Full wwPDB EM Validation Report ⓘ

Oct 26, 2024 – 05:34 PM EDT

PDB ID	:	6NZK
EMDB ID	:	EMD-0557
Title	:	Structural basis for human coronavirus attachment to sialic acid receptors
Authors	:	Tortorici, M.A.; Walls, A.C.; Lang, Y.; Wang, C.; Li, Z.; Koerhuis, D.; Boons, G.J.; Bosch, B.J.; Rey, F.A.; de Groot, R.; Veesler, D.
Deposited on	:	2019-02-13
Resolution	:	2.80 Å(reported)

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:

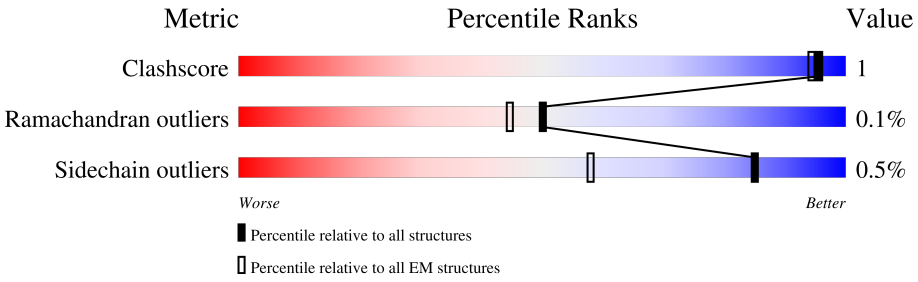
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1322	6% 81% 7% 11%
1	B	1322	6% 82% 7% 11%
1	C	1322	6% 82% 7% 11%
2	D	3	100% 33% 67%
2	E	3	67% 33% 67%
2	G	3	67% 33% 67%
2	H	3	100% 33% 33% 33%
2	M	3	100% 33% 67%

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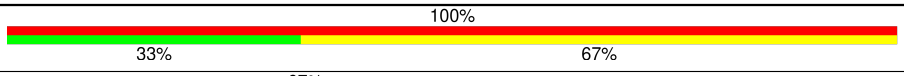
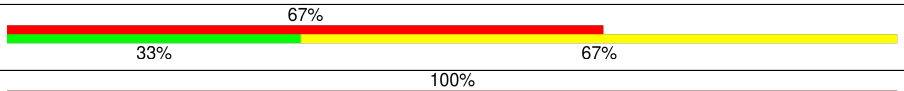
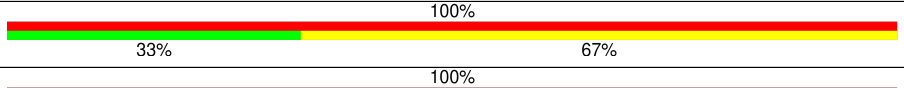
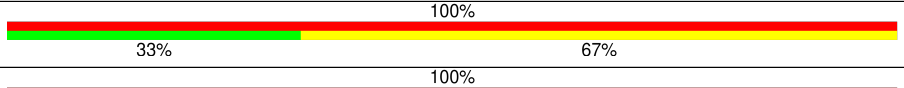
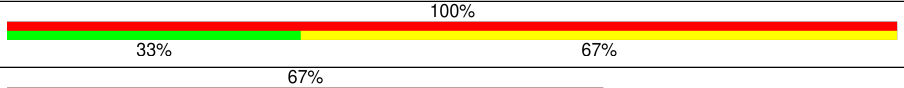
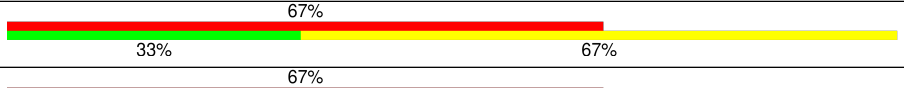
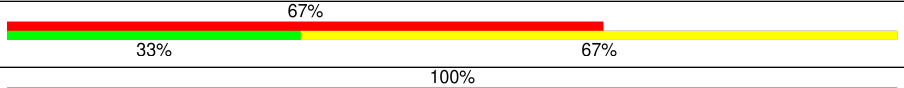
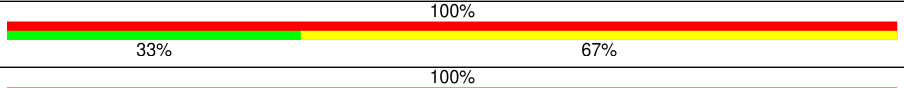
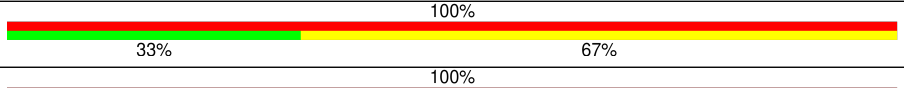
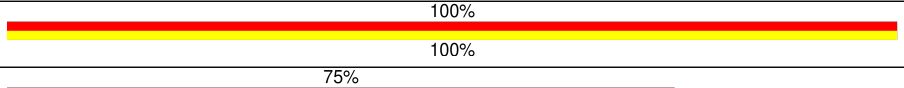
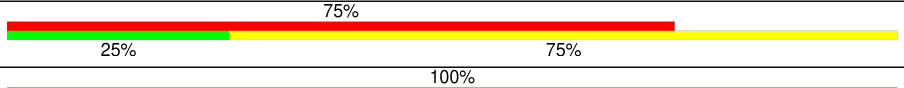
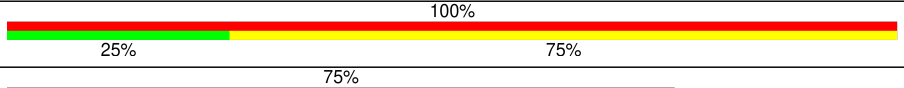
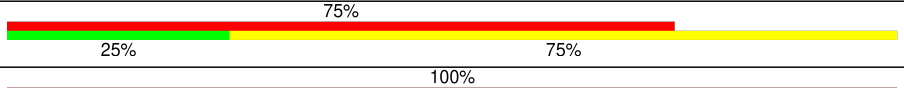
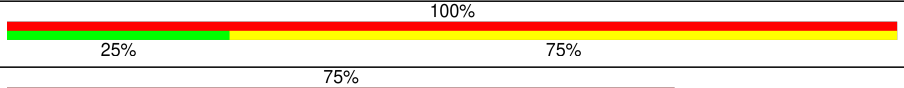
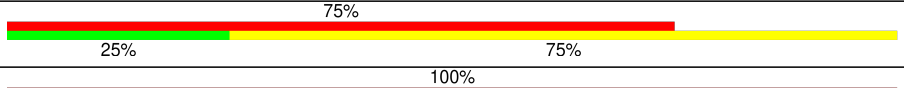
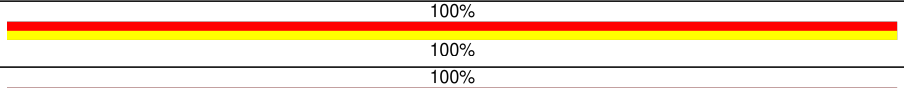
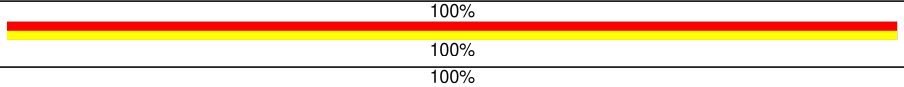
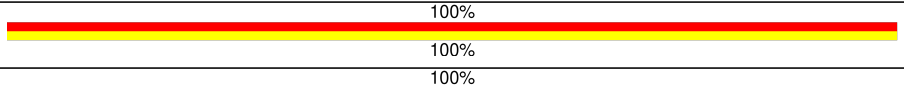
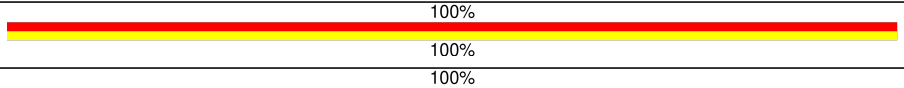
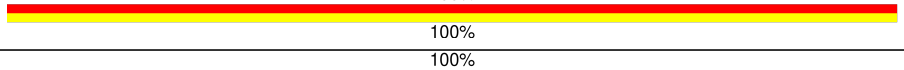
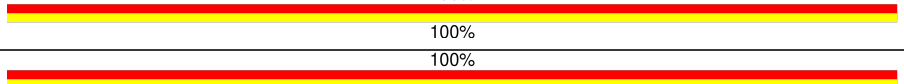
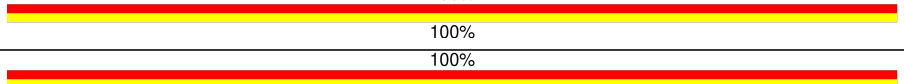
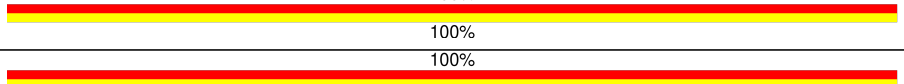
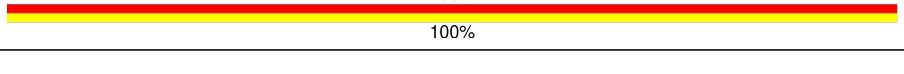
Mol	Chain	Length	Quality of chain
2	N	3	
2	O	3	
2	Q	3	
2	R	3	
2	W	3	
2	X	3	
2	Y	3	
2	a	3	
2	b	3	
2	g	3	
3	F	4	
3	J	4	
3	P	4	
3	T	4	
3	Z	4	
3	d	4	
4	I	2	
4	K	2	
4	L	2	
4	S	2	
4	U	2	
4	V	2	
4	c	2	
4	e	2	
4	f	2	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 29268 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 surface glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1175	Total	C	N	O	S	0	0
			9150	5832	1506	1751	61		
1	B	1175	Total	C	N	O	S	0	0
			9150	5832	1506	1751	61		
1	C	1175	Total	C	N	O	S	0	0
			9150	5832	1506	1751	61		

There are 225 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP Q696P8
A	-8	PRO	-	expression tag	UNP Q696P8
A	-7	MET	-	expression tag	UNP Q696P8
A	-6	GLY	-	expression tag	UNP Q696P8
A	-5	SER	-	expression tag	UNP Q696P8
A	-4	LEU	-	expression tag	UNP Q696P8
A	-3	GLN	-	expression tag	UNP Q696P8
A	-2	PRO	-	expression tag	UNP Q696P8
A	-1	LEU	-	expression tag	UNP Q696P8
A	0	ALA	-	expression tag	UNP Q696P8
A	1	THR	-	expression tag	UNP Q696P8
A	2	LEU	-	expression tag	UNP Q696P8
A	3	TYR	-	expression tag	UNP Q696P8
A	4	LEU	-	expression tag	UNP Q696P8
A	5	LEU	-	expression tag	UNP Q696P8
A	6	GLY	-	expression tag	UNP Q696P8
A	7	MET	-	expression tag	UNP Q696P8
A	8	LEU	-	expression tag	UNP Q696P8
A	9	VAL	-	expression tag	UNP Q696P8
A	10	ALA	-	expression tag	UNP Q696P8
A	11	SER	-	expression tag	UNP Q696P8
A	12	VAL	-	expression tag	UNP Q696P8
A	13	LEU	-	expression tag	UNP Q696P8
A	764	GLY	ARG	engineered mutation	UNP Q696P8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	765	GLY	ARG	engineered mutation	UNP Q696P8
A	767	GLY	ARG	engineered mutation	UNP Q696P8
A	1274	LEU	-	expression tag	UNP Q696P8
A	1275	ILE	-	expression tag	UNP Q696P8
A	1276	LYS	-	expression tag	UNP Q696P8
A	1277	ARG	-	expression tag	UNP Q696P8
A	1278	MET	-	expression tag	UNP Q696P8
A	1279	LYS	-	expression tag	UNP Q696P8
A	1280	GLN	-	expression tag	UNP Q696P8
A	1281	ILE	-	expression tag	UNP Q696P8
A	1282	GLU	-	expression tag	UNP Q696P8
A	1283	ASP	-	expression tag	UNP Q696P8
A	1284	LYS	-	expression tag	UNP Q696P8
A	1285	ILE	-	expression tag	UNP Q696P8
A	1286	GLU	-	expression tag	UNP Q696P8
A	1287	GLU	-	expression tag	UNP Q696P8
A	1288	ILE	-	expression tag	UNP Q696P8
A	1289	GLU	-	expression tag	UNP Q696P8
A	1290	SER	-	expression tag	UNP Q696P8
A	1291	LYS	-	expression tag	UNP Q696P8
A	1292	GLN	-	expression tag	UNP Q696P8
A	1293	LYS	-	expression tag	UNP Q696P8
A	1294	LYS	-	expression tag	UNP Q696P8
A	1295	ILE	-	expression tag	UNP Q696P8
A	1296	GLU	-	expression tag	UNP Q696P8
A	1297	ASN	-	expression tag	UNP Q696P8
A	1298	GLU	-	expression tag	UNP Q696P8
A	1299	ILE	-	expression tag	UNP Q696P8
A	1300	ALA	-	expression tag	UNP Q696P8
A	1301	ARG	-	expression tag	UNP Q696P8
A	1302	ILE	-	expression tag	UNP Q696P8
A	1303	LYS	-	expression tag	UNP Q696P8
A	1304	LYS	-	expression tag	UNP Q696P8
A	1305	ILE	-	expression tag	UNP Q696P8
A	1306	LYS	-	expression tag	UNP Q696P8
A	1307	LEU	-	expression tag	UNP Q696P8
A	1308	VAL	-	expression tag	UNP Q696P8
A	1309	PRO	-	expression tag	UNP Q696P8
A	1310	ARG	-	expression tag	UNP Q696P8
A	1311	GLY	-	expression tag	UNP Q696P8
A	1312	SER	-	expression tag	UNP Q696P8
A	1313	LEU	-	expression tag	UNP Q696P8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1314	GLU	-	expression tag	UNP Q696P8
A	1315	TRP	-	expression tag	UNP Q696P8
A	1316	SER	-	expression tag	UNP Q696P8
A	1317	HIS	-	expression tag	UNP Q696P8
A	1318	PRO	-	expression tag	UNP Q696P8
A	1319	GLN	-	expression tag	UNP Q696P8
A	1320	PHE	-	expression tag	UNP Q696P8
A	1321	GLU	-	expression tag	UNP Q696P8
A	1322	LYS	-	expression tag	UNP Q696P8
B	-9	MET	-	initiating methionine	UNP Q696P8
B	-8	PRO	-	expression tag	UNP Q696P8
B	-7	MET	-	expression tag	UNP Q696P8
B	-6	GLY	-	expression tag	UNP Q696P8
B	-5	SER	-	expression tag	UNP Q696P8
B	-4	LEU	-	expression tag	UNP Q696P8
B	-3	GLN	-	expression tag	UNP Q696P8
B	-2	PRO	-	expression tag	UNP Q696P8
B	-1	LEU	-	expression tag	UNP Q696P8
B	0	ALA	-	expression tag	UNP Q696P8
B	1	THR	-	expression tag	UNP Q696P8
B	2	LEU	-	expression tag	UNP Q696P8
B	3	TYR	-	expression tag	UNP Q696P8
B	4	LEU	-	expression tag	UNP Q696P8
B	5	LEU	-	expression tag	UNP Q696P8
B	6	GLY	-	expression tag	UNP Q696P8
B	7	MET	-	expression tag	UNP Q696P8
B	8	LEU	-	expression tag	UNP Q696P8
B	9	VAL	-	expression tag	UNP Q696P8
B	10	ALA	-	expression tag	UNP Q696P8
B	11	SER	-	expression tag	UNP Q696P8
B	12	VAL	-	expression tag	UNP Q696P8
B	13	LEU	-	expression tag	UNP Q696P8
B	764	GLY	ARG	engineered mutation	UNP Q696P8
B	765	GLY	ARG	engineered mutation	UNP Q696P8
B	767	GLY	ARG	engineered mutation	UNP Q696P8
B	1274	LEU	-	expression tag	UNP Q696P8
B	1275	ILE	-	expression tag	UNP Q696P8
B	1276	LYS	-	expression tag	UNP Q696P8
B	1277	ARG	-	expression tag	UNP Q696P8
B	1278	MET	-	expression tag	UNP Q696P8
B	1279	LYS	-	expression tag	UNP Q696P8
B	1280	GLN	-	expression tag	UNP Q696P8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1281	ILE	-	expression tag	UNP Q696P8
B	1282	GLU	-	expression tag	UNP Q696P8
B	1283	ASP	-	expression tag	UNP Q696P8
B	1284	LYS	-	expression tag	UNP Q696P8
B	1285	ILE	-	expression tag	UNP Q696P8
B	1286	GLU	-	expression tag	UNP Q696P8
B	1287	GLU	-	expression tag	UNP Q696P8
B	1288	ILE	-	expression tag	UNP Q696P8
B	1289	GLU	-	expression tag	UNP Q696P8
B	1290	SER	-	expression tag	UNP Q696P8
B	1291	LYS	-	expression tag	UNP Q696P8
B	1292	GLN	-	expression tag	UNP Q696P8
B	1293	LYS	-	expression tag	UNP Q696P8
B	1294	LYS	-	expression tag	UNP Q696P8
B	1295	ILE	-	expression tag	UNP Q696P8
B	1296	GLU	-	expression tag	UNP Q696P8
B	1297	ASN	-	expression tag	UNP Q696P8
B	1298	GLU	-	expression tag	UNP Q696P8
B	1299	ILE	-	expression tag	UNP Q696P8
B	1300	ALA	-	expression tag	UNP Q696P8
B	1301	ARG	-	expression tag	UNP Q696P8
B	1302	ILE	-	expression tag	UNP Q696P8
B	1303	LYS	-	expression tag	UNP Q696P8
B	1304	LYS	-	expression tag	UNP Q696P8
B	1305	ILE	-	expression tag	UNP Q696P8
B	1306	LYS	-	expression tag	UNP Q696P8
B	1307	LEU	-	expression tag	UNP Q696P8
B	1308	VAL	-	expression tag	UNP Q696P8
B	1309	PRO	-	expression tag	UNP Q696P8
B	1310	ARG	-	expression tag	UNP Q696P8
B	1311	GLY	-	expression tag	UNP Q696P8
B	1312	SER	-	expression tag	UNP Q696P8
B	1313	LEU	-	expression tag	UNP Q696P8
B	1314	GLU	-	expression tag	UNP Q696P8
B	1315	TRP	-	expression tag	UNP Q696P8
B	1316	SER	-	expression tag	UNP Q696P8
B	1317	HIS	-	expression tag	UNP Q696P8
B	1318	PRO	-	expression tag	UNP Q696P8
B	1319	GLN	-	expression tag	UNP Q696P8
B	1320	PHE	-	expression tag	UNP Q696P8
B	1321	GLU	-	expression tag	UNP Q696P8
B	1322	LYS	-	expression tag	UNP Q696P8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	MET	-	initiating methionine	UNP Q696P8
C	-8	PRO	-	expression tag	UNP Q696P8
C	-7	MET	-	expression tag	UNP Q696P8
C	-6	GLY	-	expression tag	UNP Q696P8
C	-5	SER	-	expression tag	UNP Q696P8
C	-4	LEU	-	expression tag	UNP Q696P8
C	-3	GLN	-	expression tag	UNP Q696P8
C	-2	PRO	-	expression tag	UNP Q696P8
C	-1	LEU	-	expression tag	UNP Q696P8
C	0	ALA	-	expression tag	UNP Q696P8
C	1	THR	-	expression tag	UNP Q696P8
C	2	LEU	-	expression tag	UNP Q696P8
C	3	TYR	-	expression tag	UNP Q696P8
C	4	LEU	-	expression tag	UNP Q696P8
C	5	LEU	-	expression tag	UNP Q696P8
C	6	GLY	-	expression tag	UNP Q696P8
C	7	MET	-	expression tag	UNP Q696P8
C	8	LEU	-	expression tag	UNP Q696P8
C	9	VAL	-	expression tag	UNP Q696P8
C	10	ALA	-	expression tag	UNP Q696P8
C	11	SER	-	expression tag	UNP Q696P8
C	12	VAL	-	expression tag	UNP Q696P8
C	13	LEU	-	expression tag	UNP Q696P8
C	764	GLY	ARG	engineered mutation	UNP Q696P8
C	765	GLY	ARG	engineered mutation	UNP Q696P8
C	767	GLY	ARG	engineered mutation	UNP Q696P8
C	1274	LEU	-	expression tag	UNP Q696P8
C	1275	ILE	-	expression tag	UNP Q696P8
C	1276	LYS	-	expression tag	UNP Q696P8
C	1277	ARG	-	expression tag	UNP Q696P8
C	1278	MET	-	expression tag	UNP Q696P8
C	1279	LYS	-	expression tag	UNP Q696P8
C	1280	GLN	-	expression tag	UNP Q696P8
C	1281	ILE	-	expression tag	UNP Q696P8
C	1282	GLU	-	expression tag	UNP Q696P8
C	1283	ASP	-	expression tag	UNP Q696P8
C	1284	LYS	-	expression tag	UNP Q696P8
C	1285	ILE	-	expression tag	UNP Q696P8
C	1286	GLU	-	expression tag	UNP Q696P8
C	1287	GLU	-	expression tag	UNP Q696P8
C	1288	ILE	-	expression tag	UNP Q696P8
C	1289	GLU	-	expression tag	UNP Q696P8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1290	SER	-	expression tag	UNP Q696P8
C	1291	LYS	-	expression tag	UNP Q696P8
C	1292	GLN	-	expression tag	UNP Q696P8
C	1293	LYS	-	expression tag	UNP Q696P8
C	1294	LYS	-	expression tag	UNP Q696P8
C	1295	ILE	-	expression tag	UNP Q696P8
C	1296	GLU	-	expression tag	UNP Q696P8
C	1297	ASN	-	expression tag	UNP Q696P8
C	1298	GLU	-	expression tag	UNP Q696P8
C	1299	ILE	-	expression tag	UNP Q696P8
C	1300	ALA	-	expression tag	UNP Q696P8
C	1301	ARG	-	expression tag	UNP Q696P8
C	1302	ILE	-	expression tag	UNP Q696P8
C	1303	LYS	-	expression tag	UNP Q696P8
C	1304	LYS	-	expression tag	UNP Q696P8
C	1305	ILE	-	expression tag	UNP Q696P8
C	1306	LYS	-	expression tag	UNP Q696P8
C	1307	LEU	-	expression tag	UNP Q696P8
C	1308	VAL	-	expression tag	UNP Q696P8
C	1309	PRO	-	expression tag	UNP Q696P8
C	1310	ARG	-	expression tag	UNP Q696P8
C	1311	GLY	-	expression tag	UNP Q696P8
C	1312	SER	-	expression tag	UNP Q696P8
C	1313	LEU	-	expression tag	UNP Q696P8
C	1314	GLU	-	expression tag	UNP Q696P8
C	1315	TRP	-	expression tag	UNP Q696P8
C	1316	SER	-	expression tag	UNP Q696P8
C	1317	HIS	-	expression tag	UNP Q696P8
C	1318	PRO	-	expression tag	UNP Q696P8
C	1319	GLN	-	expression tag	UNP Q696P8
C	1320	PHE	-	expression tag	UNP Q696P8
C	1321	GLU	-	expression tag	UNP Q696P8
C	1322	LYS	-	expression tag	UNP Q696P8

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	E	3	Total	C	N	O	0	0
			39	22	2	15		
2	G	3	Total	C	N	O	0	0
			39	22	2	15		
2	H	3	Total	C	N	O	0	0
			39	22	2	15		
2	M	3	Total	C	N	O	0	0
			39	22	2	15		
2	N	3	Total	C	N	O	0	0
			39	22	2	15		
2	O	3	Total	C	N	O	0	0
			39	22	2	15		
2	Q	3	Total	C	N	O	0	0
			39	22	2	15		
2	R	3	Total	C	N	O	0	0
			39	22	2	15		
2	W	3	Total	C	N	O	0	0
			39	22	2	15		
2	X	3	Total	C	N	O	0	0
			39	22	2	15		
2	Y	3	Total	C	N	O	0	0
			39	22	2	15		
2	a	3	Total	C	N	O	0	0
			39	22	2	15		
2	b	3	Total	C	N	O	0	0
			39	22	2	15		
2	g	3	Total	C	N	O	0	0
			39	22	2	15		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	4	Total	C	N	O	0	0
			50	28	2	20		
3	J	4	Total	C	N	O	0	0
			50	28	2	20		

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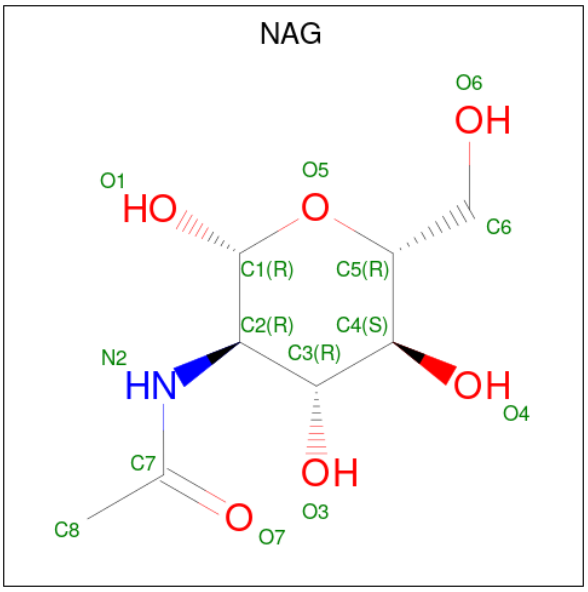
Mol	Chain	Residues	Atoms				AltConf	Trace
3	P	4	Total 50	C 28	N 2	O 20	0	0
3	T	4	Total 50	C 28	N 2	O 20	0	0
3	Z	4	Total 50	C 28	N 2	O 20	0	0
3	d	4	Total 50	C 28	N 2	O 20	0	0

- Molecule 4 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
4	I	2	Total 28	C 16	N 2	O 10	0	0
4	K	2	Total 28	C 16	N 2	O 10	0	0
4	L	2	Total 28	C 16	N 2	O 10	0	0
4	S	2	Total 28	C 16	N 2	O 10	0	0
4	U	2	Total 28	C 16	N 2	O 10	0	0
4	V	2	Total 28	C 16	N 2	O 10	0	0
4	c	2	Total 28	C 16	N 2	O 10	0	0
4	e	2	Total 28	C 16	N 2	O 10	0	0
4	f	2	Total 28	C 16	N 2	O 10	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	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
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	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	

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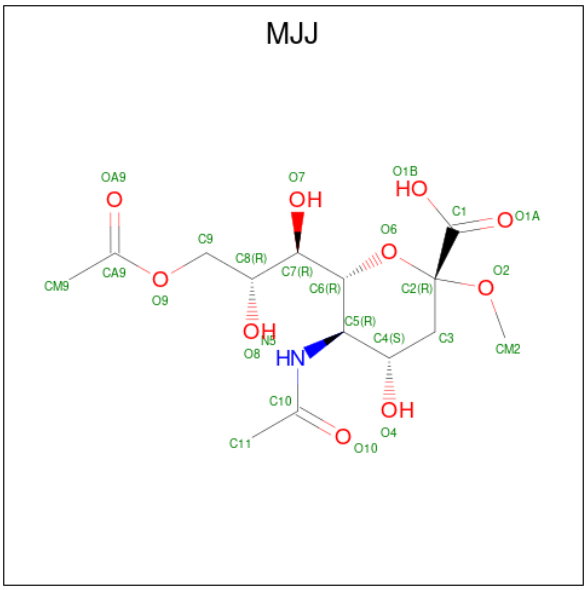
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is methyl 9-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosidonic acid (three-letter code: MJJ) (formula: $C_{14}H_{23}NO_{10}$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			25	14	1	10	
6	B	1	Total	C	N	O	0
			25	14	1	10	
6	C	1	Total	C	N	O	0
			25	14	1	10	

- Molecule 7 is water.

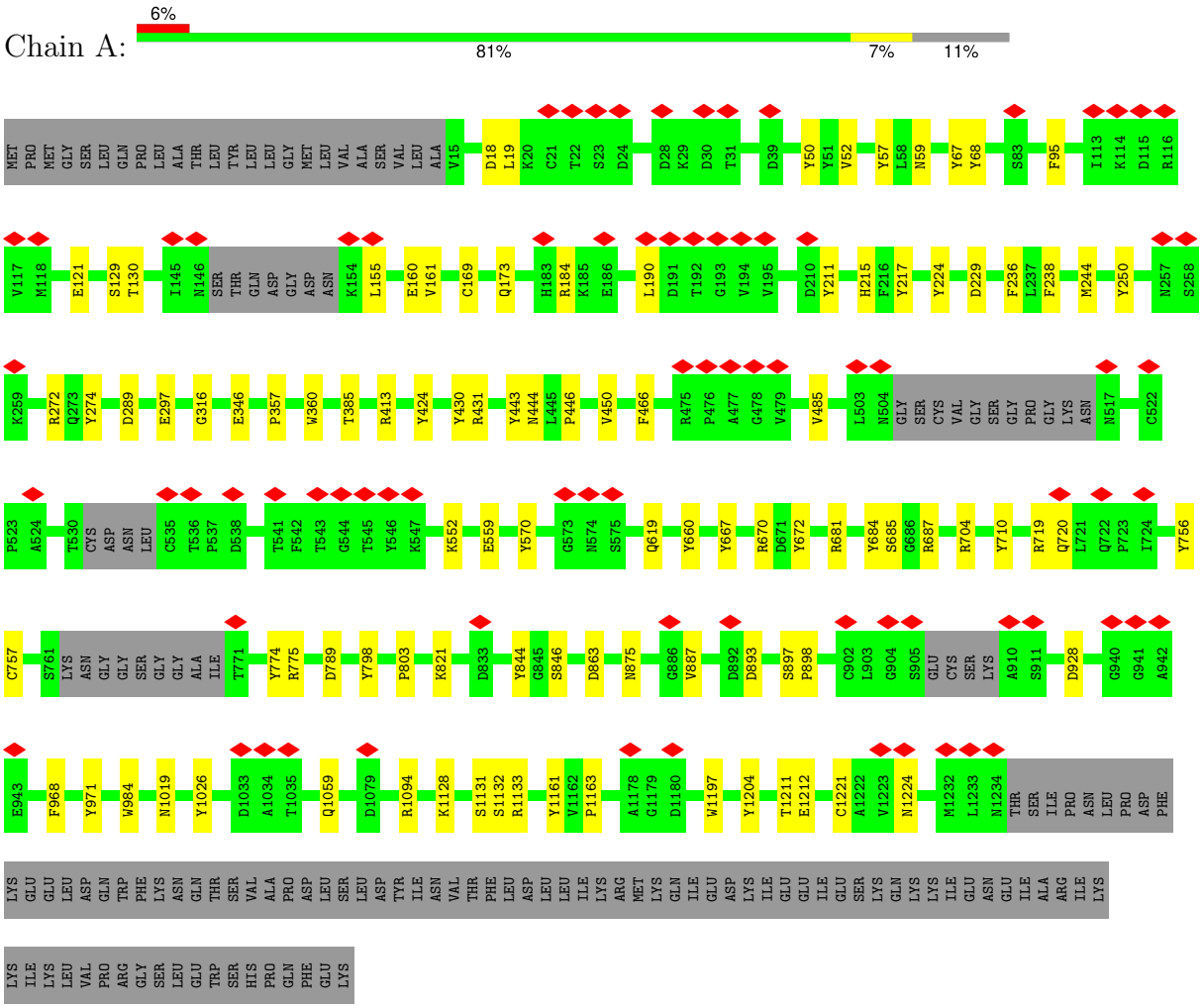
Mol	Chain	Residues	Atoms		AltConf
7	A	132	Total	O	0
			132	132	
7	B	132	Total	O	0
			132	132	
7	C	132	Total	O	0
			132	132	

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.

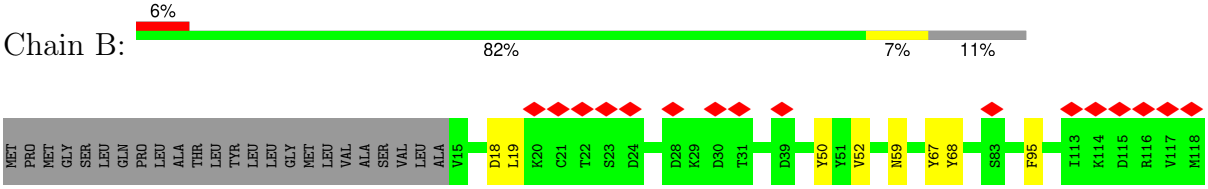
• Molecule 1: Spike surface glycoprotein

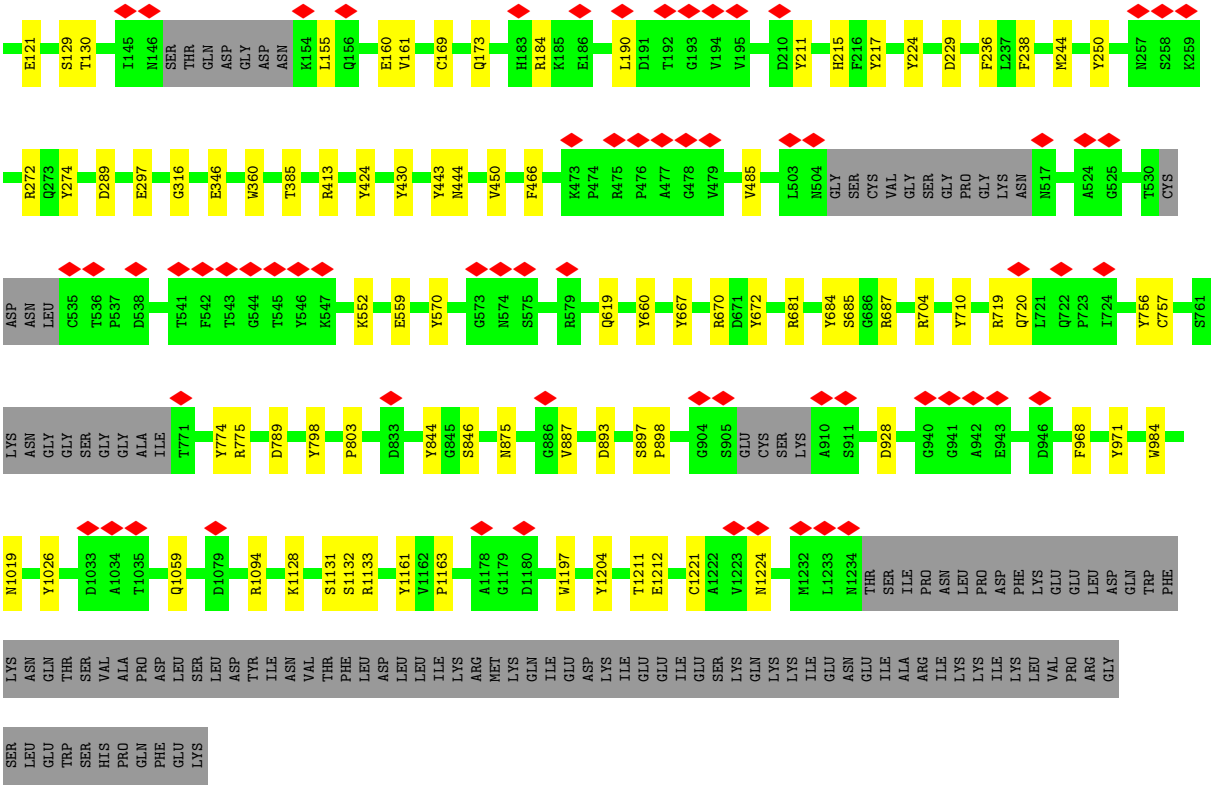
Chain A:



• Molecule 1: Spike surface glycoprotein

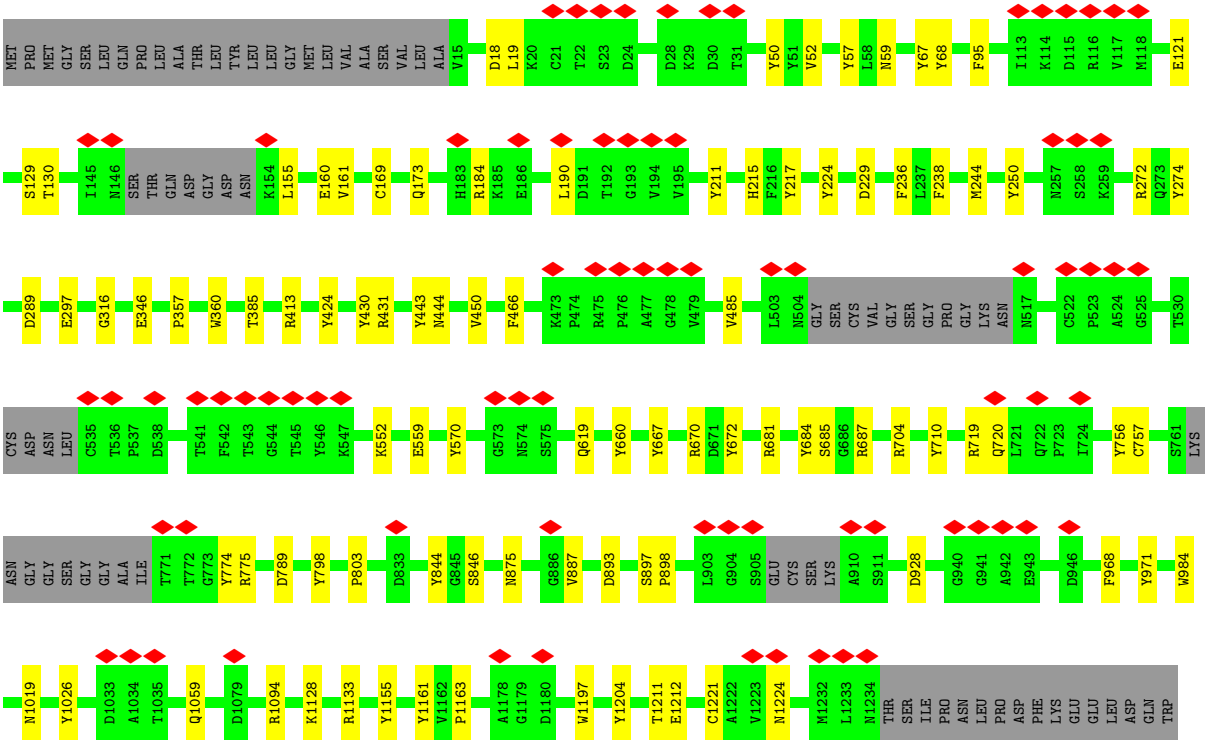
Chain B:





• Molecule 1: Spike surface glycoprotein

Chain C:



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

GLY SER LEU GLU TRP SER HIS PRO GLN PHE GLU LYS

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

Chain D:

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

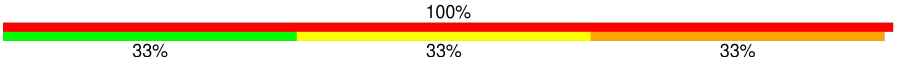
Chain E:

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

Chain G:

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

Chain H:



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

Chain M:

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

Chain N:

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

Chain O:

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

Chain Q:

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

Chain R:

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

Chain W:

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

Chain X:

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

Chain Y:

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

Chain a:

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

Chain b:

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

Chain g:

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

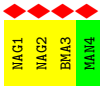
Chain F:

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

Chain J:

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

Chain P:

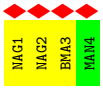


• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

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

Chain Z:



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

Chain d:

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

Chain I:

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

Chain K:

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

Chain L:

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

Chain S:

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

Chain U:

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

Chain V:

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

Chain c:

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

Chain e:

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

Chain f:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	178356	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.030	Depositor
Minimum map value	-4.580	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	1	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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, MJJ, MAN, 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	1.36	51/9359 (0.5%)	0.96	31/12744 (0.2%)
1	B	1.36	52/9359 (0.6%)	0.96	29/12744 (0.2%)
1	C	1.36	52/9359 (0.6%)	0.96	31/12744 (0.2%)
All	All	1.36	155/28077 (0.6%)	0.96	91/38232 (0.2%)

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	757	CYS	CB-SG	-9.05	1.66	1.82
1	B	757	CYS	CB-SG	-9.05	1.66	1.82
1	C	757	CYS	CB-SG	-9.03	1.66	1.82
1	C	169	CYS	CB-SG	-8.30	1.68	1.82
1	B	169	CYS	CB-SG	-8.30	1.68	1.82
1	A	169	CYS	CB-SG	-8.28	1.68	1.82
1	A	485	VAL	CB-CG1	-7.42	1.37	1.52
1	C	485	VAL	CB-CG1	-7.41	1.37	1.52
1	B	485	VAL	CB-CG1	-7.41	1.37	1.52
1	B	444	ASN	CB-CG	-6.84	1.35	1.51
1	C	444	ASN	CB-CG	-6.84	1.35	1.51
1	A	444	ASN	CB-CG	-6.83	1.35	1.51
1	A	1161	TYR	CB-CG	-6.66	1.41	1.51
1	B	1161	TYR	CB-CG	-6.66	1.41	1.51
1	C	1161	TYR	CB-CG	-6.66	1.41	1.51
1	B	67	TYR	CB-CG	-6.26	1.42	1.51
1	C	67	TYR	CB-CG	-6.26	1.42	1.51
1	A	67	TYR	CB-CG	-6.25	1.42	1.51
1	B	844	TYR	CB-CG	-6.10	1.42	1.51
1	A	844	TYR	CB-CG	-6.07	1.42	1.51
1	C	844	TYR	CB-CG	-6.07	1.42	1.51
1	B	1128	LYS	CE-NZ	-6.03	1.33	1.49
1	C	160	GLU	CD-OE1	-6.03	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	215	HIS	CB-CG	-6.02	1.39	1.50
1	A	215	HIS	CB-CG	-6.01	1.39	1.50
1	B	215	HIS	CB-CG	-6.01	1.39	1.50
1	C	1161	TYR	CG-CD1	-6.00	1.31	1.39
1	A	1128	LYS	CE-NZ	-6.00	1.34	1.49
1	C	1128	LYS	CE-NZ	-6.00	1.34	1.49
1	A	1161	TYR	CG-CD1	-6.00	1.31	1.39
1	C	756	TYR	CB-CG	-5.99	1.42	1.51
1	A	756	TYR	CB-CG	-5.98	1.42	1.51
1	B	1221	CYS	CB-SG	-5.98	1.72	1.81
1	B	1161	TYR	CG-CD1	-5.97	1.31	1.39
1	A	160	GLU	CD-OE1	-5.97	1.19	1.25
1	A	1221	CYS	CB-SG	-5.96	1.72	1.81
1	C	1221	CYS	CB-SG	-5.92	1.72	1.81
1	B	756	TYR	CB-CG	-5.92	1.42	1.51
1	B	160	GLU	CD-OE1	-5.92	1.19	1.25
1	B	798	TYR	CB-CG	-5.91	1.42	1.51
1	C	798	TYR	CB-CG	-5.91	1.42	1.51
1	B	297	GLU	CD-OE1	-5.90	1.19	1.25
1	A	798	TYR	CB-CG	-5.90	1.42	1.51
1	C	968	PHE	CB-CG	-5.90	1.41	1.51
1	B	968	PHE	CB-CG	-5.90	1.41	1.51
1	A	968	PHE	CB-CG	-5.89	1.41	1.51
1	C	297	GLU	CD-OE1	-5.85	1.19	1.25
1	A	297	GLU	CD-OE1	-5.83	1.19	1.25
1	B	1026	TYR	CB-CG	-5.80	1.43	1.51
1	A	1026	TYR	CB-CG	-5.79	1.43	1.51
1	C	660	TYR	CG-CD2	-5.79	1.31	1.39
1	C	1026	TYR	CB-CG	-5.77	1.43	1.51
1	A	660	TYR	CG-CD2	-5.77	1.31	1.39
1	B	443	TYR	CD2-CE2	-5.77	1.30	1.39
1	B	660	TYR	CG-CD2	-5.76	1.31	1.39
1	A	443	TYR	CD2-CE2	-5.75	1.30	1.39
1	C	443	TYR	CD2-CE2	-5.71	1.30	1.39
1	A	559	GLU	CD-OE1	-5.67	1.19	1.25
1	B	430	TYR	CG-CD1	-5.67	1.31	1.39
1	B	430	TYR	CD2-CE2	-5.66	1.30	1.39
1	B	430	TYR	CE2-CZ	-5.65	1.31	1.38
1	C	430	TYR	CE2-CZ	-5.65	1.31	1.38
1	C	430	TYR	CG-CD1	-5.65	1.31	1.39
1	A	430	TYR	CE2-CZ	-5.64	1.31	1.38
1	A	430	TYR	CG-CD1	-5.64	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	559	GLU	CD-OE1	-5.64	1.19	1.25
1	B	95	PHE	CB-CG	-5.63	1.41	1.51
1	B	485	VAL	CB-CG2	-5.63	1.41	1.52
1	A	430	TYR	CD2-CE2	-5.62	1.30	1.39
1	C	95	PHE	CB-CG	-5.62	1.41	1.51
1	A	95	PHE	CB-CG	-5.61	1.41	1.51
1	A	485	VAL	CB-CG2	-5.60	1.41	1.52
1	C	430	TYR	CD2-CE2	-5.60	1.30	1.39
1	A	774	TYR	CG-CD2	-5.59	1.31	1.39
1	C	485	VAL	CB-CG2	-5.59	1.41	1.52
1	C	774	TYR	CG-CD2	-5.57	1.31	1.39
1	B	559	GLU	CD-OE1	-5.57	1.19	1.25
1	B	984	TRP	CD2-CE2	-5.57	1.34	1.41
1	C	984	TRP	CD2-CE2	-5.56	1.34	1.41
1	B	660	TYR	CE2-CZ	-5.55	1.31	1.38
1	C	660	TYR	CE2-CZ	-5.55	1.31	1.38
1	C	685	SER	CB-OG	-5.54	1.35	1.42
1	A	984	TRP	CD2-CE2	-5.53	1.34	1.41
1	B	774	TYR	CG-CD2	-5.53	1.31	1.39
1	C	250	TYR	CB-CG	-5.52	1.43	1.51
1	A	660	TYR	CE2-CZ	-5.51	1.31	1.38
1	B	685	SER	CB-OG	-5.50	1.35	1.42
1	A	685	SER	CB-OG	-5.50	1.35	1.42
1	A	250	TYR	CB-CG	-5.48	1.43	1.51
1	B	450	VAL	CB-CG2	-5.48	1.41	1.52
1	C	224	TYR	CB-CG	-5.47	1.43	1.51
1	B	250	TYR	CB-CG	-5.45	1.43	1.51
1	A	450	VAL	CB-CG2	-5.45	1.41	1.52
1	B	217	TYR	CB-CG	-5.44	1.43	1.51
1	C	217	TYR	CB-CG	-5.44	1.43	1.51
1	A	217	TYR	CB-CG	-5.43	1.43	1.51
1	A	224	TYR	CB-CG	-5.43	1.43	1.51
1	C	450	VAL	CB-CG2	-5.41	1.41	1.52
1	C	1204	TYR	CB-CG	-5.41	1.43	1.51
1	A	887	VAL	CB-CG1	-5.40	1.41	1.52
1	B	887	VAL	CB-CG1	-5.39	1.41	1.52
1	C	887	VAL	CB-CG1	-5.39	1.41	1.52
1	A	360	TRP	CZ3-CH2	-5.39	1.31	1.40
1	B	224	TYR	CB-CG	-5.39	1.43	1.51
1	A	1204	TYR	CB-CG	-5.38	1.43	1.51
1	B	346	GLU	CD-OE2	-5.37	1.19	1.25
1	B	1204	TYR	CB-CG	-5.37	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	360	TRP	CZ3-CH2	-5.35	1.31	1.40
1	A	68	TYR	CE2-CZ	-5.35	1.31	1.38
1	B	68	TYR	CE2-CZ	-5.35	1.31	1.38
1	C	360	TRP	CZ3-CH2	-5.35	1.31	1.40
1	C	570	TYR	CB-CG	-5.35	1.43	1.51
1	A	570	TYR	CB-CG	-5.33	1.43	1.51
1	C	68	TYR	CE2-CZ	-5.33	1.31	1.38
1	A	346	GLU	CD-OE2	-5.32	1.19	1.25
1	C	672	TYR	CG-CD1	-5.31	1.32	1.39
1	C	1197	TRP	CD2-CE2	-5.31	1.34	1.41
1	B	570	TYR	CB-CG	-5.30	1.43	1.51
1	B	1197	TRP	CD2-CE2	-5.30	1.34	1.41
1	B	672	TYR	CG-CD1	-5.30	1.32	1.39
1	A	1197	TRP	CD2-CE2	-5.29	1.35	1.41
1	A	672	TYR	CG-CD1	-5.28	1.32	1.39
1	C	346	GLU	CD-OE2	-5.24	1.19	1.25
1	C	274	TYR	CE2-CZ	-5.21	1.31	1.38
1	A	250	TYR	CD1-CE1	-5.20	1.31	1.39
1	B	250	TYR	CD1-CE1	-5.19	1.31	1.39
1	A	274	TYR	CE2-CZ	-5.18	1.31	1.38
1	C	250	TYR	CD1-CE1	-5.17	1.31	1.39
1	C	236	PHE	CB-CG	-5.16	1.42	1.51
1	A	236	PHE	CB-CG	-5.15	1.42	1.51
1	B	236	PHE	CB-CG	-5.14	1.42	1.51
1	C	173	GLN	CG-CD	-5.13	1.39	1.51
1	A	173	GLN	CG-CD	-5.12	1.39	1.51
1	B	274	TYR	CE2-CZ	-5.12	1.31	1.38
1	C	466	PHE	CG-CD1	-5.12	1.31	1.38
1	B	121	GLU	CD-OE1	-5.11	1.20	1.25
1	C	18	ASP	CB-CG	5.10	1.62	1.51
1	B	173	GLN	CG-CD	-5.10	1.39	1.51
1	A	466	PHE	CG-CD1	-5.09	1.31	1.38
1	A	18	ASP	CB-CG	5.09	1.62	1.51
1	B	18	ASP	CB-CG	5.09	1.62	1.51
1	A	121	GLU	CD-OE1	-5.08	1.20	1.25
1	B	360	TRP	NE1-CE2	-5.07	1.30	1.37
1	A	360	TRP	NE1-CE2	-5.05	1.30	1.37
1	B	466	PHE	CG-CD1	-5.05	1.31	1.38
1	C	121	GLU	CD-OE1	-5.05	1.20	1.25
1	A	1204	TYR	CG-CD2	-5.03	1.32	1.39
1	C	360	TRP	NE1-CE2	-5.03	1.31	1.37
1	A	357	PRO	N-CD	-5.03	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1204	TYR	CG-CD2	-5.03	1.32	1.39
1	C	357	PRO	N-CD	-5.03	1.40	1.47
1	C	1204	TYR	CG-CD2	-5.03	1.32	1.39
1	C	1155	TYR	CE2-CZ	-5.02	1.32	1.38
1	B	466	PHE	CB-CG	-5.01	1.42	1.51
1	B	50	TYR	CB-CG	-5.00	1.44	1.51

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	52	VAL	CA-CB-CG2	10.30	126.34	110.90
1	A	52	VAL	CA-CB-CG2	10.29	126.34	110.90
1	B	52	VAL	CA-CB-CG2	10.28	126.32	110.90
1	C	272	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	B	272	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	A	272	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	B	704	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	A	704	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	C	704	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	C	274	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	A	274	TYR	CB-CG-CD2	-8.17	116.10	121.00
1	B	274	TYR	CB-CG-CD2	-8.15	116.11	121.00
1	C	413	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	A	413	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	50	TYR	CB-CG-CD2	-6.95	116.83	121.00
1	B	50	TYR	CB-CG-CD2	-6.94	116.84	121.00
1	C	775	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	413	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	50	TYR	CB-CG-CD2	-6.88	116.88	121.00
1	A	775	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	775	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	A	660	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	C	1094	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	C	660	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	B	660	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	B	1094	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	1094	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	184	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	184	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	184	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	C	1094	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	1094	ARG	NE-CZ-NH2	-6.39	117.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1094	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	684	TYR	CB-CG-CD1	-6.34	117.20	121.00
1	B	684	TYR	CB-CG-CD1	-6.29	117.23	121.00
1	C	684	TYR	CB-CG-CD1	-6.28	117.23	121.00
1	A	893	ASP	N-CA-C	6.15	127.61	111.00
1	C	893	ASP	N-CA-C	6.15	127.60	111.00
1	B	893	ASP	N-CA-C	6.14	127.58	111.00
1	A	971	TYR	CB-CG-CD1	-6.12	117.33	121.00
1	B	971	TYR	CB-CG-CD1	-6.11	117.34	121.00
1	A	704	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	704	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	316	GLY	N-CA-C	6.04	128.19	113.10
1	A	316	GLY	N-CA-C	6.03	128.18	113.10
1	C	971	TYR	CB-CG-CD1	-6.03	117.39	121.00
1	B	316	GLY	N-CA-C	6.00	128.11	113.10
1	C	704	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	C	184	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	184	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	184	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	52	VAL	CG1-CB-CG2	-5.79	101.64	110.90
1	B	52	VAL	CG1-CB-CG2	-5.79	101.64	110.90
1	C	52	VAL	CG1-CB-CG2	-5.78	101.64	110.90
1	B	289	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	289	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	289	ASP	CB-CG-OD1	5.63	123.36	118.30
1	C	670	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	670	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	670	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	C	789	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	789	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	424	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	B	789	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	424	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	B	211	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	211	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	B	424	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	C	211	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	A	67	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	B	67	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	C	67	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	C	719	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	710	TYR	CB-CG-CD1	-5.26	117.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1133	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	B	719	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	C	710	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	A	667	TYR	CB-CG-CD1	-5.21	117.88	121.00
1	A	719	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	1133	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	710	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	C	681	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	667	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	C	667	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	A	681	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	1133	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	681	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	57	TYR	CB-CG-CD2	-5.06	117.97	121.00
1	C	431	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	431	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	57	TYR	CB-CG-CD2	-5.01	117.99	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9150	0	8848	20	0
1	B	9150	0	8848	18	0
1	C	9150	0	8848	17	0
2	D	39	0	34	0	0
2	E	39	0	34	0	0
2	G	39	0	34	0	0
2	H	39	0	34	1	0
2	M	39	0	34	0	0
2	N	39	0	34	0	0
2	O	39	0	34	0	0
2	Q	39	0	34	0	0
2	R	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	39	0	34	0	0
2	X	39	0	34	0	0
2	Y	39	0	34	0	0
2	a	39	0	34	0	0
2	b	39	0	34	0	0
2	g	39	0	34	0	0
3	F	50	0	43	0	0
3	J	50	0	43	0	0
3	P	50	0	43	0	0
3	T	50	0	43	0	0
3	Z	50	0	43	0	0
3	d	50	0	43	0	0
4	I	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	S	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	c	28	0	25	0	0
4	e	28	0	25	0	0
4	f	28	0	25	0	0
5	A	70	0	65	1	0
5	B	70	0	65	1	0
5	C	70	0	65	1	0
6	A	25	0	0	0	0
6	B	25	0	0	0	0
6	C	25	0	0	0	0
7	A	132	0	0	5	0
7	B	132	0	0	5	0
7	C	132	0	0	5	0
All	All	29268	0	27732	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:LEU:HD12	7:C:5043:HOH:O	1.62	1.00
1:A:190:LEU:HD12	7:A:5043:HOH:O	1.62	0.98
1:B:190:LEU:HD12	7:B:5043:HOH:O	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:HA	7:A:5043:HOH:O	1.77	0.84
1:C:190:LEU:HA	7:C:5043:HOH:O	1.77	0.83
1:B:190:LEU:HA	7:B:5043:HOH:O	1.77	0.82
1:B:1059:GLN:NE2	1:C:846:SER:OG	2.28	0.67
1:A:846:SER:OG	1:C:1059:GLN:NE2	2.28	0.67
1:A:1059:GLN:NE2	1:B:846:SER:OG	2.28	0.66
1:A:687:ARG:O	7:A:5057:HOH:O	2.14	0.65
1:C:687:ARG:O	7:C:5057:HOH:O	2.14	0.64
1:B:687:ARG:O	7:B:5057:HOH:O	2.14	0.64
1:A:1019:ASN:HB3	7:A:5129:HOH:O	2.05	0.57
1:C:1019:ASN:HB3	7:C:5129:HOH:O	2.05	0.56
1:B:1019:ASN:HB3	7:B:5129:HOH:O	2.05	0.56
1:B:229:ASP:N	1:B:229:ASP:OD1	2.41	0.53
1:A:229:ASP:OD1	1:A:229:ASP:N	2.41	0.52
1:C:229:ASP:OD1	1:C:229:ASP:N	2.41	0.49
1:C:897:SER:N	1:C:898:PRO:CD	2.78	0.47
1:A:897:SER:N	1:A:898:PRO:CD	2.78	0.46
1:A:552:LYS:NZ	1:B:619:GLN:OE1	2.49	0.46
1:B:897:SER:N	1:B:898:PRO:CD	2.78	0.46
1:A:619:GLN:OE1	1:C:552:LYS:NZ	2.49	0.46
1:B:552:LYS:NZ	1:C:619:GLN:OE1	2.49	0.45
1:A:385:THR:HG22	7:A:5069:HOH:O	2.16	0.45
1:C:385:THR:HG22	7:C:5069:HOH:O	2.16	0.45
1:A:129:SER:OG	1:A:130:THR:N	2.49	0.45
1:A:821:LYS:NZ	1:A:863:ASP:OD2	2.40	0.45
1:B:129:SER:OG	1:B:130:THR:N	2.49	0.44
1:B:155:LEU:HD21	5:B:3198:NAG:H82	2.00	0.44
1:B:385:THR:HG22	7:B:5069:HOH:O	2.16	0.43
1:A:155:LEU:HD21	5:A:3198:NAG:H82	2.00	0.43
1:C:155:LEU:HD21	5:C:3198:NAG:H82	2.00	0.43
1:B:928:ASP:N	1:B:928:ASP:OD1	2.52	0.43
1:C:129:SER:OG	1:C:130:THR:N	2.49	0.43
1:C:928:ASP:OD1	1:C:928:ASP:N	2.52	0.43
1:A:928:ASP:N	1:A:928:ASP:OD1	2.52	0.43
1:C:161:VAL:HG11	1:C:238:PHE:CE2	2.54	0.42
1:B:161:VAL:HG11	1:B:238:PHE:CE2	2.54	0.42
1:A:161:VAL:HG11	1:A:238:PHE:CE2	2.54	0.42
1:A:1211:THR:OG1	1:A:1212:GLU:N	2.53	0.42
1:B:1131:SER:OG	1:B:1132:SER:N	2.52	0.42
1:A:1131:SER:OG	1:A:1132:SER:N	2.52	0.42
1:C:803:PRO:HB3	1:C:1163:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1211:THR:OG1	1:C:1212:GLU:N	2.53	0.41
1:A:803:PRO:HB3	1:A:1163:PRO:HB3	2.03	0.41
1:B:803:PRO:HB3	1:B:1163:PRO:HB3	2.03	0.41
1:B:1211:THR:OG1	1:B:1212:GLU:N	2.53	0.41
1:A:446:PRO:HG2	2:H:1:NAG:H82	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1163/1322 (88%)	1143 (98%)	19 (2%)	1 (0%)	48	77
1	B	1163/1322 (88%)	1143 (98%)	19 (2%)	1 (0%)	48	77
1	C	1163/1322 (88%)	1143 (98%)	19 (2%)	1 (0%)	48	77
All	All	3489/3966 (88%)	3429 (98%)	57 (2%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	875	ASN
1	B	875	ASN
1	C	875	ASN

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	1022/1151 (89%)	1017 (100%)	5 (0%)	86 95
1	B	1022/1151 (89%)	1017 (100%)	5 (0%)	86 95
1	C	1022/1151 (89%)	1017 (100%)	5 (0%)	86 95
All	All	3066/3453 (89%)	3051 (100%)	15 (0%)	85 95

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	59	ASN
1	A	244	MET
1	A	720	GLN
1	A	1224	ASN
1	B	19	LEU
1	B	59	ASN
1	B	244	MET
1	B	720	GLN
1	B	1224	ASN
1	C	19	LEU
1	C	59	ASN
1	C	244	MET
1	C	720	GLN
1	C	1224	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	1059	GLN
1	A	1104	GLN
1	B	183	HIS
1	B	1059	GLN
1	B	1104	GLN
1	C	183	HIS
1	C	1059	GLN
1	C	1104	GLN

5.3.3 RNA

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)

87 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	0.66	0	17,19,21	0.86	1 (5%)
2	NAG	D	2	2	14,14,15	0.83	1 (7%)	17,19,21	1.23	2 (11%)
2	BMA	D	3	2	11,11,12	0.70	0	15,15,17	0.74	0
2	NAG	E	1	2,1	14,14,15	0.78	1 (7%)	17,19,21	0.86	0
2	NAG	E	2	2	14,14,15	0.72	0	17,19,21	1.20	2 (11%)
2	BMA	E	3	2	11,11,12	0.68	0	15,15,17	0.75	0
3	NAG	F	1	3,1	14,14,15	0.80	1 (7%)	17,19,21	1.08	2 (11%)
3	NAG	F	2	3	14,14,15	0.82	0	17,19,21	1.53	2 (11%)
3	BMA	F	3	3	11,11,12	0.68	0	15,15,17	0.94	1 (6%)
3	MAN	F	4	3	11,11,12	0.73	0	15,15,17	0.80	1 (6%)
2	NAG	G	1	2,1	14,14,15	0.65	0	17,19,21	1.23	3 (17%)
2	NAG	G	2	2	14,14,15	0.84	1 (7%)	17,19,21	1.12	1 (5%)
2	BMA	G	3	2	11,11,12	0.59	0	15,15,17	0.74	0
2	NAG	H	1	2,1	14,14,15	0.80	1 (7%)	17,19,21	0.79	1 (5%)
2	NAG	H	2	2	14,14,15	0.85	0	17,19,21	1.43	3 (17%)
2	BMA	H	3	2	11,11,12	0.70	0	15,15,17	0.75	0
4	NAG	I	1	4,1	14,14,15	0.86	1 (7%)	17,19,21	1.30	2 (11%)
4	NAG	I	2	4	14,14,15	0.77	1 (7%)	17,19,21	0.93	1 (5%)
3	NAG	J	1	3,1	14,14,15	0.55	0	17,19,21	0.65	0
3	NAG	J	2	3	14,14,15	0.66	0	17,19,21	0.98	1 (5%)
3	BMA	J	3	3	11,11,12	0.82	1 (9%)	15,15,17	1.04	1 (6%)
3	MAN	J	4	3	11,11,12	0.70	0	15,15,17	0.77	1 (6%)
4	NAG	K	1	4,1	14,14,15	0.76	1 (7%)	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	K	2	4	14,14,15	0.81	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	L	1	4,1	14,14,15	0.79	1 (7%)	17,19,21	0.94	2 (11%)
4	NAG	L	2	4	14,14,15	0.99	1 (7%)	17,19,21	0.75	0
2	NAG	M	1	2,1	14,14,15	0.69	1 (7%)	17,19,21	1.39	3 (17%)
2	NAG	M	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.31	2 (11%)
2	BMA	M	3	2	11,11,12	0.72	0	15,15,17	0.68	0
2	NAG	N	1	2,1	14,14,15	0.66	0	17,19,21	0.85	1 (5%)
2	NAG	N	2	2	14,14,15	0.83	1 (7%)	17,19,21	1.23	2 (11%)
2	BMA	N	3	2	11,11,12	0.69	0	15,15,17	0.74	0
2	NAG	O	1	2,1	14,14,15	0.78	1 (7%)	17,19,21	0.87	0
2	NAG	O	2	2	14,14,15	0.73	0	17,19,21	1.20	2 (11%)
2	BMA	O	3	2	11,11,12	0.68	0	15,15,17	0.75	0
3	NAG	P	1	3,1	14,14,15	0.80	1 (7%)	17,19,21	1.08	2 (11%)
3	NAG	P	2	3	14,14,15	0.81	0	17,19,21	1.53	2 (11%)
3	BMA	P	3	3	11,11,12	0.68	0	15,15,17	0.94	1 (6%)
3	MAN	P	4	3	11,11,12	0.72	0	15,15,17	0.79	0
2	NAG	Q	1	2,1	14,14,15	0.65	0	17,19,21	1.23	3 (17%)
2	NAG	Q	2	2	14,14,15	0.84	1 (7%)	17,19,21	1.12	1 (5%)
2	BMA	Q	3	2	11,11,12	0.59	0	15,15,17	0.73	0
2	NAG	R	1	2,1	14,14,15	0.80	1 (7%)	17,19,21	0.78	1 (5%)
2	NAG	R	2	2	14,14,15	0.85	0	17,19,21	1.44	3 (17%)
2	BMA	R	3	2	11,11,12	0.71	0	15,15,17	0.75	0
4	NAG	S	1	4,1	14,14,15	0.86	1 (7%)	17,19,21	1.30	2 (11%)
4	NAG	S	2	4	14,14,15	0.78	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	T	1	3,1	14,14,15	0.55	0	17,19,21	0.65	0
3	NAG	T	2	3	14,14,15	0.66	0	17,19,21	0.98	1 (5%)
3	BMA	T	3	3	11,11,12	0.82	1 (9%)	15,15,17	1.04	1 (6%)
3	MAN	T	4	3	11,11,12	0.71	0	15,15,17	0.77	1 (6%)
4	NAG	U	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	0.79	0
4	NAG	U	2	4	14,14,15	0.80	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	V	1	4,1	14,14,15	0.79	1 (7%)	17,19,21	0.94	2 (11%)
4	NAG	V	2	4	14,14,15	1.00	1 (7%)	17,19,21	0.74	0
2	NAG	W	1	2,1	14,14,15	0.68	0	17,19,21	1.39	3 (17%)
2	NAG	W	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.31	2 (11%)
2	BMA	W	3	2	11,11,12	0.72	0	15,15,17	0.68	0
2	NAG	X	1	2,1	14,14,15	0.66	0	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	X	2	2	14,14,15	0.82	1 (7%)	17,19,21	1.23	2 (11%)
2	BMA	X	3	2	11,11,12	0.70	0	15,15,17	0.74	0
2	NAG	Y	1	2,1	14,14,15	0.79	1 (7%)	17,19,21	0.86	0
2	NAG	Y	2	2	14,14,15	0.73	0	17,19,21	1.20	2 (11%)
2	BMA	Y	3	2	11,11,12	0.68	0	15,15,17	0.75	0
3	NAG	Z	1	3,1	14,14,15	0.81	1 (7%)	17,19,21	1.08	2 (11%)
3	NAG	Z	2	3	14,14,15	0.82	0	17,19,21	1.53	2 (11%)
3	BMA	Z	3	3	11,11,12	0.67	0	15,15,17	0.94	1 (6%)
3	MAN	Z	4	3	11,11,12	0.73	0	15,15,17	0.80	0
2	NAG	a	1	2,1	14,14,15	0.65	0	17,19,21	1.24	3 (17%)
2	NAG	a	2	2	14,14,15	0.84	1 (7%)	17,19,21	1.12	1 (5%)
2	BMA	a	3	2	11,11,12	0.58	0	15,15,17	0.74	0
2	NAG	b	1	2,1	14,14,15	0.80	1 (7%)	17,19,21	0.78	1 (5%)
2	NAG	b	2	2	14,14,15	0.86	0	17,19,21	1.43	3 (17%)
2	BMA	b	3	2	11,11,12	0.71	0	15,15,17	0.75	0
4	NAG	c	1	4,1	14,14,15	0.86	1 (7%)	17,19,21	1.31	2 (11%)
4	NAG	c	2	4	14,14,15	0.77	1 (7%)	17,19,21	0.93	1 (5%)
3	NAG	d	1	3,1	14,14,15	0.55	0	17,19,21	0.65	0
3	NAG	d	2	3	14,14,15	0.66	0	17,19,21	0.98	1 (5%)
3	BMA	d	3	3	11,11,12	0.82	1 (9%)	15,15,17	1.05	1 (6%)
3	MAN	d	4	3	11,11,12	0.72	0	15,15,17	0.76	1 (6%)
4	NAG	e	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	0.79	0
4	NAG	e	2	4	14,14,15	0.80	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	f	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	0.93	2 (11%)
4	NAG	f	2	4	14,14,15	0.99	1 (7%)	17,19,21	0.75	0
2	NAG	g	1	2,1	14,14,15	0.69	1 (7%)	17,19,21	1.39	3 (17%)
2	NAG	g	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.31	2 (11%)
2	BMA	g	3	2	11,11,12	0.71	0	15,15,17	0.68	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
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	e	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	e	2	4	-	1/6/23/26	0/1/1/1
4	NAG	f	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	f	2	4	-	1/6/23/26	0/1/1/1
2	NAG	g	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	g	2	2	-	2/6/23/26	0/1/1/1
2	BMA	g	3	2	-	1/2/19/22	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	2	NAG	C1-C2	3.34	1.56	1.52
4	f	2	NAG	C1-C2	3.30	1.56	1.52
4	L	2	NAG	C1-C2	3.30	1.56	1.52
2	a	2	NAG	C1-C2	2.75	1.56	1.52
2	Q	2	NAG	C1-C2	2.74	1.56	1.52
2	G	2	NAG	C1-C2	2.74	1.56	1.52
2	b	1	NAG	C1-C2	2.68	1.56	1.52
2	R	1	NAG	C1-C2	2.66	1.56	1.52
4	K	2	NAG	C1-C2	2.66	1.56	1.52
2	H	1	NAG	C1-C2	2.65	1.56	1.52
4	U	2	NAG	C1-C2	2.63	1.55	1.52
4	e	2	NAG	C1-C2	2.63	1.55	1.52
4	c	1	NAG	C1-C2	2.58	1.55	1.52
3	Z	1	NAG	C1-C2	2.58	1.55	1.52
4	I	1	NAG	C1-C2	2.58	1.55	1.52
4	S	1	NAG	C1-C2	2.57	1.55	1.52
3	F	1	NAG	C1-C2	2.56	1.55	1.52
3	P	1	NAG	C1-C2	2.56	1.55	1.52
4	S	2	NAG	C1-C2	2.54	1.55	1.52
4	I	2	NAG	C1-C2	2.51	1.55	1.52
4	c	2	NAG	C1-C2	2.51	1.55	1.52
2	W	2	NAG	C1-C2	2.42	1.55	1.52
2	M	2	NAG	C1-C2	2.41	1.55	1.52
2	g	2	NAG	C1-C2	2.40	1.55	1.52
2	N	2	NAG	C1-C2	2.40	1.55	1.52
2	Y	1	NAG	C1-C2	2.39	1.55	1.52
2	O	1	NAG	C1-C2	2.39	1.55	1.52
4	V	1	NAG	C1-C2	2.39	1.55	1.52
2	D	2	NAG	C1-C2	2.38	1.55	1.52
4	L	1	NAG	C1-C2	2.38	1.55	1.52
2	E	1	NAG	C1-C2	2.37	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	2	NAG	C1-C2	2.35	1.55	1.52
4	f	1	NAG	C1-C2	2.30	1.55	1.52
4	U	1	NAG	C1-C2	2.15	1.55	1.52
3	T	3	BMA	C1-C2	2.14	1.57	1.52
3	d	3	BMA	C1-C2	2.12	1.57	1.52
4	K	1	NAG	C1-C2	2.12	1.55	1.52
4	e	1	NAG	C1-C2	2.12	1.55	1.52
3	J	3	BMA	C1-C2	2.10	1.57	1.52
2	g	1	NAG	C1-C2	2.02	1.55	1.52
2	M	1	NAG	C1-C2	2.01	1.55	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	2	NAG	C4-C3-C2	-4.36	104.63	111.02
3	P	2	NAG	C4-C3-C2	-4.36	104.63	111.02
3	F	2	NAG	C4-C3-C2	-4.35	104.64	111.02
2	W	1	NAG	C3-C4-C5	-3.57	103.76	110.23
2	M	1	NAG	C3-C4-C5	-3.57	103.77	110.23
4	c	1	NAG	C1-O5-C5	-3.57	107.41	112.19
2	g	1	NAG	C3-C4-C5	-3.56	103.77	110.23
4	I	1	NAG	C1-O5-C5	-3.55	107.42	112.19
4	S	1	NAG	C1-O5-C5	-3.55	107.43	112.19
2	a	1	NAG	C1-C2-N2	-3.18	105.43	110.43
2	G	1	NAG	C1-C2-N2	-3.14	105.48	110.43
2	Q	1	NAG	C1-C2-N2	-3.13	105.50	110.43
2	M	1	NAG	C4-C3-C2	3.05	115.49	111.02
3	Z	3	BMA	C2-C3-C4	-3.04	105.51	110.86
2	g	1	NAG	C4-C3-C2	3.04	115.48	111.02
2	W	1	NAG	C4-C3-C2	3.04	115.47	111.02
3	F	3	BMA	C2-C3-C4	-3.02	105.55	110.86
3	P	3	BMA	C2-C3-C4	-3.02	105.55	110.86
2	H	2	NAG	C3-C4-C5	-2.91	104.96	110.23
2	R	2	NAG	C3-C4-C5	-2.90	104.97	110.23
2	b	2	NAG	C3-C4-C5	-2.90	104.98	110.23
3	d	3	BMA	C2-C3-C4	-2.87	105.81	110.86
3	J	3	BMA	C2-C3-C4	-2.86	105.84	110.86
3	T	3	BMA	C2-C3-C4	-2.85	105.85	110.86
2	R	2	NAG	O4-C4-C3	2.70	116.75	110.38
2	H	2	NAG	O4-C4-C3	2.70	116.74	110.38
2	b	2	NAG	O4-C4-C3	2.70	116.74	110.38
2	M	2	NAG	C3-C4-C5	-2.62	105.48	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	g	2	NAG	C3-C4-C5	-2.62	105.48	110.23
4	e	2	NAG	C4-C3-C2	-2.61	107.20	111.02
2	W	2	NAG	C3-C4-C5	-2.60	105.51	110.23
2	W	2	NAG	O4-C4-C3	2.60	116.50	110.38
2	g	2	NAG	O4-C4-C3	2.59	116.48	110.38
4	U	2	NAG	C4-C3-C2	-2.59	107.22	111.02
3	P	2	NAG	O4-C4-C3	2.59	116.48	110.38
4	K	2	NAG	C4-C3-C2	-2.59	107.22	111.02
2	M	2	NAG	O4-C4-C3	2.58	116.47	110.38
3	F	2	NAG	O4-C4-C3	2.58	116.45	110.38
3	Z	2	NAG	O4-C4-C3	2.56	116.42	110.38
2	a	1	NAG	C3-C4-C5	-2.54	105.62	110.23
2	G	1	NAG	C3-C4-C5	-2.54	105.63	110.23
2	Q	1	NAG	C3-C4-C5	-2.53	105.65	110.23
4	f	1	NAG	C3-C4-C5	-2.45	105.78	110.23
4	V	1	NAG	C3-C4-C5	-2.45	105.79	110.23
4	L	1	NAG	C3-C4-C5	-2.45	105.80	110.23
4	c	2	NAG	C4-C3-C2	-2.45	107.43	111.02
4	S	2	NAG	C4-C3-C2	-2.44	107.44	111.02
2	g	1	NAG	O4-C4-C3	-2.43	104.64	110.38
4	I	2	NAG	C4-C3-C2	-2.43	107.46	111.02
2	M	1	NAG	O4-C4-C3	-2.42	104.68	110.38
2	W	1	NAG	O4-C4-C3	-2.41	104.69	110.38
2	Q	2	NAG	C3-C4-C5	-2.38	105.91	110.23
2	G	2	NAG	C3-C4-C5	-2.38	105.91	110.23
4	c	1	NAG	C3-C4-C5	-2.37	105.93	110.23
4	S	1	NAG	C3-C4-C5	-2.37	105.93	110.23
2	R	2	NAG	O3-C3-C2	-2.37	104.48	109.40
4	I	1	NAG	C3-C4-C5	-2.37	105.94	110.23
2	a	2	NAG	C3-C4-C5	-2.37	105.94	110.23
2	H	2	NAG	O3-C3-C2	-2.37	104.48	109.40
3	T	2	NAG	C3-C4-C5	-2.36	105.94	110.23
3	P	1	NAG	C3-C4-C5	-2.36	105.96	110.23
2	b	2	NAG	O3-C3-C2	-2.35	104.51	109.40
3	J	2	NAG	C3-C4-C5	-2.35	105.97	110.23
3	d	2	NAG	C3-C4-C5	-2.35	105.97	110.23
3	F	1	NAG	C3-C4-C5	-2.34	105.98	110.23
2	N	2	NAG	C3-C4-C5	-2.34	105.99	110.23
3	Z	1	NAG	C3-C4-C5	-2.33	106.01	110.23
2	D	2	NAG	C3-C4-C5	-2.33	106.02	110.23
2	X	2	NAG	C3-C4-C5	-2.30	106.06	110.23
2	b	1	NAG	C3-C4-C5	-2.29	106.07	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	NAG	C3-C4-C5	-2.28	106.09	110.23
2	R	1	NAG	C3-C4-C5	-2.28	106.09	110.23
3	F	1	NAG	C1-O5-C5	-2.28	109.13	112.19
3	P	1	NAG	C1-O5-C5	-2.27	109.14	112.19
4	V	1	NAG	C1-O5-C5	2.26	115.21	112.19
3	Z	1	NAG	C1-O5-C5	-2.25	109.17	112.19
4	L	1	NAG	C1-O5-C5	2.25	115.20	112.19
2	Q	1	NAG	C1-O5-C5	-2.25	109.17	112.19
2	G	1	NAG	C1-O5-C5	-2.24	109.18	112.19
4	f	1	NAG	C1-O5-C5	2.23	115.18	112.19
2	a	1	NAG	C1-O5-C5	-2.23	109.20	112.19
2	Y	2	NAG	C4-C3-C2	-2.16	107.86	111.02
2	E	2	NAG	C4-C3-C2	-2.14	107.89	111.02
2	O	2	NAG	C4-C3-C2	-2.10	107.94	111.02
2	D	1	NAG	C3-C4-C5	-2.08	106.46	110.23
2	X	1	NAG	C3-C4-C5	-2.08	106.46	110.23
2	N	1	NAG	C3-C4-C5	-2.07	106.48	110.23
3	J	4	MAN	C2-C3-C4	-2.05	107.26	110.86
3	T	4	MAN	C2-C3-C4	-2.04	107.28	110.86
2	D	2	NAG	C4-C3-C2	-2.04	108.03	111.02
3	d	4	MAN	C2-C3-C4	-2.04	107.28	110.86
2	O	2	NAG	C3-C4-C5	-2.03	106.55	110.23
2	X	2	NAG	C4-C3-C2	-2.03	108.05	111.02
2	Y	2	NAG	C3-C4-C5	-2.02	106.57	110.23
3	F	4	MAN	C2-C3-C4	-2.02	107.31	110.86
2	N	2	NAG	C4-C3-C2	-2.01	108.07	111.02
2	E	2	NAG	C3-C4-C5	-2.01	106.59	110.23

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	1	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	d	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	d	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	b	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	Z	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
3	J	4	MAN	O5-C5-C6-O6
3	T	4	MAN	O5-C5-C6-O6
3	d	4	MAN	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
2	g	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	b	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	d	2	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	b	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	L	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	a	2	NAG	C4-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	P	3	BMA	O5-C5-C6-O6
3	Z	3	BMA	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
2	Y	3	BMA	O5-C5-C6-O6
2	a	3	BMA	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	M	3	BMA	O5-C5-C6-O6
2	R	3	BMA	O5-C5-C6-O6
2	W	3	BMA	O5-C5-C6-O6
2	b	3	BMA	O5-C5-C6-O6
2	g	3	BMA	O5-C5-C6-O6
2	Q	3	BMA	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
3	P	4	MAN	O5-C5-C6-O6
3	Z	4	MAN	O5-C5-C6-O6
3	Z	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	T	3	BMA	O5-C5-C6-O6
3	d	3	BMA	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	N	3	BMA	O5-C5-C6-O6
2	X	3	BMA	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	Q	1	NAG	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
3	J	4	MAN	C4-C5-C6-O6
3	d	4	MAN	C4-C5-C6-O6
3	T	4	MAN	C4-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	g	1	NAG	O5-C5-C6-O6

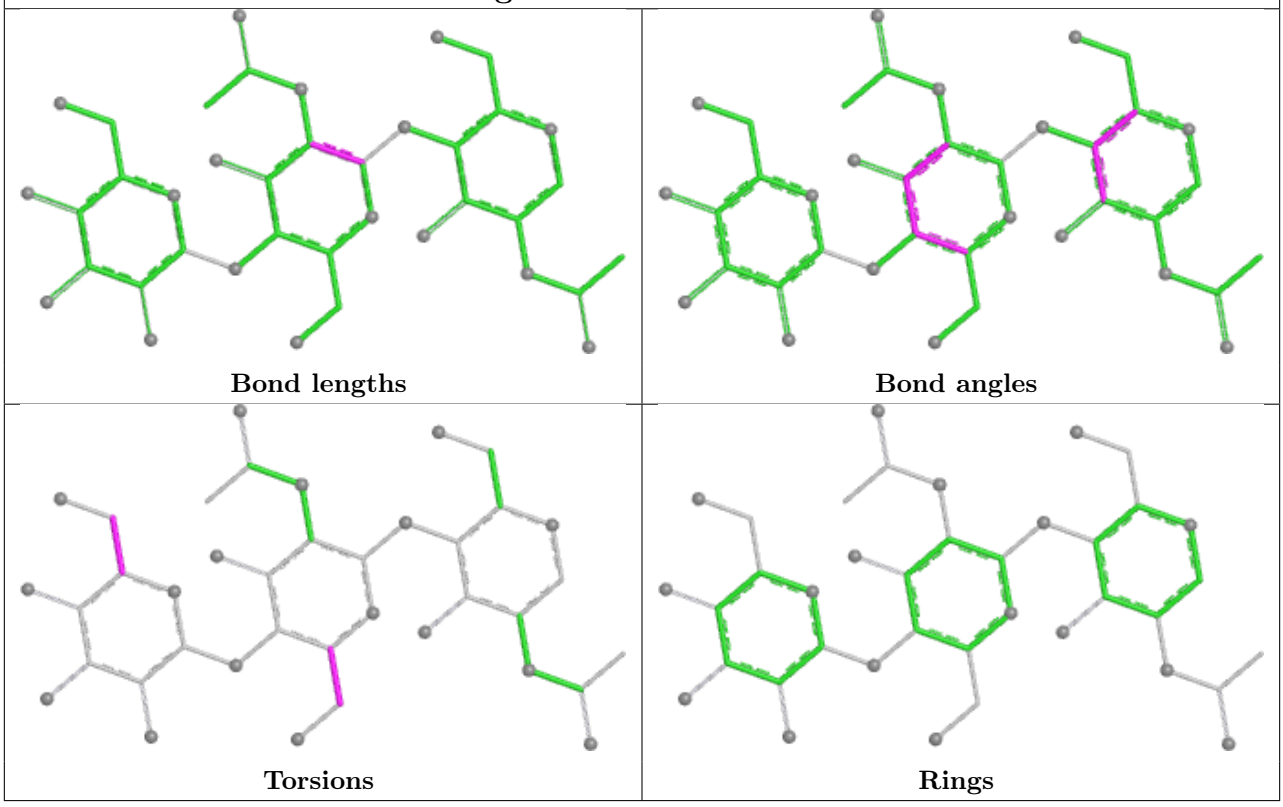
There are no ring outliers.

1 monomer is involved in 1 short contact:

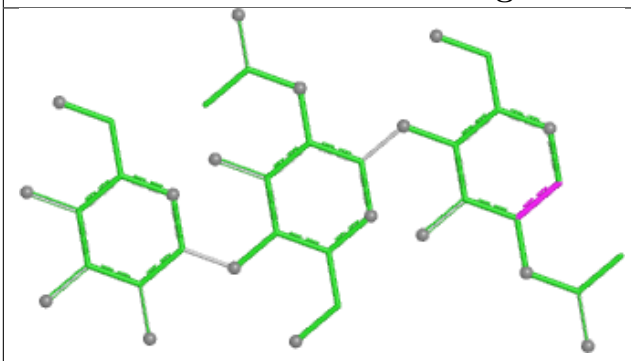
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0

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

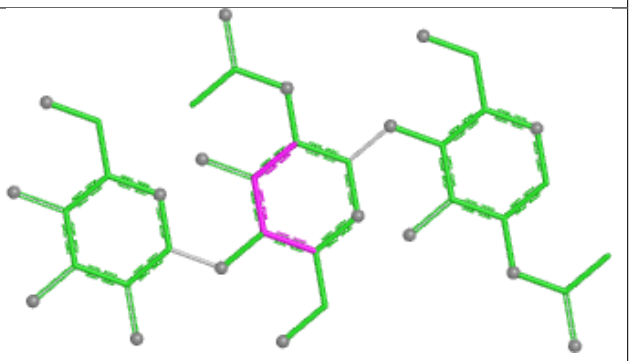
Oligosaccharide Chain D



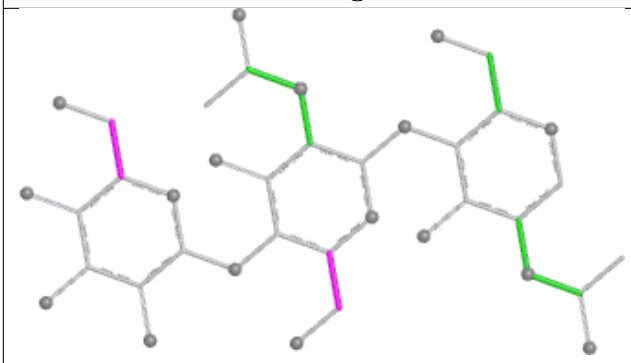
Oligosaccharide Chain E



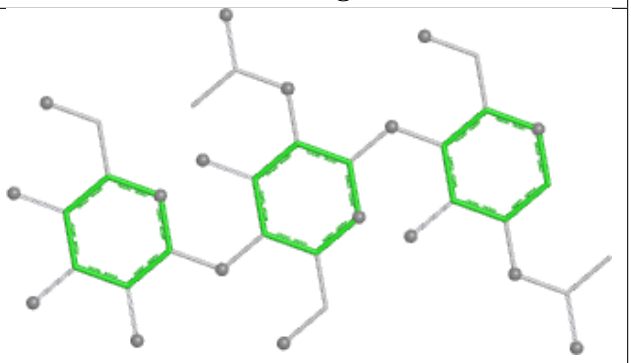
Bond lengths



Bond angles

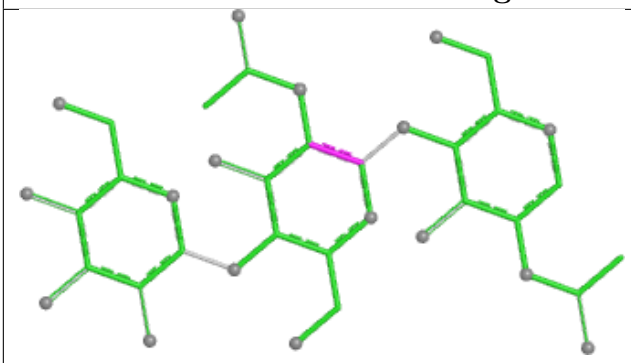


Torsions

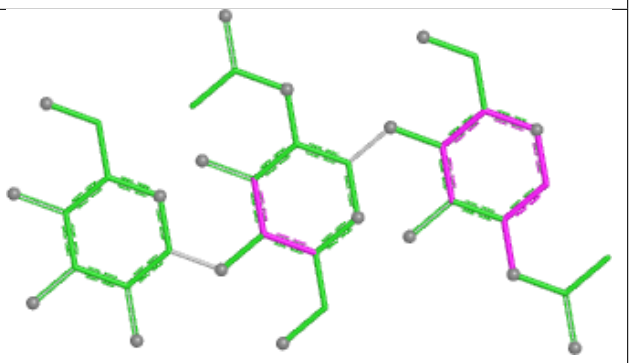


Rings

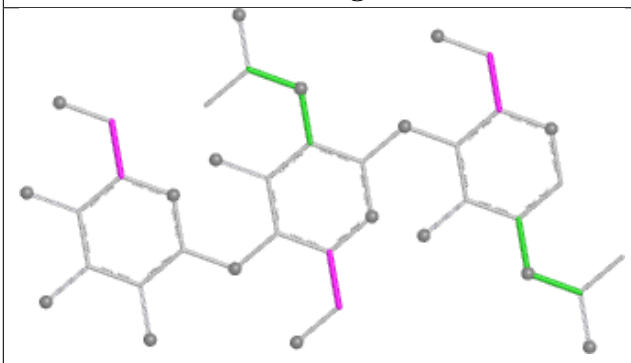
Oligosaccharide Chain G



Bond lengths



Bond angles



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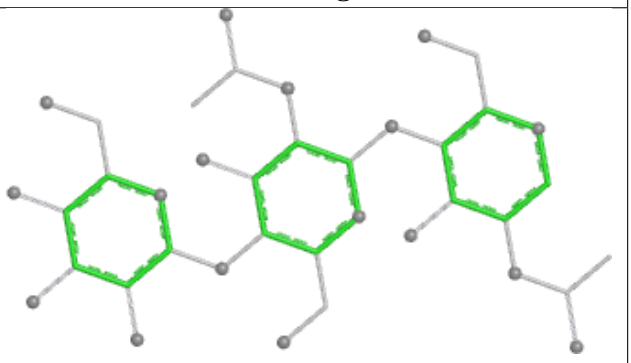
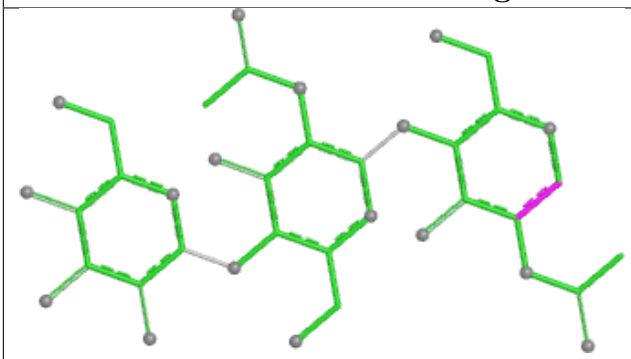


Rings

Oligosaccharide Chain H



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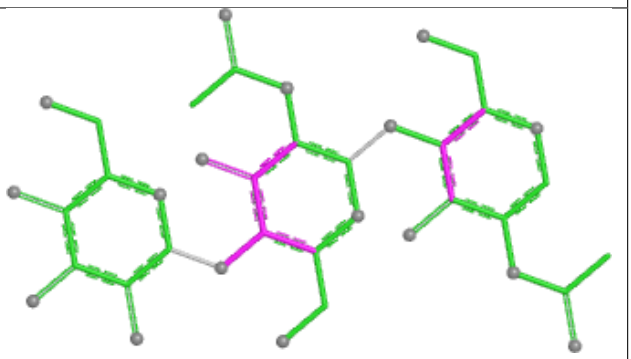
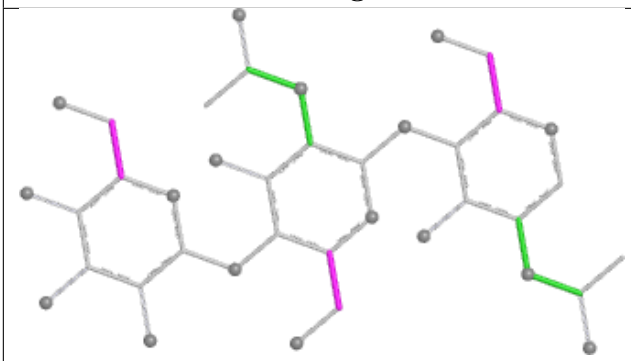


Bond angles



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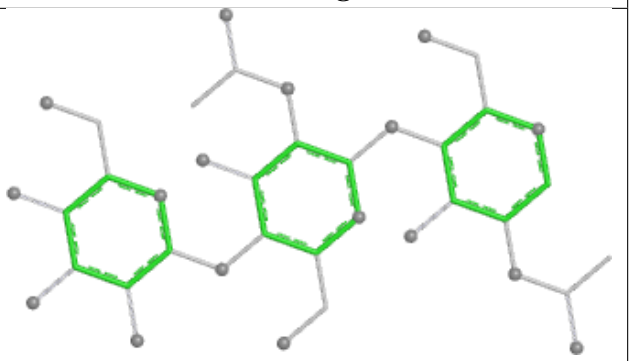
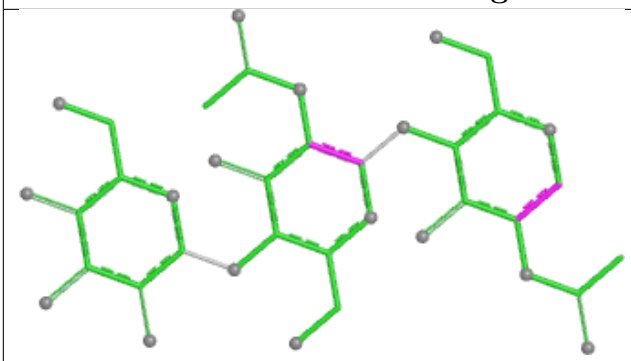


Rings

Oligosaccharide Chain M



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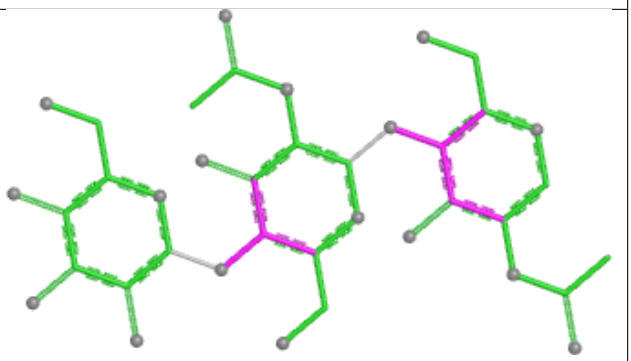
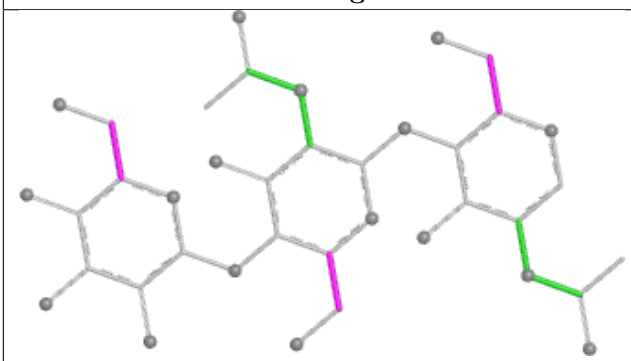


Bond angles



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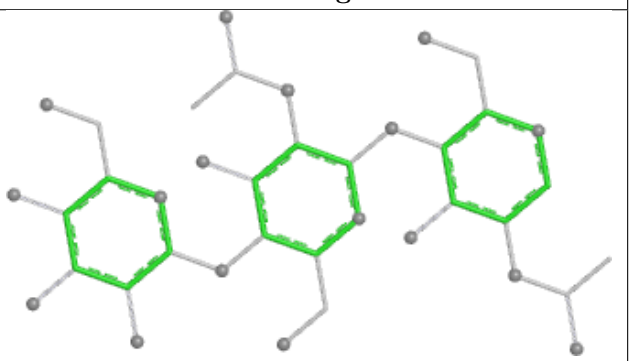
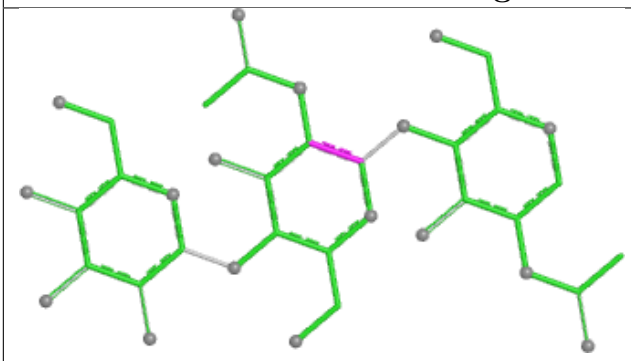


Rings

Oligosaccharide Chain N



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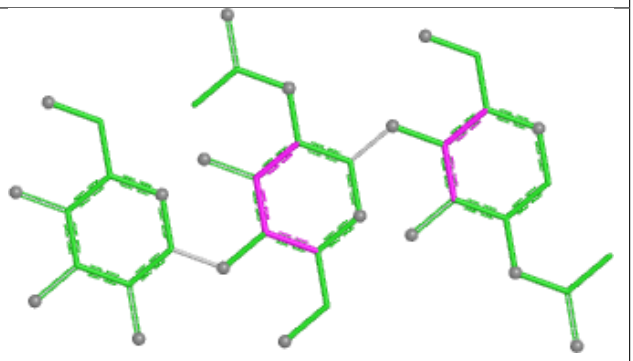
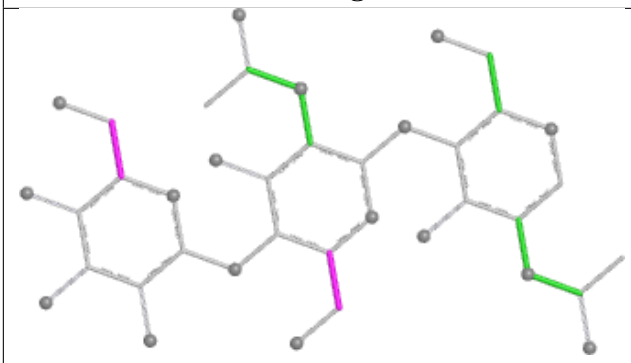


Bond angles



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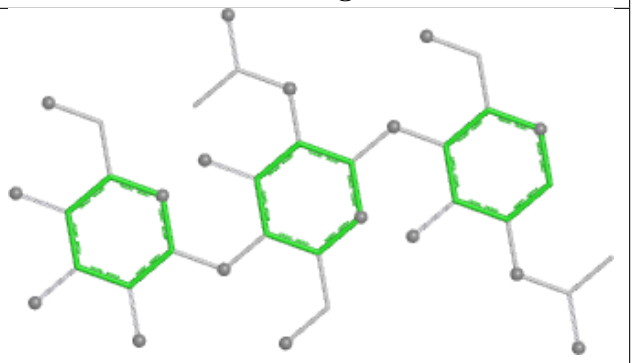
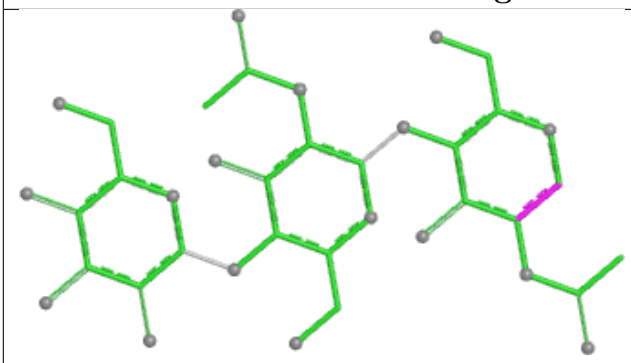


Rings

Oligosaccharide Chain O



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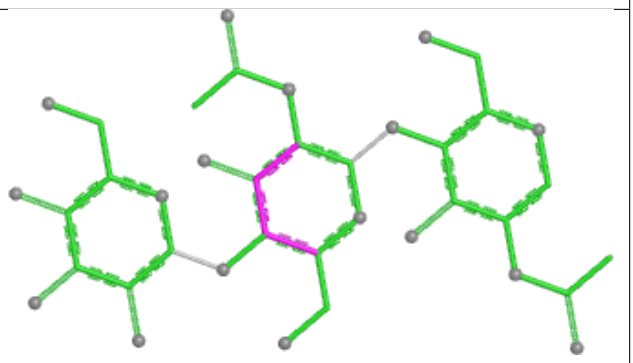
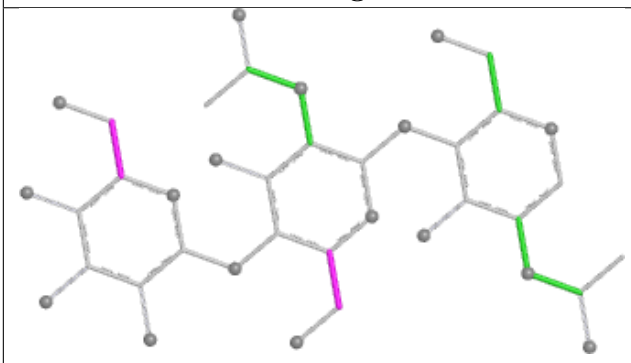


Bond angles



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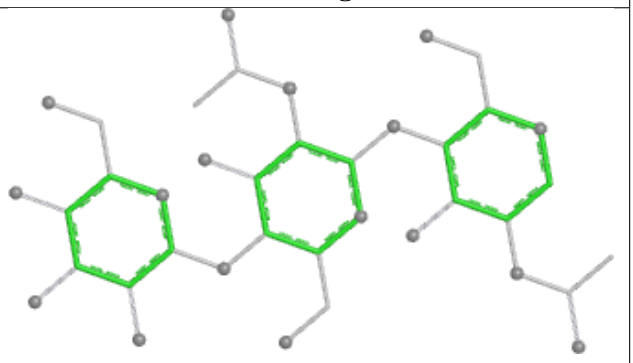
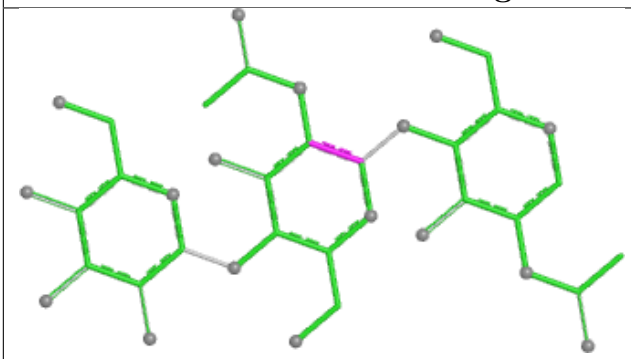


Rings

Oligosaccharide Chain Q



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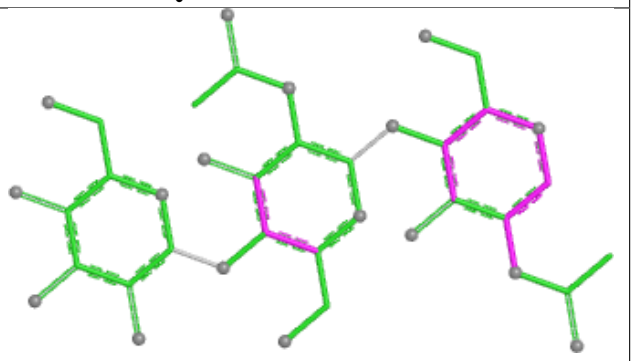
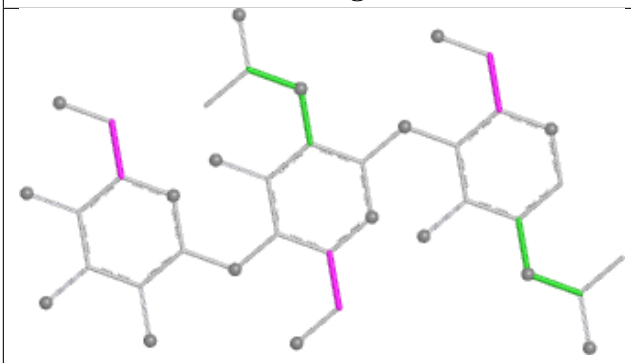


Bond angles



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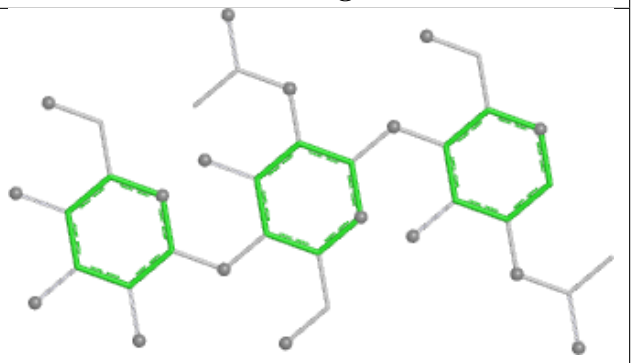
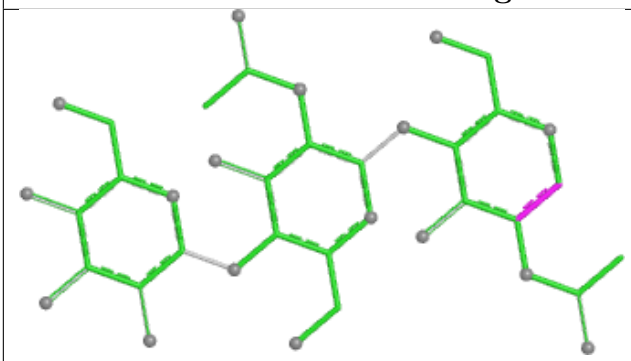


Rings

Oligosaccharide Chain R



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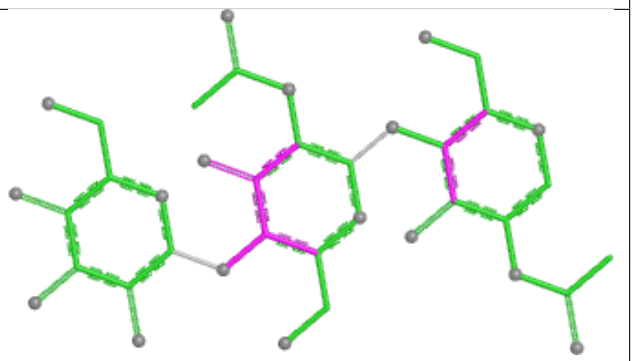
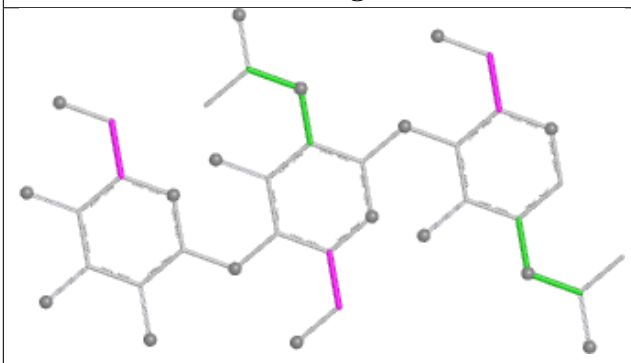


Bond angles



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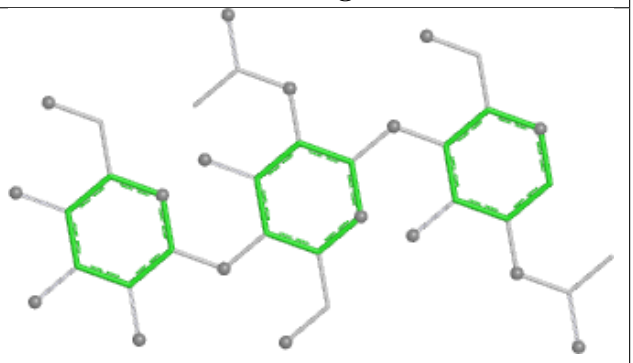
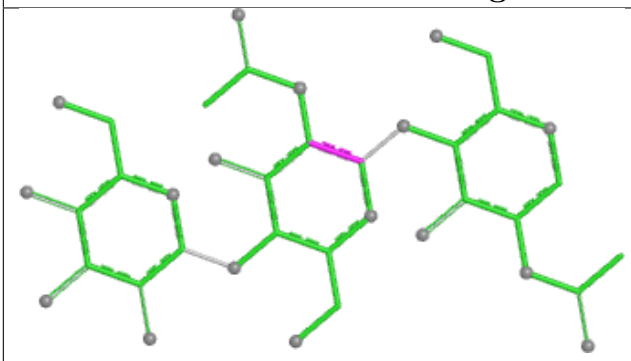


Rings

Oligosaccharide Chain W



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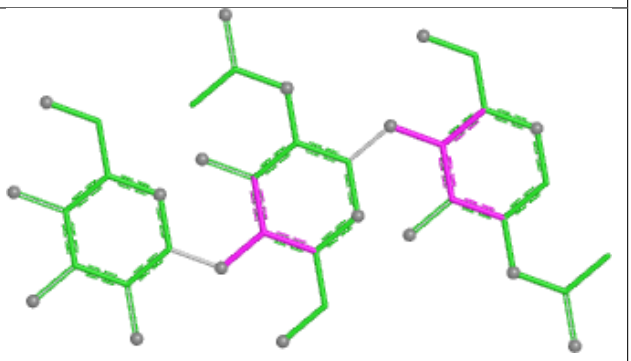

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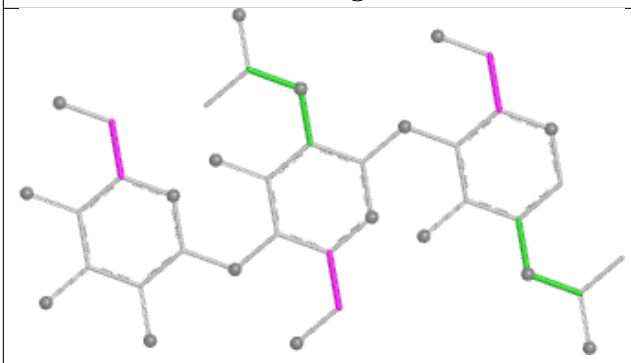

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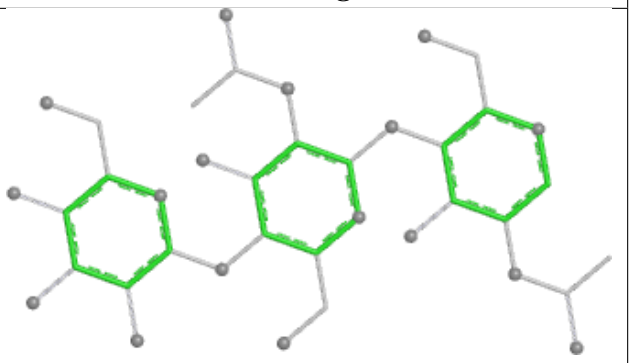
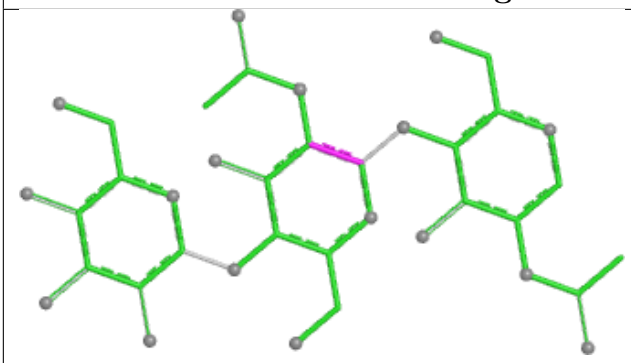


Rings

Oligosaccharide Chain X



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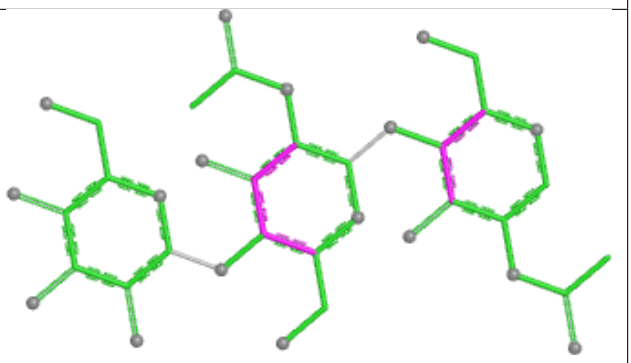

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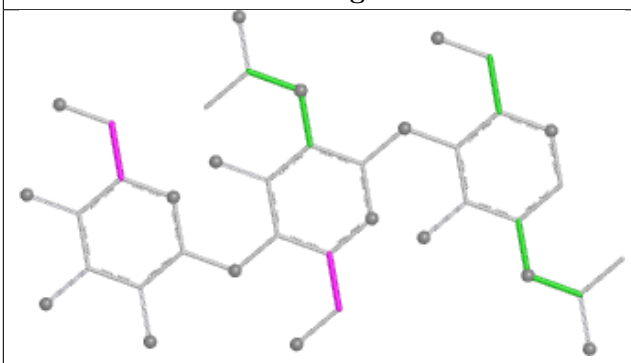

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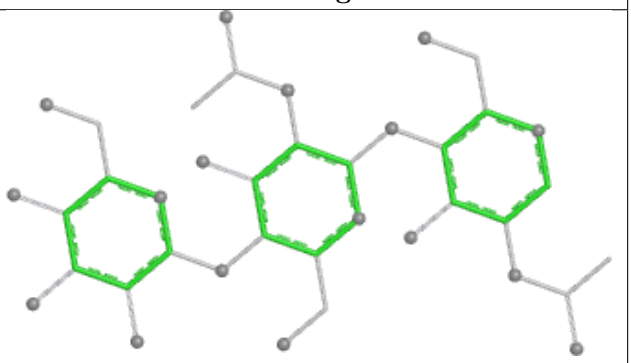
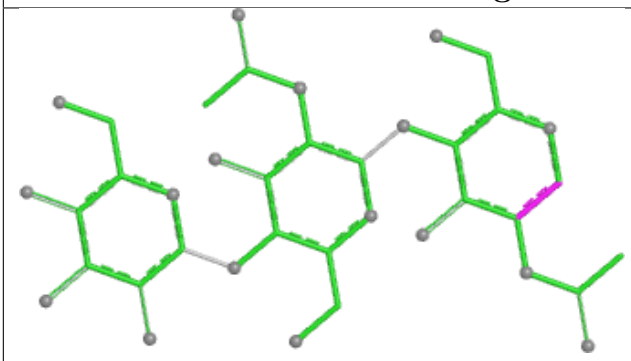


Rings

Oligosaccharide Chain Y



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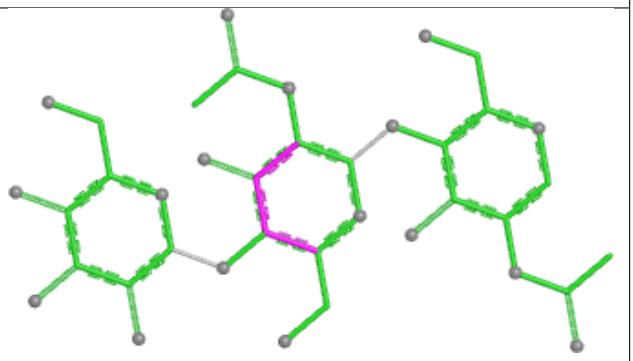

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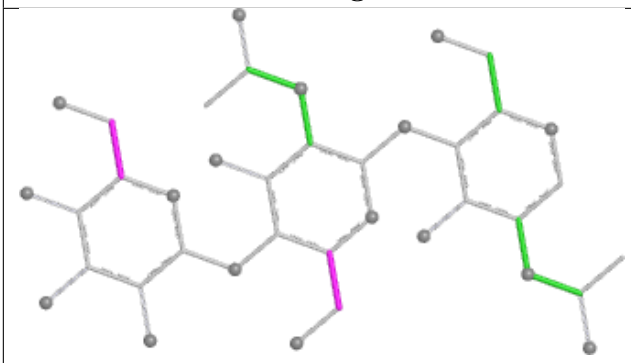

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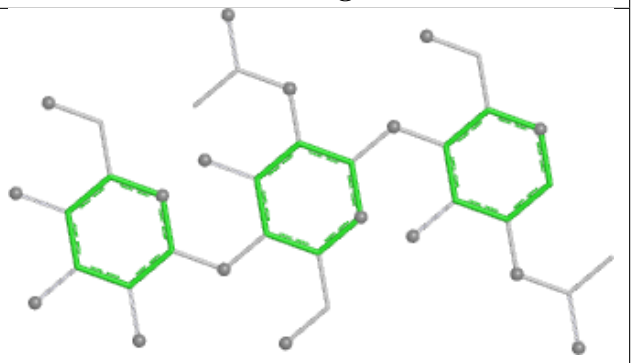
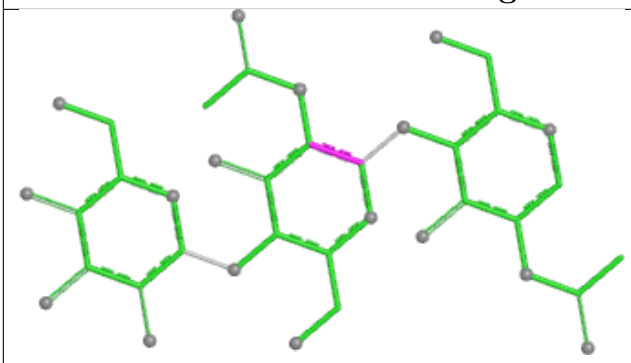


Rings

Oligosaccharide Chain a



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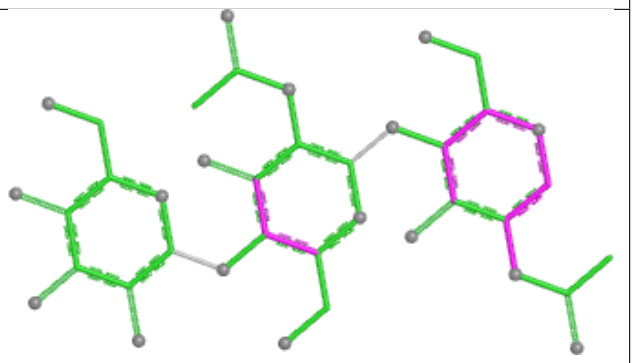

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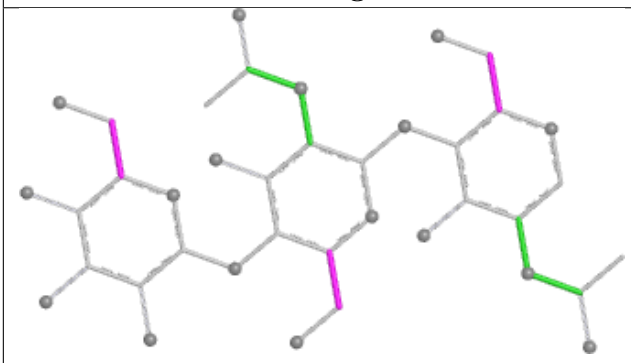

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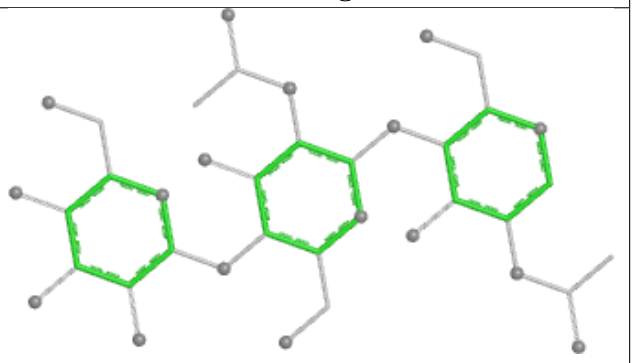
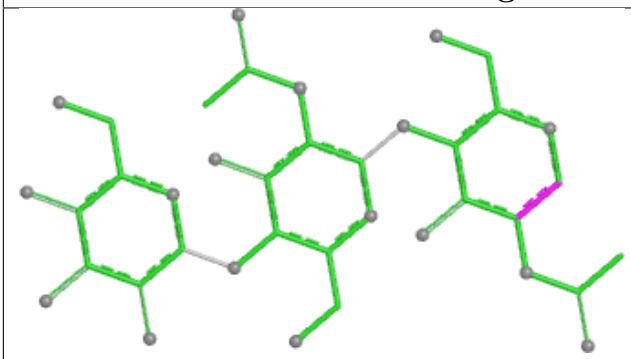


Rings

Oligosaccharide Chain b



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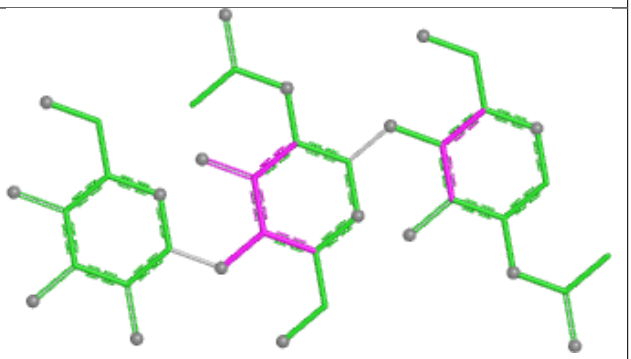
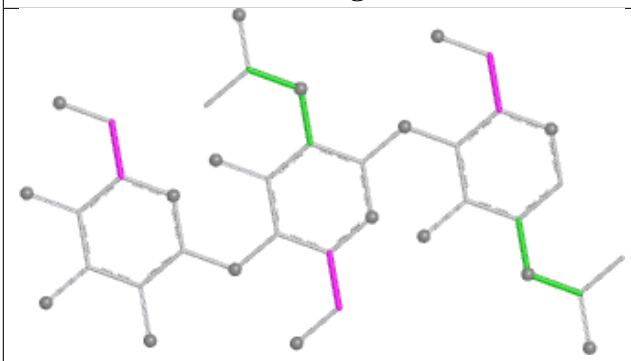


Bond angles



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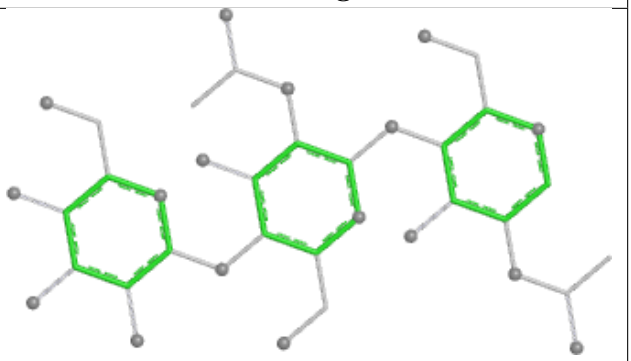
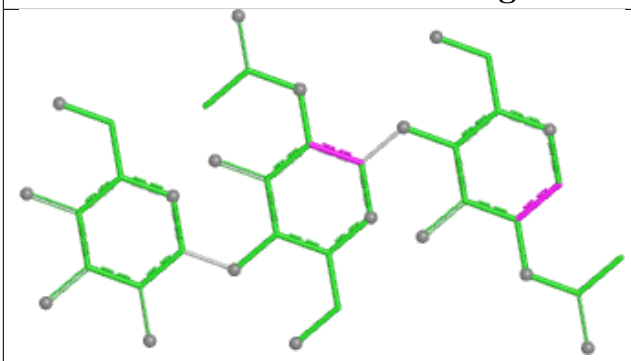


Rings

Oligosaccharide Chain g



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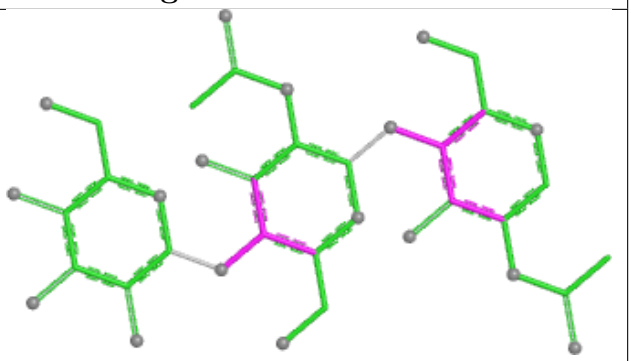
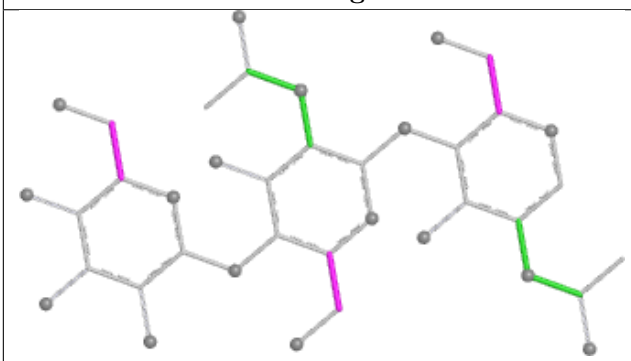


Bond angles



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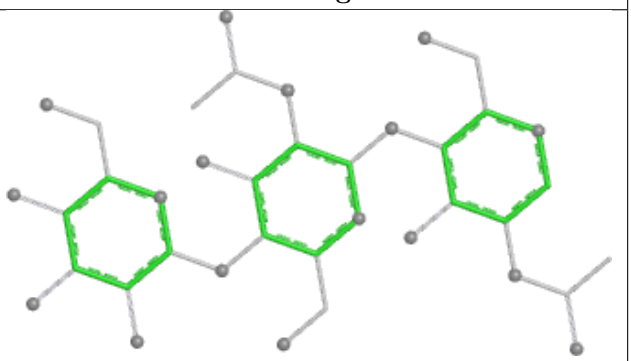
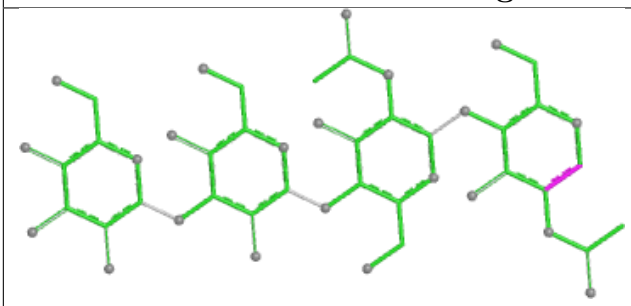
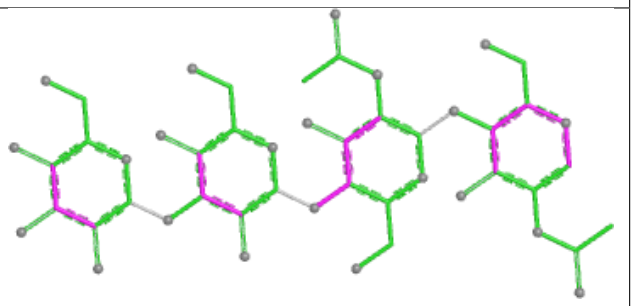
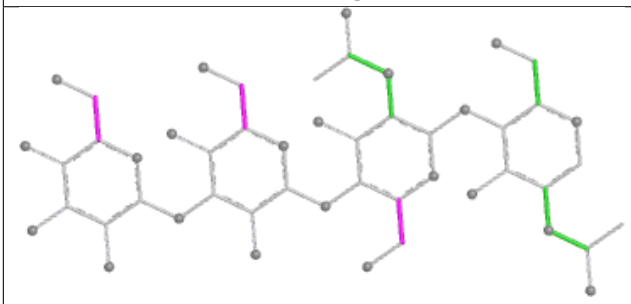
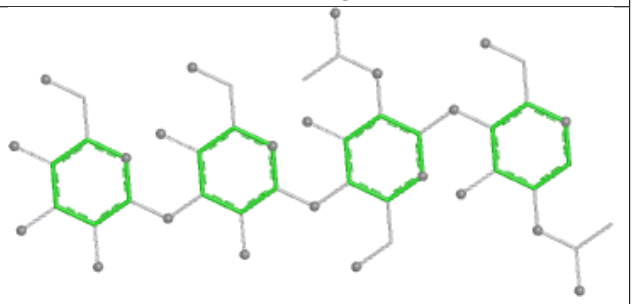
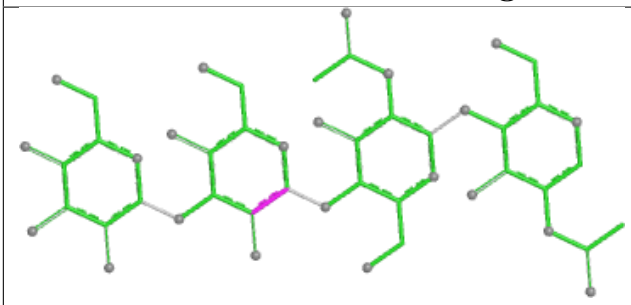
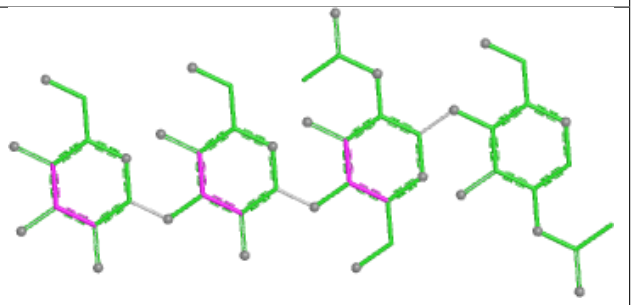
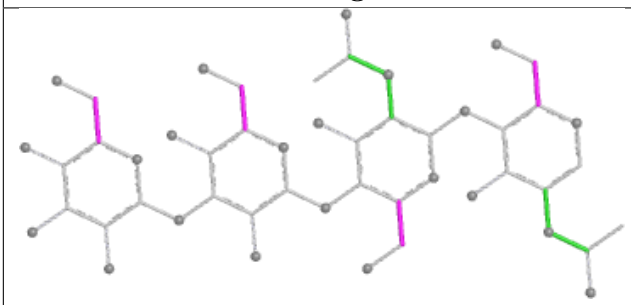
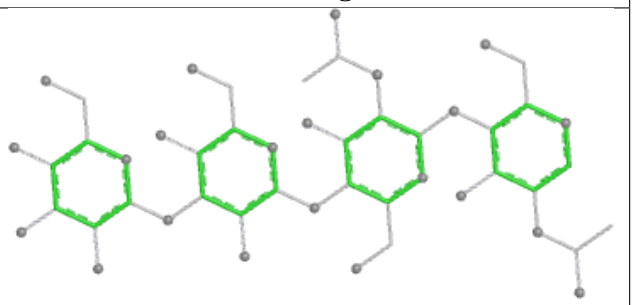
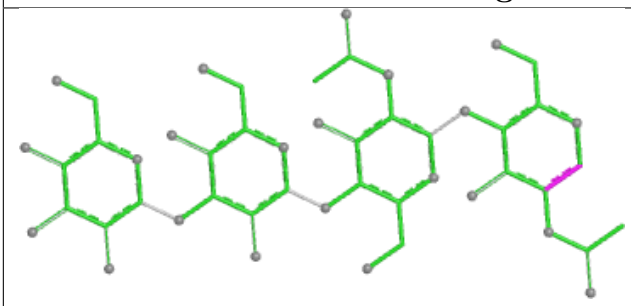


Rings

Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain J	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain P



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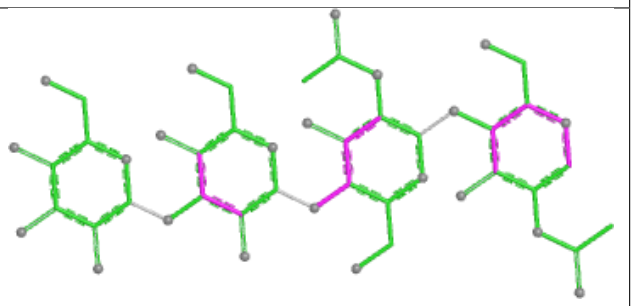

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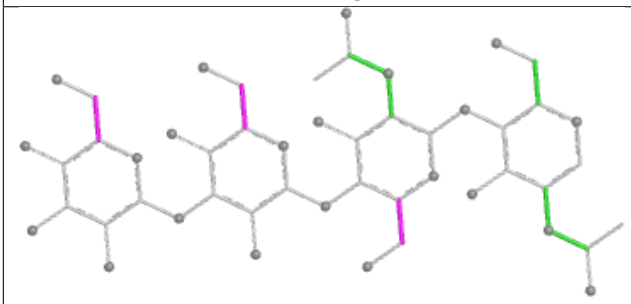

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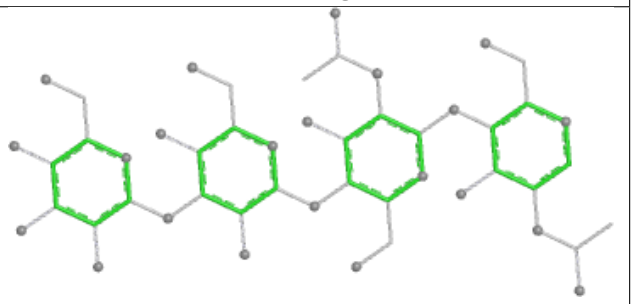
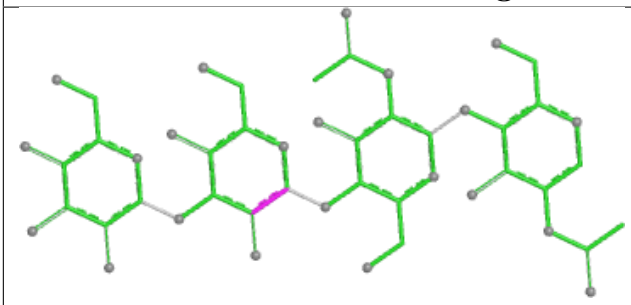


Rings

Oligosaccharide Chain T



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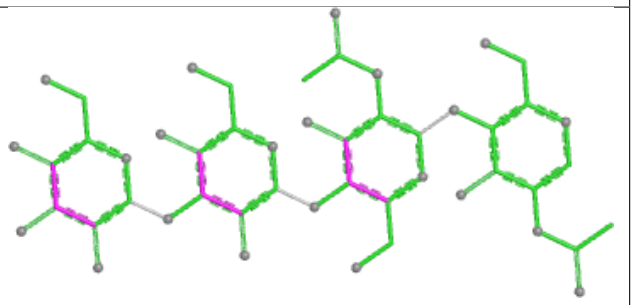
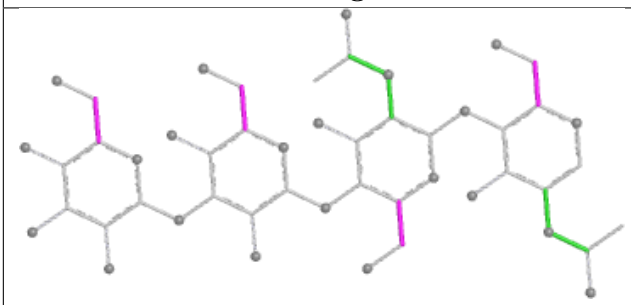


Bond angles



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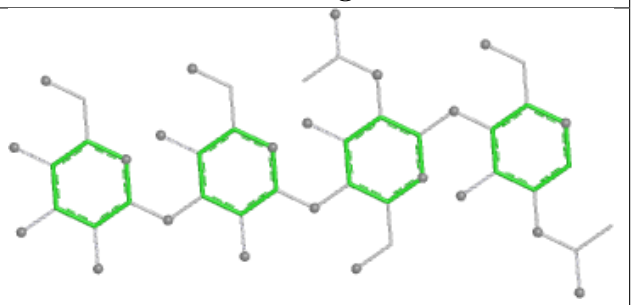
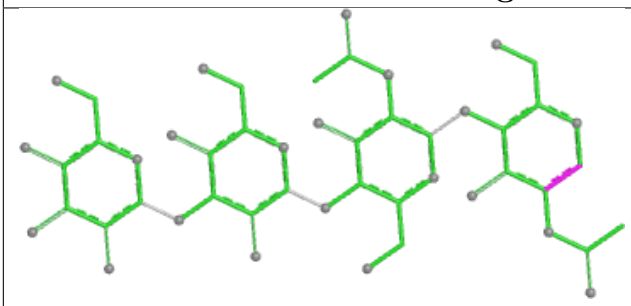
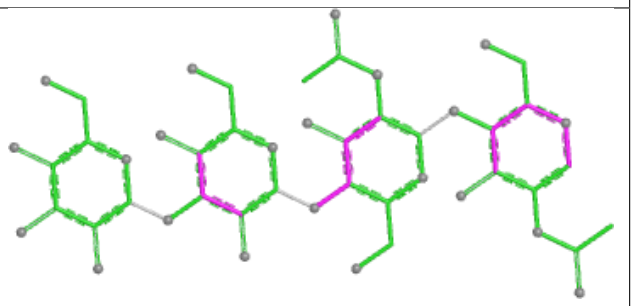


Rings

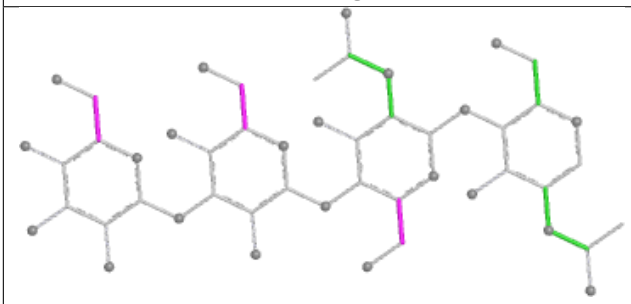
Oligosaccharide Chain Z



Bond lengths



Bond angles



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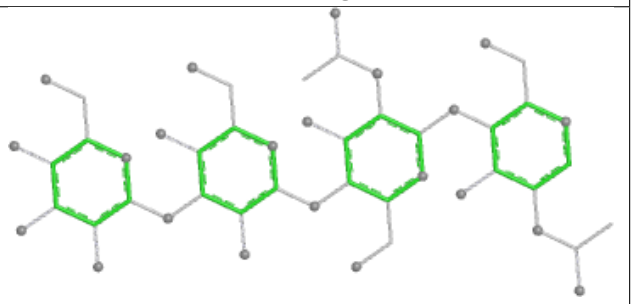
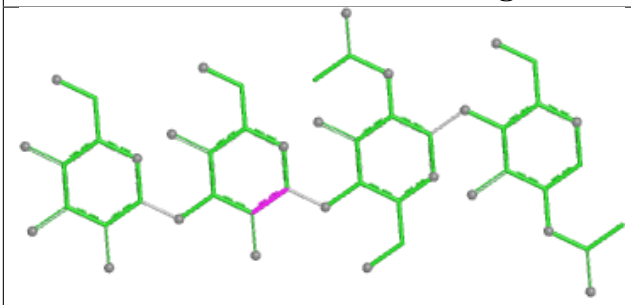
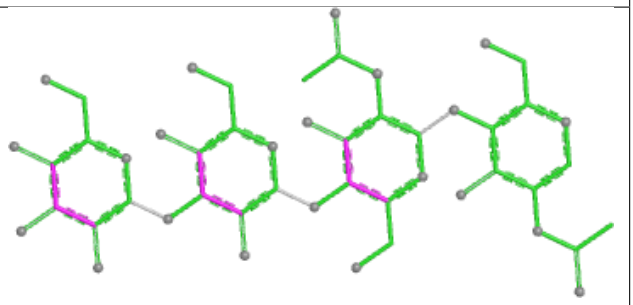


Rings

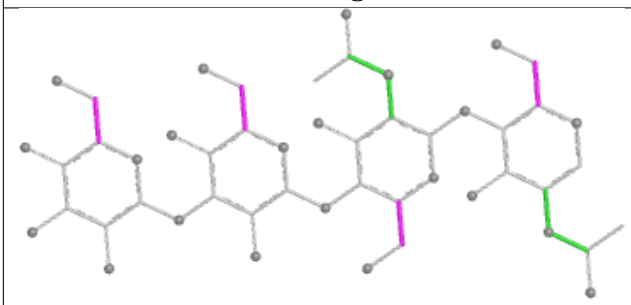
Oligosaccharide Chain d



Bond lengths



Bond angles



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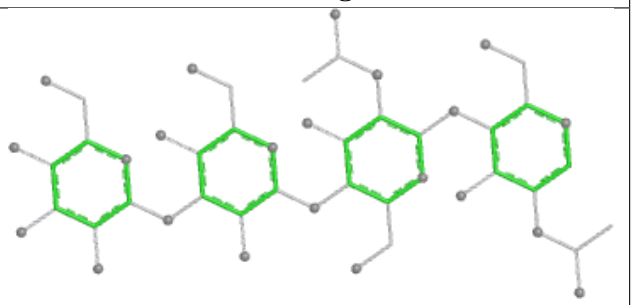
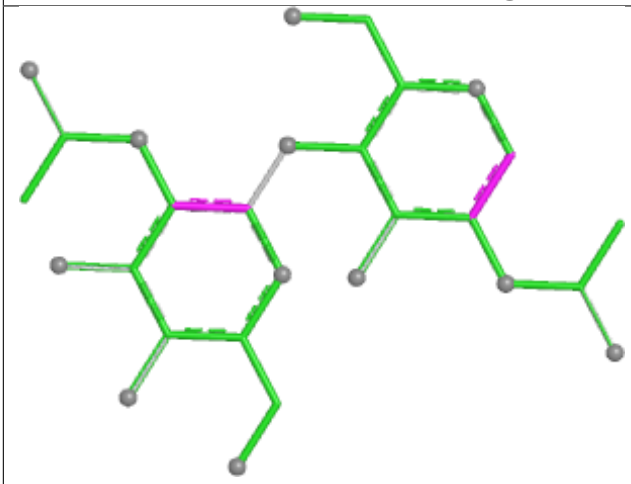
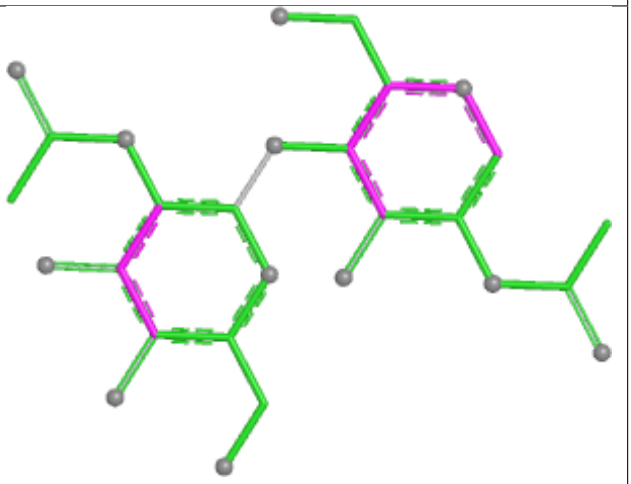


Rings

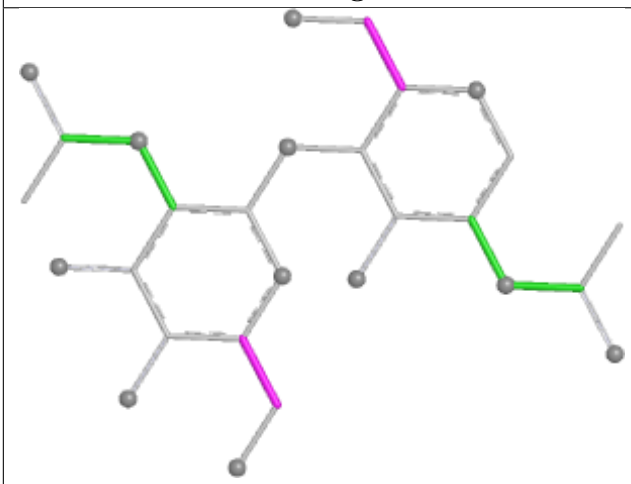
Oligosaccharide Chain I



Bond lengths



Bond angles



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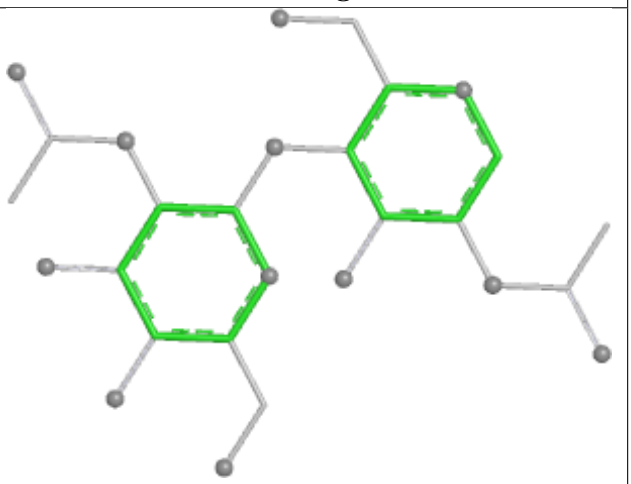
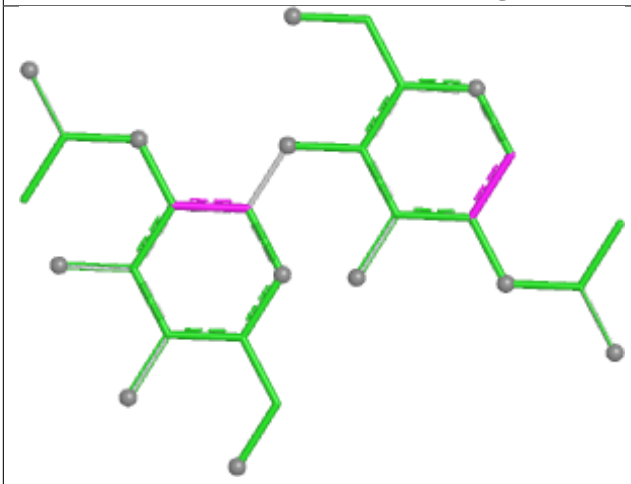
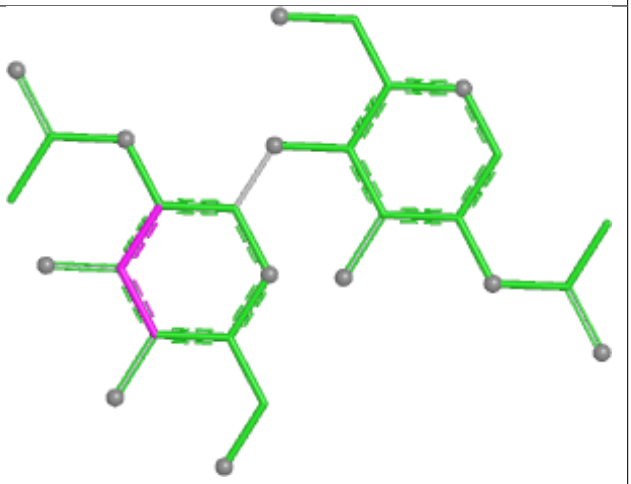


Rings

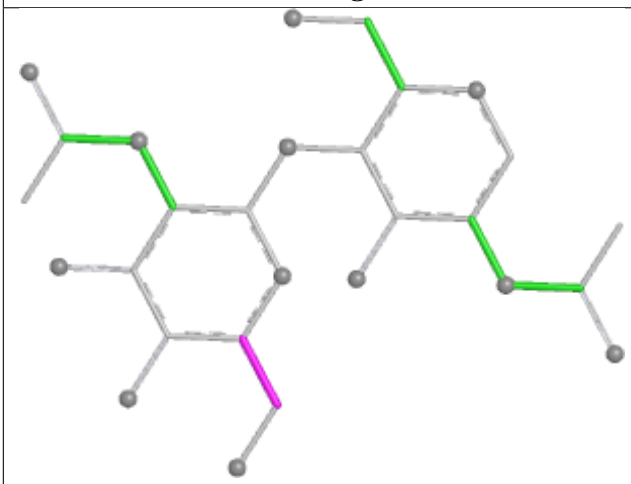
Oligosaccharide Chain K



Bond lengths



Bond angles



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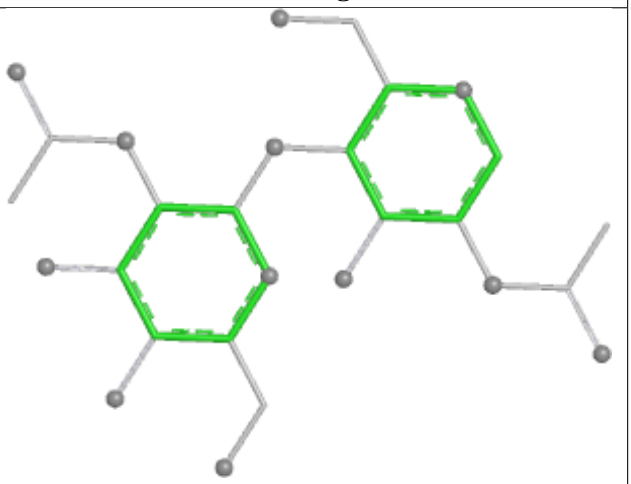
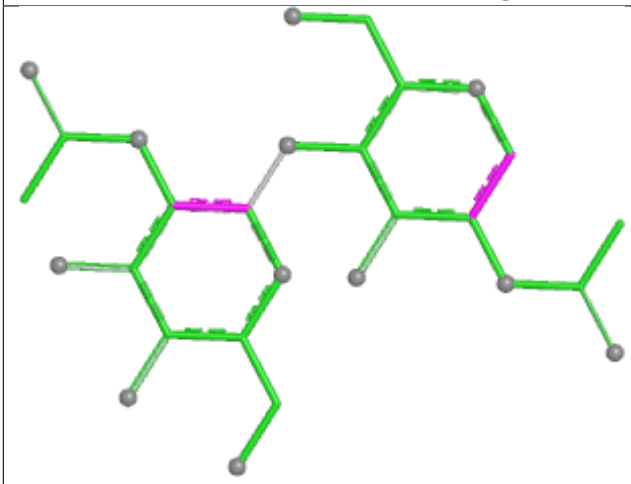


Rings

Oligosaccharide Chain L



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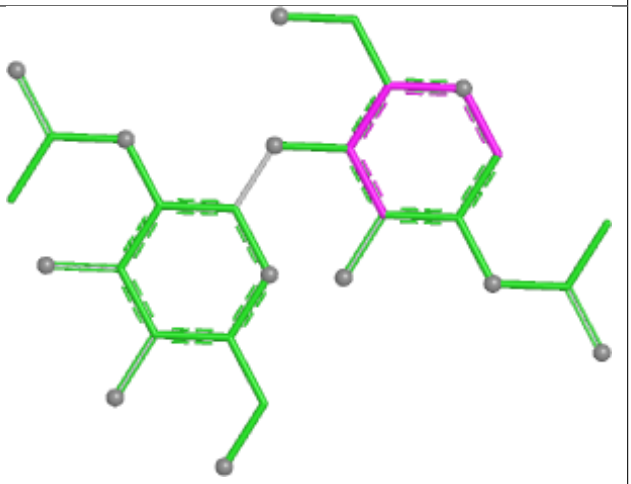

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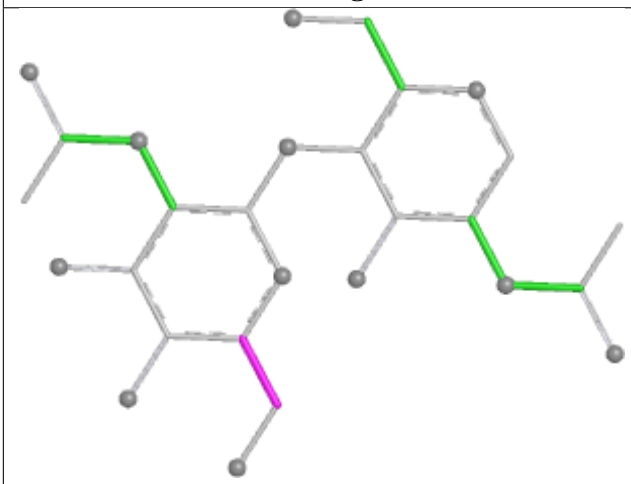

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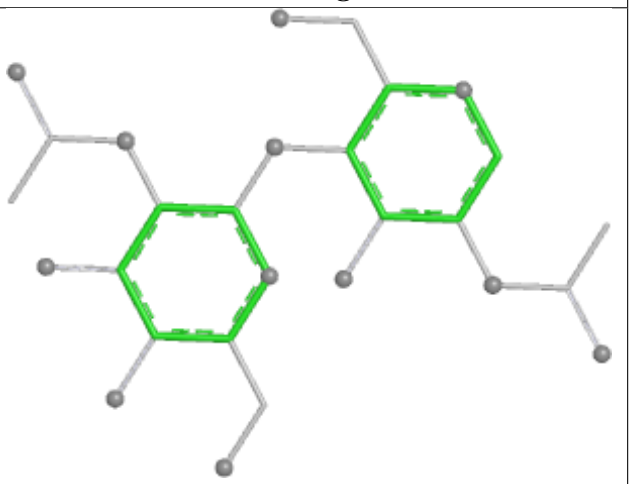
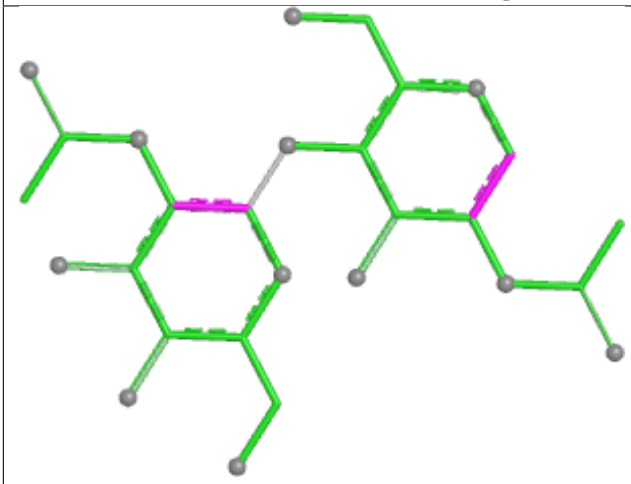


Rings

Oligosaccharide Chain S



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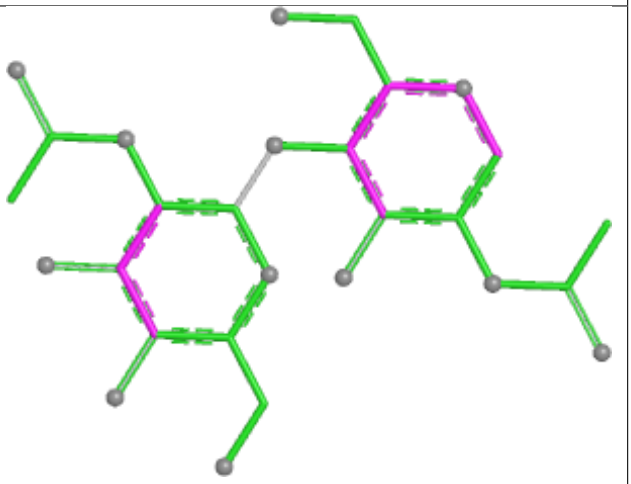
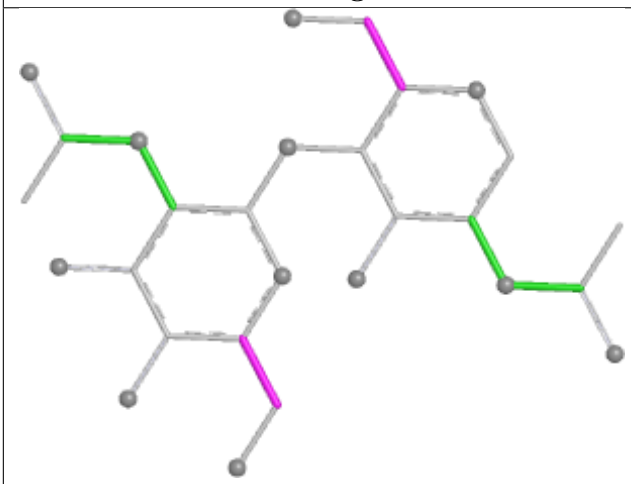


Bond angles



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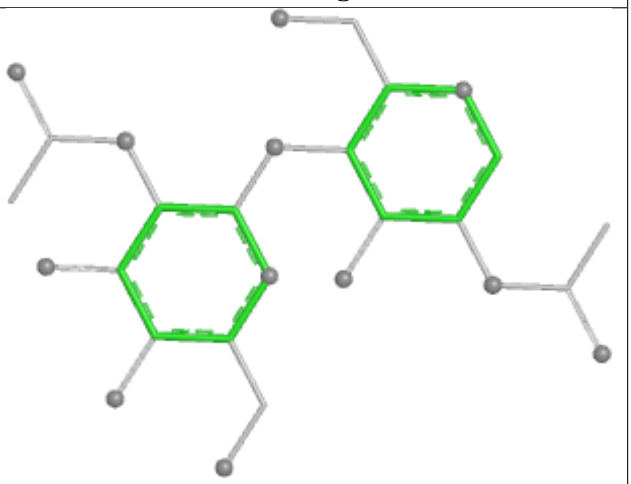
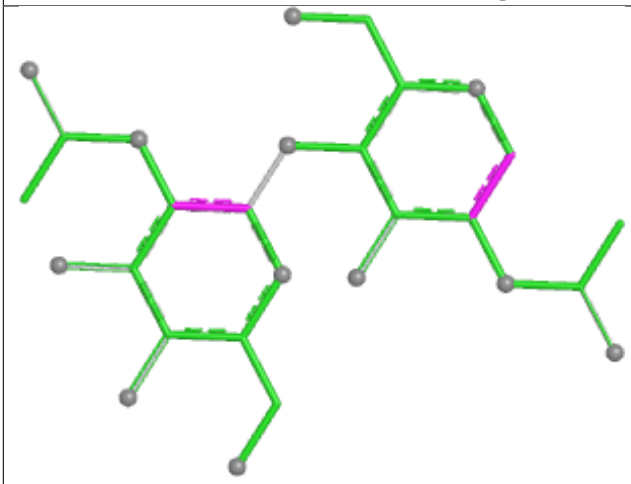
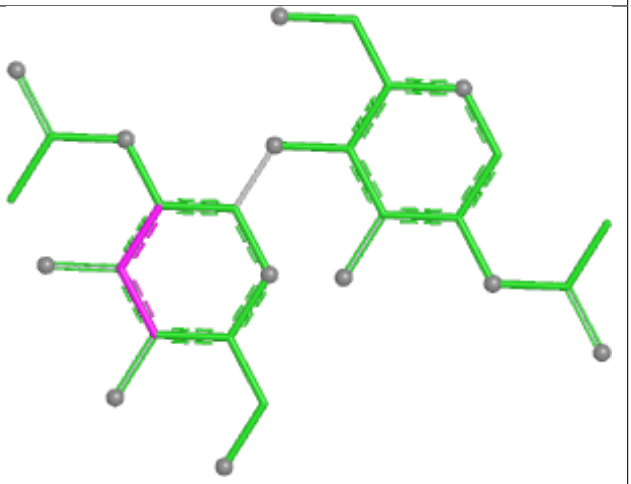


Rings

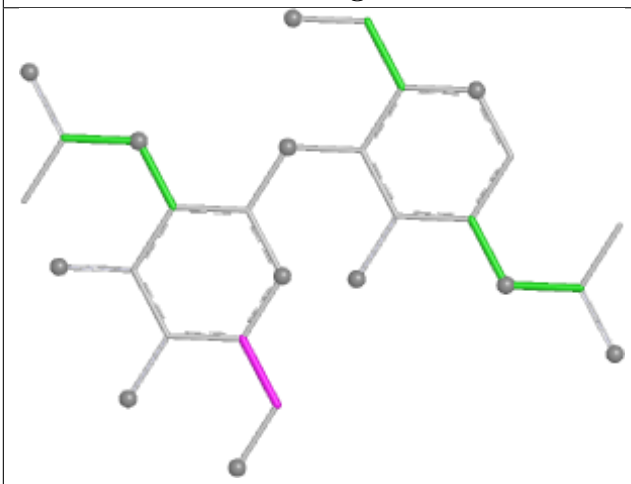
Oligosaccharide Chain U



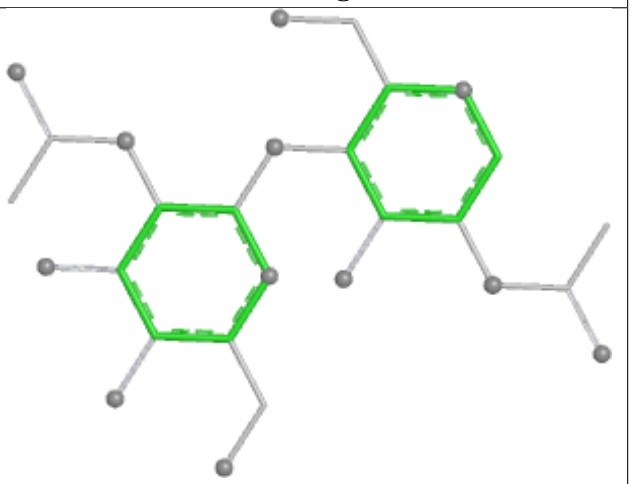
Bond lengths



Bond angles

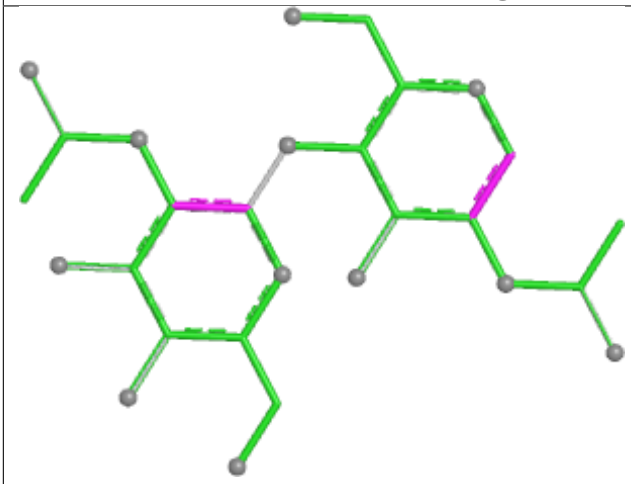


Torsions



Rings

Oligosaccharide Chain V



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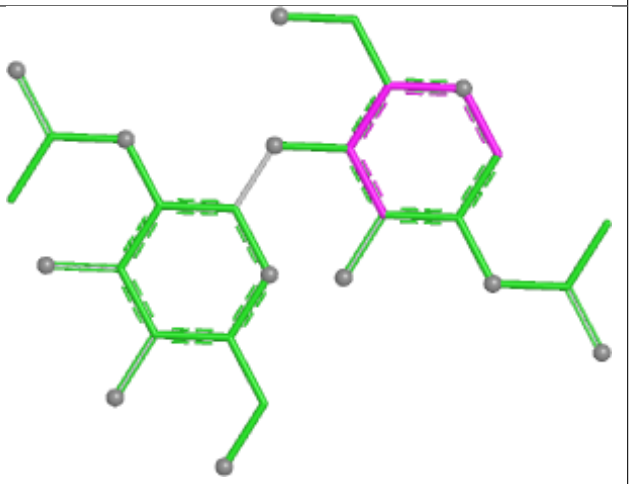
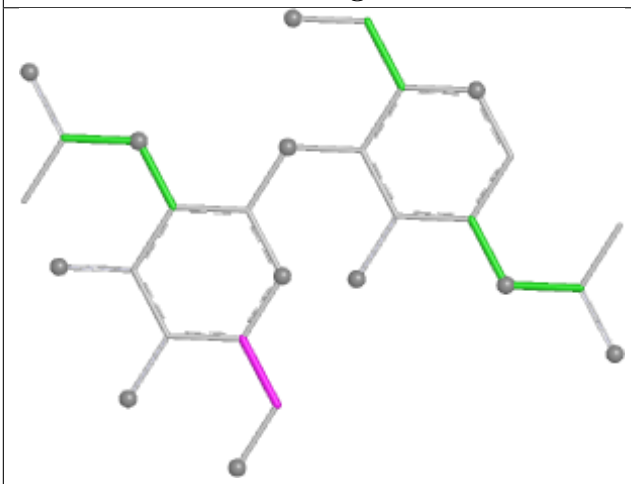


Bond angles



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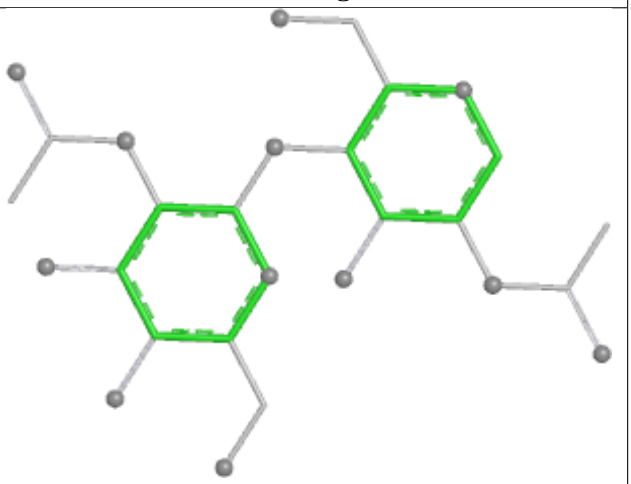
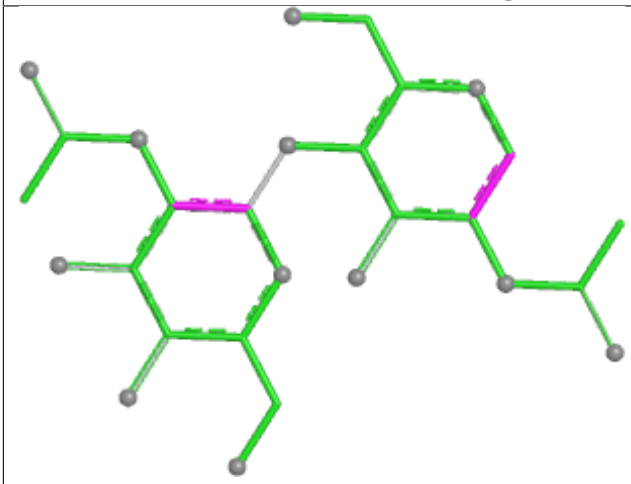
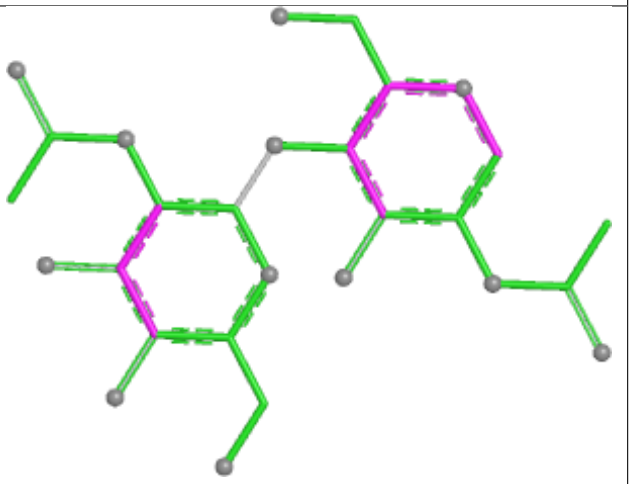


Rings

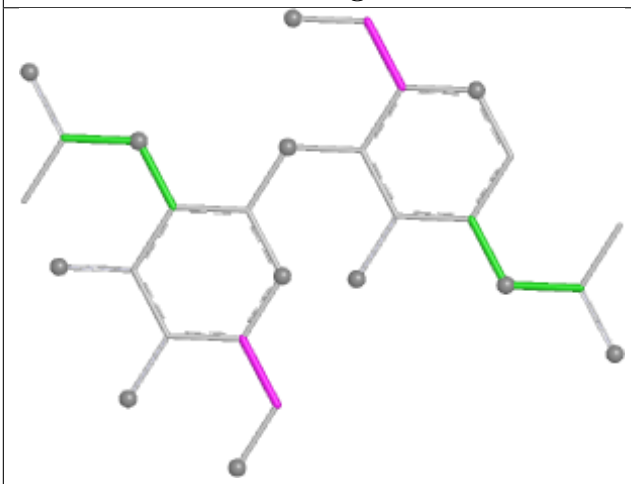
Oligosaccharide Chain c



Bond lengths



Bond angles



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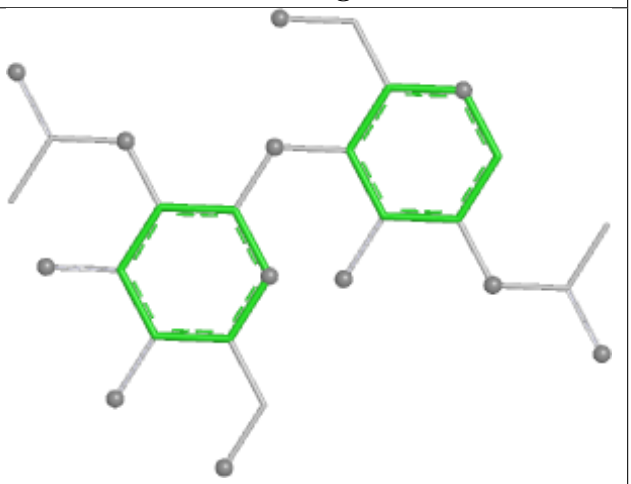
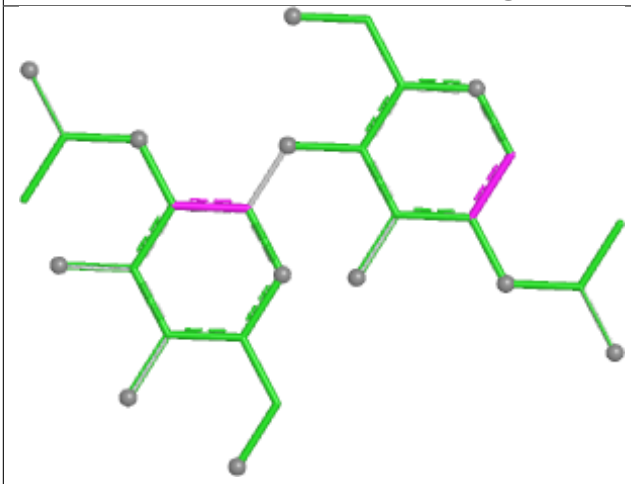
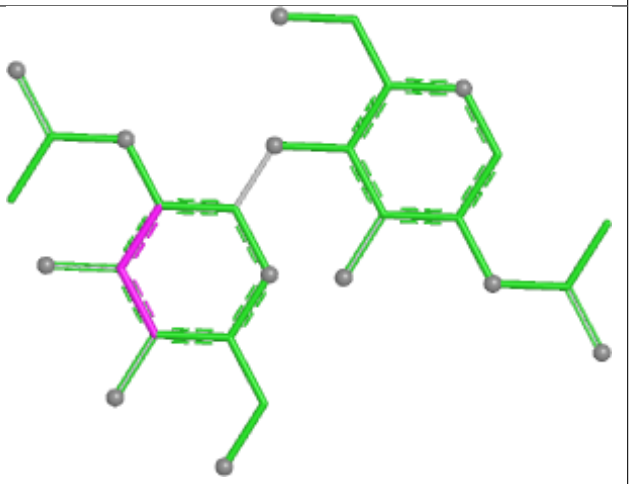


Rings

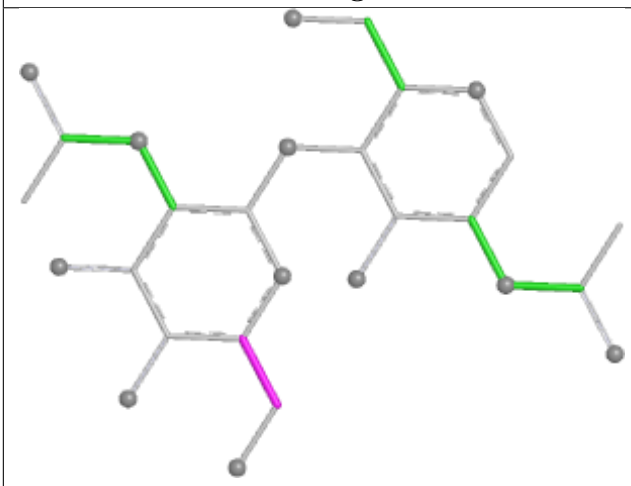
Oligosaccharide Chain e



Bond lengths



Bond angles



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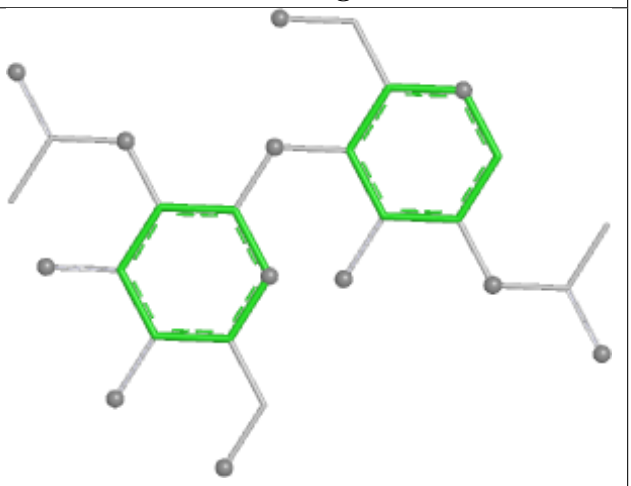
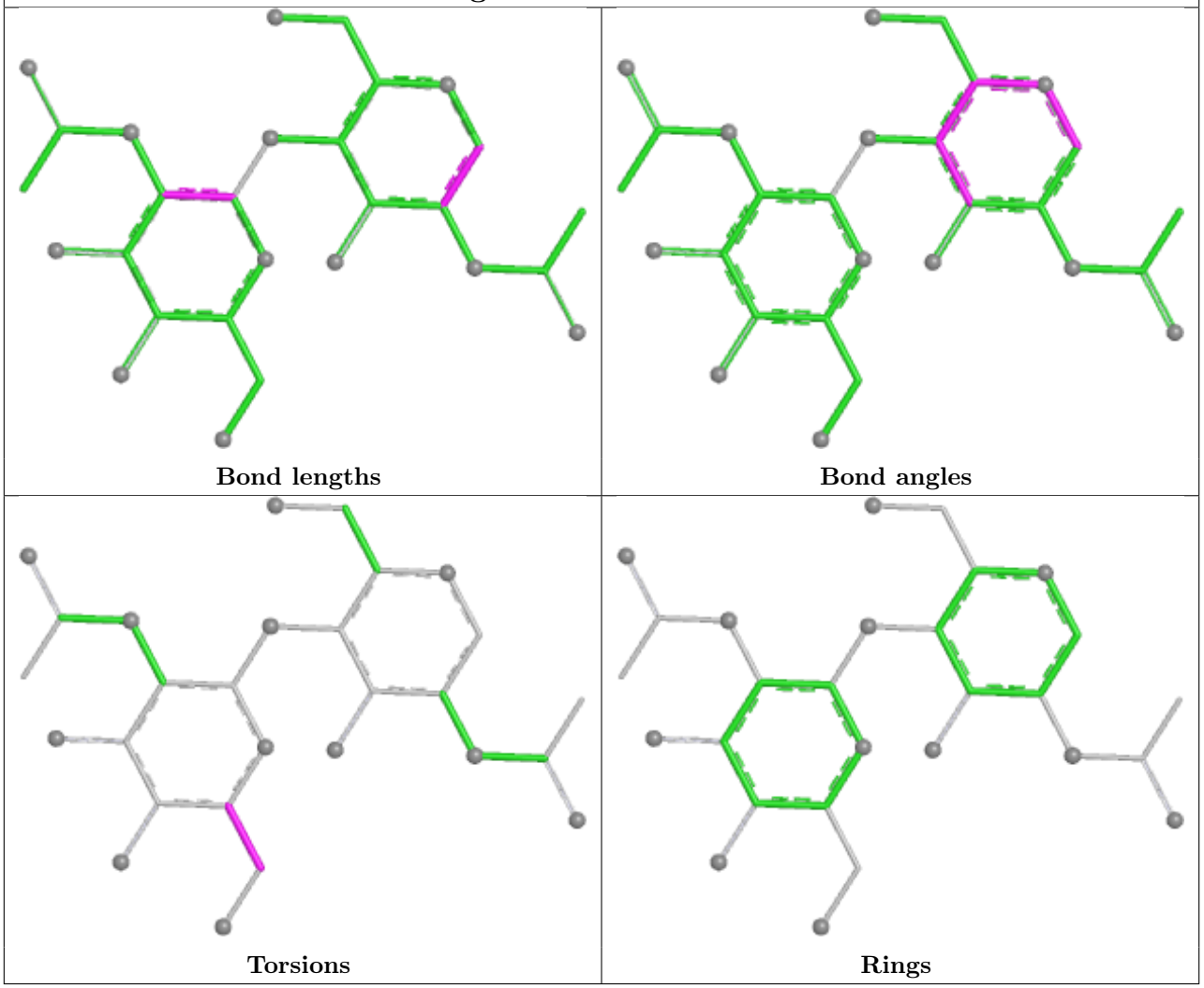


Rings

Oligosaccharide Chain f



5.6 Ligand geometry (i)

18 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	A	3197	1	14,14,15	0.86	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	C	3201	1	14,14,15	1.03	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	A	3199	1	14,14,15	0.70	1 (7%)	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	3199	1	14,14,15	0.71	1 (7%)	17,19,21	0.96	1 (5%)
5	NAG	A	3198	1	14,14,15	0.82	1 (7%)	17,19,21	0.61	0
6	MJJ	A	9999	-	25,25,25	2.34	8 (32%)	30,36,36	1.69	4 (13%)
6	MJJ	C	9999	-	25,25,25	2.35	8 (32%)	30,36,36	1.69	4 (13%)
5	NAG	A	3200	1	14,14,15	0.76	1 (7%)	17,19,21	0.80	1 (5%)
5	NAG	C	3197	1	14,14,15	0.85	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	C	3200	1	14,14,15	0.76	1 (7%)	17,19,21	0.80	1 (5%)
5	NAG	A	3201	1	14,14,15	1.03	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	B	3197	1	14,14,15	0.86	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	B	3200	1	14,14,15	0.77	1 (7%)	17,19,21	0.81	1 (5%)
6	MJJ	B	9999	-	25,25,25	2.34	8 (32%)	30,36,36	1.69	4 (13%)
5	NAG	B	3198	1	14,14,15	0.82	1 (7%)	17,19,21	0.61	0
5	NAG	C	3199	1	14,14,15	0.71	1 (7%)	17,19,21	0.95	1 (5%)
5	NAG	C	3198	1	14,14,15	0.83	1 (7%)	17,19,21	0.61	0
5	NAG	B	3201	1	14,14,15	1.03	1 (7%)	17,19,21	0.87	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	3197	1	-	2/6/23/26	0/1/1/1
5	NAG	C	3201	1	-	1/6/23/26	0/1/1/1
5	NAG	A	3199	1	-	1/6/23/26	0/1/1/1
5	NAG	B	3199	1	-	1/6/23/26	0/1/1/1
5	NAG	A	3198	1	-	1/6/23/26	0/1/1/1
6	MJJ	A	9999	-	-	1/26/44/44	0/1/1/1
6	MJJ	C	9999	-	-	1/26/44/44	0/1/1/1
5	NAG	A	3200	1	-	2/6/23/26	0/1/1/1
5	NAG	C	3197	1	-	2/6/23/26	0/1/1/1
5	NAG	C	3200	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3201	1	-	1/6/23/26	0/1/1/1
5	NAG	B	3197	1	-	2/6/23/26	0/1/1/1
5	NAG	B	3200	1	-	2/6/23/26	0/1/1/1
6	MJJ	B	9999	-	-	1/26/44/44	0/1/1/1
5	NAG	B	3198	1	-	1/6/23/26	0/1/1/1
5	NAG	C	3199	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	3198	1	-	1/6/23/26	0/1/1/1
5	NAG	B	3201	1	-	1/6/23/26	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	9999	MJJ	C4-C5	7.37	1.59	1.53
6	A	9999	MJJ	C4-C5	7.35	1.59	1.53
6	B	9999	MJJ	C4-C5	7.26	1.59	1.53
6	A	9999	MJJ	O1A-C1	3.77	1.33	1.22
6	C	9999	MJJ	O1A-C1	3.75	1.33	1.22
6	B	9999	MJJ	O1A-C1	3.75	1.33	1.22
5	C	3201	NAG	C1-C2	3.52	1.57	1.52
5	B	3201	NAG	C1-C2	3.52	1.57	1.52
5	A	3201	NAG	C1-C2	3.52	1.57	1.52
6	C	9999	MJJ	C6-C5	3.41	1.58	1.53
6	A	9999	MJJ	C6-C5	3.37	1.58	1.53
6	B	9999	MJJ	C6-C5	3.36	1.58	1.53
6	A	9999	MJJ	C8-C7	3.19	1.59	1.53
6	B	9999	MJJ	C8-C7	3.18	1.59	1.53
6	C	9999	MJJ	C8-C7	3.16	1.59	1.53
6	B	9999	MJJ	C7-C6	3.16	1.56	1.52
6	C	9999	MJJ	C7-C6	3.14	1.56	1.52
6	A	9999	MJJ	C7-C6	3.11	1.56	1.52
6	C	9999	MJJ	C3-C2	3.08	1.56	1.52
6	A	9999	MJJ	C3-C2	3.08	1.56	1.52
6	B	9999	MJJ	C3-C2	3.07	1.56	1.52
5	C	3198	NAG	C1-C2	2.77	1.56	1.52
5	A	3198	NAG	C1-C2	2.75	1.56	1.52
5	B	3198	NAG	C1-C2	2.75	1.56	1.52
5	A	3197	NAG	C1-C2	2.72	1.56	1.52
5	B	3197	NAG	C1-C2	2.71	1.56	1.52
5	C	3197	NAG	C1-C2	2.71	1.56	1.52
5	B	3200	NAG	C1-C2	2.53	1.55	1.52
5	A	3200	NAG	C1-C2	2.51	1.55	1.52
5	C	3200	NAG	C1-C2	2.51	1.55	1.52
6	C	9999	MJJ	O6-C6	2.39	1.47	1.44
6	A	9999	MJJ	O6-C6	2.36	1.47	1.44
6	B	9999	MJJ	O6-C6	2.34	1.47	1.44
6	C	9999	MJJ	O1B-C1	-2.18	1.22	1.30
6	A	9999	MJJ	O1B-C1	-2.18	1.22	1.30
6	B	9999	MJJ	O1B-C1	-2.18	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3199	NAG	C1-C2	2.15	1.55	1.52
5	B	3199	NAG	C1-C2	2.15	1.55	1.52
5	A	3199	NAG	C1-C2	2.10	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	9999	MJJ	O1B-C1-O1A	-4.98	107.93	123.86
6	C	9999	MJJ	O1B-C1-O1A	-4.97	107.95	123.86
6	B	9999	MJJ	O1B-C1-O1A	-4.97	107.95	123.86
6	A	9999	MJJ	CM2-O2-C2	4.86	121.78	115.46
6	C	9999	MJJ	CM2-O2-C2	4.84	121.75	115.46
6	B	9999	MJJ	CM2-O2-C2	4.84	121.75	115.46
5	B	3197	NAG	C4-C3-C2	-3.36	106.09	111.02
5	C	3197	NAG	C4-C3-C2	-3.35	106.11	111.02
5	A	3197	NAG	C4-C3-C2	-3.35	106.11	111.02
5	A	3201	NAG	C4-C3-C2	-2.89	106.78	111.02
5	C	3201	NAG	C4-C3-C2	-2.89	106.78	111.02
5	B	3201	NAG	C4-C3-C2	-2.89	106.79	111.02
5	A	3199	NAG	C4-C3-C2	-2.74	107.00	111.02
5	B	3199	NAG	C4-C3-C2	-2.73	107.02	111.02
5	C	3199	NAG	C4-C3-C2	-2.70	107.06	111.02
5	B	3200	NAG	C4-C3-C2	-2.63	107.17	111.02
5	A	3200	NAG	C4-C3-C2	-2.62	107.18	111.02
5	C	3200	NAG	C4-C3-C2	-2.61	107.19	111.02
6	C	9999	MJJ	O6-C2-C3	-2.32	108.23	111.35
6	A	9999	MJJ	O6-C2-C3	-2.31	108.24	111.35
6	B	9999	MJJ	O6-C2-C3	-2.30	108.26	111.35
6	C	9999	MJJ	C9-O9-CA9	2.18	122.47	117.08
6	B	9999	MJJ	C9-O9-CA9	2.17	122.43	117.08
6	A	9999	MJJ	C9-O9-CA9	2.16	122.42	117.08

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	9999	MJJ	O1B-C1-C2-O2
6	B	9999	MJJ	O1B-C1-C2-O2
6	C	9999	MJJ	O1B-C1-C2-O2
5	A	3197	NAG	C4-C5-C6-O6
5	B	3197	NAG	C4-C5-C6-O6
5	C	3197	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	3200	NAG	O5-C5-C6-O6
5	B	3200	NAG	O5-C5-C6-O6
5	C	3200	NAG	O5-C5-C6-O6
5	A	3197	NAG	O5-C5-C6-O6
5	B	3197	NAG	O5-C5-C6-O6
5	C	3197	NAG	O5-C5-C6-O6
5	A	3201	NAG	O5-C5-C6-O6
5	B	3201	NAG	O5-C5-C6-O6
5	C	3201	NAG	O5-C5-C6-O6
5	A	3200	NAG	C4-C5-C6-O6
5	B	3200	NAG	C4-C5-C6-O6
5	C	3200	NAG	C4-C5-C6-O6
5	A	3198	NAG	O5-C5-C6-O6
5	B	3198	NAG	O5-C5-C6-O6
5	C	3198	NAG	O5-C5-C6-O6
5	A	3199	NAG	O5-C5-C6-O6
5	B	3199	NAG	O5-C5-C6-O6
5	C	3199	NAG	O5-C5-C6-O6

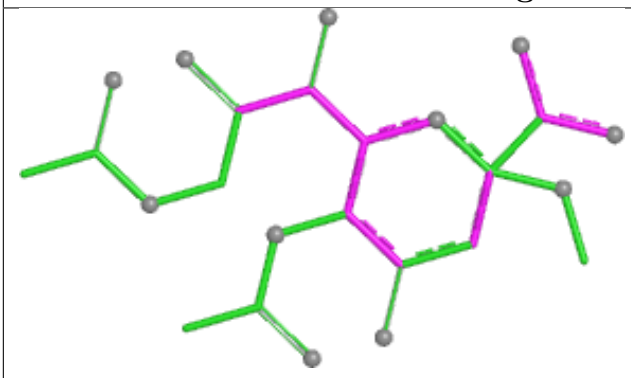
There are no ring outliers.

3 monomers are involved in 3 short contacts:

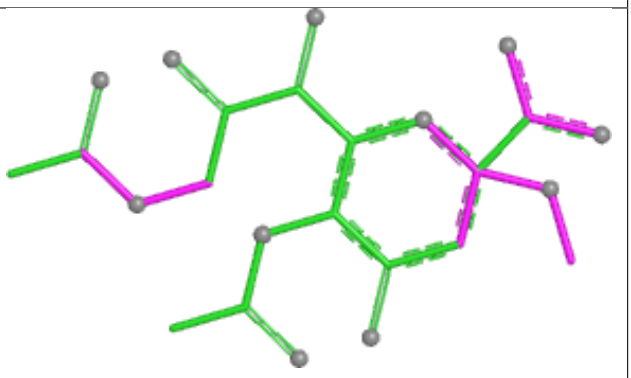
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3198	NAG	1	0
5	B	3198	NAG	1	0
5	C	3198	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

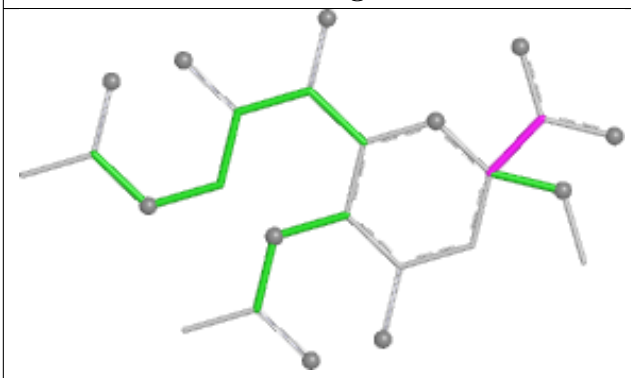
Ligand MJJ A 9999



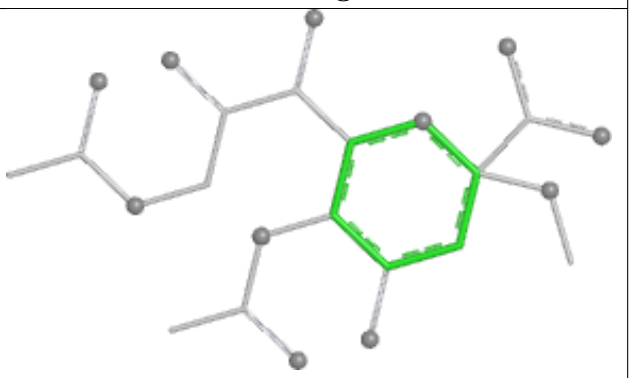
Bond lengths



Bond angles

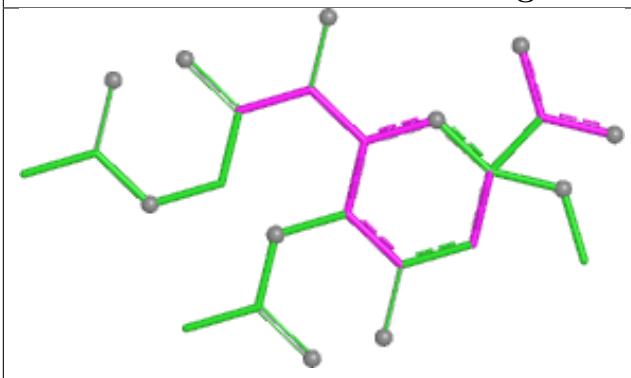


Torsions

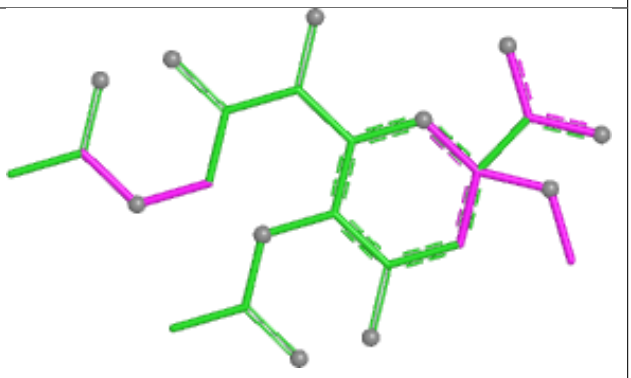


Rings

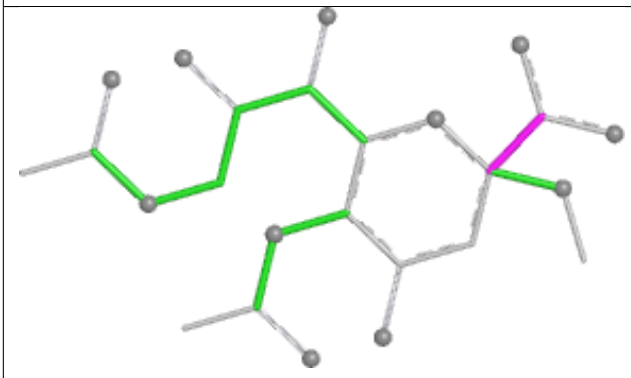
Ligand MJJ C 9999



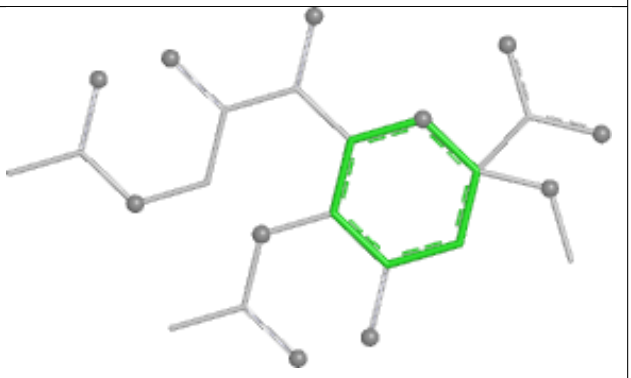
Bond lengths



Bond angles

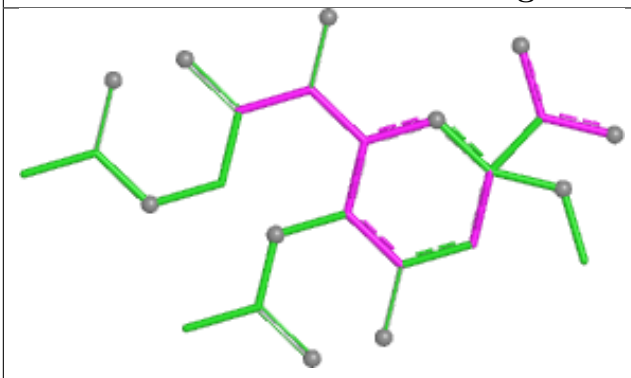


Torsions

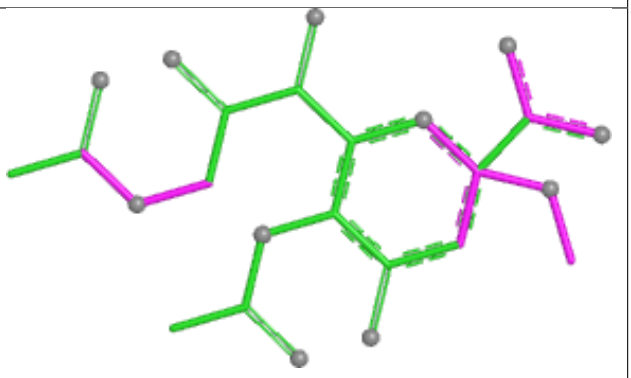


Rings

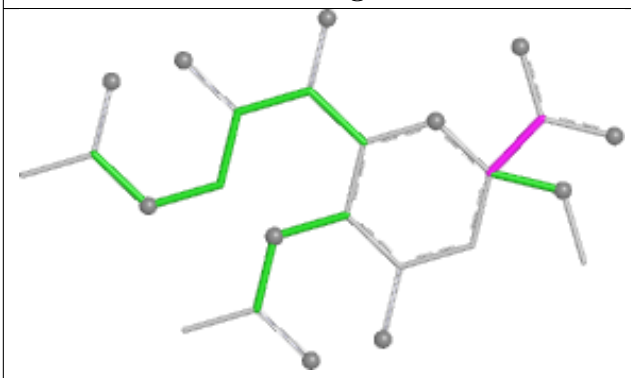
Ligand MJJ B 9999



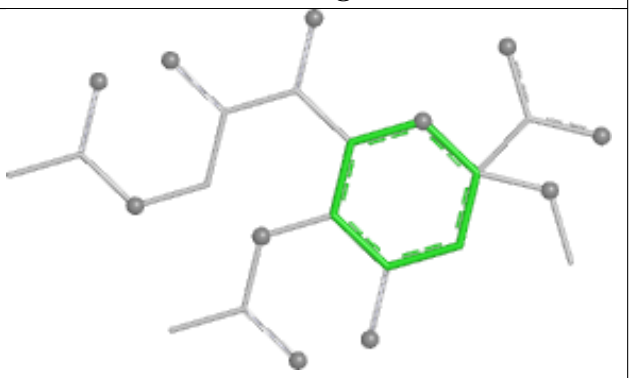
Bond lengths



Bond angles



Torsions



Rings

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.

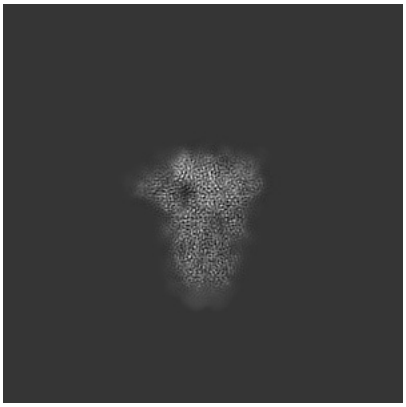
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0557. These allow visual inspection of the internal detail of the map and identification of artifacts.

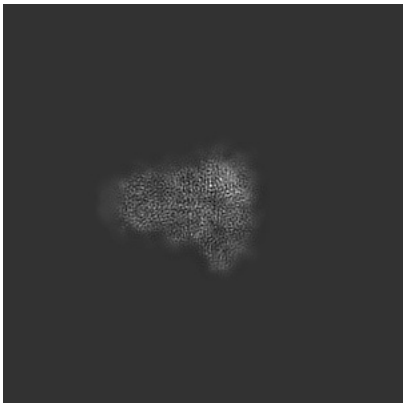
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

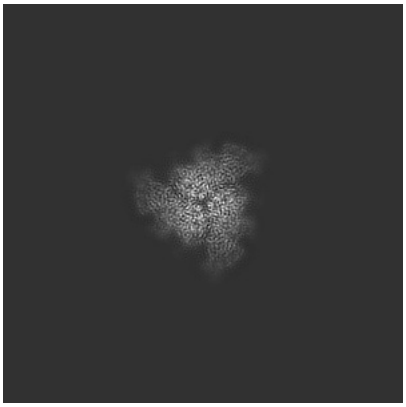
6.1.1 Primary map



X



Y

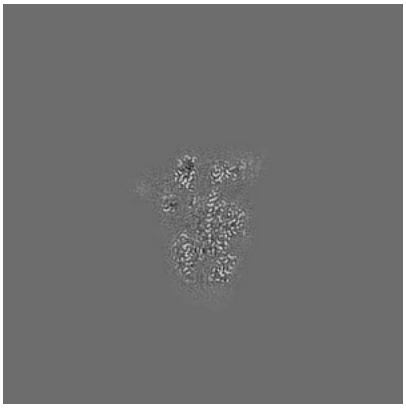


Z

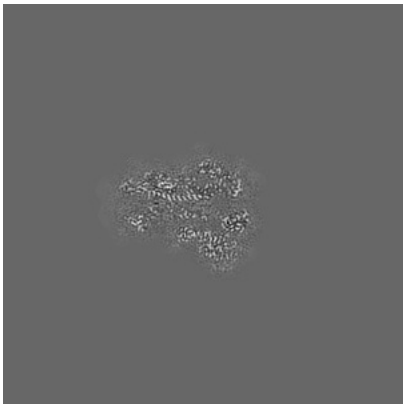
The images above show the map projected in three orthogonal directions.

6.2 Central slices

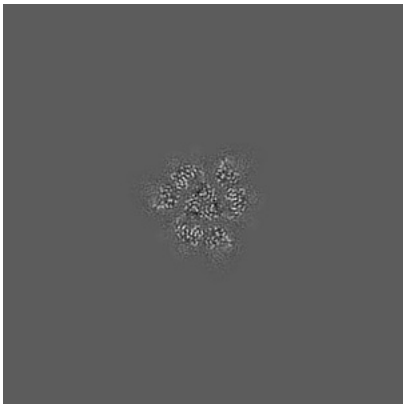
6.2.1 Primary map



X Index: 200



Y Index: 200



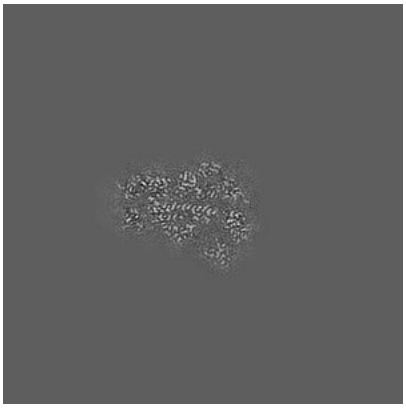
Z Index: 200

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

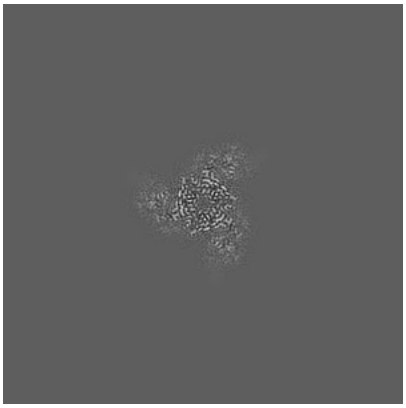
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 213



Y Index: 194

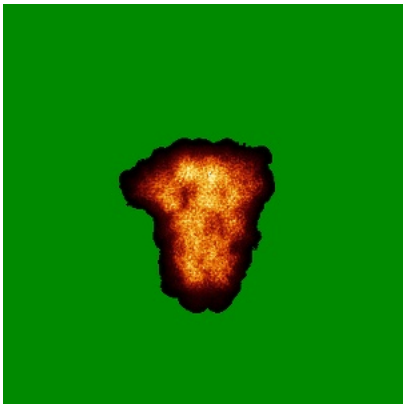


Z Index: 228

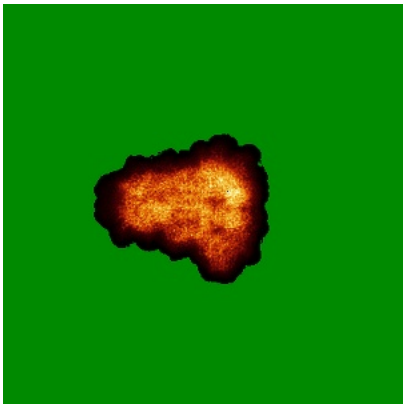
The images above show the largest variance slices of the map in three orthogonal directions.

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

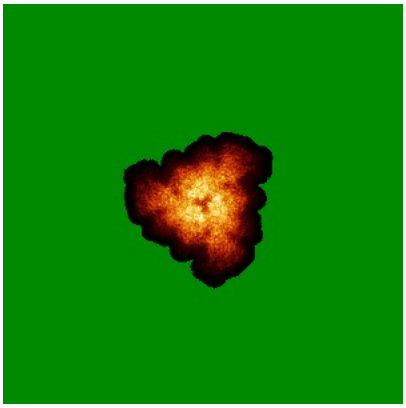
6.4.1 Primary map



X



Y



Z

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 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

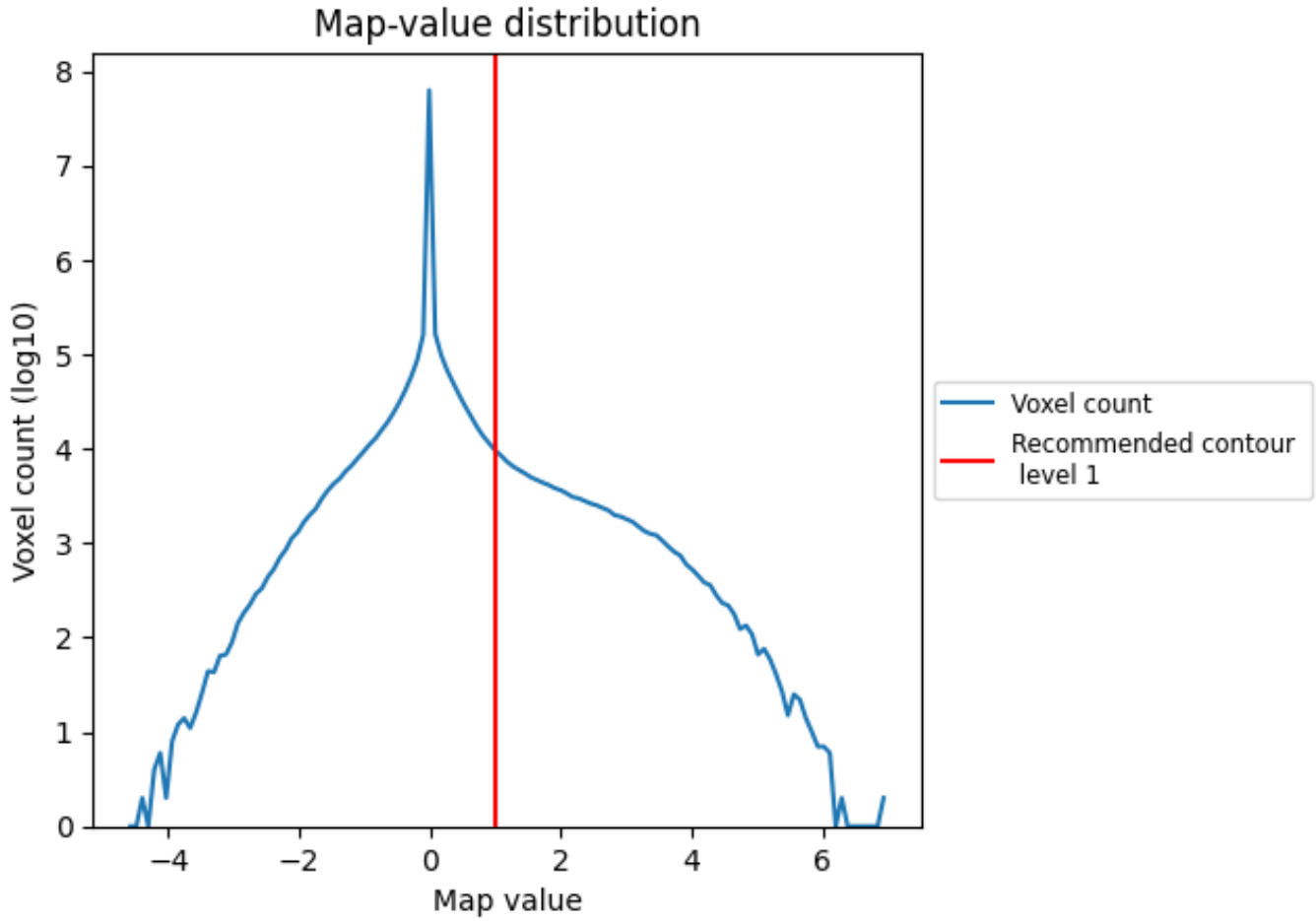
6.6 Mask visualisation (i)

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

7 Map analysis

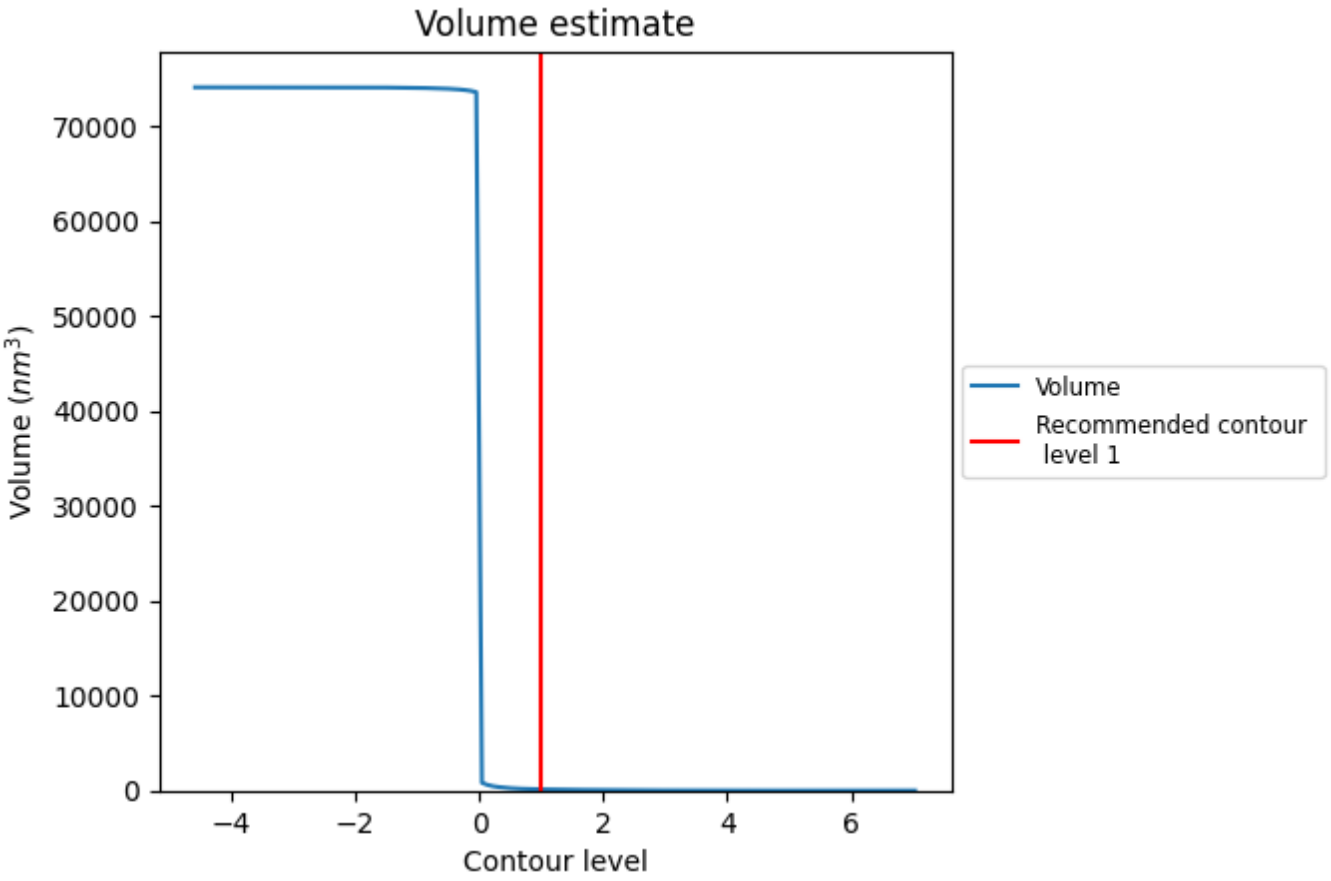
This section contains the results of statistical analysis of the map.

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.

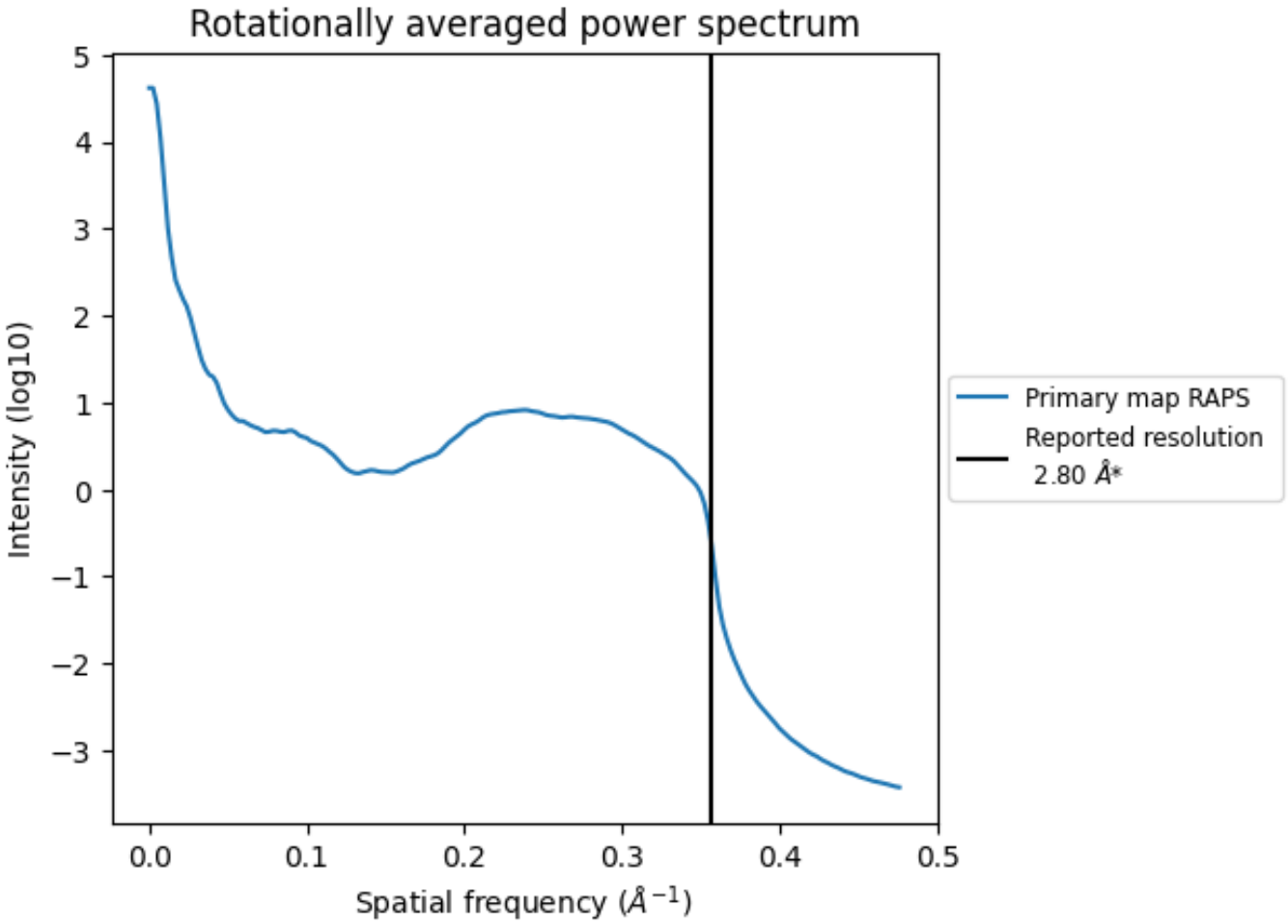
7.2 Volume estimate (i)



The volume at the recommended contour level is 128 nm^3; this corresponds to an approximate mass of 116 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}

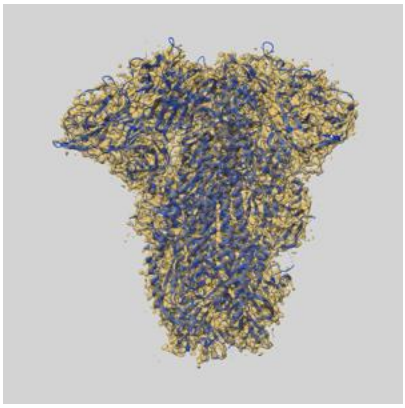
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

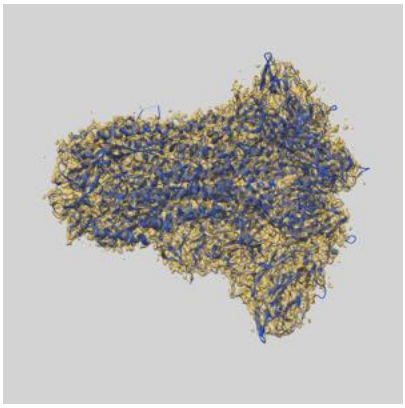
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0557 and PDB model 6NZK. Per-residue inclusion information can be found in section 3 on page 14.

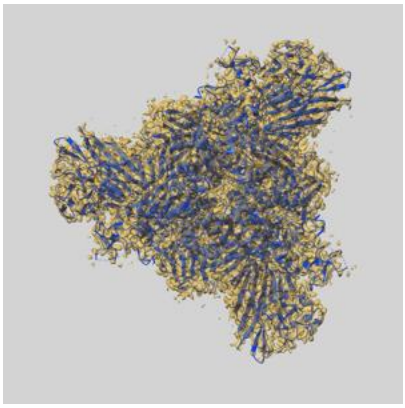
9.1 Map-model overlay



X



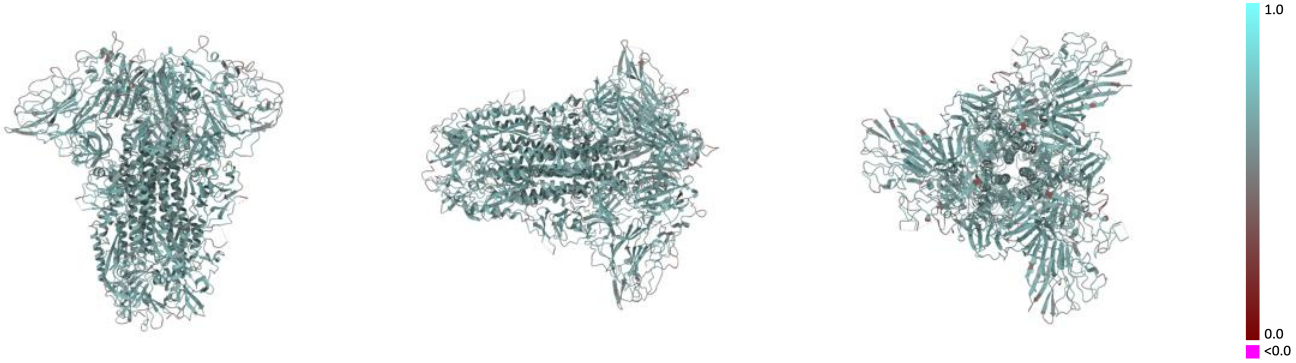
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

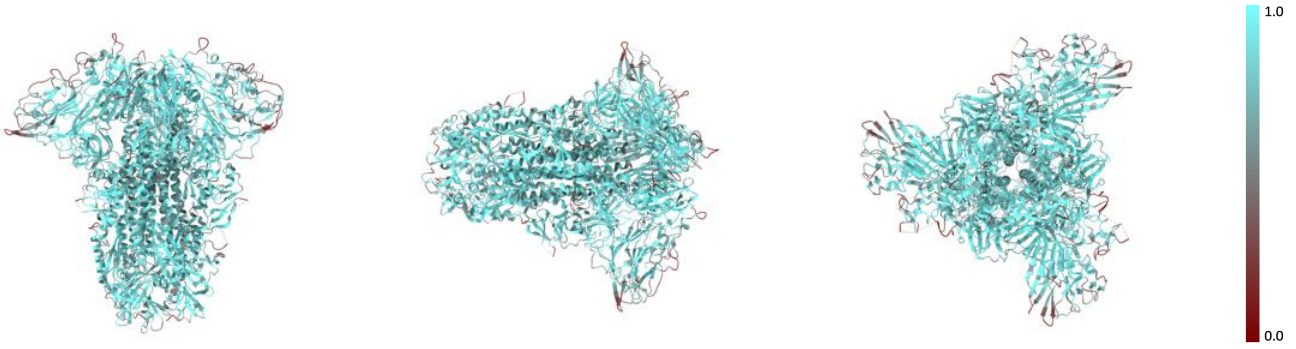
9.2 Q-score mapped to coordinate model (i)



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.

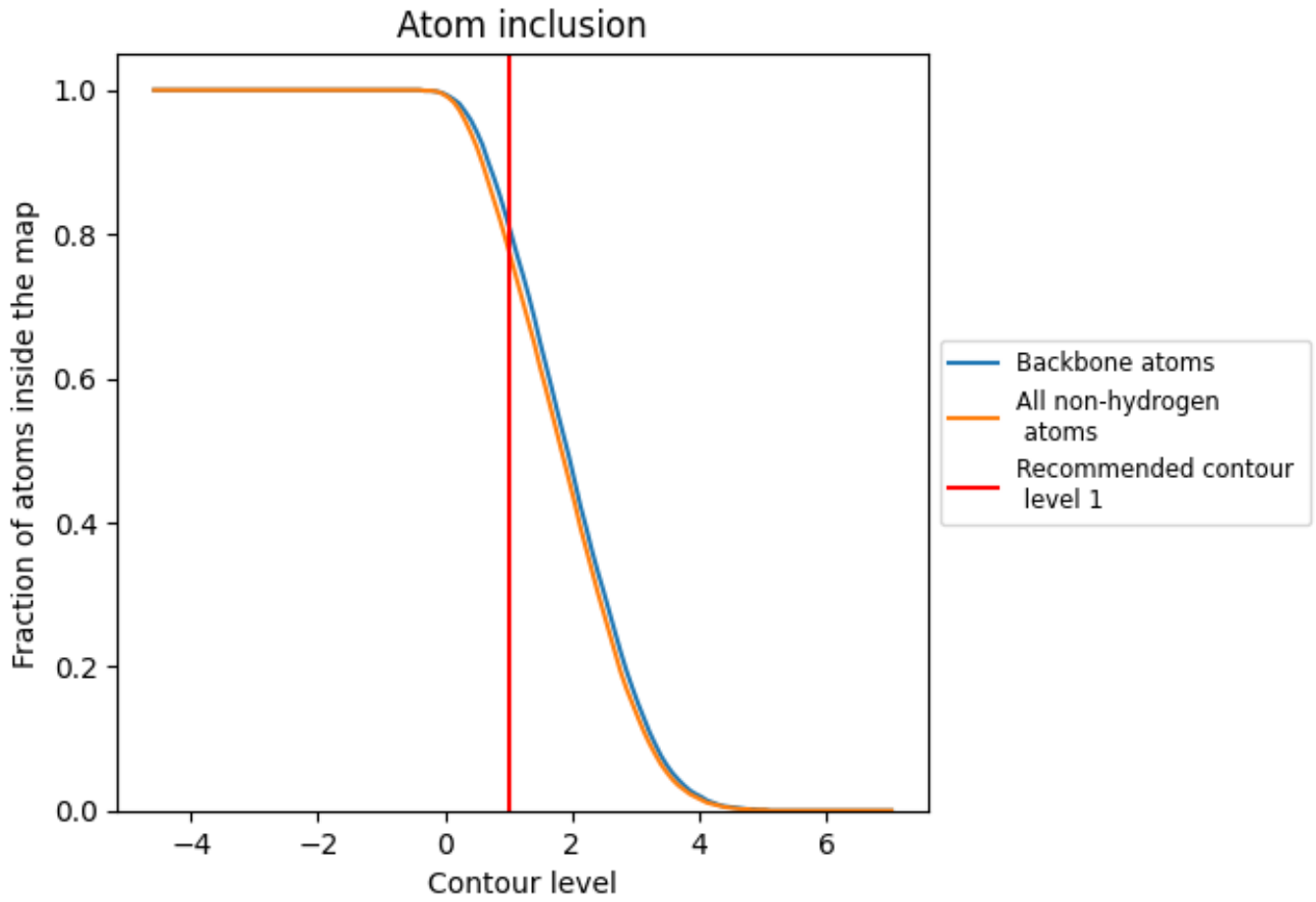
9.3 Atom inclusion mapped to coordinate model (i)



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 (1).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 78% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7790	0.5910
A	0.8090	0.6030
B	0.8070	0.6030
C	0.8100	0.6030
D	0.1030	0.3390
E	0.2310	0.3880
F	0.0400	0.2490
G	0.3330	0.3100
H	0.0260	0.2520
I	0.0000	0.3210
J	0.1600	0.2880
K	0.0000	0.2340
L	0.1790	0.3520
M	0.1030	0.3800
N	0.1030	0.3190
O	0.2310	0.3980
P	0.0400	0.2670
Q	0.3330	0.3080
R	0.0260	0.2590
S	0.0360	0.3270
T	0.1800	0.2930
U	0.0000	0.2410
V	0.1790	0.3240
W	0.0770	0.3730
X	0.1030	0.3340
Y	0.2050	0.3910
Z	0.0400	0.2460
a	0.3330	0.2970
b	0.0260	0.2640
c	0.0000	0.3300
d	0.1600	0.2860
e	0.0000	0.2510
f	0.1790	0.3360
g	0.0510	0.3710