Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 06:14 am GMT

PDB ID	:	7ZRV
EMDB ID	:	EMD-14922
Title	:	cryo-EM structure of omicron spike in complex with de novo designed binder, full map
Authors	:	Pablo, G.; Sarah, W.; Alexandra, V.H.; Anthony, M.; Andreas, S.; Zander, H.; Dongchun, N.; Shuguang, T.; Freyr, S.; Casper, G.; Priscilla, T.; Alexandra, T.; Stephane, R.; Sandrine, G.; Jane, M.; Aaron, P.; Zepeng, X.; Yan, C.; Pu, H.; George, G.; Elisa, O.; Beat, F.; Didier, T.; Henning, S.; Michael, B.; Bruno, E.C.
Deposited on	:	2022-05-05
Resolution	:	2.80 Å(reported)
Based on initial model	:	7QO7

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 ⓘ symbol.

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

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

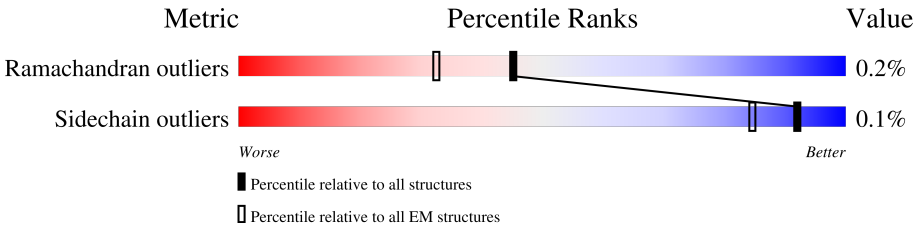
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 2.80 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	1285	86% 14%
1	B	1285	85% 15%
1	C	1285	8% 85% 14%
2	E	79	63% 81% 18%
2	F	79	20% 80% 18%
3	D	2	100%
3	H	2	100%
3	L	2	100%

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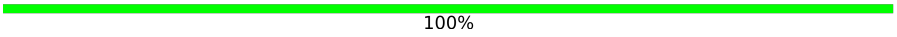
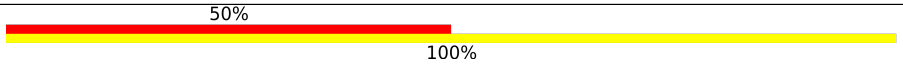
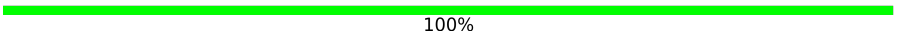
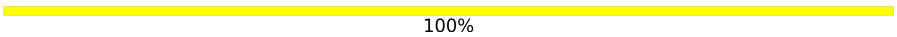
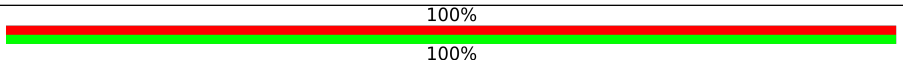
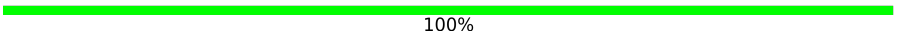
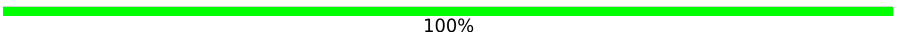
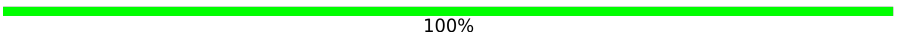
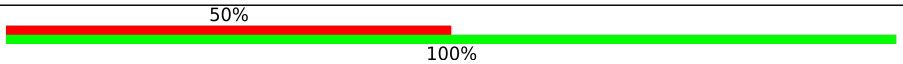
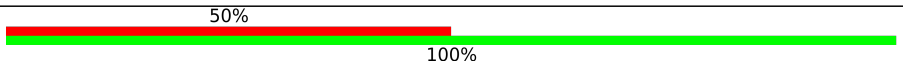
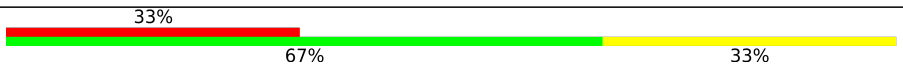
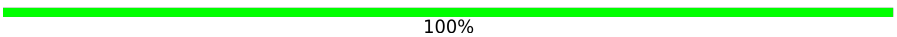
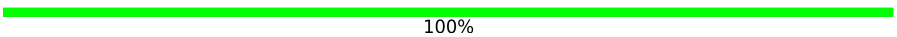
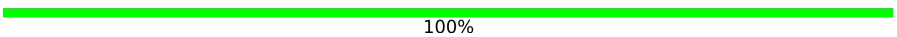
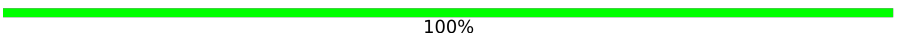
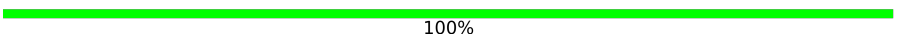
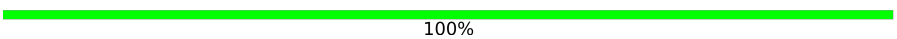
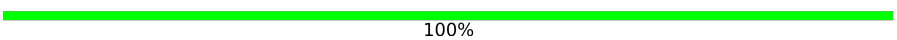
Mol	Chain	Length	Quality of chain
3	M	2	
3	O	2	
3	P	2	
3	U	2	
3	V	2	
3	W	2	
3	X	2	
3	Y	2	
3	Z	2	
3	d	2	
3	e	2	
3	f	2	
3	g	2	
3	h	2	
3	i	2	
4	G	3	
4	I	3	
4	J	3	
4	K	3	
4	N	3	
4	Q	3	
4	R	3	
4	S	3	
4	T	3	
4	a	3	

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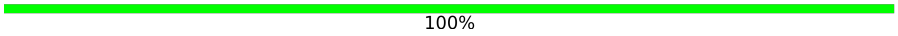
Mol	Chain	Length	Quality of chain
4	b	3	
4	c	3	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 28055 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,Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1103	Total	C	N	O	S	0	0
			8623	5510	1442	1632	39		
1	B	1096	Total	C	N	O	S	0	0
			8589	5490	1435	1625	39		
1	C	1100	Total	C	N	O	S	0	0
			8609	5502	1439	1629	39		

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	VAL	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	96	ILE	THR	conflict	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	143	ASP	TYR	conflict	UNP P0DTC2
A	209	ILE	-	insertion	UNP P0DTC2
A	210	VAL	-	insertion	UNP P0DTC2
A	211	ARG	ASN	conflict	UNP P0DTC2
A	212	GLU	LEU	conflict	UNP P0DTC2
A	213	PRO	VAL	conflict	UNP P0DTC2
A	214	GLU	ARG	conflict	UNP P0DTC2
A	339	ASP	GLY	conflict	UNP P0DTC2
A	371	LEU	SER	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	conflict	UNP P0DTC2
A	496	SER	GLY	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2
A	547	LYS	THR	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	655	TYR	HIS	conflict	UNP P0DTC2
A	679	LYS	ASN	conflict	UNP P0DTC2
A	681	HIS	PRO	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	conflict	UNP P0DTC2
A	796	TYR	ASP	conflict	UNP P0DTC2
A	856	LYS	ASN	conflict	UNP P0DTC2
A	954	HIS	GLN	conflict	UNP P0DTC2
A	969	LYS	ASN	conflict	UNP P0DTC2
A	981	PHE	LEU	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1239	ARG	SER	conflict	UNP M1E1E4
A	1241	LEU	-	expression tag	UNP M1E1E4
A	1242	GLU	-	expression tag	UNP M1E1E4
A	1243	VAL	-	expression tag	UNP M1E1E4
A	1244	LEU	-	expression tag	UNP M1E1E4
A	1245	PHE	-	expression tag	UNP M1E1E4
A	1246	GLN	-	expression tag	UNP M1E1E4
A	1247	GLY	-	expression tag	UNP M1E1E4
A	1248	PRO	-	expression tag	UNP M1E1E4
A	1249	GLY	-	expression tag	UNP M1E1E4
A	1250	HIS	-	expression tag	UNP M1E1E4
A	1251	HIS	-	expression tag	UNP M1E1E4
A	1252	HIS	-	expression tag	UNP M1E1E4
A	1253	HIS	-	expression tag	UNP M1E1E4
A	1254	HIS	-	expression tag	UNP M1E1E4
A	1255	HIS	-	expression tag	UNP M1E1E4
A	1256	HIS	-	expression tag	UNP M1E1E4
A	1257	HIS	-	expression tag	UNP M1E1E4
A	1258	SER	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1259	ALA	-	expression tag	UNP M1E1E4
A	1260	TRP	-	expression tag	UNP M1E1E4
A	1261	SER	-	expression tag	UNP M1E1E4
A	1262	HIS	-	expression tag	UNP M1E1E4
A	1263	PRO	-	expression tag	UNP M1E1E4
A	1264	GLN	-	expression tag	UNP M1E1E4
A	1265	PHE	-	expression tag	UNP M1E1E4
A	1266	GLU	-	expression tag	UNP M1E1E4
A	1267	LYS	-	expression tag	UNP M1E1E4
A	1268	GLY	-	expression tag	UNP M1E1E4
A	1269	GLY	-	expression tag	UNP M1E1E4
A	1270	GLY	-	expression tag	UNP M1E1E4
A	1271	SER	-	expression tag	UNP M1E1E4
A	1272	GLY	-	expression tag	UNP M1E1E4
A	1273	GLY	-	expression tag	UNP M1E1E4
A	1274	GLY	-	expression tag	UNP M1E1E4
A	1275	GLY	-	expression tag	UNP M1E1E4
A	1276	SER	-	expression tag	UNP M1E1E4
A	1277	GLY	-	expression tag	UNP M1E1E4
A	1278	GLY	-	expression tag	UNP M1E1E4
A	1279	SER	-	expression tag	UNP M1E1E4
A	1280	ALA	-	expression tag	UNP M1E1E4
A	1281	TRP	-	expression tag	UNP M1E1E4
A	1282	SER	-	expression tag	UNP M1E1E4
A	1283	HIS	-	expression tag	UNP M1E1E4
A	1284	PRO	-	expression tag	UNP M1E1E4
A	1285	GLN	-	expression tag	UNP M1E1E4
A	1286	PHE	-	expression tag	UNP M1E1E4
A	1287	GLU	-	expression tag	UNP M1E1E4
A	1288	LYS	-	expression tag	UNP M1E1E4
B	70	VAL	ALA	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	96	ILE	THR	conflict	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	143	ASP	TYR	conflict	UNP P0DTC2
B	209	ILE	-	insertion	UNP P0DTC2
B	210	VAL	-	insertion	UNP P0DTC2
B	211	ARG	ASN	conflict	UNP P0DTC2
B	212	GLU	LEU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	213	PRO	VAL	conflict	UNP P0DTC2
B	214	GLU	ARG	conflict	UNP P0DTC2
B	339	ASP	GLY	conflict	UNP P0DTC2
B	371	LEU	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2
B	375	PHE	SER	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2
B	484	ALA	GLU	conflict	UNP P0DTC2
B	493	ARG	GLN	conflict	UNP P0DTC2
B	496	SER	GLY	conflict	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	505	HIS	TYR	conflict	UNP P0DTC2
B	547	LYS	THR	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	655	TYR	HIS	conflict	UNP P0DTC2
B	679	LYS	ASN	conflict	UNP P0DTC2
B	681	HIS	PRO	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	conflict	UNP P0DTC2
B	796	TYR	ASP	conflict	UNP P0DTC2
B	856	LYS	ASN	conflict	UNP P0DTC2
B	954	HIS	GLN	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	981	PHE	LEU	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
B	1239	ARG	SER	conflict	UNP M1E1E4
B	1241	LEU	-	expression tag	UNP M1E1E4
B	1242	GLU	-	expression tag	UNP M1E1E4
B	1243	VAL	-	expression tag	UNP M1E1E4
B	1244	LEU	-	expression tag	UNP M1E1E4
B	1245	PHE	-	expression tag	UNP M1E1E4
B	1246	GLN	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1247	GLY	-	expression tag	UNP M1E1E4
B	1248	PRO	-	expression tag	UNP M1E1E4
B	1249	GLY	-	expression tag	UNP M1E1E4
B	1250	HIS	-	expression tag	UNP M1E1E4
B	1251	HIS	-	expression tag	UNP M1E1E4
B	1252	HIS	-	expression tag	UNP M1E1E4
B	1253	HIS	-	expression tag	UNP M1E1E4
B	1254	HIS	-	expression tag	UNP M1E1E4
B	1255	HIS	-	expression tag	UNP M1E1E4
B	1256	HIS	-	expression tag	UNP M1E1E4
B	1257	HIS	-	expression tag	UNP M1E1E4
B	1258	SER	-	expression tag	UNP M1E1E4
B	1259	ALA	-	expression tag	UNP M1E1E4
B	1260	TRP	-	expression tag	UNP M1E1E4
B	1261	SER	-	expression tag	UNP M1E1E4
B	1262	HIS	-	expression tag	UNP M1E1E4
B	1263	PRO	-	expression tag	UNP M1E1E4
B	1264	GLN	-	expression tag	UNP M1E1E4
B	1265	PHE	-	expression tag	UNP M1E1E4
B	1266	GLU	-	expression tag	UNP M1E1E4
B	1267	LYS	-	expression tag	UNP M1E1E4
B	1268	GLY	-	expression tag	UNP M1E1E4
B	1269	GLY	-	expression tag	UNP M1E1E4
B	1270	GLY	-	expression tag	UNP M1E1E4
B	1271	SER	-	expression tag	UNP M1E1E4
B	1272	GLY	-	expression tag	UNP M1E1E4
B	1273	GLY	-	expression tag	UNP M1E1E4
B	1274	GLY	-	expression tag	UNP M1E1E4
B	1275	GLY	-	expression tag	UNP M1E1E4
B	1276	SER	-	expression tag	UNP M1E1E4
B	1277	GLY	-	expression tag	UNP M1E1E4
B	1278	GLY	-	expression tag	UNP M1E1E4
B	1279	SER	-	expression tag	UNP M1E1E4
B	1280	ALA	-	expression tag	UNP M1E1E4
B	1281	TRP	-	expression tag	UNP M1E1E4
B	1282	SER	-	expression tag	UNP M1E1E4
B	1283	HIS	-	expression tag	UNP M1E1E4
B	1284	PRO	-	expression tag	UNP M1E1E4
B	1285	GLN	-	expression tag	UNP M1E1E4
B	1286	PHE	-	expression tag	UNP M1E1E4
B	1287	GLU	-	expression tag	UNP M1E1E4
B	1288	LYS	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	70	VAL	ALA	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	96	ILE	THR	conflict	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	143	ASP	TYR	conflict	UNP P0DTC2
C	209	ILE	-	insertion	UNP P0DTC2
C	210	VAL	-	insertion	UNP P0DTC2
C	211	ARG	ASN	conflict	UNP P0DTC2
C	212	GLU	LEU	conflict	UNP P0DTC2
C	213	PRO	VAL	conflict	UNP P0DTC2
C	214	GLU	ARG	conflict	UNP P0DTC2
C	339	ASP	GLY	conflict	UNP P0DTC2
C	371	LEU	SER	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	484	ALA	GLU	conflict	UNP P0DTC2
C	493	ARG	GLN	conflict	UNP P0DTC2
C	496	SER	GLY	conflict	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	505	HIS	TYR	conflict	UNP P0DTC2
C	547	LYS	THR	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	HIS	PRO	conflict	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	UNP P0DTC2
C	856	LYS	ASN	conflict	UNP P0DTC2
C	954	HIS	GLN	conflict	UNP P0DTC2
C	969	LYS	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	981	PHE	LEU	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
C	1239	ARG	SER	conflict	UNP M1E1E4
C	1241	LEU	-	expression tag	UNP M1E1E4
C	1242	GLU	-	expression tag	UNP M1E1E4
C	1243	VAL	-	expression tag	UNP M1E1E4
C	1244	LEU	-	expression tag	UNP M1E1E4
C	1245	PHE	-	expression tag	UNP M1E1E4
C	1246	GLN	-	expression tag	UNP M1E1E4
C	1247	GLY	-	expression tag	UNP M1E1E4
C	1248	PRO	-	expression tag	UNP M1E1E4
C	1249	GLY	-	expression tag	UNP M1E1E4
C	1250	HIS	-	expression tag	UNP M1E1E4
C	1251	HIS	-	expression tag	UNP M1E1E4
C	1252	HIS	-	expression tag	UNP M1E1E4
C	1253	HIS	-	expression tag	UNP M1E1E4
C	1254	HIS	-	expression tag	UNP M1E1E4
C	1255	HIS	-	expression tag	UNP M1E1E4
C	1256	HIS	-	expression tag	UNP M1E1E4
C	1257	HIS	-	expression tag	UNP M1E1E4
C	1258	SER	-	expression tag	UNP M1E1E4
C	1259	ALA	-	expression tag	UNP M1E1E4
C	1260	TRP	-	expression tag	UNP M1E1E4
C	1261	SER	-	expression tag	UNP M1E1E4
C	1262	HIS	-	expression tag	UNP M1E1E4
C	1263	PRO	-	expression tag	UNP M1E1E4
C	1264	GLN	-	expression tag	UNP M1E1E4
C	1265	PHE	-	expression tag	UNP M1E1E4
C	1266	GLU	-	expression tag	UNP M1E1E4
C	1267	LYS	-	expression tag	UNP M1E1E4
C	1268	GLY	-	expression tag	UNP M1E1E4
C	1269	GLY	-	expression tag	UNP M1E1E4
C	1270	GLY	-	expression tag	UNP M1E1E4
C	1271	SER	-	expression tag	UNP M1E1E4
C	1272	GLY	-	expression tag	UNP M1E1E4
C	1273	GLY	-	expression tag	UNP M1E1E4
C	1274	GLY	-	expression tag	UNP M1E1E4
C	1275	GLY	-	expression tag	UNP M1E1E4
C	1276	SER	-	expression tag	UNP M1E1E4

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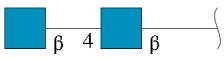
Chain	Residue	Modelled	Actual	Comment	Reference
C	1277	GLY	-	expression tag	UNP M1E1E4
C	1278	GLY	-	expression tag	UNP M1E1E4
C	1279	SER	-	expression tag	UNP M1E1E4
C	1280	ALA	-	expression tag	UNP M1E1E4
C	1281	TRP	-	expression tag	UNP M1E1E4
C	1282	SER	-	expression tag	UNP M1E1E4
C	1283	HIS	-	expression tag	UNP M1E1E4
C	1284	PRO	-	expression tag	UNP M1E1E4
C	1285	GLN	-	expression tag	UNP M1E1E4
C	1286	PHE	-	expression tag	UNP M1E1E4
C	1287	GLU	-	expression tag	UNP M1E1E4
C	1288	LYS	-	expression tag	UNP M1E1E4

- Molecule 2 is a protein called de novo designed binder.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	65	Total	C	N	O	S	0	0
			519	332	95	91	1		
2	F	65	Total	C	N	O	S	0	0
			519	332	95	91	1		

- 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	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		
3	e	2	Total	C	N	O	0	0
			28	16	2	10		
3	f	2	Total	C	N	O	0	0
			28	16	2	10		
3	g	2	Total	C	N	O	0	0
			28	16	2	10		
3	h	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	3	Total	C	N	O	0	0
			39	22	2	15		
4	I	3	Total	C	N	O	0	0
			39	22	2	15		
4	J	3	Total	C	N	O	0	0
			39	22	2	15		
4	K	3	Total	C	N	O	0	0
			39	22	2	15		
4	N	3	Total	C	N	O	0	0
			39	22	2	15		

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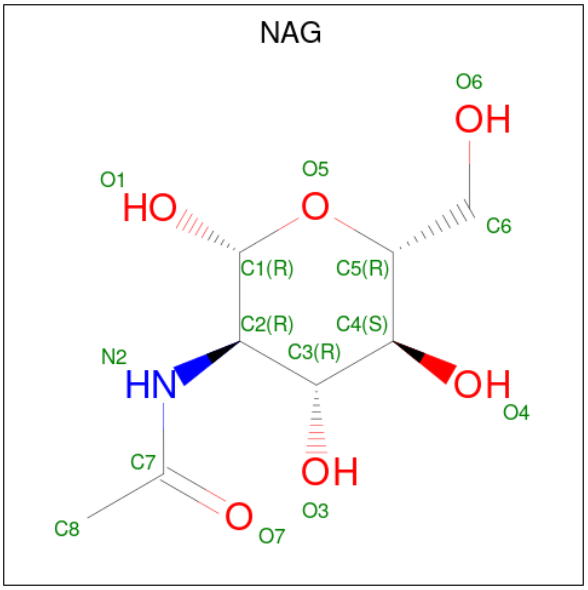
Mol	Chain	Residues	Atoms	AltConf	Trace
4	Q	3	Total C N O 39 22 2 15	0	0
4	R	3	Total C N O 39 22 2 15	0	0
4	S	3	Total C N O 39 22 2 15	0	0
4	T	3	Total C N O 39 22 2 15	0	0
4	a	3	Total C N O 39 22 2 15	0	0
4	b	3	Total C N O 39 22 2 15	0	0
4	c	3	Total C N O 39 22 2 15	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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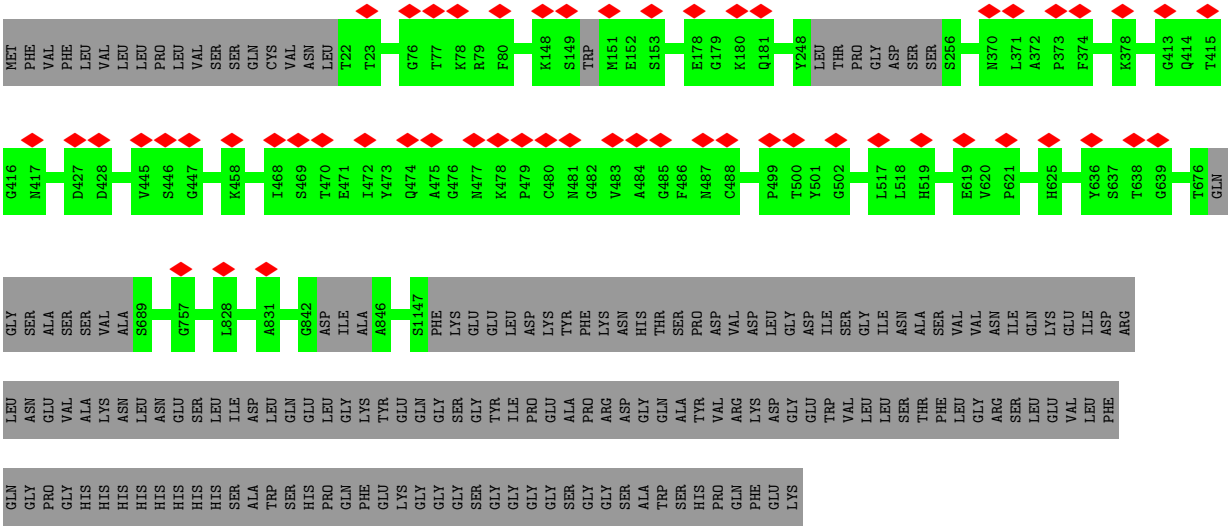
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5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

3 Residue-property plots (i)

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

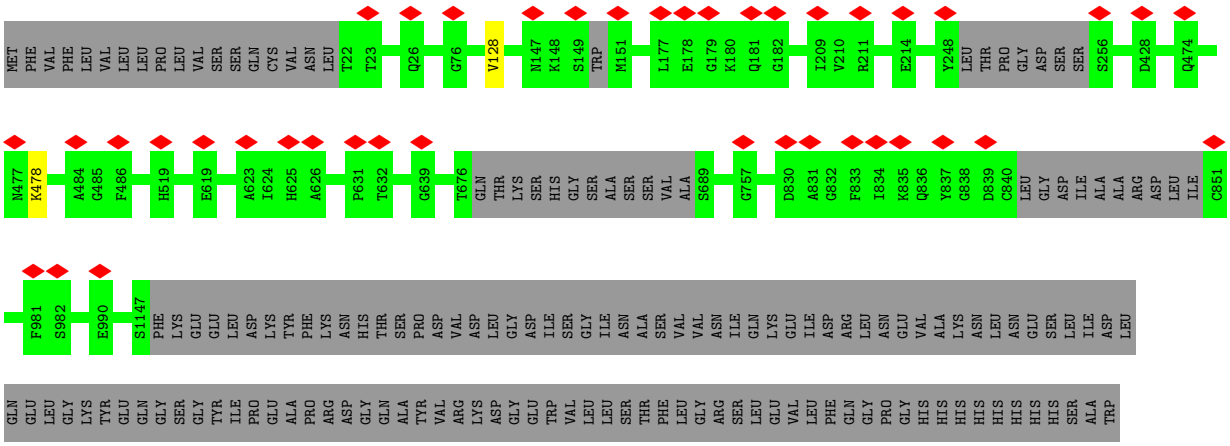
• Molecule 1: Spike glycoprotein,Envelope glycoprotein

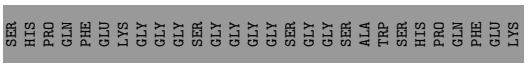
Chain A:



• Molecule 1: Spike glycoprotein,Envelope glycoprotein

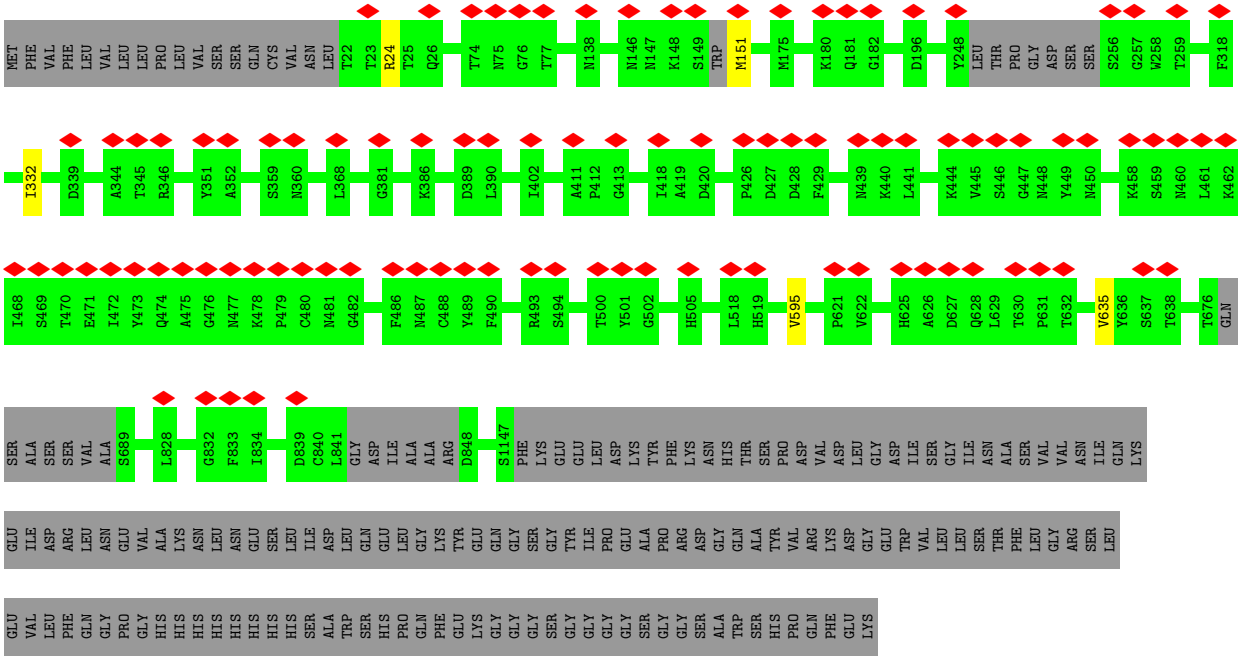
Chain B:





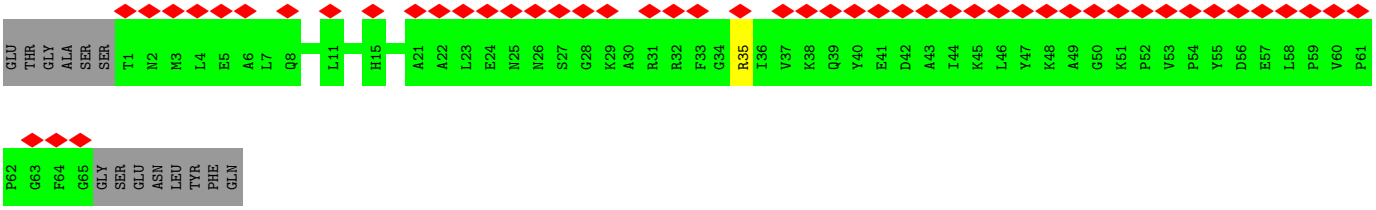
• Molecule 1: Spike glycoprotein,Envelope glycoprotein

Chain C:



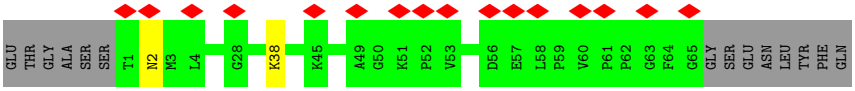
• Molecule 2: de novo designed binder

Chain E:



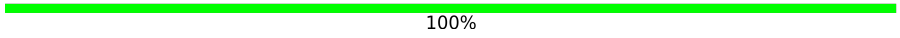
• Molecule 2: de novo designed binder

Chain F:



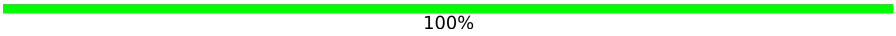
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



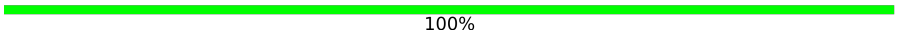
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



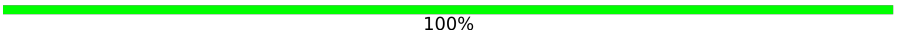
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



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

Chain M:



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

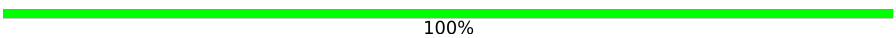
Chain O:

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

Chain P:

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

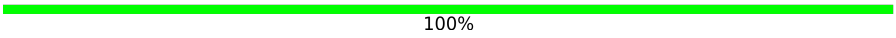
Chain U:



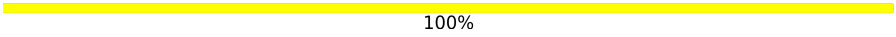
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

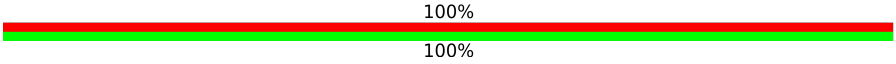
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 

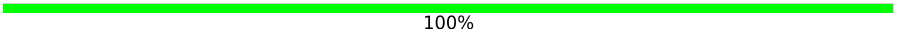
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

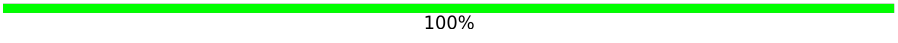
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 

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

Chain Z: 

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

Chain d: 

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

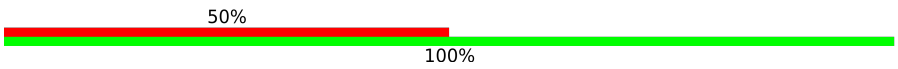
Chain e:

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

Chain f:

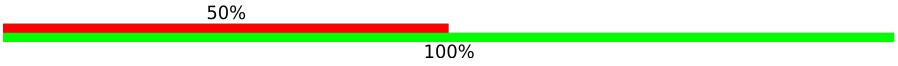
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



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

Chain h:



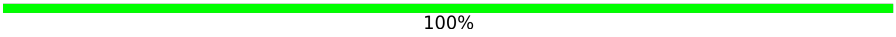
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

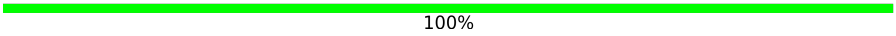
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

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

Chain I: 

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

Chain J: 

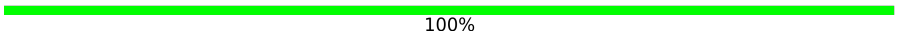
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

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

Chain N:

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

Chain Q: 

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

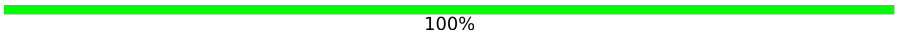
Chain R:

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

Chain S:

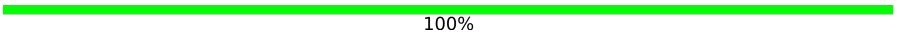
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



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

Chain a:

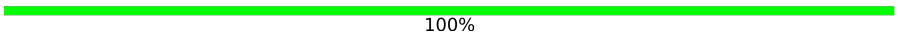


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

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

Chain c:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.841	Depositor
Minimum map value	-0.344	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	345.576, 345.576, 345.576	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2342, 1.2342, 1.2342	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.25	0/8827	0.47	0/12008
1	B	0.25	0/8793	0.48	0/11961
1	C	0.25	0/8814	0.47	0/11992
2	E	0.25	0/531	0.46	0/715
2	F	0.29	0/531	0.55	0/715
All	All	0.25	0/27496	0.48	0/37391

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1093/1285 (85%)	1043 (95%)	50 (5%)	0	100	100
1	B	1086/1285 (84%)	1030 (95%)	55 (5%)	1 (0%)	48	77
1	C	1092/1285 (85%)	1037 (95%)	51 (5%)	4 (0%)	30	61
2	E	63/79 (80%)	60 (95%)	3 (5%)	0	100	100
2	F	63/79 (80%)	60 (95%)	2 (3%)	1 (2%)	8	27
All	All	3397/4013 (85%)	3230 (95%)	161 (5%)	6 (0%)	45	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	595	VAL
2	F	2	ASN
1	B	128	VAL
1	C	151	MET
1	C	635	VAL
1	C	332	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	956/1113 (86%)	956 (100%)	0	100	100
1	B	956/1113 (86%)	955 (100%)	1 (0%)	92	98
1	C	956/1113 (86%)	955 (100%)	1 (0%)	92	98
2	E	52/63 (82%)	51 (98%)	1 (2%)	52	82
2	F	52/63 (82%)	51 (98%)	1 (2%)	52	82
All	All	2972/3465 (86%)	2968 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	478	LYS
1	C	24	ARG

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Mol	Chain	Res	Type
2	E	35	ARG
2	F	38	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	ASN
1	C	135	GLN
1	C	144	HIS

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)

72 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	$\#\|Z\| > 2$
3	NAG	D	1	1,3	14,14,15	0.38	0	17,19,21	0.39	0
3	NAG	D	2	3	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	G	1	1,4	14,14,15	0.65	0	17,19,21	0.90	1 (5%)
4	NAG	G	2	4	14,14,15	0.22	0	17,19,21	0.43	0
4	BMA	G	3	4	11,11,12	0.61	0	15,15,17	0.78	0
3	NAG	H	1	1,3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	H	2	3	14,14,15	0.25	0	17,19,21	0.52	0
4	NAG	I	1	1,4	14,14,15	0.22	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	I	2	4	14,14,15	0.18	0	17,19,21	0.40	0
4	BMA	I	3	4	11,11,12	0.55	0	15,15,17	0.80	0
4	NAG	J	1	1,4	14,14,15	0.23	0	17,19,21	0.47	0
4	NAG	J	2	4	14,14,15	0.21	0	17,19,21	0.39	0
4	BMA	J	3	4	11,11,12	0.55	0	15,15,17	0.74	0
4	NAG	K	1	1,4	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	K	2	4	14,14,15	0.25	0	17,19,21	0.48	0
4	BMA	K	3	4	11,11,12	0.57	0	15,15,17	0.74	0
3	NAG	L	1	1,3	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	L	2	3	14,14,15	0.29	0	17,19,21	0.45	0
3	NAG	M	1	1,3	14,14,15	0.23	0	17,19,21	0.49	0
3	NAG	M	2	3	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	N	1	1,4	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	N	2	4	14,14,15	0.41	0	17,19,21	0.38	0
4	BMA	N	3	4	11,11,12	0.88	0	15,15,17	0.95	0
3	NAG	O	1	1,3	14,14,15	0.24	0	17,19,21	0.48	0
3	NAG	O	2	3	14,14,15	0.48	0	17,19,21	1.26	1 (5%)
3	NAG	P	1	1,3	14,14,15	0.43	0	17,19,21	1.25	1 (5%)
3	NAG	P	2	3	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	Q	1	1,4	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	Q	2	4	14,14,15	0.20	0	17,19,21	0.38	0
4	BMA	Q	3	4	11,11,12	0.61	0	15,15,17	0.74	0
4	NAG	R	1	1,4	14,14,15	0.39	0	17,19,21	1.27	2 (11%)
4	NAG	R	2	4	14,14,15	0.22	0	17,19,21	0.50	0
4	BMA	R	3	4	11,11,12	0.55	0	15,15,17	0.74	0
4	NAG	S	1	1,4	14,14,15	0.63	1 (7%)	17,19,21	0.74	0
4	NAG	S	2	4	14,14,15	0.34	0	17,19,21	0.48	0
4	BMA	S	3	4	11,11,12	0.95	0	15,15,17	0.94	0
4	NAG	T	1	1,4	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	T	2	4	14,14,15	0.24	0	17,19,21	0.51	0
4	BMA	T	3	4	11,11,12	0.60	0	15,15,17	0.75	0
3	NAG	U	1	1,3	14,14,15	0.18	0	17,19,21	0.49	0
3	NAG	U	2	3	14,14,15	0.57	0	17,19,21	0.44	0
3	NAG	V	1	1,3	14,14,15	0.43	0	17,19,21	1.28	2 (11%)
3	NAG	V	2	3	14,14,15	0.96	1 (7%)	17,19,21	1.28	1 (5%)
3	NAG	W	1	1,3	14,14,15	0.38	0	17,19,21	0.55	0
3	NAG	W	2	3	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	X	1	1,3	14,14,15	0.76	1 (7%)	17,19,21	0.87	0
3	NAG	X	2	3	14,14,15	0.74	1 (7%)	17,19,21	1.27	1 (5%)
3	NAG	Y	1	1,3	14,14,15	0.18	0	17,19,21	0.40	0
3	NAG	Y	2	3	14,14,15	0.25	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	Z	1	1,3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	Z	2	3	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	a	1	1,4	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	a	2	4	14,14,15	0.21	0	17,19,21	0.40	0
4	BMA	a	3	4	11,11,12	0.57	0	15,15,17	0.82	0
4	NAG	b	1	1,4	14,14,15	0.39	0	17,19,21	1.28	2 (11%)
4	NAG	b	2	4	14,14,15	0.19	0	17,19,21	0.45	0
4	BMA	b	3	4	11,11,12	0.57	0	15,15,17	0.73	0
4	NAG	c	1	1,4	14,14,15	0.19	0	17,19,21	0.45	0
4	NAG	c	2	4	14,14,15	0.22	0	17,19,21	0.39	0
4	BMA	c	3	4	11,11,12	0.58	0	15,15,17	0.75	0
3	NAG	d	1	1,3	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	d	2	3	14,14,15	0.25	0	17,19,21	0.51	0
3	NAG	e	1	1,3	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	e	2	3	14,14,15	0.25	0	17,19,21	0.51	0
3	NAG	f	1	1,3	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	f	2	3	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	g	1	1,3	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	g	2	3	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	h	1	1,3	14,14,15	0.23	0	17,19,21	0.36	0
3	NAG	h	2	3	14,14,15	0.26	0	17,19,21	0.40	0
3	NAG	i	1	1,3	14,14,15	0.91	1 (7%)	17,19,21	1.49	2 (11%)
3	NAG	i	2	3	14,14,15	0.19	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
4	NAG	a	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	0/6/23/26	0/1/1/1
4	BMA	a	3	4	-	0/2/19/22	0/1/1/1
4	NAG	b	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	b	2	4	-	2/6/23/26	0/1/1/1
4	BMA	b	3	4	-	2/2/19/22	0/1/1/1
4	NAG	c	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	c	2	4	-	2/6/23/26	0/1/1/1
4	BMA	c	3	4	-	0/2/19/22	0/1/1/1
3	NAG	d	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	d	2	3	-	3/6/23/26	0/1/1/1
3	NAG	e	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	e	2	3	-	3/6/23/26	0/1/1/1
3	NAG	f	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	NAG	g	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	NAG	h	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	2	NAG	O5-C1	3.23	1.48	1.43
3	i	1	NAG	C1-C2	2.62	1.56	1.52
3	X	2	NAG	O5-C1	2.61	1.47	1.43
3	X	1	NAG	O5-C1	-2.39	1.39	1.43
4	S	1	NAG	O5-C1	-2.25	1.40	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	2	NAG	C1-O5-C5	4.96	118.91	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	2	NAG	C1-O5-C5	4.87	118.78	112.19
3	i	1	NAG	C1-O5-C5	4.79	118.68	112.19
4	b	1	NAG	C2-N2-C7	4.33	129.06	122.90
3	P	1	NAG	C2-N2-C7	4.31	129.04	122.90
4	R	1	NAG	C2-N2-C7	4.30	129.02	122.90
3	V	1	NAG	C2-N2-C7	4.26	128.97	122.90
3	O	2	NAG	C2-N2-C7	4.25	128.96	122.90
4	G	1	NAG	C1-O5-C5	3.00	116.26	112.19
3	i	1	NAG	C2-N2-C7	2.21	126.05	122.90
3	V	1	NAG	C1-C2-N2	2.03	113.96	110.49
4	R	1	NAG	C1-C2-N2	2.01	113.92	110.49
4	b	1	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Z	2	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	e	1	NAG	O5-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
3	Z	2	NAG	C4-C5-C6-O6
3	e	2	NAG	C4-C5-C6-O6
3	e	1	NAG	C4-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
3	d	2	NAG	C4-C5-C6-O6
3	e	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	L	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
3	X	2	NAG	C8-C7-N2-C2
3	X	2	NAG	O7-C7-N2-C2
3	e	1	NAG	C8-C7-N2-C2
3	e	1	NAG	O7-C7-N2-C2
3	f	1	NAG	C8-C7-N2-C2
3	f	1	NAG	O7-C7-N2-C2
3	g	1	NAG	C8-C7-N2-C2
3	g	1	NAG	O7-C7-N2-C2
3	i	2	NAG	C8-C7-N2-C2
3	i	2	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	T	1	NAG	C8-C7-N2-C2
4	T	1	NAG	O7-C7-N2-C2
4	b	1	NAG	C8-C7-N2-C2
4	b	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	b	2	NAG	C4-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
3	g	2	NAG	C4-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	X	1	NAG	C1-C2-N2-C7
3	i	1	NAG	C1-C2-N2-C7
4	Q	2	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
3	d	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C3-C2-N2-C7
3	M	1	NAG	C3-C2-N2-C7
3	W	1	NAG	C3-C2-N2-C7
3	d	2	NAG	C3-C2-N2-C7
3	e	2	NAG	C3-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7
4	K	2	NAG	C3-C2-N2-C7
4	R	2	NAG	C3-C2-N2-C7
4	S	1	NAG	C3-C2-N2-C7
4	S	2	NAG	C3-C2-N2-C7
4	T	2	NAG	C3-C2-N2-C7
3	d	1	NAG	O5-C5-C6-O6
4	b	3	BMA	O5-C5-C6-O6
4	b	3	BMA	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C3-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7

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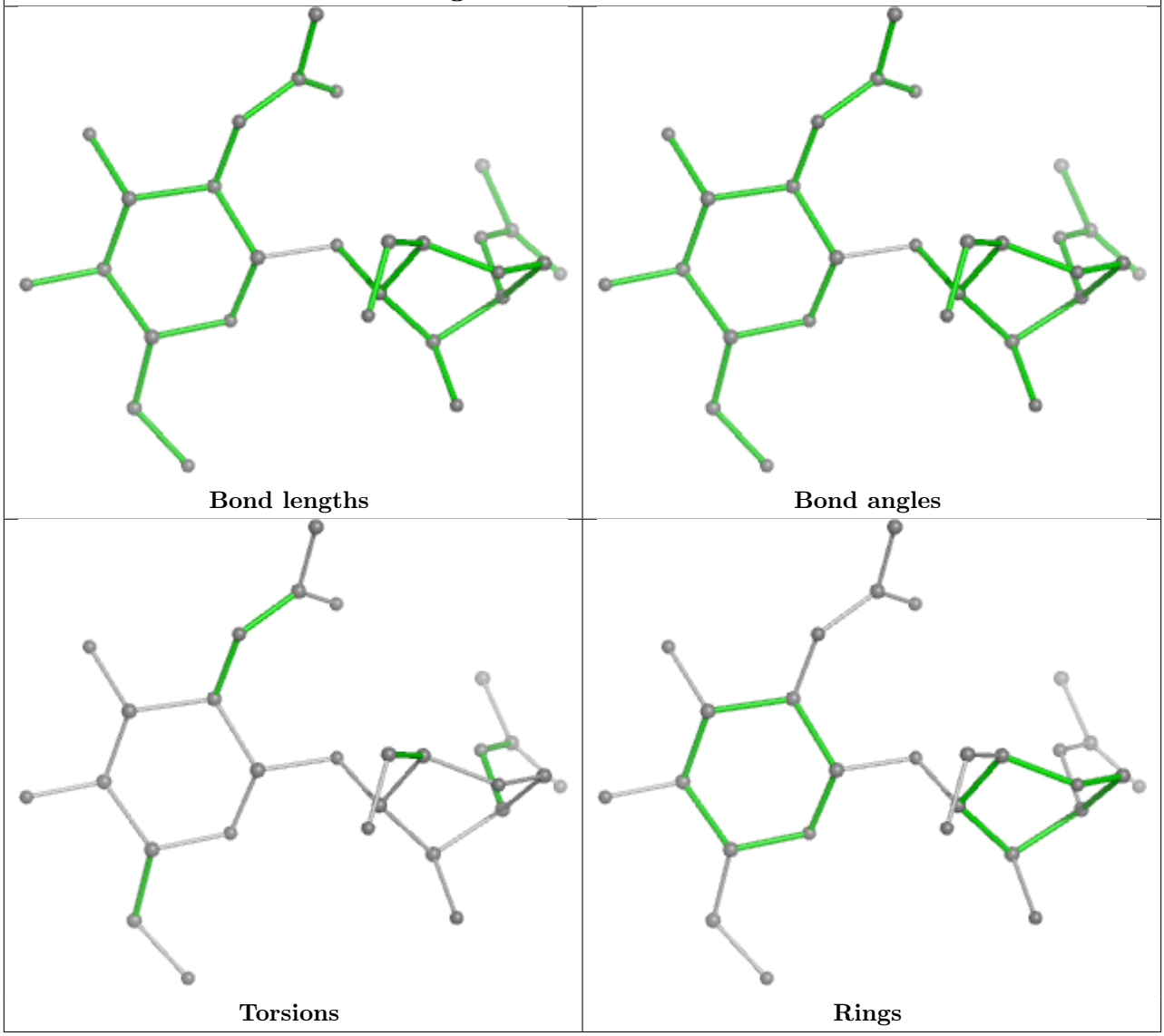
Mol	Chain	Res	Type	Atoms
3	V	1	NAG	C3-C2-N2-C7
4	R	1	NAG	C3-C2-N2-C7
4	b	1	NAG	C3-C2-N2-C7
3	f	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6

There are no ring outliers.

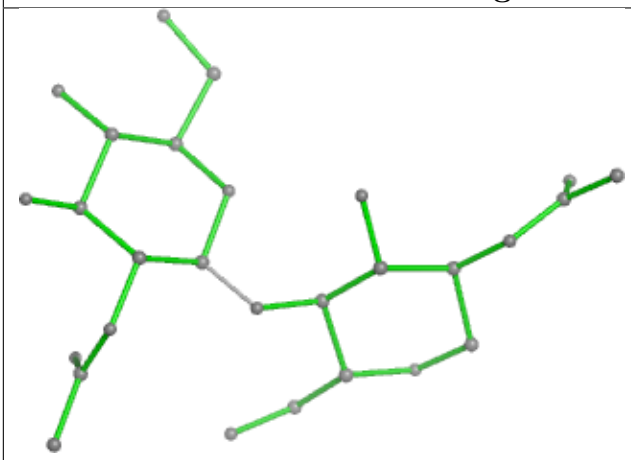
No monomer is involved in short contacts.

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

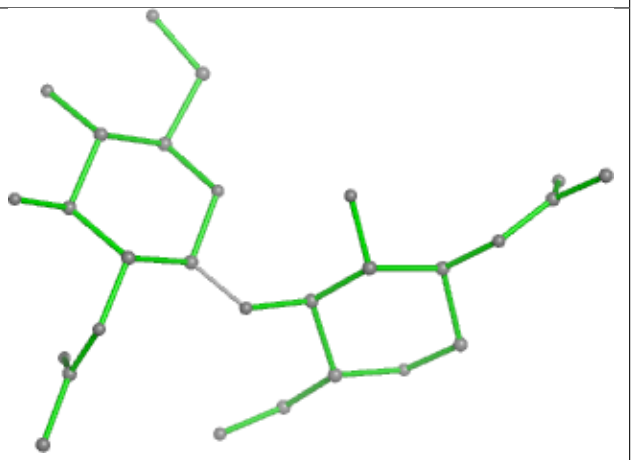
Oligosaccharide Chain D



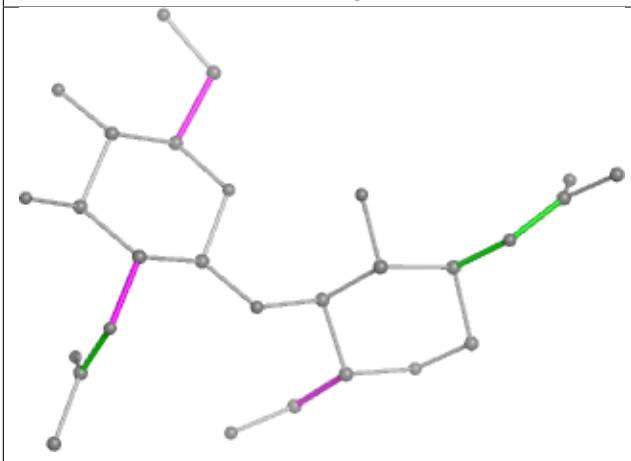
Oligosaccharide Chain H



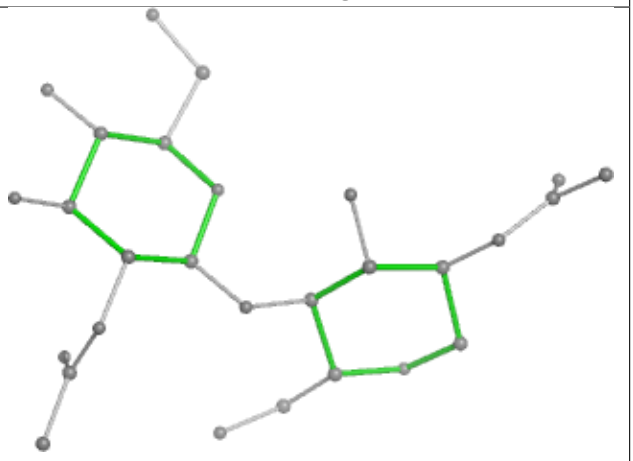
Bond lengths



Bond angles

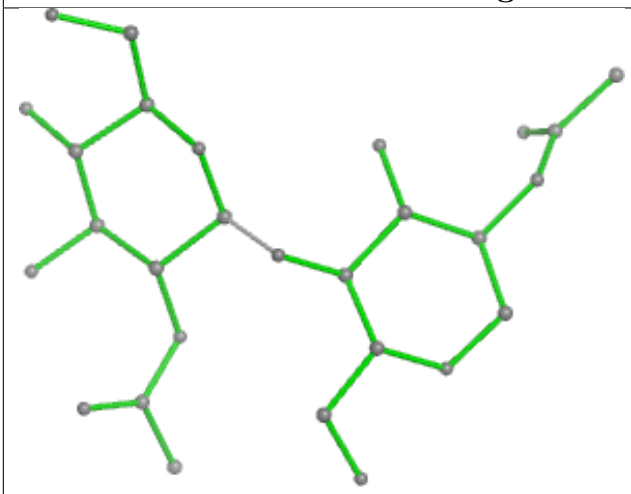


Torsions

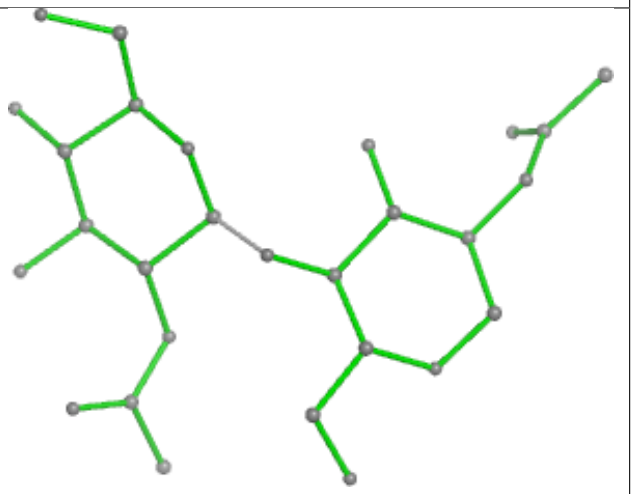


Rings

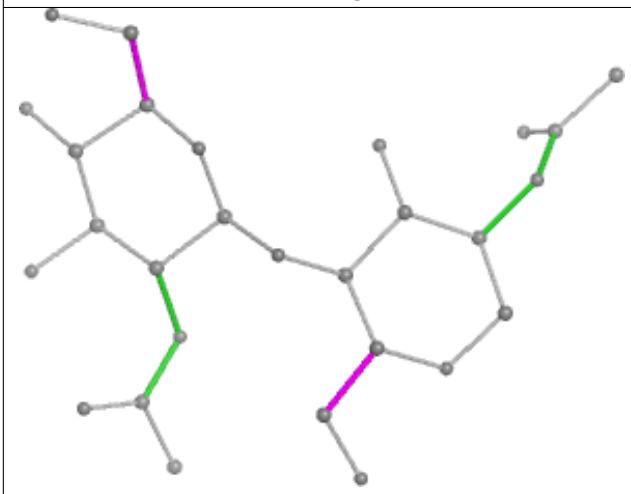
Oligosaccharide Chain L



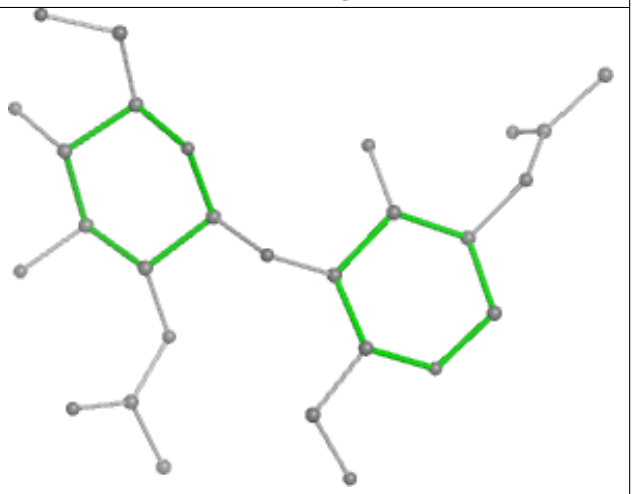
Bond lengths



Bond angles

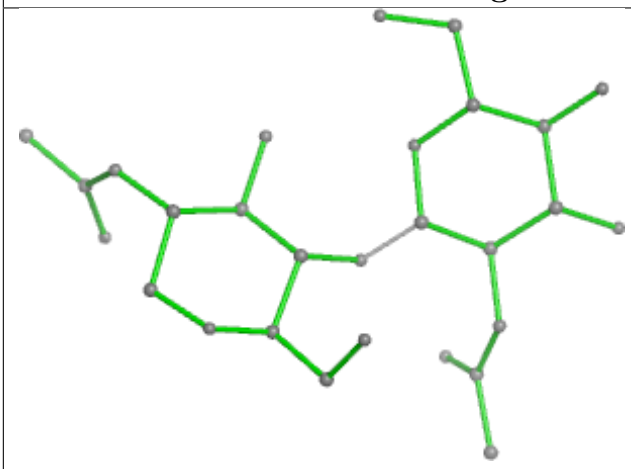


Torsions

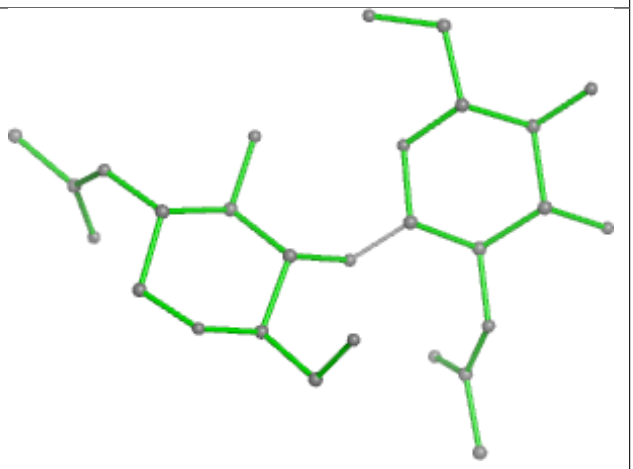


Rings

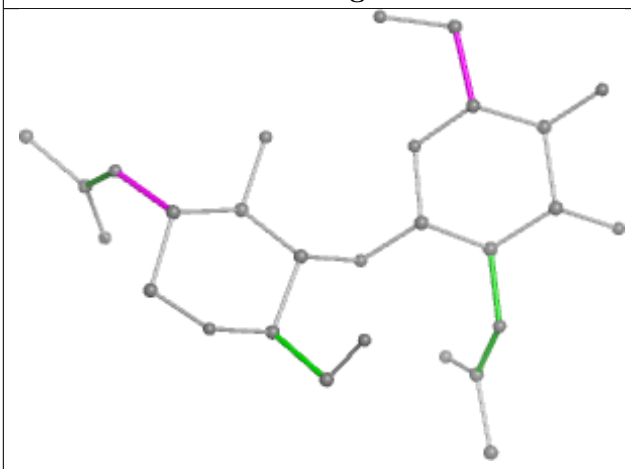
Oligosaccharide Chain M



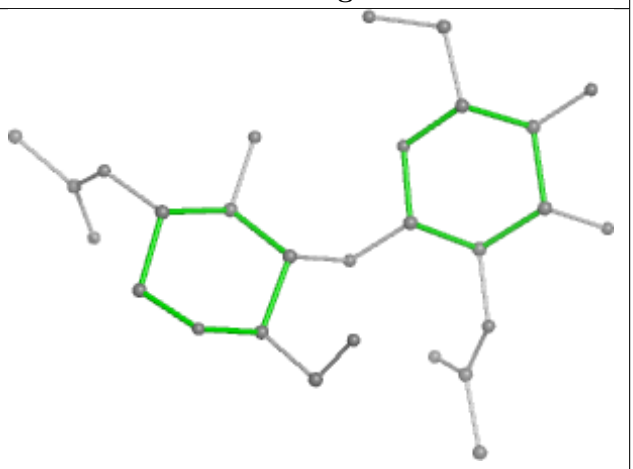
Bond lengths



Bond angles

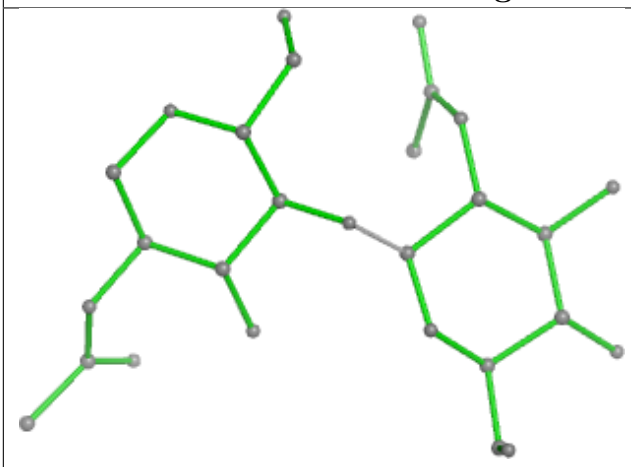


Torsions

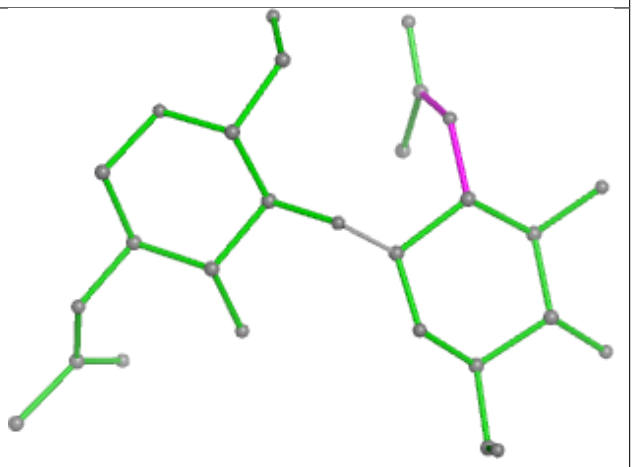


Rings

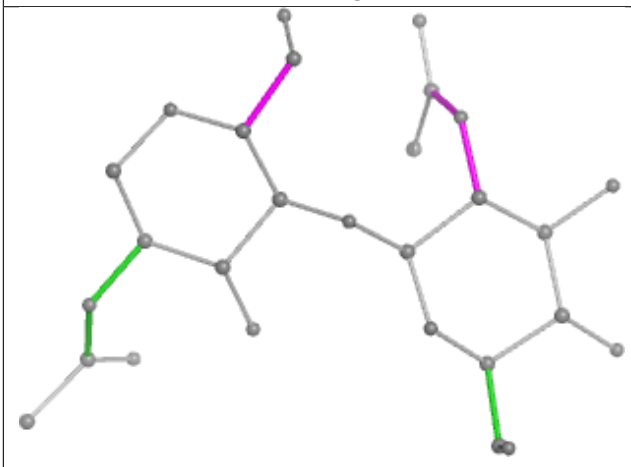
Oligosaccharide Chain O



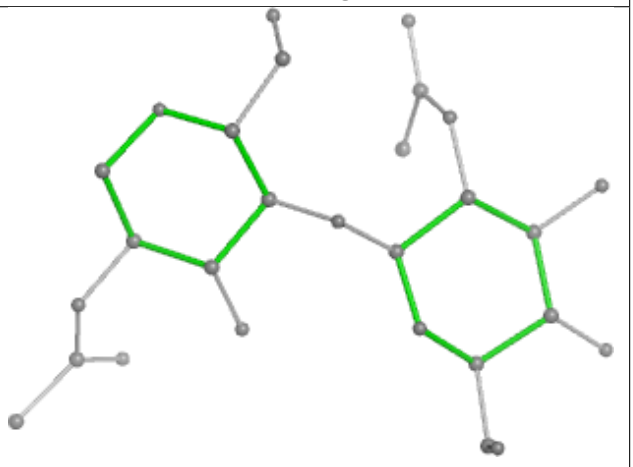
Bond lengths



Bond angles

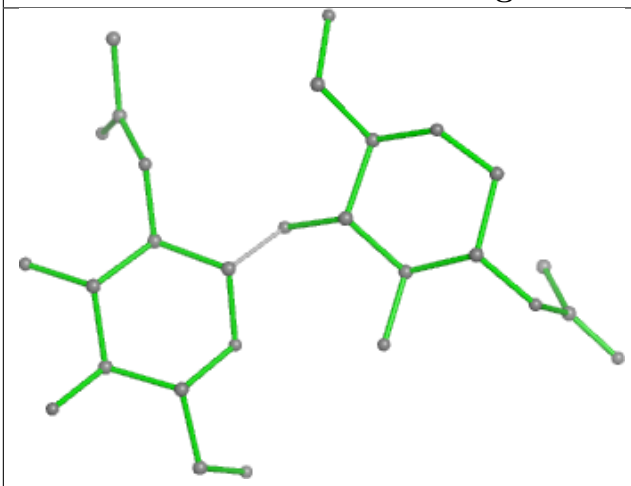


Torsions

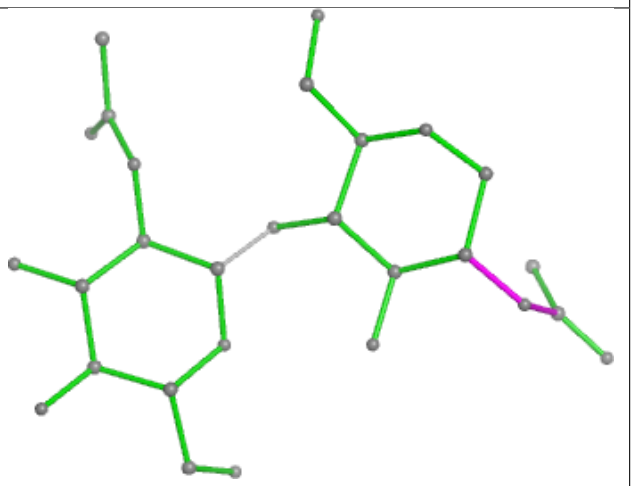


Rings

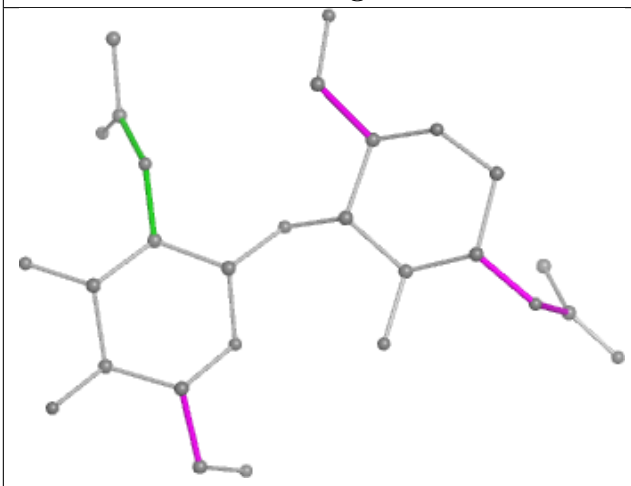
Oligosaccharide Chain P



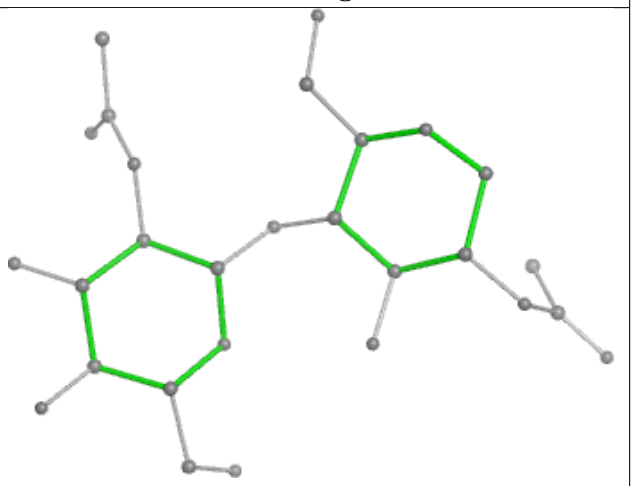
Bond lengths



Bond angles

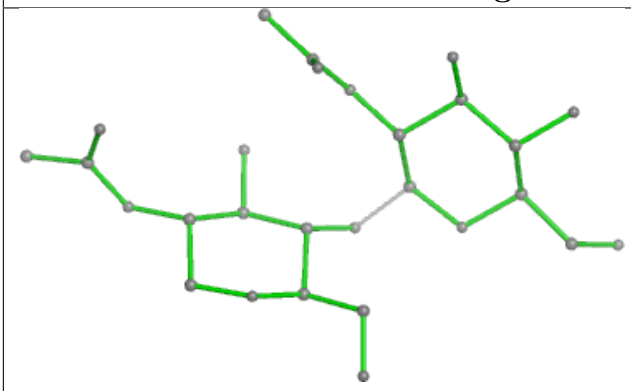


Torsions

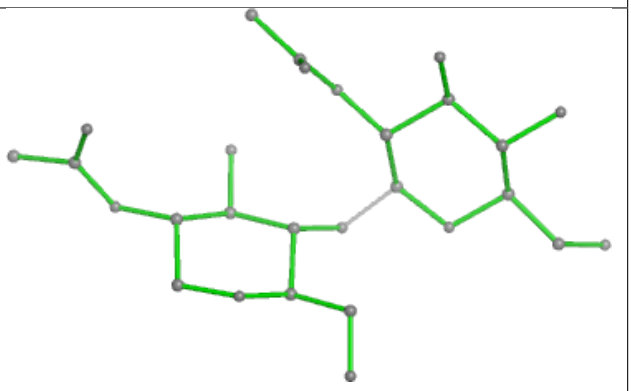


Rings

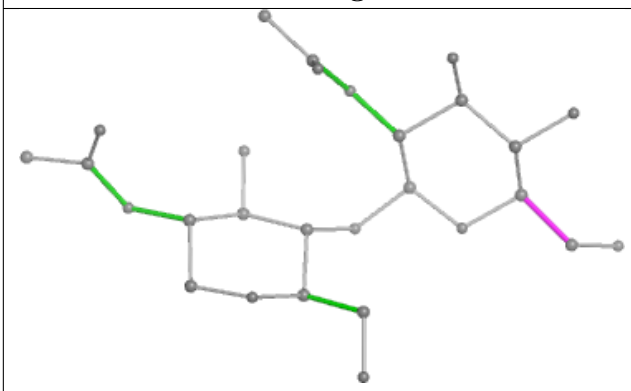
Oligosaccharide Chain U



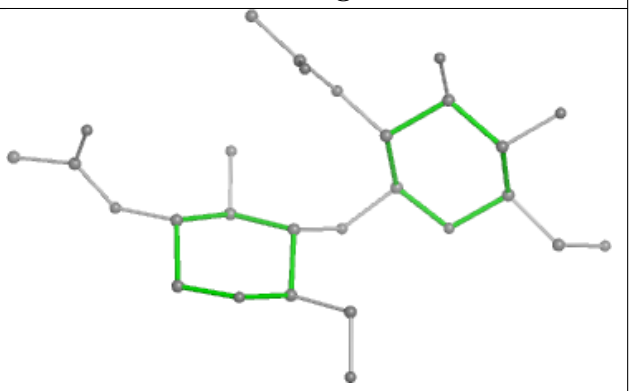
Bond lengths



Bond angles

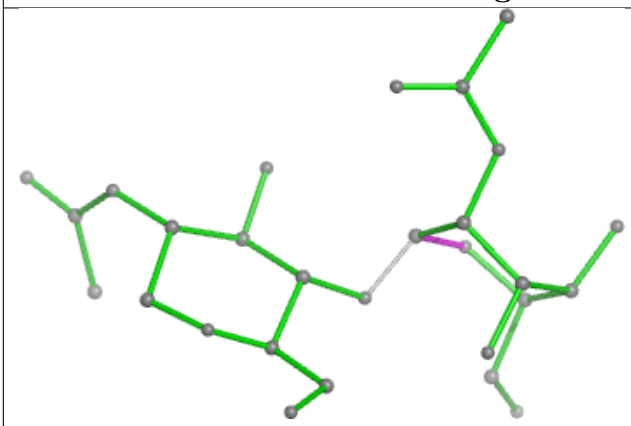


Torsions

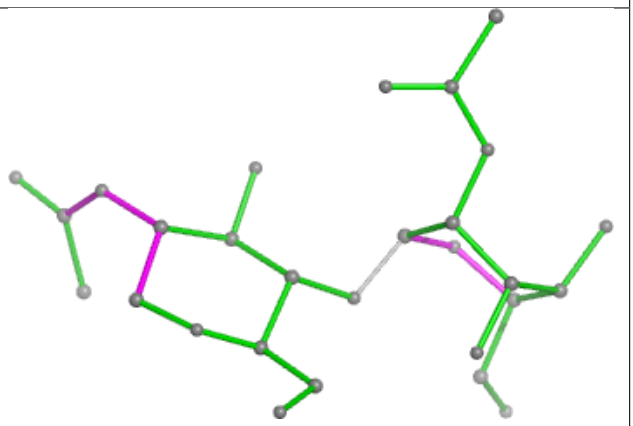


Rings

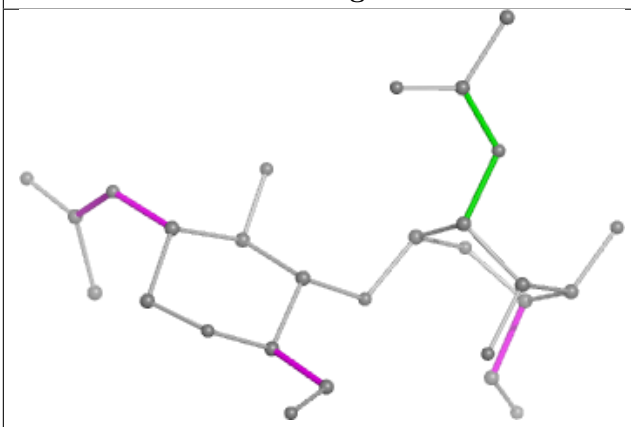
Oligosaccharide Chain V



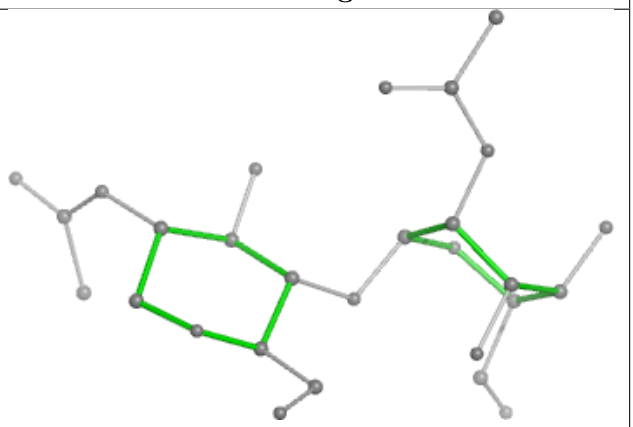
Bond lengths



Bond angles

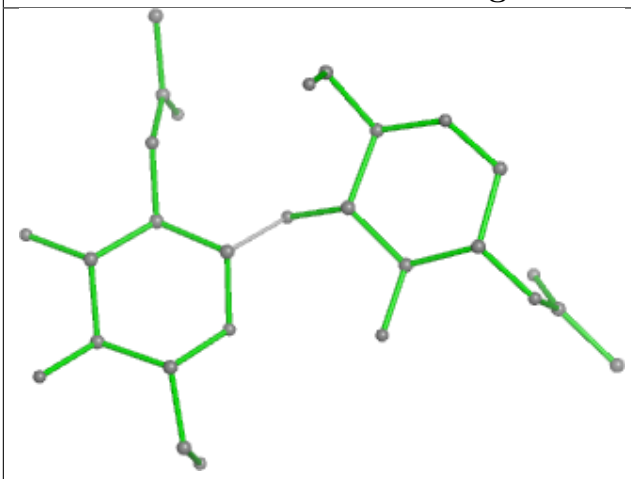


Torsions



Rings

Oligosaccharide Chain W



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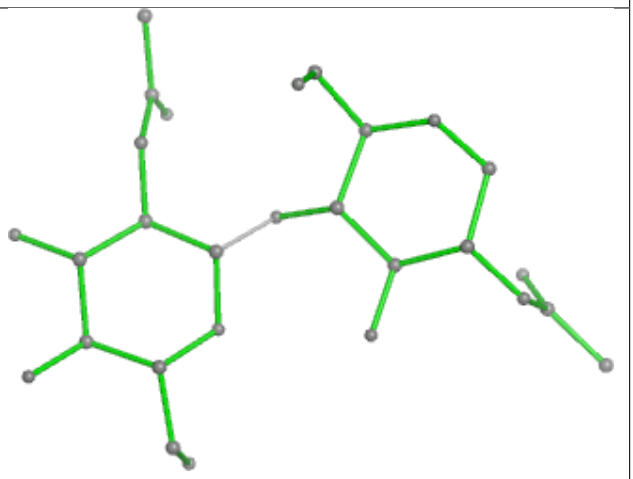

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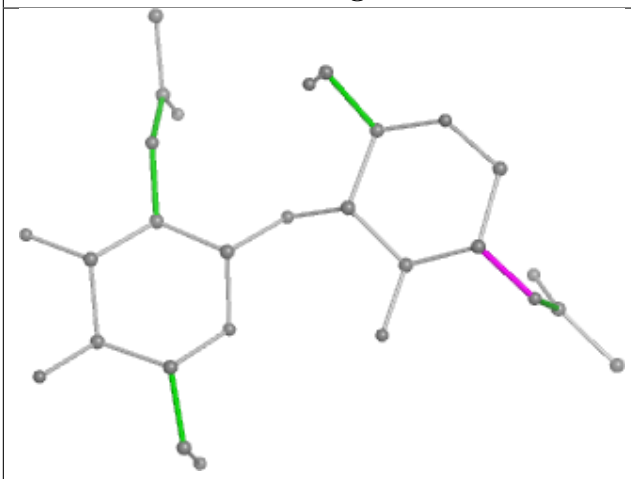

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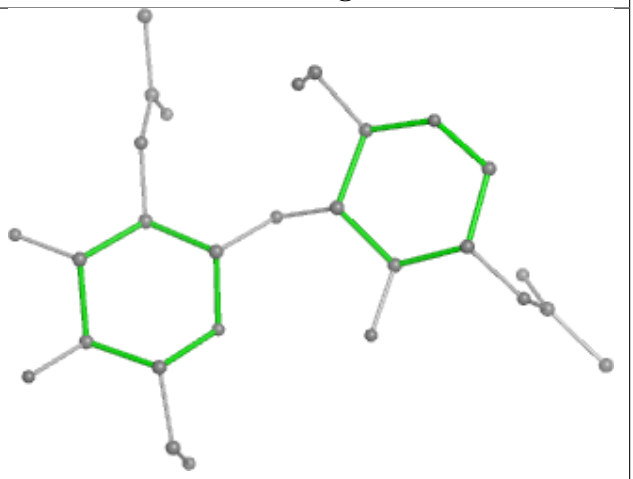
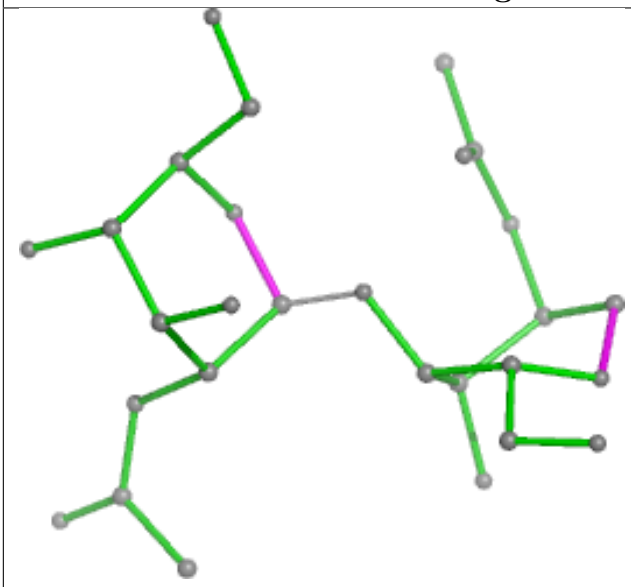


Rings

Oligosaccharide Chain X



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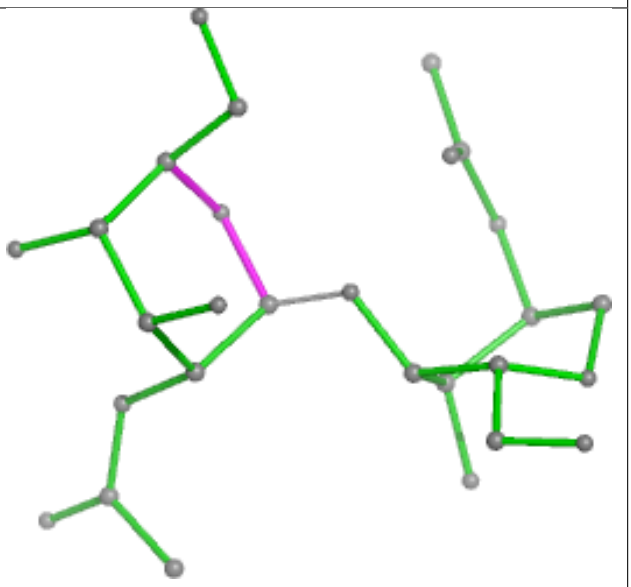

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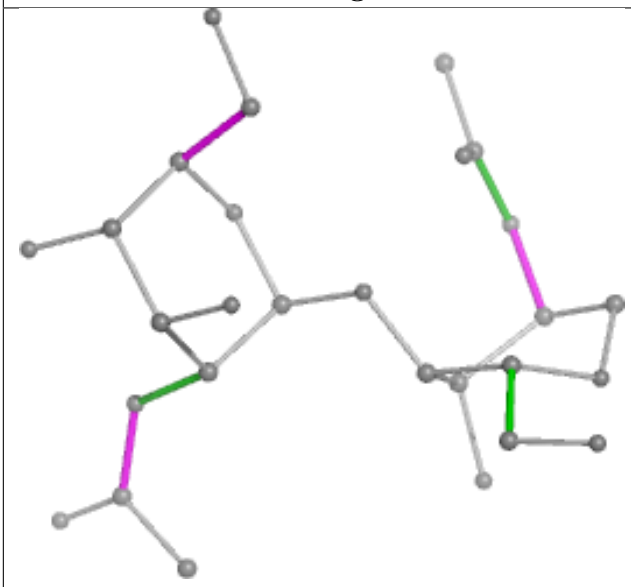

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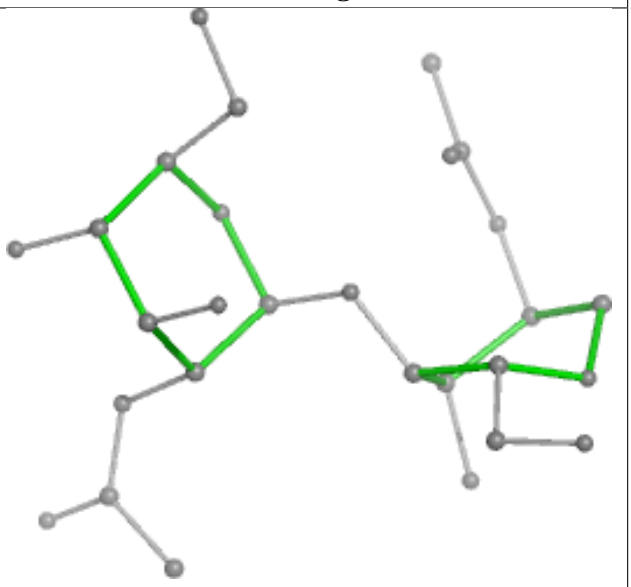
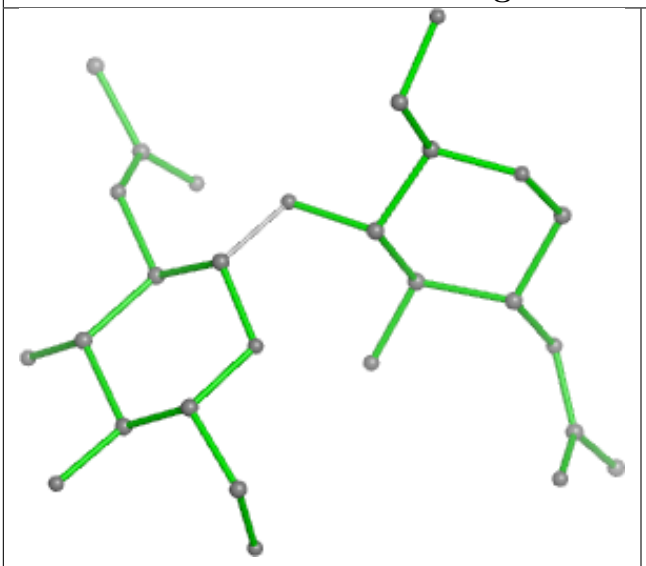


Rings

Oligosaccharide Chain Y



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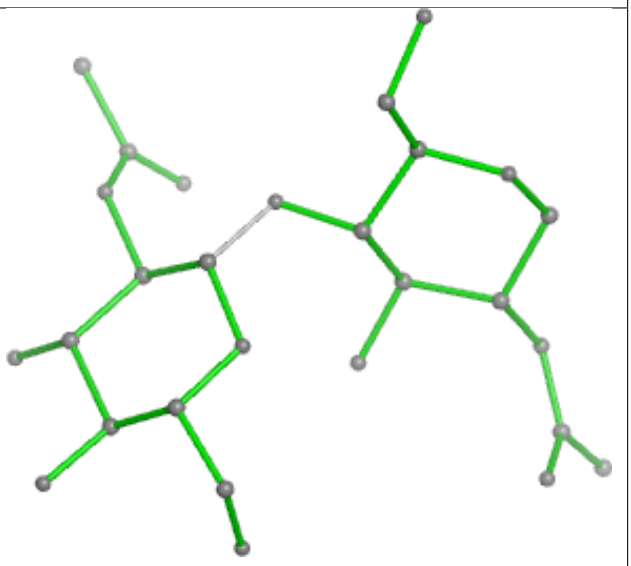

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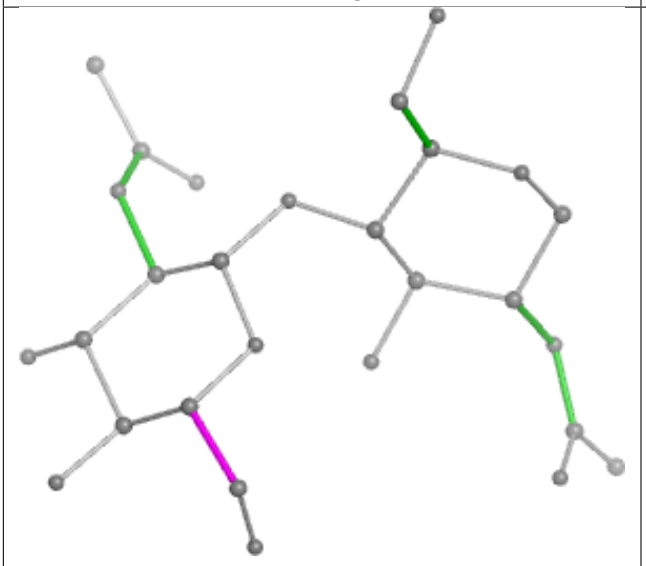

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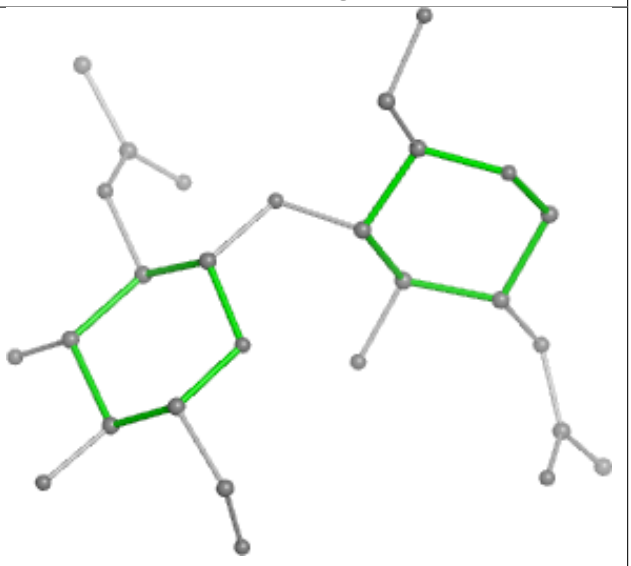
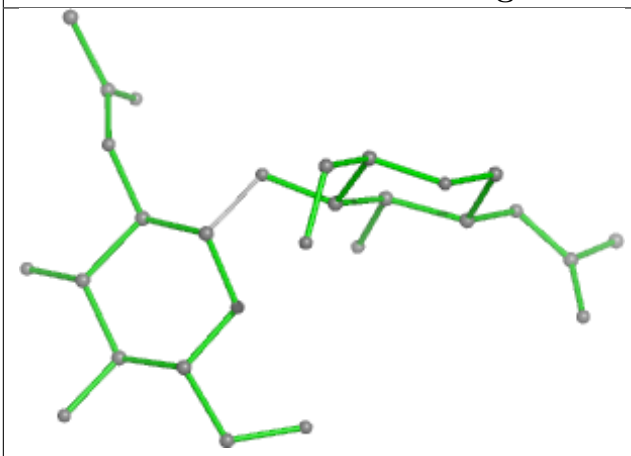


Rings

Oligosaccharide Chain Z



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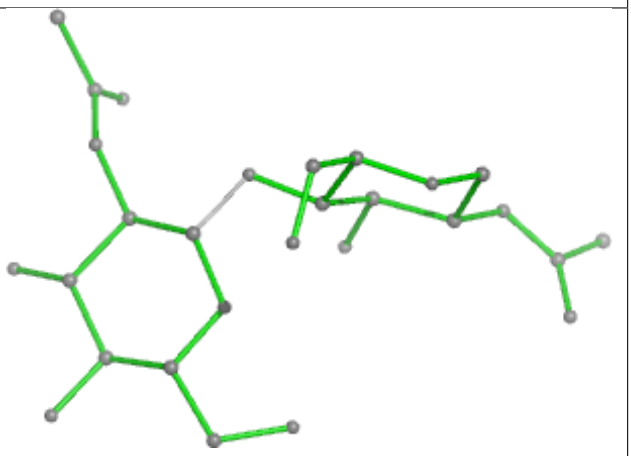
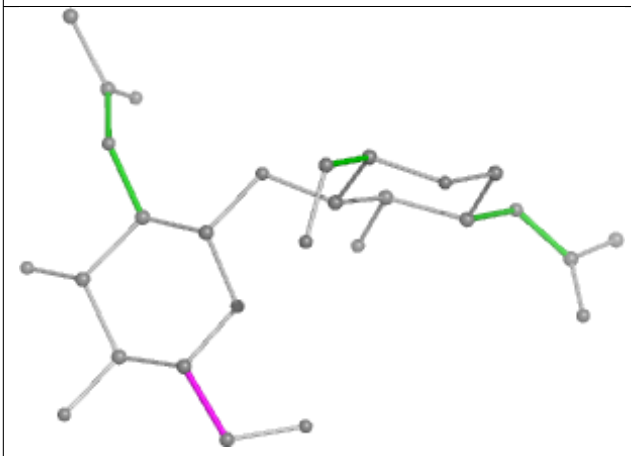


Bond angles



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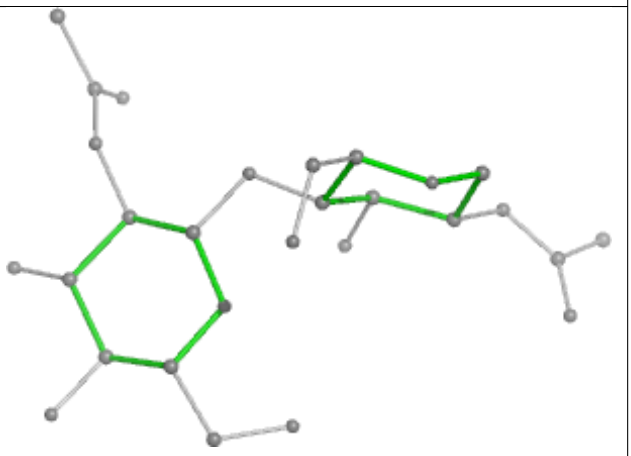
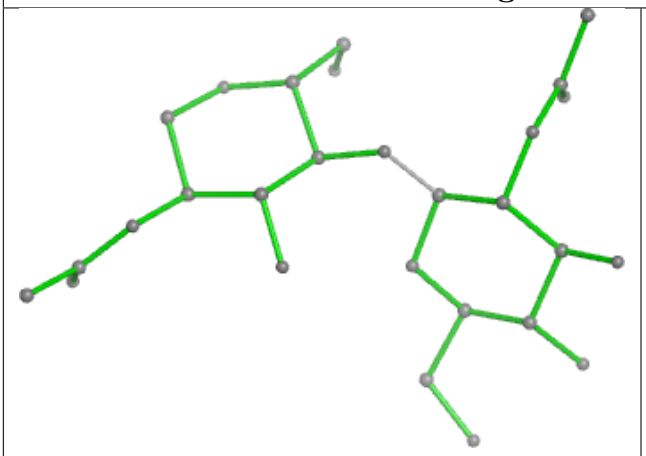


Rings

Oligosaccharide Chain d



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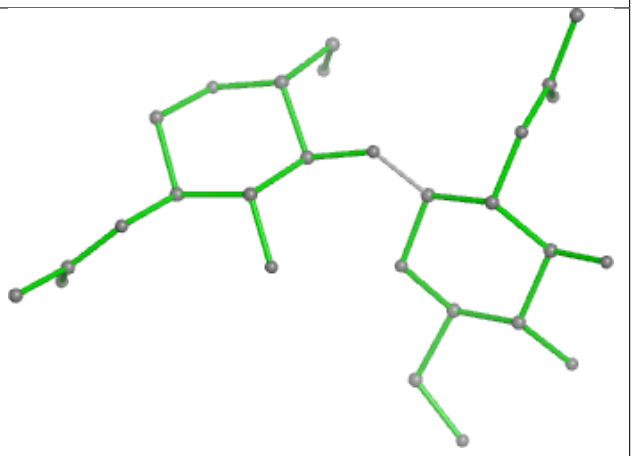

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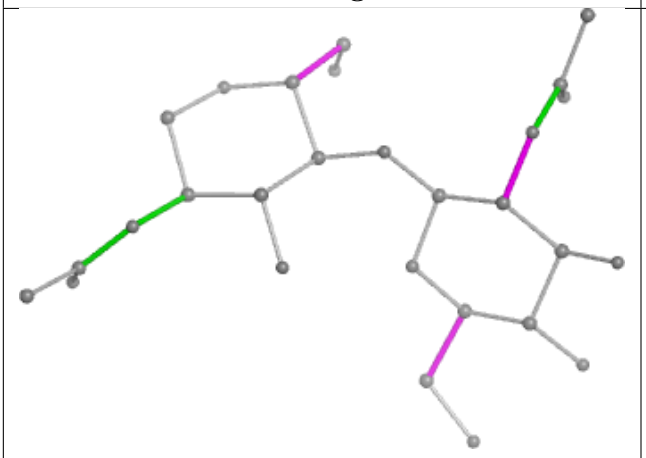

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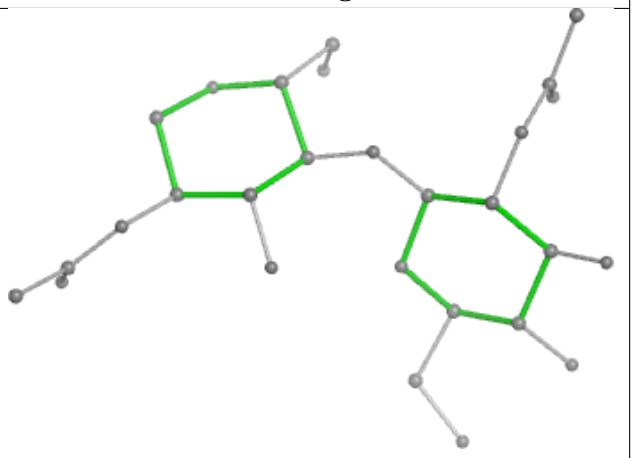
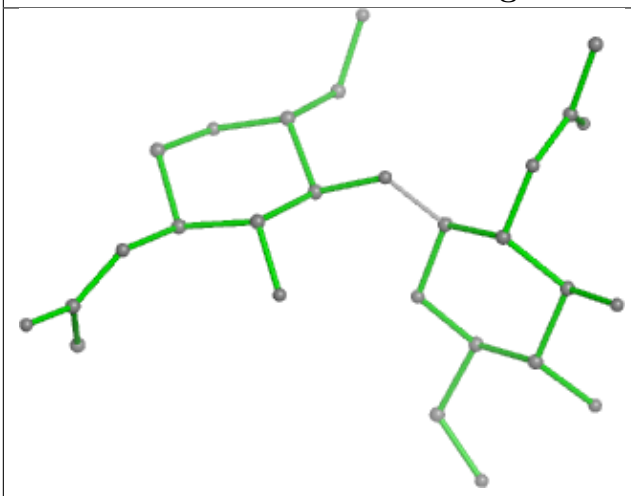


Rings

Oligosaccharide Chain e



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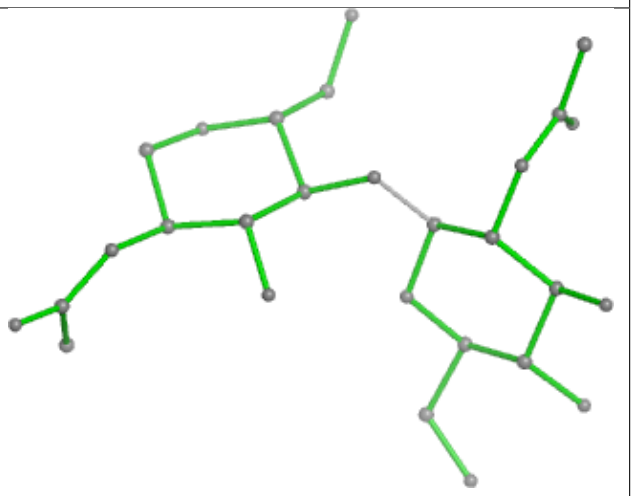

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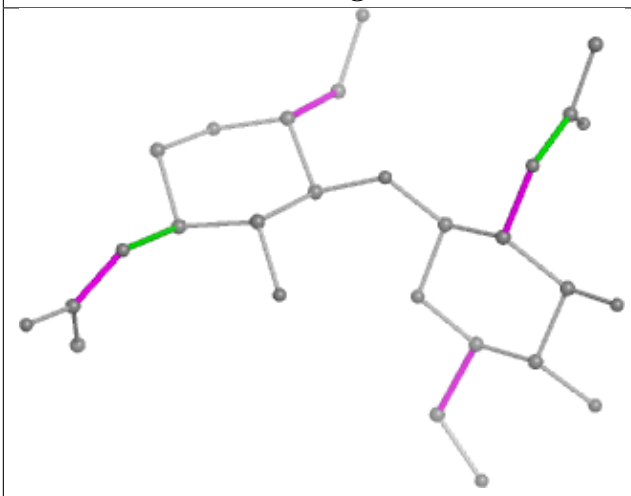

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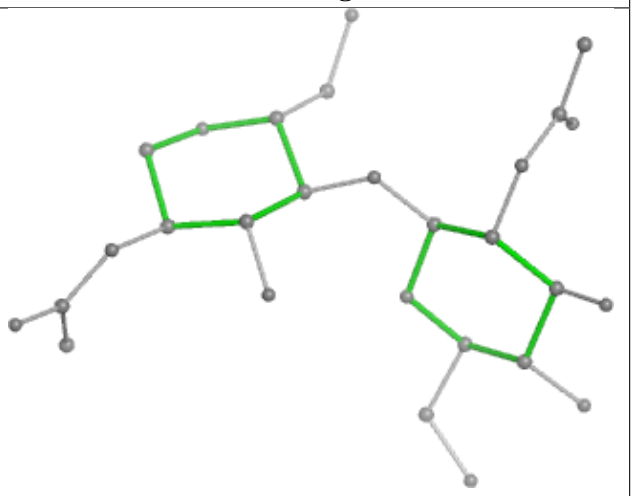
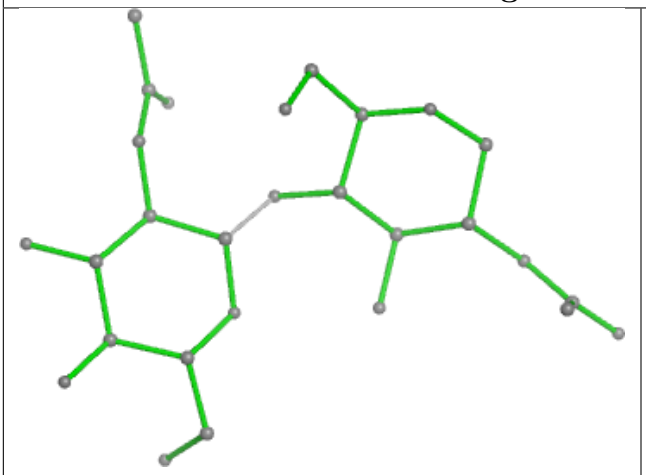


Rings

Oligosaccharide Chain f



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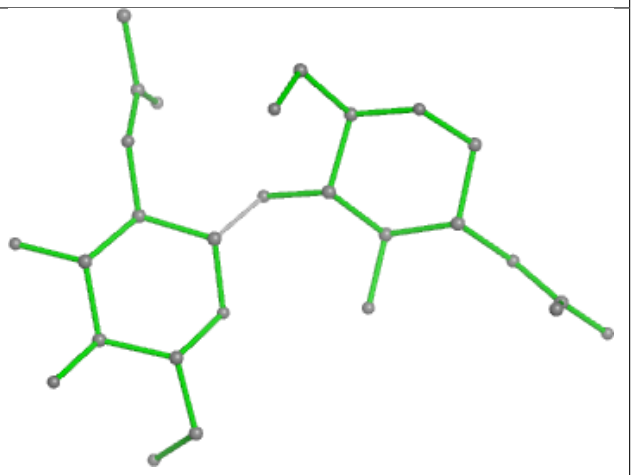

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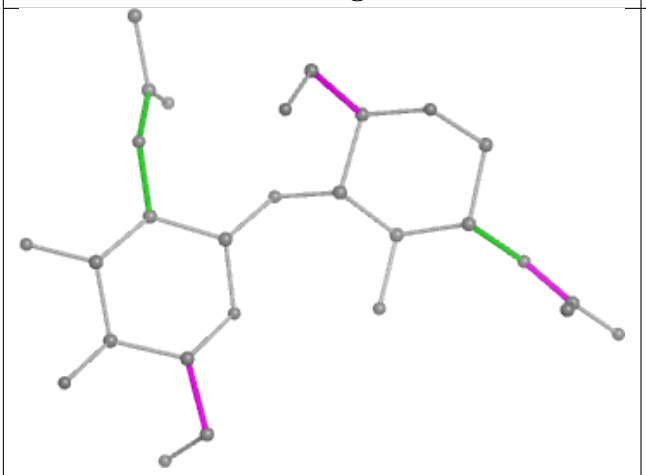

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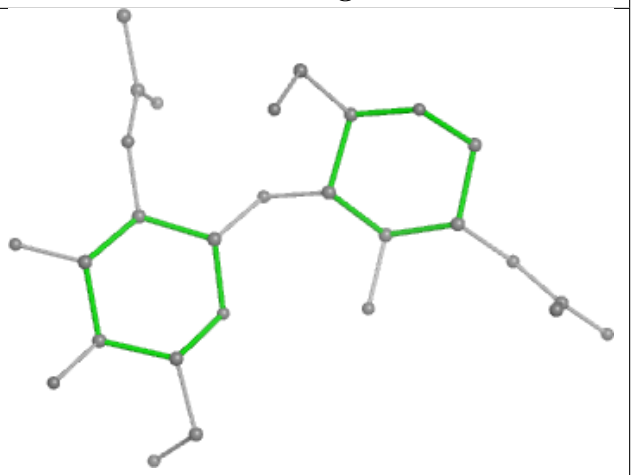
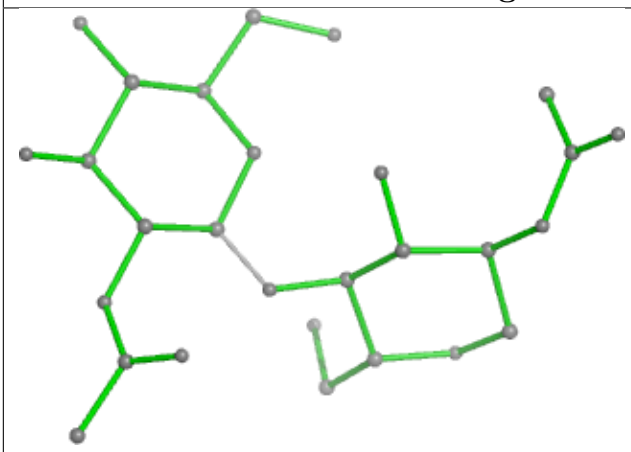


Rings

Oligosaccharide Chain g



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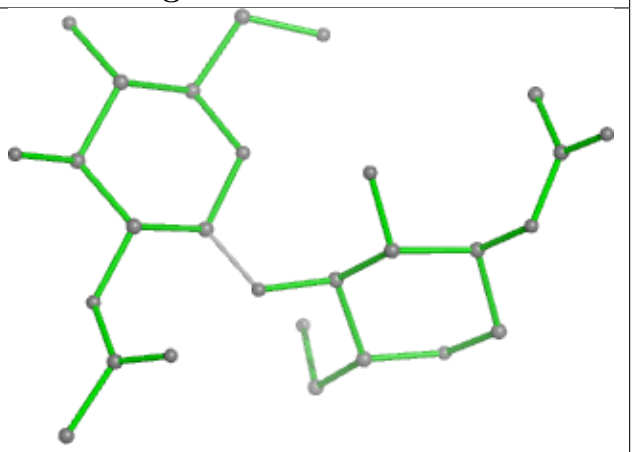
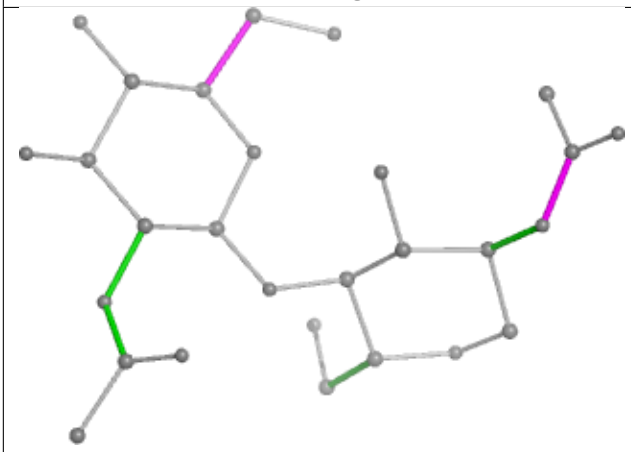


Bond angles



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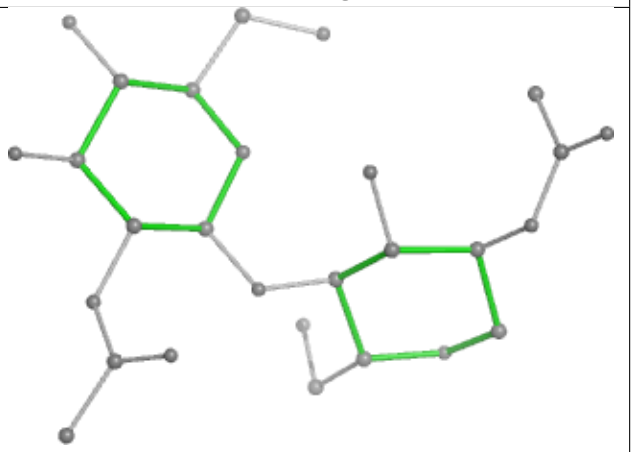
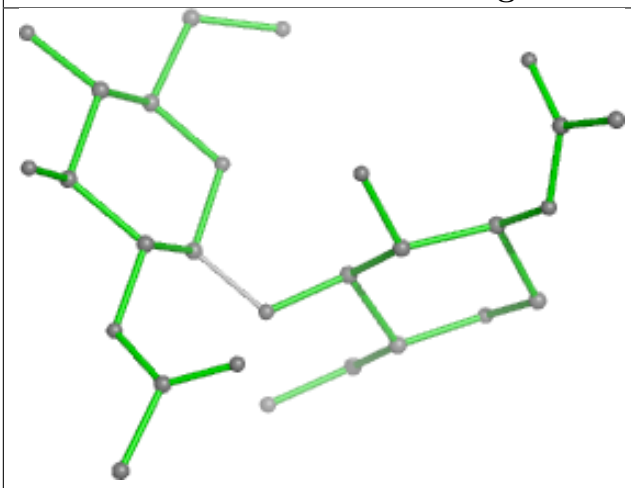


Rings

Oligosaccharide Chain h



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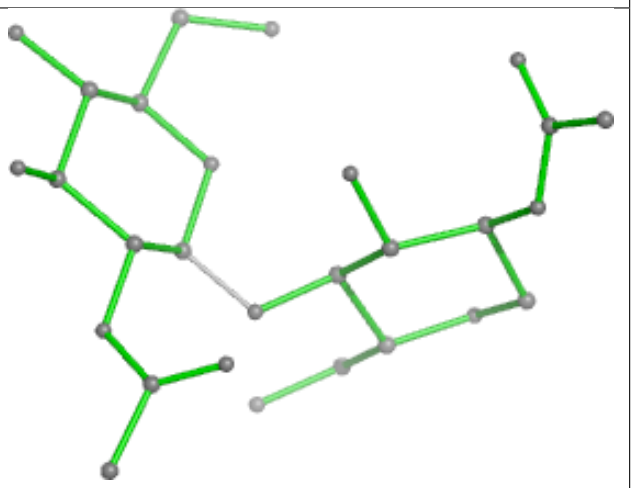

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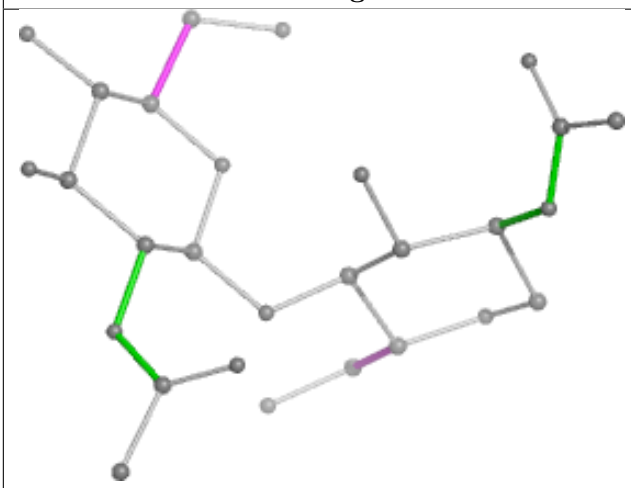

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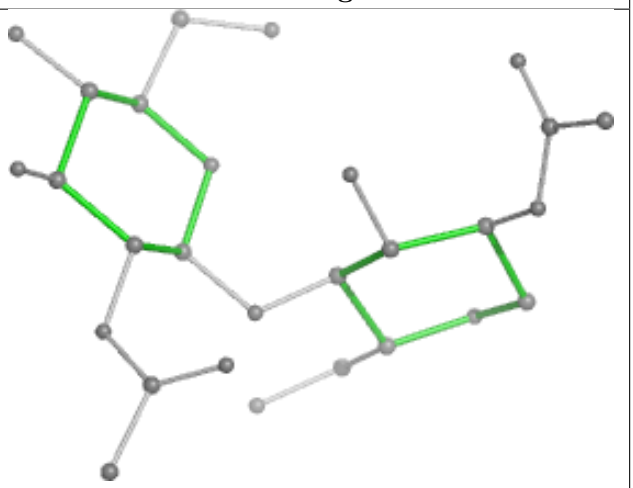
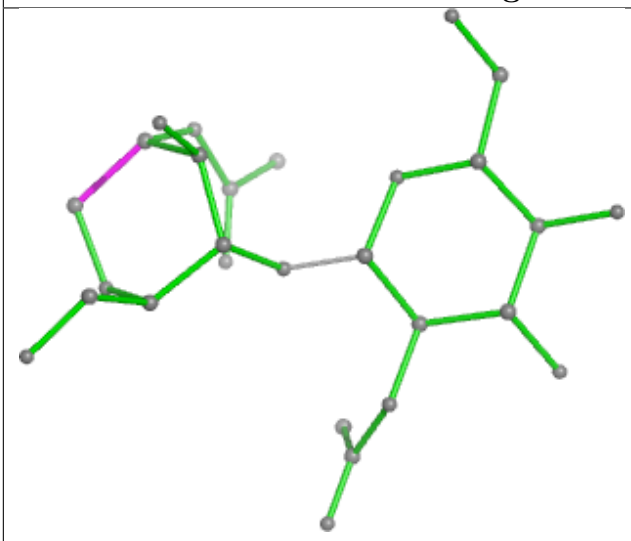


Rings

Oligosaccharide Chain i



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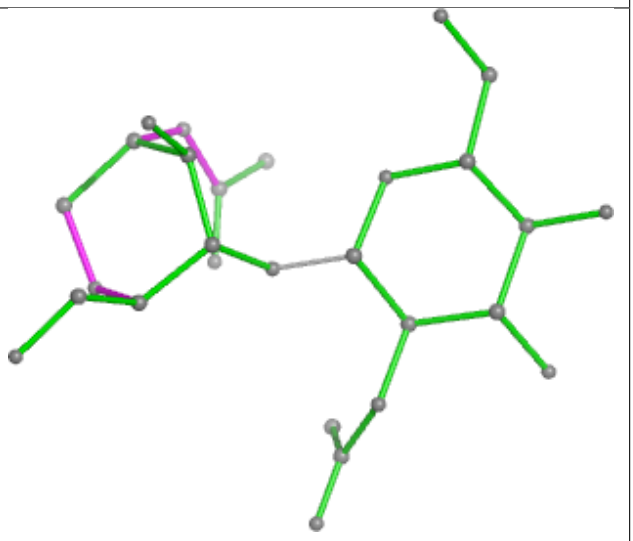

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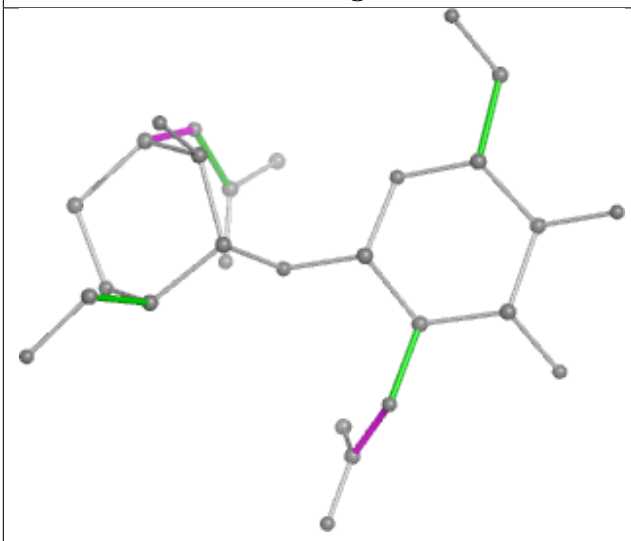

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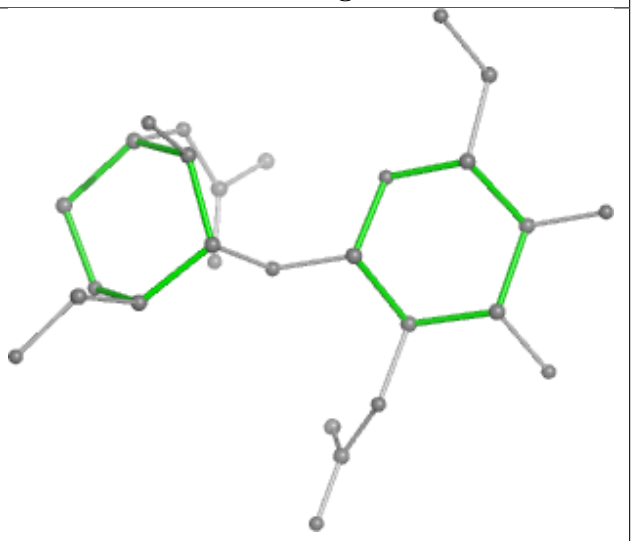
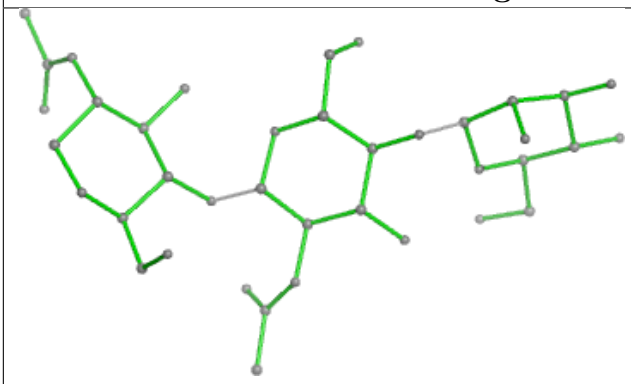


Rings

Oligosaccharide Chain G



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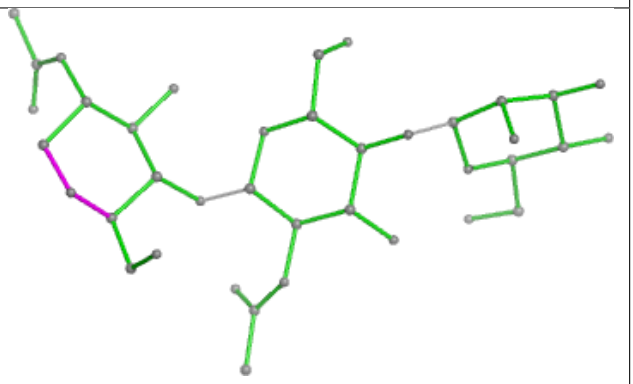
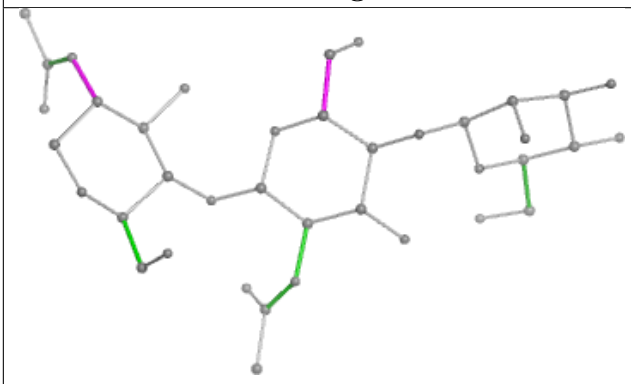


Bond angles



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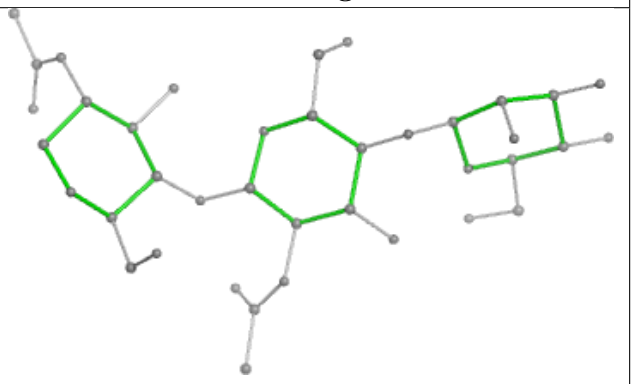
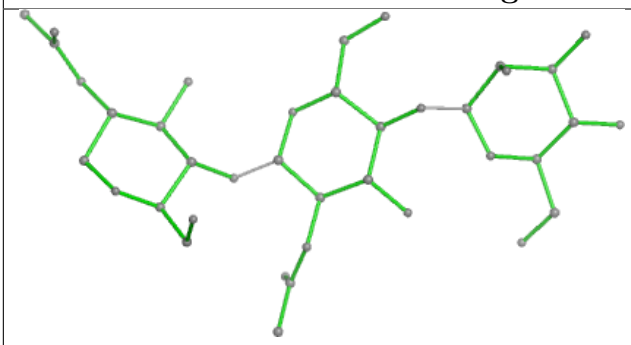


Rings

Oligosaccharide Chain I



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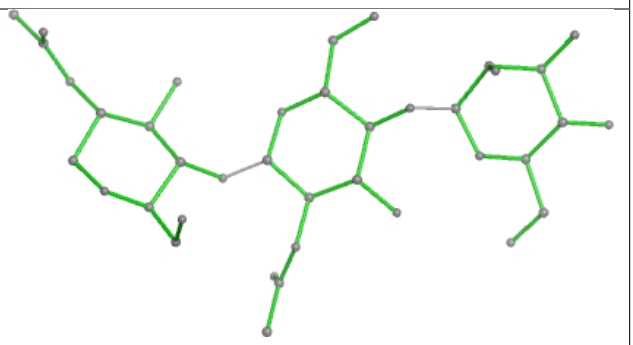
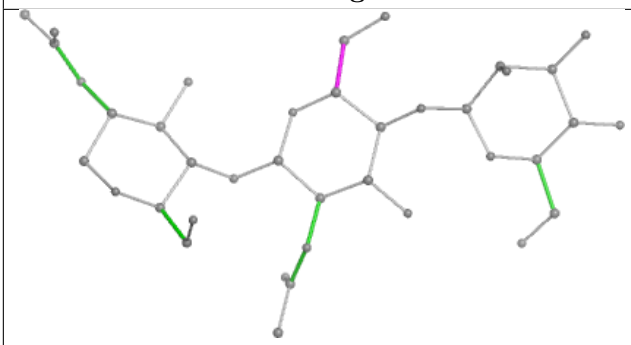
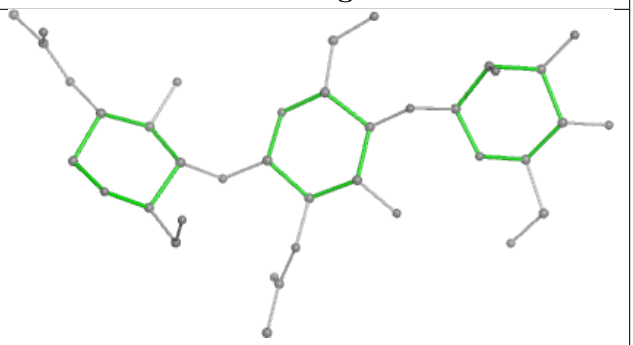


Bond angles

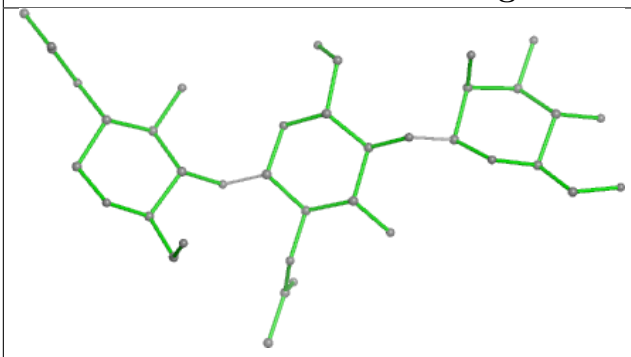


Torsions



Rings

Oligosaccharide Chain J



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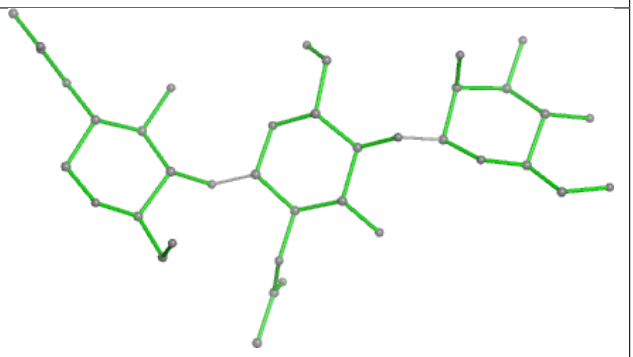
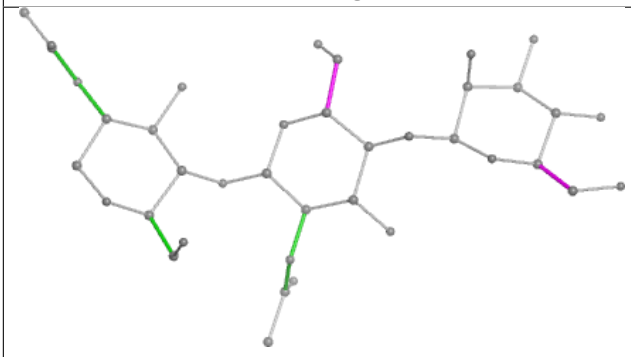
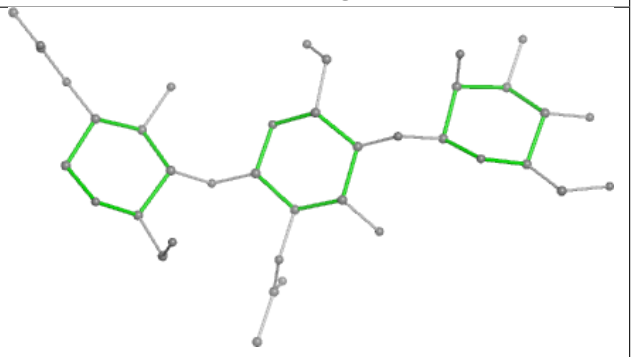


Bond angles

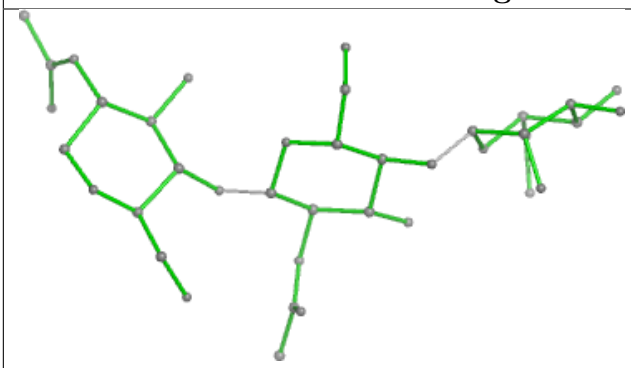


Torsions

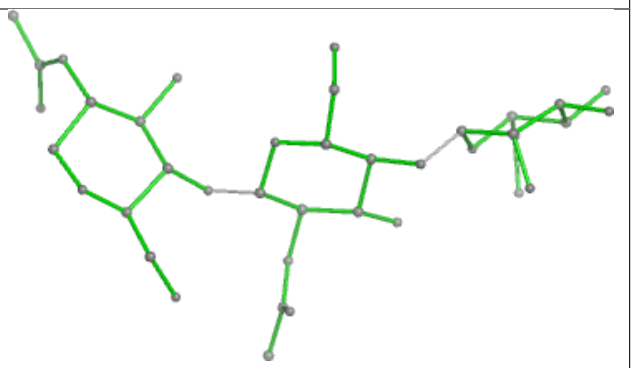


Rings

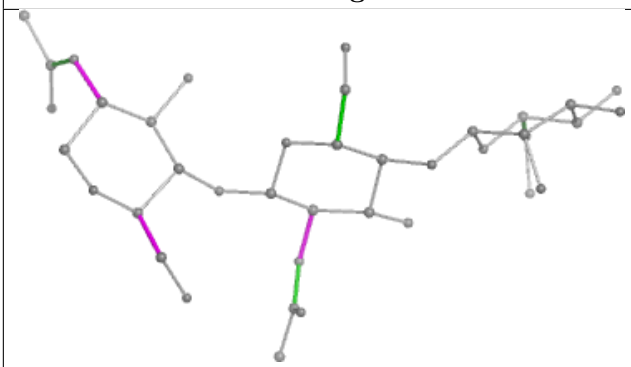
Oligosaccharide Chain K



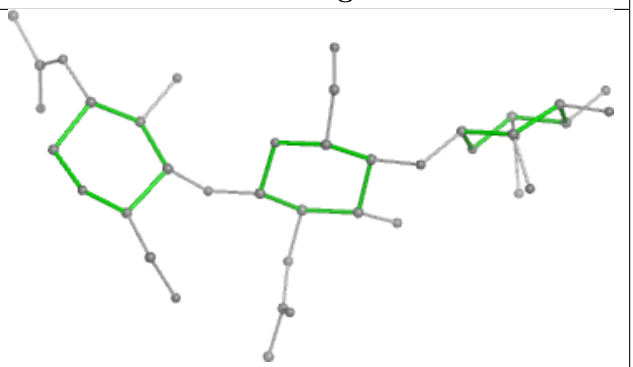
Bond lengths



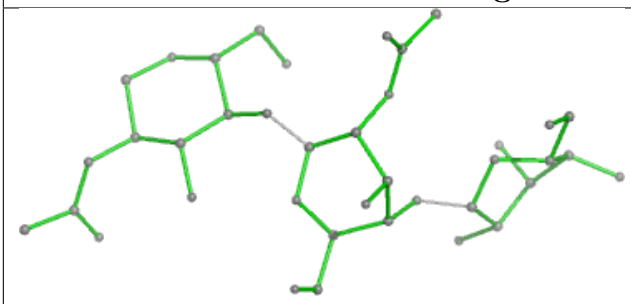
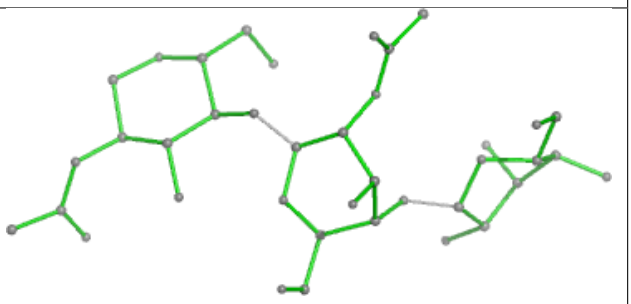
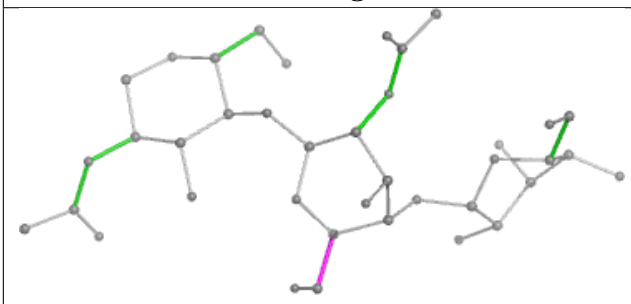
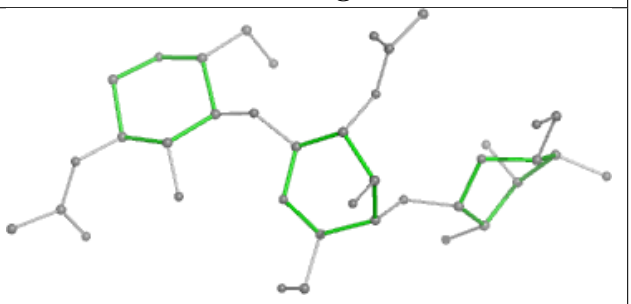
Bond angles

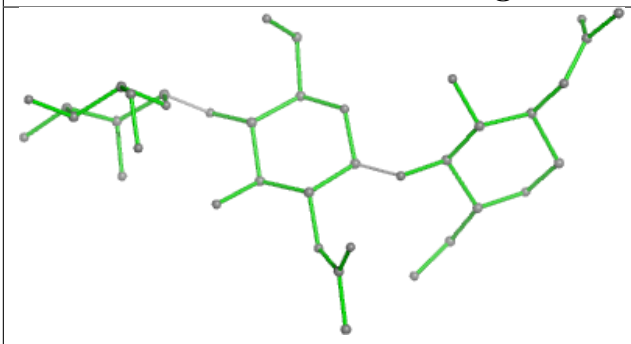
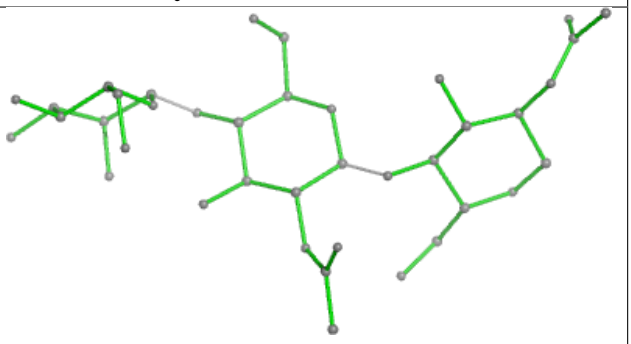
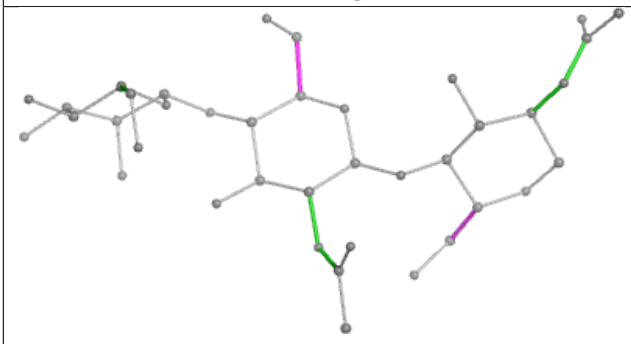
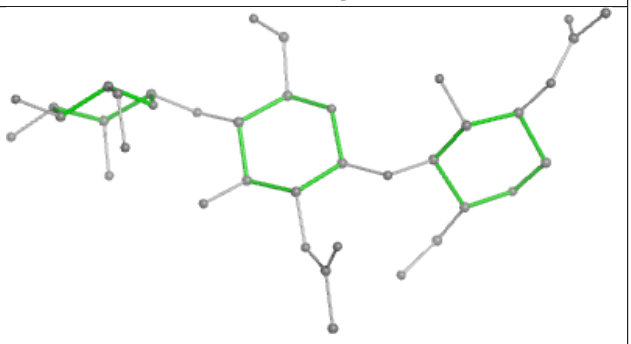


Torsions

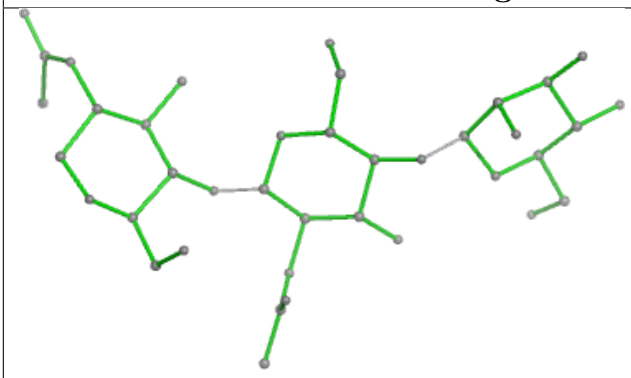


Rings

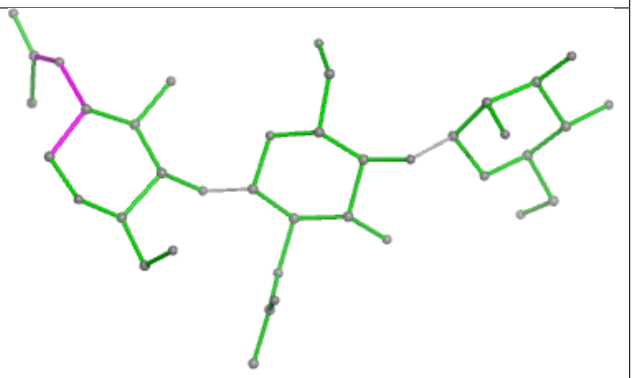
Oligosaccharide Chain N	
	
Bond lengths	Bond angles
	
Torsions	Rings

Oligosaccharide Chain Q	
	
Bond lengths	Bond angles
	
Torsions	Rings

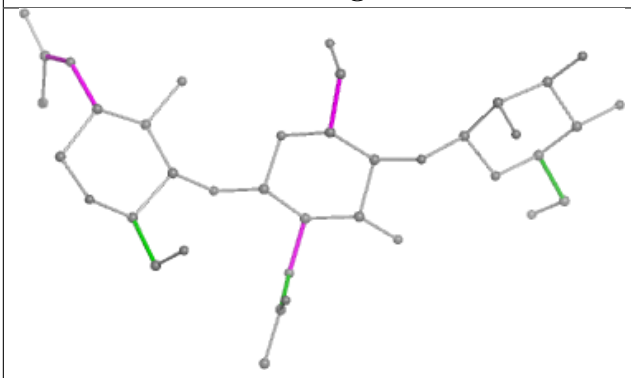
Oligosaccharide Chain R



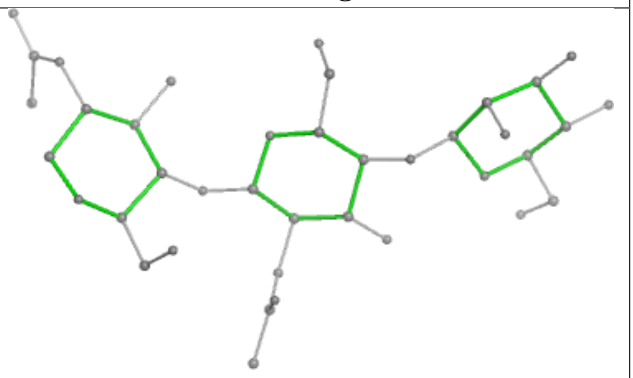
Bond lengths



Bond angles

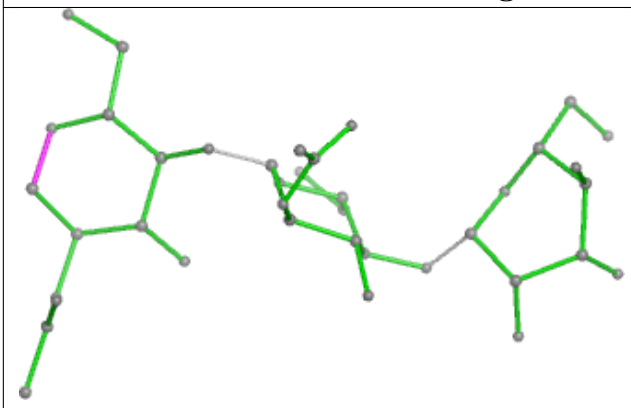


Torsions

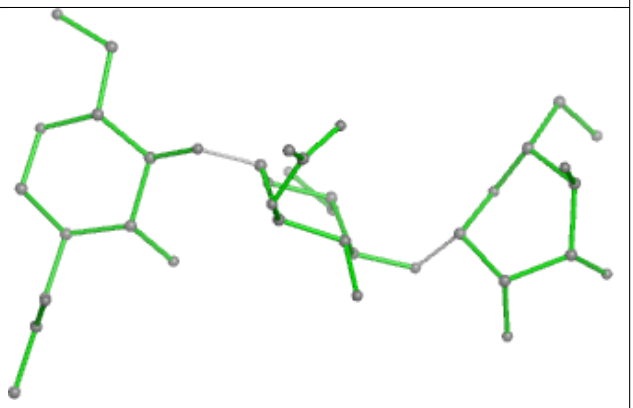


Rings

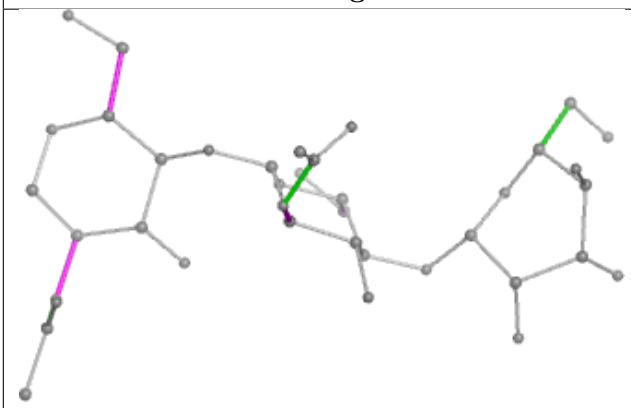
Oligosaccharide Chain S



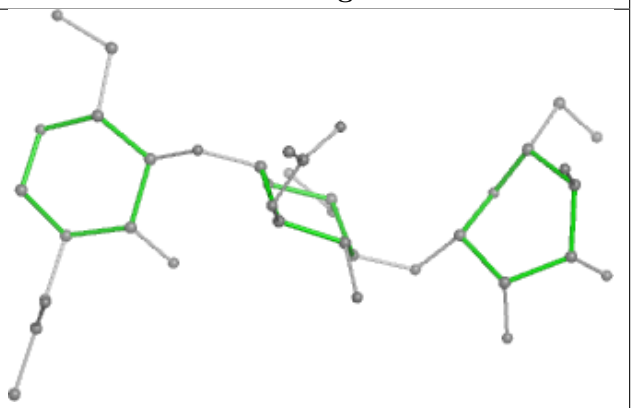
Bond lengths



Bond angles

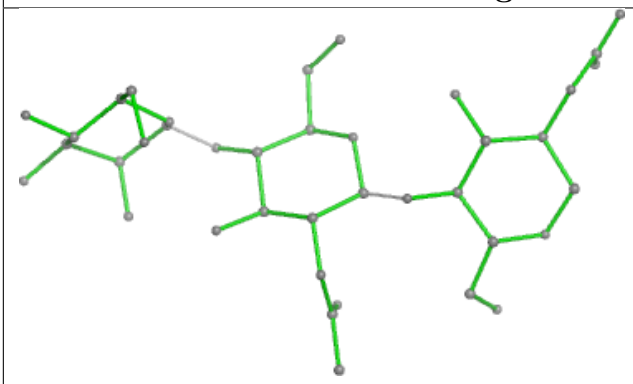


Torsions

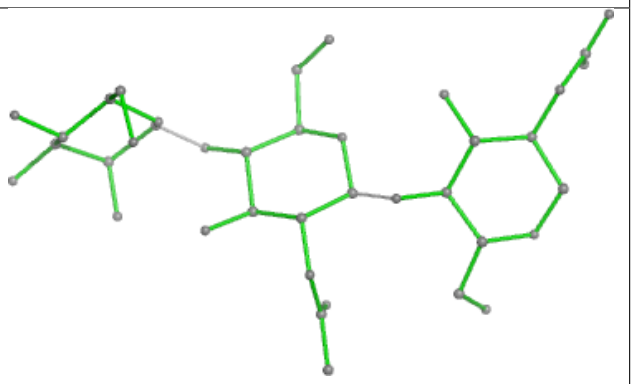


Rings

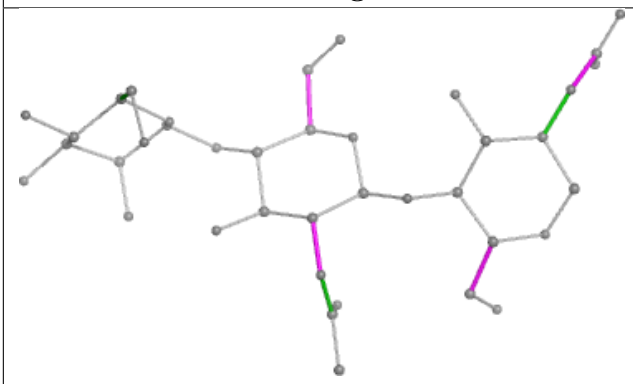
Oligosaccharide Chain T



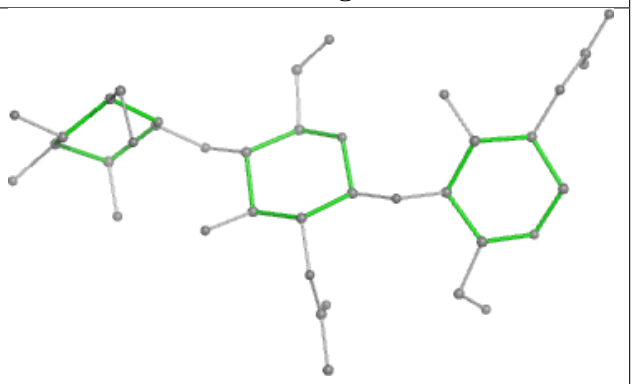
Bond lengths



Bond angles

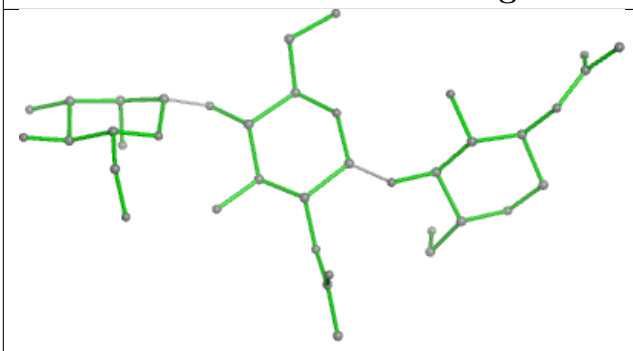


Torsions

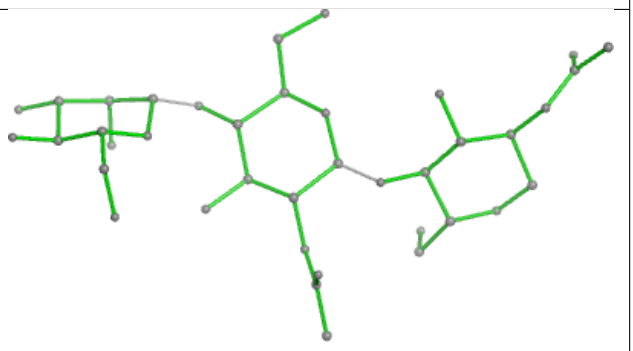


Rings

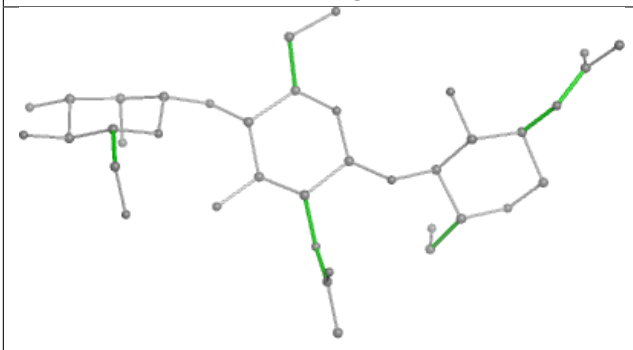
Oligosaccharide Chain a



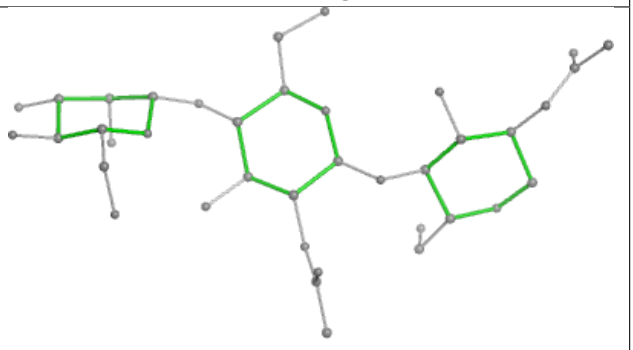
Bond lengths



Bond angles

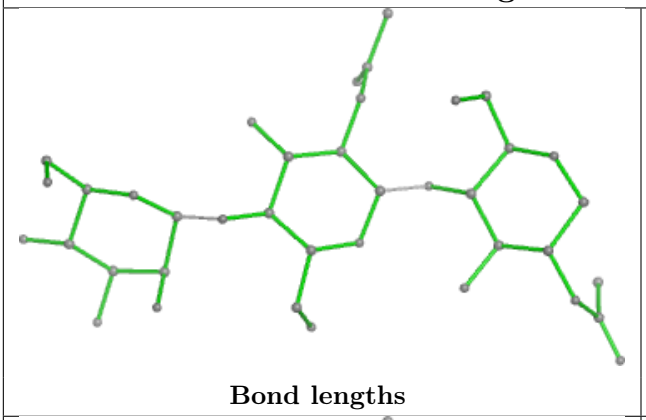


Torsions

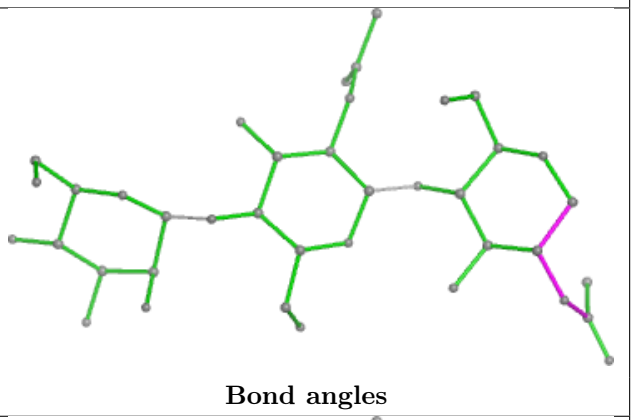


Rings

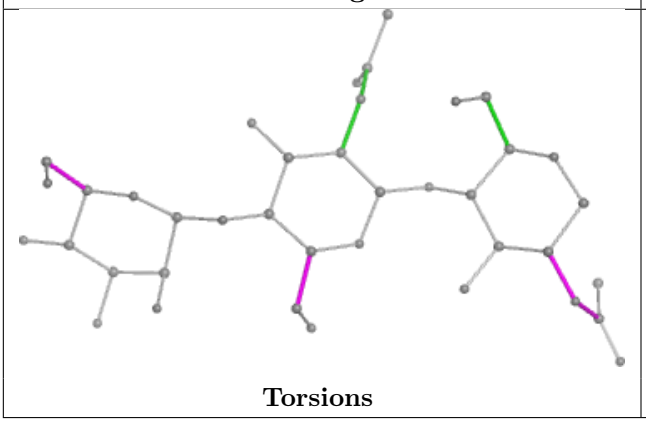
Oligosaccharide Chain b



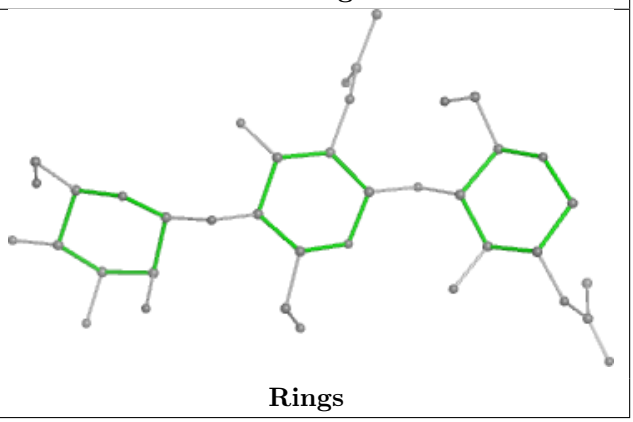
Bond lengths



Bond angles

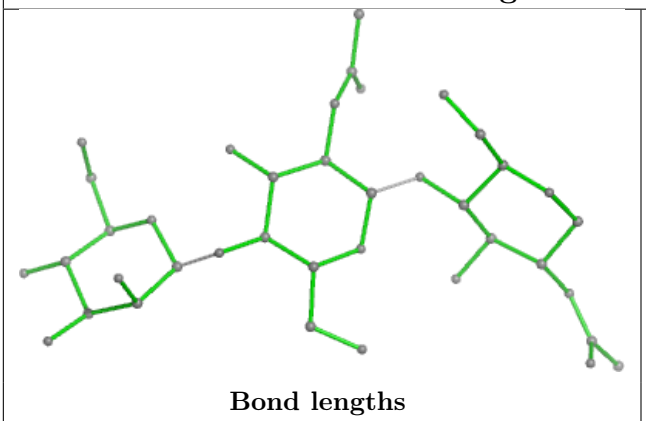


Torsions

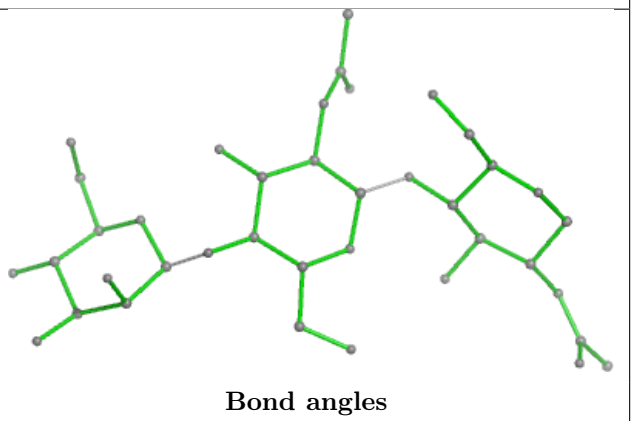


Rings

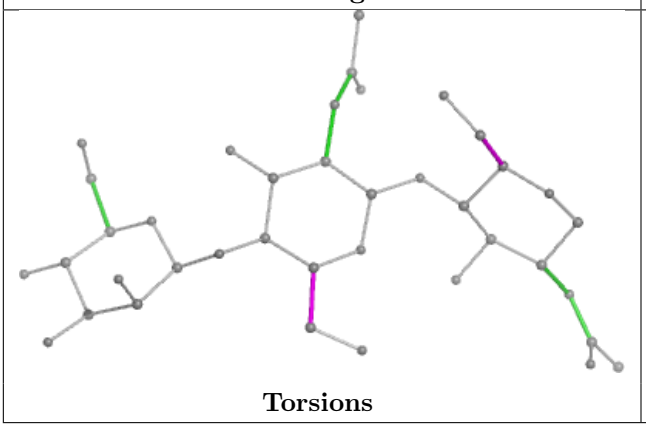
Oligosaccharide Chain c



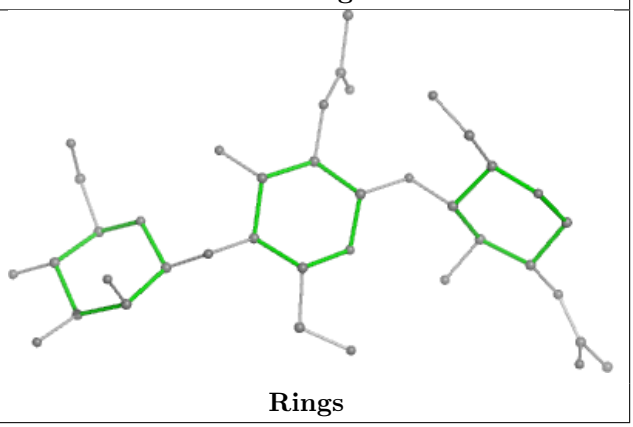
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
5	NAG	B	1305	1	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	C	1301	1	14,14,15	0.32	0	17,19,21	0.42	0
5	NAG	B	1302	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	B	1306	1	14,14,15	0.33	0	17,19,21	0.47	0
5	NAG	A	1303	1	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	C	1302	1	14,14,15	0.27	0	17,19,21	0.52	0
5	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	C	1304	1	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	B	1304	1	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	A	1301	1	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	A	1302	1	14,14,15	0.19	0	17,19,21	0.46	0
5	NAG	C	1303	1	14,14,15	0.19	0	17,19,21	0.42	0
5	NAG	A	1305	1	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	B	1301	1	14,14,15	0.49	0	17,19,21	1.24	1 (5%)
5	NAG	B	1307	1	14,14,15	0.23	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1301	NAG	C1-O5-C5	4.76	118.65	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1305	NAG	C4-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	A	1301	NAG	C4-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	B	1305	NAG	C4-C5-C6-O6
5	A	1302	NAG	C8-C7-N2-C2
5	A	1302	NAG	O7-C7-N2-C2
5	C	1301	NAG	C8-C7-N2-C2
5	C	1301	NAG	O7-C7-N2-C2
5	C	1302	NAG	C4-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	B	1306	NAG	C4-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1304	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	B	1306	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	B	1303	NAG	C4-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	C	1302	NAG	C3-C2-N2-C7
5	C	1304	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.

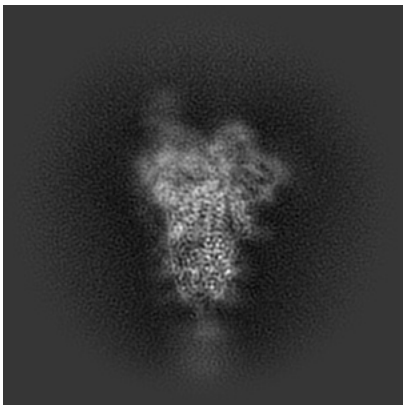
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14922. These allow visual inspection of the internal detail of the map and identification of artifacts.

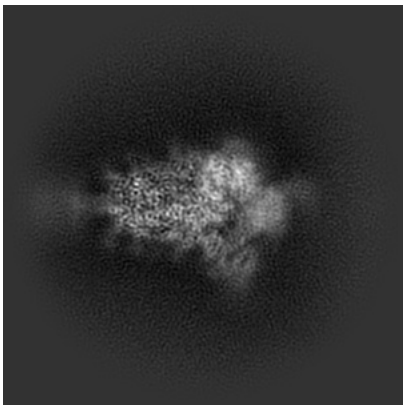
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

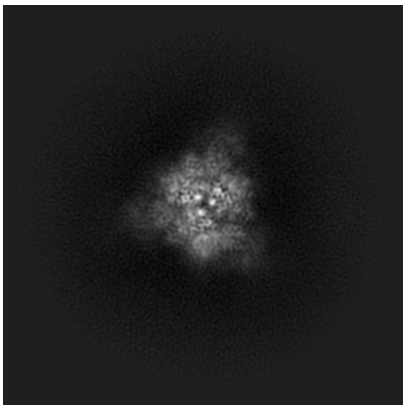
6.1.1 Primary map



X

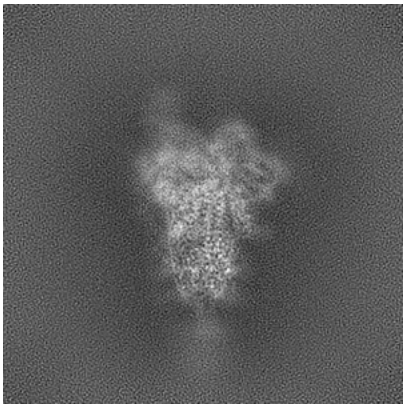


Y

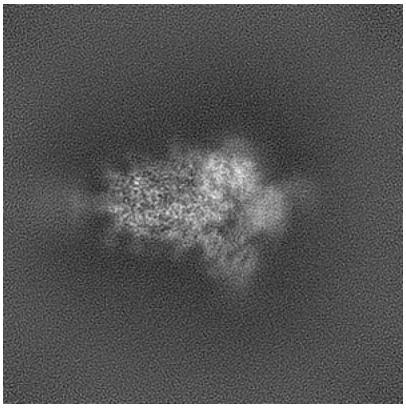


Z

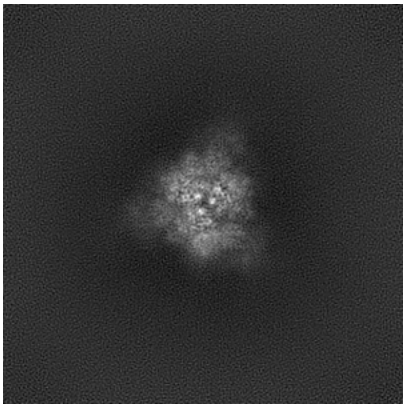
6.1.2 Raw map



X



Y

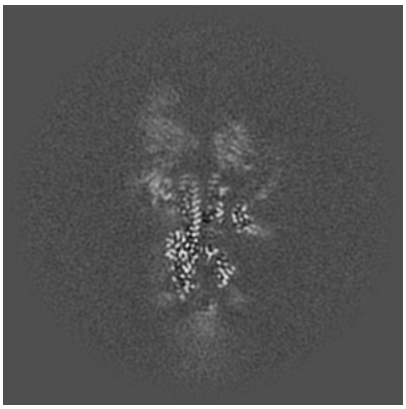


Z

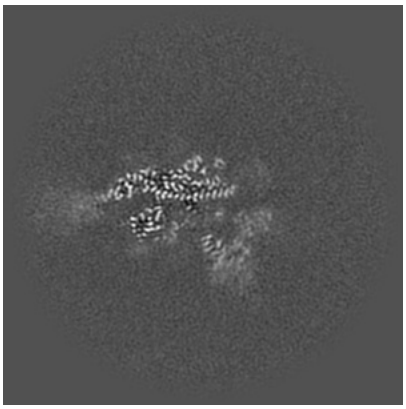
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

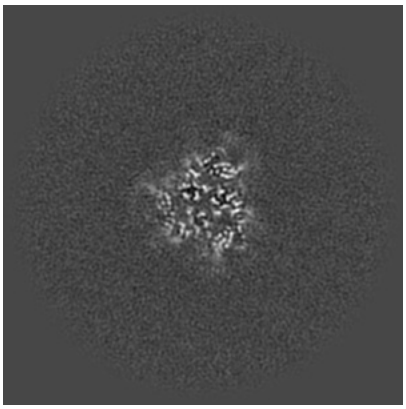
6.2.1 Primary map



X Index: 140



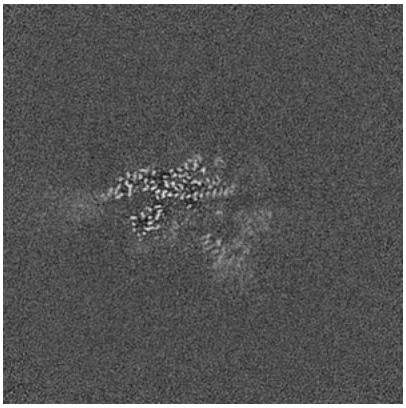
Y Index: 140



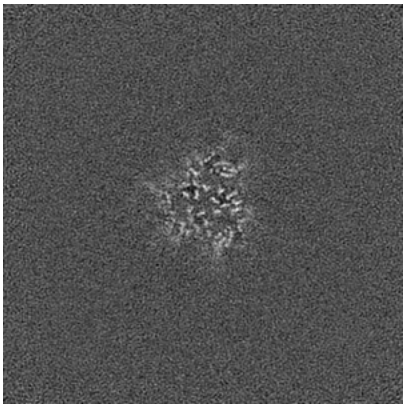
Z Index: 140

6.2.2 Raw map

X Index: 140



Y Index: 140

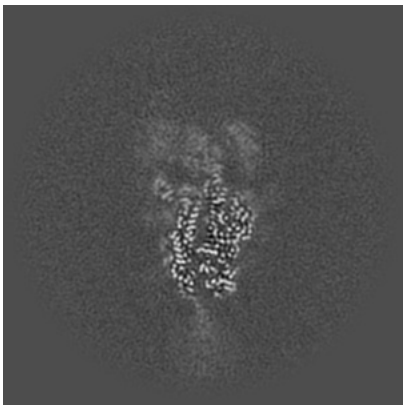


Z Index: 140

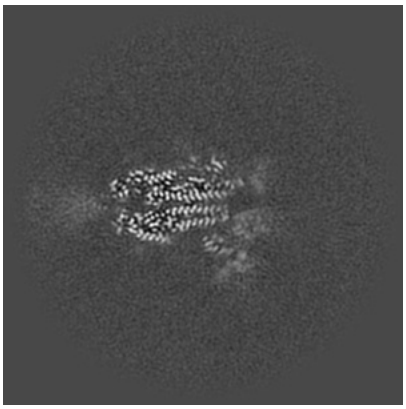
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

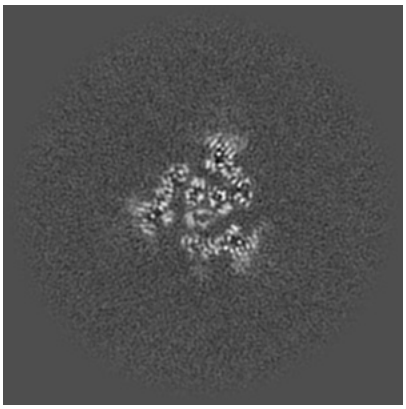
6.3.1 Primary map



X Index: 132

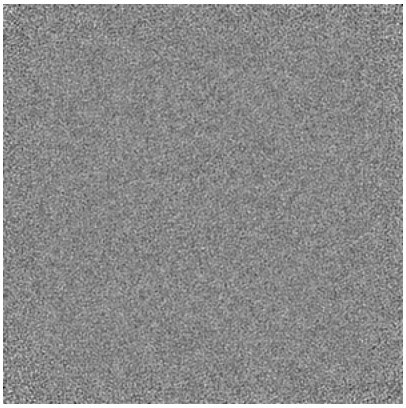


Y Index: 143

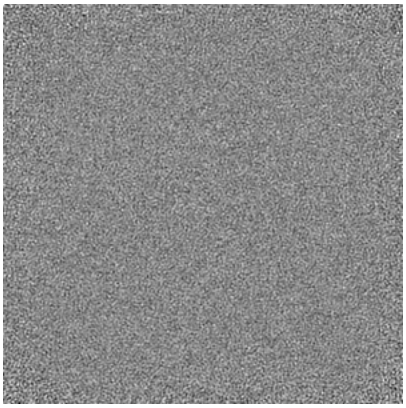


Z Index: 151

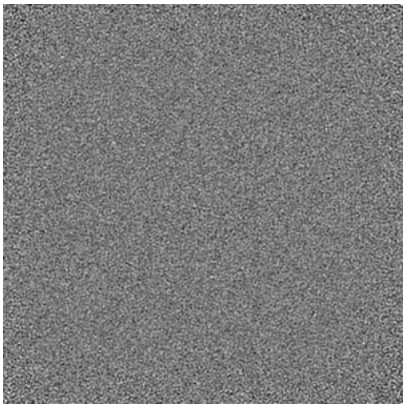
6.3.2 Raw map



X Index: 0



Y Index: 0

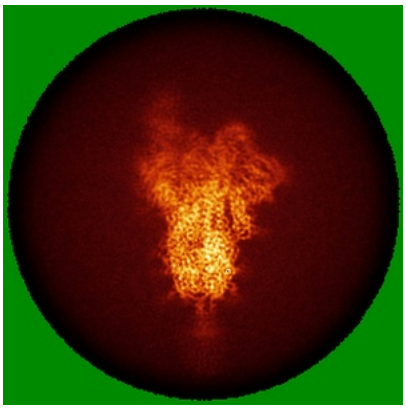


Z Index: 0

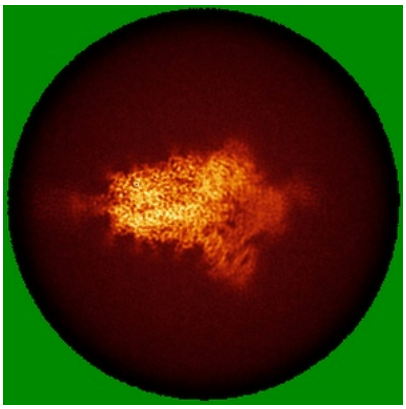
The images above show the largest variance slices of the map in three orthogonal directions.

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

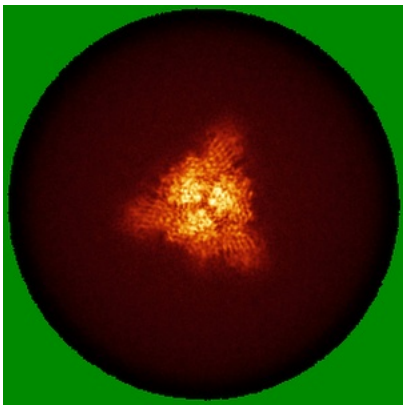
6.4.1 Primary map



X

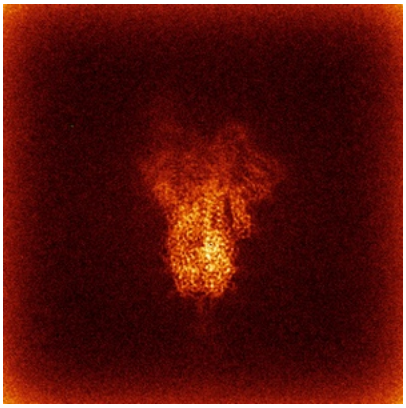


Y

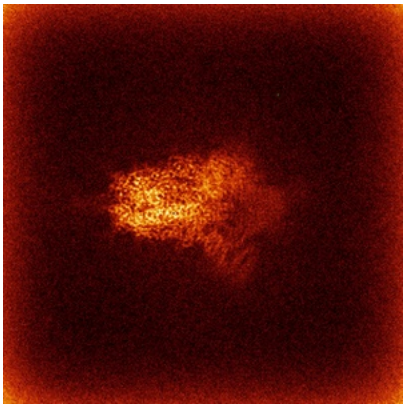


Z

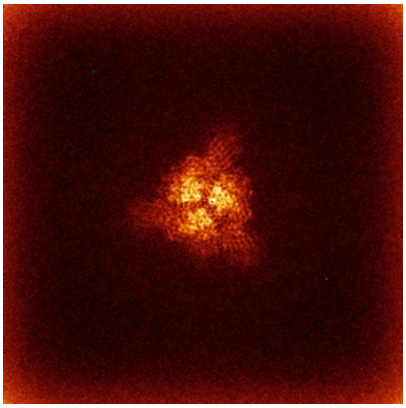
6.4.2 Raw map



X



Y

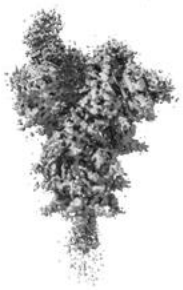


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X

Y

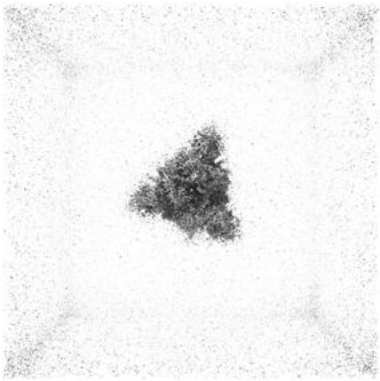
Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

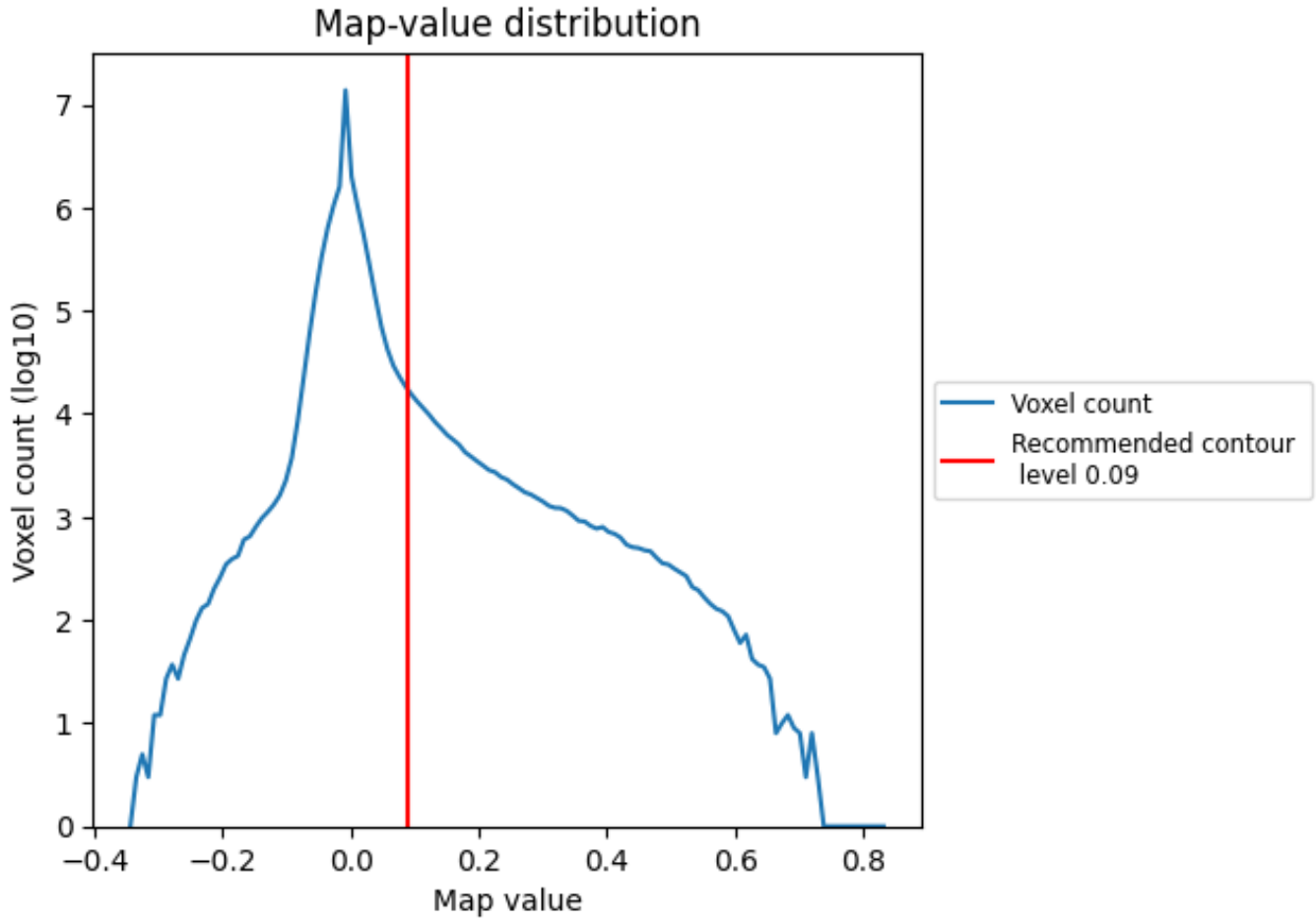
6.6 Mask visualisation (i)

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

7 Map analysis

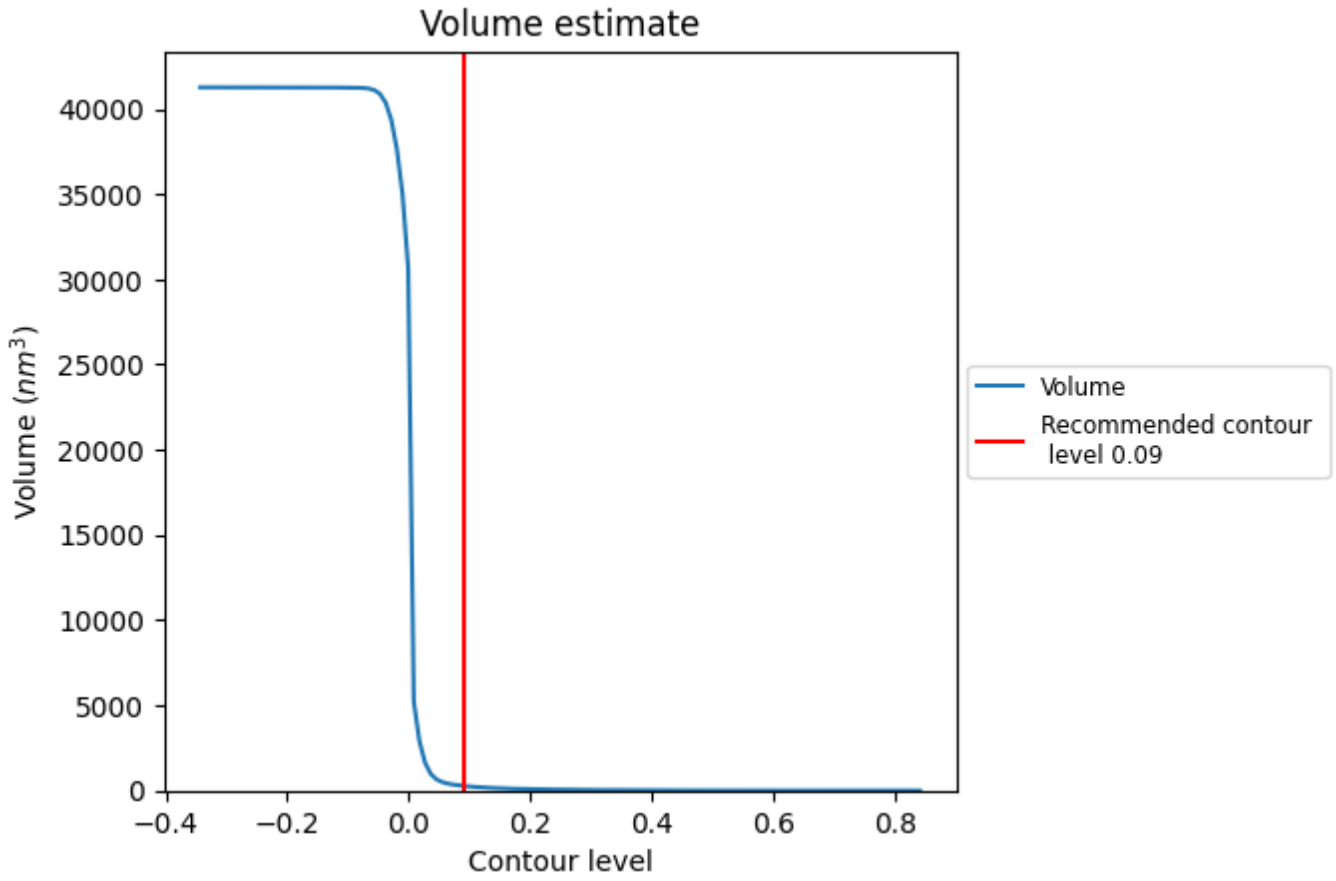
This section contains the results of statistical analysis of the map.

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.

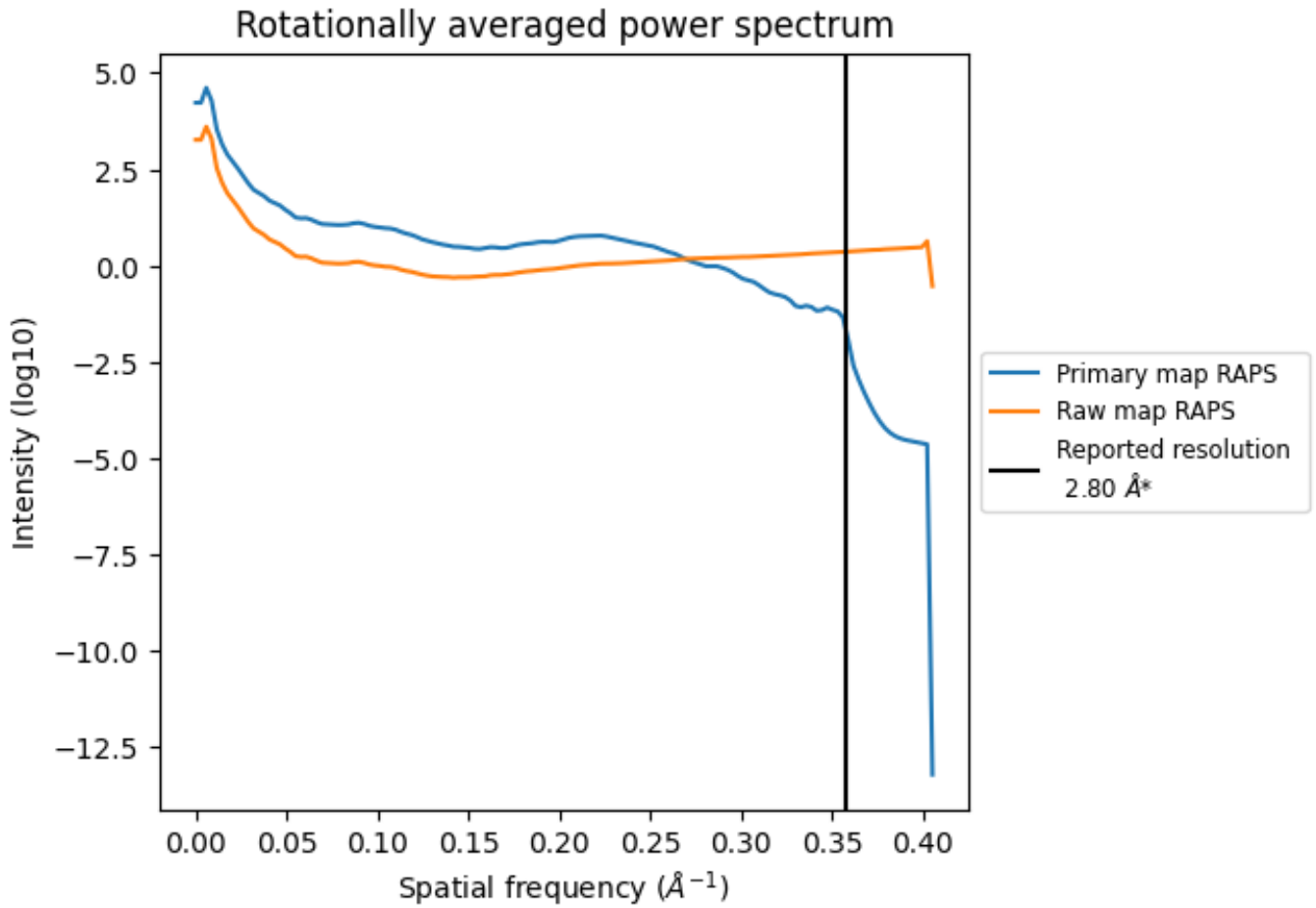
7.2 Volume estimate



The volume at the recommended contour level is 273 nm^3; this corresponds to an approximate mass of 246 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)

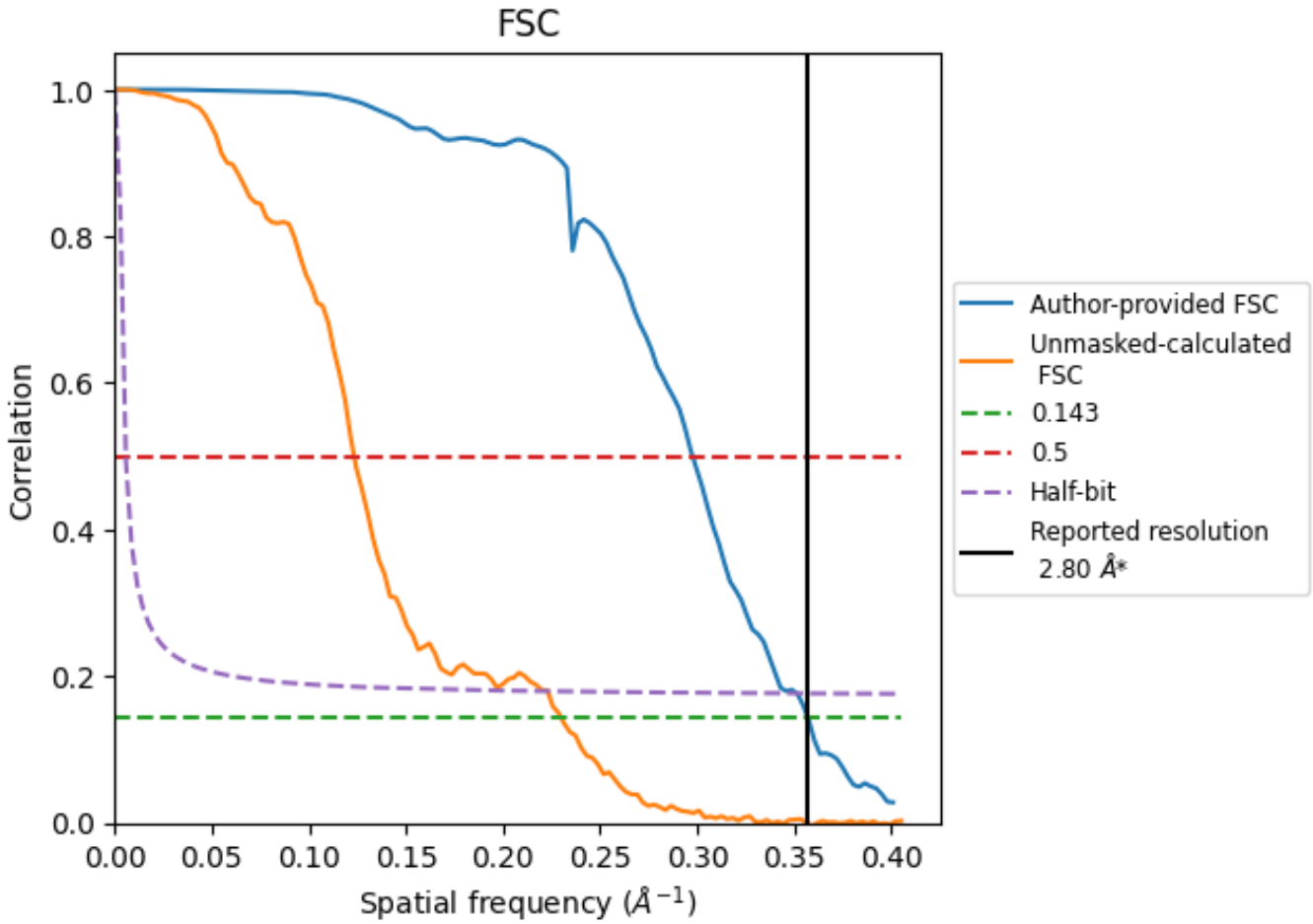


*Reported resolution corresponds to spatial frequency of 0.357 $Å^{-1}$

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

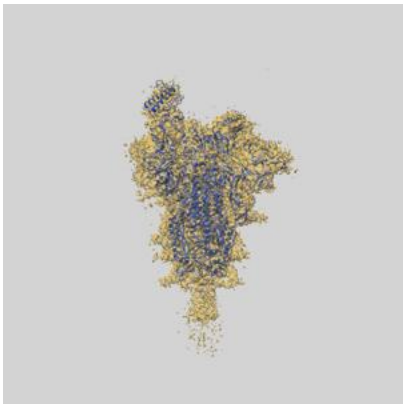
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.36	2.85
Unmasked-calculated*	4.35	8.11	4.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 2.8 by more than 10 %

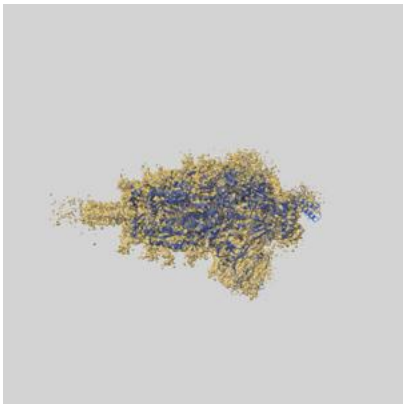
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14922 and PDB model 7ZRV. Per-residue inclusion information can be found in section 3 on page 16.

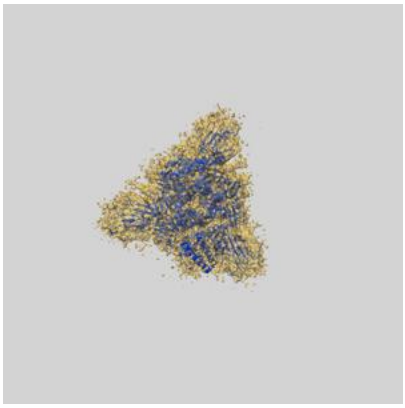
9.1 Map-model overlay



X



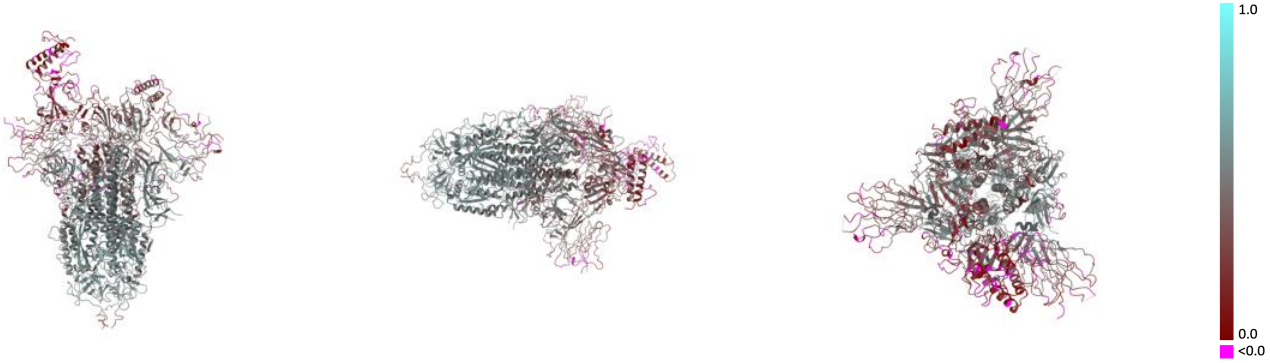
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

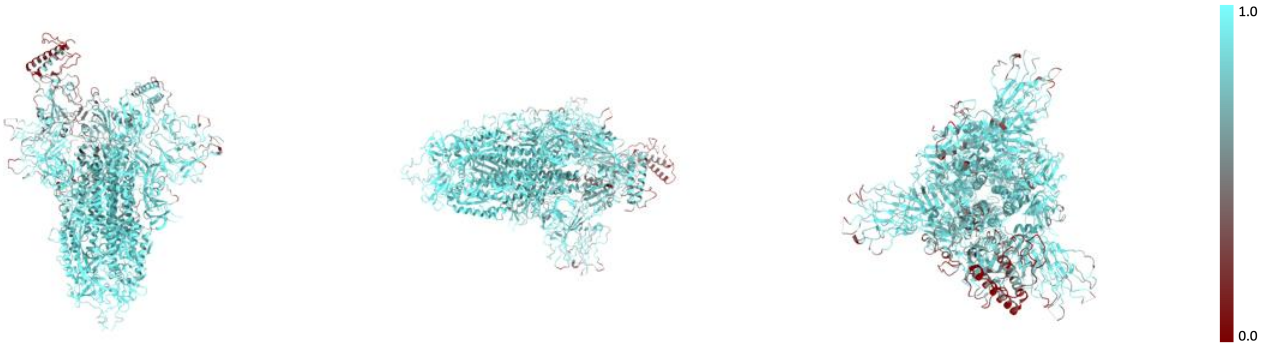
9.2 Q-score mapped to coordinate model (i)



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.

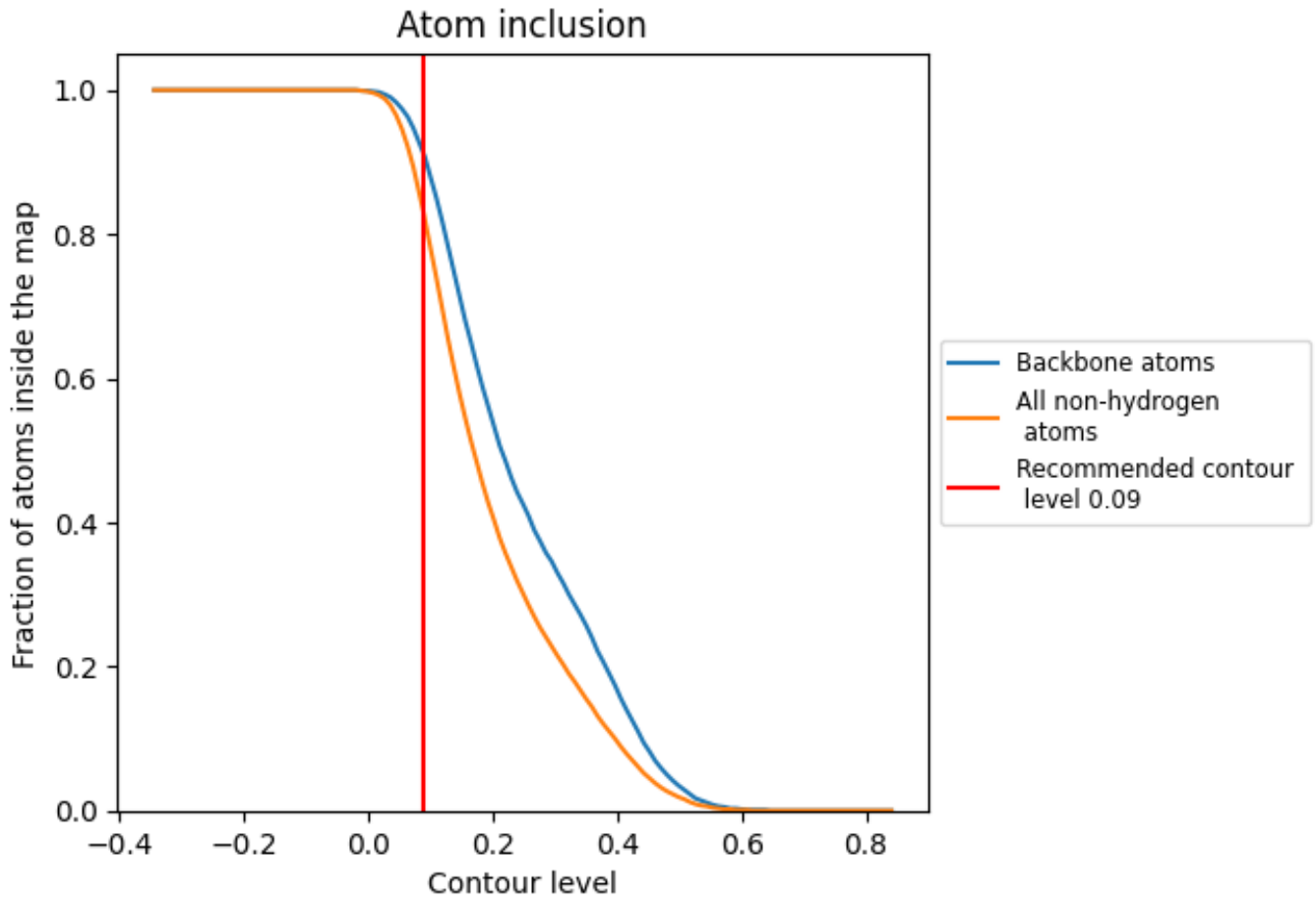
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 83% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8270	0.4000
A	0.8510	0.4200
B	0.8700	0.4270
C	0.8160	0.3850
D	0.6070	0.2560
E	0.2020	0.1360
F	0.6530	0.2090
G	0.5640	0.3160
H	0.7500	0.4410
I	0.8460	0.3950
J	0.8720	0.4730
K	0.9490	0.4510
L	0.8930	0.3670
M	0.7500	0.3060
N	0.6150	0.0730
O	0.8570	0.3930
P	0.5710	0.2530
Q	0.7950	0.4250
R	0.9490	0.4500
S	0.7180	0.3330
T	0.8970	0.4210
U	0.6430	0.2650
V	0.6790	0.2670
W	0.6430	0.1740
X	0.6790	0.2730
Y	0.2500	0.1250
Z	0.7140	0.3940
a	0.8460	0.4090
b	1.0000	0.4810
c	0.8720	0.4500
d	0.8570	0.3830
e	0.6790	0.4100
f	0.8570	0.4210
g	0.4640	0.3230
h	0.6070	0.3170
i	0.3210	0.1610