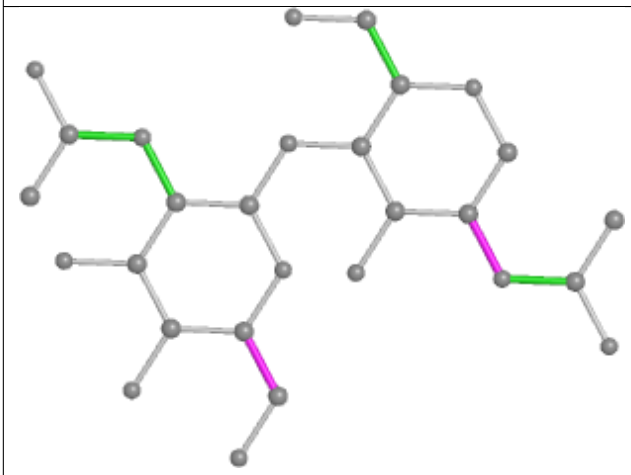
Oligosaccharide Chain H



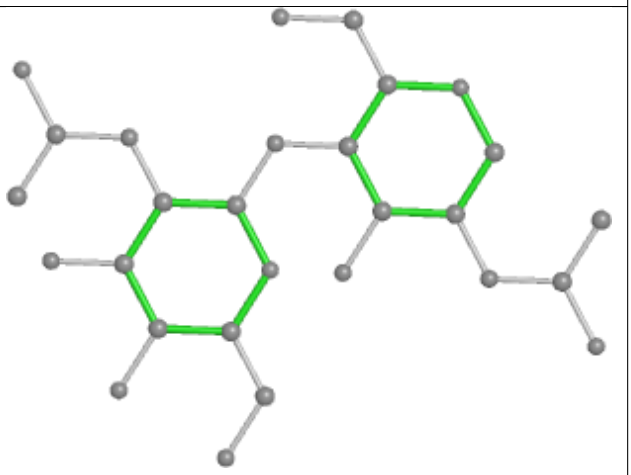
Bond lengths



Bond angles

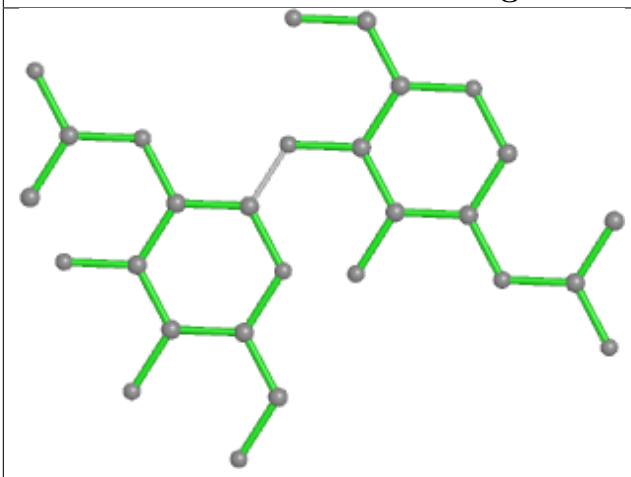


Torsions

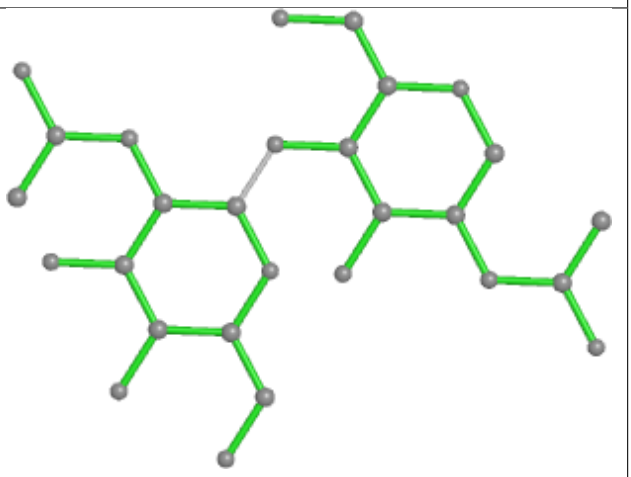


Rings

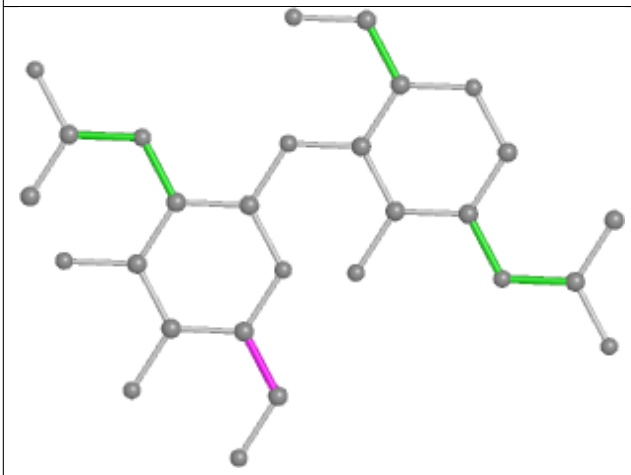
Oligosaccharide Chain I



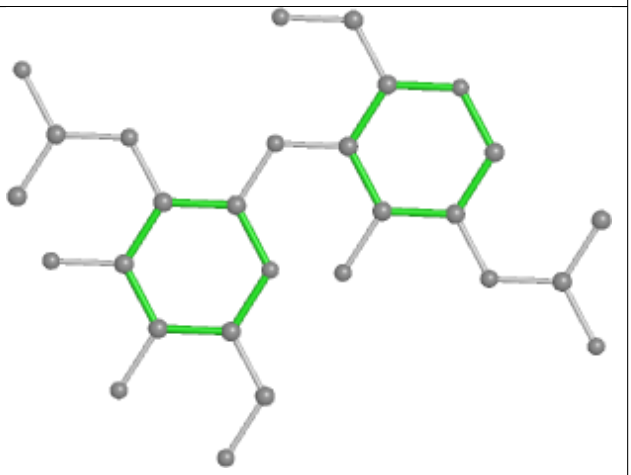
Bond lengths



Bond angles

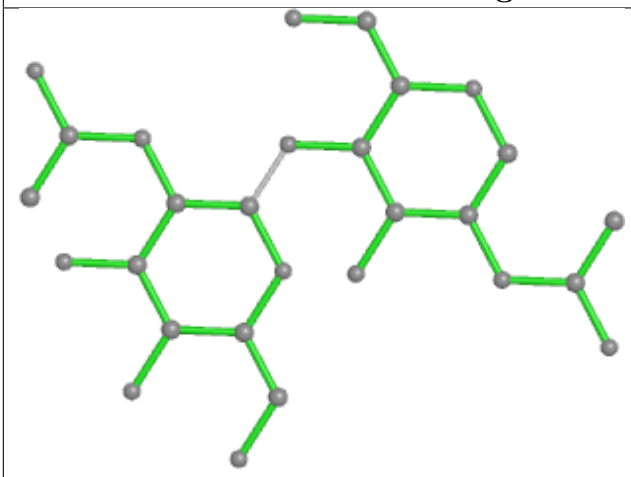


Torsions

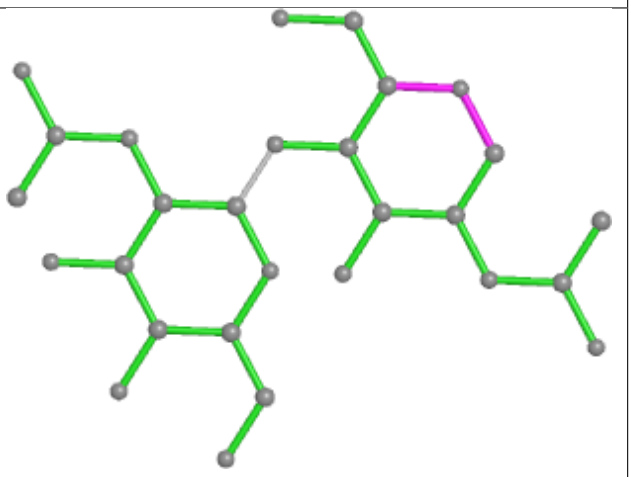


Rings

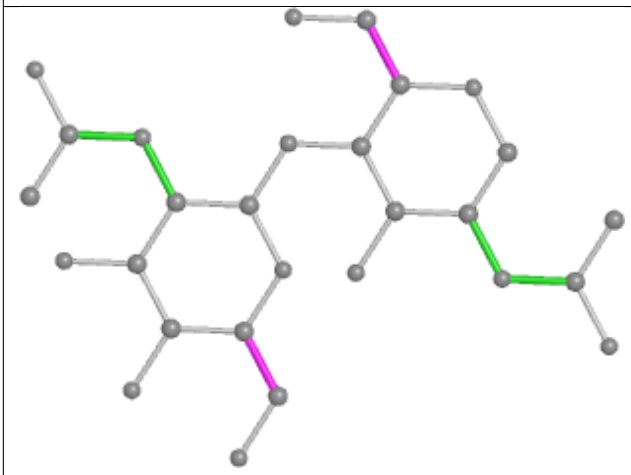
Oligosaccharide Chain P



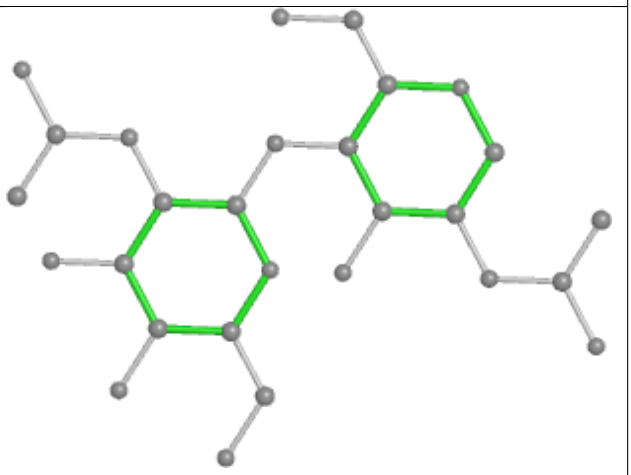
Bond lengths



Bond angles

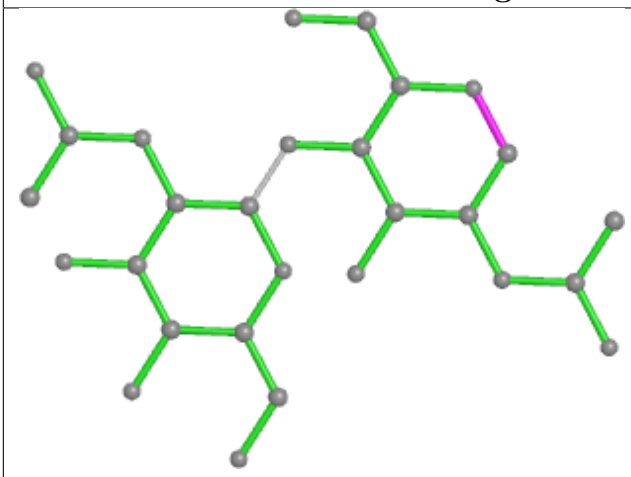


Torsions

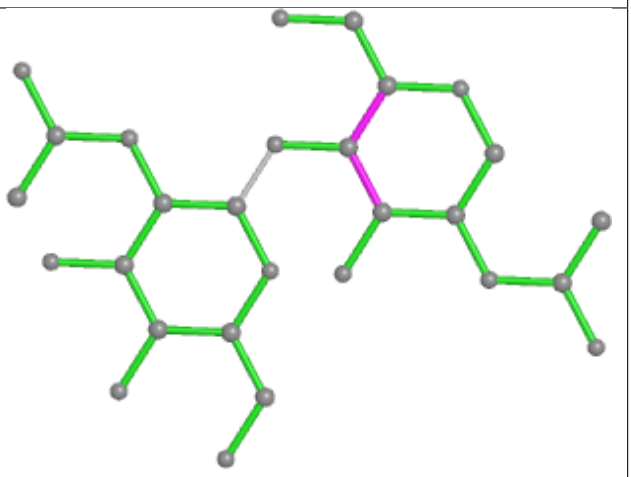


Rings

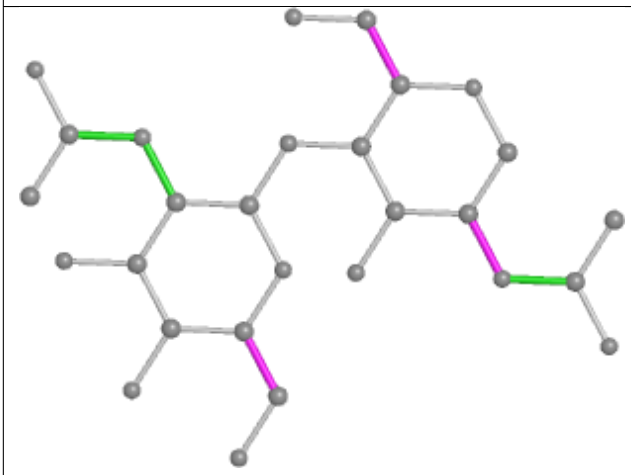
Oligosaccharide Chain R



Bond lengths



Bond angles



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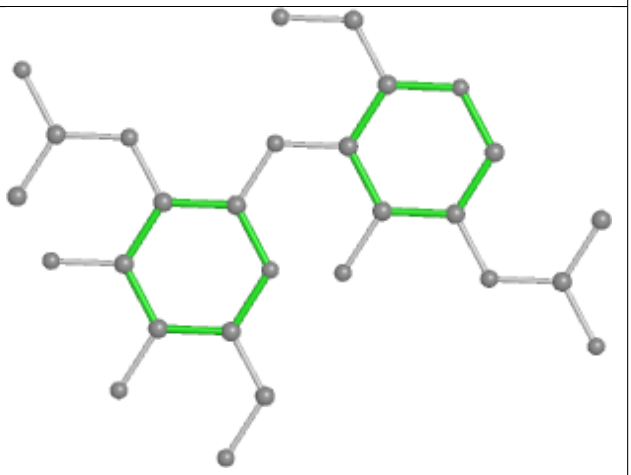
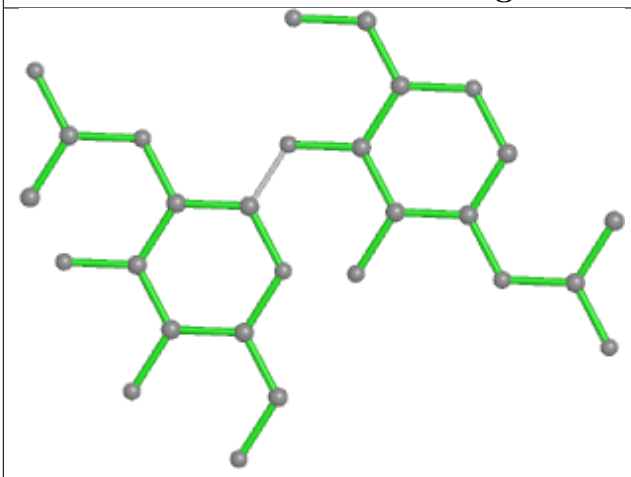
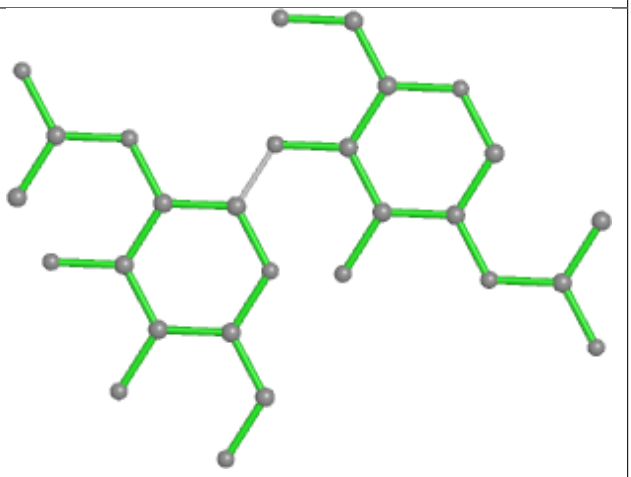


Rings

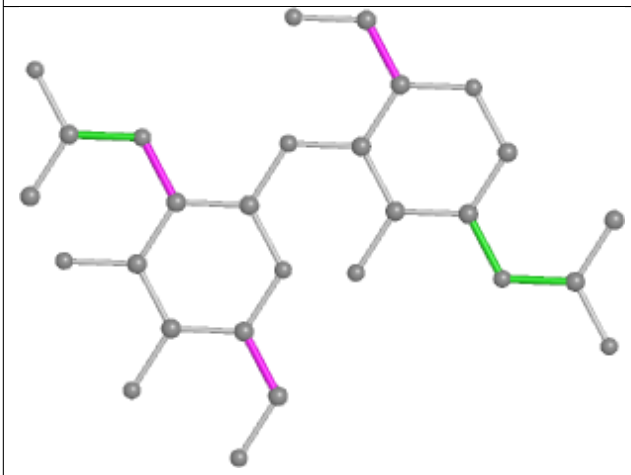
Oligosaccharide Chain T



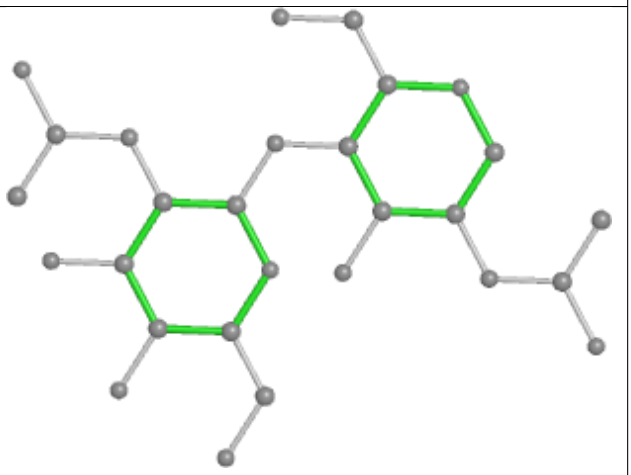
Bond lengths



Bond angles

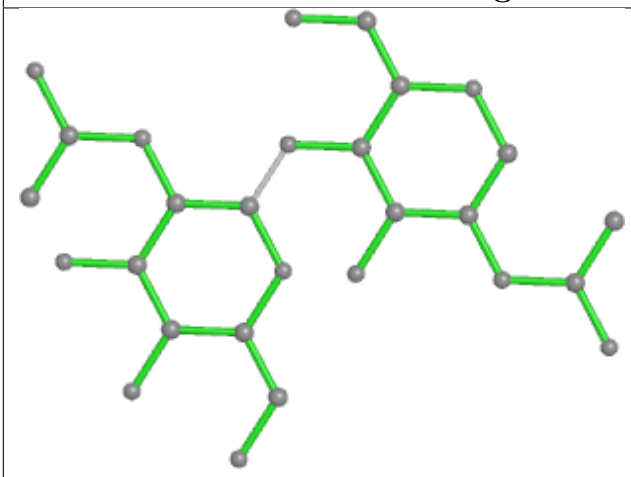


Torsions



Rings

Oligosaccharide Chain V



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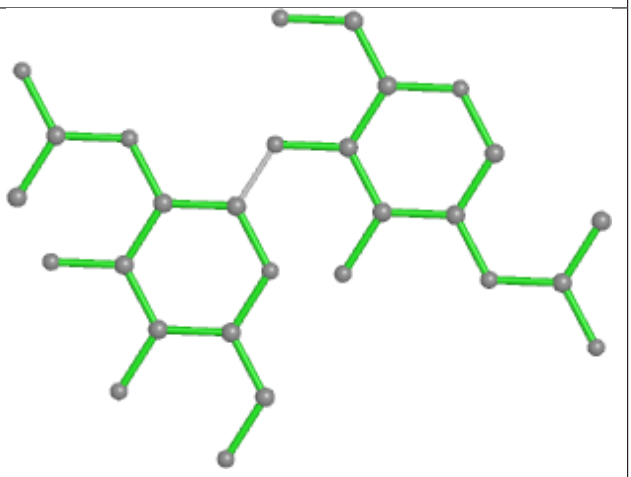
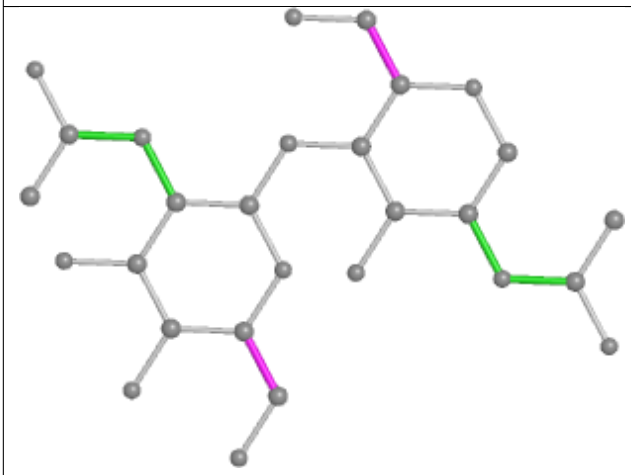


Bond angles



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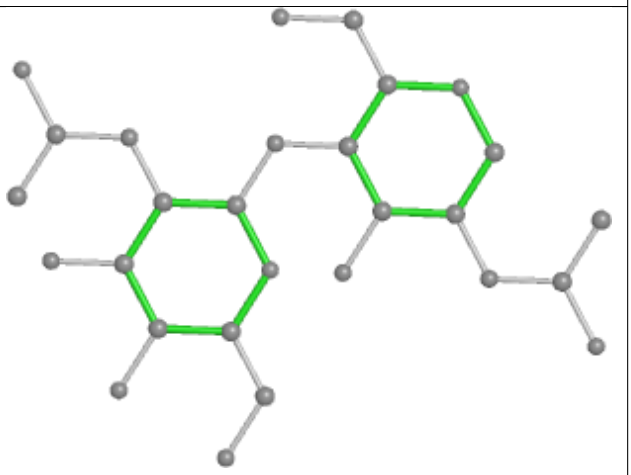
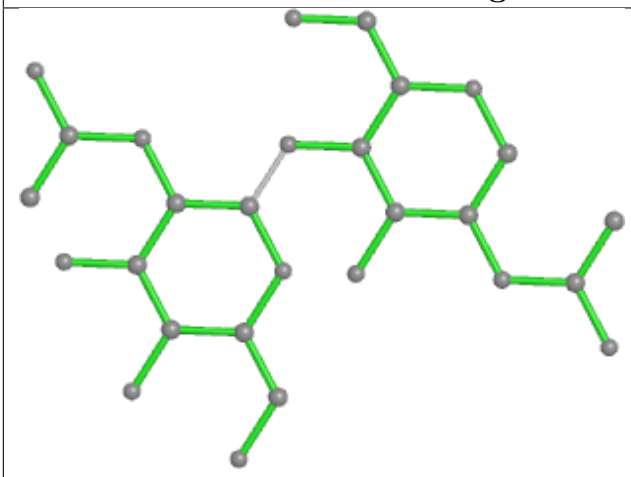


Rings

Oligosaccharide Chain W



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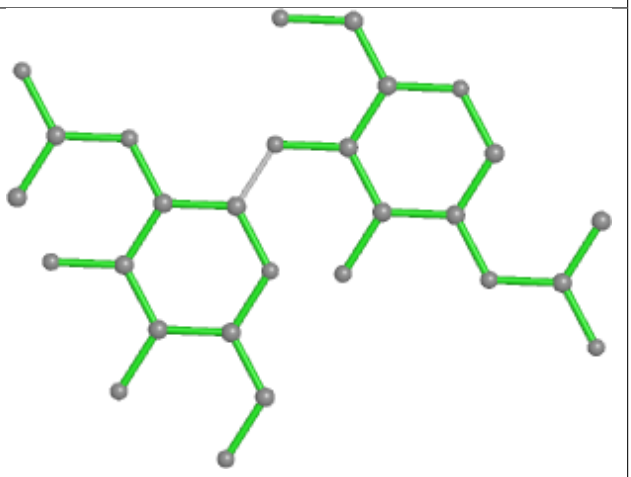

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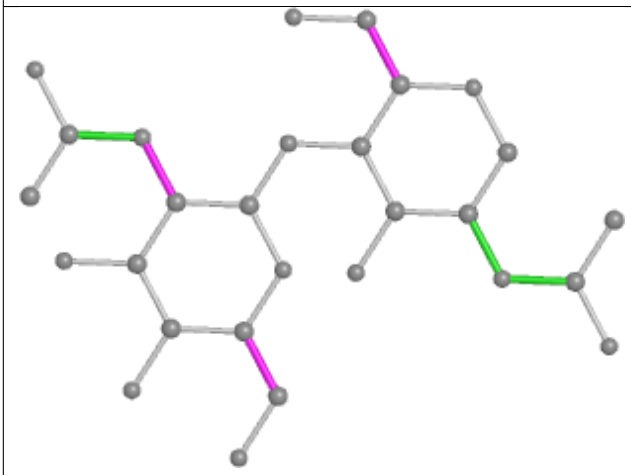

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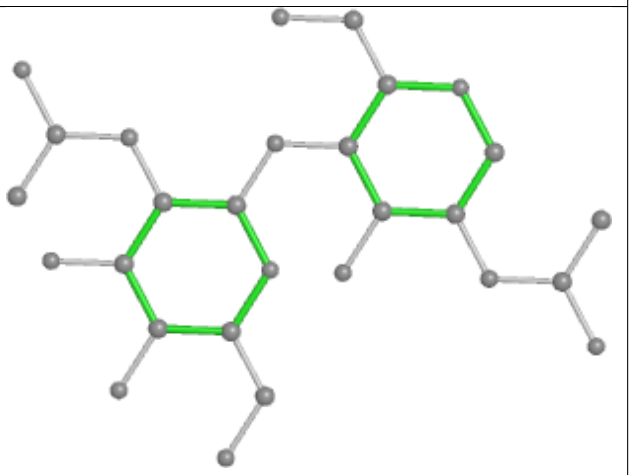
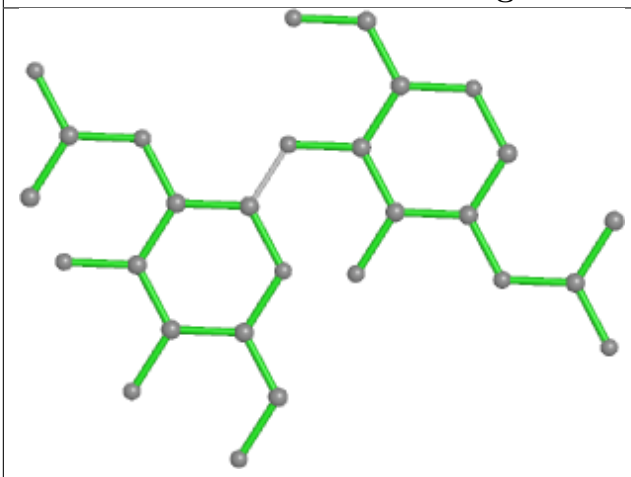


Rings

Oligosaccharide Chain Z



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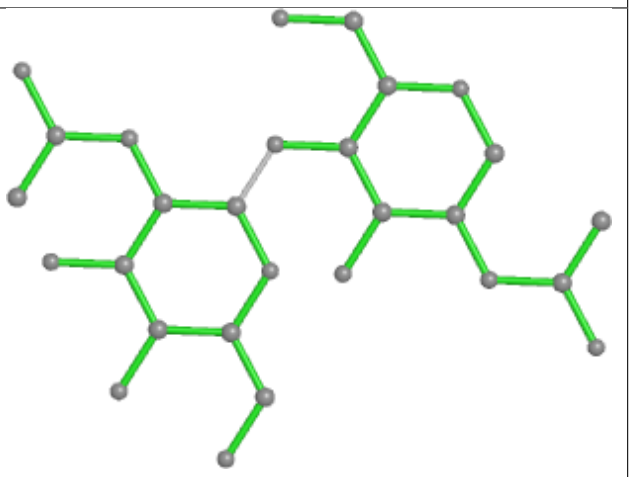

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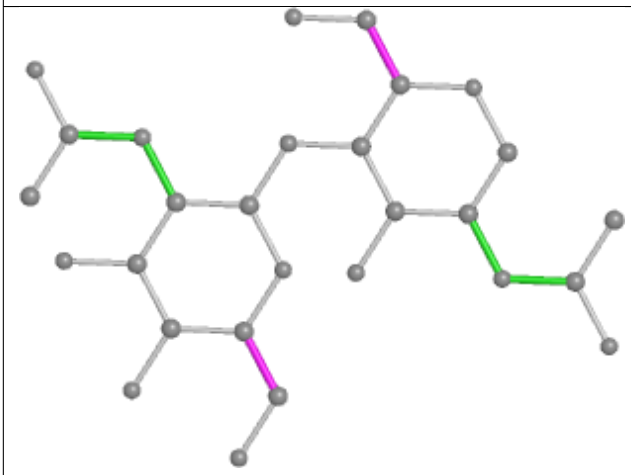

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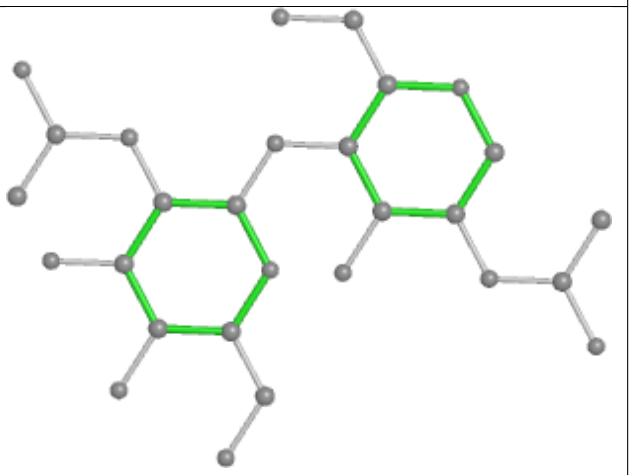
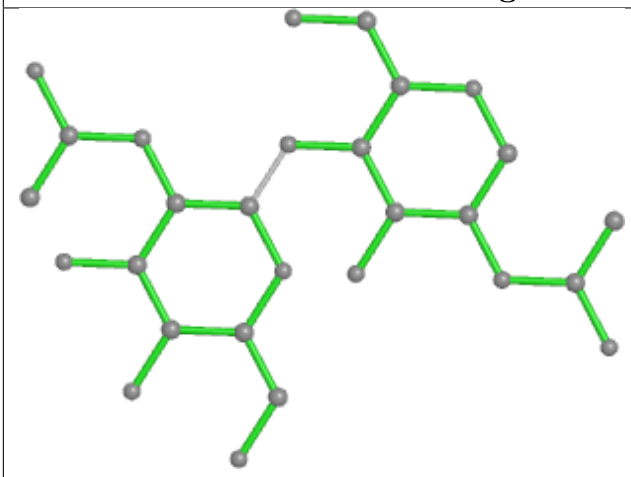


Rings

Oligosaccharide Chain a



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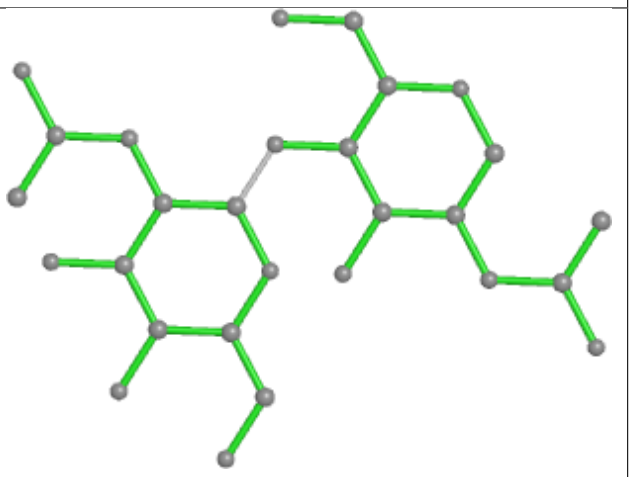

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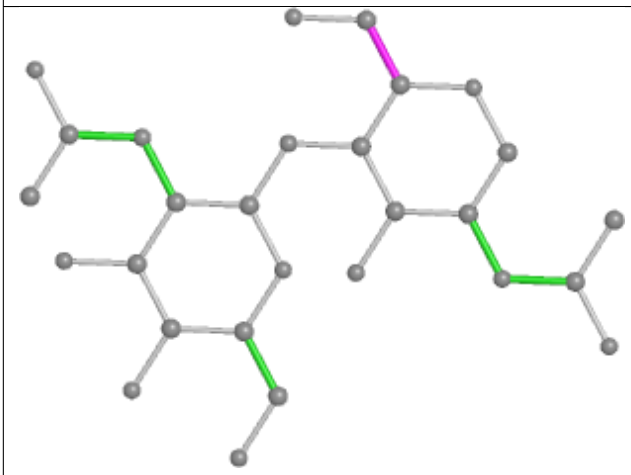

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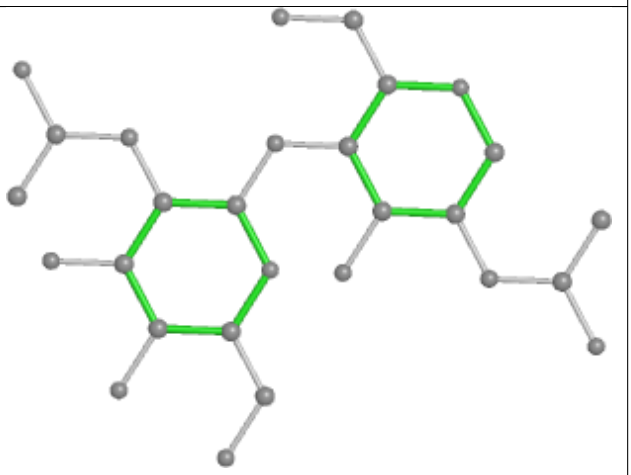
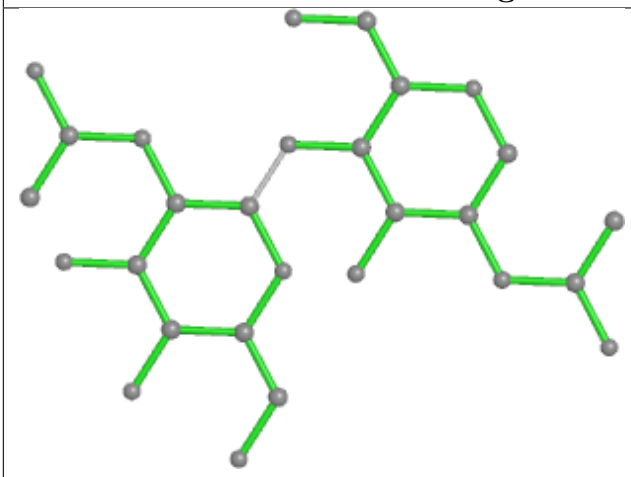


Rings

Oligosaccharide Chain b



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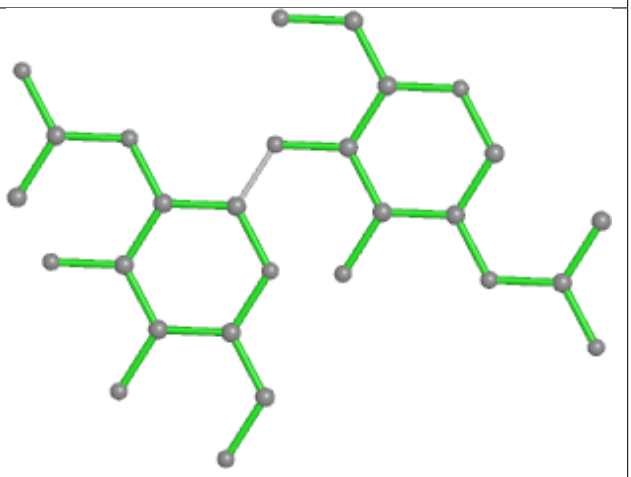

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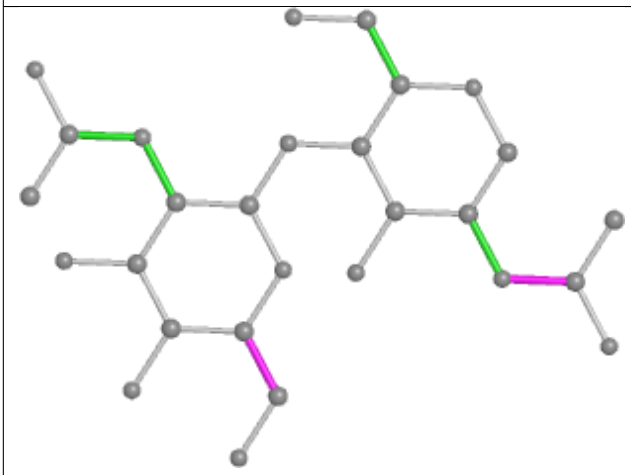

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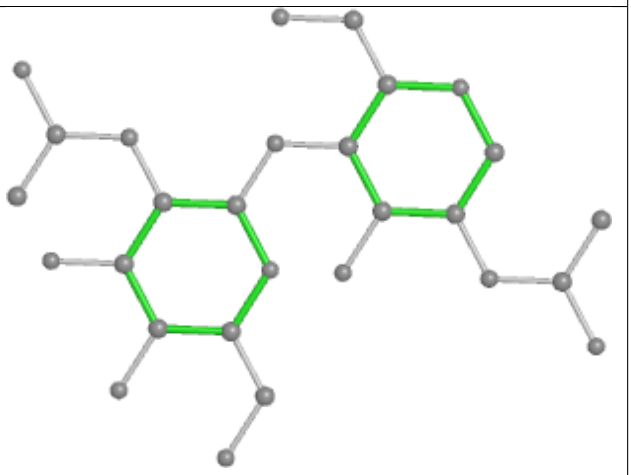
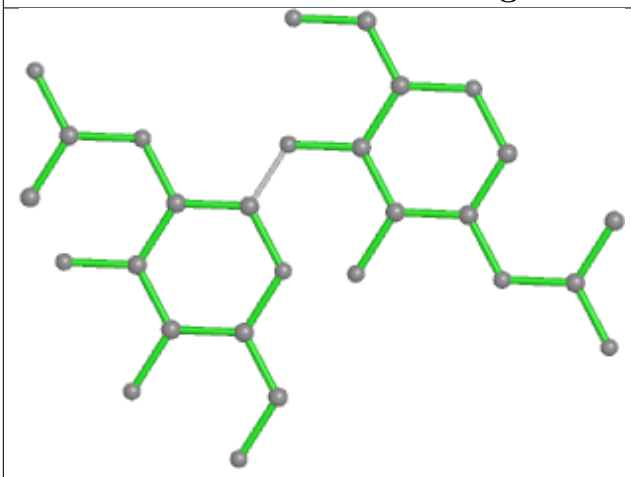


Rings

Oligosaccharide Chain c



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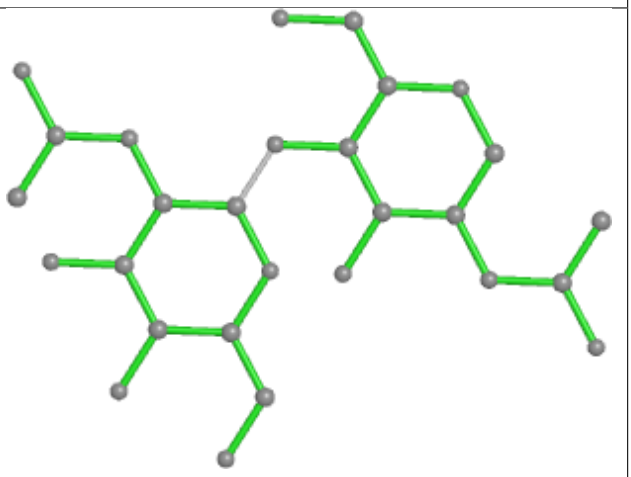

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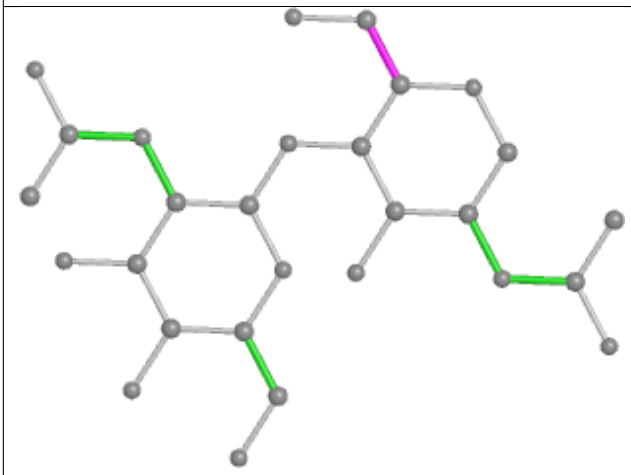

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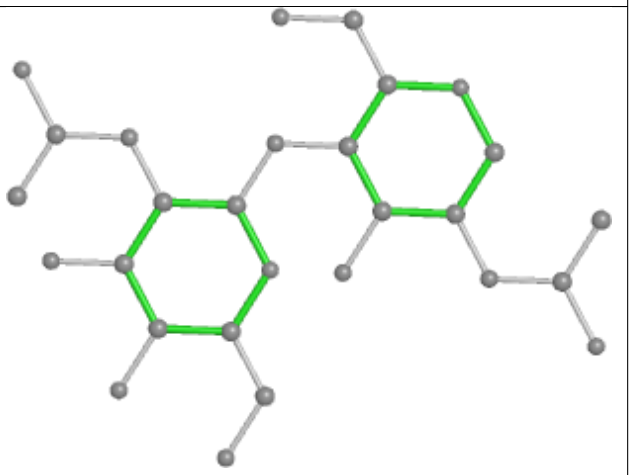
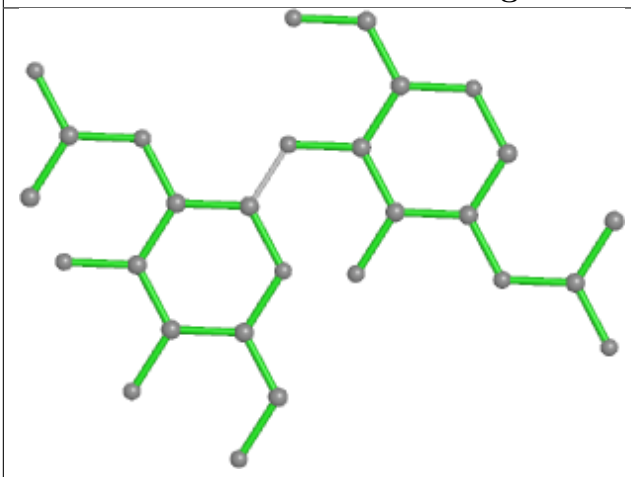


Rings

Oligosaccharide Chain f



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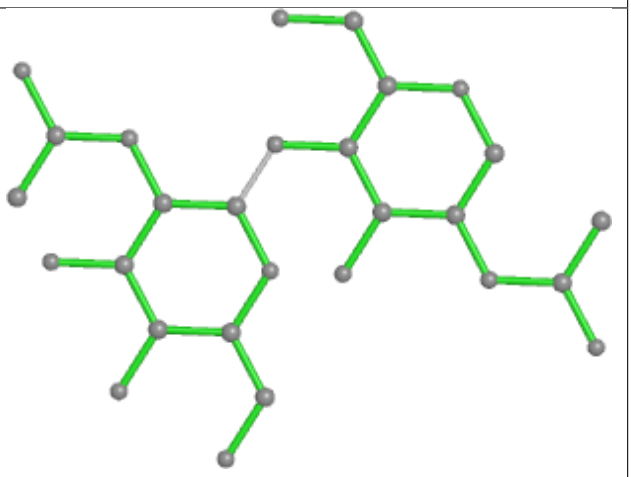

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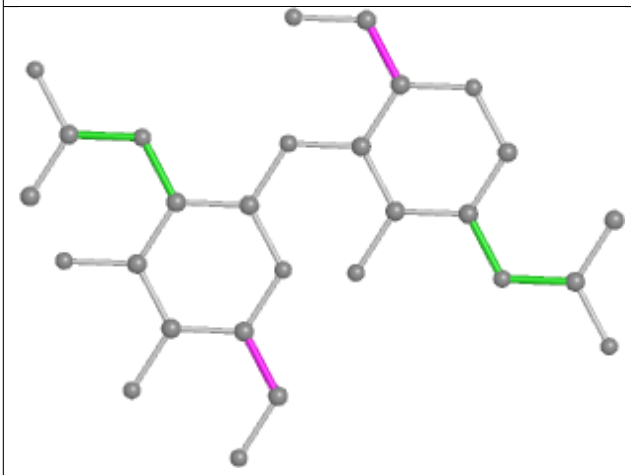

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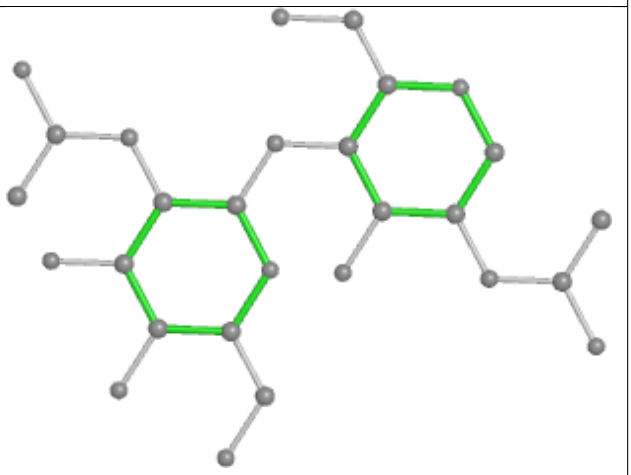
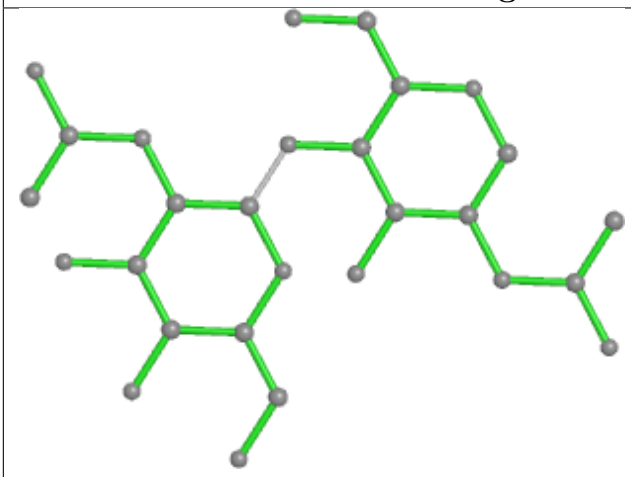


Rings

Oligosaccharide Chain g



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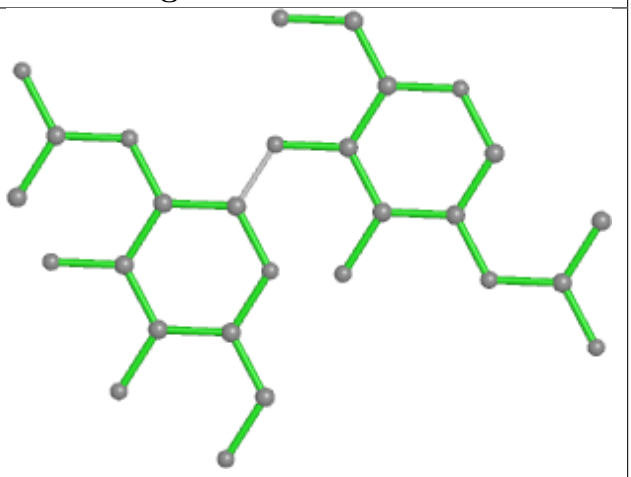

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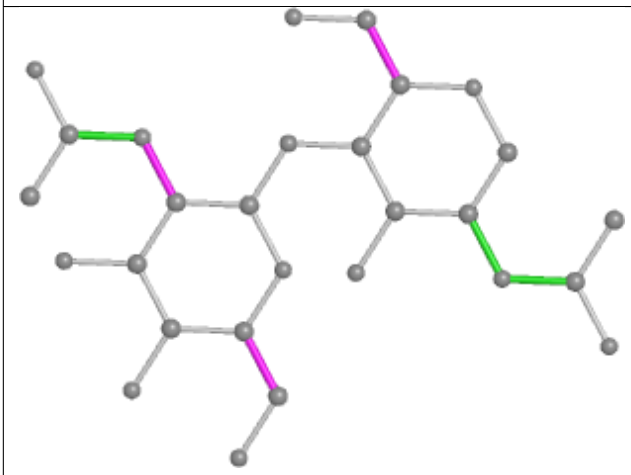

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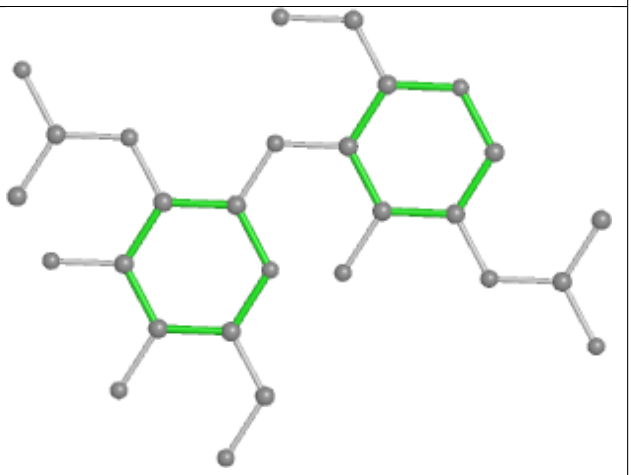
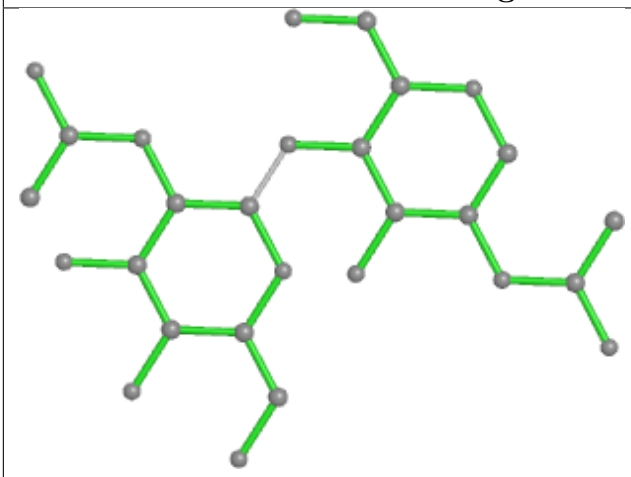


Rings

Oligosaccharide Chain h



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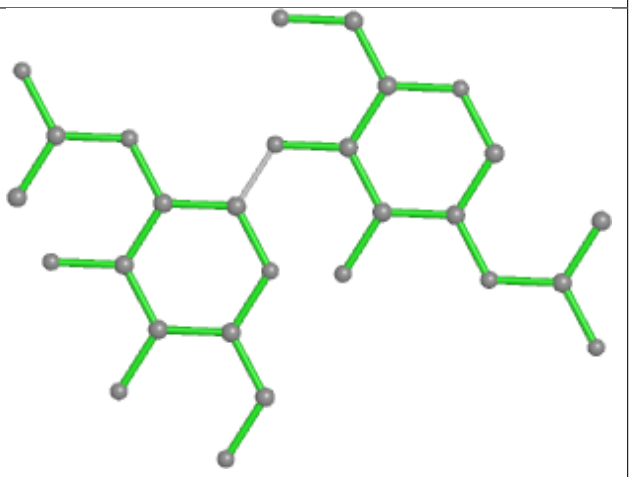

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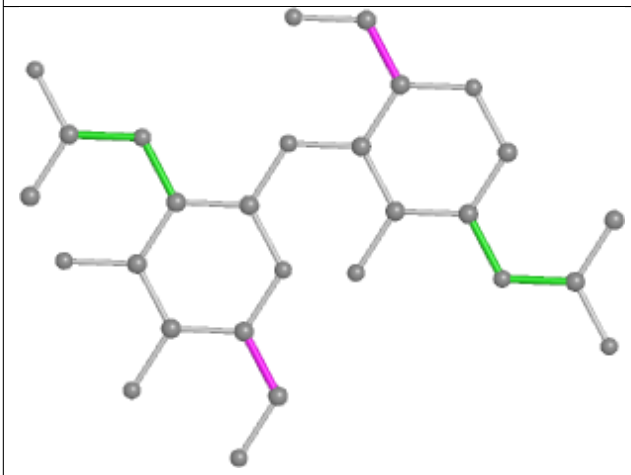

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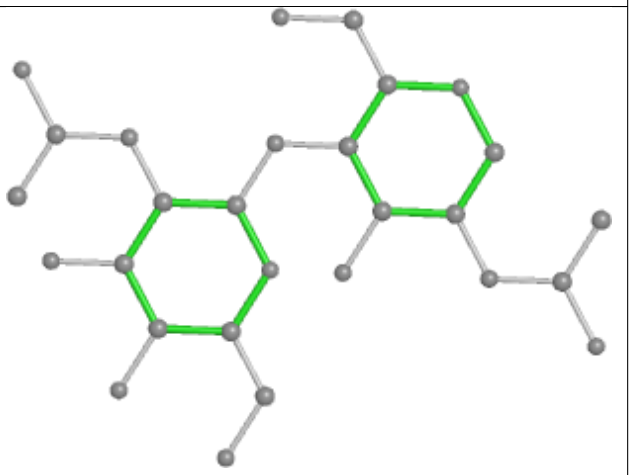
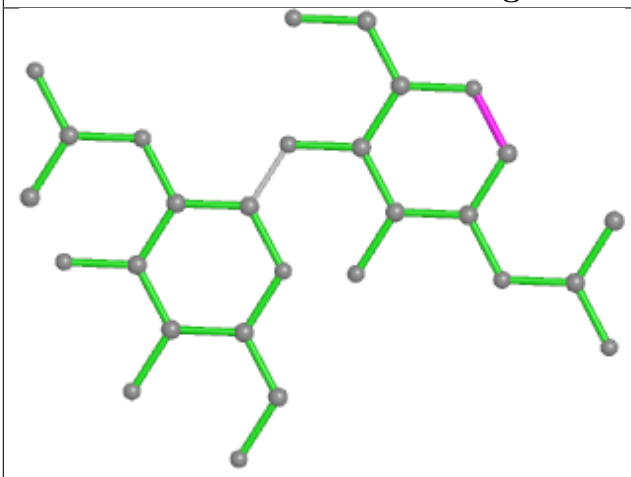


Rings

Oligosaccharide Chain i



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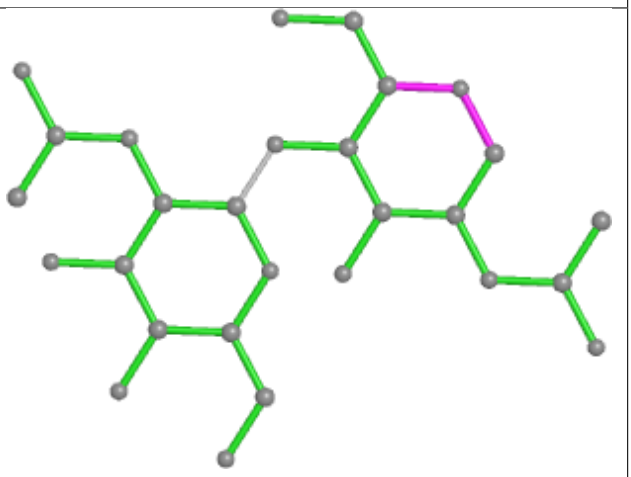

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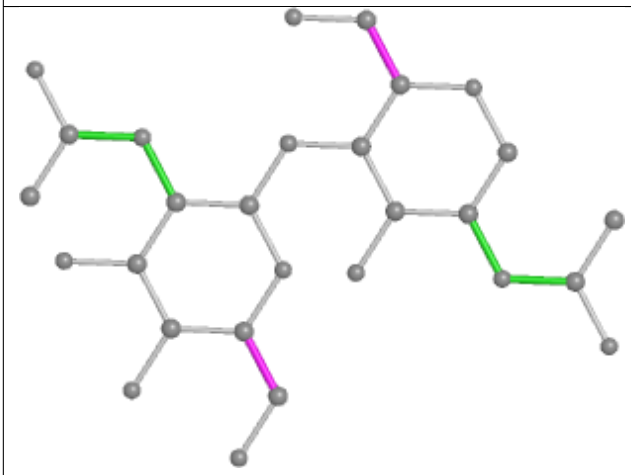

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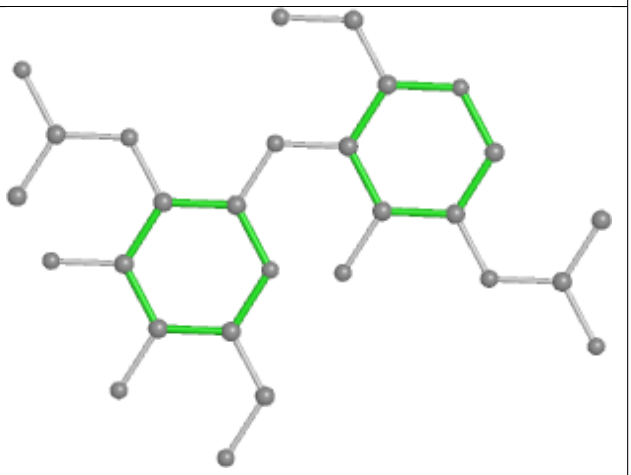
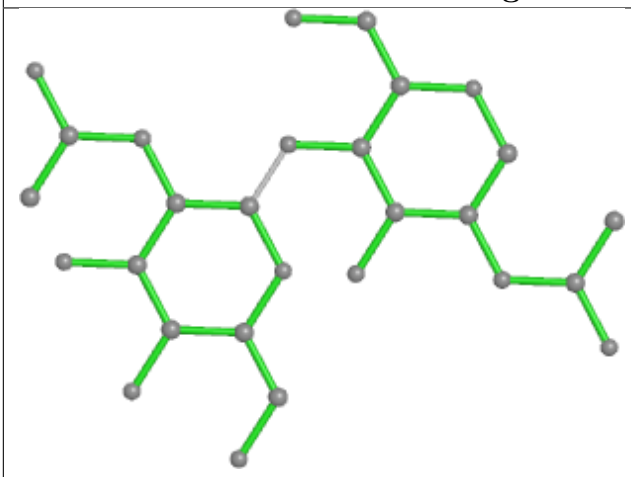


Rings

Oligosaccharide Chain j



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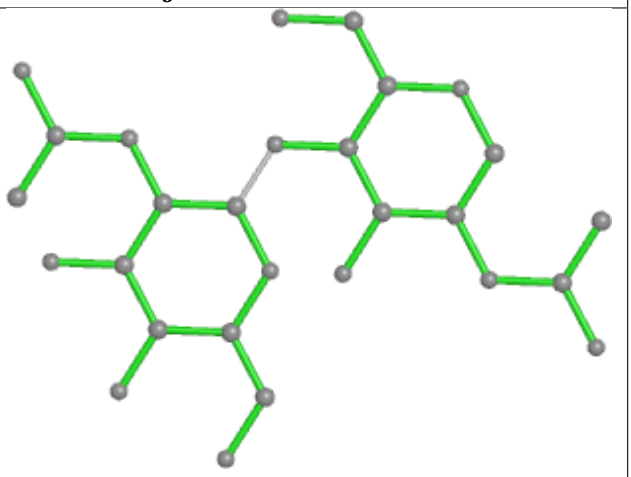

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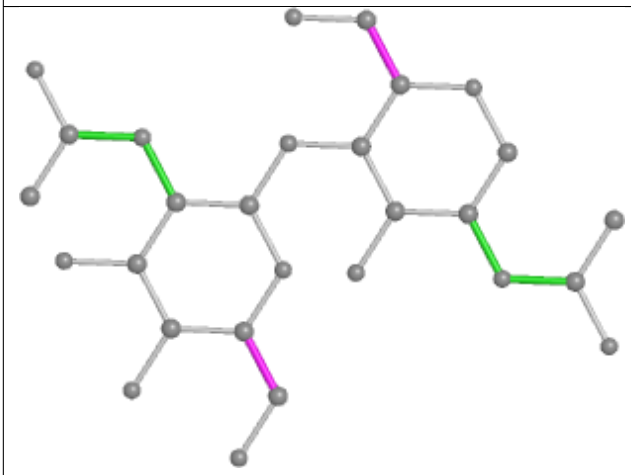

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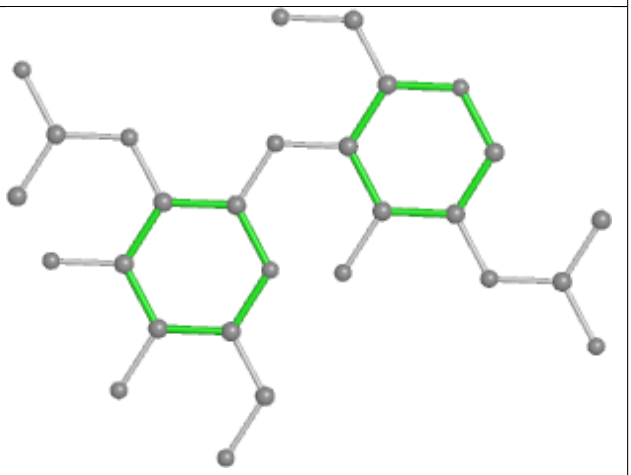
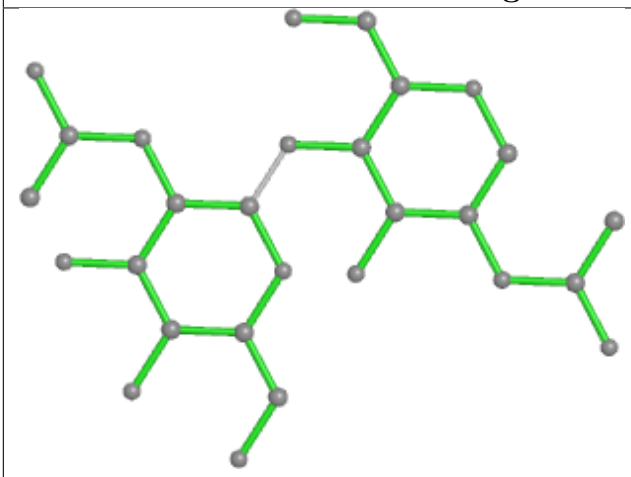


Rings

Oligosaccharide Chain l



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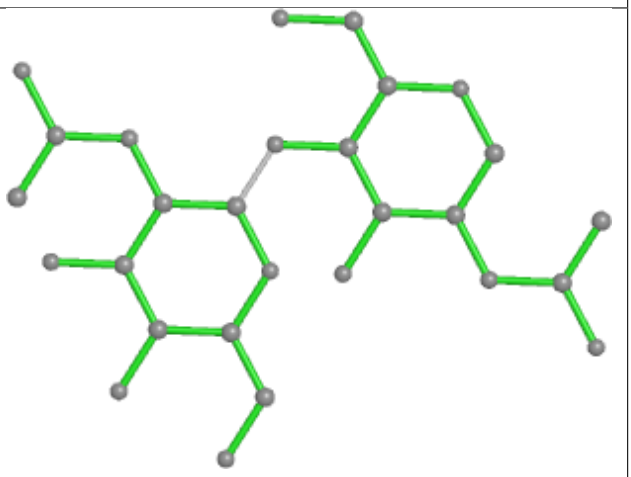

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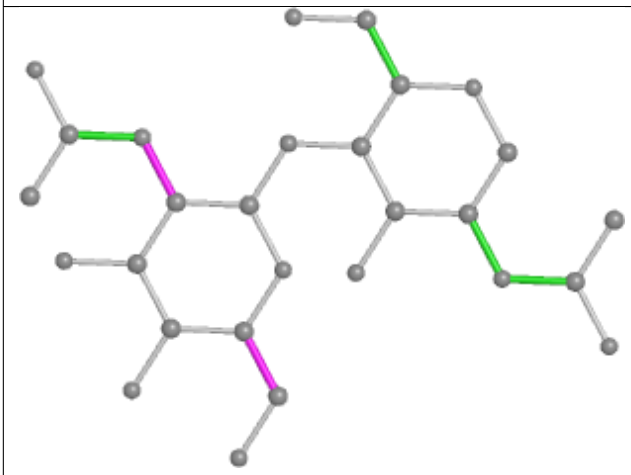

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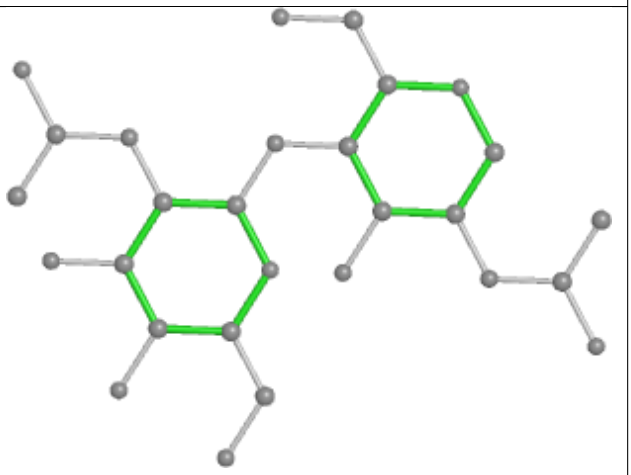
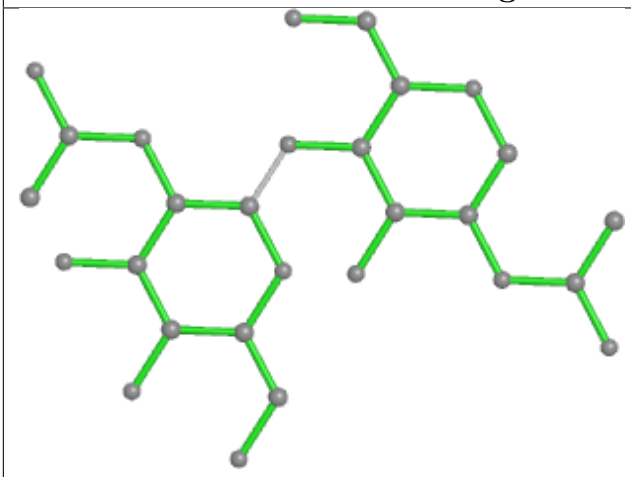


Rings

Oligosaccharide Chain o



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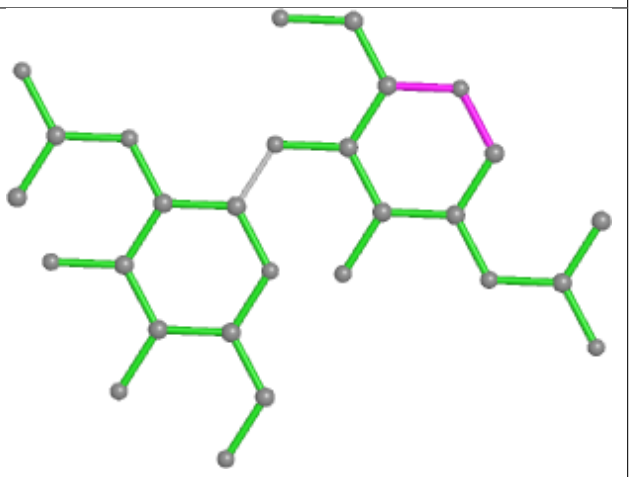

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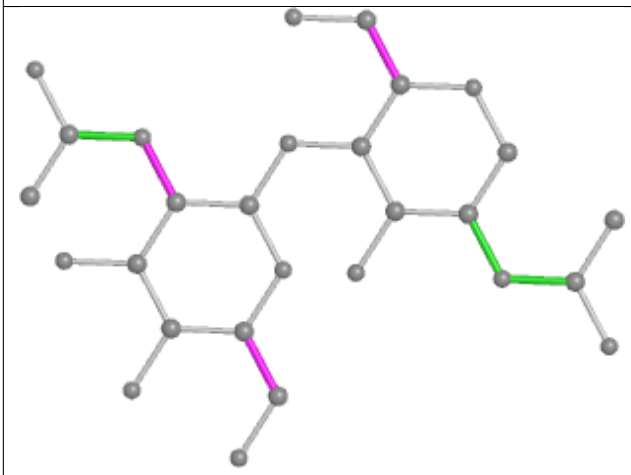

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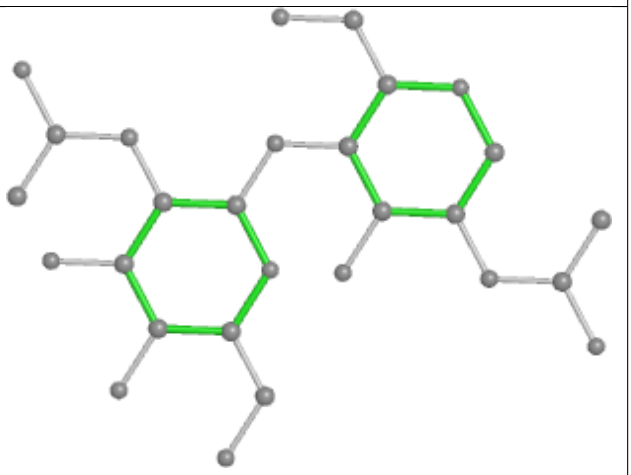
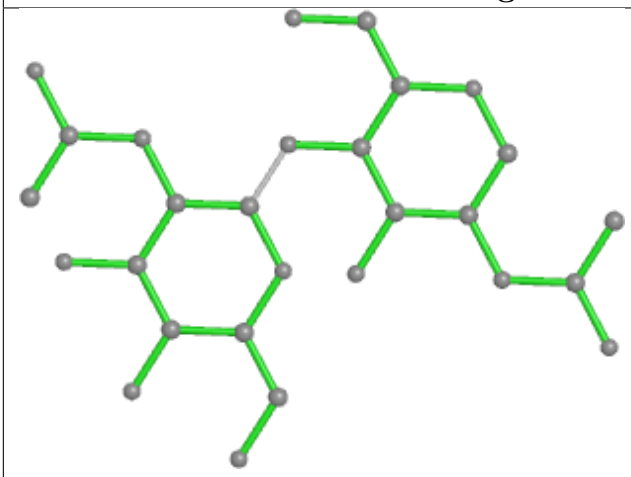
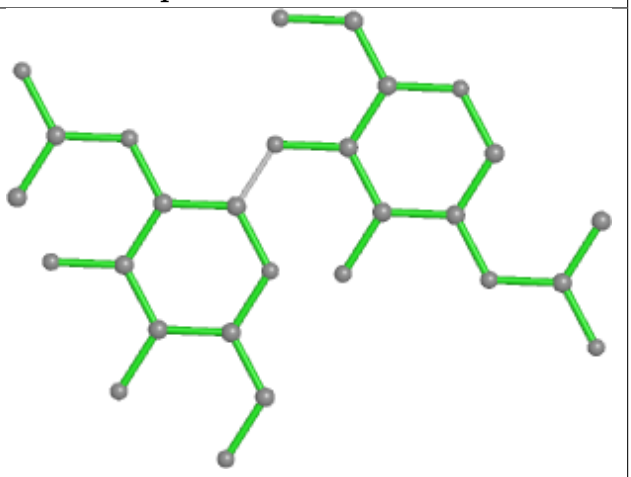


Rings

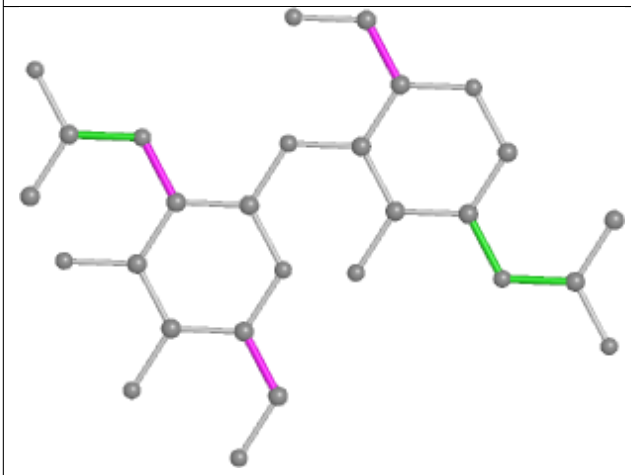
Oligosaccharide Chain p



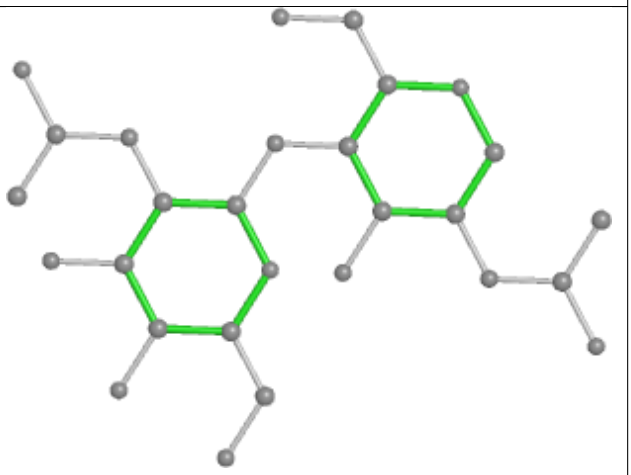
Bond lengths



Bond angles

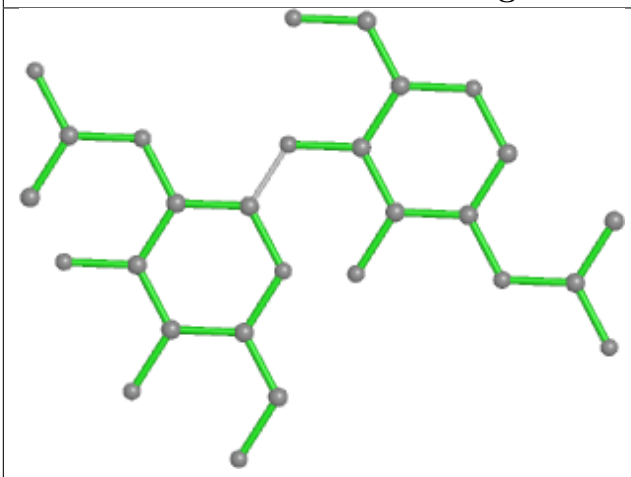


Torsions



Rings

Oligosaccharide Chain q



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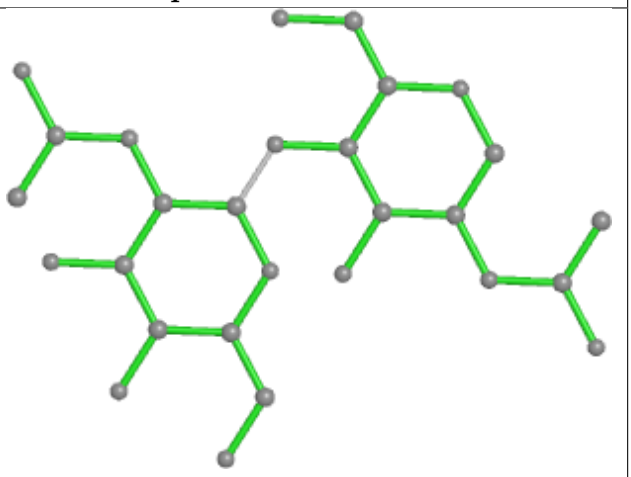

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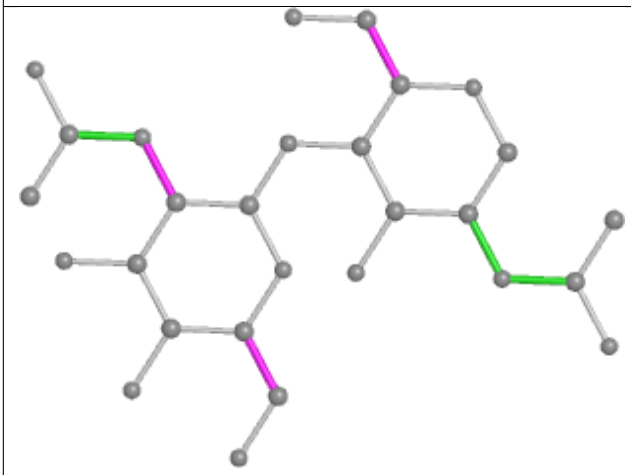

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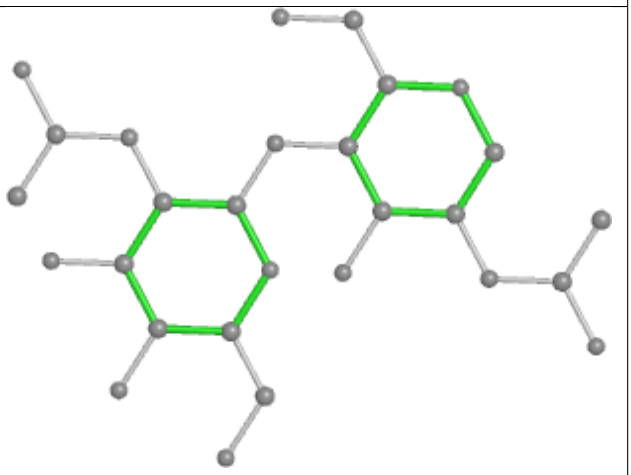
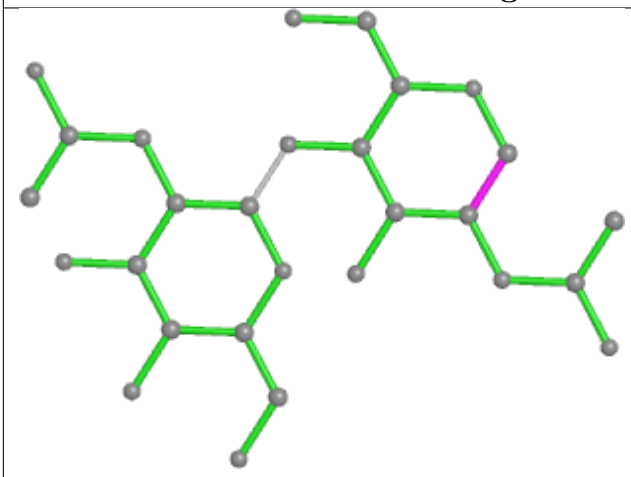


Rings

Oligosaccharide Chain r



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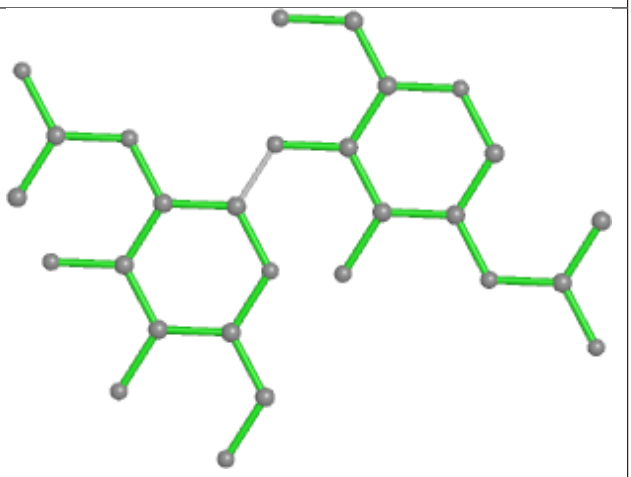

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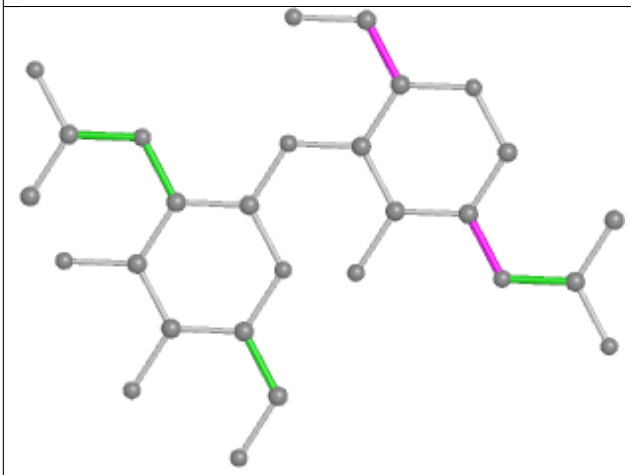

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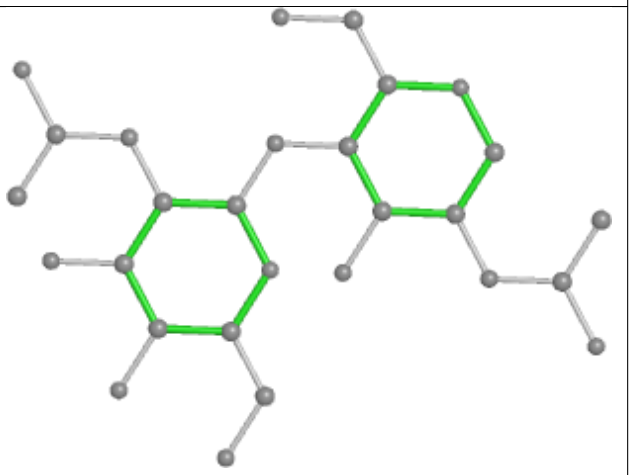
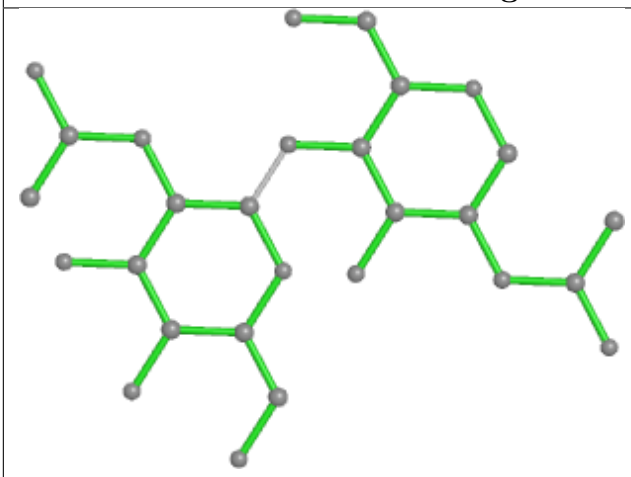


Rings

Oligosaccharide Chain s



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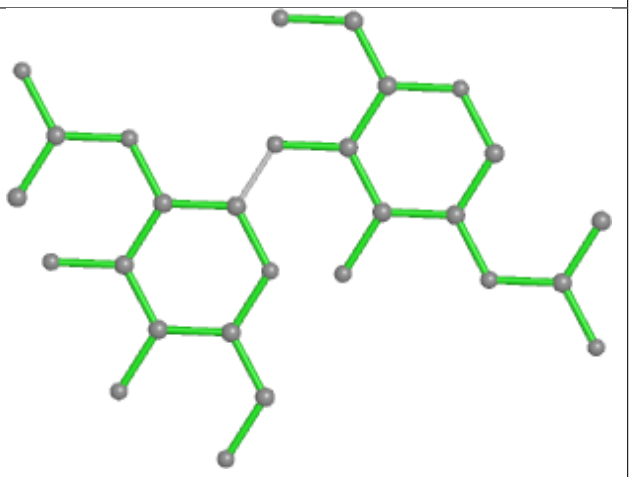
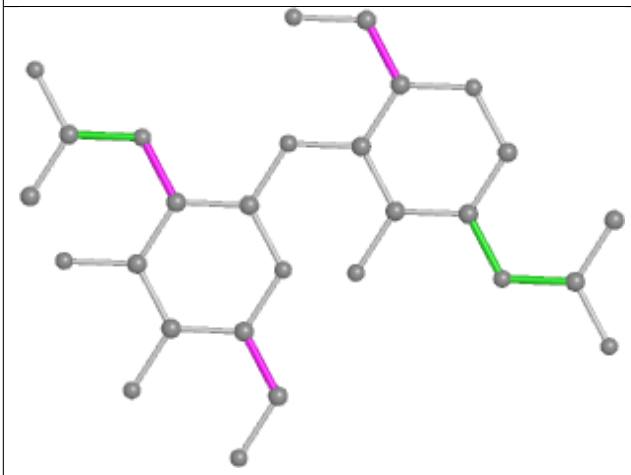


Bond angles



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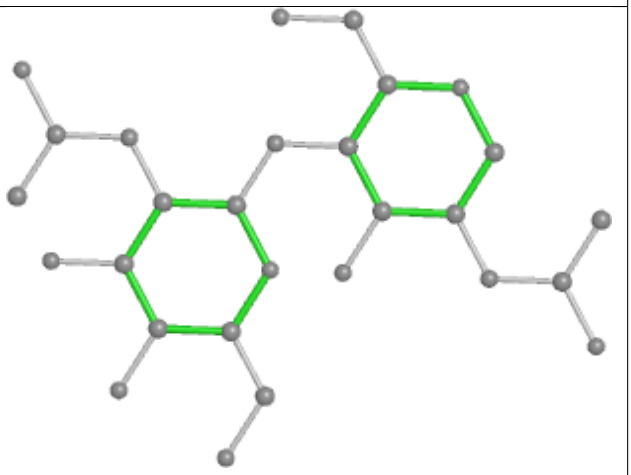
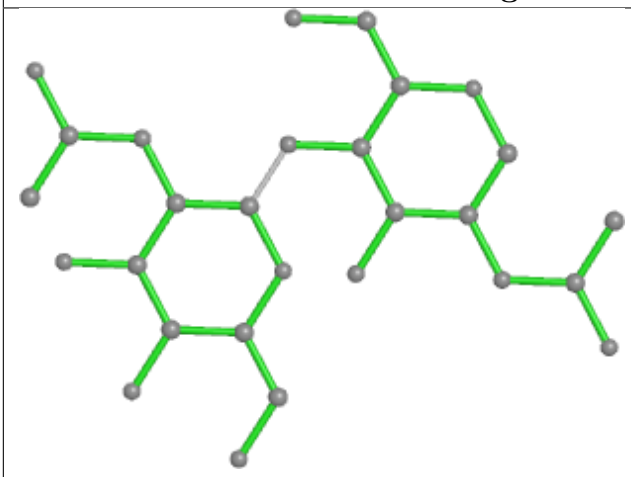


Rings

Oligosaccharide Chain t



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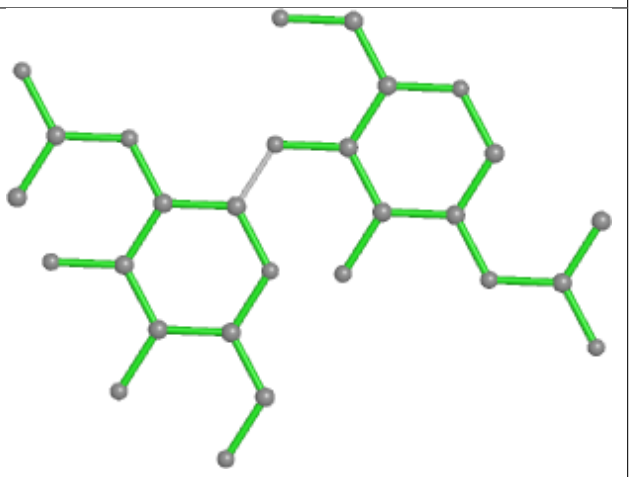
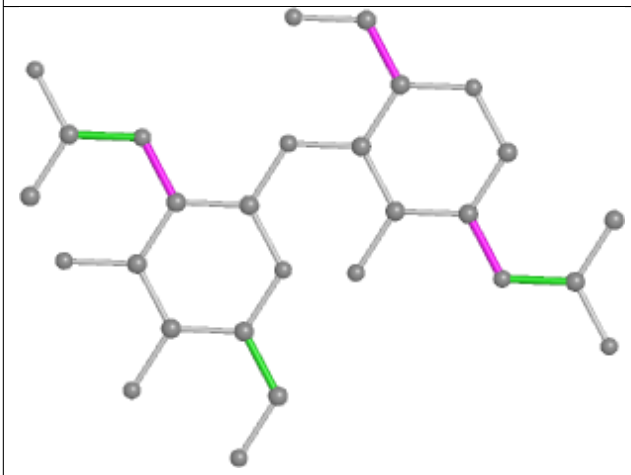


Bond angles



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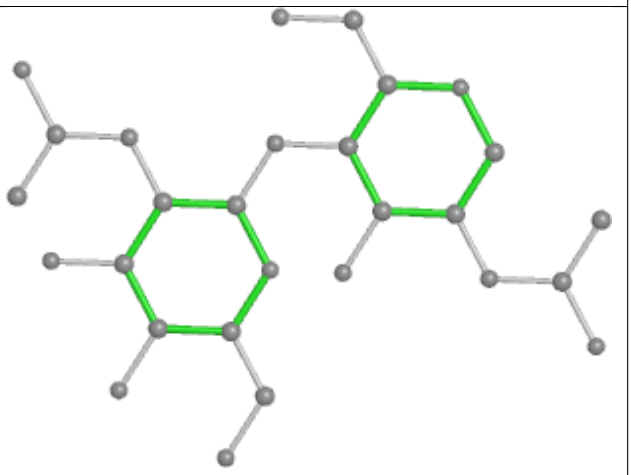
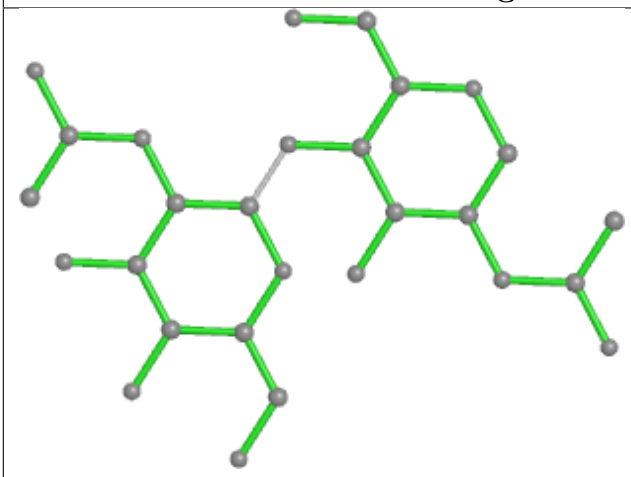
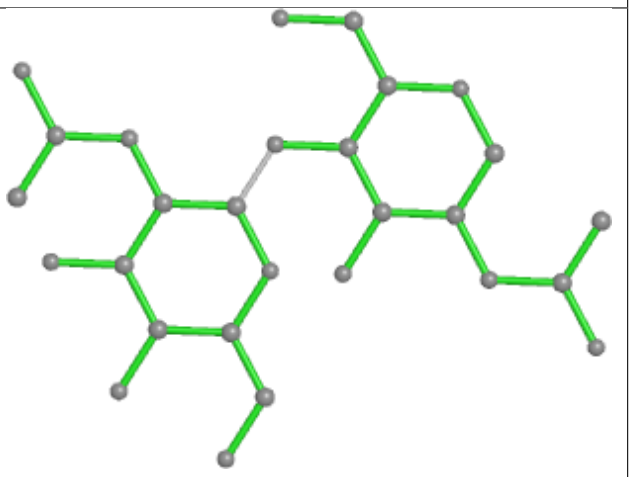


Rings

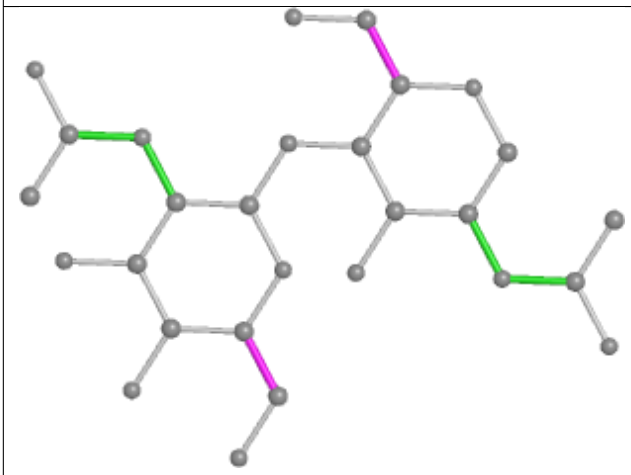
Oligosaccharide Chain u



Bond lengths



Bond angles



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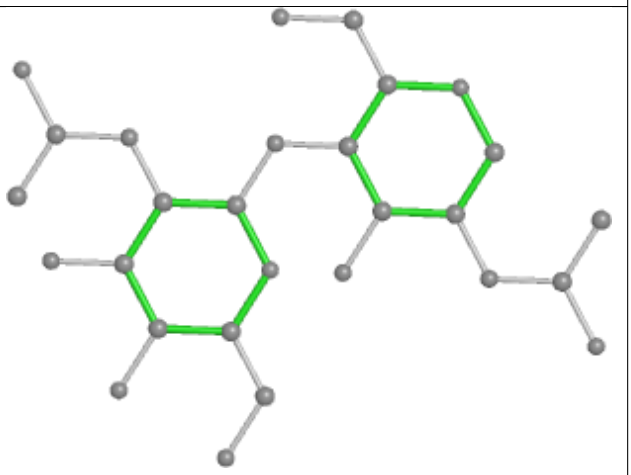
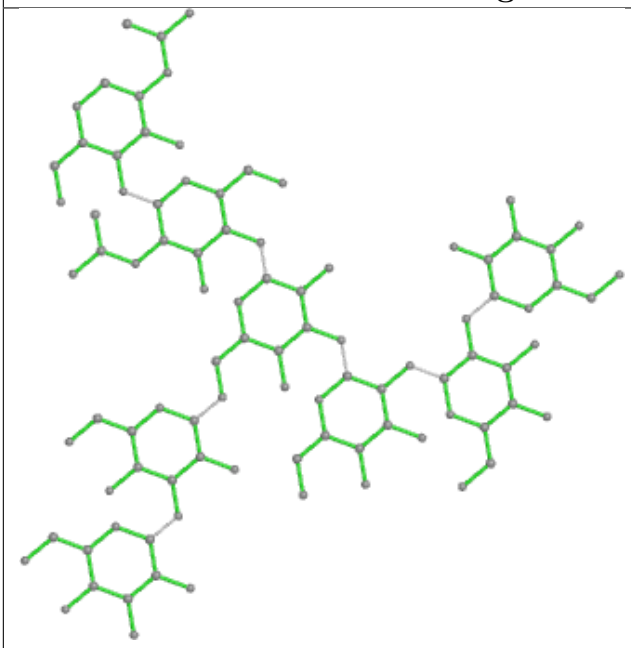
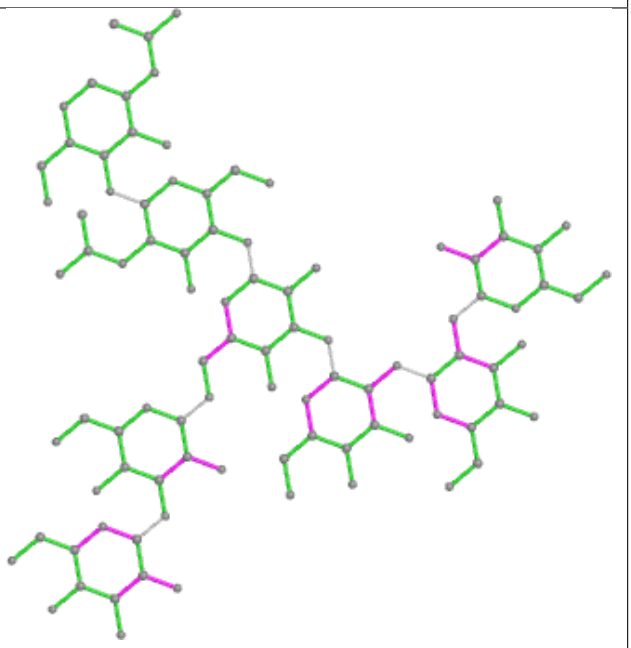
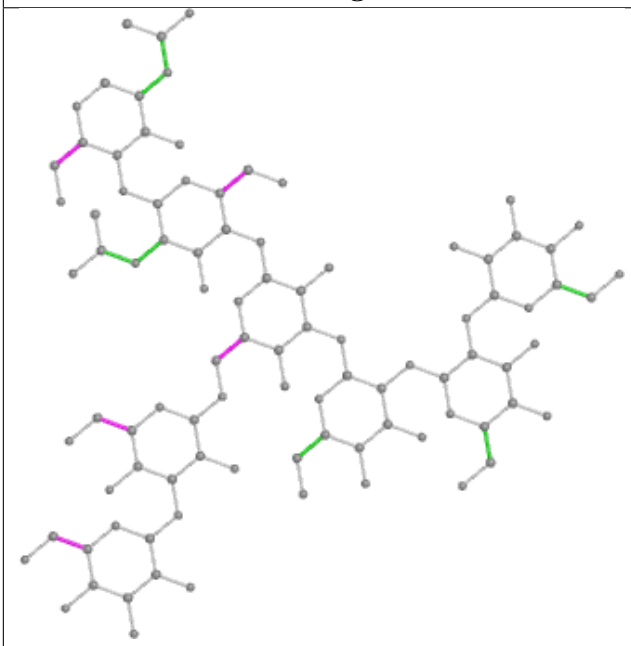
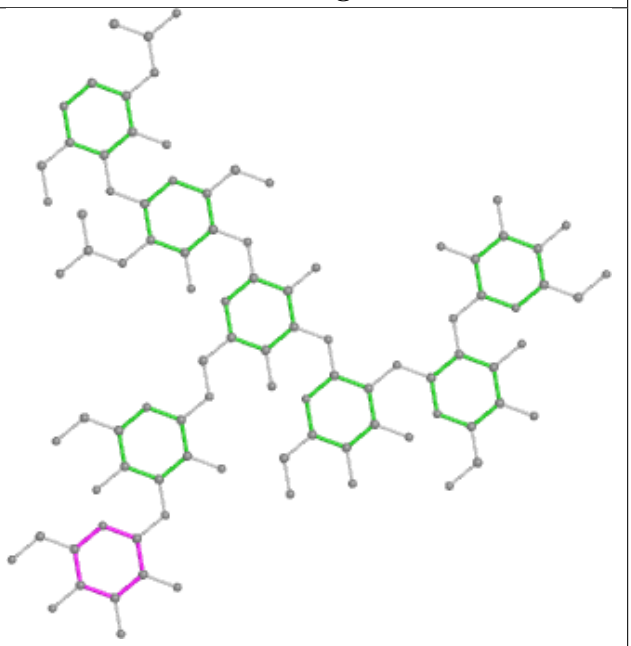
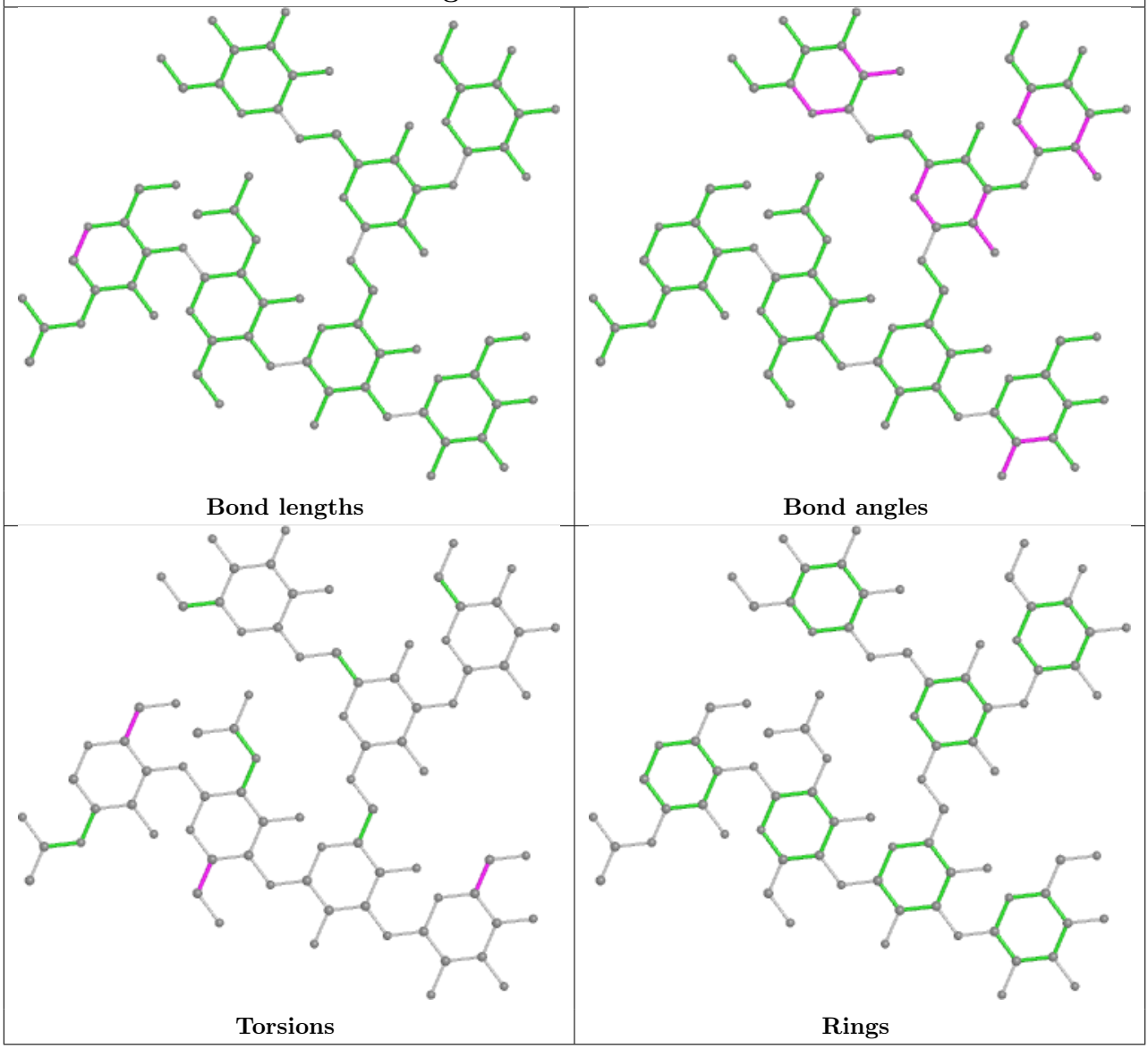


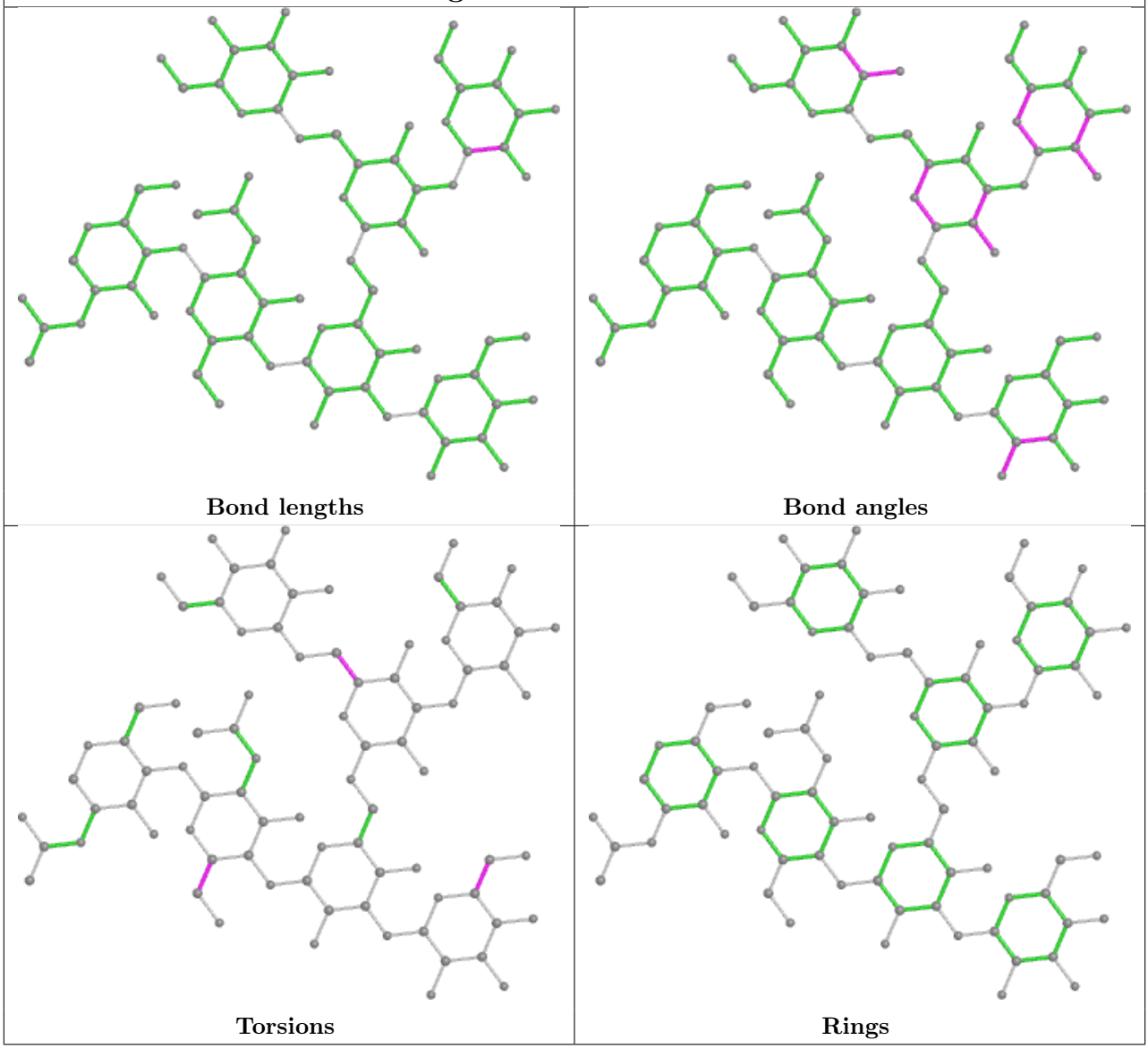
Rings

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

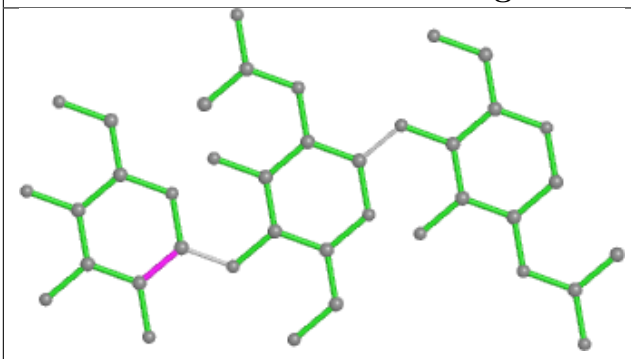
Oligosaccharide Chain O



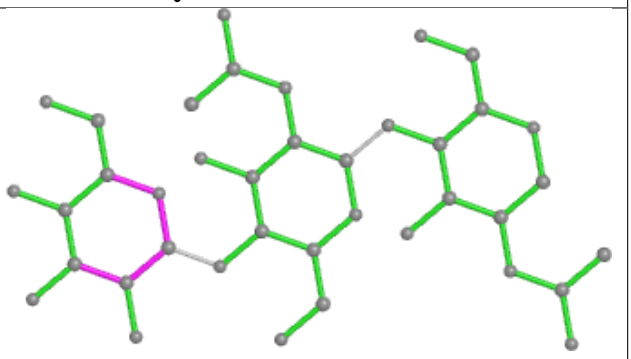
Oligosaccharide Chain e



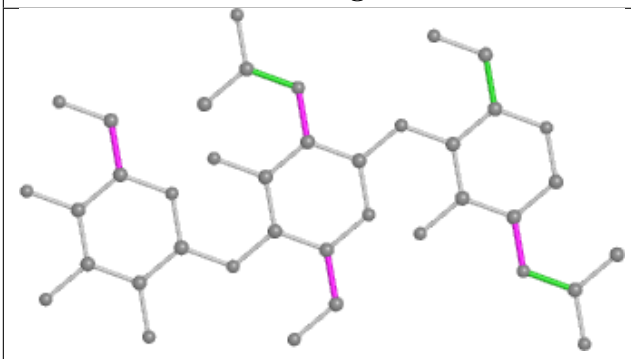
Oligosaccharide Chain Q



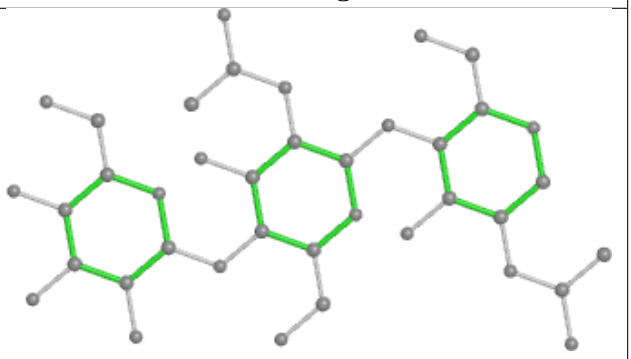
Bond lengths



Bond angles

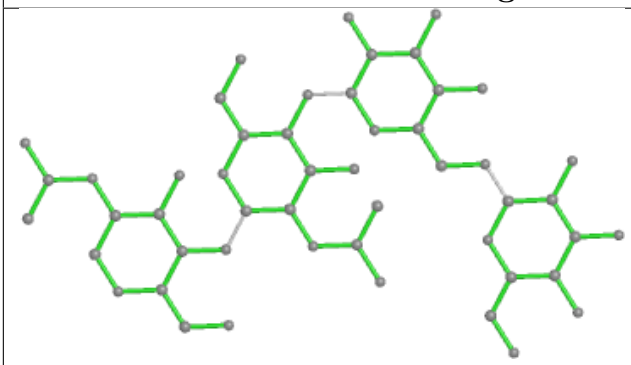


Torsions

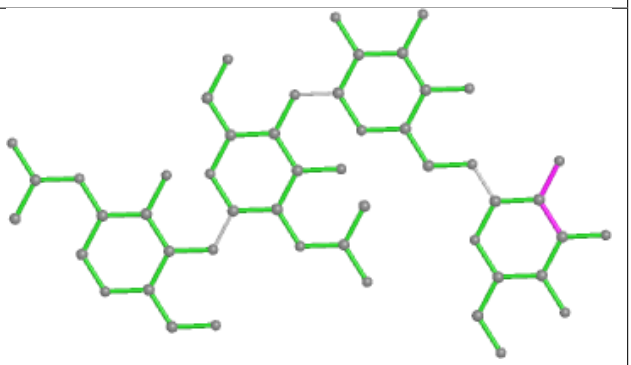


Rings

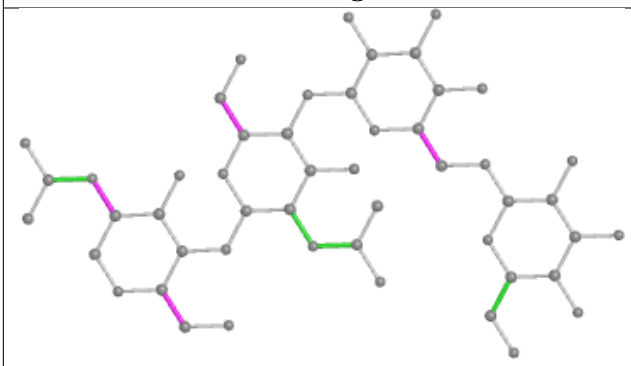
Oligosaccharide Chain d



Bond lengths



Bond angles



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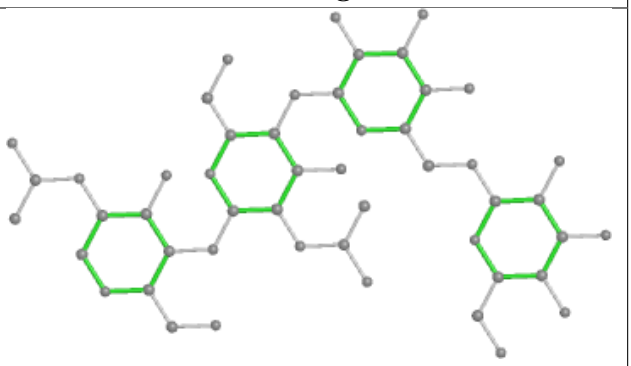
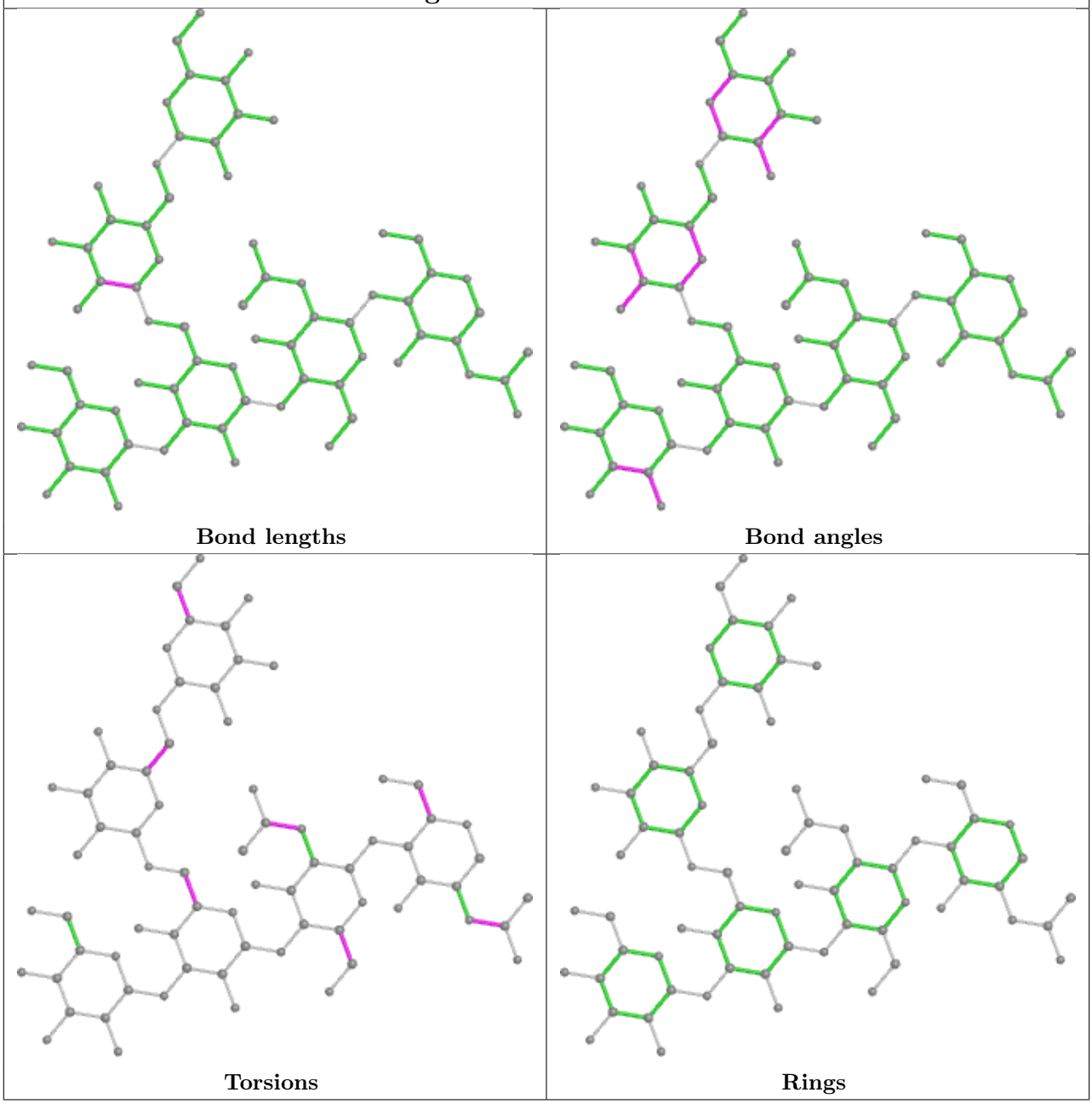
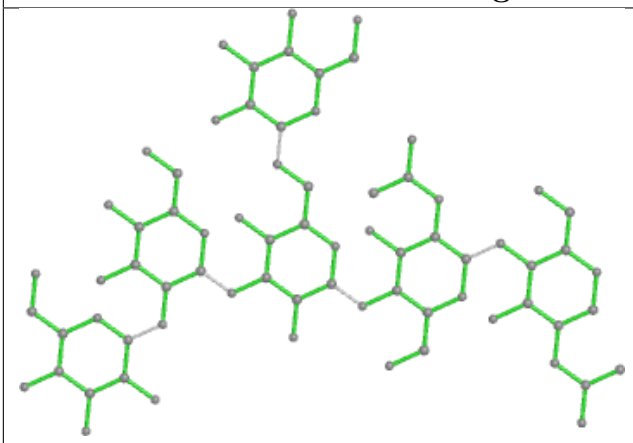


Rings

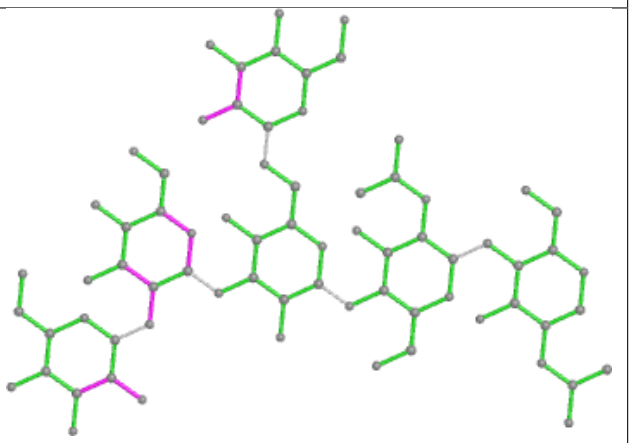
Oligosaccharide Chain k



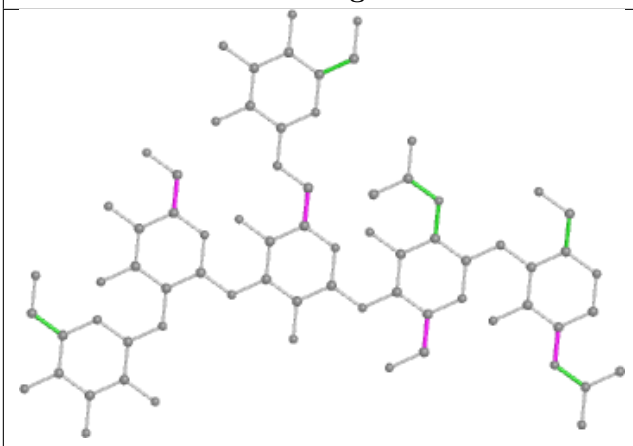
Oligosaccharide Chain m



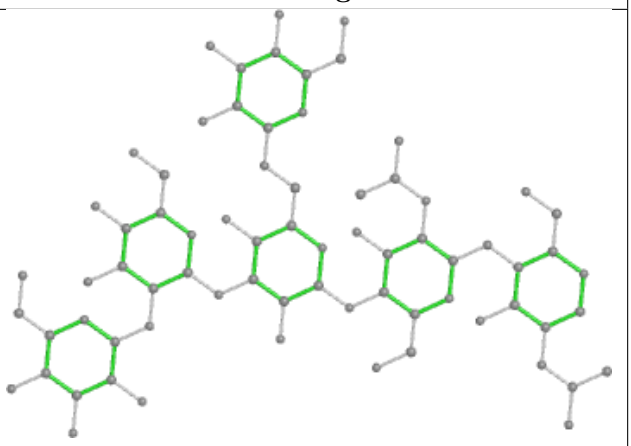
Bond lengths



Bond angles

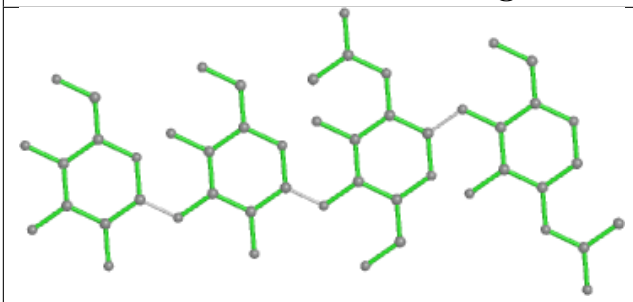


Torsions

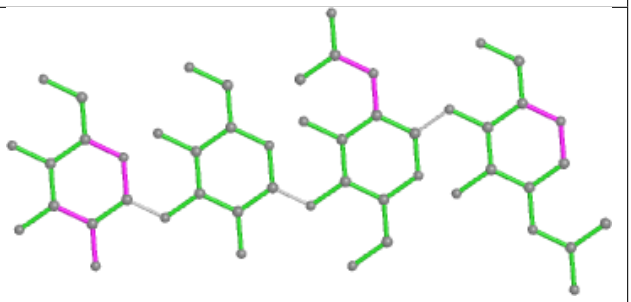


Rings

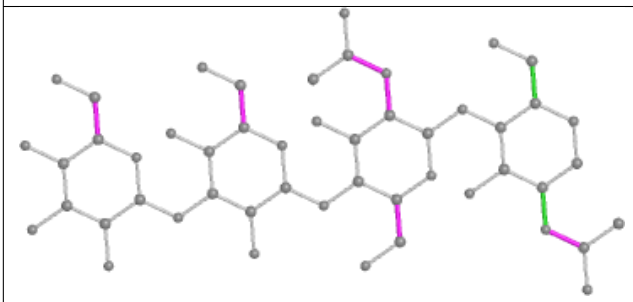
Oligosaccharide Chain n



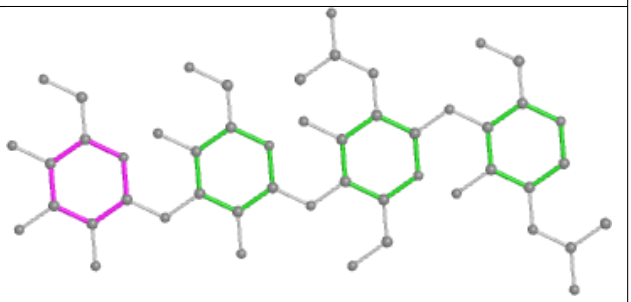
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

45 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	NAG	N	702	6	14,14,15	0.20	0	17,19,21	0.48	0
15	NAG	F	606	1	14,14,15	0.33	0	17,19,21	0.54	0
15	NAG	G	601	1	14,14,15	0.40	0	17,19,21	0.51	0
15	NAG	N	701	6	14,14,15	0.50	0	17,19,21	0.34	0
15	NAG	B	704	6	14,14,15	0.22	0	17,19,21	0.42	0
15	NAG	U	301	3	14,14,15	0.43	0	17,19,21	0.44	0
15	NAG	B	702	6	14,14,15	0.61	0	17,19,21	0.77	1 (5%)
15	NAG	G	603	1	14,14,15	0.21	0	17,19,21	0.53	0
15	NAG	D	301	3	14,14,15	0.29	0	17,19,21	1.31	2 (11%)
15	NAG	A	605	1	14,14,15	0.33	0	17,19,21	0.58	0
15	NAG	F	609	1	14,14,15	0.31	0	17,19,21	0.53	0
15	NAG	A	608	1	14,14,15	0.42	0	17,19,21	0.49	0
15	NAG	B	701	6	14,14,15	0.20	0	17,19,21	0.37	0
15	NAG	G	608	1	14,14,15	0.23	0	17,19,21	0.46	0
15	NAG	A	604	1	14,14,15	1.06	1 (7%)	17,19,21	1.13	1 (5%)
15	NAG	A	607	1	14,14,15	1.31	1 (7%)	17,19,21	1.45	1 (5%)
15	NAG	G	607	1	14,14,15	0.35	0	17,19,21	0.64	0
15	NAG	A	603	1	14,14,15	0.91	1 (7%)	17,19,21	0.90	1 (5%)
15	NAG	F	610	1	14,14,15	0.30	0	17,19,21	0.59	0
15	NAG	F	603	1	14,14,15	0.23	0	17,19,21	0.42	0
15	NAG	K	301	3	14,14,15	0.49	0	17,19,21	1.23	1 (5%)
15	NAG	M	701	6	14,14,15	0.24	0	17,19,21	0.38	0
15	NAG	A	602	1	14,14,15	0.41	0	17,19,21	0.67	0
15	NAG	B	703	6	14,14,15	0.18	0	17,19,21	0.41	0
15	NAG	G	604	1	14,14,15	0.19	0	17,19,21	0.59	0
17	MAN	X	301	-	11,11,12	0.73	0	15,15,17	1.00	1 (6%)
15	NAG	F	608	1	14,14,15	0.26	0	17,19,21	0.50	0
15	NAG	F	607	1	14,14,15	0.22	0	17,19,21	0.48	0
15	NAG	G	605	1	14,14,15	0.36	0	17,19,21	0.45	0
15	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	PO4	A	609	-	4,4,4	0.94	0	6,6,6	0.44	0
15	NAG	G	609	1	14,14,15	0.30	0	17,19,21	0.43	0
17	MAN	S	301	-	11,11,12	0.66	0	15,15,17	1.05	2 (13%)
16	PO4	F	601	-	4,4,4	0.96	0	6,6,6	0.43	0
15	NAG	F	611	1	14,14,15	0.20	0	17,19,21	0.41	0
15	NAG	G	606	1	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
15	NAG	M	703	6	14,14,15	0.25	0	17,19,21	0.47	0
15	NAG	M	702	6	14,14,15	0.45	0	17,19,21	0.67	1 (5%)
15	NAG	F	604	1	14,14,15	0.18	0	17,19,21	0.45	0
15	NAG	N	703	6	14,14,15	0.62	1 (7%)	17,19,21	0.57	0
15	NAG	F	605	1	14,14,15	0.25	0	17,19,21	0.49	0
15	NAG	A	606	1	14,14,15	0.42	0	17,19,21	0.40	0
16	PO4	F	602	-	4,4,4	0.94	0	6,6,6	0.43	0
15	NAG	F	612	1	14,14,15	0.20	0	17,19,21	0.40	0
15	NAG	G	602	1	14,14,15	0.21	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	N	702	6	-	3/6/23/26	0/1/1/1
15	NAG	F	606	1	-	2/6/23/26	0/1/1/1
15	NAG	G	601	1	-	1/6/23/26	0/1/1/1
15	NAG	N	701	6	-	0/6/23/26	0/1/1/1
15	NAG	B	704	6	-	2/6/23/26	0/1/1/1
15	NAG	U	301	3	-	4/6/23/26	0/1/1/1
15	NAG	B	702	6	-	3/6/23/26	0/1/1/1
15	NAG	G	603	1	-	3/6/23/26	0/1/1/1
15	NAG	D	301	3	-	5/6/23/26	0/1/1/1
15	NAG	A	605	1	-	1/6/23/26	0/1/1/1
15	NAG	F	609	1	-	2/6/23/26	0/1/1/1
15	NAG	A	608	1	-	3/6/23/26	0/1/1/1
15	NAG	B	701	6	-	2/6/23/26	0/1/1/1
15	NAG	G	608	1	-	4/6/23/26	0/1/1/1
15	NAG	A	604	1	-	2/6/23/26	0/1/1/1
15	NAG	A	607	1	-	0/6/23/26	0/1/1/1
15	NAG	G	607	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	A	603	1	-	4/6/23/26	0/1/1/1
15	NAG	F	610	1	-	3/6/23/26	0/1/1/1
15	NAG	F	603	1	-	2/6/23/26	0/1/1/1
15	NAG	K	301	3	-	4/6/23/26	0/1/1/1
15	NAG	M	701	6	-	2/6/23/26	0/1/1/1
15	NAG	A	602	1	-	2/6/23/26	0/1/1/1
15	NAG	B	703	6	-	2/6/23/26	0/1/1/1
15	NAG	G	604	1	-	0/6/23/26	0/1/1/1
17	MAN	X	301	-	-	0/2/19/22	0/1/1/1
15	NAG	F	608	1	-	3/6/23/26	0/1/1/1
15	NAG	F	607	1	-	0/6/23/26	0/1/1/1
15	NAG	G	605	1	-	2/6/23/26	0/1/1/1
15	NAG	A	601	1	-	2/6/23/26	0/1/1/1
15	NAG	G	609	1	-	0/6/23/26	0/1/1/1
17	MAN	S	301	-	-	0/2/19/22	0/1/1/1
15	NAG	F	611	1	-	2/6/23/26	0/1/1/1
15	NAG	G	606	1	-	3/6/23/26	0/1/1/1
15	NAG	M	703	6	-	2/6/23/26	0/1/1/1
15	NAG	M	702	6	-	3/6/23/26	0/1/1/1
15	NAG	F	604	1	-	2/6/23/26	0/1/1/1
15	NAG	N	703	6	-	0/6/23/26	0/1/1/1
15	NAG	F	605	1	-	2/6/23/26	0/1/1/1
15	NAG	A	606	1	-	2/6/23/26	0/1/1/1
15	NAG	F	612	1	-	1/6/23/26	0/1/1/1
15	NAG	G	602	1	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	607	NAG	O5-C1	4.54	1.51	1.43
15	A	604	NAG	O5-C1	3.64	1.49	1.43
15	A	603	NAG	O5-C1	3.04	1.48	1.43
15	N	703	NAG	O5-C1	2.11	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	607	NAG	C1-O5-C5	5.55	119.71	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	301	NAG	C2-N2-C7	4.37	129.13	122.90
15	A	604	NAG	C1-O5-C5	4.36	118.10	112.19
15	K	301	NAG	C2-N2-C7	4.33	129.07	122.90
15	A	603	NAG	C1-O5-C5	3.36	116.75	112.19
15	B	702	NAG	C1-O5-C5	2.54	115.64	112.19
15	D	301	NAG	C1-C2-N2	2.46	114.70	110.49
17	S	301	MAN	O2-C2-C3	-2.34	105.46	110.14
17	S	301	MAN	C1-O5-C5	2.32	115.34	112.19
17	X	301	MAN	O2-C2-C3	-2.18	105.77	110.14
15	G	606	NAG	C1-O5-C5	2.08	115.01	112.19
15	M	702	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	B	702	NAG	C4-C5-C6-O6
15	A	603	NAG	C4-C5-C6-O6
15	A	603	NAG	O5-C5-C6-O6
15	B	702	NAG	O5-C5-C6-O6
15	B	704	NAG	O5-C5-C6-O6
15	A	606	NAG	C4-C5-C6-O6
15	G	606	NAG	C4-C5-C6-O6
15	A	608	NAG	O5-C5-C6-O6
15	U	301	NAG	O5-C5-C6-O6
15	A	602	NAG	C4-C5-C6-O6
15	D	301	NAG	C4-C5-C6-O6
15	F	608	NAG	O5-C5-C6-O6
15	G	603	NAG	O5-C5-C6-O6
15	F	611	NAG	O5-C5-C6-O6
15	F	610	NAG	C4-C5-C6-O6
15	G	602	NAG	C4-C5-C6-O6
15	B	704	NAG	C4-C5-C6-O6
15	D	301	NAG	O5-C5-C6-O6
15	F	610	NAG	O5-C5-C6-O6
15	G	608	NAG	O5-C5-C6-O6
15	B	701	NAG	O5-C5-C6-O6
15	G	603	NAG	C4-C5-C6-O6
15	G	605	NAG	C4-C5-C6-O6
15	A	602	NAG	O5-C5-C6-O6
15	A	606	NAG	O5-C5-C6-O6
15	G	606	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
15	A	608	NAG	C4-C5-C6-O6
15	A	601	NAG	C1-C2-N2-C7
15	M	702	NAG	O5-C5-C6-O6
15	F	608	NAG	C4-C5-C6-O6
15	M	703	NAG	O5-C5-C6-O6
15	G	608	NAG	C4-C5-C6-O6
15	D	301	NAG	C8-C7-N2-C2
15	D	301	NAG	O7-C7-N2-C2
15	G	602	NAG	C8-C7-N2-C2
15	G	602	NAG	O7-C7-N2-C2
15	K	301	NAG	C8-C7-N2-C2
15	K	301	NAG	O7-C7-N2-C2
15	U	301	NAG	C8-C7-N2-C2
15	U	301	NAG	O7-C7-N2-C2
15	B	701	NAG	C4-C5-C6-O6
15	M	701	NAG	O5-C5-C6-O6
15	F	604	NAG	O5-C5-C6-O6
15	M	703	NAG	C4-C5-C6-O6
15	F	604	NAG	C4-C5-C6-O6
15	G	602	NAG	O5-C5-C6-O6
15	U	301	NAG	C4-C5-C6-O6
15	B	703	NAG	O5-C5-C6-O6
15	G	605	NAG	O5-C5-C6-O6
15	F	611	NAG	C4-C5-C6-O6
15	F	605	NAG	O5-C5-C6-O6
15	A	604	NAG	O5-C5-C6-O6
15	A	603	NAG	C1-C2-N2-C7
15	G	607	NAG	O5-C5-C6-O6
15	F	606	NAG	O5-C5-C6-O6
15	K	301	NAG	O5-C5-C6-O6
15	F	612	NAG	O5-C5-C6-O6
15	N	702	NAG	O5-C5-C6-O6
15	F	609	NAG	O5-C5-C6-O6
15	F	603	NAG	C4-C5-C6-O6
15	G	601	NAG	O5-C5-C6-O6
15	F	603	NAG	O5-C5-C6-O6
15	M	701	NAG	C4-C5-C6-O6
15	A	601	NAG	C3-C2-N2-C7
15	A	604	NAG	C3-C2-N2-C7
15	F	606	NAG	C3-C2-N2-C7
15	F	608	NAG	C3-C2-N2-C7
15	F	609	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
15	F	610	NAG	C3-C2-N2-C7
15	G	603	NAG	C3-C2-N2-C7
15	G	606	NAG	C3-C2-N2-C7
15	G	607	NAG	C3-C2-N2-C7
15	M	702	NAG	C3-C2-N2-C7
15	B	702	NAG	C3-C2-N2-C7
15	N	702	NAG	C3-C2-N2-C7
15	B	703	NAG	C4-C5-C6-O6
15	M	702	NAG	C4-C5-C6-O6
15	A	608	NAG	C1-C2-N2-C7
15	N	702	NAG	C1-C2-N2-C7
15	A	603	NAG	C3-C2-N2-C7
15	A	605	NAG	C3-C2-N2-C7
15	D	301	NAG	C3-C2-N2-C7
15	F	605	NAG	C3-C2-N2-C7
15	G	608	NAG	C3-C2-N2-C7
15	K	301	NAG	C3-C2-N2-C7
15	G	608	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

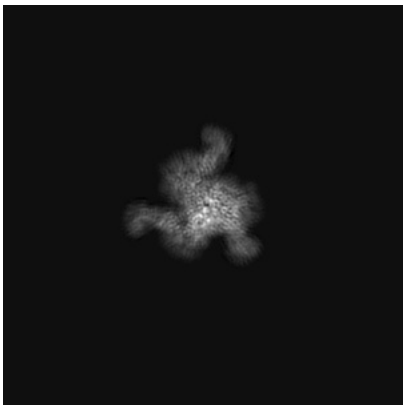
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24128. These allow visual inspection of the internal detail of the map and identification of artifacts.

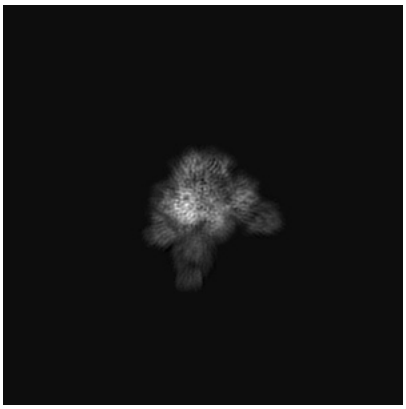
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

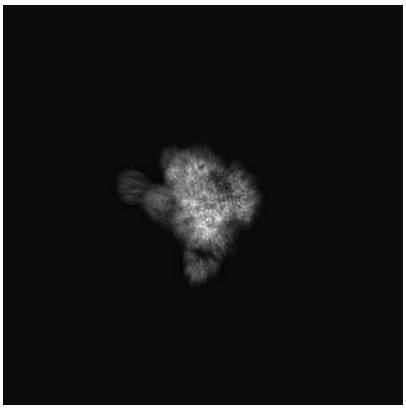
6.1.1 Primary map



X

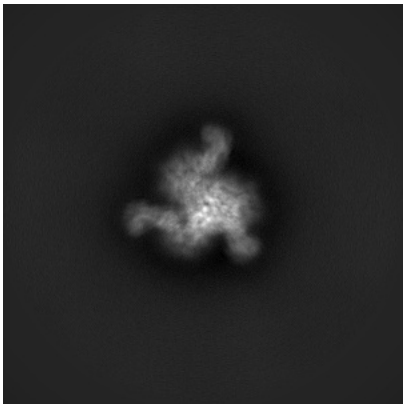


Y

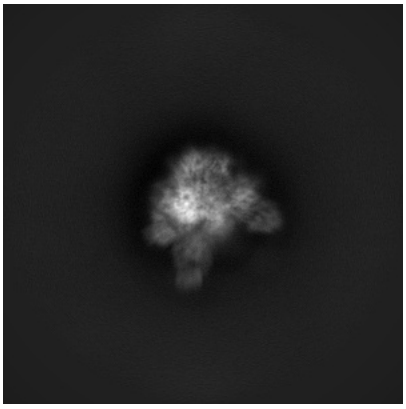


Z

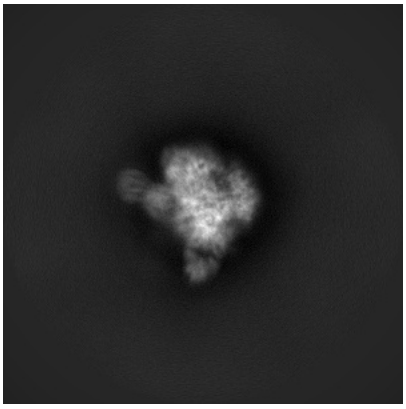
6.1.2 Raw map



X



Y

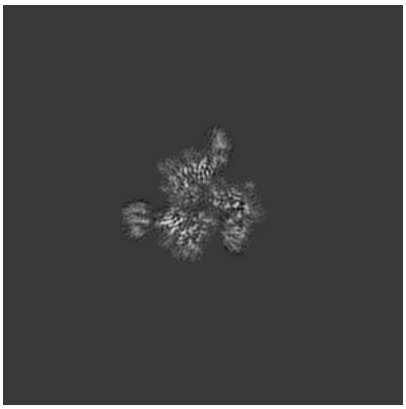


Z

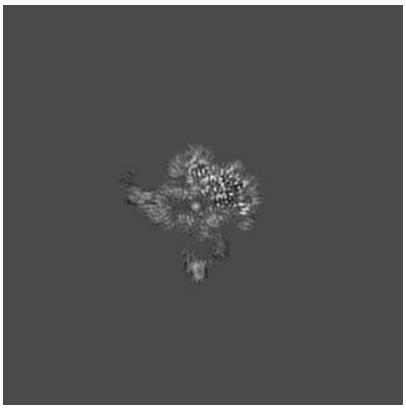
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

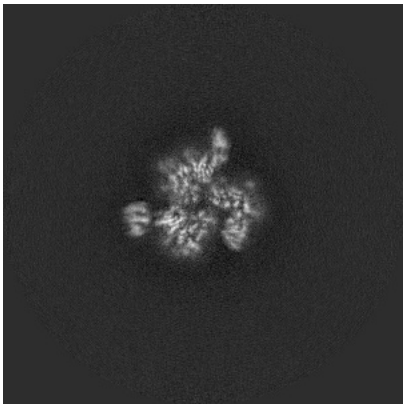
6.2.1 Primary map

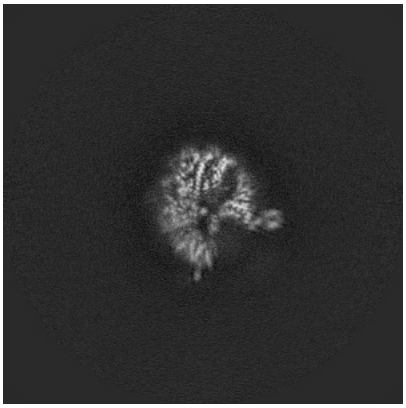

X Index: 240

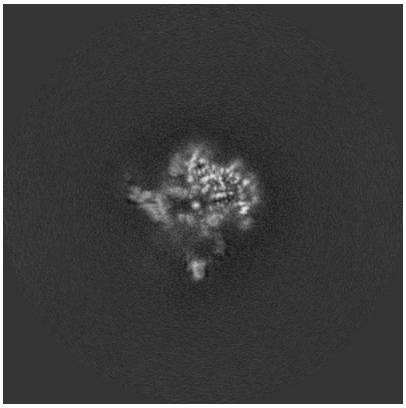
Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

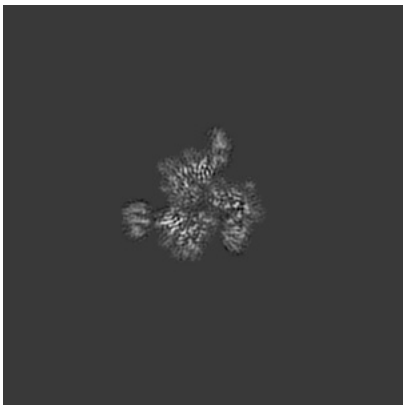

Y Index: 240


Z Index: 240

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

6.3 Largest variance slices (i)

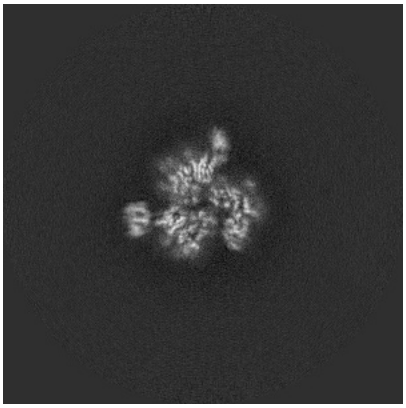
6.3.1 Primary map

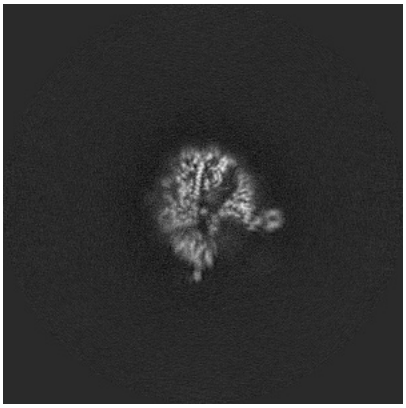

X Index: 240

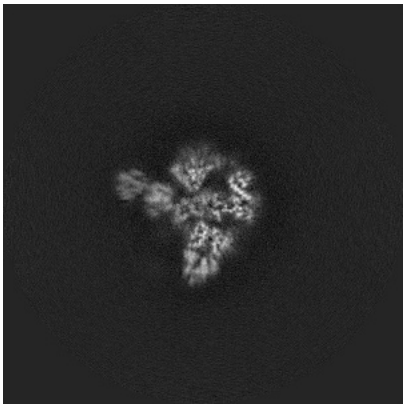
Y Index: 241

Z Index: 222

6.3.2 Raw map


X Index: 239


Y Index: 241


Z Index: 221

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

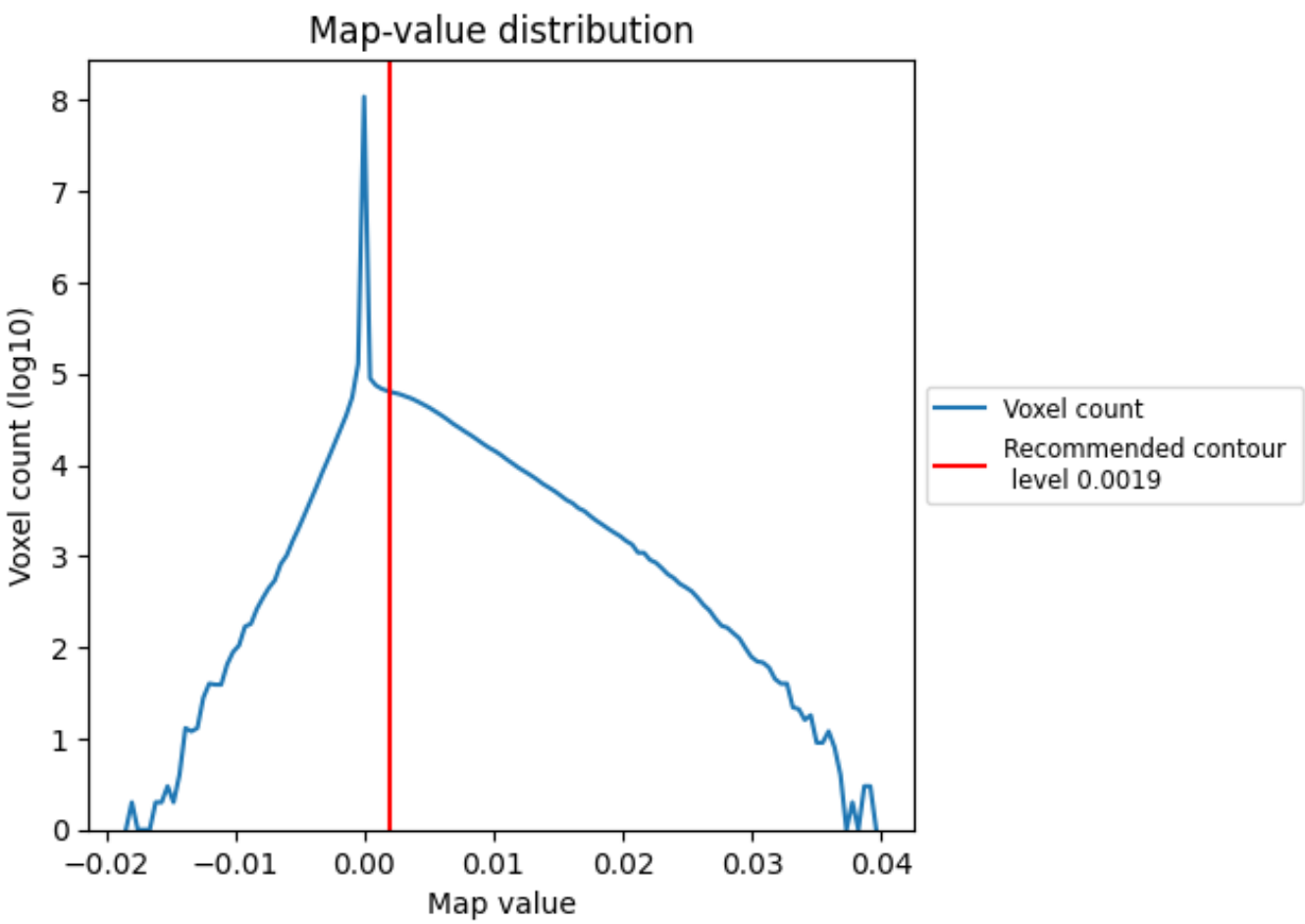
6.5 Mask visualisation (i)

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

7 Map analysis (i)

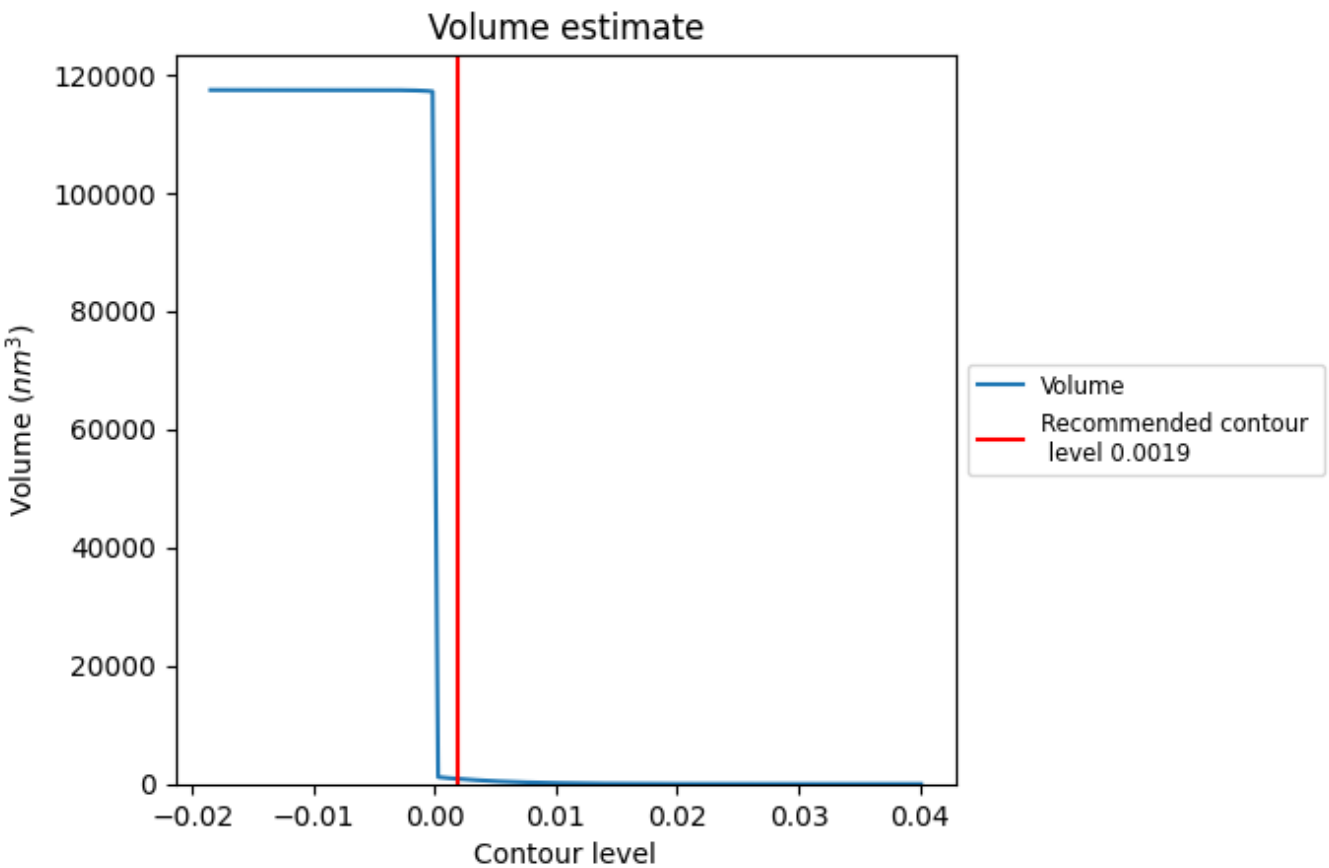
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

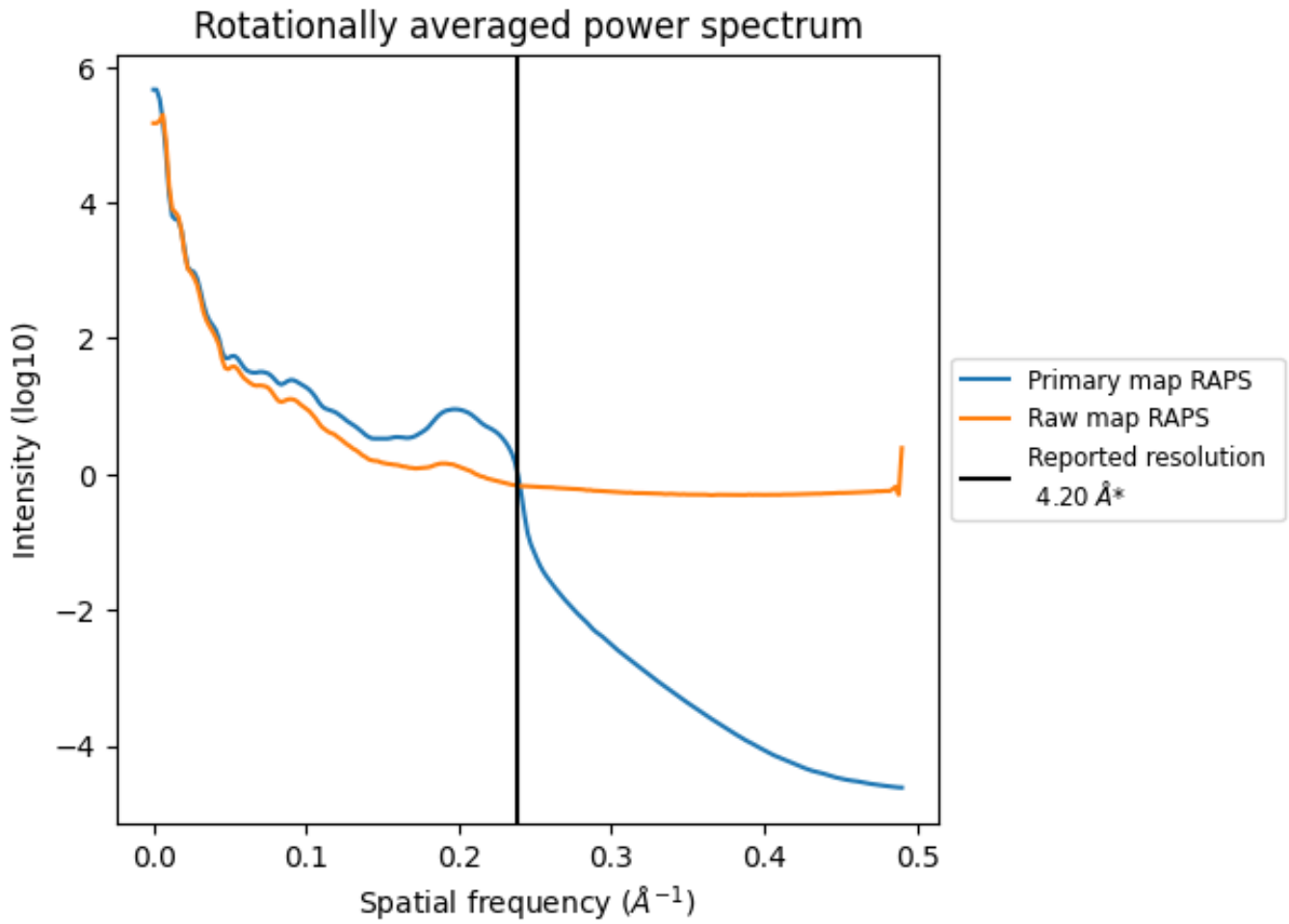
7.2 Volume estimate (i)



The volume at the recommended contour level is 870 nm^3; this corresponds to an approximate mass of 786 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)

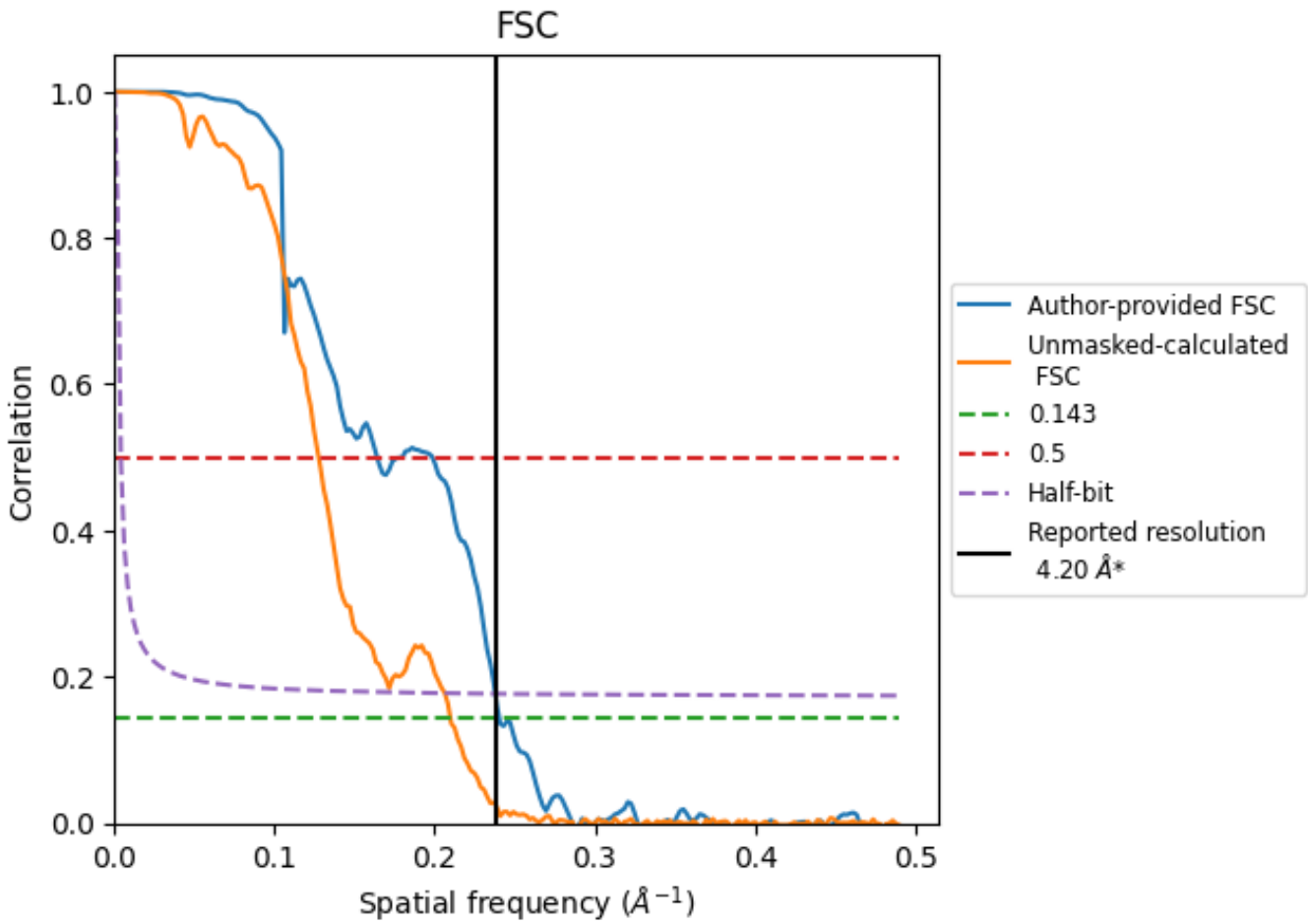


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

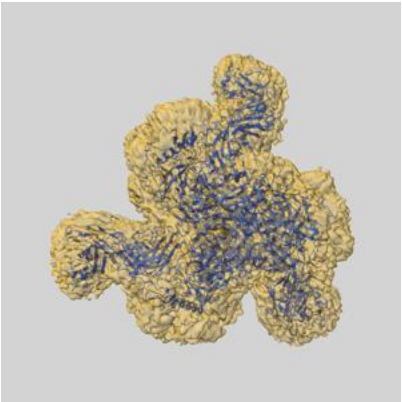
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.16	6.10	4.20
Unmasked-calculated*	4.77	7.84	4.84

*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 4.77 differs from the reported value 4.2 by more than 10 %

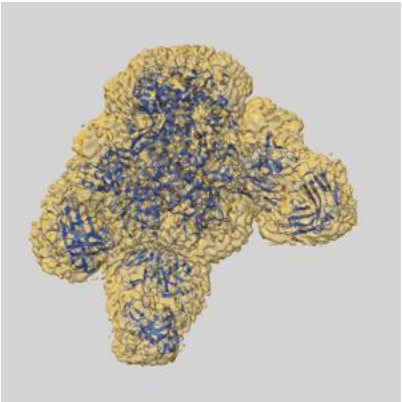
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24128 and PDB model 7N28. Per-residue inclusion information can be found in section 3 on page 17.

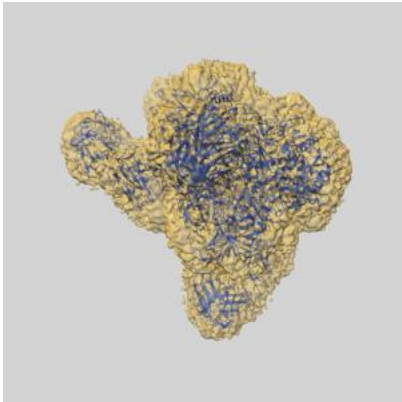
9.1 Map-model overlay (i)



X



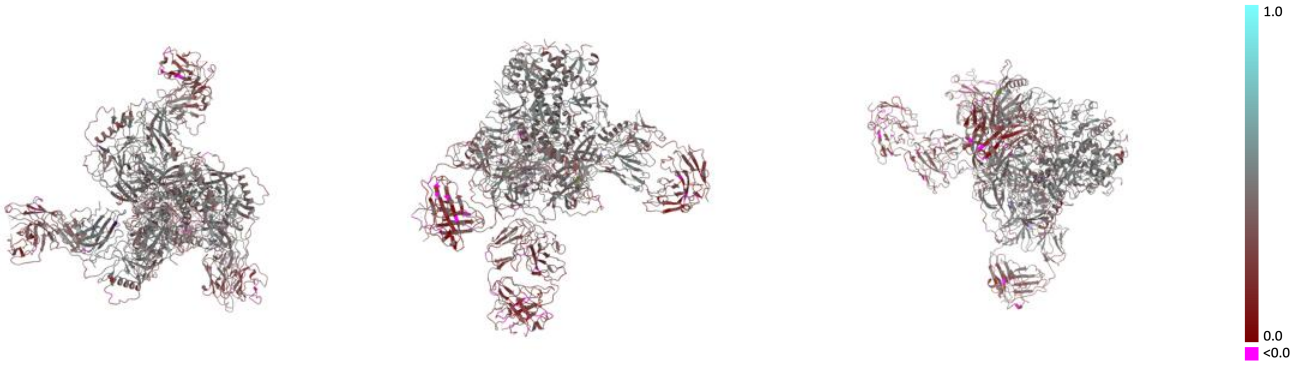
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0019 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

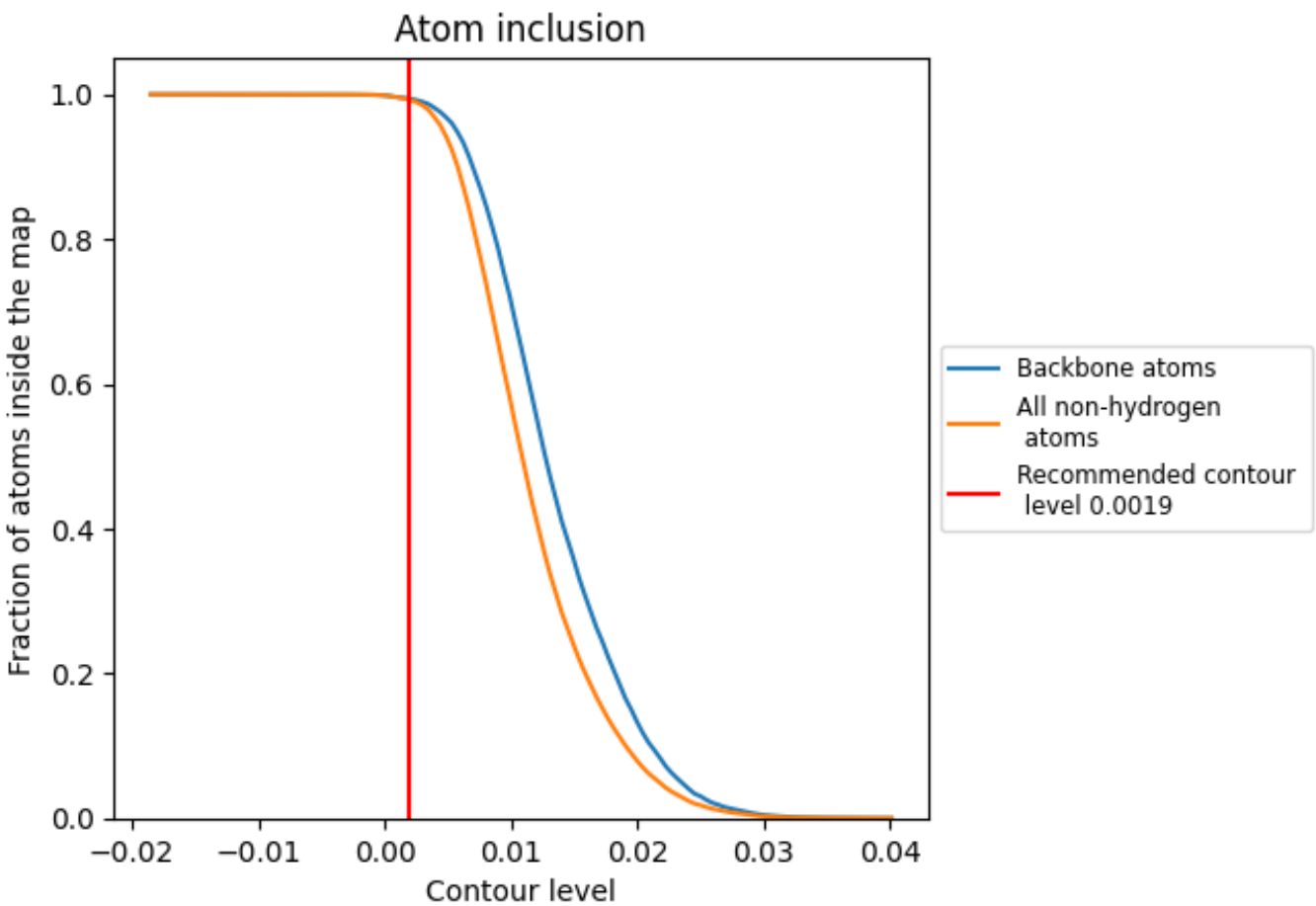
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0019).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9930	0.3850
A	0.9982	0.4230
B	0.9965	0.4290
C	0.9988	0.3850
D	0.9975	0.3230
E	1.0000	0.3330
F	0.9976	0.4240
G	0.9984	0.4260
H	0.8929	0.2980
I	0.9643	0.2840
J	0.9982	0.4060
K	0.9994	0.3420
L	1.0000	0.3810
M	0.9982	0.4290
N	0.9919	0.4280
O	1.0000	0.3840
P	1.0000	0.4020
Q	1.0000	0.4200
R	1.0000	0.4050
S	0.9994	0.3850
T	1.0000	0.3480
U	0.9968	0.3180
V	1.0000	0.4070
W	1.0000	0.3620
X	0.9730	0.2800
Y	0.9380	0.2750
Z	1.0000	0.4110
a	1.0000	0.3360
b	0.9643	0.3170
c	1.0000	0.3020
d	1.0000	0.4760
e	1.0000	0.4130
f	1.0000	0.4520
g	1.0000	0.4650
h	1.0000	0.4380

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Chain	Atom inclusion	Q-score
i	1.0000	0.3850
j	1.0000	0.4540
k	0.9861	0.4020
l	1.0000	0.3210
m	1.0000	0.4240
n	1.0000	0.3890
o	1.0000	0.3240
p	1.0000	0.4040
q	1.0000	0.3660
r	1.0000	0.3780
s	1.0000	0.2650
t	1.0000	0.3000
u	1.0000	0.4350