Full wwPDB EM Validation Report

Mar 8, 2025 – 12:59 PM EST

PDB ID	:	9CSS
EMDB ID	:	EMD-45893
Title	:	Cryo-EM structure of SARS-CoV-2 spike protein Ecto-domain with internal tag, 1UP RBD conformation
Authors	:	Singh, S.; Hasan, S.S.
Deposited on	:	2024-07-24
Resolution	:	2.72 Å(reported)
Based on initial models	:	., 7KRR

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

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

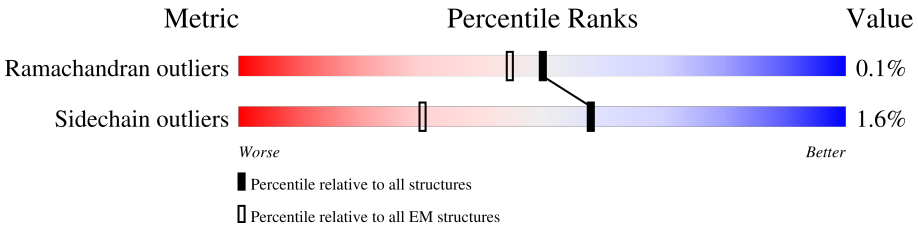
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.72 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	1275	7% 81% 18%
1	B	1275	81% 18%
1	C	1275	7% 82% 17%
2	D	3	33% 33% 67%
2	E	3	33% 67%
2	J	3	33% 67%
2	T	3	33% 67%
2	Z	3	33% 33% 67%
2	b	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	F	2	50% 100%
3	G	2	50% 100%
3	H	2	100%
3	I	2	50% 100%
3	R	2	50% 100%
3	U	2	100%
3	X	2	100%
3	c	2	100%
4	K	3	33% 100%
4	V	3	33% 100%
4	d	3	33% 33% 67%
5	L	3	100%
5	M	3	33% 100%
5	W	3	100%
5	e	3	100%
5	f	3	33% 100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25719 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1043	Total	C	N	O	S	0	0
			8158	5216	1355	1550	37		
1	C	1061	Total	C	N	O	S	0	0
			8294	5305	1376	1575	38		
1	A	1045	Total	C	N	O	S	0	0
			8164	5219	1355	1554	36		

There are 219 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	insertion	UNP P0DTC2
B	-19	ALA	-	insertion	UNP P0DTC2
B	-18	TRP	-	insertion	UNP P0DTC2
B	-17	SER	-	insertion	UNP P0DTC2
B	-16	HIS	-	insertion	UNP P0DTC2
B	-15	PRO	-	insertion	UNP P0DTC2
B	-14	GLN	-	insertion	UNP P0DTC2
B	-13	PHE	-	insertion	UNP P0DTC2
B	-12	GLU	-	insertion	UNP P0DTC2
B	-11	LYS	-	insertion	UNP P0DTC2
B	-10	GLY	-	insertion	UNP P0DTC2
B	-9	GLY	-	insertion	UNP P0DTC2
B	-8	GLY	-	insertion	UNP P0DTC2
B	-7	SER	-	insertion	UNP P0DTC2
B	-6	GLY	-	insertion	UNP P0DTC2
B	-5	GLY	-	insertion	UNP P0DTC2
B	-4	GLY	-	insertion	UNP P0DTC2
B	-3	SER	-	insertion	UNP P0DTC2
B	-2	GLY	-	insertion	UNP P0DTC2
B	-1	GLY	-	insertion	UNP P0DTC2
B	0	SER	-	insertion	UNP P0DTC2
B	1	SER	-	insertion	UNP P0DTC2
B	2	ALA	-	insertion	UNP P0DTC2
B	3	TRP	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	insertion	UNP P0DTC2
B	5	HIS	-	insertion	UNP P0DTC2
B	6	PRO	-	insertion	UNP P0DTC2
B	7	GLN	-	insertion	UNP P0DTC2
B	8	PHE	-	insertion	UNP P0DTC2
B	9	GLU	-	insertion	UNP P0DTC2
B	10	LYS	-	insertion	UNP P0DTC2
B	11	SER	-	insertion	UNP P0DTC2
B	12	ALA	-	insertion	UNP P0DTC2
B	13	LEU	-	insertion	UNP P0DTC2
B	14	VAL	-	insertion	UNP P0DTC2
B	15	PRO	-	insertion	UNP P0DTC2
B	16	ARG	-	insertion	UNP P0DTC2
B	17	GLY	-	insertion	UNP P0DTC2
B	18	SER	-	insertion	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
C	-20	SER	-	insertion	UNP P0DTC2
C	-19	ALA	-	insertion	UNP P0DTC2
C	-18	TRP	-	insertion	UNP P0DTC2
C	-17	SER	-	insertion	UNP P0DTC2
C	-16	HIS	-	insertion	UNP P0DTC2
C	-15	PRO	-	insertion	UNP P0DTC2
C	-14	GLN	-	insertion	UNP P0DTC2
C	-13	PHE	-	insertion	UNP P0DTC2
C	-12	GLU	-	insertion	UNP P0DTC2
C	-11	LYS	-	insertion	UNP P0DTC2
C	-10	GLY	-	insertion	UNP P0DTC2
C	-9	GLY	-	insertion	UNP P0DTC2
C	-8	GLY	-	insertion	UNP P0DTC2
C	-7	SER	-	insertion	UNP P0DTC2
C	-6	GLY	-	insertion	UNP P0DTC2
C	-5	GLY	-	insertion	UNP P0DTC2
C	-4	GLY	-	insertion	UNP P0DTC2
C	-3	SER	-	insertion	UNP P0DTC2
C	-2	GLY	-	insertion	UNP P0DTC2
C	-1	GLY	-	insertion	UNP P0DTC2
C	0	SER	-	insertion	UNP P0DTC2
C	1	SER	-	insertion	UNP P0DTC2
C	2	ALA	-	insertion	UNP P0DTC2
C	3	TRP	-	insertion	UNP P0DTC2
C	4	SER	-	insertion	UNP P0DTC2
C	5	HIS	-	insertion	UNP P0DTC2
C	6	PRO	-	insertion	UNP P0DTC2
C	7	GLN	-	insertion	UNP P0DTC2
C	8	PHE	-	insertion	UNP P0DTC2
C	9	GLU	-	insertion	UNP P0DTC2
C	10	LYS	-	insertion	UNP P0DTC2
C	11	SER	-	insertion	UNP P0DTC2
C	12	ALA	-	insertion	UNP P0DTC2
C	13	LEU	-	insertion	UNP P0DTC2
C	14	VAL	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	15	PRO	-	insertion	UNP P0DTC2
C	16	ARG	-	insertion	UNP P0DTC2
C	17	GLY	-	insertion	UNP P0DTC2
C	18	SER	-	insertion	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
A	-20	SER	-	insertion	UNP P0DTC2
A	-19	ALA	-	insertion	UNP P0DTC2
A	-18	TRP	-	insertion	UNP P0DTC2
A	-17	SER	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	insertion	UNP P0DTC2
A	-15	PRO	-	insertion	UNP P0DTC2
A	-14	GLN	-	insertion	UNP P0DTC2
A	-13	PHE	-	insertion	UNP P0DTC2
A	-12	GLU	-	insertion	UNP P0DTC2
A	-11	LYS	-	insertion	UNP P0DTC2
A	-10	GLY	-	insertion	UNP P0DTC2
A	-9	GLY	-	insertion	UNP P0DTC2
A	-8	GLY	-	insertion	UNP P0DTC2
A	-7	SER	-	insertion	UNP P0DTC2
A	-6	GLY	-	insertion	UNP P0DTC2
A	-5	GLY	-	insertion	UNP P0DTC2
A	-4	GLY	-	insertion	UNP P0DTC2
A	-3	SER	-	insertion	UNP P0DTC2
A	-2	GLY	-	insertion	UNP P0DTC2
A	-1	GLY	-	insertion	UNP P0DTC2
A	0	SER	-	insertion	UNP P0DTC2
A	1	SER	-	insertion	UNP P0DTC2
A	2	ALA	-	insertion	UNP P0DTC2
A	3	TRP	-	insertion	UNP P0DTC2
A	4	SER	-	insertion	UNP P0DTC2
A	5	HIS	-	insertion	UNP P0DTC2
A	6	PRO	-	insertion	UNP P0DTC2
A	7	GLN	-	insertion	UNP P0DTC2
A	8	PHE	-	insertion	UNP P0DTC2
A	9	GLU	-	insertion	UNP P0DTC2
A	10	LYS	-	insertion	UNP P0DTC2
A	11	SER	-	insertion	UNP P0DTC2
A	12	ALA	-	insertion	UNP P0DTC2
A	13	LEU	-	insertion	UNP P0DTC2
A	14	VAL	-	insertion	UNP P0DTC2
A	15	PRO	-	insertion	UNP P0DTC2
A	16	ARG	-	insertion	UNP P0DTC2
A	17	GLY	-	insertion	UNP P0DTC2
A	18	SER	-	insertion	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2

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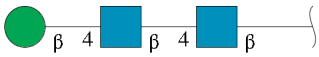
Chain	Residue	Modelled	Actual	Comment	Reference
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	E	3	Total	C	N	O	0	0
			39	22	2	15		
2	J	3	Total	C	N	O	0	0
			39	22	2	15		

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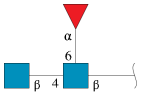
Mol	Chain	Residues	Atoms	AltConf	Trace
2	T	3	Total C N O 39 22 2 15	0	0
2	Z	3	Total C N O 39 22 2 15	0	0
2	b	3	Total C N O 39 22 2 15	0	0

- Molecule 3 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
3	F	2	Total C N O 28 16 2 10	0	0
3	G	2	Total C N O 28 16 2 10	0	0
3	H	2	Total C N O 28 16 2 10	0	0
3	I	2	Total C N O 28 16 2 10	0	0
3	R	2	Total C N O 28 16 2 10	0	0
3	U	2	Total C N O 28 16 2 10	0	0
3	X	2	Total C N O 28 16 2 10	0	0
3	c	2	Total C N O 28 16 2 10	0	0

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



Mol	Chain	Residues	Atoms	AltConf	Trace
4	K	3	Total C N O 38 22 2 14	0	0

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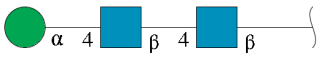
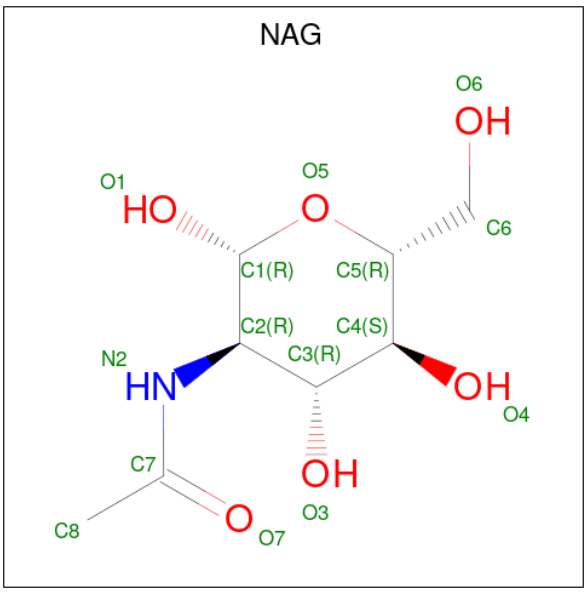
Mol	Chain	Residues	Atoms	AltConf	Trace
4	V	3	Total C N O 38 22 2 14	0	0
4	d	3	Total C N O 38 22 2 14	0	0

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



Mol	Chain	Residues	Atoms	AltConf	Trace
5	L	3	Total C N O 39 22 2 15	0	0
5	M	3	Total C N O 39 22 2 15	0	0
5	W	3	Total C N O 39 22 2 15	0	0
5	e	3	Total C N O 39 22 2 15	0	0
5	f	3	Total C N O 39 22 2 15	0	0

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



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

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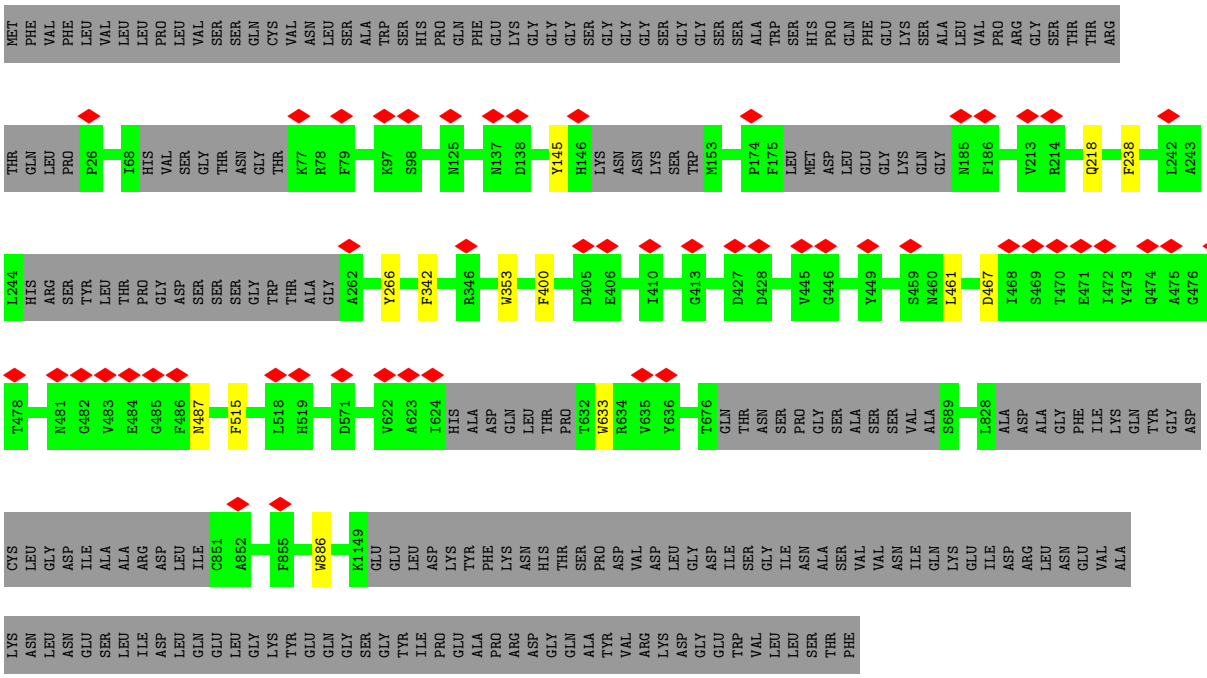
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	

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.

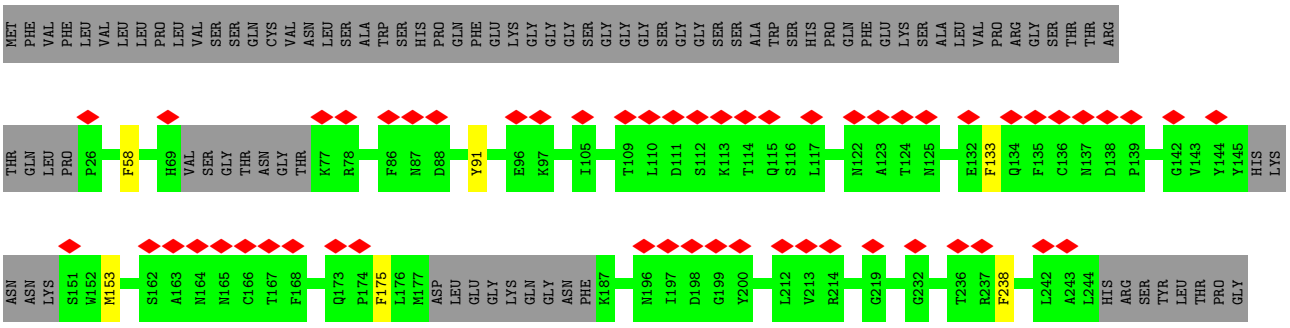
• Molecule 1: Spike glycoprotein

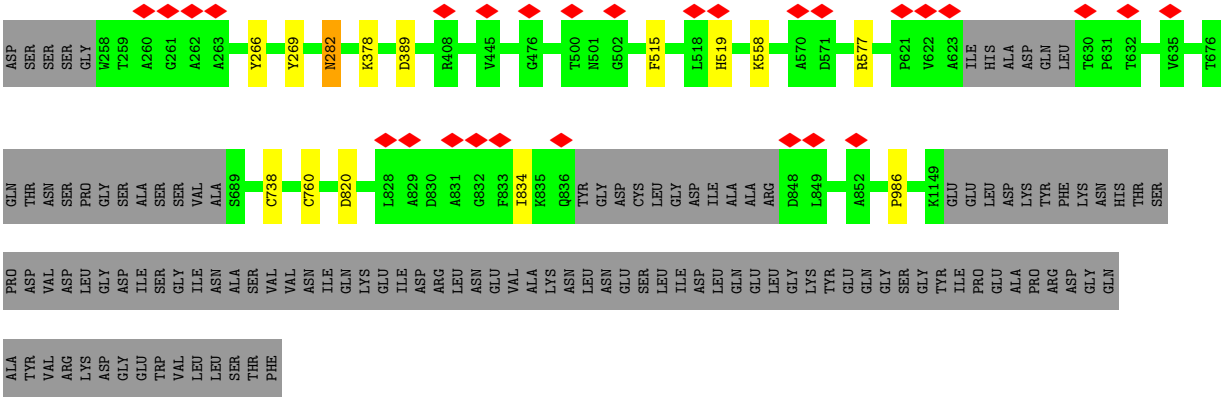
Chain B:



• Molecule 1: Spike glycoprotein

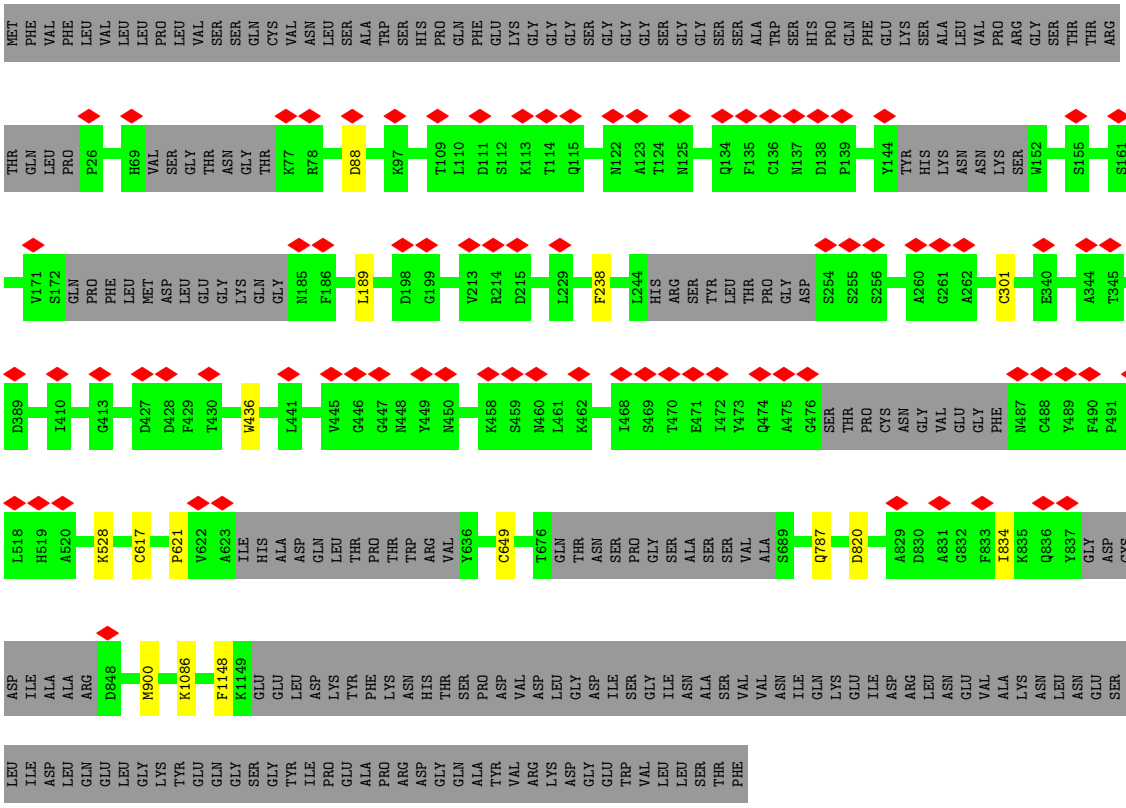
Chain C:





• Molecule 1: Spike glycoprotein

Chain A:

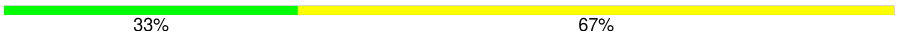


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

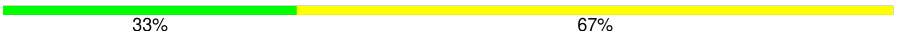
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



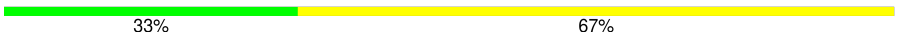
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain T:



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

Chain Z:

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

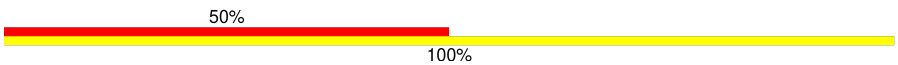
Chain b:

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

Chain F:

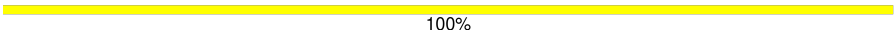
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



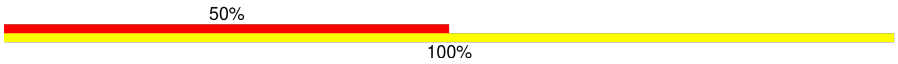
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



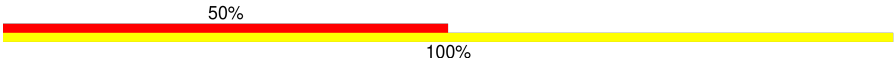
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



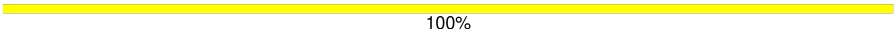
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



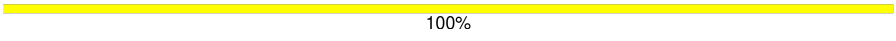
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



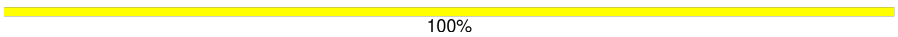
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



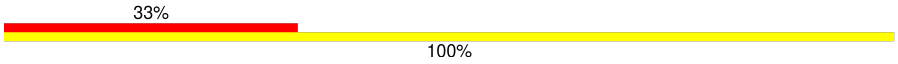
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



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

Chain K:



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

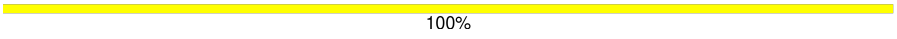
Chain V:

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

Chain d:

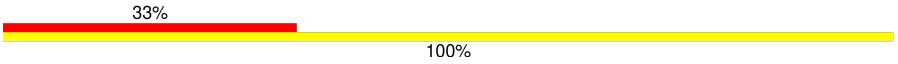
• Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



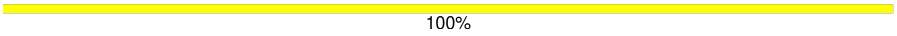
• Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

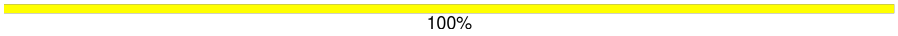


• Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

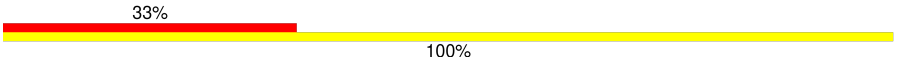
Chain W:



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

Chain e: 

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

Chain f: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111897	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43.97	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	191780	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.987	Depositor
Minimum map value	-0.463	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	377.0018, 377.0018, 377.0018	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.99211, 0.99211, 0.99211	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	2/8350 (0.0%)	0.54	4/11357 (0.0%)
1	B	0.27	0/8346	0.50	1/11355 (0.0%)
1	C	0.27	0/8487	0.48	0/11549
All	All	0.29	2/25183 (0.0%)	0.51	5/34261 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	621	PRO	CB-CG	-11.75	0.91	1.50
1	A	621	PRO	CG-CD	-8.25	1.23	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	621	PRO	CB-CG-CD	18.44	178.41	106.50
1	A	621	PRO	N-CD-CG	-16.30	78.75	103.20
1	A	621	PRO	CA-CB-CG	-14.83	75.83	104.00
1	A	621	PRO	CA-N-CD	-7.59	100.88	111.50
1	B	461	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	617	CYS	Peptide
1	C	282	ASN	Peptide

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	1027/1275 (80%)	983 (96%)	43 (4%)	1 (0%)	48	72
1	B	1027/1275 (80%)	973 (95%)	53 (5%)	1 (0%)	48	72
1	C	1045/1275 (82%)	994 (95%)	50 (5%)	1 (0%)	48	72
All	All	3099/3825 (81%)	2950 (95%)	146 (5%)	3 (0%)	50	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	487	ASN
1	A	834	ILE
1	C	834	ILE

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	909/1101 (83%)	894 (98%)	15 (2%)	56 80
1	B	911/1101 (83%)	900 (99%)	11 (1%)	67 85
1	C	924/1101 (84%)	905 (98%)	19 (2%)	48 75
All	All	2744/3303 (83%)	2699 (98%)	45 (2%)	58 81

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	145	TYR
1	B	218	GLN
1	B	238	PHE
1	B	266	TYR
1	B	342	PHE
1	B	353	TRP
1	B	400	PHE
1	B	467	ASP
1	B	515	PHE
1	B	633	TRP
1	B	886	TRP
1	C	58	PHE
1	C	91	TYR
1	C	133	PHE
1	C	153	MET
1	C	175	PHE
1	C	238	PHE
1	C	266	TYR
1	C	269	TYR
1	C	282	ASN
1	C	378	LYS
1	C	389	ASP
1	C	515	PHE
1	C	519	HIS
1	C	558	LYS
1	C	577	ARG
1	C	738	CYS
1	C	760	CYS
1	C	820	ASP
1	C	986	PRO
1	A	88	ASP
1	A	168	PHE

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Mol	Chain	Res	Type
1	A	189	LEU
1	A	238	PHE
1	A	301	CYS
1	A	386	LYS
1	A	436	TRP
1	A	515	PHE
1	A	528	LYS
1	A	649	CYS
1	A	787	GLN
1	A	820	ASP
1	A	900	MET
1	A	1086	LYS
1	A	1148	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	ASN
1	B	115	GLN
1	B	493	GLN
1	B	540	ASN
1	B	563	GLN
1	B	658	ASN
1	B	751	ASN
1	B	955	ASN
1	C	394	ASN
1	C	440	ASN
1	C	460	ASN
1	C	481	ASN
1	C	580	GLN
1	C	613	GLN
1	C	901	GLN
1	C	919	ASN
1	C	965	GLN
1	C	1119	ASN
1	A	30	ASN
1	A	164	ASN
1	A	196	ASN
1	A	207	HIS
1	A	394	ASN
1	A	474	GLN
1	A	493	GLN

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Mol	Chain	Res	Type
1	A	563	GLN
1	A	580	GLN
1	A	717	ASN
1	A	762	GLN
1	A	764	ASN
1	A	804	GLN
1	A	907	ASN
1	A	935	GLN
1	A	955	ASN
1	A	957	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

58 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	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	1.98	4 (28%)	17,19,21	2.09	5 (29%)
2	NAG	D	2	2	14,14,15	2.04	3 (21%)	17,19,21	1.24	2 (11%)
2	BMA	D	3	2	11,11,12	0.58	0	15,15,17	0.77	0
2	NAG	E	1	1,2	14,14,15	1.91	3 (21%)	17,19,21	1.14	2 (11%)
2	NAG	E	2	2	14,14,15	1.95	4 (28%)	17,19,21	1.06	2 (11%)
2	BMA	E	3	2	11,11,12	0.54	0	15,15,17	0.66	0
3	NAG	F	1	1,3	14,14,15	2.22	5 (35%)	17,19,21	2.19	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	F	2	3	14,14,15	2.02	4 (28%)	17,19,21	1.13	2 (11%)
3	NAG	G	1	1,3	14,14,15	1.91	3 (21%)	17,19,21	1.32	2 (11%)
3	NAG	G	2	3	14,14,15	2.15	4 (28%)	17,19,21	1.26	2 (11%)
3	NAG	H	1	1,3	14,14,15	1.96	4 (28%)	17,19,21	1.19	2 (11%)
3	NAG	H	2	3	14,14,15	1.99	4 (28%)	17,19,21	1.13	2 (11%)
3	NAG	I	1	1,3	14,14,15	2.20	4 (28%)	17,19,21	1.59	4 (23%)
3	NAG	I	2	3	14,14,15	2.09	4 (28%)	17,19,21	1.05	1 (5%)
2	NAG	J	1	2	14,14,15	1.95	5 (35%)	17,19,21	1.99	6 (35%)
2	NAG	J	2	2	14,14,15	2.13	4 (28%)	17,19,21	0.94	0
2	BMA	J	3	2	11,11,12	0.58	0	15,15,17	0.67	0
4	NAG	K	1	1,4	14,14,15	1.96	3 (21%)	17,19,21	1.34	1 (5%)
4	NAG	K	2	4	14,14,15	1.98	4 (28%)	17,19,21	1.09	2 (11%)
4	FUC	K	3	4	10,10,11	0.95	0	14,14,16	1.05	1 (7%)
5	NAG	L	1	1,5	14,14,15	2.00	4 (28%)	17,19,21	1.31	2 (11%)
5	NAG	L	2	5	14,14,15	1.93	4 (28%)	17,19,21	1.47	3 (17%)
5	MAN	L	3	5	11,11,12	0.70	0	15,15,17	1.00	2 (13%)
5	NAG	M	1	1,5	14,14,15	2.08	4 (28%)	17,19,21	1.61	3 (17%)
5	NAG	M	2	5	14,14,15	1.99	4 (28%)	17,19,21	1.38	2 (11%)
5	MAN	M	3	5	11,11,12	0.77	0	15,15,17	1.15	2 (13%)
3	NAG	R	1	1,3	14,14,15	2.00	4 (28%)	17,19,21	2.15	5 (29%)
3	NAG	R	2	3	14,14,15	2.10	4 (28%)	17,19,21	1.18	3 (17%)
2	NAG	T	1	2	14,14,15	1.93	4 (28%)	17,19,21	1.24	2 (11%)
2	NAG	T	2	2	14,14,15	1.97	4 (28%)	17,19,21	1.06	2 (11%)
2	BMA	T	3	2	11,11,12	0.55	0	15,15,17	0.68	0
3	NAG	U	1	1,3	14,14,15	1.92	3 (21%)	17,19,21	1.52	4 (23%)
3	NAG	U	2	3	14,14,15	1.98	4 (28%)	17,19,21	1.14	2 (11%)
4	NAG	V	1	1,4	14,14,15	2.12	5 (35%)	17,19,21	1.71	4 (23%)
4	NAG	V	2	4	14,14,15	2.00	4 (28%)	17,19,21	1.10	2 (11%)
4	FUC	V	3	4	10,10,11	0.99	1 (10%)	14,14,16	1.16	2 (14%)
5	NAG	W	1	1,5	14,14,15	2.01	4 (28%)	17,19,21	1.18	2 (11%)
5	NAG	W	2	5	14,14,15	1.95	4 (28%)	17,19,21	1.32	2 (11%)
5	MAN	W	3	5	11,11,12	0.80	0	15,15,17	1.14	2 (13%)
3	NAG	X	1	1,3	14,14,15	1.97	4 (28%)	17,19,21	1.13	2 (11%)
3	NAG	X	2	3	14,14,15	1.99	4 (28%)	17,19,21	1.20	2 (11%)
2	NAG	Z	1	2	14,14,15	1.93	4 (28%)	17,19,21	1.44	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	Z	2	2	14,14,15	1.96	4 (28%)	17,19,21	1.12	2 (11%)
2	BMA	Z	3	2	11,11,12	0.50	0	15,15,17	0.72	0
2	NAG	b	1	2	14,14,15	1.90	3 (21%)	17,19,21	1.28	1 (5%)
2	NAG	b	2	2	14,14,15	1.95	4 (28%)	17,19,21	1.21	2 (11%)
2	BMA	b	3	2	11,11,12	0.53	0	15,15,17	0.66	0
3	NAG	c	1	1,3	14,14,15	1.93	3 (21%)	17,19,21	1.18	2 (11%)
3	NAG	c	2	3	14,14,15	1.99	4 (28%)	17,19,21	1.20	2 (11%)
4	NAG	d	1	1,4	14,14,15	1.98	4 (28%)	17,19,21	1.29	2 (11%)
4	NAG	d	2	4	14,14,15	1.98	4 (28%)	17,19,21	1.11	2 (11%)
4	FUC	d	3	4	10,10,11	0.75	0	14,14,16	0.87	0
5	NAG	e	1	1,5	14,14,15	2.06	4 (28%)	17,19,21	0.87	0
5	NAG	e	2	5	14,14,15	1.96	4 (28%)	17,19,21	1.39	3 (17%)
5	MAN	e	3	5	11,11,12	0.77	0	15,15,17	1.06	2 (13%)
5	NAG	f	1	1,5	14,14,15	1.94	4 (28%)	17,19,21	1.17	2 (11%)
5	NAG	f	2	5	14,14,15	1.97	4 (28%)	17,19,21	1.21	2 (11%)
5	MAN	f	3	5	11,11,12	0.73	0	15,15,17	1.13	2 (13%)

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
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	BMA	J	3	2	-	1/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	FUC	K	3	4	-	-	0/1/1/1
5	NAG	L	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	MAN	L	3	5	-	2/2/19/22	1/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	MAN	M	3	5	-	0/2/19/22	1/1/1/1
3	NAG	R	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
2	NAG	T	1	2	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	BMA	T	3	2	-	0/2/19/22	0/1/1/1
3	NAG	U	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	FUC	V	3	4	-	-	0/1/1/1
5	NAG	W	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	1/6/23/26	0/1/1/1
5	MAN	W	3	5	-	1/2/19/22	1/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1
2	NAG	Z	1	2	-	1/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	1/6/23/26	0/1/1/1
2	BMA	Z	3	2	-	0/2/19/22	0/1/1/1
2	NAG	b	1	2	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	2/6/23/26	0/1/1/1
2	BMA	b	3	2	-	0/2/19/22	0/1/1/1
3	NAG	c	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
4	NAG	d	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	2/6/23/26	0/1/1/1
4	FUC	d	3	4	-	-	0/1/1/1
5	NAG	e	1	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	e	2	5	-	0/6/23/26	0/1/1/1
5	MAN	e	3	5	-	2/2/19/22	1/1/1/1
5	NAG	f	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	f	2	5	-	2/6/23/26	0/1/1/1
5	MAN	f	3	5	-	2/2/19/22	1/1/1/1

All (173) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	4.92	1.51	1.43
3	I	2	NAG	O5-C1	4.72	1.51	1.43
5	M	1	NAG	O5-C1	4.69	1.51	1.43
3	R	2	NAG	O5-C1	4.68	1.51	1.43
3	G	2	NAG	O5-C1	4.67	1.51	1.43
2	J	2	NAG	O5-C1	4.64	1.51	1.43
4	V	1	NAG	O5-C1	4.62	1.51	1.43
5	e	1	NAG	O5-C1	4.47	1.51	1.43
4	K	1	NAG	O5-C1	4.42	1.51	1.43
3	I	1	NAG	O5-C1	4.40	1.51	1.43
2	D	2	NAG	O5-C1	4.38	1.51	1.43
5	L	1	NAG	O5-C1	4.33	1.51	1.43
3	F	2	NAG	O5-C1	4.30	1.50	1.43
4	V	2	NAG	O5-C1	4.29	1.50	1.43
3	H	2	NAG	O5-C1	4.28	1.50	1.43
3	U	1	NAG	O5-C1	4.26	1.50	1.43
3	X	2	NAG	O5-C1	4.25	1.50	1.43
4	K	2	NAG	O5-C1	4.24	1.50	1.43
4	d	1	NAG	O5-C1	4.24	1.50	1.43
3	c	2	NAG	O5-C1	4.23	1.50	1.43
3	R	1	NAG	C7-N2	4.23	1.48	1.34
4	d	2	NAG	O5-C1	4.22	1.50	1.43
3	U	2	NAG	O5-C1	4.22	1.50	1.43
3	X	1	NAG	O5-C1	4.19	1.50	1.43
2	E	1	NAG	O5-C1	4.18	1.50	1.43
5	f	2	NAG	O5-C1	4.18	1.50	1.43
5	W	1	NAG	O5-C1	4.18	1.50	1.43
5	M	2	NAG	O5-C1	4.16	1.50	1.43
2	T	2	NAG	O5-C1	4.16	1.50	1.43
5	f	1	NAG	O5-C1	4.14	1.50	1.43
3	c	1	NAG	O5-C1	4.14	1.50	1.43
3	R	1	NAG	O5-C1	4.14	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	4.13	1.50	1.43
2	Z	2	NAG	O5-C1	4.11	1.50	1.43
2	b	2	NAG	O5-C1	4.11	1.50	1.43
2	D	1	NAG	O5-C1	4.10	1.50	1.43
2	E	2	NAG	O5-C1	4.09	1.50	1.43
5	e	2	NAG	O5-C1	4.07	1.50	1.43
3	G	2	NAG	C7-N2	4.04	1.47	1.34
5	W	2	NAG	O5-C1	4.02	1.50	1.43
2	J	2	NAG	C7-N2	4.02	1.47	1.34
2	D	2	NAG	C7-N2	4.01	1.47	1.34
3	G	1	NAG	O5-C1	3.98	1.50	1.43
2	Z	1	NAG	O5-C1	3.97	1.50	1.43
2	T	1	NAG	O5-C1	3.96	1.50	1.43
2	D	1	NAG	C7-N2	3.95	1.47	1.34
3	I	1	NAG	C7-N2	3.94	1.47	1.34
3	R	2	NAG	C7-N2	3.94	1.47	1.34
3	I	2	NAG	C7-N2	3.93	1.47	1.34
3	G	1	NAG	C7-N2	3.92	1.47	1.34
3	F	2	NAG	C7-N2	3.92	1.47	1.34
5	L	2	NAG	O5-C1	3.90	1.50	1.43
2	T	1	NAG	C7-N2	3.89	1.46	1.34
4	d	2	NAG	C7-N2	3.88	1.46	1.34
5	M	1	NAG	C7-N2	3.88	1.46	1.34
3	X	2	NAG	C7-N2	3.88	1.46	1.34
2	E	2	NAG	C7-N2	3.87	1.46	1.34
2	T	2	NAG	C7-N2	3.86	1.46	1.34
3	H	2	NAG	C7-N2	3.86	1.46	1.34
2	b	2	NAG	C7-N2	3.86	1.46	1.34
4	K	2	NAG	C7-N2	3.86	1.46	1.34
2	b	1	NAG	O5-C1	3.86	1.50	1.43
2	Z	2	NAG	C7-N2	3.85	1.46	1.34
5	M	2	NAG	C7-N2	3.85	1.46	1.34
3	U	2	NAG	C7-N2	3.85	1.46	1.34
3	c	2	NAG	C7-N2	3.85	1.46	1.34
5	f	1	NAG	C7-N2	3.85	1.46	1.34
4	V	2	NAG	C7-N2	3.84	1.46	1.34
5	L	1	NAG	C7-N2	3.84	1.46	1.34
3	X	1	NAG	C7-N2	3.84	1.46	1.34
3	U	1	NAG	C7-N2	3.84	1.46	1.34
2	Z	1	NAG	C7-N2	3.84	1.46	1.34
5	L	2	NAG	C7-N2	3.84	1.46	1.34
4	d	1	NAG	C7-N2	3.84	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	2	NAG	C7-N2	3.84	1.46	1.34
2	E	1	NAG	C7-N2	3.83	1.46	1.34
5	f	2	NAG	C7-N2	3.83	1.46	1.34
3	F	1	NAG	C7-N2	3.83	1.46	1.34
2	b	1	NAG	C7-N2	3.83	1.46	1.34
4	K	1	NAG	C7-N2	3.83	1.46	1.34
2	J	1	NAG	C7-N2	3.82	1.46	1.34
5	W	2	NAG	C7-N2	3.81	1.46	1.34
5	e	1	NAG	C7-N2	3.81	1.46	1.34
3	c	1	NAG	C7-N2	3.80	1.46	1.34
2	J	1	NAG	O5-C1	3.78	1.50	1.43
3	H	1	NAG	C7-N2	3.67	1.46	1.34
5	W	1	NAG	C7-N2	3.66	1.46	1.34
4	V	1	NAG	C7-N2	3.61	1.46	1.34
3	I	1	NAG	O5-C5	3.42	1.50	1.43
3	G	2	NAG	C2-N2	2.95	1.51	1.46
3	F	1	NAG	O5-C5	2.94	1.49	1.43
4	V	1	NAG	O5-C5	2.88	1.49	1.43
2	J	2	NAG	C2-N2	2.83	1.50	1.46
3	R	1	NAG	C2-N2	2.73	1.50	1.46
3	I	1	NAG	C2-N2	2.72	1.50	1.46
5	W	1	NAG	O5-C5	2.70	1.48	1.43
2	D	2	NAG	C2-N2	2.66	1.50	1.46
5	M	1	NAG	O5-C5	2.61	1.48	1.43
3	R	2	NAG	C2-N2	2.57	1.50	1.46
3	F	2	NAG	C2-N2	2.56	1.50	1.46
3	F	1	NAG	C2-N2	2.56	1.50	1.46
3	G	1	NAG	C2-N2	2.52	1.50	1.46
5	e	1	NAG	C2-N2	2.52	1.50	1.46
3	I	2	NAG	C2-N2	2.51	1.50	1.46
5	M	2	NAG	O5-C5	2.51	1.48	1.43
4	K	2	NAG	C2-N2	2.49	1.50	1.46
5	e	1	NAG	O5-C5	2.48	1.48	1.43
3	U	2	NAG	C2-N2	2.47	1.50	1.46
3	R	2	NAG	O5-C5	2.46	1.48	1.43
2	b	2	NAG	C2-N2	2.45	1.50	1.46
2	E	2	NAG	C2-N2	2.45	1.50	1.46
5	W	1	NAG	C2-N2	2.45	1.50	1.46
2	D	1	NAG	O5-C5	2.44	1.48	1.43
2	J	1	NAG	O5-C5	2.44	1.48	1.43
3	F	1	NAG	C3-C2	-2.44	1.47	1.52
2	J	2	NAG	O5-C5	2.43	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	2	NAG	C2-N2	2.43	1.50	1.46
4	d	2	NAG	C2-N2	2.42	1.50	1.46
3	X	2	NAG	C2-N2	2.42	1.50	1.46
3	U	1	NAG	C2-N2	2.42	1.50	1.46
2	T	2	NAG	C2-N2	2.41	1.50	1.46
3	H	2	NAG	C2-N2	2.41	1.50	1.46
5	L	1	NAG	O5-C5	2.41	1.48	1.43
5	M	1	NAG	C2-N2	2.41	1.50	1.46
3	c	2	NAG	C2-N2	2.40	1.50	1.46
5	f	1	NAG	C2-N2	2.40	1.50	1.46
3	H	1	NAG	C2-N2	2.40	1.50	1.46
5	M	2	NAG	C2-N2	2.39	1.50	1.46
4	d	1	NAG	C2-N2	2.39	1.50	1.46
2	Z	1	NAG	C2-N2	2.38	1.50	1.46
5	L	2	NAG	C2-N2	2.38	1.50	1.46
3	X	1	NAG	C2-N2	2.37	1.50	1.46
5	f	2	NAG	C2-N2	2.37	1.50	1.46
4	V	2	NAG	C2-N2	2.36	1.50	1.46
2	b	1	NAG	C2-N2	2.36	1.50	1.46
5	e	2	NAG	C2-N2	2.34	1.50	1.46
3	c	1	NAG	C2-N2	2.34	1.50	1.46
4	V	1	NAG	C2-N2	2.33	1.50	1.46
5	W	2	NAG	C2-N2	2.33	1.50	1.46
2	J	1	NAG	C2-N2	2.33	1.50	1.46
3	F	2	NAG	O5-C5	2.33	1.48	1.43
4	V	2	NAG	O5-C5	2.32	1.48	1.43
2	T	1	NAG	C2-N2	2.32	1.50	1.46
3	I	2	NAG	O5-C5	2.32	1.47	1.43
5	e	2	NAG	O5-C5	2.30	1.47	1.43
5	L	2	NAG	O5-C5	2.30	1.47	1.43
5	f	2	NAG	O5-C5	2.29	1.47	1.43
3	X	2	NAG	O5-C5	2.29	1.47	1.43
4	K	1	NAG	C2-N2	2.29	1.50	1.46
3	c	2	NAG	O5-C5	2.29	1.47	1.43
2	E	1	NAG	C2-N2	2.28	1.50	1.46
2	D	1	NAG	C2-N2	2.27	1.50	1.46
3	H	2	NAG	O5-C5	2.26	1.47	1.43
5	W	2	NAG	O5-C5	2.25	1.47	1.43
5	L	1	NAG	C2-N2	2.24	1.50	1.46
3	H	1	NAG	O5-C5	2.20	1.47	1.43
2	Z	1	NAG	O5-C5	2.19	1.47	1.43
2	Z	2	NAG	O5-C5	2.19	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	2	NAG	O5-C5	2.19	1.47	1.43
3	G	2	NAG	O5-C5	2.19	1.47	1.43
4	d	1	NAG	O5-C5	2.18	1.47	1.43
3	U	2	NAG	O5-C5	2.18	1.47	1.43
2	T	2	NAG	O5-C5	2.17	1.47	1.43
4	V	3	FUC	C2-C3	2.14	1.55	1.52
2	T	1	NAG	O5-C5	2.13	1.47	1.43
3	X	1	NAG	O5-C5	2.11	1.47	1.43
4	K	2	NAG	O5-C5	2.09	1.47	1.43
3	R	1	NAG	O5-C5	2.07	1.47	1.43
4	V	1	NAG	C3-C2	-2.07	1.48	1.52
2	b	2	NAG	O5-C5	2.06	1.47	1.43
2	J	1	NAG	C3-C2	-2.03	1.48	1.52
5	f	1	NAG	O5-C5	2.02	1.47	1.43
2	E	2	NAG	O5-C5	2.00	1.47	1.43

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	1	NAG	C4-C3-C2	6.69	120.82	111.02
3	F	1	NAG	C1-O5-C5	6.02	120.25	112.19
4	V	1	NAG	C1-O5-C5	4.53	118.26	112.19
2	J	1	NAG	C3-C4-C5	4.22	117.88	110.23
2	D	1	NAG	C4-C3-C2	3.95	116.81	111.02
2	D	1	NAG	C3-C4-C5	3.95	117.39	110.23
3	F	1	NAG	C2-N2-C7	3.85	128.05	122.90
5	M	1	NAG	C2-N2-C7	-3.56	118.13	122.90
5	M	3	MAN	C1-O5-C5	3.45	116.81	112.19
2	D	1	NAG	C8-C7-N2	3.44	121.83	116.12
3	I	1	NAG	C1-O5-C5	-3.42	107.60	112.19
4	K	1	NAG	C1-O5-C5	3.39	116.73	112.19
5	f	3	MAN	C1-O5-C5	3.37	116.70	112.19
5	W	3	MAN	C1-O5-C5	3.35	116.68	112.19
3	U	1	NAG	C2-N2-C7	-3.27	118.52	122.90
2	D	2	NAG	C4-C3-C2	3.24	115.76	111.02
3	G	2	NAG	C1-O5-C5	3.09	116.33	112.19
5	e	3	MAN	C1-O5-C5	3.02	116.23	112.19
5	M	1	NAG	C1-O5-C5	2.95	116.14	112.19
5	L	1	NAG	C2-N2-C7	-2.95	118.95	122.90
2	J	1	NAG	O5-C5-C4	2.94	117.97	110.83
2	J	1	NAG	C4-C3-C2	2.90	115.27	111.02
3	R	1	NAG	O5-C1-C2	-2.90	106.81	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	2	NAG	C2-N2-C7	-2.87	119.05	122.90
4	V	1	NAG	C2-N2-C7	-2.84	119.09	122.90
5	M	2	NAG	C2-N2-C7	-2.84	119.09	122.90
5	W	2	NAG	C2-N2-C7	-2.84	119.09	122.90
4	d	1	NAG	C1-O5-C5	2.84	115.99	112.19
5	M	1	NAG	C8-C7-N2	2.80	120.76	116.12
3	U	1	NAG	O5-C1-C2	-2.80	106.97	111.29
5	e	2	NAG	C2-N2-C7	-2.78	119.18	122.90
5	L	3	MAN	C1-O5-C5	2.77	115.90	112.19
5	L	2	NAG	C2-N2-C7	-2.74	119.23	122.90
2	J	1	NAG	C2-N2-C7	-2.72	119.25	122.90
3	F	1	NAG	O5-C5-C4	2.72	117.45	110.83
3	U	1	NAG	C8-C7-N2	2.69	120.59	116.12
3	H	1	NAG	C2-N2-C7	-2.68	119.30	122.90
3	X	2	NAG	C2-N2-C7	-2.66	119.34	122.90
3	R	1	NAG	C1-C2-N2	2.64	114.60	110.43
3	F	1	NAG	C1-C2-N2	2.64	114.59	110.43
2	Z	1	NAG	C3-C4-C5	2.63	115.00	110.23
5	W	1	NAG	C1-O5-C5	2.62	115.69	112.19
4	V	1	NAG	O5-C5-C4	2.61	117.18	110.83
3	I	1	NAG	O5-C1-C2	-2.58	107.30	111.29
3	G	1	NAG	C4-C3-C2	2.55	114.75	111.02
3	I	1	NAG	O5-C5-C4	2.54	117.00	110.83
2	b	2	NAG	C8-C7-N2	2.49	120.25	116.12
2	J	1	NAG	C8-C7-N2	2.48	120.24	116.12
2	D	1	NAG	O5-C1-C2	-2.48	107.45	111.29
3	X	2	NAG	C8-C7-N2	2.47	120.21	116.12
3	U	1	NAG	C4-C3-C2	2.47	114.63	111.02
3	c	2	NAG	C8-C7-N2	2.46	120.20	116.12
2	T	2	NAG	C2-N2-C7	-2.46	119.60	122.90
3	F	2	NAG	C8-C7-N2	2.46	120.20	116.12
3	H	1	NAG	C8-C7-N2	2.45	120.18	116.12
5	L	2	NAG	C8-C7-N2	2.43	120.16	116.12
3	U	2	NAG	C8-C7-N2	2.43	120.15	116.12
2	T	2	NAG	C8-C7-N2	2.43	120.14	116.12
3	I	1	NAG	C8-C7-N2	2.42	120.13	116.12
3	U	2	NAG	C2-N2-C7	-2.42	119.66	122.90
3	G	2	NAG	O5-C1-C2	2.42	115.03	111.29
4	K	2	NAG	C8-C7-N2	2.42	120.13	116.12
2	E	2	NAG	C8-C7-N2	2.42	120.12	116.12
2	b	1	NAG	C8-C7-N2	2.41	120.11	116.12
3	X	1	NAG	C8-C7-N2	2.40	120.10	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1	NAG	C8-C7-N2	2.39	120.08	116.12
5	f	2	NAG	C8-C7-N2	2.38	120.07	116.12
2	Z	2	NAG	C8-C7-N2	2.38	120.06	116.12
5	M	2	NAG	C8-C7-N2	2.36	120.03	116.12
3	G	1	NAG	C8-C7-N2	2.35	120.02	116.12
3	R	2	NAG	C8-C7-N2	2.33	119.99	116.12
5	f	2	NAG	C2-N2-C7	-2.33	119.77	122.90
4	V	3	FUC	C1-C2-C3	2.33	113.03	109.64
2	Z	1	NAG	C8-C7-N2	2.33	119.98	116.12
3	I	2	NAG	C8-C7-N2	2.33	119.98	116.12
3	c	1	NAG	C2-N2-C7	-2.32	119.79	122.90
3	H	2	NAG	C8-C7-N2	2.32	119.96	116.12
2	D	1	NAG	O4-C4-C3	-2.32	104.92	110.38
3	X	1	NAG	C2-N2-C7	-2.31	119.80	122.90
3	c	1	NAG	C8-C7-N2	2.31	119.94	116.12
3	R	2	NAG	C2-N2-C7	-2.30	119.81	122.90
4	V	2	NAG	C8-C7-N2	2.30	119.94	116.12
5	f	1	NAG	C8-C7-N2	2.30	119.93	116.12
2	b	2	NAG	C2-N2-C7	-2.29	119.83	122.90
4	d	2	NAG	C8-C7-N2	2.29	119.92	116.12
5	L	2	NAG	C3-C4-C5	2.28	114.37	110.23
5	f	1	NAG	C2-N2-C7	-2.28	119.84	122.90
5	e	2	NAG	C8-C7-N2	2.28	119.89	116.12
5	W	1	NAG	O5-C5-C4	2.27	116.34	110.83
5	W	2	NAG	C8-C7-N2	2.26	119.86	116.12
2	Z	2	NAG	C2-N2-C7	-2.25	119.88	122.90
3	H	2	NAG	C2-N2-C7	-2.25	119.89	122.90
4	V	3	FUC	C1-O5-C5	2.24	118.25	112.97
2	T	1	NAG	C8-C7-N2	2.23	119.82	116.12
3	F	2	NAG	C2-N2-C7	-2.23	119.91	122.90
2	J	1	NAG	O5-C1-C2	-2.22	107.85	111.29
2	Z	1	NAG	C2-N2-C7	-2.22	119.92	122.90
3	F	1	NAG	O4-C4-C3	-2.21	105.17	110.38
4	V	2	NAG	C2-N2-C7	-2.21	119.94	122.90
2	D	2	NAG	C8-C7-N2	2.20	119.77	116.12
2	T	1	NAG	C2-N2-C7	-2.19	119.96	122.90
2	E	1	NAG	C8-C7-N2	2.18	119.74	116.12
4	d	1	NAG	C8-C7-N2	2.17	119.72	116.12
5	W	3	MAN	O2-C2-C3	-2.17	105.65	110.15
5	f	3	MAN	O2-C2-C3	-2.16	105.68	110.15
5	e	2	NAG	C3-C4-C5	2.15	114.13	110.23
5	e	3	MAN	O2-C2-C3	-2.15	105.70	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	1	NAG	O7-C7-C8	-2.14	118.24	122.05
5	L	3	MAN	O2-C2-C3	-2.13	105.73	110.15
2	E	1	NAG	C1-O5-C5	2.11	115.02	112.19
5	M	3	MAN	O2-C2-C3	-2.11	105.78	110.15
4	K	2	NAG	C2-N2-C7	-2.07	120.12	122.90
4	V	1	NAG	C6-C5-C4	-2.07	107.93	113.02
4	K	3	FUC	C1-O5-C5	2.06	117.83	112.97
3	R	1	NAG	C1-O5-C5	-2.05	109.44	112.19
4	d	2	NAG	C2-N2-C7	-2.02	120.19	122.90
3	R	2	NAG	C6-C5-C4	-2.01	108.07	113.02
2	Z	1	NAG	C4-C3-C2	2.01	113.96	111.02
2	E	2	NAG	C2-N2-C7	-2.01	120.21	122.90

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C1-C2-N2-C7
4	V	2	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
5	f	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
4	d	2	NAG	O5-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	K	2	NAG	C4-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
2	b	2	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	d	2	NAG	C4-C5-C6-O6
5	f	3	MAN	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
5	e	3	MAN	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
5	L	3	MAN	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	f	3	MAN	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
5	W	3	MAN	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	Z	1	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
2	J	2	NAG	C1-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
5	e	3	MAN	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
5	f	1	NAG	C4-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
3	R	1	NAG	C3-C2-N2-C7
2	E	2	NAG	O5-C5-C6-O6
5	f	1	NAG	O5-C5-C6-O6
5	L	3	MAN	C4-C5-C6-O6

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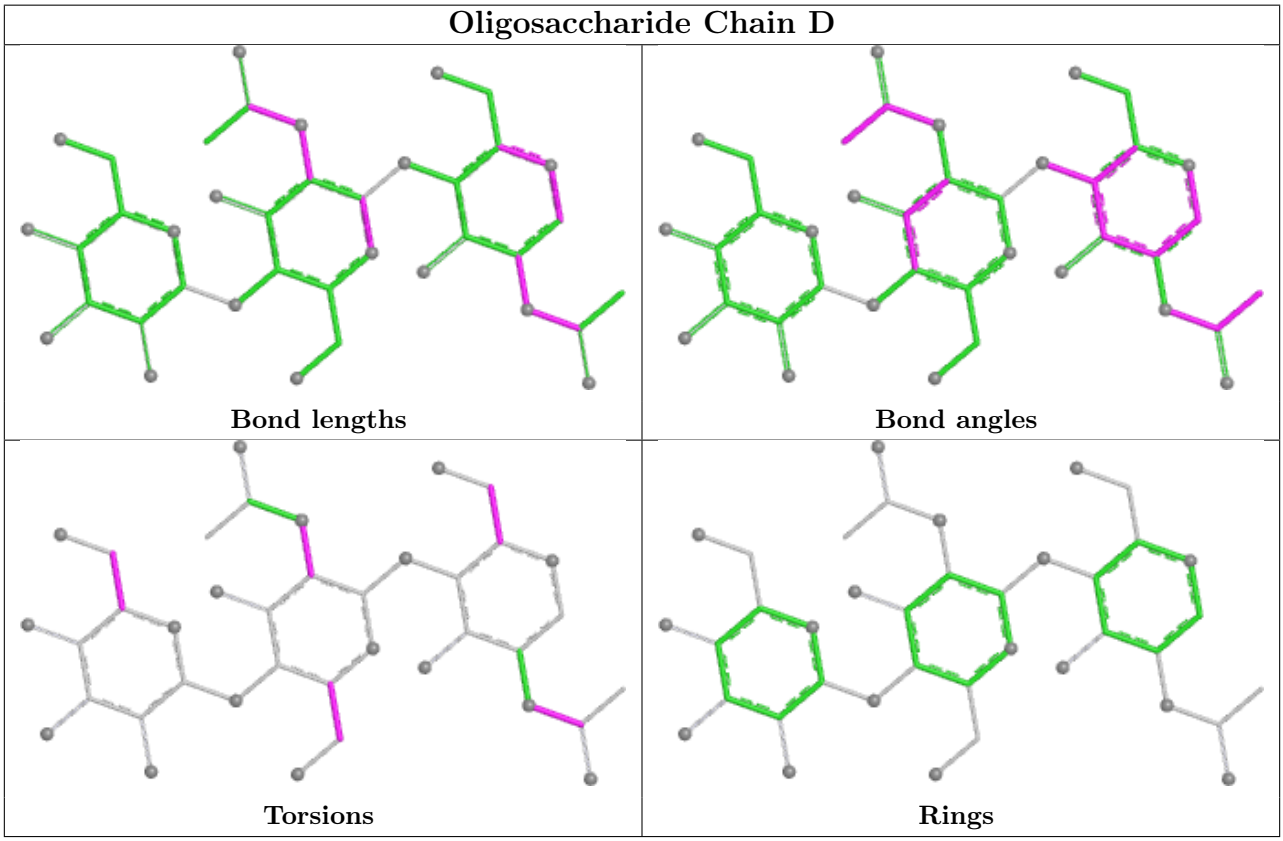
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C3-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7
3	G	2	NAG	C3-C2-N2-C7
5	W	2	NAG	C4-C5-C6-O6

All (5) ring outliers are listed below:

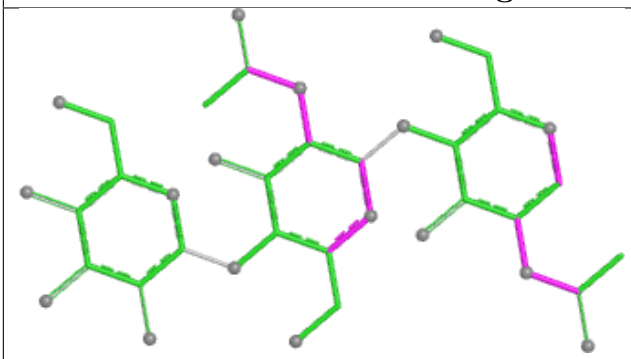
Mol	Chain	Res	Type	Atoms
5	L	3	MAN	C1-C2-C3-C4-C5-O5
5	M	3	MAN	C1-C2-C3-C4-C5-O5
5	e	3	MAN	C1-C2-C3-C4-C5-O5
5	f	3	MAN	C1-C2-C3-C4-C5-O5
5	W	3	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

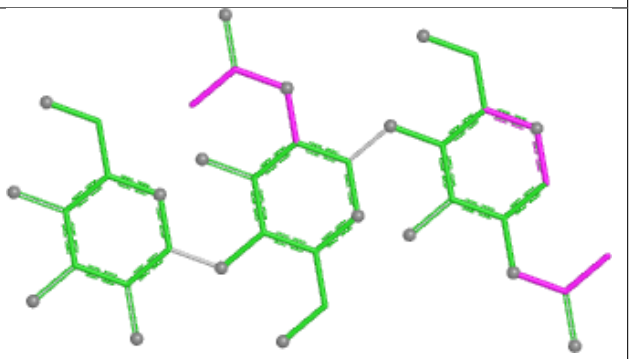
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



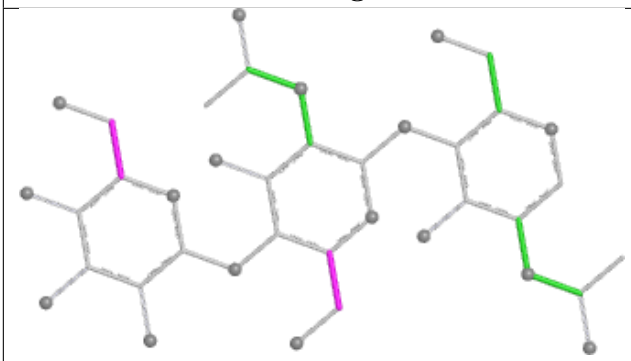
Oligosaccharide Chain E



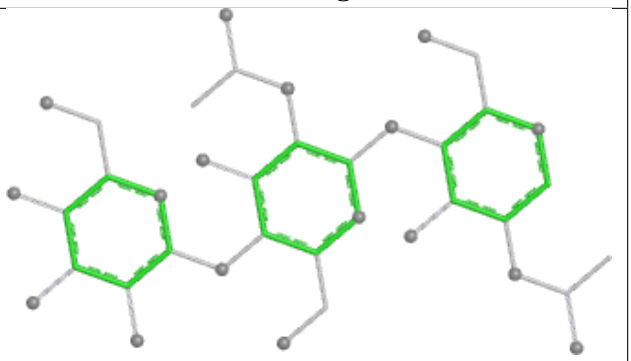
Bond lengths



Bond angles

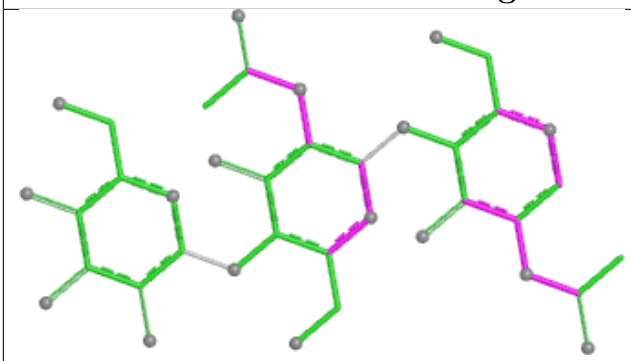


Torsions

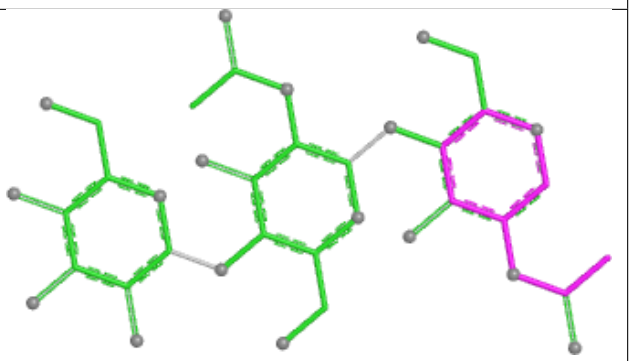


Rings

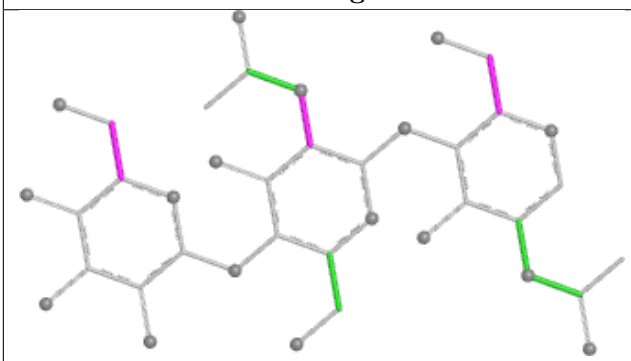
Oligosaccharide Chain J



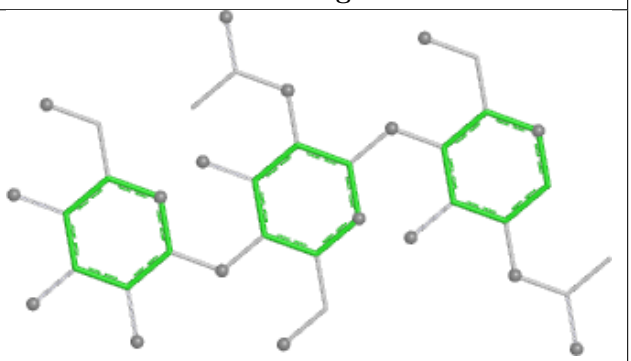
Bond lengths



Bond angles

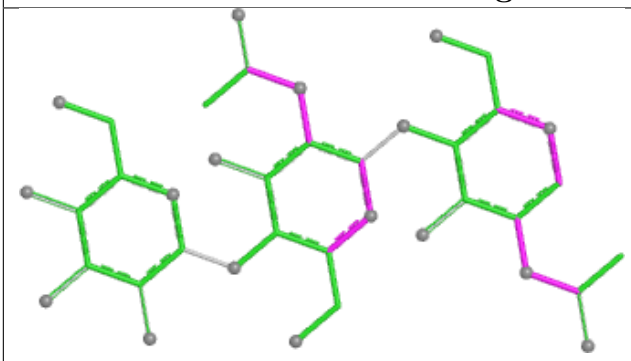


Torsions

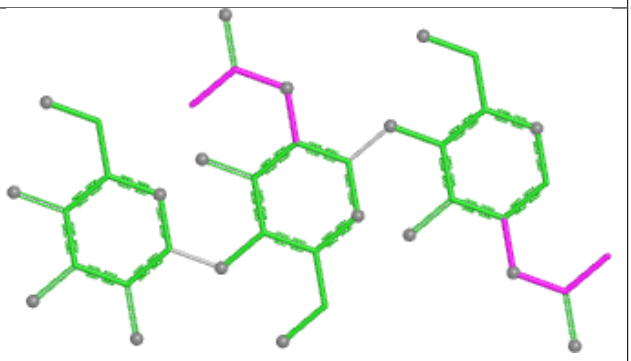


Rings

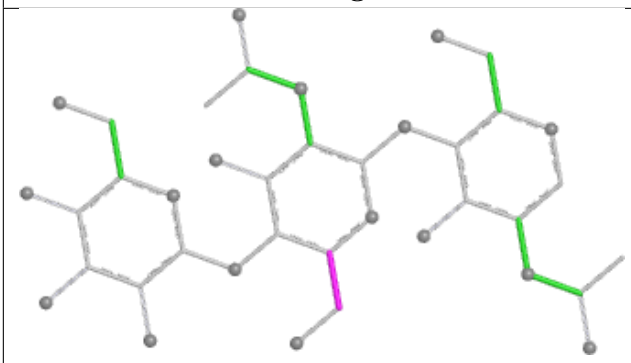
Oligosaccharide Chain T



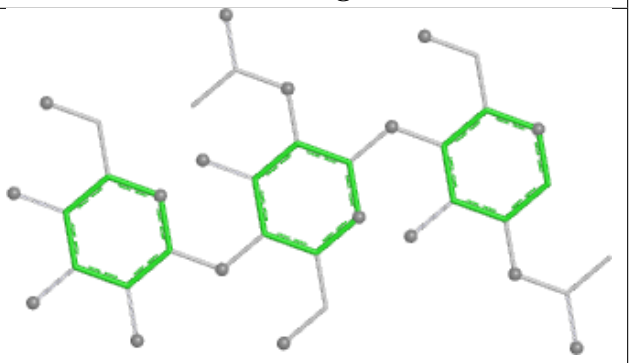
Bond lengths



Bond angles

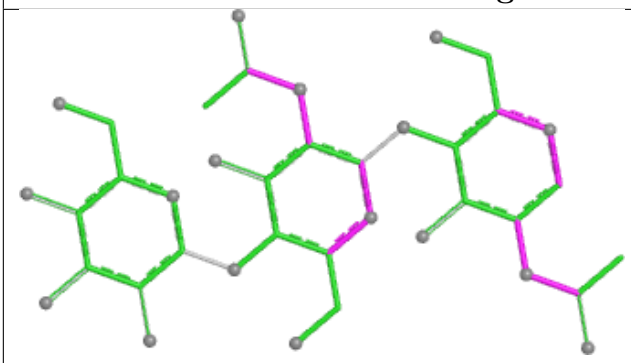


Torsions

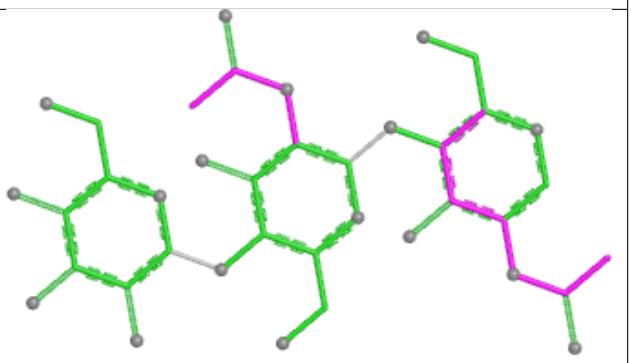


Rings

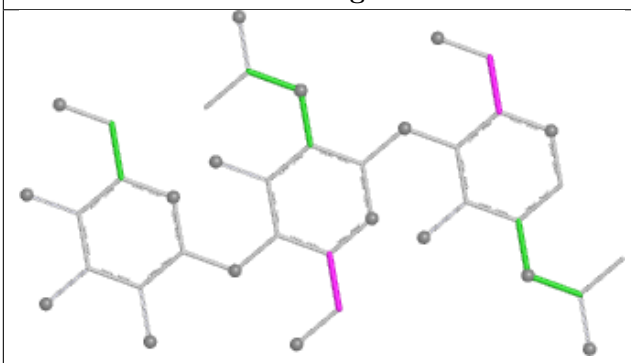
Oligosaccharide Chain Z



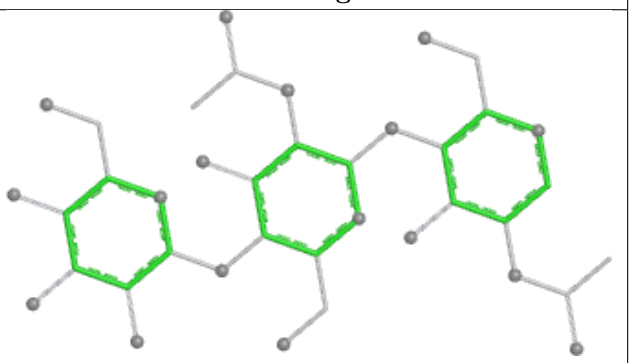
Bond lengths



Bond angles

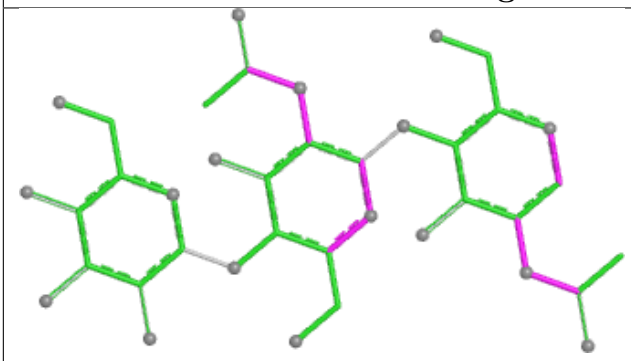


Torsions



Rings

Oligosaccharide Chain b



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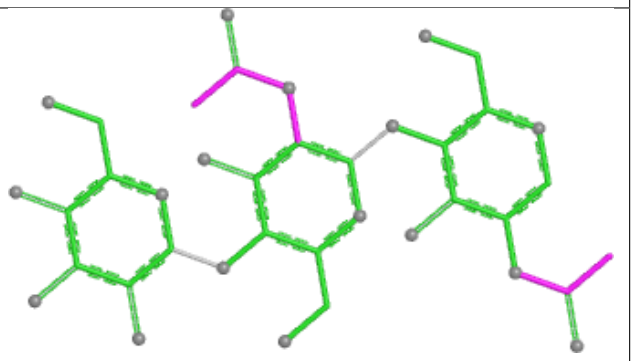
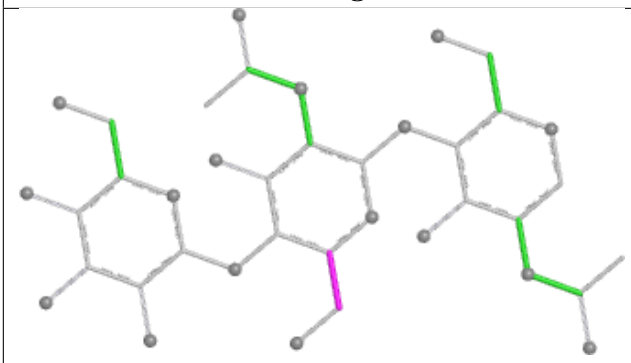
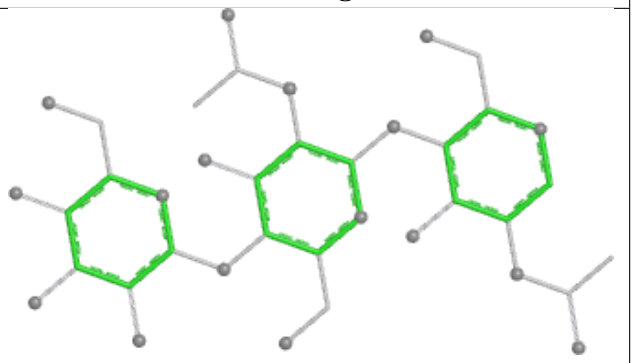


Bond angles

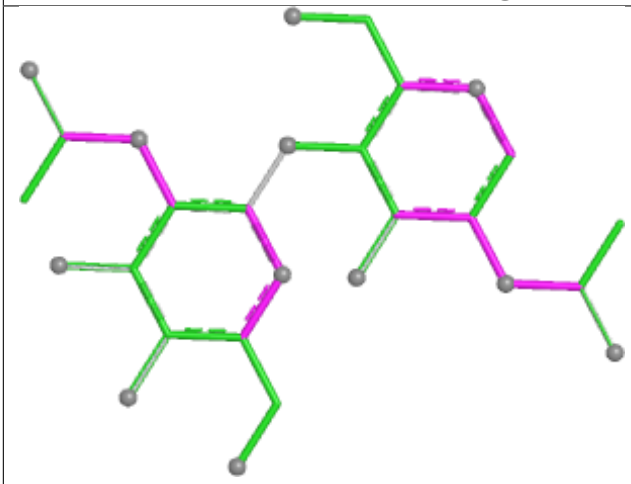


Torsions



Rings

Oligosaccharide Chain F



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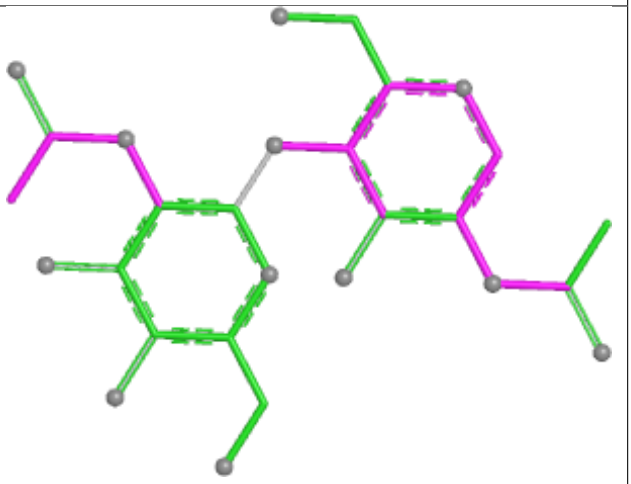
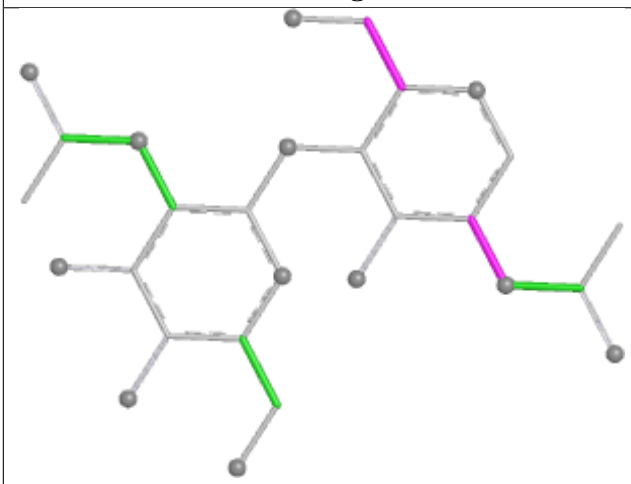
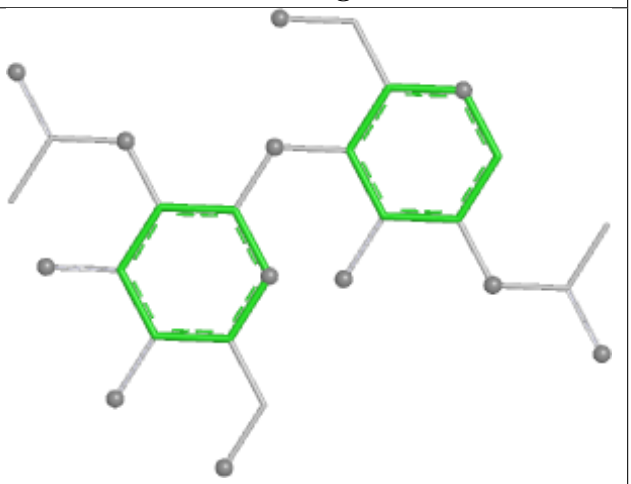


Bond angles

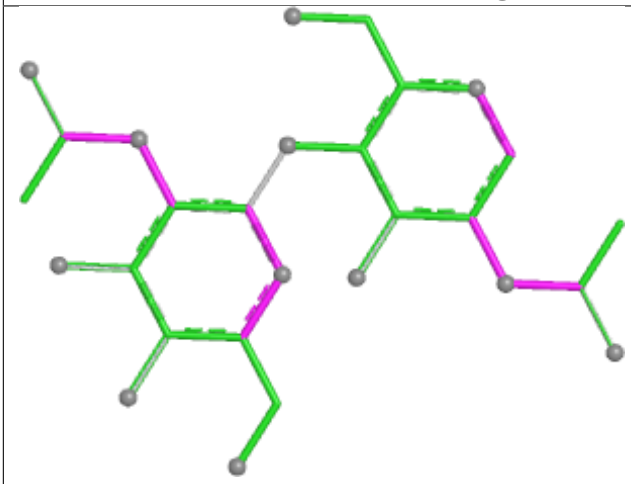


Torsions



Rings

Oligosaccharide Chain G



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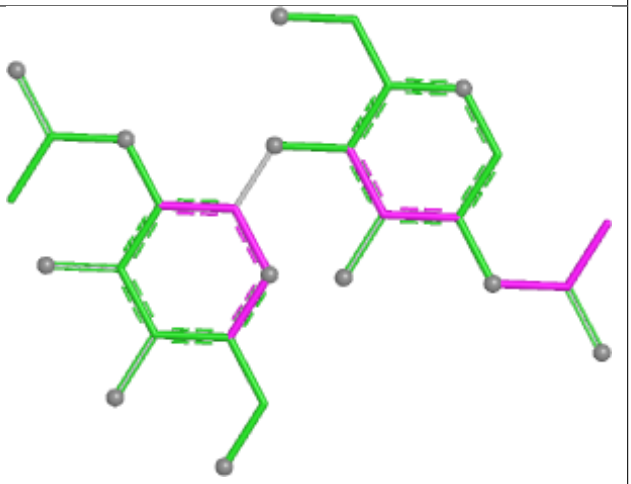
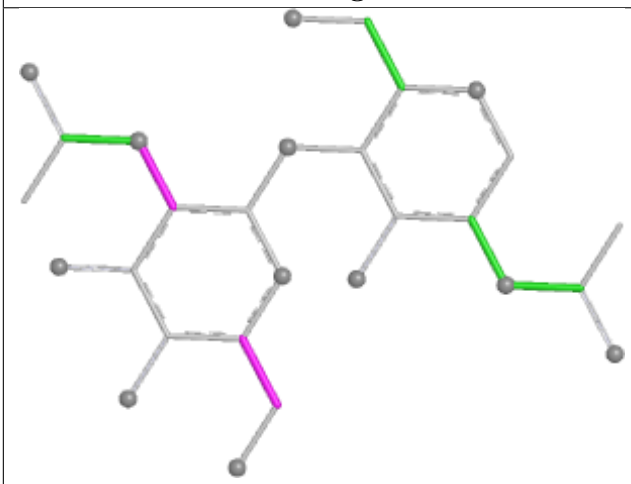
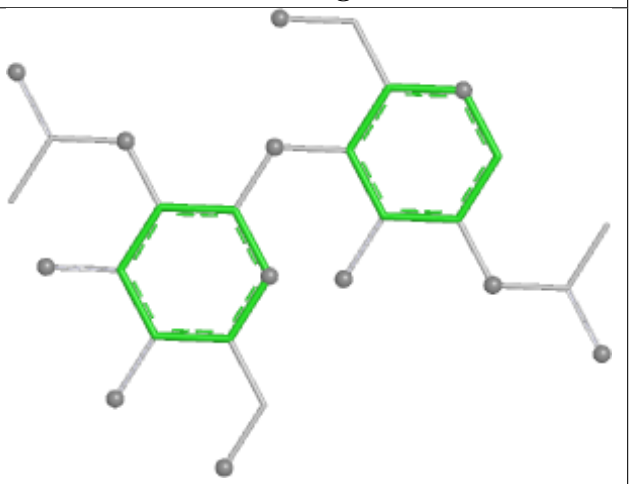


Bond angles

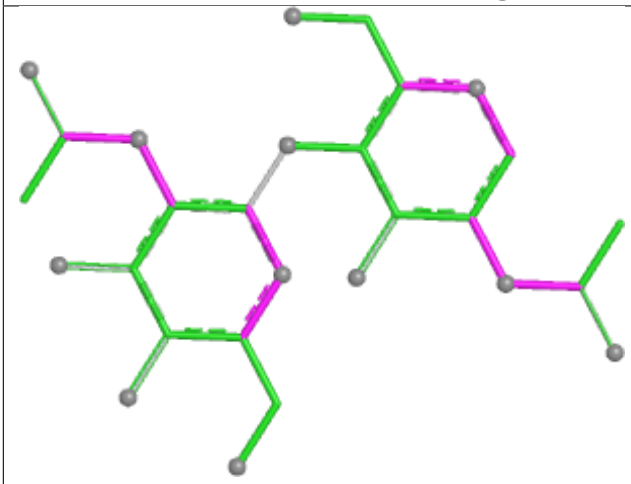


Torsions



Rings

Oligosaccharide Chain H



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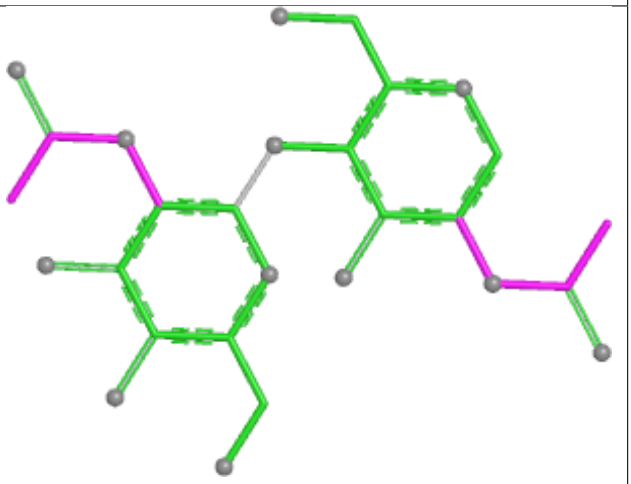
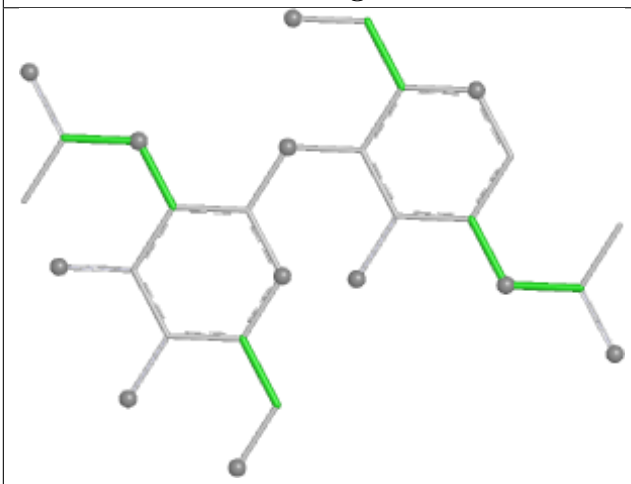
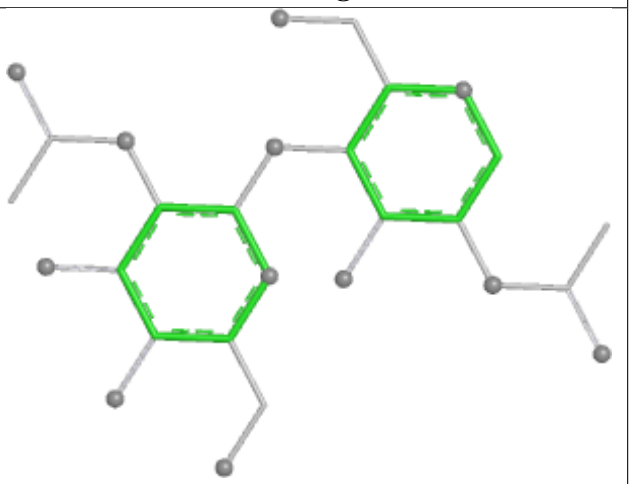


Bond angles

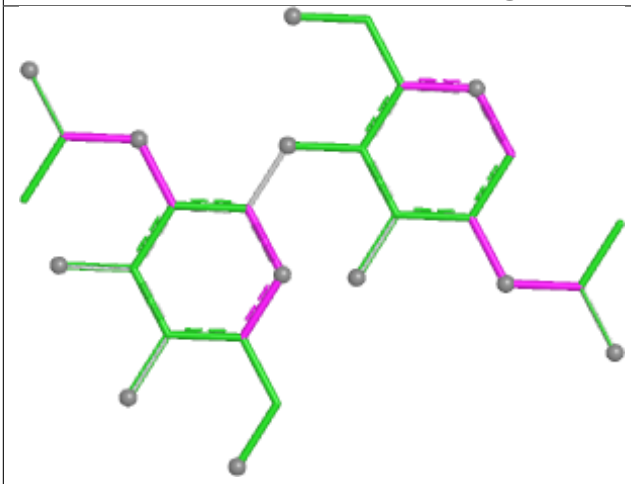


Torsions



Rings

Oligosaccharide Chain I



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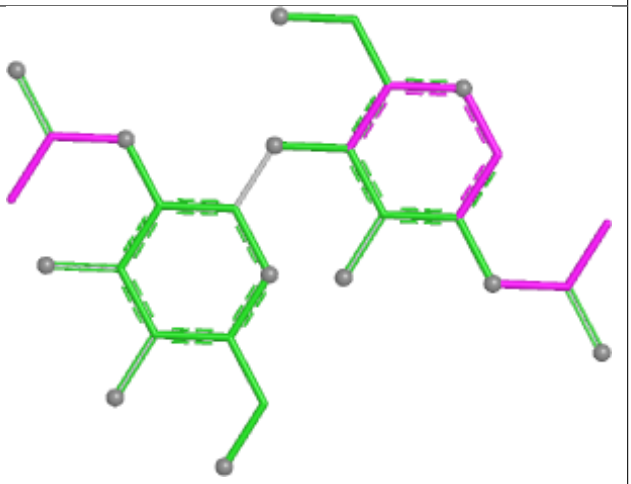
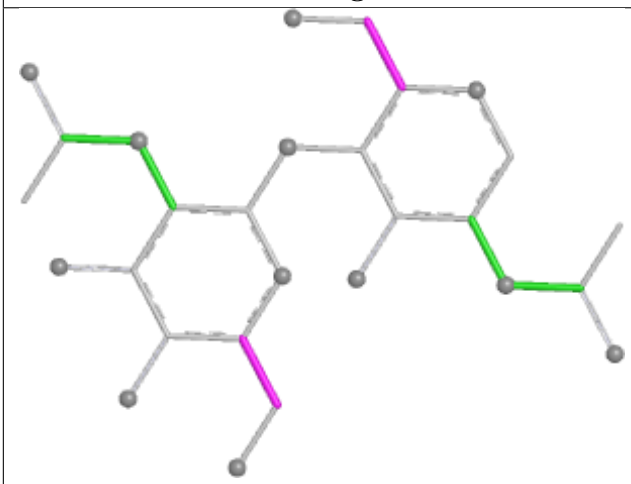


Bond angles



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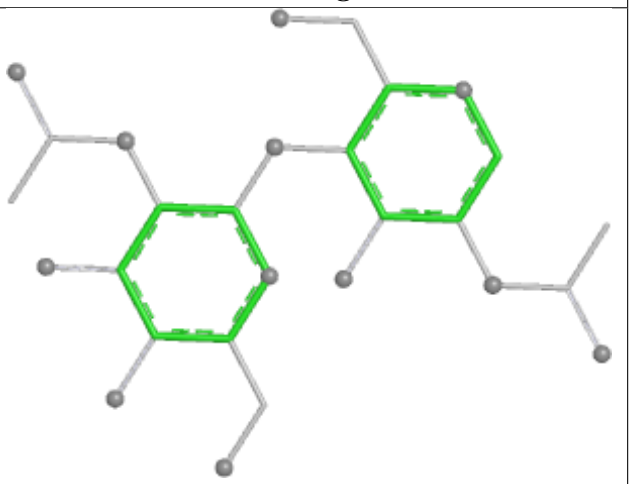
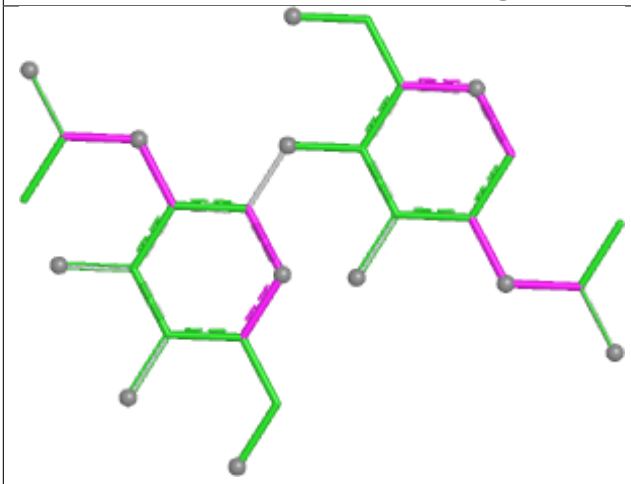


Rings

Oligosaccharide Chain R



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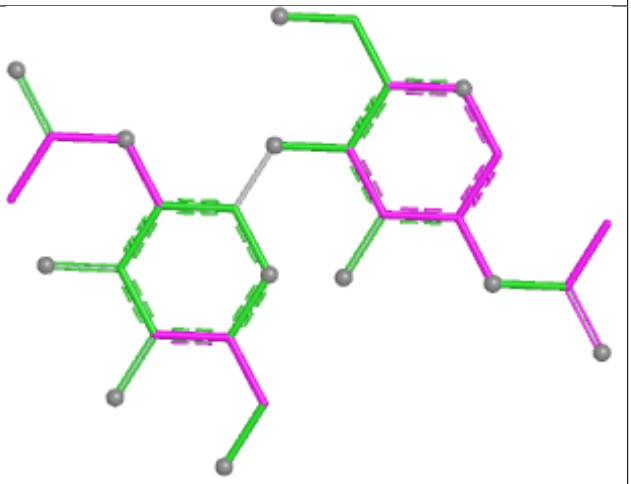
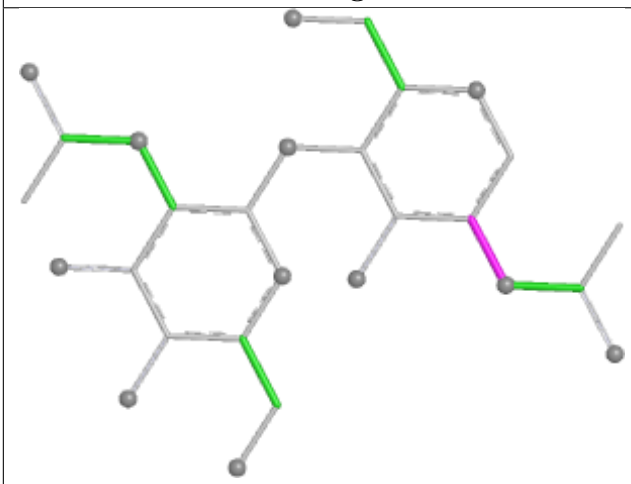
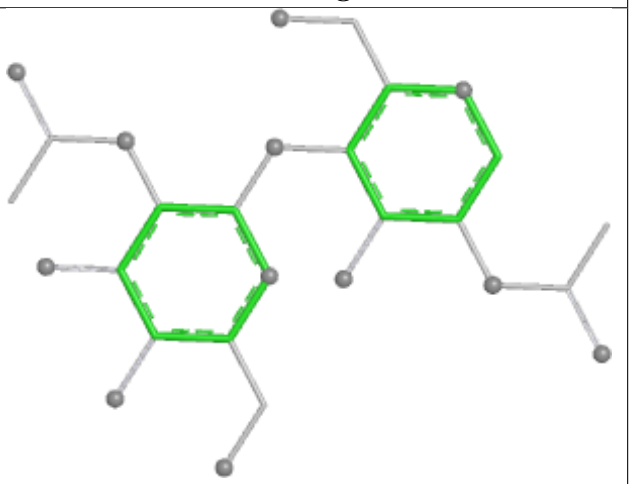


Bond angles

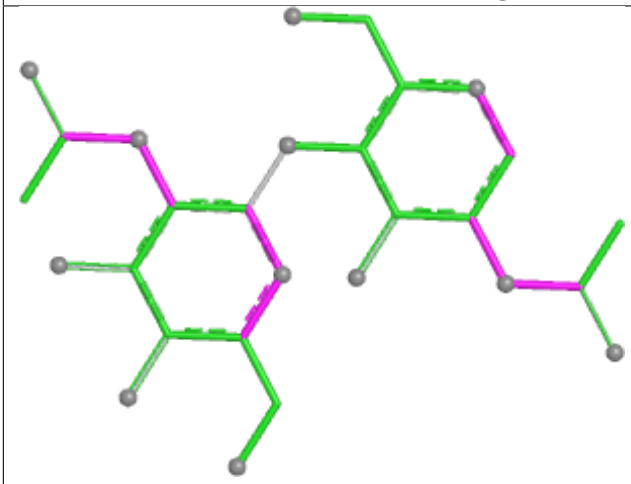


Torsions



Rings

Oligosaccharide Chain U



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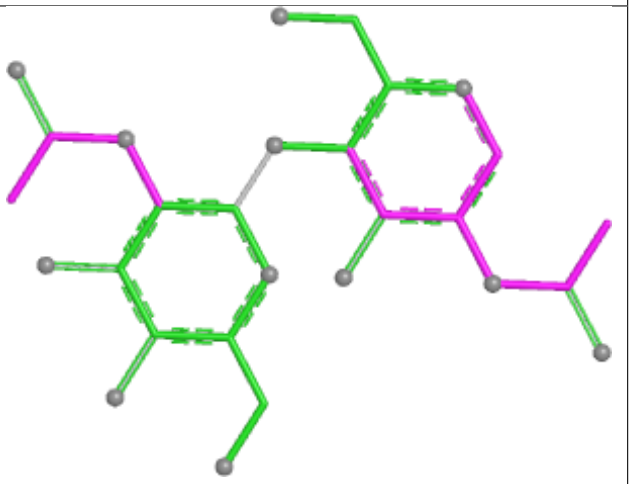
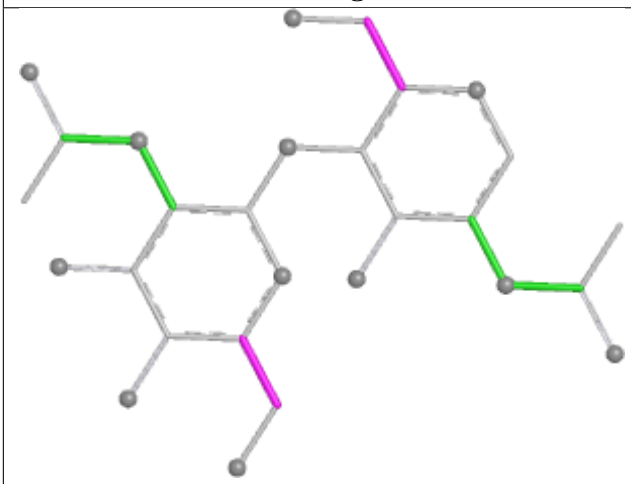
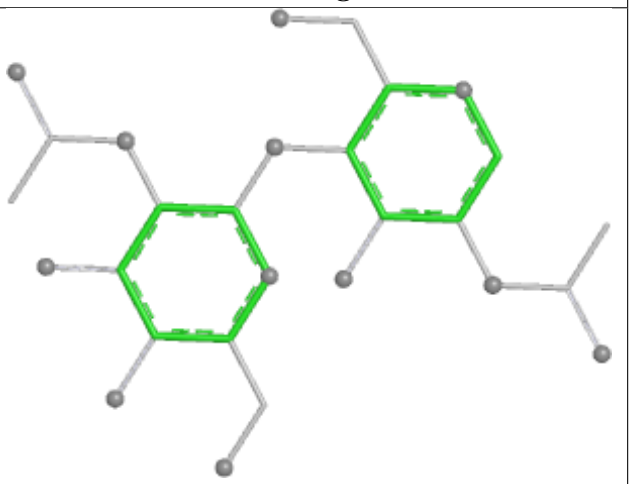


Bond angles

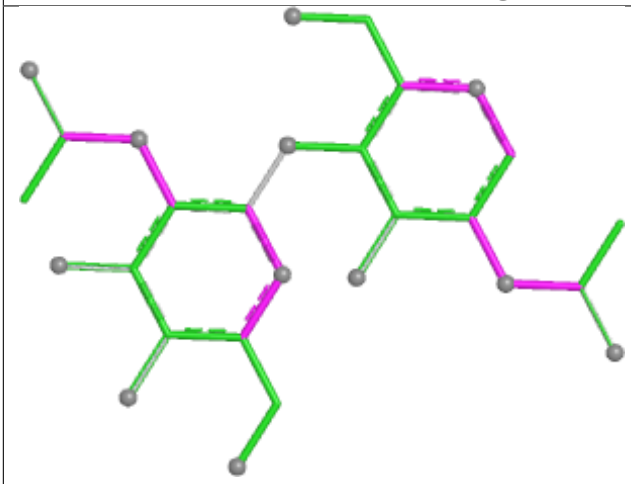


Torsions



Rings

Oligosaccharide Chain X



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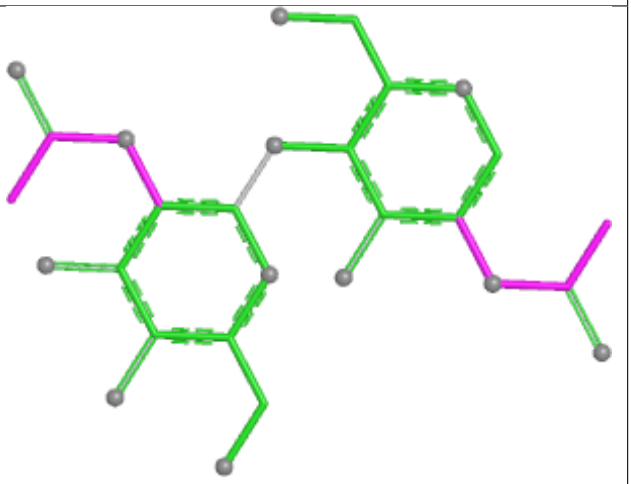
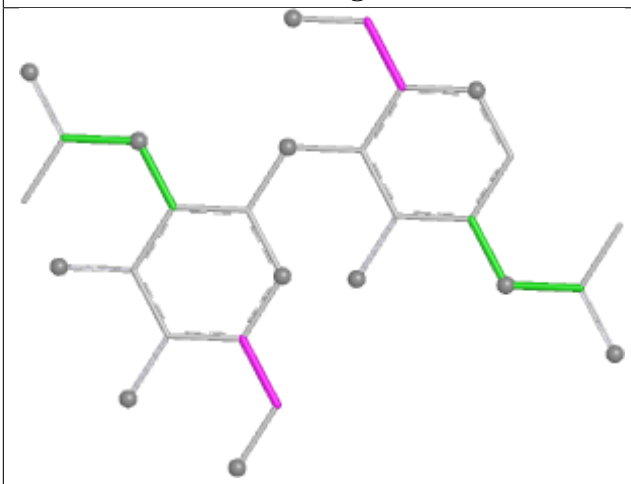
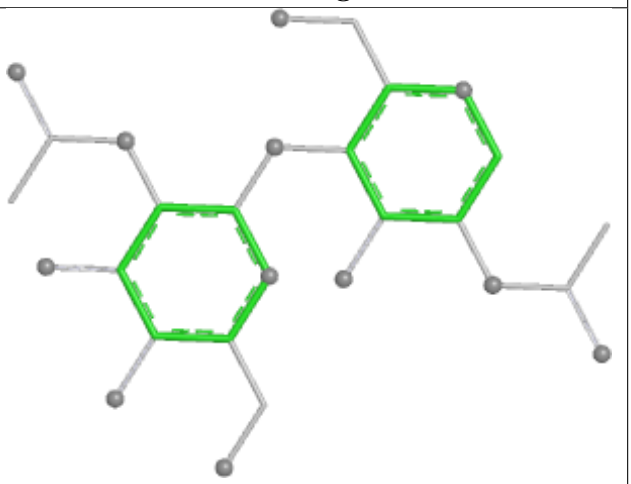


Bond angles

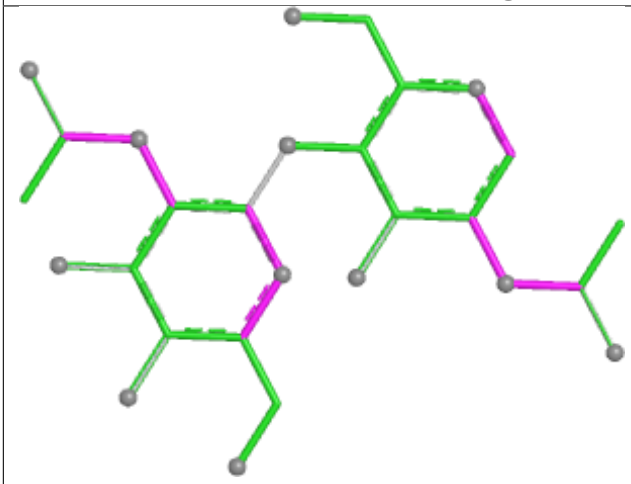


Torsions



Rings

Oligosaccharide Chain c



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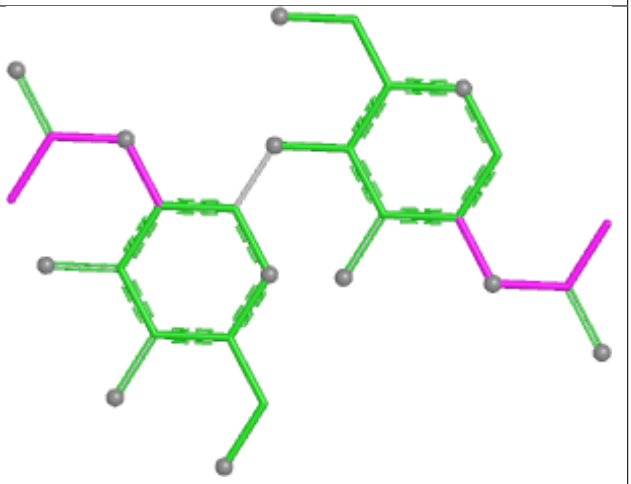
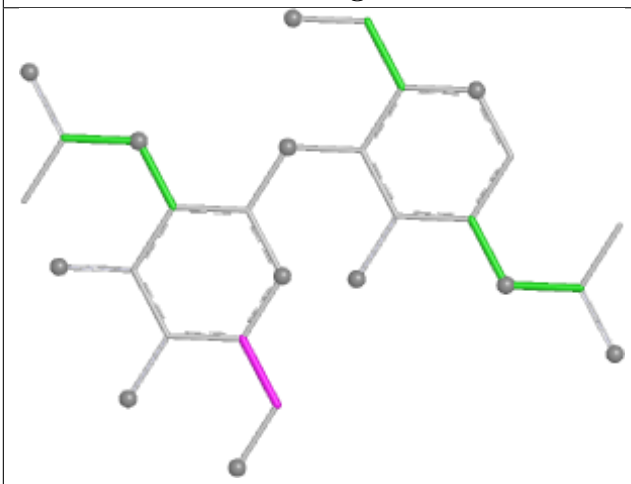
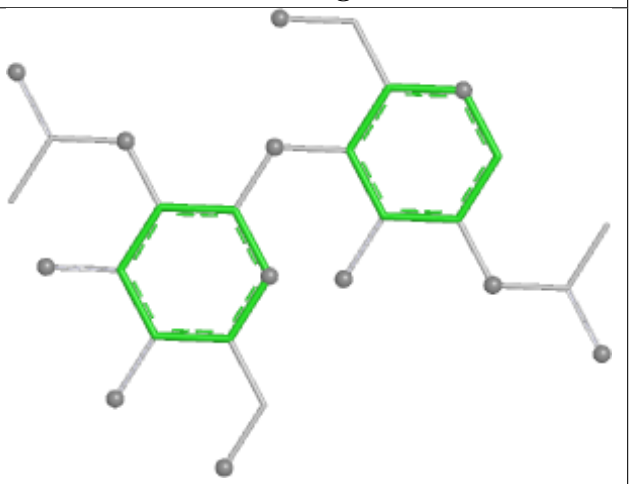


Bond angles

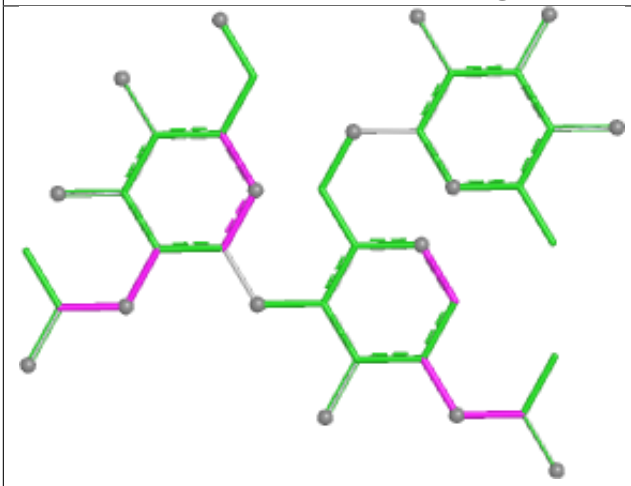


Torsions



Rings

Oligosaccharide Chain K



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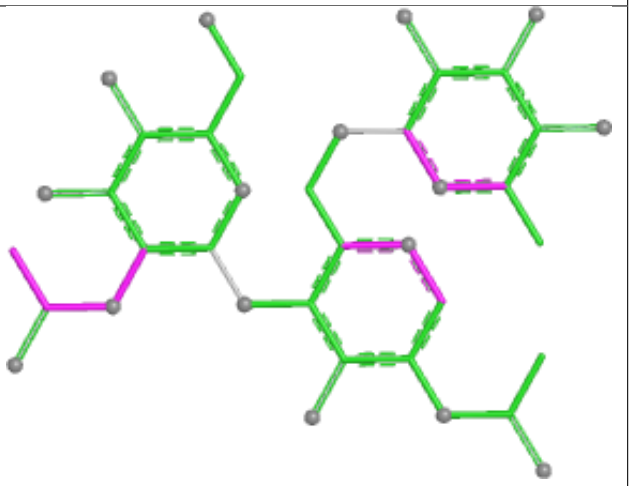
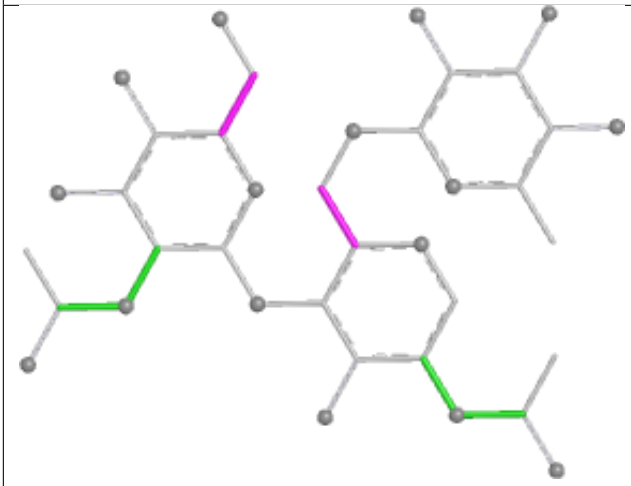


Bond angles



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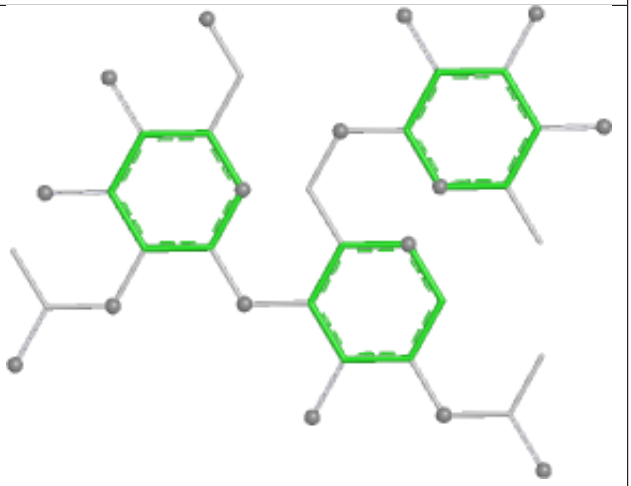
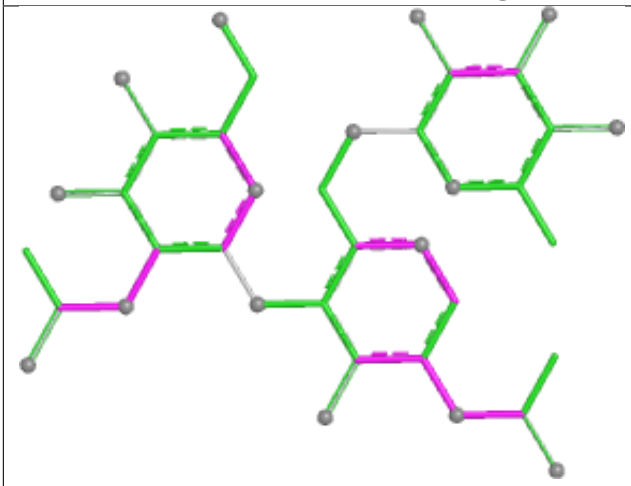


Rings

Oligosaccharide Chain V



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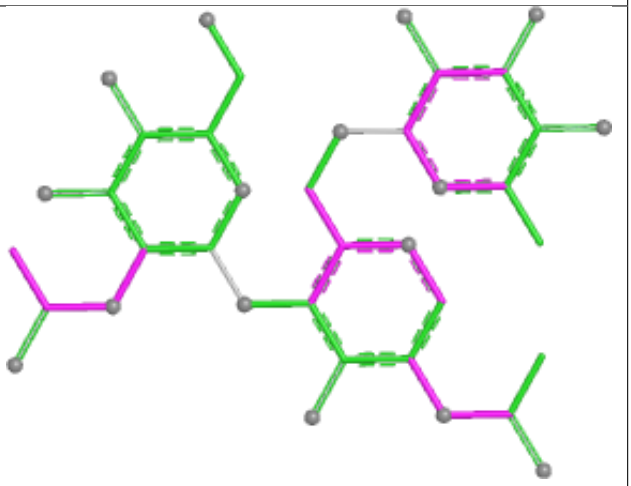
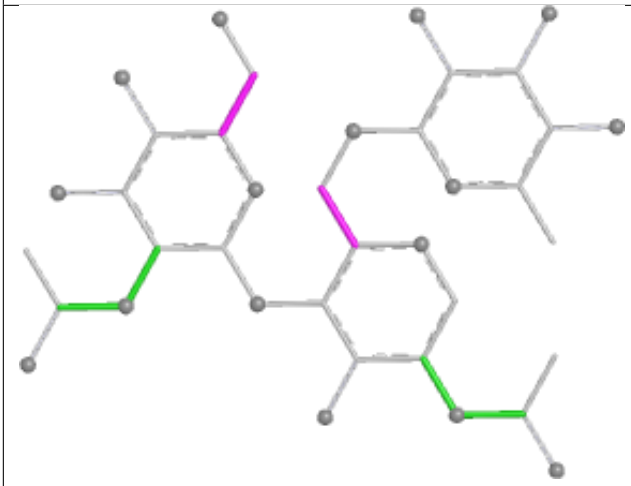
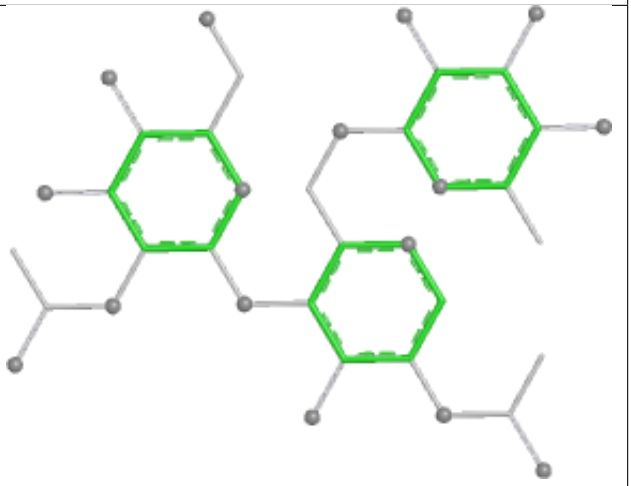


Bond angles

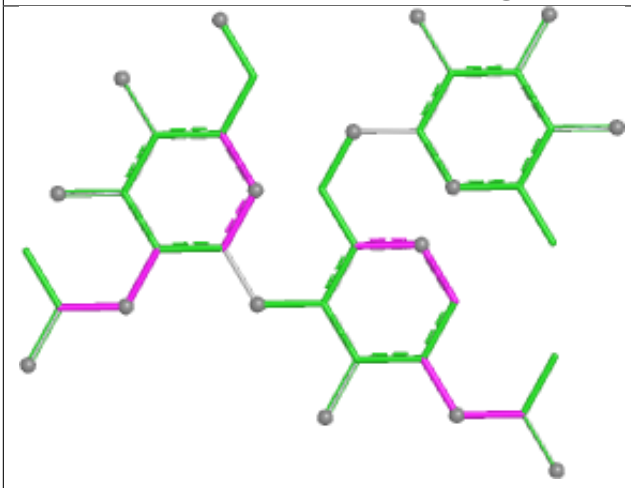


Torsions

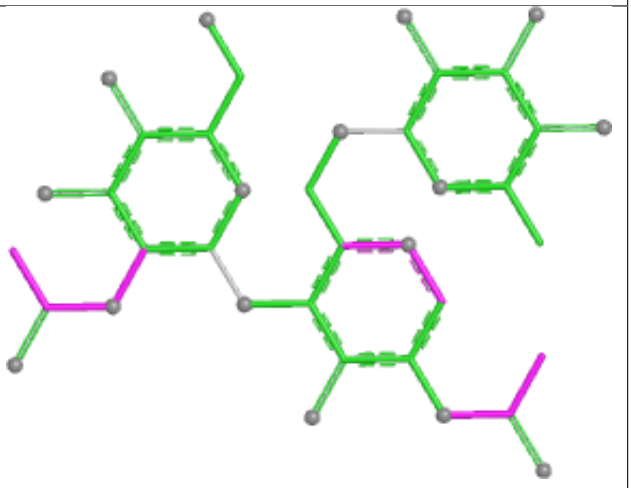


Rings

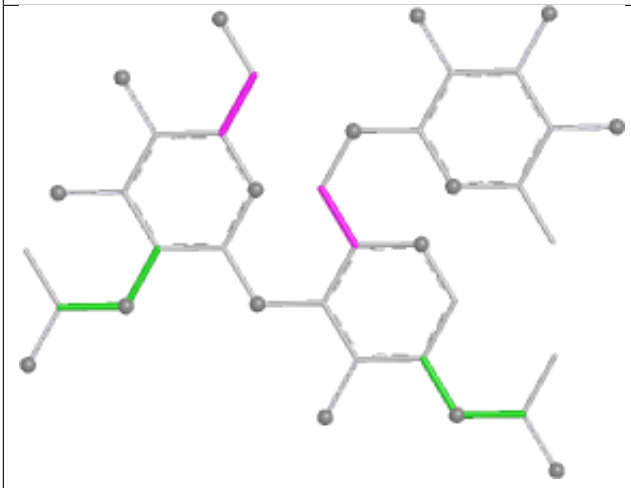
Oligosaccharide Chain d



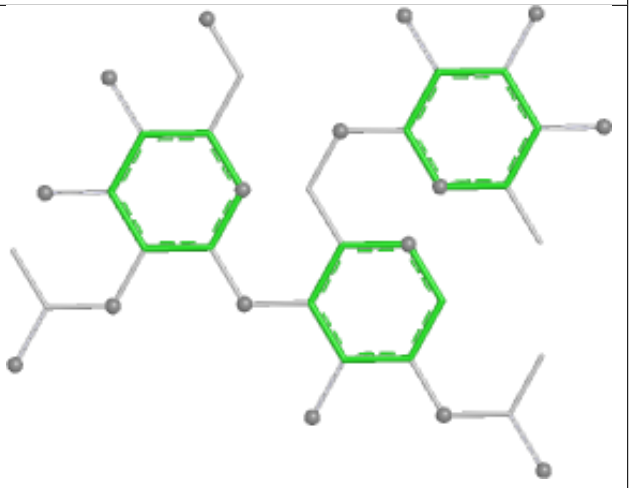
Bond lengths



Bond angles

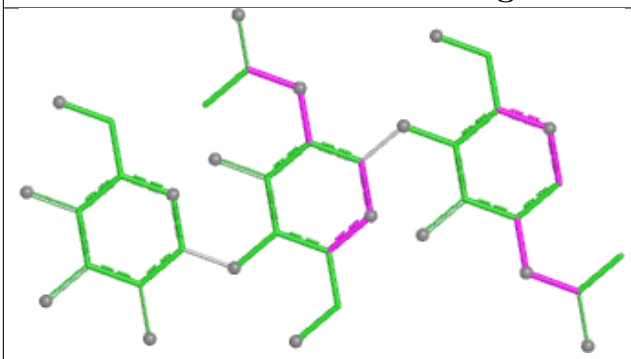


Torsions

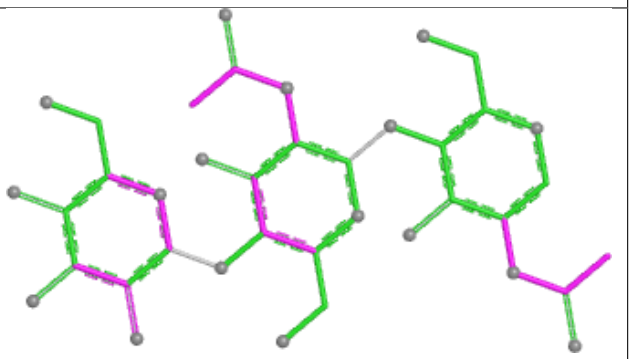


Rings

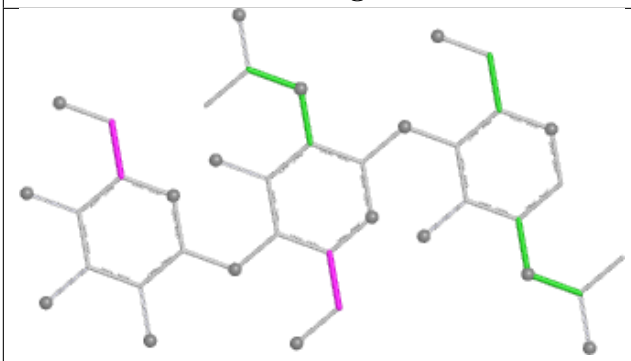
Oligosaccharide Chain L



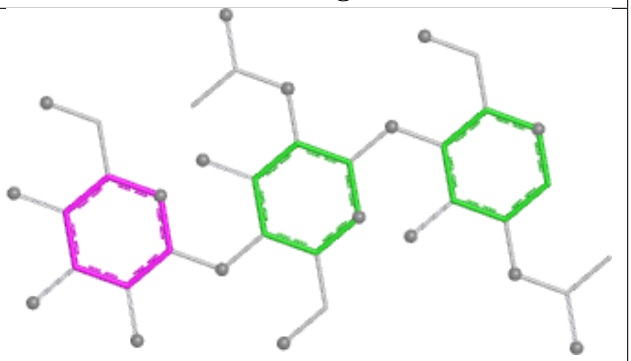
Bond lengths



Bond angles

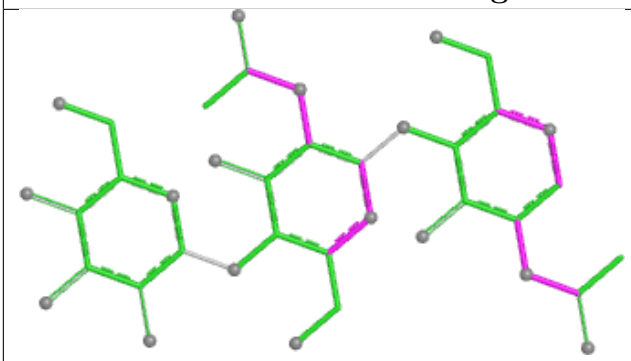


Torsions

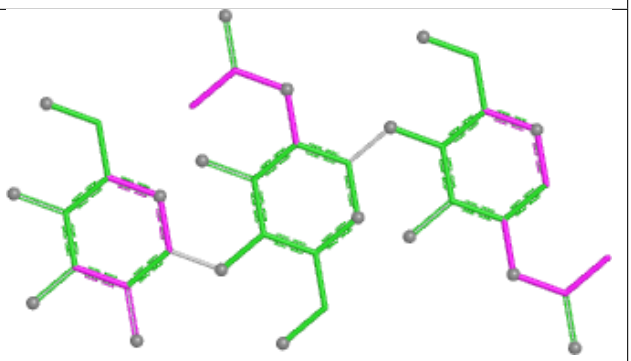


Rings

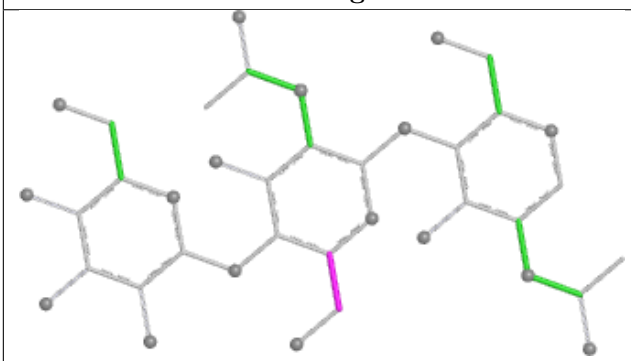
Oligosaccharide Chain M



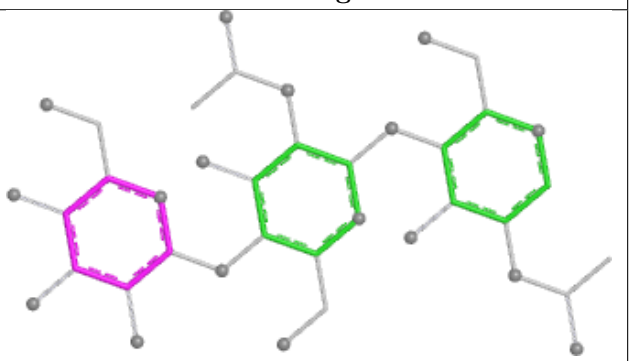
Bond lengths



Bond angles

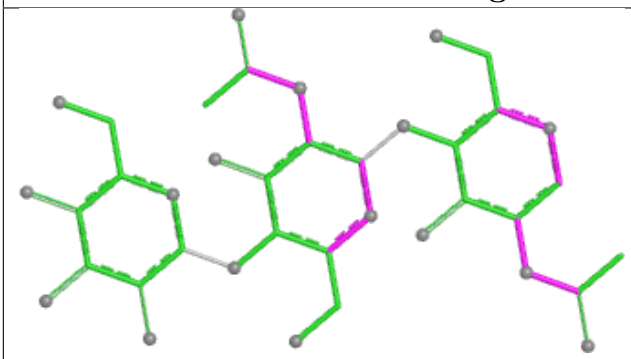


Torsions

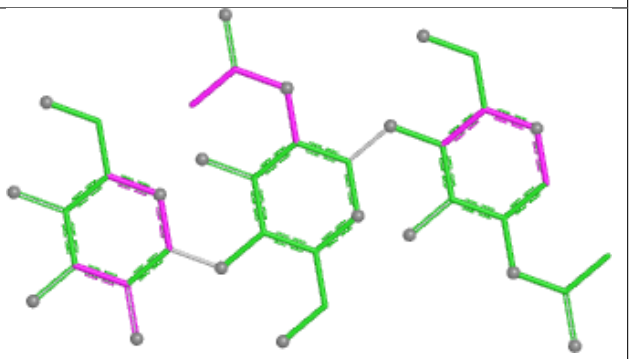


Rings

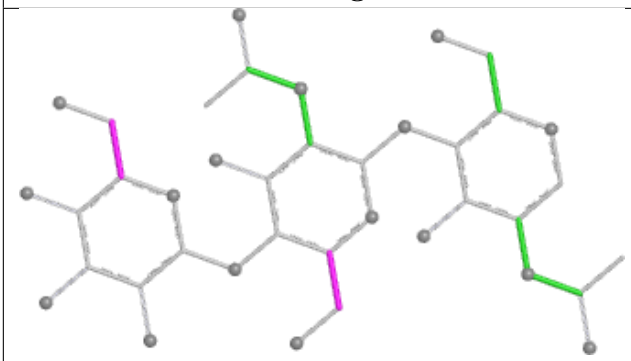
Oligosaccharide Chain W



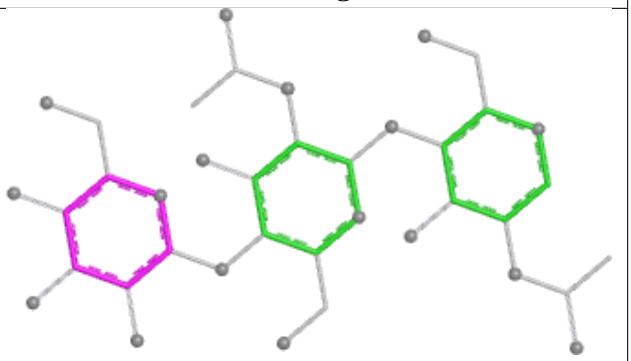
Bond lengths



Bond angles

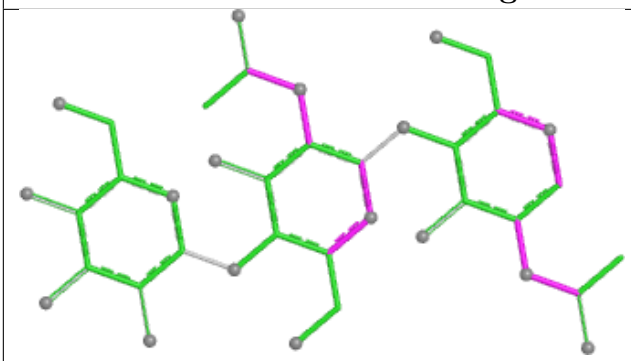


Torsions

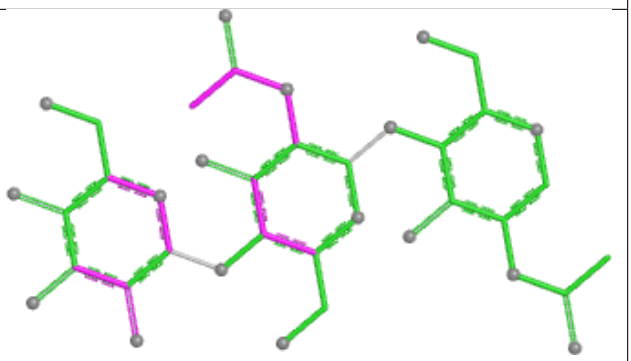


Rings

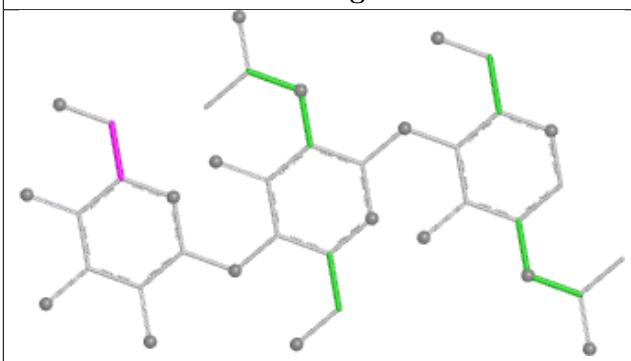
Oligosaccharide Chain e



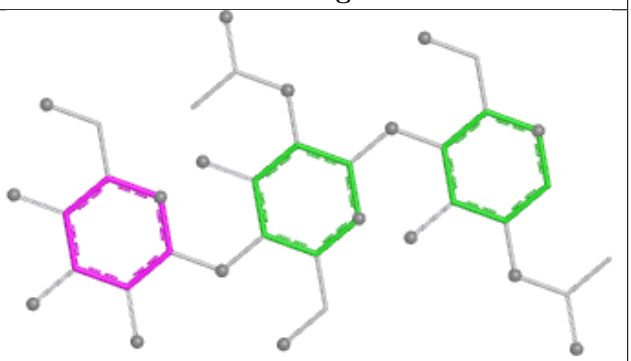
Bond lengths



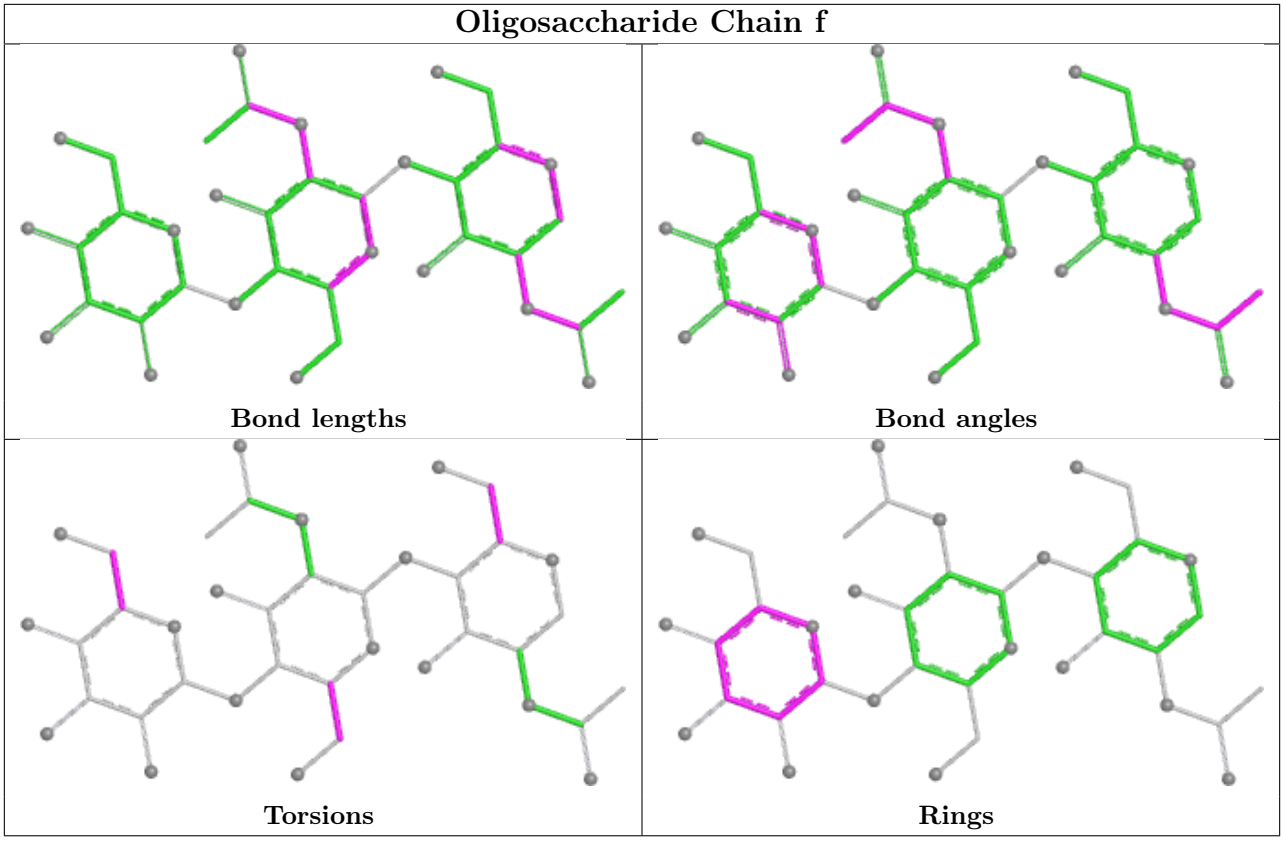
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	B	1405	1	14,14,15	2.06	4 (28%)	17,19,21	0.93	0
6	NAG	C	1408	1	14,14,15	2.01	3 (21%)	17,19,21	1.71	3 (17%)
6	NAG	C	1407	1	14,14,15	2.00	4 (28%)	17,19,21	1.11	1 (5%)
6	NAG	A	1407	1	14,14,15	2.04	4 (28%)	17,19,21	1.17	1 (5%)
6	NAG	B	1403	1	14,14,15	2.02	4 (28%)	17,19,21	1.13	1 (5%)
6	NAG	A	1406	1	14,14,15	1.98	4 (28%)	17,19,21	1.28	2 (11%)
6	NAG	C	1405	1	14,14,15	2.00	4 (28%)	17,19,21	1.07	1 (5%)
6	NAG	A	1403	1	14,14,15	2.00	4 (28%)	17,19,21	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	C	1401	1	14,14,15	2.00	4 (28%)	17,19,21	1.07	2 (11%)
6	NAG	B	1404	1	14,14,15	2.00	4 (28%)	17,19,21	1.22	2 (11%)
6	NAG	A	1405	1	14,14,15	1.95	4 (28%)	17,19,21	1.57	3 (17%)
6	NAG	C	1406	1	14,14,15	1.95	3 (21%)	17,19,21	1.22	2 (11%)
6	NAG	B	1402	1	14,14,15	2.03	4 (28%)	17,19,21	1.07	2 (11%)
6	NAG	A	1402	1	14,14,15	2.03	4 (28%)	17,19,21	1.21	2 (11%)
6	NAG	B	1401	1	14,14,15	2.00	4 (28%)	17,19,21	1.10	2 (11%)
6	NAG	A	1401	1	14,14,15	2.01	4 (28%)	17,19,21	1.16	2 (11%)
6	NAG	B	1408	-	14,14,15	1.99	4 (28%)	17,19,21	1.11	1 (5%)
6	NAG	A	1404	1	14,14,15	2.01	4 (28%)	17,19,21	1.08	2 (11%)
6	NAG	B	1406	1	14,14,15	1.97	4 (28%)	17,19,21	1.23	2 (11%)
6	NAG	B	1407	1	14,14,15	2.13	4 (28%)	17,19,21	1.95	4 (23%)
6	NAG	A	1408	1	14,14,15	2.00	4 (28%)	17,19,21	1.03	1 (5%)
6	NAG	C	1404	1	14,14,15	2.02	4 (28%)	17,19,21	1.43	3 (17%)
6	NAG	C	1402	1	14,14,15	1.96	4 (28%)	17,19,21	1.27	3 (17%)
6	NAG	C	1403	1	14,14,15	1.92	3 (21%)	17,19,21	1.58	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1405	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1407	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1407	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1404	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1402	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1401	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1408	-	-	0/6/23/26	0/1/1/1
6	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1406	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1407	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1403	1	-	0/6/23/26	0/1/1/1

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1407	NAG	O5-C1	4.84	1.51	1.43
6	C	1408	NAG	O5-C1	4.57	1.51	1.43
6	A	1407	NAG	O5-C1	4.50	1.51	1.43
6	B	1402	NAG	O5-C1	4.45	1.51	1.43
6	B	1403	NAG	O5-C1	4.41	1.51	1.43
6	C	1405	NAG	O5-C1	4.39	1.51	1.43
6	A	1404	NAG	O5-C1	4.37	1.51	1.43
6	A	1402	NAG	O5-C1	4.37	1.51	1.43
6	C	1401	NAG	O5-C1	4.37	1.51	1.43
6	C	1407	NAG	O5-C1	4.36	1.51	1.43
6	A	1408	NAG	O5-C1	4.35	1.51	1.43
6	B	1405	NAG	O5-C1	4.35	1.51	1.43
6	C	1404	NAG	O5-C1	4.31	1.50	1.43
6	A	1406	NAG	O5-C1	4.30	1.50	1.43
6	A	1401	NAG	O5-C1	4.29	1.50	1.43
6	B	1401	NAG	O5-C1	4.28	1.50	1.43
6	B	1406	NAG	O5-C1	4.27	1.50	1.43
6	B	1408	NAG	O5-C1	4.27	1.50	1.43
6	C	1406	NAG	O5-C1	4.24	1.50	1.43
6	A	1403	NAG	O5-C1	4.23	1.50	1.43
6	B	1404	NAG	O5-C1	4.23	1.50	1.43
6	C	1402	NAG	O5-C1	4.16	1.50	1.43
6	C	1403	NAG	O5-C1	4.11	1.50	1.43
6	B	1405	NAG	C7-N2	4.06	1.47	1.34
6	A	1405	NAG	O5-C1	4.00	1.50	1.43
6	A	1403	NAG	C7-N2	3.93	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1404	NAG	C7-N2	3.91	1.47	1.34
6	A	1407	NAG	C7-N2	3.91	1.47	1.34
6	B	1408	NAG	C7-N2	3.90	1.46	1.34
6	B	1403	NAG	C7-N2	3.90	1.46	1.34
6	C	1407	NAG	C7-N2	3.89	1.46	1.34
6	B	1401	NAG	C7-N2	3.89	1.46	1.34
6	A	1402	NAG	C7-N2	3.89	1.46	1.34
6	A	1401	NAG	C7-N2	3.89	1.46	1.34
6	C	1408	NAG	C7-N2	3.89	1.46	1.34
6	A	1405	NAG	C7-N2	3.88	1.46	1.34
6	B	1404	NAG	C7-N2	3.88	1.46	1.34
6	C	1402	NAG	C7-N2	3.88	1.46	1.34
6	B	1402	NAG	C7-N2	3.87	1.46	1.34
6	B	1407	NAG	C7-N2	3.87	1.46	1.34
6	C	1405	NAG	C7-N2	3.87	1.46	1.34
6	C	1401	NAG	C7-N2	3.87	1.46	1.34
6	C	1403	NAG	C7-N2	3.87	1.46	1.34
6	A	1404	NAG	C7-N2	3.86	1.46	1.34
6	A	1406	NAG	C7-N2	3.85	1.46	1.34
6	C	1406	NAG	C7-N2	3.83	1.46	1.34
6	A	1408	NAG	C7-N2	3.82	1.46	1.34
6	B	1406	NAG	C7-N2	3.79	1.46	1.34
6	B	1405	NAG	C2-N2	2.87	1.51	1.46
6	A	1403	NAG	C2-N2	2.54	1.50	1.46
6	A	1407	NAG	C2-N2	2.53	1.50	1.46
6	B	1403	NAG	C2-N2	2.53	1.50	1.46
6	B	1408	NAG	C2-N2	2.50	1.50	1.46
6	C	1403	NAG	C2-N2	2.50	1.50	1.46
6	A	1402	NAG	C2-N2	2.50	1.50	1.46
6	C	1407	NAG	C2-N2	2.49	1.50	1.46
6	C	1405	NAG	C2-N2	2.49	1.50	1.46
6	A	1401	NAG	C2-N2	2.49	1.50	1.46
6	B	1407	NAG	C2-N2	2.49	1.50	1.46
6	C	1404	NAG	C2-N2	2.48	1.50	1.46
6	B	1402	NAG	C2-N2	2.48	1.50	1.46
6	B	1401	NAG	C2-N2	2.48	1.50	1.46
6	B	1404	NAG	C2-N2	2.46	1.50	1.46
6	C	1402	NAG	C2-N2	2.46	1.50	1.46
6	C	1401	NAG	C2-N2	2.45	1.50	1.46
6	A	1404	NAG	C2-N2	2.43	1.50	1.46
6	A	1406	NAG	C2-N2	2.42	1.50	1.46
6	A	1408	NAG	C2-N2	2.41	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1408	NAG	C2-N2	2.40	1.50	1.46
6	A	1402	NAG	O5-C5	2.40	1.48	1.43
6	C	1406	NAG	C2-N2	2.36	1.50	1.46
6	A	1405	NAG	C2-N2	2.35	1.50	1.46
6	B	1407	NAG	O5-C5	2.34	1.48	1.43
6	B	1404	NAG	O5-C5	2.33	1.48	1.43
6	A	1401	NAG	O5-C5	2.31	1.47	1.43
6	B	1402	NAG	O5-C5	2.29	1.47	1.43
6	B	1406	NAG	C2-N2	2.29	1.50	1.46
6	B	1406	NAG	O5-C5	2.27	1.47	1.43
6	C	1404	NAG	O5-C5	2.27	1.47	1.43
6	A	1404	NAG	O5-C5	2.27	1.47	1.43
6	A	1405	NAG	O5-C5	2.27	1.47	1.43
6	B	1401	NAG	O5-C5	2.25	1.47	1.43
6	B	1405	NAG	O5-C5	2.22	1.47	1.43
6	A	1406	NAG	O5-C5	2.18	1.47	1.43
6	C	1401	NAG	O5-C5	2.18	1.47	1.43
6	A	1408	NAG	O5-C5	2.18	1.47	1.43
6	A	1403	NAG	O5-C5	2.14	1.47	1.43
6	B	1403	NAG	O5-C5	2.13	1.47	1.43
6	C	1407	NAG	O5-C5	2.13	1.47	1.43
6	B	1408	NAG	O5-C5	2.11	1.47	1.43
6	C	1405	NAG	O5-C5	2.09	1.47	1.43
6	C	1402	NAG	O5-C5	2.07	1.47	1.43
6	A	1407	NAG	O5-C5	2.07	1.47	1.43

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1407	NAG	C1-O5-C5	5.68	119.79	112.19
6	C	1403	NAG	C4-C3-C2	4.00	116.88	111.02
6	C	1408	NAG	O5-C1-C2	3.93	117.38	111.29
6	C	1408	NAG	C1-O5-C5	3.78	117.26	112.19
6	C	1404	NAG	C2-N2-C7	-3.30	118.47	122.90
6	A	1405	NAG	C3-C4-C5	3.28	116.17	110.23
6	B	1406	NAG	C2-N2-C7	-3.07	118.79	122.90
6	B	1407	NAG	O5-C1-C2	2.89	115.77	111.29
6	A	1402	NAG	C2-N2-C7	-2.70	119.28	122.90
6	B	1407	NAG	C2-N2-C7	-2.70	119.28	122.90
6	C	1404	NAG	C8-C7-N2	2.57	120.38	116.12
6	C	1403	NAG	C1-C2-N2	-2.57	106.38	110.43
6	A	1405	NAG	C2-N2-C7	-2.54	119.50	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1402	NAG	C8-C7-N2	2.52	120.30	116.12
6	A	1401	NAG	C2-N2-C7	-2.52	119.53	122.90
6	C	1408	NAG	C1-C2-N2	-2.51	106.47	110.43
6	A	1406	NAG	C2-N2-C7	-2.46	119.60	122.90
6	B	1404	NAG	C2-N2-C7	-2.45	119.61	122.90
6	A	1405	NAG	C8-C7-N2	2.44	120.17	116.12
6	B	1407	NAG	C8-C7-N2	2.43	120.15	116.12
6	A	1401	NAG	C8-C7-N2	2.42	120.13	116.12
6	B	1401	NAG	C8-C7-N2	2.41	120.12	116.12
6	B	1404	NAG	C8-C7-N2	2.39	120.09	116.12
6	B	1406	NAG	C8-C7-N2	2.38	120.07	116.12
6	B	1402	NAG	C2-N2-C7	-2.37	119.72	122.90
6	B	1402	NAG	C8-C7-N2	2.36	120.03	116.12
6	A	1406	NAG	C8-C7-N2	2.36	120.03	116.12
6	C	1406	NAG	C1-C2-N2	-2.35	106.73	110.43
6	C	1402	NAG	C8-C7-N2	2.33	119.99	116.12
6	A	1404	NAG	C8-C7-N2	2.32	119.96	116.12
6	C	1407	NAG	C8-C7-N2	2.31	119.95	116.12
6	A	1403	NAG	C8-C7-N2	2.30	119.94	116.12
6	B	1403	NAG	C8-C7-N2	2.29	119.92	116.12
6	B	1401	NAG	C2-N2-C7	-2.29	119.83	122.90
6	C	1405	NAG	C8-C7-N2	2.28	119.90	116.12
6	C	1401	NAG	C8-C7-N2	2.27	119.88	116.12
6	A	1407	NAG	C8-C7-N2	2.23	119.82	116.12
6	B	1408	NAG	C8-C7-N2	2.23	119.81	116.12
6	A	1404	NAG	C2-N2-C7	-2.22	119.92	122.90
6	A	1408	NAG	C8-C7-N2	2.17	119.72	116.12
6	C	1404	NAG	C1-O5-C5	-2.09	109.39	112.19
6	C	1401	NAG	C2-N2-C7	-2.06	120.14	122.90
6	C	1402	NAG	C2-N2-C7	-2.06	120.15	122.90
6	C	1402	NAG	C3-C4-C5	2.05	113.96	110.23
6	C	1406	NAG	C8-C7-N2	2.05	119.51	116.12

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1405	NAG	O5-C5-C6-O6
6	C	1407	NAG	O5-C5-C6-O6
6	B	1402	NAG	C4-C5-C6-O6
6	C	1401	NAG	O5-C5-C6-O6
6	C	1408	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	1402	NAG	O5-C5-C6-O6
6	B	1407	NAG	O5-C5-C6-O6
6	A	1408	NAG	O5-C5-C6-O6
6	C	1407	NAG	C4-C5-C6-O6
6	A	1405	NAG	C4-C5-C6-O6
6	B	1401	NAG	O5-C5-C6-O6
6	B	1403	NAG	O5-C5-C6-O6
6	A	1405	NAG	O5-C5-C6-O6
6	C	1408	NAG	C4-C5-C6-O6
6	A	1408	NAG	C4-C5-C6-O6
6	C	1404	NAG	O5-C5-C6-O6
6	A	1406	NAG	C4-C5-C6-O6
6	C	1405	NAG	C4-C5-C6-O6
6	A	1403	NAG	O5-C5-C6-O6
6	C	1401	NAG	C4-C5-C6-O6
6	B	1407	NAG	C4-C5-C6-O6
6	A	1402	NAG	C4-C5-C6-O6
6	A	1402	NAG	O5-C5-C6-O6
6	B	1403	NAG	C4-C5-C6-O6
6	A	1406	NAG	O5-C5-C6-O6
6	C	1404	NAG	C4-C5-C6-O6
6	B	1401	NAG	C4-C5-C6-O6
6	C	1402	NAG	O5-C5-C6-O6
6	B	1405	NAG	C4-C5-C6-O6
6	A	1407	NAG	C4-C5-C6-O6
6	A	1407	NAG	O5-C5-C6-O6
6	C	1406	NAG	O5-C5-C6-O6
6	A	1401	NAG	O5-C5-C6-O6
6	A	1403	NAG	C4-C5-C6-O6
6	B	1405	NAG	O5-C5-C6-O6
6	B	1404	NAG	C4-C5-C6-O6
6	B	1405	NAG	C3-C2-N2-C7
6	C	1402	NAG	C4-C5-C6-O6
6	B	1405	NAG	C1-C2-N2-C7
6	C	1406	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

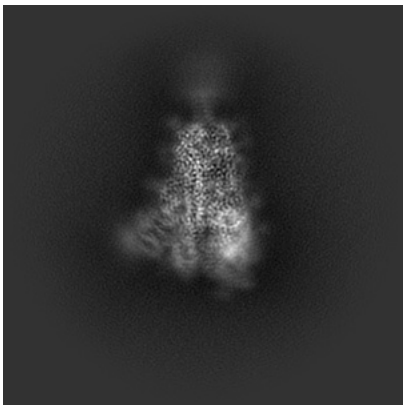
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45893. These allow visual inspection of the internal detail of the map and identification of artifacts.

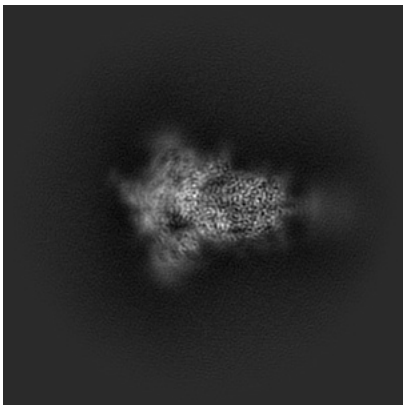
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

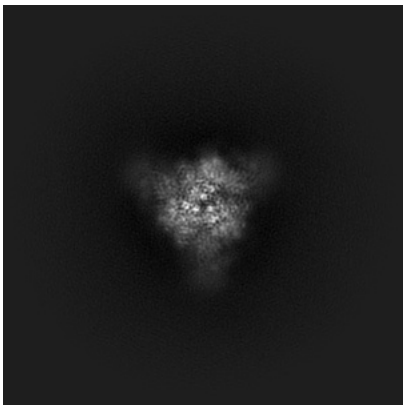
6.1.1 Primary map



X

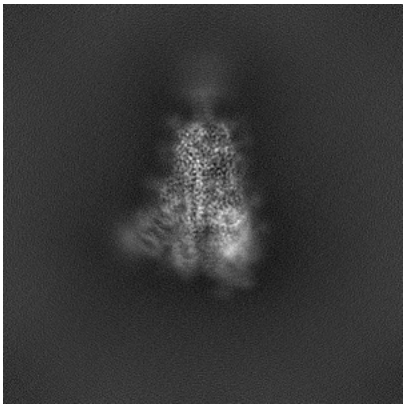


Y

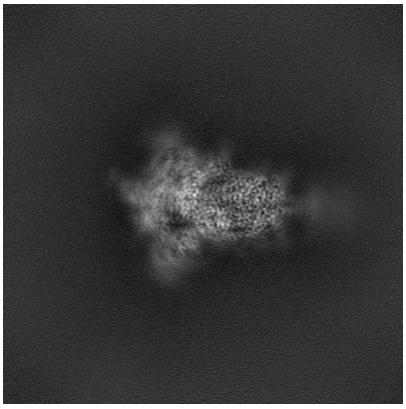


Z

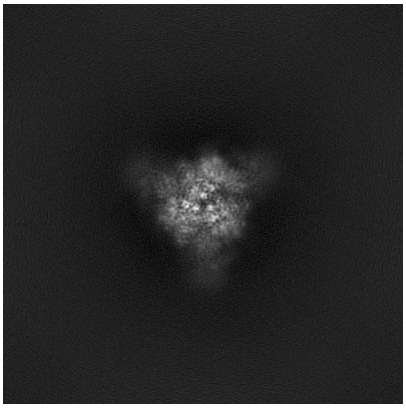
6.1.2 Raw map



X



Y

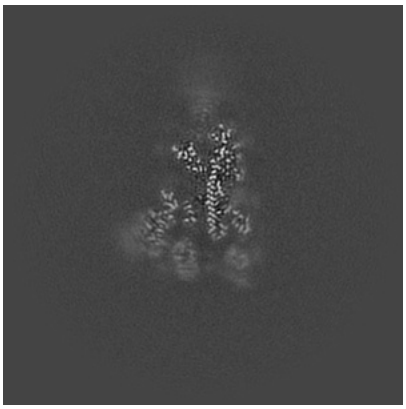


Z

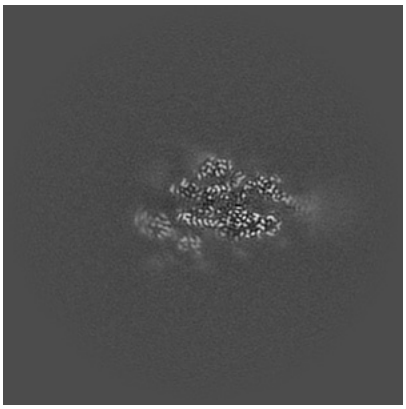
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

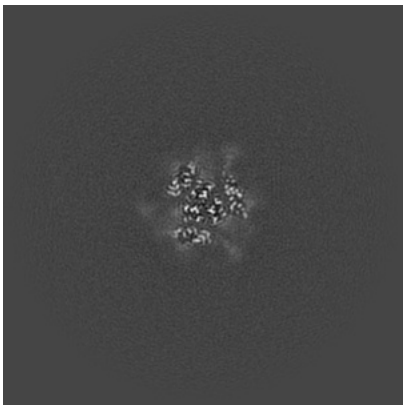
6.2.1 Primary map



X Index: 190

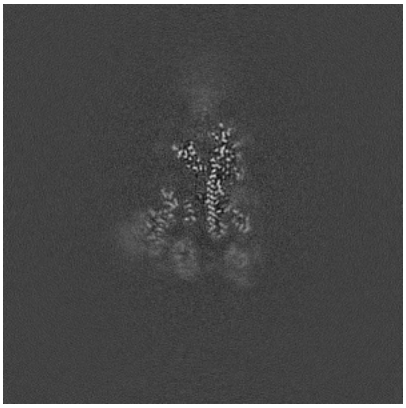


Y Index: 190

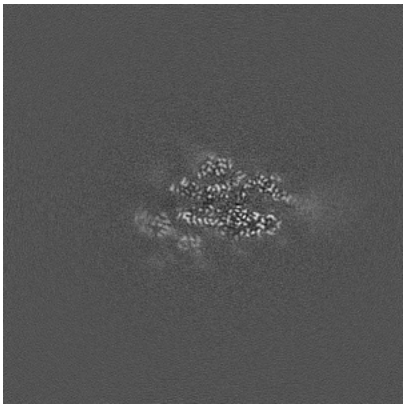


Z Index: 190

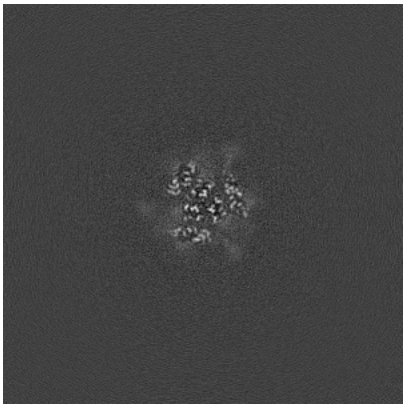
6.2.2 Raw map



X Index: 190



Y Index: 190

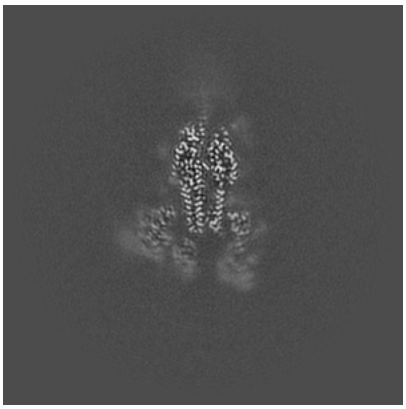


Z Index: 190

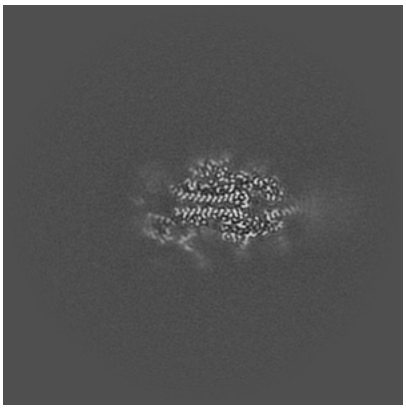
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

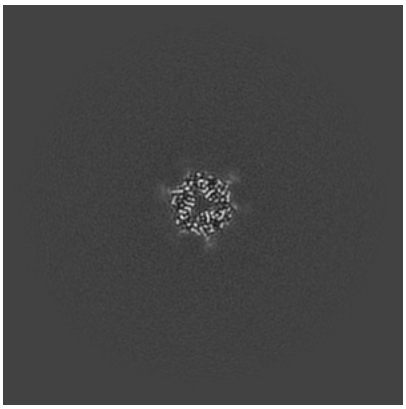
6.3.1 Primary map



X Index: 198

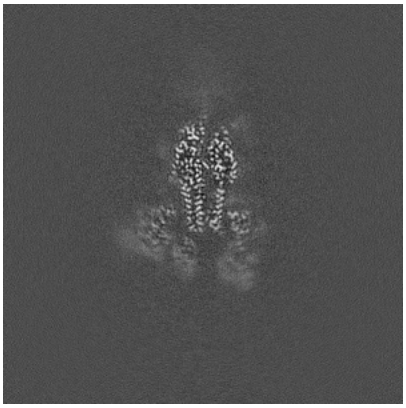


Y Index: 185

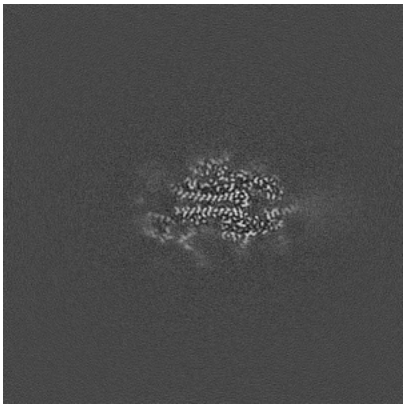


Z Index: 241

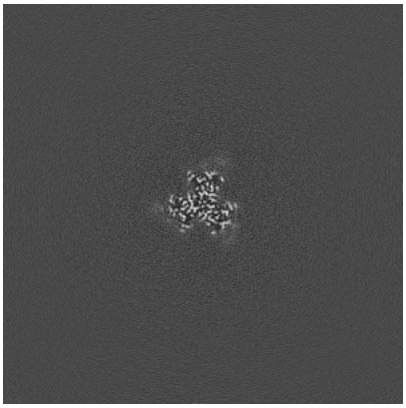
6.3.2 Raw map



X Index: 198



Y Index: 185

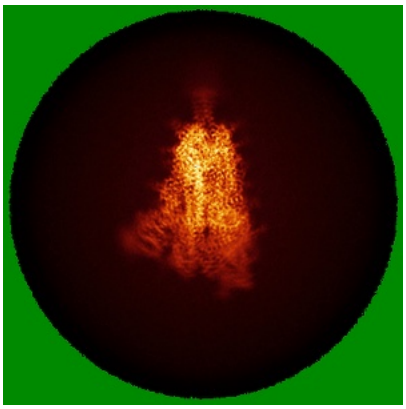


Z Index: 225

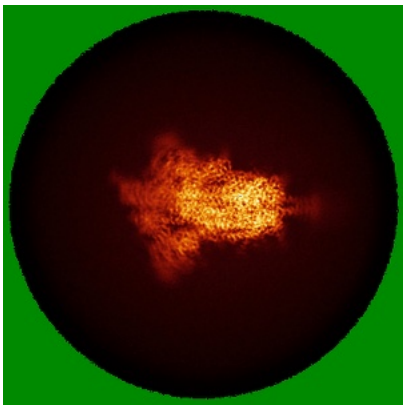
The images above show the largest variance slices of the map in three orthogonal directions.

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

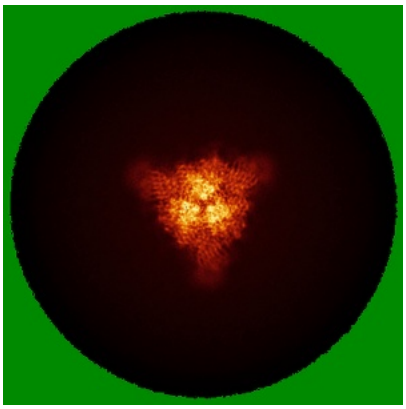
6.4.1 Primary map



X

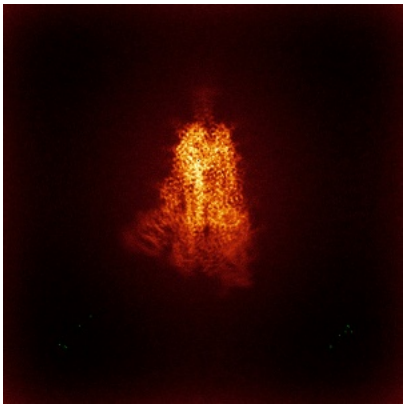


Y

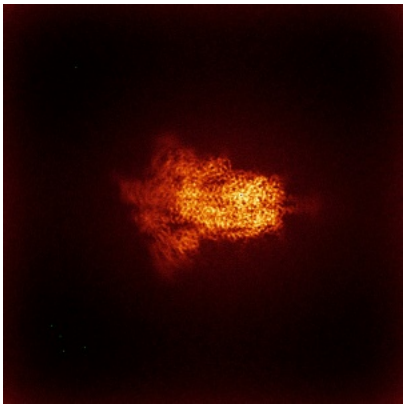


Z

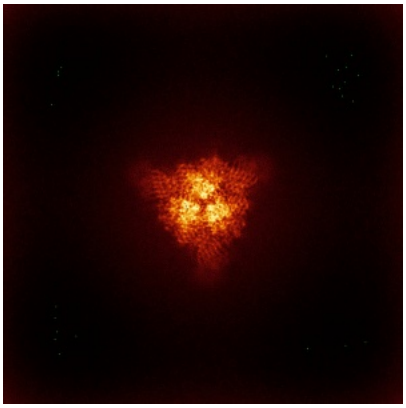
6.4.2 Raw map



X



Y

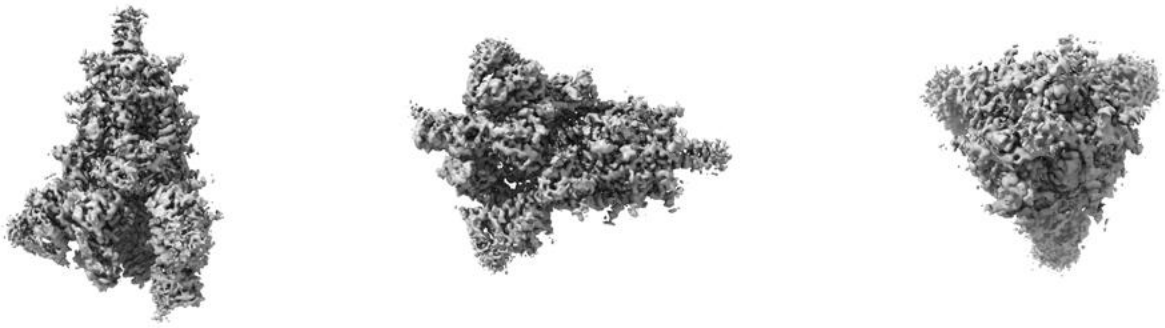


Z

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)

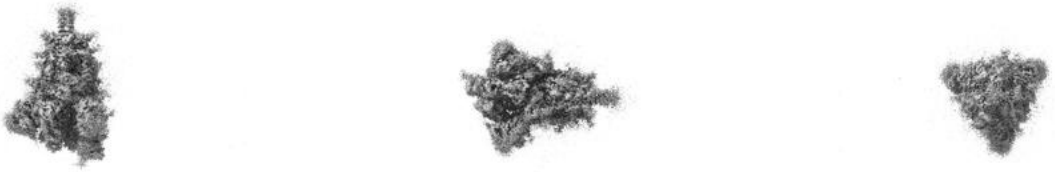
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

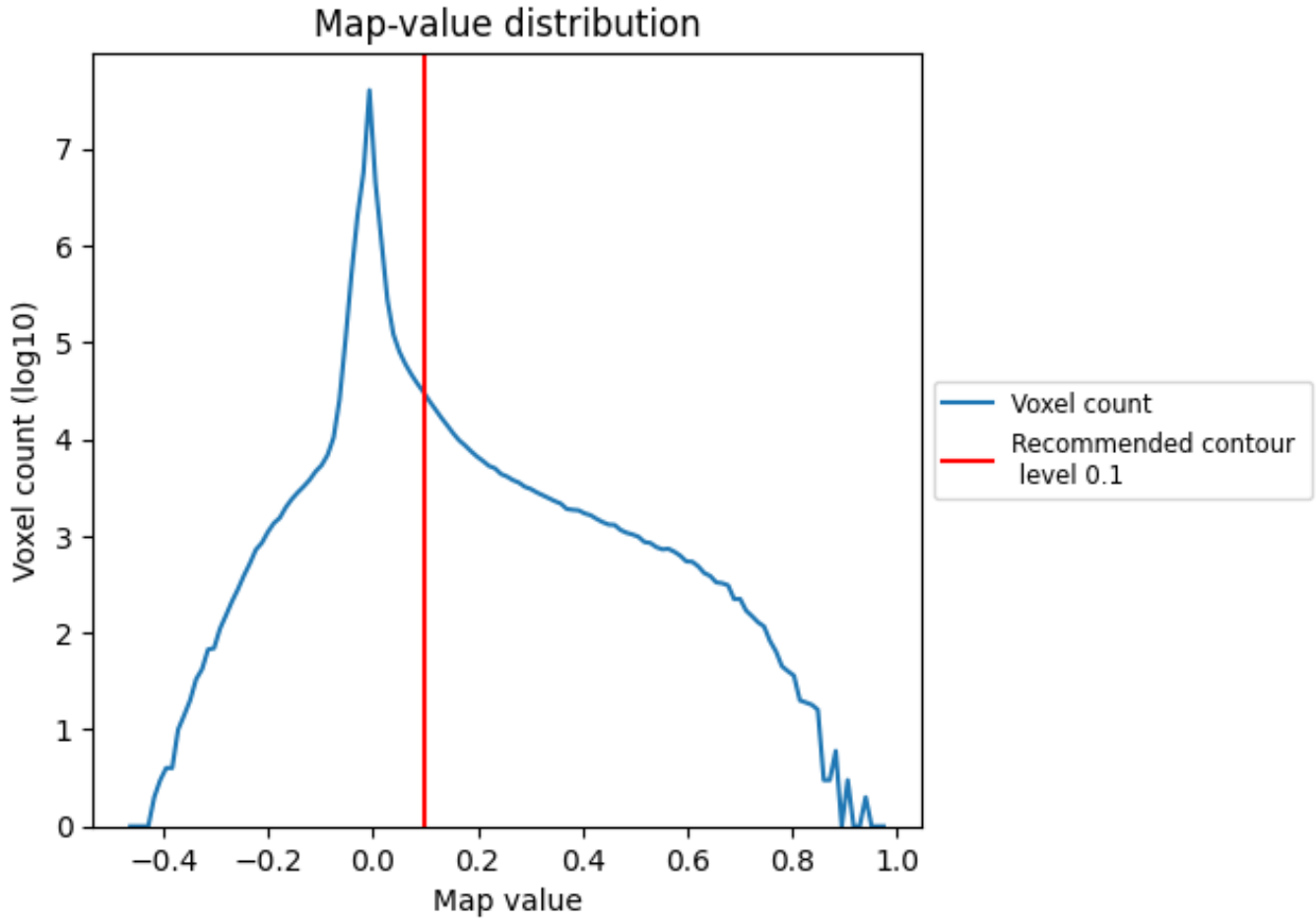
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

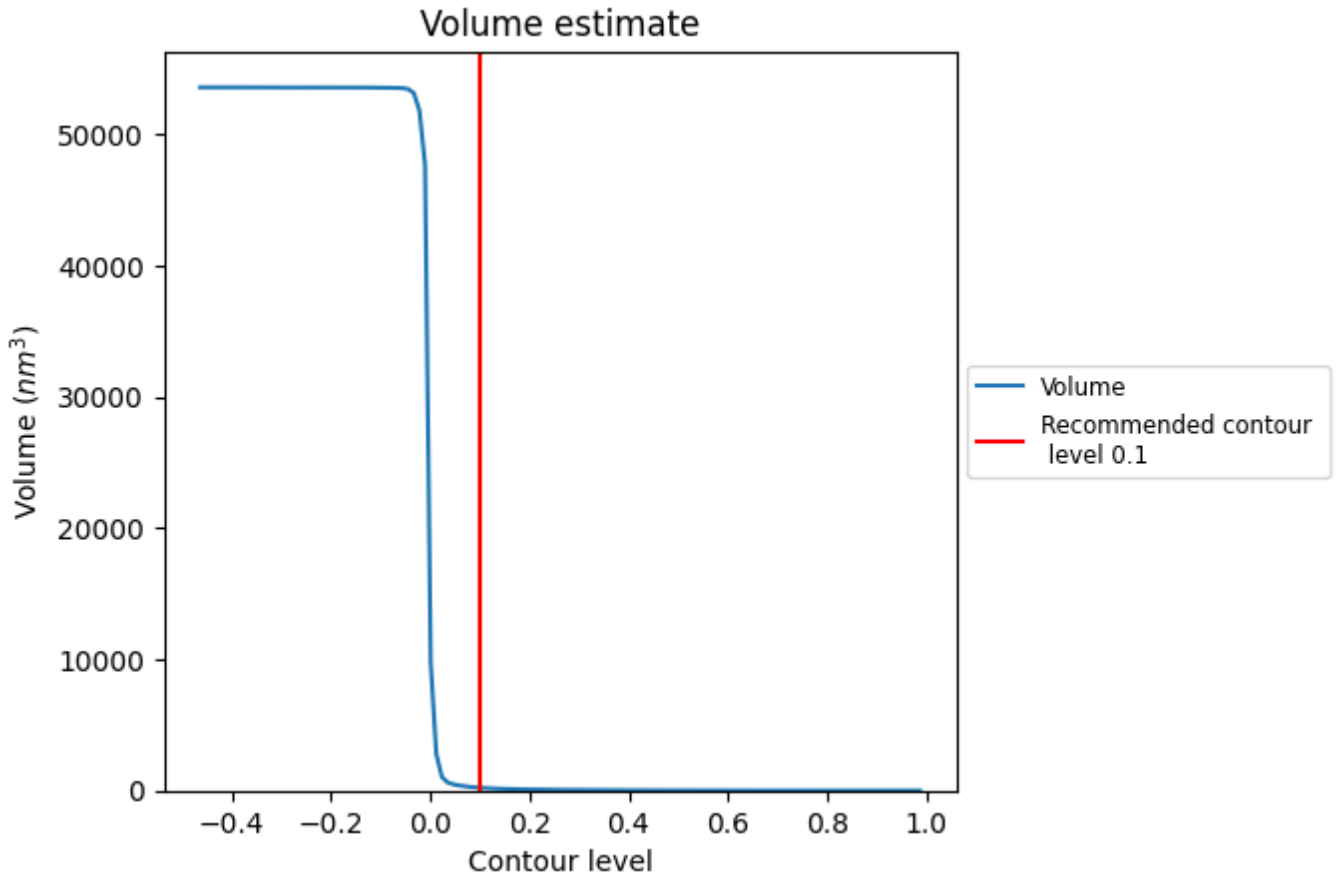
This section contains the results of statistical analysis of the map.

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.

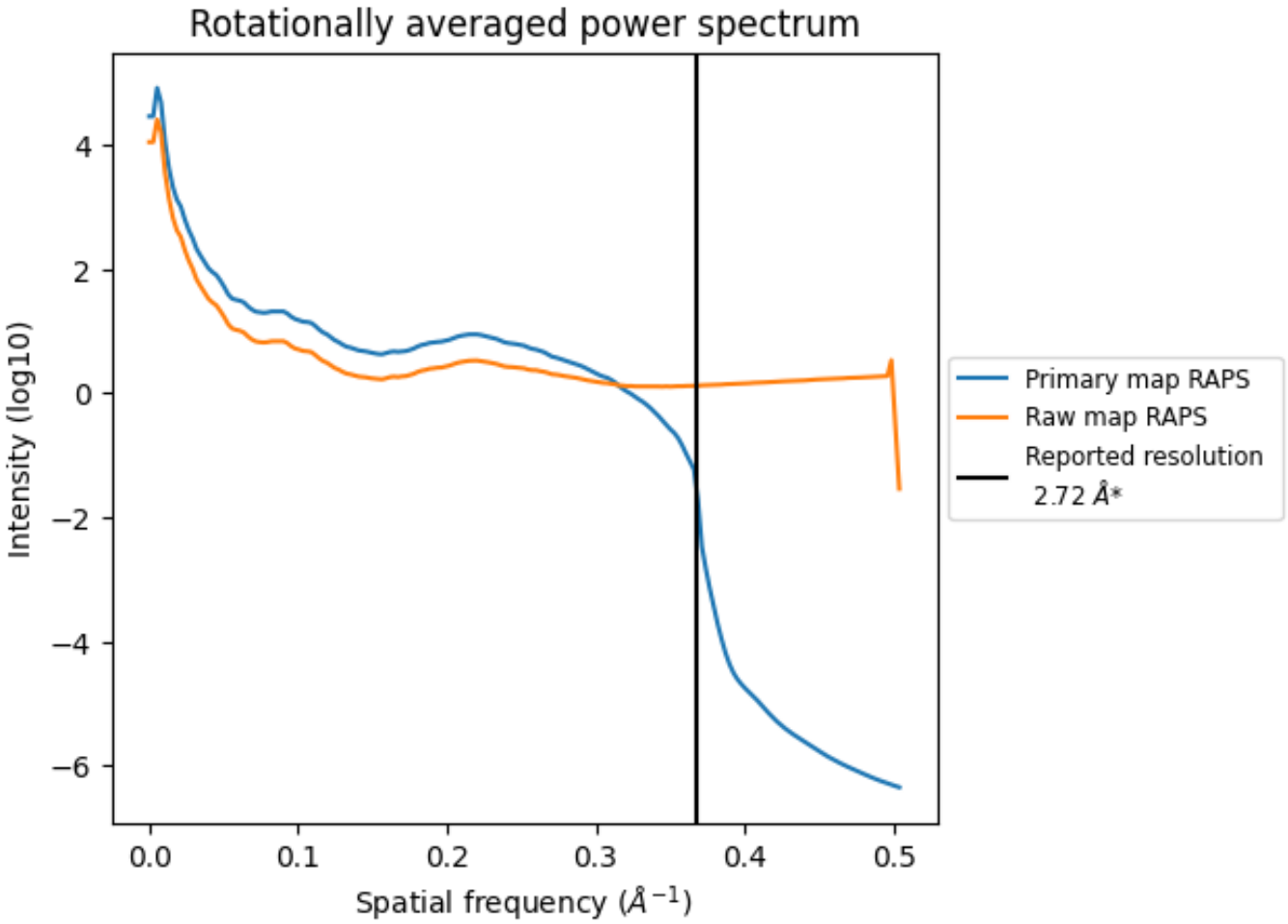
7.2 Volume estimate



The volume at the recommended contour level is 214 nm^3; this corresponds to an approximate mass of 193 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)

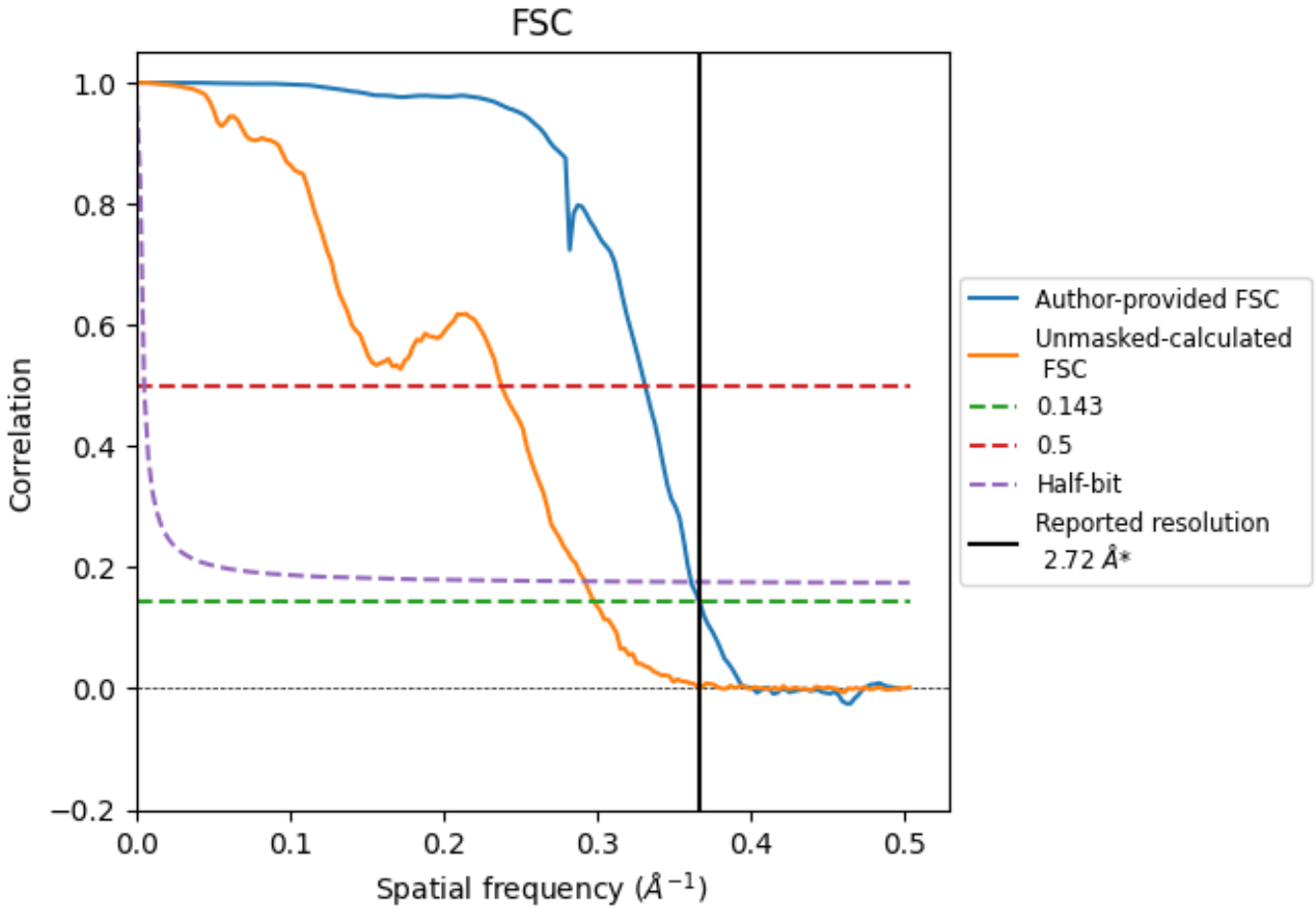


*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

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 0.368 Å^{-1}

8.2 Resolution estimates (i)

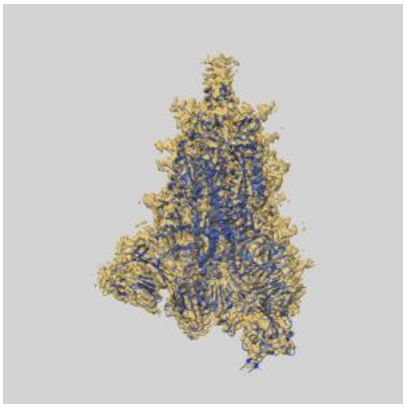
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.72	3.01	2.76
Unmasked-calculated*	3.35	4.20	3.42

*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 3.35 differs from the reported value 2.72 by more than 10 %

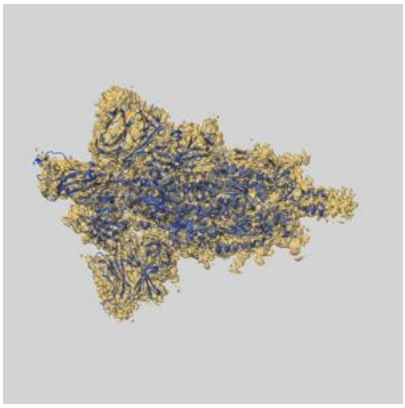
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45893 and PDB model 9CSS. Per-residue inclusion information can be found in section 3 on page 14.

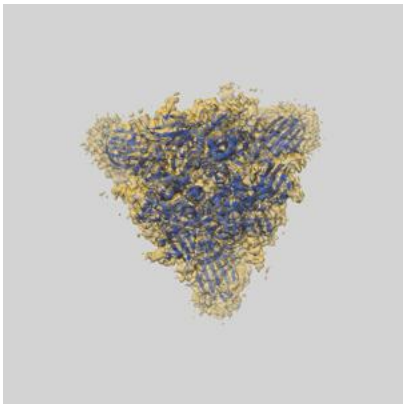
9.1 Map-model overlay



X



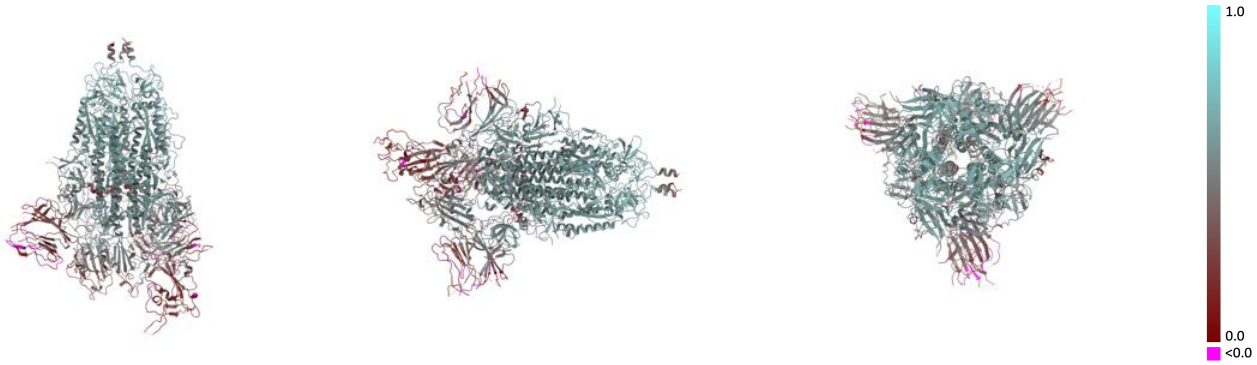
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

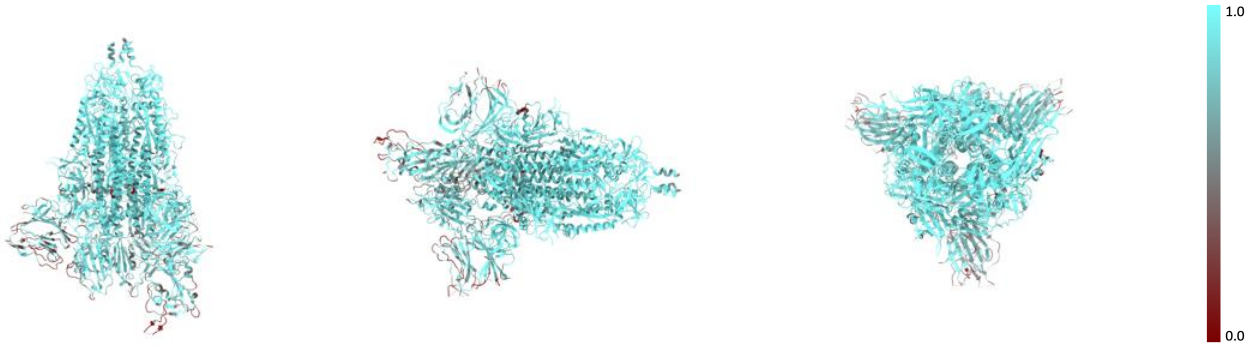
9.2 Q-score mapped to coordinate model (i)



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.

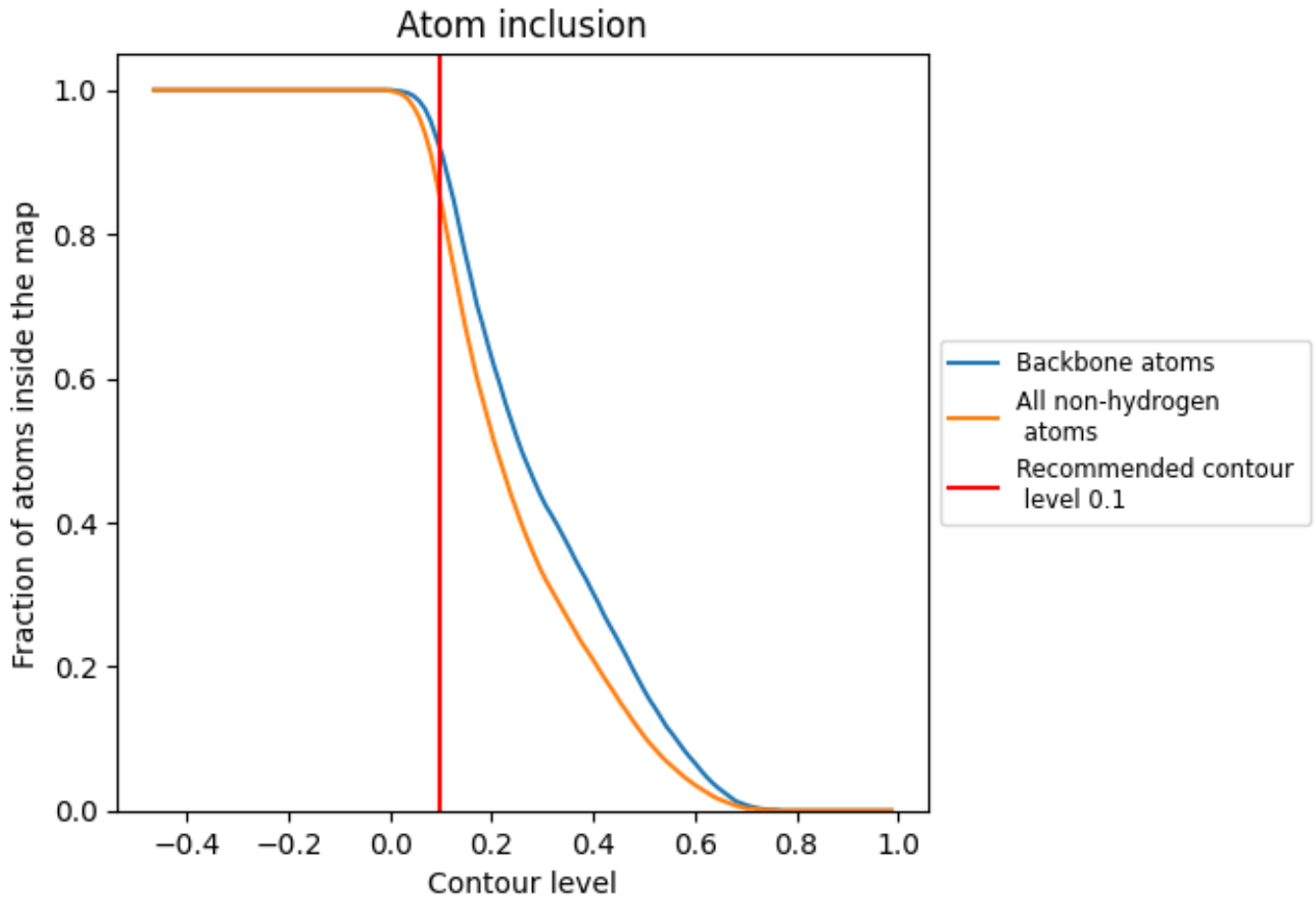
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 85% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.4730
A	0.8390	0.4610
B	0.8730	0.4950
C	0.8440	0.4710
D	0.3850	0.2260
E	0.8970	0.4900
F	0.5360	0.2310
G	0.4290	0.2410
H	0.6790	0.3790
I	0.5000	0.3320
J	0.7180	0.4250
K	0.4740	0.4290
L	0.8720	0.5200
M	0.7180	0.3710
R	0.4290	0.2440
T	0.8720	0.5150
U	0.8570	0.4790
V	0.6580	0.4760
W	0.8460	0.4260
X	0.9290	0.4790
Z	0.7180	0.3680
b	0.8210	0.4470
c	0.7860	0.4410
d	0.6320	0.4430
e	0.7440	0.4220
f	0.6920	0.4340