wwPDB EM Validation Summary Report (i)

Nov 4, 2024 – 05:46 PM EST

PDB ID	:	8FK5
EMDB ID	:	EMD-29248
Title	:	Cryo-EM Structure of PG9RSH DU011 Fab in complex with BG505 DS-SOSIP.664
Authors	:	Gorman, J.; Kwong, P.D.
Deposited on	:	2022-12-20
Resolution	:	3.40 Å(reported)
Based on initial model	:	6NNF

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 (i) symbol.

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

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

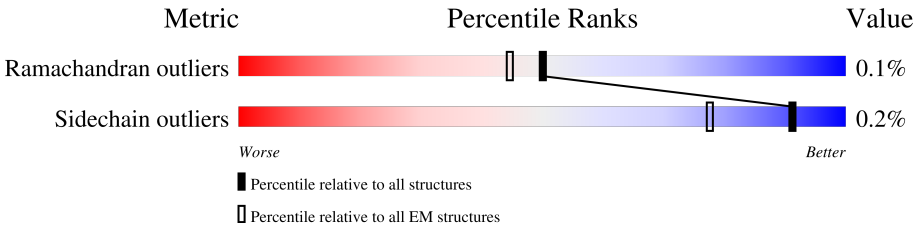
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	153	81% 18%
1	B	153	5% 81% 19%
1	F	153	82% 18%
2	C	481	93% 6%
2	G	481	5% 93% 6%
2	I	481	94% 6%
3	H	248	6% 54% 45%
4	L	216	10% 50% 50%
5	D	2	100%

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Mol	Chain	Length	Quality of chain
5	E	2	50% 100%
5	K	2	100%
5	M	2	50% 50% 50%
5	N	2	100%
5	O	2	100%
5	P	2	50% 100%
5	R	2	50% 50% 50%
5	S	2	100%
5	T	2	100%
5	U	2	100%
5	W	2	50% 100%
5	Y	2	50% 100%
5	Z	2	50% 50% 50%
5	b	2	50% 50%
5	c	2	100%
6	J	6	33% 50% 50%
6	Q	6	33% 33% 67%
6	X	6	33% 50% 50%
7	V	5	60% 40% 60%
7	a	5	60% 60% 40%
7	d	5	20% 60% 40%
8	e	9	11% 33% 67%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16980 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	125	Total	C	N	O	S	0	0
			997	631	171	189	6		
1	B	124	Total	C	N	O	S	0	0
			990	626	170	188	6		
1	F	126	Total	C	N	O	S	0	0
			1001	633	172	190	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	PRO	ILE	conflict	UNP Q2N0S6
A	605	CYS	THR	conflict	UNP Q2N0S6
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	450	Total	C	N	O	S	0	0
			3535	2215	626	664	30		
2	G	450	Total	C	N	O	S	0	0
			3535	2215	626	664	30		
2	I	450	Total	C	N	O	S	0	0
			3535	2215	626	664	30		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	201	CYS	ILE	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	433	CYS	ALA	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	509	ARG	GLU	conflict	UNP Q2N0S6
C	510	ARG	LYS	conflict	UNP Q2N0S6
C	512	ARG	ALA	conflict	UNP Q2N0S6
C	513	ARG	VAL	conflict	UNP Q2N0S6
G	201	CYS	ILE	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	433	CYS	ALA	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	GLU	conflict	UNP Q2N0S6
G	510	ARG	LYS	conflict	UNP Q2N0S6
G	512	ARG	ALA	conflict	UNP Q2N0S6
G	513	ARG	VAL	conflict	UNP Q2N0S6
I	201	CYS	ILE	conflict	UNP Q2N0S6
I	332	ASN	THR	conflict	UNP Q2N0S6
I	433	CYS	ALA	conflict	UNP Q2N0S6
I	501	CYS	ALA	conflict	UNP Q2N0S6
I	509	ARG	GLU	conflict	UNP Q2N0S6
I	510	ARG	LYS	conflict	UNP Q2N0S6
I	512	ARG	ALA	conflict	UNP Q2N0S6
I	513	ARG	VAL	conflict	UNP Q2N0S6

- Molecule 3 is a protein called Immunoblobulin G1 Fab heavy chain variable region (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	136	Total	C	N	O	S	0	0
			1102	692	186	217	7		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	2	GLU	-	expression tag	UNP A4F255
H	3	ARG	-	expression tag	UNP A4F255
H	5	VAL	GLU	conflict	UNP A4F255
H	16	SER	LYS	conflict	UNP A4F255
H	23	ALA	THR	conflict	UNP A4F255
H	28	ASP	ILE	conflict	UNP A4F255
H	31	ARG	ASP	conflict	UNP A4F255
H	32	GLN	PHE	conflict	UNP A4F255
H	43	GLN	LYS	conflict	UNP A4F255
H	47	TRP	SER	conflict	UNP A4F255

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Chain	Residue	Modelled	Actual	Comment	Reference
H	50	PHE	THR	conflict	UNP A4F255
H	52	LYS	TRP	conflict	UNP A4F255
H	52A	TYR	SER	conflict	UNP A4F255
H	56	GLU	ASN	conflict	UNP A4F255
H	57	LYS	GLU	conflict	UNP A4F255
H	58	TYR	LYS	conflict	UNP A4F255
H	59	HIS	TYR	conflict	UNP A4F255
H	64	TRP	THR	conflict	UNP A4F255
H	67	LEU	PHE	conflict	UNP A4F255
H	68	SER	ALA	conflict	UNP A4F255
H	76	ASP	ASN	conflict	UNP A4F255
H	77	THR	MET	conflict	UNP A4F255
H	81	GLN	HIS	conflict	UNP A4F255
H	82A	ASN	ASP	conflict	UNP A4F255
H	82B	SER	ASN	conflict	UNP A4F255
H	84	VAL	ALA	conflict	UNP A4F255
H	89	THR	VAL	conflict	UNP A4F255
H	91	PHE	TYR	conflict	UNP A4F255
H	93	VAL	ALA	conflict	UNP A4F255
H	95	GLU	ASP	conflict	UNP A4F255
H	97	GLY	-	insertion	UNP A4F255
H	98	GLY	-	insertion	UNP A4F255
H	99	PRO	-	insertion	UNP A4F255
H	100A	TYR	MET	conflict	UNP A4F255
H	100B	ARG	ILE	conflict	UNP A4F255
H	100C	ASN	THR	conflict	UNP A4F255
H	100D	GLY	PHE	conflict	UNP A4F255
H	100E	TYR	ALA	conflict	UNP A4F255
H	100F	TYR	ARG	conflict	UNP A4F255
H	100G	TYS	ILE	conflict	UNP A4F255
H	100H	TYS	LEU	conflict	UNP A4F255
H	?	-	PRO	deletion	UNP A4F255
H	?	-	PRO	deletion	UNP A4F255
H	100K	TYR	HIS	conflict	UNP A4F255
H	100L	ASP	LYS	conflict	UNP A4F255
H	100N	TYR	-	insertion	UNP A4F255
H	100O	TYR	-	insertion	UNP A4F255
H	100P	ASN	-	insertion	UNP A4F255
H	100Q	TYR	-	insertion	UNP A4F255
H	100R	HIS	-	insertion	UNP A4F255
H	100S	TYR	-	insertion	UNP A4F255
H	105	LYS	GLN	conflict	UNP A4F255

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Chain	Residue	Modelled	Actual	Comment	Reference
H	110	THR	ILE	conflict	UNP A4F255
H	219	GLY	-	expression tag	UNP A4F255
H	220	LEU	-	expression tag	UNP A4F255
H	221	GLU	-	expression tag	UNP A4F255
H	222	VAL	-	expression tag	UNP A4F255
H	223	LEU	-	expression tag	UNP A4F255
H	224	PHE	-	expression tag	UNP A4F255
H	225	GLN	-	expression tag	UNP A4F255

- Molecule 4 is a protein called Immunoglobulin lambda-1 light chain-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	109	Total	C	N	O	S	0	0
			801	492	141	166	2		

There are 22 discrepancies between the modelled and reference sequences:

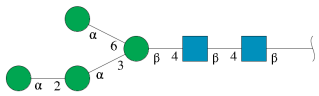
Chain	Residue	Modelled	Actual	Comment	Reference
L	24	GLN	THR	conflict	UNP Q6PJG0
L	27A	ASN	THR	conflict	UNP Q6PJG0
L	29	GLY	SER	conflict	UNP Q6PJG0
L	30	TYR	HIS	conflict	UNP Q6PJG0
L	31	GLU	SER	conflict	UNP Q6PJG0
L	32	SER	LEU	conflict	UNP Q6PJG0
L	46	VAL	PHE	conflict	UNP Q6PJG0
L	47	VAL	LEU	conflict	UNP Q6PJG0
L	49	TYR	PHE	conflict	UNP Q6PJG0
L	50	ASP	GLU	conflict	UNP Q6PJG0
L	51	VAL	GLY	conflict	UNP Q6PJG0
L	84	GLY	ALA	conflict	UNP Q6PJG0
L	89	LYS	CYS	conflict	UNP Q6PJG0
L	91	LEU	TYR	conflict	UNP Q6PJG0
L	92	THR	VAL	conflict	UNP Q6PJG0
L	93	SER	GLY	conflict	UNP Q6PJG0
L	94	ARG	SER	conflict	UNP Q6PJG0
L	95	SER	GLY	conflict	UNP Q6PJG0
L	95A	HIS	THR	conflict	UNP Q6PJG0
L	96	ARG	VAL	conflict	UNP Q6PJG0
L	100	THR	GLY	conflict	UNP Q6PJG0
L	189	LYS	ARG	conflict	UNP Q6PJG0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.

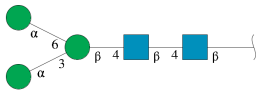
Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		

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



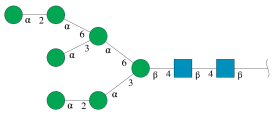
Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	6	Total	C	N	O	0	0
			72	40	2	30		
6	Q	6	Total	C	N	O	0	0
			72	40	2	30		
6	X	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 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.



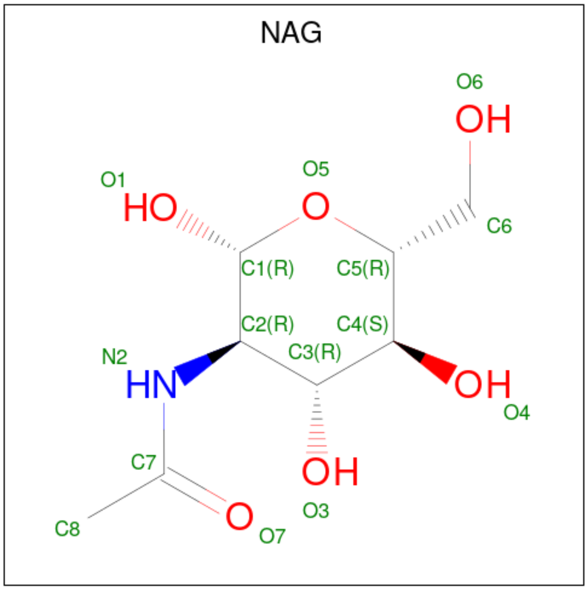
Mol	Chain	Residues	Atoms				AltConf	Trace
7	V	5	Total	C	N	O	0	0
			61	34	2	25		
7	a	5	Total	C	N	O	0	0
			61	34	2	25		
7	d	5	Total	C	N	O	0	0
			61	34	2	25		

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



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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms	AltConf
9	C	1	Total C N O 14 8 1 5	0
9	C	1	Total C N O 14 8 1 5	0
9	F	1	Total C N O 14 8 1 5	0
9	F	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	I	1	Total C N O 14 8 1 5	0
9	I	1	Total C N O 14 8 1 5	0
9	I	1	Total C N O 14 8 1 5	0
9	I	1	Total C N O 14 8 1 5	0
9	I	1	Total C N O 14 8 1 5	0
9	I	1	Total C N O 14 8 1 5	0

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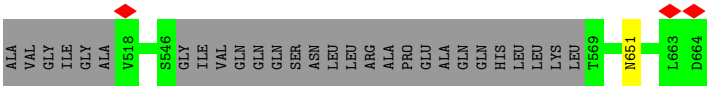
Mol	Chain	Residues	Atoms				AltConf
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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

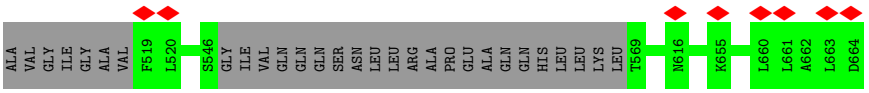
• Molecule 1: Envelope glycoprotein gp41

Chain A:



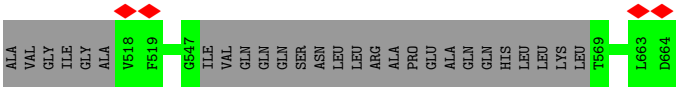
• Molecule 1: Envelope glycoprotein gp41

Chain B:



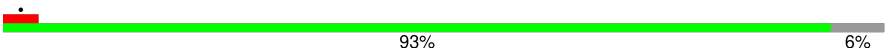
• Molecule 1: Envelope glycoprotein gp41

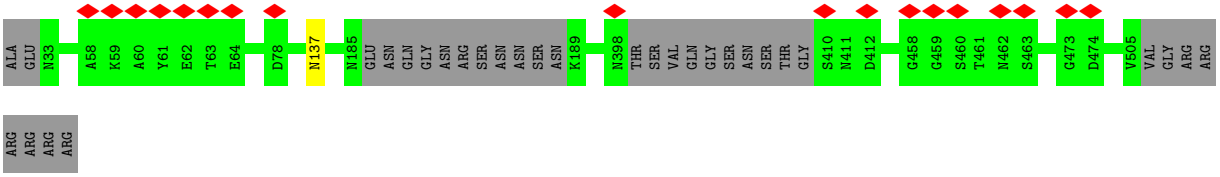
Chain F:



• Molecule 2: Envelope glycoprotein gp120

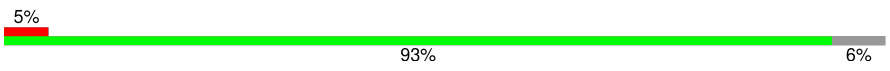
Chain C:

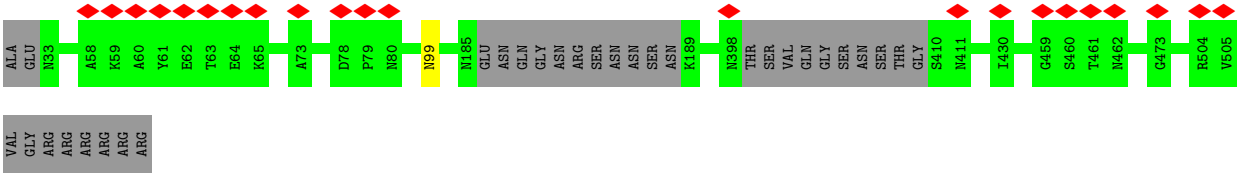




• Molecule 2: Envelope glycoprotein gp120

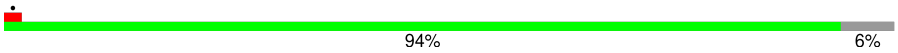
Chain G:

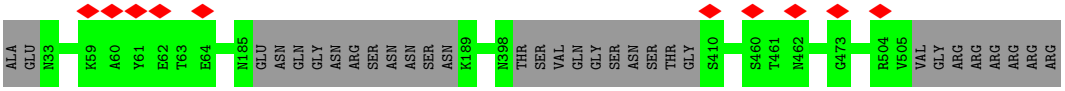




• Molecule 2: Envelope glycoprotein gp120

Chain I:



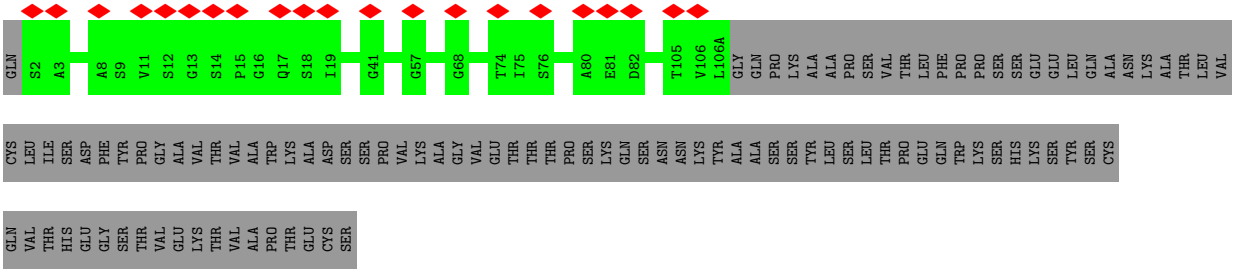


• Molecule 3: Immunoblobulin G1 Fab heavy chain variable region (Fragment)

Chain H:

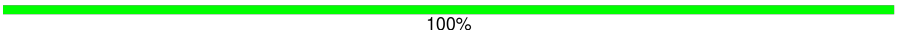
• Molecule 4: Immunoglobulin lambda-1 light chain-like

Chain L:



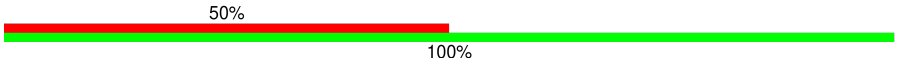
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



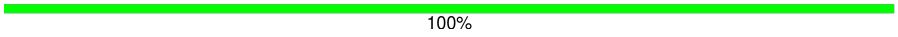
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain K:

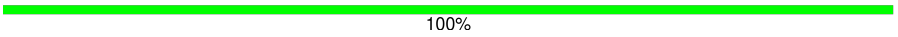


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

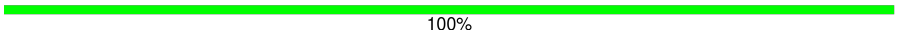
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain O:



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

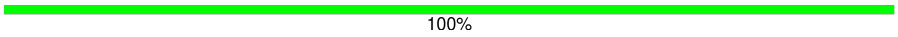
Chain P:

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

Chain R:

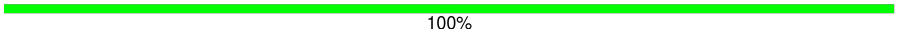
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



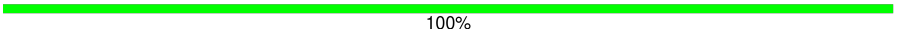
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



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

Chain U:

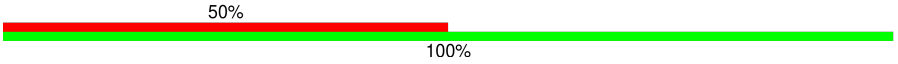


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

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

Chain Y:



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

Chain Z:

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

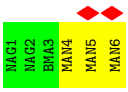
Chain b:

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

Chain c:

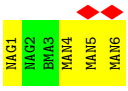
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



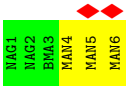
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



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

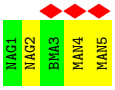
Chain X:



• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra

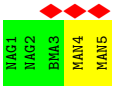
nose

Chain V:



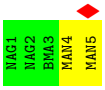
• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 7: 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 d:



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

Chain e:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230180	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	63.75	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.175	Depositor
Minimum map value	-2.551	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	368.21997, 368.21997, 368.21997	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	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, TYS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.23	0/1015	0.42	0/1377
1	B	0.22	0/1008	0.43	0/1367
1	F	0.23	0/1019	0.44	0/1382
2	C	0.25	0/3608	0.50	0/4898
2	G	0.25	0/3608	0.50	0/4898
2	I	0.26	0/3608	0.52	0/4898
3	H	0.26	0/1099	0.51	0/1486
4	L	0.24	0/816	0.49	0/1105
All	All	0.25	0/15781	0.49	0/21411

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	121/153 (79%)	119 (98%)	2 (2%)	0	100	100
1	B	120/153 (78%)	119 (99%)	1 (1%)	0	100	100
1	F	122/153 (80%)	118 (97%)	4 (3%)	0	100	100
2	C	444/481 (92%)	427 (96%)	17 (4%)	0	100	100
2	G	444/481 (92%)	431 (97%)	13 (3%)	0	100	100
2	I	444/481 (92%)	428 (96%)	16 (4%)	0	100	100
3	H	132/248 (53%)	127 (96%)	4 (3%)	1 (1%)	16	44
4	L	107/216 (50%)	106 (99%)	1 (1%)	0	100	100
All	All	1934/2366 (82%)	1875 (97%)	58 (3%)	1 (0%)	50	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	100(I)	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	108/129 (84%)	107 (99%)	1 (1%)	75	86
1	B	107/129 (83%)	107 (100%)	0	100	100
1	F	108/129 (84%)	108 (100%)	0	100	100
2	C	402/429 (94%)	401 (100%)	1 (0%)	92	96
2	G	402/429 (94%)	401 (100%)	1 (0%)	92	96
2	I	402/429 (94%)	402 (100%)	0	100	100
3	H	111/208 (53%)	111 (100%)	0	100	100
4	L	91/183 (50%)	91 (100%)	0	100	100
All	All	1731/2065 (84%)	1728 (100%)	3 (0%)	91	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	651	ASN
2	C	137	ASN
2	G	99	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TYS	H	100(G)	3	15,16,17	0.73	0	15,22,24	0.92	0
3	TYS	H	100(H)	3	15,16,17	0.60	0	15,22,24	0.96	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
3	TYS	H	100(G)	3	-	1/10/11/13	0/1/1/1
3	TYS	H	100(H)	3	-	2/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	100(H)	TYS	CE1-CZ-OH-S
3	H	100(H)	TYS	CE2-CZ-OH-S
3	H	100(G)	TYS	CE1-CZ-OH-S

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

74 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	D	1	2,5	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	D	2	5	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	E	1	2,5	14,14,15	0.22	0	17,19,21	0.47	0
5	NAG	E	2	5	14,14,15	0.20	0	17,19,21	0.45	0
6	NAG	J	1	2,6	14,14,15	0.24	0	17,19,21	0.51	0
6	NAG	J	2	6	14,14,15	0.20	0	17,19,21	0.43	0
6	BMA	J	3	6	11,11,12	0.57	0	15,15,17	0.79	0
6	MAN	J	4	6	11,11,12	0.67	0	15,15,17	1.07	2 (13%)
6	MAN	J	5	6	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
6	MAN	J	6	6	11,11,12	0.62	0	15,15,17	0.95	2 (13%)
5	NAG	K	1	2,5	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	K	2	5	14,14,15	0.22	0	17,19,21	0.55	0
5	NAG	M	1	2,5	14,14,15	0.32	0	17,19,21	1.23	2 (11%)
5	NAG	M	2	5	14,14,15	0.22	0	17,19,21	0.46	0
5	NAG	N	1	2,5	14,14,15	0.25	0	17,19,21	0.40	0
5	NAG	N	2	5	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	O	1	2,5	14,14,15	0.25	0	17,19,21	0.52	0
5	NAG	O	2	5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	P	1	2,5	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	P	2	5	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	Q	1	2,6	14,14,15	0.36	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	Q	2	6	14,14,15	0.21	0	17,19,21	0.45	0
6	BMA	Q	3	6	11,11,12	0.56	0	15,15,17	0.78	0
6	MAN	Q	4	6	11,11,12	0.61	0	15,15,17	0.90	1 (6%)
6	MAN	Q	5	6	11,11,12	0.62	0	15,15,17	0.98	2 (13%)
6	MAN	Q	6	6	11,11,12	0.59	0	15,15,17	0.93	2 (13%)
5	NAG	R	1	2,5	14,14,15	0.34	0	17,19,21	1.25	2 (11%)
5	NAG	R	2	5	14,14,15	0.22	0	17,19,21	0.47	0
5	NAG	S	1	2,5	14,14,15	0.18	0	17,19,21	0.44	0
5	NAG	S	2	5	14,14,15	0.20	0	17,19,21	0.45	0
5	NAG	T	1	2,5	14,14,15	0.21	0	17,19,21	0.52	0
5	NAG	T	2	5	14,14,15	0.19	0	17,19,21	0.43	0
5	NAG	U	1	2,5	14,14,15	0.56	0	17,19,21	0.67	0
5	NAG	U	2	5	14,14,15	0.25	0	17,19,21	0.55	0
7	NAG	V	1	2,7	14,14,15	0.19	0	17,19,21	0.45	0
7	NAG	V	2	7	14,14,15	0.28	0	17,19,21	1.27	2 (11%)
7	BMA	V	3	7	11,11,12	0.52	0	15,15,17	0.73	0
7	MAN	V	4	7	11,11,12	0.60	0	15,15,17	0.93	2 (13%)
7	MAN	V	5	7	11,11,12	0.63	0	15,15,17	0.94	2 (13%)
5	NAG	W	1	2,5	14,14,15	0.26	0	17,19,21	0.49	0
5	NAG	W	2	5	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	X	1	2,6	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	X	2	6	14,14,15	0.21	0	17,19,21	0.43	0
6	BMA	X	3	6	11,11,12	0.59	0	15,15,17	0.81	0
6	MAN	X	4	6	11,11,12	0.58	0	15,15,17	0.98	2 (13%)
6	MAN	X	5	6	11,11,12	0.59	0	15,15,17	0.92	2 (13%)
6	MAN	X	6	6	11,11,12	0.62	0	15,15,17	0.93	2 (13%)
5	NAG	Y	1	2,5	14,14,15	0.22	0	17,19,21	0.46	0
5	NAG	Y	2	5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	Z	1	2,5	14,14,15	0.36	0	17,19,21	1.25	2 (11%)
5	NAG	Z	2	5	14,14,15	0.22	0	17,19,21	0.46	0
7	NAG	a	1	2,7	14,14,15	0.22	0	17,19,21	0.48	0
7	NAG	a	2	7	14,14,15	0.21	0	17,19,21	0.45	0
7	BMA	a	3	7	11,11,12	0.61	0	15,15,17	0.75	0
7	MAN	a	4	7	11,11,12	0.63	0	15,15,17	0.93	2 (13%)
7	MAN	a	5	7	11,11,12	0.61	0	15,15,17	0.92	2 (13%)
5	NAG	b	1	2,5	14,14,15	0.36	0	17,19,21	0.63	1 (5%)
5	NAG	b	2	5	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	c	1	2,5	14,14,15	0.25	0	17,19,21	0.57	0
5	NAG	c	2	5	14,14,15	0.24	0	17,19,21	0.45	0
7	NAG	d	1	2,7	14,14,15	0.26	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	d	2	7	14,14,15	0.35	0	17,19,21	0.55	0
7	BMA	d	3	7	11,11,12	0.48	0	15,15,17	0.73	0
7	MAN	d	4	7	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
7	MAN	d	5	7	11,11,12	0.67	0	15,15,17	1.04	2 (13%)
8	NAG	e	1	2,8	14,14,15	0.20	0	17,19,21	0.44	0
8	NAG	e	2	8	14,14,15	0.20	0	17,19,21	0.42	0
8	BMA	e	3	8	11,11,12	0.50	0	15,15,17	0.80	0
8	MAN	e	4	8	11,11,12	0.60	0	15,15,17	1.01	2 (13%)
8	MAN	e	5	8	11,11,12	0.60	0	15,15,17	0.96	2 (13%)
8	MAN	e	6	8	11,11,12	0.57	0	15,15,17	0.93	2 (13%)
8	MAN	e	7	8	11,11,12	0.55	0	15,15,17	0.93	2 (13%)
8	MAN	e	8	8	11,11,12	0.58	0	15,15,17	1.04	2 (13%)
8	MAN	e	9	8	11,11,12	2.92	2 (18%)	15,15,17	1.09	1 (6%)

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	c	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
7	NAG	d	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	d	2	7	-	2/6/23/26	0/1/1/1
7	BMA	d	3	7	-	0/2/19/22	0/1/1/1
7	MAN	d	4	7	-	0/2/19/22	0/1/1/1
7	MAN	d	5	7	-	0/2/19/22	0/1/1/1
8	NAG	e	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	e	2	8	-	2/6/23/26	0/1/1/1
8	BMA	e	3	8	-	0/2/19/22	0/1/1/1
8	MAN	e	4	8	-	2/2/19/22	0/1/1/1
8	MAN	e	5	8	-	0/2/19/22	0/1/1/1
8	MAN	e	6	8	-	2/2/19/22	0/1/1/1
8	MAN	e	7	8	-	0/2/19/22	0/1/1/1
8	MAN	e	8	8	-	2/2/19/22	0/1/1/1
8	MAN	e	9	8	-	2/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	e	9	MAN	O5-C1	7.10	1.55	1.43
8	e	9	MAN	C1-C2	6.26	1.67	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	2	NAG	C2-N2-C7	4.01	128.27	122.90
5	Z	1	NAG	C2-N2-C7	3.96	128.21	122.90
5	R	1	NAG	C2-N2-C7	3.90	128.12	122.90
6	Q	1	NAG	C2-N2-C7	3.88	128.11	122.90
5	M	1	NAG	C2-N2-C7	3.84	128.05	122.90

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1	NAG	C1-C2-N2-C7
5	R	1	NAG	C1-C2-N2-C7
5	Z	1	NAG	C1-C2-N2-C7

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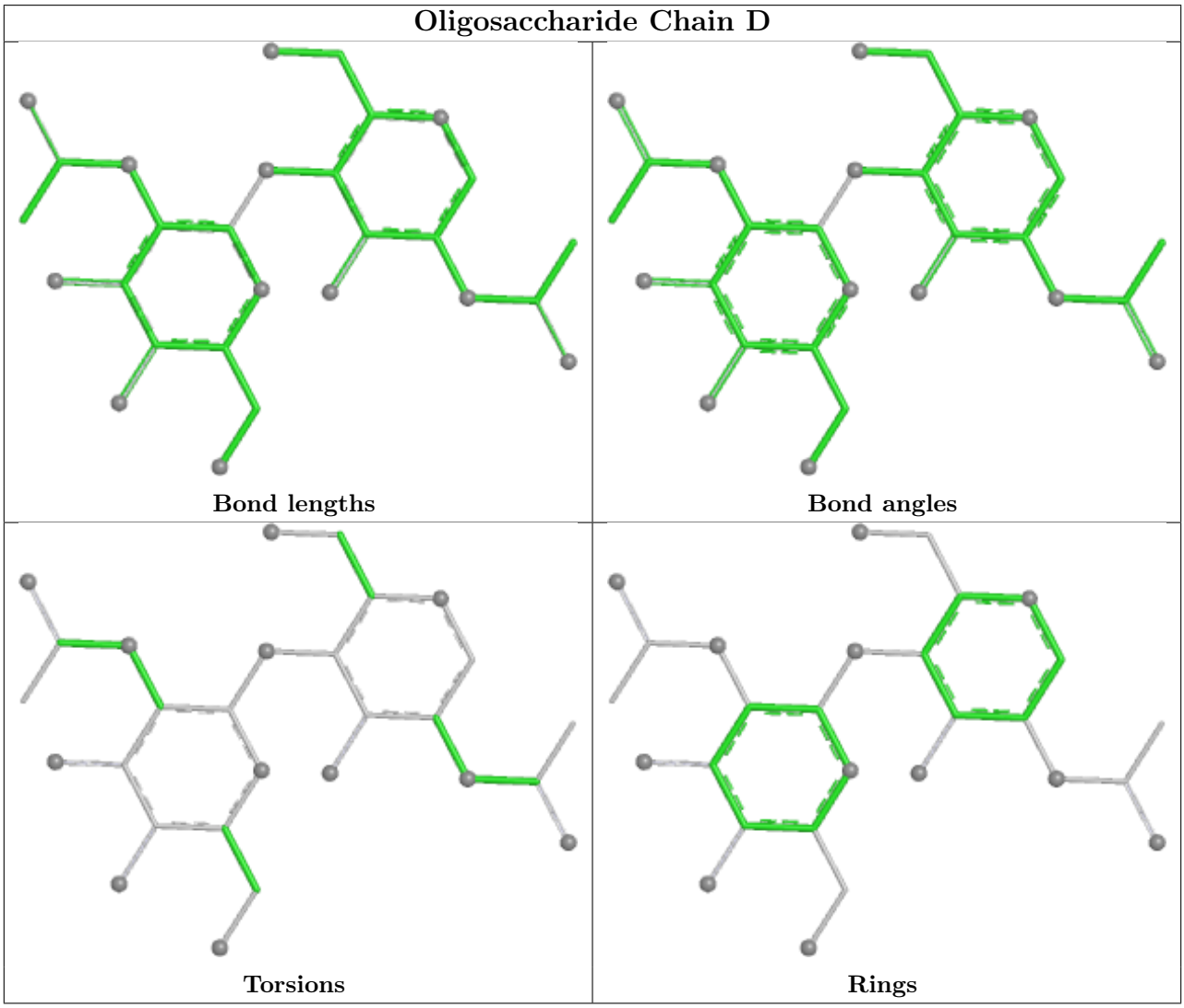
Mol	Chain	Res	Type	Atoms
8	e	1	NAG	O5-C5-C6-O6
8	e	4	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

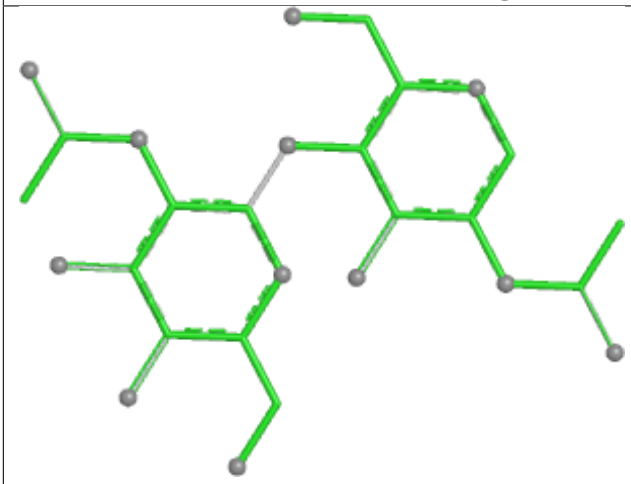
Mol	Chain	Res	Type	Atoms
8	e	9	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

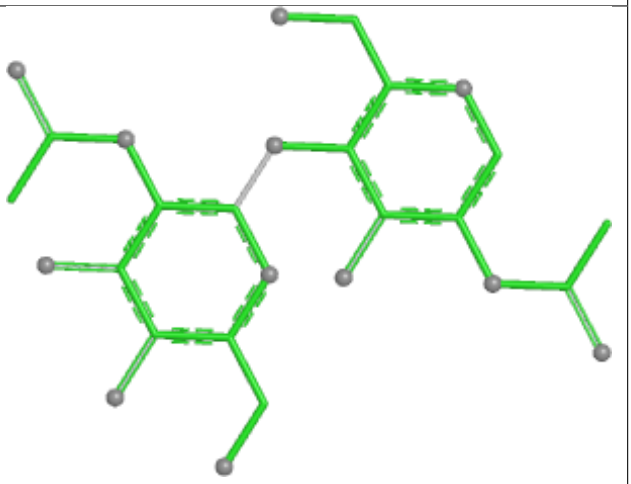
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



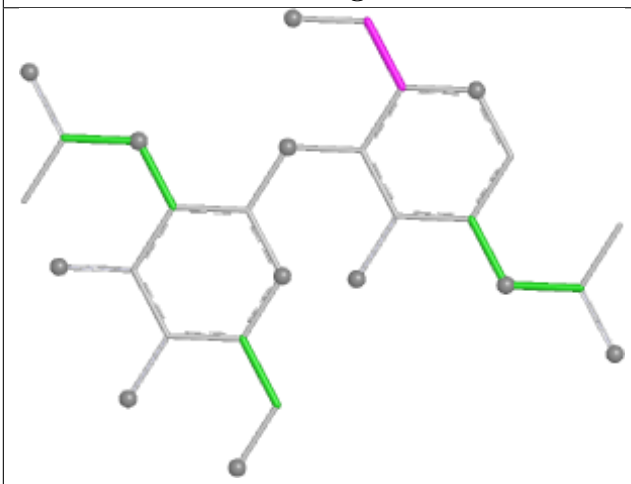
Oligosaccharide Chain E



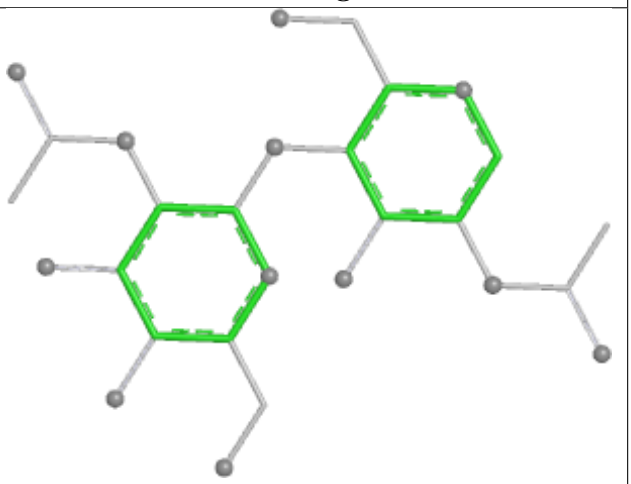
Bond lengths



Bond angles

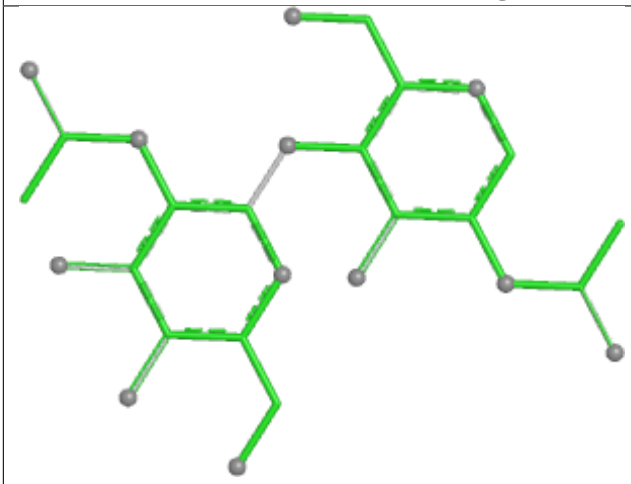


Torsions

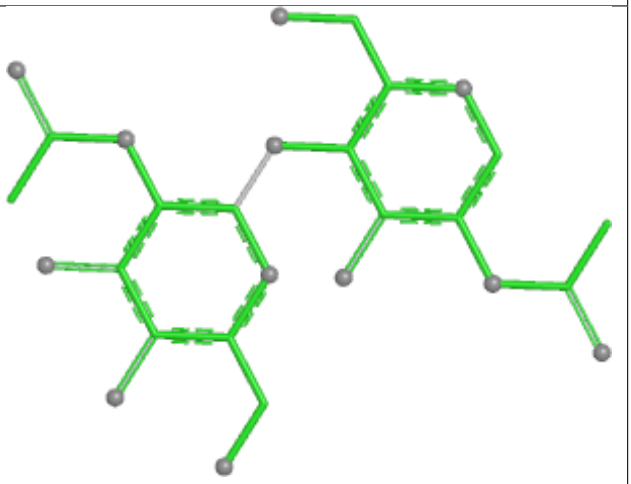


Rings

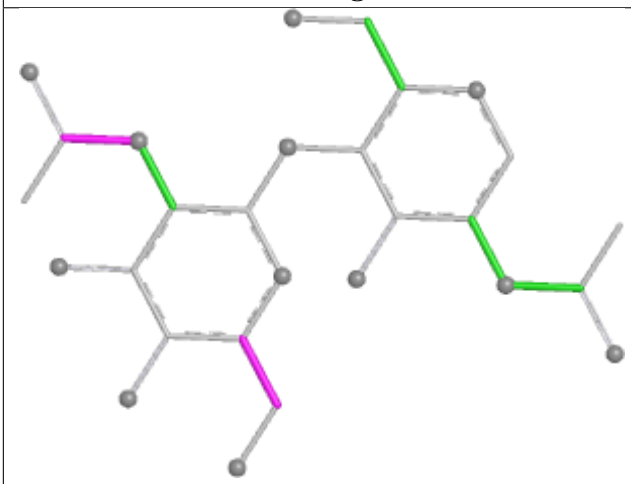
Oligosaccharide Chain K



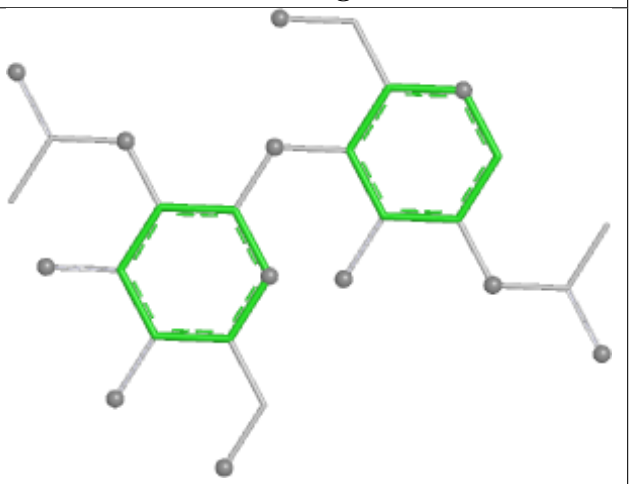
Bond lengths



Bond angles

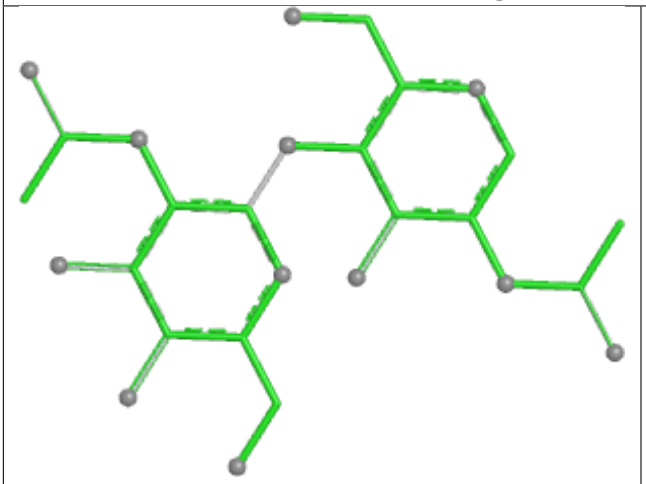


Torsions

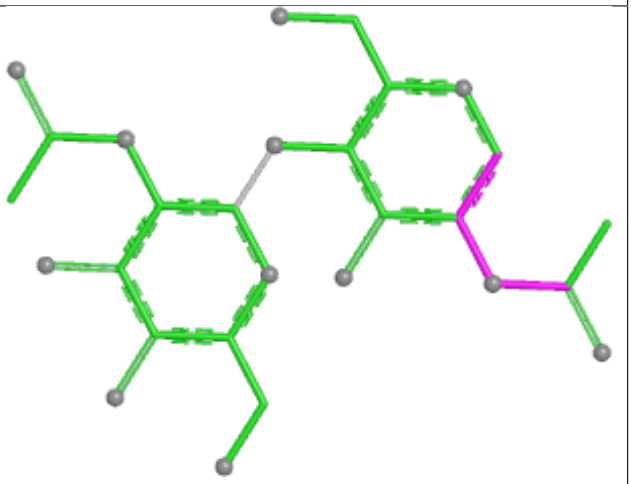


Rings

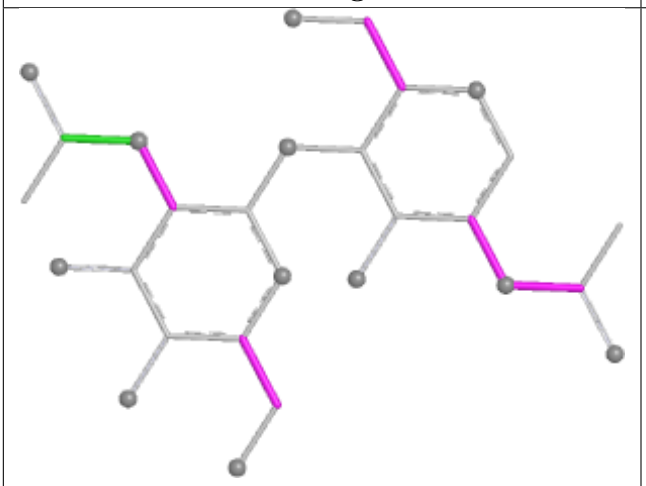
Oligosaccharide Chain M



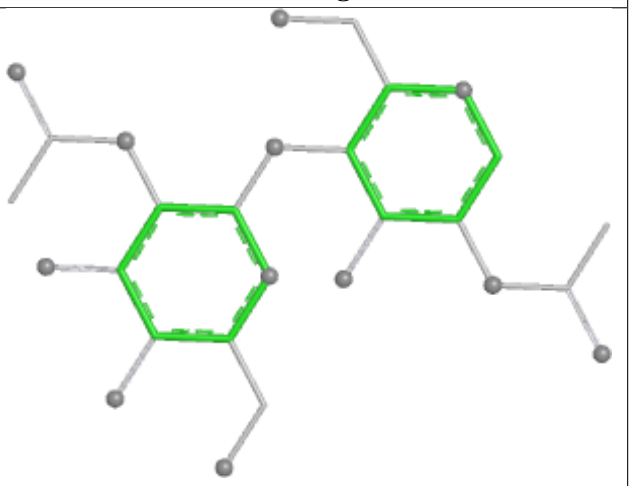
Bond lengths



Bond angles

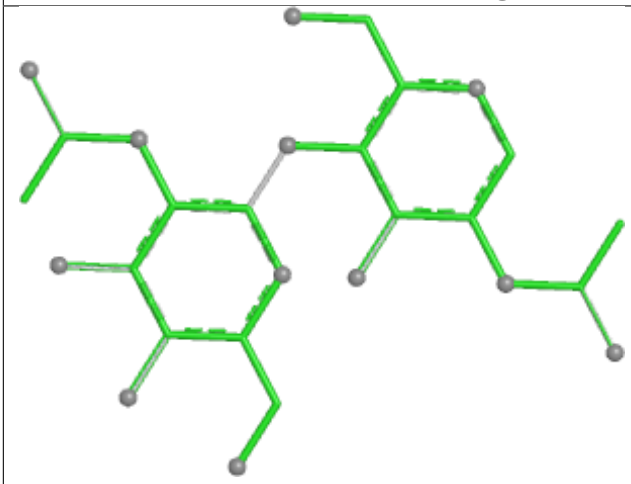


Torsions

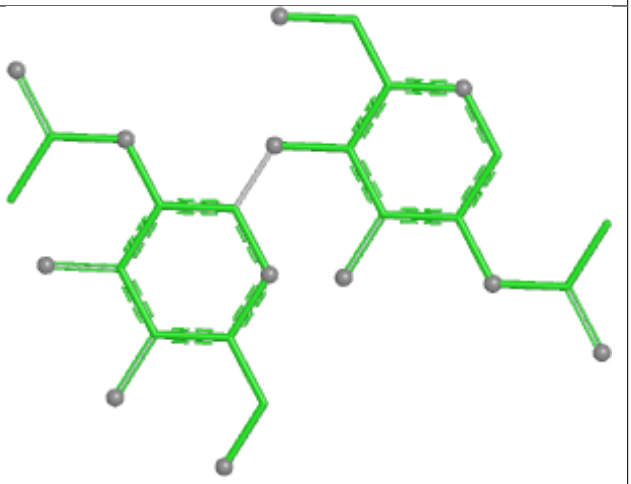


Rings

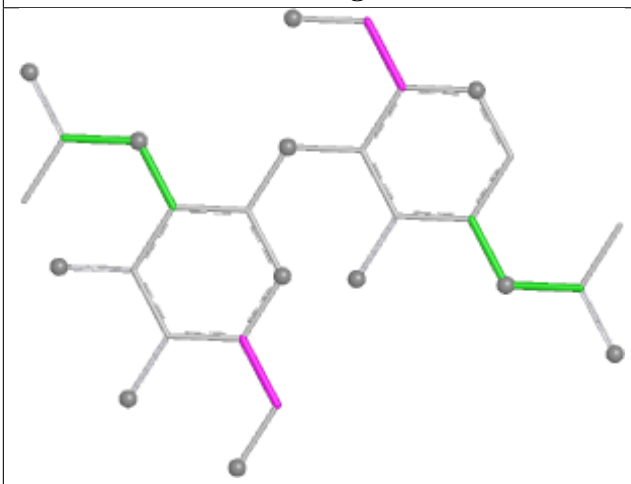
Oligosaccharide Chain N



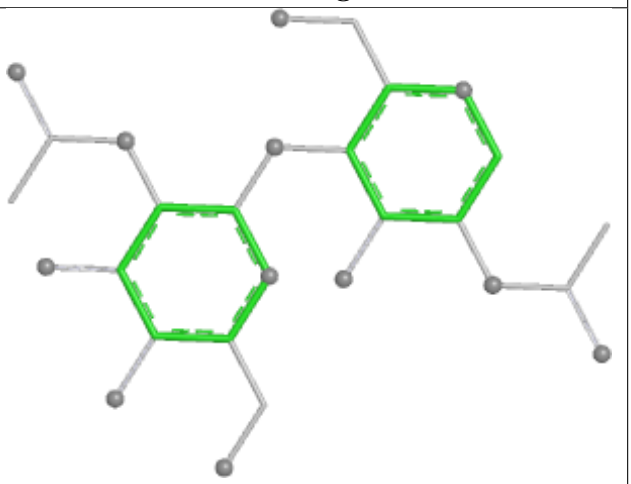
Bond lengths



Bond angles

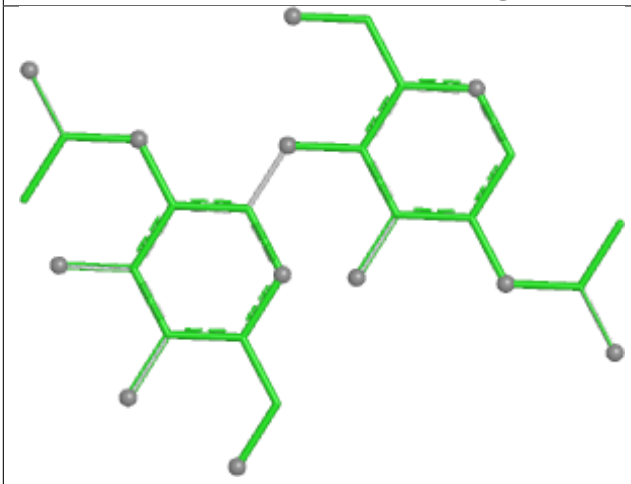


Torsions

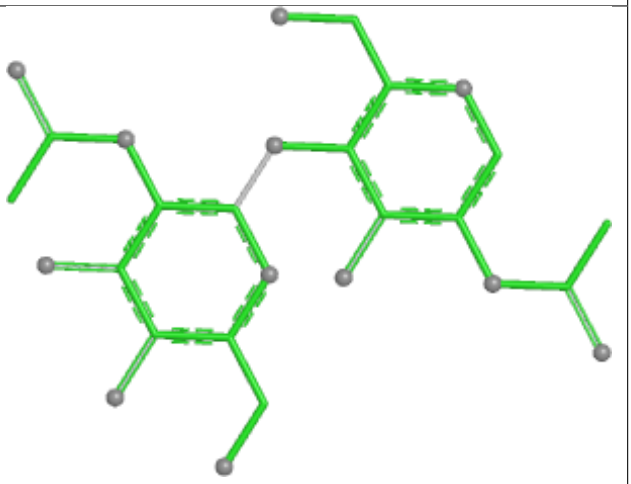


Rings

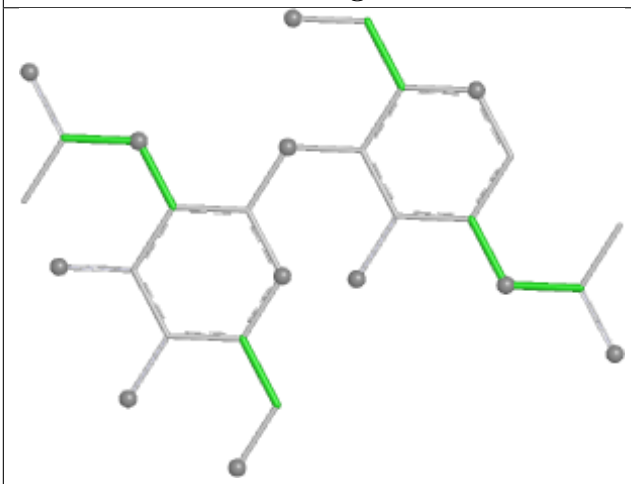
Oligosaccharide Chain O



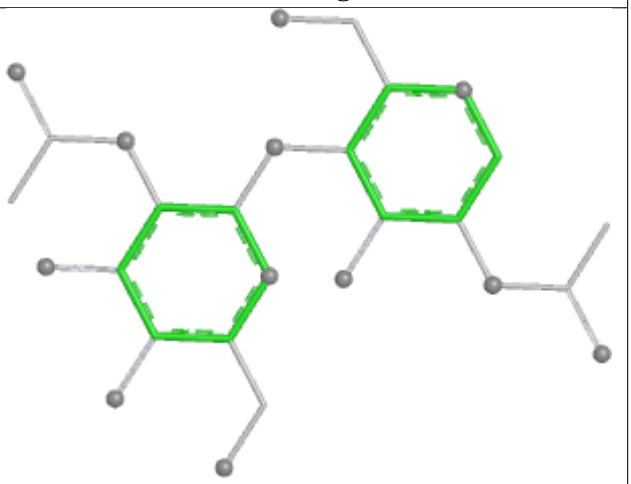
Bond lengths



Bond angles

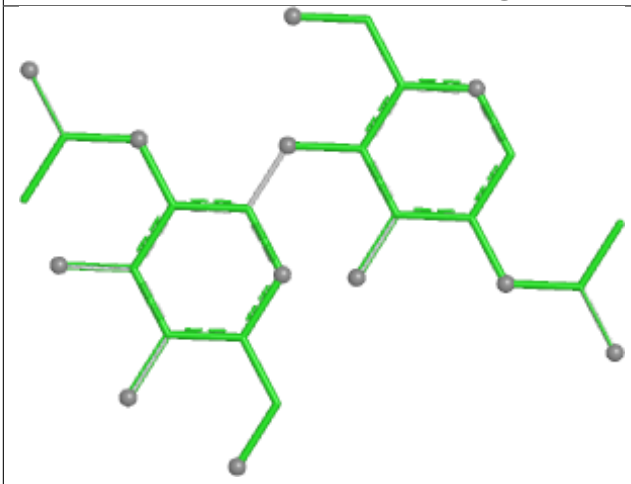


Torsions

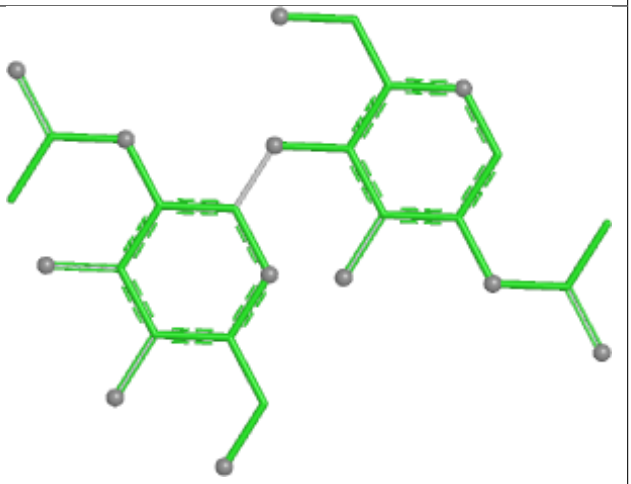


Rings

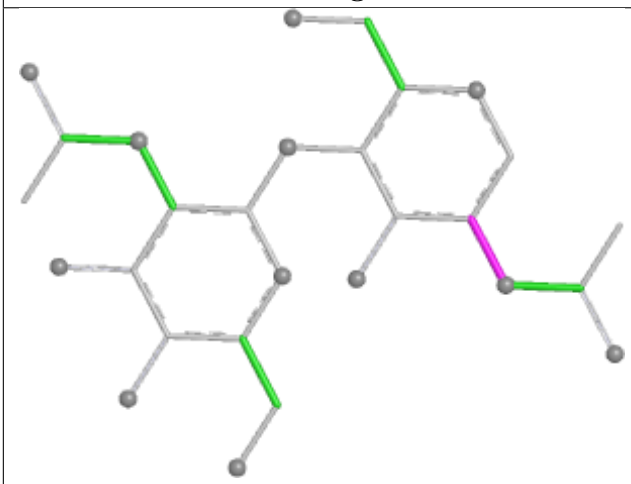
Oligosaccharide Chain P



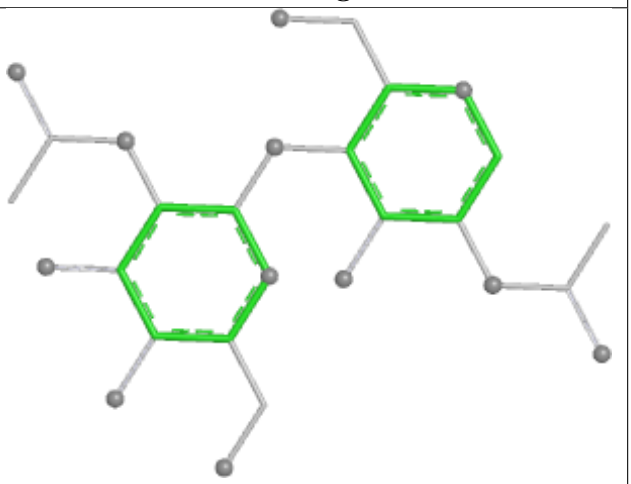
Bond lengths



Bond angles

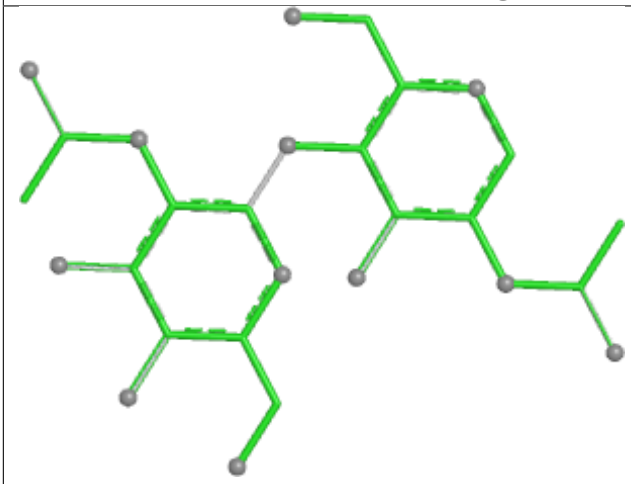


Torsions

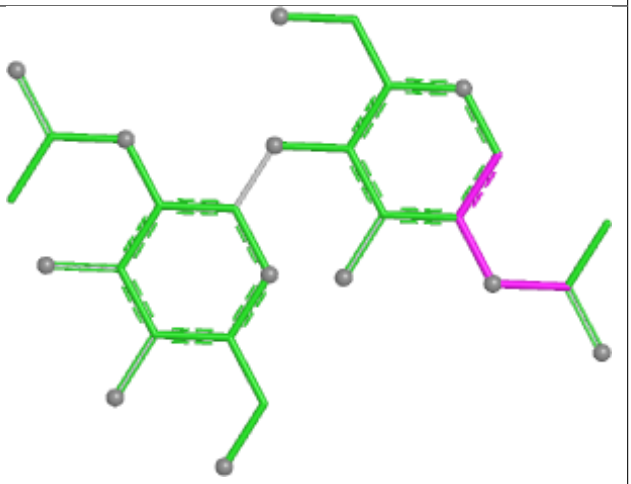


Rings

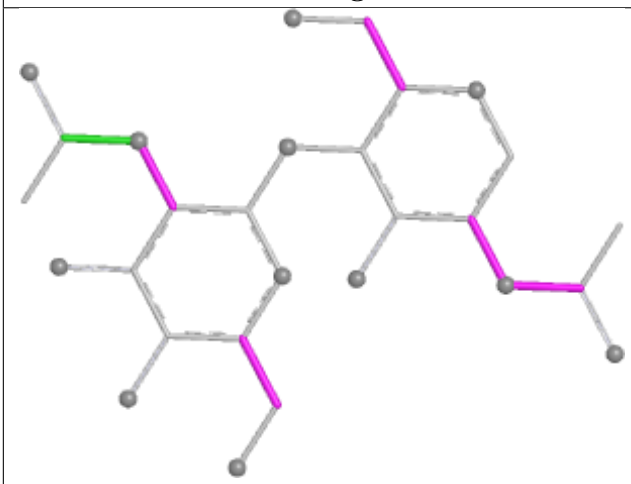
Oligosaccharide Chain R



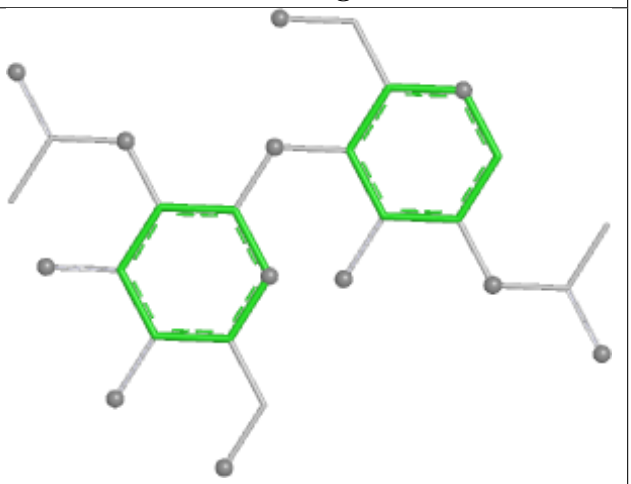
Bond lengths



Bond angles

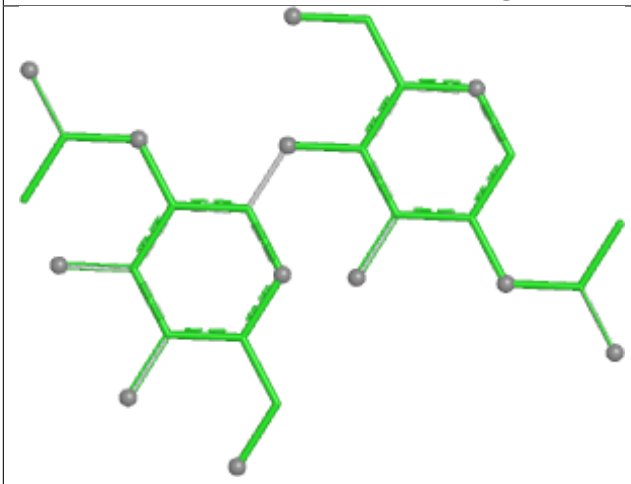


Torsions

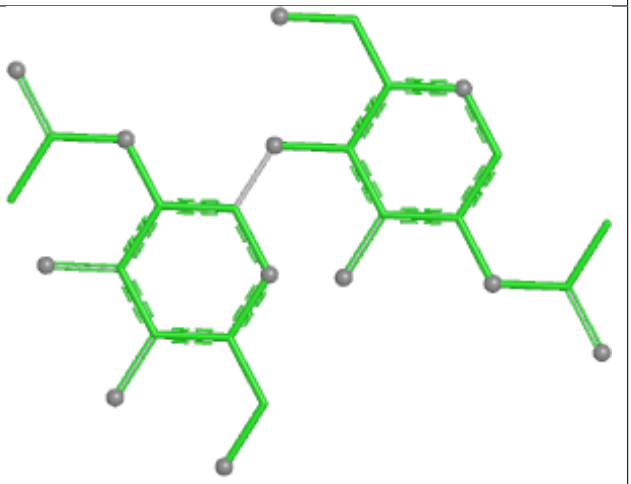


Rings

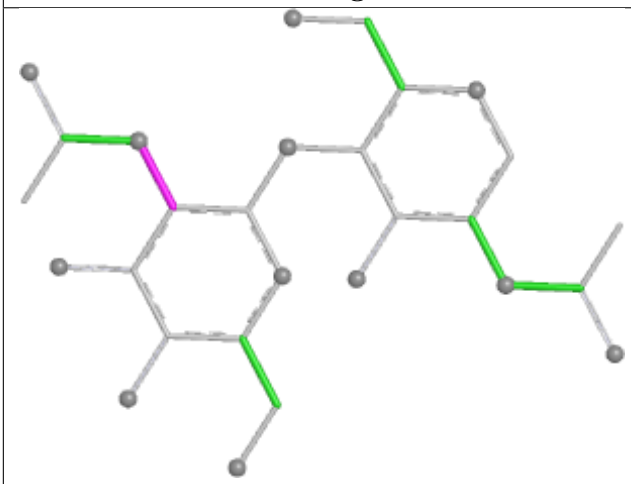
Oligosaccharide Chain S



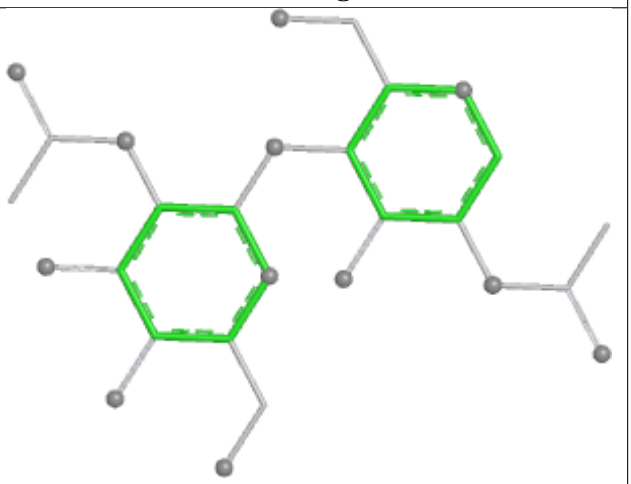
Bond lengths



Bond angles

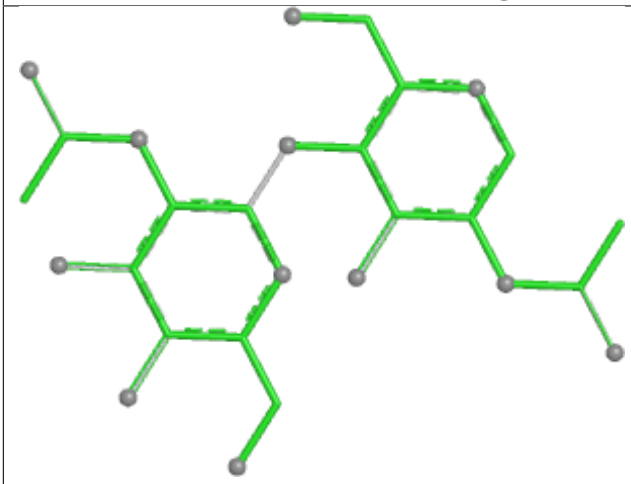


Torsions



Rings

Oligosaccharide Chain T



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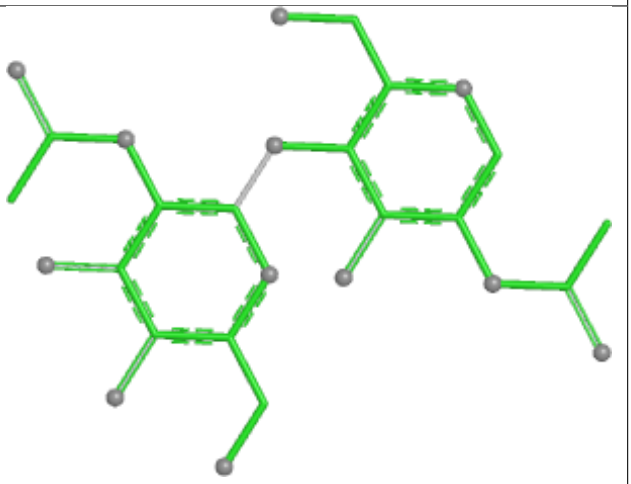
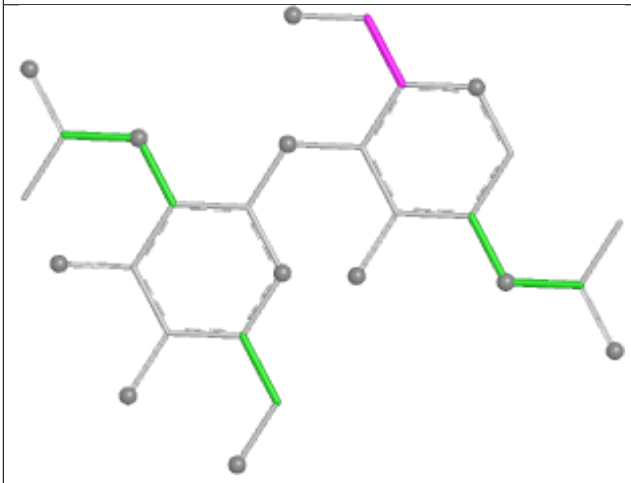
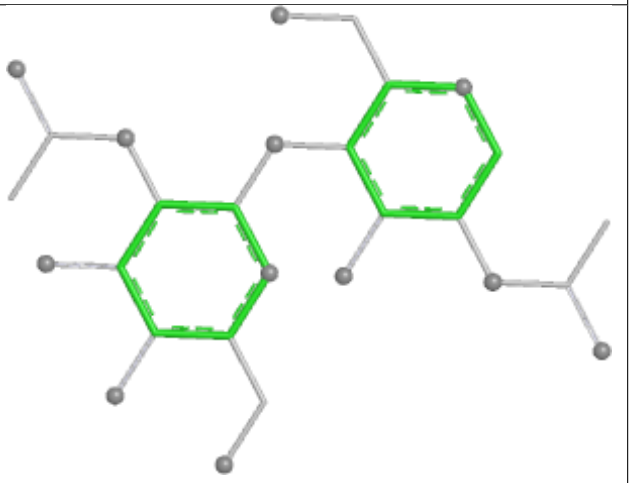


Bond angles

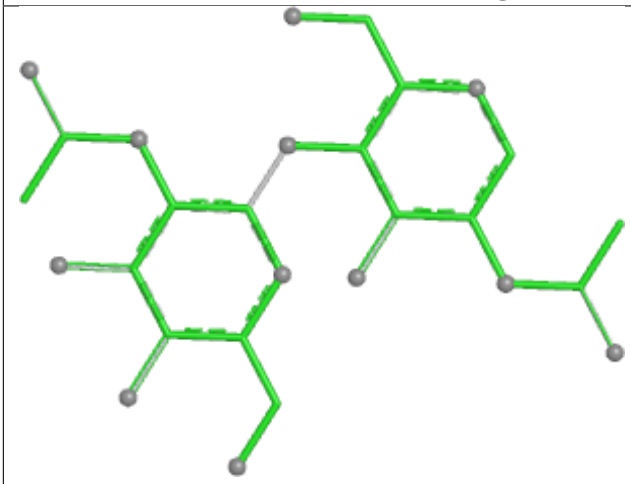


Torsions



Rings

Oligosaccharide Chain U



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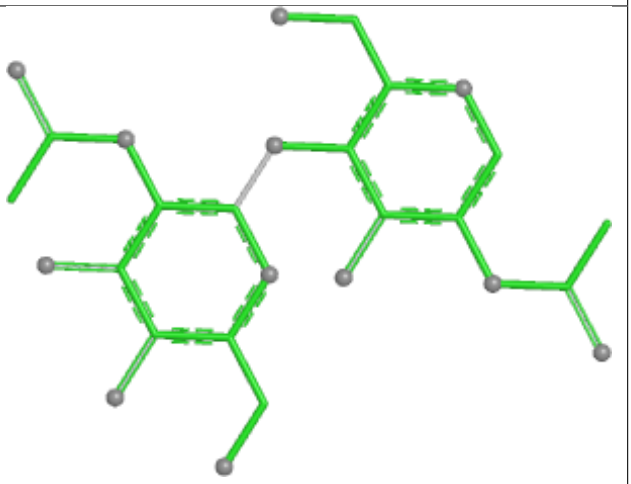
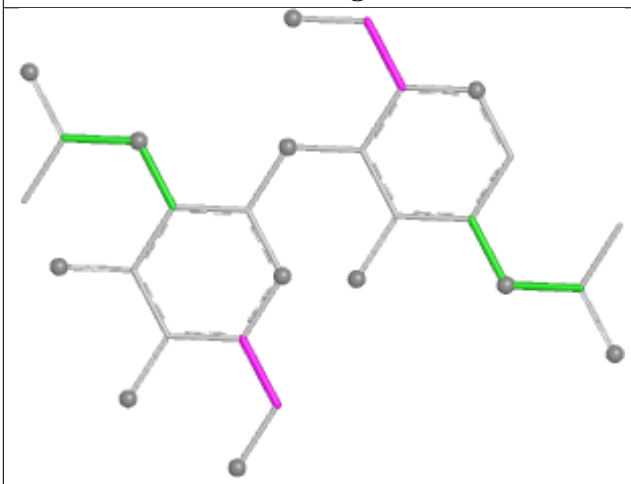


Bond angles



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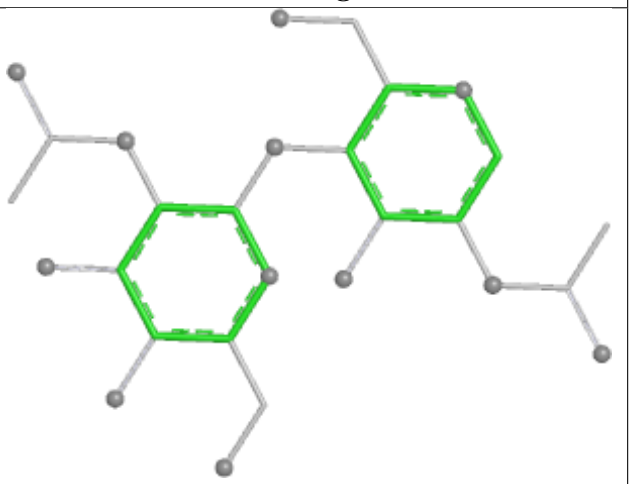
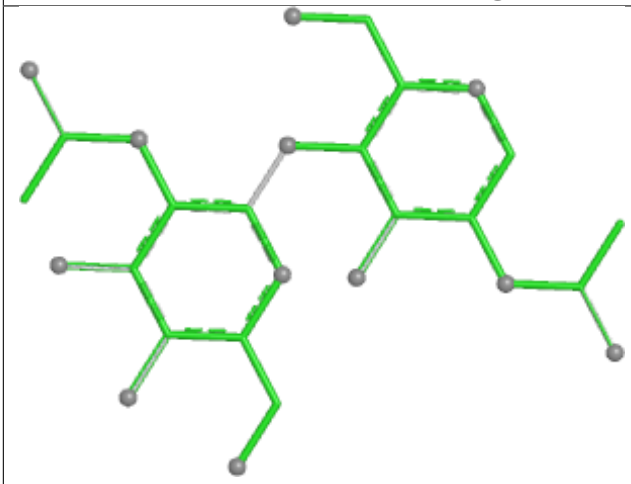


Rings

Oligosaccharide Chain W



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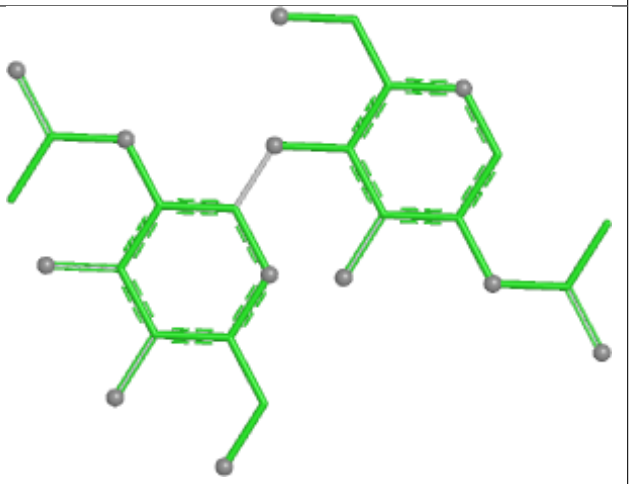
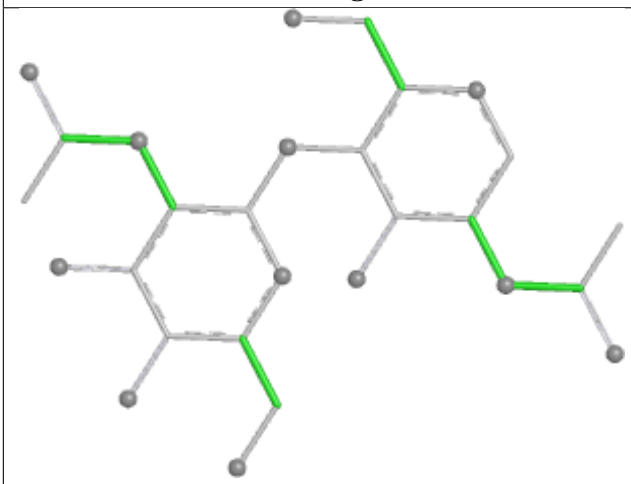


Bond angles



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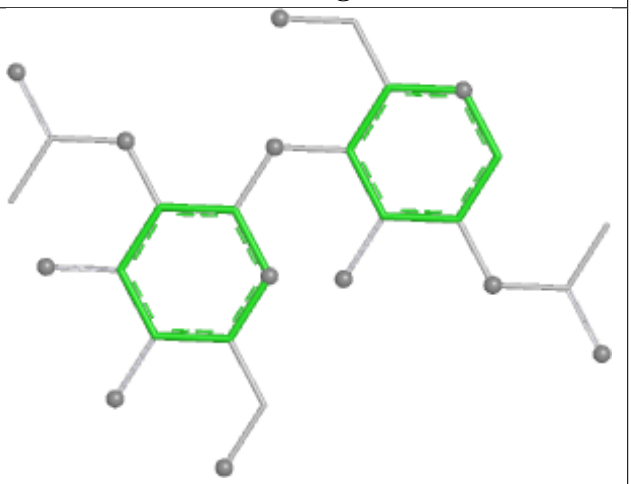
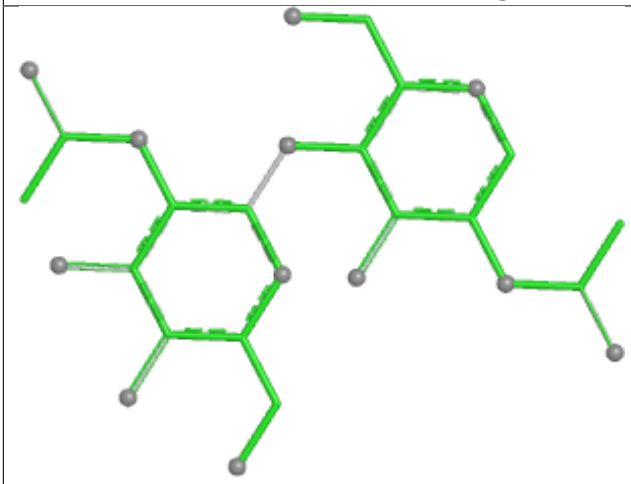


Rings

Oligosaccharide Chain Y



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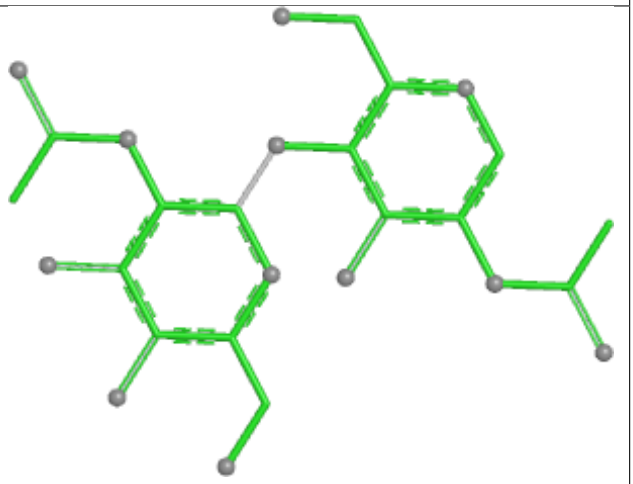
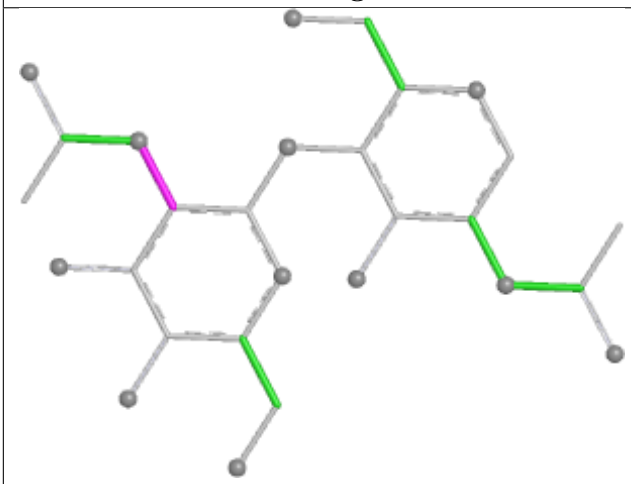


Bond angles



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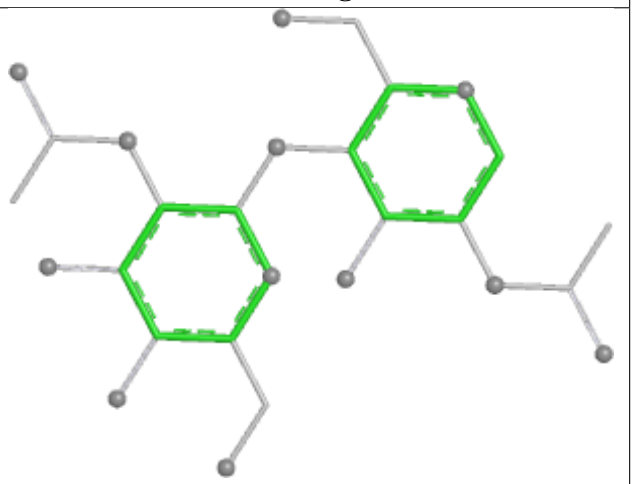
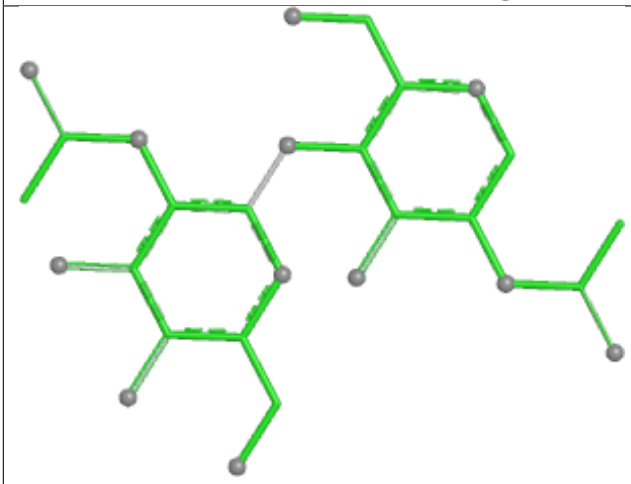


Rings

Oligosaccharide Chain Z



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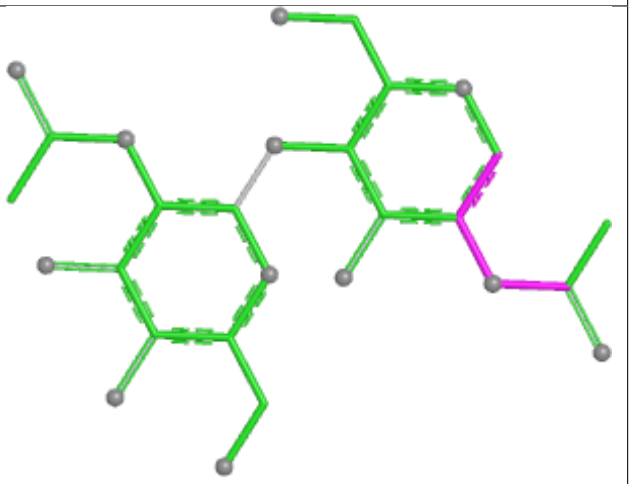
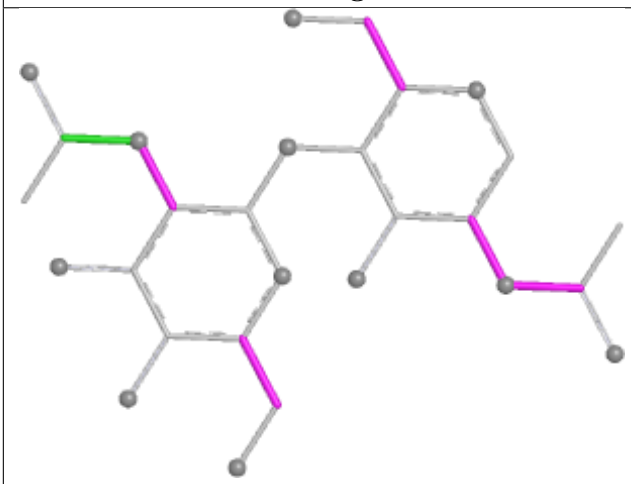


Bond angles



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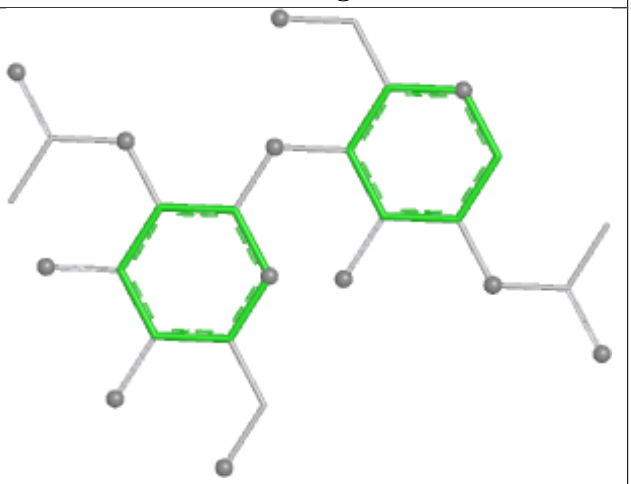
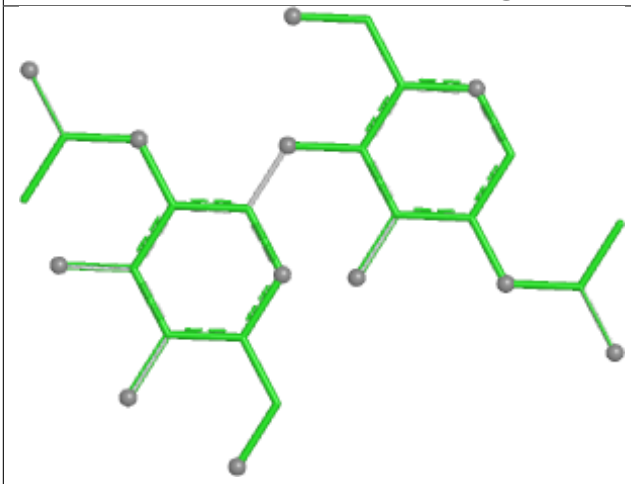


Rings

Oligosaccharide Chain b



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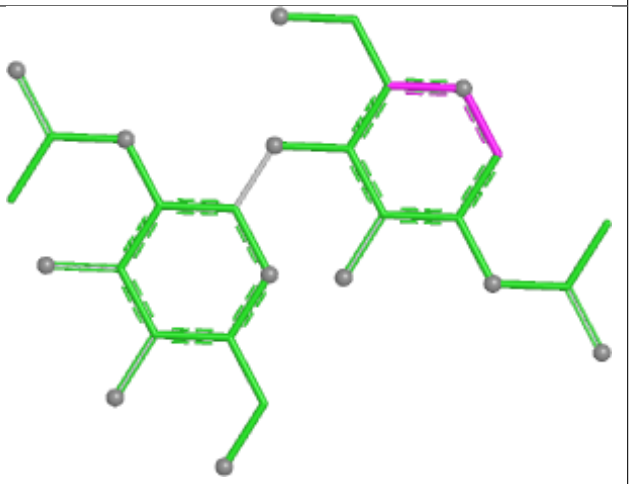
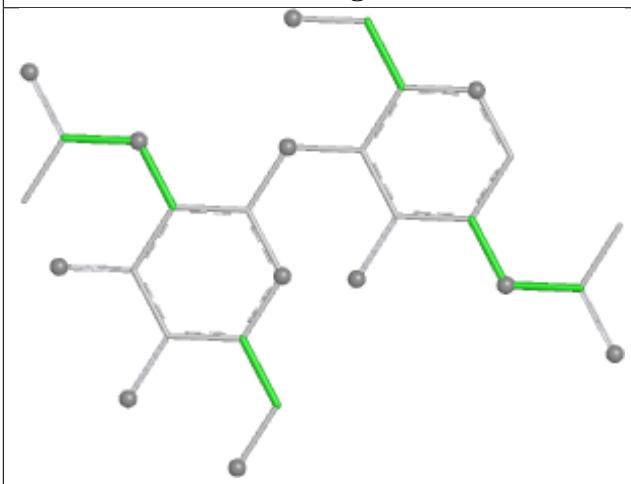


Bond angles



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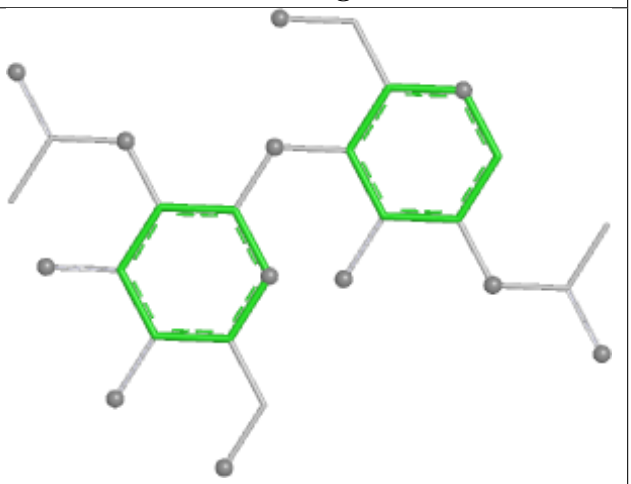
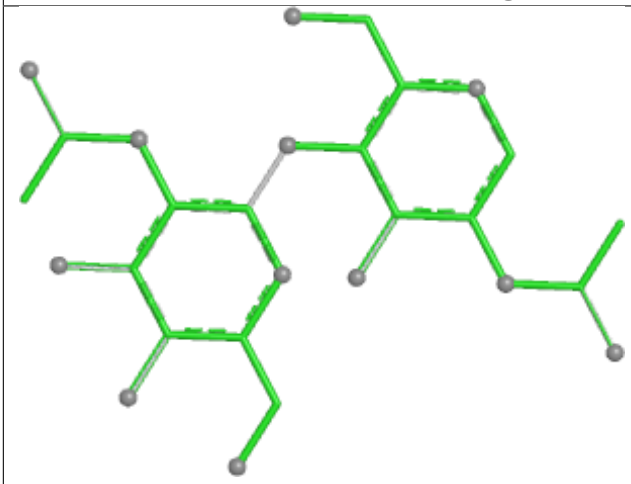


Rings

Oligosaccharide Chain c



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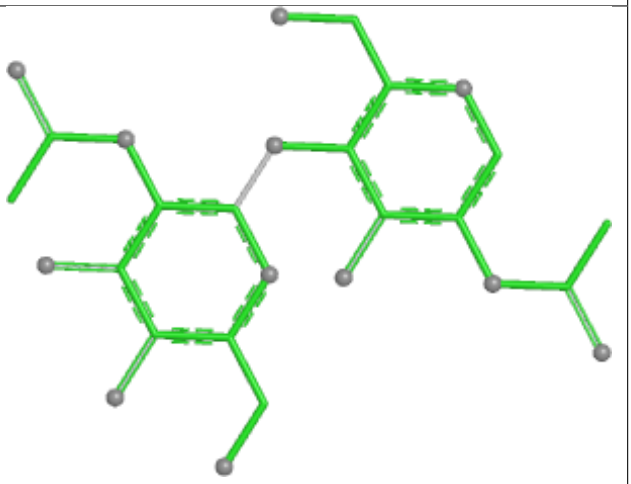
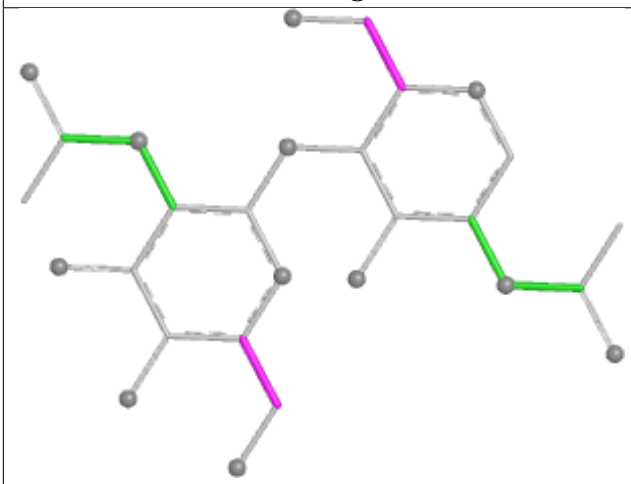


Bond angles



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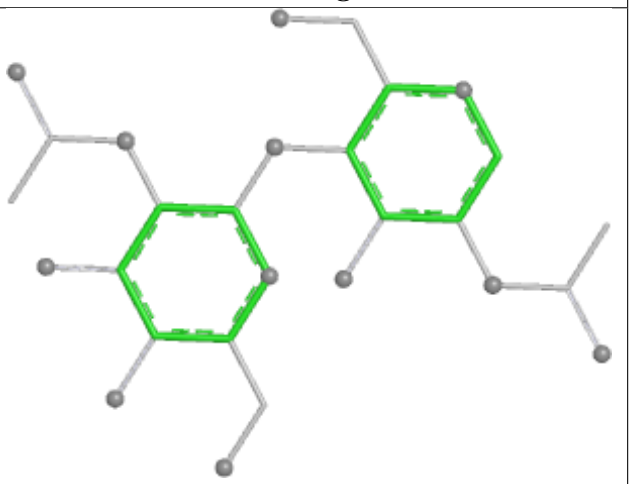
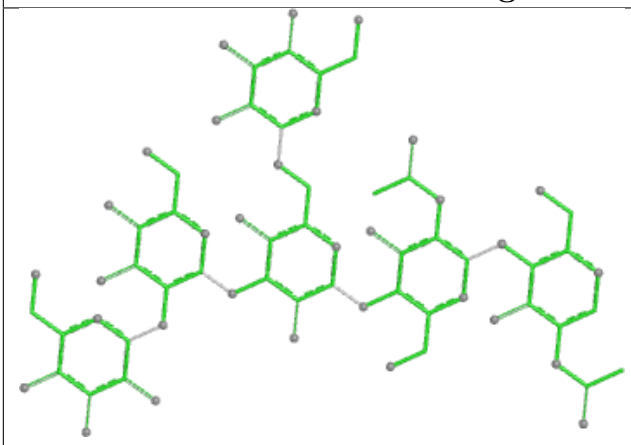


Rings

Oligosaccharide Chain J



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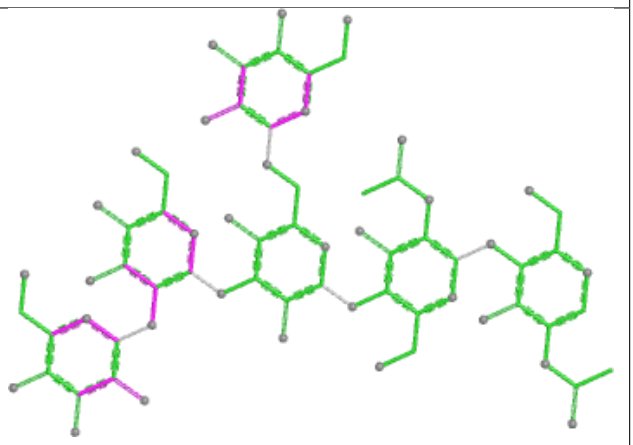
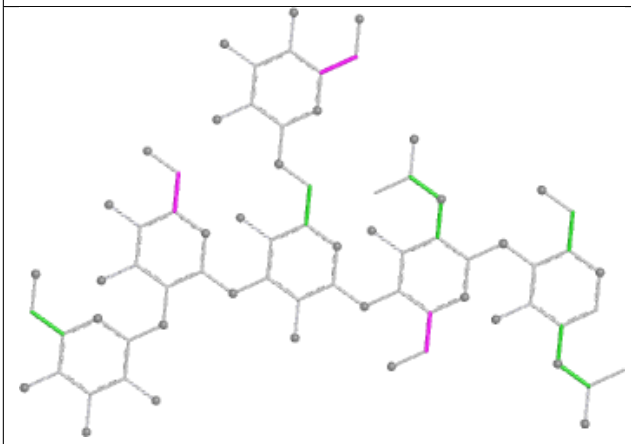


Bond angles



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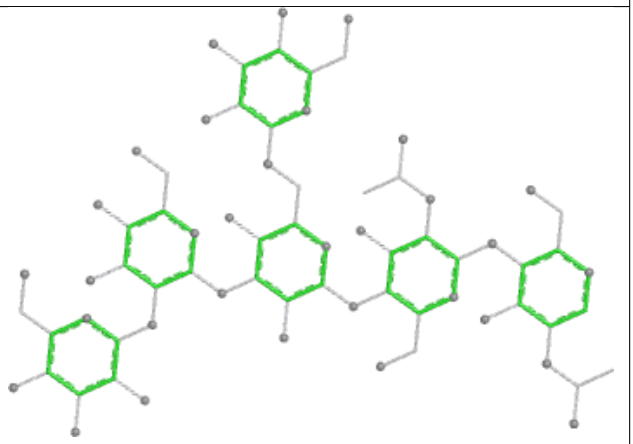
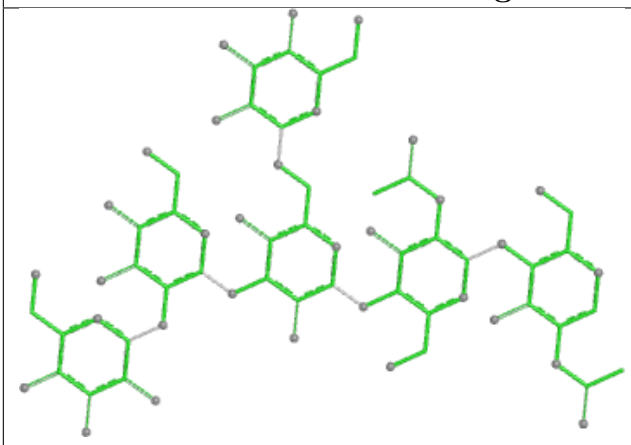


Rings

Oligosaccharide Chain Q



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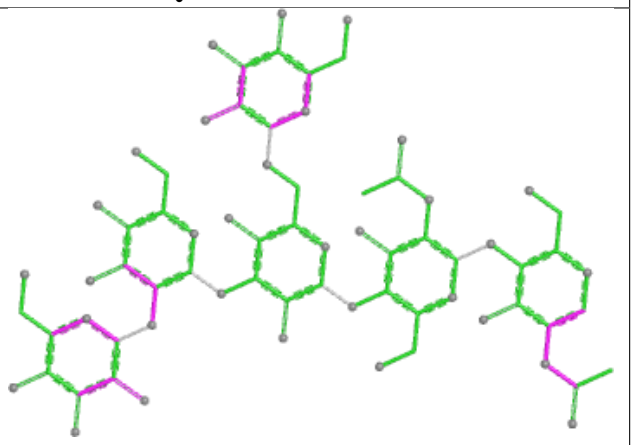
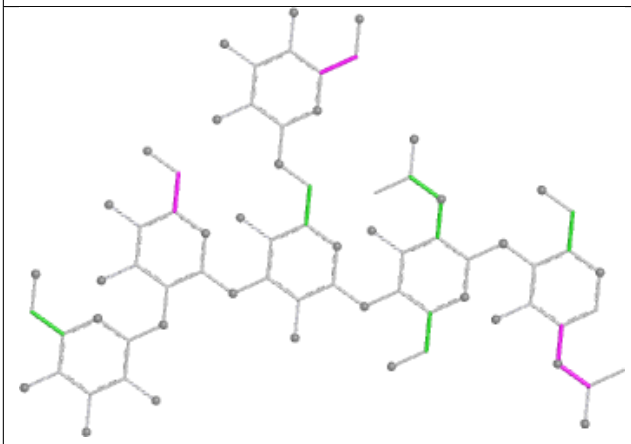


Bond angles



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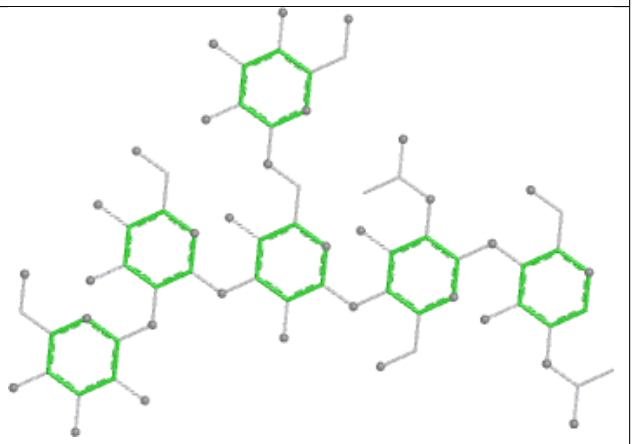
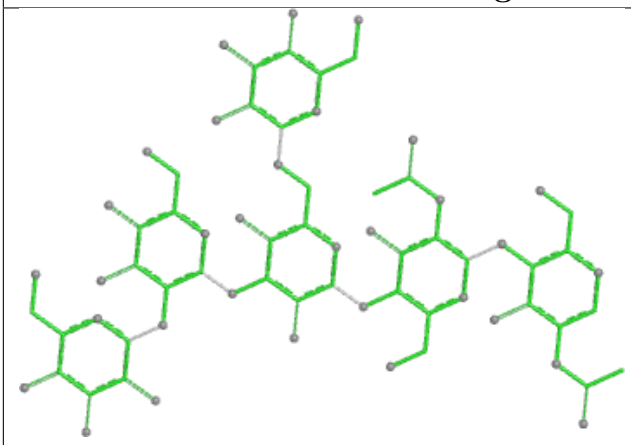


Rings

Oligosaccharide Chain X



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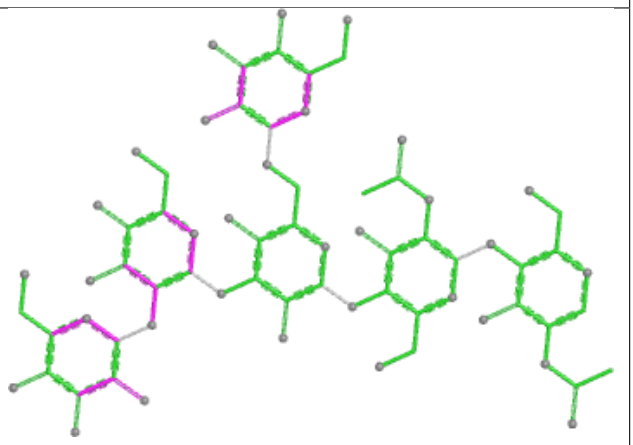
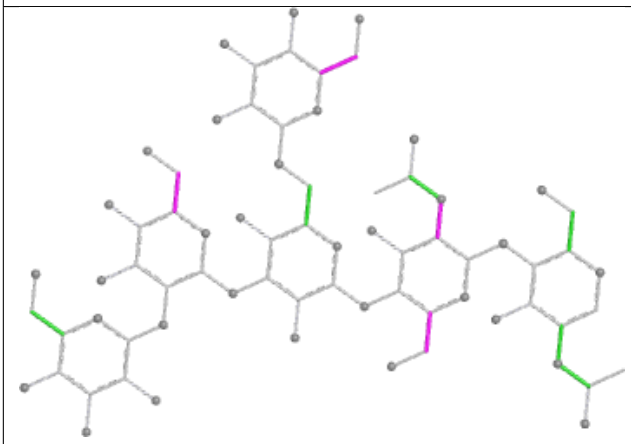


Bond angles



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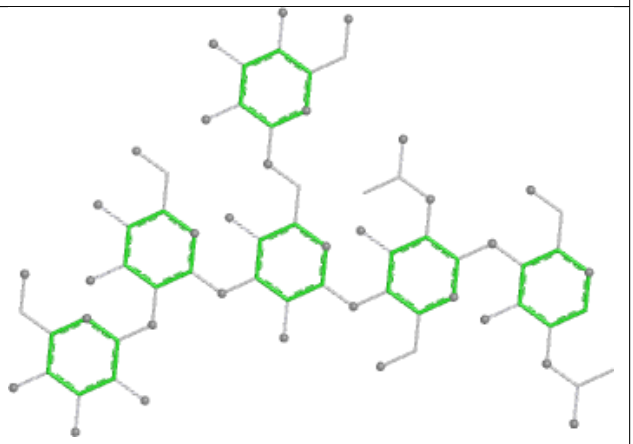
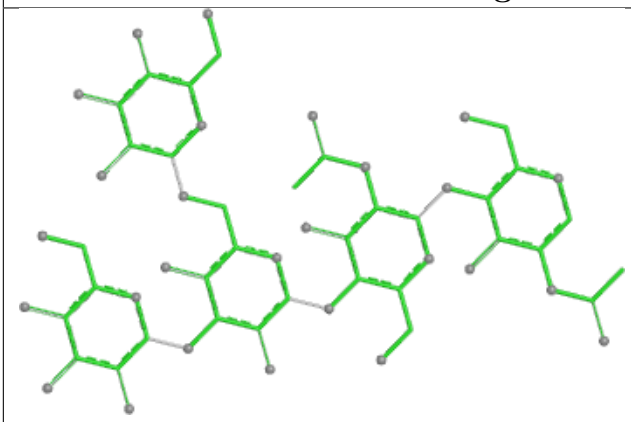


Rings

Oligosaccharide Chain V



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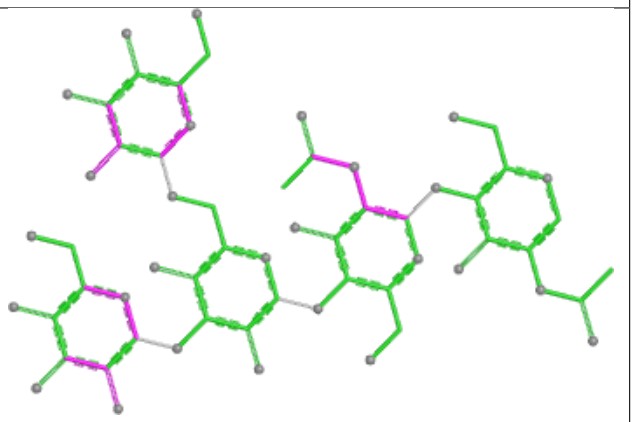
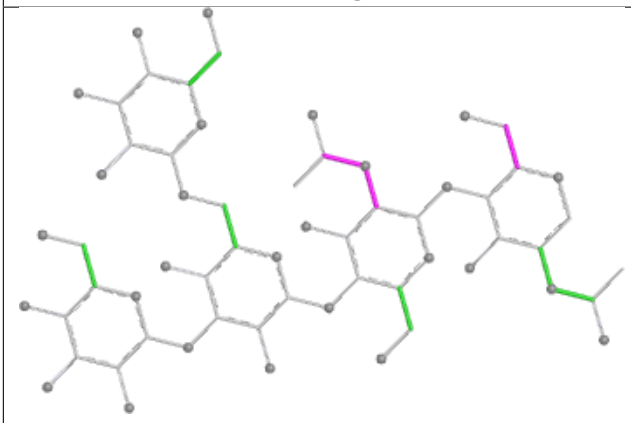


Bond angles



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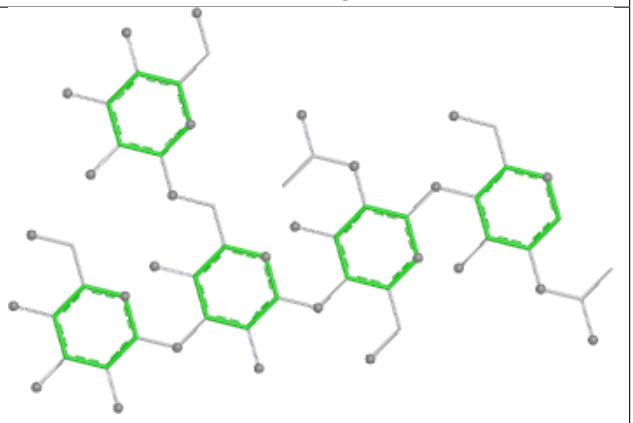
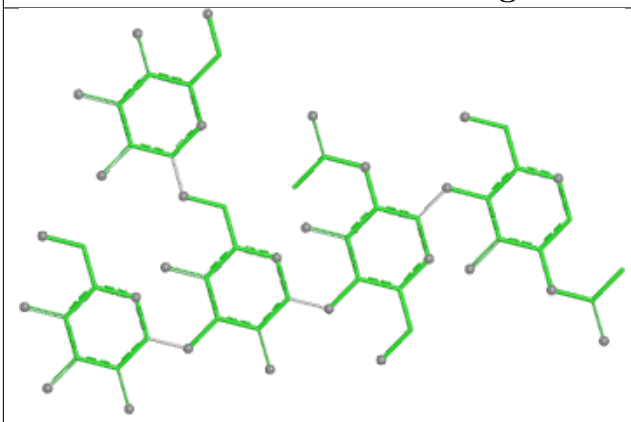


Rings

Oligosaccharide Chain a



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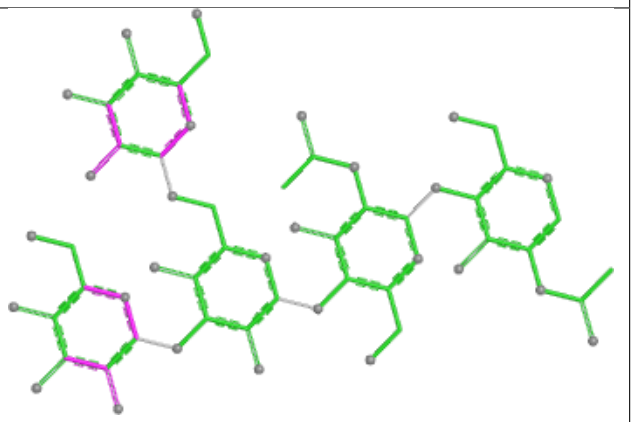
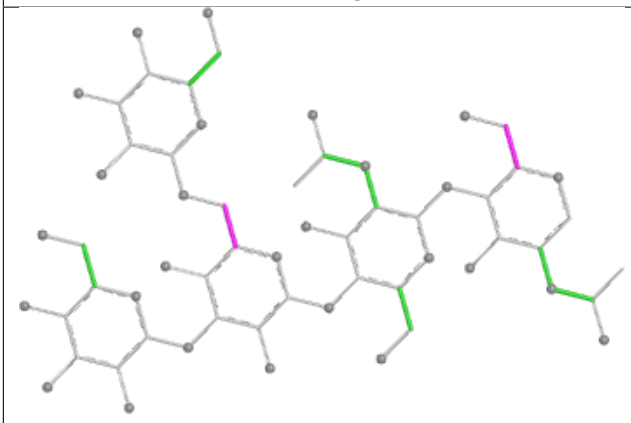
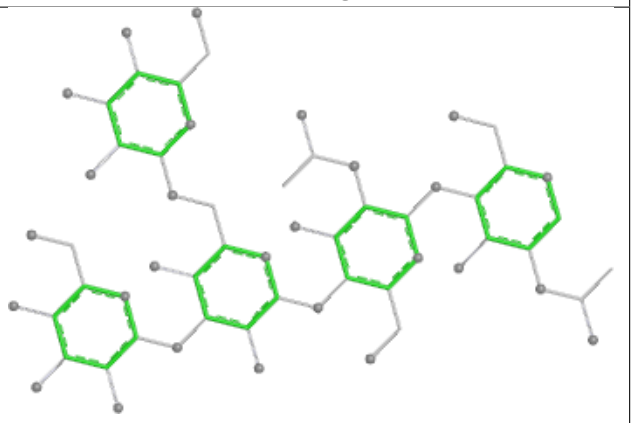


Bond angles

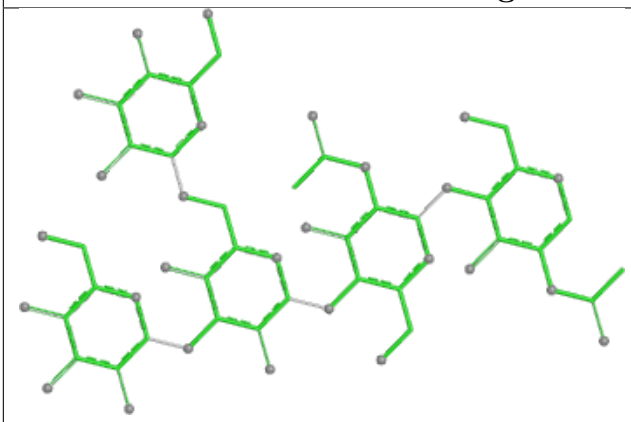


Torsions

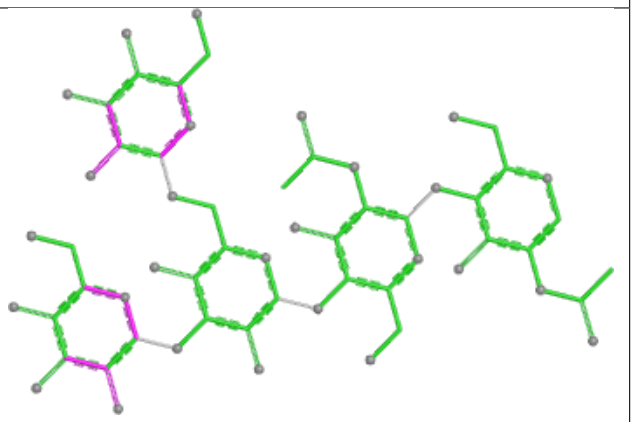


Rings

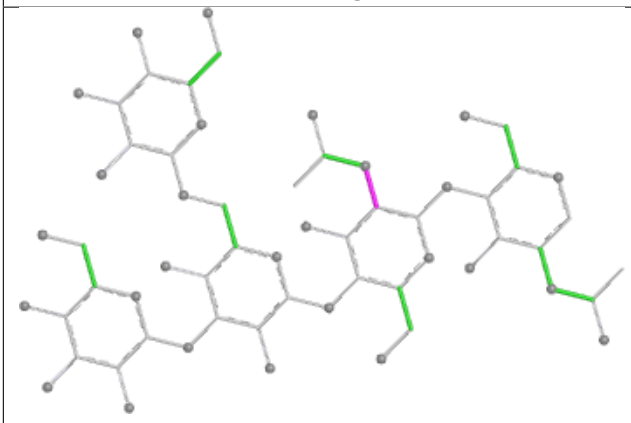
Oligosaccharide Chain d



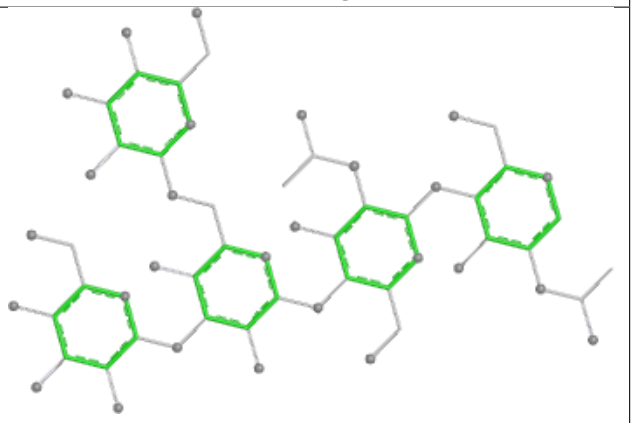
Bond lengths



Bond angles

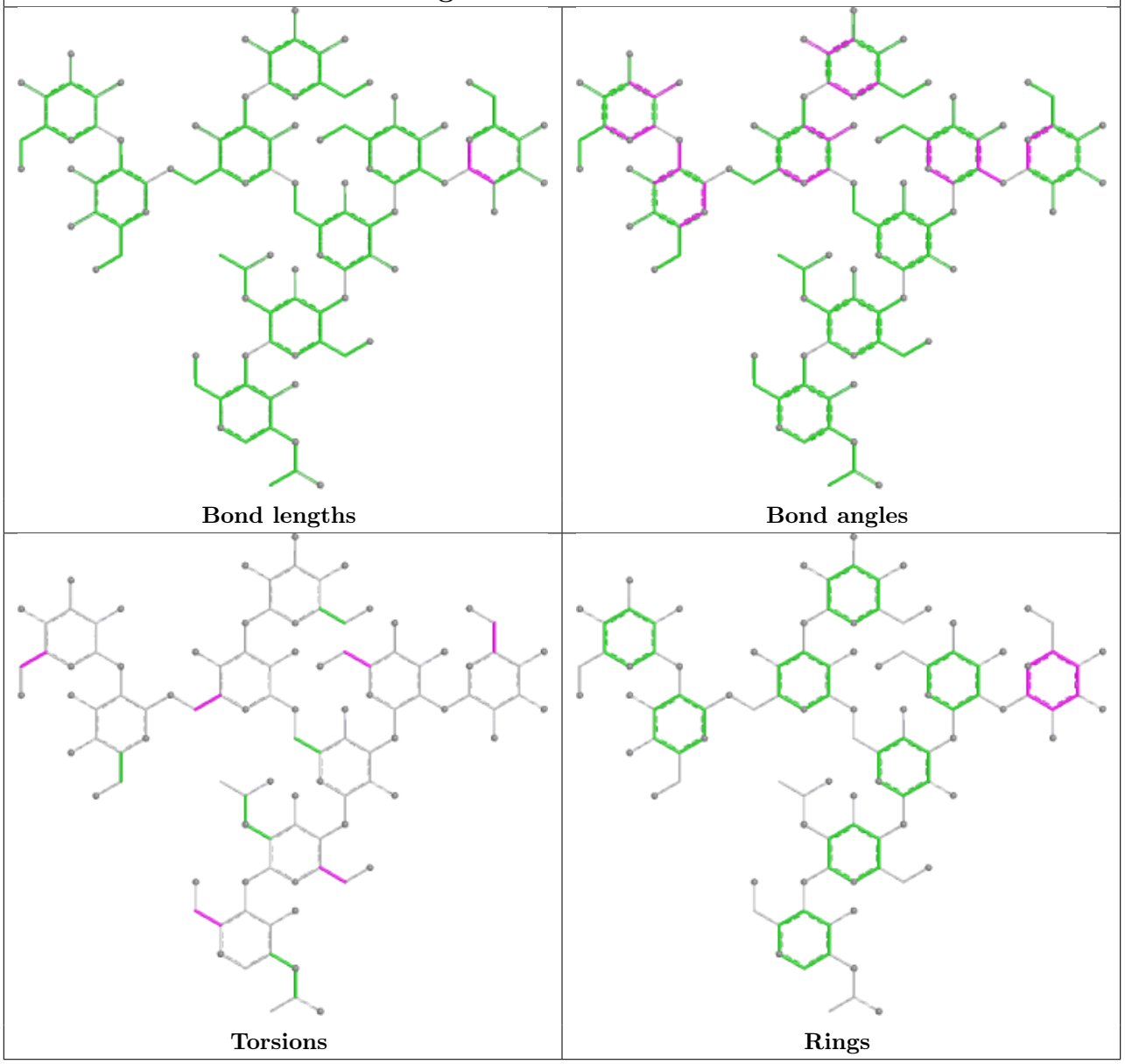


Torsions



Rings

Oligosaccharide Chain e



5.6 Ligand geometry (i)

38 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	$\#\|Z\|>2$
9	NAG	B	702	1	14,14,15	0.23	0	17,19,21	0.43	0
9	NAG	I	603	2	14,14,15	0.30	0	17,19,21	0.40	0
9	NAG	C	607	2	14,14,15	0.26	0	17,19,21	0.43	0
9	NAG	C	610	2	14,14,15	0.18	0	17,19,21	0.44	0
9	NAG	I	607	2	14,14,15	0.23	0	17,19,21	0.43	0
9	NAG	C	604	2	14,14,15	0.22	0	17,19,21	0.46	0
9	NAG	G	608	2	14,14,15	0.27	0	17,19,21	0.41	0
9	NAG	I	604	2	14,14,15	0.22	0	17,19,21	0.47	0
9	NAG	C	602	2	14,14,15	0.21	0	17,19,21	0.44	0
9	NAG	C	603	2	14,14,15	0.23	0	17,19,21	0.45	0
9	NAG	C	605	2	14,14,15	0.21	0	17,19,21	0.44	0
9	NAG	G	601	2	14,14,15	0.22	0	17,19,21	0.49	0
9	NAG	F	701	1	14,14,15	0.23	0	17,19,21	0.40	0
9	NAG	I	609	2	14,14,15	0.23	0	17,19,21	0.49	0
9	NAG	G	611	2	14,14,15	0.21	0	17,19,21	0.47	0
9	NAG	G	606	2	14,14,15	0.17	0	17,19,21	0.47	0
9	NAG	G	610	2	14,14,15	0.22	0	17,19,21	0.40	0
9	NAG	C	601	2	14,14,15	0.22	0	17,19,21	0.47	0
9	NAG	A	703	1	14,14,15	0.22	0	17,19,21	0.42	0
9	NAG	G	603	2	14,14,15	0.21	0	17,19,21	0.44	0
9	NAG	C	609	2	14,14,15	0.18	0	17,19,21	0.42	0
9	NAG	I	605	2	14,14,15	0.17	0	17,19,21	0.48	0
9	NAG	C	608	2	14,14,15	0.21	0	17,19,21	0.43	0
9	NAG	C	611	2	14,14,15	0.22	0	17,19,21	0.48	0
9	NAG	B	701	1	14,14,15	0.20	0	17,19,21	0.44	0
9	NAG	G	602	2	14,14,15	0.21	0	17,19,21	0.44	0
9	NAG	C	606	2	14,14,15	0.19	0	17,19,21	0.45	0
9	NAG	G	604	2	14,14,15	0.24	0	17,19,21	0.45	0
9	NAG	I	606	2	14,14,15	0.24	0	17,19,21	0.47	0
9	NAG	A	701	1	14,14,15	0.24	0	17,19,21	0.46	0
9	NAG	I	602	2	14,14,15	0.22	0	17,19,21	0.46	0
9	NAG	I	608	2	14,14,15	0.20	0	17,19,21	0.42	0
9	NAG	G	609	2	14,14,15	0.18	0	17,19,21	0.41	0
9	NAG	G	607	2	14,14,15	0.24	0	17,19,21	0.44	0
9	NAG	I	601	2	14,14,15	0.21	0	17,19,21	0.48	0
9	NAG	A	702	1	14,14,15	0.21	0	17,19,21	0.44	0
9	NAG	F	702	1	14,14,15	0.24	0	17,19,21	0.44	0
9	NAG	G	605	2	14,14,15	0.20	0	17,19,21	0.44	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	B	702	1	-	0/6/23/26	0/1/1/1
9	NAG	I	603	2	-	1/6/23/26	0/1/1/1
9	NAG	C	607	2	-	2/6/23/26	0/1/1/1
9	NAG	C	610	2	-	2/6/23/26	0/1/1/1
9	NAG	I	607	2	-	1/6/23/26	0/1/1/1
9	NAG	C	604	2	-	2/6/23/26	0/1/1/1
9	NAG	G	608	2	-	1/6/23/26	0/1/1/1
9	NAG	I	604	2	-	0/6/23/26	0/1/1/1
9	NAG	C	602	2	-	0/6/23/26	0/1/1/1
9	NAG	C	603	2	-	2/6/23/26	0/1/1/1
9	NAG	C	605	2	-	0/6/23/26	0/1/1/1
9	NAG	G	601	2	-	3/6/23/26	0/1/1/1
9	NAG	F	701	1	-	3/6/23/26	0/1/1/1
9	NAG	I	609	2	-	2/6/23/26	0/1/1/1
9	NAG	G	611	2	-	3/6/23/26	0/1/1/1
9	NAG	G	606	2	-	3/6/23/26	0/1/1/1
9	NAG	G	610	2	-	0/6/23/26	0/1/1/1
9	NAG	C	601	2	-	3/6/23/26	0/1/1/1
9	NAG	A	703	1	-	0/6/23/26	0/1/1/1
9	NAG	G	603	2	-	0/6/23/26	0/1/1/1
9	NAG	C	609	2	-	2/6/23/26	0/1/1/1
9	NAG	I	605	2	-	4/6/23/26	0/1/1/1
9	NAG	C	608	2	-	1/6/23/26	0/1/1/1
9	NAG	C	611	2	-	2/6/23/26	0/1/1/1
9	NAG	B	701	1	-	0/6/23/26	0/1/1/1
9	NAG	G	602	2	-	0/6/23/26	0/1/1/1
9	NAG	C	606	2	-	3/6/23/26	0/1/1/1
9	NAG	G	604	2	-	1/6/23/26	0/1/1/1
9	NAG	I	606	2	-	0/6/23/26	0/1/1/1
9	NAG	A	701	1	-	0/6/23/26	0/1/1/1
9	NAG	I	602	2	-	2/6/23/26	0/1/1/1
9	NAG	I	608	2	-	3/6/23/26	0/1/1/1
9	NAG	G	609	2	-	0/6/23/26	0/1/1/1
9	NAG	G	607	2	-	1/6/23/26	0/1/1/1
9	NAG	I	601	2	-	2/6/23/26	0/1/1/1
9	NAG	A	702	1	-	0/6/23/26	0/1/1/1
9	NAG	F	702	1	-	0/6/23/26	0/1/1/1
9	NAG	G	605	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	610	NAG	O5-C5-C6-O6
9	I	605	NAG	O5-C5-C6-O6
9	C	607	NAG	O5-C5-C6-O6
9	C	610	NAG	C4-C5-C6-O6
9	C	603	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

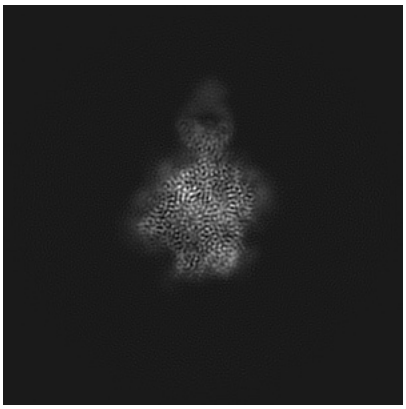
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29248. These allow visual inspection of the internal detail of the map and identification of artifacts.

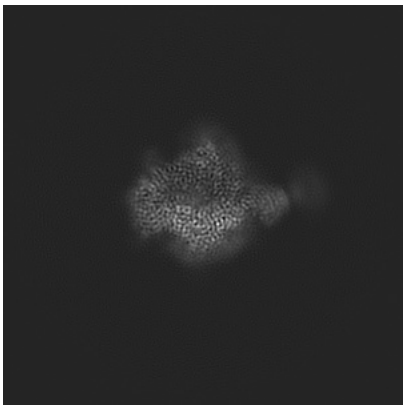
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

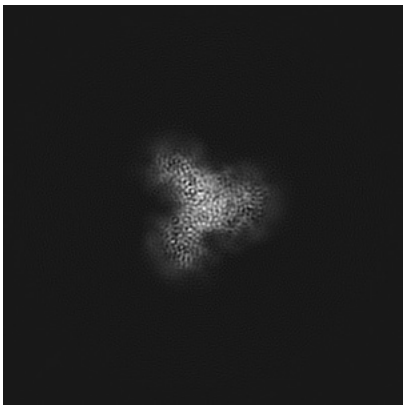
6.1.1 Primary map



X

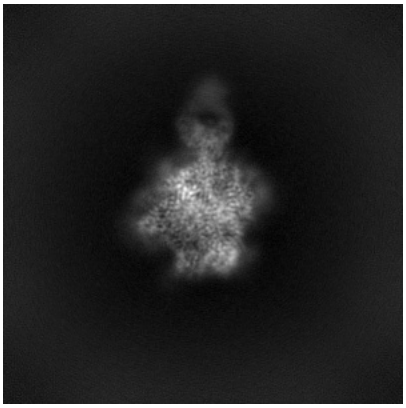


Y

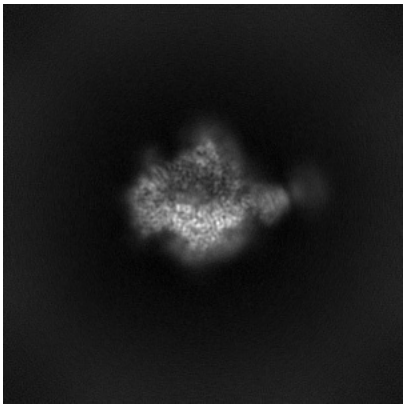


Z

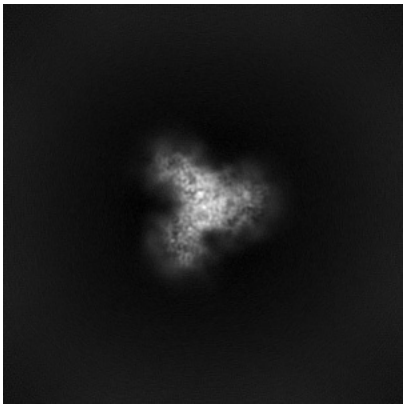
6.1.2 Raw map



X



Y

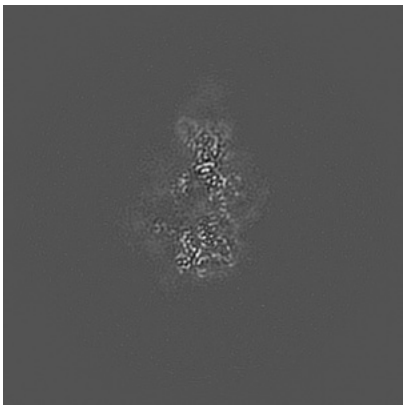


Z

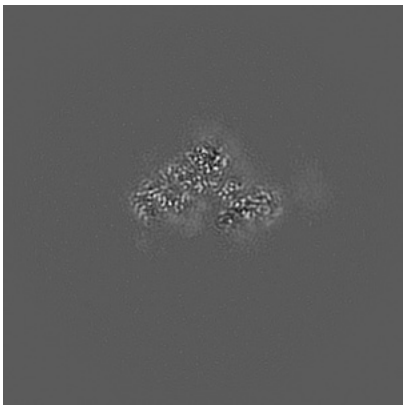
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

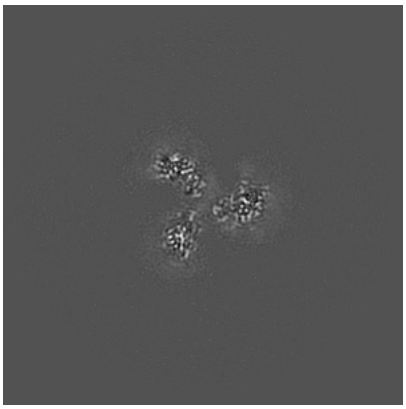
6.2.1 Primary map



X Index: 170

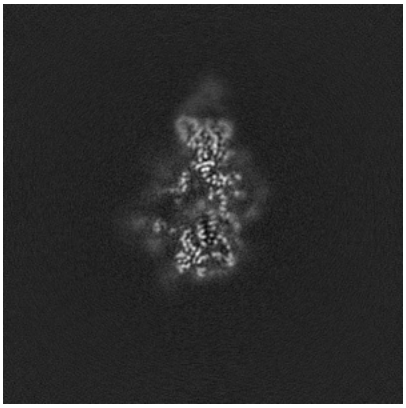


Y Index: 170

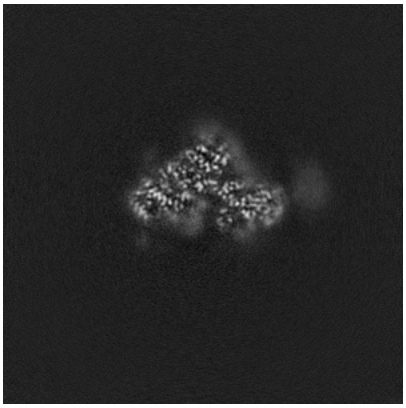


Z Index: 170

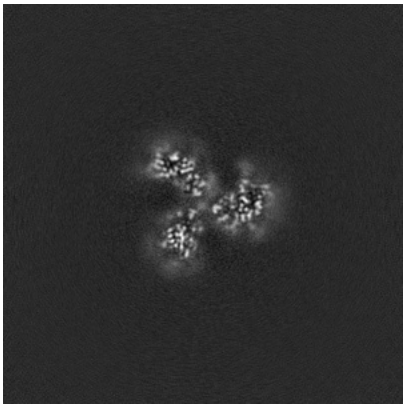
6.2.2 Raw map



X Index: 170



Y Index: 170

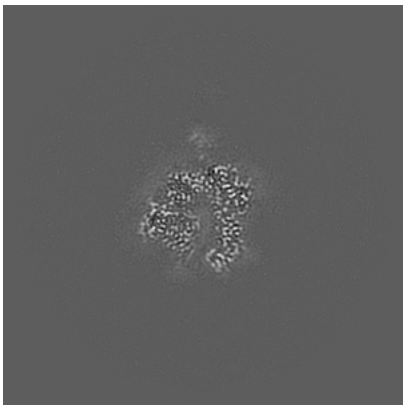


Z Index: 170

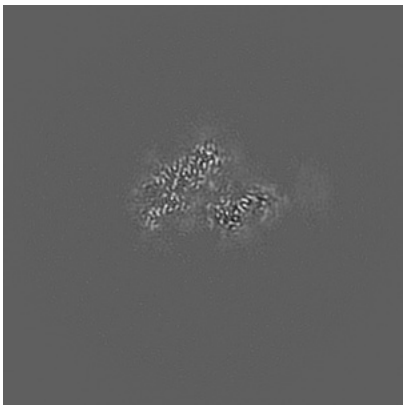
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

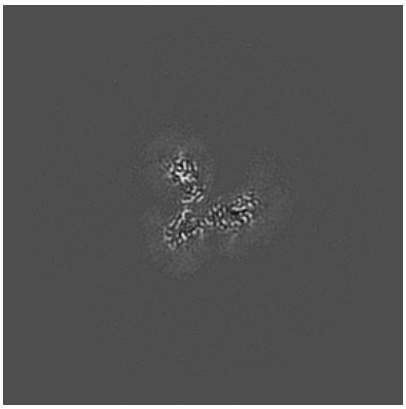
6.3.1 Primary map



X Index: 156

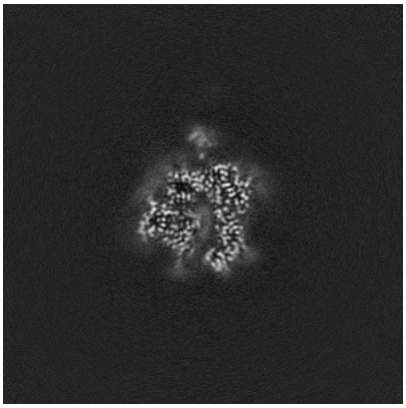


Y Index: 175

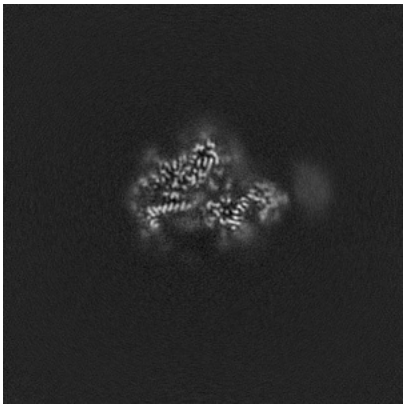


Z Index: 182

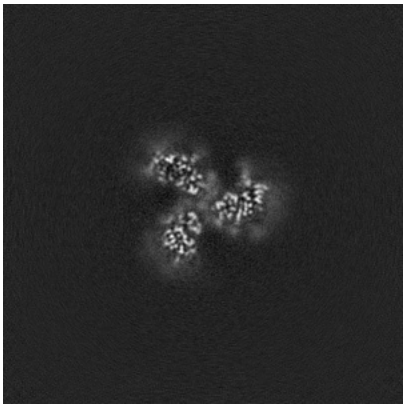
6.3.2 Raw map



X Index: 156



Y Index: 176

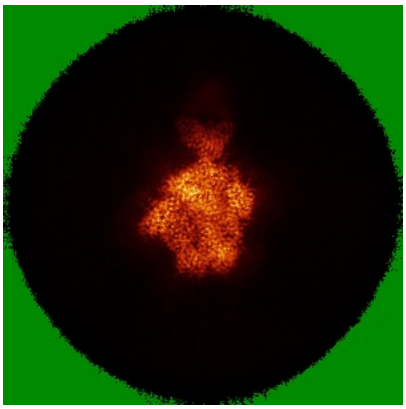


Z Index: 167

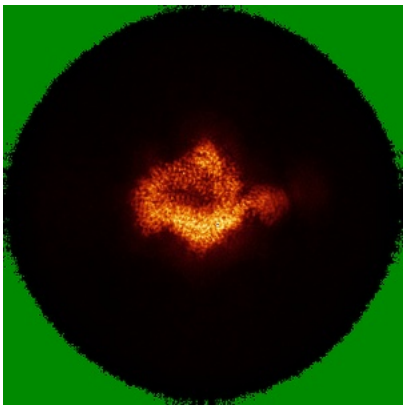
The images above show the largest variance slices of the map in three orthogonal directions.

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

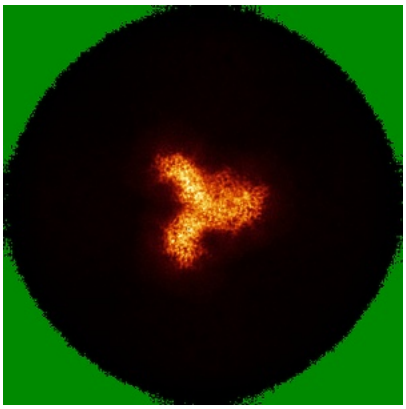
6.4.1 Primary map



X

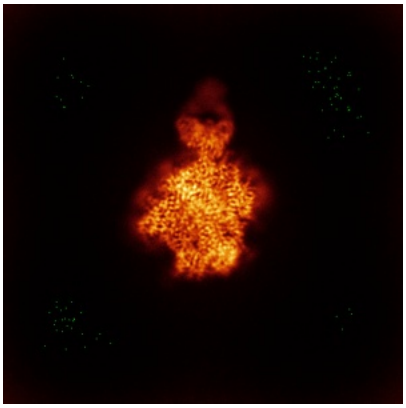


Y

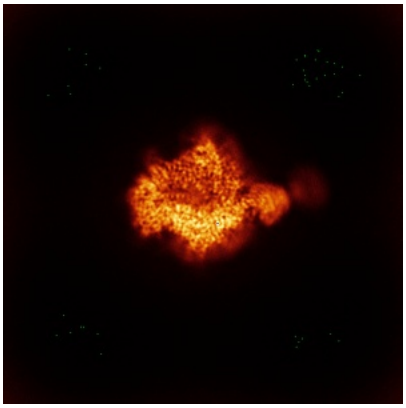


Z

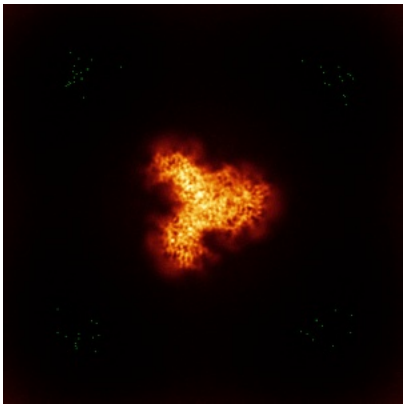
6.4.2 Raw map



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.

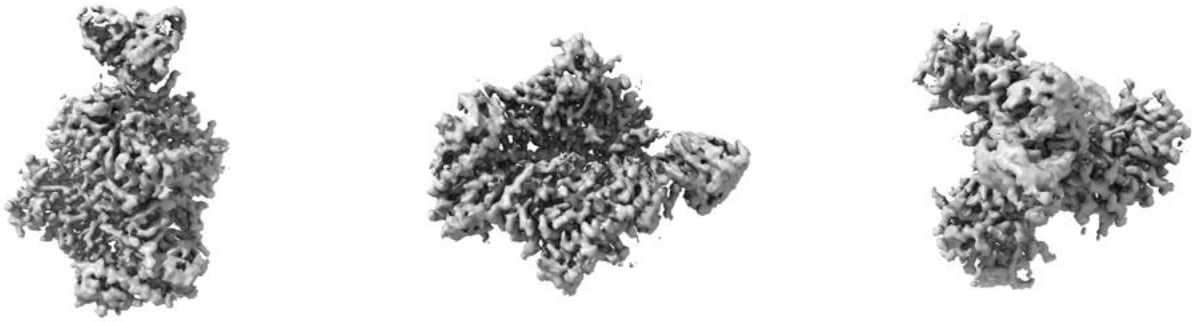
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

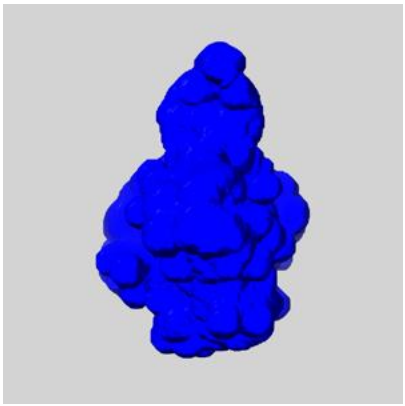
6.6 Mask visualisation

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

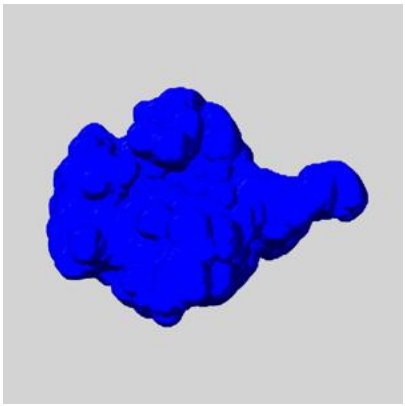
A mask typically either:

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

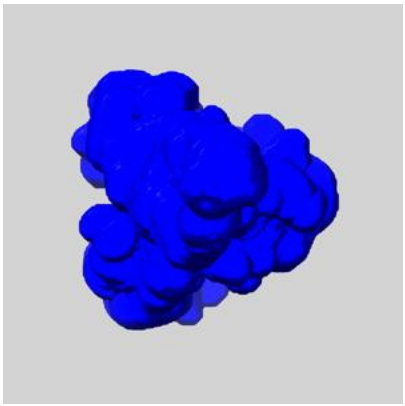
6.6.1 emd_29248_msk_1.map



X



Y

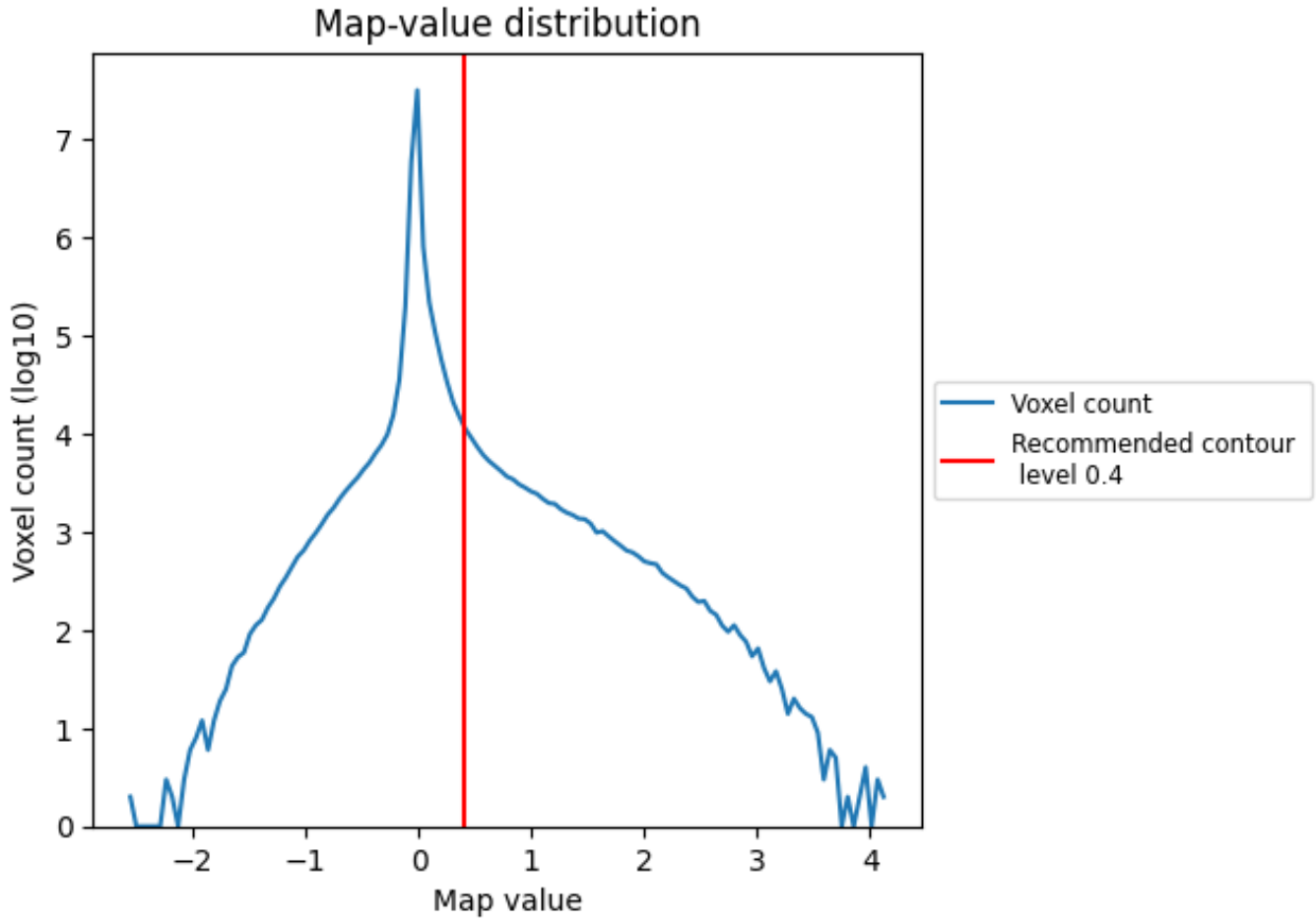


Z

7 Map analysis

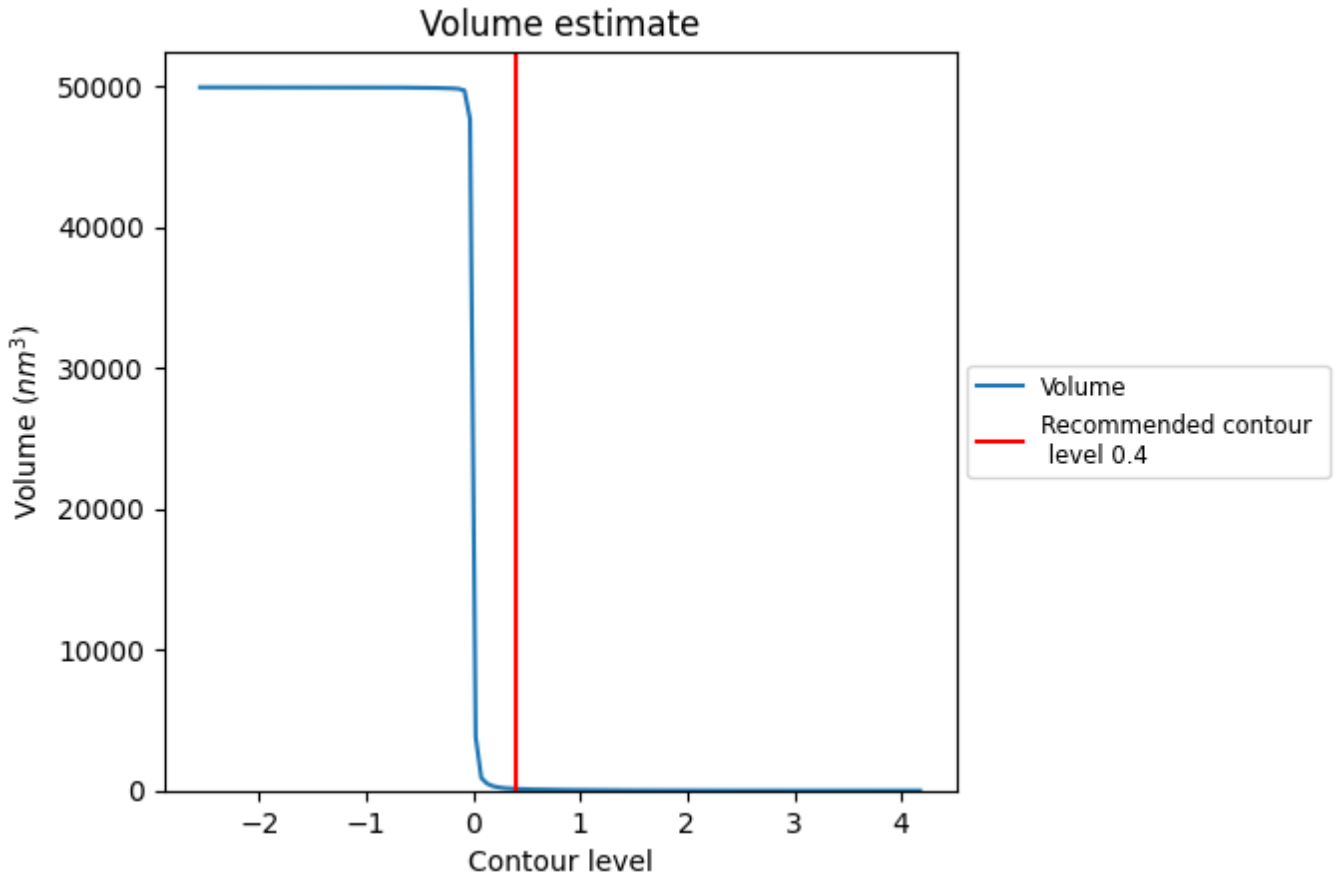
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

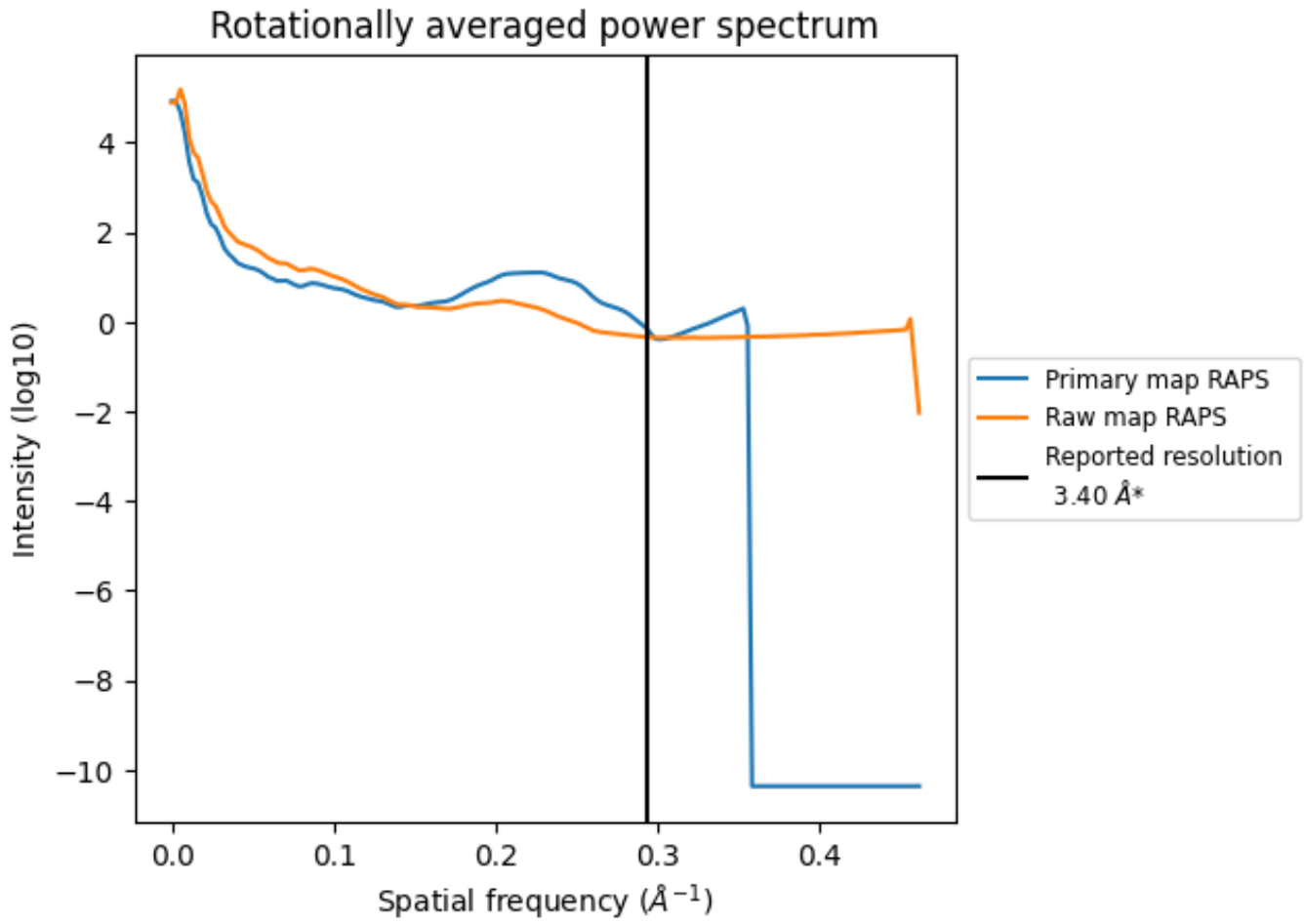
7.2 Volume estimate



The volume at the recommended contour level is 122 nm^3; this corresponds to an approximate mass of 110 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)

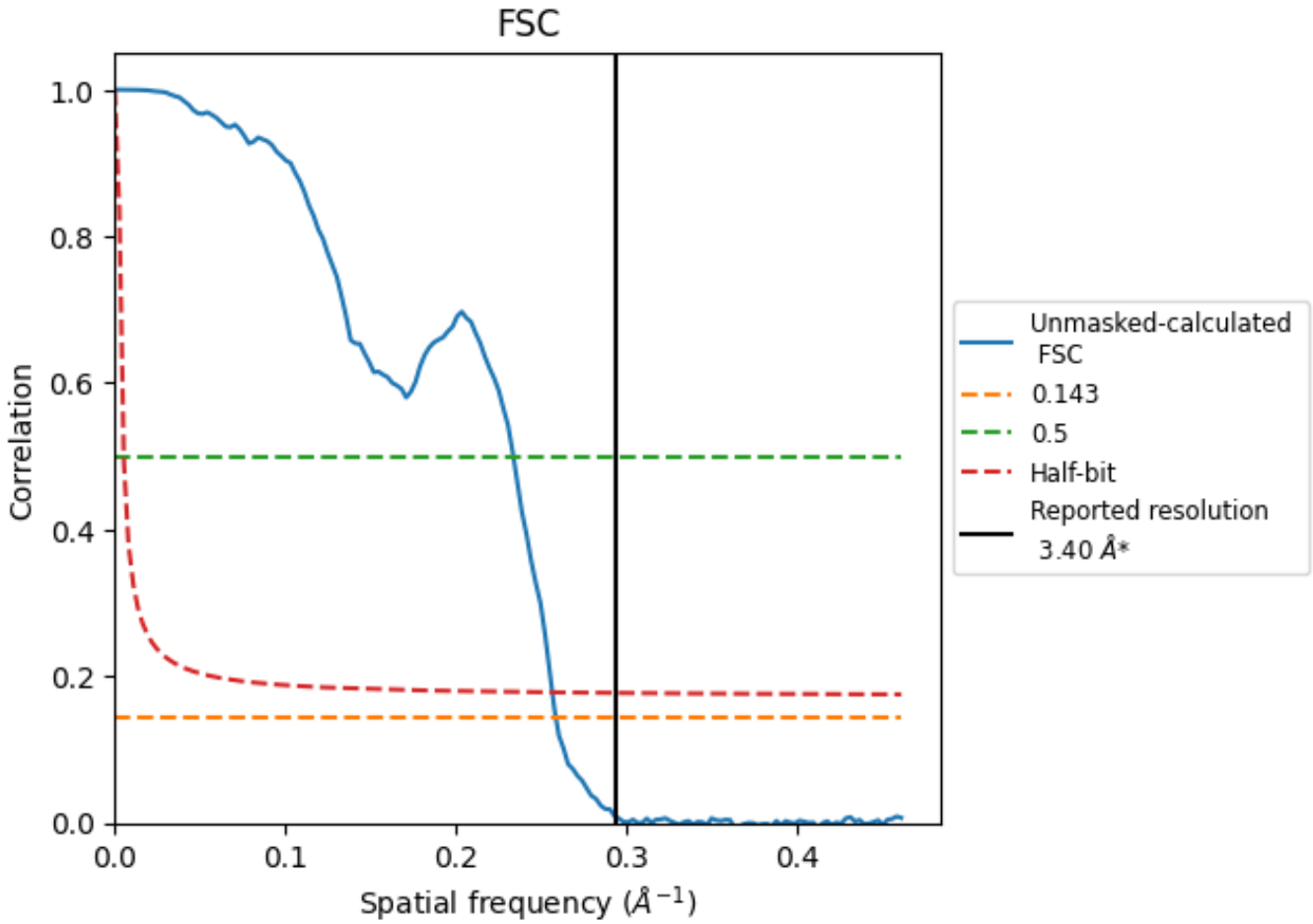


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

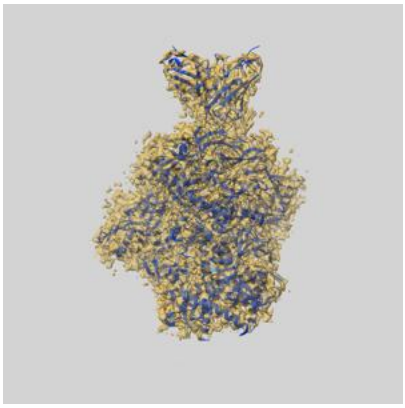
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	4.28	3.89

*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 3.86 differs from the reported value 3.4 by more than 10 %

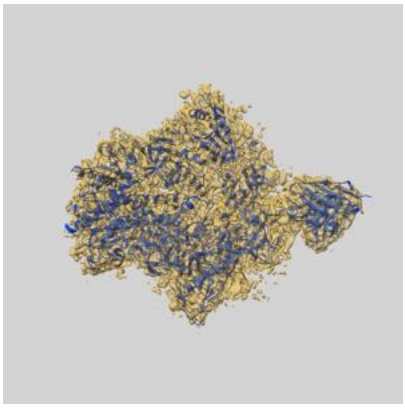
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29248 and PDB model 8FK5. Per-residue inclusion information can be found in section 3 on page 13.

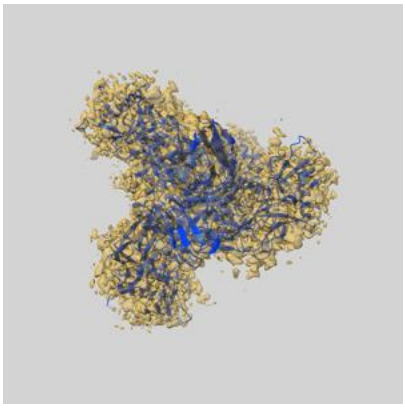
9.1 Map-model overlay



X



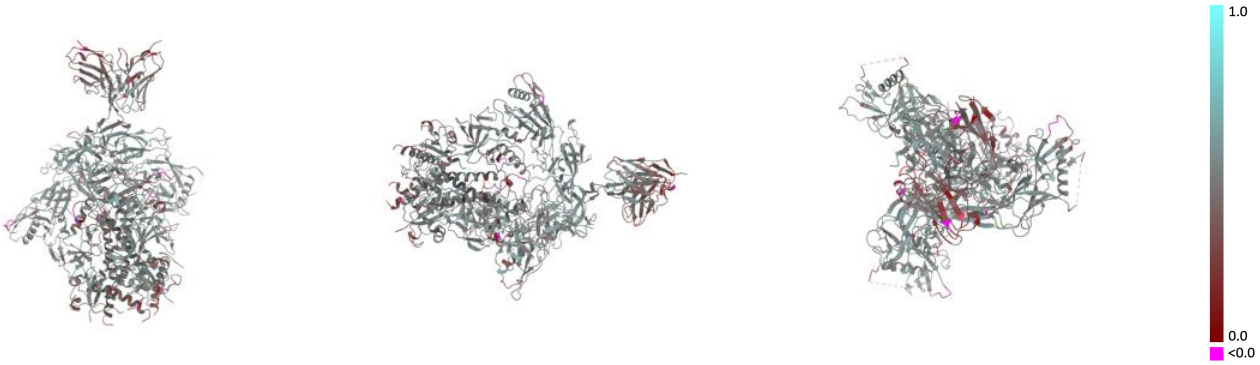
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

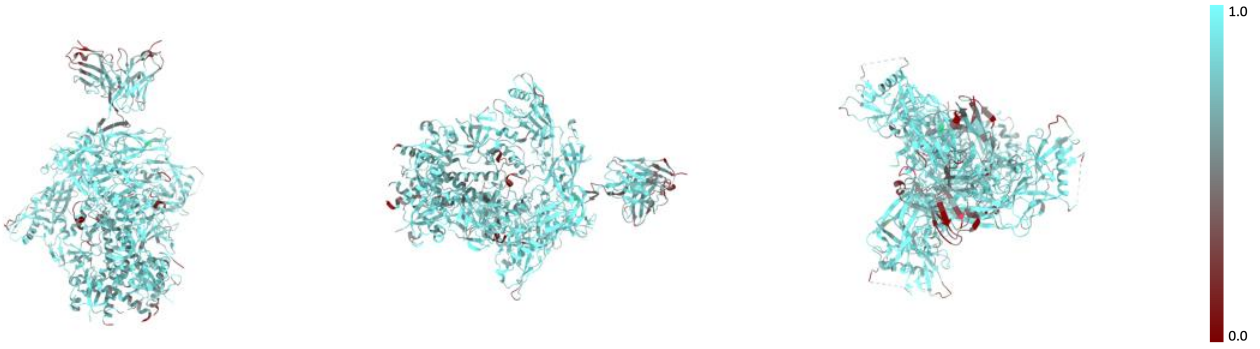
9.2 Q-score mapped to coordinate model



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.

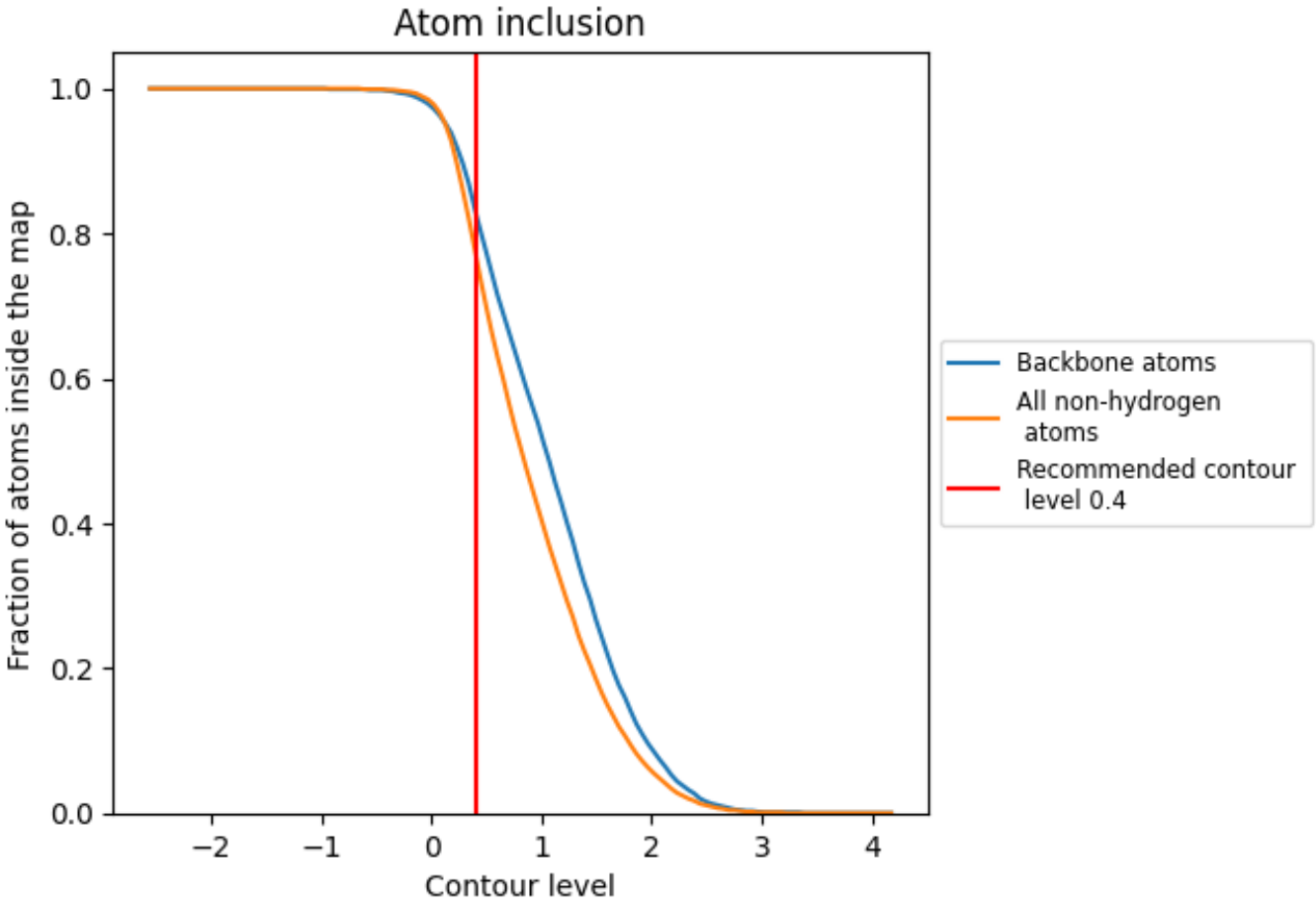
9.3 Atom inclusion mapped to coordinate model



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 83% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7740	0.4560
A	0.7540	0.4440
B	0.7420	0.4390
C	0.8140	0.4730
D	0.6070	0.3870
E	0.4640	0.4090
F	0.7680	0.4410
G	0.8070	0.4770
H	0.7540	0.4370
I	0.8150	0.4820
J	0.6250	0.4200
K	0.5710	0.3200
L	0.6050	0.3480
M	0.6430	0.3210
N	0.6070	0.3390
O	0.7500	0.4850
P	0.4290	0.3660
Q	0.5420	0.3660
R	0.5710	0.3040
S	0.6070	0.3720
T	0.6790	0.3750
U	0.4640	0.2770
V	0.3110	0.3160
W	0.4640	0.3840
X	0.5970	0.3740
Y	0.5710	0.3840
Z	0.6070	0.3450
a	0.3440	0.3220
b	0.7140	0.4660
c	0.5000	0.2850
d	0.6230	0.3170
e	0.6760	0.4370