wwPDB EM Validation Summary Report

May 6, 2025 – 03:27 AM EDT

PDB ID	:	9AYS / pdb_00009ays
EMDB ID	:	EMD-43998
Title	:	HIV BG505.v5.2 (N289/N241) SOSIP Env in Complex with V5, gp120-Interface, and Anti-Immune Complex pAbs from Rh.33203
Authors	:	Brown, S.; Antansijevic, A.; Ward, A.B.
Deposited on	:	2024-03-08
Resolution	:	4.60 Å(reported)

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

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

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

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

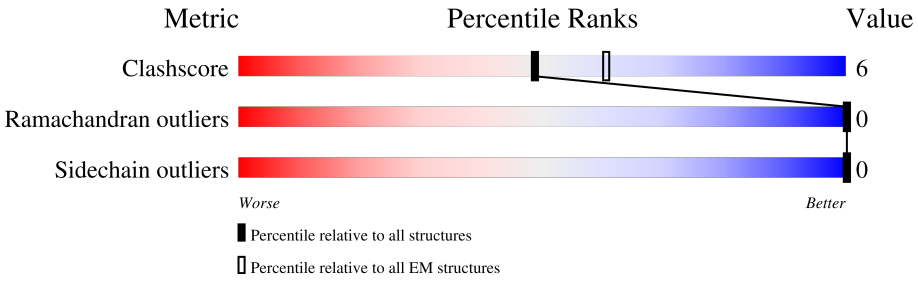
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	H	121	6% 100%
2	L	101	6% 100%
3	A	514	74% 14% 11%
3	C	514	75% 13% 12%
3	E	514	77% 11% 11%
4	B	155	82% 10% 8%
4	D	155	5% 77% 16% 7%
4	F	155	81% 12% 8%

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Mol	Chain	Length	Quality of chain
5	G	102	96%
6	I	115	97%
7	J	104	27% 100%
8	K	94	27% 98%
9	M	3	33% 67%
10	N	2	100%
10	P	2	100%
10	R	2	100%
10	S	2	100%
10	T	2	100%
10	U	2	50% 50%
10	X	2	100%
10	Y	2	100%
10	Z	2	100%
10	a	2	50% 50%
10	b	2	100%
10	d	2	100%
10	e	2	100%
10	g	2	100%
10	h	2	50% 50% 50%
11	O	2	50% 50%
11	V	2	50% 50%
12	Q	6	33% 67%
13	W	5	20% 80%
13	c	5	20% 60% 20%

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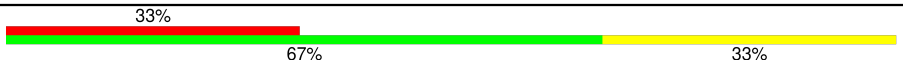
Mol	Chain	Length	Quality of chain
14	f	3	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 18710 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 NHP gp120-Interface Epitope pAb - Predicted Heavy Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	H	121	Total	C	N	O	0	0
			605	363	121	121		

- Molecule 2 is a protein called NHP gp120-Interface Epitope pAb - Predicted Light Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	L	101	Total	C	N	O	0	0
			505	303	101	101		

- Molecule 3 is a protein called Surface protein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	455	Total	C	N	O	S	0	0
			3591	2249	635	679	28		
3	C	451	Total	C	N	O	S	0	0
			3564	2235	631	670	28		
3	E	455	Total	C	N	O	S	0	0
			3586	2248	634	676	28		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	64	LYS	GLU	conflict	UNP Q2N0S6
A	73	CYS	ALA	conflict	UNP Q2N0S6
A	240	THR	PRO	conflict	UNP Q2N0S6
A	241	ASN	SER	conflict	UNP Q2N0S6
A	271	ILE	MET	conflict	UNP Q2N0S6
A	288	LEU	PHE	conflict	UNP Q2N0S6
A	290	GLU	THR	conflict	UNP Q2N0S6
A	291	SER	PRO	conflict	UNP Q2N0S6
A	314	TRP	ALA	conflict	UNP Q2N0S6
A	331	ASN	THR	conflict	UNP Q2N0S6
A	500	CYS	ALA	conflict	UNP Q2N0S6
A	508	ARG	GLU	conflict	UNP Q2N0S6
A	509	ARG	LYS	conflict	UNP Q2N0S6
C	-4	MET	-	initiating methionine	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	64	LYS	GLU	conflict	UNP Q2N0S6
C	73	CYS	ALA	conflict	UNP Q2N0S6
C	240	THR	PRO	conflict	UNP Q2N0S6
C	241	ASN	SER	conflict	UNP Q2N0S6
C	271	ILE	MET	conflict	UNP Q2N0S6
C	288	LEU	PHE	conflict	UNP Q2N0S6
C	290	GLU	THR	conflict	UNP Q2N0S6
C	291	SER	PRO	conflict	UNP Q2N0S6
C	314	TRP	ALA	conflict	UNP Q2N0S6
C	331	ASN	THR	conflict	UNP Q2N0S6
C	500	CYS	ALA	conflict	UNP Q2N0S6
C	508	ARG	GLU	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	509	ARG	LYS	conflict	UNP Q2N0S6
E	-4	MET	-	initiating methionine	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
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	64	LYS	GLU	conflict	UNP Q2N0S6
E	73	CYS	ALA	conflict	UNP Q2N0S6
E	240	THR	PRO	conflict	UNP Q2N0S6
E	241	ASN	SER	conflict	UNP Q2N0S6
E	271	ILE	MET	conflict	UNP Q2N0S6
E	288	LEU	PHE	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	290	GLU	THR	conflict	UNP Q2N0S6
E	291	SER	PRO	conflict	UNP Q2N0S6
E	314	TRP	ALA	conflict	UNP Q2N0S6
E	331	ASN	THR	conflict	UNP Q2N0S6
E	500	CYS	ALA	conflict	UNP Q2N0S6
E	508	ARG	GLU	conflict	UNP Q2N0S6
E	509	ARG	LYS	conflict	UNP Q2N0S6

- Molecule 4 is a protein called Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	143	Total	C	N	O	S	0	0
			1139	717	201	214	7		
4	D	144	Total	C	N	O	S	0	0
			1147	723	202	215	7		
4	F	143	Total	C	N	O	S	0	0
			1145	723	201	214	7		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	510	ARG	LYS	conflict	UNP Q2N0S6
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	561	CYS	ALA	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
B	613	THR	SER	conflict	UNP Q2N0S6
D	510	ARG	LYS	conflict	UNP Q2N0S6
D	559	PRO	ILE	conflict	UNP Q2N0S6
D	561	CYS	ALA	conflict	UNP Q2N0S6
D	605	CYS	THR	conflict	UNP Q2N0S6
D	613	THR	SER	conflict	UNP Q2N0S6
F	510	ARG	LYS	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	561	CYS	ALA	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6
F	613	THR	SER	conflict	UNP Q2N0S6

- Molecule 5 is a protein called NHP V5 Epitope pAb - Predicted Light Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	102	Total	C	N	O	0	0
			510	306	102	102		

- Molecule 6 is a protein called NHP V5 Epitope pAb - Predicted Heavy Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	115	Total	C	N	O	0	0
			575	345	115	115		

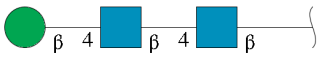
- Molecule 7 is a protein called NHP Anti-Immune Complex pAb - Predicted Heavy Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	104	Total	C	N	O	0	0
			520	312	104	104		

- Molecule 8 is a protein called NHP Anti-Immune Complex pAb - Predicted Light Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	94	Total	C	N	O	0	0
			470	282	94	94		

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



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

- Molecule 10 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
10	N	2	Total	C	N	O	0	0
			28	16	2	10		
10	P	2	Total	C	N	O	0	0
			28	16	2	10		
10	R	2	Total	C	N	O	0	0
			28	16	2	10		

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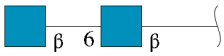
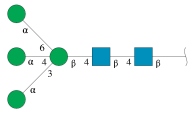
Mol	Chain	Residues	Atoms				AltConf	Trace
10	S	2	Total	C	N	O	0	0
			28	16	2	10		
10	T	2	Total	C	N	O	0	0
			28	16	2	10		
10	U	2	Total	C	N	O	0	0
			28	16	2	10		
10	X	2	Total	C	N	O	0	0
			28	16	2	10		
10	Y	2	Total	C	N	O	0	0
			28	16	2	10		
10	Z	2	Total	C	N	O	0	0
			28	16	2	10		
10	a	2	Total	C	N	O	0	0
			28	16	2	10		
10	b	2	Total	C	N	O	0	0
			28	16	2	10		
10	d	2	Total	C	N	O	0	0
			28	16	2	10		
10	e	2	Total	C	N	O	0	0
			28	16	2	10		
10	g	2	Total	C	N	O	0	0
			28	16	2	10		
10	h	2	Total	C	N	O	0	0
			28	16	2	10		

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



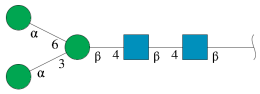
Mol	Chain	Residues	Atoms				AltConf	Trace
11	O	2	Total	C	N	O	0	0
			28	16	2	10		
11	V	2	Total	C	N	O	0	0
			28	16	2	10		

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



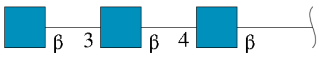
Mol	Chain	Residues	Atoms				AltConf	Trace
12	Q	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



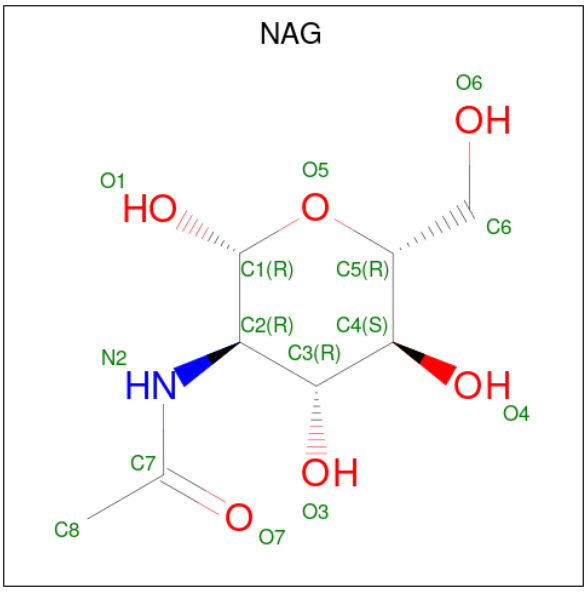
Mol	Chain	Residues	Atoms				AltConf	Trace
13	W	5	Total	C	N	O	0	0
			61	34	2	25		
13	c	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 14 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	3	Total	C	N	O	0	0
			42	24	3	15		

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



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

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

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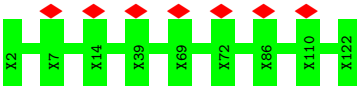
Mol	Chain	Residues	Atoms				AltConf
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	F	1	Total	C	N	O	0
			14	8	1	5	
15	F	1	Total	C	N	O	0
			14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

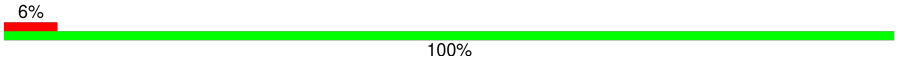
• Molecule 1: NHP gp120-Interface Epitope pAb - Predicted Heavy Chain

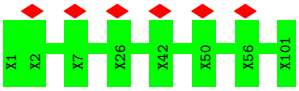
Chain H:



• Molecule 2: NHP gp120-Interface Epitope pAb - Predicted Light Chain

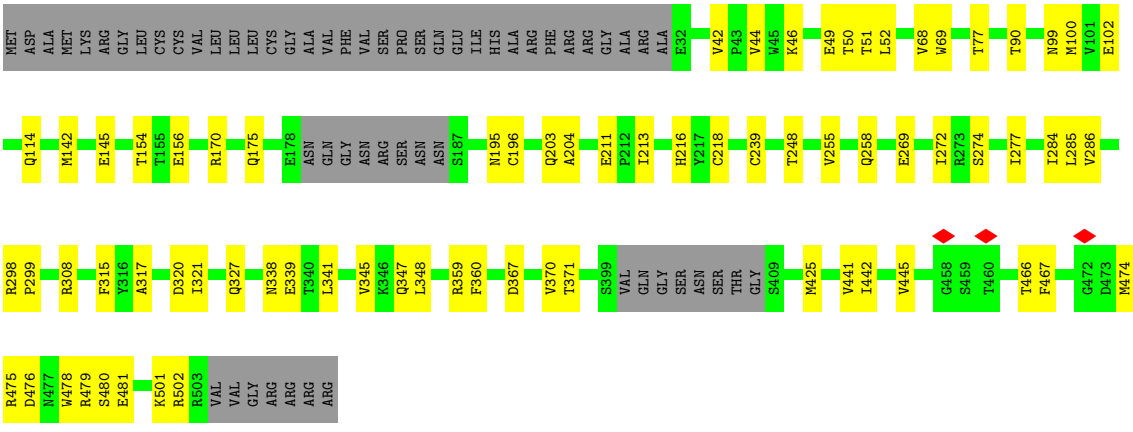
Chain L:





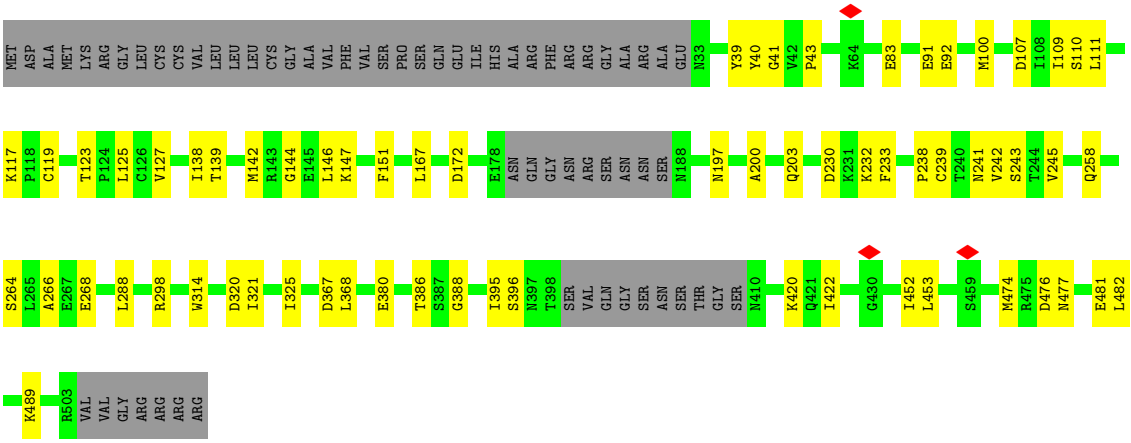
• Molecule 3: Surface protein gp120

Chain A:



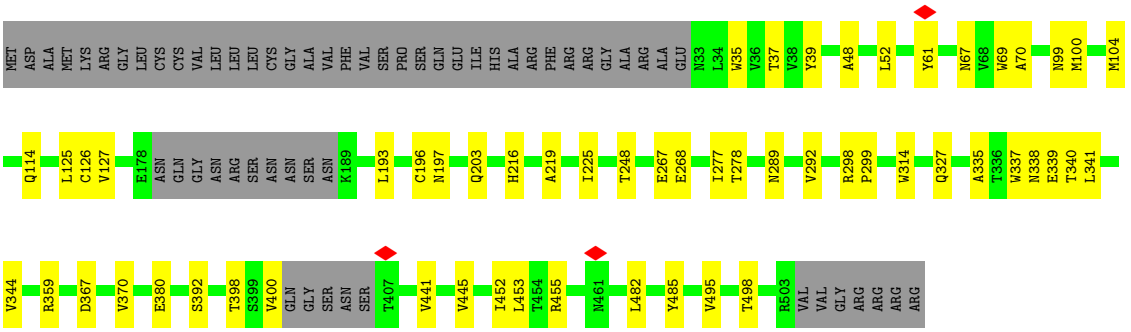
• Molecule 3: Surface protein gp120

Chain C:



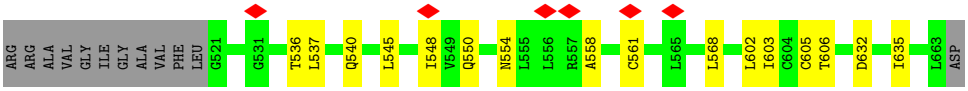
• Molecule 3: Surface protein gp120

Chain E:



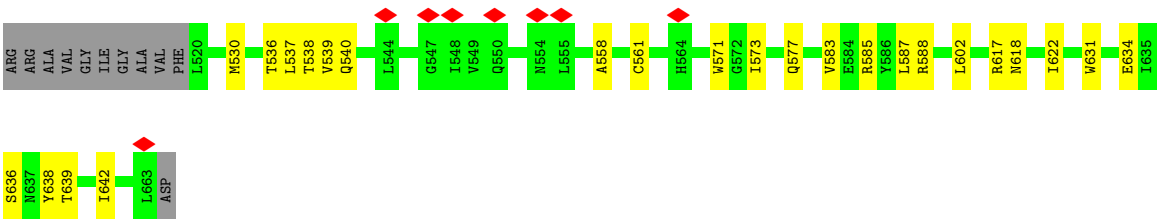
• Molecule 4: Transmembrane protein gp41

Chain B:



• Molecule 4: Transmembrane protein gp41

Chain D:

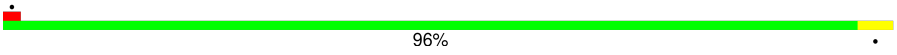


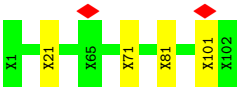
• Molecule 4: Transmembrane protein gp41

Chain F:

• Molecule 5: NHP V5 Epitope pAb - Predicted Light Chain

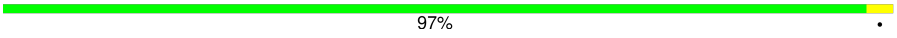
Chain G:

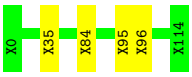




• Molecule 6: NHP V5 Epitope pAb - Predicted Heavy Chain

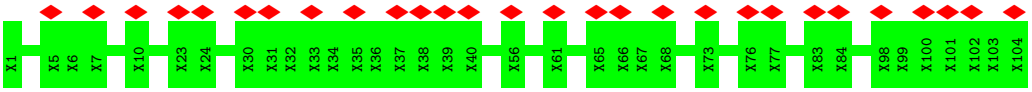
Chain I:





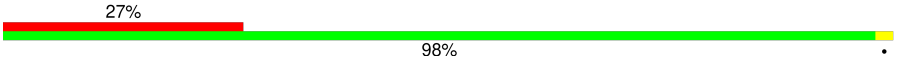
• Molecule 7: NHP Anti-Immune Complex pAb - Predicted Heavy Chain

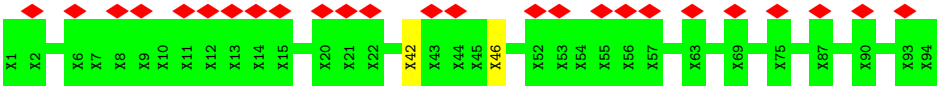
Chain J:



• Molecule 8: NHP Anti-Immune Complex pAb - Predicted Light Chain

Chain K:





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

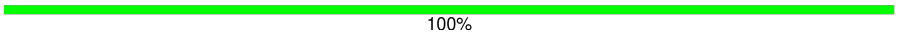
Chain M:

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

Chain N:

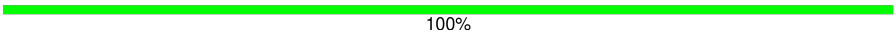
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



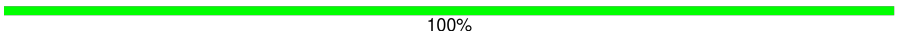
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



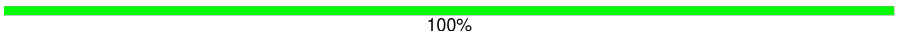
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



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

Chain T:

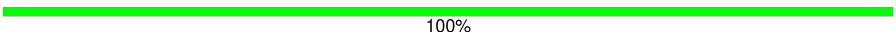


• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

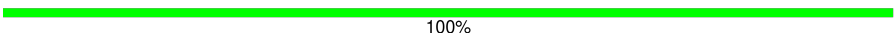
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

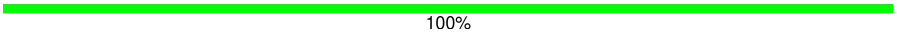


• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



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

Chain Z: 

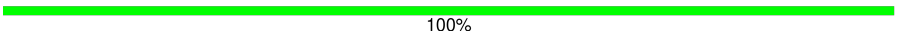
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

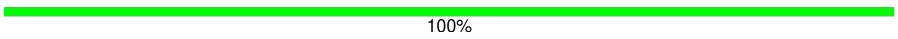
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

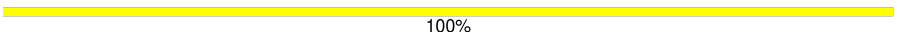
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 

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

Chain e: 

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

Chain g: 

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

Chain h:

• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

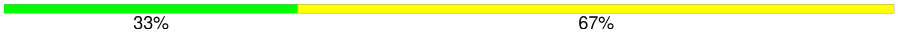
Chain O:

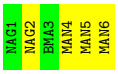
• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

• Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][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

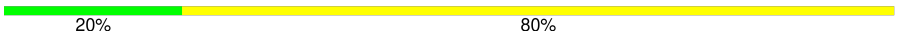
Chain Q:





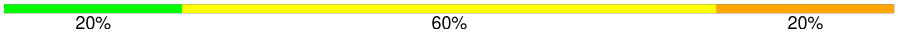
• Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



• Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



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

Chain f:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12893	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	376.19998, 376.19998, 376.19998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	A	0.28	0/3664	0.52	0/4973
3	C	0.34	0/3637	0.56	0/4937
3	E	0.26	0/3659	0.51	0/4967
4	B	0.26	0/1159	0.52	0/1573
4	D	0.40	0/1167	0.63	0/1584
4	F	0.30	0/1166	0.53	0/1582
All	All	0.30	0/14452	0.54	0/19616

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	605	0	147	0	0
2	L	505	0	124	0	0
3	A	3591	0	3518	48	0
3	C	3564	0	3496	67	0
3	E	3586	0	3520	42	0
4	B	1139	0	1129	12	0
4	D	1147	0	1139	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1145	0	1133	15	0
5	G	510	0	119	2	0
6	I	575	0	140	3	0
7	J	520	0	125	0	0
8	K	470	0	118	1	0
9	M	39	0	34	1	0
10	N	28	0	25	0	0
10	P	28	0	25	0	0
10	R	28	0	25	0	0
10	S	28	0	25	0	0
10	T	28	0	25	0	0
10	U	28	0	25	2	0
10	X	28	0	25	0	0
10	Y	28	0	25	0	0
10	Z	28	0	25	0	0
10	a	28	0	25	2	0
10	b	28	0	25	0	0
10	d	28	0	25	0	0
10	e	28	0	25	0	0
10	g	28	0	25	1	0
10	h	28	0	25	3	0
11	O	28	0	25	0	0
11	V	28	0	25	2	0
12	Q	72	0	61	1	0
13	W	61	0	52	0	0
13	c	61	0	52	2	0
14	f	42	0	37	0	0
15	A	154	0	143	0	0
15	B	28	0	26	0	0
15	C	182	0	169	1	0
15	D	28	0	26	0	0
15	E	182	0	169	2	0
15	F	28	0	26	0	0
All	All	18710	0	15928	195	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 195 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:MET:HG2	3:C:325:ILE:CG2	1.77	1.14
3:C:92:GLU:HA	3:C:238:PRO:HA	1.53	0.90
3:C:146:LEU:HD11	3:C:167:LEU:HB3	1.52	0.88
3:C:142:MET:HG2	3:C:325:ILE:HG22	1.52	0.88
3:C:139:THR:HG23	3:C:142:MET:H	1.39	0.88

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	449/514 (87%)	434 (97%)	15 (3%)	0	100	100
3	C	445/514 (87%)	433 (97%)	12 (3%)	0	100	100
3	E	449/514 (87%)	436 (97%)	13 (3%)	0	100	100
4	B	141/155 (91%)	138 (98%)	3 (2%)	0	100	100
4	D	142/155 (92%)	133 (94%)	9 (6%)	0	100	100
4	F	141/155 (91%)	137 (97%)	4 (3%)	0	100	100
All	All	1767/2007 (88%)	1711 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	409/456 (90%)	409 (100%)	0	100	100
3	C	405/456 (89%)	405 (100%)	0	100	100
3	E	408/456 (90%)	408 (100%)	0	100	100
4	B	124/132 (94%)	124 (100%)	0	100	100
4	D	125/132 (95%)	125 (100%)	0	100	100
4	F	125/132 (95%)	125 (100%)	0	100	100
All	All	1596/1764 (90%)	1596 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	577	GLN
3	E	98	ASN
3	E	195	ASN
3	E	114	GLN
3	A	327	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

56 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	$\#\|Z\|>2$
9	NAG	M	1	3,9	14,14,15	0.19	0	17,19,21	0.48	0
9	NAG	M	2	9	14,14,15	0.45	0	17,19,21	0.77	1 (5%)
9	BMA	M	3	9	11,11,12	1.14	1 (9%)	15,15,17	0.82	0
10	NAG	N	1	3,10	14,14,15	0.23	0	17,19,21	0.48	0
10	NAG	N	2	10	14,14,15	0.56	0	17,19,21	0.55	0
11	NAG	O	1	11,3	14,14,15	0.34	0	17,19,21	0.87	1 (5%)
11	NAG	O	2	11	14,14,15	0.16	0	17,19,21	0.44	0
10	NAG	P	1	3,10	14,14,15	0.26	0	17,19,21	0.49	0
10	NAG	P	2	10	14,14,15	0.18	0	17,19,21	0.49	0
12	NAG	Q	1	3,12	14,14,15	0.26	0	17,19,21	0.53	0
12	NAG	Q	2	12	14,14,15	0.19	0	17,19,21	0.47	0
12	BMA	Q	3	12	11,11,12	0.62	0	15,15,17	0.76	0
12	MAN	Q	4	12	11,11,12	0.61	0	15,15,17	0.90	1 (6%)
12	MAN	Q	5	12	11,11,12	0.69	0	15,15,17	1.03	2 (13%)
12	MAN	Q	6	12	11,11,12	0.56	0	15,15,17	1.07	2 (13%)
10	NAG	R	1	3,10	14,14,15	0.19	0	17,19,21	0.58	0
10	NAG	R	2	10	14,14,15	0.20	0	17,19,21	0.44	0
10	NAG	S	1	3,10	14,14,15	0.28	0	17,19,21	0.38	0
10	NAG	S	2	10	14,14,15	0.49	0	17,19,21	0.51	0
10	NAG	T	1	3,10	14,14,15	0.21	0	17,19,21	0.48	0
10	NAG	T	2	10	14,14,15	0.37	0	17,19,21	0.44	0
10	NAG	U	1	3,10	14,14,15	0.39	0	17,19,21	0.52	0
10	NAG	U	2	10	14,14,15	0.45	0	17,19,21	0.47	0
11	NAG	V	1	11,3	14,14,15	0.71	1 (7%)	17,19,21	0.51	0
11	NAG	V	2	11	14,14,15	0.46	0	17,19,21	0.42	0
13	NAG	W	1	3,13	14,14,15	0.20	0	17,19,21	0.64	0
13	NAG	W	2	13	14,14,15	0.72	1 (7%)	17,19,21	0.62	0
13	BMA	W	3	13	11,11,12	0.76	0	15,15,17	1.52	2 (13%)
13	MAN	W	4	13	11,11,12	0.51	0	15,15,17	1.03	2 (13%)
13	MAN	W	5	13	11,11,12	0.51	0	15,15,17	1.21	2 (13%)
10	NAG	X	1	3,10	14,14,15	0.16	0	17,19,21	0.57	0
10	NAG	X	2	10	14,14,15	0.16	0	17,19,21	0.50	0
10	NAG	Y	1	3,10	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	Y	2	10	14,14,15	0.47	0	17,19,21	0.50	0
10	NAG	Z	1	3,10	14,14,15	0.25	0	17,19,21	0.48	0
10	NAG	Z	2	10	14,14,15	0.17	0	17,19,21	0.41	0
10	NAG	a	1	3,10	14,14,15	0.70	1 (7%)	17,19,21	0.72	0
10	NAG	a	2	10	14,14,15	0.65	0	17,19,21	0.40	0
10	NAG	b	1	10,4	14,14,15	0.17	0	17,19,21	0.61	0
10	NAG	b	2	10	14,14,15	0.30	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	NAG	c	1	3,13	14,14,15	0.30	0	17,19,21	0.45	0
13	NAG	c	2	13	14,14,15	0.51	0	17,19,21	1.02	2 (11%)
13	BMA	c	3	13	11,11,12	0.40	0	15,15,17	1.36	1 (6%)
13	MAN	c	4	13	11,11,12	0.50	0	15,15,17	1.01	2 (13%)
13	MAN	c	5	13	11,11,12	0.83	0	15,15,17	1.44	2 (13%)
10	NAG	d	1	3,10	14,14,15	0.26	0	17,19,21	0.50	0
10	NAG	d	2	10	14,14,15	0.19	0	17,19,21	0.41	0
10	NAG	e	1	3,10	14,14,15	0.21	0	17,19,21	0.53	0
10	NAG	e	2	10	14,14,15	0.16	0	17,19,21	0.41	0
14	NAG	f	1	14,3	14,14,15	0.23	0	17,19,21	0.62	0
14	NAG	f	2	14	14,14,15	0.71	1 (7%)	17,19,21	0.83	1 (5%)
14	NAG	f	3	14	14,14,15	0.58	0	17,19,21	0.52	0
10	NAG	g	1	3,10	14,14,15	0.35	0	17,19,21	0.40	0
10	NAG	g	2	10	14,14,15	0.26	0	17,19,21	0.59	0
10	NAG	h	1	3,10	14,14,15	0.25	0	17,19,21	0.73	1 (5%)
10	NAG	h	2	10	14,14,15	0.27	0	17,19,21	0.61	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	S	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	S	2	10	-	0/6/23/26	0/1/1/1
10	NAG	T	1	3,10	-	1/6/23/26	0/1/1/1
10	NAG	T	2	10	-	1/6/23/26	0/1/1/1
10	NAG	U	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	U	2	10	-	2/6/23/26	0/1/1/1
11	NAG	V	1	11,3	-	3/6/23/26	0/1/1/1
11	NAG	V	2	11	-	1/6/23/26	0/1/1/1
13	NAG	W	1	3,13	-	0/6/23/26	0/1/1/1
13	NAG	W	2	13	-	0/6/23/26	0/1/1/1
13	BMA	W	3	13	-	2/2/19/22	0/1/1/1
13	MAN	W	4	13	-	1/2/19/22	0/1/1/1
13	MAN	W	5	13	-	1/2/19/22	0/1/1/1
10	NAG	X	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	X	2	10	-	2/6/23/26	0/1/1/1
10	NAG	Y	1	3,10	-	1/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	0/6/23/26	0/1/1/1
10	NAG	Z	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	0/6/23/26	0/1/1/1
10	NAG	a	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	a	2	10	-	3/6/23/26	0/1/1/1
10	NAG	b	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	b	2	10	-	1/6/23/26	0/1/1/1
13	NAG	c	1	3,13	-	1/6/23/26	0/1/1/1
13	NAG	c	2	13	-	2/6/23/26	0/1/1/1
13	BMA	c	3	13	-	2/2/19/22	0/1/1/1
13	MAN	c	4	13	-	1/2/19/22	0/1/1/1
13	MAN	c	5	13	-	1/2/19/22	0/1/1/1
10	NAG	d	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	d	2	10	-	1/6/23/26	0/1/1/1
10	NAG	e	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	e	2	10	-	1/6/23/26	0/1/1/1
14	NAG	f	1	14,3	-	0/6/23/26	0/1/1/1
14	NAG	f	2	14	-	4/6/23/26	0/1/1/1
14	NAG	f	3	14	-	1/6/23/26	0/1/1/1
10	NAG	g	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	g	2	10	-	1/6/23/26	0/1/1/1
10	NAG	h	1	3,10	-	4/6/23/26	0/1/1/1
10	NAG	h	2	10	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	3	BMA	C1-C2	2.67	1.58	1.52
10	a	1	NAG	O5-C1	-2.50	1.39	1.43
14	f	2	NAG	O5-C1	2.45	1.47	1.43
11	V	1	NAG	C1-C2	2.40	1.55	1.52
13	W	2	NAG	O5-C1	2.01	1.47	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	c	5	MAN	C1-O5-C5	4.73	118.52	112.19
13	W	3	BMA	C1-O5-C5	4.69	118.47	112.19
13	c	3	BMA	C1-O5-C5	4.38	118.06	112.19
13	W	5	MAN	C1-O5-C5	3.79	117.26	112.19
12	Q	6	MAN	C1-O5-C5	2.97	116.17	112.19

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

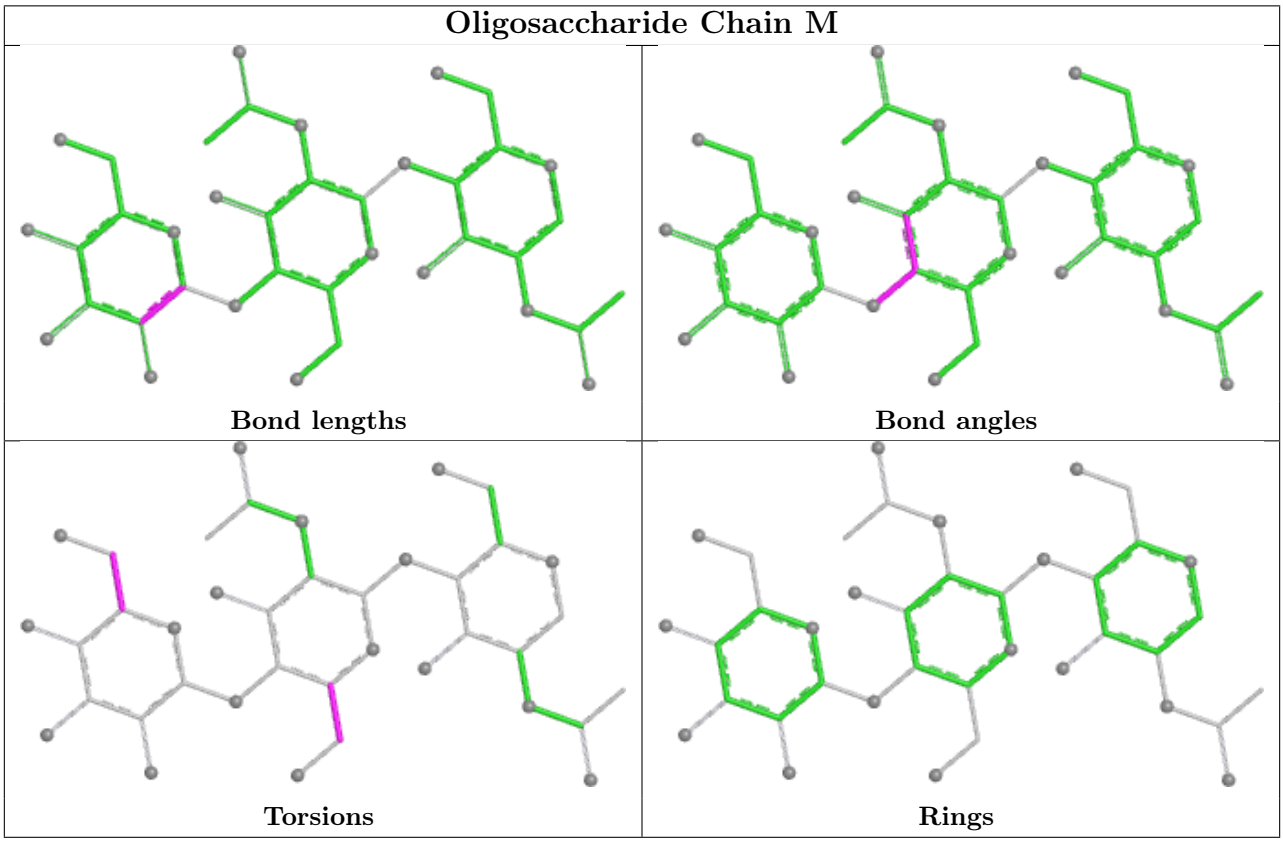
Mol	Chain	Res	Type	Atoms
14	f	2	NAG	C1-C2-N2-C7
13	c	3	BMA	C4-C5-C6-O6
10	X	2	NAG	O5-C5-C6-O6
12	Q	3	BMA	O5-C5-C6-O6
10	h	2	NAG	C8-C7-N2-C2

There are no ring outliers.

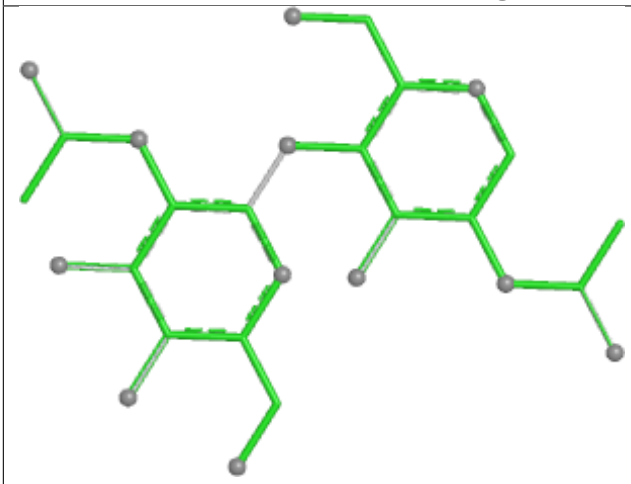
11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	U	1	NAG	2	0
11	V	1	NAG	2	0
13	c	2	NAG	2	0
10	h	1	NAG	3	0
9	M	2	NAG	1	0
10	h	2	NAG	1	0
10	a	1	NAG	2	0
10	g	2	NAG	1	0
9	M	3	BMA	1	0
12	Q	2	NAG	1	0
10	g	1	NAG	1	0

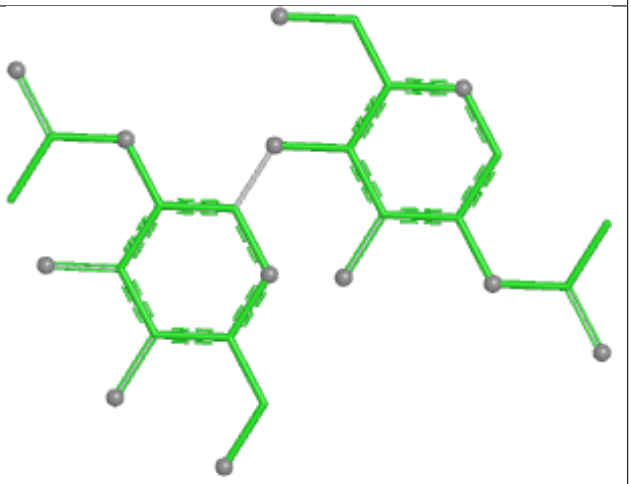
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



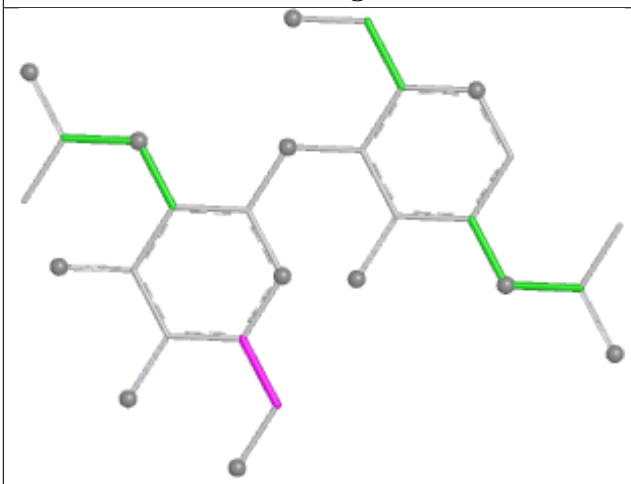
Oligosaccharide Chain N



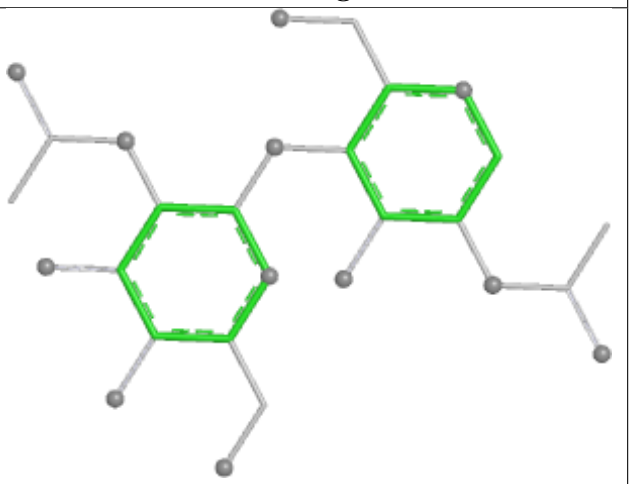
Bond lengths



Bond angles

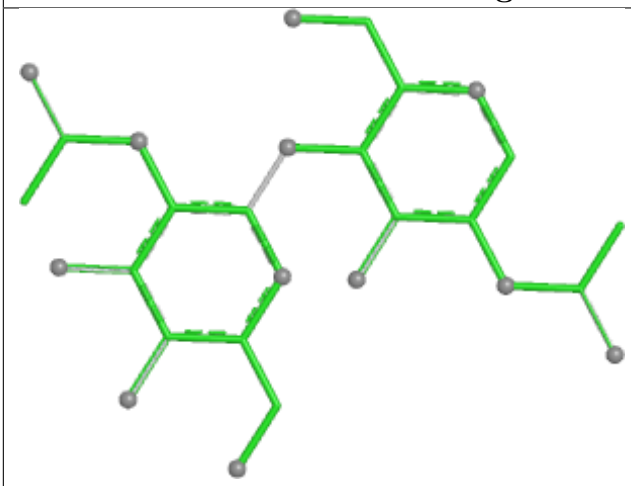


Torsions

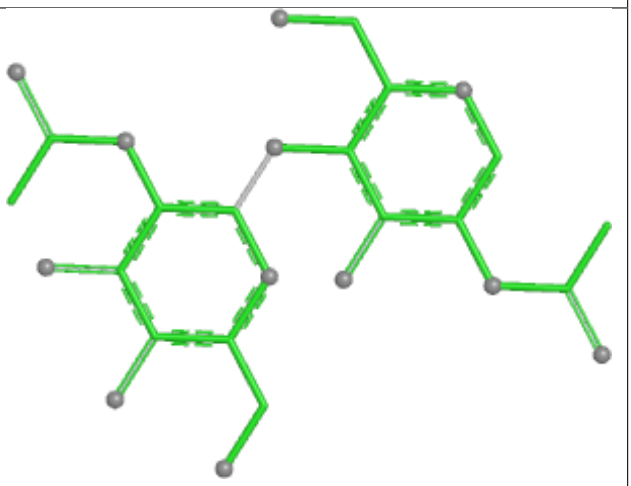


Rings

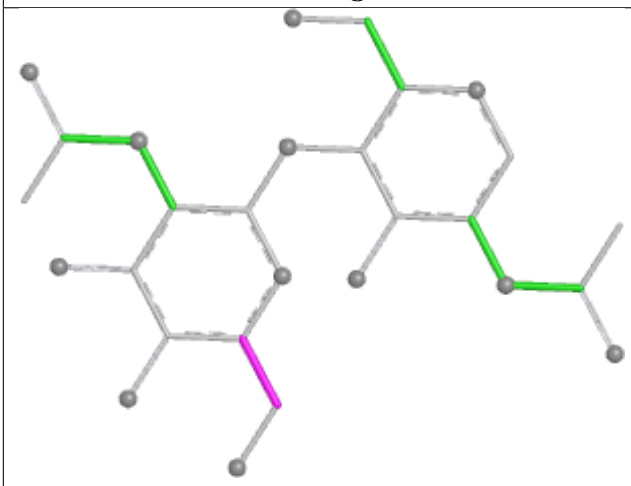
Oligosaccharide Chain P



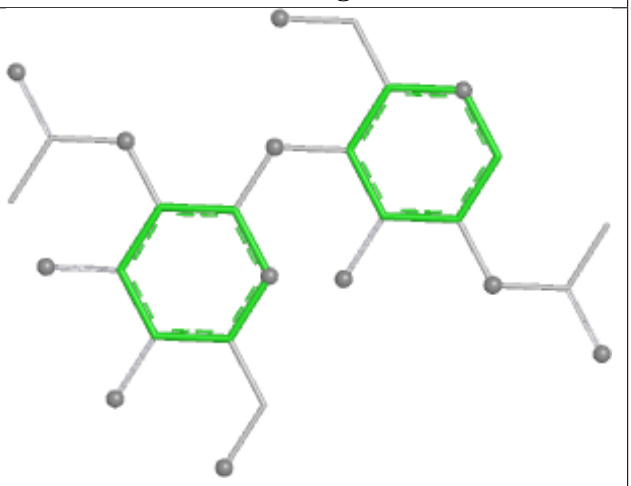
Bond lengths



Bond angles

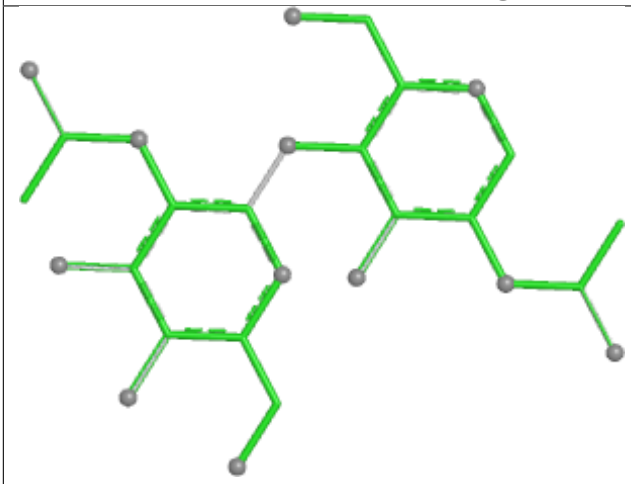


Torsions

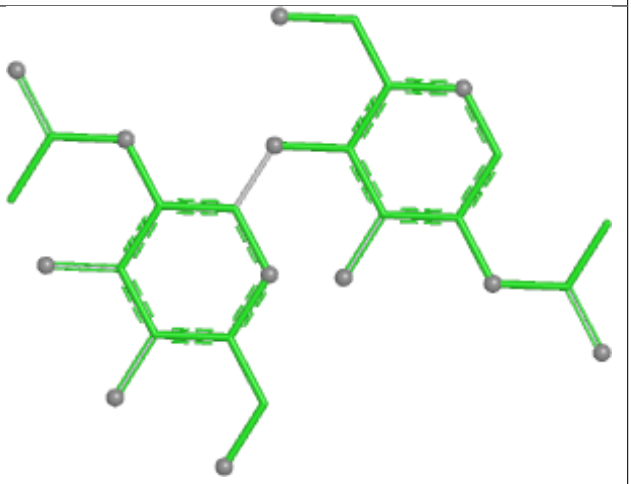


Rings

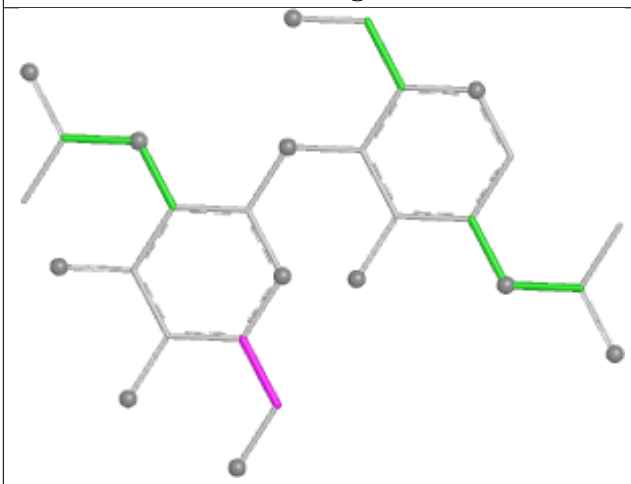
Oligosaccharide Chain R



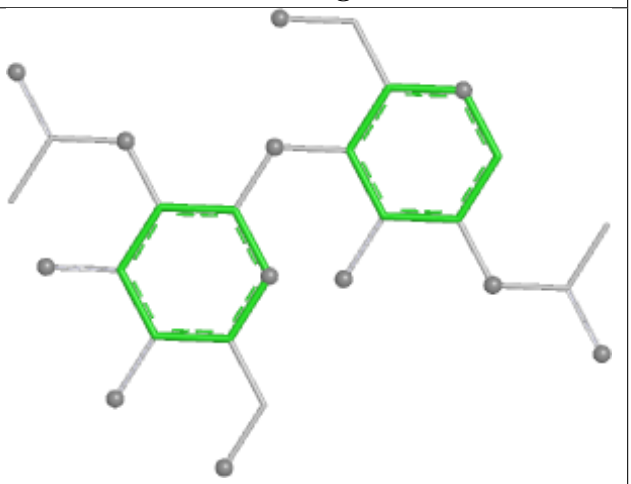
Bond lengths



Bond angles

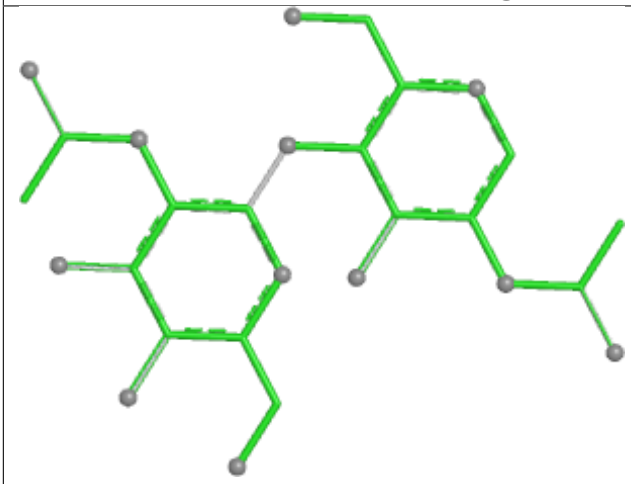


Torsions



Rings

Oligosaccharide Chain S



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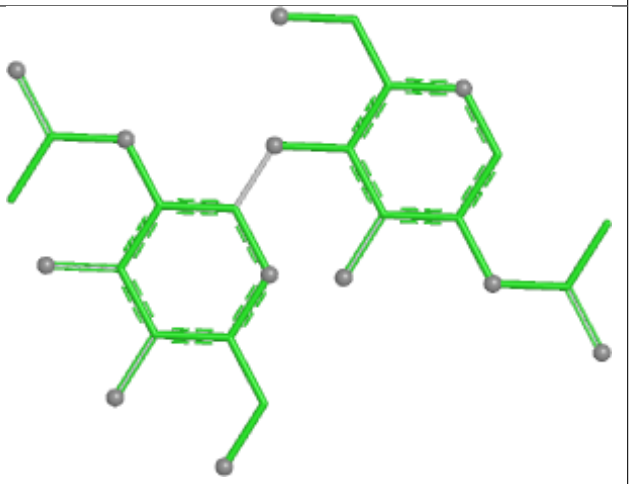

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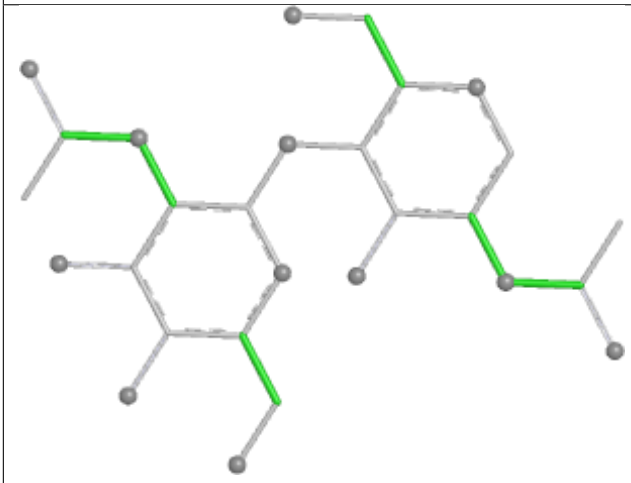

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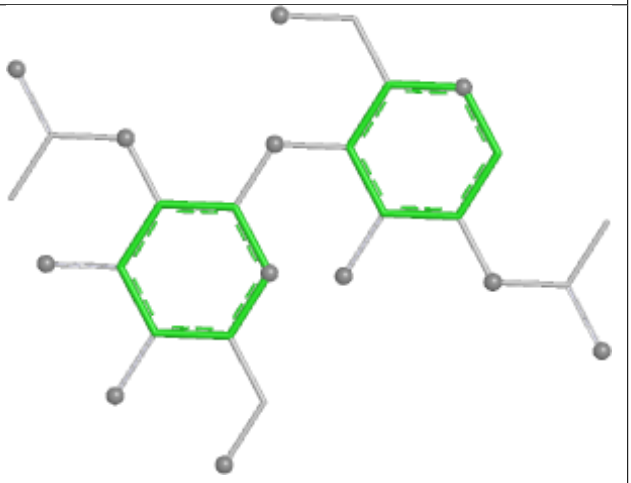
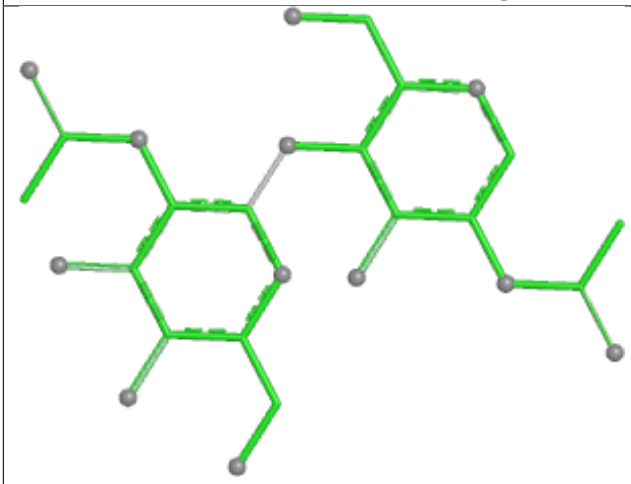


Rings

Oligosaccharide Chain T



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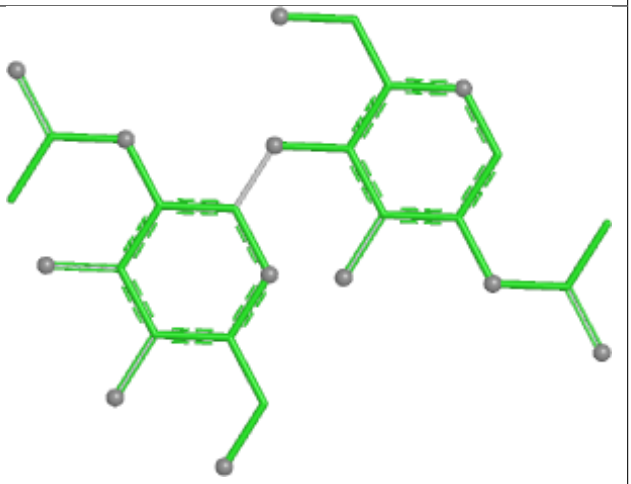

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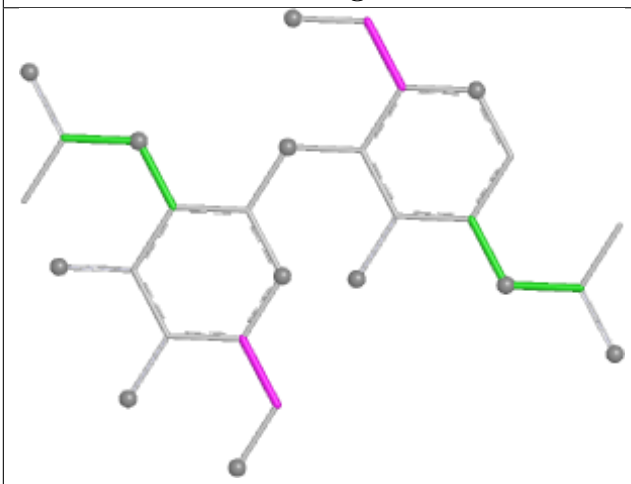

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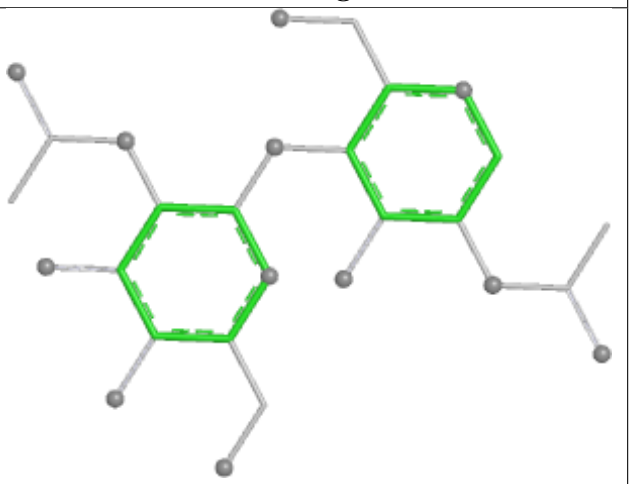
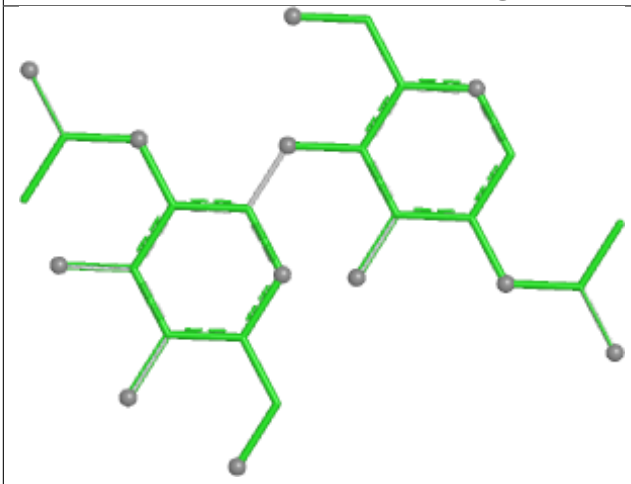


Rings

Oligosaccharide Chain U



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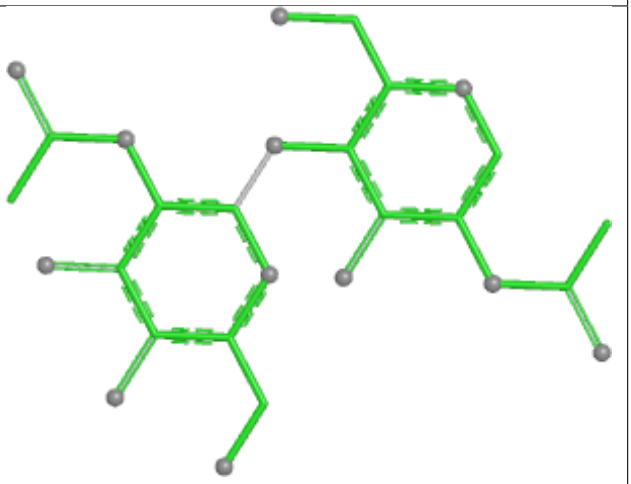

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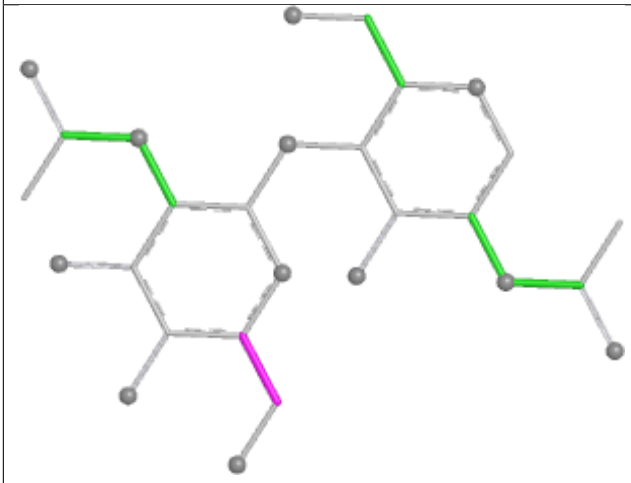

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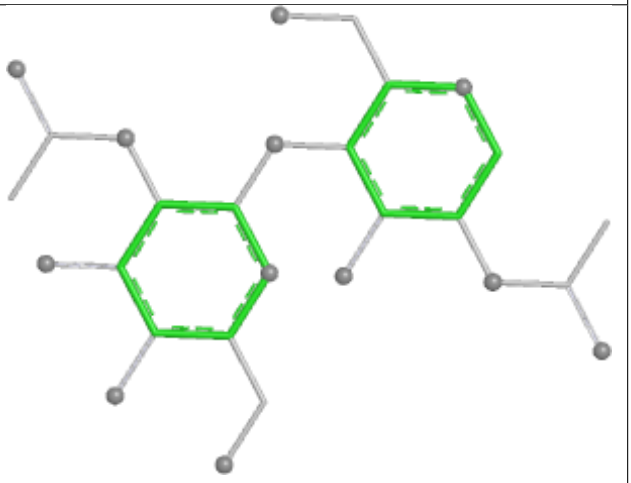
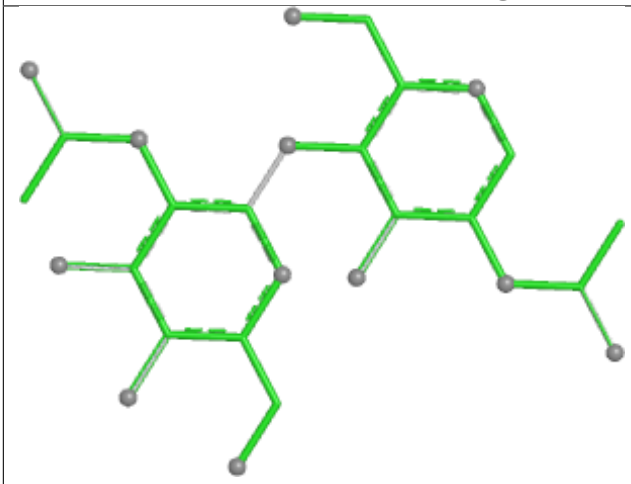


Rings

Oligosaccharide Chain X



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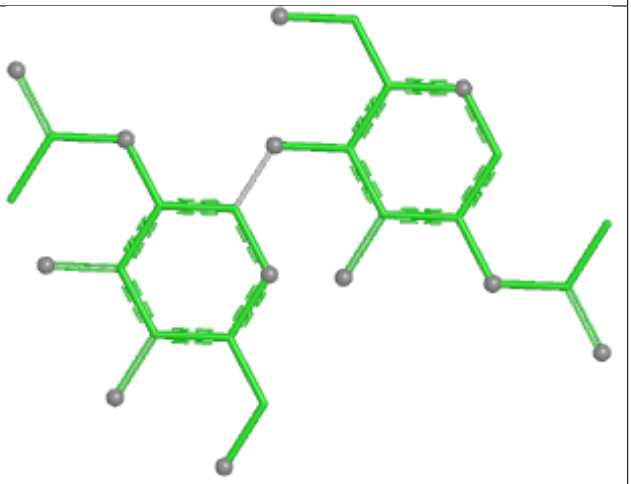

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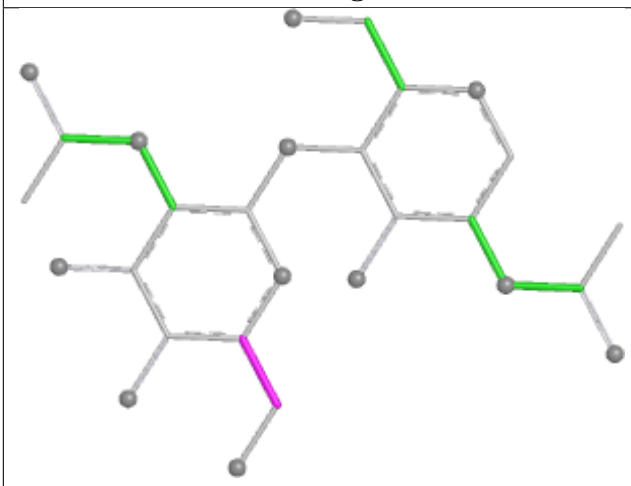

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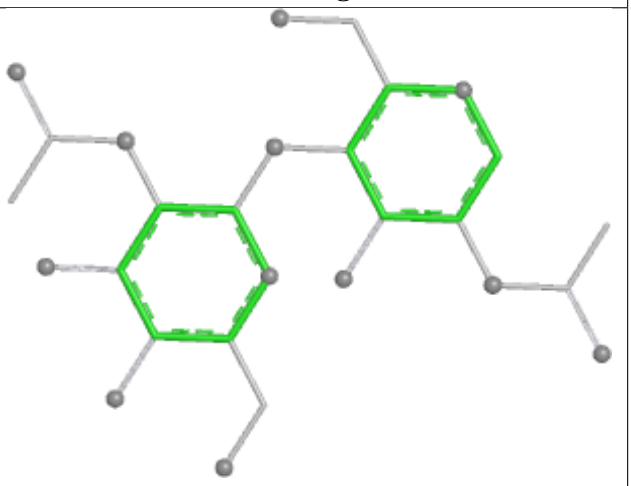

Rings

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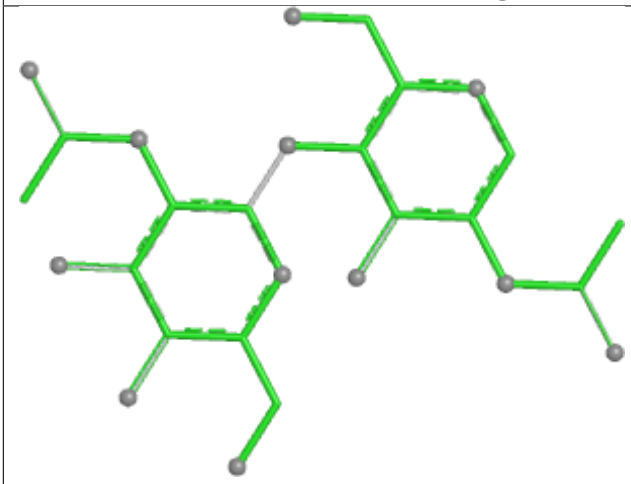

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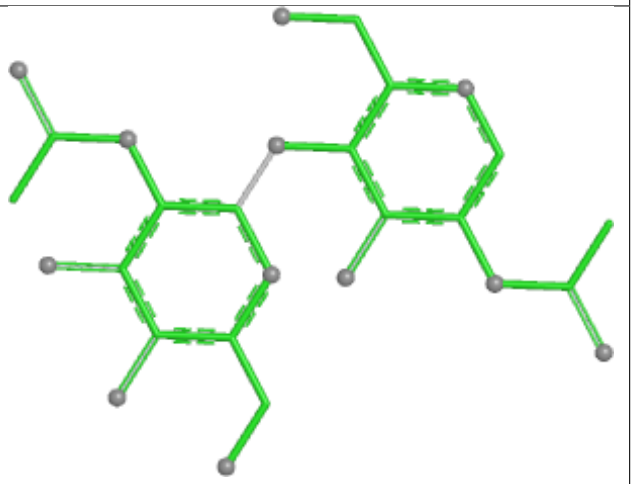

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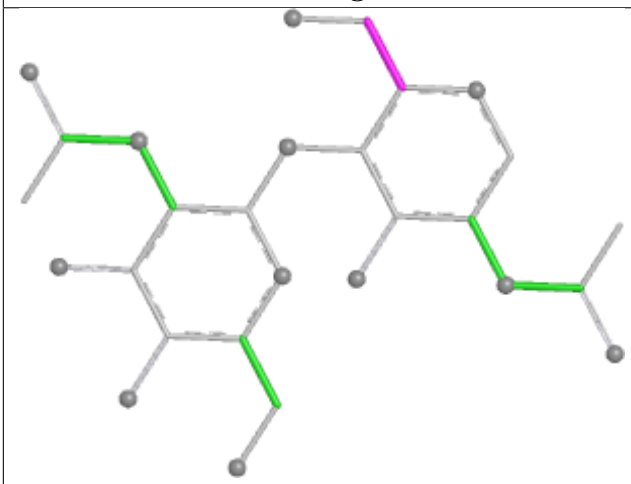

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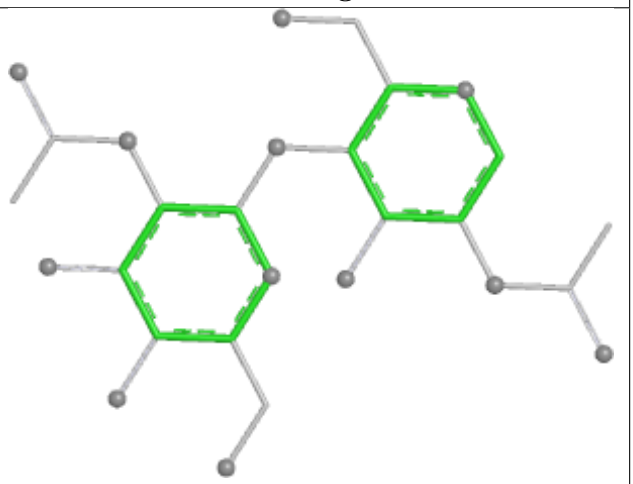

Rings

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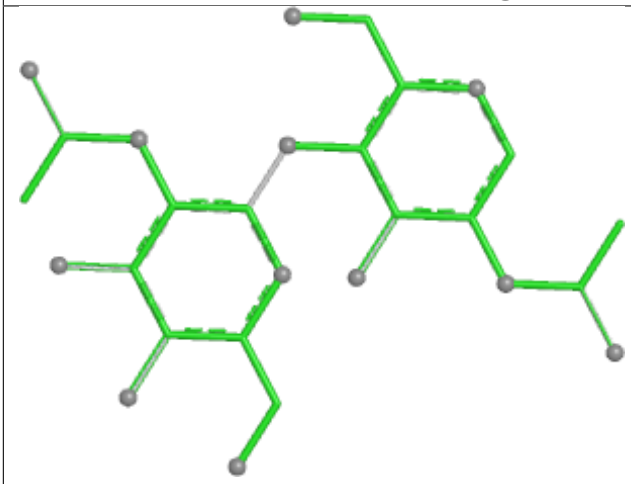

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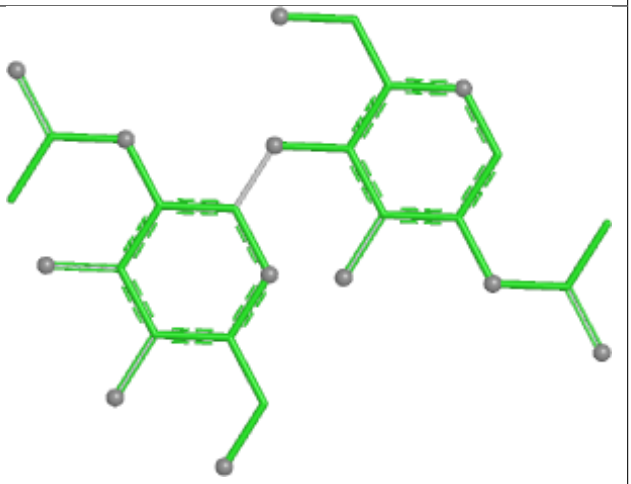
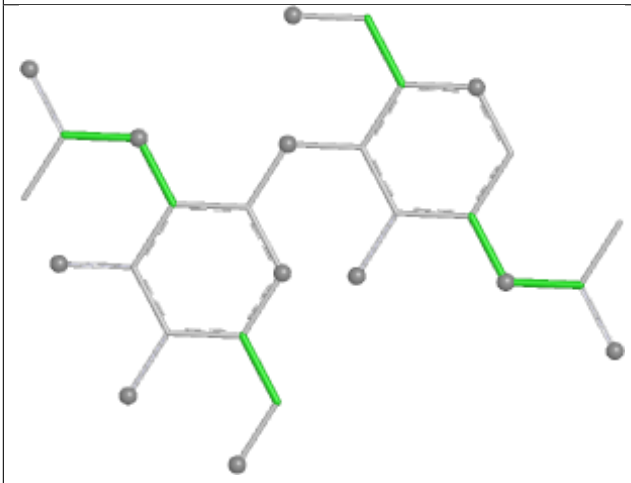


Bond angles



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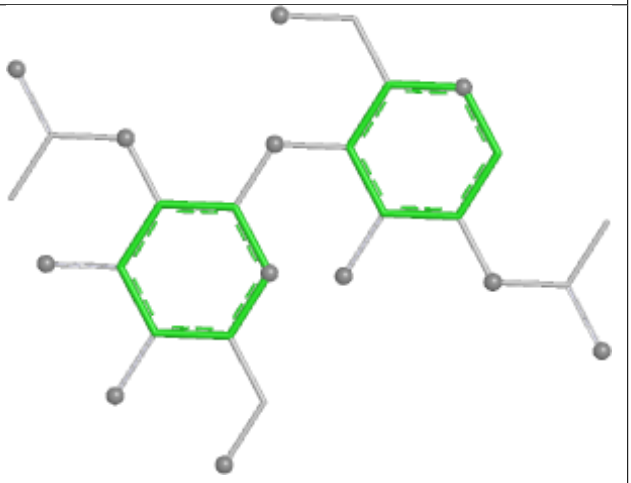
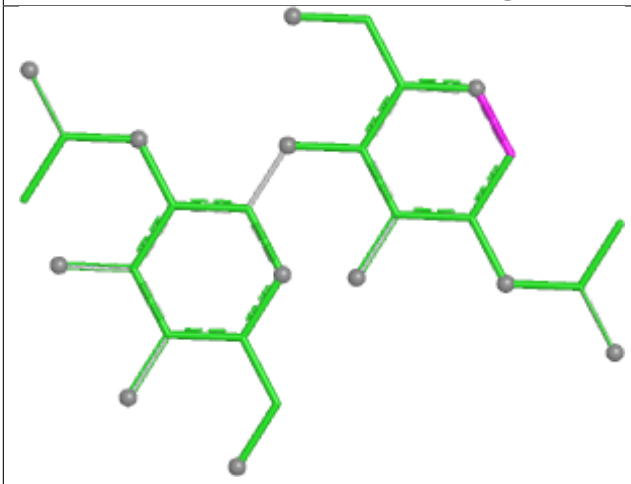


Rings

Oligosaccharide Chain a



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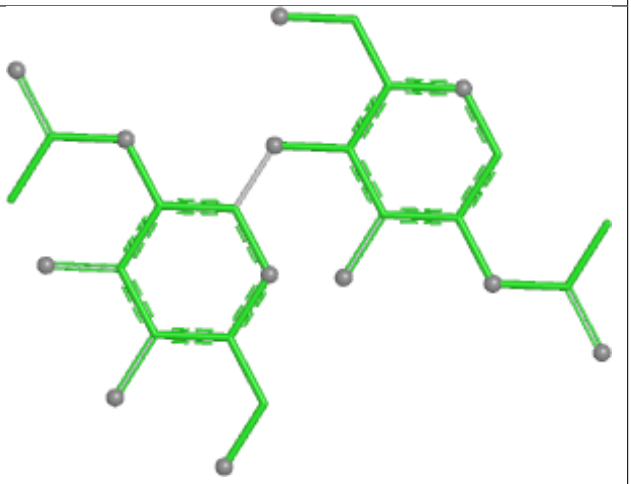

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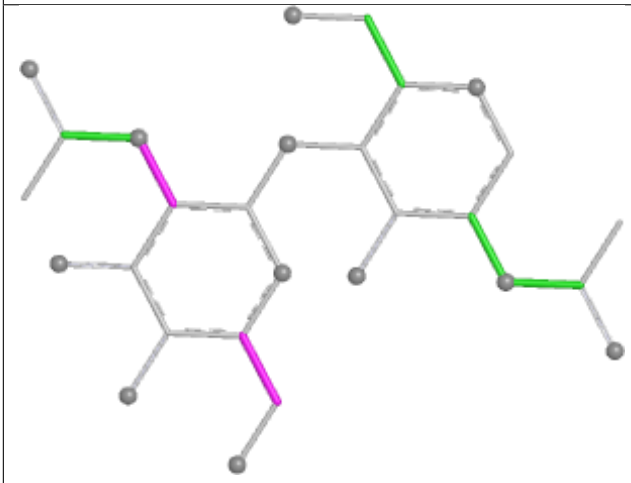

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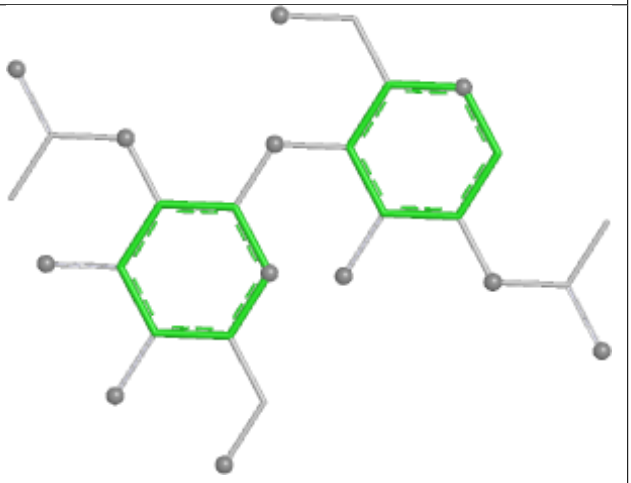
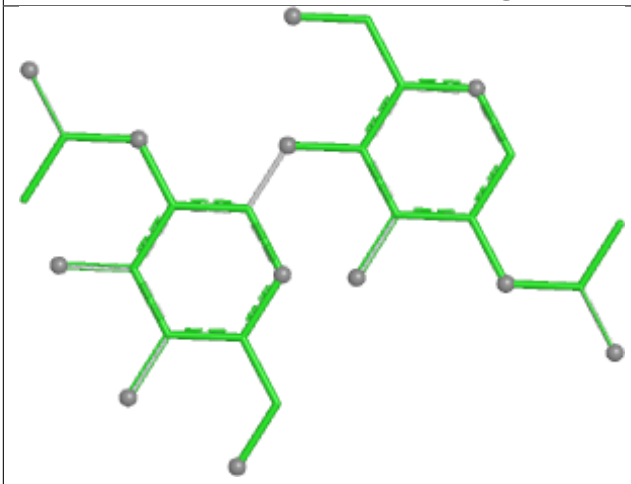


Rings

Oligosaccharide Chain b



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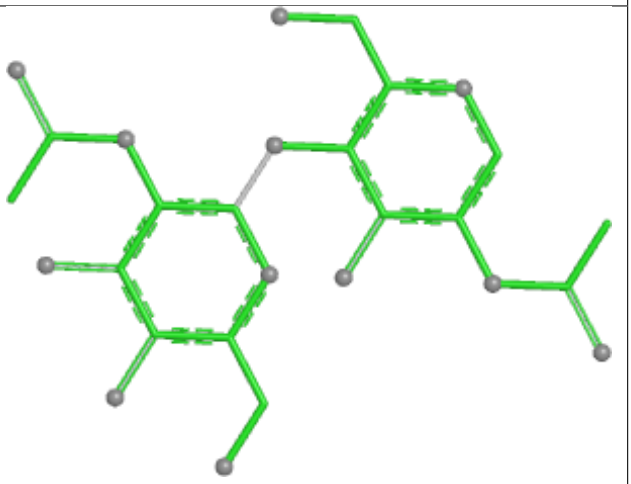

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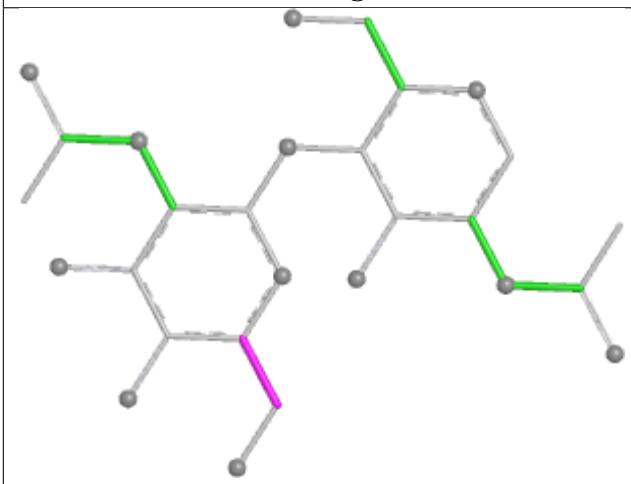

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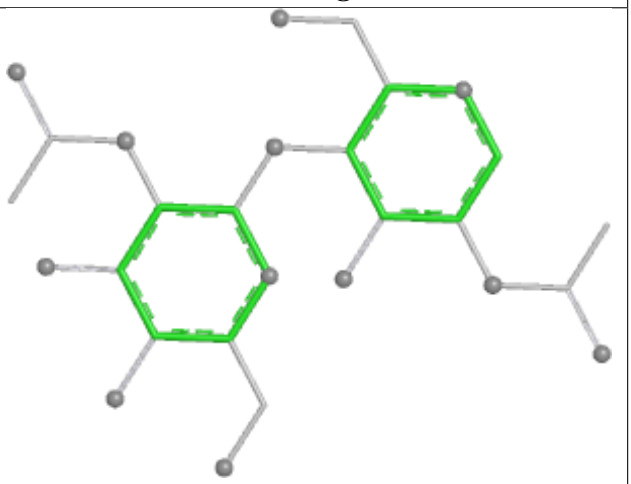
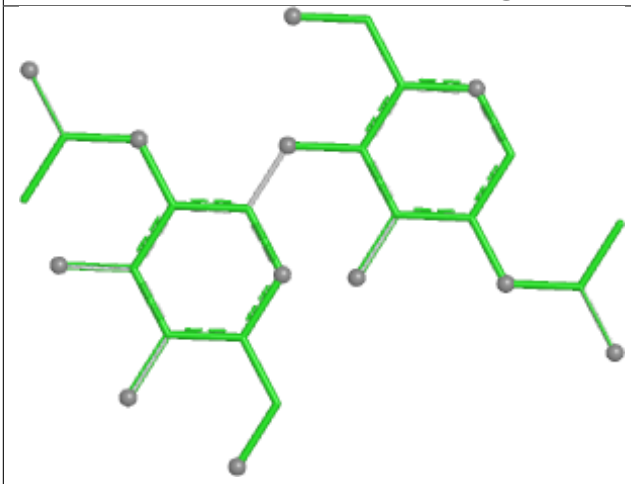


Rings

Oligosaccharide Chain d



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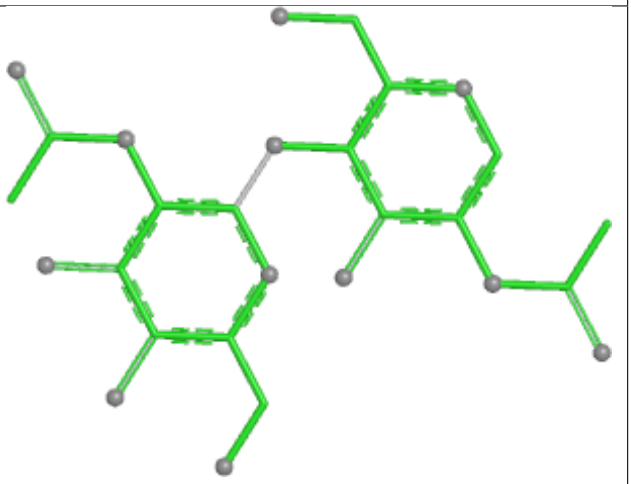

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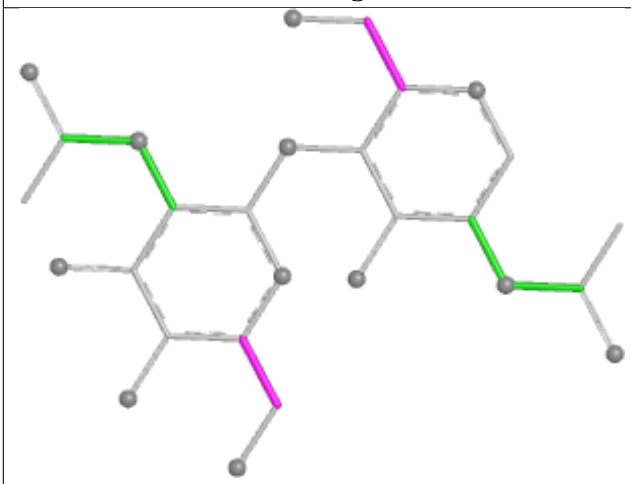

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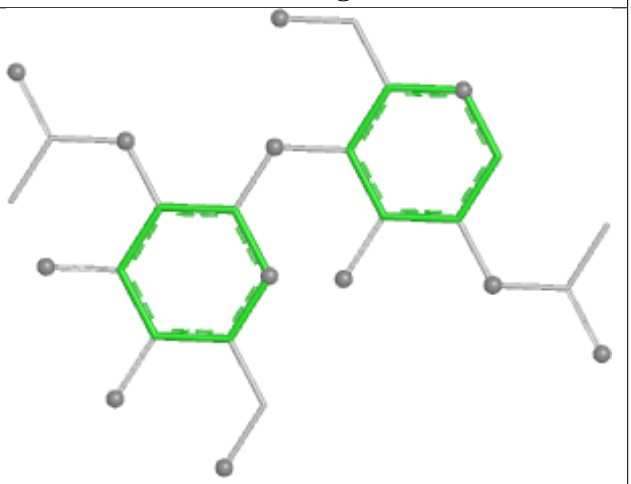
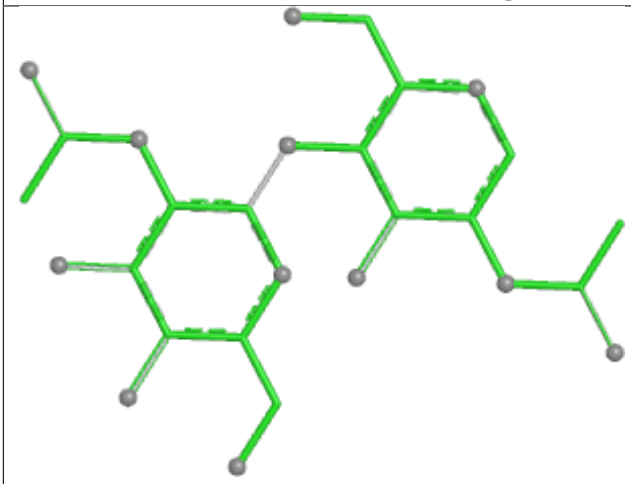


Rings

Oligosaccharide Chain e



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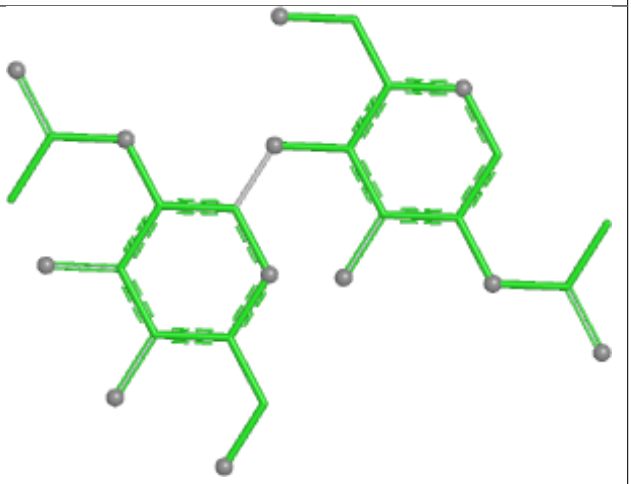

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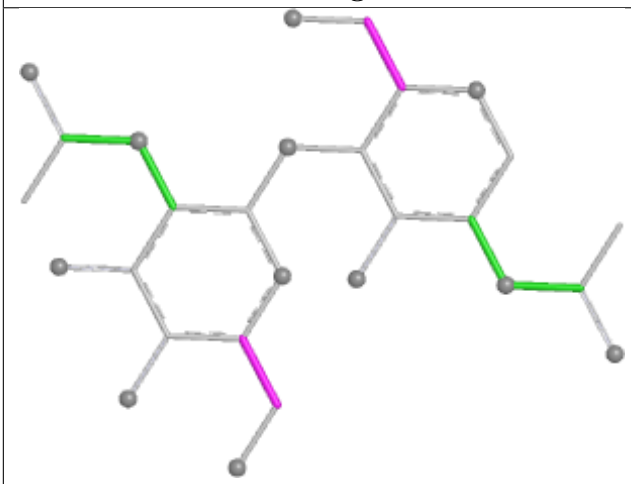

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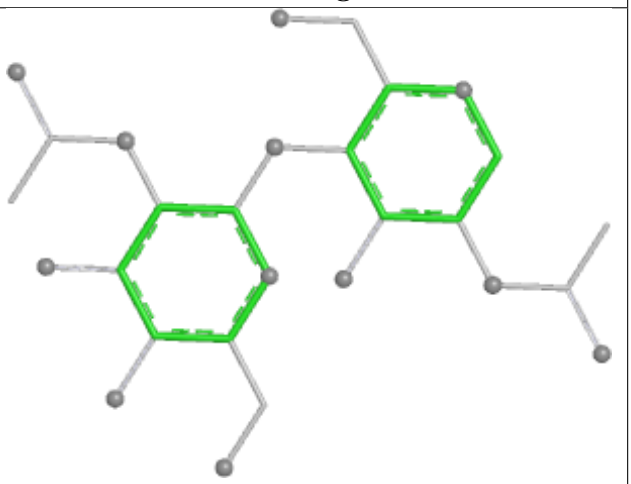
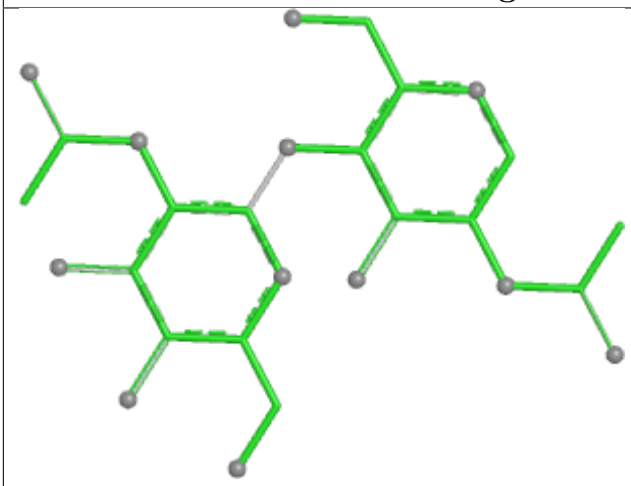


Rings

Oligosaccharide Chain g



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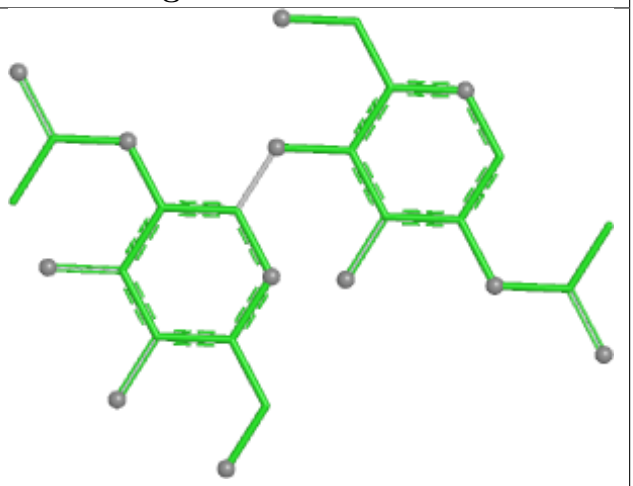

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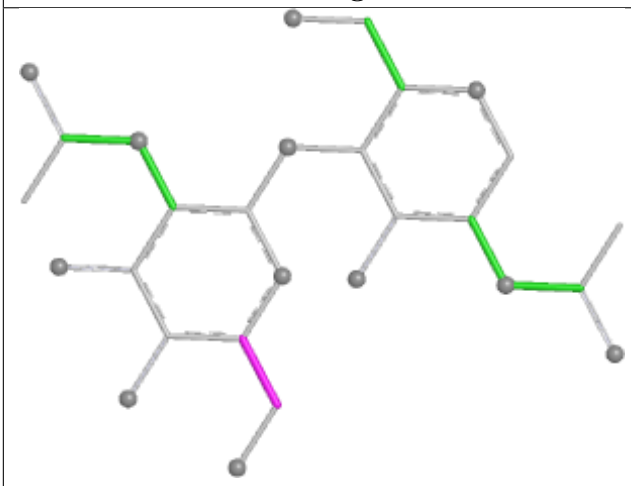

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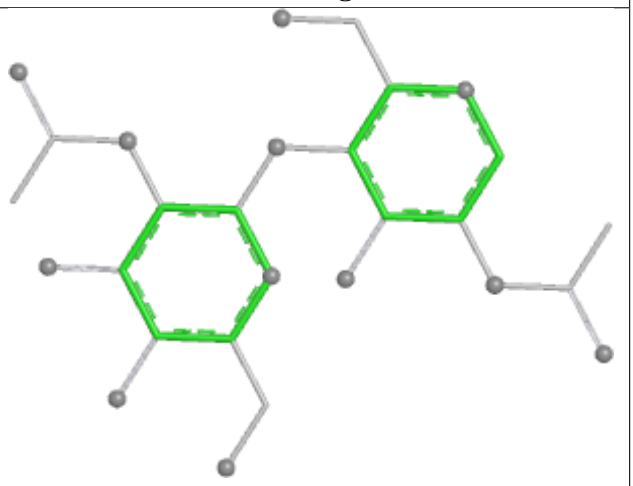
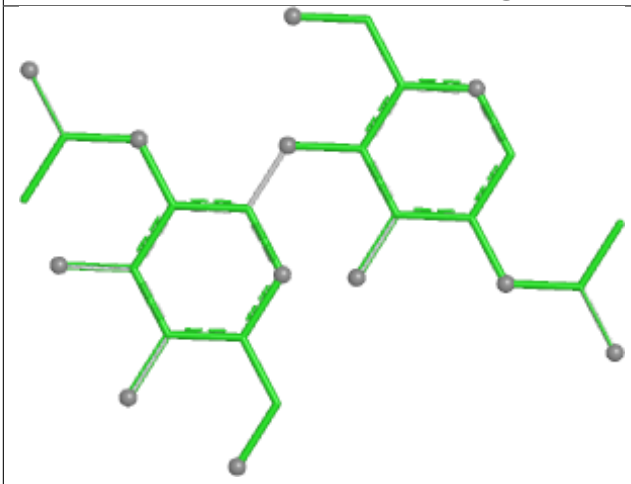


Rings

Oligosaccharide Chain h



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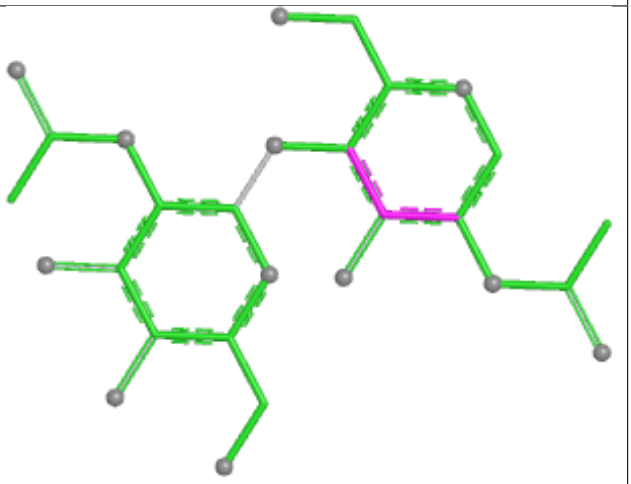
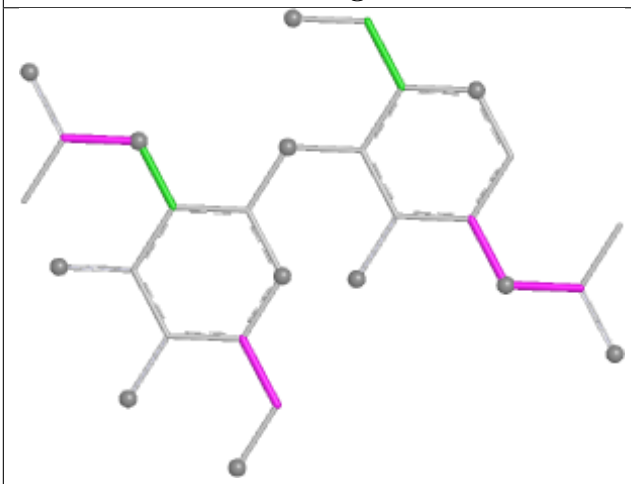


Bond angles



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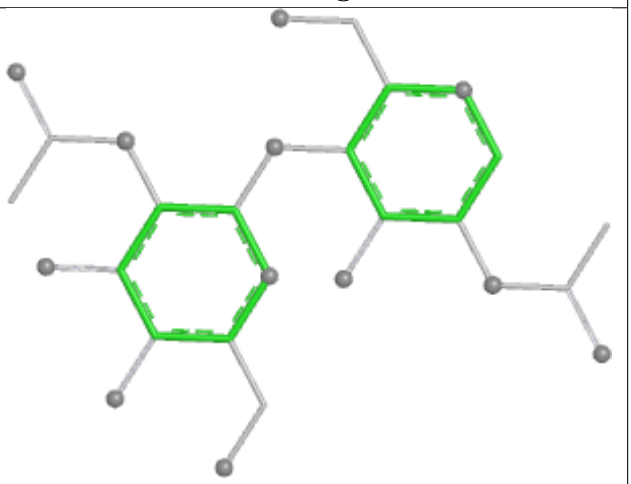
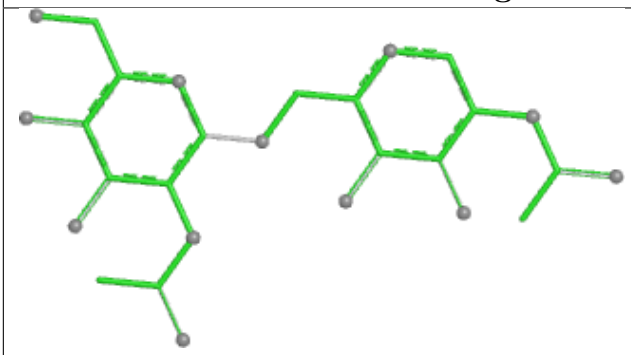


Rings

Oligosaccharide Chain O



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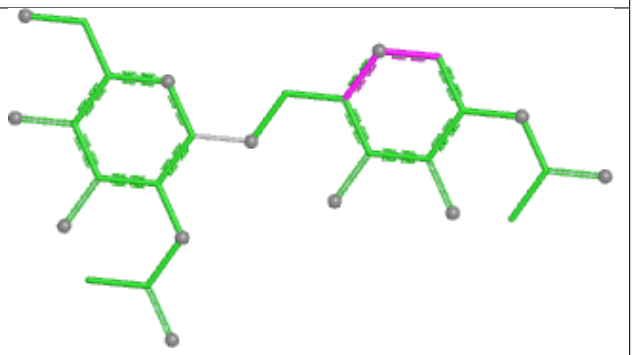
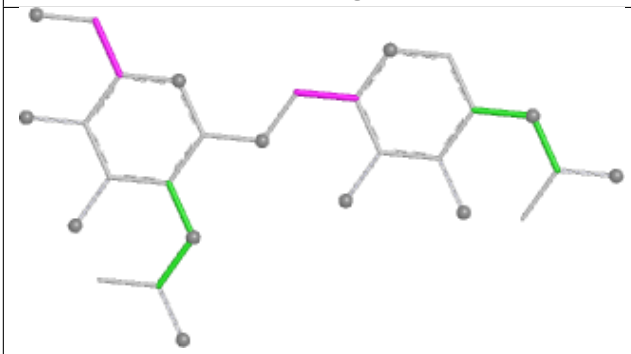
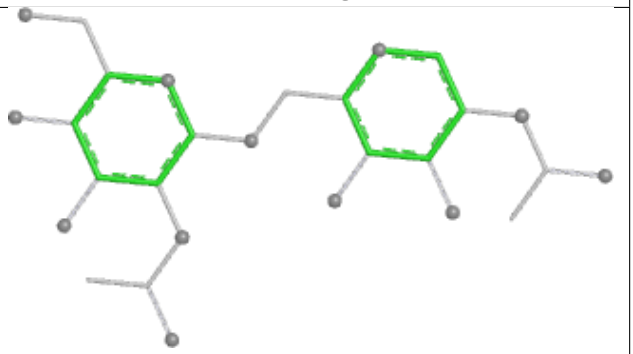


Bond angles

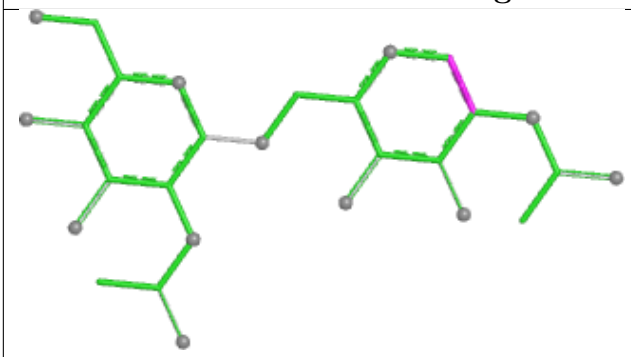


Torsions

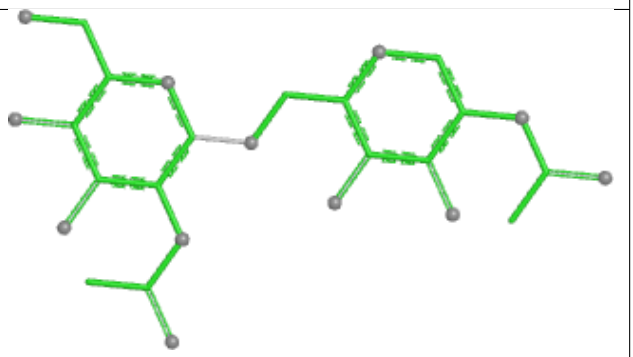


Rings

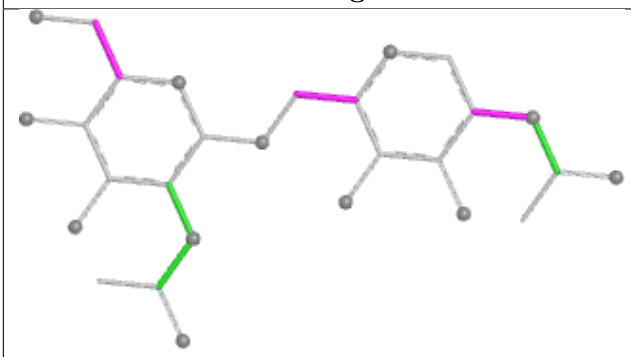
Oligosaccharide Chain V



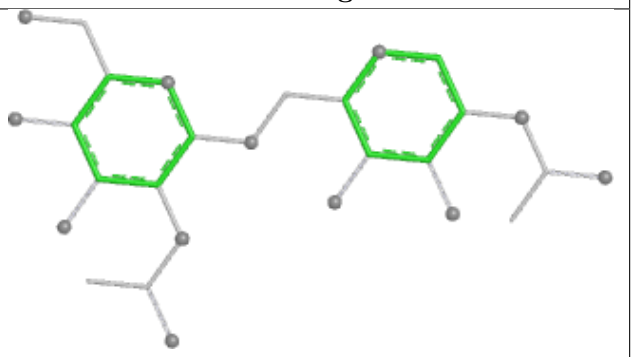
Bond lengths



Bond angles

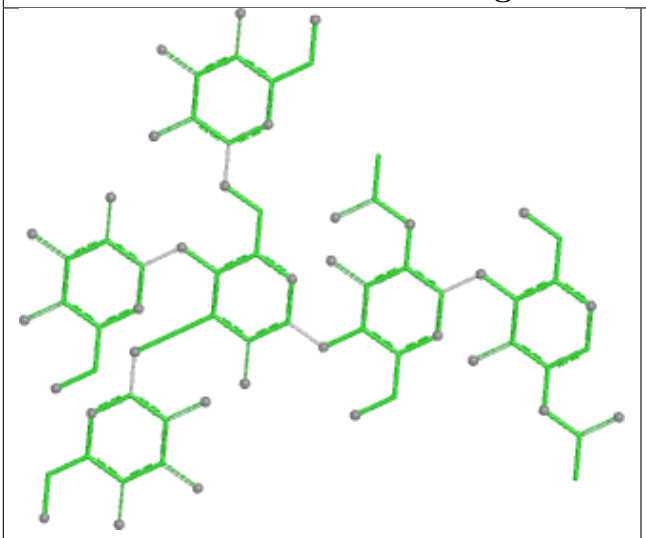


Torsions

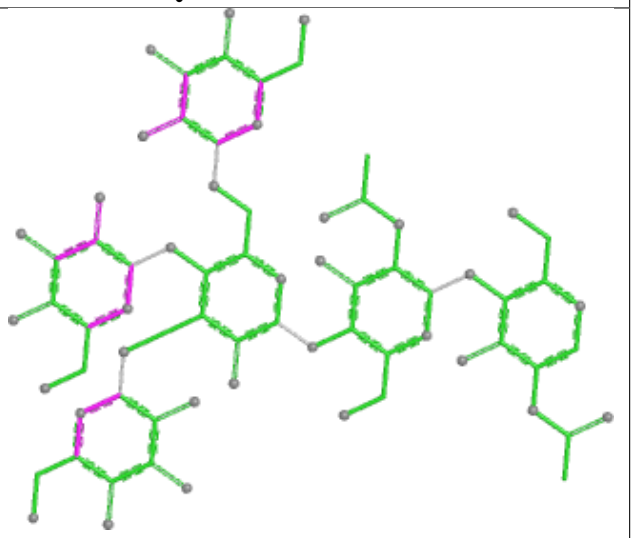


Rings

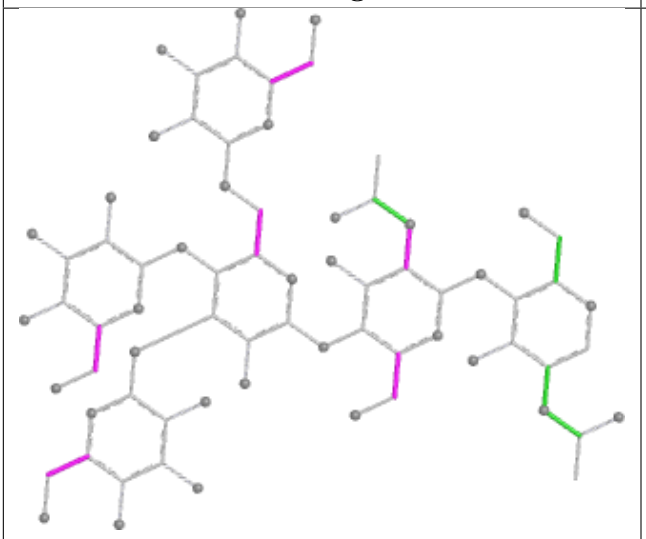
Oligosaccharide Chain Q



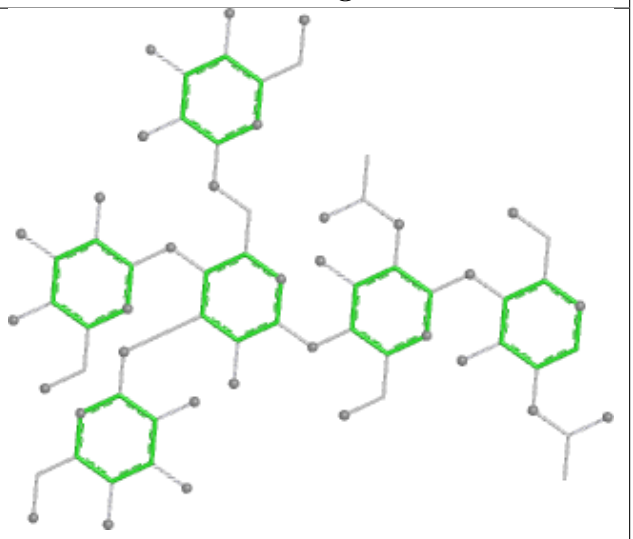
Bond lengths



Bond angles

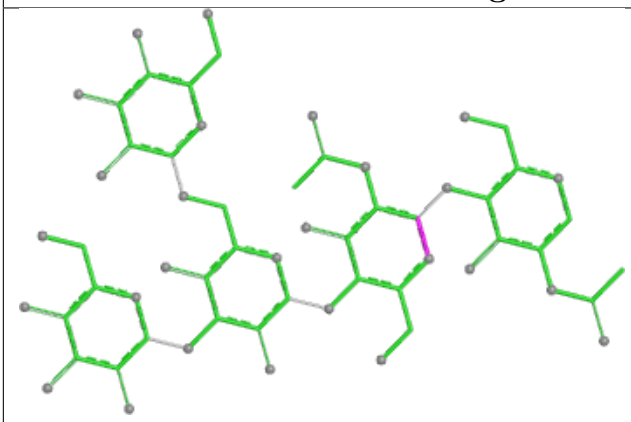


Torsions

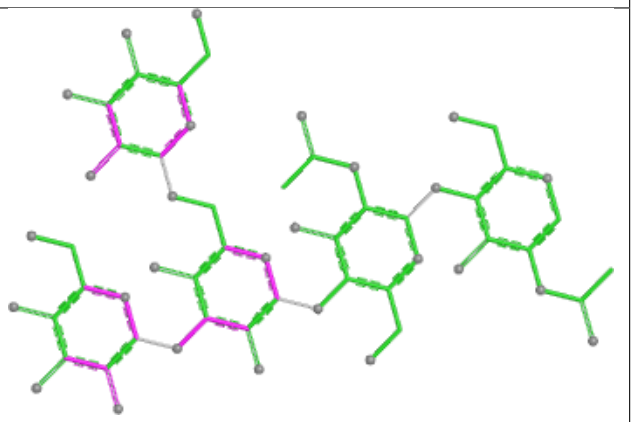


Rings

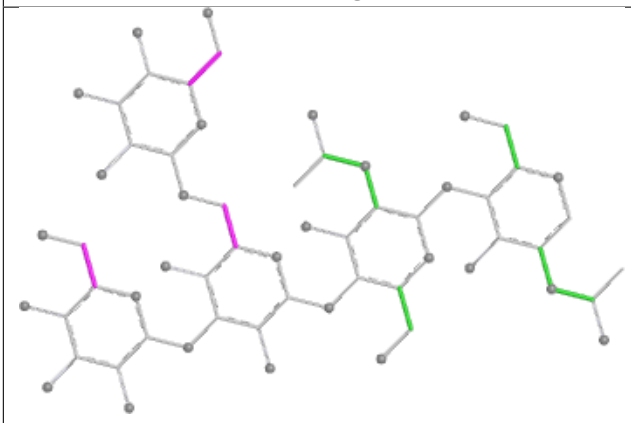
Oligosaccharide Chain W



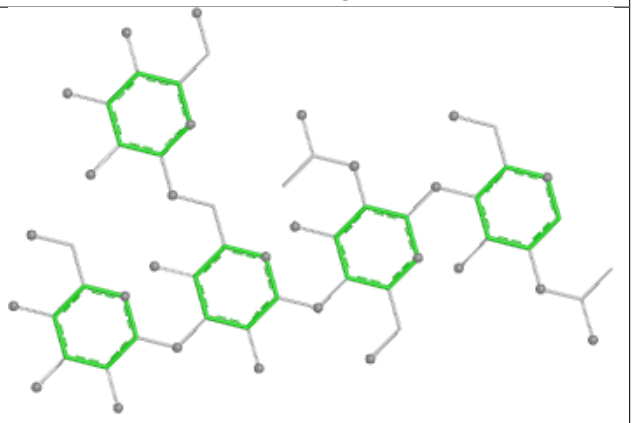
Bond lengths



Bond angles

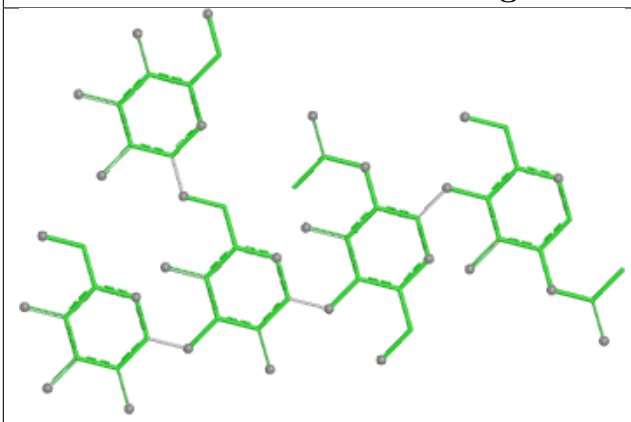


Torsions

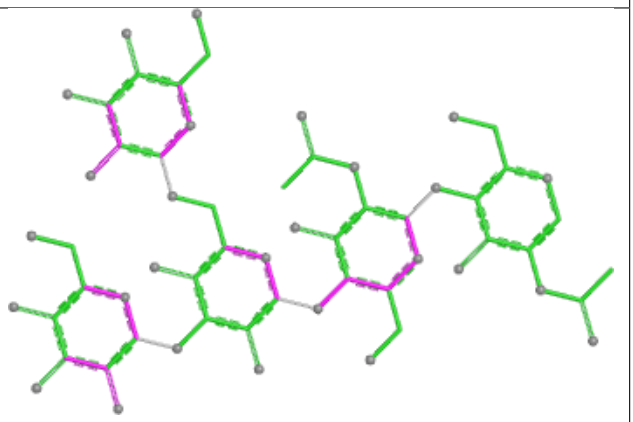


Rings

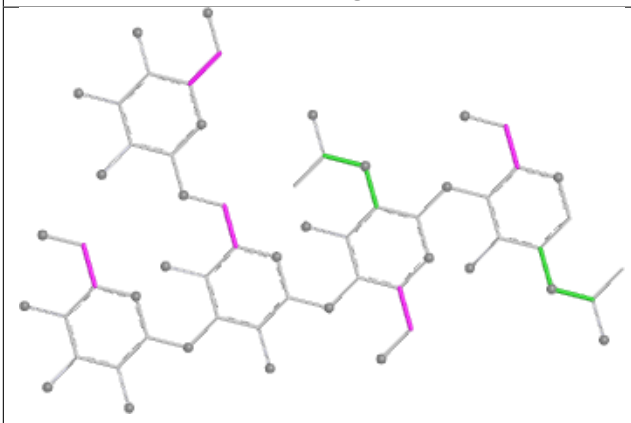
Oligosaccharide Chain c



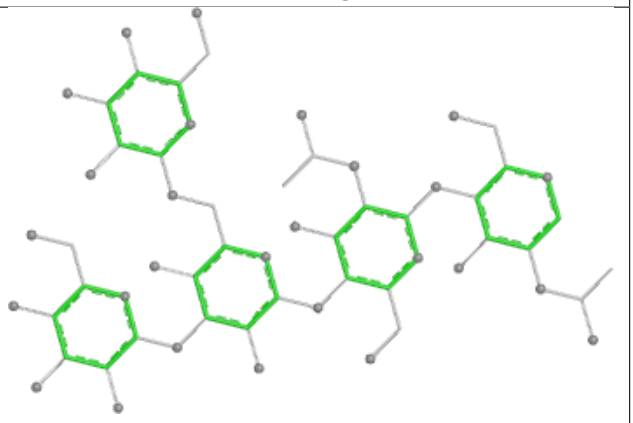
Bond lengths



Bond angles

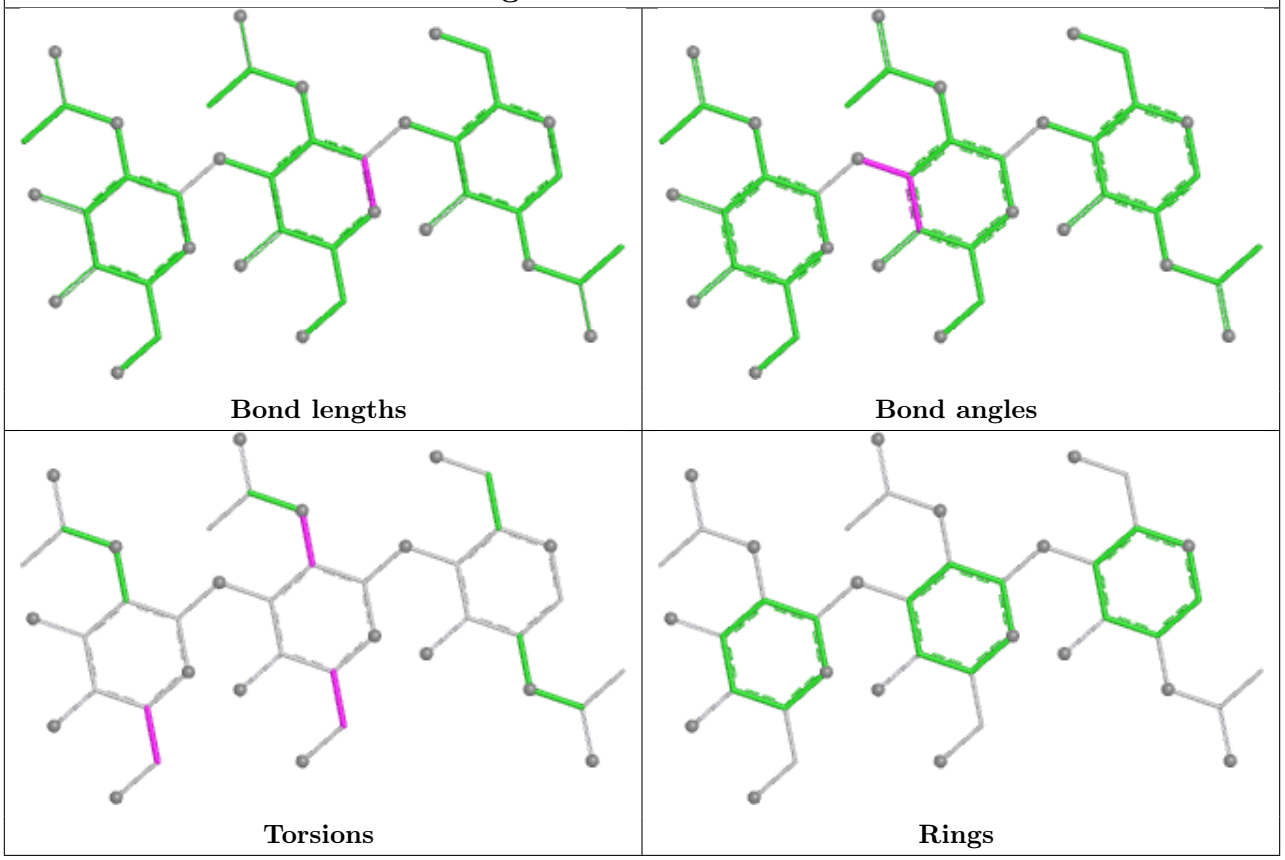


Torsions



Rings

Oligosaccharide Chain f



5.6 Ligand geometry (i)

43 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	NAG	C	607	3	14,14,15	0.28	0	17,19,21	0.46	0
15	NAG	F	701	4	14,14,15	0.18	0	17,19,21	0.38	0
15	NAG	A	610	3	14,14,15	0.42	0	17,19,21	0.46	0
15	NAG	C	613	3	14,14,15	0.77	1 (7%)	17,19,21	0.37	0
15	NAG	A	605	3	14,14,15	0.19	0	17,19,21	0.54	0
15	NAG	E	612	3	14,14,15	0.28	0	17,19,21	0.63	0
15	NAG	A	608	3	14,14,15	0.23	0	17,19,21	0.38	0
15	NAG	E	608	3	14,14,15	0.36	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	NAG	F	702	4	14,14,15	0.17	0	17,19,21	0.43	0
15	NAG	A	611	3	14,14,15	0.29	0	17,19,21	0.42	0
15	NAG	E	605	3	14,14,15	0.17	0	17,19,21	0.62	0
15	NAG	A	606	3	14,14,15	0.14	0	17,19,21	0.47	0
15	NAG	E	602	3	14,14,15	0.29	0	17,19,21	0.65	1 (5%)
15	NAG	C	603	3	14,14,15	0.26	0	17,19,21	0.48	0
15	NAG	E	604	3	14,14,15	0.20	0	17,19,21	0.45	0
15	NAG	E	606	3	14,14,15	0.25	0	17,19,21	0.44	0
15	NAG	E	607	3	14,14,15	0.19	0	17,19,21	0.49	0
15	NAG	E	613	3	14,14,15	0.21	0	17,19,21	0.57	0
15	NAG	C	612	3	14,14,15	0.20	0	17,19,21	0.47	0
15	NAG	B	702	4	14,14,15	0.40	0	17,19,21	0.44	0
15	NAG	C	608	3	14,14,15	0.22	0	17,19,21	0.34	0
15	NAG	E	611	3	14,14,15	0.39	0	17,19,21	0.49	0
15	NAG	A	604	3	14,14,15	0.32	0	17,19,21	0.37	0
15	NAG	C	611	3	14,14,15	0.16	0	17,19,21	0.51	0
15	NAG	A	609	3	14,14,15	0.17	0	17,19,21	0.54	0
15	NAG	E	609	3	14,14,15	0.16	0	17,19,21	0.50	0
15	NAG	D	701	4	14,14,15	0.39	0	17,19,21	0.42	0
15	NAG	A	603	3	14,14,15	0.35	0	17,19,21	0.45	0
15	NAG	C	602	3	14,14,15	0.39	0	17,19,21	0.50	0
15	NAG	D	702	4	14,14,15	0.42	0	17,19,21	0.40	0
15	NAG	E	603	3	14,14,15	0.19	0	17,19,21	0.45	0
15	NAG	C	601	3	14,14,15	0.49	0	17,19,21	0.49	0
15	NAG	B	701	4	14,14,15	0.19	0	17,19,21	0.50	0
15	NAG	C	610	3	14,14,15	0.23	0	17,19,21	0.46	0
15	NAG	E	601	3	14,14,15	0.63	1 (7%)	17,19,21	0.73	1 (5%)
15	NAG	C	609	3	14,14,15	0.30	0	17,19,21	0.39	0
15	NAG	A	607	3	14,14,15	0.25	0	17,19,21	0.50	0
15	NAG	A	602	3	14,14,15	0.21	0	17,19,21	0.54	0
15	NAG	C	606	3	14,14,15	0.23	0	17,19,21	0.42	0
15	NAG	C	605	3	14,14,15	0.22	0	17,19,21	0.44	0
15	NAG	A	601	3	14,14,15	0.19	0	17,19,21	0.39	0
15	NAG	C	604	3	14,14,15	0.21	0	17,19,21	0.38	0
15	NAG	E	610	3	14,14,15	0.18	0	17,19,21	0.41	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	C	604	3	-	1/6/23/26	0/1/1/1
15	NAG	E	610	3	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	613	NAG	C1-C2	2.81	1.56	1.52
15	E	601	NAG	C1-C2	2.08	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	E	601	NAG	C1-O5-C5	2.55	115.60	112.19
15	E	602	NAG	C1-O5-C5	2.16	115.08	112.19

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	E	612	NAG	C8-C7-N2-C2
15	E	612	NAG	O7-C7-N2-C2
15	E	613	NAG	C1-C2-N2-C7
15	E	613	NAG	C8-C7-N2-C2
15	E	613	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	613	NAG	2	0
15	C	611	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

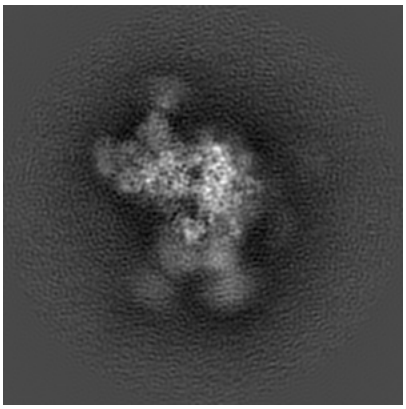
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43998. These allow visual inspection of the internal detail of the map and identification of artifacts.

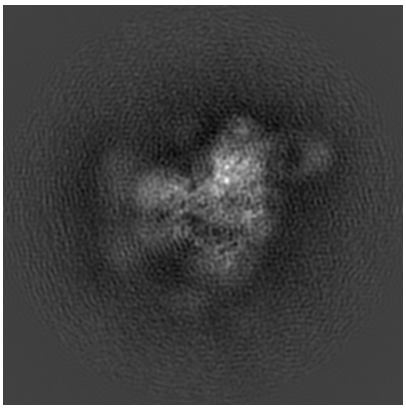
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

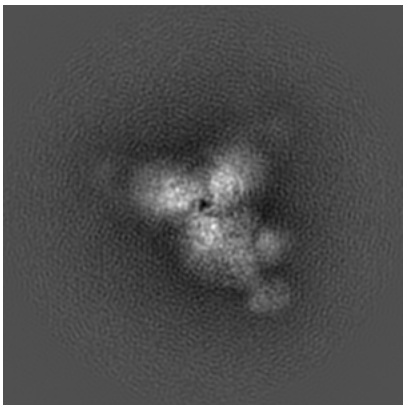
6.1.1 Primary map



X

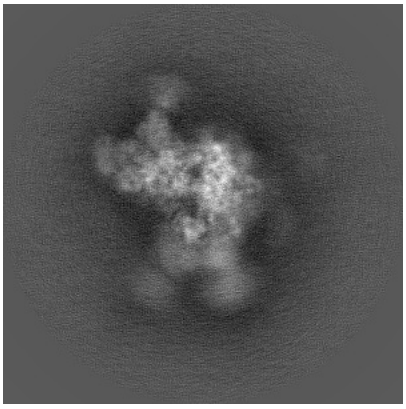


Y

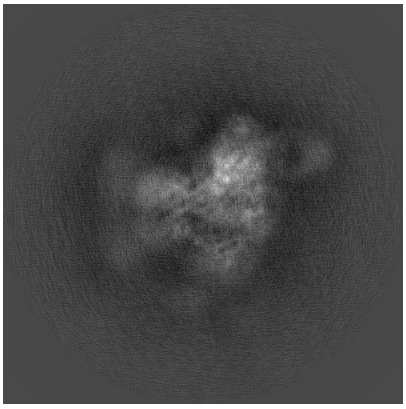


Z

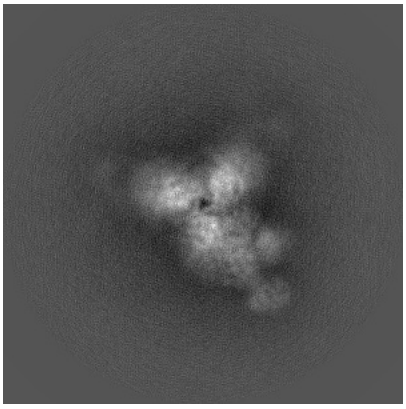
6.1.2 Raw map



X



Y

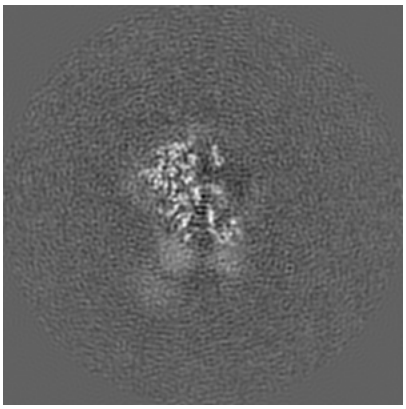


Z

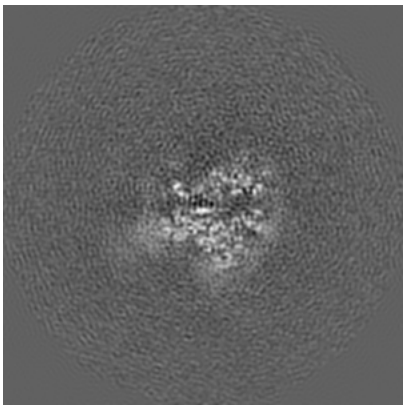
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

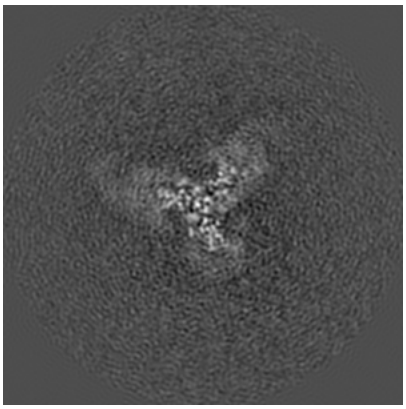
6.2.1 Primary map



X Index: 180

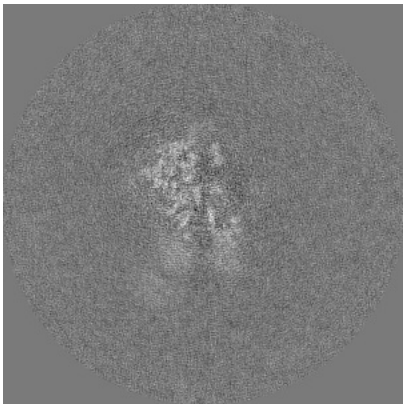


Y Index: 180

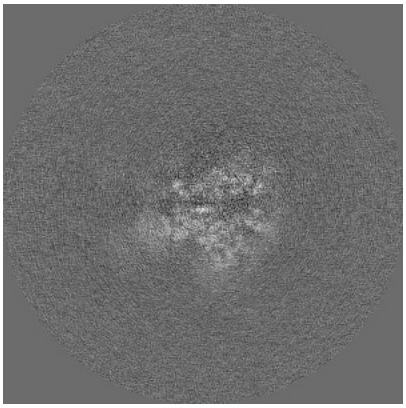


Z Index: 180

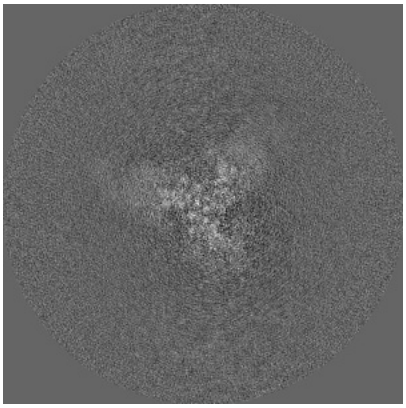
6.2.2 Raw map



X Index: 180



Y Index: 180

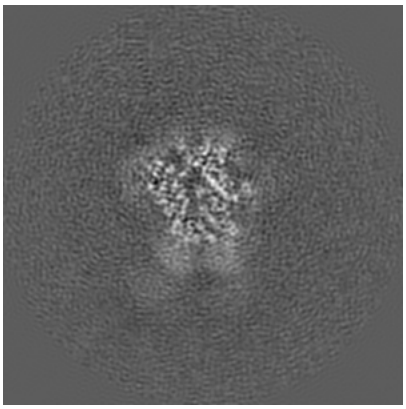


Z Index: 180

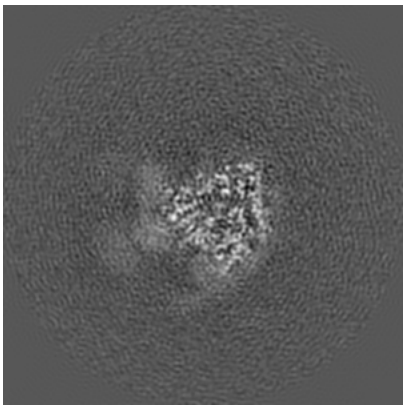
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

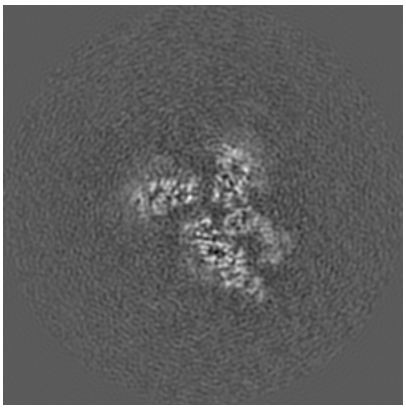
6.3.1 Primary map



X Index: 192

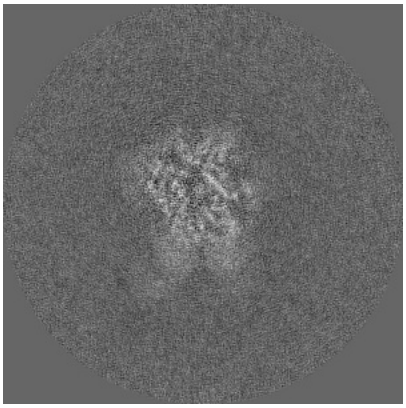


Y Index: 189

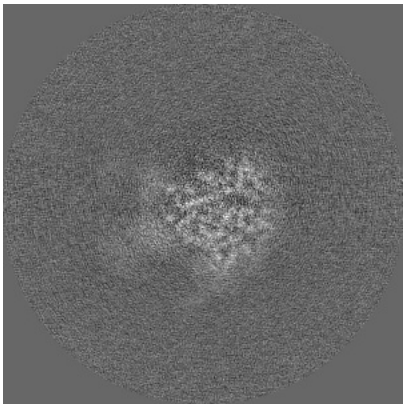


Z Index: 200

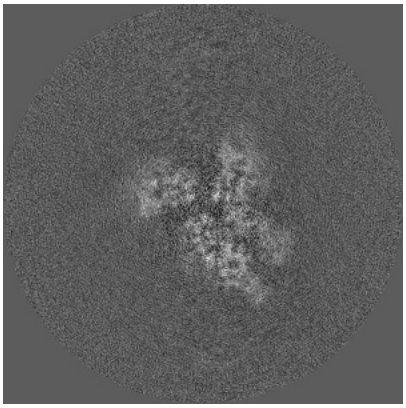
6.3.2 Raw map



X Index: 191



Y Index: 186

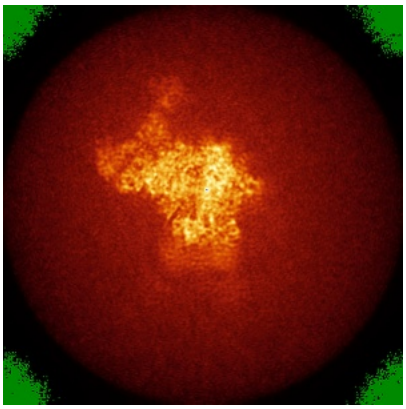


Z Index: 202

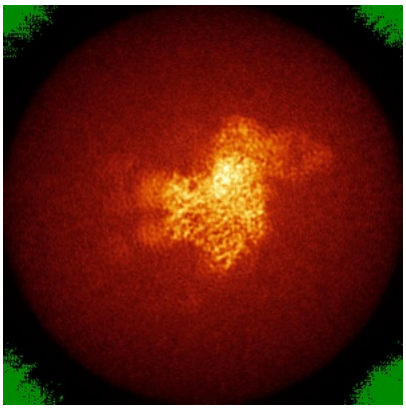
The images above show the largest variance slices of the map in three orthogonal directions.

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

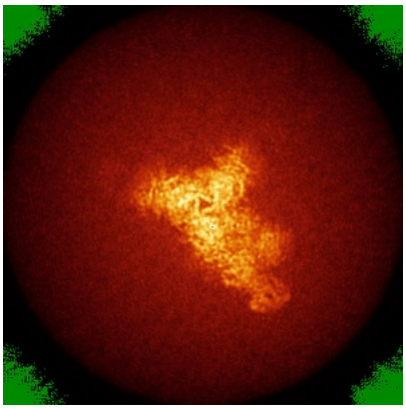
6.4.1 Primary map



X

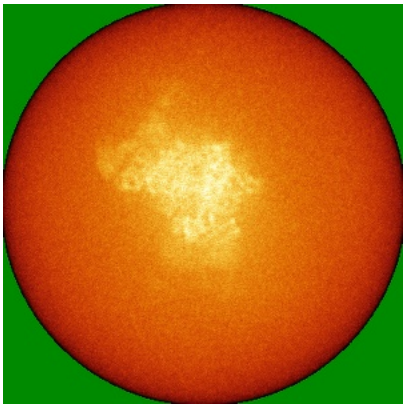


Y

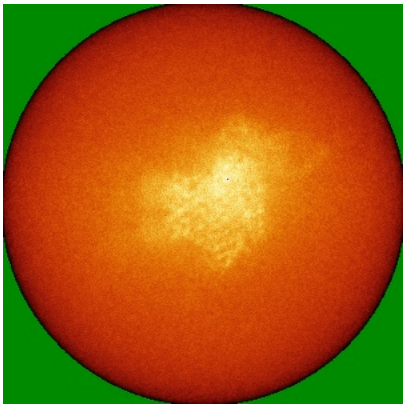


Z

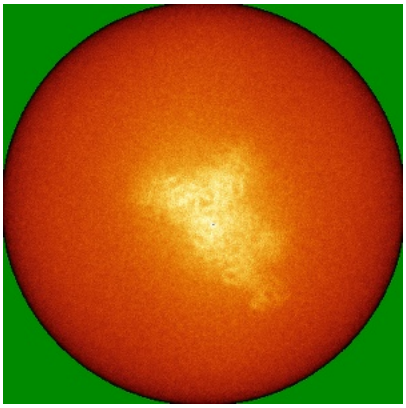
6.4.2 Raw map



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.

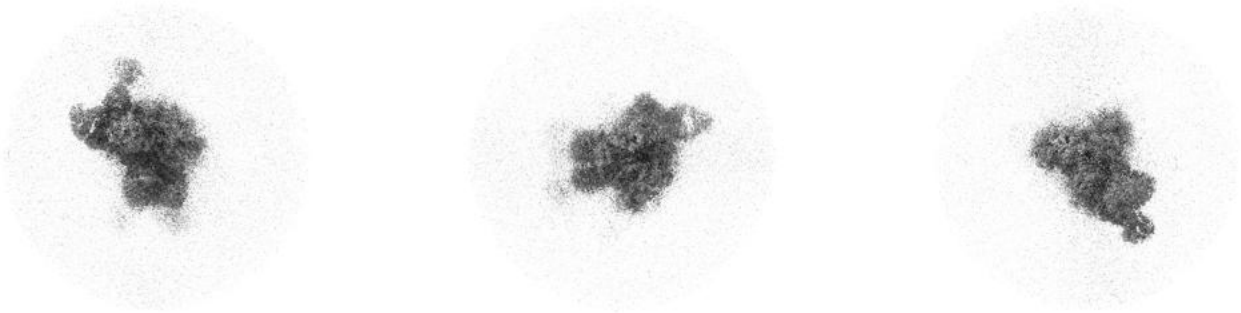
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

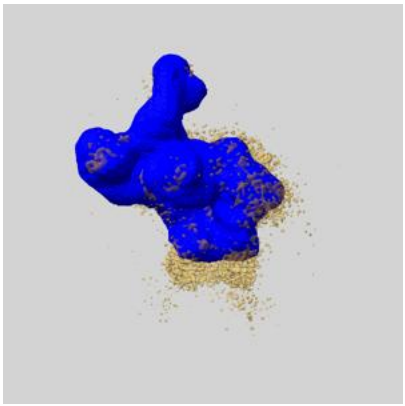
6.6 Mask visualisation (i)

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

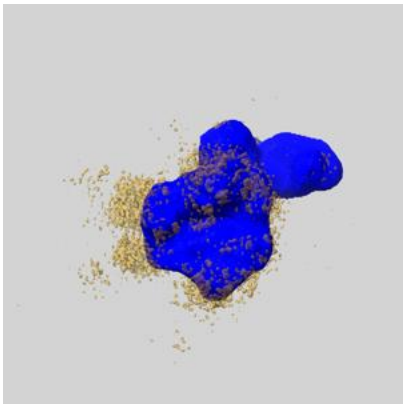
A mask typically either:

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

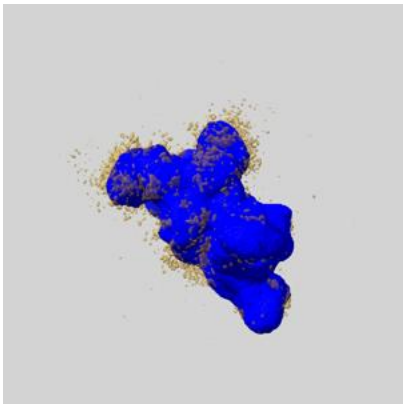
6.6.1 emd_43998_msk_1.map (i)



X



Y

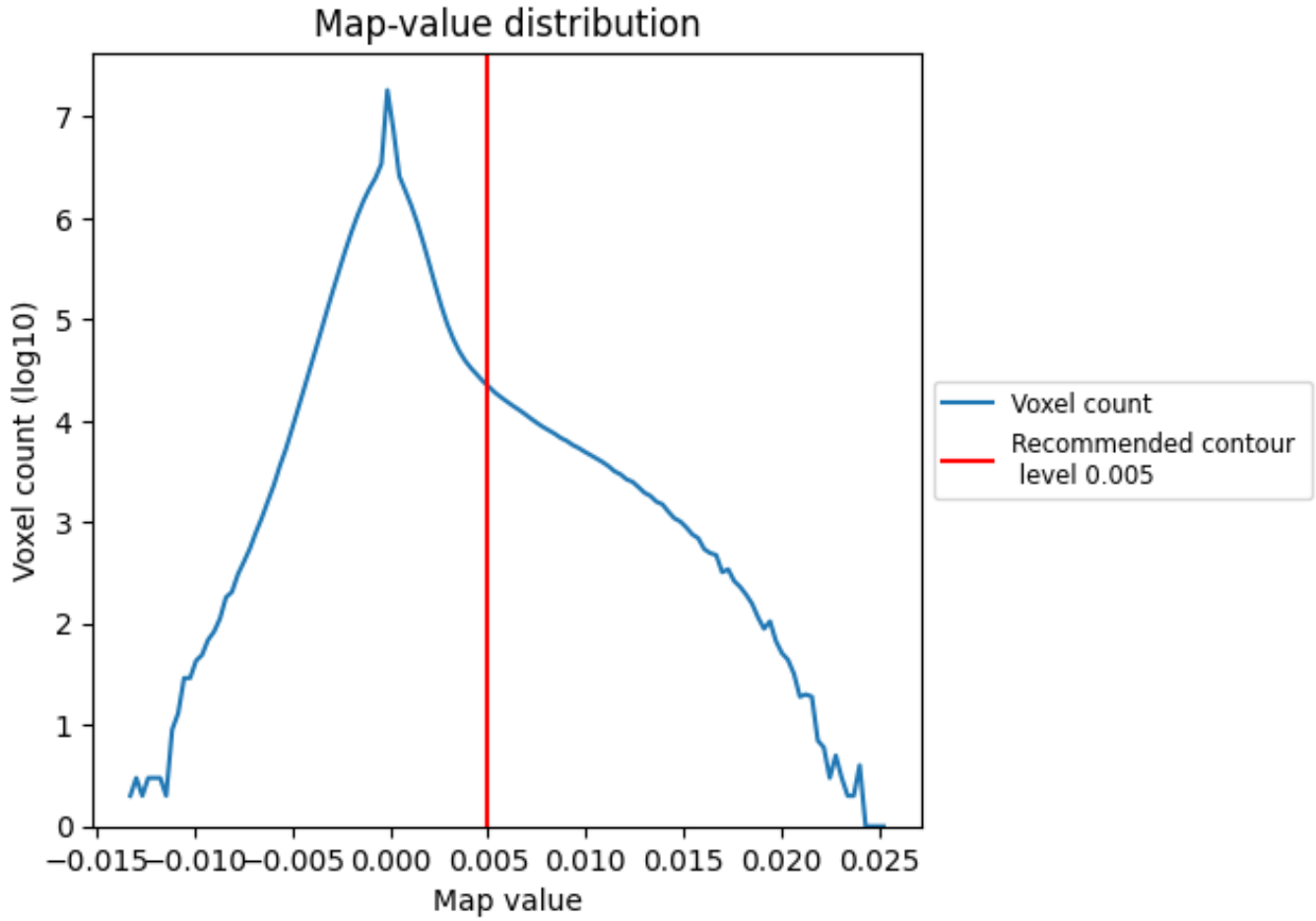


Z

7 Map analysis

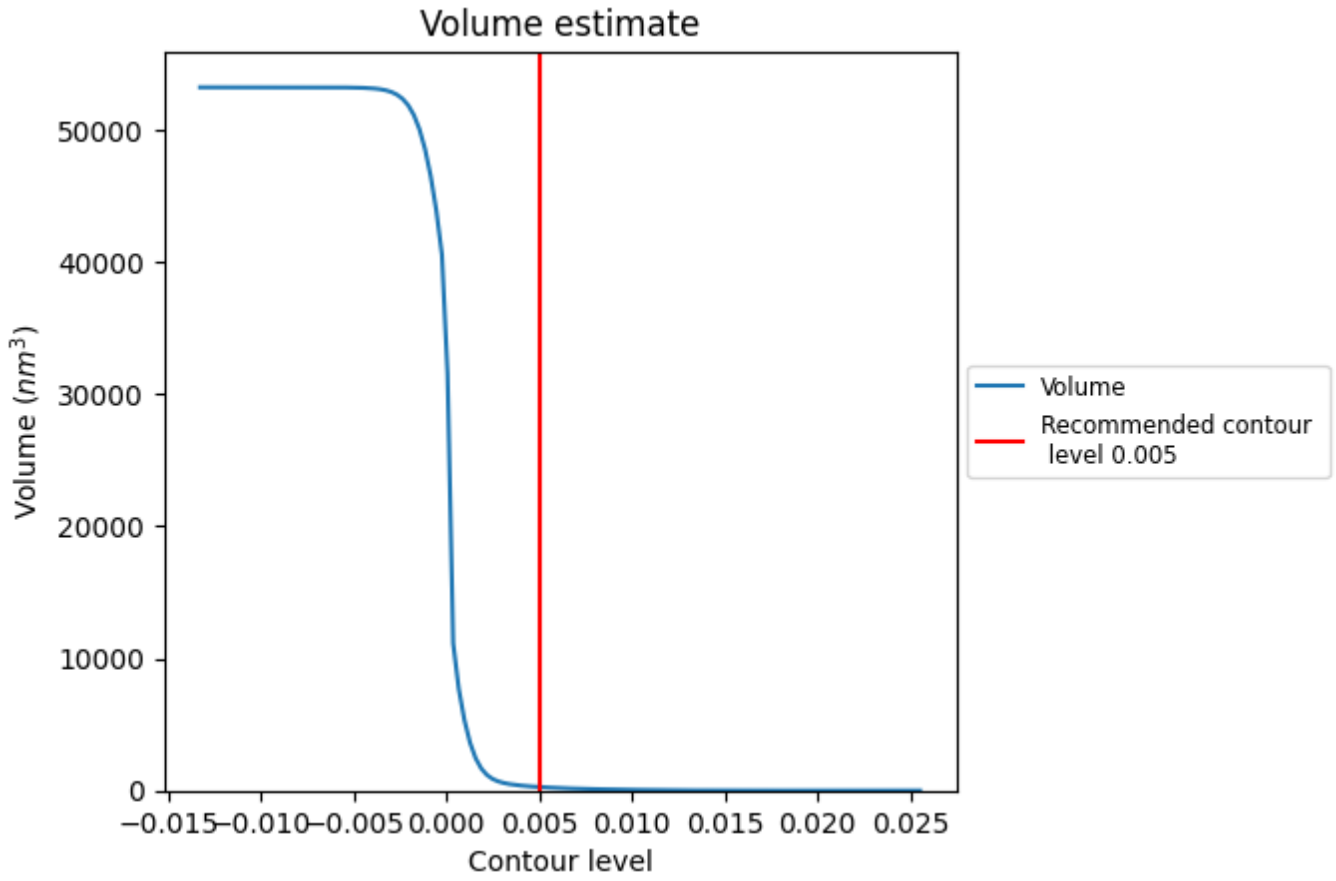
This section contains the results of statistical analysis of the map.

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.

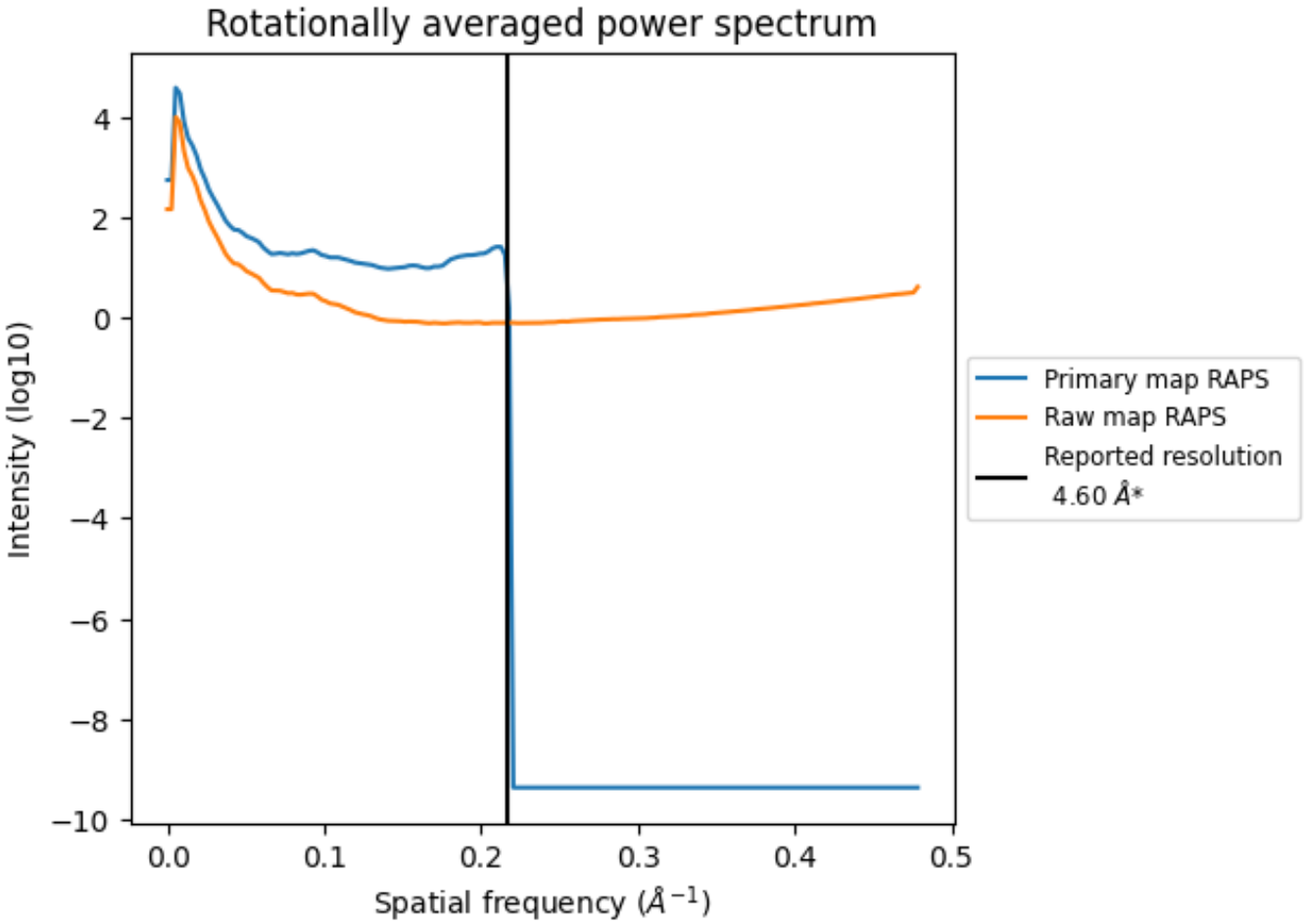
7.2 Volume estimate (i)



The volume at the recommended contour level is 269 nm^3; this corresponds to an approximate mass of 243 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)

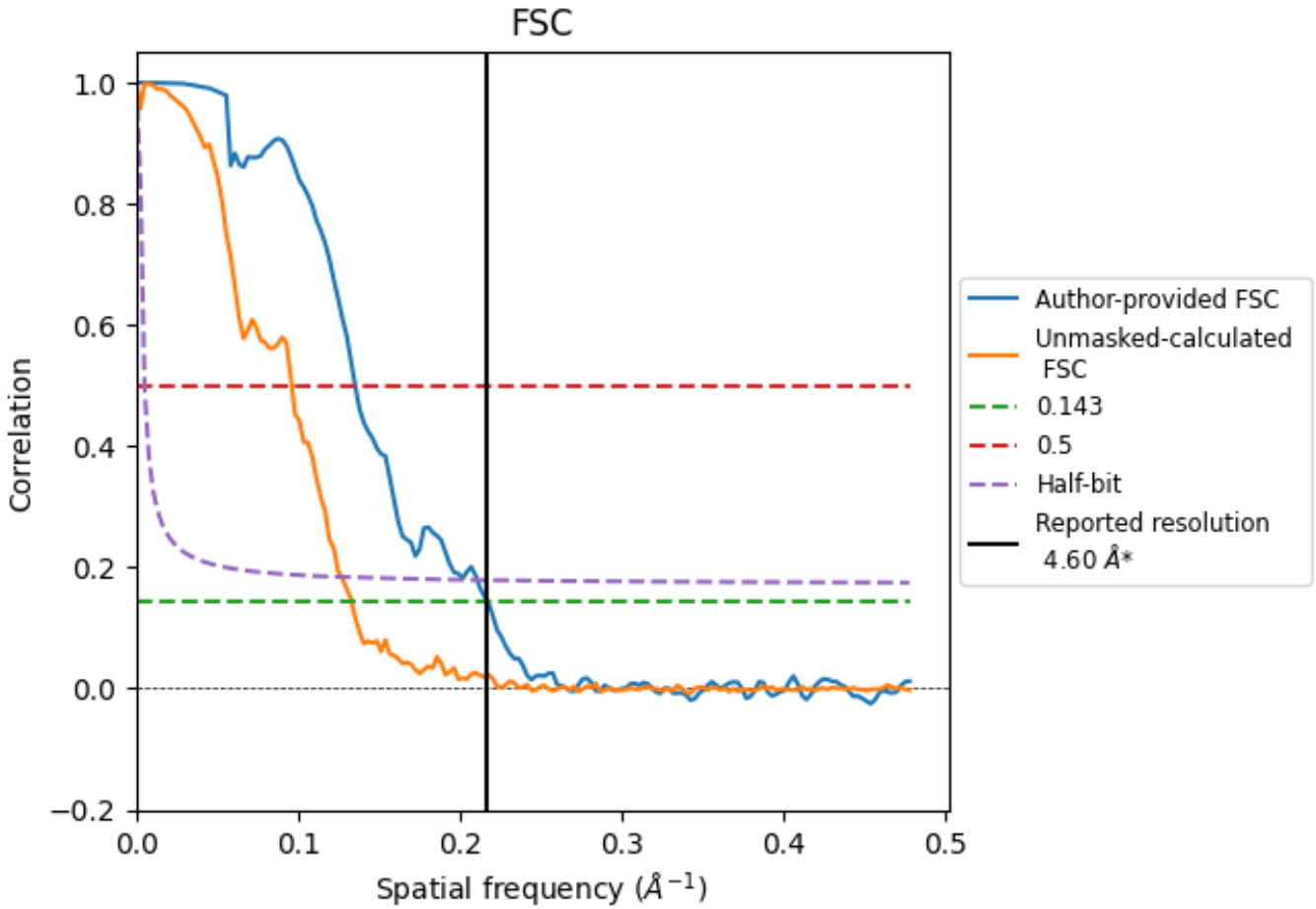


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

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 0.217 $Å^{-1}$

8.2 Resolution estimates (i)

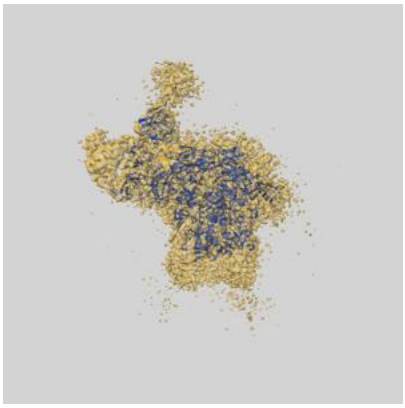
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.59	7.38	4.74
Unmasked-calculated*	7.50	10.38	7.87

*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 7.50 differs from the reported value 4.6 by more than 10 %

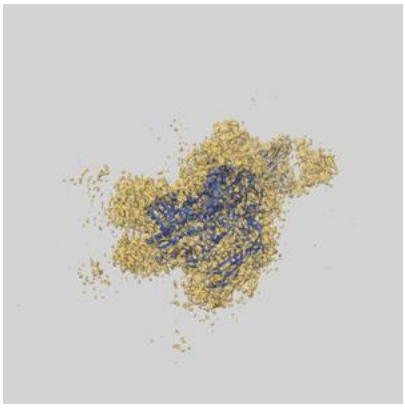
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43998 and PDB model 9AYS. Per-residue inclusion information can be found in section 3 on page 16.

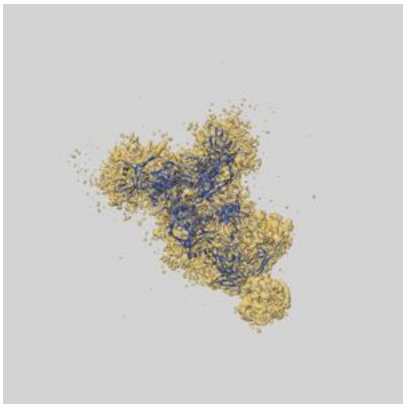
9.1 Map-model overlay



X



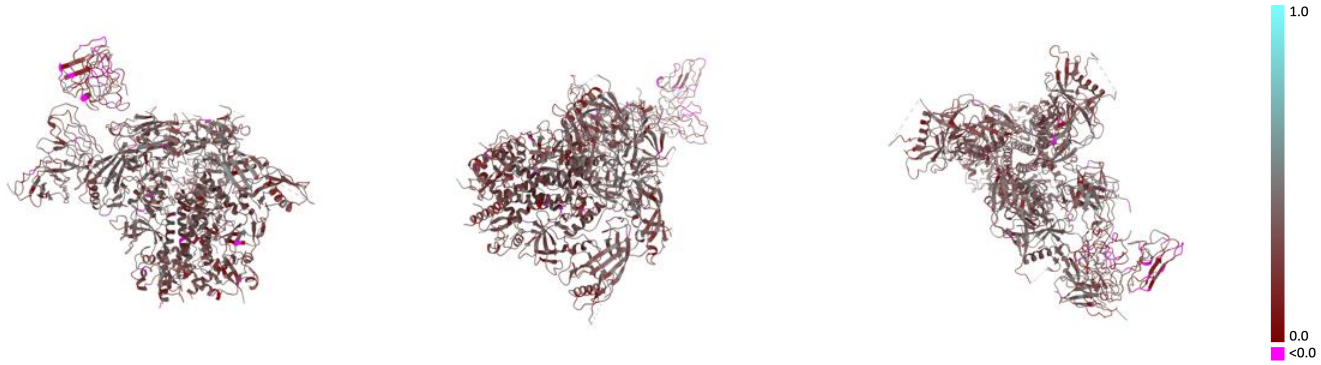
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

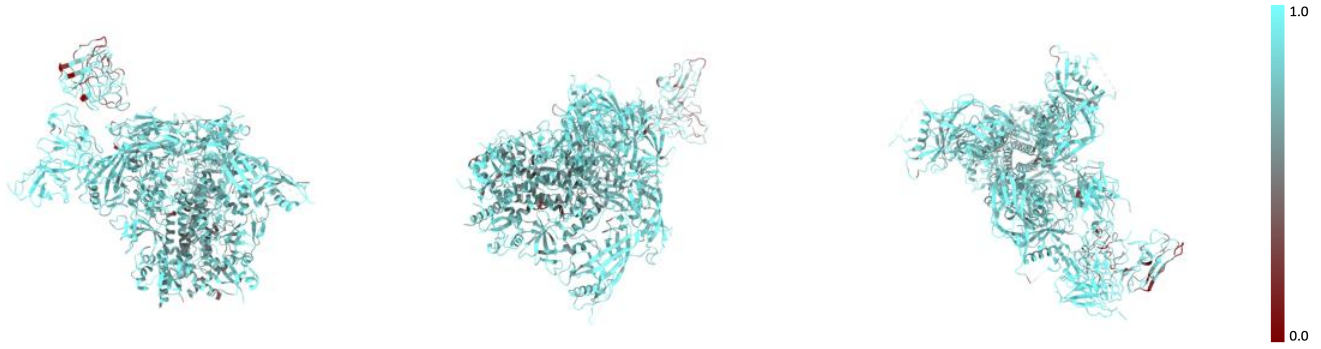
9.2 Q-score mapped to coordinate model (i)



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.

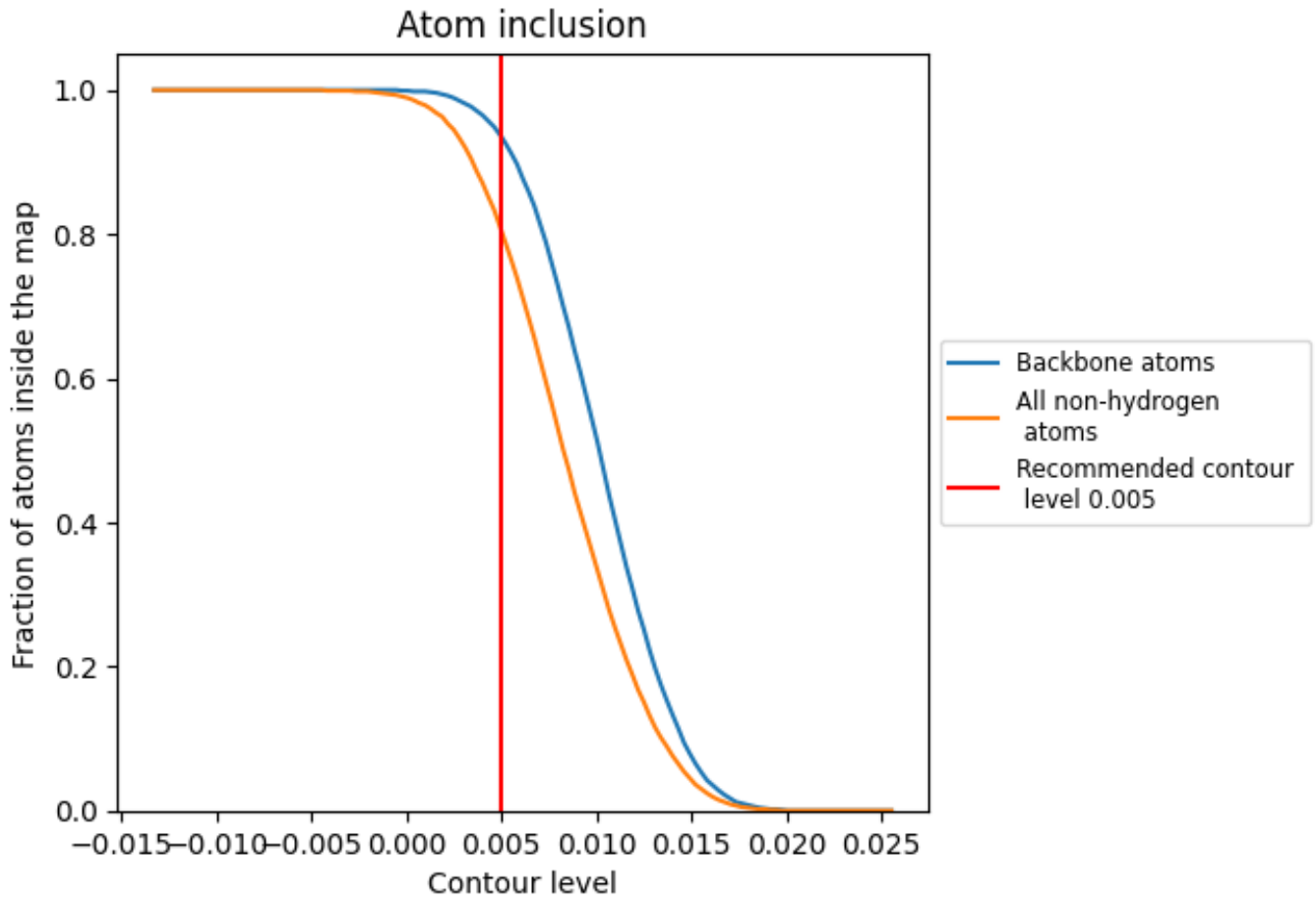
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 80% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.3210
A	0.8140	0.3320
B	0.7540	0.2790
C	0.8130	0.3230
D	0.7650	0.2940
E	0.8290	0.3530
F	0.7780	0.2860
G	0.8920	0.3370
H	0.8280	0.3430
I	0.9340	0.3400
J	0.6580	0.2130
K	0.6700	0.2340
L	0.8550	0.3440
M	0.6920	0.3270
N	0.6070	0.3400
O	0.8210	0.3740
P	0.6790	0.3830
Q	0.8060	0.3410
R	0.8210	0.3600
S	0.9640	0.2910
T	0.7860	0.3330
U	0.8930	0.3850
V	0.6430	0.2590
W	0.8360	0.3840
X	0.9640	0.4320
Y	0.8210	0.3220
Z	0.6790	0.2700
a	0.7500	0.2460
b	0.6790	0.3350
c	0.8360	0.3950
d	0.7140	0.3690
e	0.7860	0.3580
f	0.6910	0.2690
g	0.7860	0.3500
h	0.4640	0.1540