Full wwPDB EM Validation Report

Oct 12, 2024 – 10:55 PM EDT

PDB ID	:	6PW6
EMDB ID	:	EMD-20500
Title	:	The HIV-1 Envelope Glycoprotein Clone BG505 SOSIP.664 in Complex with Three Copies of the Bovine Broadly Neutralizing Antibody, NC-Cow1, Fragment Antigen Binding Domain
Authors	:	Berndsen, Z.T.; Ward, A.B.
Deposited on	:	2019-07-22
Resolution	:	4.50 Å(reported)
Based on initial model	:	5CEZ

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

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

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

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

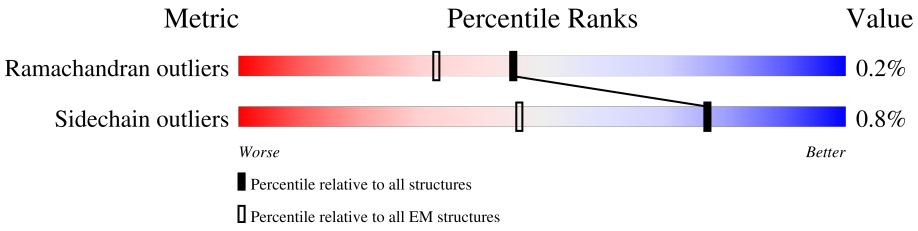
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 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	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	516	81% 15%
1	C	516	81% 15%
1	E	516	81% 15%
2	B	153	5% 78% 5% 18%
2	D	153	5% 78% 5% 18%
2	F	153	5% 78% 5% 18%
3	G	268	17% 82%
3	H	268	16% 82%
3	I	268	16% 82%

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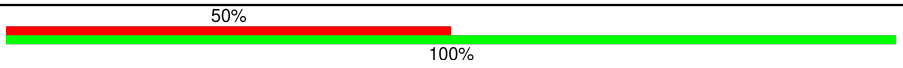
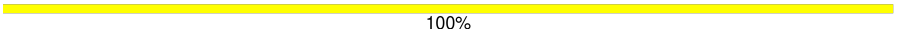
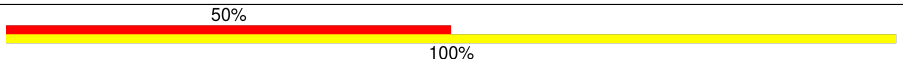
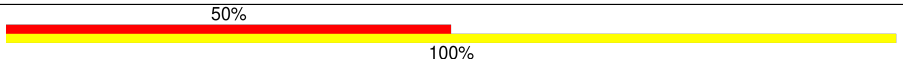
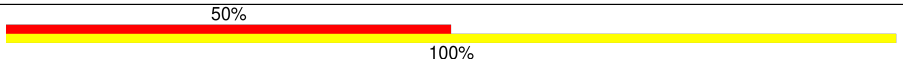
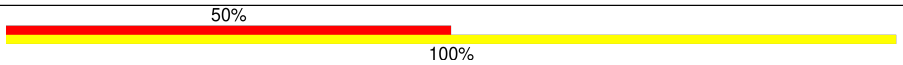
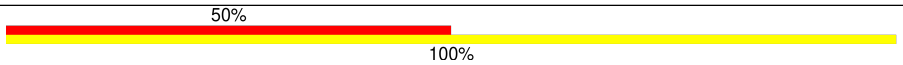
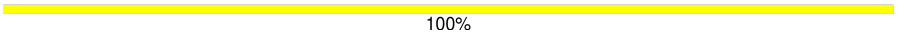
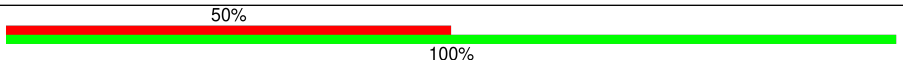
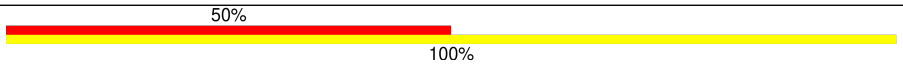
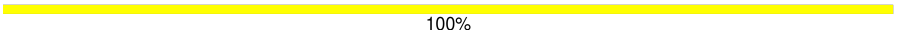
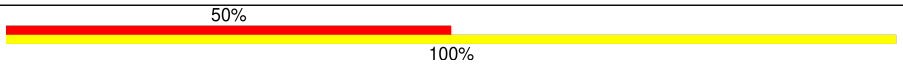
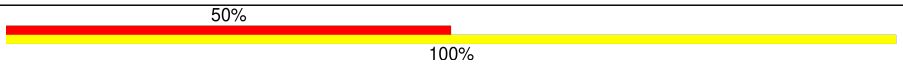
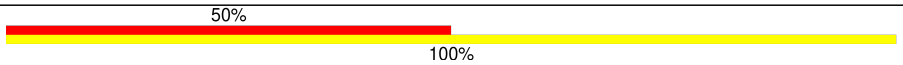
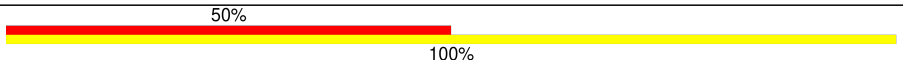
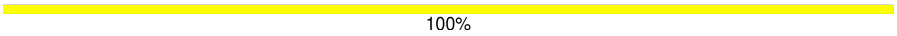
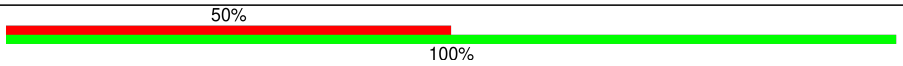
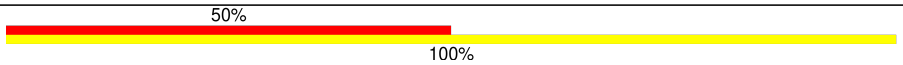
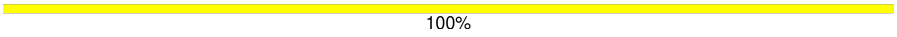
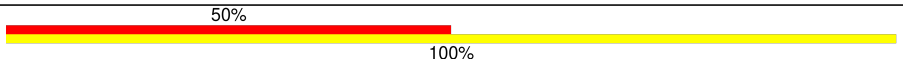
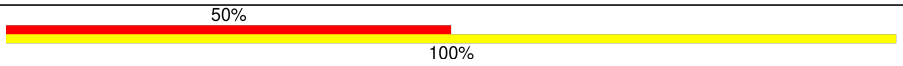
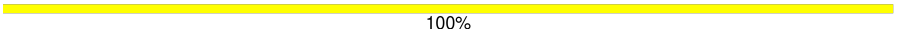
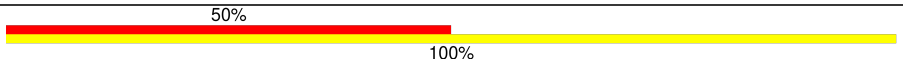
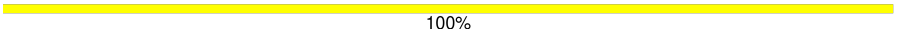
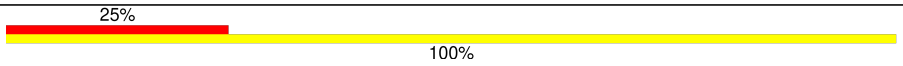
Mol	Chain	Length	Quality of chain
4	J	2	
4	K	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	S	2	
4	T	2	
4	U	2	
4	W	2	
4	X	2	
4	Y	2	
4	Z	2	
4	a	2	
4	c	2	
4	d	2	
4	e	2	
4	g	2	
4	h	2	
4	i	2	
4	j	2	
4	k	2	
4	m	2	
5	L	4	

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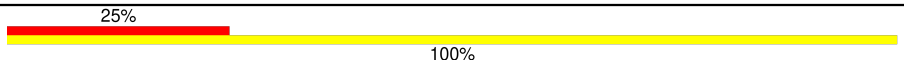
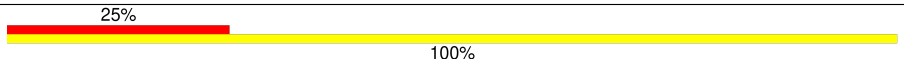
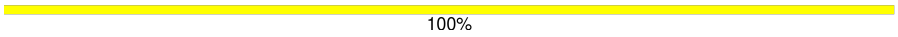
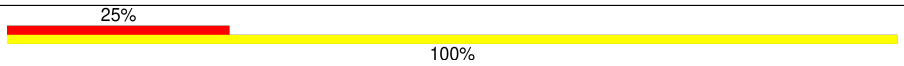
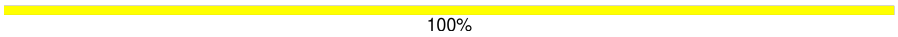
Mol	Chain	Length	Quality of chain
5	R	4	
5	V	4	
5	b	4	
5	f	4	
5	l	4	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15942 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
1	A	439	Total 3454	C 2170	N 609	O 647	S 28	0	0
1	C	439	Total 3454	C 2170	N 609	O 647	S 28	0	0
1	E	439	Total 3454	C 2170	N 609	O 647	S 28	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP Q2N0S6
A	-3	ASP	-	expression tag	UNP Q2N0S6
A	-2	ALA	-	expression tag	UNP Q2N0S6
A	-1	MET	-	expression tag	UNP Q2N0S6
A	0	LYS	-	expression tag	UNP Q2N0S6
A	1	ARG	-	expression tag	UNP Q2N0S6
A	2	GLY	-	expression tag	UNP Q2N0S6
A	3	LEU	-	expression tag	UNP Q2N0S6
A	4	CYS	-	expression tag	UNP Q2N0S6
A	5	CYS	-	expression tag	UNP Q2N0S6
A	6	VAL	-	expression tag	UNP Q2N0S6
A	7	LEU	-	expression tag	UNP Q2N0S6
A	8	LEU	-	expression tag	UNP Q2N0S6
A	9	LEU	-	expression tag	UNP Q2N0S6
A	10	CYS	-	expression tag	UNP Q2N0S6
A	11	GLY	-	expression tag	UNP Q2N0S6
A	12	ALA	-	expression tag	UNP Q2N0S6
A	13	VAL	-	expression tag	UNP Q2N0S6
A	14	PHE	-	expression tag	UNP Q2N0S6
A	15	VAL	-	expression tag	UNP Q2N0S6
A	16	SER	-	expression tag	UNP Q2N0S6
A	17	PRO	-	expression tag	UNP Q2N0S6
A	18	SER	-	expression tag	UNP Q2N0S6
A	19	GLN	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLU	-	expression tag	UNP Q2N0S6
A	21	ILE	-	expression tag	UNP Q2N0S6
A	22	HIS	-	expression tag	UNP Q2N0S6
A	23	ALA	-	expression tag	UNP Q2N0S6
A	24	ARG	-	expression tag	UNP Q2N0S6
A	25	PHE	-	expression tag	UNP Q2N0S6
A	26	ARG	-	expression tag	UNP Q2N0S6
A	27	ARG	-	expression tag	UNP Q2N0S6
A	28	GLY	-	expression tag	UNP Q2N0S6
A	29	ALA	-	expression tag	UNP Q2N0S6
A	30	ARG	-	expression tag	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
C	-4	MET	-	expression tag	UNP Q2N0S6
C	-3	ASP	-	expression tag	UNP Q2N0S6
C	-2	ALA	-	expression tag	UNP Q2N0S6
C	-1	MET	-	expression tag	UNP Q2N0S6
C	0	LYS	-	expression tag	UNP Q2N0S6
C	1	ARG	-	expression tag	UNP Q2N0S6
C	2	GLY	-	expression tag	UNP Q2N0S6
C	3	LEU	-	expression tag	UNP Q2N0S6
C	4	CYS	-	expression tag	UNP Q2N0S6
C	5	CYS	-	expression tag	UNP Q2N0S6
C	6	VAL	-	expression tag	UNP Q2N0S6
C	7	LEU	-	expression tag	UNP Q2N0S6
C	8	LEU	-	expression tag	UNP Q2N0S6
C	9	LEU	-	expression tag	UNP Q2N0S6
C	10	CYS	-	expression tag	UNP Q2N0S6
C	11	GLY	-	expression tag	UNP Q2N0S6
C	12	ALA	-	expression tag	UNP Q2N0S6
C	13	VAL	-	expression tag	UNP Q2N0S6
C	14	PHE	-	expression tag	UNP Q2N0S6
C	15	VAL	-	expression tag	UNP Q2N0S6
C	16	SER	-	expression tag	UNP Q2N0S6
C	17	PRO	-	expression tag	UNP Q2N0S6
C	18	SER	-	expression tag	UNP Q2N0S6
C	19	GLN	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	GLU	-	expression tag	UNP Q2N0S6
C	21	ILE	-	expression tag	UNP Q2N0S6
C	22	HIS	-	expression tag	UNP Q2N0S6
C	23	ALA	-	expression tag	UNP Q2N0S6
C	24	ARG	-	expression tag	UNP Q2N0S6
C	25	PHE	-	expression tag	UNP Q2N0S6
C	26	ARG	-	expression tag	UNP Q2N0S6
C	27	ARG	-	expression tag	UNP Q2N0S6
C	28	GLY	-	expression tag	UNP Q2N0S6
C	29	ALA	-	expression tag	UNP Q2N0S6
C	30	ARG	-	expression tag	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	509	ARG	-	expression tag	UNP Q2N0S6
C	510	ARG	-	expression tag	UNP Q2N0S6
C	511	ARG	-	expression tag	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6
E	-4	MET	-	expression tag	UNP Q2N0S6
E	-3	ASP	-	expression tag	UNP Q2N0S6
E	-2	ALA	-	expression tag	UNP Q2N0S6
E	-1	MET	-	expression tag	UNP Q2N0S6
E	0	LYS	-	expression tag	UNP Q2N0S6
E	1	ARG	-	expression tag	UNP Q2N0S6
E	2	GLY	-	expression tag	UNP Q2N0S6
E	3	LEU	-	expression tag	UNP Q2N0S6
E	4	CYS	-	expression tag	UNP Q2N0S6
E	5	CYS	-	expression tag	UNP Q2N0S6
E	6	VAL	-	expression tag	UNP Q2N0S6
E	7	LEU	-	expression tag	UNP Q2N0S6
E	8	LEU	-	expression tag	UNP Q2N0S6
E	9	LEU	-	expression tag	UNP Q2N0S6
E	10	CYS	-	expression tag	UNP Q2N0S6
E	11	GLY	-	expression tag	UNP Q2N0S6
E	12	ALA	-	expression tag	UNP Q2N0S6
E	13	VAL	-	expression tag	UNP Q2N0S6
E	14	PHE	-	expression tag	UNP Q2N0S6
E	15	VAL	-	expression tag	UNP Q2N0S6
E	16	SER	-	expression tag	UNP Q2N0S6
E	17	PRO	-	expression tag	UNP Q2N0S6
E	18	SER	-	expression tag	UNP Q2N0S6
E	19	GLN	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	20	GLU	-	expression tag	UNP Q2N0S6
E	21	ILE	-	expression tag	UNP Q2N0S6
E	22	HIS	-	expression tag	UNP Q2N0S6
E	23	ALA	-	expression tag	UNP Q2N0S6
E	24	ARG	-	expression tag	UNP Q2N0S6
E	25	PHE	-	expression tag	UNP Q2N0S6
E	26	ARG	-	expression tag	UNP Q2N0S6
E	27	ARG	-	expression tag	UNP Q2N0S6
E	28	GLY	-	expression tag	UNP Q2N0S6
E	29	ALA	-	expression tag	UNP Q2N0S6
E	30	ARG	-	expression tag	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6
E	509	ARG	-	expression tag	UNP Q2N0S6
E	510	ARG	-	expression tag	UNP Q2N0S6
E	511	ARG	-	expression tag	UNP Q2N0S6
E	512	ARG	-	expression tag	UNP Q2N0S6
E	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	126	Total	C	N	O	S	0	0
			970	612	167	185	6		
2	D	126	Total	C	N	O	S	0	0
			970	612	167	185	6		
2	F	126	Total	C	N	O	S	0	0
			970	612	167	185	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	567J	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
D	567J	PRO	ILE	conflict	UNP Q2N0S6
D	605	CYS	THR	conflict	UNP Q2N0S6
F	567J	PRO	ILE	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called Broadly Neutralizing Antibody NC-Cow1 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	49	Total	C	N	O	S	0	0
			398	239	72	80	7		
3	H	49	Total	C	N	O	S	0	0
			398	239	72	80	7		
3	I	49	Total	C	N	O	S	0	0
			398	239	72	80	7		

- Molecule 4 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
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		

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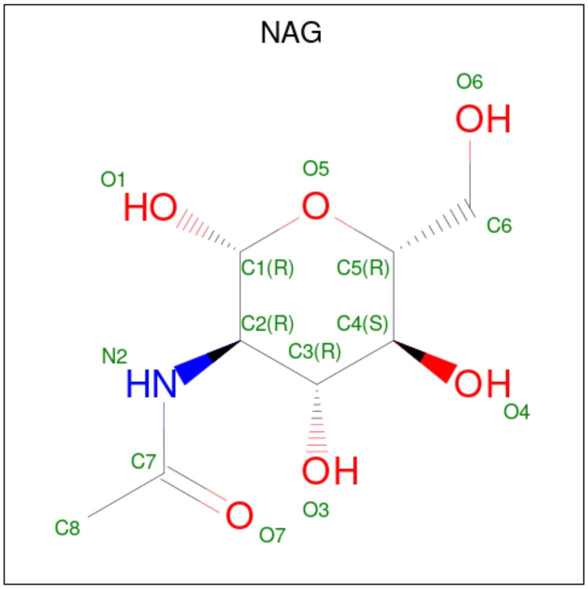
Mol	Chain	Residues	Atoms				AltConf	Trace
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	h	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	2	Total	C	N	O	0	0
			28	16	2	10		
4	k	2	Total	C	N	O	0	0
			28	16	2	10		
4	m	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 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
5	L	4	Total	C	N	O	0	0
			50	28	2	20		
5	R	4	Total	C	N	O	0	0
			50	28	2	20		
5	V	4	Total	C	N	O	0	0
			50	28	2	20		
5	b	4	Total	C	N	O	0	0
			50	28	2	20		
5	f	4	Total	C	N	O	0	0
			50	28	2	20		
5	l	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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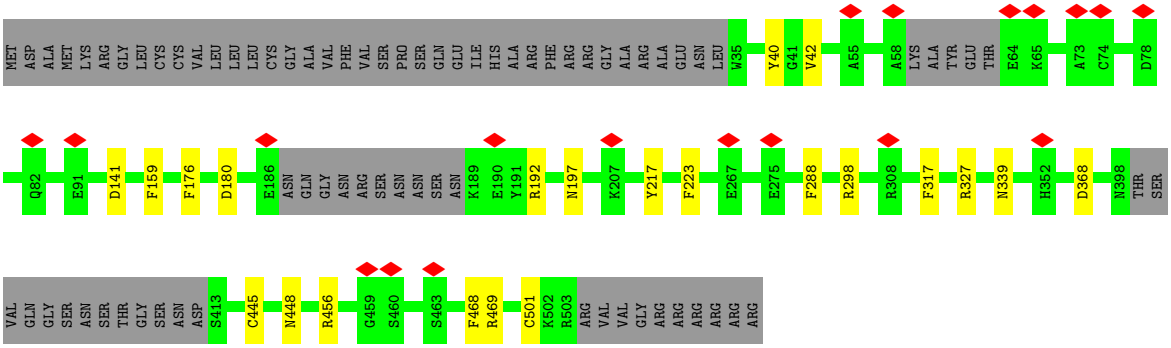
Mol	Chain	Residues	Atoms				AltConf
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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

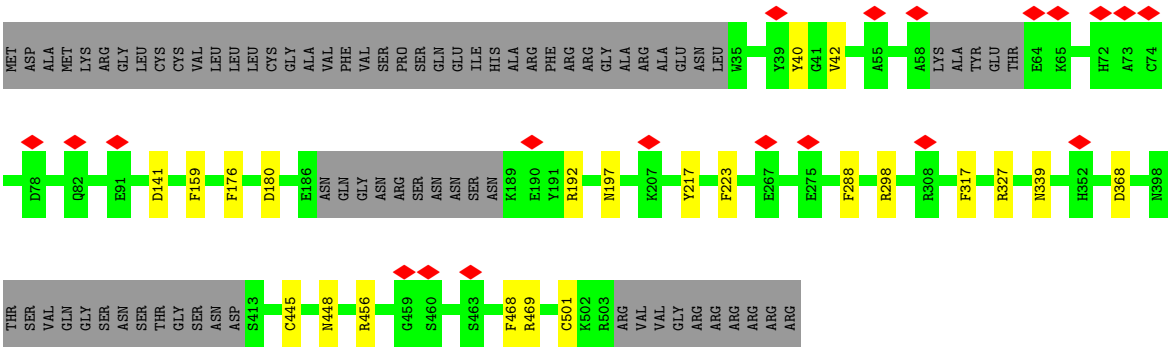
• Molecule 1: Envelope glycoprotein gp120

Chain A:



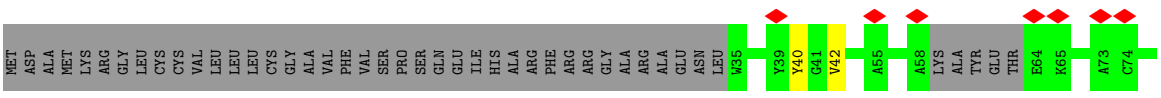
• Molecule 1: Envelope glycoprotein gp120

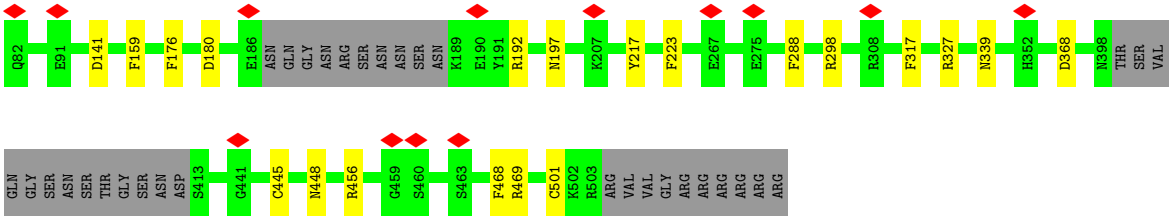
Chain C:



• Molecule 1: Envelope glycoprotein gp120

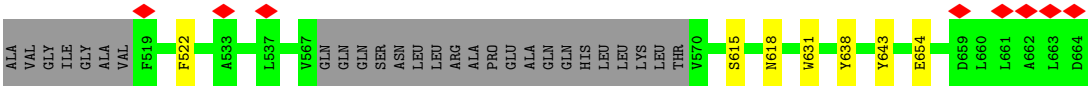
Chain E:





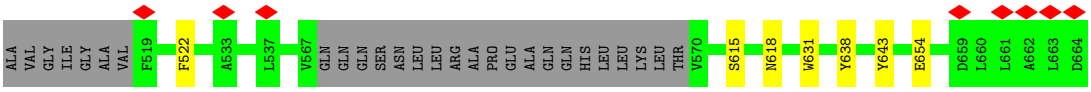
• Molecule 2: Envelope glycoprotein gp41

Chain B:



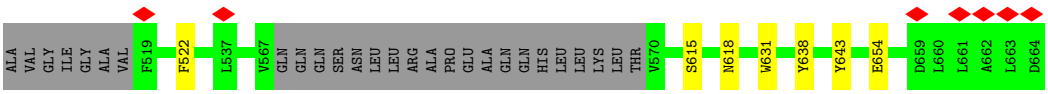
• Molecule 2: Envelope glycoprotein gp41

Chain D:



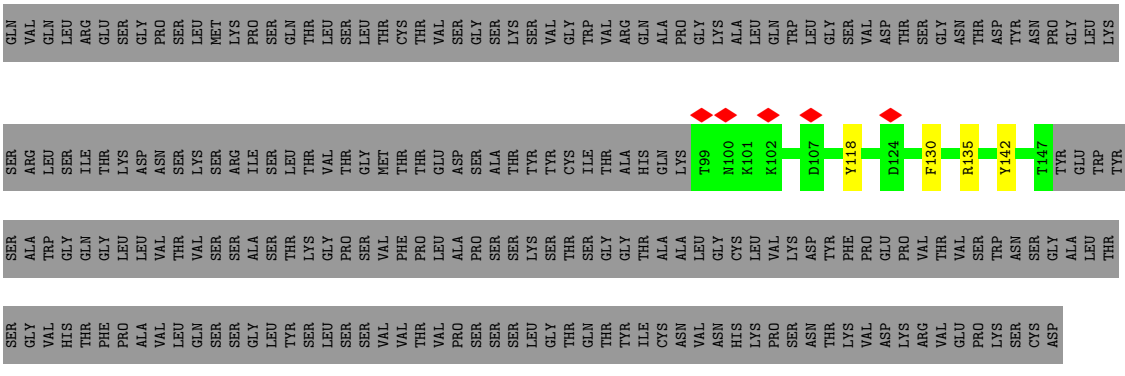
• Molecule 2: Envelope glycoprotein gp41

Chain F:



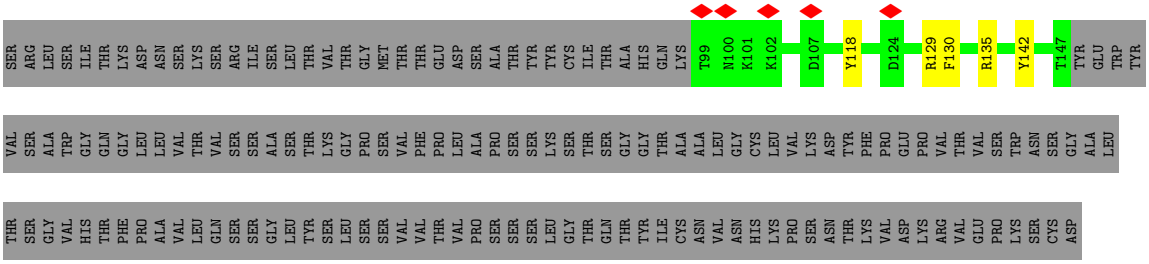
• Molecule 3: Broadly Neutralizing Antibody NC-Cow1 Heavy Chain

Chain G:



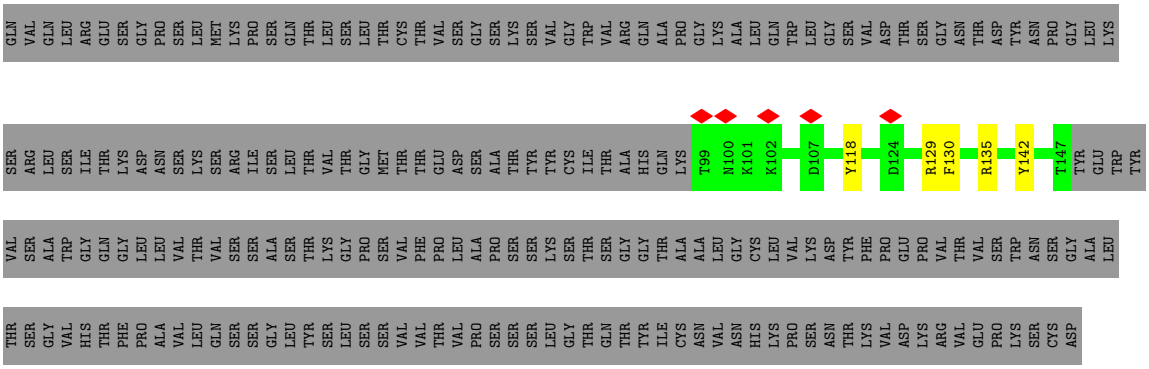
• Molecule 3: Broadly Neutralizing Antibody NC-Cow1 Heavy Chain

Chain H:



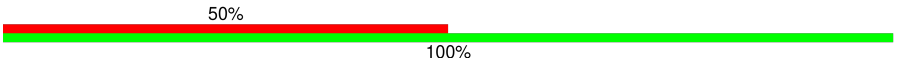
• Molecule 3: Broadly Neutralizing Antibody NC-Cow1 Heavy Chain

Chain I:



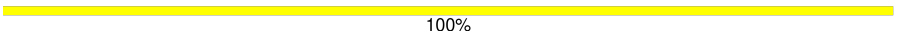
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain K:



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

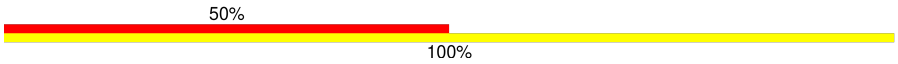
Chain M:

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

Chain N:

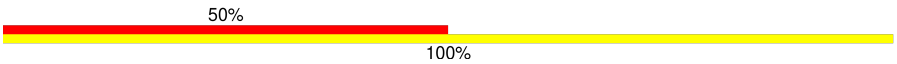
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



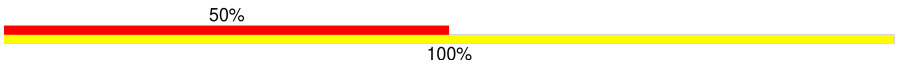
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



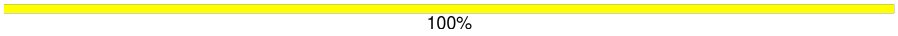
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



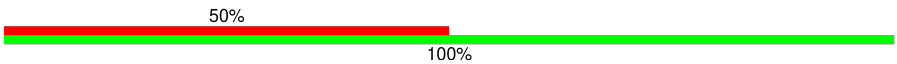
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



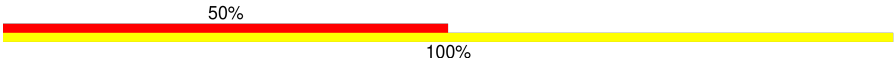
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



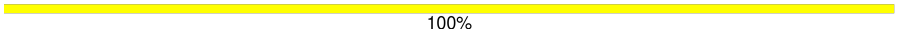
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



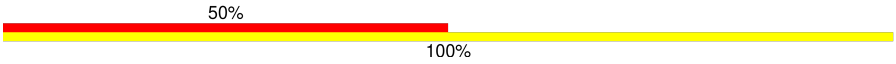
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



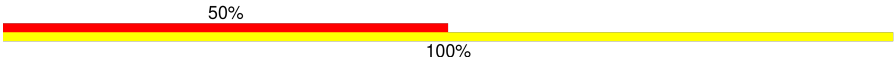
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



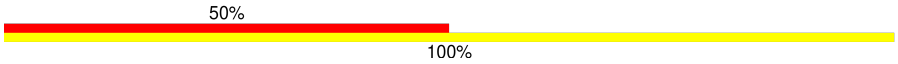
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



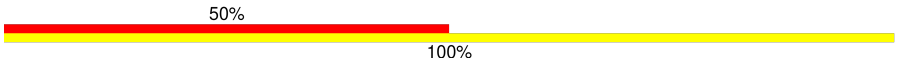
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



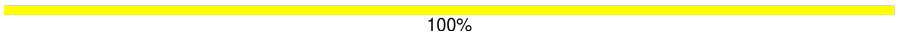
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



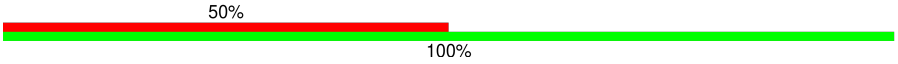
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



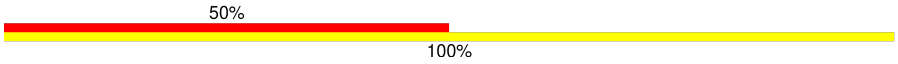
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



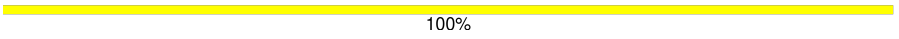
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



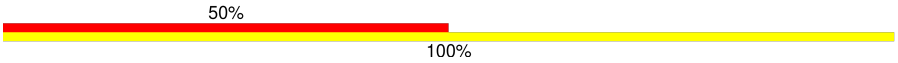
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



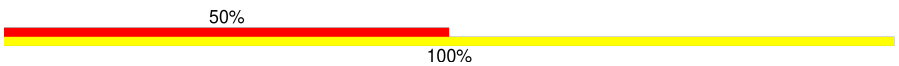
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



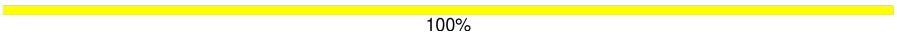
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



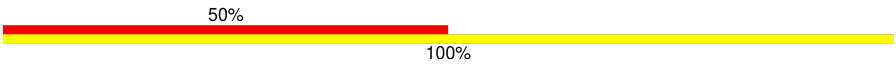
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



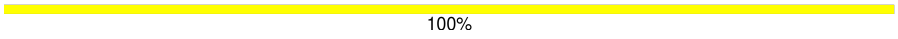
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



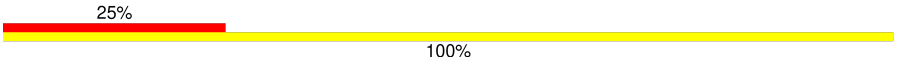
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



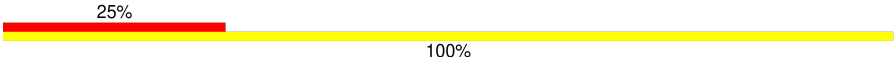
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



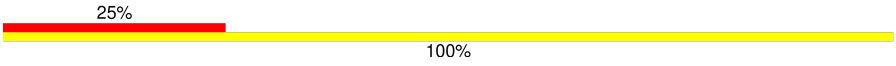
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 5: 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 V:

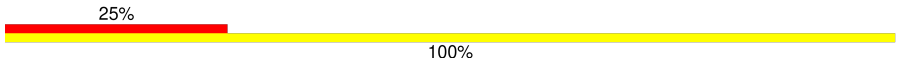


• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

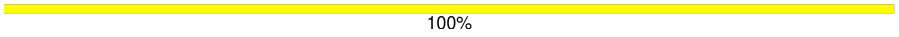
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



• Molecule 5: 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:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	21427	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.167	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	322.0, 322.0, 322.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, 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	1.13	10/3526 (0.3%)	0.94	11/4786 (0.2%)
1	C	1.13	10/3526 (0.3%)	0.94	11/4786 (0.2%)
1	E	1.13	10/3526 (0.3%)	0.94	11/4786 (0.2%)
2	B	1.14	3/988 (0.3%)	0.87	2/1341 (0.1%)
2	D	1.14	3/988 (0.3%)	0.87	2/1341 (0.1%)
2	F	1.14	3/988 (0.3%)	0.87	2/1341 (0.1%)
3	G	1.28	3/409 (0.7%)	1.03	1/551 (0.2%)
3	H	1.28	3/409 (0.7%)	1.03	2/551 (0.4%)
3	I	1.28	3/409 (0.7%)	1.02	2/551 (0.4%)
All	All	1.15	48/14769 (0.3%)	0.94	44/20034 (0.2%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	654	GLU	CD-OE2	-8.29	1.16	1.25
2	D	654	GLU	CD-OE2	-8.28	1.16	1.25
2	B	654	GLU	CD-OE2	-8.25	1.16	1.25
1	A	159	PHE	CB-CG	-7.45	1.38	1.51
1	C	159	PHE	CB-CG	-7.44	1.38	1.51
1	E	159	PHE	CB-CG	-7.44	1.38	1.51
2	F	522	PHE	CB-CG	-7.27	1.39	1.51
2	D	522	PHE	CB-CG	-7.27	1.39	1.51
2	B	522	PHE	CB-CG	-7.25	1.39	1.51
1	A	176	PHE	CB-CG	-6.88	1.39	1.51
1	E	176	PHE	CB-CG	-6.87	1.39	1.51
1	C	176	PHE	CB-CG	-6.85	1.39	1.51
1	C	468	PHE	CB-CG	-6.79	1.39	1.51
1	E	468	PHE	CB-CG	-6.78	1.39	1.51
1	A	468	PHE	CB-CG	-6.78	1.39	1.51
2	F	631	TRP	CB-CG	-6.37	1.38	1.50
2	D	631	TRP	CB-CG	-6.37	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	631	TRP	CB-CG	-6.37	1.38	1.50
3	I	135	ARG	CG-CD	-6.36	1.36	1.51
3	H	135	ARG	CG-CD	-6.36	1.36	1.51
3	G	135	ARG	CG-CD	-6.36	1.36	1.51
1	C	223	PHE	CB-CG	-6.34	1.40	1.51
1	A	223	PHE	CB-CG	-6.30	1.40	1.51
1	E	223	PHE	CB-CG	-6.28	1.40	1.51
1	C	501	CYS	CB-SG	-5.90	1.72	1.81
1	A	501	CYS	CB-SG	-5.89	1.72	1.81
1	E	501	CYS	CB-SG	-5.89	1.72	1.81
1	A	317	PHE	CB-CG	-5.70	1.41	1.51
1	C	317	PHE	CB-CG	-5.68	1.41	1.51
1	E	317	PHE	CB-CG	-5.65	1.41	1.51
3	H	142	TYR	CB-CG	-5.44	1.43	1.51
3	G	142	TYR	CB-CG	-5.42	1.43	1.51
1	E	42	VAL	CB-CG1	-5.42	1.41	1.52
1	C	445	CYS	CB-SG	-5.41	1.73	1.81
1	A	445	CYS	CB-SG	-5.40	1.73	1.81
3	I	142	TYR	CB-CG	-5.40	1.43	1.51
1	E	445	CYS	CB-SG	-5.39	1.73	1.81
1	A	42	VAL	CB-CG1	-5.38	1.41	1.52
1	E	40	TYR	CB-CG	-5.37	1.43	1.51
1	A	40	TYR	CB-CG	-5.36	1.43	1.51
1	C	42	VAL	CB-CG1	-5.35	1.41	1.52
1	C	40	TYR	CB-CG	-5.34	1.43	1.51
1	C	141	ASP	CB-CG	5.12	1.62	1.51
1	A	141	ASP	CB-CG	5.12	1.62	1.51
3	G	130	PHE	CB-CG	-5.11	1.42	1.51
3	H	130	PHE	CB-CG	-5.10	1.42	1.51
1	E	141	ASP	CB-CG	5.08	1.62	1.51
3	I	130	PHE	CB-CG	-5.08	1.42	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	327	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	A	327	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	E	327	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	E	298	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	298	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	C	298	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	C	40	TYR	CB-CG-CD1	-7.89	116.27	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	40	TYR	CB-CG-CD1	-7.81	116.31	121.00
1	E	40	TYR	CB-CG-CD1	-7.76	116.34	121.00
1	C	456	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	A	456	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	E	456	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	E	469	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	C	469	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	469	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	E	217	TYR	CB-CG-CD2	-6.71	116.98	121.00
1	A	217	TYR	CB-CG-CD2	-6.70	116.98	121.00
1	C	217	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	E	368	ASP	CB-CG-OD1	6.57	124.21	118.30
1	C	368	ASP	CB-CG-OD1	6.55	124.20	118.30
1	A	368	ASP	CB-CG-OD1	6.53	124.18	118.30
1	E	192	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	192	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	C	192	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	F	643	TYR	CB-CG-CD2	-6.10	117.34	121.00
2	B	643	TYR	CB-CG-CD2	-6.09	117.35	121.00
2	F	638	TYR	CB-CG-CD1	-6.04	117.38	121.00
2	B	638	TYR	CB-CG-CD1	-6.03	117.38	121.00
2	D	638	TYR	CB-CG-CD1	-6.01	117.40	121.00
2	D	643	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	180	ASP	CB-CG-OD1	5.58	123.32	118.30
1	E	180	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	180	ASP	CB-CG-OD1	5.55	123.29	118.30
1	C	288	PHE	CB-CG-CD2	-5.24	117.13	120.80
3	I	118	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	E	288	PHE	CB-CG-CD2	-5.18	117.18	120.80
1	A	288	PHE	CB-CG-CD2	-5.18	117.18	120.80
3	G	118	TYR	CB-CG-CD2	-5.17	117.90	121.00
3	H	118	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	C	469	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	469	ARG	NE-CZ-NH1	5.02	122.81	120.30
3	H	129	ARG	NE-CZ-NH2	-5.02	117.79	120.30
3	I	129	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	E	469	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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	431/516 (84%)	419 (97%)	12 (3%)	0	100	100
1	C	431/516 (84%)	419 (97%)	12 (3%)	0	100	100
1	E	431/516 (84%)	419 (97%)	12 (3%)	0	100	100
2	B	122/153 (80%)	118 (97%)	3 (2%)	1 (1%)	16	54
2	D	122/153 (80%)	118 (97%)	3 (2%)	1 (1%)	16	54
2	F	122/153 (80%)	118 (97%)	3 (2%)	1 (1%)	16	54
3	G	47/268 (18%)	46 (98%)	1 (2%)	0	100	100
3	H	47/268 (18%)	46 (98%)	1 (2%)	0	100	100
3	I	47/268 (18%)	46 (98%)	1 (2%)	0	100	100
All	All	1800/2811 (64%)	1749 (97%)	48 (3%)	3 (0%)	45	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	615	SER
2	D	615	SER
2	F	615	SER

5.3.2 Protein sidechains

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	392/456 (86%)	389 (99%)	3 (1%)	79 84
1	C	392/456 (86%)	389 (99%)	3 (1%)	79 84
1	E	392/456 (86%)	389 (99%)	3 (1%)	79 84
2	B	97/129 (75%)	96 (99%)	1 (1%)	73 81
2	D	97/129 (75%)	96 (99%)	1 (1%)	73 81
2	F	97/129 (75%)	96 (99%)	1 (1%)	73 81
3	G	44/234 (19%)	44 (100%)	0	100 100
3	H	44/234 (19%)	44 (100%)	0	100 100
3	I	44/234 (19%)	44 (100%)	0	100 100
All	All	1599/2457 (65%)	1587 (99%)	12 (1%)	77 84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	339	ASN
1	A	448	ASN
2	B	618	ASN
1	C	197	ASN
1	C	339	ASN
1	C	448	ASN
2	D	618	ASN
1	E	197	ASN
1	E	339	ASN
1	E	448	ASN
2	F	618	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	658	GLN
2	D	658	GLN
2	F	658	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

72 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	$\#\|Z\| > 2$
4	NAG	J	1	4,1	14,14,15	0.28	0	17,19,21	0.59	0
4	NAG	J	2	4	14,14,15	0.28	0	17,19,21	0.62	0
4	NAG	K	1	4,1	14,14,15	0.82	1 (7%)	17,19,21	1.68	3 (17%)
4	NAG	K	2	4	14,14,15	0.85	0	17,19,21	1.23	2 (11%)
5	NAG	L	1	1,5	14,14,15	0.81	0	17,19,21	1.12	2 (11%)
5	NAG	L	2	5	14,14,15	0.97	1 (7%)	17,19,21	1.95	6 (35%)
5	BMA	L	3	5	11,11,12	1.96	2 (18%)	15,15,17	1.49	4 (26%)
5	MAN	L	4	5	11,11,12	1.83	2 (18%)	15,15,17	0.94	0
4	NAG	M	1	4,1	14,14,15	0.68	0	17,19,21	1.58	2 (11%)
4	NAG	M	2	4	14,14,15	0.71	0	17,19,21	1.08	1 (5%)
4	NAG	N	1	4,1	14,14,15	0.81	1 (7%)	17,19,21	1.88	5 (29%)
4	NAG	N	2	4	14,14,15	0.78	0	17,19,21	0.97	1 (5%)
4	NAG	O	1	4,1	14,14,15	0.82	0	17,19,21	1.20	1 (5%)
4	NAG	O	2	4	14,14,15	0.82	0	17,19,21	0.95	1 (5%)
4	NAG	P	1	4,1	14,14,15	0.92	1 (7%)	17,19,21	2.20	5 (29%)
4	NAG	P	2	4	14,14,15	0.81	0	17,19,21	1.21	1 (5%)
4	NAG	Q	1	4,1	14,14,15	0.73	0	17,19,21	1.18	2 (11%)
4	NAG	Q	2	4	14,14,15	0.75	0	17,19,21	1.22	1 (5%)
5	NAG	R	1	1,5	14,14,15	0.84	0	17,19,21	1.39	2 (11%)
5	NAG	R	2	5	14,14,15	0.90	1 (7%)	17,19,21	1.12	1 (5%)
5	BMA	R	3	5	11,11,12	1.92	2 (18%)	15,15,17	2.08	5 (33%)
5	MAN	R	4	5	11,11,12	1.80	2 (18%)	15,15,17	1.15	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	S	1	4,1	14,14,15	0.98	1 (7%)	17,19,21	1.41	3 (17%)
4	NAG	S	2	4	14,14,15	0.93	0	17,19,21	1.08	1 (5%)
4	NAG	T	1	4,1	14,14,15	0.29	0	17,19,21	0.60	0
4	NAG	T	2	4	14,14,15	0.28	0	17,19,21	0.62	0
4	NAG	U	1	4,1	14,14,15	0.81	1 (7%)	17,19,21	1.68	3 (17%)
4	NAG	U	2	4	14,14,15	0.86	0	17,19,21	1.23	2 (11%)
5	NAG	V	1	1,5	14,14,15	0.81	0	17,19,21	1.11	2 (11%)
5	NAG	V	2	5	14,14,15	0.96	1 (7%)	17,19,21	1.96	6 (35%)
5	BMA	V	3	5	11,11,12	1.97	2 (18%)	15,15,17	1.49	4 (26%)
5	MAN	V	4	5	11,11,12	1.83	2 (18%)	15,15,17	0.94	0
4	NAG	W	1	4,1	14,14,15	0.68	0	17,19,21	1.58	2 (11%)
4	NAG	W	2	4	14,14,15	0.71	0	17,19,21	1.08	1 (5%)
4	NAG	X	1	4,1	14,14,15	0.81	1 (7%)	17,19,21	1.88	5 (29%)
4	NAG	X	2	4	14,14,15	0.79	0	17,19,21	0.97	1 (5%)
4	NAG	Y	1	4,1	14,14,15	0.82	0	17,19,21	1.20	1 (5%)
4	NAG	Y	2	4	14,14,15	0.82	0	17,19,21	0.95	1 (5%)
4	NAG	Z	1	4,1	14,14,15	0.91	1 (7%)	17,19,21	2.20	5 (29%)
4	NAG	Z	2	4	14,14,15	0.79	0	17,19,21	1.21	1 (5%)
4	NAG	a	1	4,1	14,14,15	0.73	0	17,19,21	1.18	2 (11%)
4	NAG	a	2	4	14,14,15	0.75	0	17,19,21	1.22	1 (5%)
5	NAG	b	1	1,5	14,14,15	0.85	0	17,19,21	1.39	2 (11%)
5	NAG	b	2	5	14,14,15	0.91	1 (7%)	17,19,21	1.13	1 (5%)
5	BMA	b	3	5	11,11,12	1.92	2 (18%)	15,15,17	2.08	5 (33%)
5	MAN	b	4	5	11,11,12	1.80	2 (18%)	15,15,17	1.14	2 (13%)
4	NAG	c	1	4,1	14,14,15	0.97	1 (7%)	17,19,21	1.42	3 (17%)
4	NAG	c	2	4	14,14,15	0.93	0	17,19,21	1.08	1 (5%)
4	NAG	d	1	4,1	14,14,15	0.29	0	17,19,21	0.59	0
4	NAG	d	2	4	14,14,15	0.28	0	17,19,21	0.61	0
4	NAG	e	1	4,1	14,14,15	0.82	1 (7%)	17,19,21	1.68	3 (17%)
4	NAG	e	2	4	14,14,15	0.84	0	17,19,21	1.22	2 (11%)
5	NAG	f	1	1,5	14,14,15	0.81	0	17,19,21	1.12	2 (11%)
5	NAG	f	2	5	14,14,15	0.96	1 (7%)	17,19,21	1.95	6 (35%)
5	BMA	f	3	5	11,11,12	1.97	2 (18%)	15,15,17	1.49	4 (26%)
5	MAN	f	4	5	11,11,12	1.82	2 (18%)	15,15,17	0.95	0
4	NAG	g	1	4,1	14,14,15	0.68	0	17,19,21	1.58	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	g	2	4	14,14,15	0.71	0	17,19,21	1.09	1 (5%)
4	NAG	h	1	4,1	14,14,15	0.81	1 (7%)	17,19,21	1.88	5 (29%)
4	NAG	h	2	4	14,14,15	0.78	0	17,19,21	0.97	1 (5%)
4	NAG	i	1	4,1	14,14,15	0.83	0	17,19,21	1.19	1 (5%)
4	NAG	i	2	4	14,14,15	0.82	0	17,19,21	0.95	1 (5%)
4	NAG	j	1	4,1	14,14,15	0.92	1 (7%)	17,19,21	2.20	5 (29%)
4	NAG	j	2	4	14,14,15	0.81	0	17,19,21	1.21	1 (5%)
4	NAG	k	1	4,1	14,14,15	0.73	0	17,19,21	1.18	2 (11%)
4	NAG	k	2	4	14,14,15	0.74	0	17,19,21	1.23	1 (5%)
5	NAG	l	1	1,5	14,14,15	0.84	0	17,19,21	1.38	2 (11%)
5	NAG	l	2	5	14,14,15	0.90	1 (7%)	17,19,21	1.12	1 (5%)
5	BMA	l	3	5	11,11,12	1.93	2 (18%)	15,15,17	2.07	5 (33%)
5	MAN	l	4	5	11,11,12	1.79	2 (18%)	15,15,17	1.14	2 (13%)
4	NAG	m	1	4,1	14,14,15	0.97	1 (7%)	17,19,21	1.41	3 (17%)
4	NAG	m	2	4	14,14,15	0.93	0	17,19,21	1.09	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	1/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1

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

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

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	l	3	BMA	O2-C2	-4.43	1.34	1.43
5	R	3	BMA	O2-C2	-4.43	1.34	1.43
5	b	3	BMA	O2-C2	-4.43	1.34	1.43
5	R	4	MAN	O2-C2	-4.27	1.34	1.43
5	b	4	MAN	O2-C2	-4.26	1.34	1.43
5	l	4	MAN	O2-C2	-4.26	1.34	1.43
5	V	3	BMA	O2-C2	-4.24	1.34	1.43
5	f	3	BMA	O2-C2	-4.24	1.34	1.43
5	L	3	BMA	O2-C2	-4.24	1.34	1.43
5	V	4	MAN	O2-C2	-4.19	1.34	1.43
5	L	4	MAN	O2-C2	-4.18	1.34	1.43
5	f	4	MAN	O2-C2	-4.15	1.34	1.43
5	f	3	BMA	C2-C3	-2.92	1.48	1.52
5	V	3	BMA	C2-C3	-2.91	1.48	1.52
5	L	3	BMA	C2-C3	-2.87	1.48	1.52
4	X	1	NAG	C3-C2	-2.37	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	h	1	NAG	C3-C2	-2.37	1.47	1.52
4	c	1	NAG	C3-C2	-2.36	1.47	1.52
4	N	1	NAG	C3-C2	-2.36	1.47	1.52
4	S	1	NAG	C3-C2	-2.35	1.47	1.52
4	m	1	NAG	C3-C2	-2.33	1.47	1.52
5	V	4	MAN	C2-C3	-2.30	1.49	1.52
5	L	4	MAN	C2-C3	-2.29	1.49	1.52
5	f	4	MAN	C2-C3	-2.27	1.49	1.52
4	j	1	NAG	C3-C2	-2.23	1.47	1.52
5	b	2	NAG	C3-C2	-2.22	1.47	1.52
5	R	2	NAG	C3-C2	-2.20	1.47	1.52
4	P	1	NAG	C3-C2	-2.20	1.47	1.52
5	l	4	MAN	C2-C3	-2.19	1.49	1.52
5	l	2	NAG	C3-C2	-2.19	1.47	1.52
5	R	4	MAN	C2-C3	-2.19	1.49	1.52
5	b	4	MAN	C2-C3	-2.18	1.49	1.52
4	Z	1	NAG	C3-C2	-2.18	1.47	1.52
4	e	1	NAG	C3-C2	-2.18	1.47	1.52
4	K	1	NAG	C3-C2	-2.18	1.47	1.52
5	l	3	BMA	C2-C3	-2.18	1.49	1.52
4	U	1	NAG	C3-C2	-2.17	1.48	1.52
5	R	3	BMA	C2-C3	-2.13	1.49	1.52
5	b	3	BMA	C2-C3	-2.12	1.49	1.52
5	L	2	NAG	C3-C2	-2.10	1.48	1.52
5	f	2	NAG	C3-C2	-2.09	1.48	1.52
5	V	2	NAG	C3-C2	-2.07	1.48	1.52

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Z	1	NAG	O4-C4-C3	-4.83	98.98	110.38
4	j	1	NAG	O4-C4-C3	-4.82	99.01	110.38
4	P	1	NAG	O4-C4-C3	-4.82	99.02	110.38
4	P	1	NAG	O5-C5-C6	-4.35	99.20	107.66
4	j	1	NAG	O5-C5-C6	-4.35	99.20	107.66
4	Z	1	NAG	O5-C5-C6	-4.33	99.23	107.66
5	V	2	NAG	C4-C3-C2	-4.30	104.71	111.02
5	f	2	NAG	C4-C3-C2	-4.28	104.75	111.02
5	L	2	NAG	C4-C3-C2	-4.27	104.76	111.02
4	X	1	NAG	O5-C5-C6	-4.16	99.57	107.66
4	N	1	NAG	O5-C5-C6	-4.15	99.58	107.66
4	h	1	NAG	O5-C5-C6	-4.13	99.62	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	e	1	NAG	O4-C4-C3	-4.10	100.72	110.38
5	b	3	BMA	C2-C3-C4	-4.09	103.67	110.86
4	K	1	NAG	O4-C4-C3	-4.09	100.74	110.38
5	R	3	BMA	C2-C3-C4	-4.09	103.67	110.86
4	U	1	NAG	O4-C4-C3	-4.08	100.76	110.38
5	l	3	BMA	C2-C3-C4	-4.07	103.70	110.86
4	U	1	NAG	O5-C5-C6	-4.03	99.82	107.66
4	K	1	NAG	O5-C5-C6	-4.01	99.86	107.66
4	e	1	NAG	O5-C5-C6	-4.00	99.88	107.66
5	b	3	BMA	O3-C3-C2	-3.96	101.96	110.05
5	R	3	BMA	O3-C3-C2	-3.96	101.96	110.05
5	l	3	BMA	O3-C3-C2	-3.94	102.00	110.05
4	j	1	NAG	C3-C4-C5	-3.94	103.09	110.23
4	P	1	NAG	C3-C4-C5	-3.93	103.10	110.23
4	Z	1	NAG	C3-C4-C5	-3.93	103.11	110.23
4	k	2	NAG	C4-C3-C2	-3.83	105.40	111.02
4	a	2	NAG	C4-C3-C2	-3.82	105.42	111.02
4	Q	2	NAG	C4-C3-C2	-3.81	105.43	111.02
4	g	1	NAG	C2-N2-C7	3.79	127.97	122.90
4	M	1	NAG	C2-N2-C7	3.74	127.92	122.90
4	W	1	NAG	C2-N2-C7	3.74	127.91	122.90
5	l	3	BMA	C1-C2-C3	3.60	114.88	109.64
5	R	3	BMA	C1-C2-C3	3.59	114.87	109.64
5	b	3	BMA	C1-C2-C3	3.59	114.87	109.64
4	P	2	NAG	C4-C3-C2	-3.58	105.78	111.02
4	j	2	NAG	C4-C3-C2	-3.58	105.78	111.02
4	X	1	NAG	C2-N2-C7	-3.58	118.11	122.90
4	Z	2	NAG	C4-C3-C2	-3.57	105.78	111.02
4	N	1	NAG	C2-N2-C7	-3.57	118.12	122.90
4	h	1	NAG	C2-N2-C7	-3.55	118.15	122.90
4	K	2	NAG	C4-C3-C2	-3.49	105.91	111.02
4	e	2	NAG	C4-C3-C2	-3.48	105.92	111.02
4	U	2	NAG	C4-C3-C2	-3.48	105.92	111.02
5	V	2	NAG	C1-O5-C5	3.34	116.67	112.19
4	S	2	NAG	C4-C3-C2	-3.32	106.16	111.02
4	c	2	NAG	C4-C3-C2	-3.32	106.16	111.02
4	c	1	NAG	C3-C4-C5	-3.32	104.22	110.23
4	m	2	NAG	C4-C3-C2	-3.31	106.17	111.02
5	L	2	NAG	C1-O5-C5	3.31	116.62	112.19
4	S	1	NAG	C3-C4-C5	-3.30	104.24	110.23
5	f	2	NAG	C1-O5-C5	3.30	116.61	112.19
4	m	1	NAG	C3-C4-C5	-3.30	104.26	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	1	NAG	C4-C3-C2	-3.27	106.22	111.02
4	M	1	NAG	C4-C3-C2	-3.24	106.27	111.02
4	g	1	NAG	C4-C3-C2	-3.23	106.28	111.02
4	P	1	NAG	O4-C4-C5	3.23	117.28	109.32
4	j	1	NAG	O4-C4-C5	3.23	117.27	109.32
4	Z	1	NAG	O4-C4-C5	3.22	117.26	109.32
5	R	1	NAG	O5-C5-C6	-3.21	101.41	107.66
5	b	1	NAG	O5-C5-C6	-3.21	101.41	107.66
5	l	1	NAG	O5-C5-C6	-3.19	101.45	107.66
5	L	2	NAG	O4-C4-C5	3.01	116.74	109.32
5	V	2	NAG	O4-C4-C5	3.01	116.74	109.32
5	f	2	NAG	O4-C4-C5	3.01	116.73	109.32
5	f	1	NAG	C3-C4-C5	-2.98	104.83	110.23
5	L	1	NAG	C3-C4-C5	-2.97	104.84	110.23
5	V	1	NAG	C3-C4-C5	-2.95	104.88	110.23
4	N	1	NAG	C4-C3-C2	-2.94	106.71	111.02
4	h	1	NAG	C4-C3-C2	-2.93	106.72	111.02
4	X	1	NAG	C4-C3-C2	-2.92	106.74	111.02
5	b	2	NAG	C3-C4-C5	-2.87	105.02	110.23
5	b	3	BMA	O3-C3-C4	2.86	117.12	110.38
5	R	2	NAG	C3-C4-C5	-2.86	105.05	110.23
5	R	3	BMA	O3-C3-C4	2.86	117.11	110.38
5	l	2	NAG	C3-C4-C5	-2.85	105.06	110.23
4	g	2	NAG	C4-C3-C2	-2.85	106.84	111.02
4	M	2	NAG	C4-C3-C2	-2.85	106.85	111.02
4	W	2	NAG	C4-C3-C2	-2.84	106.85	111.02
5	l	3	BMA	O3-C3-C4	2.84	117.08	110.38
4	X	2	NAG	C4-C3-C2	-2.82	106.89	111.02
5	V	2	NAG	O5-C5-C4	-2.81	103.98	110.83
4	h	2	NAG	C4-C3-C2	-2.81	106.89	111.02
4	N	2	NAG	C4-C3-C2	-2.81	106.91	111.02
5	f	2	NAG	O5-C5-C4	-2.80	104.01	110.83
5	L	2	NAG	O5-C5-C4	-2.80	104.02	110.83
4	S	1	NAG	C2-N2-C7	-2.65	119.35	122.90
4	c	1	NAG	C2-N2-C7	-2.65	119.35	122.90
4	m	1	NAG	C2-N2-C7	-2.60	119.42	122.90
4	i	2	NAG	C4-C3-C2	-2.59	107.22	111.02
4	Y	2	NAG	C4-C3-C2	-2.59	107.22	111.02
4	O	2	NAG	C4-C3-C2	-2.58	107.23	111.02
4	S	1	NAG	O5-C1-C2	-2.56	107.32	111.29
5	R	4	MAN	C2-C3-C4	-2.55	106.37	110.86
4	c	1	NAG	O5-C1-C2	-2.55	107.35	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	b	4	MAN	C2-C3-C4	-2.55	106.38	110.86
5	l	4	MAN	C2-C3-C4	-2.55	106.38	110.86
4	m	1	NAG	O5-C1-C2	-2.53	107.38	111.29
4	h	1	NAG	O5-C1-C2	-2.52	107.39	111.29
4	N	1	NAG	O5-C1-C2	-2.52	107.40	111.29
4	X	1	NAG	O5-C1-C2	-2.50	107.42	111.29
4	O	1	NAG	O5-C5-C6	-2.48	102.83	107.66
4	Y	1	NAG	O5-C5-C6	-2.48	102.84	107.66
4	i	1	NAG	O5-C5-C6	-2.48	102.84	107.66
4	h	1	NAG	O7-C7-N2	-2.45	117.64	121.98
4	N	1	NAG	O7-C7-N2	-2.43	117.69	121.98
4	X	1	NAG	O7-C7-N2	-2.42	117.71	121.98
4	P	1	NAG	C4-C3-C2	2.40	114.54	111.02
4	j	1	NAG	C4-C3-C2	2.40	114.53	111.02
4	U	2	NAG	O5-C1-C2	-2.38	107.60	111.29
5	V	3	BMA	C1-O5-C5	2.38	115.38	112.19
5	f	3	BMA	C1-O5-C5	2.38	115.38	112.19
5	L	3	BMA	C1-O5-C5	2.38	115.37	112.19
4	Z	1	NAG	C4-C3-C2	2.38	114.50	111.02
5	V	3	BMA	C2-C3-C4	-2.37	106.69	110.86
5	L	3	BMA	C2-C3-C4	-2.37	106.70	110.86
5	f	3	BMA	C2-C3-C4	-2.35	106.72	110.86
4	K	2	NAG	O5-C1-C2	-2.35	107.66	111.29
5	R	4	MAN	C1-C2-C3	2.34	113.05	109.64
5	b	4	MAN	C1-C2-C3	2.34	113.05	109.64
5	l	4	MAN	C1-C2-C3	2.34	113.05	109.64
4	e	2	NAG	O5-C1-C2	-2.33	107.68	111.29
5	V	2	NAG	O5-C1-C2	-2.33	107.69	111.29
5	f	2	NAG	O5-C1-C2	-2.32	107.70	111.29
5	L	2	NAG	O5-C1-C2	-2.32	107.71	111.29
5	f	1	NAG	O5-C1-C2	-2.31	107.72	111.29
5	L	1	NAG	O5-C1-C2	-2.30	107.73	111.29
4	Q	1	NAG	C1-O5-C5	-2.29	109.12	112.19
4	a	1	NAG	C1-O5-C5	-2.28	109.13	112.19
5	V	1	NAG	O5-C1-C2	-2.27	107.77	111.29
4	k	1	NAG	C1-O5-C5	-2.27	109.15	112.19
4	Q	1	NAG	O5-C5-C6	-2.21	103.36	107.66
4	k	1	NAG	O5-C5-C6	-2.21	103.36	107.66
4	U	1	NAG	C3-C4-C5	-2.20	106.25	110.23
4	a	1	NAG	O5-C5-C6	-2.20	103.39	107.66
4	K	1	NAG	C3-C4-C5	-2.19	106.25	110.23
4	e	1	NAG	C3-C4-C5	-2.17	106.29	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	f	3	BMA	C1-C2-C3	2.14	112.76	109.64
5	l	3	BMA	O2-C2-C3	-2.13	105.73	110.15
5	b	3	BMA	O2-C2-C3	-2.13	105.74	110.15
5	R	3	BMA	O2-C2-C3	-2.13	105.74	110.15
5	V	3	BMA	C1-C2-C3	2.12	112.73	109.64
5	L	3	BMA	C1-C2-C3	2.12	112.73	109.64
5	V	3	BMA	O5-C1-C2	-2.11	105.76	110.79
5	R	1	NAG	O4-C4-C3	-2.11	105.41	110.38
5	l	1	NAG	O4-C4-C3	-2.11	105.41	110.38
5	b	1	NAG	O4-C4-C3	-2.10	105.42	110.38
5	L	3	BMA	O5-C1-C2	-2.10	105.77	110.79
5	f	3	BMA	O5-C1-C2	-2.10	105.77	110.79
5	f	2	NAG	C1-C2-N2	-2.03	107.23	110.43
5	L	2	NAG	C1-C2-N2	-2.02	107.25	110.43
5	V	2	NAG	C1-C2-N2	-2.00	107.28	110.43

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1	NAG	C3-C2-N2-C7
4	W	1	NAG	C3-C2-N2-C7
4	g	1	NAG	C3-C2-N2-C7
5	R	3	BMA	C4-C5-C6-O6
5	b	3	BMA	C4-C5-C6-O6
5	l	3	BMA	C4-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	e	1	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	i	2	NAG	O5-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
5	f	1	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
4	h	2	NAG	O5-C5-C6-O6
5	R	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	b	4	MAN	O5-C5-C6-O6
5	l	4	MAN	O5-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
5	b	3	BMA	O5-C5-C6-O6
5	l	3	BMA	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	k	2	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	j	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	k	2	NAG	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
5	V	3	BMA	O5-C5-C6-O6
5	f	3	BMA	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	h	1	NAG	O5-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
5	V	3	BMA	C4-C5-C6-O6
5	f	3	BMA	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	e	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
5	L	4	MAN	O5-C5-C6-O6
5	V	4	MAN	O5-C5-C6-O6
5	f	4	MAN	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	j	1	NAG	C4-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	f	1	NAG	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	h	1	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	g	2	NAG	O5-C5-C6-O6
4	m	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	d	2	NAG	O5-C5-C6-O6
4	j	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	i	1	NAG	O5-C5-C6-O6
4	i	2	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
4	m	1	NAG	O5-C5-C6-O6
5	R	4	MAN	C4-C5-C6-O6
5	b	4	MAN	C4-C5-C6-O6
5	l	4	MAN	C4-C5-C6-O6
4	e	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	h	2	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	j	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C8-C7-N2-C2
4	T	1	NAG	C8-C7-N2-C2
4	d	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	T	1	NAG	O7-C7-N2-C2
4	d	1	NAG	O7-C7-N2-C2
4	O	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	i	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2

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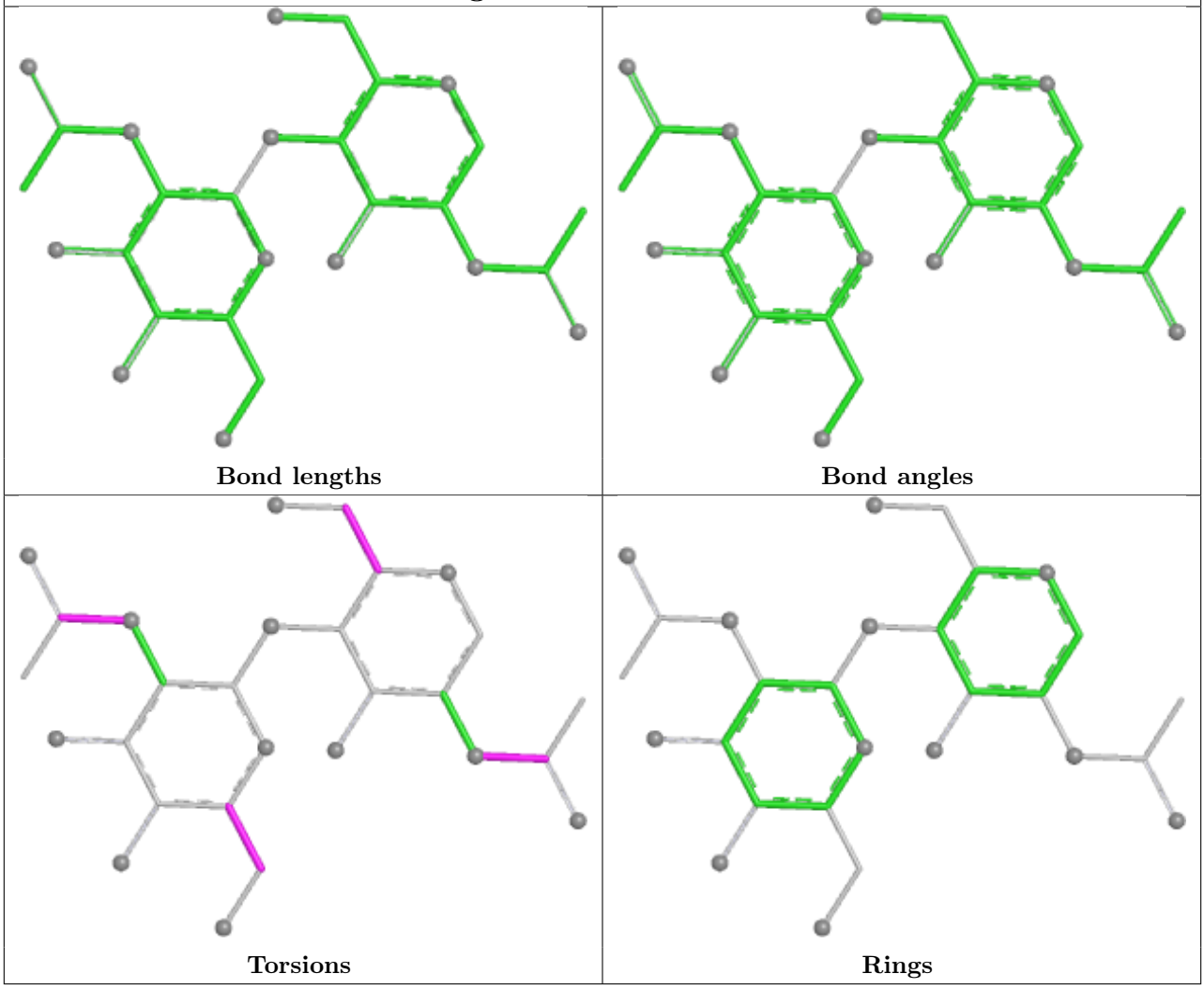
Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O7-C7-N2-C2
4	T	2	NAG	C8-C7-N2-C2
4	T	2	NAG	O7-C7-N2-C2
4	d	2	NAG	C8-C7-N2-C2
4	d	2	NAG	O7-C7-N2-C2

There are no ring outliers.

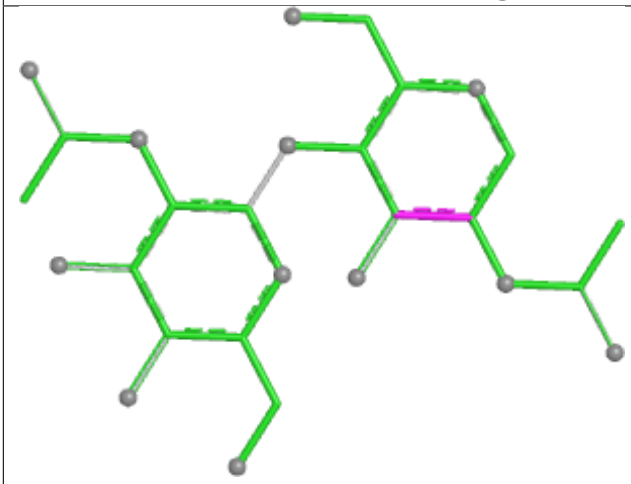
No monomer is involved in short contacts.

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

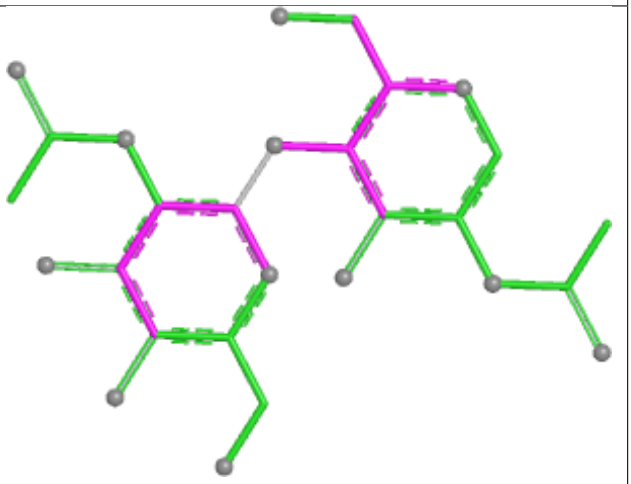
Oligosaccharide Chain J



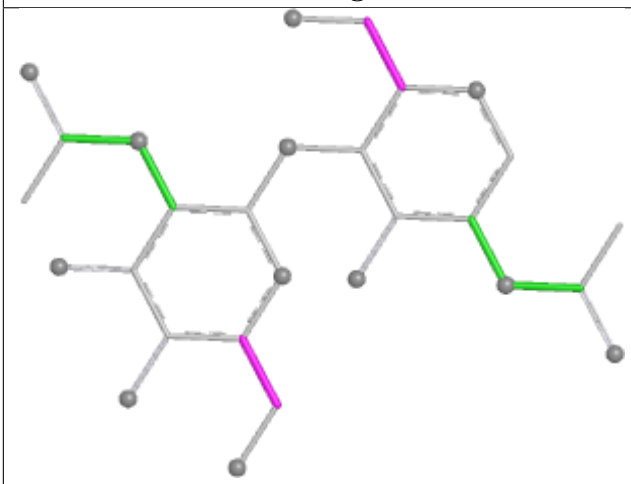
Oligosaccharide Chain K



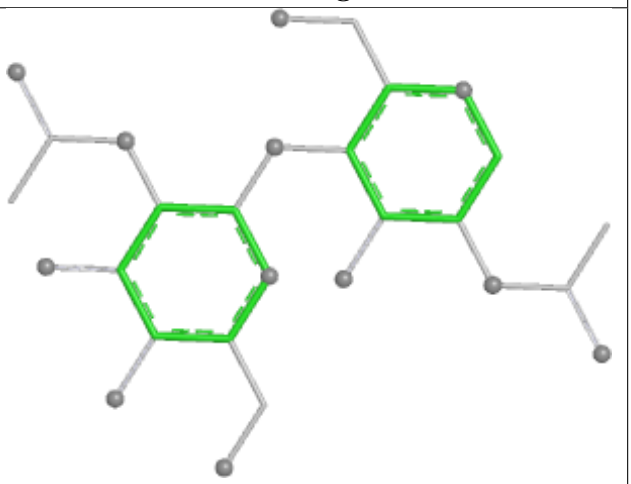
Bond lengths



Bond angles

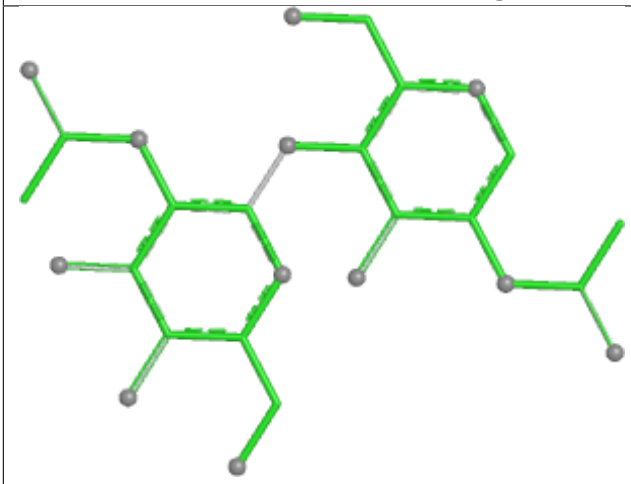


Torsions

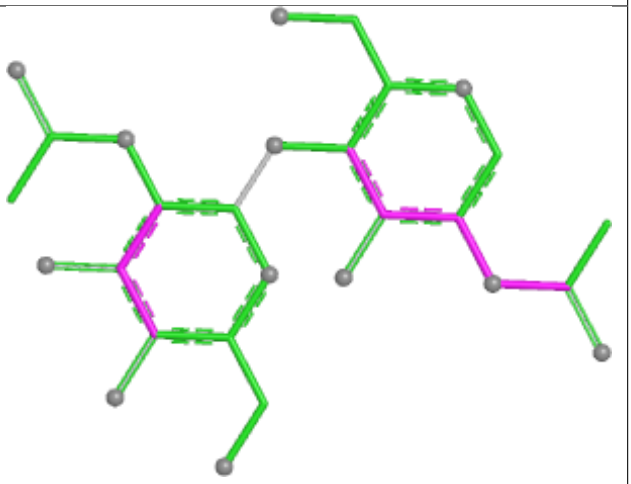


Rings

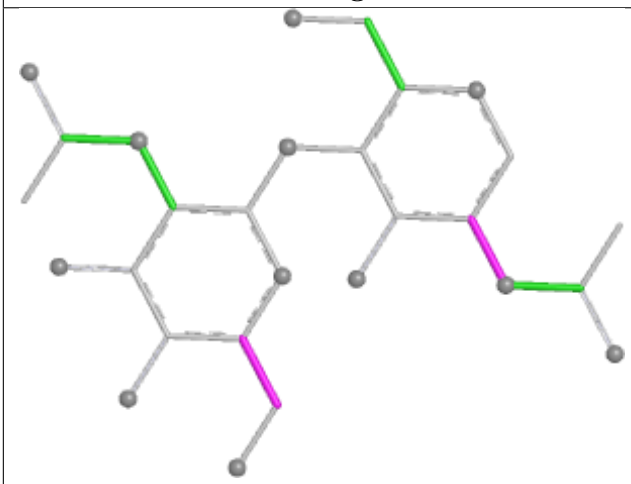
Oligosaccharide Chain M



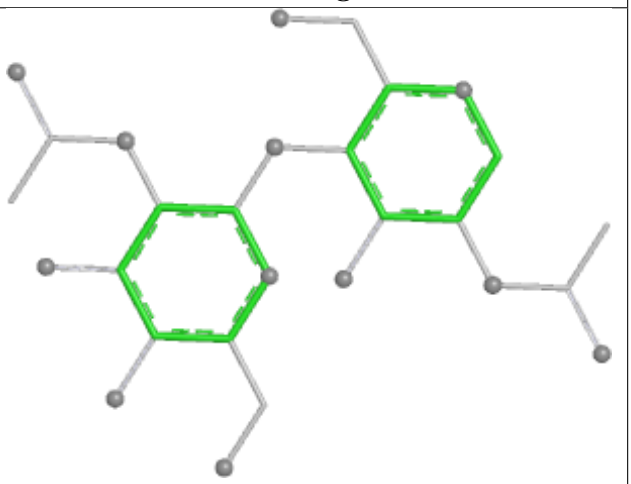
Bond lengths



Bond angles

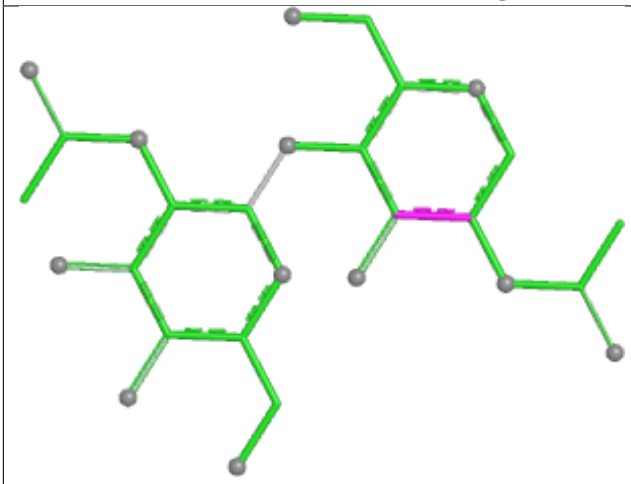


Torsions

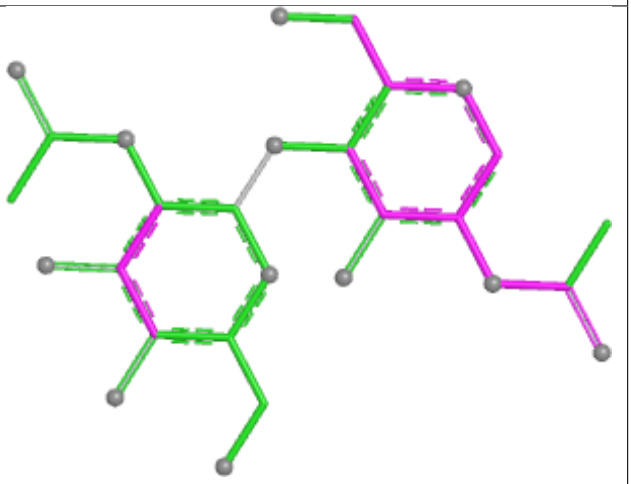


Rings

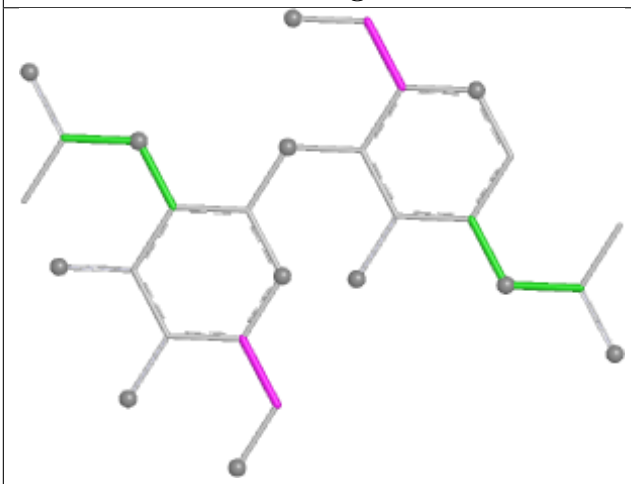
Oligosaccharide Chain N



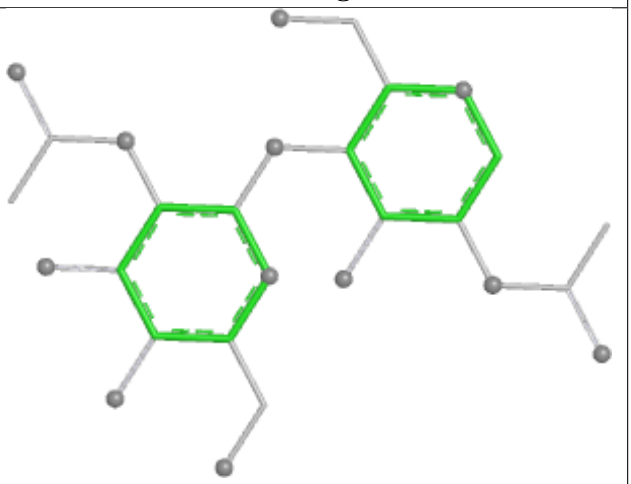
Bond lengths



Bond angles

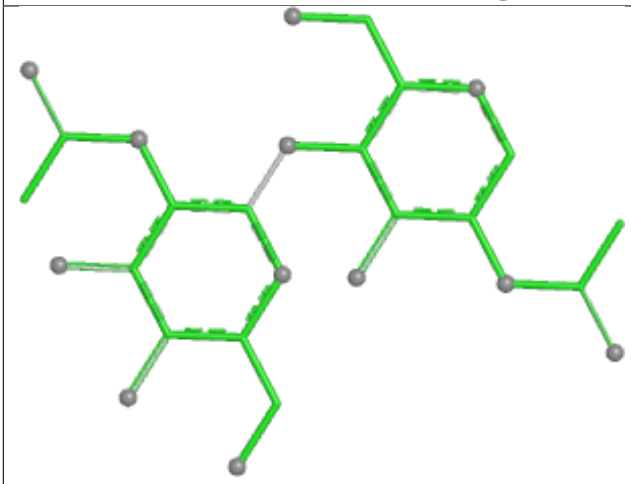


Torsions

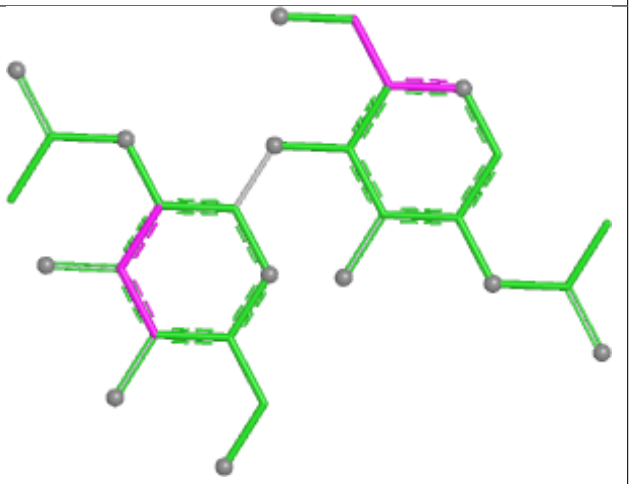


Rings

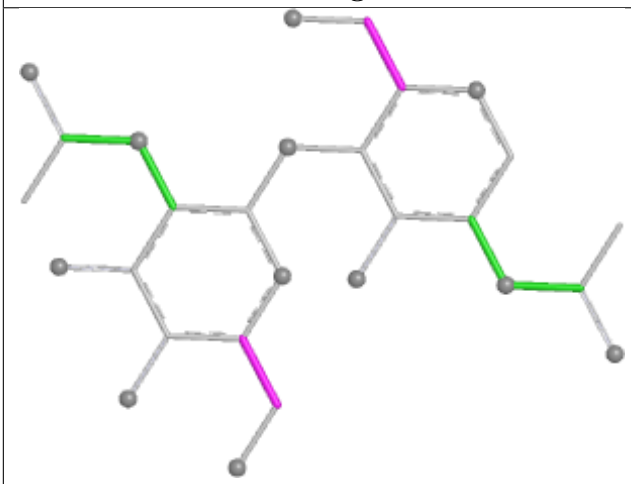
Oligosaccharide Chain O



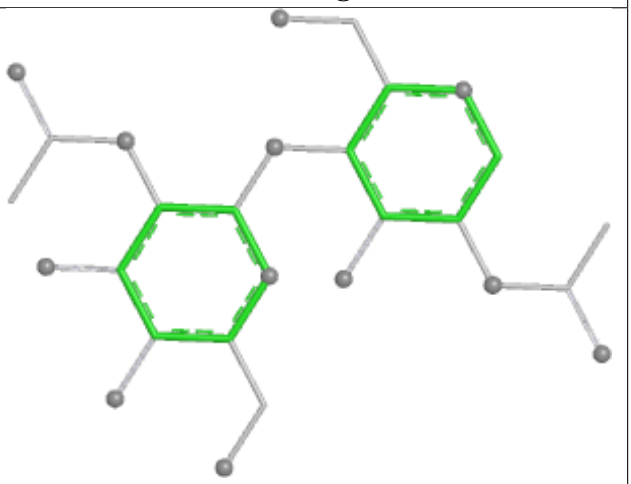
Bond lengths



Bond angles

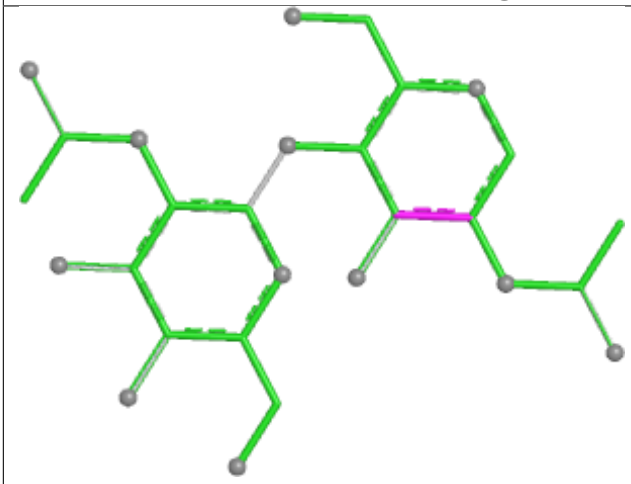


Torsions

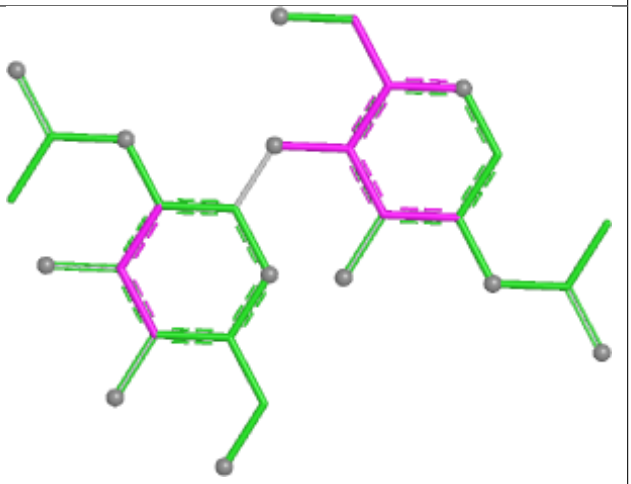


Rings

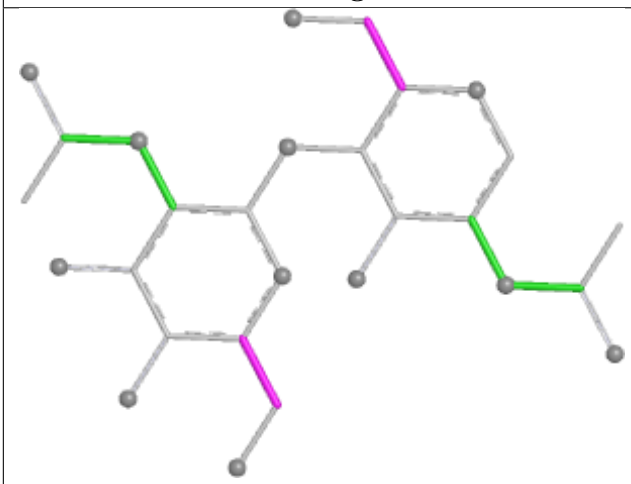
Oligosaccharide Chain P



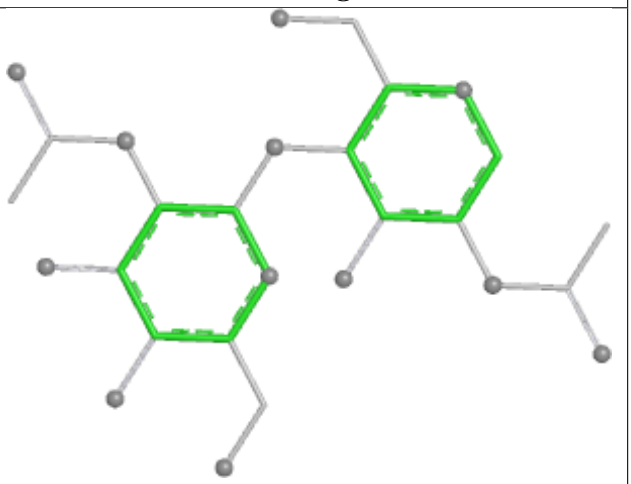
Bond lengths



Bond angles

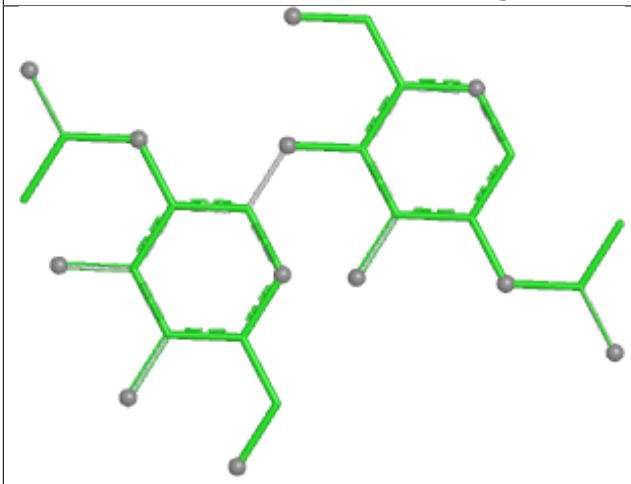


Torsions

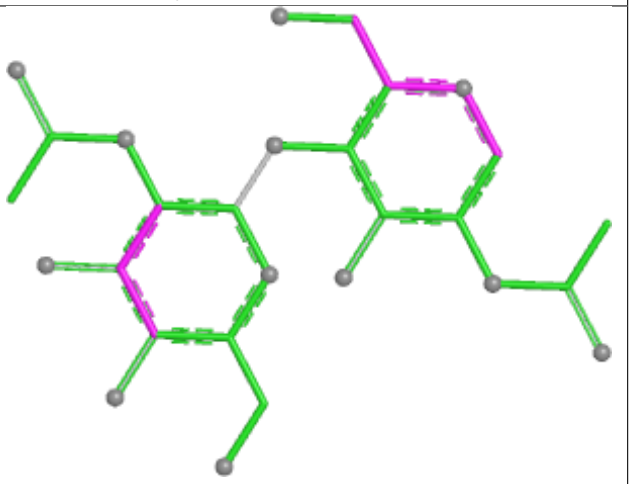


Rings

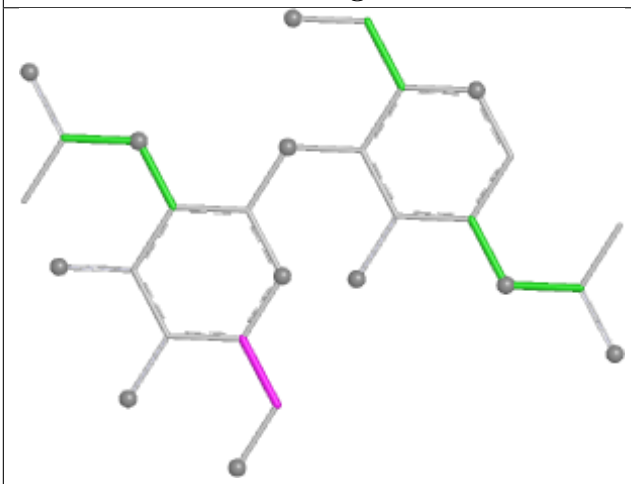
Oligosaccharide Chain Q



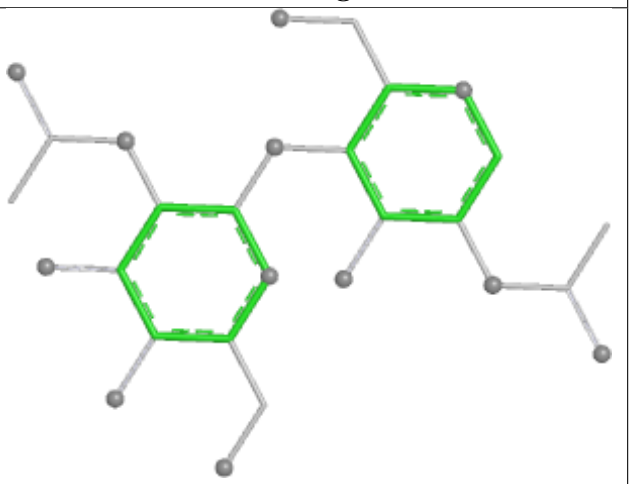
Bond lengths



Bond angles

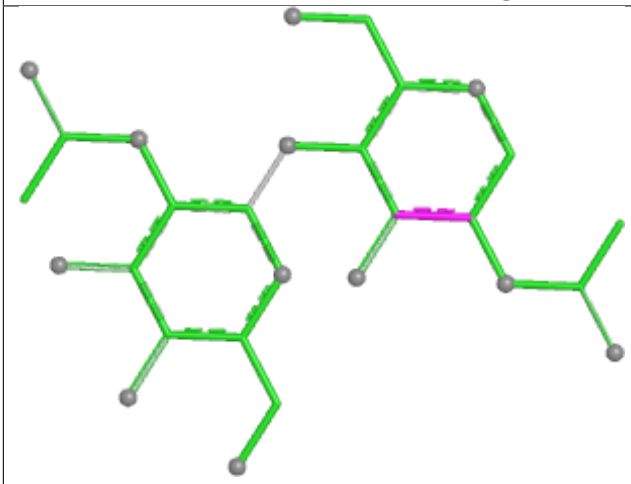


Torsions

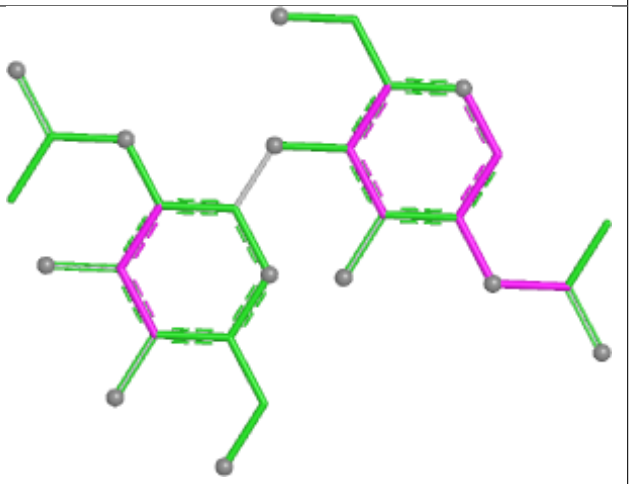


Rings

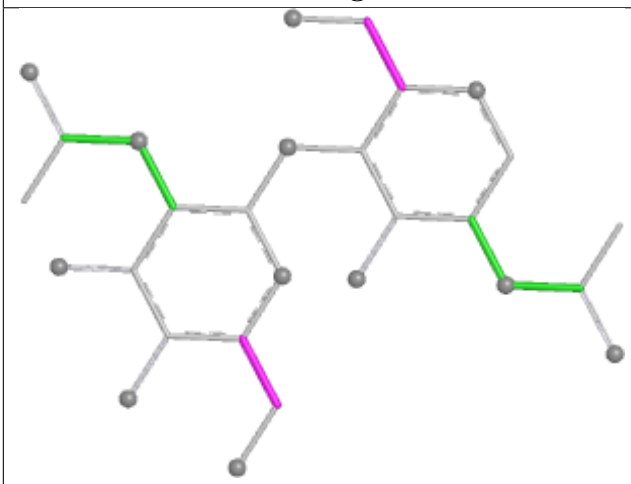
Oligosaccharide Chain S



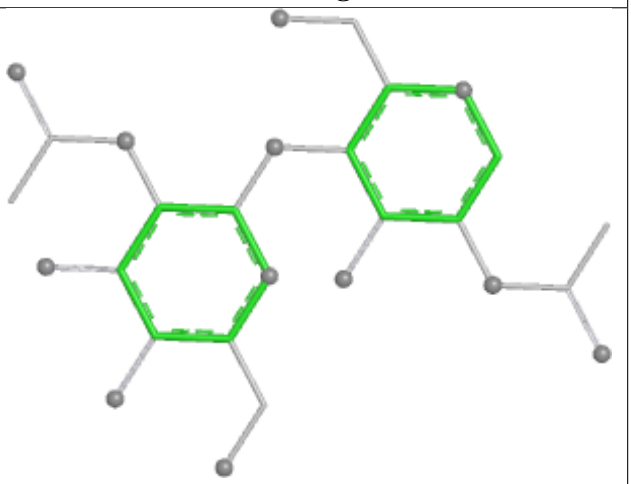
Bond lengths



Bond angles

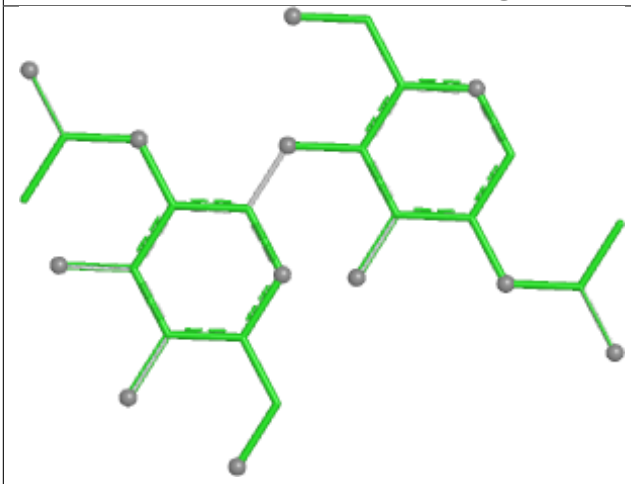


Torsions

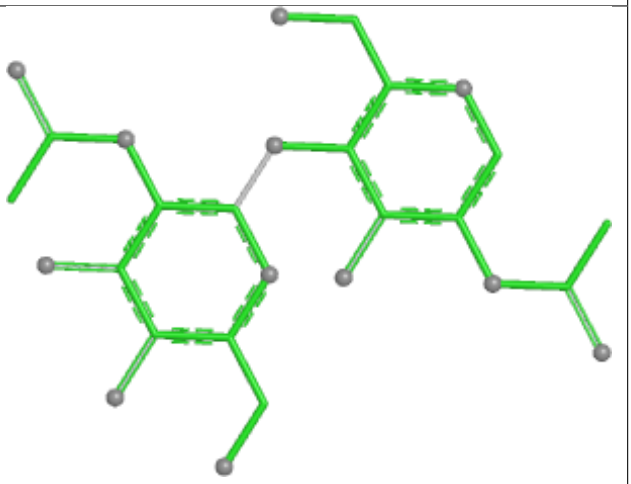


Rings

Oligosaccharide Chain T



Bond lengths



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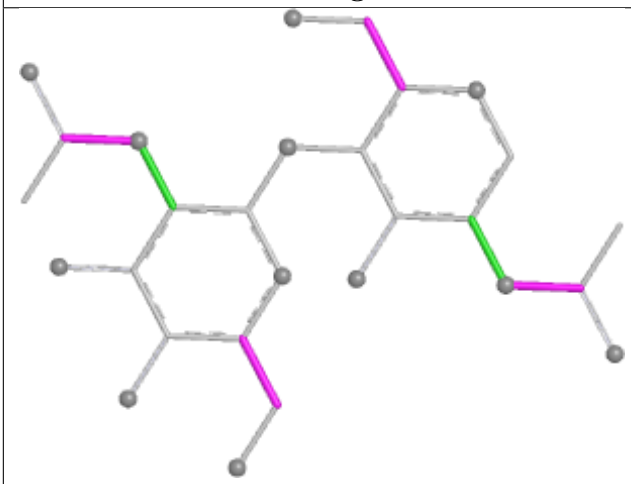

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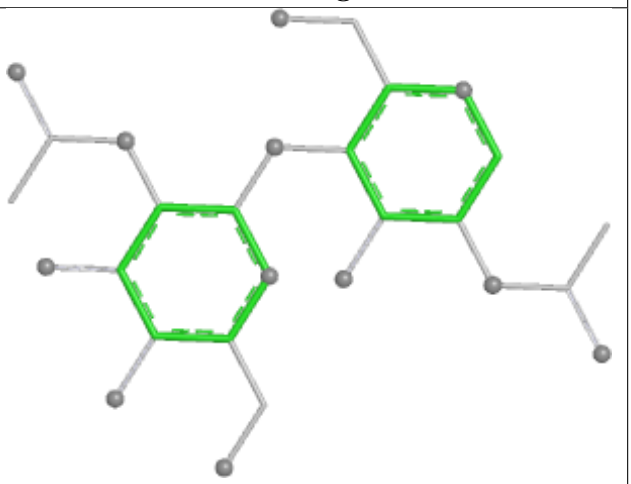
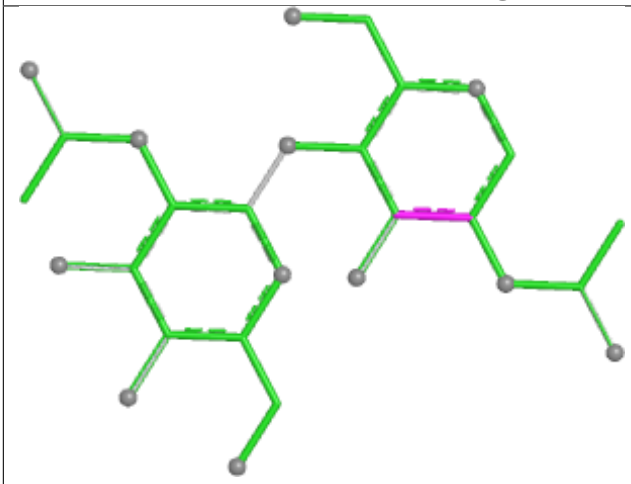


Rings

Oligosaccharide Chain U



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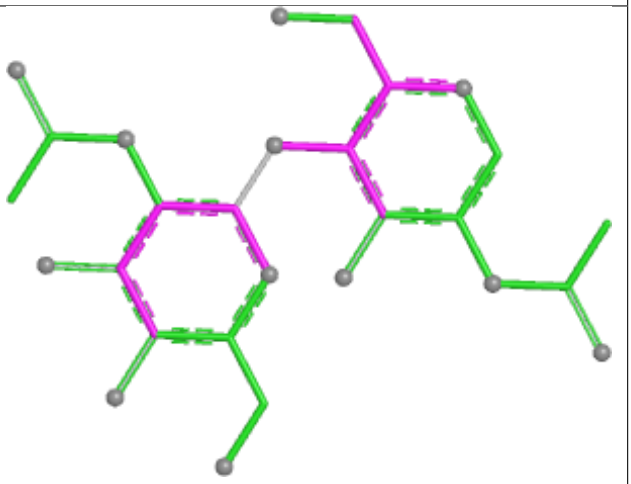
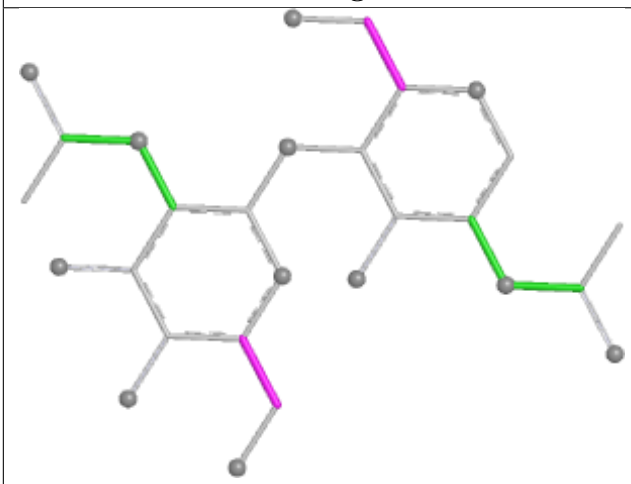


Bond angles



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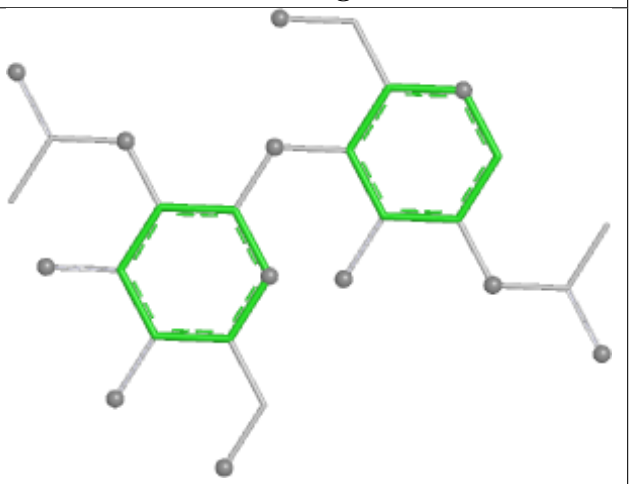
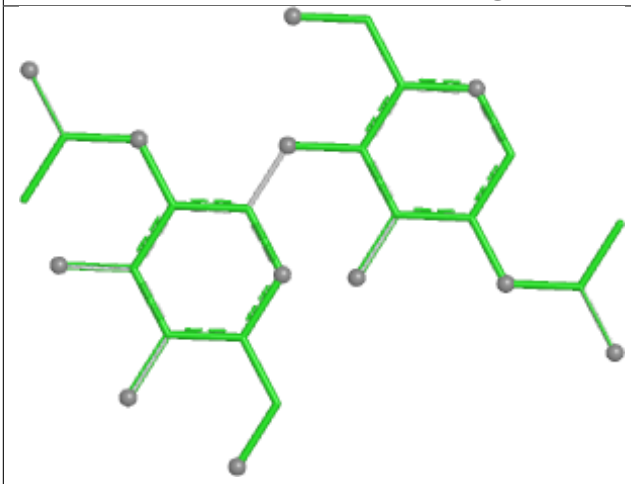


Rings

Oligosaccharide Chain W



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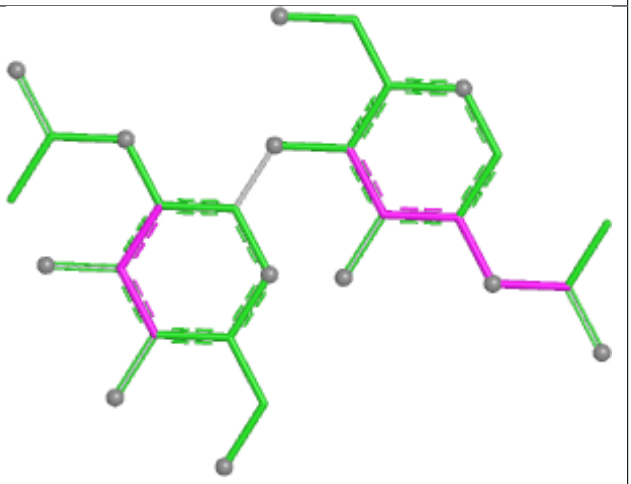
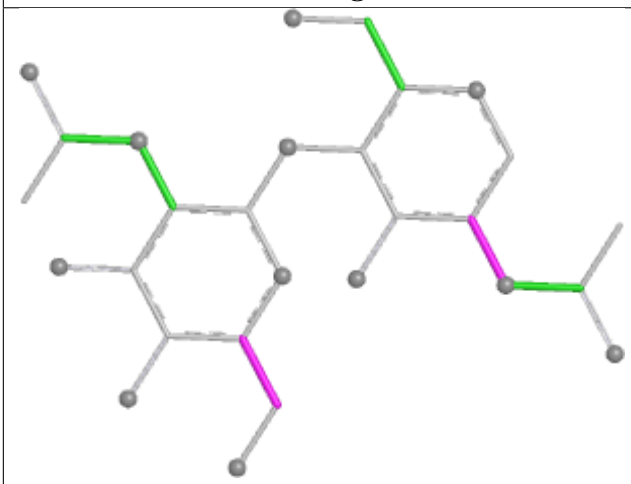


Bond angles



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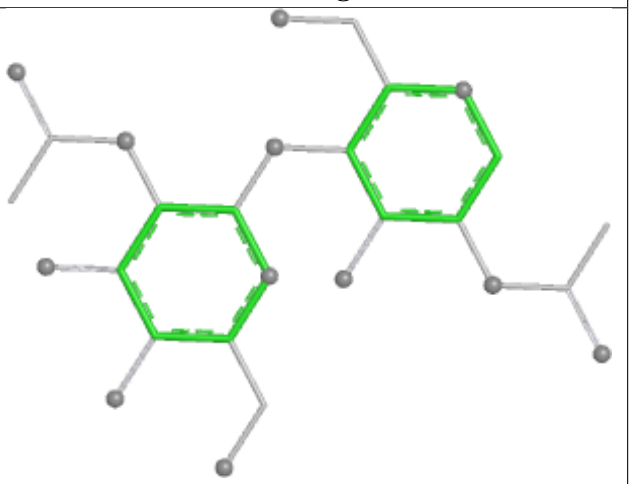
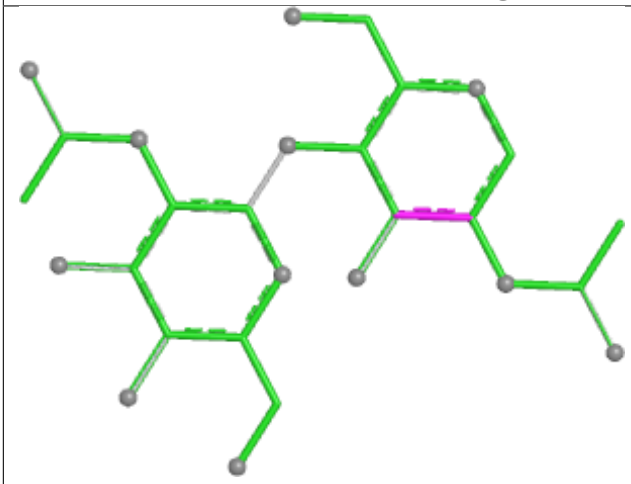
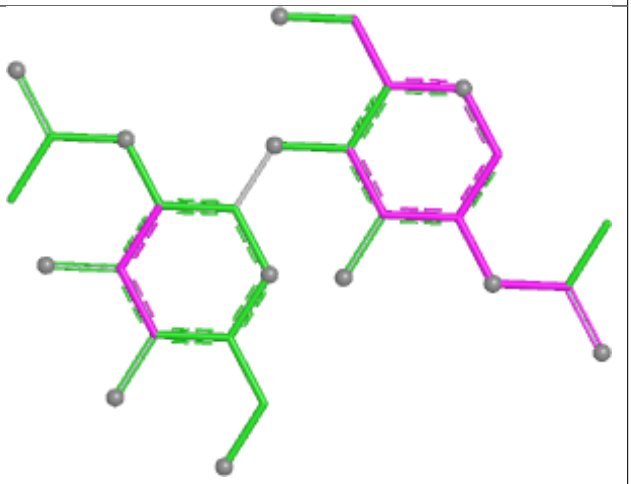


Rings

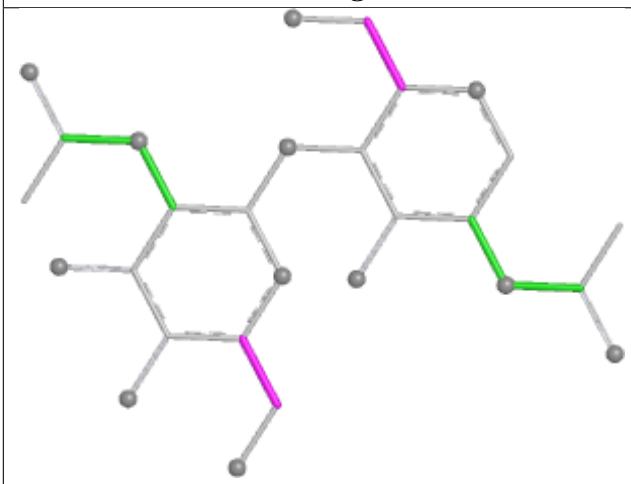
Oligosaccharide Chain X



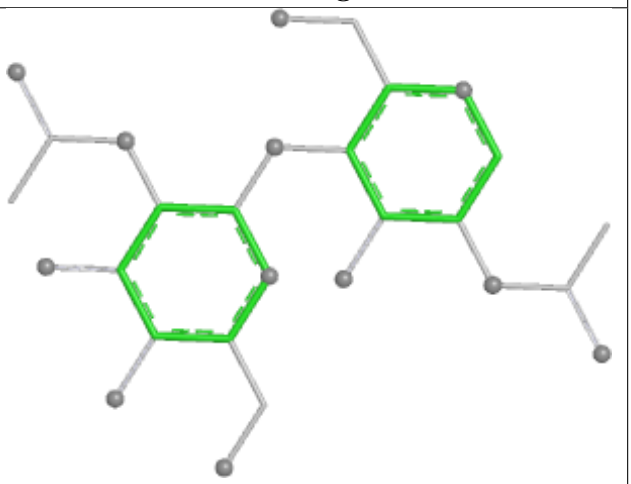
Bond lengths



Bond angles

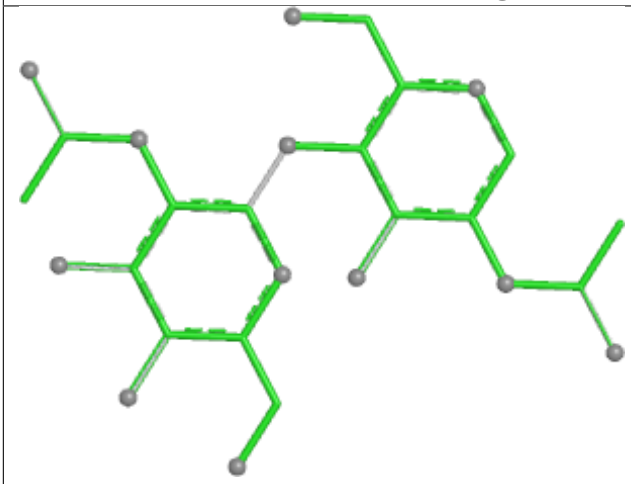


Torsions



Rings

Oligosaccharide Chain Y



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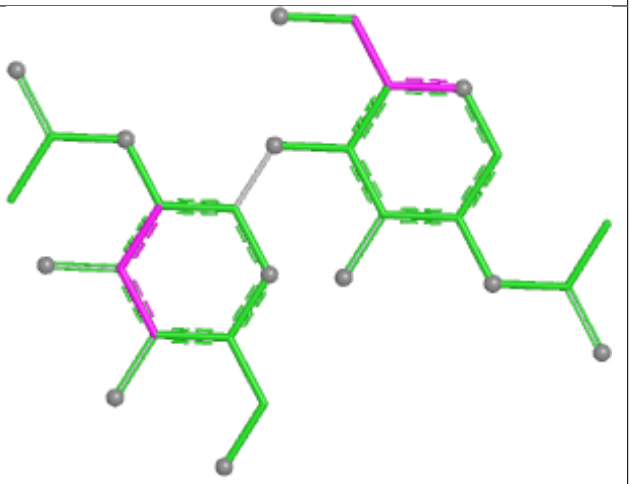
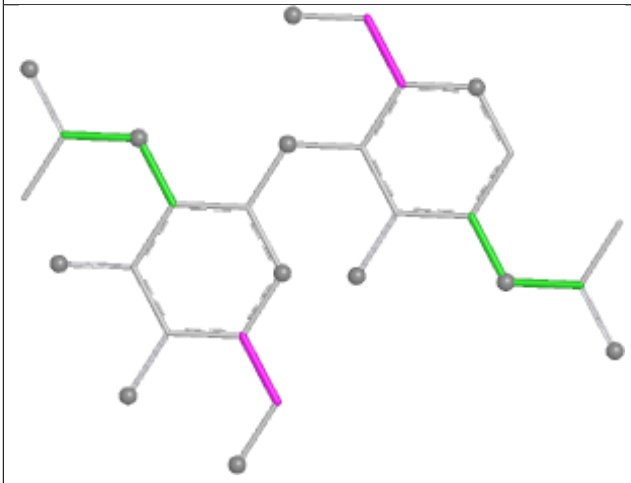


Bond angles



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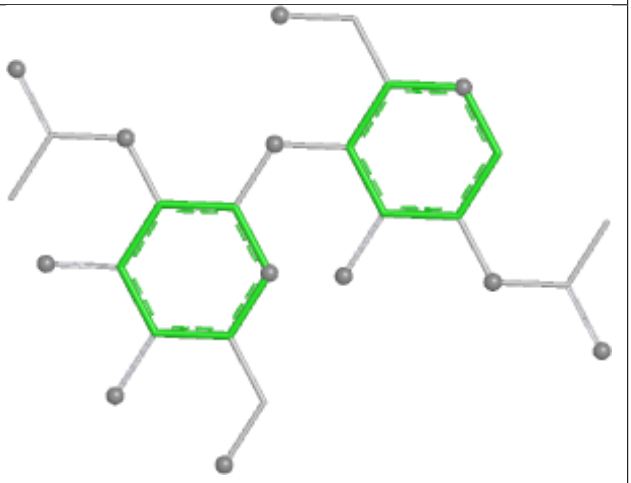
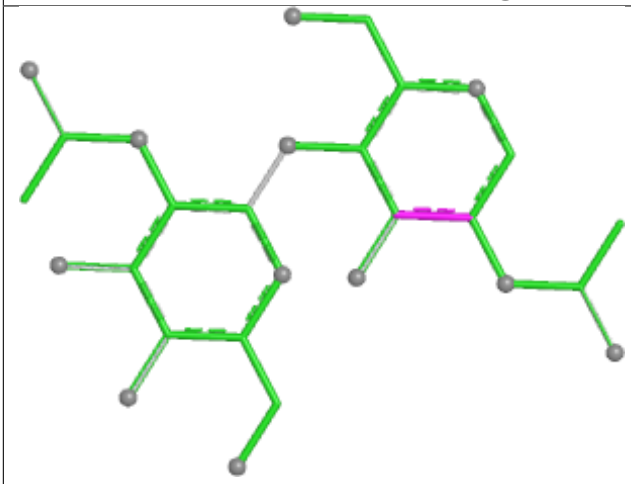


Rings

Oligosaccharide Chain Z



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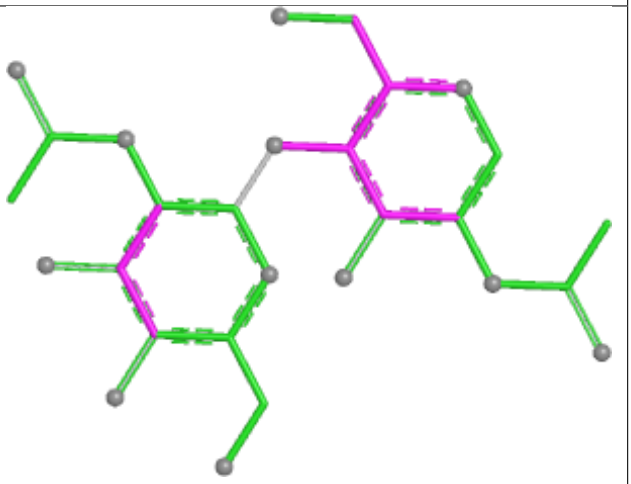
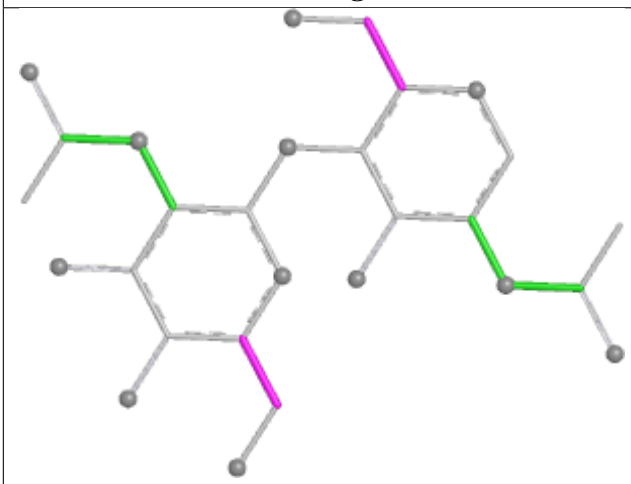
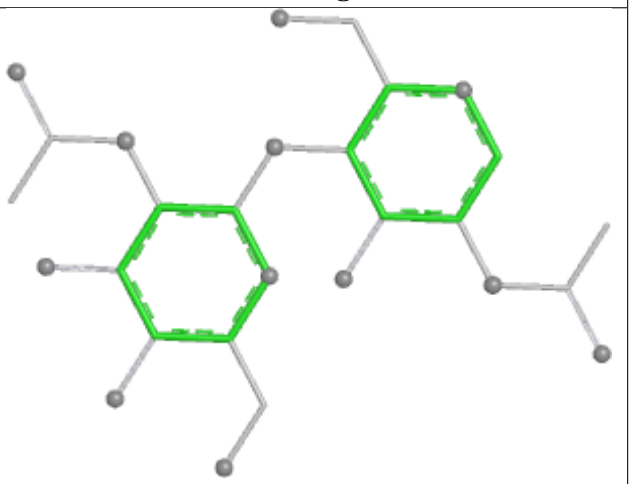


Bond angles

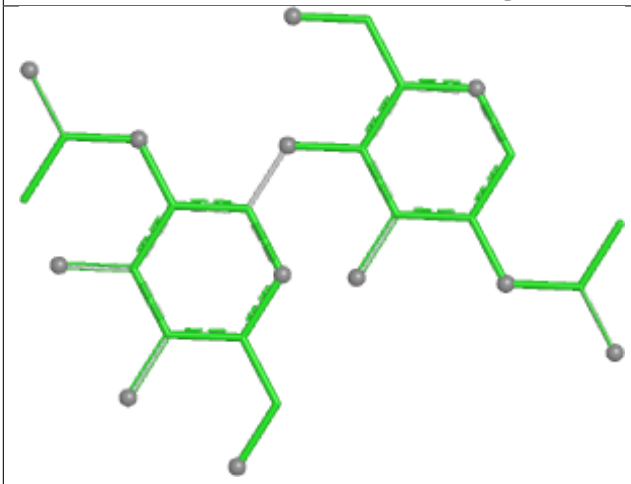


Torsions



Rings

Oligosaccharide Chain a



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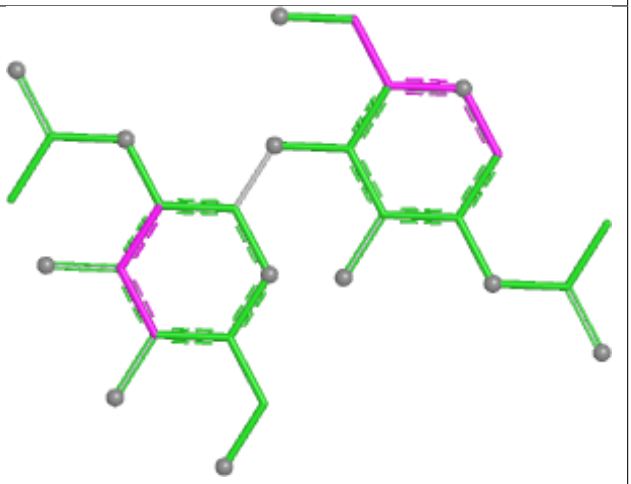
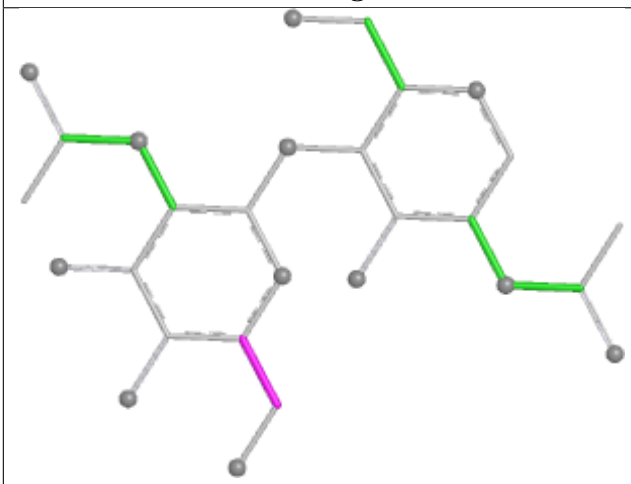


Bond angles



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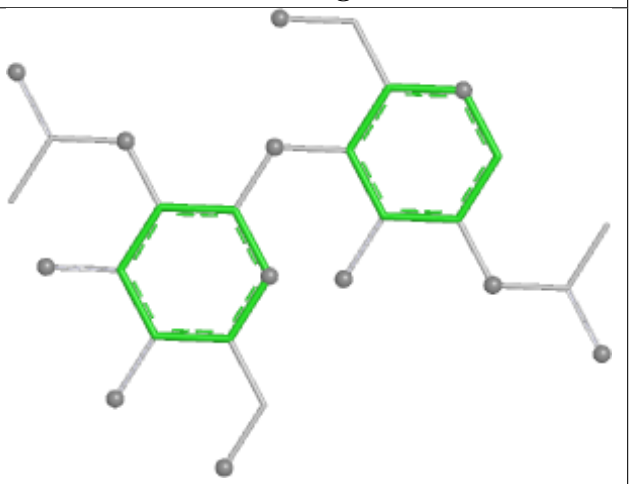
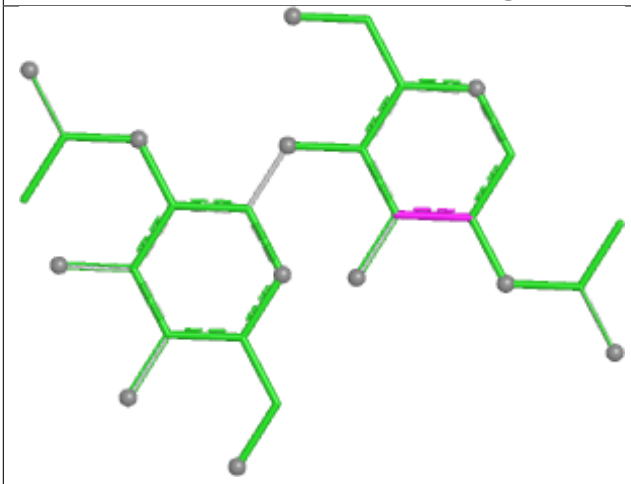


Rings

Oligosaccharide Chain c



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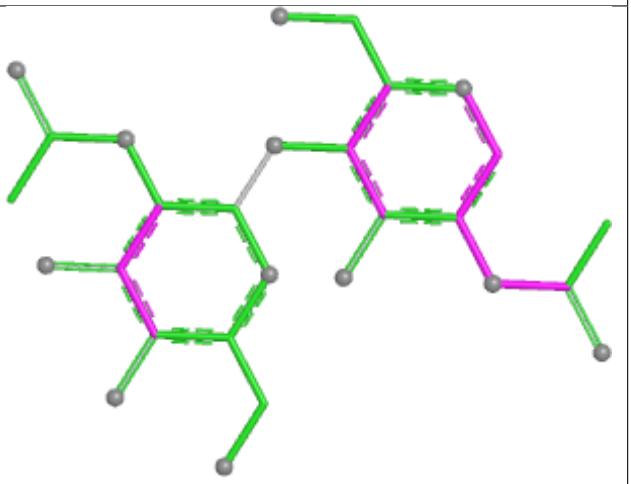
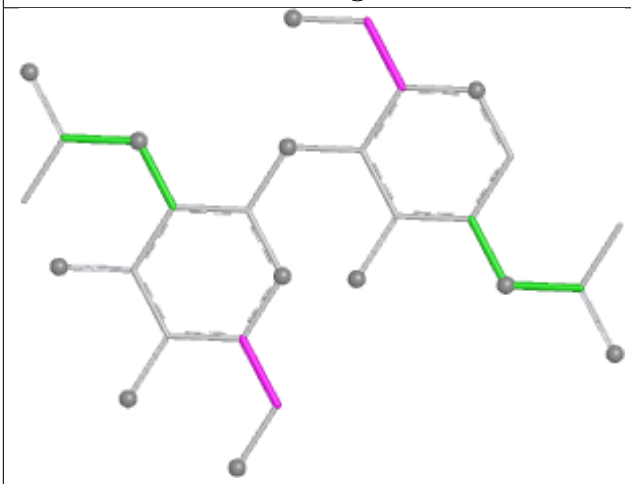


Bond angles



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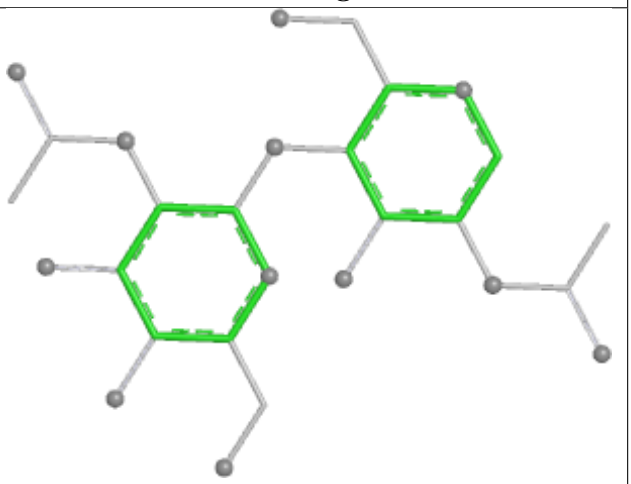
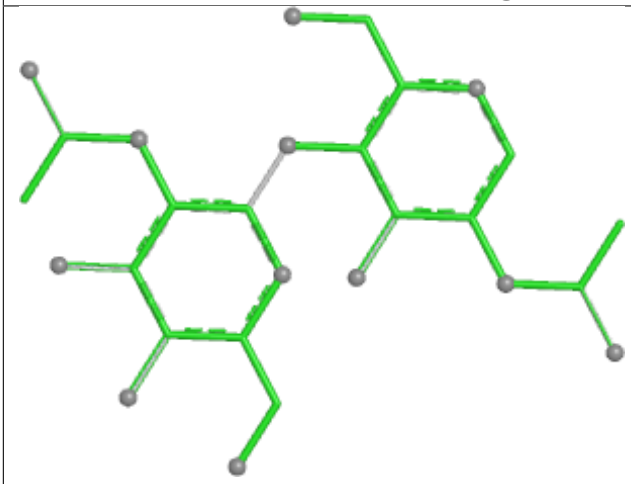


Rings

Oligosaccharide Chain d



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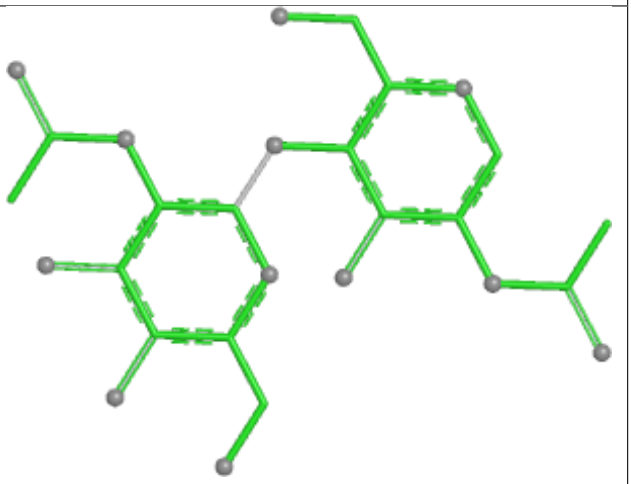
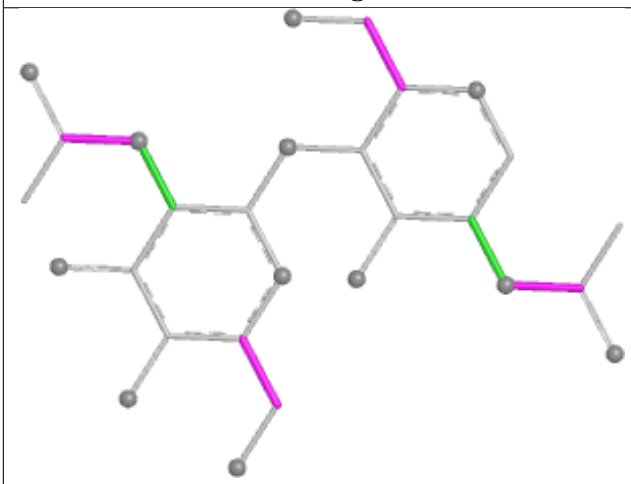
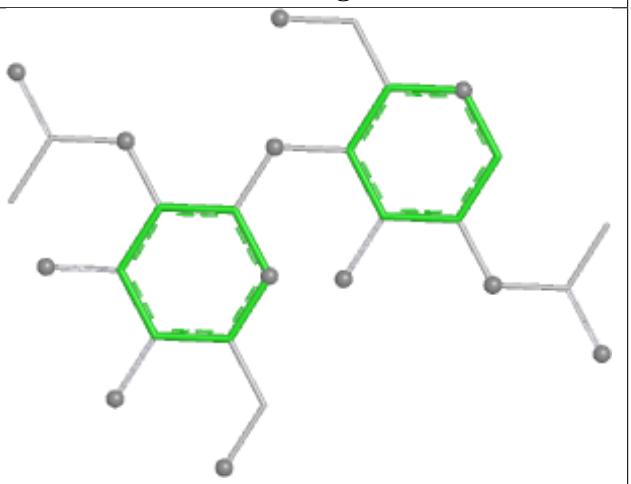


Bond angles

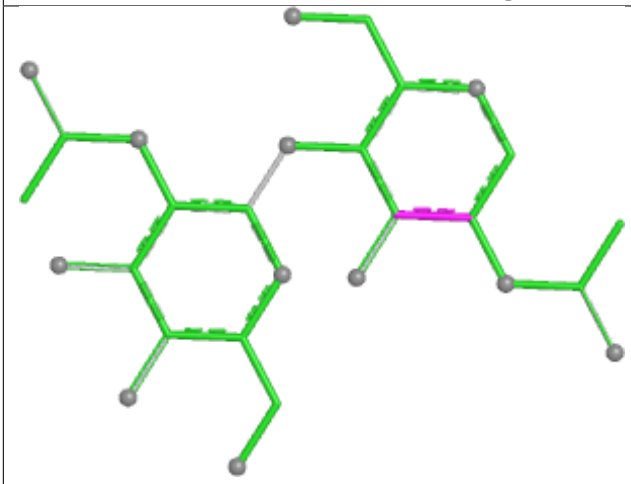


Torsions



Rings

Oligosaccharide Chain e



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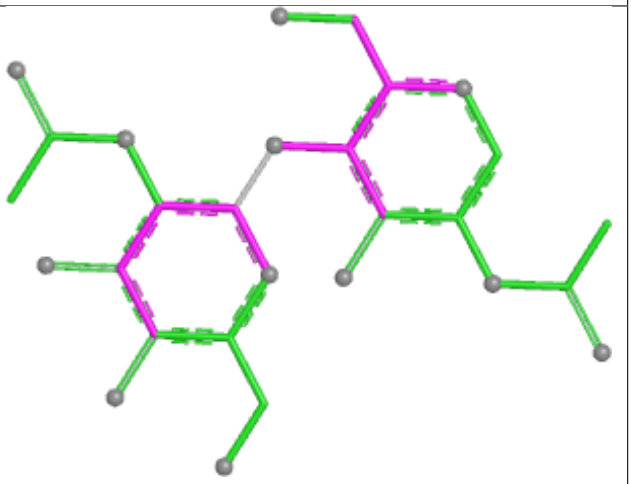
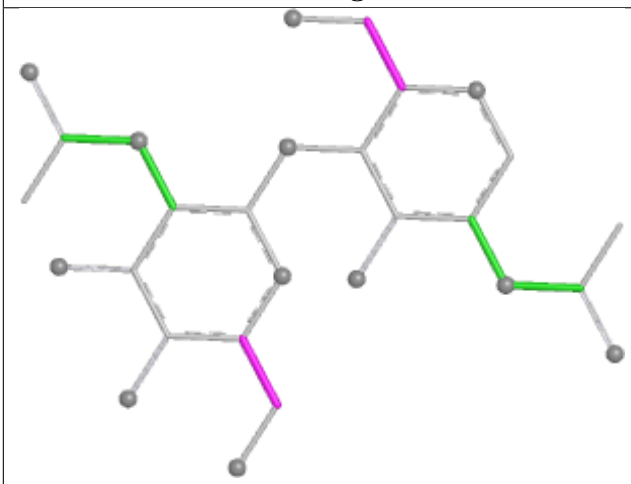


Bond angles



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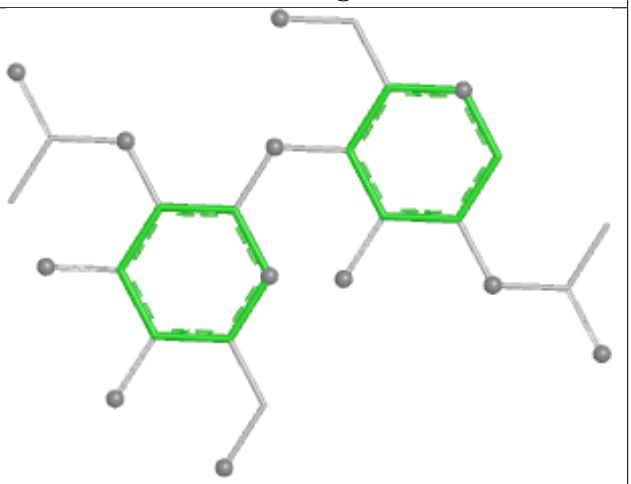
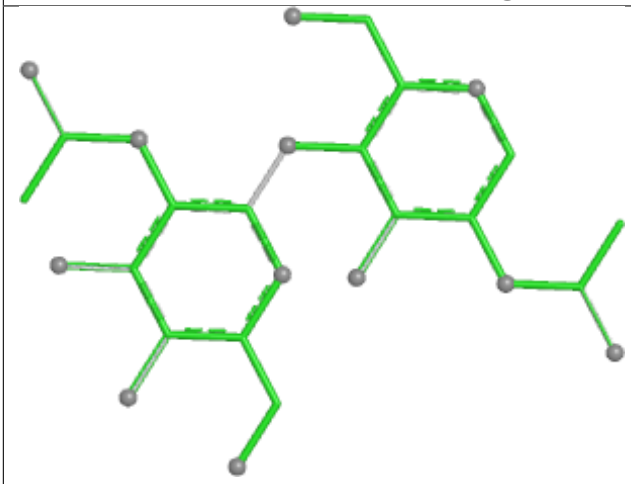


Rings

Oligosaccharide Chain g



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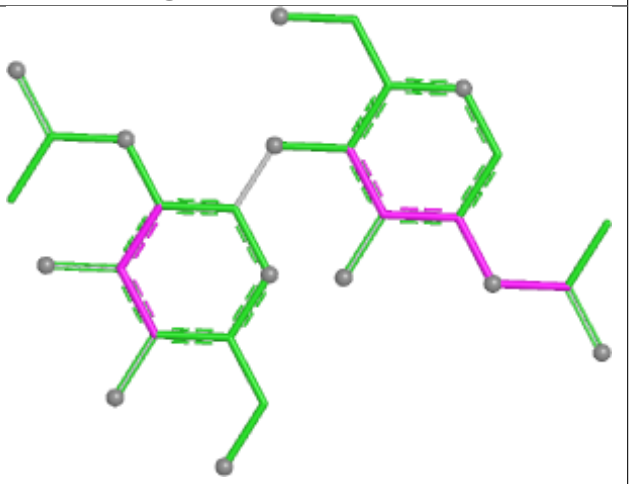
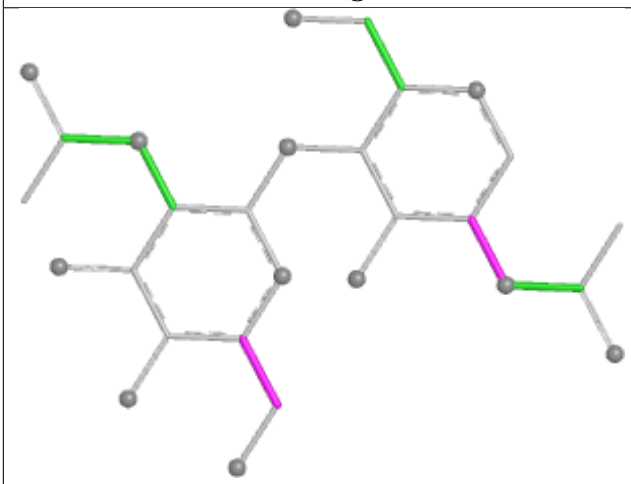


Bond angles



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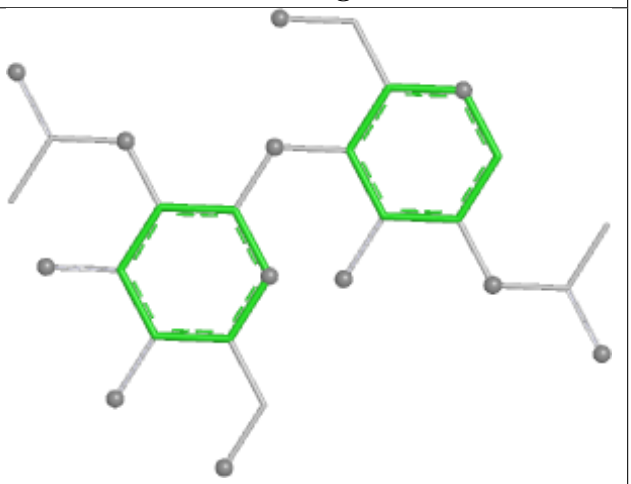
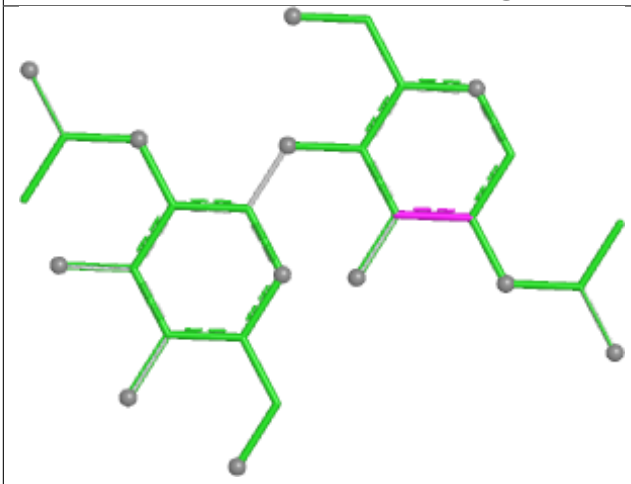


Rings

Oligosaccharide Chain h



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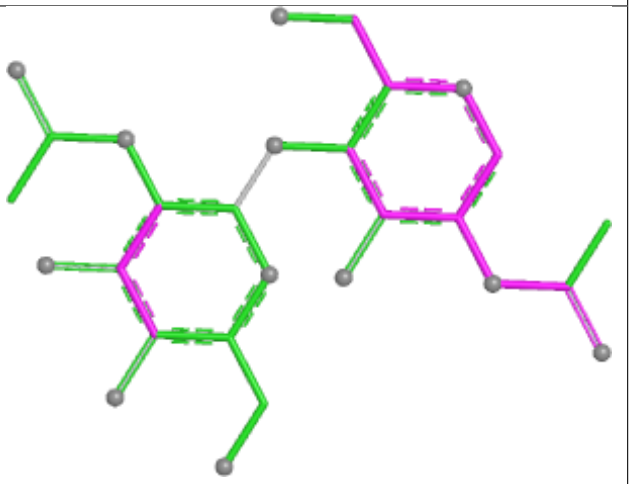
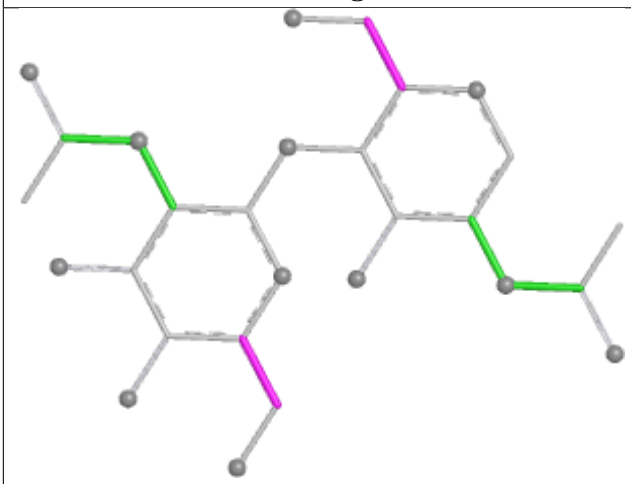
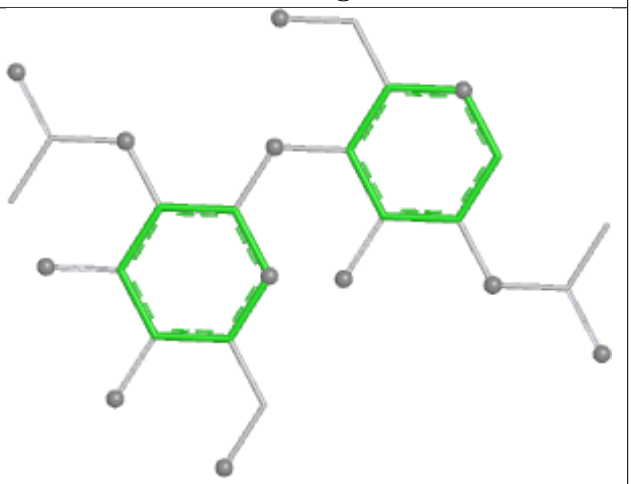


Bond angles

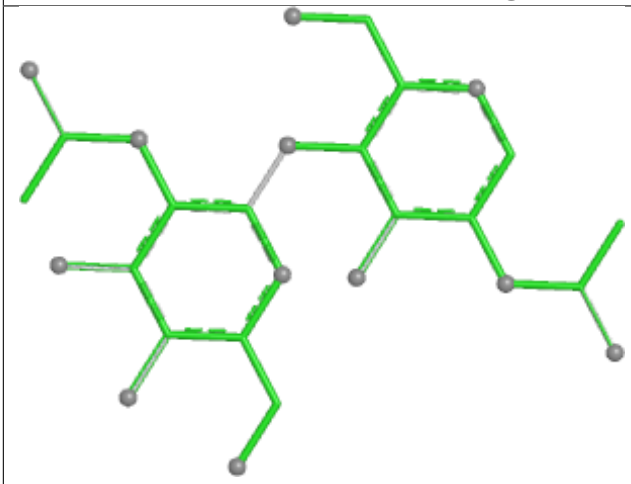


Torsions

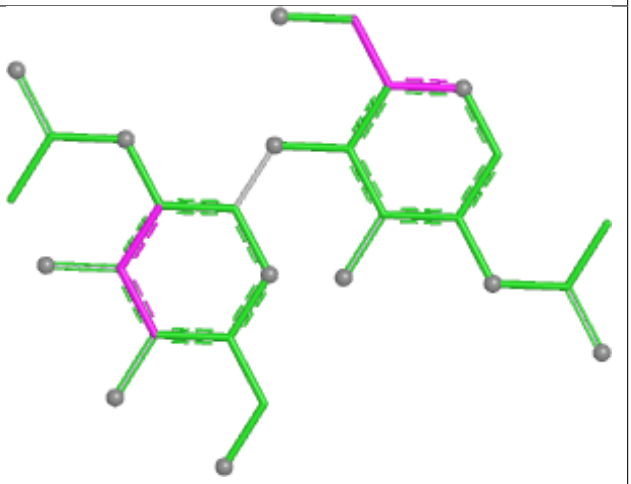


Rings

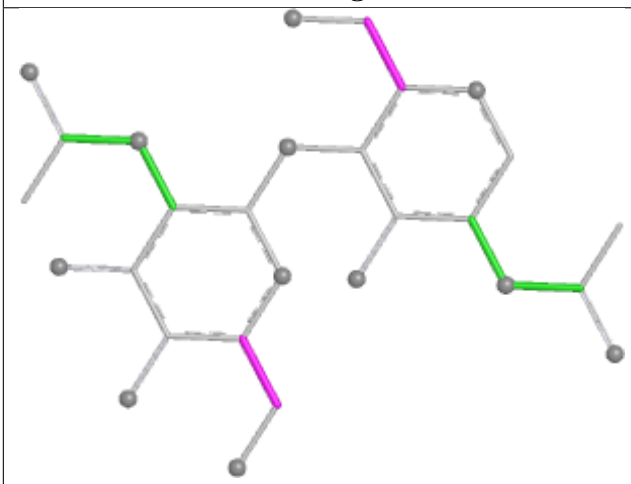
Oligosaccharide Chain i



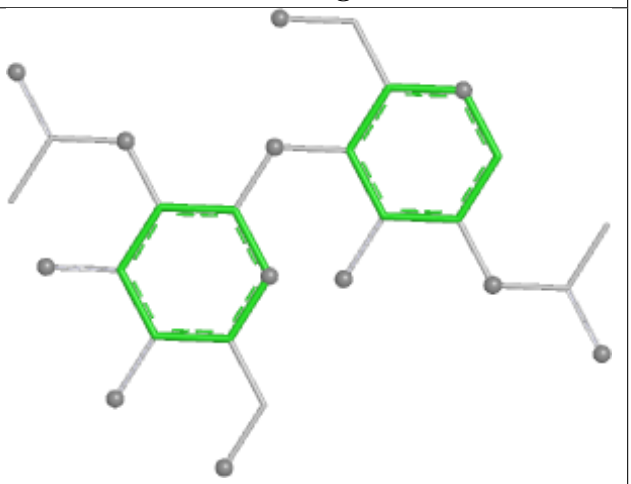
Bond lengths



Bond angles

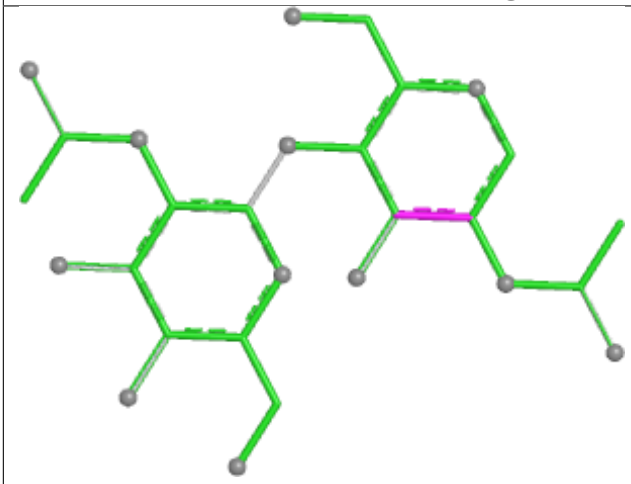


Torsions

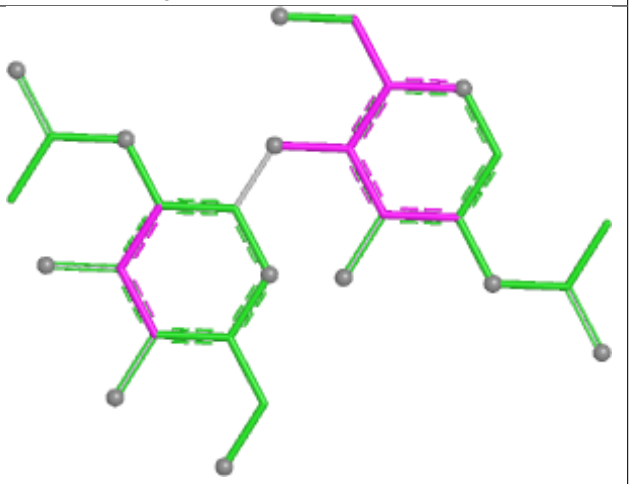


Rings

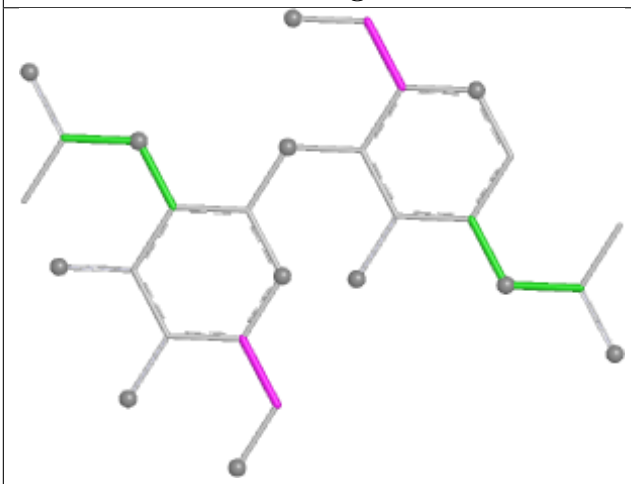
Oligosaccharide Chain j



Bond lengths



Bond angles



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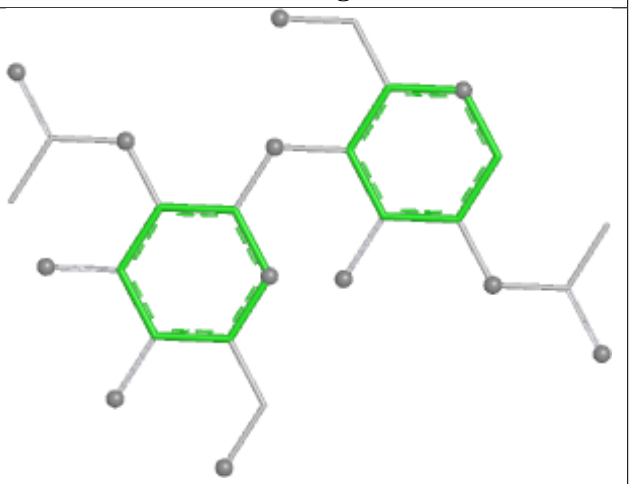
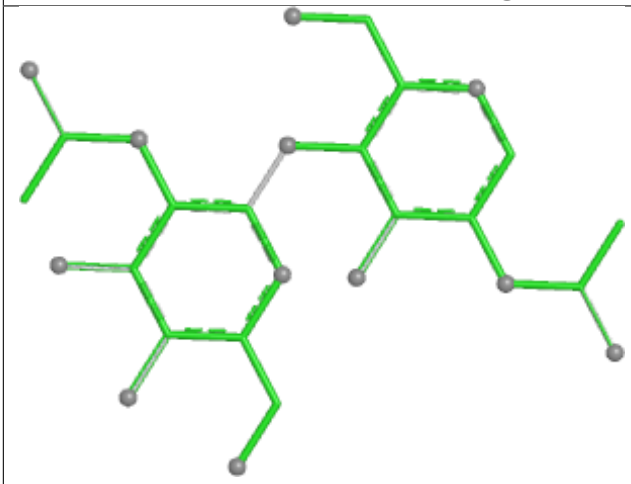
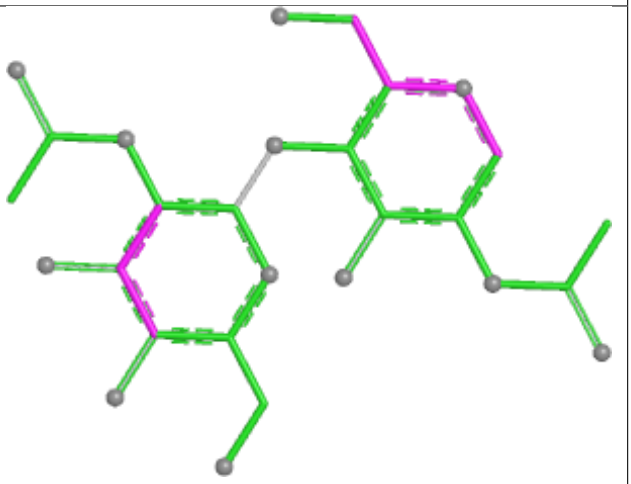


Rings

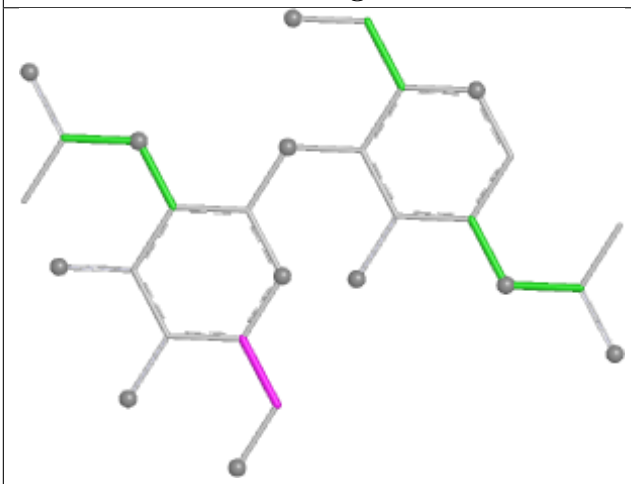
Oligosaccharide Chain k



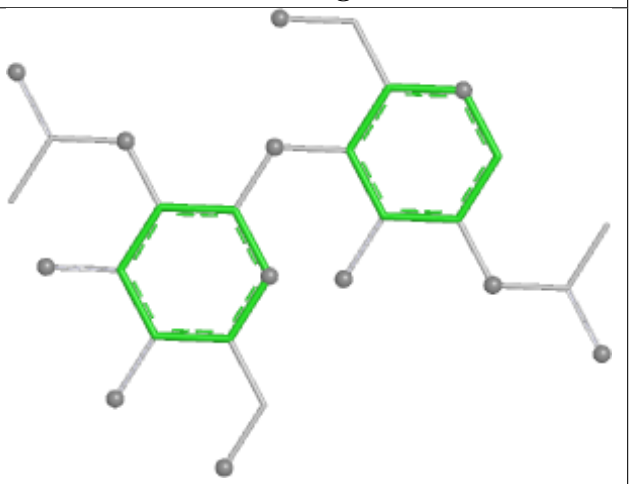
Bond lengths



Bond angles

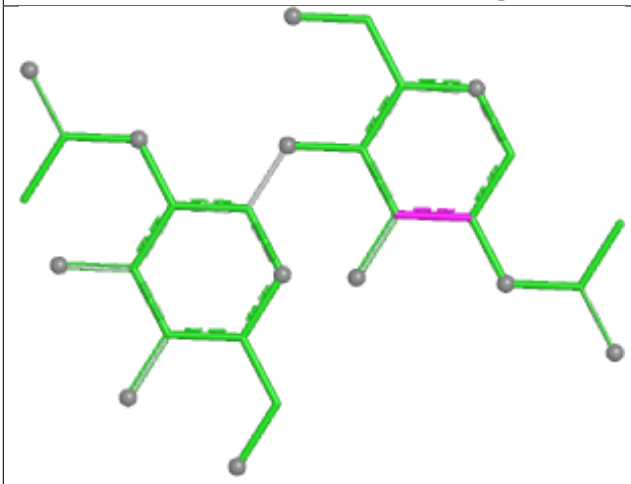


Torsions

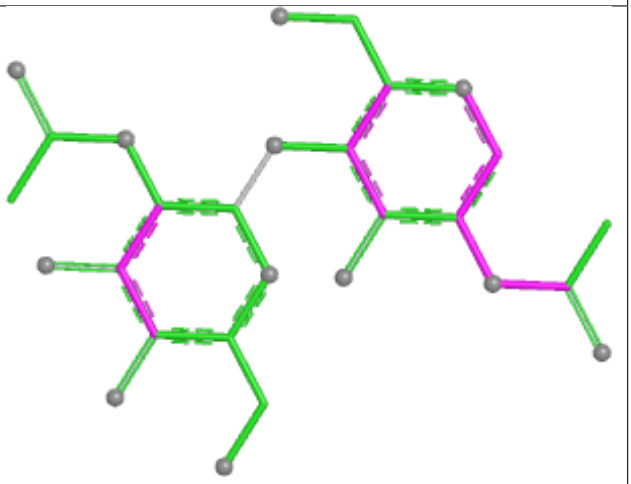


Rings

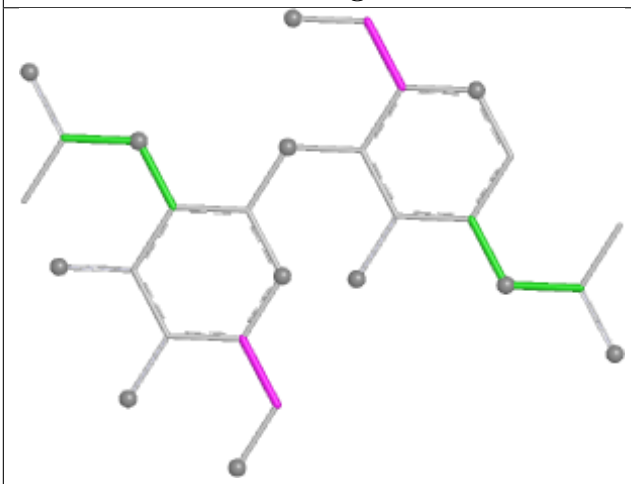
Oligosaccharide Chain m



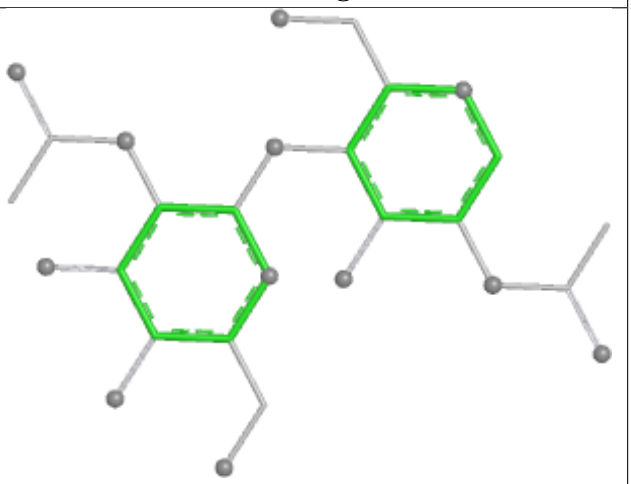
Bond lengths



Bond angles

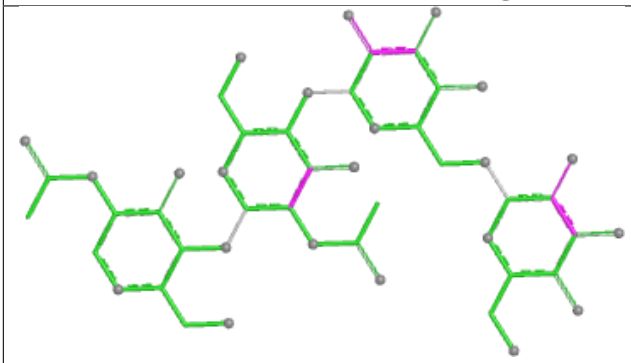


Torsions

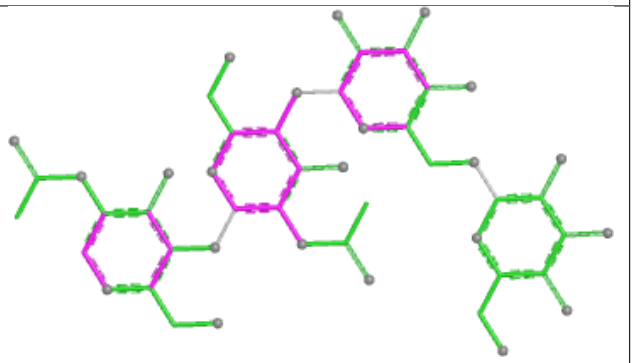


Rings

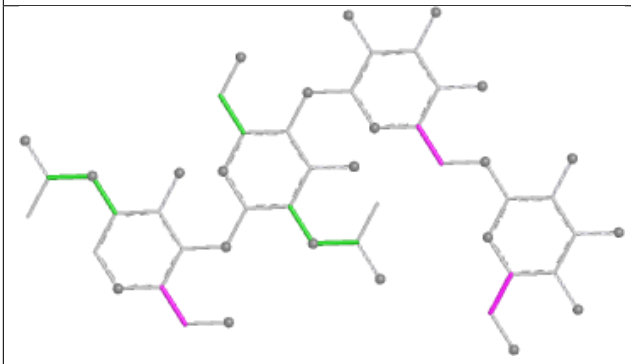
Oligosaccharide Chain L



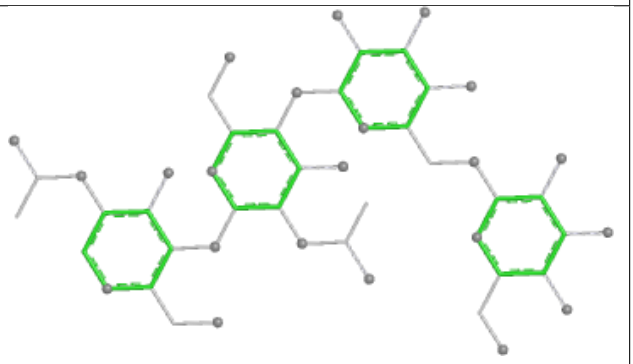
Bond lengths



Bond angles

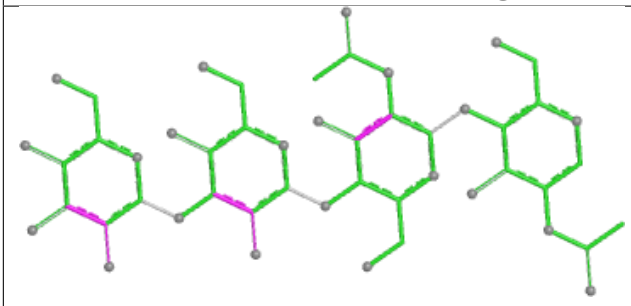


Torsions

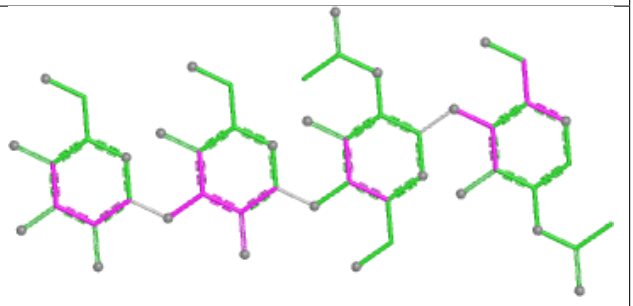


Rings

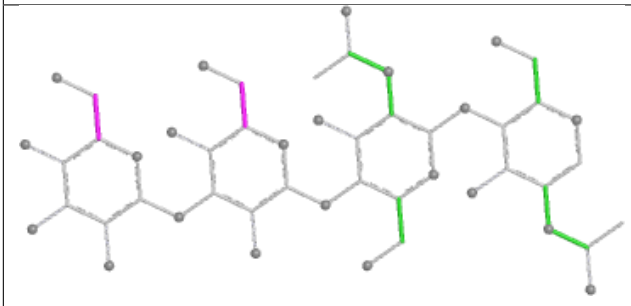
Oligosaccharide Chain R



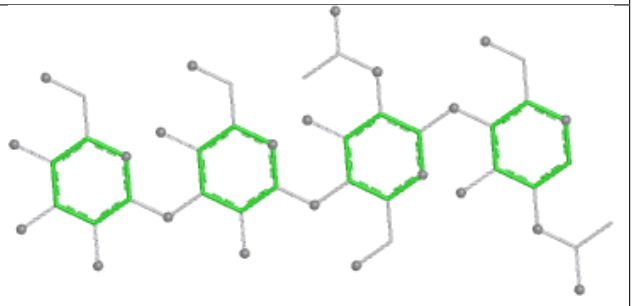
Bond lengths



Bond angles

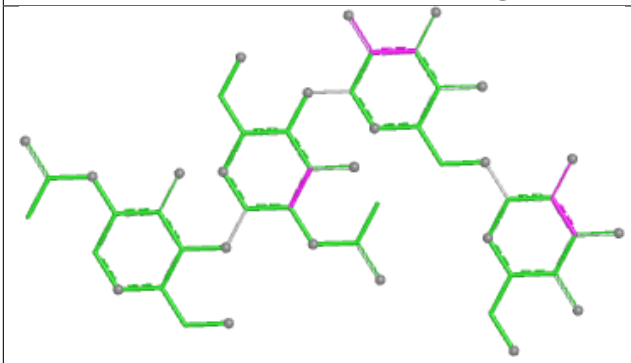


Torsions

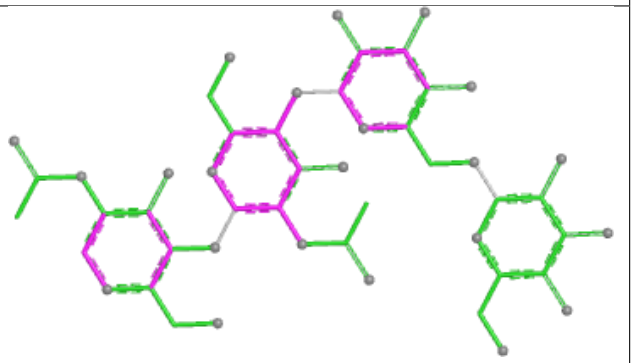


Rings

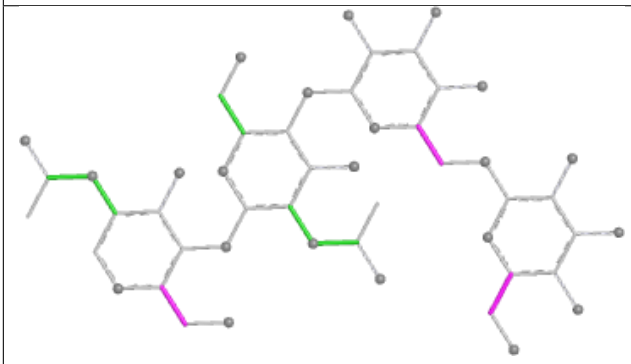
Oligosaccharide Chain V



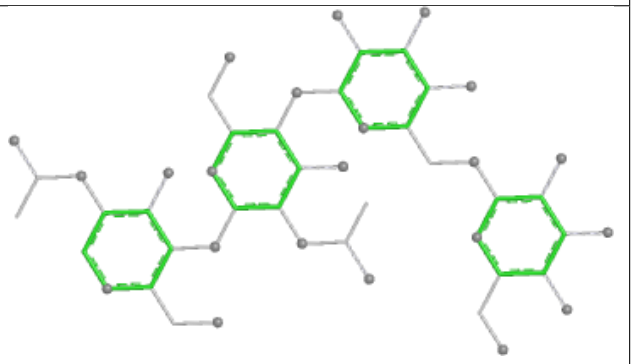
Bond lengths



Bond angles

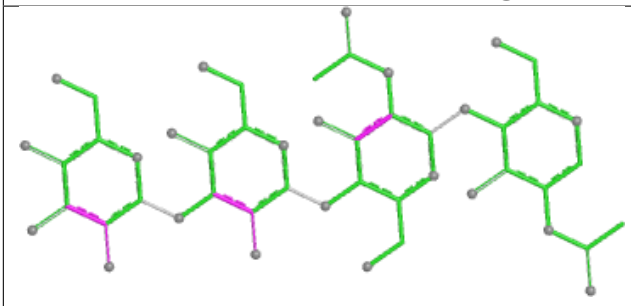


Torsions

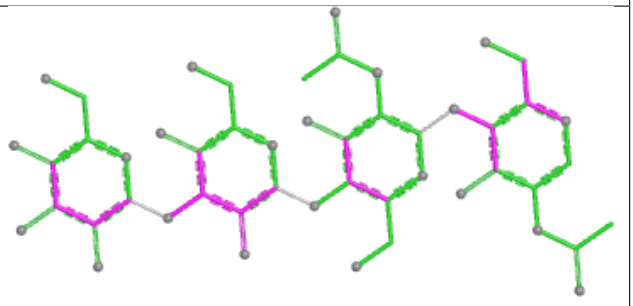


Rings

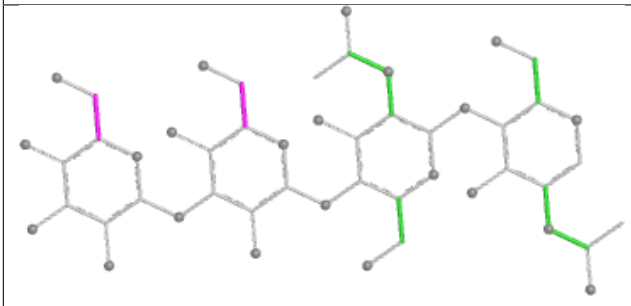
Oligosaccharide Chain b



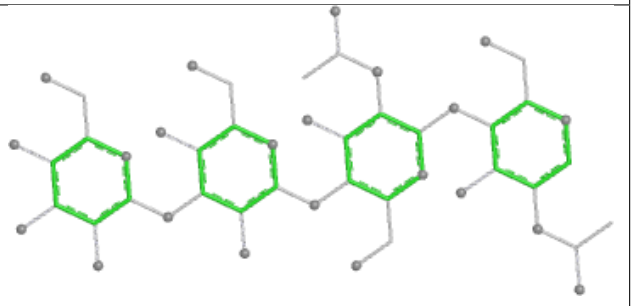
Bond lengths



Bond angles

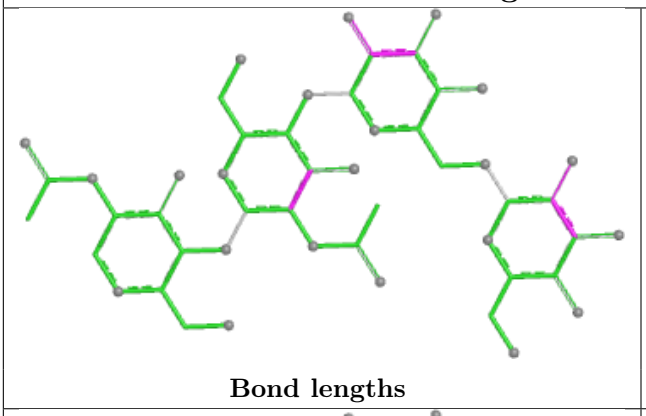


Torsions

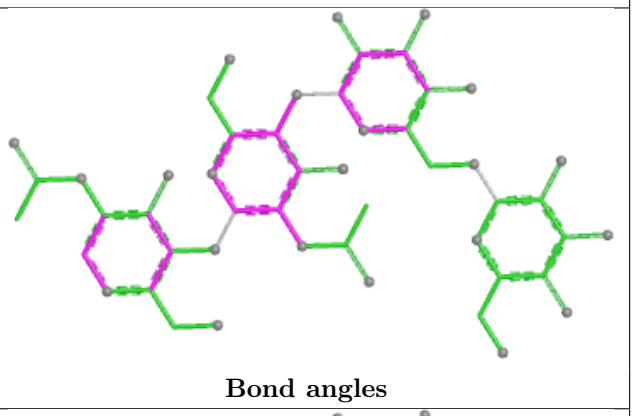


Rings

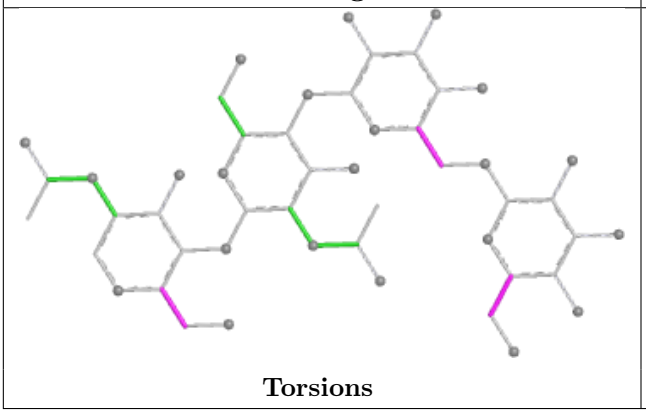
Oligosaccharide Chain f



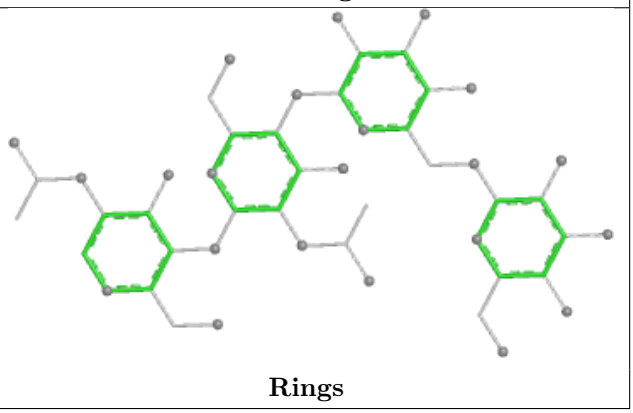
Bond lengths



Bond angles

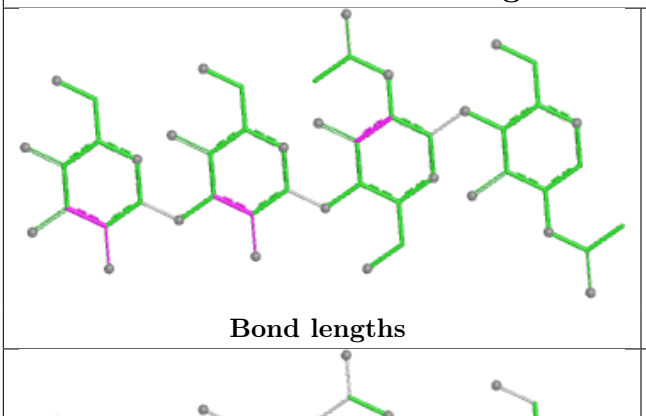


Torsions

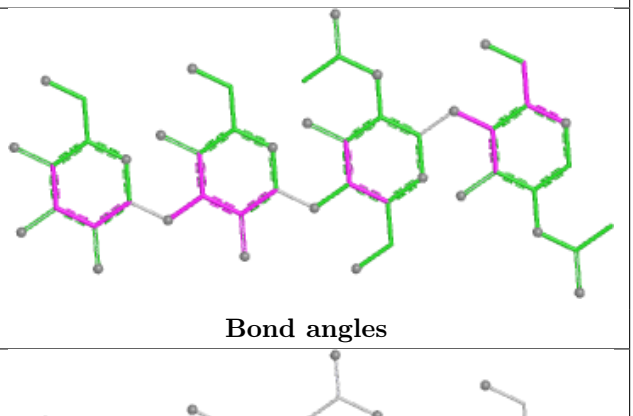


Rings

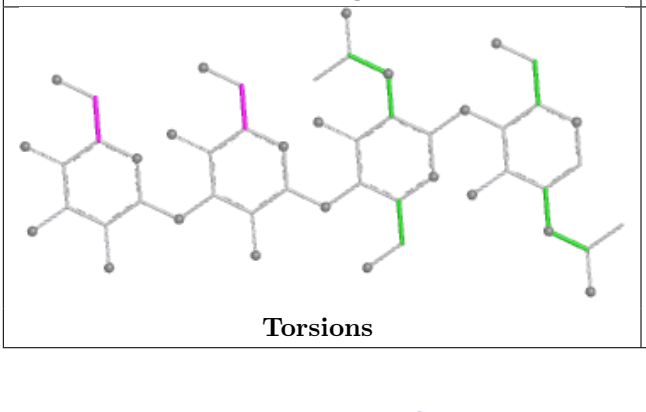
Oligosaccharide Chain l



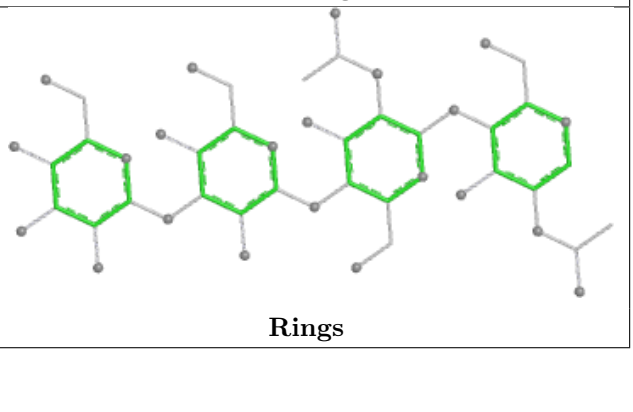
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

36 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	$\#\|Z\| > 2$
6	NAG	C	630	1	14,14,15	0.86	0	17,19,21	0.99	1 (5%)
6	NAG	E	611	1	14,14,15	0.81	1 (7%)	17,19,21	1.02	1 (5%)
6	NAG	A	630	1	14,14,15	0.85	0	17,19,21	0.99	1 (5%)
6	NAG	B	702	2	14,14,15	0.84	0	17,19,21	0.82	1 (5%)
6	NAG	D	703	2	14,14,15	0.83	0	17,19,21	1.22	1 (5%)
6	NAG	A	611	1	14,14,15	0.80	1 (7%)	17,19,21	1.02	1 (5%)
6	NAG	E	625	1	14,14,15	0.88	0	17,19,21	0.98	1 (5%)
6	NAG	E	605	1	14,14,15	0.87	1 (7%)	17,19,21	0.97	2 (11%)
6	NAG	E	612	1	14,14,15	0.85	0	17,19,21	1.22	2 (11%)
6	NAG	B	701	2	14,14,15	0.81	0	17,19,21	0.95	1 (5%)
6	NAG	D	701	2	14,14,15	0.80	0	17,19,21	0.95	1 (5%)
6	NAG	F	701	2	14,14,15	0.81	0	17,19,21	0.95	1 (5%)
6	NAG	F	702	2	14,14,15	0.84	0	17,19,21	0.82	1 (5%)
6	NAG	C	605	1	14,14,15	0.86	1 (7%)	17,19,21	0.98	2 (11%)
6	NAG	B	704	2	14,14,15	0.88	1 (7%)	17,19,21	1.04	1 (5%)
6	NAG	C	619	1	14,14,15	0.82	0	17,19,21	1.25	1 (5%)
6	NAG	B	703	2	14,14,15	0.83	0	17,19,21	1.22	1 (5%)
6	NAG	C	610	1	14,14,15	0.93	1 (7%)	17,19,21	1.14	1 (5%)
6	NAG	C	612	1	14,14,15	0.84	0	17,19,21	1.22	2 (11%)
6	NAG	A	610	1	14,14,15	0.93	1 (7%)	17,19,21	1.14	1 (5%)
6	NAG	C	620	1	14,14,15	0.86	0	17,19,21	0.97	1 (5%)
6	NAG	F	704	2	14,14,15	0.88	1 (7%)	17,19,21	1.04	1 (5%)
6	NAG	E	619	1	14,14,15	0.83	0	17,19,21	1.25	1 (5%)
6	NAG	E	630	1	14,14,15	0.85	0	17,19,21	0.99	1 (5%)
6	NAG	F	703	2	14,14,15	0.83	0	17,19,21	1.22	1 (5%)
6	NAG	E	610	1	14,14,15	0.93	1 (7%)	17,19,21	1.14	1 (5%)
6	NAG	D	702	2	14,14,15	0.84	0	17,19,21	0.82	1 (5%)
6	NAG	A	605	1	14,14,15	0.86	1 (7%)	17,19,21	0.98	2 (11%)
6	NAG	A	620	1	14,14,15	0.86	0	17,19,21	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	625	1	14,14,15	0.87	0	17,19,21	0.98	1 (5%)
6	NAG	D	704	2	14,14,15	0.87	1 (7%)	17,19,21	1.04	1 (5%)
6	NAG	C	611	1	14,14,15	0.81	1 (7%)	17,19,21	1.02	1 (5%)
6	NAG	A	619	1	14,14,15	0.82	0	17,19,21	1.25	1 (5%)
6	NAG	E	620	1	14,14,15	0.87	0	17,19,21	0.98	1 (5%)
6	NAG	A	612	1	14,14,15	0.84	0	17,19,21	1.22	2 (11%)
6	NAG	C	625	1	14,14,15	0.88	0	17,19,21	0.97	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	630	1	-	1/6/23/26	0/1/1/1
6	NAG	E	611	1	-	1/6/23/26	0/1/1/1
6	NAG	A	630	1	-	1/6/23/26	0/1/1/1
6	NAG	B	702	2	-	2/6/23/26	0/1/1/1
6	NAG	D	703	2	-	2/6/23/26	0/1/1/1
6	NAG	A	611	1	-	1/6/23/26	0/1/1/1
6	NAG	E	625	1	-	1/6/23/26	0/1/1/1
6	NAG	E	605	1	-	1/6/23/26	0/1/1/1
6	NAG	E	612	1	-	2/6/23/26	0/1/1/1
6	NAG	B	701	2	-	1/6/23/26	0/1/1/1
6	NAG	D	701	2	-	1/6/23/26	0/1/1/1
6	NAG	F	701	2	-	1/6/23/26	0/1/1/1
6	NAG	F	702	2	-	2/6/23/26	0/1/1/1
6	NAG	C	605	1	-	1/6/23/26	0/1/1/1
6	NAG	B	704	2	-	1/6/23/26	0/1/1/1
6	NAG	C	619	1	-	1/6/23/26	0/1/1/1
6	NAG	B	703	2	-	2/6/23/26	0/1/1/1
6	NAG	C	610	1	-	2/6/23/26	0/1/1/1
6	NAG	C	612	1	-	2/6/23/26	0/1/1/1
6	NAG	A	610	1	-	2/6/23/26	0/1/1/1
6	NAG	C	620	1	-	1/6/23/26	0/1/1/1
6	NAG	F	704	2	-	1/6/23/26	0/1/1/1
6	NAG	E	619	1	-	1/6/23/26	0/1/1/1
6	NAG	E	630	1	-	1/6/23/26	0/1/1/1
6	NAG	F	703	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	610	1	-	2/6/23/26	0/1/1/1
6	NAG	D	702	2	-	2/6/23/26	0/1/1/1
6	NAG	A	605	1	-	1/6/23/26	0/1/1/1
6	NAG	A	620	1	-	1/6/23/26	0/1/1/1
6	NAG	A	625	1	-	1/6/23/26	0/1/1/1
6	NAG	D	704	2	-	1/6/23/26	0/1/1/1
6	NAG	C	611	1	-	1/6/23/26	0/1/1/1
6	NAG	A	619	1	-	1/6/23/26	0/1/1/1
6	NAG	E	620	1	-	1/6/23/26	0/1/1/1
6	NAG	A	612	1	-	2/6/23/26	0/1/1/1
6	NAG	C	625	1	-	1/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	610	NAG	C3-C2	-2.19	1.47	1.52
6	E	610	NAG	C3-C2	-2.19	1.47	1.52
6	A	610	NAG	C3-C2	-2.19	1.47	1.52
6	F	704	NAG	C3-C2	-2.07	1.48	1.52
6	B	704	NAG	C3-C2	-2.06	1.48	1.52
6	A	605	NAG	C3-C2	-2.05	1.48	1.52
6	C	605	NAG	C3-C2	-2.05	1.48	1.52
6	C	611	NAG	C3-C2	-2.05	1.48	1.52
6	E	605	NAG	C3-C2	-2.05	1.48	1.52
6	A	611	NAG	C3-C2	-2.04	1.48	1.52
6	E	611	NAG	C3-C2	-2.04	1.48	1.52
6	D	704	NAG	C3-C2	-2.01	1.48	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	619	NAG	C4-C3-C2	-3.91	105.29	111.02
6	C	619	NAG	C4-C3-C2	-3.90	105.30	111.02
6	E	619	NAG	C4-C3-C2	-3.90	105.30	111.02
6	D	703	NAG	C4-C3-C2	-3.71	105.58	111.02
6	F	703	NAG	C4-C3-C2	-3.70	105.59	111.02
6	B	703	NAG	C4-C3-C2	-3.70	105.60	111.02
6	A	612	NAG	C4-C3-C2	-3.36	106.09	111.02
6	C	612	NAG	C4-C3-C2	-3.36	106.10	111.02
6	E	612	NAG	C4-C3-C2	-3.36	106.10	111.02
6	C	610	NAG	C4-C3-C2	-3.18	106.36	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	610	NAG	C4-C3-C2	-3.18	106.36	111.02
6	A	610	NAG	C4-C3-C2	-3.17	106.36	111.02
6	F	704	NAG	C4-C3-C2	-3.15	106.41	111.02
6	D	704	NAG	C4-C3-C2	-3.14	106.41	111.02
6	B	704	NAG	C4-C3-C2	-3.14	106.41	111.02
6	A	625	NAG	C4-C3-C2	-2.99	106.64	111.02
6	E	625	NAG	C4-C3-C2	-2.98	106.65	111.02
6	C	625	NAG	C4-C3-C2	-2.97	106.67	111.02
6	E	620	NAG	C4-C3-C2	-2.83	106.87	111.02
6	C	620	NAG	C4-C3-C2	-2.82	106.88	111.02
6	A	620	NAG	C4-C3-C2	-2.82	106.89	111.02
6	A	630	NAG	C4-C3-C2	-2.72	107.03	111.02
6	E	630	NAG	C4-C3-C2	-2.71	107.05	111.02
6	C	630	NAG	C4-C3-C2	-2.69	107.07	111.02
6	C	611	NAG	C4-C3-C2	-2.51	107.34	111.02
6	A	611	NAG	C4-C3-C2	-2.50	107.35	111.02
6	C	605	NAG	C4-C3-C2	-2.50	107.35	111.02
6	E	611	NAG	C4-C3-C2	-2.50	107.35	111.02
6	A	605	NAG	C4-C3-C2	-2.49	107.37	111.02
6	E	605	NAG	C4-C3-C2	-2.47	107.39	111.02
6	E	612	NAG	O5-C1-C2	-2.38	107.61	111.29
6	A	612	NAG	O5-C1-C2	-2.37	107.62	111.29
6	C	612	NAG	O5-C1-C2	-2.37	107.63	111.29
6	D	701	NAG	C4-C3-C2	-2.29	107.66	111.02
6	B	701	NAG	C4-C3-C2	-2.28	107.67	111.02
6	F	701	NAG	C4-C3-C2	-2.28	107.68	111.02
6	D	702	NAG	C4-C3-C2	-2.03	108.05	111.02
6	B	702	NAG	C4-C3-C2	-2.02	108.06	111.02
6	A	605	NAG	O5-C1-C2	-2.02	108.17	111.29
6	C	605	NAG	O5-C1-C2	-2.01	108.17	111.29
6	F	702	NAG	C4-C3-C2	-2.01	108.07	111.02
6	E	605	NAG	O5-C1-C2	-2.01	108.18	111.29

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	610	NAG	O5-C5-C6-O6
6	C	610	NAG	O5-C5-C6-O6
6	E	610	NAG	O5-C5-C6-O6
6	A	612	NAG	O5-C5-C6-O6
6	C	612	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	E	612	NAG	O5-C5-C6-O6
6	B	702	NAG	O5-C5-C6-O6
6	B	703	NAG	O5-C5-C6-O6
6	D	702	NAG	O5-C5-C6-O6
6	D	703	NAG	O5-C5-C6-O6
6	F	702	NAG	O5-C5-C6-O6
6	F	703	NAG	O5-C5-C6-O6
6	A	605	NAG	O5-C5-C6-O6
6	A	611	NAG	O5-C5-C6-O6
6	C	605	NAG	O5-C5-C6-O6
6	C	611	NAG	O5-C5-C6-O6
6	E	605	NAG	O5-C5-C6-O6
6	E	611	NAG	O5-C5-C6-O6
6	A	610	NAG	C4-C5-C6-O6
6	C	610	NAG	C4-C5-C6-O6
6	E	610	NAG	C4-C5-C6-O6
6	B	701	NAG	O5-C5-C6-O6
6	D	701	NAG	O5-C5-C6-O6
6	F	701	NAG	O5-C5-C6-O6
6	A	619	NAG	O5-C5-C6-O6
6	C	619	NAG	O5-C5-C6-O6
6	E	619	NAG	O5-C5-C6-O6
6	A	625	NAG	O5-C5-C6-O6
6	C	625	NAG	O5-C5-C6-O6
6	E	625	NAG	O5-C5-C6-O6
6	A	612	NAG	C4-C5-C6-O6
6	C	612	NAG	C4-C5-C6-O6
6	E	612	NAG	C4-C5-C6-O6
6	B	704	NAG	O5-C5-C6-O6
6	D	704	NAG	O5-C5-C6-O6
6	F	704	NAG	O5-C5-C6-O6
6	A	630	NAG	O5-C5-C6-O6
6	C	630	NAG	O5-C5-C6-O6
6	E	630	NAG	O5-C5-C6-O6
6	A	620	NAG	O5-C5-C6-O6
6	C	620	NAG	O5-C5-C6-O6
6	E	620	NAG	O5-C5-C6-O6
6	B	703	NAG	C4-C5-C6-O6
6	D	703	NAG	C4-C5-C6-O6
6	F	703	NAG	C4-C5-C6-O6
6	F	702	NAG	C4-C5-C6-O6
6	B	702	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	D	702	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

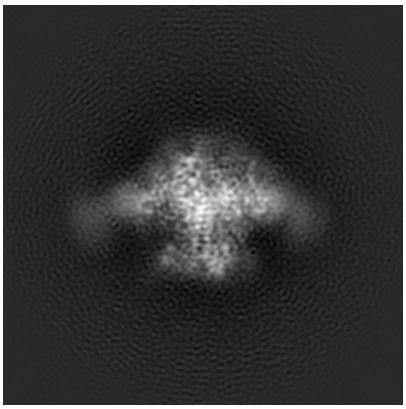
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20500. These allow visual inspection of the internal detail of the map and identification of artifacts.

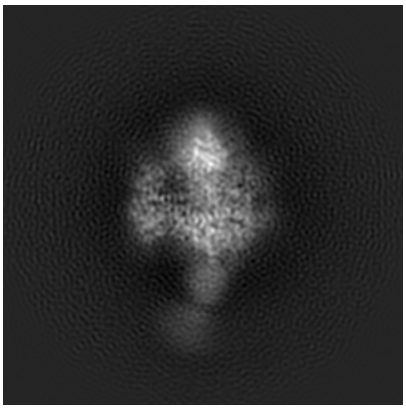
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

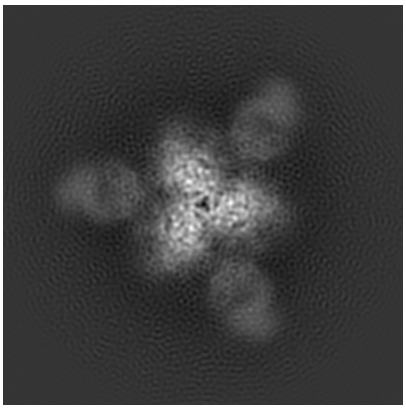
6.1.1 Primary map



X

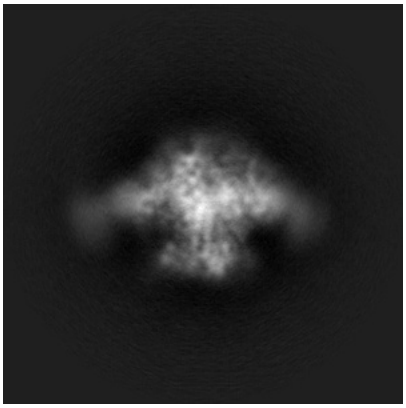


Y

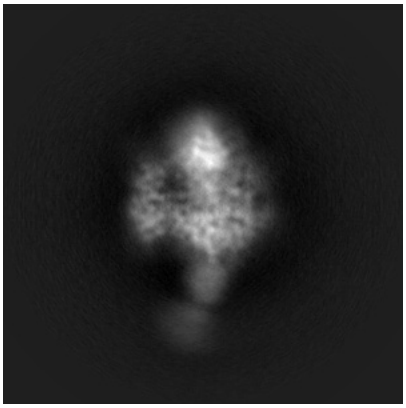


Z

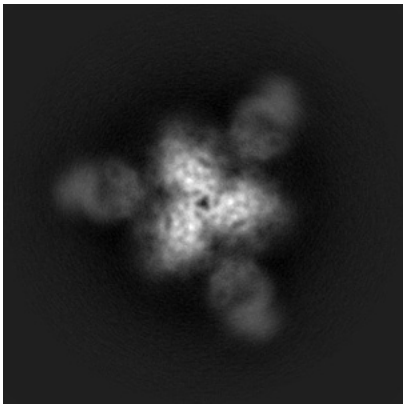
6.1.2 Raw map



X



Y

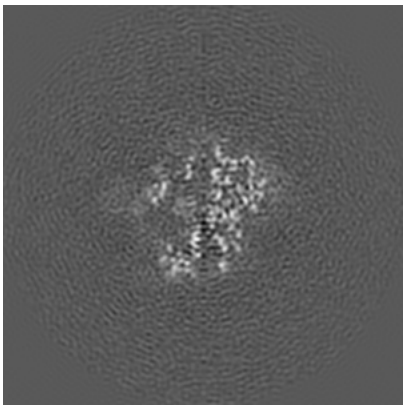


Z

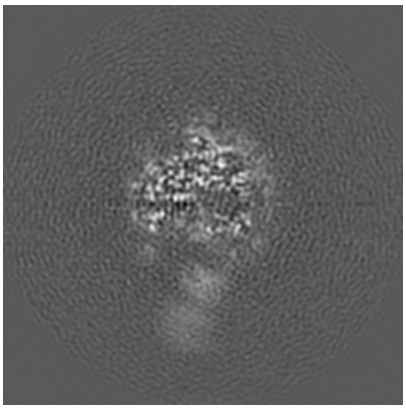
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

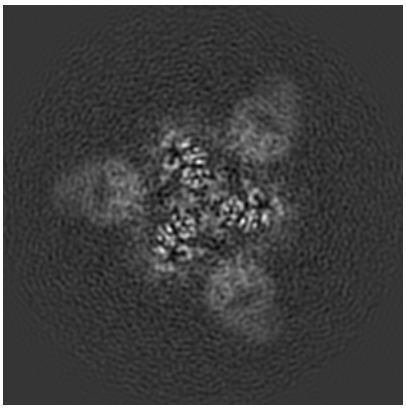
6.2.1 Primary map



X Index: 140

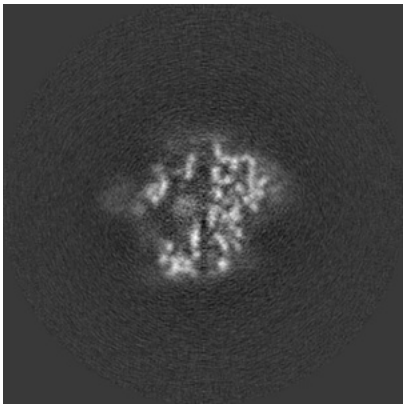


Y Index: 140

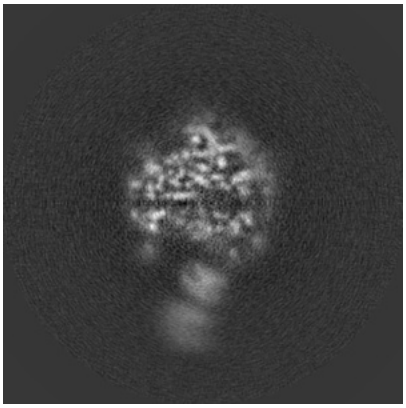


Z Index: 140

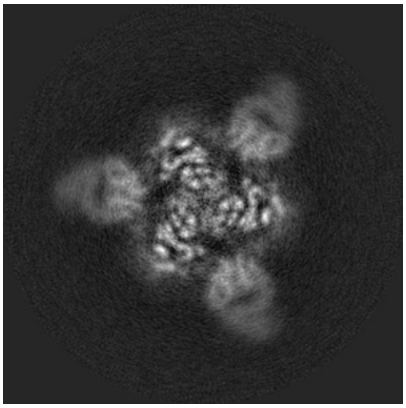
6.2.2 Raw map



X Index: 140



Y Index: 140

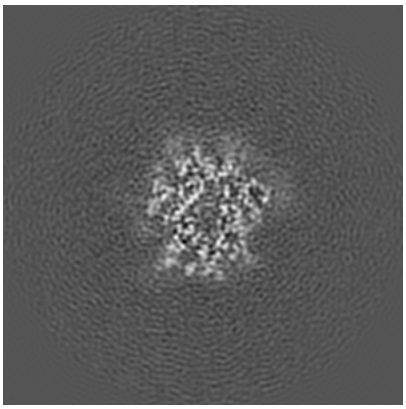


Z Index: 140

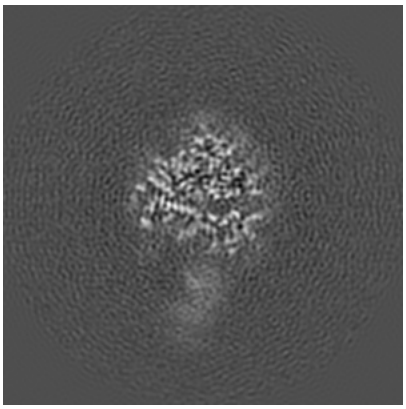
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

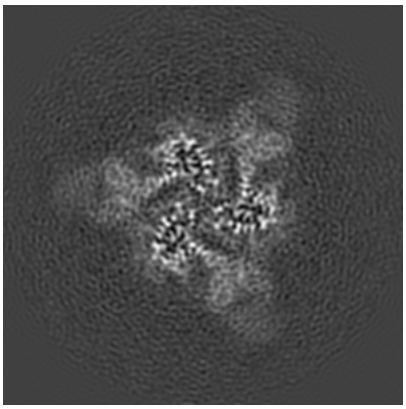
6.3.1 Primary map



X Index: 131

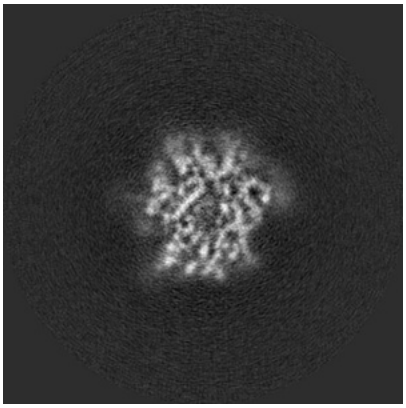


Y Index: 135

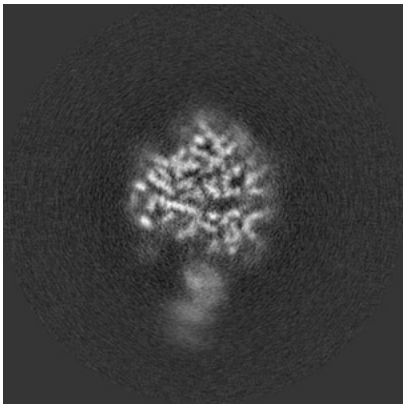


Z Index: 144

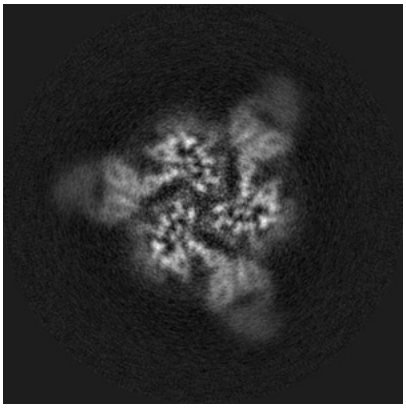
6.3.2 Raw map



X Index: 131



Y Index: 135

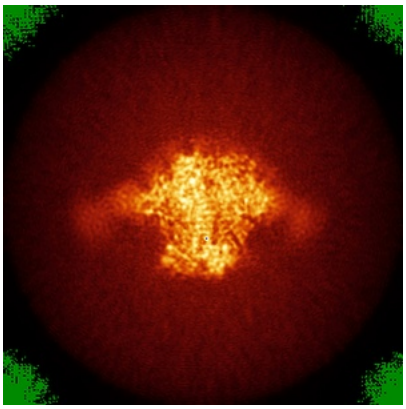


Z Index: 144

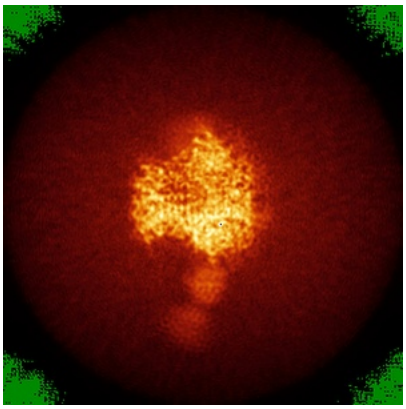
The images above show the largest variance slices of the map in three orthogonal directions.

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

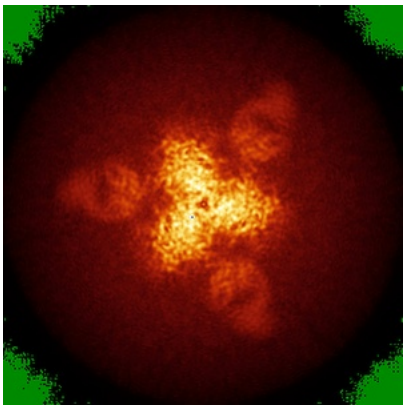
6.4.1 Primary map



X

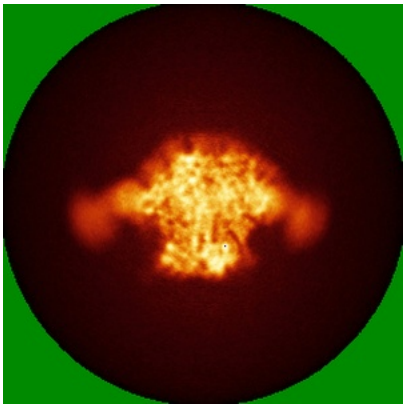


Y

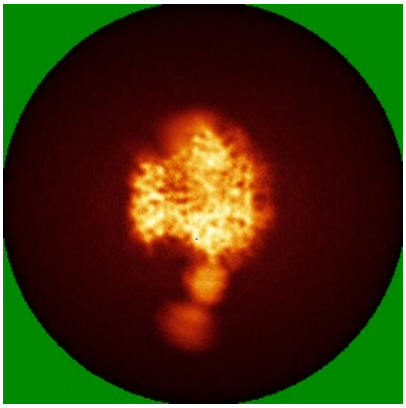


Z

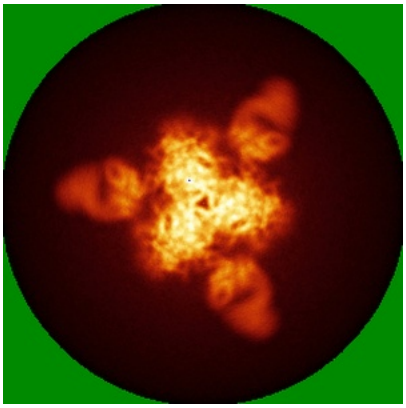
6.4.2 Raw map



X



Y



Z

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

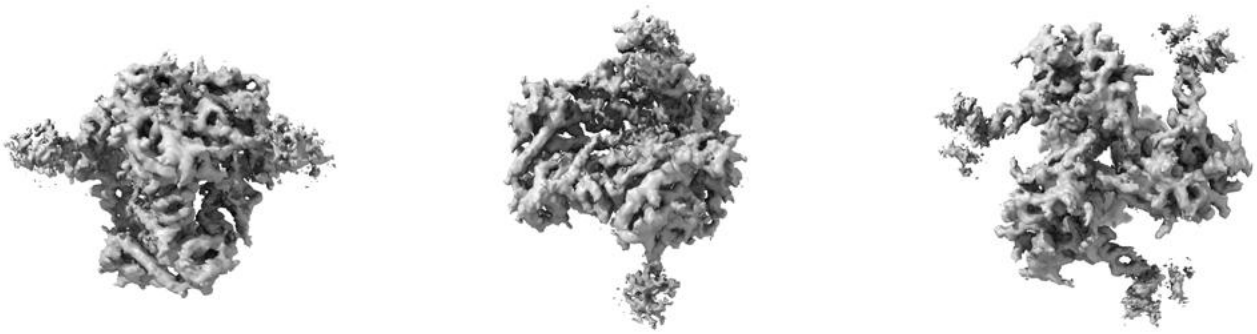
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

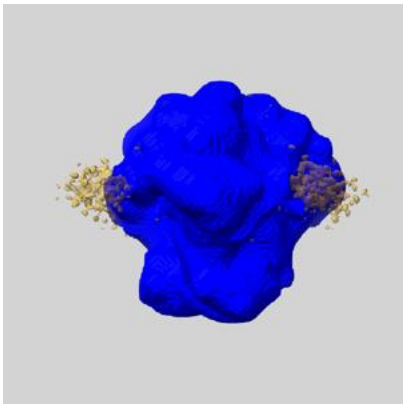
6.6 Mask visualisation

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

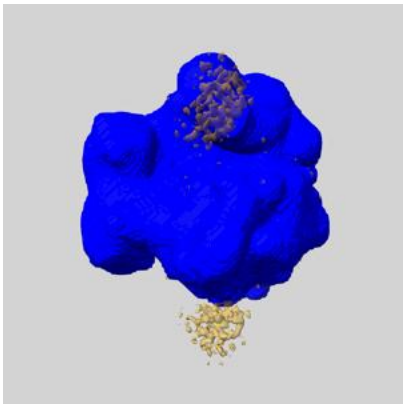
A mask typically either:

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

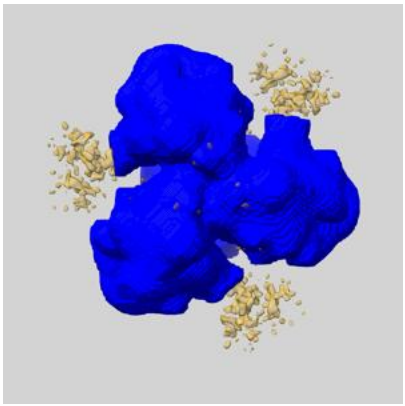
6.6.1 emd_20500_msk_1.map



X



Y

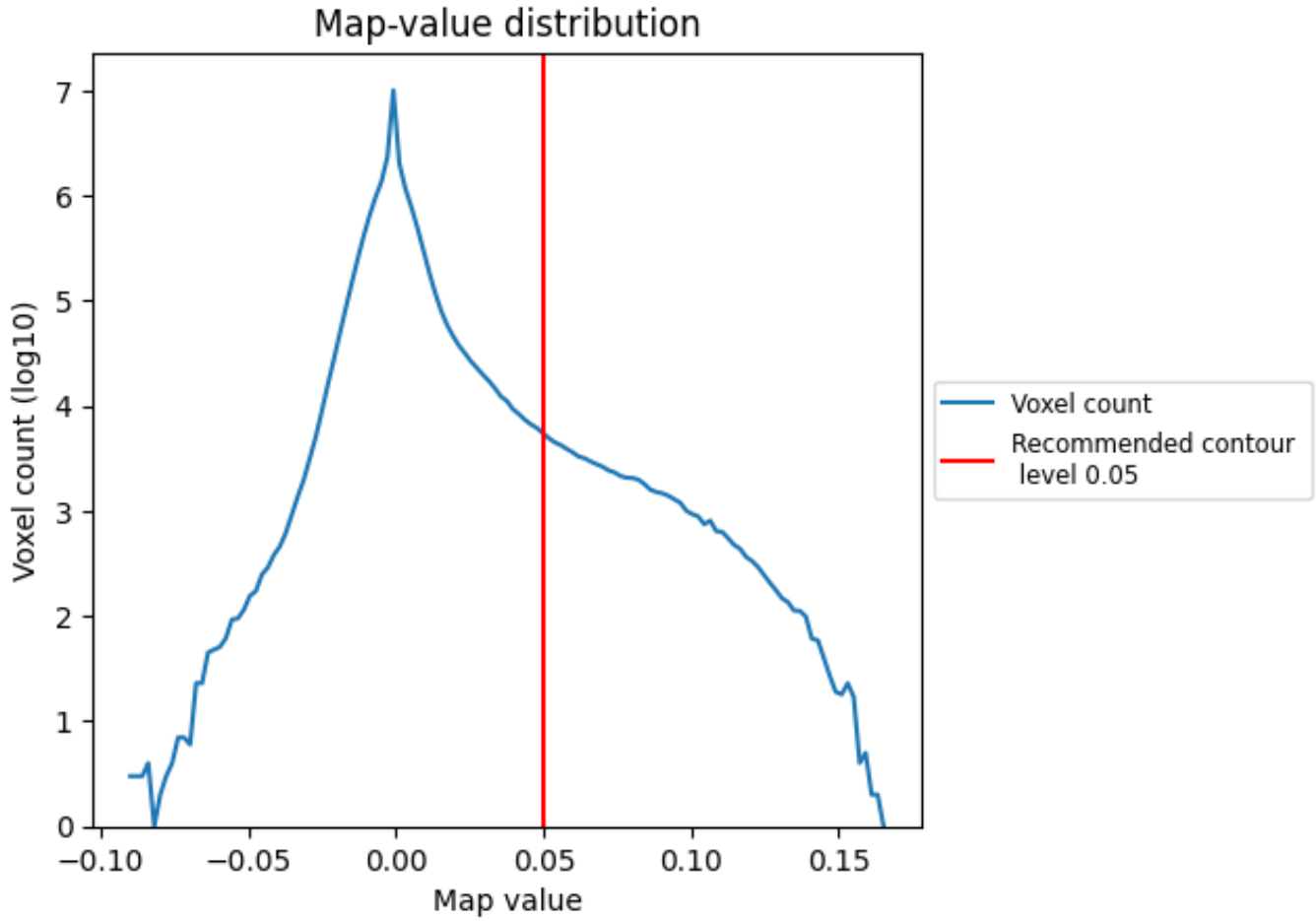


Z

7 Map analysis

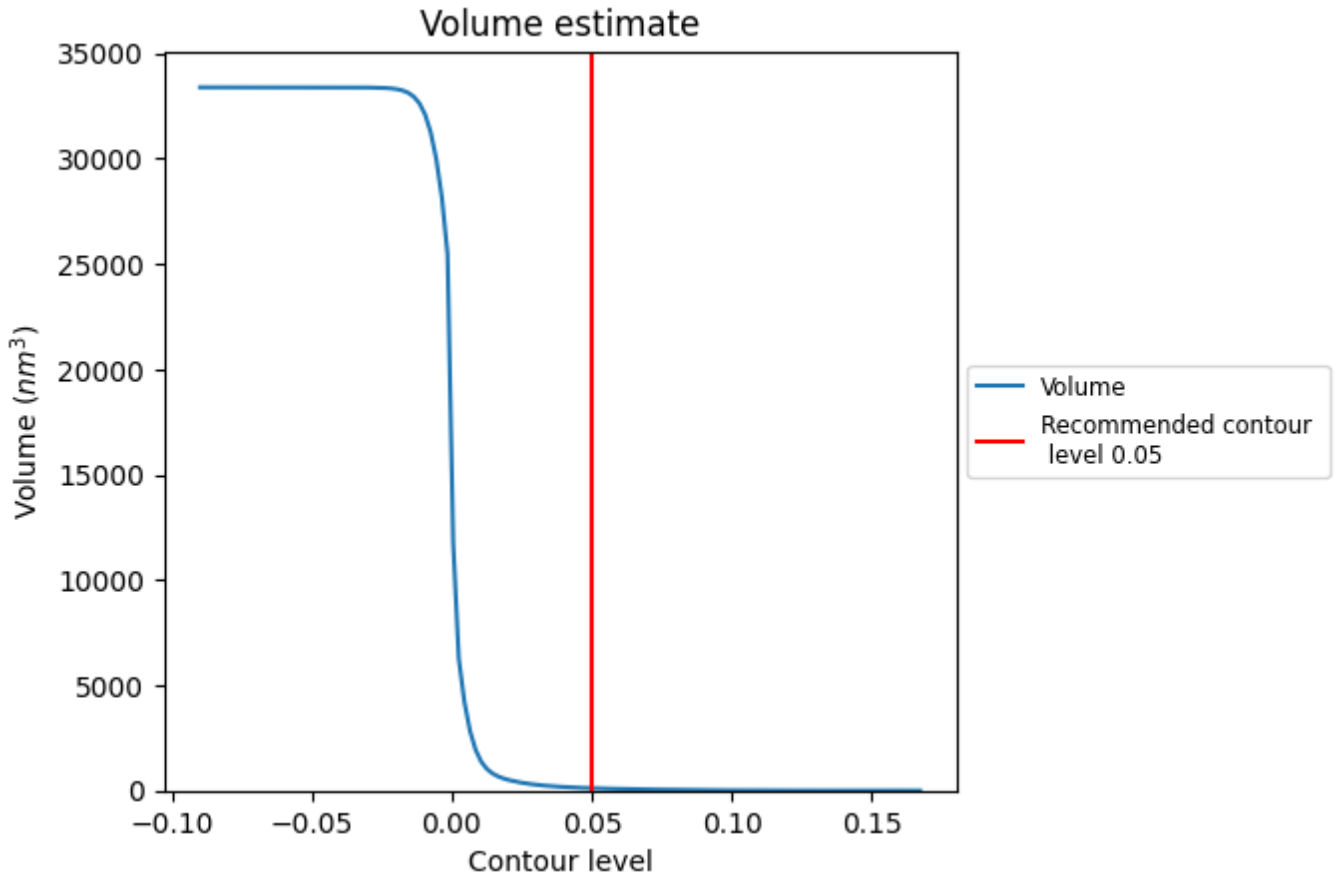
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

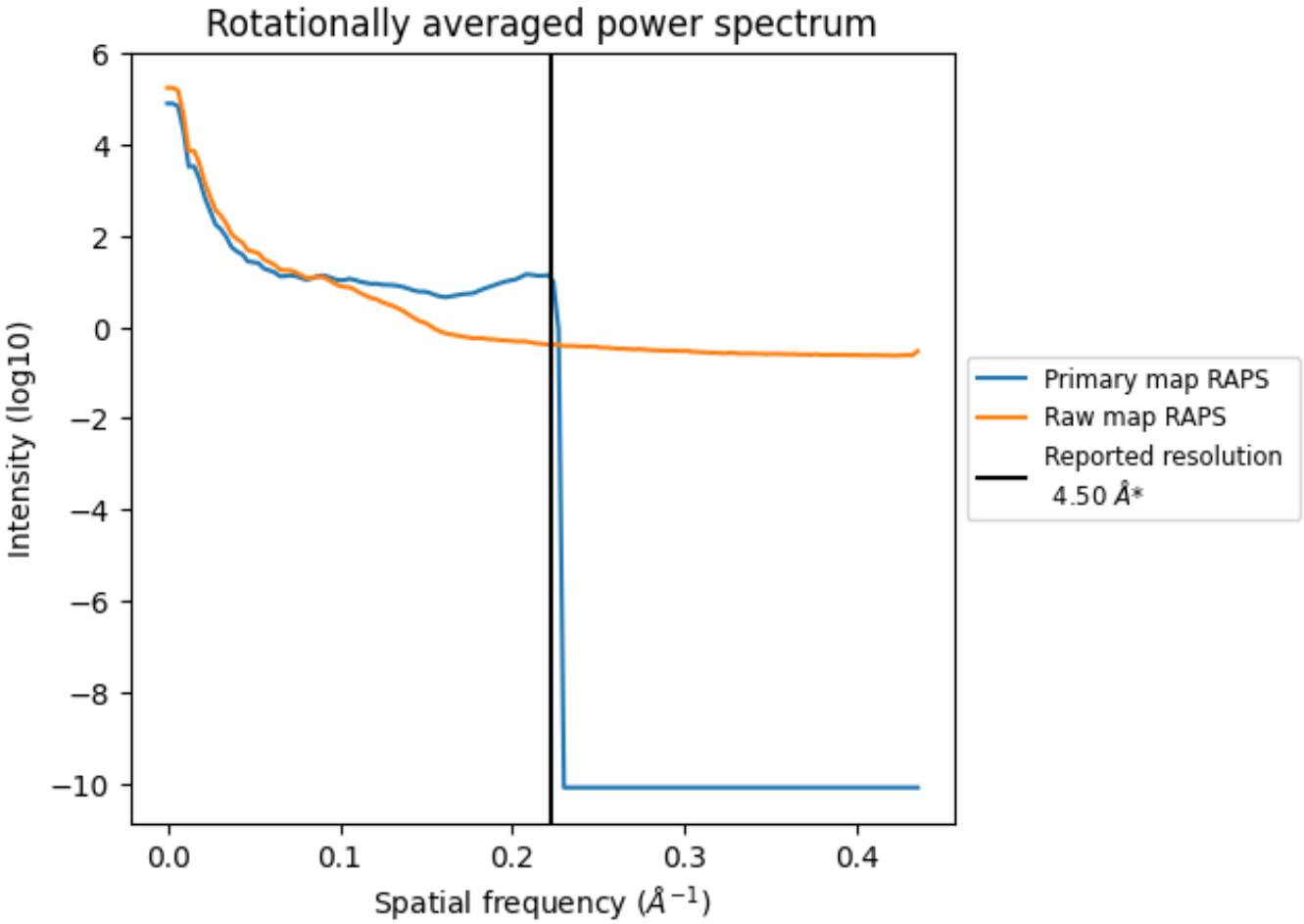
7.2 Volume estimate



The volume at the recommended contour level is 113 nm^3; this corresponds to an approximate mass of 102 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)

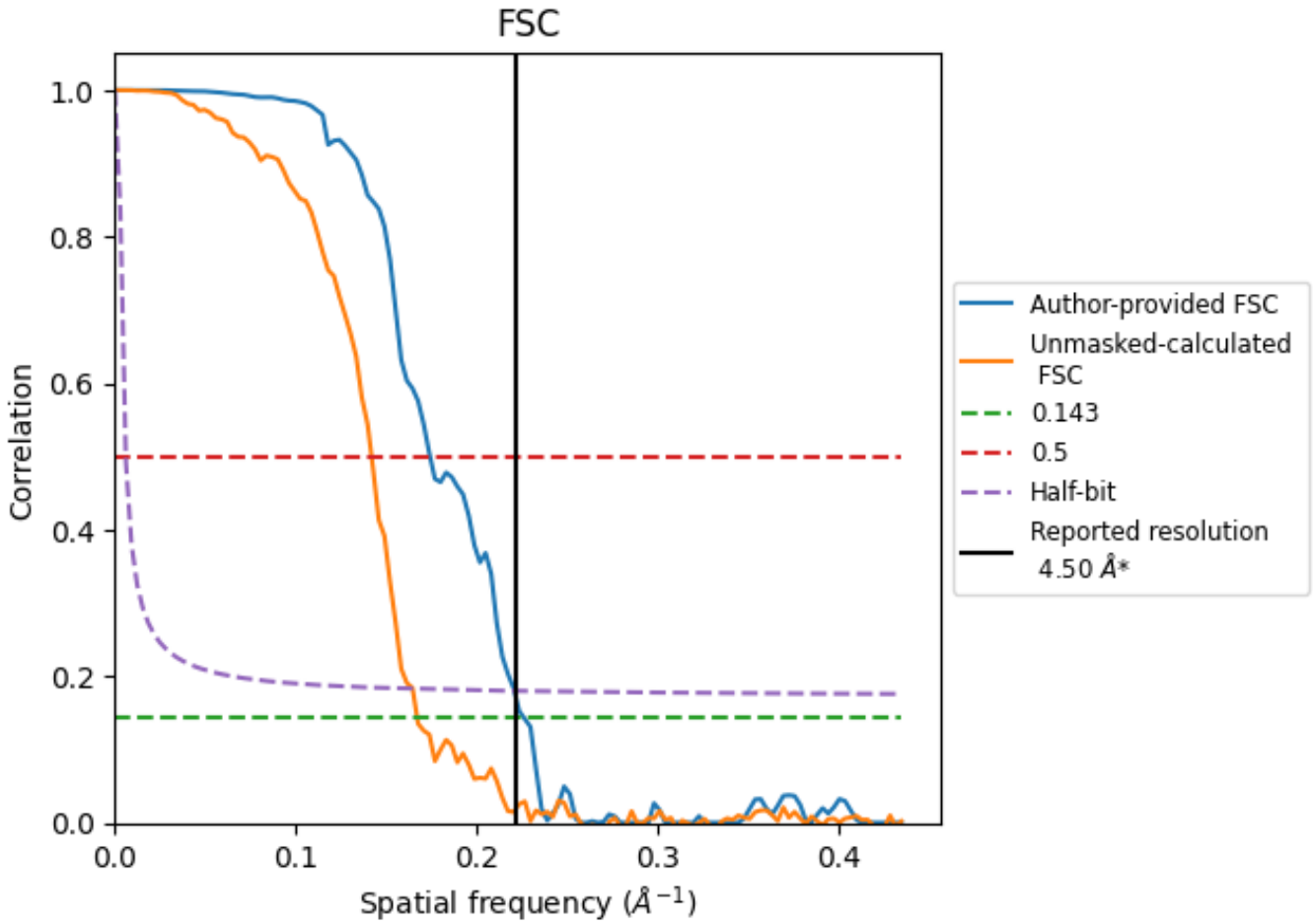


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8.2 Resolution estimates (i)

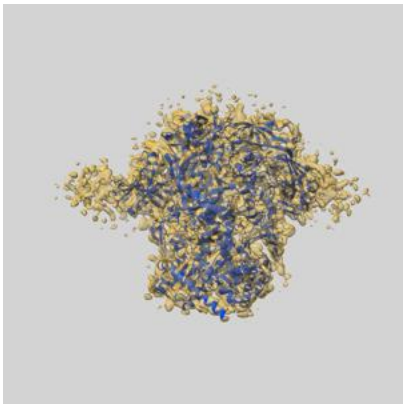
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.42	5.74	4.53
Unmasked-calculated*	5.98	7.05	6.07

*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 5.98 differs from the reported value 4.5 by more than 10 %

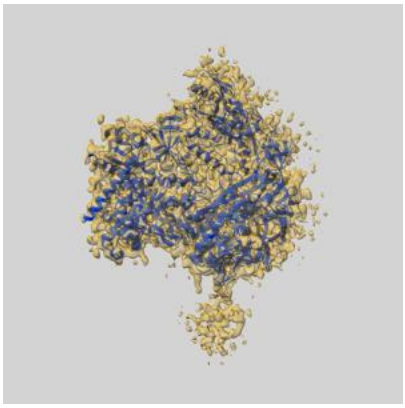
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20500 and PDB model 6PW6. Per-residue inclusion information can be found in section 3 on page 14.

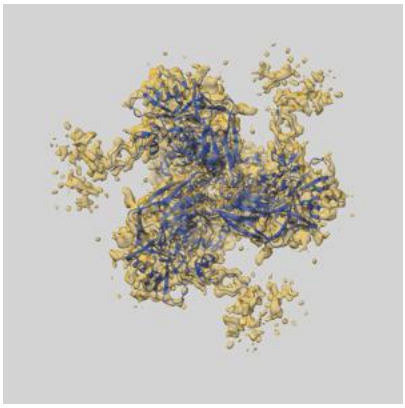
9.1 Map-model overlay



X



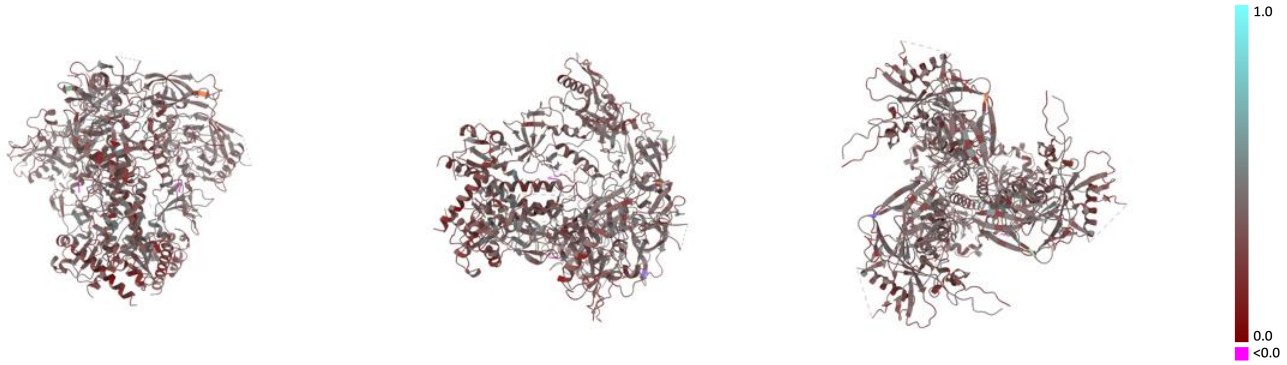
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

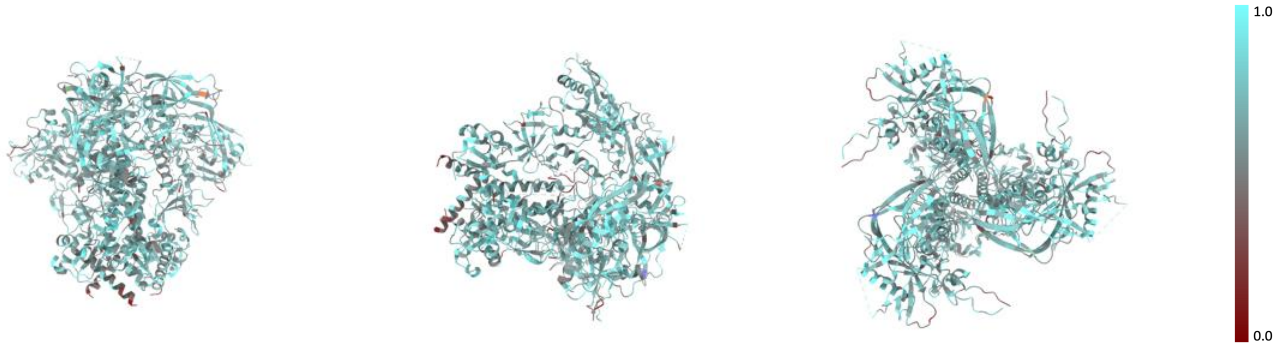
9.2 Q-score mapped to coordinate model (i)



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.

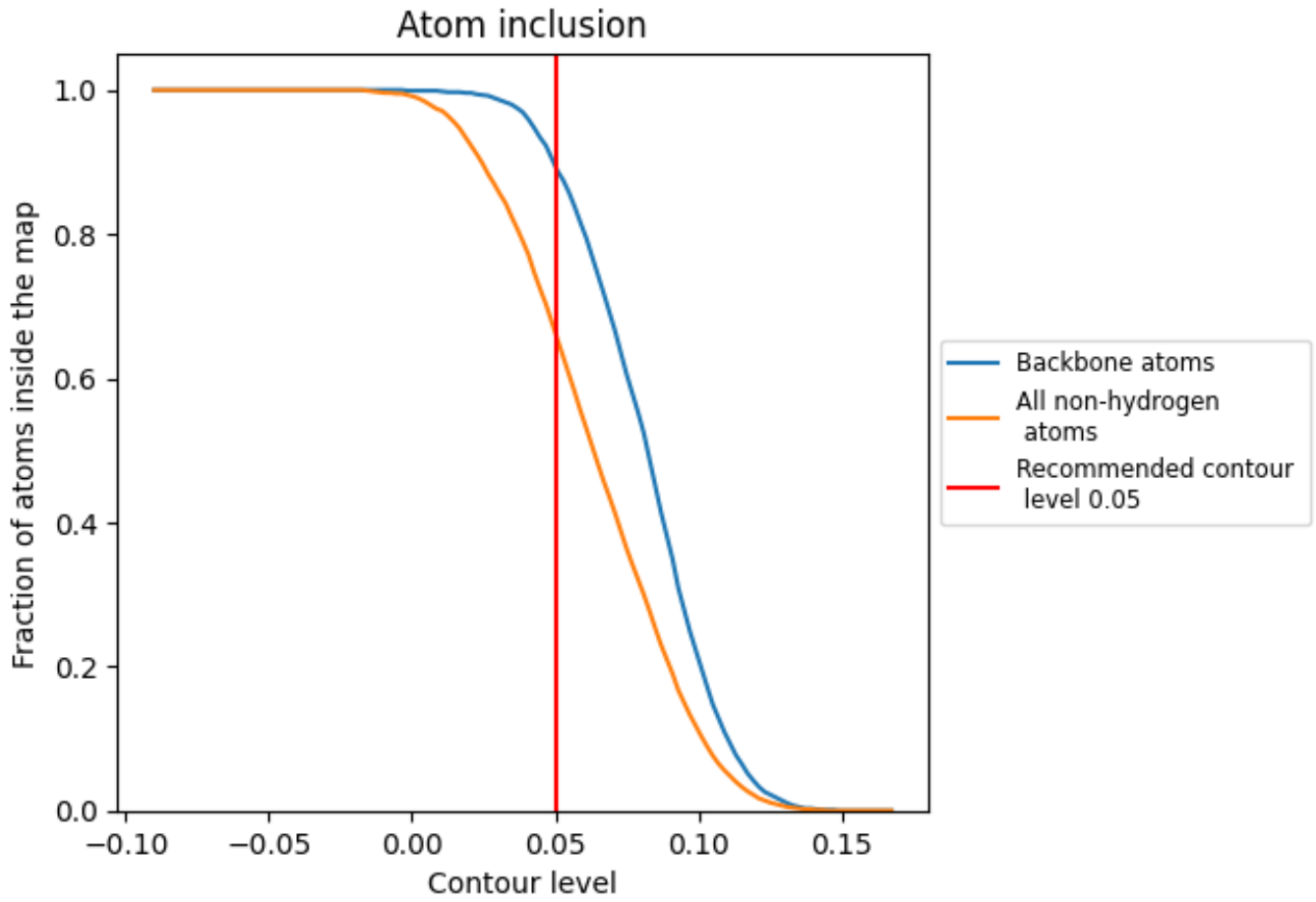
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6630	0.3540
A	0.6810	0.3680
B	0.6510	0.3140
C	0.6820	0.3680
D	0.6480	0.3150
E	0.6820	0.3680
F	0.6480	0.3140
G	0.6670	0.3440
H	0.6640	0.3430
I	0.6610	0.3450
J	0.3930	0.2660
K	0.6430	0.3420
L	0.5800	0.4420
M	0.5710	0.3310
N	0.5000	0.2780
O	0.3210	0.3250
P	0.4640	0.3510
Q	0.3570	0.3350
R	0.5600	0.3840
S	0.5360	0.3180
T	0.3930	0.2820
U	0.6070	0.3550
V	0.5800	0.4450
W	0.6070	0.3280
X	0.4640	0.2730
Y	0.3570	0.3340
Z	0.4640	0.3580
a	0.3570	0.3270
b	0.5600	0.3930
c	0.5000	0.3080
d	0.3930	0.2750
e	0.6070	0.3590
f	0.5800	0.4530
g	0.6070	0.3100
h	0.4640	0.2700

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Chain	Atom inclusion	Q-score
i	0.3570	0.3370
j	0.5360	0.3590
k	0.3570	0.3320
l	0.5600	0.3830
m	0.5360	0.3280