wwPDB EM Validation Summary Report

May 5, 2025 – 10:34 AM EDT

PDB ID	:	9AXI / pdb_00009axi
EMDB ID	:	EMD-43967
Title	:	HIV 16055.v8.3 SOSIP Env in Complex with Base and N625 Epitope pAbs from Rabbit 2463
Authors	:	Brown, S.; Antanasijevic, A.; Ward, A.B.
Deposited on	:	2024-03-06
Resolution	:	3.30 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:

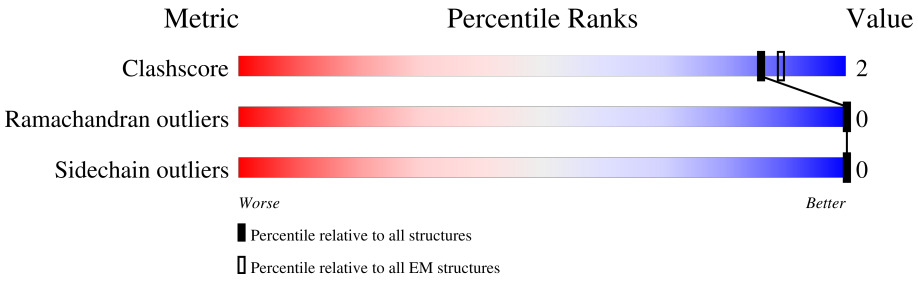
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 3.30 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	D	155	77% 6% 16%
1	I	155	5% 81% 6% 14%
1	M	155	85% 12%
2	F	110	100%
3	H	119	100%
4	A	122	100%
5	B	109	100%
6	J	514	79% 6% 15%

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Mol	Chain	Length	Quality of chain
6	K	514	81% 5% 15%
6	L	514	80% 17%
7	C	2	100%
7	E	2	50% 50% 50%
7	N	2	100%
7	O	2	50% 100%
7	P	2	50% 100%
7	Q	2	50% 100%
7	S	2	50% 100%
7	T	2	100%
7	U	2	50% 100%
7	V	2	50% 100%
7	X	2	100%
7	Y	2	50% 100%
7	Z	2	100%
7	a	2	100%
7	c	2	100%
7	d	2	100%
7	e	2	50% 50%
8	G	5	40% 60%
8	b	5	60% 40%
9	R	2	50% 50% 50%
10	W	4	75% 25%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17031 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 Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	136	Total	C	N	O	S	0	0
			1075	674	189	205	7		
1	D	130	Total	C	N	O	S	0	0
			1043	654	183	199	7		
1	I	134	Total	C	N	O	S	0	0
			1067	670	187	203	7		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	512	ARG	LYS	conflict	UNP A0A0B5KUY7
M	521	SER	ILE	conflict	UNP A0A0B5KUY7
M	561	PRO	ILE	conflict	UNP A0A0B5KUY7
M	563	CYS	ALA	conflict	UNP A0A0B5KUY7
M	570	ASP	LEU	conflict	UNP A0A0B5KUY7
M	571	GLY	THR	conflict	UNP A0A0B5KUY7
M	572	HIS	VAL	conflict	UNP A0A0B5KUY7
M	587	HIS	ARG	conflict	UNP A0A0B5KUY7
M	607	CYS	THR	conflict	UNP A0A0B5KUY7
D	512	ARG	LYS	conflict	UNP A0A0B5KUY7
D	521	SER	ILE	conflict	UNP A0A0B5KUY7
D	548M	PRO	ILE	conflict	UNP A0A0B5KUY7
D	562	CYS	ALA	conflict	UNP A0A0B5KUY7
D	569	ASP	LEU	conflict	UNP A0A0B5KUY7
D	570	GLY	THR	conflict	UNP A0A0B5KUY7
D	571	HIS	VAL	conflict	UNP A0A0B5KUY7
D	586	HIS	ARG	conflict	UNP A0A0B5KUY7
D	606	CYS	THR	conflict	UNP A0A0B5KUY7
I	512	ARG	LYS	conflict	UNP A0A0B5KUY7
I	521	SER	ILE	conflict	UNP A0A0B5KUY7
I	561	PRO	ILE	conflict	UNP A0A0B5KUY7
I	563	CYS	ALA	conflict	UNP A0A0B5KUY7
I	570	ASP	LEU	conflict	UNP A0A0B5KUY7
I	571	GLY	THR	conflict	UNP A0A0B5KUY7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	572	HIS	VAL	conflict	UNP A0A0B5KUY7
I	587	HIS	ARG	conflict	UNP A0A0B5KUY7
I	607	CYS	THR	conflict	UNP A0A0B5KUY7

- Molecule 2 is a protein called Rabbit Polyclonal Antibody N625 Epitope - Predicted Light Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	110	Total 550	C 330	N 110	O 110	0	0

- Molecule 3 is a protein called Rabbit Polyclonal Antibody N625 Epitope - Predicted Heavy Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	119	Total 595	C 357	N 119	O 119	0	0

- Molecule 4 is a protein called Rabbit Polyclonal Antibody Base Epitope - Predicted Heavy Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	A	122	Total 610	C 366	N 122	O 122	0	0

- Molecule 5 is a protein called Rabbit Polyclonal Antibody Base Epitope - Predicted Light Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	B	109	Total 545	C 327	N 109	O 109	0	0

- Molecule 6 is a protein called Surface protein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	439	Total 3496	C 2207	N 614	O 648	S 27	0	0
6	L	429	Total 3425	C 2165	N 602	O 631	S 27	0	0
6	J	436	Total 3476	C 2195	N 610	O 644	S 27	0	0

There are 153 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	MET	-	initiating methionine	UNP A1EAI1
K	-3	ASP	-	expression tag	UNP A1EAI1
K	-2	ALA	-	expression tag	UNP A1EAI1
K	-1	MET	-	expression tag	UNP A1EAI1
K	0	LYS	-	expression tag	UNP A1EAI1
K	1	ARG	-	expression tag	UNP A1EAI1
K	2	GLY	-	expression tag	UNP A1EAI1
K	3	LEU	-	expression tag	UNP A1EAI1
K	4	CYS	-	expression tag	UNP A1EAI1
K	5	CYS	-	expression tag	UNP A1EAI1
K	6	VAL	-	expression tag	UNP A1EAI1
K	7	LEU	-	expression tag	UNP A1EAI1
K	8	LEU	-	expression tag	UNP A1EAI1
K	9	LEU	-	expression tag	UNP A1EAI1
K	10	CYS	-	expression tag	UNP A1EAI1
K	11	GLY	-	expression tag	UNP A1EAI1
K	12	ALA	-	expression tag	UNP A1EAI1
K	13	VAL	-	expression tag	UNP A1EAI1
K	14	PHE	-	expression tag	UNP A1EAI1
K	15	VAL	-	expression tag	UNP A1EAI1
K	16	SER	-	expression tag	UNP A1EAI1
K	17	PRO	-	expression tag	UNP A1EAI1
K	18	SER	-	expression tag	UNP A1EAI1
K	19	GLN	-	expression tag	UNP A1EAI1
K	20	GLU	-	expression tag	UNP A1EAI1
K	21	ILE	-	expression tag	UNP A1EAI1
K	22	HIS	-	expression tag	UNP A1EAI1
K	23	ALA	-	expression tag	UNP A1EAI1
K	24	ARG	-	expression tag	UNP A1EAI1
K	25	PHE	-	expression tag	UNP A1EAI1
K	26	ARG	-	expression tag	UNP A1EAI1
K	27	ARG	-	expression tag	UNP A1EAI1
K	28	GLY	-	expression tag	UNP A1EAI1
K	29	ALA	-	expression tag	UNP A1EAI1
K	30	ARG	-	expression tag	UNP A1EAI1
K	47	ASP	GLU	conflict	UNP A1EAI1
K	49	GLU	LYS	conflict	UNP A1EAI1
K	65	LYS	VAL	conflict	UNP A1EAI1
K	66	ARG	HIS	conflict	UNP A1EAI1
K	73	CYS	ALA	conflict	UNP A1EAI1
K	165	LEU	ILE	conflict	UNP A1EAI1
K	308	VAL	ARG	conflict	UNP A1EAI1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	318	TRP	THR	conflict	UNP A1EAI1
K	321	TYR	ALA	conflict	UNP A1EAI1
K	365	GLN	SER	conflict	UNP A1EAI1
K	431	ARG	GLU	conflict	UNP A1EAI1
K	434	GLN	ARG	conflict	UNP A1EAI1
K	502	ARG	ALA	conflict	UNP A1EAI1
K	503	CYS	ALA	conflict	UNP A1EAI1
K	511	ARG	GLU	conflict	UNP A1EAI1
K	512	ARG	LYS	conflict	UNP A1EAI1
L	-4	MET	-	initiating methionine	UNP A1EAI1
L	-3	ASP	-	expression tag	UNP A1EAI1
L	-2	ALA	-	expression tag	UNP A1EAI1
L	-1	MET	-	expression tag	UNP A1EAI1
L	0	LYS	-	expression tag	UNP A1EAI1
L	1	ARG	-	expression tag	UNP A1EAI1
L	2	GLY	-	expression tag	UNP A1EAI1
L	3	LEU	-	expression tag	UNP A1EAI1
L	4	CYS	-	expression tag	UNP A1EAI1
L	5	CYS	-	expression tag	UNP A1EAI1
L	6	VAL	-	expression tag	UNP A1EAI1
L	7	LEU	-	expression tag	UNP A1EAI1
L	8	LEU	-	expression tag	UNP A1EAI1
L	9	LEU	-	expression tag	UNP A1EAI1
L	10	CYS	-	expression tag	UNP A1EAI1
L	11	GLY	-	expression tag	UNP A1EAI1
L	12	ALA	-	expression tag	UNP A1EAI1
L	13	VAL	-	expression tag	UNP A1EAI1
L	14	PHE	-	expression tag	UNP A1EAI1
L	15	VAL	-	expression tag	UNP A1EAI1
L	16	SER	-	expression tag	UNP A1EAI1
L	17	PRO	-	expression tag	UNP A1EAI1
L	18	SER	-	expression tag	UNP A1EAI1
L	19	GLN	-	expression tag	UNP A1EAI1
L	20	GLU	-	expression tag	UNP A1EAI1
L	21	ILE	-	expression tag	UNP A1EAI1
L	22	HIS	-	expression tag	UNP A1EAI1
L	23	ALA	-	expression tag	UNP A1EAI1
L	24	ARG	-	expression tag	UNP A1EAI1
L	25	PHE	-	expression tag	UNP A1EAI1
L	26	ARG	-	expression tag	UNP A1EAI1
L	27	ARG	-	expression tag	UNP A1EAI1
L	28	GLY	-	expression tag	UNP A1EAI1

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Chain	Residue	Modelled	Actual	Comment	Reference
L	29	ALA	-	expression tag	UNP A1EAI1
L	30	ARG	-	expression tag	UNP A1EAI1
L	47	ASP	GLU	conflict	UNP A1EAI1
L	49	GLU	LYS	conflict	UNP A1EAI1
L	65	LYS	VAL	conflict	UNP A1EAI1
L	66	ARG	HIS	conflict	UNP A1EAI1
L	73	CYS	ALA	conflict	UNP A1EAI1
L	165	LEU	ILE	conflict	UNP A1EAI1
L	308	VAL	ARG	conflict	UNP A1EAI1
L	318	TRP	THR	conflict	UNP A1EAI1
L	321	TYR	ALA	conflict	UNP A1EAI1
L	365	GLN	SER	conflict	UNP A1EAI1
L	431	ARG	GLU	conflict	UNP A1EAI1
L	434	GLN	ARG	conflict	UNP A1EAI1
L	502	ARG	ALA	conflict	UNP A1EAI1
L	503	CYS	ALA	conflict	UNP A1EAI1
L	511	ARG	GLU	conflict	UNP A1EAI1
L	512	ARG	LYS	conflict	UNP A1EAI1
J	-4	MET	-	initiating methionine	UNP A1EAI1
J	-3	ASP	-	expression tag	UNP A1EAI1
J	-2	ALA	-	expression tag	UNP A1EAI1
J	-1	MET	-	expression tag	UNP A1EAI1
J	0	LYS	-	expression tag	UNP A1EAI1
J	1	ARG	-	expression tag	UNP A1EAI1
J	2	GLY	-	expression tag	UNP A1EAI1
J	3	LEU	-	expression tag	UNP A1EAI1
J	4	CYS	-	expression tag	UNP A1EAI1
J	5	CYS	-	expression tag	UNP A1EAI1
J	6	VAL	-	expression tag	UNP A1EAI1
J	7	LEU	-	expression tag	UNP A1EAI1
J	8	LEU	-	expression tag	UNP A1EAI1
J	9	LEU	-	expression tag	UNP A1EAI1
J	10	CYS	-	expression tag	UNP A1EAI1
J	11	GLY	-	expression tag	UNP A1EAI1
J	12	ALA	-	expression tag	UNP A1EAI1
J	13	VAL	-	expression tag	UNP A1EAI1
J	14	PHE	-	expression tag	UNP A1EAI1
J	15	VAL	-	expression tag	UNP A1EAI1
J	16	SER	-	expression tag	UNP A1EAI1
J	17	PRO	-	expression tag	UNP A1EAI1
J	18	SER	-	expression tag	UNP A1EAI1
J	19	GLN	-	expression tag	UNP A1EAI1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	20	GLU	-	expression tag	UNP A1EAI1
J	21	ILE	-	expression tag	UNP A1EAI1
J	22	HIS	-	expression tag	UNP A1EAI1
J	23	ALA	-	expression tag	UNP A1EAI1
J	24	ARG	-	expression tag	UNP A1EAI1
J	25	PHE	-	expression tag	UNP A1EAI1
J	26	ARG	-	expression tag	UNP A1EAI1
J	27	ARG	-	expression tag	UNP A1EAI1
J	28	GLY	-	expression tag	UNP A1EAI1
J	29	ALA	-	expression tag	UNP A1EAI1
J	30	ARG	-	expression tag	UNP A1EAI1
J	47	ASP	GLU	conflict	UNP A1EAI1
J	49	GLU	LYS	conflict	UNP A1EAI1
J	65	LYS	VAL	conflict	UNP A1EAI1
J	66	ARG	HIS	conflict	UNP A1EAI1
J	73	CYS	ALA	conflict	UNP A1EAI1
J	165	LEU	ILE	conflict	UNP A1EAI1
J	308	VAL	ARG	conflict	UNP A1EAI1
J	318	TRP	THR	conflict	UNP A1EAI1
J	321	TYR	ALA	conflict	UNP A1EAI1
J	365	GLN	SER	conflict	UNP A1EAI1
J	431	ARG	GLU	conflict	UNP A1EAI1
J	434	GLN	ARG	conflict	UNP A1EAI1
J	502	ARG	ALA	conflict	UNP A1EAI1
J	503	CYS	ALA	conflict	UNP A1EAI1
J	511	ARG	GLU	conflict	UNP A1EAI1
J	512	ARG	LYS	conflict	UNP A1EAI1

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	C	2	Total	C	N	O	0	0
			28	16	2	10		
7	E	2	Total	C	N	O	0	0
			28	16	2	10		
7	N	2	Total	C	N	O	0	0
			28	16	2	10		

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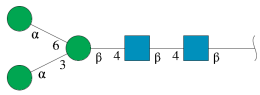
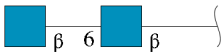
Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	2	Total	C	N	O	0	0
			28	16	2	10		
7	P	2	Total	C	N	O	0	0
			28	16	2	10		
7	Q	2	Total	C	N	O	0	0
			28	16	2	10		
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		
7	Y	2	Total	C	N	O	0	0
			28	16	2	10		
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	a	2	Total	C	N	O	0	0
			28	16	2	10		
7	c	2	Total	C	N	O	0	0
			28	16	2	10		
7	d	2	Total	C	N	O	0	0
			28	16	2	10		
7	e	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 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
8	G	5	Total	C	N	O	0	0
			61	34	2	25		
8	b	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

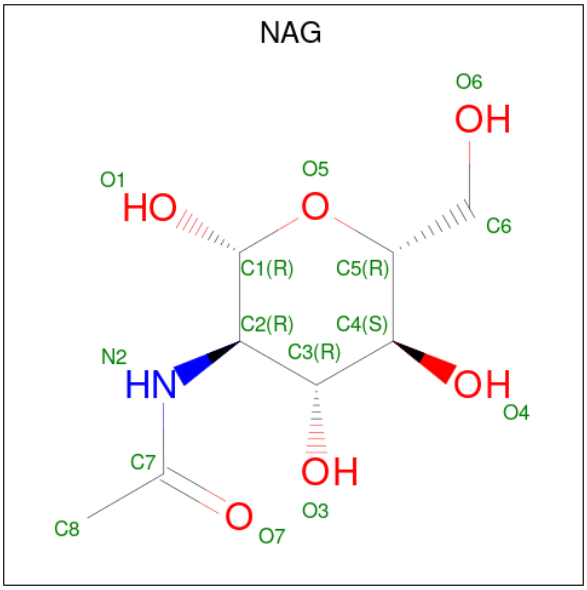


Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	2	Total	C	N	O	0	0
			28	16	2	10		

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

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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
11	M	1	Total	C	N	O	0
			14	8	1	5	
11	M	1	Total	C	N	O	0
			14	8	1	5	
11	M	1	Total	C	N	O	0
			14	8	1	5	
11	M	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	I	1	Total	C	N	O	0
			14	8	1	5	
11	I	1	Total	C	N	O	0
			14	8	1	5	
11	I	1	Total	C	N	O	0
			14	8	1	5	
11	K	1	Total	C	N	O	0
			14	8	1	5	
11	K	1	Total	C	N	O	0
			14	8	1	5	
11	K	1	Total	C	N	O	0
			14	8	1	5	
11	K	1	Total	C	N	O	0
			14	8	1	5	
11	K	1	Total	C	N	O	0
			14	8	1	5	
11	K	1	Total	C	N	O	0
			14	8	1	5	
11	K	1	Total	C	N	O	0
			14	8	1	5	
11	K	1	Total	C	N	O	0
			14	8	1	5	
11	K	1	Total	C	N	O	0
			14	8	1	5	
11	L	1	Total	C	N	O	0
			14	8	1	5	
11	L	1	Total	C	N	O	0
			14	8	1	5	
11	L	1	Total	C	N	O	0
			14	8	1	5	
11	L	1	Total	C	N	O	0
			14	8	1	5	
11	L	1	Total	C	N	O	0
			14	8	1	5	

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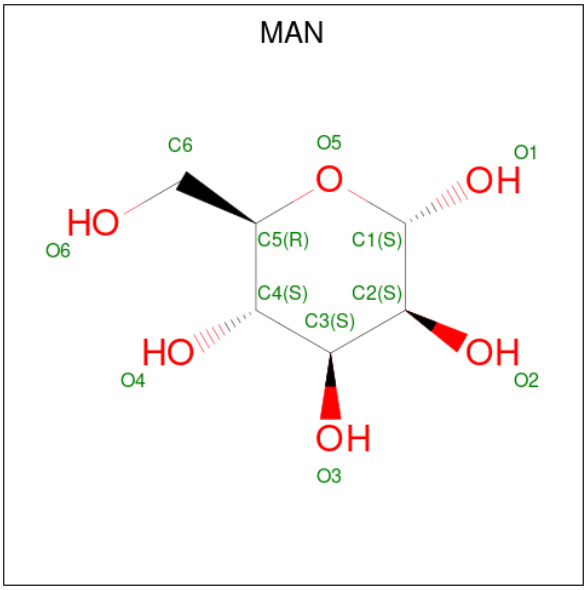
Mol	Chain	Residues	Atoms				AltConf
11	L	1	Total	C	N	O	0
			14	8	1	5	
11	L	1	Total	C	N	O	0
			14	8	1	5	
11	J	1	Total	C	N	O	0
			14	8	1	5	
11	J	1	Total	C	N	O	0
			14	8	1	5	
11	J	1	Total	C	N	O	0
			14	8	1	5	
11	J	1	Total	C	N	O	0
			14	8	1	5	
11	J	1	Total	C	N	O	0
			14	8	1	5	
11	J	1	Total	C	N	O	0
			14	8	1	5	
11	J	1	Total	C	N	O	0
			14	8	1	5	
11	J	1	Total	C	N	O	0
			14	8	1	5	
11	J	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 12 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



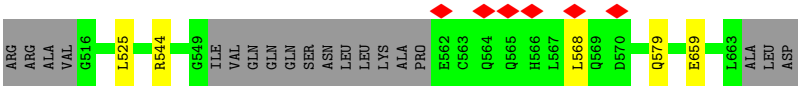
Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			11	6	5	

3 Residue-property plots (i)

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

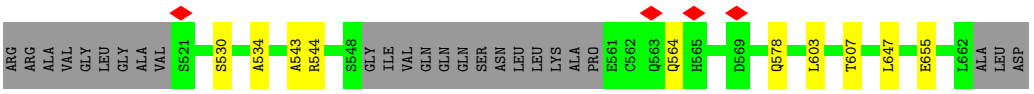
• Molecule 1: Transmembrane protein gp41

Chain M:



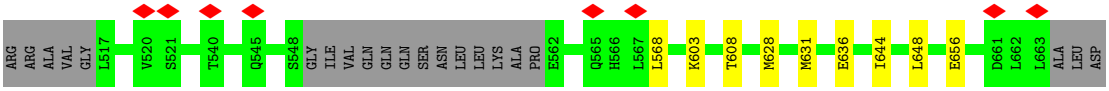
• Molecule 1: Transmembrane protein gp41

Chain D:



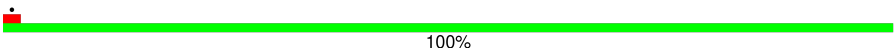
• Molecule 1: Transmembrane protein gp41

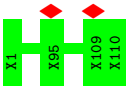
Chain I:



• Molecule 2: Rabbit Polyclonal Antibody N625 Epitope - Predicted Light Chain

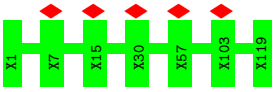
Chain F:





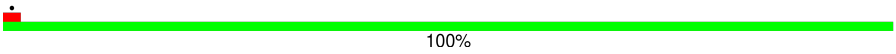
• Molecule 3: Rabbit Polyclonal Antibody N625 Epitope - Predicted Heavy Chain

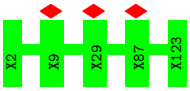
Chain H:



• Molecule 4: Rabbit Polyclonal Antibody Base Epitope - Predicted Heavy Chain

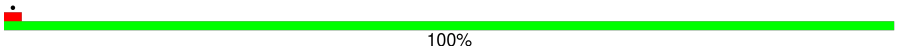
Chain A:

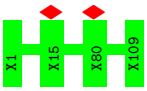




• Molecule 5: Rabbit Polyclonal Antibody Base Epitope - Predicted Light Chain

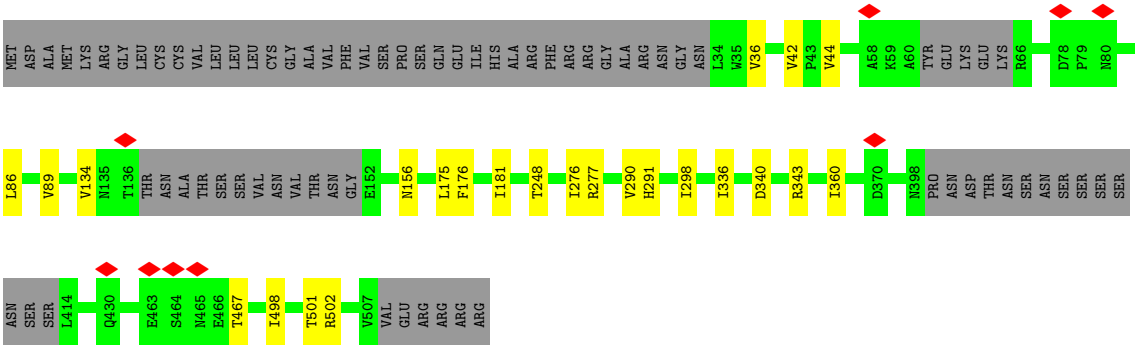
Chain B:





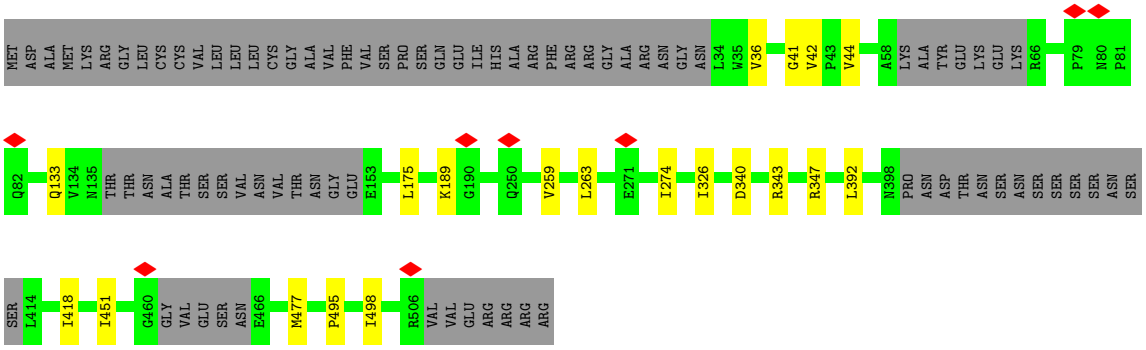
• Molecule 6: Surface protein gp120

Chain K:



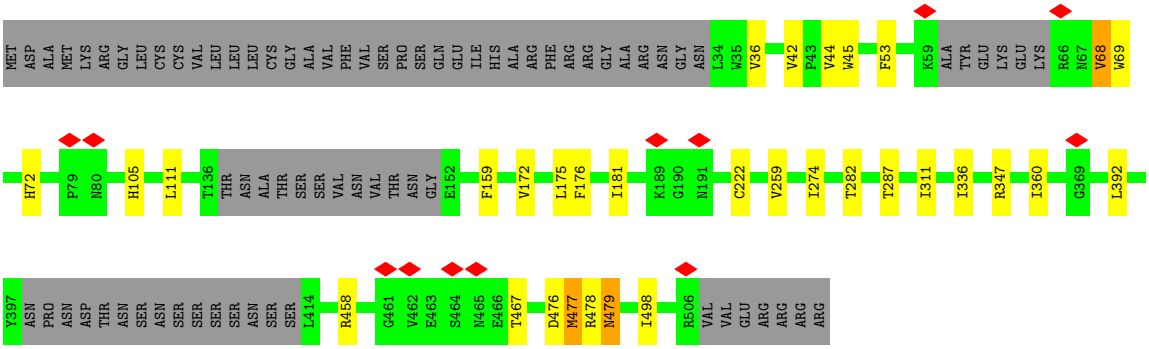
• Molecule 6: Surface protein gp120

Chain L:



• Molecule 6: Surface protein gp120

Chain J:



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

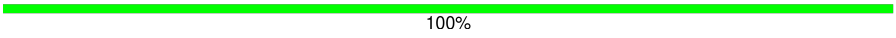
Chain C:

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

Chain E:

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

Chain N:



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

Chain O:

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

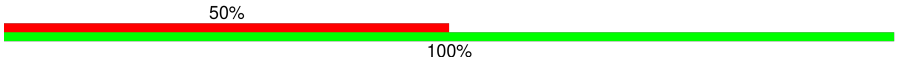
Chain P:

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

Chain Q:

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

Chain S:

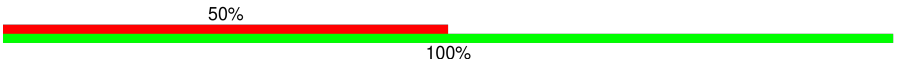


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

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

Chain U:

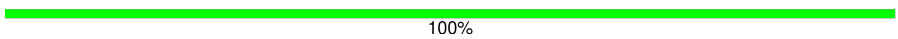


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

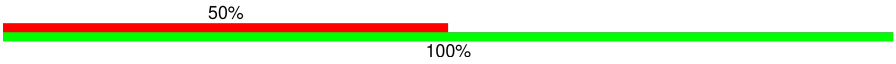
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



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

Chain Y:

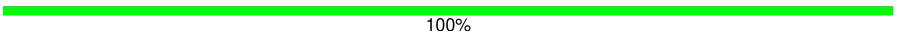


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

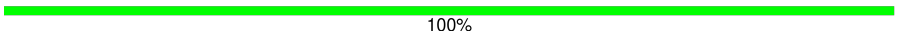
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



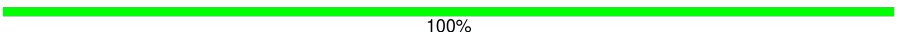
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



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

Chain d:

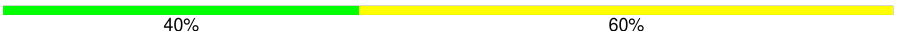


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

• Molecule 8: 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 G:



• Molecule 8: 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 b:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

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

Chain W:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51733	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 ($e^-/Å^2$)	40.3	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.078	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	384.72, 384.72, 384.72	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8015, 0.8015, 0.8015	Depositor

5 Model quality

5.1 Standard geometry

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

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	D	0.25	0/1065	0.51	0/1442
1	I	0.29	0/1089	0.60	0/1475
1	M	0.29	0/1097	0.57	0/1485
6	J	0.31	0/3549	0.62	3/4817 (0.1%)
6	K	0.27	0/3569	0.58	0/4845
6	L	0.26	0/3497	0.59	0/4746
All	All	0.28	0/13866	0.59	3/18810 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	477	MET	N-CA-C	-8.96	102.34	113.18
6	J	479	ASN	N-CA-C	-8.16	103.34	113.38
6	J	68	VAL	N-CA-C	-5.67	101.61	108.53

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	D	1043	0	998	9	0
1	I	1067	0	1024	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1075	0	1028	6	0
2	F	550	0	133	0	0
3	H	595	0	147	0	0
4	A	610	0	147	0	0
5	B	545	0	127	0	0
6	J	3476	0	3433	25	0
6	K	3496	0	3451	15	0
6	L	3425	0	3383	12	0
7	C	28	0	25	0	0
7	E	28	0	25	0	0
7	N	28	0	25	0	0
7	O	28	0	25	0	0
7	P	28	0	25	0	0
7	Q	28	0	25	0	0
7	S	28	0	25	0	0
7	T	28	0	25	0	0
7	U	28	0	25	0	0
7	V	28	0	25	0	0
7	X	28	0	25	0	0
7	Y	28	0	25	0	0
7	Z	28	0	25	0	0
7	a	28	0	25	0	0
7	c	28	0	25	0	0
7	d	28	0	25	0	0
7	e	28	0	25	1	0
8	G	61	0	52	0	0
8	b	61	0	52	0	0
9	R	28	0	25	1	0
10	W	50	0	43	0	0
11	D	14	0	13	0	0
11	I	42	0	39	0	0
11	J	126	0	117	1	0
11	K	126	0	117	1	0
11	L	98	0	91	1	0
11	M	56	0	52	0	0
12	L	11	0	10	0	0
All	All	17031	0	14907	64	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 2.

The worst 5 of 64 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)
1:D:544:ARG:NH2	1:I:656:GLU:OE1	2.22	0.72
6:K:176:PHE:HB2	6:K:181:ILE:HD11	1.74	0.69
6:K:277:ARG:HH11	6:K:291:HIS:CE1	2.11	0.68
6:J:175:LEU:HD21	7:e:1:NAG:H82	1.77	0.67
6:L:392:LEU:HD11	6:L:418:ILE:HD11	1.80	0.63

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	126/155 (81%)	125 (99%)	1 (1%)	0	100	100
1	I	130/155 (84%)	130 (100%)	0	0	100	100
1	M	132/155 (85%)	130 (98%)	2 (2%)	0	100	100
6	J	428/514 (83%)	422 (99%)	6 (1%)	0	100	100
6	K	431/514 (84%)	427 (99%)	4 (1%)	0	100	100
6	L	419/514 (82%)	414 (99%)	5 (1%)	0	100	100
All	All	1666/2007 (83%)	1648 (99%)	18 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	113/131 (86%)	113 (100%)	0	100	100
1	I	115/131 (88%)	115 (100%)	0	100	100
1	M	115/131 (88%)	115 (100%)	0	100	100
6	J	393/460 (85%)	393 (100%)	0	100	100
6	K	395/460 (86%)	395 (100%)	0	100	100
6	L	387/460 (84%)	387 (100%)	0	100	100
All	All	1518/1773 (86%)	1518 (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 9 such sidechains are listed below:

Mol	Chain	Res	Type
6	J	346	GLN
6	J	434	GLN
1	I	593	GLN
6	K	92	ASN
6	K	434	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)

50 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	C	1	6,7	14,14,15	0.28	0	17,19,21	0.50	0
7	NAG	C	2	7	14,14,15	0.26	0	17,19,21	0.64	0
7	NAG	E	1	6,7	14,14,15	0.44	0	17,19,21	1.13	3 (17%)
7	NAG	E	2	7	14,14,15	0.30	0	17,19,21	0.63	0
8	NAG	G	1	6,8	14,14,15	0.20	0	17,19,21	0.71	0
8	NAG	G	2	8	14,14,15	0.16	0	17,19,21	0.62	0
8	BMA	G	3	8	11,11,12	0.69	0	15,15,17	1.16	1 (6%)
8	MAN	G	4	8	11,11,12	0.77	1 (9%)	15,15,17	0.88	1 (6%)
8	MAN	G	5	8	11,11,12	1.42	3 (27%)	15,15,17	2.13	3 (20%)
7	NAG	N	1	6,7	14,14,15	0.20	0	17,19,21	0.61	0
7	NAG	N	2	7	14,14,15	0.23	0	17,19,21	0.64	0
7	NAG	O	1	6,7	14,14,15	0.14	0	17,19,21	0.58	0
7	NAG	O	2	7	14,14,15	0.30	0	17,19,21	0.59	0
7	NAG	P	1	6,7	14,14,15	0.18	0	17,19,21	0.68	0
7	NAG	P	2	7	14,14,15	0.21	0	17,19,21	0.58	0
7	NAG	Q	1	6,7	14,14,15	0.18	0	17,19,21	0.58	0
7	NAG	Q	2	7	14,14,15	0.20	0	17,19,21	0.60	0
9	NAG	R	1	6,9	14,14,15	0.34	0	17,19,21	0.63	0
9	NAG	R	2	9	14,14,15	0.32	0	17,19,21	0.58	0
7	NAG	S	1	6,7	14,14,15	0.18	0	17,19,21	0.64	0
7	NAG	S	2	7	14,14,15	0.22	0	17,19,21	0.64	0
7	NAG	T	1	6,7	14,14,15	0.27	0	17,19,21	0.60	0
7	NAG	T	2	7	14,14,15	0.30	0	17,19,21	0.65	0
7	NAG	U	1	6,7	14,14,15	0.23	0	17,19,21	0.48	0
7	NAG	U	2	7	14,14,15	0.56	0	17,19,21	0.41	0
7	NAG	V	1	6,7	14,14,15	0.19	0	17,19,21	0.79	1 (5%)
7	NAG	V	2	7	14,14,15	0.23	0	17,19,21	0.66	1 (5%)
10	NAG	W	1	6,10	14,14,15	0.19	0	17,19,21	0.61	0
10	NAG	W	2	10	14,14,15	0.16	0	17,19,21	0.55	0
10	BMA	W	3	10	11,11,12	0.60	0	15,15,17	0.82	0
10	MAN	W	4	10	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
7	NAG	X	1	6,7	14,14,15	0.18	0	17,19,21	0.61	0
7	NAG	X	2	7	14,14,15	0.22	0	17,19,21	0.66	0
7	NAG	Y	1	6,7	14,14,15	0.13	0	17,19,21	0.62	0
7	NAG	Y	2	7	14,14,15	0.43	0	17,19,21	0.54	0
7	NAG	Z	1	6,7	14,14,15	0.23	0	17,19,21	0.69	0
7	NAG	Z	2	7	14,14,15	0.31	0	17,19,21	0.64	0
7	NAG	a	1	6,7	14,14,15	0.21	0	17,19,21	0.59	0
7	NAG	a	2	7	14,14,15	0.23	0	17,19,21	0.66	0
8	NAG	b	1	6,8	14,14,15	0.23	0	17,19,21	0.60	0
8	NAG	b	2	8	14,14,15	0.28	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BMA	b	3	8	11,11,12	0.45	0	15,15,17	0.81	0
8	MAN	b	4	8	11,11,12	0.60	0	15,15,17	0.93	2 (13%)
8	MAN	b	5	8	11,11,12	0.67	0	15,15,17	0.85	1 (6%)
7	NAG	c	1	6,7	14,14,15	0.17	0	17,19,21	0.58	0
7	NAG	c	2	7	14,14,15	0.20	0	17,19,21	0.62	0
7	NAG	d	1	6,7	14,14,15	0.17	0	17,19,21	0.58	0
7	NAG	d	2	7	14,14,15	0.24	0	17,19,21	0.70	0
7	NAG	e	1	6,7	14,14,15	0.19	0	17,19,21	0.62	0
7	NAG	e	2	7	14,14,15	0.18	0	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	1	6,7	-	0/6/23/26	0/1/1/1
7	NAG	C	2	7	-	2/6/23/26	0/1/1/1
7	NAG	E	1	6,7	-	2/6/23/26	0/1/1/1
7	NAG	E	2	7	-	2/6/23/26	0/1/1/1
8	NAG	G	1	6,8	-	0/6/23/26	0/1/1/1
8	NAG	G	2	8	-	0/6/23/26	0/1/1/1
8	BMA	G	3	8	-	0/2/19/22	0/1/1/1
8	MAN	G	4	8	-	1/2/19/22	0/1/1/1
8	MAN	G	5	8	-	0/2/19/22	0/1/1/1
7	NAG	N	1	6,7	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	1/6/23/26	0/1/1/1
7	NAG	O	1	6,7	-	2/6/23/26	0/1/1/1
7	NAG	O	2	7	-	1/6/23/26	0/1/1/1
7	NAG	P	1	6,7	-	1/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	NAG	Q	1	6,7	-	0/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	3/6/23/26	0/1/1/1
9	NAG	R	1	6,9	-	2/6/23/26	0/1/1/1
9	NAG	R	2	9	-	1/6/23/26	0/1/1/1
7	NAG	S	1	6,7	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1
7	NAG	T	1	6,7	-	0/6/23/26	0/1/1/1
7	NAG	T	2	7	-	2/6/23/26	0/1/1/1
7	NAG	U	1	6,7	-	0/6/23/26	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	5	MAN	C1-C2	3.02	1.59	1.52
8	G	5	MAN	O5-C1	2.90	1.48	1.43
8	G	4	MAN	O5-C1	-2.14	1.40	1.43
8	G	5	MAN	O5-C5	2.03	1.47	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	5	MAN	C1-O5-C5	7.35	122.04	112.19
7	E	1	NAG	O4-C4-C5	2.50	115.47	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	3	BMA	C1-O5-C5	2.39	115.39	112.19
10	W	4	MAN	C1-O5-C5	2.28	115.24	112.19
10	W	4	MAN	O2-C2-C3	-2.27	105.46	110.15

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	R	1	NAG	C4-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6
7	C	2	NAG	O5-C5-C6-O6
7	E	2	NAG	O5-C5-C6-O6
7	Z	2	NAG	O5-C5-C6-O6

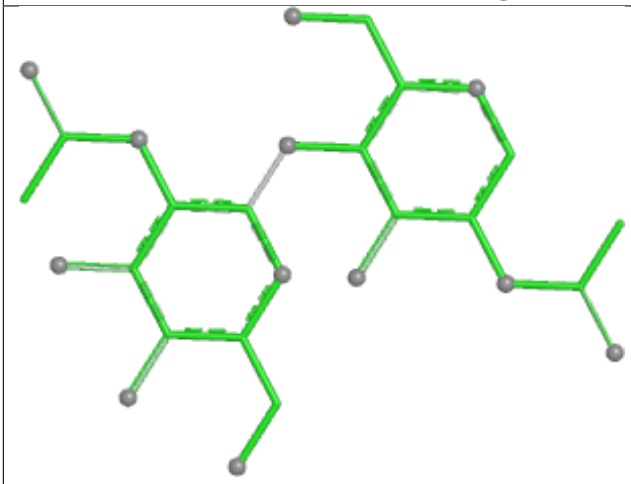
There are no ring outliers.

2 monomers are involved in 2 short contacts:

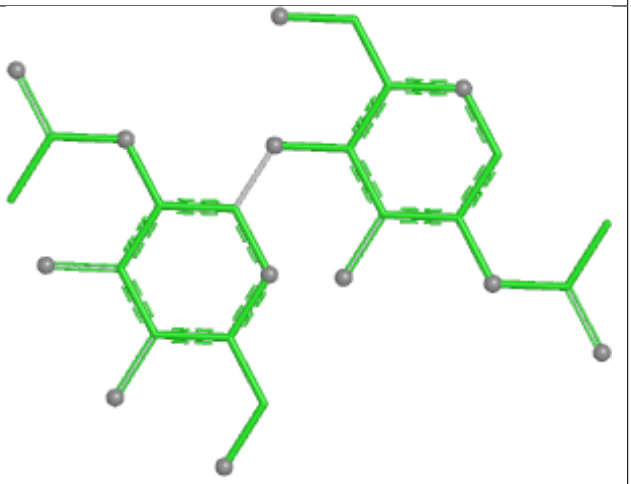
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	1	NAG	1	0
7	e	1	NAG	1	0

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

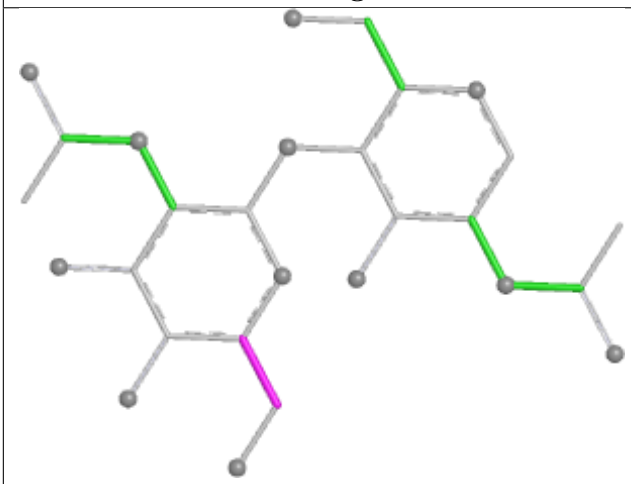
Oligosaccharide Chain C



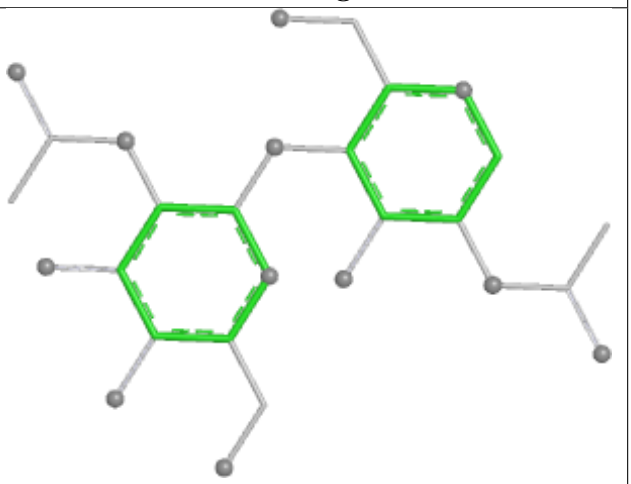
Bond lengths



Bond angles

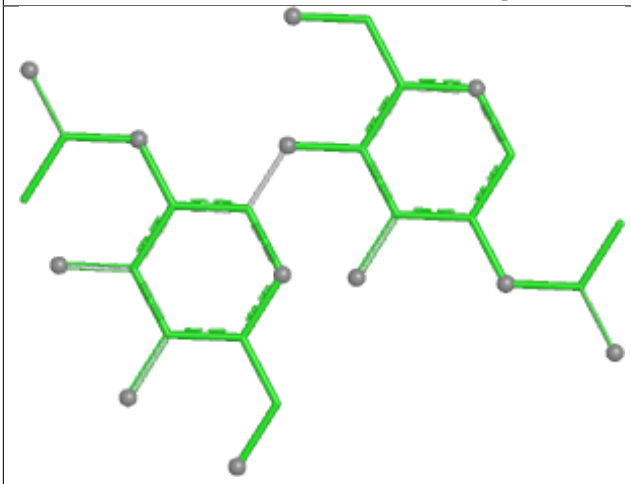


Torsions

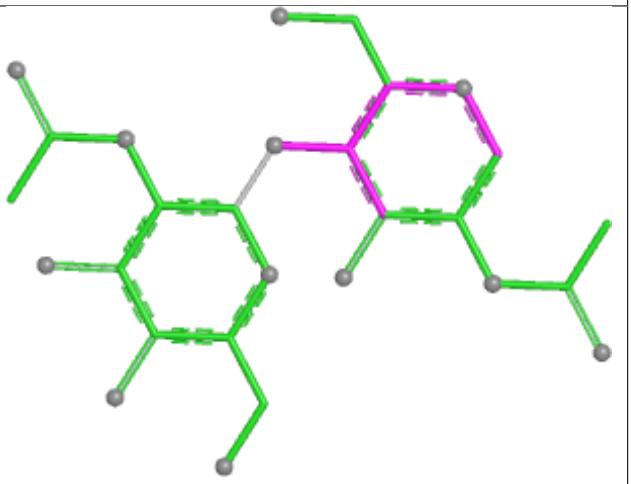


Rings

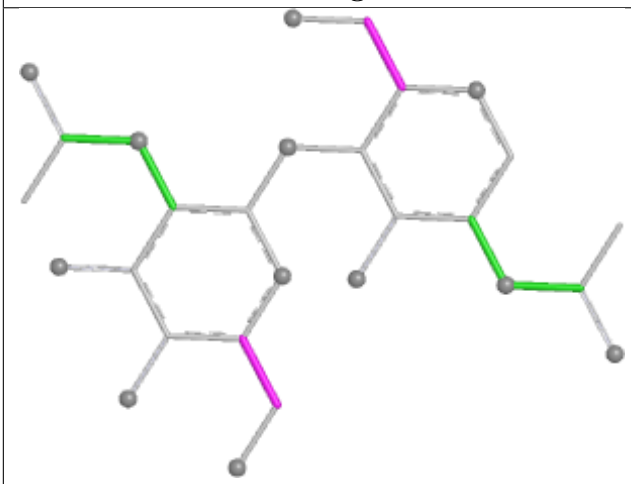
Oligosaccharide Chain E



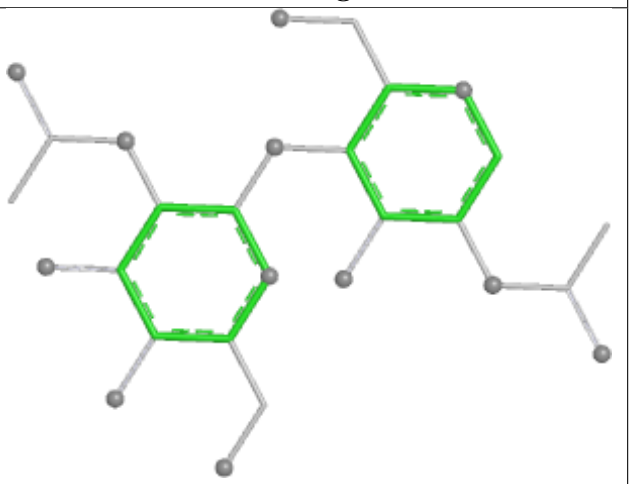
Bond lengths



Bond angles

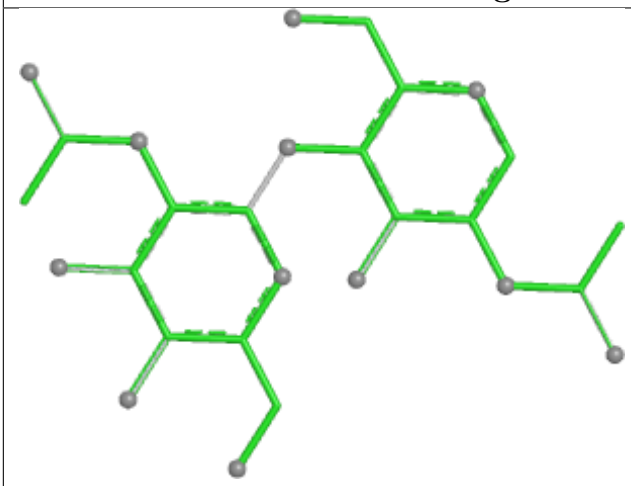


Torsions

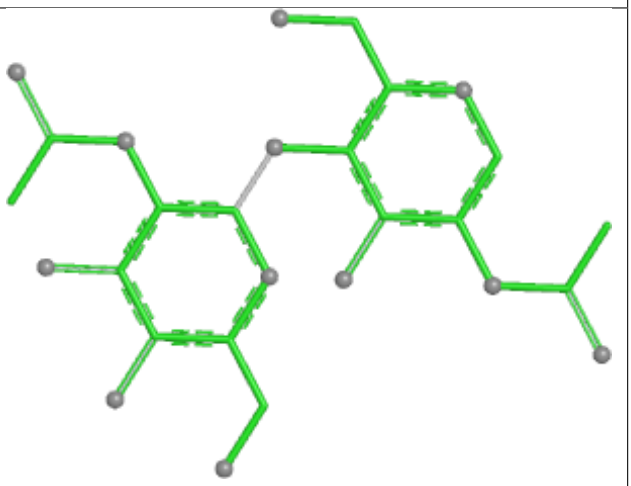


Rings

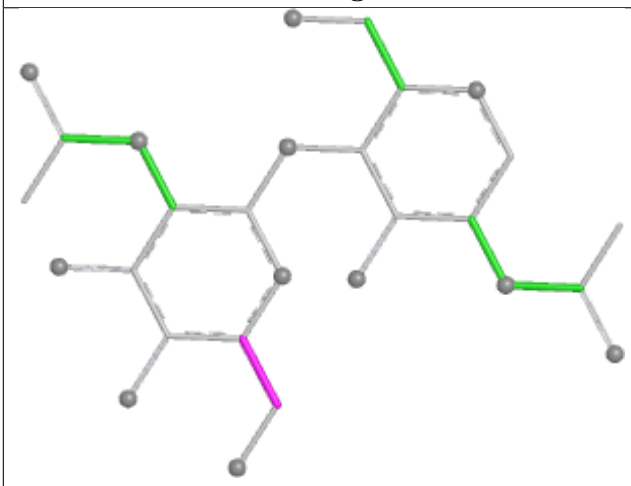
Oligosaccharide Chain N



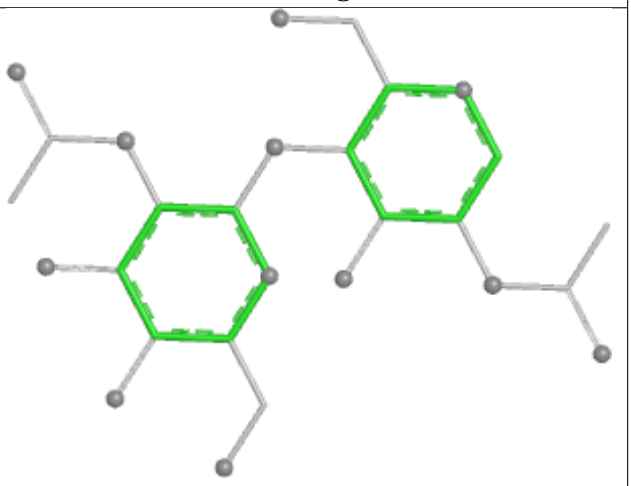
Bond lengths



Bond angles

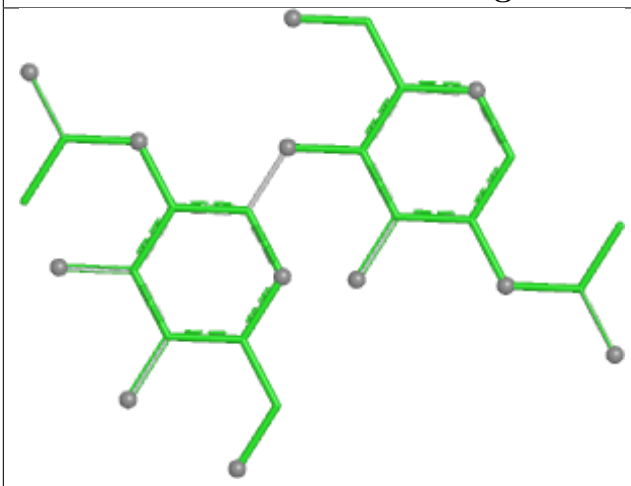


Torsions

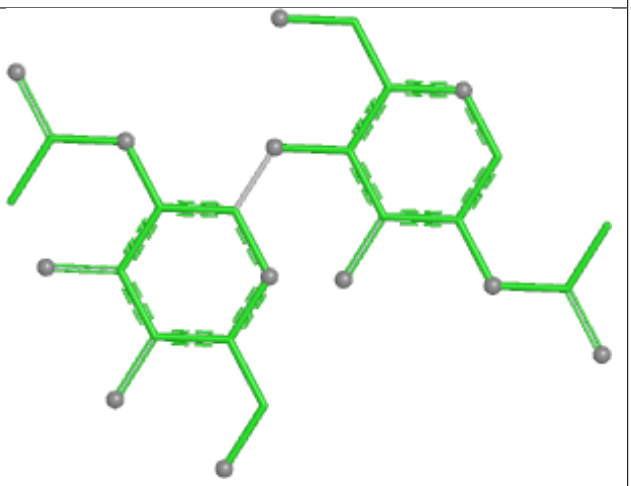


Rings

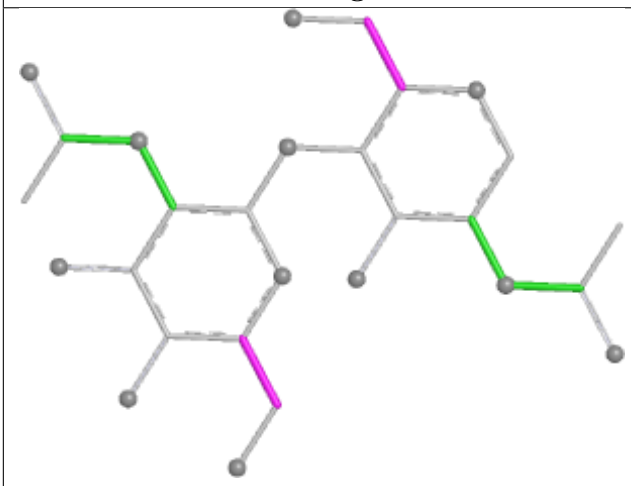
Oligosaccharide Chain O



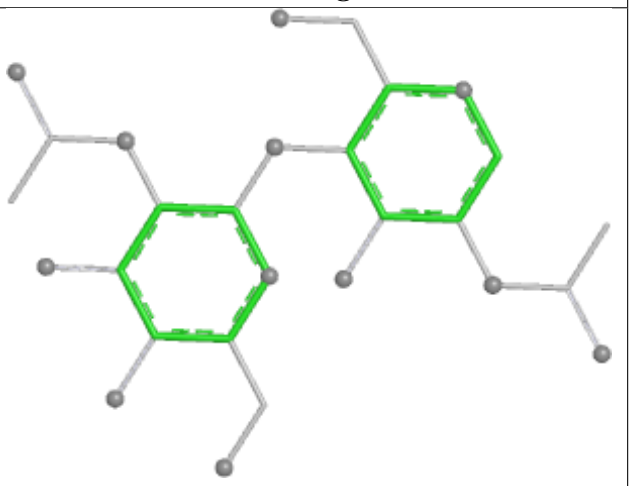
Bond lengths



Bond angles

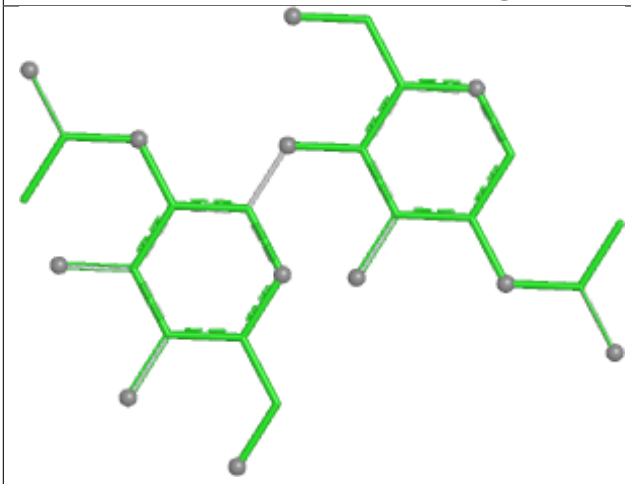


Torsions

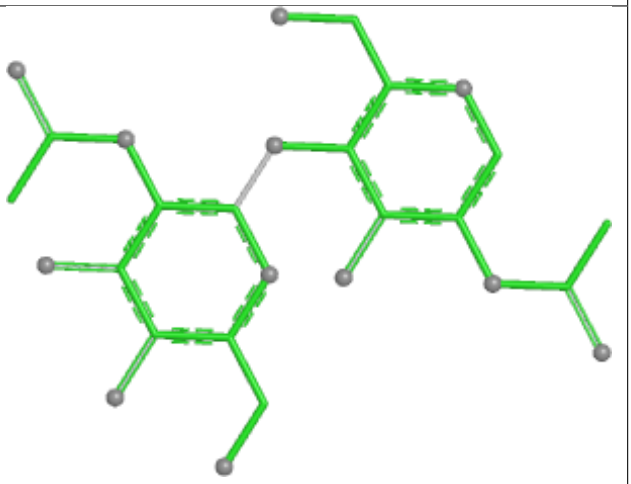


Rings

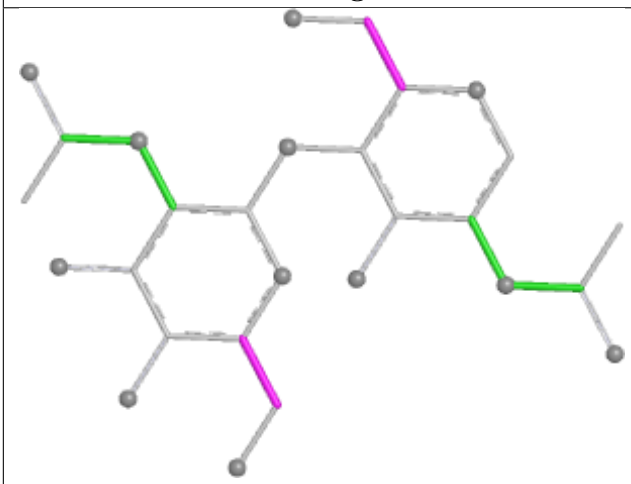
Oligosaccharide Chain P



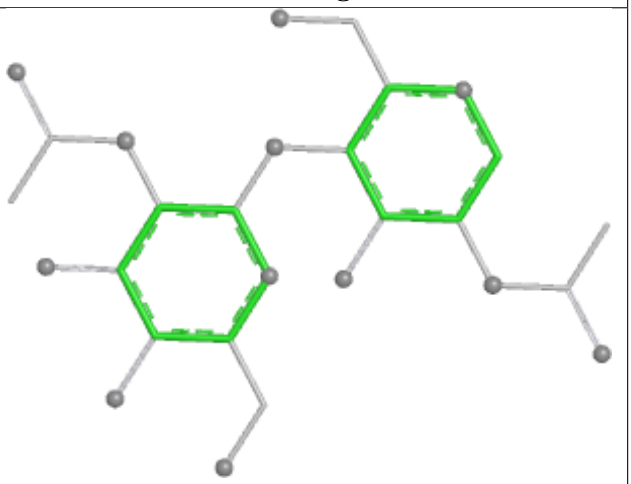
Bond lengths



Bond angles

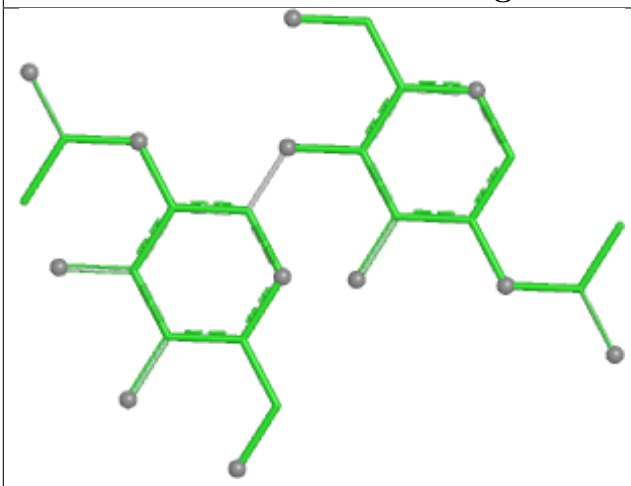


Torsions

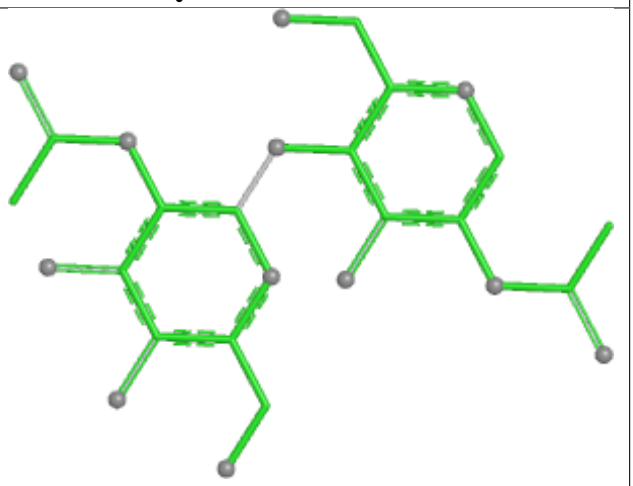


Rings

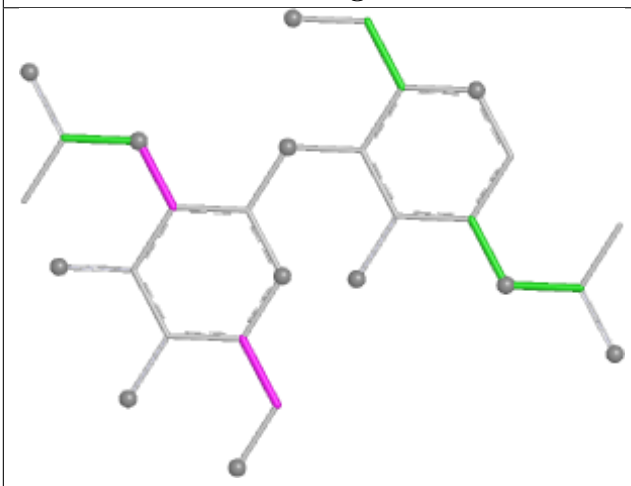
Oligosaccharide Chain Q



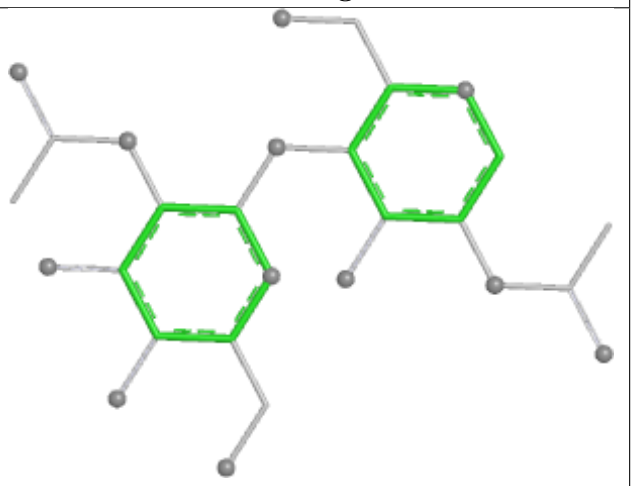
Bond lengths



Bond angles

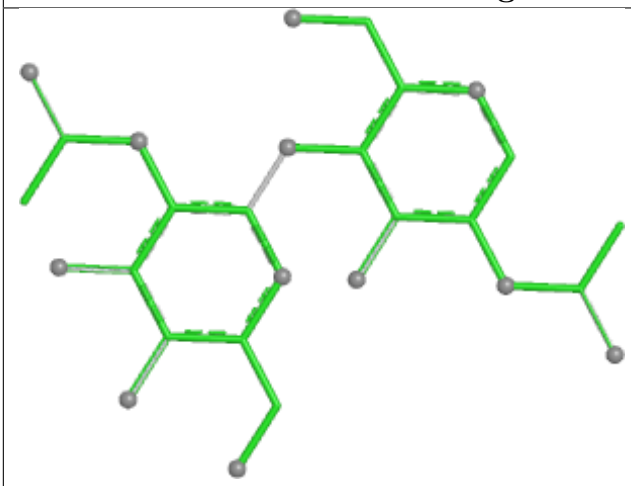


Torsions

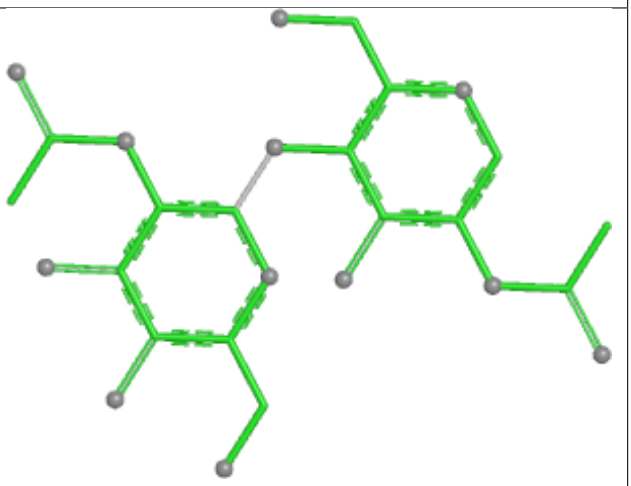


Rings

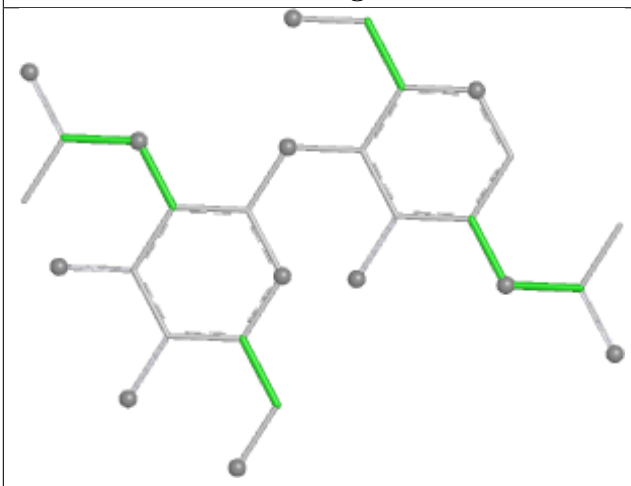
Oligosaccharide Chain S



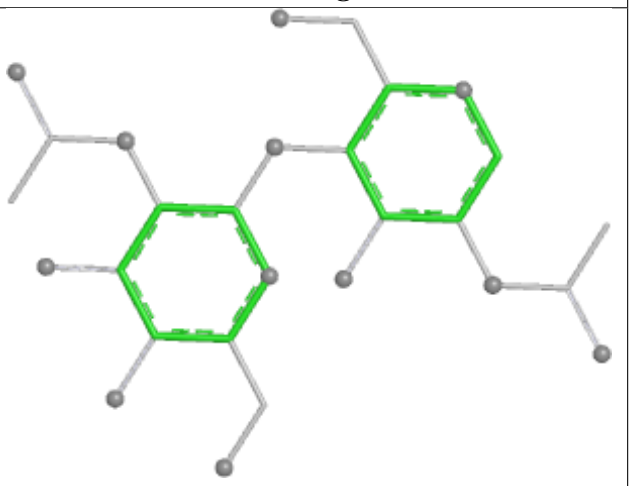
Bond lengths



Bond angles

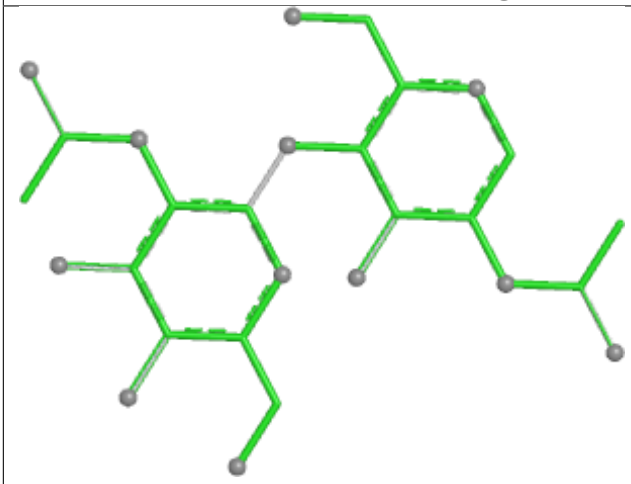


Torsions



Rings

Oligosaccharide Chain T



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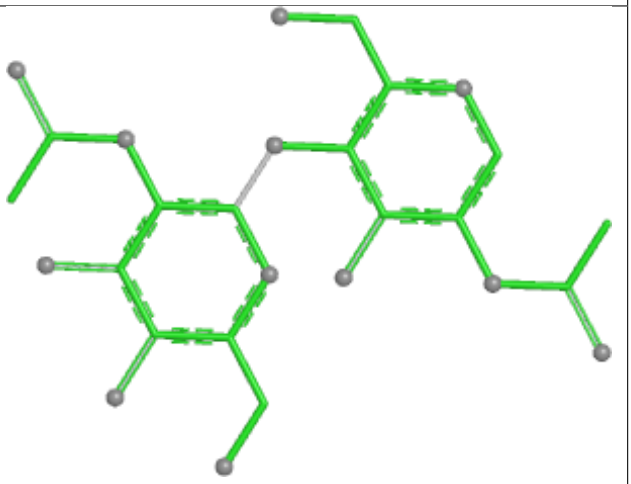

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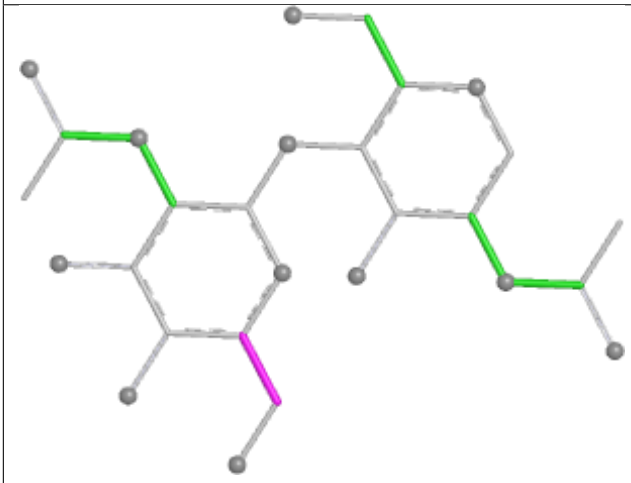

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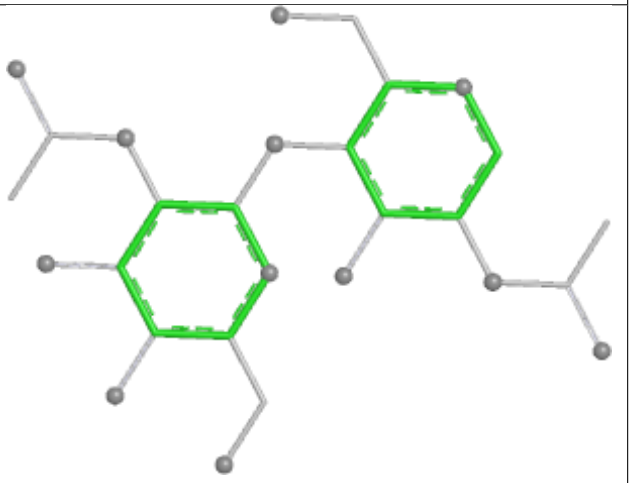
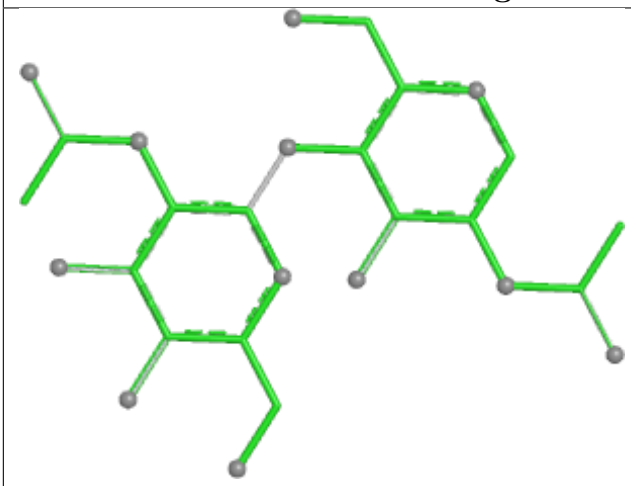


Rings

Oligosaccharide Chain U



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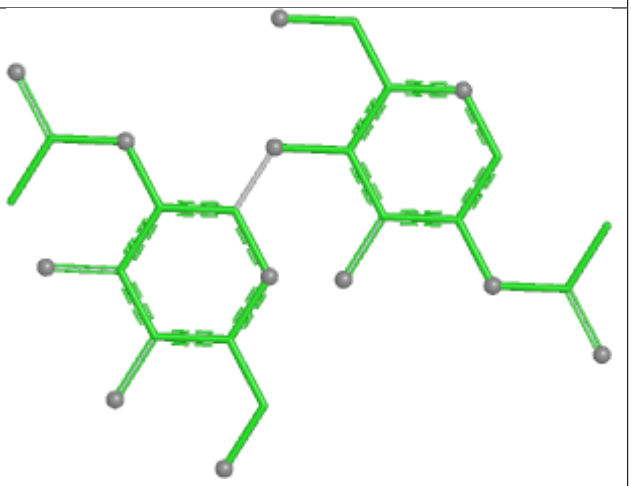

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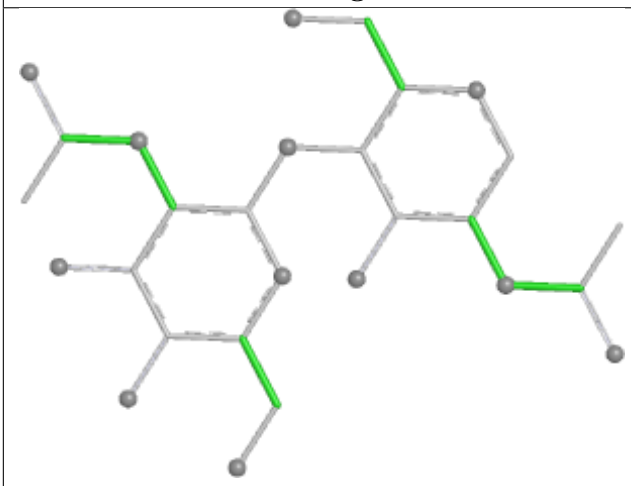

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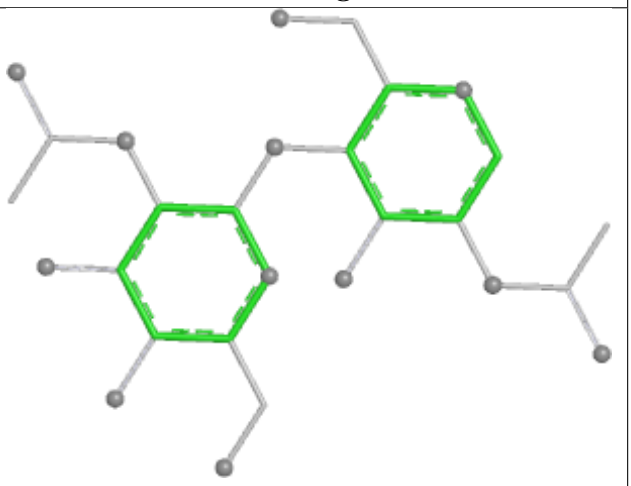
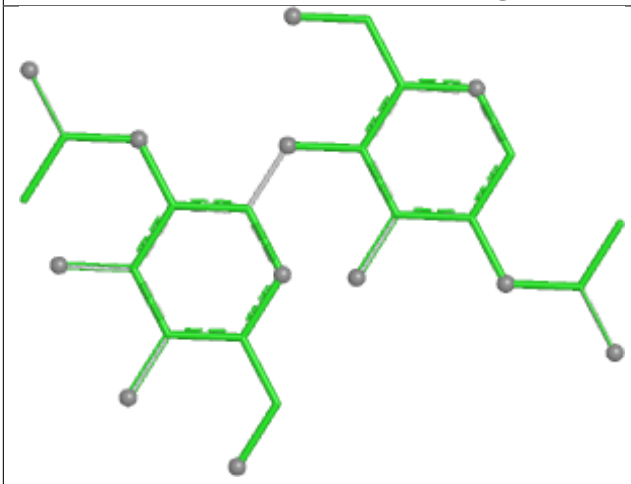


Rings

Oligosaccharide Chain V



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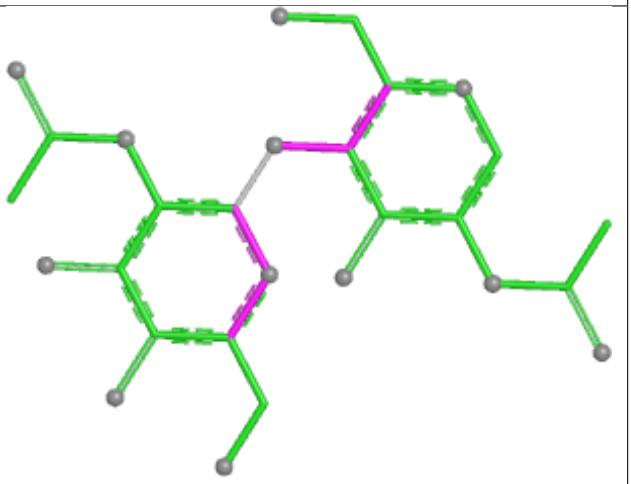
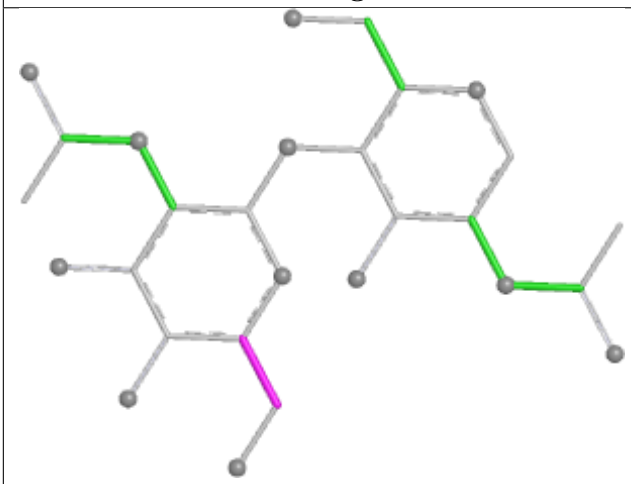


Bond angles



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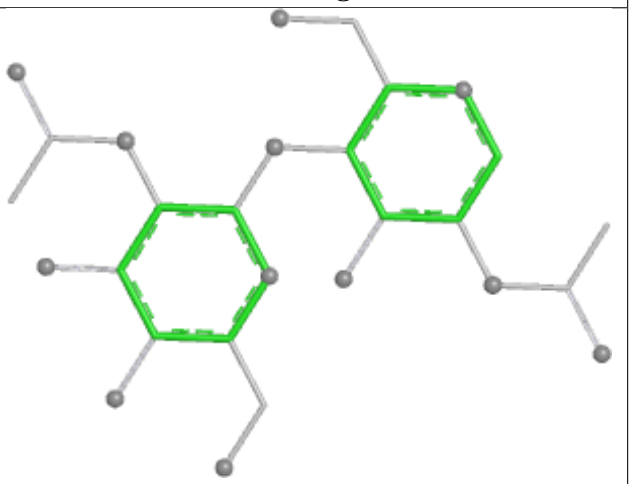
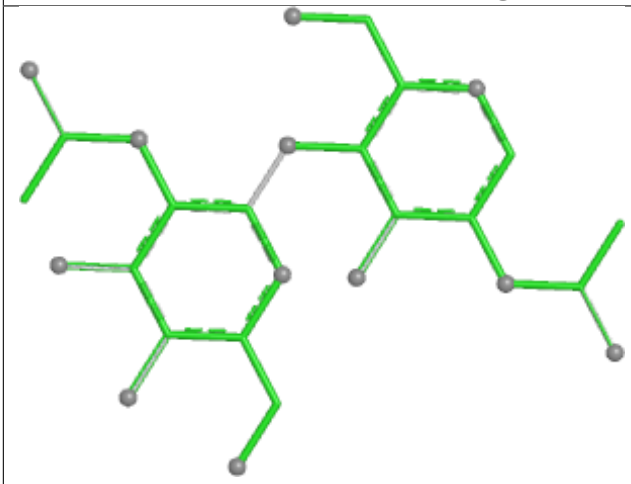


Rings

Oligosaccharide Chain X



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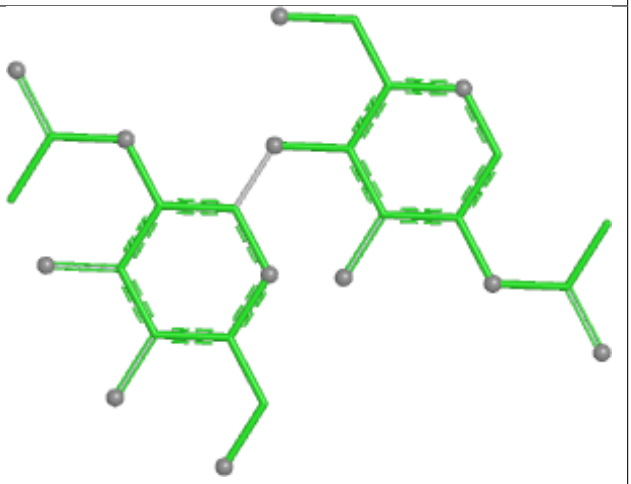

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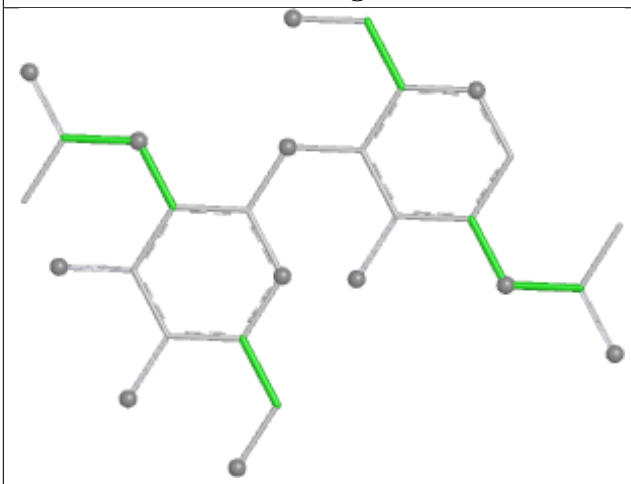

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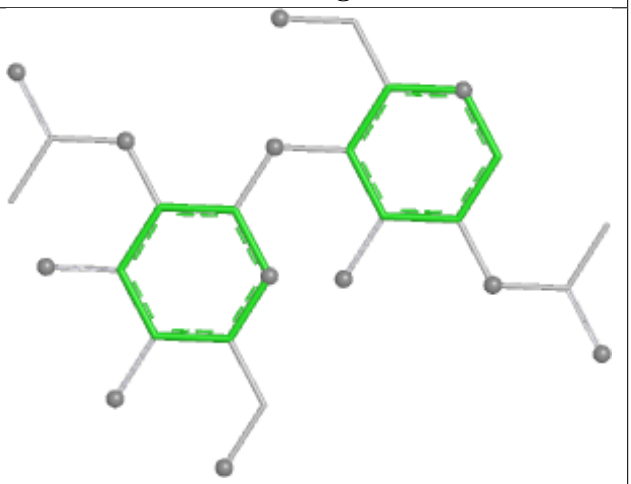
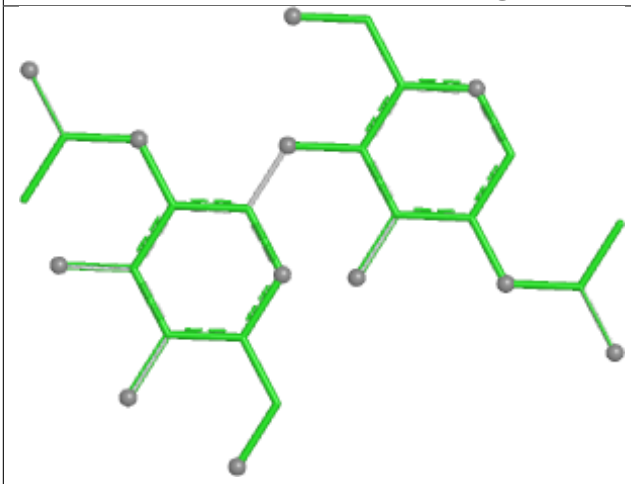


Rings

Oligosaccharide Chain Y



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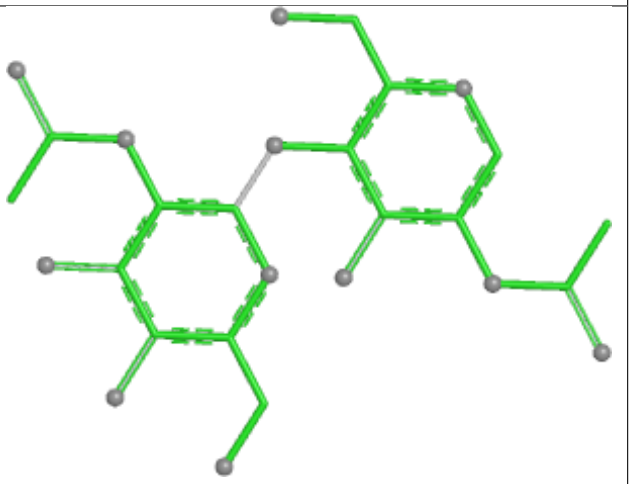

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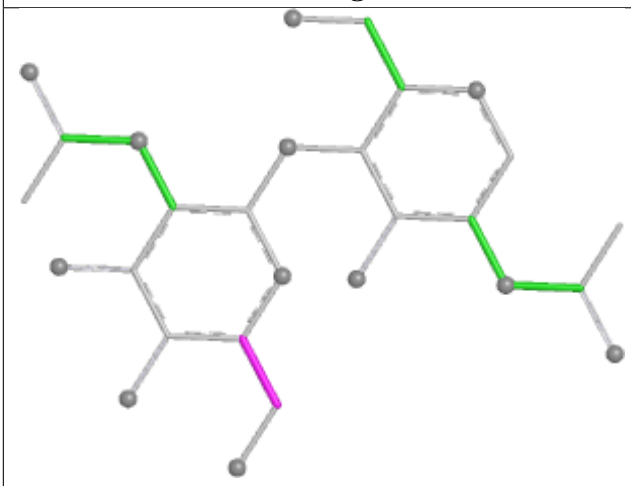

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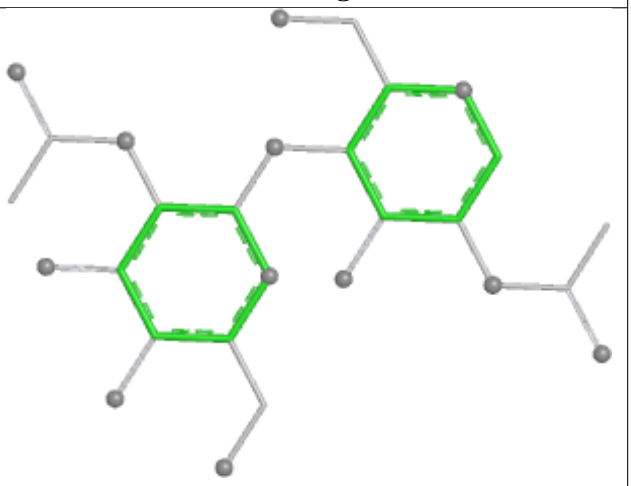
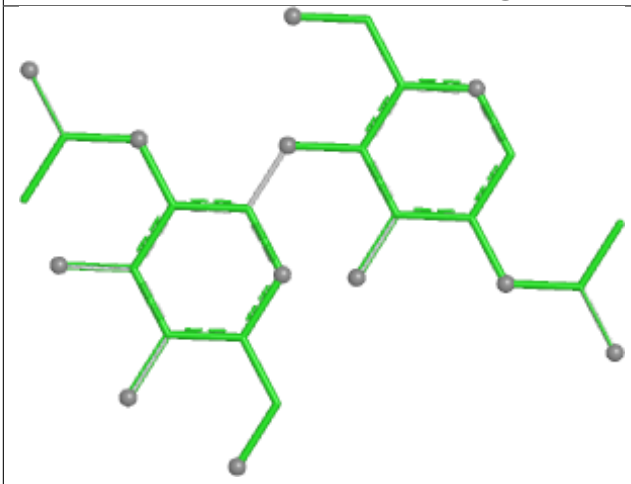


Rings

Oligosaccharide Chain Z



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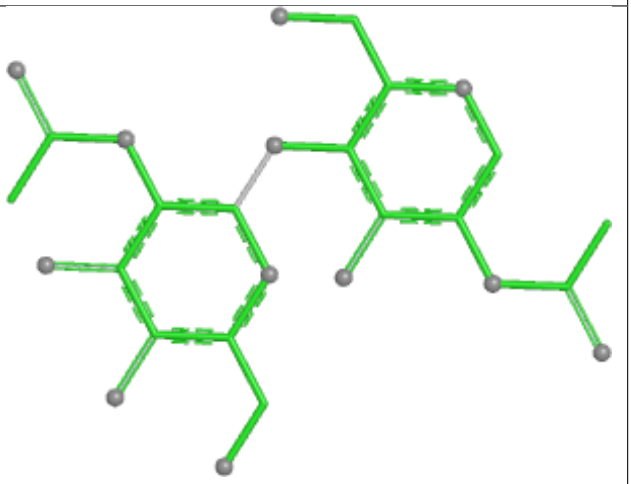

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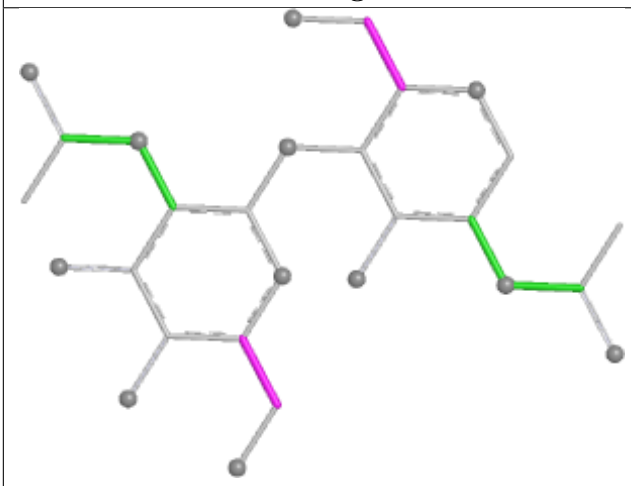

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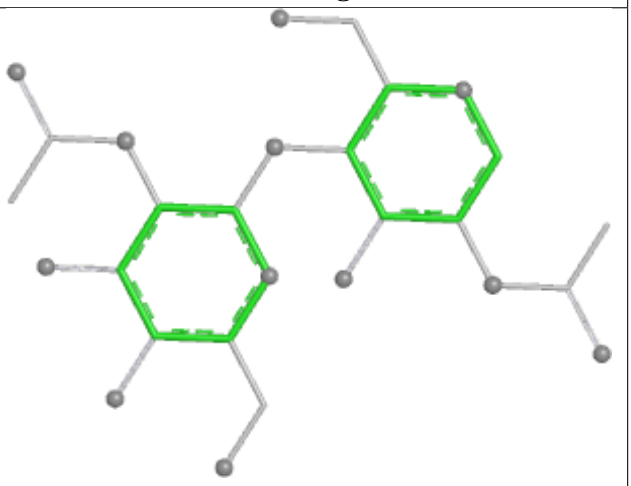
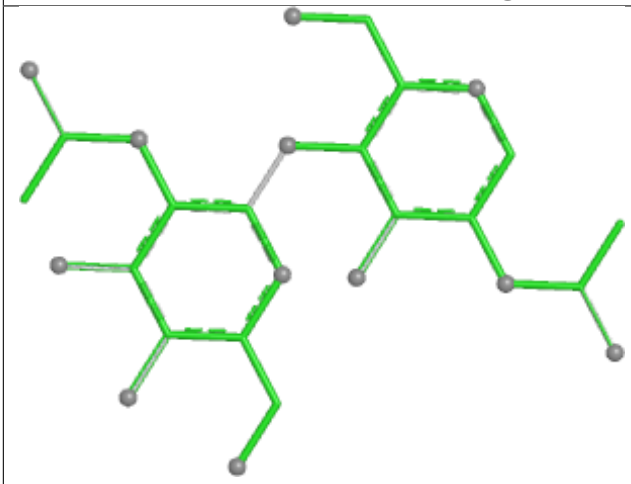


Rings

Oligosaccharide Chain a



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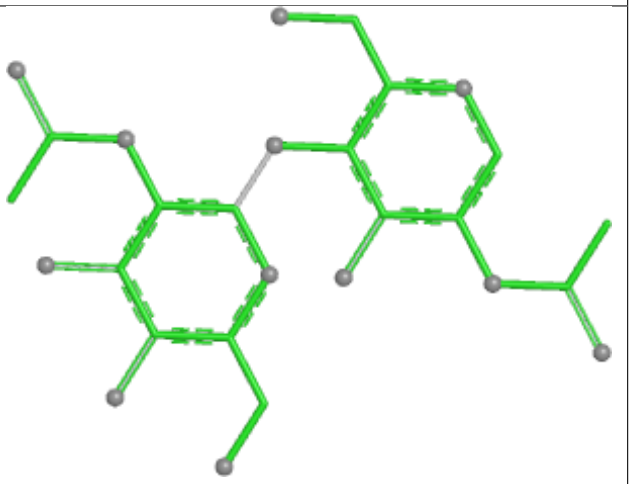

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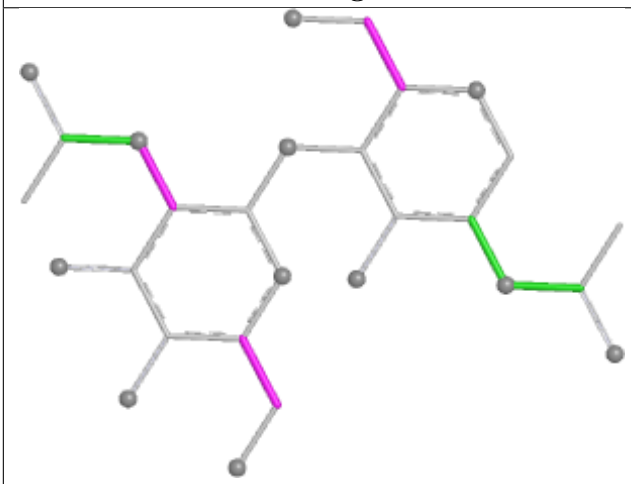

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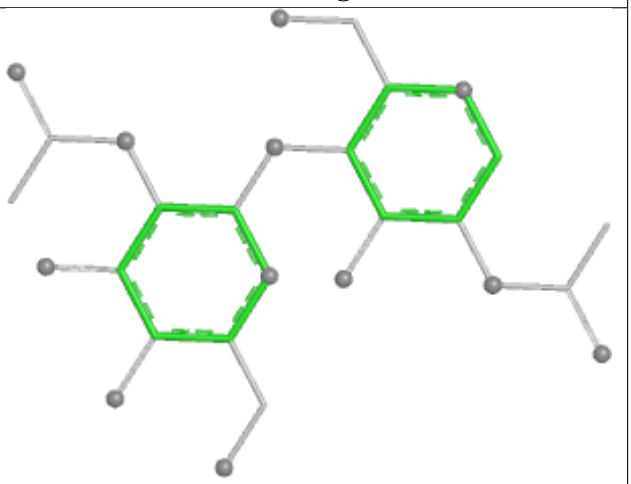
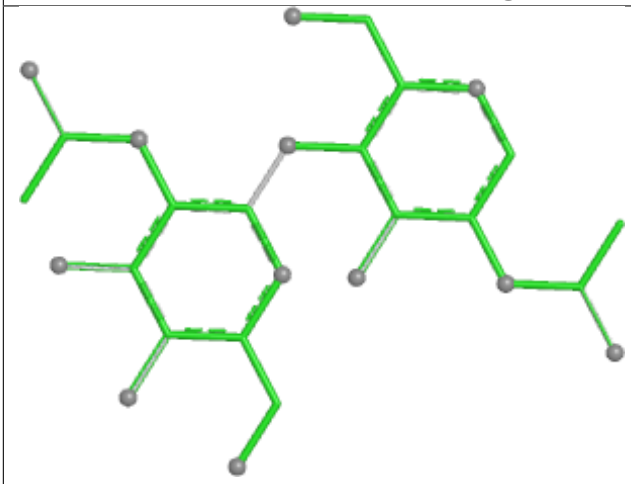


Rings

Oligosaccharide Chain c



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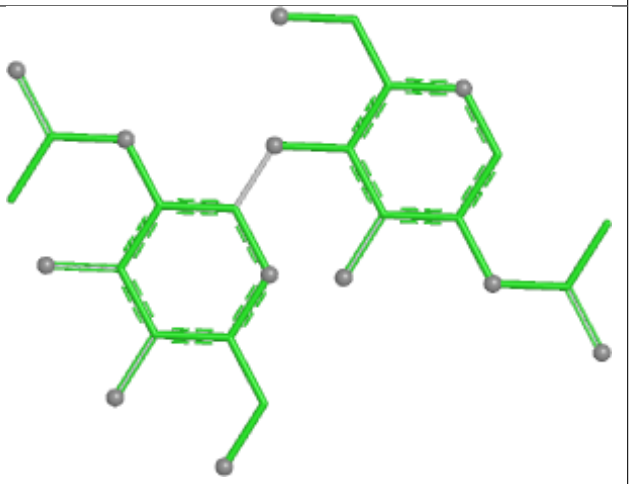

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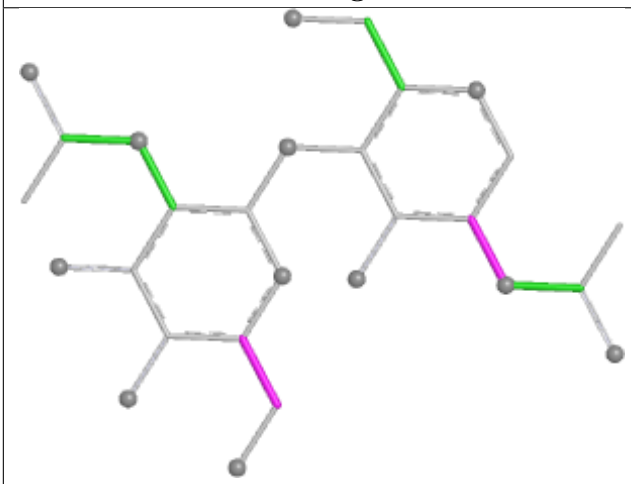

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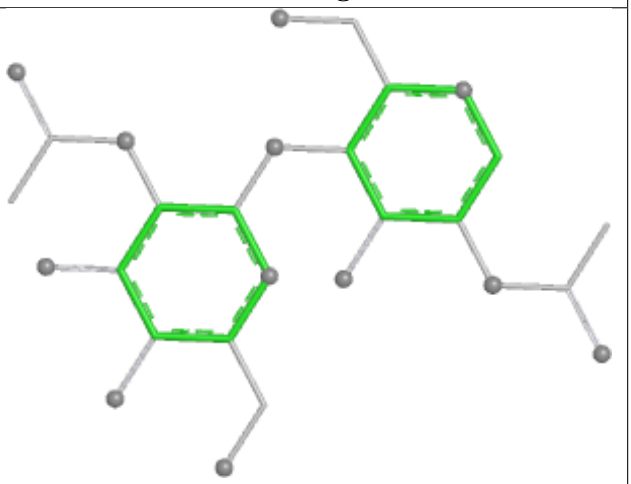
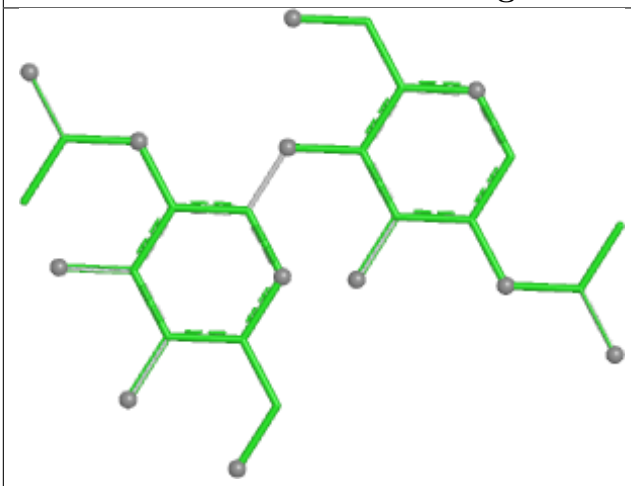


Rings

Oligosaccharide Chain d



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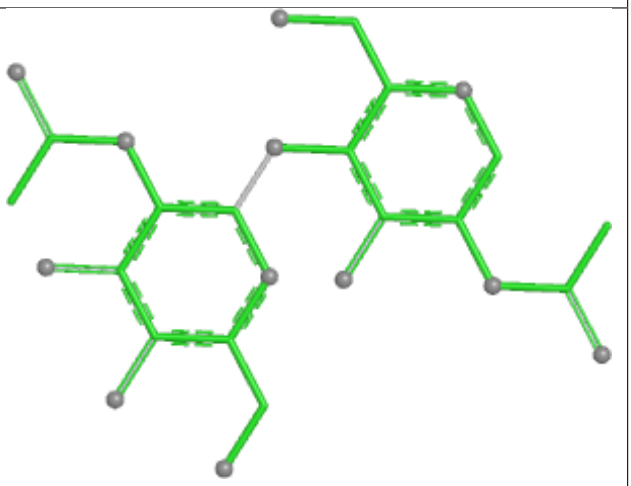

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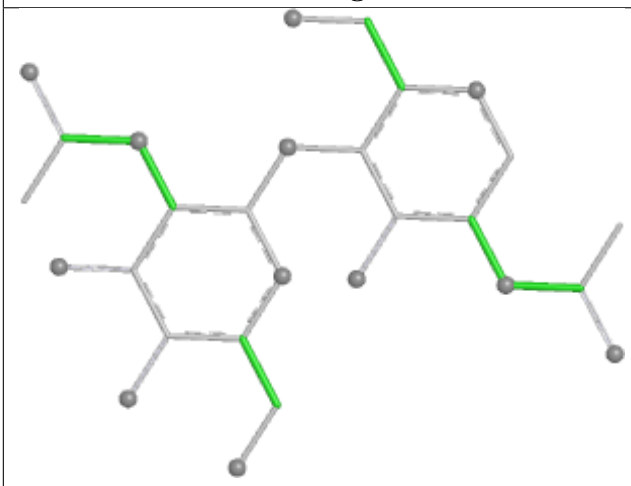

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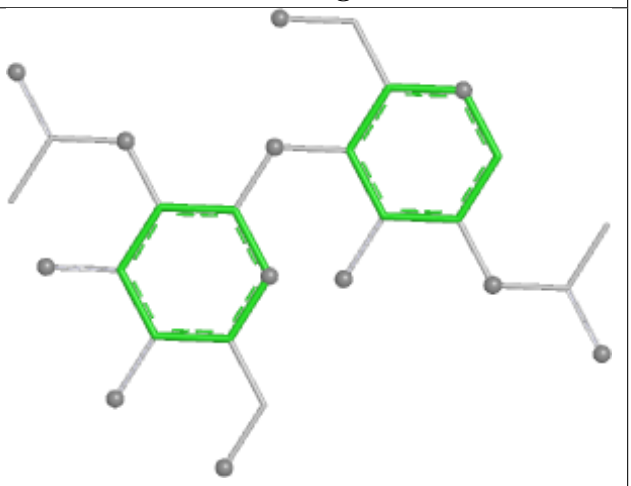
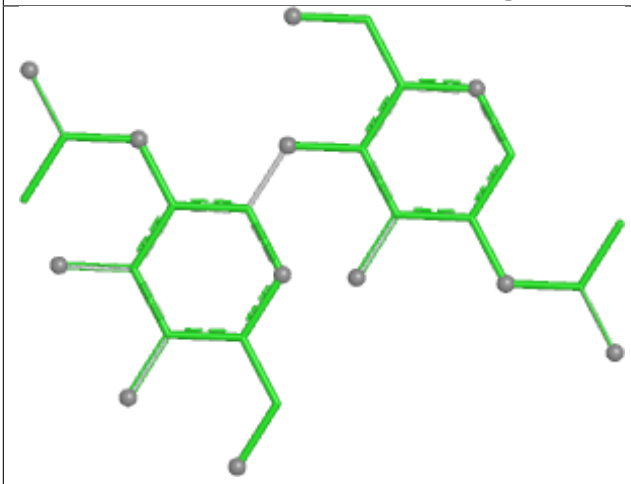


Rings

Oligosaccharide Chain e



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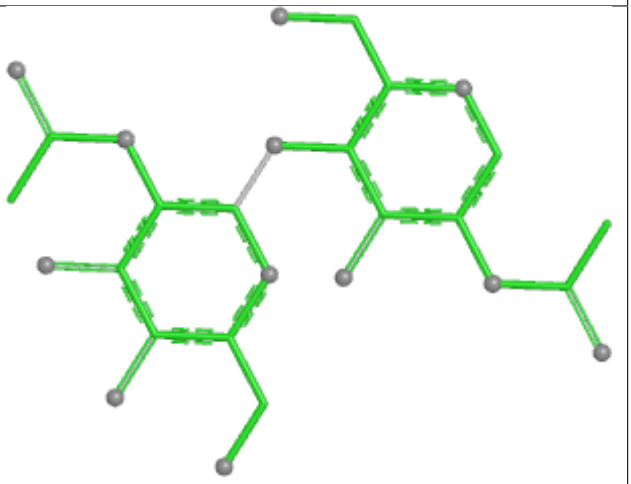

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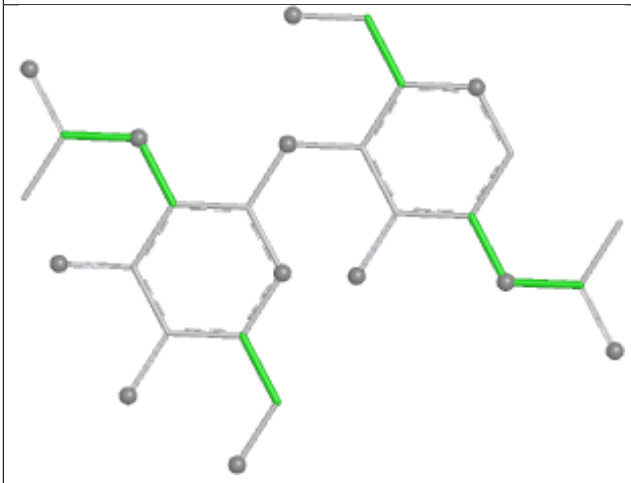

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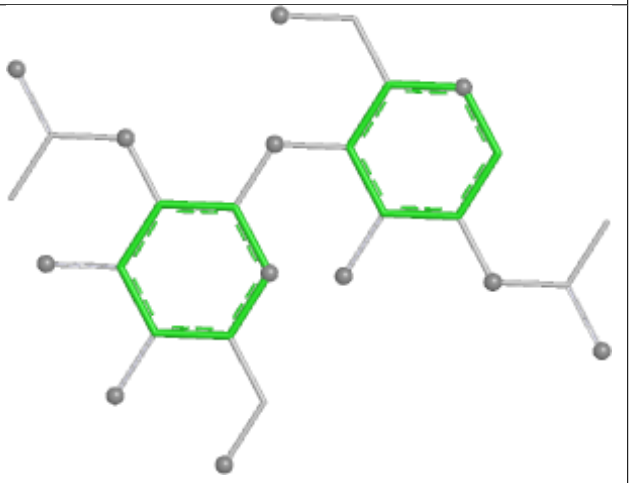
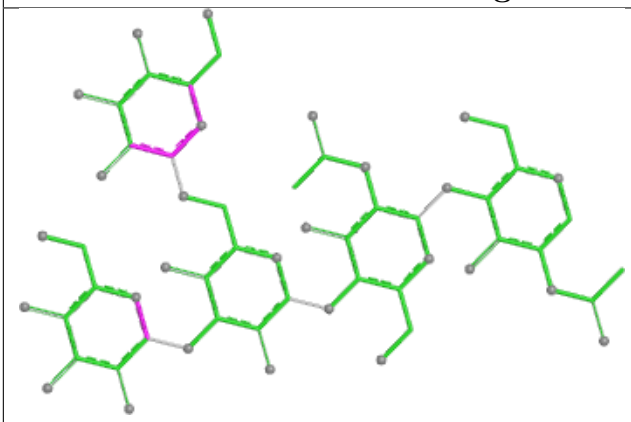


Rings

Oligosaccharide Chain G



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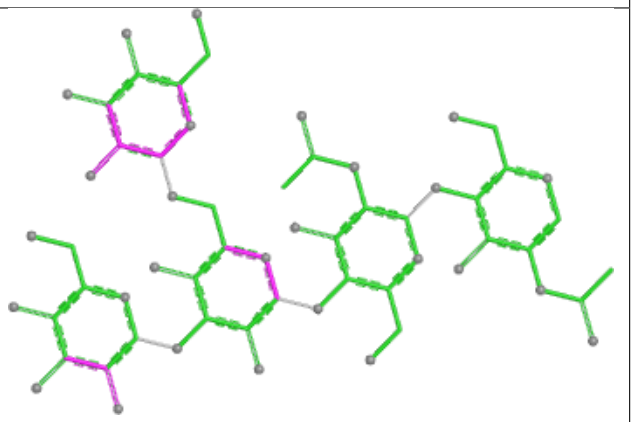

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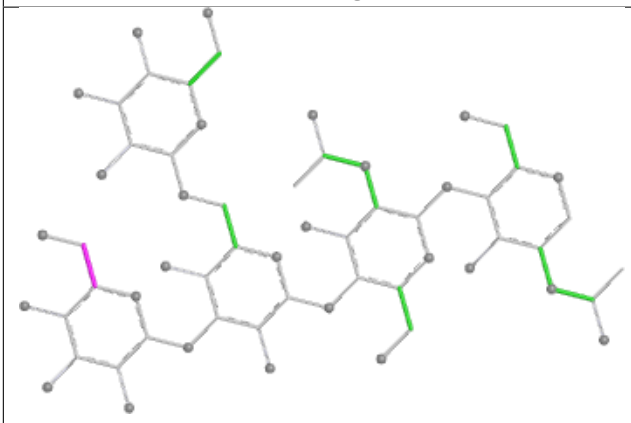

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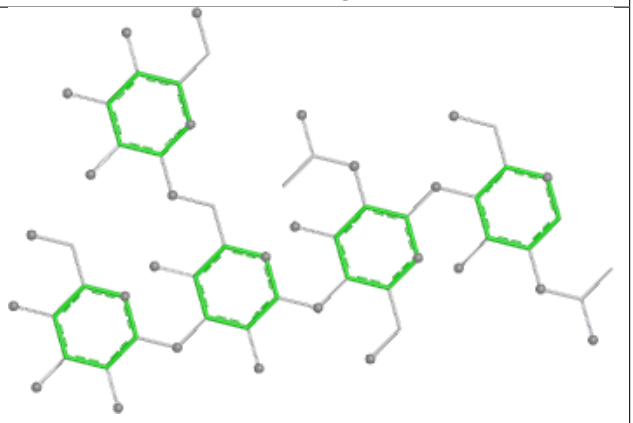
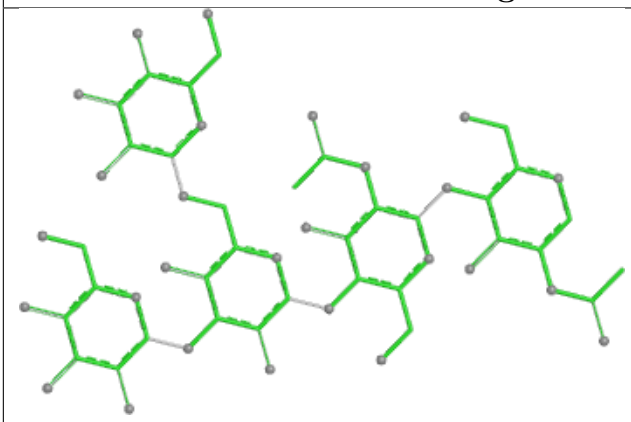


Rings

Oligosaccharide Chain b



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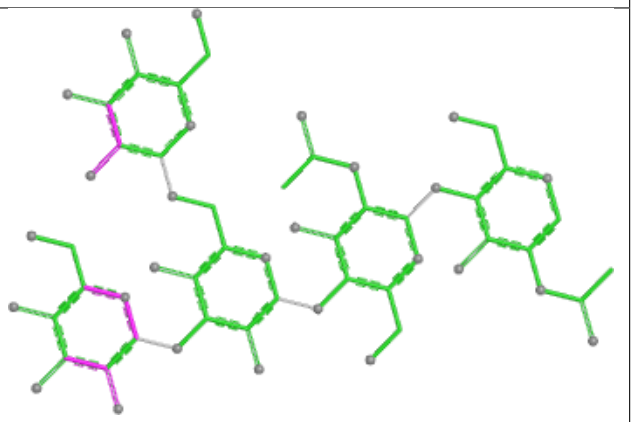
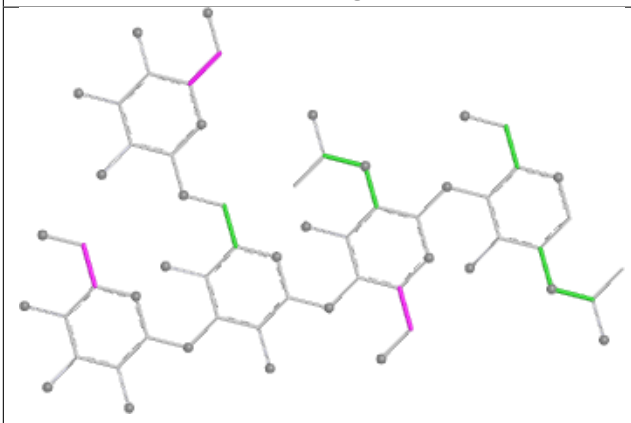


Bond angles



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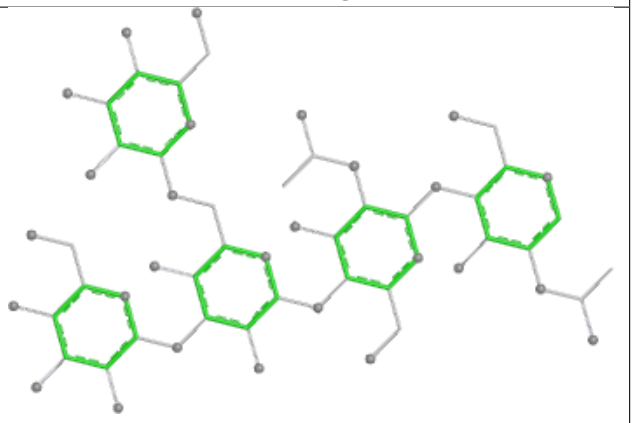
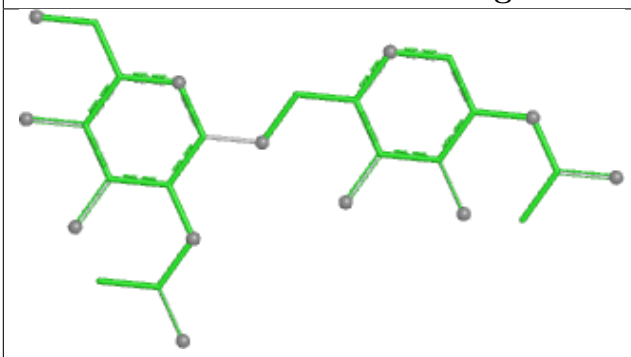


Rings

Oligosaccharide Chain R



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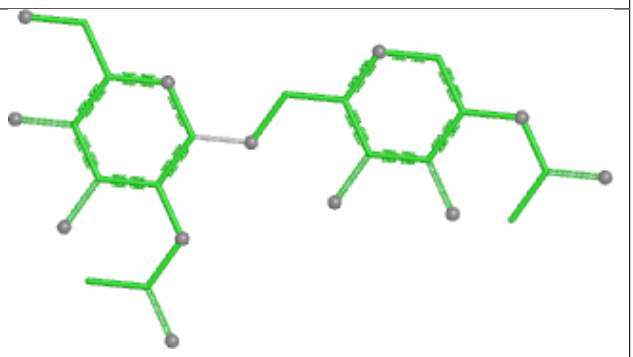
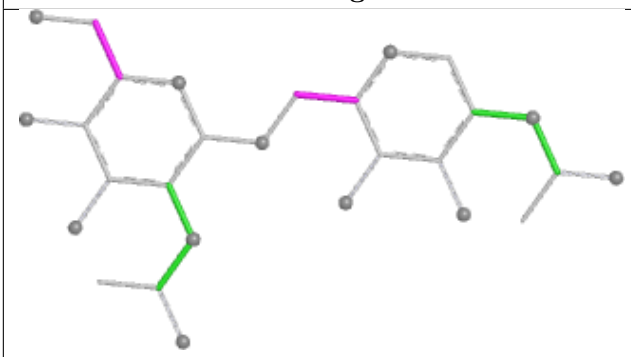


Bond angles



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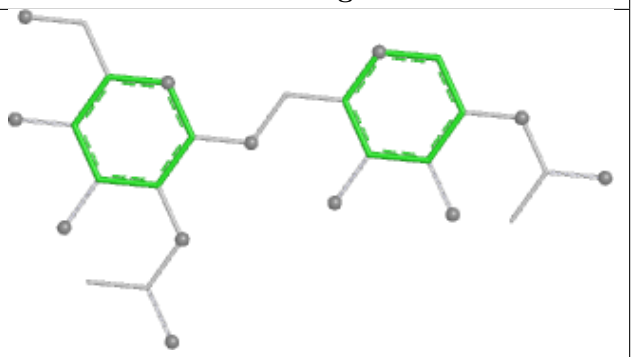
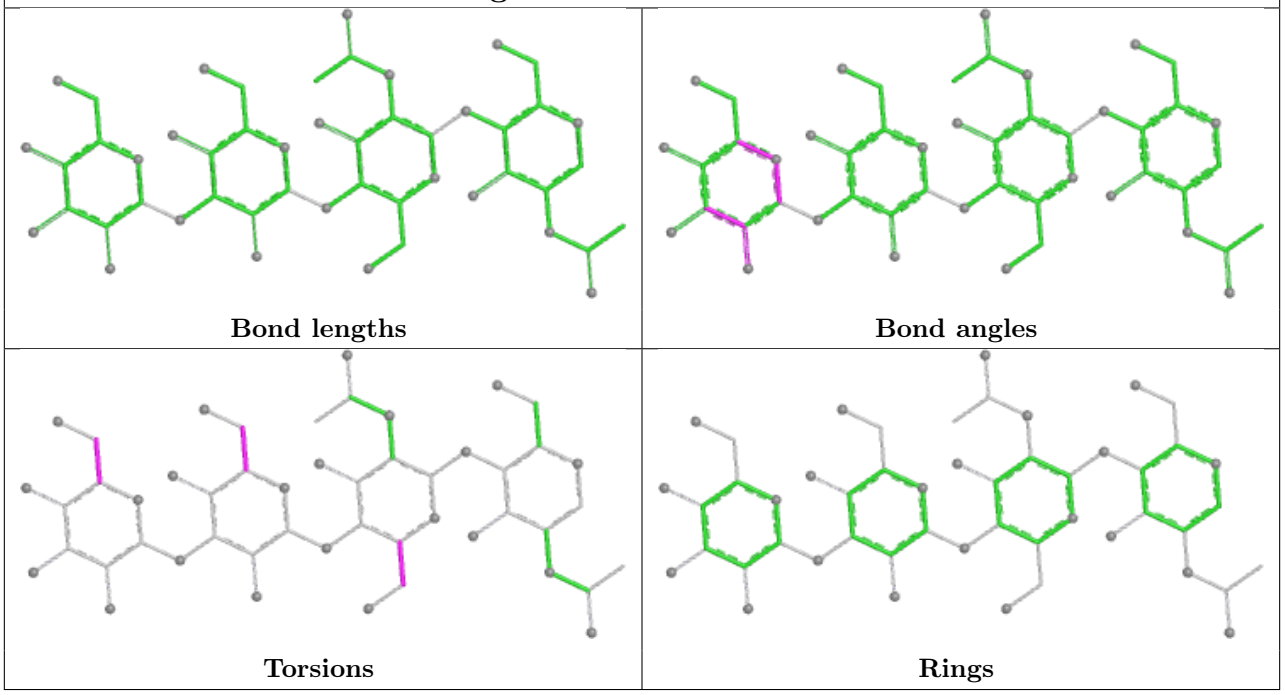


Rings

Oligosaccharide Chain W



5.6 Ligand geometry (i)

34 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	$\#\|Z\| > 2$
11	NAG	K	607	6	14,14,15	0.41	0	17,19,21	0.63	0
11	NAG	M	703	1	14,14,15	0.17	0	17,19,21	0.56	0
12	MAN	L	607	-	11,11,12	0.70	0	15,15,17	1.04	2 (13%)
11	NAG	M	701	1	14,14,15	0.22	0	17,19,21	0.57	0
11	NAG	L	603	6	14,14,15	0.23	0	17,19,21	0.57	0
11	NAG	J	606	6	14,14,15	0.23	0	17,19,21	0.55	0
11	NAG	K	609	6	14,14,15	0.24	0	17,19,21	0.54	0
11	NAG	I	701	1	14,14,15	0.16	0	17,19,21	0.60	0
11	NAG	K	602	6	14,14,15	0.18	0	17,19,21	0.49	0
11	NAG	J	604	6	14,14,15	0.22	0	17,19,21	0.55	0
11	NAG	I	703	1	14,14,15	0.23	0	17,19,21	0.39	0
11	NAG	M	702	1	14,14,15	0.18	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	NAG	K	606	6	14,14,15	0.26	0	17,19,21	0.56	0
11	NAG	K	608	6	14,14,15	0.20	0	17,19,21	0.41	0
11	NAG	J	607	6	14,14,15	0.25	0	17,19,21	0.61	0
11	NAG	L	601	6	14,14,15	0.17	0	17,19,21	0.63	0
11	NAG	K	605	6	14,14,15	0.20	0	17,19,21	0.50	0
11	NAG	L	606	6	14,14,15	0.35	0	17,19,21	0.70	0
11	NAG	K	603	6	14,14,15	0.17	0	17,19,21	0.56	0
11	NAG	D	701	1	14,14,15	0.21	0	17,19,21	0.61	0
11	NAG	K	601	6	14,14,15	0.21	0	17,19,21	0.52	0
11	NAG	J	602	6	14,14,15	0.19	0	17,19,21	0.61	0
11	NAG	J	601	6	14,14,15	0.21	0	17,19,21	0.66	0
11	NAG	L	604	6	14,14,15	0.27	0	17,19,21	0.58	0
11	NAG	M	704	1	14,14,15	0.26	0	17,19,21	0.44	0
11	NAG	L	608	6	14,14,15	0.24	0	17,19,21	0.64	1 (5%)
11	NAG	J	609	6	14,14,15	0.30	0	17,19,21	0.88	1 (5%)
11	NAG	K	604	6	14,14,15	0.18	0	17,19,21	0.57	0
11	NAG	J	605	6	14,14,15	0.19	0	17,19,21	0.62	0
11	NAG	L	602	6	14,14,15	0.14	0	17,19,21	0.61	0
11	NAG	J	608	6	14,14,15	0.20	0	17,19,21	0.46	0
11	NAG	L	605	6	14,14,15	0.23	0	17,19,21	0.60	0
11	NAG	I	702	1	14,14,15	0.21	0	17,19,21	0.57	0
11	NAG	J	603	6	14,14,15	0.14	0	17,19,21	0.64	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
11	NAG	K	607	6	-	1/6/23/26	0/1/1/1
11	NAG	M	703	1	-	1/6/23/26	0/1/1/1
12	MAN	L	607	-	-	0/2/19/22	0/1/1/1
11	NAG	M	701	1	-	0/6/23/26	0/1/1/1
11	NAG	L	603	6	-	1/6/23/26	0/1/1/1
11	NAG	J	606	6	-	1/6/23/26	0/1/1/1
11	NAG	K	609	6	-	2/6/23/26	0/1/1/1
11	NAG	I	701	1	-	0/6/23/26	0/1/1/1
11	NAG	K	602	6	-	2/6/23/26	0/1/1/1
11	NAG	J	604	6	-	1/6/23/26	0/1/1/1
11	NAG	I	703	1	-	1/6/23/26	0/1/1/1
11	NAG	M	702	1	-	1/6/23/26	0/1/1/1
11	NAG	K	606	6	-	1/6/23/26	0/1/1/1

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	K	608	6	-	2/6/23/26	0/1/1/1
11	NAG	J	607	6	-	1/6/23/26	0/1/1/1
11	NAG	L	601	6	-	1/6/23/26	0/1/1/1
11	NAG	K	605	6	-	1/6/23/26	0/1/1/1
11	NAG	L	606	6	-	1/6/23/26	0/1/1/1
11	NAG	K	603	6	-	0/6/23/26	0/1/1/1
11	NAG	D	701	1	-	0/6/23/26	0/1/1/1
11	NAG	K	601	6	-	1/6/23/26	0/1/1/1
11	NAG	J	602	6	-	2/6/23/26	0/1/1/1
11	NAG	J	601	6	-	2/6/23/26	0/1/1/1
11	NAG	L	604	6	-	1/6/23/26	0/1/1/1
11	NAG	M	704	1	-	1/6/23/26	0/1/1/1
11	NAG	L	608	6	-	0/6/23/26	0/1/1/1
11	NAG	J	609	6	-	2/6/23/26	0/1/1/1
11	NAG	K	604	6	-	2/6/23/26	0/1/1/1
11	NAG	J	605	6	-	2/6/23/26	0/1/1/1
11	NAG	L	602	6	-	0/6/23/26	0/1/1/1
11	NAG	J	608	6	-	1/6/23/26	0/1/1/1
11	NAG	L	605	6	-	1/6/23/26	0/1/1/1
11	NAG	I	702	1	-	0/6/23/26	0/1/1/1
11	NAG	J	603	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	J	609	NAG	C1-O5-C5	3.34	116.67	112.19
12	L	607	MAN	C1-O5-C5	2.61	115.69	112.19
11	L	608	NAG	C1-O5-C5	2.18	115.10	112.19
12	L	607	MAN	O2-C2-C3	-2.03	105.96	110.15

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	608	NAG	O5-C5-C6-O6
11	J	603	NAG	O5-C5-C6-O6
11	J	605	NAG	O5-C5-C6-O6
11	J	605	NAG	C4-C5-C6-O6
11	K	602	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	606	NAG	1	0
11	K	601	NAG	1	0
11	J	608	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

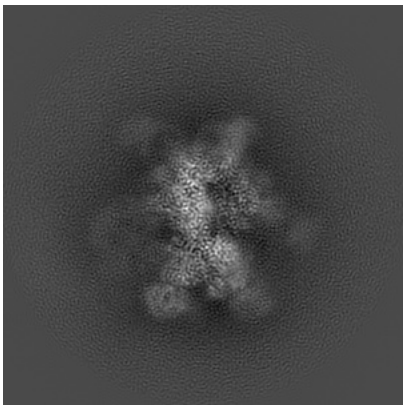
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43967. These allow visual inspection of the internal detail of the map and identification of artifacts.

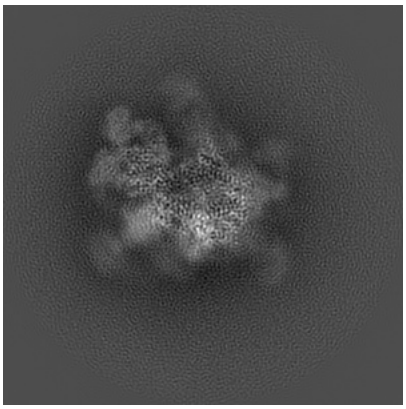
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

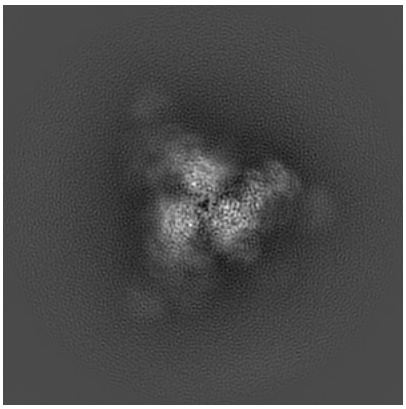
6.1.1 Primary map



X

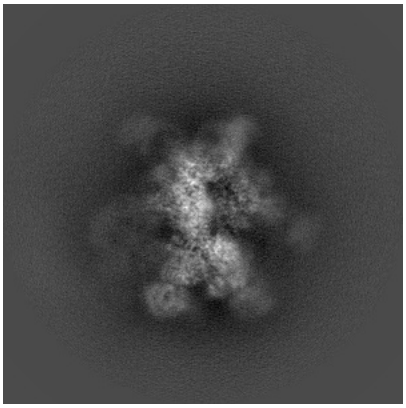


Y

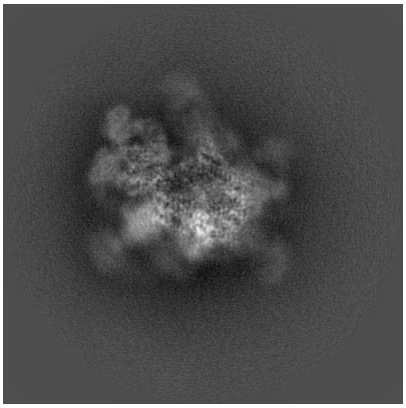


Z

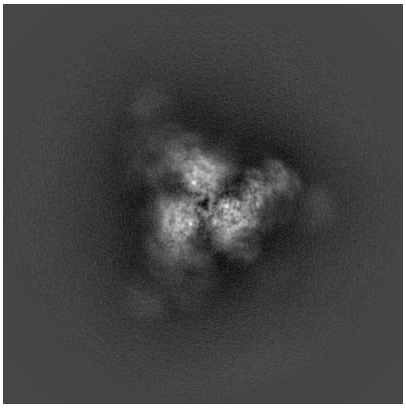
6.1.2 Raw map



X



Y

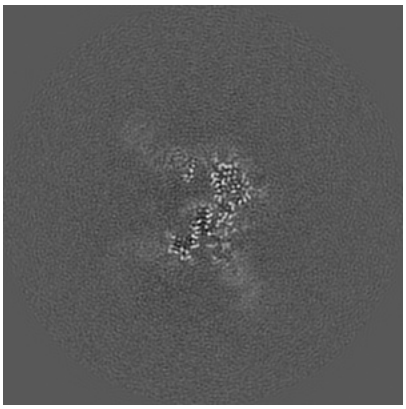


Z

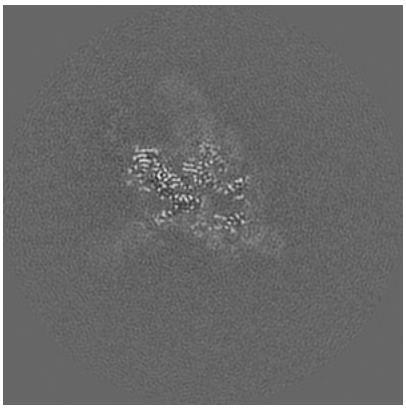
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

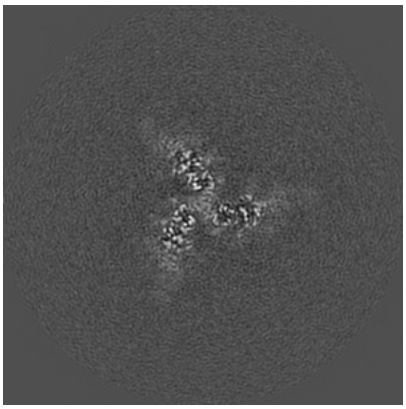
6.2.1 Primary map



X Index: 240

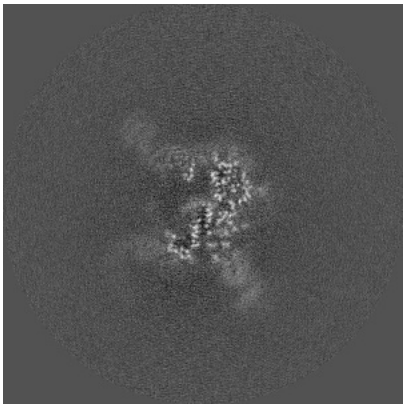


Y Index: 240

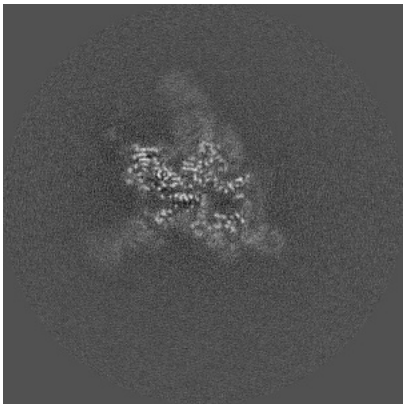


Z Index: 240

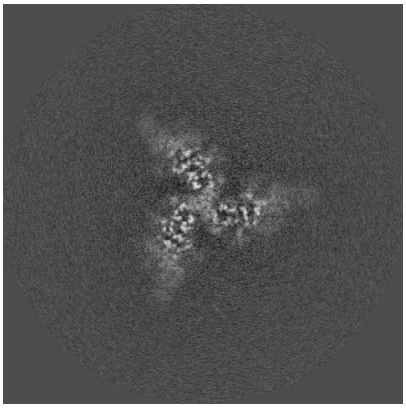
6.2.2 Raw map



X Index: 240



Y Index: 240

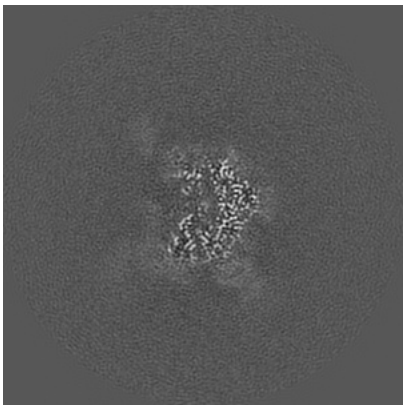


Z Index: 240

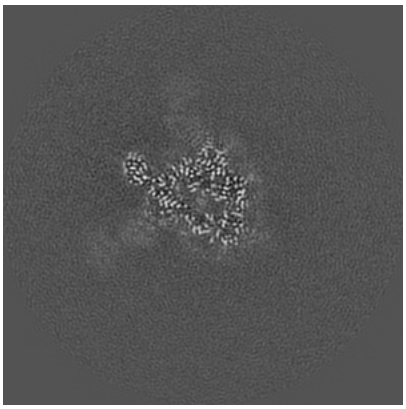
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

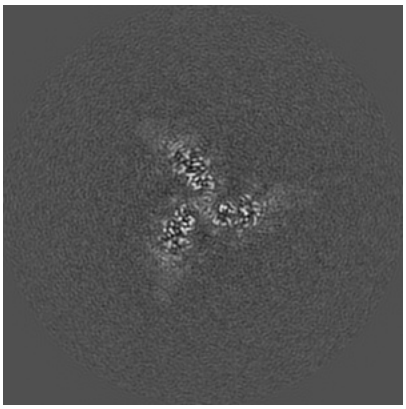
6.3.1 Primary map



X Index: 230

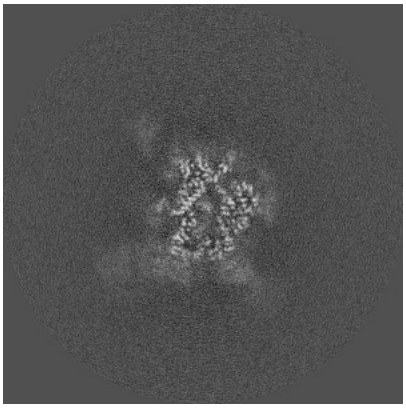


Y Index: 228

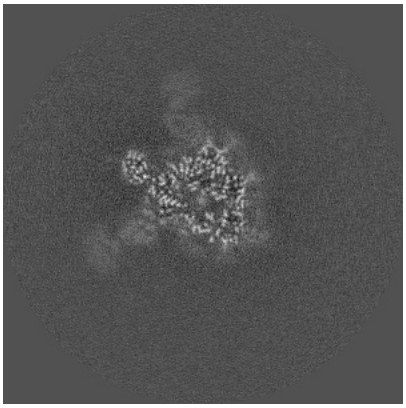


Z Index: 241

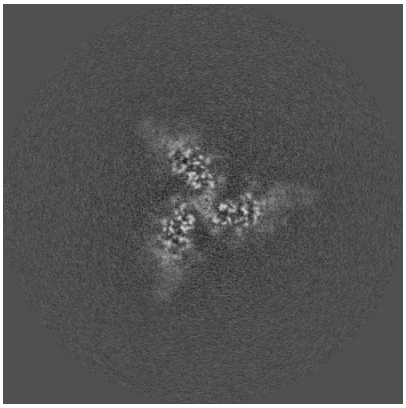
6.3.2 Raw map



X Index: 225



Y Index: 228

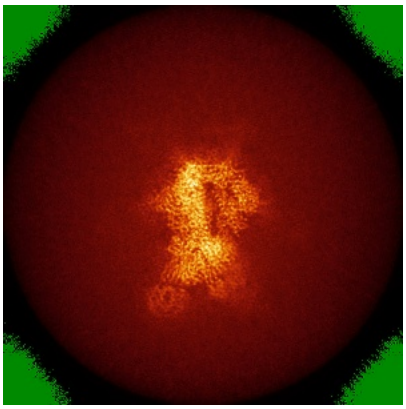


Z Index: 241

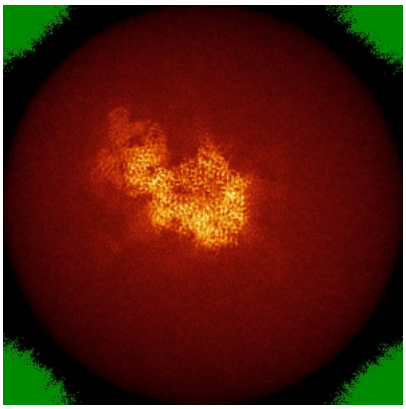
The images above show the largest variance slices of the map in three orthogonal directions.

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

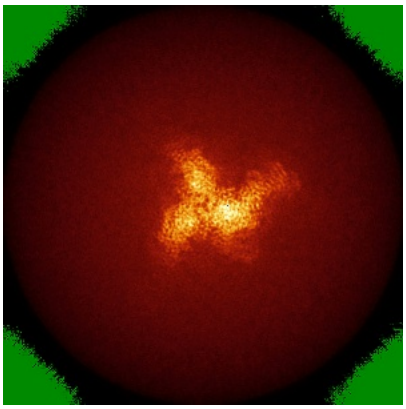
6.4.1 Primary map



X

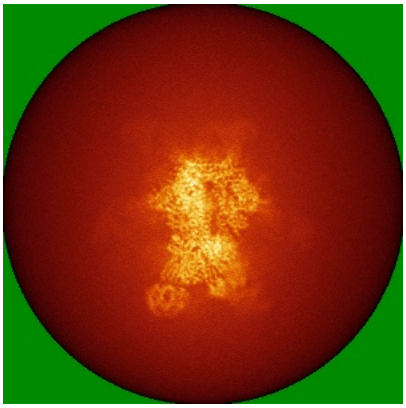


Y

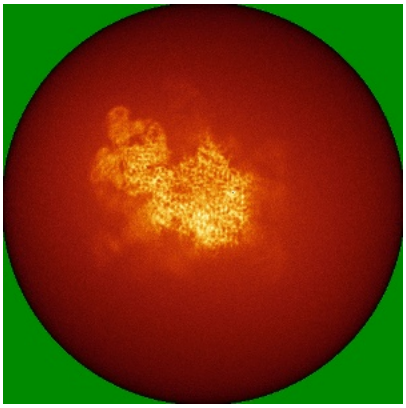


Z

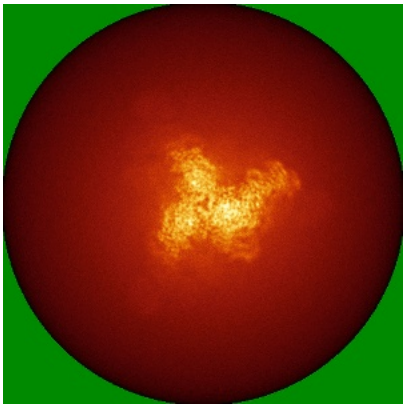
6.4.2 Raw map



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 0.012. 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.

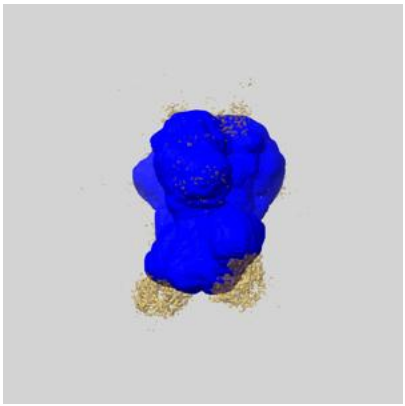
6.6 Mask visualisation (i)

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

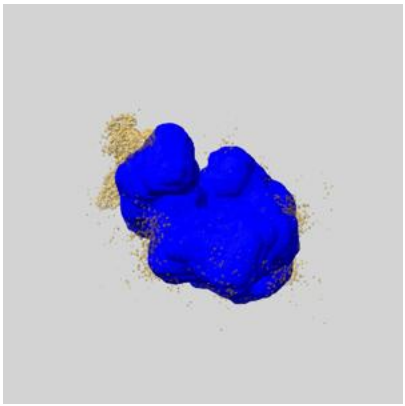
A mask typically either:

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

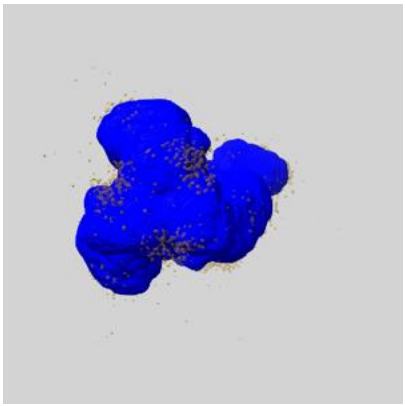
6.6.1 emd_43967_msk_1.map (i)



X



Y

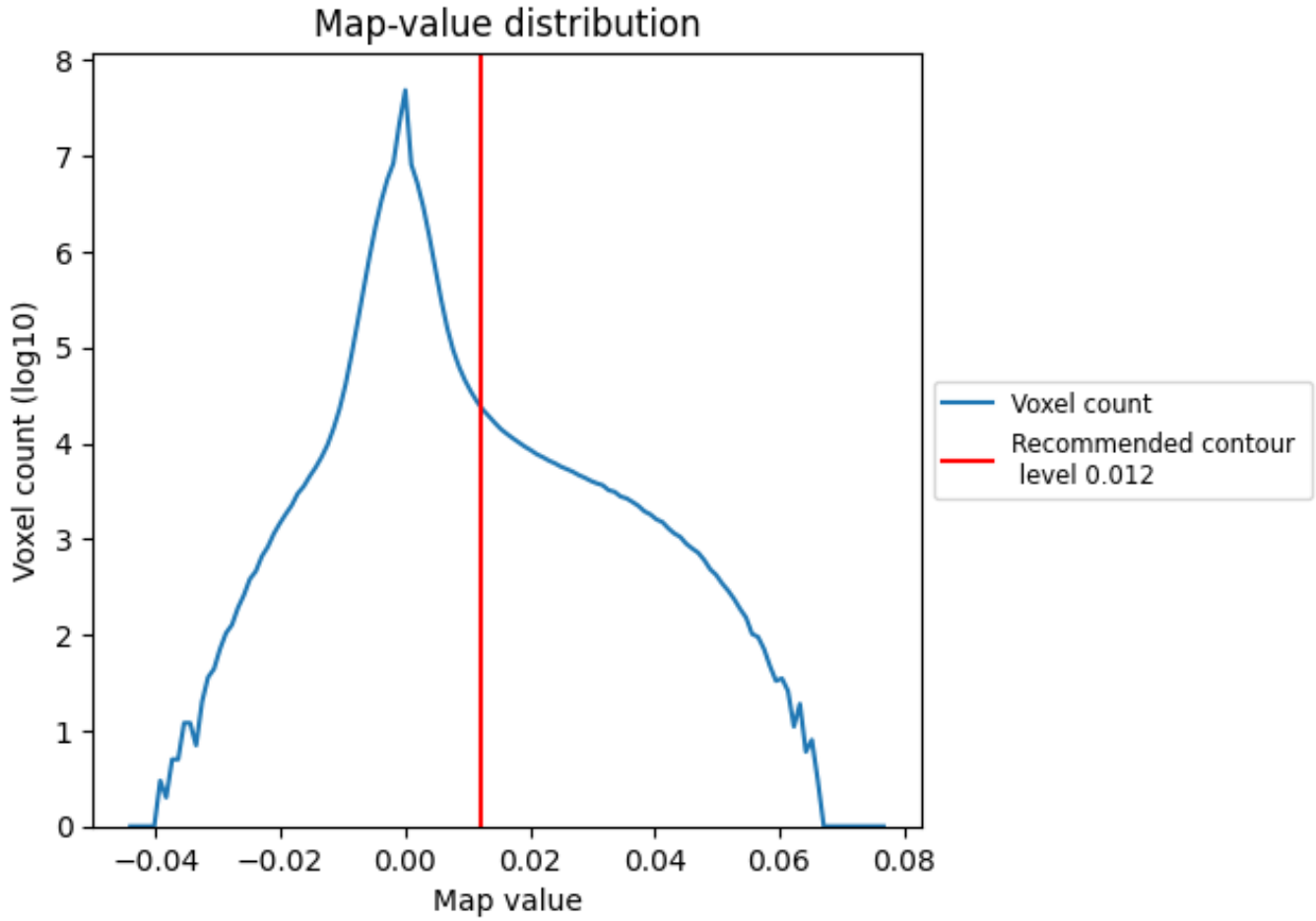


Z

7 Map analysis

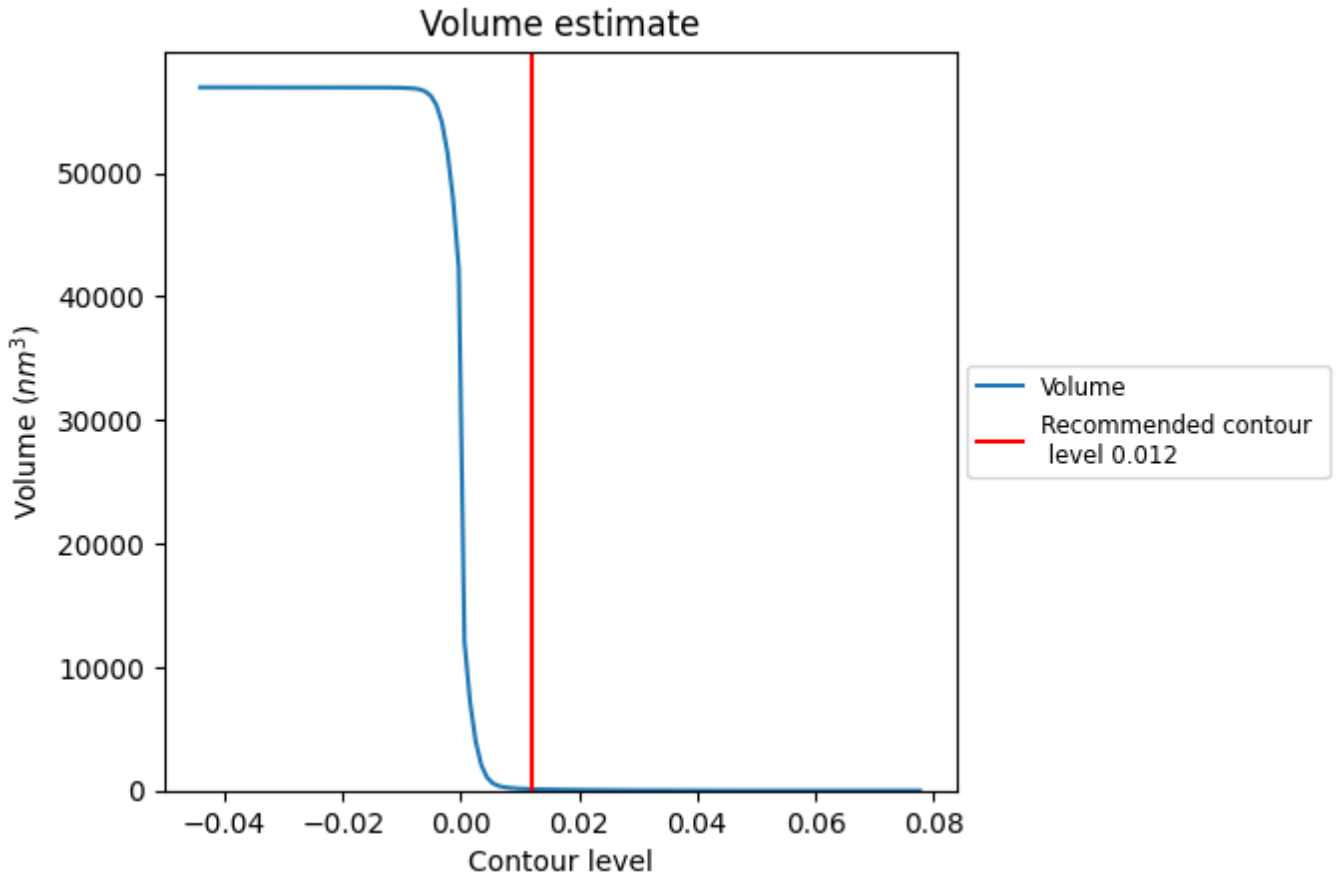
This section contains the results of statistical analysis of the map.

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.

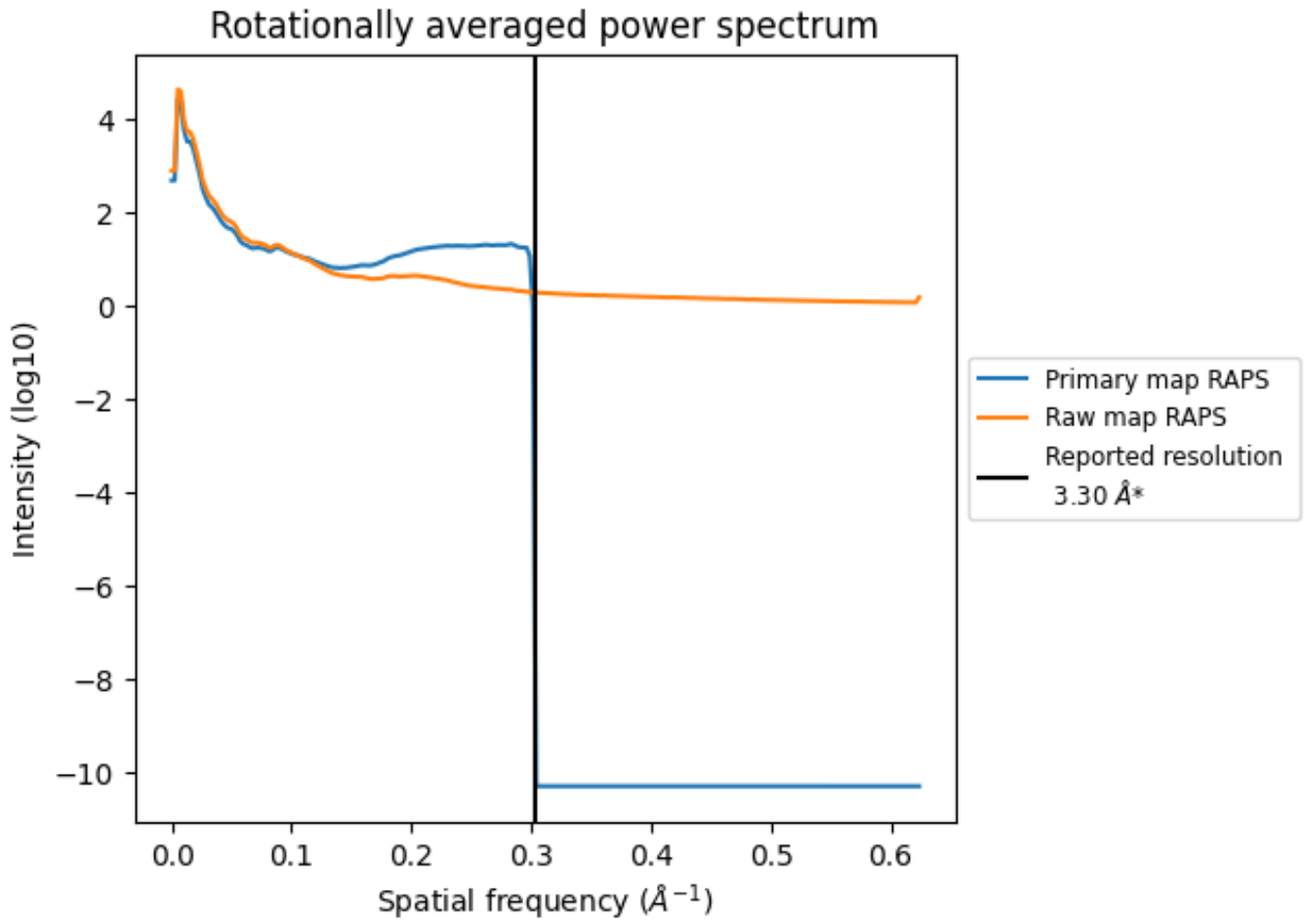
7.2 Volume estimate (i)



The volume at the recommended contour level is 120 nm^3; this corresponds to an approximate mass of 108 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)

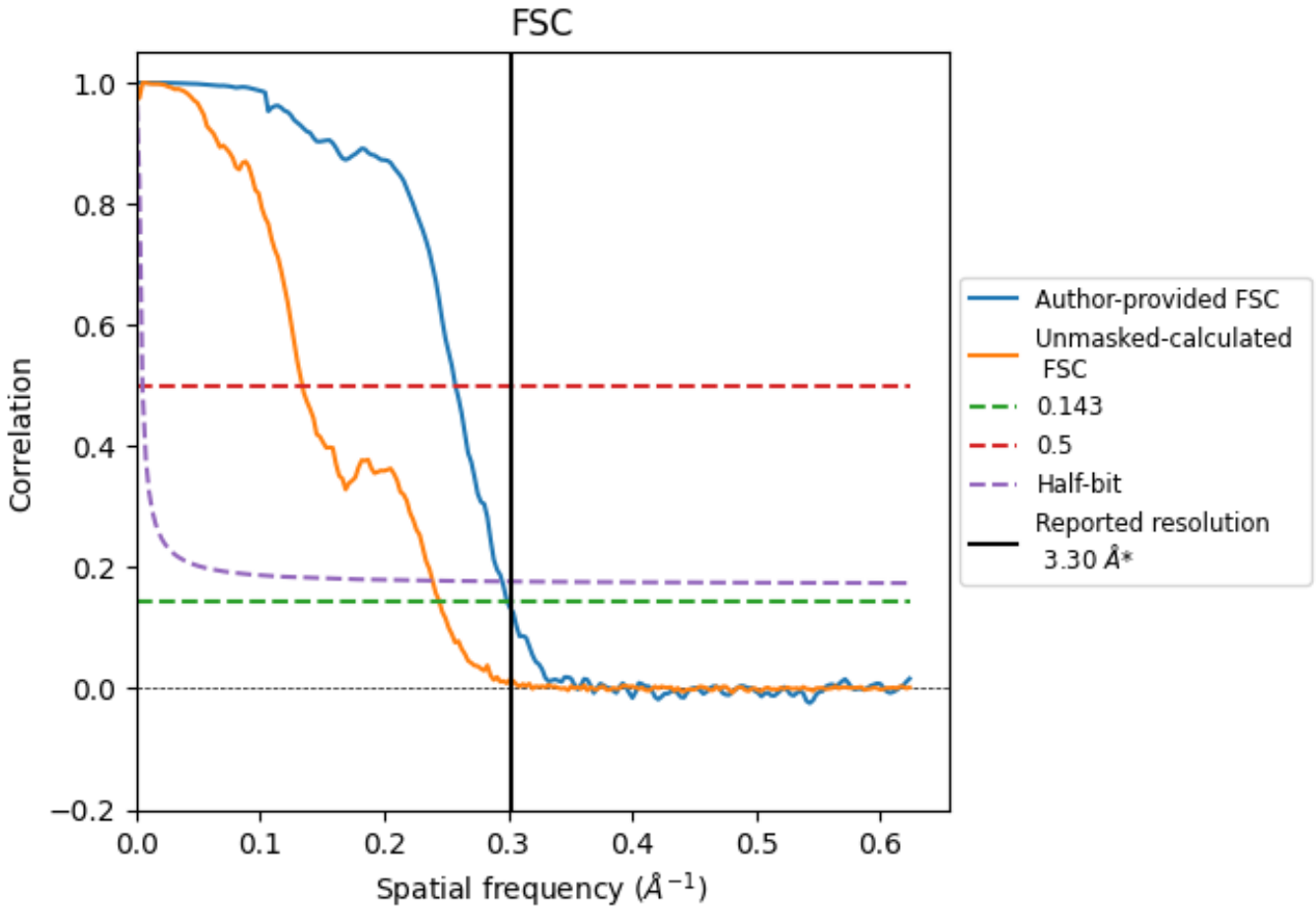


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 $Å^{-1}$

8.2 Resolution estimates (i)

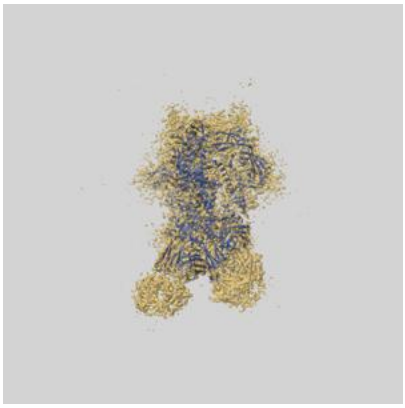
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.34	3.88	3.39
Unmasked-calculated*	4.09	7.46	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.3 by more than 10 %

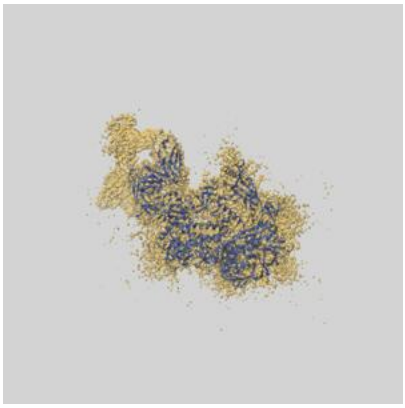
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43967 and PDB model 9AXI. Per-residue inclusion information can be found in section 3 on page 15.

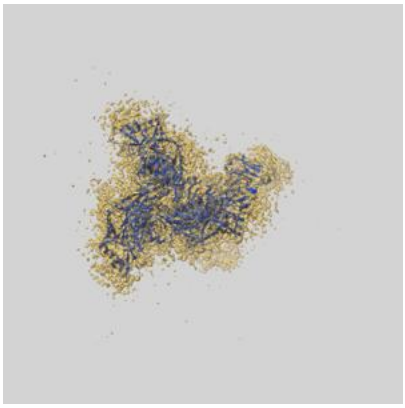
9.1 Map-model overlay



X



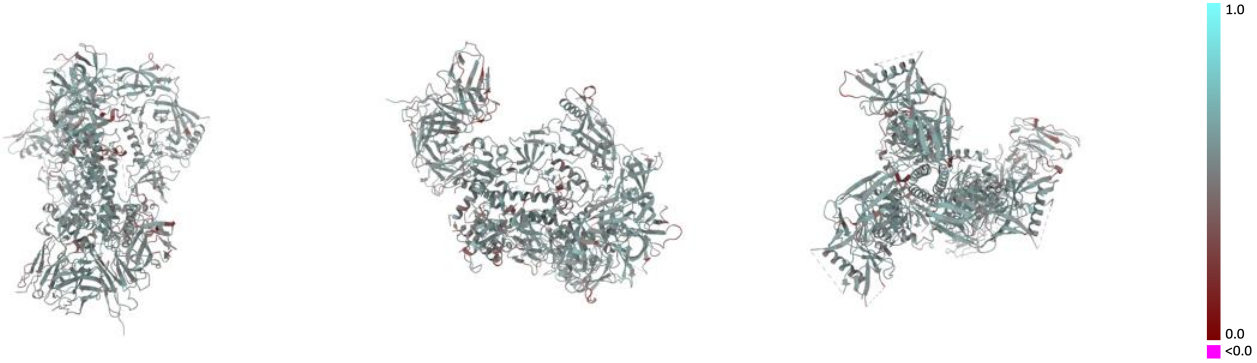
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

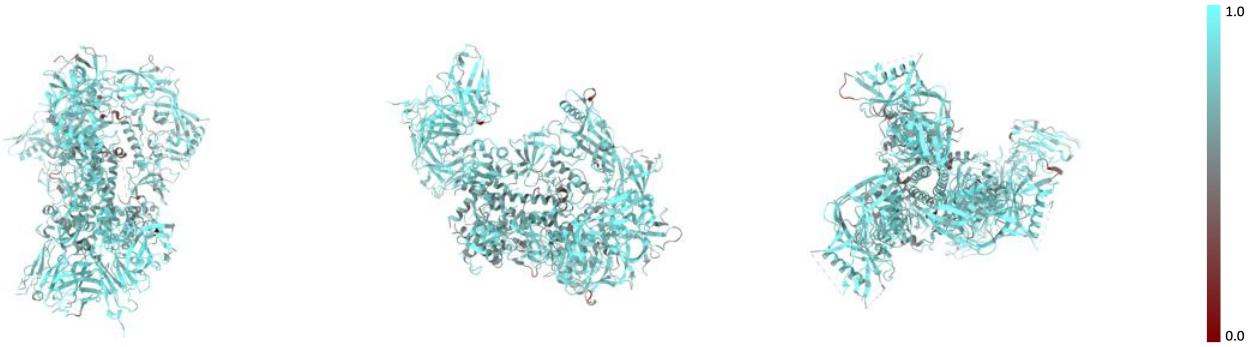
9.2 Q-score mapped to coordinate model



X Y Z

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

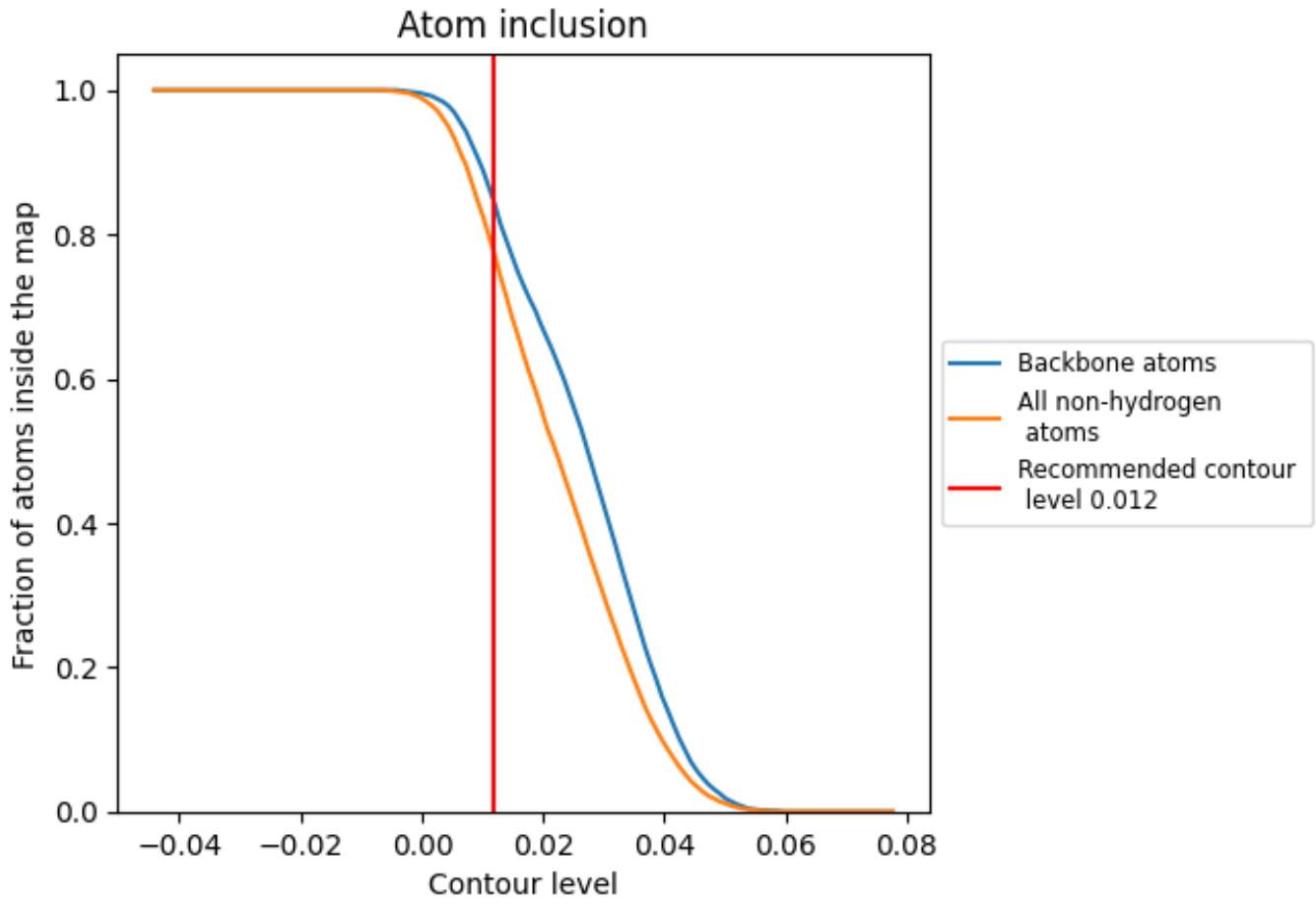
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7720	0.5110
A	0.8180	0.5170
B	0.7980	0.4880
C	0.7860	0.4800
D	0.7300	0.4990
E	0.3570	0.2620
F	0.8600	0.5110
G	0.8030	0.5240
H	0.8030	0.4570
I	0.6960	0.4710
J	0.7700	0.5170
K	0.7930	0.5250
L	0.7880	0.5250
M	0.7630	0.5190
N	0.7140	0.4490
O	0.6070	0.4570
P	0.5000	0.4210
Q	0.4640	0.4130
R	0.3930	0.2670
S	0.6790	0.5180
T	0.6070	0.5140
U	0.3930	0.3840
V	0.3930	0.2070
W	0.8800	0.5520
X	0.6790	0.5200
Y	0.5000	0.4100
Z	0.7140	0.4930
a	0.5360	0.4890
b	0.7700	0.5290
c	0.6430	0.4590
d	0.7140	0.5030
e	0.6790	0.4240