wwPDB EM Validation Summary Report

Oct 27, 2026 – 12:41 PM EDT

PDB ID	:	9YYY / pdb_00009yyy
EMDB ID	:	EMD-73659
Title	:	Cryo-EM structure of HKU1 spike with antibody HKU1-2 (conformation 1)
Authors	:	Bangaru, S.; Feng, Z.; Ward, A.B.
Deposited on	:	2025-10-29
Resolution	:	3.55 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:

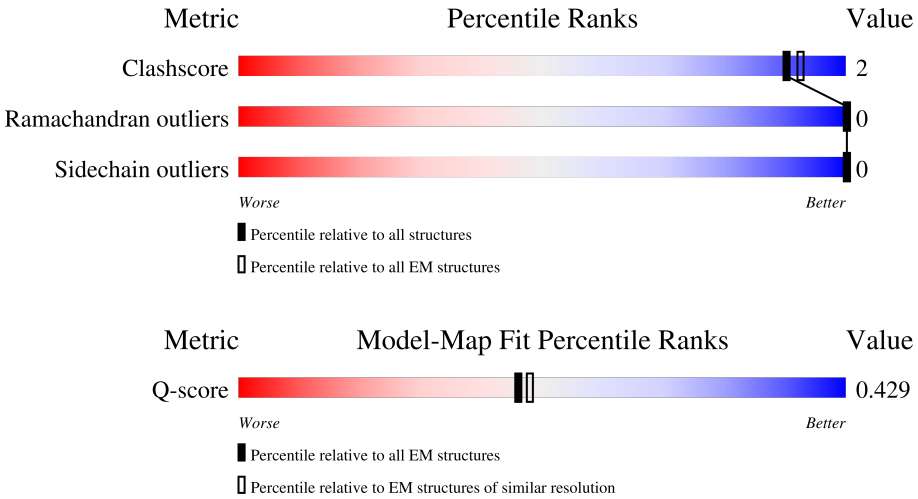
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.55 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12819 (3.05 - 4.05)

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

Mol	Chain	Length	Quality of chain
1	H	130	42% 91% 8%
2	L	108	54% 85% 14%
3	A	1299	88% 8%
3	B	1299	5% 87% 5% 8%

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Mol	Chain	Length	Quality of chain
3	C	1299	87% 5% 8%
4	D	3	33% 100%
4	F	3	67% 100%
4	M	3	67% 100%
4	N	3	33% 100%
4	P	3	100% 100%
4	T	3	67% 100%
4	U	3	33% 100%
4	Z	3	67% 100%
5	E	2	50% 100%
5	I	2	100%
5	J	2	50% 50% 50%
5	K	2	50% 50% 50%
5	O	2	50% 100%
5	R	2	50% 100%
5	S	2	50% 100%
5	V	2	50% 50% 50%
5	X	2	50% 100%
5	Y	2	50% 100%
6	G	5	40% 100%
6	Q	5	60% 100%
6	W	5	60% 100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 31125 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 HKU1-2 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	128	Total	C	N	O	S	0	0
			995	622	164	201	8		

- Molecule 2 is a protein called HKU1-2 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	107	Total	C	N	O	S	0	0
			821	516	141	162	2		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1194	Total	C	N	O	S	0	0
			9332	5949	1532	1794	57		
3	B	1194	Total	C	N	O	S	0	0
			9328	5946	1532	1793	57		
3	C	1193	Total	C	N	O	S	0	0
			9314	5940	1525	1792	57		

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	752	GLY	ARG	conflict	UNP Q0ZME7
A	753	GLY	ARG	conflict	UNP Q0ZME7
A	754	SER	LYS	conflict	UNP Q0ZME7
A	755	GLY	ARG	conflict	UNP Q0ZME7
A	756	SER	ARG	conflict	UNP Q0ZME7
A	1277	GLY	-	expression tag	UNP Q0ZME7
A	1278	SER	-	expression tag	UNP Q0ZME7
A	1279	GLY	-	expression tag	UNP Q0ZME7
A	1280	TYR	-	expression tag	UNP Q0ZME7
A	1281	ILE	-	expression tag	UNP Q0ZME7
A	1282	PRO	-	expression tag	UNP Q0ZME7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1283	GLU	-	expression tag	UNP Q0ZME7
A	1284	ALA	-	expression tag	UNP Q0ZME7
A	1285	PRO	-	expression tag	UNP Q0ZME7
A	1286	ARG	-	expression tag	UNP Q0ZME7
A	1287	ASP	-	expression tag	UNP Q0ZME7
A	1288	GLY	-	expression tag	UNP Q0ZME7
A	1289	GLN	-	expression tag	UNP Q0ZME7
A	1290	ALA	-	expression tag	UNP Q0ZME7
A	1291	TYR	-	expression tag	UNP Q0ZME7
A	1292	VAL	-	expression tag	UNP Q0ZME7
A	1293	ARG	-	expression tag	UNP Q0ZME7
A	1294	LYS	-	expression tag	UNP Q0ZME7
A	1295	ASP	-	expression tag	UNP Q0ZME7
A	1296	GLY	-	expression tag	UNP Q0ZME7
A	1297	GLU	-	expression tag	UNP Q0ZME7
A	1298	TRP	-	expression tag	UNP Q0ZME7
A	1299	VAL	-	expression tag	UNP Q0ZME7
A	1300	LEU	-	expression tag	UNP Q0ZME7
A	1301	LEU	-	expression tag	UNP Q0ZME7
A	1302	SER	-	expression tag	UNP Q0ZME7
A	1303	THR	-	expression tag	UNP Q0ZME7
A	1304	PHE	-	expression tag	UNP Q0ZME7
A	1305	LEU	-	expression tag	UNP Q0ZME7
A	1306	GLY	-	expression tag	UNP Q0ZME7
A	1307	LEU	-	expression tag	UNP Q0ZME7
A	1308	GLU	-	expression tag	UNP Q0ZME7
A	1309	VAL	-	expression tag	UNP Q0ZME7
A	1310	LEU	-	expression tag	UNP Q0ZME7
A	1311	PHE	-	expression tag	UNP Q0ZME7
A	1312	GLN	-	expression tag	UNP Q0ZME7
B	752	GLY	ARG	conflict	UNP Q0ZME7
B	753	GLY	ARG	conflict	UNP Q0ZME7
B	754	SER	LYS	conflict	UNP Q0ZME7
B	755	GLY	ARG	conflict	UNP Q0ZME7
B	756	SER	ARG	conflict	UNP Q0ZME7
B	1277	GLY	-	expression tag	UNP Q0ZME7
B	1278	SER	-	expression tag	UNP Q0ZME7
B	1279	GLY	-	expression tag	UNP Q0ZME7
B	1280	TYR	-	expression tag	UNP Q0ZME7
B	1281	ILE	-	expression tag	UNP Q0ZME7
B	1282	PRO	-	expression tag	UNP Q0ZME7
B	1283	GLU	-	expression tag	UNP Q0ZME7

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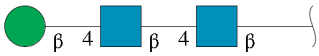
Chain	Residue	Modelled	Actual	Comment	Reference
B	1284	ALA	-	expression tag	UNP Q0ZME7
B	1285	PRO	-	expression tag	UNP Q0ZME7
B	1286	ARG	-	expression tag	UNP Q0ZME7
B	1287	ASP	-	expression tag	UNP Q0ZME7
B	1288	GLY	-	expression tag	UNP Q0ZME7
B	1289	GLN	-	expression tag	UNP Q0ZME7
B	1290	ALA	-	expression tag	UNP Q0ZME7
B	1291	TYR	-	expression tag	UNP Q0ZME7
B	1292	VAL	-	expression tag	UNP Q0ZME7
B	1293	ARG	-	expression tag	UNP Q0ZME7
B	1294	LYS	-	expression tag	UNP Q0ZME7
B	1295	ASP	-	expression tag	UNP Q0ZME7
B	1296	GLY	-	expression tag	UNP Q0ZME7
B	1297	GLU	-	expression tag	UNP Q0ZME7
B	1298	TRP	-	expression tag	UNP Q0ZME7
B	1299	VAL	-	expression tag	UNP Q0ZME7
B	1300	LEU	-	expression tag	UNP Q0ZME7
B	1301	LEU	-	expression tag	UNP Q0ZME7
B	1302	SER	-	expression tag	UNP Q0ZME7
B	1303	THR	-	expression tag	UNP Q0ZME7
B	1304	PHE	-	expression tag	UNP Q0ZME7
B	1305	LEU	-	expression tag	UNP Q0ZME7
B	1306	GLY	-	expression tag	UNP Q0ZME7
B	1307	LEU	-	expression tag	UNP Q0ZME7
B	1308	GLU	-	expression tag	UNP Q0ZME7
B	1309	VAL	-	expression tag	UNP Q0ZME7
B	1310	LEU	-	expression tag	UNP Q0ZME7
B	1311	PHE	-	expression tag	UNP Q0ZME7
B	1312	GLN	-	expression tag	UNP Q0ZME7
C	752	GLY	ARG	conflict	UNP Q0ZME7
C	753	GLY	ARG	conflict	UNP Q0ZME7
C	754	SER	LYS	conflict	UNP Q0ZME7
C	755	GLY	ARG	conflict	UNP Q0ZME7
C	756	SER	ARG	conflict	UNP Q0ZME7
C	1277	GLY	-	expression tag	UNP Q0ZME7
C	1278	SER	-	expression tag	UNP Q0ZME7
C	1279	GLY	-	expression tag	UNP Q0ZME7
C	1280	TYR	-	expression tag	UNP Q0ZME7
C	1281	ILE	-	expression tag	UNP Q0ZME7
C	1282	PRO	-	expression tag	UNP Q0ZME7
C	1283	GLU	-	expression tag	UNP Q0ZME7
C	1284	ALA	-	expression tag	UNP Q0ZME7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1285	PRO	-	expression tag	UNP Q0ZME7
C	1286	ARG	-	expression tag	UNP Q0ZME7
C	1287	ASP	-	expression tag	UNP Q0ZME7
C	1288	GLY	-	expression tag	UNP Q0ZME7
C	1289	GLN	-	expression tag	UNP Q0ZME7
C	1290	ALA	-	expression tag	UNP Q0ZME7
C	1291	TYR	-	expression tag	UNP Q0ZME7
C	1292	VAL	-	expression tag	UNP Q0ZME7
C	1293	ARG	-	expression tag	UNP Q0ZME7
C	1294	LYS	-	expression tag	UNP Q0ZME7
C	1295	ASP	-	expression tag	UNP Q0ZME7
C	1296	GLY	-	expression tag	UNP Q0ZME7
C	1297	GLU	-	expression tag	UNP Q0ZME7
C	1298	TRP	-	expression tag	UNP Q0ZME7
C	1299	VAL	-	expression tag	UNP Q0ZME7
C	1300	LEU	-	expression tag	UNP Q0ZME7
C	1301	LEU	-	expression tag	UNP Q0ZME7
C	1302	SER	-	expression tag	UNP Q0ZME7
C	1303	THR	-	expression tag	UNP Q0ZME7
C	1304	PHE	-	expression tag	UNP Q0ZME7
C	1305	LEU	-	expression tag	UNP Q0ZME7
C	1306	GLY	-	expression tag	UNP Q0ZME7
C	1307	LEU	-	expression tag	UNP Q0ZME7
C	1308	GLU	-	expression tag	UNP Q0ZME7
C	1309	VAL	-	expression tag	UNP Q0ZME7
C	1310	LEU	-	expression tag	UNP Q0ZME7
C	1311	PHE	-	expression tag	UNP Q0ZME7
C	1312	GLN	-	expression tag	UNP Q0ZME7

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	3	Total	C	N	O	0	0
			39	22	2	15		
4	F	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	3	Total 39	C 22	N 2	O 15	0	0
4	N	3	Total 39	C 22	N 2	O 15	0	0
4	P	3	Total 39	C 22	N 2	O 15	0	0
4	T	3	Total 39	C 22	N 2	O 15	0	0
4	U	3	Total 39	C 22	N 2	O 15	0	0
4	Z	3	Total 39	C 22	N 2	O 15	0	0

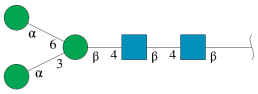
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	2	Total 28	C 16	N 2	O 10	0	0
5	I	2	Total 28	C 16	N 2	O 10	0	0
5	J	2	Total 28	C 16	N 2	O 10	0	0
5	K	2	Total 28	C 16	N 2	O 10	0	0
5	O	2	Total 28	C 16	N 2	O 10	0	0
5	R	2	Total 28	C 16	N 2	O 10	0	0
5	S	2	Total 28	C 16	N 2	O 10	0	0
5	V	2	Total 28	C 16	N 2	O 10	0	0
5	X	2	Total 28	C 16	N 2	O 10	0	0
5	Y	2	Total 28	C 16	N 2	O 10	0	0

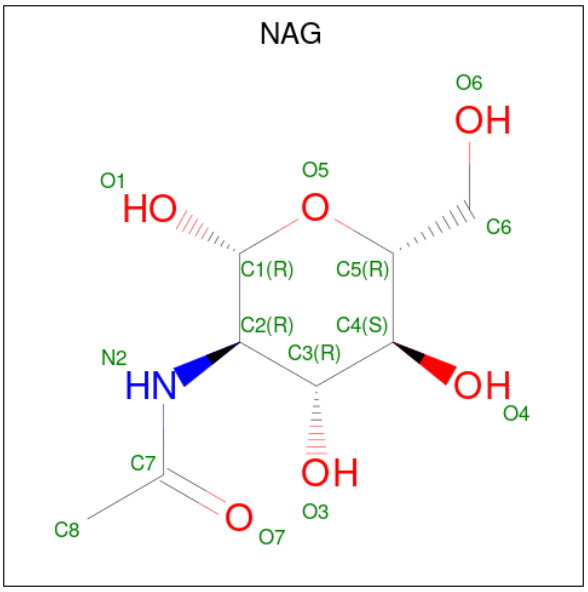
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(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	G	5	Total C N O 61 34 2 25	0	0
6	Q	5	Total C N O 61 34 2 25	0	0
6	W	5	Total C N O 61 34 2 25	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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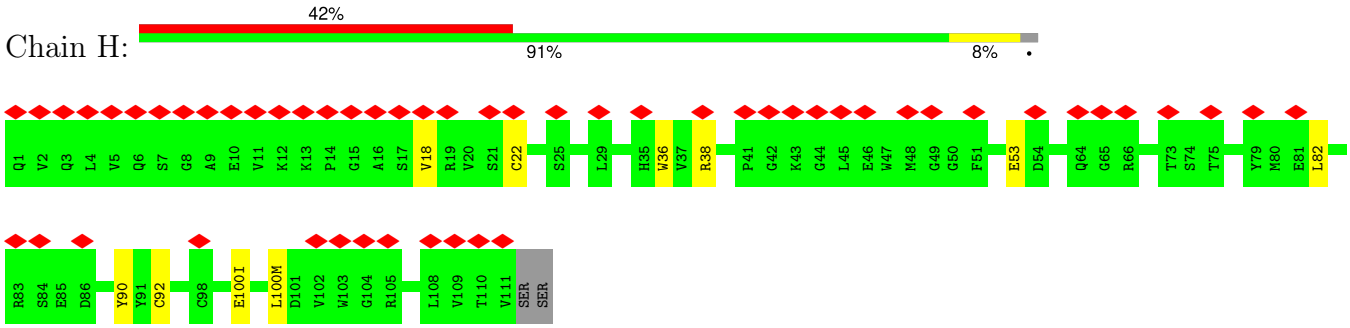
Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	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.

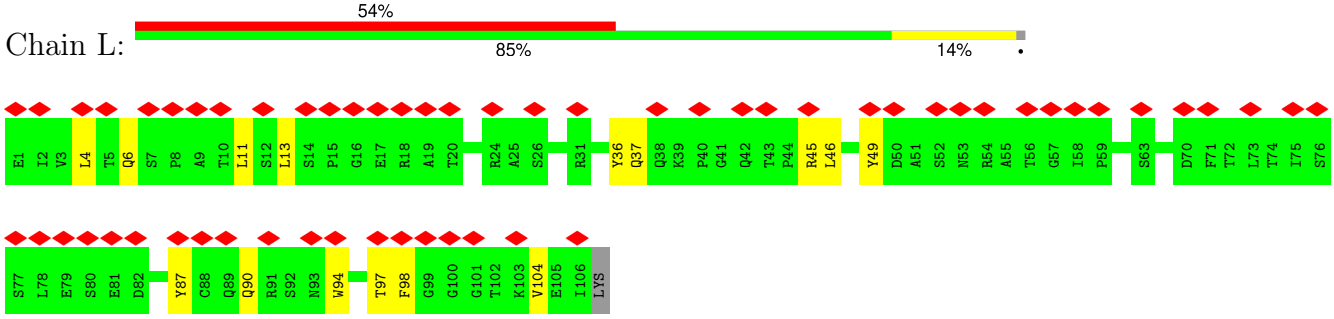
• Molecule 1: HKU1-2 Fab heavy chain

Chain H:



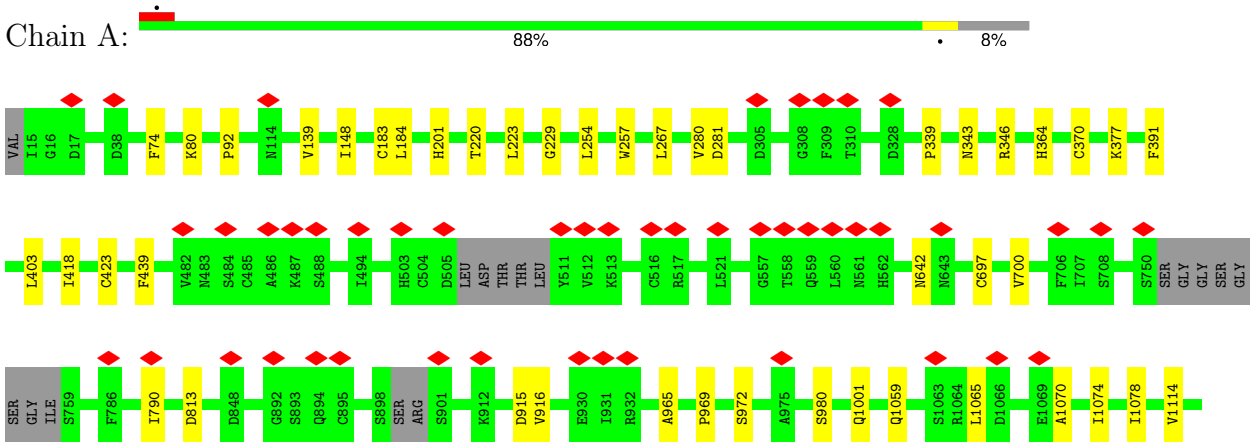
• Molecule 2: HKU1-2 Fab light chain

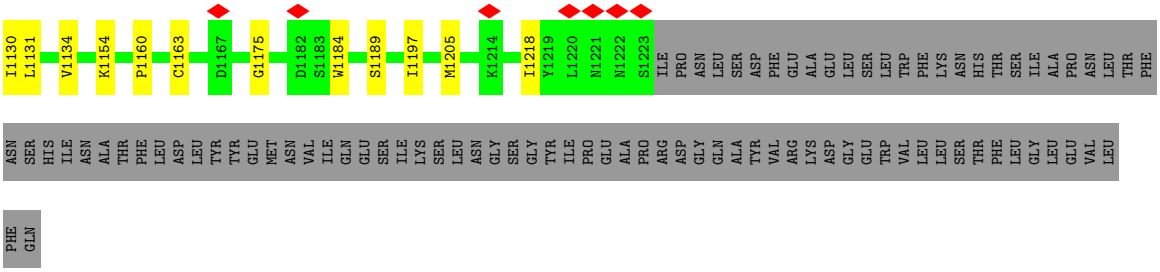
Chain L:



• Molecule 3: Spike glycoprotein

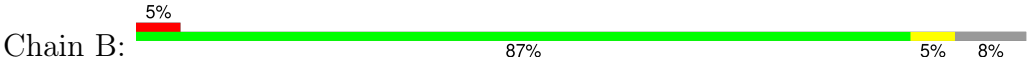
Chain A:

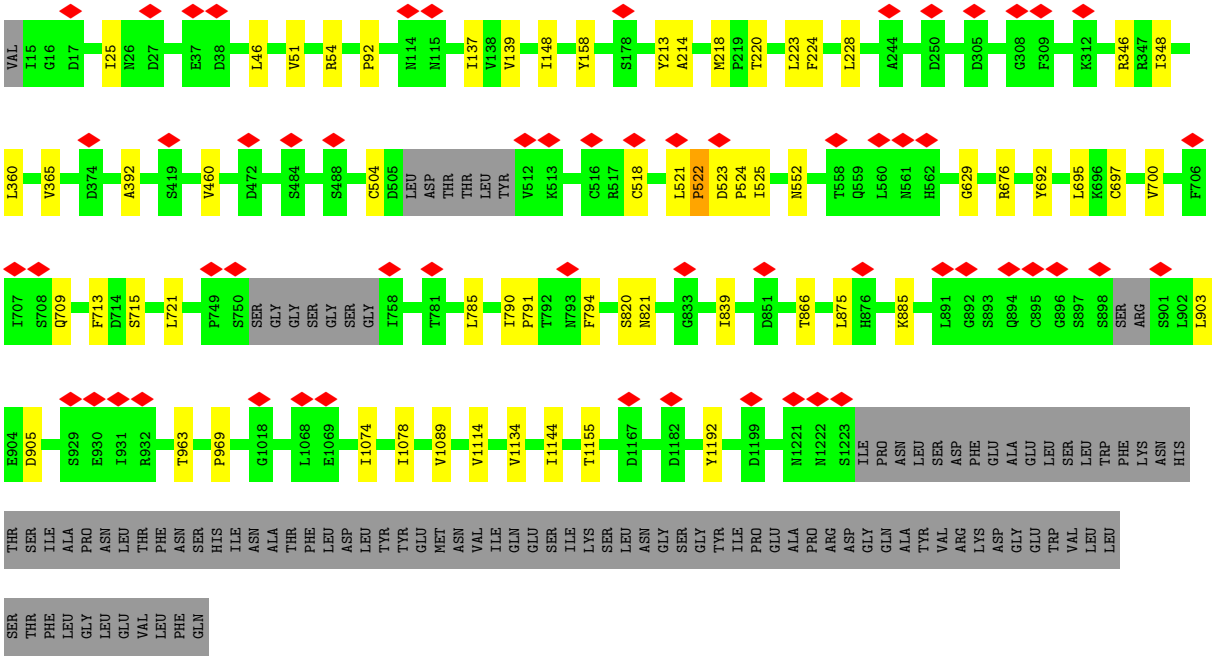




• Molecule 3: Spike glycoprotein

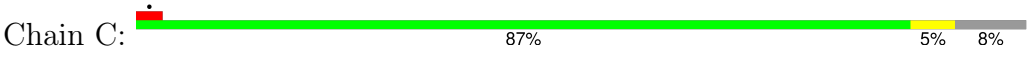
Chain B:

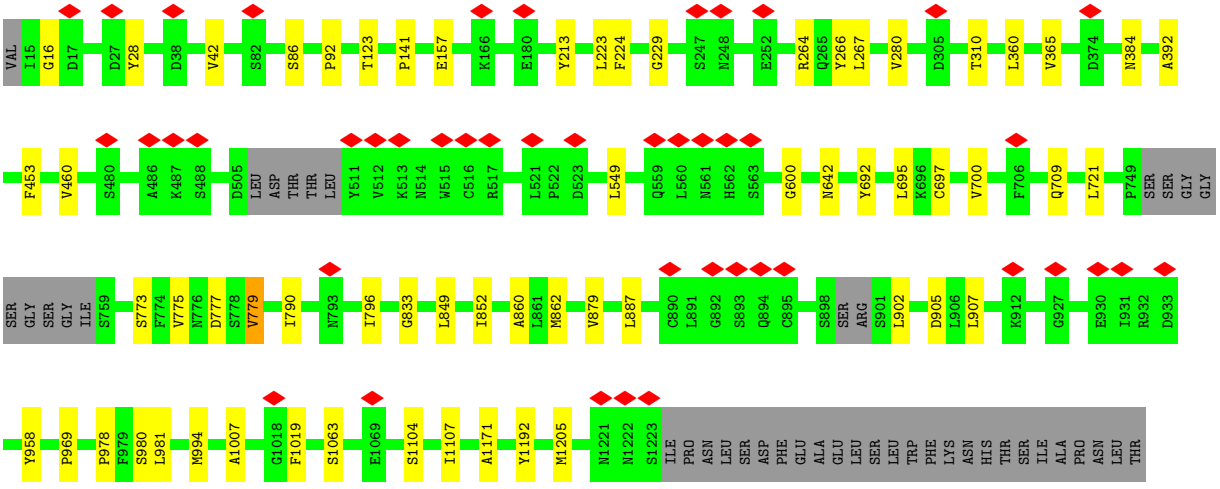




• Molecule 3: Spike glycoprotein

Chain C:



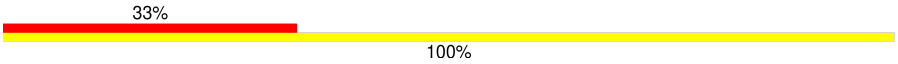


PHE ASN SER HIS ILE ASN ALA THR PHE LEU ASP LEU TYR TYR GLU MET ASN VAL ILE GLN GLU SER ILE LYS SER LEU ASN GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY LEU GLU VAL

LEU PHE GLN

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

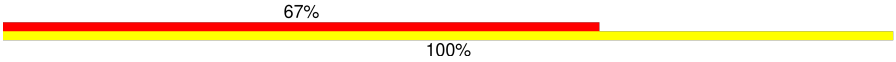
Chain D:



NAG1 NAG2 BMA3

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

Chain F:



NAG1 NAG2 BMA3

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

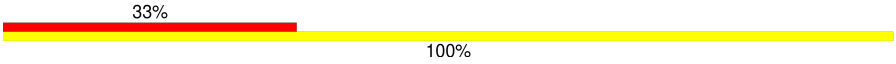
Chain M:



NAG1 NAG2 BMA3

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

Chain N:



NAG1 NAG2 BMA3

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

Chain P:



NAG1 NAG2 BMA3

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

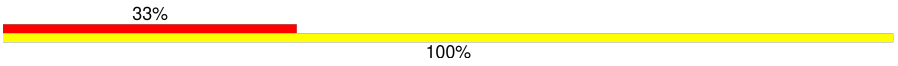
Chain T:





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

Chain U:





• Molecule 4: beta-D-mannopyranose-(1-4)-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

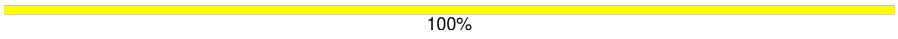
Chain E:





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

Chain I:





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

Chain J:





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

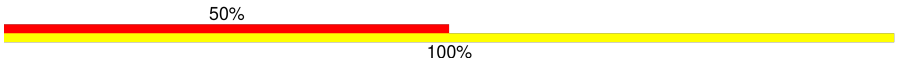
Chain K:





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

Chain O:





• 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 V:





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

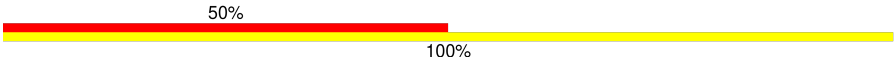
Chain X:





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

Chain Y:





• Molecule 6: 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

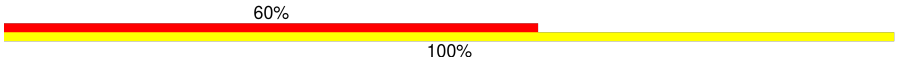
Chain G:





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

Chain W:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59894	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50.14	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.338	Depositor
Minimum map value	-0.196	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.062	Depositor
Map size (Å)	371.2, 371.2, 371.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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	H	0.37	0/1019	0.85	0/1385
2	L	0.35	0/840	0.72	1/1143 (0.1%)
3	A	0.31	1/9557 (0.0%)	0.67	8/13011 (0.1%)
3	B	0.30	0/9552	0.66	8/13004 (0.1%)
3	C	0.30	0/9539	0.68	9/12989 (0.1%)
All	All	0.31	1/30507 (0.0%)	0.68	26/41532 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1163	CYS	CB-SG	-5.25	1.64	1.81

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	183	CYS	CA-CB-SG	8.58	134.12	114.40
3	B	522	PRO	N-CA-C	-8.25	98.10	111.21
3	C	642	ASN	CA-C-N	7.71	140.09	126.45
3	C	642	ASN	C-N-CA	7.71	140.09	126.45
3	C	779	VAL	N-CA-C	-7.21	106.11	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	995	0	929	7	0
2	L	821	0	802	8	0
3	A	9332	0	8973	33	0
3	B	9328	0	8975	35	0
3	C	9314	0	8946	37	0
4	D	39	0	34	0	0
4	F	39	0	34	0	0
4	M	39	0	34	0	0
4	N	39	0	34	0	0
4	P	39	0	34	0	0
4	T	39	0	34	0	0
4	U	39	0	34	0	0
4	Z	39	0	34	0	0
5	E	28	0	25	0	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
5	K	28	0	25	0	0
5	O	28	0	25	0	0
5	R	28	0	25	0	0
5	S	28	0	25	0	0
5	V	28	0	25	0	0
5	X	28	0	25	0	0
5	Y	28	0	25	0	0
6	G	61	0	52	0	0
6	Q	61	0	52	0	0
6	W	61	0	52	0	0
7	A	168	0	156	0	0
7	B	196	0	182	0	0
7	C	196	0	182	0	0
All	All	31125	0	29823	106	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 106 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:821:ASN:HD22	3:C:310:THR:HG21	1.50	0.74
3:C:123:THR:HG22	3:C:141:PRO:HD2	1.74	0.69
3:C:978:PRO:HD2	3:C:981:LEU:HD12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:339:PRO:HG2	3:A:391:PHE:HA	1.80	0.63
3:C:879:VAL:HG21	3:C:980:SER:HB3	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	H	126/130 (97%)	120 (95%)	6 (5%)	0	100	100
2	L	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
3	A	1186/1299 (91%)	1143 (96%)	43 (4%)	0	100	100
3	B	1186/1299 (91%)	1148 (97%)	38 (3%)	0	100	100
3	C	1185/1299 (91%)	1151 (97%)	34 (3%)	0	100	100
All	All	3788/4135 (92%)	3664 (97%)	124 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	108/111 (97%)	108 (100%)	0	100	100
2	L	90/91 (99%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	1070/1161 (92%)	1070 (100%)	0	100	100
3	B	1070/1161 (92%)	1070 (100%)	0	100	100
3	C	1067/1161 (92%)	1067 (100%)	0	100	100
All	All	3405/3685 (92%)	3405 (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 35 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	559	GLN
3	C	652	ASN
3	C	1036	ASN
3	A	1045	GLN
3	A	1000	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

59 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	1	4,3	14,14,15	0.80	0	17,19,21	1.20	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	D	2	4	14,14,15	0.71	0	17,19,21	1.01	1 (5%)
4	BMA	D	3	4	11,11,12	0.79	0	15,15,17	2.42	4 (26%)
5	NAG	E	1	3,5	14,14,15	0.71	0	17,19,21	1.00	1 (5%)
5	NAG	E	2	5	14,14,15	0.70	0	17,19,21	1.10	1 (5%)
4	NAG	F	1	4,3	14,14,15	0.76	0	17,19,21	0.99	1 (5%)
4	NAG	F	2	4	14,14,15	0.78	1 (7%)	17,19,21	1.54	2 (11%)
4	BMA	F	3	4	11,11,12	0.86	0	15,15,17	2.29	3 (20%)
6	NAG	G	1	6,3	14,14,15	0.73	0	17,19,21	1.57	3 (17%)
6	NAG	G	2	6	14,14,15	0.67	0	17,19,21	1.10	2 (11%)
6	BMA	G	3	6	11,11,12	0.80	0	15,15,17	2.63	2 (13%)
6	MAN	G	4	6	11,11,12	0.76	0	15,15,17	1.14	1 (6%)
6	MAN	G	5	6	11,11,12	0.65	0	15,15,17	1.51	1 (6%)
5	NAG	I	1	3,5	14,14,15	0.70	0	17,19,21	1.41	2 (11%)
5	NAG	I	2	5	14,14,15	0.69	0	17,19,21	1.24	1 (5%)
5	NAG	J	1	3,5	14,14,15	0.76	0	17,19,21	1.47	3 (17%)
5	NAG	J	2	5	14,14,15	0.67	0	17,19,21	0.97	0
5	NAG	K	1	3,5	14,14,15	0.74	0	17,19,21	1.19	1 (5%)
5	NAG	K	2	5	14,14,15	0.73	0	17,19,21	1.01	0
4	NAG	M	1	4,3	14,14,15	0.64	0	17,19,21	1.27	3 (17%)
4	NAG	M	2	4	14,14,15	0.69	0	17,19,21	1.14	1 (5%)
4	BMA	M	3	4	11,11,12	0.86	0	15,15,17	2.45	3 (20%)
4	NAG	N	1	4,3	14,14,15	0.76	0	17,19,21	1.39	3 (17%)
4	NAG	N	2	4	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
4	BMA	N	3	4	11,11,12	0.80	0	15,15,17	2.50	3 (20%)
5	NAG	O	1	3,5	14,14,15	0.75	0	17,19,21	1.44	1 (5%)
5	NAG	O	2	5	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
4	NAG	P	1	4,3	14,14,15	0.75	0	17,19,21	1.07	1 (5%)
4	NAG	P	2	4	14,14,15	0.84	1 (7%)	17,19,21	1.69	4 (23%)
4	BMA	P	3	4	11,11,12	0.88	0	15,15,17	2.30	3 (20%)
6	NAG	Q	1	6,3	14,14,15	0.73	0	17,19,21	1.45	3 (17%)
6	NAG	Q	2	6	14,14,15	0.73	0	17,19,21	0.98	1 (5%)
6	BMA	Q	3	6	11,11,12	0.90	1 (9%)	15,15,17	2.02	2 (13%)
6	MAN	Q	4	6	11,11,12	0.69	0	15,15,17	1.53	1 (6%)
6	MAN	Q	5	6	11,11,12	0.61	0	15,15,17	1.64	1 (6%)
5	NAG	R	1	3,5	14,14,15	0.89	1 (7%)	17,19,21	1.90	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	R	2	5	14,14,15	0.83	1 (7%)	17,19,21	1.43	2 (11%)
5	NAG	S	1	3,5	14,14,15	0.72	0	17,19,21	1.06	2 (11%)
5	NAG	S	2	5	14,14,15	0.68	0	17,19,21	1.10	1 (5%)
4	NAG	T	1	4,3	14,14,15	0.71	0	17,19,21	1.00	1 (5%)
4	NAG	T	2	4	14,14,15	0.67	0	17,19,21	1.29	1 (5%)
4	BMA	T	3	4	11,11,12	0.83	0	15,15,17	2.51	2 (13%)
4	NAG	U	1	4,3	14,14,15	0.80	0	17,19,21	1.50	4 (23%)
4	NAG	U	2	4	14,14,15	0.69	0	17,19,21	1.04	1 (5%)
4	BMA	U	3	4	11,11,12	0.81	0	15,15,17	2.52	4 (26%)
5	NAG	V	1	3,5	14,14,15	0.73	0	17,19,21	1.30	2 (11%)
5	NAG	V	2	5	14,14,15	0.70	0	17,19,21	0.91	0
6	NAG	W	1	6,3	14,14,15	0.76	0	17,19,21	1.66	3 (17%)
6	NAG	W	2	6	14,14,15	0.74	0	17,19,21	1.01	1 (5%)
6	BMA	W	3	6	11,11,12	0.86	0	15,15,17	2.09	2 (13%)
6	MAN	W	4	6	11,11,12	0.79	0	15,15,17	1.10	1 (6%)
6	MAN	W	5	6	11,11,12	0.65	0	15,15,17	1.55	1 (6%)
5	NAG	X	1	3,5	14,14,15	0.71	0	17,19,21	1.40	2 (11%)
5	NAG	X	2	5	14,14,15	0.70	0	17,19,21	1.20	1 (5%)
5	NAG	Y	1	3,5	14,14,15	0.83	0	17,19,21	1.67	3 (17%)
5	NAG	Y	2	5	14,14,15	0.70	0	17,19,21	1.24	1 (5%)
4	NAG	Z	1	4,3	14,14,15	0.72	0	17,19,21	1.03	2 (11%)
4	NAG	Z	2	4	14,14,15	0.70	0	17,19,21	1.27	1 (5%)
4	BMA	Z	3	4	11,11,12	0.82	0	15,15,17	2.42	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
5	NAG	E	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	1/6/23/26	0/1/1/1
4	NAG	F	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
6	NAG	G	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	1/2/19/22	0/1/1/1
6	MAN	G	4	6	-	1/2/19/22	0/1/1/1
6	MAN	G	5	6	-	2/2/19/22	0/1/1/1
5	NAG	I	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
5	NAG	J	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	NAG	K	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
4	NAG	M	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	1/2/19/22	0/1/1/1
4	NAG	N	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	BMA	N	3	4	-	1/2/19/22	0/1/1/1
5	NAG	O	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
4	NAG	P	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	BMA	P	3	4	-	0/2/19/22	0/1/1/1
6	NAG	Q	1	6,3	-	2/6/23/26	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	-	2/2/19/22	0/1/1/1
5	NAG	R	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
5	NAG	S	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	1/6/23/26	0/1/1/1
4	NAG	T	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	BMA	T	3	4	-	1/2/19/22	0/1/1/1
4	NAG	U	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
4	BMA	U	3	4	-	1/2/19/22	0/1/1/1
5	NAG	V	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/6/23/26	0/1/1/1
6	NAG	W	1	6,3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	W	2	6	-	1/6/23/26	0/1/1/1
6	BMA	W	3	6	-	2/2/19/22	0/1/1/1
6	MAN	W	4	6	-	0/2/19/22	0/1/1/1
6	MAN	W	5	6	-	2/2/19/22	0/1/1/1
5	NAG	X	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	X	2	5	-	1/6/23/26	0/1/1/1
5	NAG	Y	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	1/6/23/26	0/1/1/1
4	NAG	Z	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	1/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	1	NAG	C1-C2	2.45	1.55	1.52
4	P	2	NAG	C1-C2	2.37	1.55	1.52
5	R	2	NAG	C1-C2	2.32	1.55	1.52
4	F	2	NAG	C1-C2	2.08	1.55	1.52
6	Q	3	BMA	C2-C3	2.03	1.55	1.52

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	3	BMA	C1-O5-C5	9.05	124.31	112.19
4	T	3	BMA	C1-O5-C5	8.36	123.39	112.19
4	U	3	BMA	C1-O5-C5	8.33	123.35	112.19
4	N	3	BMA	C1-O5-C5	8.23	123.21	112.19
4	M	3	BMA	C1-O5-C5	8.03	122.95	112.19

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

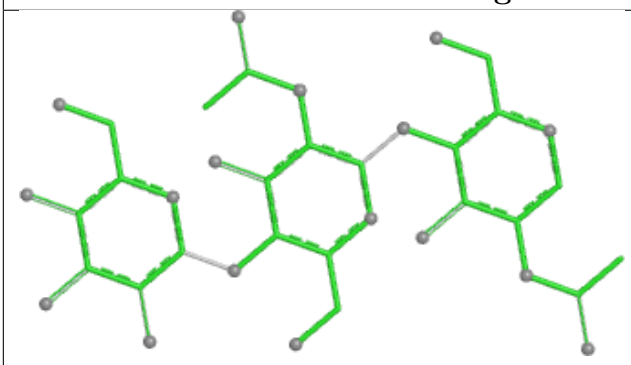
Mol	Chain	Res	Type	Atoms
4	M	3	BMA	O5-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
6	W	3	BMA	C4-C5-C6-O6
6	W	3	BMA	O5-C5-C6-O6
4	T	3	BMA	O5-C5-C6-O6

There are no ring outliers.

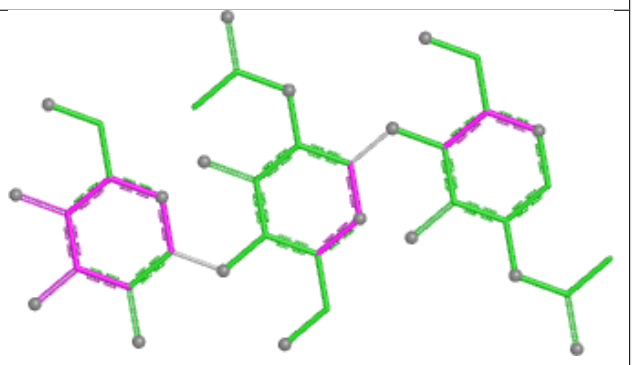
No monomer is involved in short contacts.

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

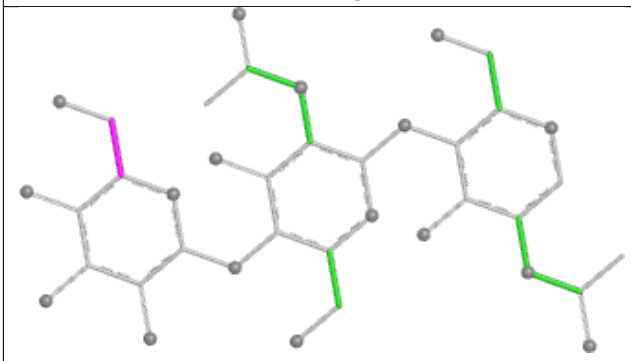
Oligosaccharide Chain D



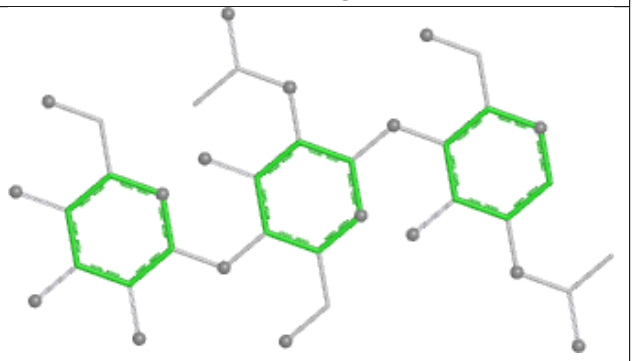
Bond lengths



Bond angles

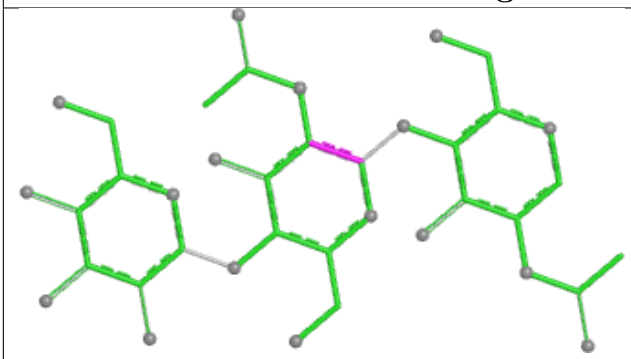


Torsions

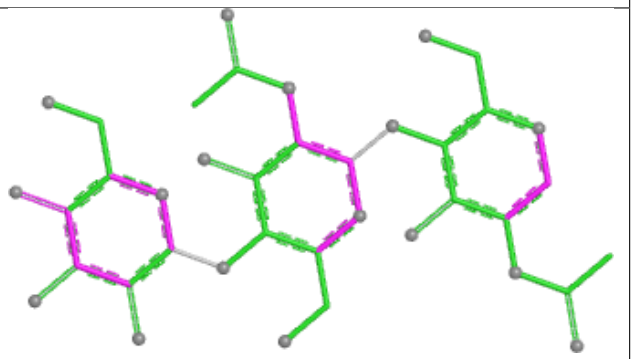


Rings

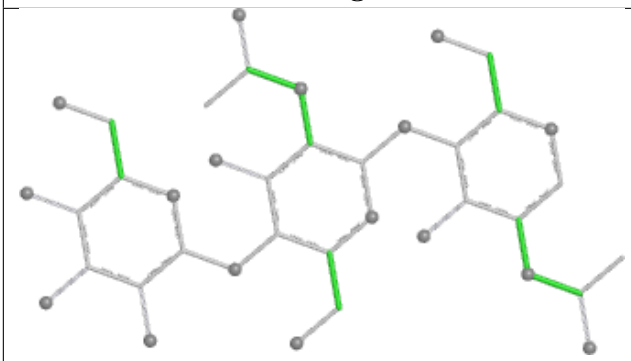
Oligosaccharide Chain F



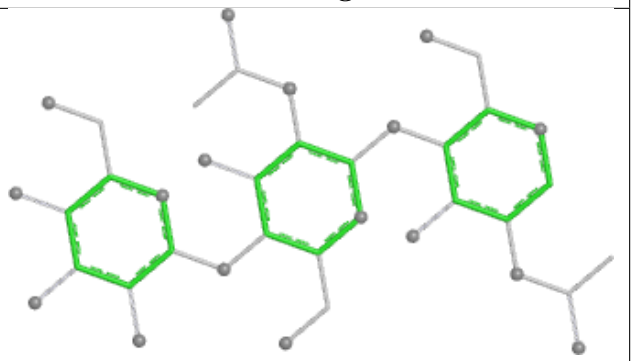
Bond lengths



Bond angles

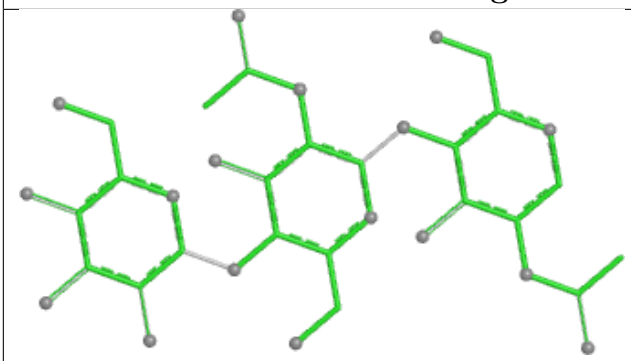


Torsions

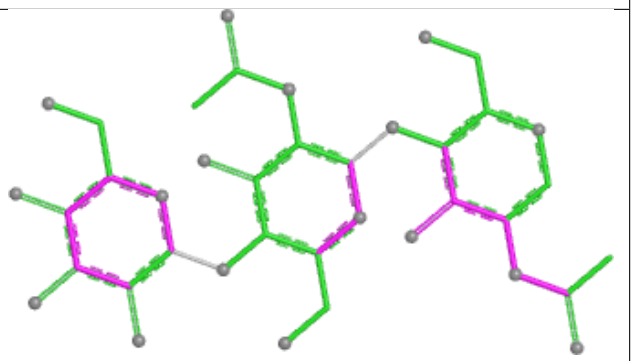


Rings

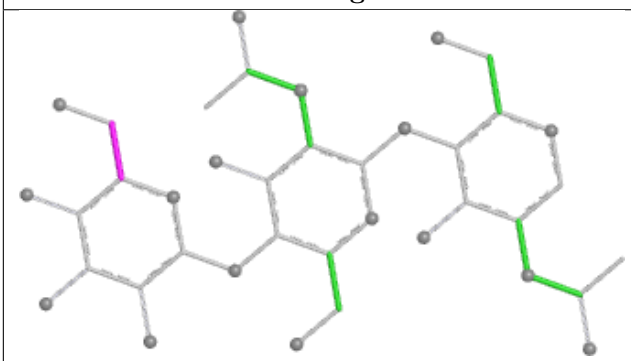
Oligosaccharide Chain M



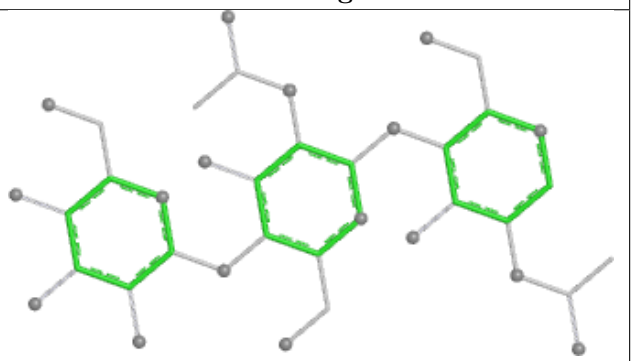
Bond lengths



Bond angles

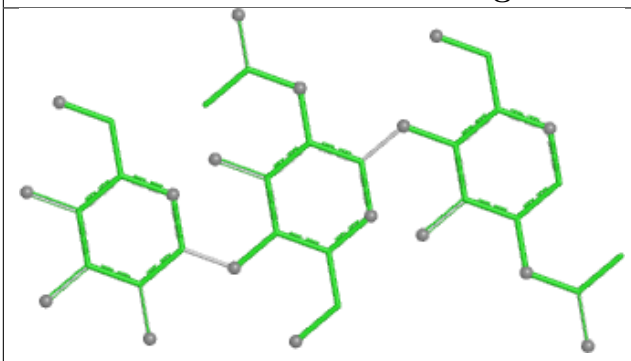


Torsions

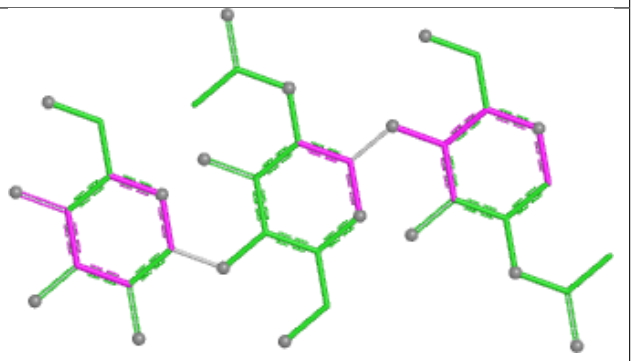


Rings

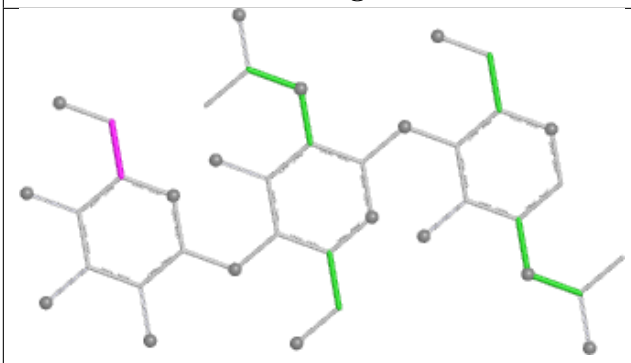
Oligosaccharide Chain N



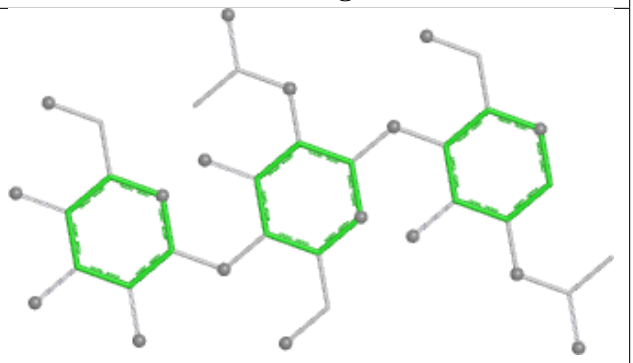
Bond lengths



Bond angles

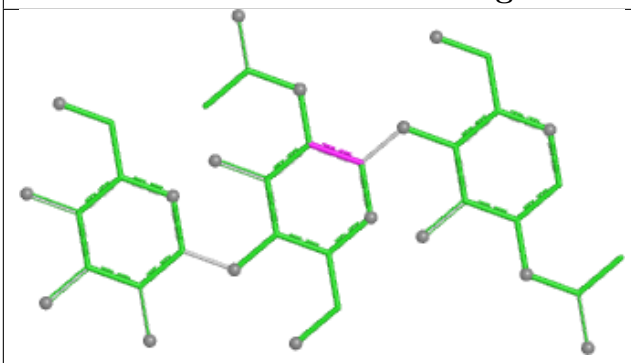


Torsions

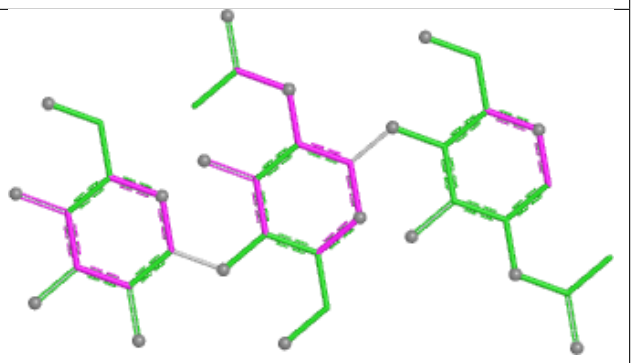


Rings

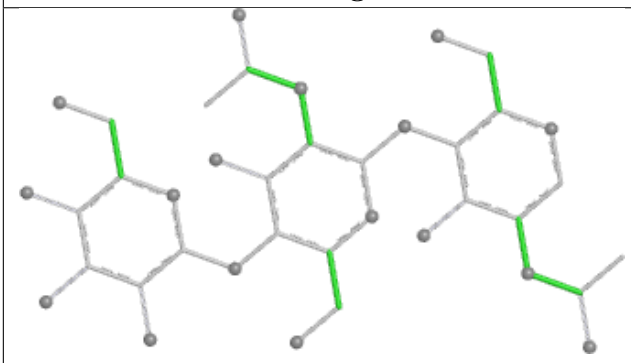
Oligosaccharide Chain P



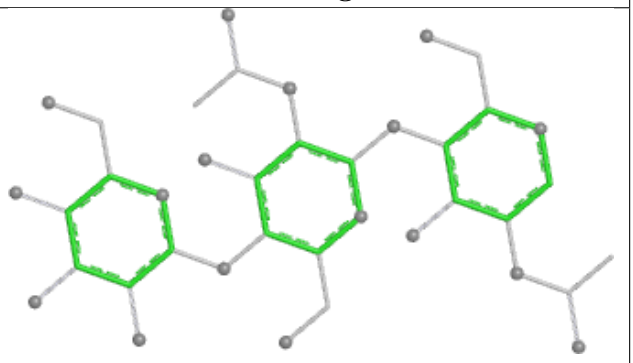
Bond lengths



Bond angles

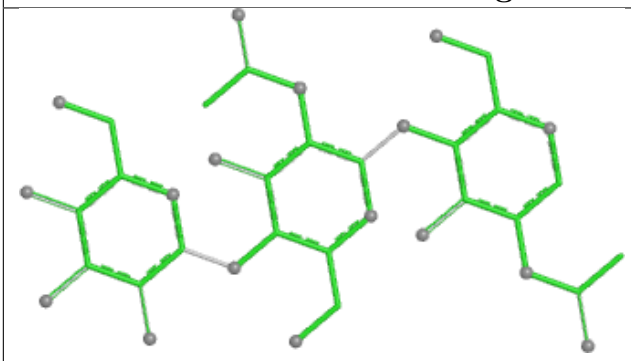


Torsions

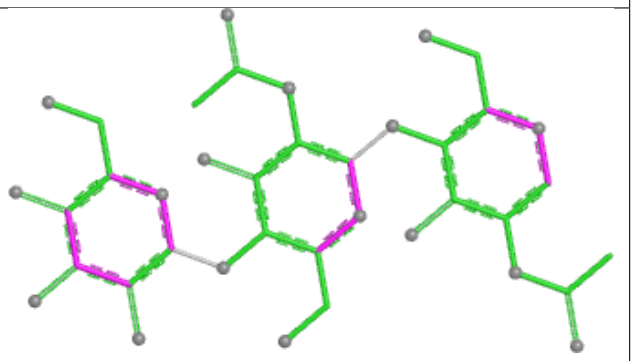


Rings

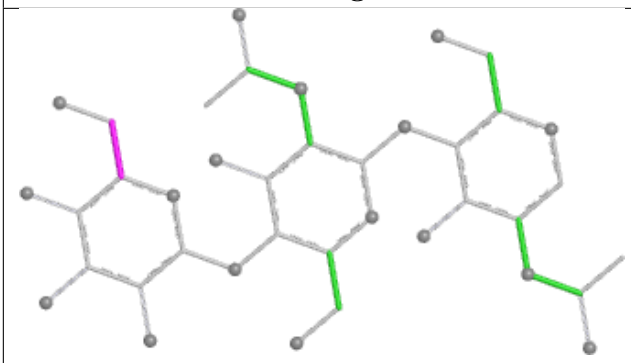
Oligosaccharide Chain T



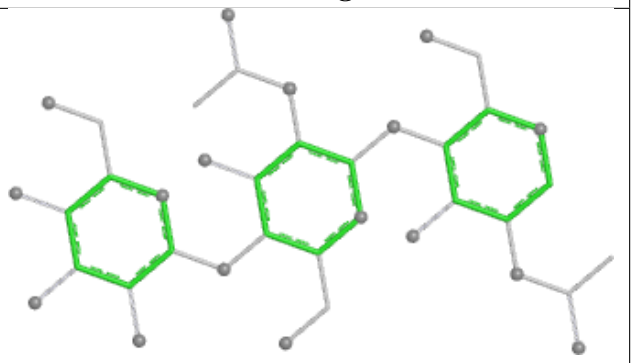
Bond lengths



Bond angles

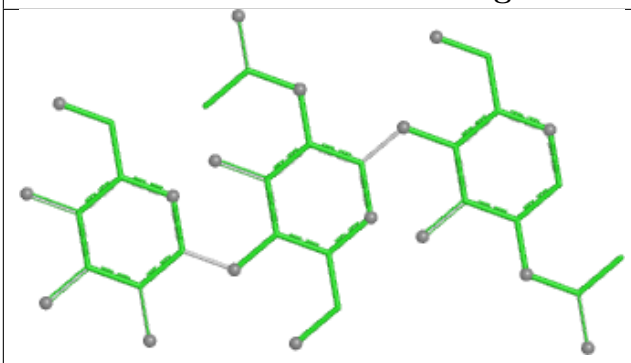


Torsions

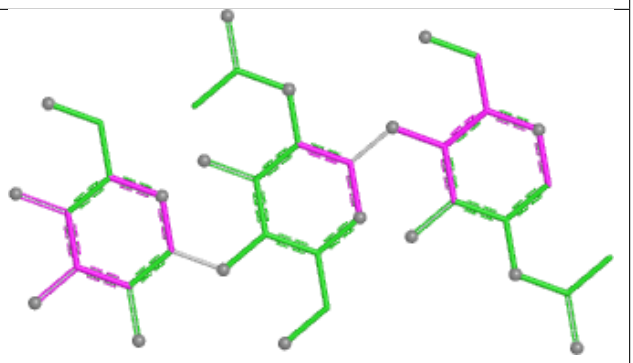


Rings

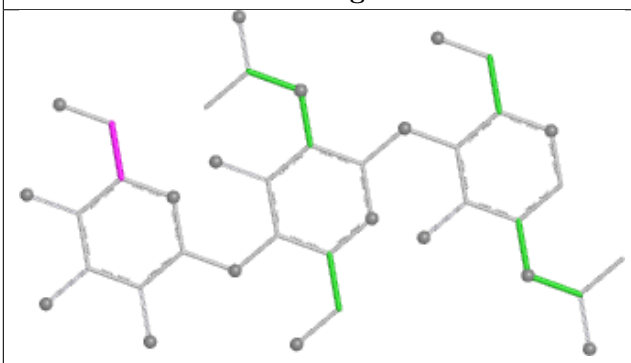
Oligosaccharide Chain U



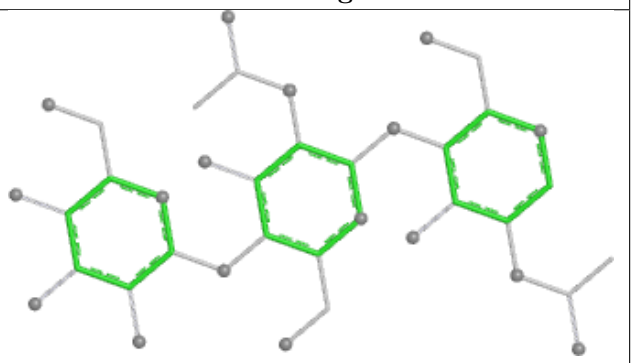
Bond lengths



Bond angles

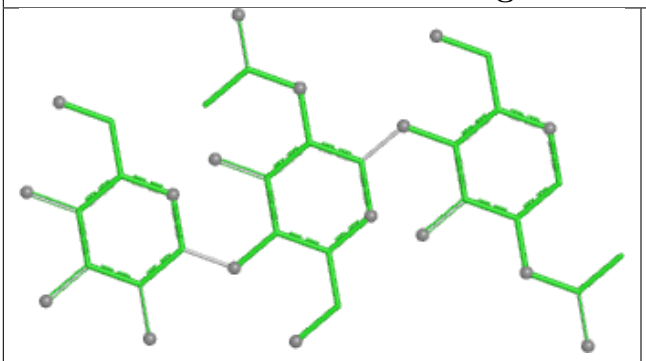


Torsions

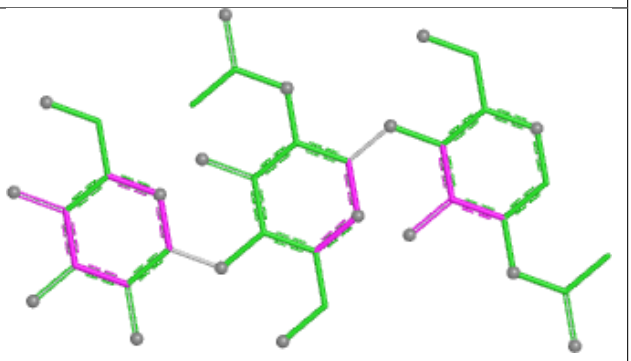


Rings

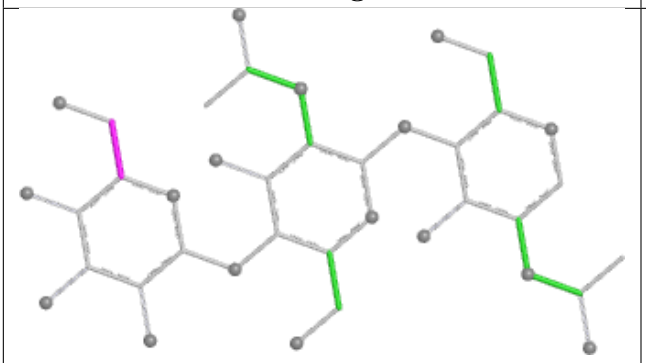
Oligosaccharide Chain Z



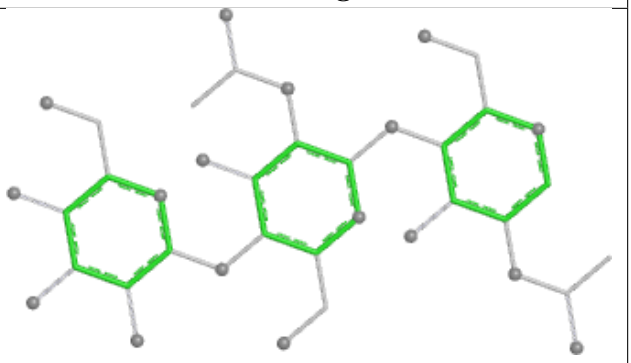
Bond lengths



Bond angles

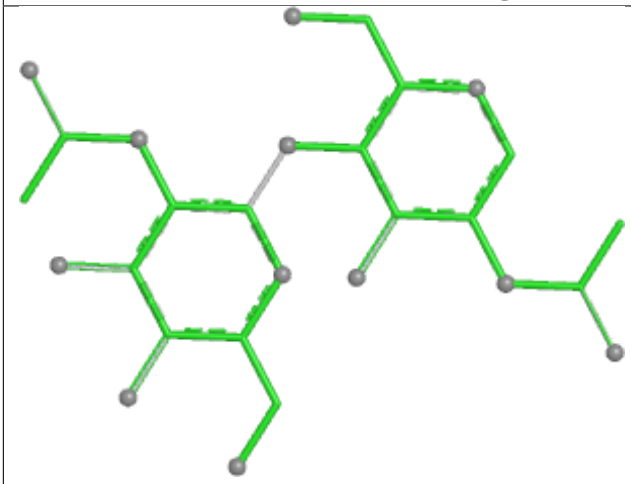


Torsions

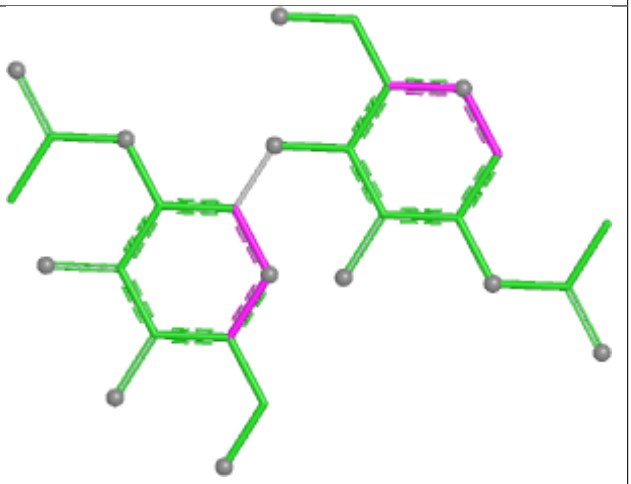


Rings

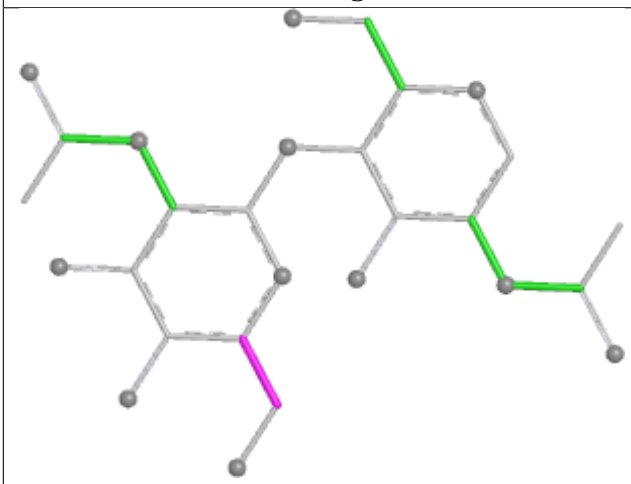
Oligosaccharide Chain E



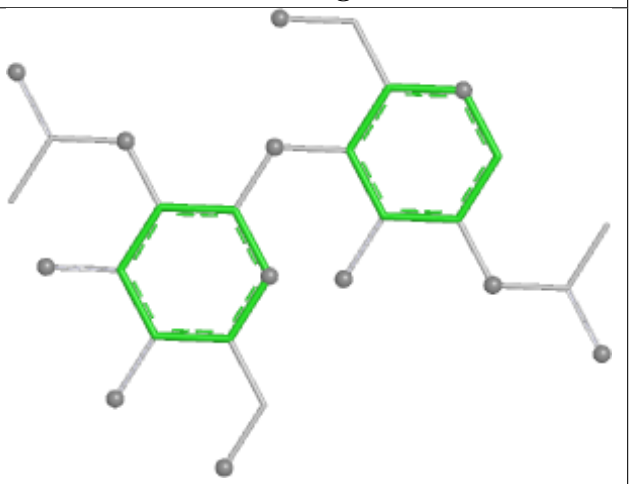
Bond lengths



Bond angles

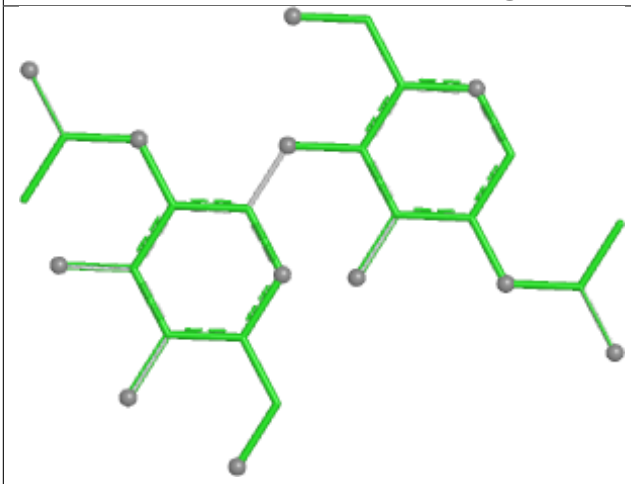


Torsions

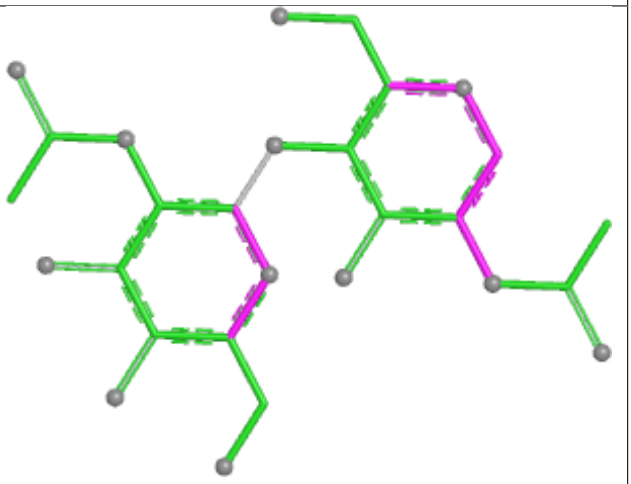


Rings

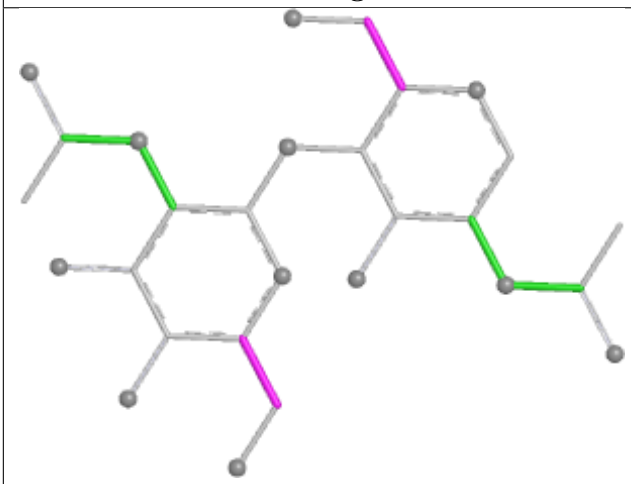
Oligosaccharide Chain I



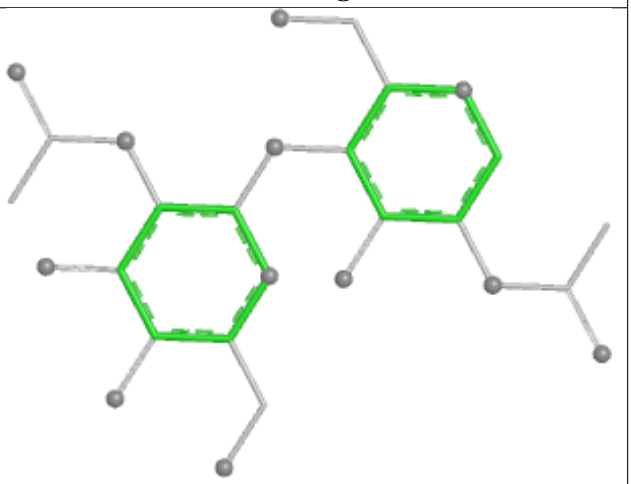
Bond lengths



Bond angles

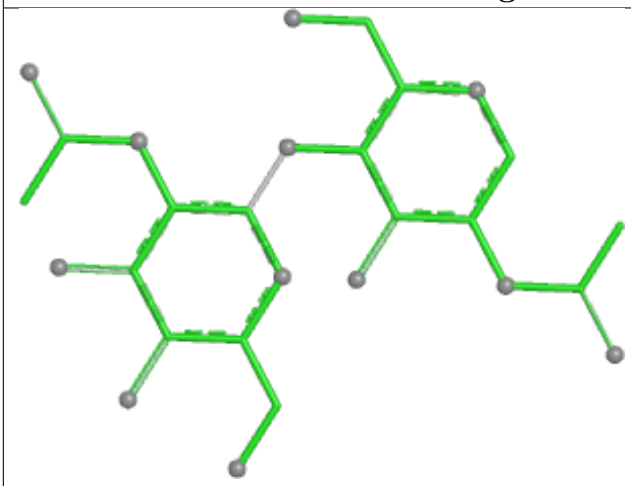


Torsions

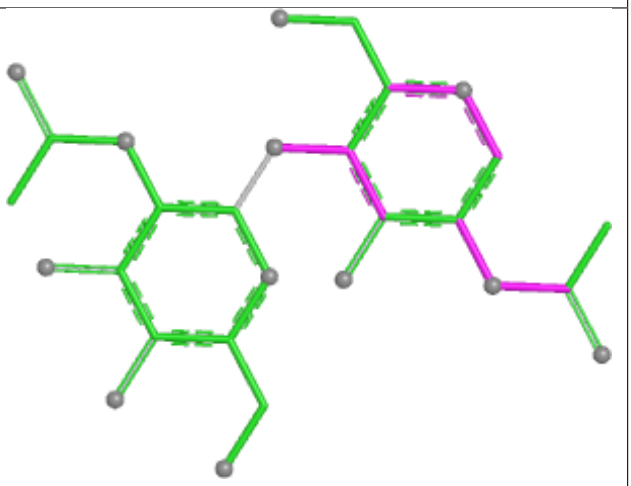


Rings

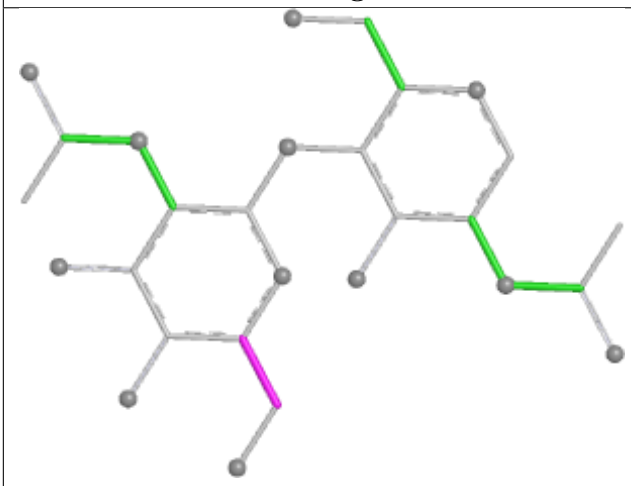
Oligosaccharide Chain J



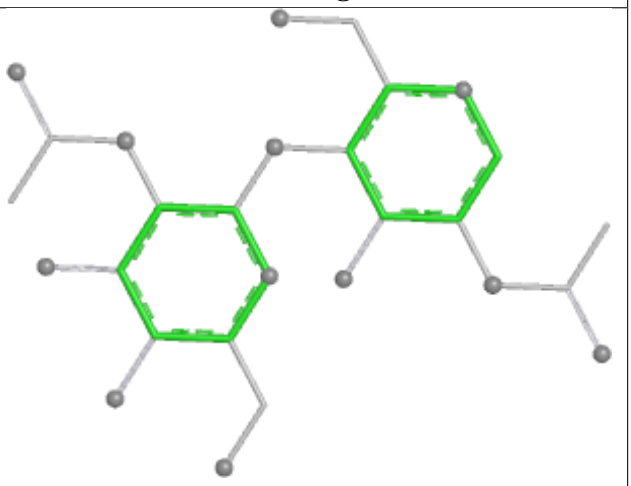
Bond lengths



Bond angles

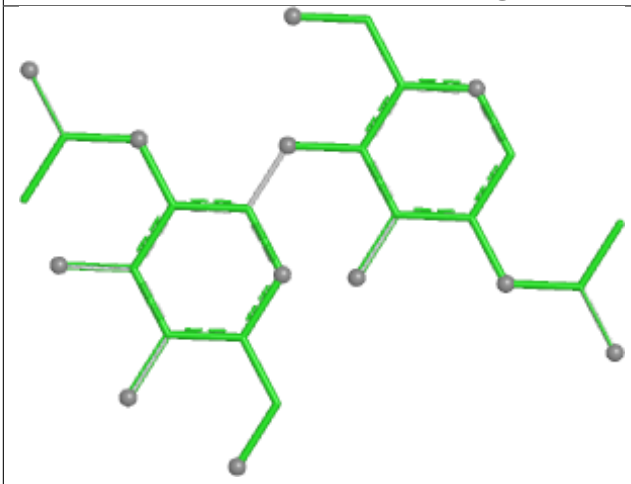


Torsions

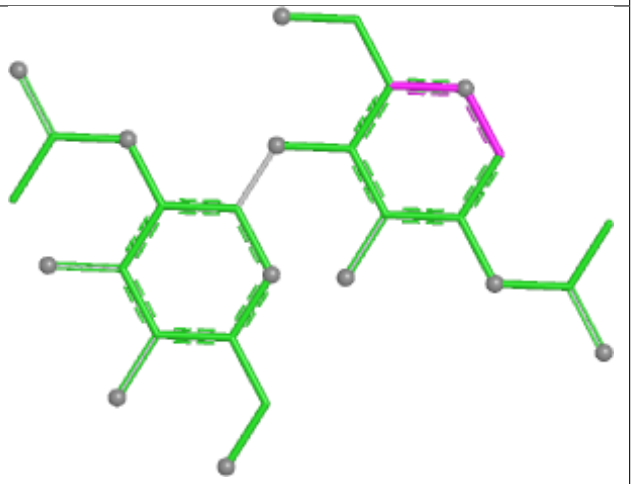


Rings

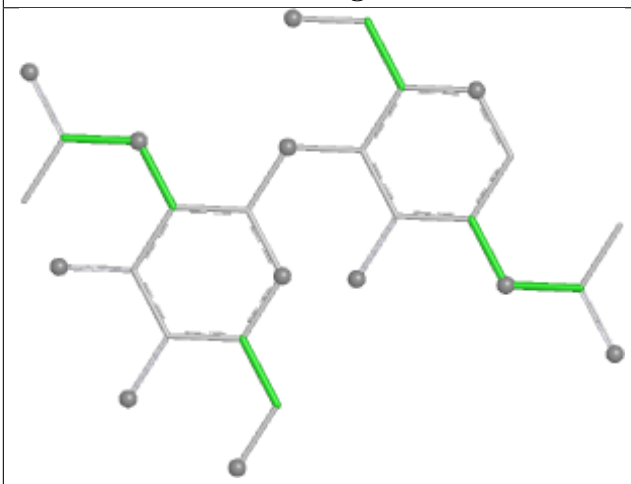
Oligosaccharide Chain K



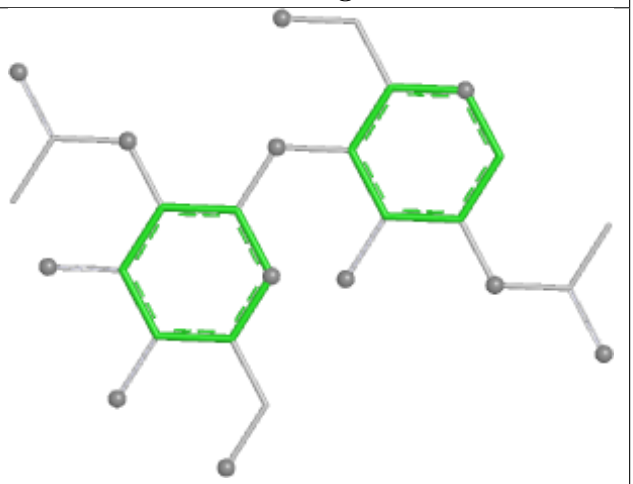
Bond lengths



Bond angles

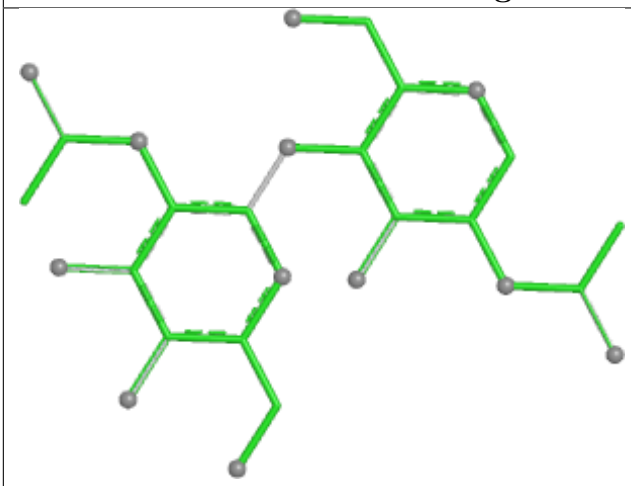


Torsions

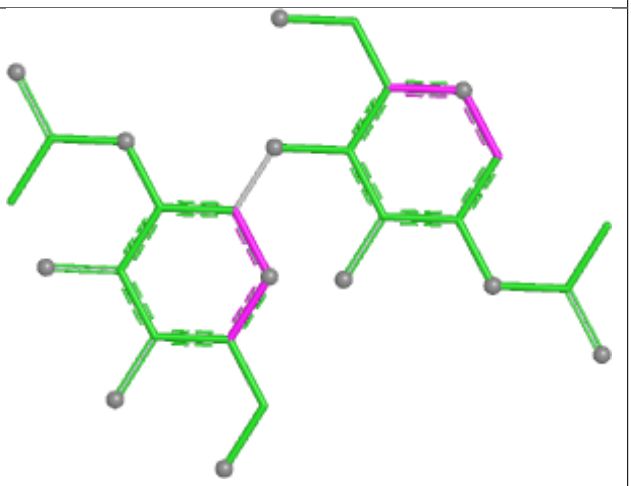


Rings

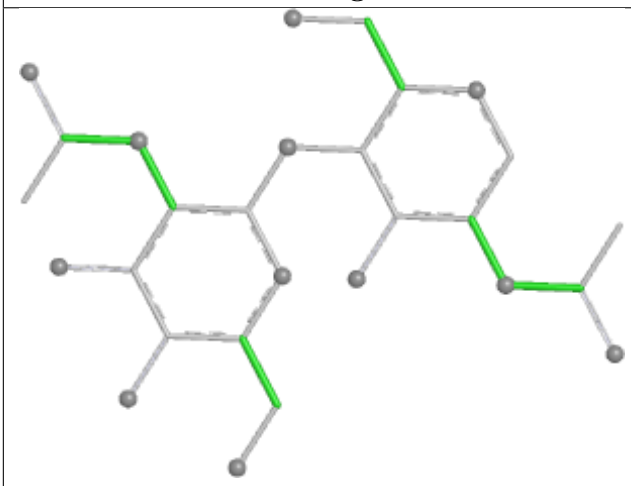
Oligosaccharide Chain O



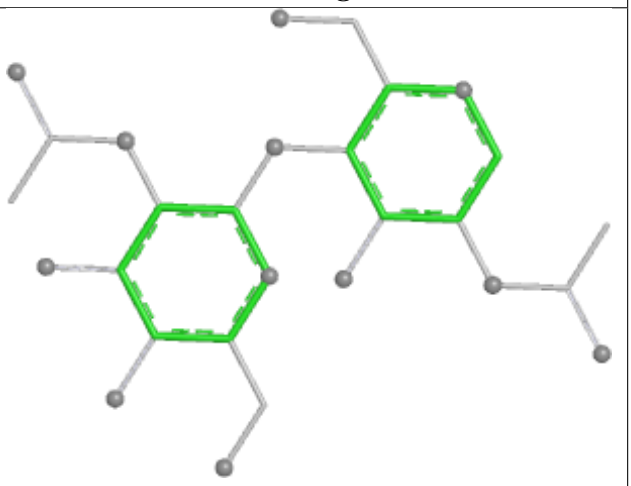
Bond lengths



Bond angles

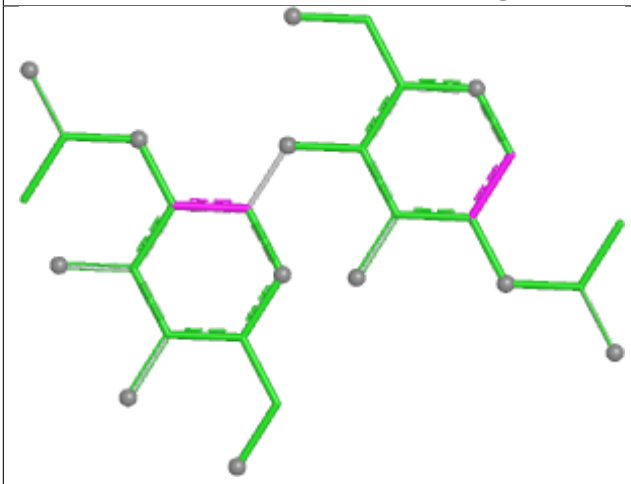


Torsions

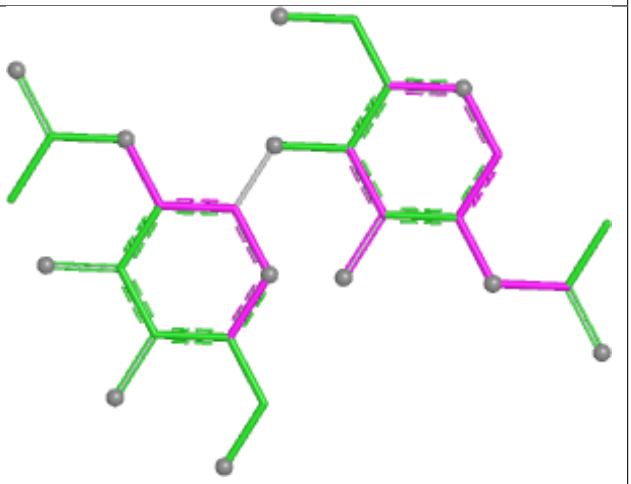


Rings

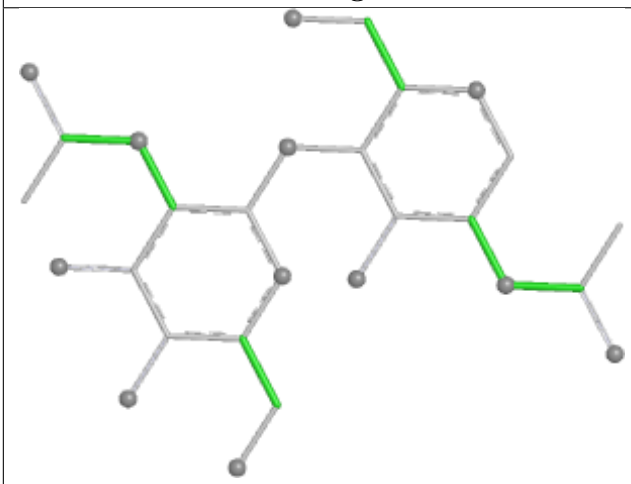
Oligosaccharide Chain R



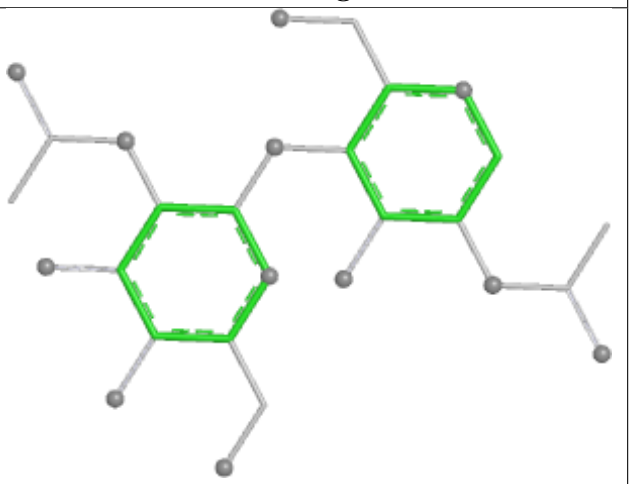
Bond lengths



Bond angles

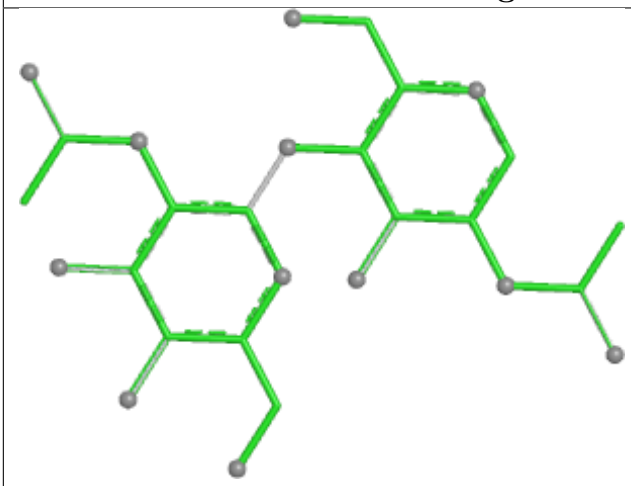


Torsions

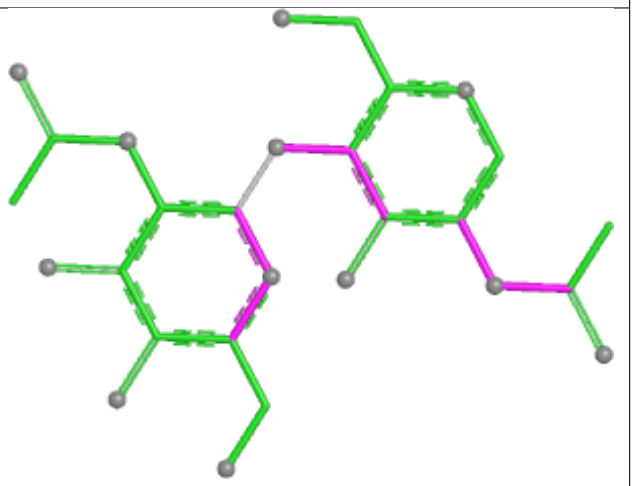


Rings

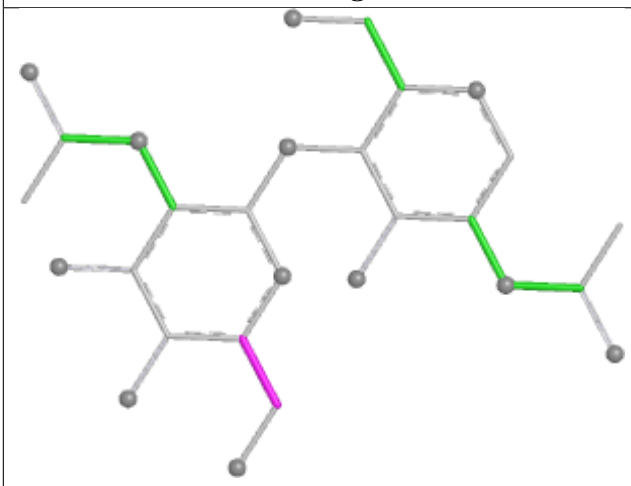
Oligosaccharide Chain S



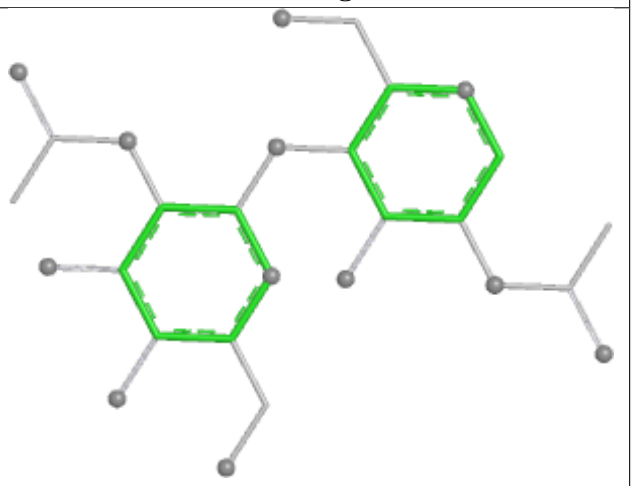
Bond lengths



Bond angles

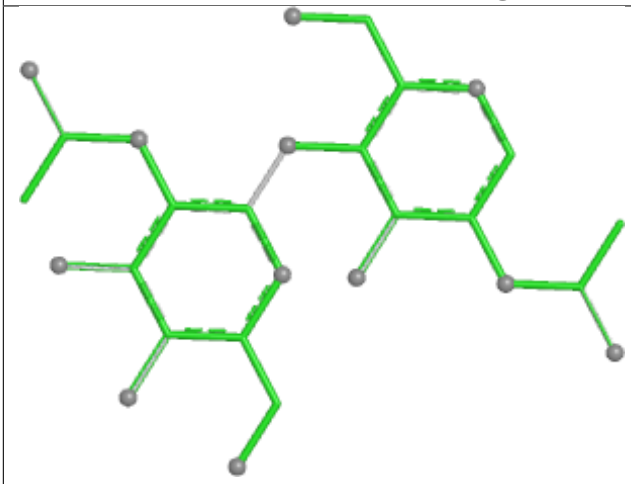


Torsions

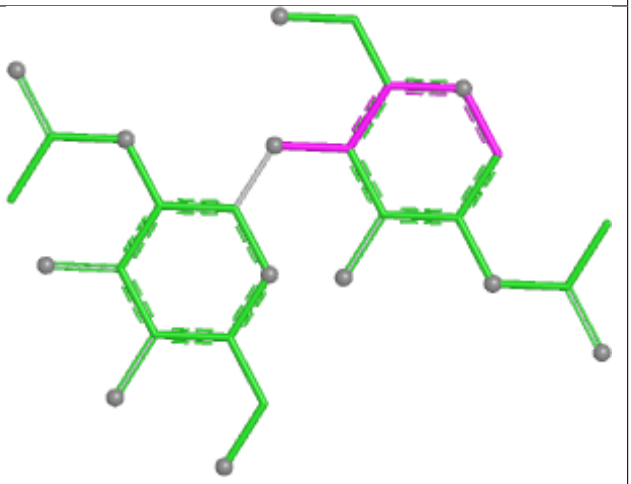


Rings

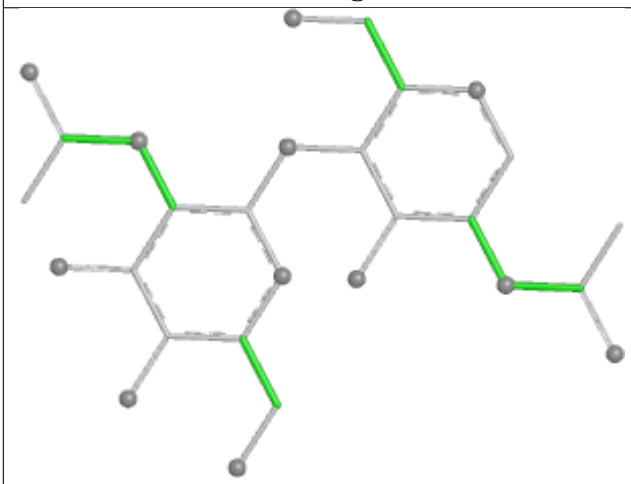
Oligosaccharide Chain V



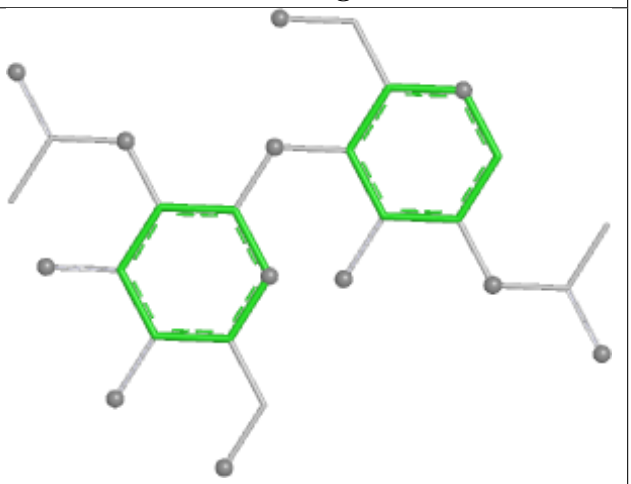
Bond lengths



Bond angles

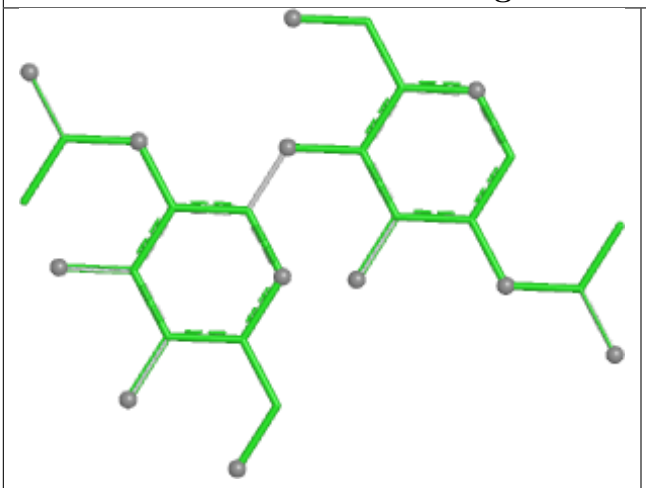


Torsions

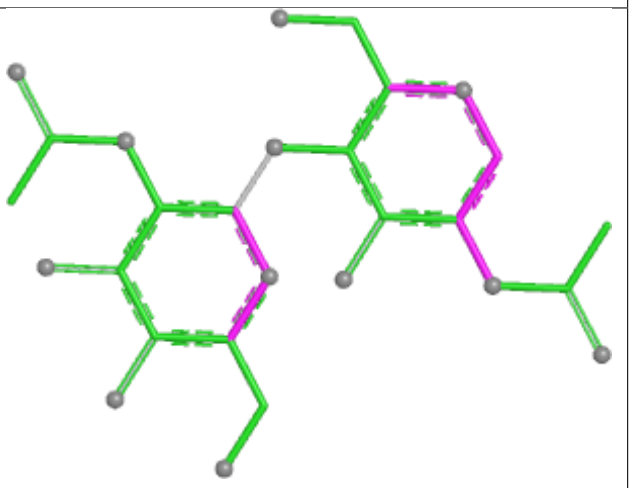


Rings

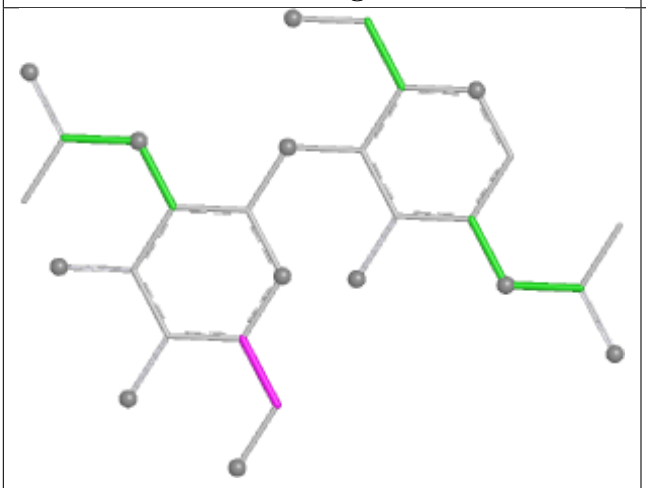
Oligosaccharide Chain X



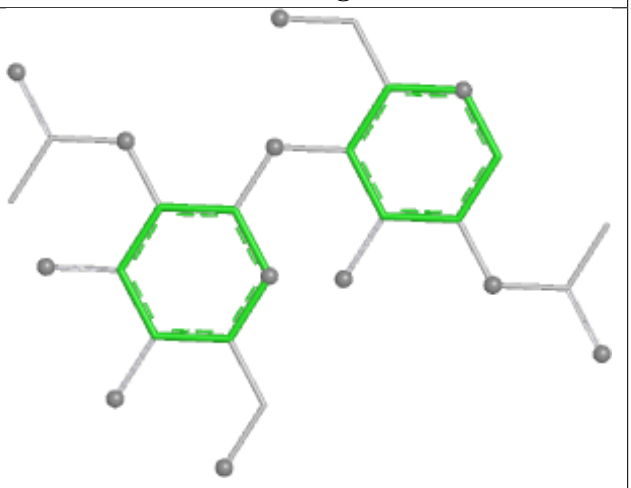
Bond lengths



Bond angles

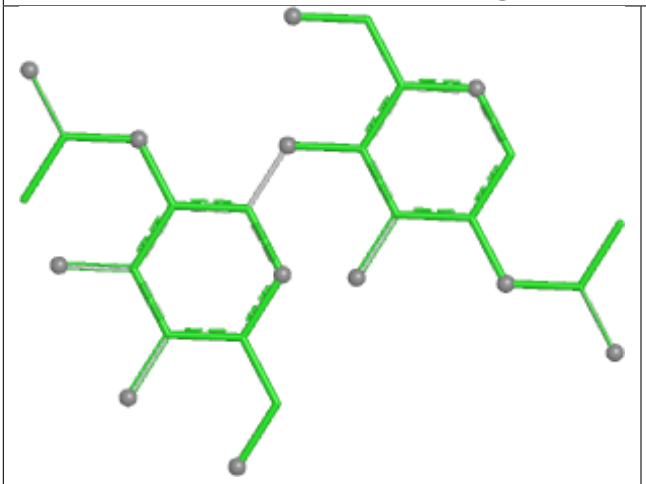


Torsions

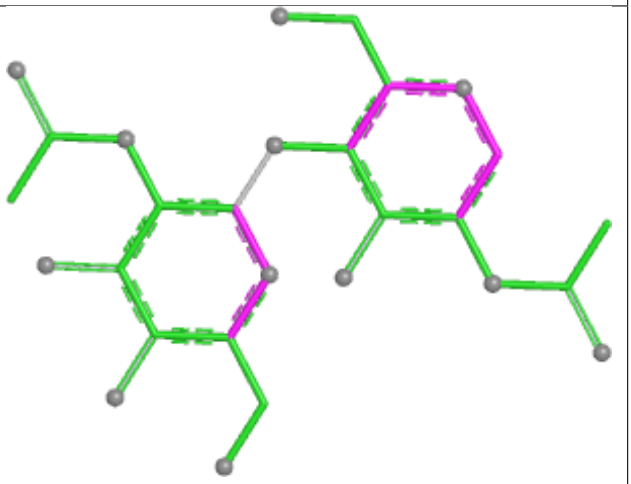


Rings

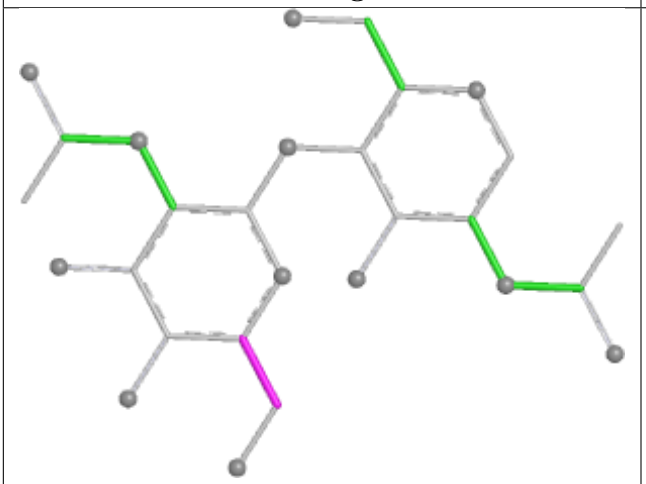
Oligosaccharide Chain Y



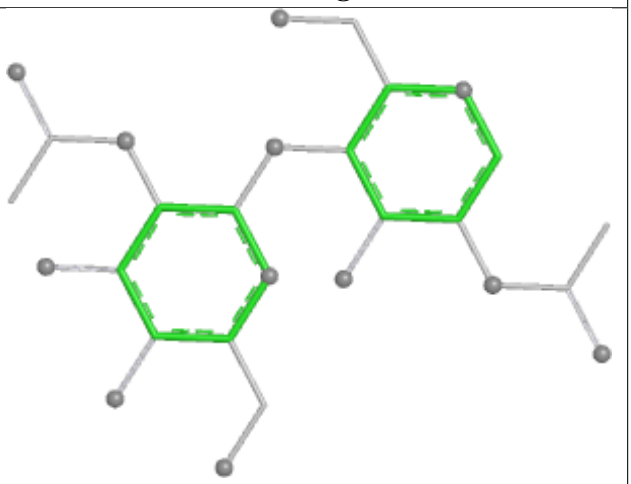
Bond lengths



Bond angles

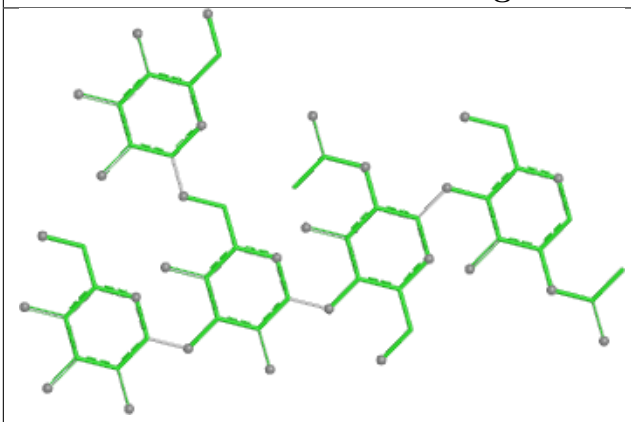


Torsions

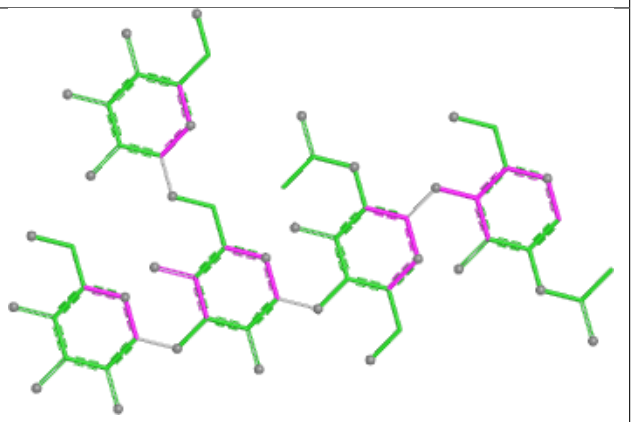


Rings

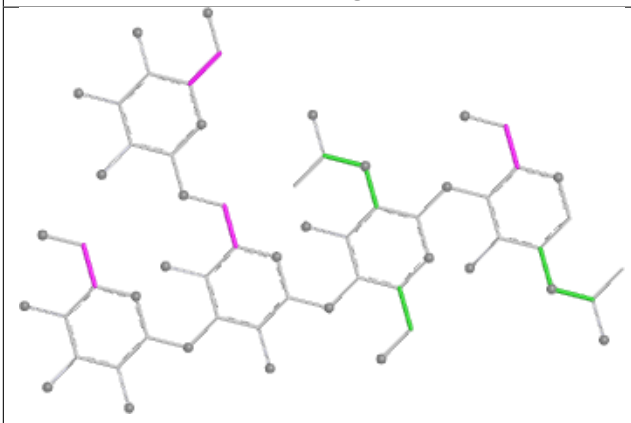
Oligosaccharide Chain G



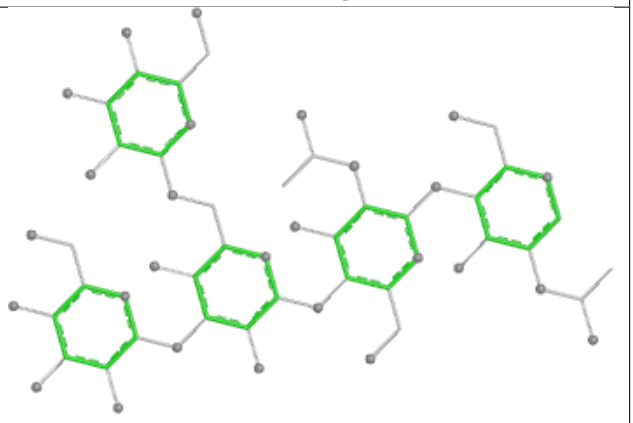
Bond lengths



Bond angles

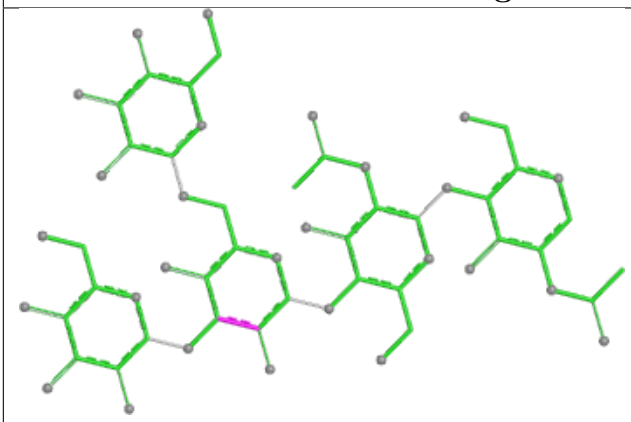


Torsions

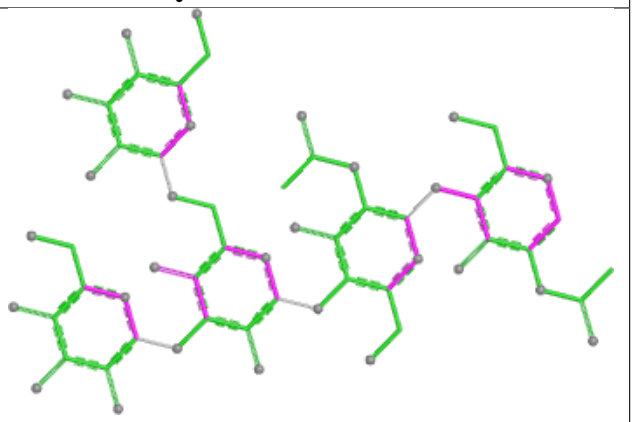


Rings

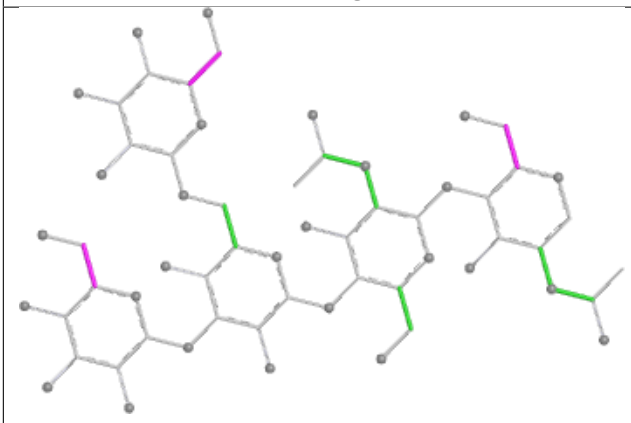
Oligosaccharide Chain Q



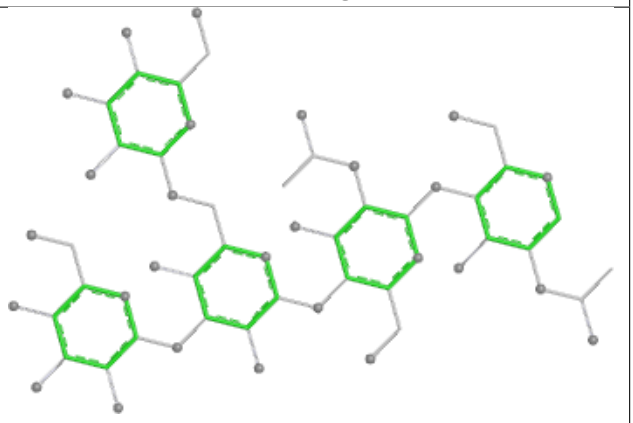
Bond lengths



Bond angles

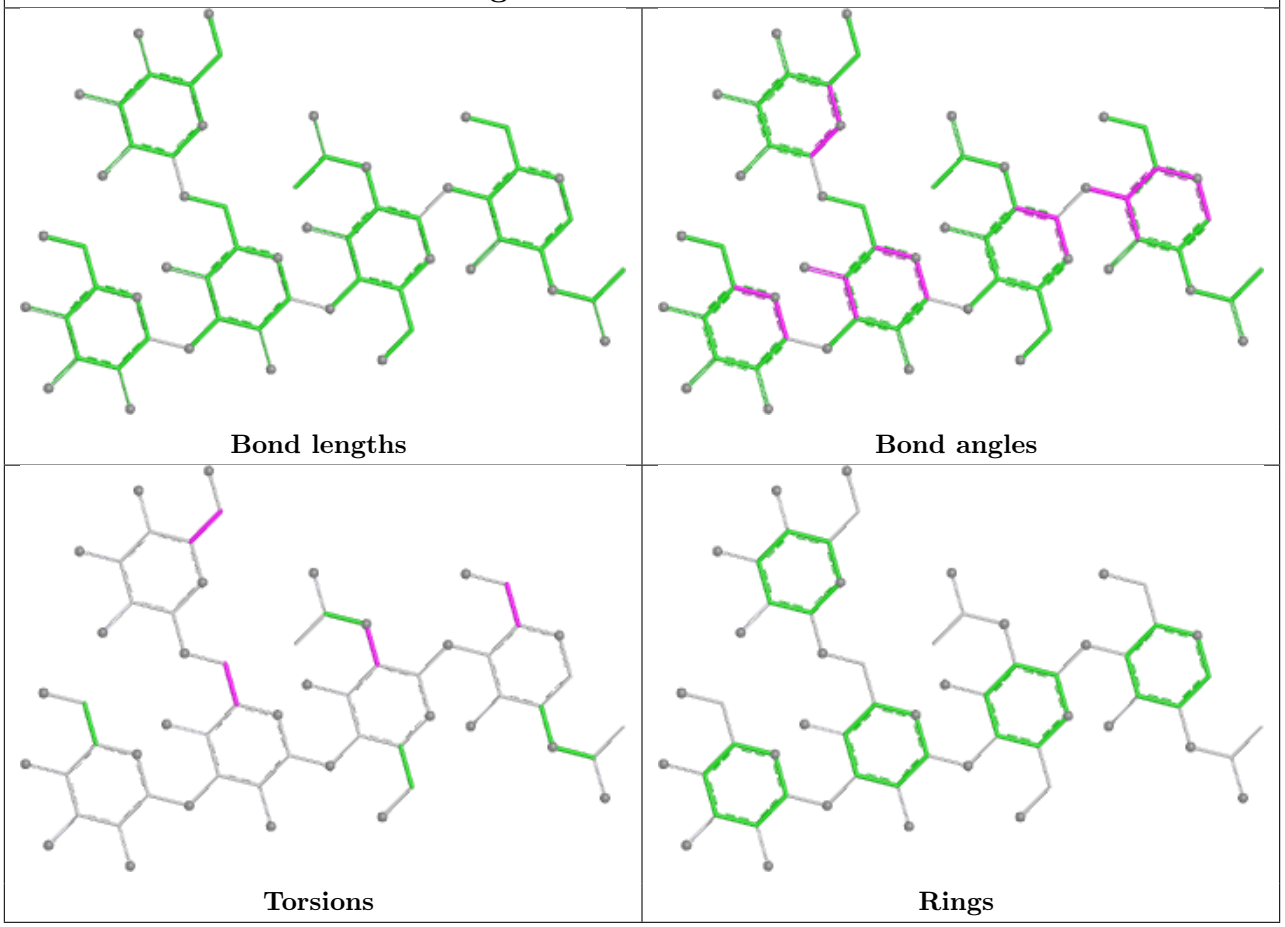


Torsions



Rings

Oligosaccharide Chain W



5.6 Ligand geometry (i)

40 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	$\#\|Z\| > 2$
7	NAG	C	1414	3	14,14,15	0.97	2 (14%)	17,19,21	1.49	2 (11%)
7	NAG	C	1412	3	14,14,15	0.73	0	17,19,21	0.99	1 (5%)
7	NAG	A	1403	3	14,14,15	0.67	0	17,19,21	0.91	0
7	NAG	A	1407	3	14,14,15	0.74	0	17,19,21	1.84	3 (17%)
7	NAG	C	1413	3	14,14,15	0.81	1 (7%)	17,19,21	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	B	1405	3	14,14,15	0.72	0	17,19,21	1.70	1 (5%)
7	NAG	A	1412	3	14,14,15	0.75	0	17,19,21	1.18	2 (11%)
7	NAG	A	1405	3	14,14,15	0.73	0	17,19,21	1.19	1 (5%)
7	NAG	A	1410	3	14,14,15	1.01	1 (7%)	17,19,21	1.63	3 (17%)
7	NAG	A	1401	3	14,14,15	0.77	1 (7%)	17,19,21	1.52	2 (11%)
7	NAG	C	1403	3	14,14,15	0.72	0	17,19,21	1.12	1 (5%)
7	NAG	C	1401	3	14,14,15	0.66	0	17,19,21	1.77	1 (5%)
7	NAG	B	1413	3	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
7	NAG	B	1404	3	14,14,15	0.68	0	17,19,21	0.89	0
7	NAG	B	1414	3	14,14,15	0.84	1 (7%)	17,19,21	1.18	2 (11%)
7	NAG	B	1403	3	14,14,15	0.71	0	17,19,21	1.10	1 (5%)
7	NAG	A	1409	3	14,14,15	0.69	0	17,19,21	0.98	1 (5%)
7	NAG	B	1407	3	14,14,15	0.70	0	17,19,21	0.84	0
7	NAG	A	1411	3	14,14,15	0.69	0	17,19,21	0.98	1 (5%)
7	NAG	A	1408	3	14,14,15	0.89	0	17,19,21	2.32	3 (17%)
7	NAG	A	1406	3	14,14,15	0.78	0	17,19,21	1.24	2 (11%)
7	NAG	C	1406	3	14,14,15	0.71	0	17,19,21	1.00	1 (5%)
7	NAG	C	1407	3	14,14,15	0.72	0	17,19,21	0.92	0
7	NAG	B	1411	3	14,14,15	0.76	0	17,19,21	0.91	1 (5%)
7	NAG	B	1406	3	14,14,15	0.70	0	17,19,21	1.02	1 (5%)
7	NAG	B	1408	3	14,14,15	0.74	0	17,19,21	1.15	1 (5%)
7	NAG	B	1410	3	14,14,15	0.70	0	17,19,21	0.95	1 (5%)
7	NAG	C	1404	3	14,14,15	0.74	0	17,19,21	0.92	1 (5%)
7	NAG	B	1402	3	14,14,15	0.70	0	17,19,21	0.87	1 (5%)
7	NAG	C	1408	3	14,14,15	0.63	0	17,19,21	1.43	1 (5%)
7	NAG	C	1411	3	14,14,15	0.68	0	17,19,21	0.90	1 (5%)
7	NAG	B	1409	3	14,14,15	0.72	0	17,19,21	1.19	2 (11%)
7	NAG	A	1402	3	14,14,15	0.71	0	17,19,21	0.96	1 (5%)
7	NAG	B	1412	3	14,14,15	0.69	0	17,19,21	0.96	1 (5%)
7	NAG	B	1401	3	14,14,15	0.76	0	17,19,21	1.22	1 (5%)
7	NAG	A	1404	3	14,14,15	0.72	0	17,19,21	1.08	1 (5%)
7	NAG	C	1405	3	14,14,15	0.69	0	17,19,21	1.05	1 (5%)
7	NAG	C	1409	3	14,14,15	0.70	0	17,19,21	1.00	1 (5%)
7	NAG	C	1410	3	14,14,15	0.78	0	17,19,21	0.90	1 (5%)
7	NAG	C	1402	3	14,14,15	0.77	0	17,19,21	1.13	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	1414	3	-	1/6/23/26	0/1/1/1
7	NAG	C	1412	3	-	1/6/23/26	0/1/1/1
7	NAG	A	1403	3	-	1/6/23/26	0/1/1/1
7	NAG	A	1407	3	-	1/6/23/26	0/1/1/1
7	NAG	C	1413	3	-	0/6/23/26	0/1/1/1
7	NAG	B	1405	3	-	1/6/23/26	0/1/1/1
7	NAG	A	1412	3	-	0/6/23/26	0/1/1/1
7	NAG	A	1405	3	-	0/6/23/26	0/1/1/1
7	NAG	A	1410	3	-	2/6/23/26	0/1/1/1
7	NAG	A	1401	3	-	0/6/23/26	0/1/1/1
7	NAG	C	1403	3	-	1/6/23/26	0/1/1/1
7	NAG	C	1401	3	-	0/6/23/26	0/1/1/1
7	NAG	B	1413	3	-	0/6/23/26	0/1/1/1
7	NAG	B	1404	3	-	1/6/23/26	0/1/1/1
7	NAG	B	1414	3	-	0/6/23/26	0/1/1/1
7	NAG	B	1403	3	-	1/6/23/26	0/1/1/1
7	NAG	A	1409	3	-	1/6/23/26	0/1/1/1
7	NAG	B	1407	3	-	1/6/23/26	0/1/1/1
7	NAG	A	1411	3	-	0/6/23/26	0/1/1/1
7	NAG	A	1408	3	-	0/6/23/26	0/1/1/1
7	NAG	A	1406	3	-	0/6/23/26	0/1/1/1
7	NAG	C	1406	3	-	0/6/23/26	0/1/1/1
7	NAG	C	1407	3	-	0/6/23/26	0/1/1/1
7	NAG	B	1411	3	-	0/6/23/26	0/1/1/1
7	NAG	B	1406	3	-	0/6/23/26	0/1/1/1
7	NAG	B	1408	3	-	1/6/23/26	0/1/1/1
7	NAG	B	1410	3	-	0/6/23/26	0/1/1/1
7	NAG	C	1404	3	-	1/6/23/26	0/1/1/1
7	NAG	B	1402	3	-	0/6/23/26	0/1/1/1
7	NAG	C	1408	3	-	0/6/23/26	0/1/1/1
7	NAG	C	1411	3	-	0/6/23/26	0/1/1/1
7	NAG	B	1409	3	-	1/6/23/26	0/1/1/1
7	NAG	A	1402	3	-	0/6/23/26	0/1/1/1
7	NAG	B	1412	3	-	1/6/23/26	0/1/1/1
7	NAG	B	1401	3	-	1/6/23/26	0/1/1/1
7	NAG	A	1404	3	-	0/6/23/26	0/1/1/1
7	NAG	C	1405	3	-	1/6/23/26	0/1/1/1
7	NAG	C	1409	3	-	0/6/23/26	0/1/1/1
7	NAG	C	1410	3	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	1402	3	-	1/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1410	NAG	C1-C2	3.31	1.56	1.52
7	A	1401	NAG	C1-C2	2.46	1.55	1.52
7	B	1414	NAG	C1-C2	2.37	1.55	1.52
7	C	1413	NAG	C1-C2	2.20	1.55	1.52
7	C	1414	NAG	C1-C2	2.07	1.55	1.52

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1408	NAG	O5-C1-C2	-6.95	100.54	111.29
7	B	1405	NAG	C1-O5-C5	6.38	120.73	112.19
7	C	1401	NAG	C1-O5-C5	6.32	120.66	112.19
7	C	1408	NAG	C1-O5-C5	5.17	119.11	112.19
7	A	1407	NAG	C1-O5-C5	5.02	118.92	112.19

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1410	NAG	C8-C7-N2-C2
7	A	1410	NAG	O7-C7-N2-C2
7	B	1404	NAG	O5-C5-C6-O6
7	A	1409	NAG	O5-C5-C6-O6
7	C	1414	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.

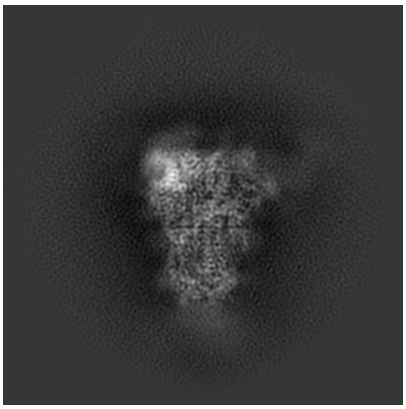
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73659. These allow visual inspection of the internal detail of the map and identification of artifacts.

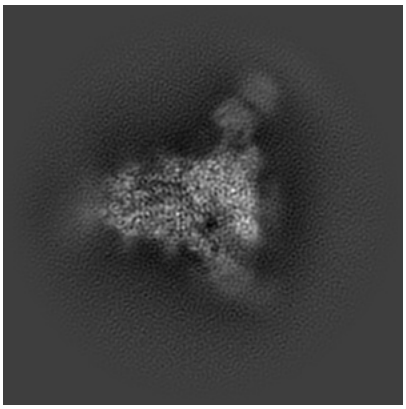
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

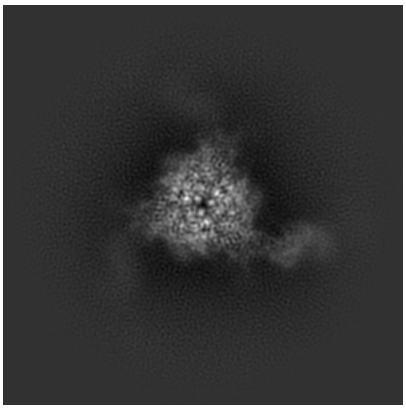
6.1.1 Primary map



X

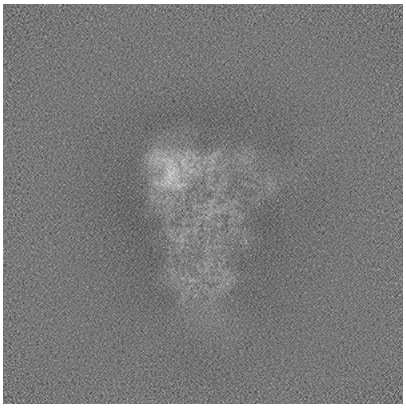


Y

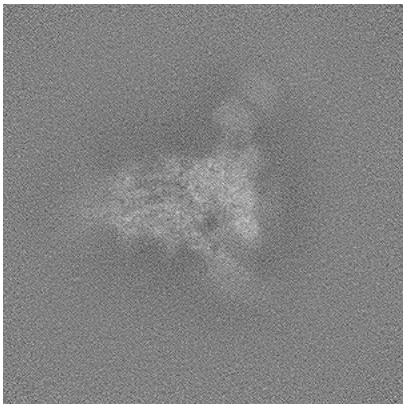


Z

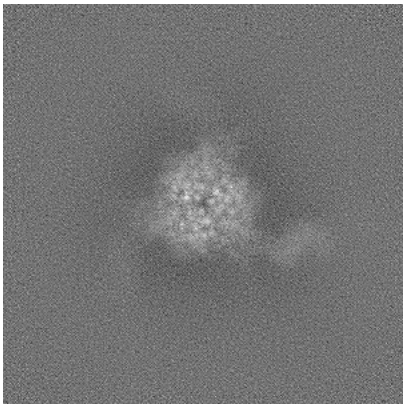
6.1.2 Raw map



X



Y

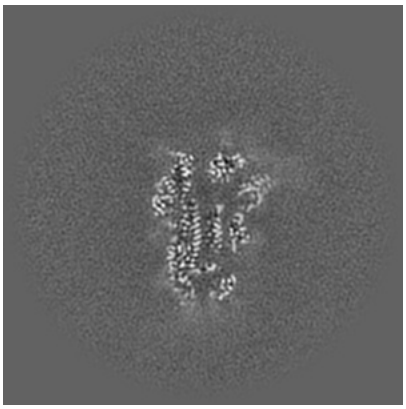


Z

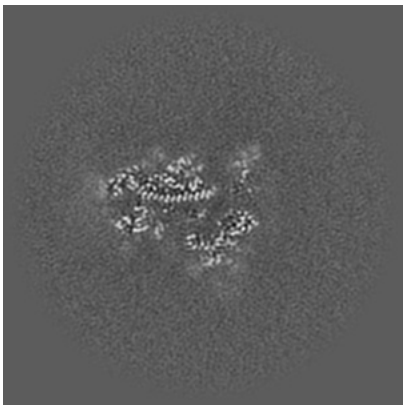
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

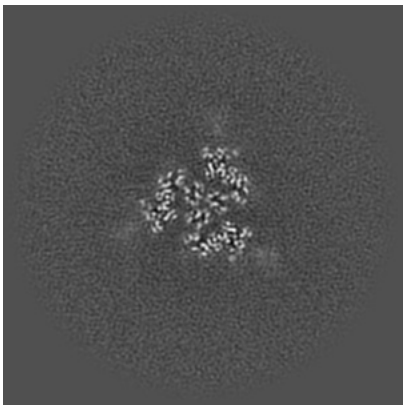
6.2.1 Primary map



X Index: 256

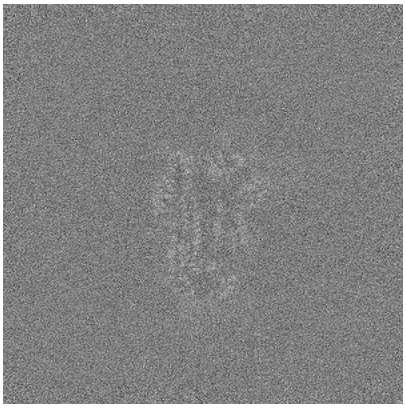


Y Index: 256

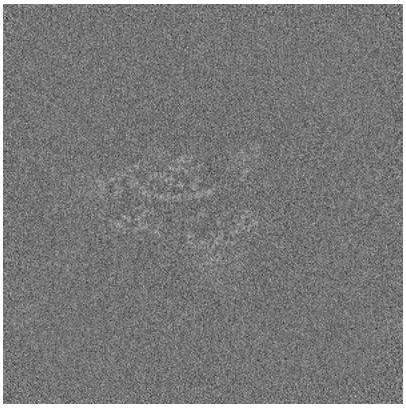


Z Index: 256

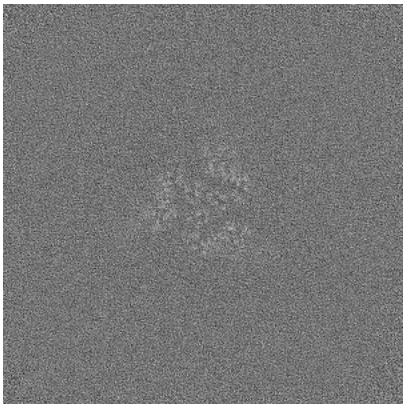
6.2.2 Raw map



X Index: 256



Y Index: 256

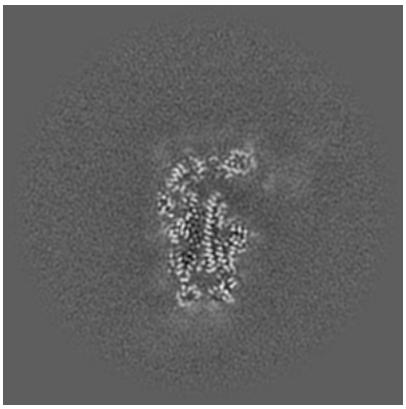


Z Index: 256

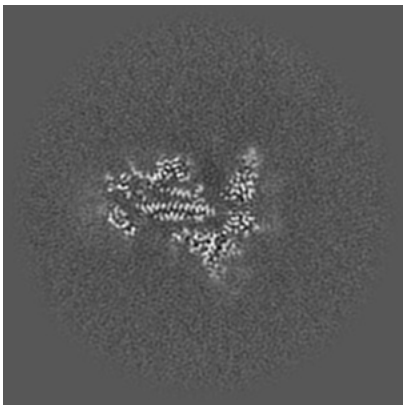
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

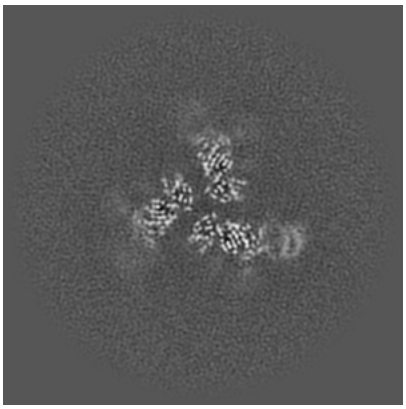
6.3.1 Primary map



X Index: 247

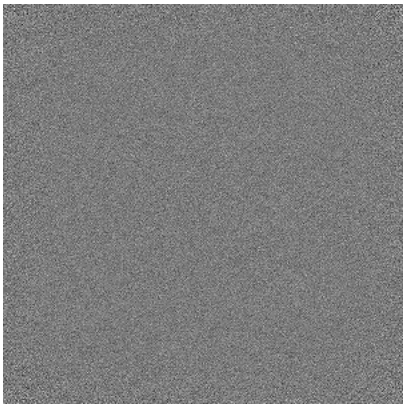


Y Index: 245

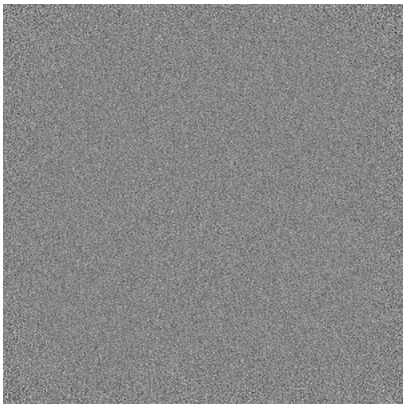


Z Index: 280

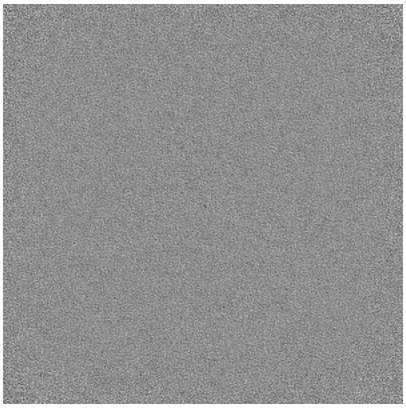
6.3.2 Raw map



X Index: 0



Y Index: 0

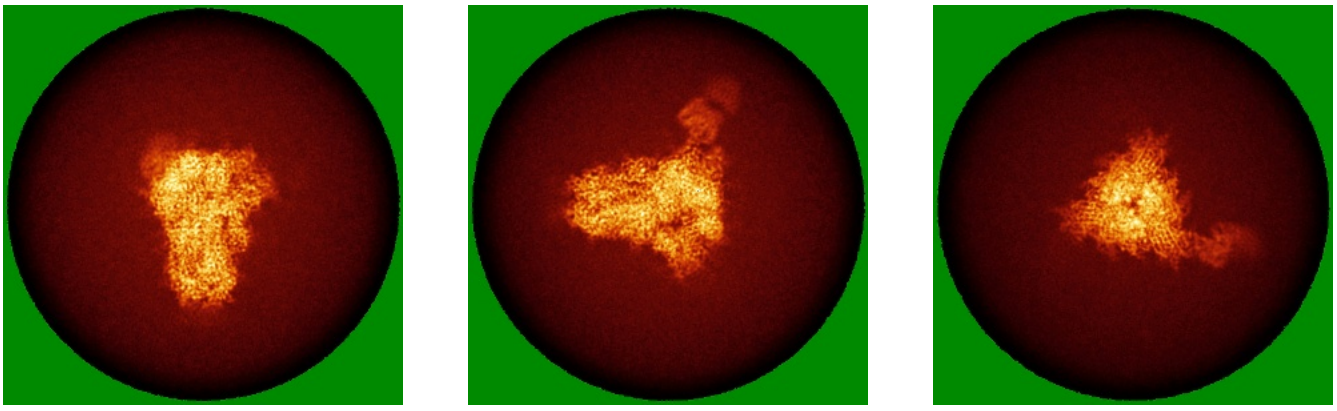


Z Index: 0

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

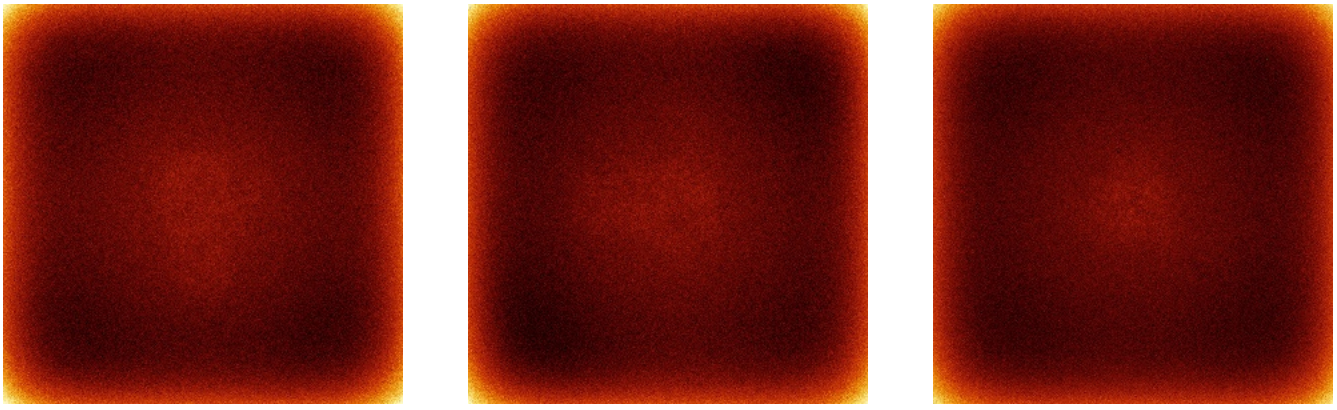
6.4 Orthogonal standard-deviation projections (False-color) (i)

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)

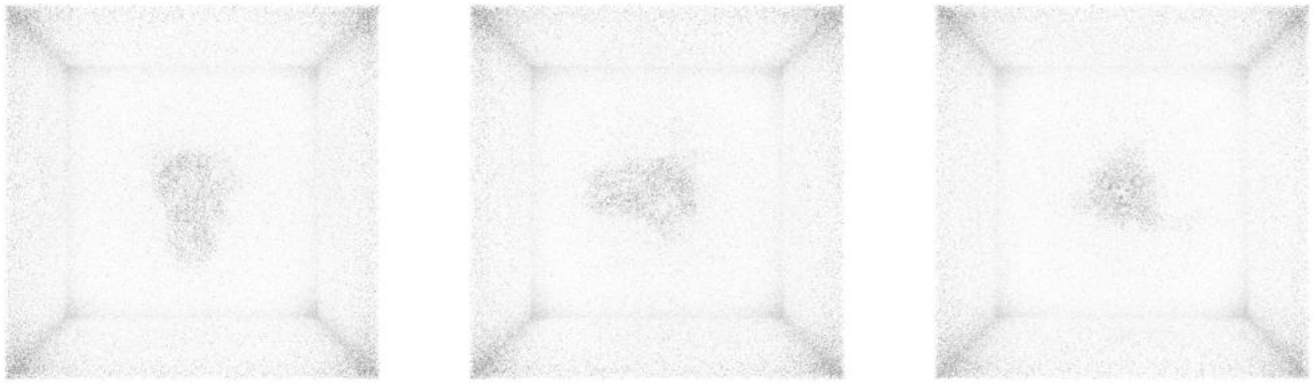
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.062. 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.

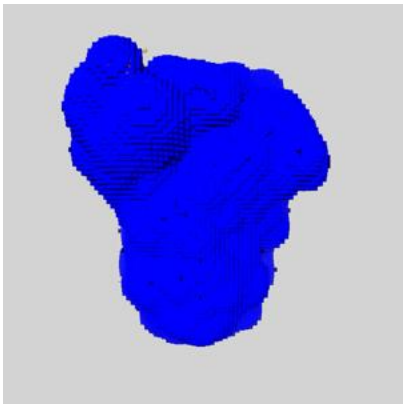
6.6 Mask visualisation (i)

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

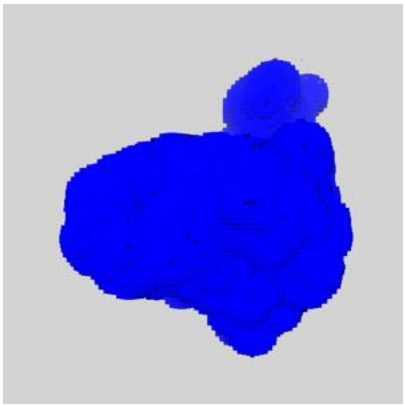
A mask typically either:

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

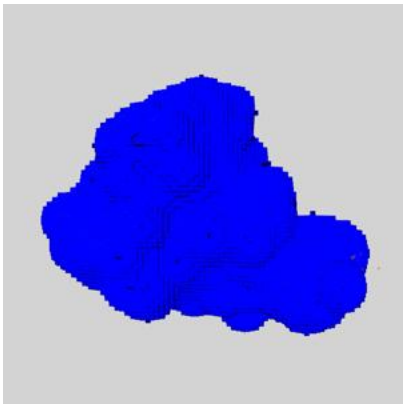
6.6.1 emd_73659_msk_1.map (i)



X



Y

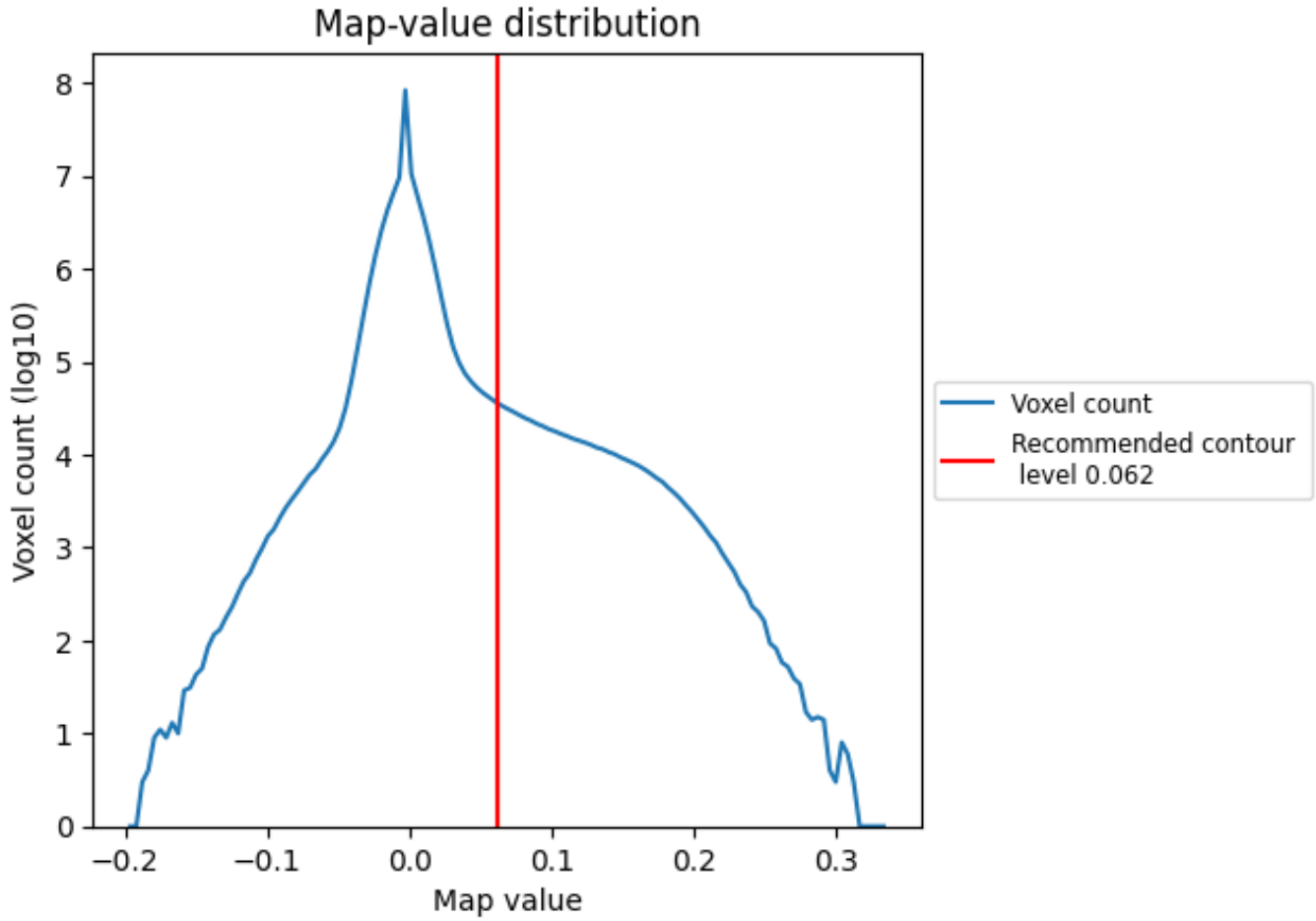


Z

7 Map analysis

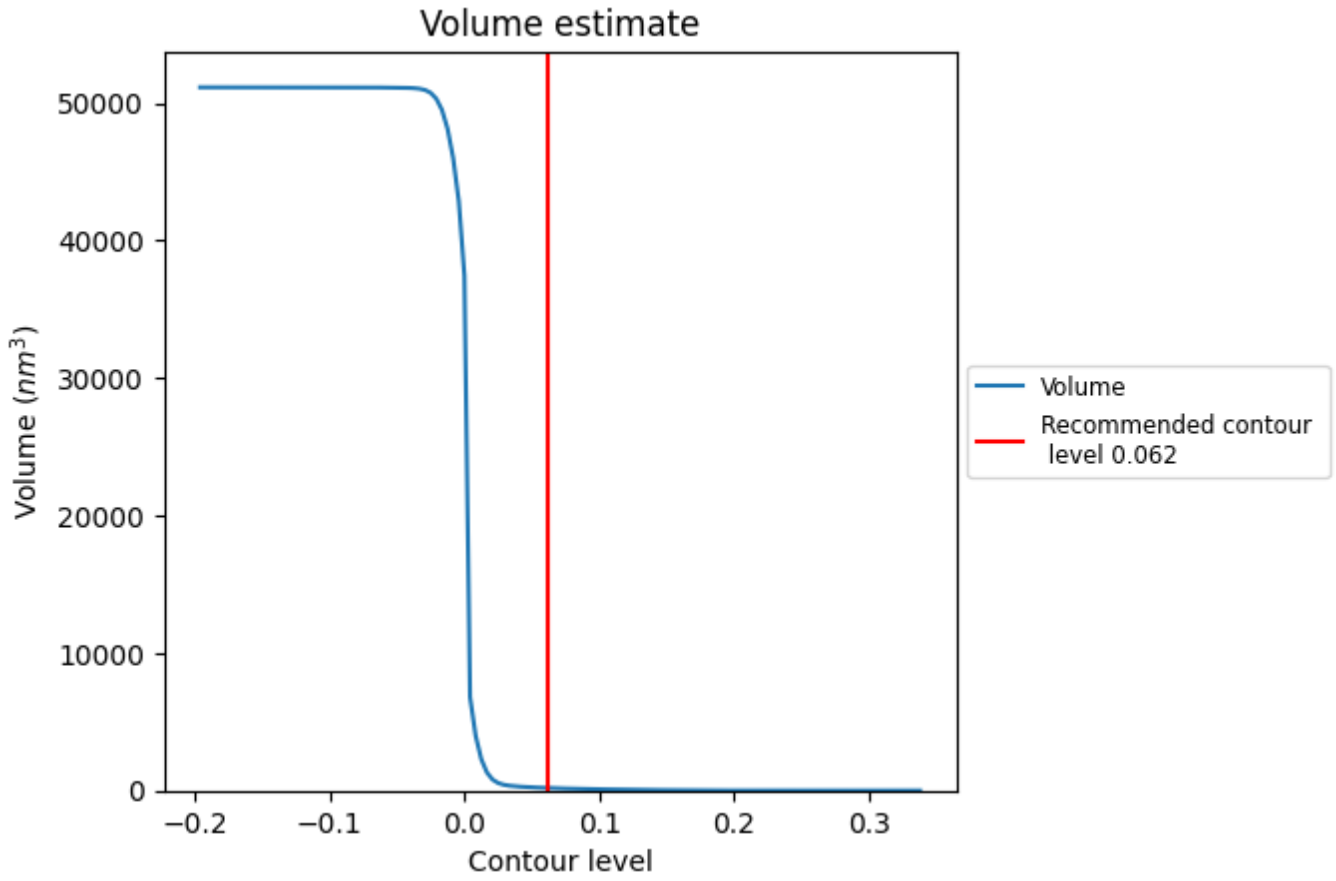
This section contains the results of statistical analysis of the map.

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.

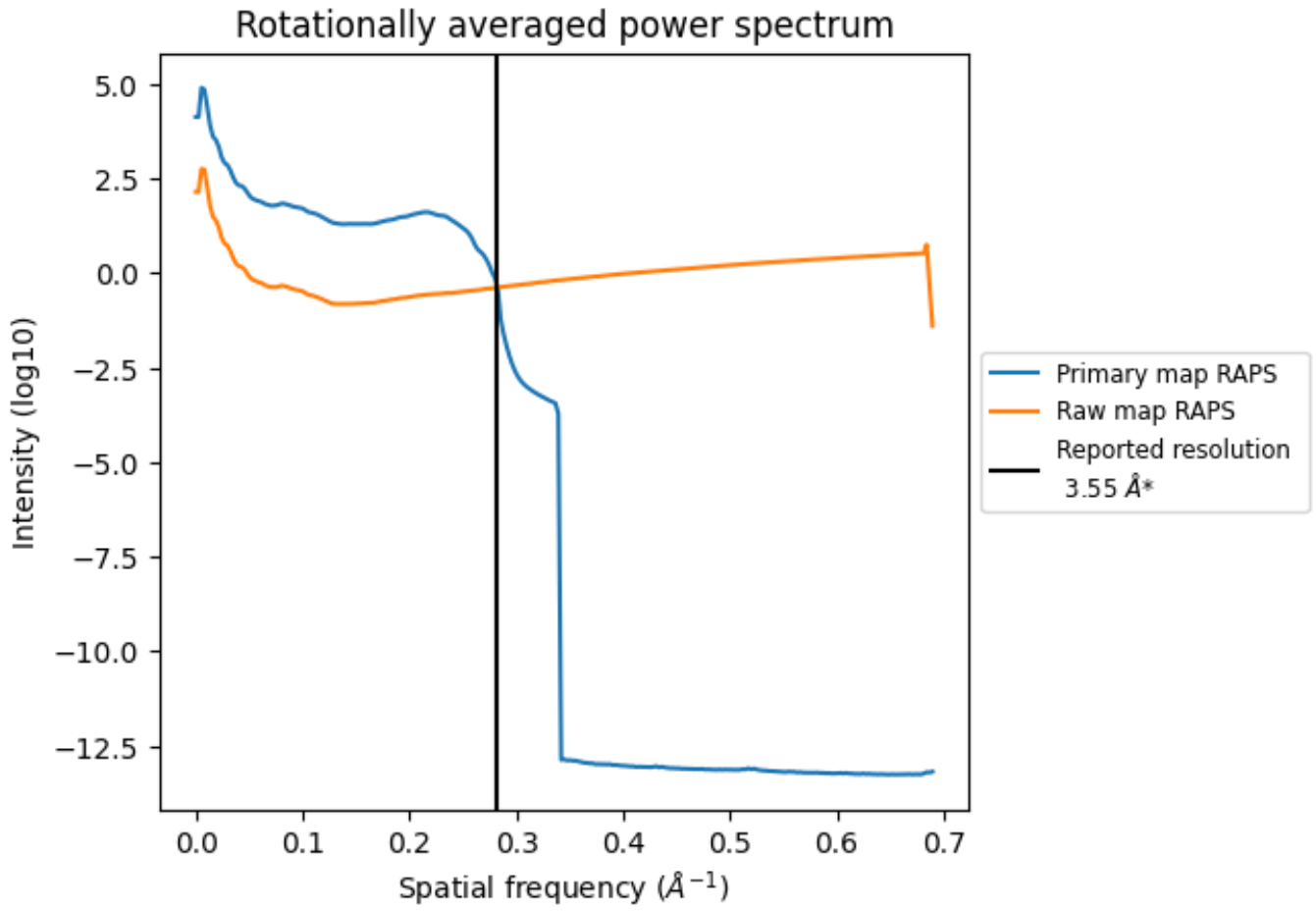
7.2 Volume estimate (i)



The volume at the recommended contour level is 185 nm^3; this corresponds to an approximate mass of 167 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)

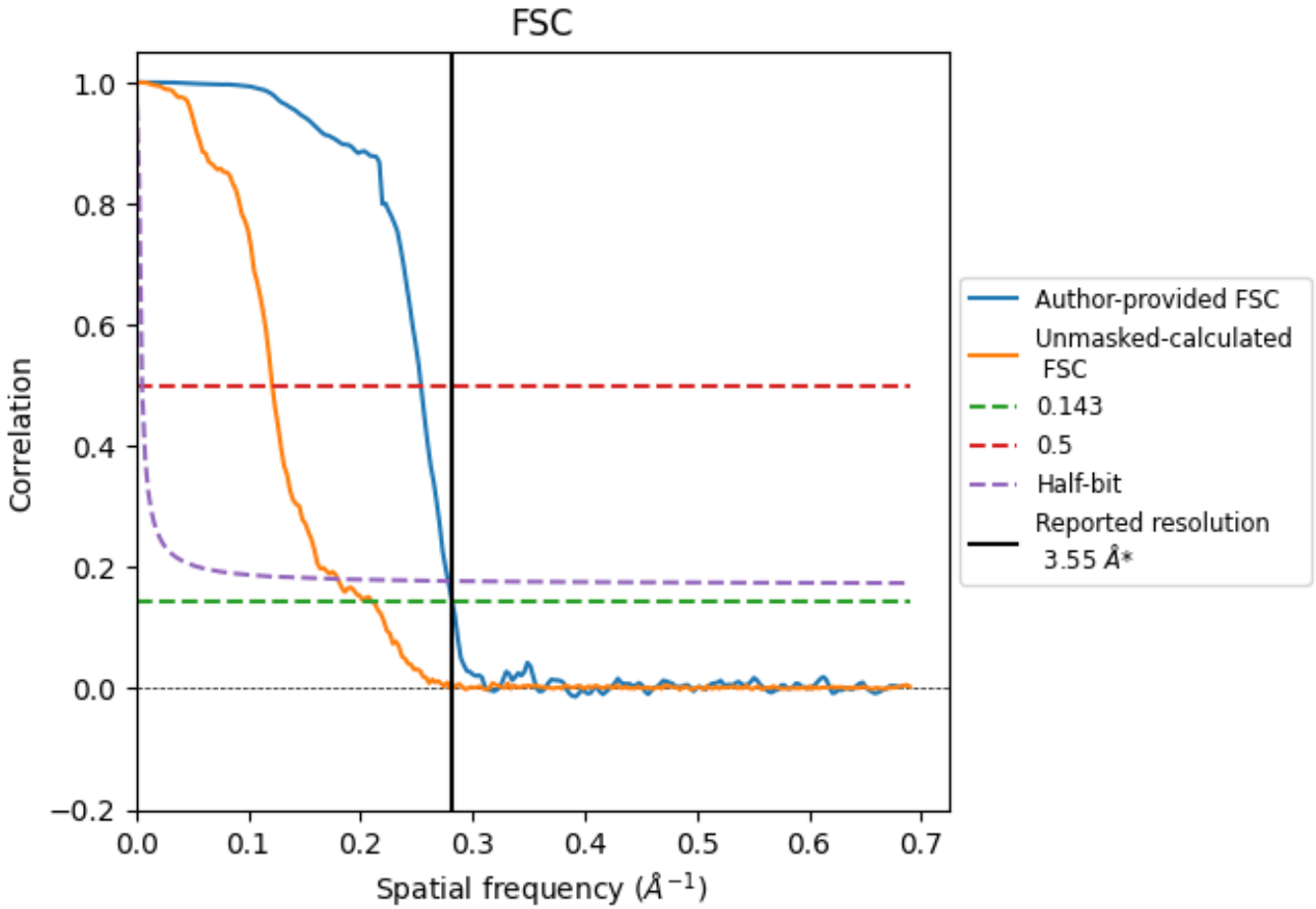


*Reported resolution corresponds to spatial frequency of 0.282 Å^{-1}

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 0.282 Å^{-1}

8.2 Resolution estimates (i)

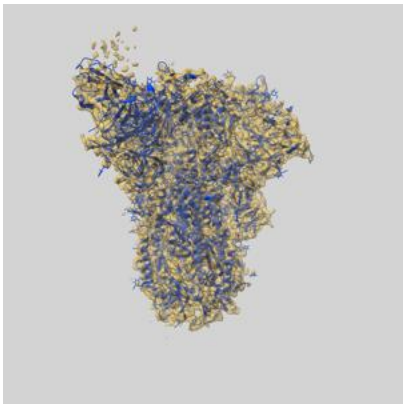
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.55	-	-
Author-provided FSC curve	3.55	3.94	3.59
Unmasked-calculated*	4.75	8.24	5.56

*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 4.75 differs from the reported value 3.55 by more than 10 %

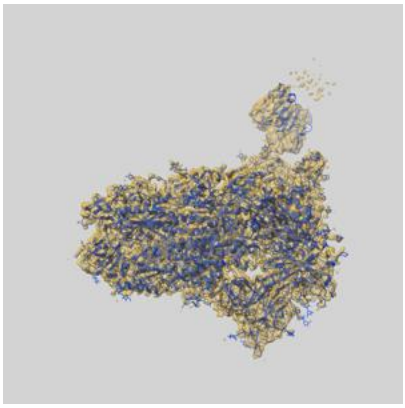
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73659 and PDB model 9YYY. Per-residue inclusion information can be found in section 3 on page 12.

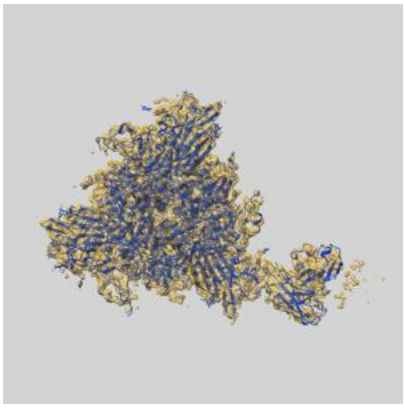
9.1 Map-model overlay



X



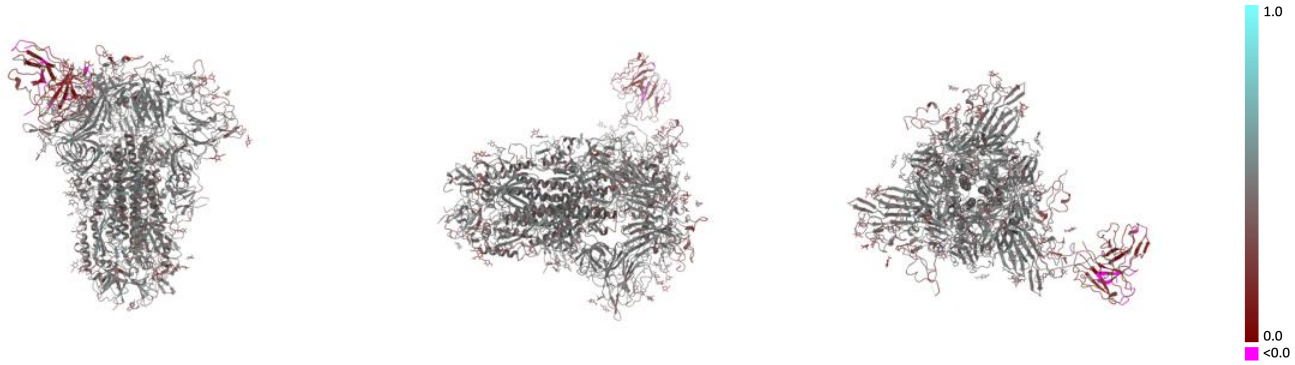
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.062 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

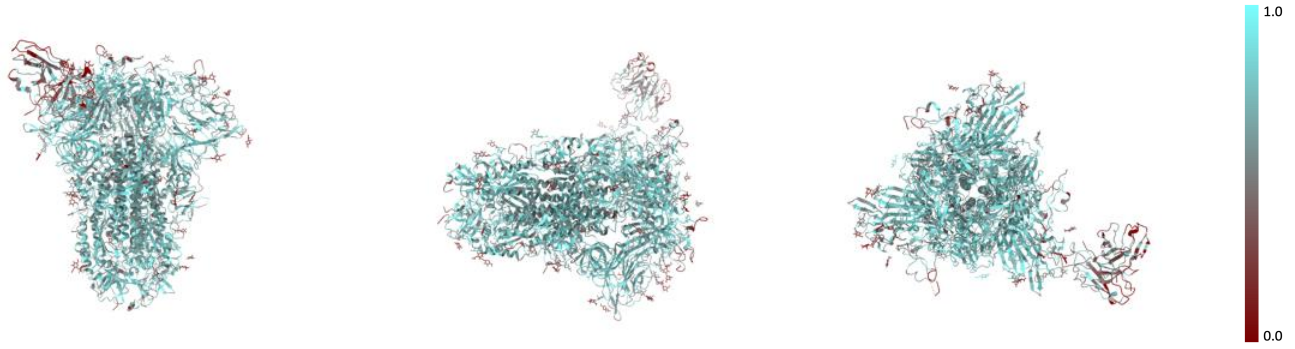
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

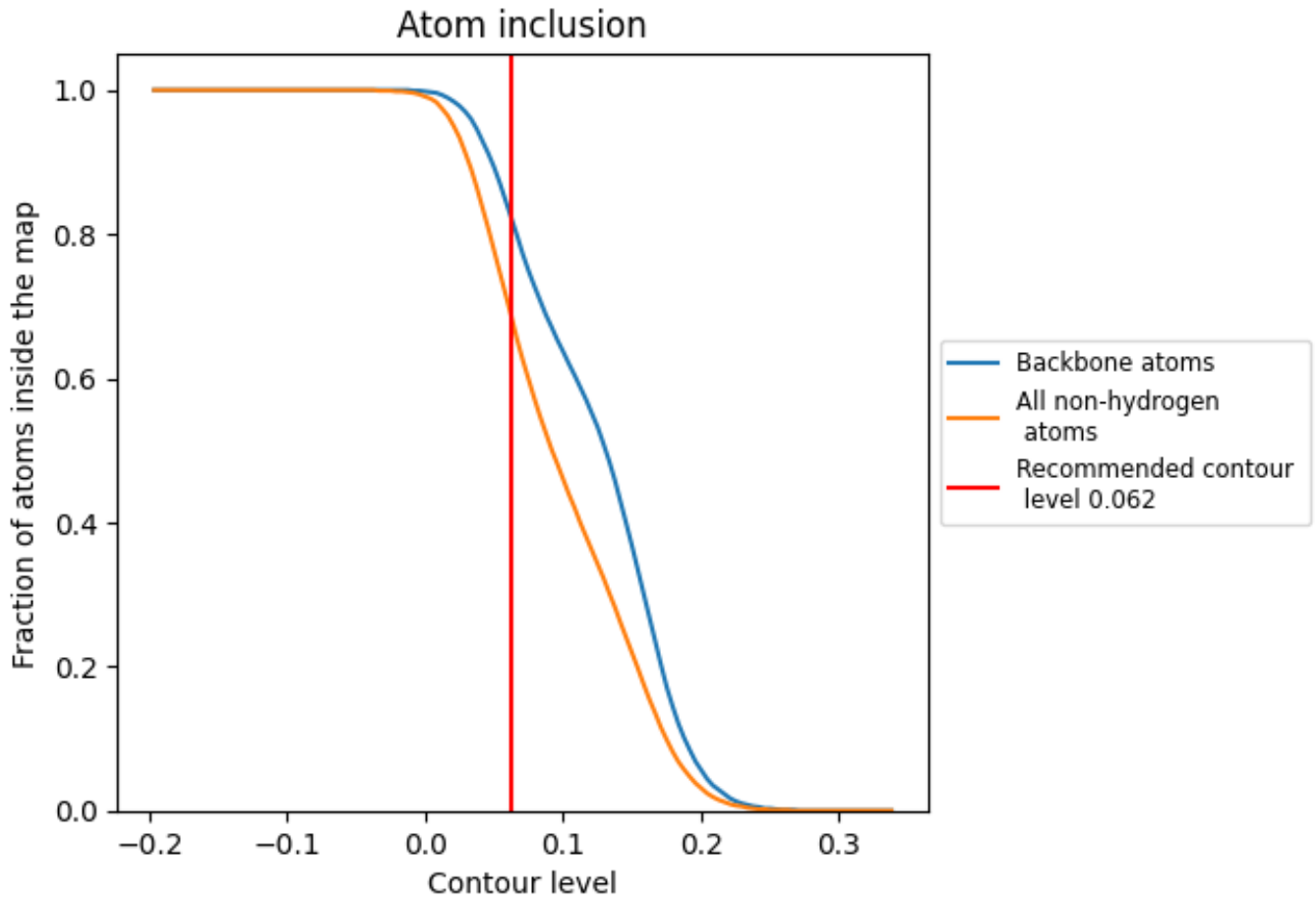
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.062).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 69% 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 (0.062) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6900	0.4290
A	0.7200	0.4480
B	0.7130	0.4460
C	0.7150	0.4450
D	0.5640	0.4420
E	0.2860	0.3080
F	0.2820	0.1920
G	0.4260	0.3470
H	0.4340	0.1930
I	0.6430	0.3280
J	0.2860	0.2400
K	0.5360	0.4230
L	0.3900	0.1900
M	0.3330	0.3470
N	0.4100	0.3670
O	0.3210	0.3690
P	0.1790	0.2250
Q	0.3280	0.3810
R	0.5710	0.3770
S	0.2140	0.3680
T	0.3080	0.3700
U	0.4620	0.3740
V	0.3930	0.2700
W	0.3110	0.2950
X	0.5360	0.3630
Y	0.3570	0.2160
Z	0.2050	0.3440

