Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 07:51 PM EST

PDB ID	:	6Q06
EMDB ID	:	EMD-20544
Title	:	MERS-CoV S structure in complex with 2,3-sialyl-N-acetyl-lactosamine
Authors	:	Park, Y.J.; Walls, A.C.; Wang, Z.; Sauer, M.; Li, W.; Tortorici, M.A.; Bosch, B.J.; DiMaio, F.D.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2019-08-01
Resolution	:	2.70 Å(reported)
Based on initial model	:	6BN3

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:

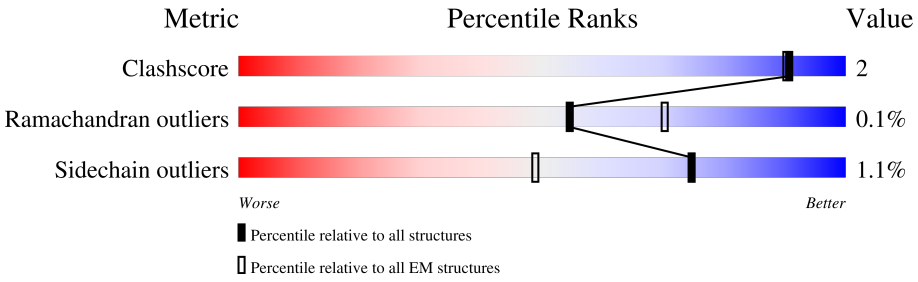
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.70 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1359	78% 6% • 15%
1	B	1359	78% 7% • 15%
1	C	1359	78% 7% • 15%
2	D	4	50% 100%
2	H	4	75% 100%
2	O	4	50% 100%
2	S	4	75% 100%
2	Z	4	50% 100%

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Mol	Chain	Length	Quality of chain
2	d	4	75% 100%
3	E	2	50% 100%
3	I	2	50% 100%
3	J	2	50% 100%
3	M	2	50% 100%
3	P	2	50% 100%
3	T	2	50% 100%
3	U	2	50% 100%
3	X	2	50% 100%
3	a	2	50% 100%
3	e	2	50% 100%
3	f	2	50% 100%
3	i	2	50% 100%
4	F	7	57% 43% 43% 14%
4	Q	7	57% 43% 57%
4	b	7	57% 43% 57%
5	G	3	67% 100%
5	R	3	100% 100%
5	c	3	67% 100%
6	K	5	40% 100%
6	L	5	60% 20% 80%
6	V	5	40% 100%
6	W	5	60% 20% 80%
6	g	5	40% 100%
6	h	5	60% 20% 80%

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Mol	Chain	Length	Quality of chain
7	N	2	50% 100%
7	Y	2	50% 100%
7	j	2	50% 100%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 28926 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1159	Total	C	N	O	S	0	0
			8952	5694	1476	1733	49		
1	B	1159	Total	C	N	O	S	0	0
			8952	5694	1476	1733	49		
1	C	1159	Total	C	N	O	S	0	0
			8952	5694	1476	1733	49		

There are 261 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP K0BRG7
A	-12	GLY	-	expression tag	UNP K0BRG7
A	-11	ILE	-	expression tag	UNP K0BRG7
A	-10	LEU	-	expression tag	UNP K0BRG7
A	-9	PRO	-	expression tag	UNP K0BRG7
A	-8	SER	-	expression tag	UNP K0BRG7
A	-7	PRO	-	expression tag	UNP K0BRG7
A	-6	GLY	-	expression tag	UNP K0BRG7
A	-5	MET	-	expression tag	UNP K0BRG7
A	-4	PRO	-	expression tag	UNP K0BRG7
A	-3	ALA	-	expression tag	UNP K0BRG7
A	-2	LEU	-	expression tag	UNP K0BRG7
A	-1	LEU	-	expression tag	UNP K0BRG7
A	0	SER	-	expression tag	UNP K0BRG7
A	1	LEU	-	expression tag	UNP K0BRG7
A	2	VAL	-	expression tag	UNP K0BRG7
A	3	SER	-	expression tag	UNP K0BRG7
A	4	LEU	-	expression tag	UNP K0BRG7
A	5	LEU	-	expression tag	UNP K0BRG7
A	6	SER	-	expression tag	UNP K0BRG7
A	7	VAL	-	expression tag	UNP K0BRG7
A	8	LEU	-	expression tag	UNP K0BRG7
A	9	LEU	-	expression tag	UNP K0BRG7
A	10	MET	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	expression tag	UNP K0BRG7
A	12	CYS	-	expression tag	UNP K0BRG7
A	13	VAL	-	expression tag	UNP K0BRG7
A	14	ALA	-	expression tag	UNP K0BRG7
A	15	GLU	-	expression tag	UNP K0BRG7
A	16	THR	-	expression tag	UNP K0BRG7
A	17	GLY	-	expression tag	UNP K0BRG7
A	18	THR	-	expression tag	UNP K0BRG7
A	748	ALA	ARG	engineered mutation	UNP K0BRG7
A	751	GLY	ARG	engineered mutation	UNP K0BRG7
A	1060	PRO	VAL	engineered mutation	UNP K0BRG7
A	1061	PRO	LEU	engineered mutation	UNP K0BRG7
A	1295	GLY	-	expression tag	UNP K0BRG7
A	1296	SER	-	expression tag	UNP K0BRG7
A	1297	GLY	-	expression tag	UNP K0BRG7
A	1298	ARG	-	expression tag	UNP K0BRG7
A	1299	GLU	-	expression tag	UNP K0BRG7
A	1300	ASN	-	expression tag	UNP K0BRG7
A	1301	LEU	-	expression tag	UNP K0BRG7
A	1302	TYR	-	expression tag	UNP K0BRG7
A	1303	PHE	-	expression tag	UNP K0BRG7
A	1304	GLN	-	expression tag	UNP K0BRG7
A	1305	GLY	-	expression tag	UNP K0BRG7
A	1306	GLY	-	expression tag	UNP K0BRG7
A	1307	GLY	-	expression tag	UNP K0BRG7
A	1308	GLY	-	expression tag	UNP K0BRG7
A	1309	SER	-	expression tag	UNP K0BRG7
A	1310	GLY	-	expression tag	UNP K0BRG7
A	1311	TYR	-	expression tag	UNP K0BRG7
A	1312	ILE	-	expression tag	UNP K0BRG7
A	1313	PRO	-	expression tag	UNP K0BRG7
A	1314	GLU	-	expression tag	UNP K0BRG7
A	1315	ALA	-	expression tag	UNP K0BRG7
A	1316	PRO	-	expression tag	UNP K0BRG7
A	1317	ARG	-	expression tag	UNP K0BRG7
A	1318	ASP	-	expression tag	UNP K0BRG7
A	1319	GLY	-	expression tag	UNP K0BRG7
A	1320	GLN	-	expression tag	UNP K0BRG7
A	1321	ALA	-	expression tag	UNP K0BRG7
A	1322	TYR	-	expression tag	UNP K0BRG7
A	1323	VAL	-	expression tag	UNP K0BRG7
A	1324	ARG	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1325	LYS	-	expression tag	UNP K0BRG7
A	1326	ASP	-	expression tag	UNP K0BRG7
A	1327	GLY	-	expression tag	UNP K0BRG7
A	1328	GLU	-	expression tag	UNP K0BRG7
A	1329	TRP	-	expression tag	UNP K0BRG7
A	1330	VAL	-	expression tag	UNP K0BRG7
A	1331	LEU	-	expression tag	UNP K0BRG7
A	1332	LEU	-	expression tag	UNP K0BRG7
A	1333	SER	-	expression tag	UNP K0BRG7
A	1334	THR	-	expression tag	UNP K0BRG7
A	1335	PHE	-	expression tag	UNP K0BRG7
A	1336	LEU	-	expression tag	UNP K0BRG7
A	1337	GLY	-	expression tag	UNP K0BRG7
A	1338	HIS	-	expression tag	UNP K0BRG7
A	1339	HIS	-	expression tag	UNP K0BRG7
A	1340	HIS	-	expression tag	UNP K0BRG7
A	1341	HIS	-	expression tag	UNP K0BRG7
A	1342	HIS	-	expression tag	UNP K0BRG7
A	1343	HIS	-	expression tag	UNP K0BRG7
A	1344	HIS	-	expression tag	UNP K0BRG7
A	1345	HIS	-	expression tag	UNP K0BRG7
B	-13	MET	-	initiating methionine	UNP K0BRG7
B	-12	GLY	-	expression tag	UNP K0BRG7
B	-11	ILE	-	expression tag	UNP K0BRG7
B	-10	LEU	-	expression tag	UNP K0BRG7
B	-9	PRO	-	expression tag	UNP K0BRG7
B	-8	SER	-	expression tag	UNP K0BRG7
B	-7	PRO	-	expression tag	UNP K0BRG7
B	-6	GLY	-	expression tag	UNP K0BRG7
B	-5	MET	-	expression tag	UNP K0BRG7
B	-4	PRO	-	expression tag	UNP K0BRG7
B	-3	ALA	-	expression tag	UNP K0BRG7
B	-2	LEU	-	expression tag	UNP K0BRG7
B	-1	LEU	-	expression tag	UNP K0BRG7
B	0	SER	-	expression tag	UNP K0BRG7
B	1	LEU	-	expression tag	UNP K0BRG7
B	2	VAL	-	expression tag	UNP K0BRG7
B	3	SER	-	expression tag	UNP K0BRG7
B	4	LEU	-	expression tag	UNP K0BRG7
B	5	LEU	-	expression tag	UNP K0BRG7
B	6	SER	-	expression tag	UNP K0BRG7
B	7	VAL	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	LEU	-	expression tag	UNP K0BRG7
B	9	LEU	-	expression tag	UNP K0BRG7
B	10	MET	-	expression tag	UNP K0BRG7
B	11	GLY	-	expression tag	UNP K0BRG7
B	12	CYS	-	expression tag	UNP K0BRG7
B	13	VAL	-	expression tag	UNP K0BRG7
B	14	ALA	-	expression tag	UNP K0BRG7
B	15	GLU	-	expression tag	UNP K0BRG7
B	16	THR	-	expression tag	UNP K0BRG7
B	17	GLY	-	expression tag	UNP K0BRG7
B	18	THR	-	expression tag	UNP K0BRG7
B	748	ALA	ARG	engineered mutation	UNP K0BRG7
B	751	GLY	ARG	engineered mutation	UNP K0BRG7
B	1060	PRO	VAL	engineered mutation	UNP K0BRG7
B	1061	PRO	LEU	engineered mutation	UNP K0BRG7
B	1295	GLY	-	expression tag	UNP K0BRG7
B	1296	SER	-	expression tag	UNP K0BRG7
B	1297	GLY	-	expression tag	UNP K0BRG7
B	1298	ARG	-	expression tag	UNP K0BRG7
B	1299	GLU	-	expression tag	UNP K0BRG7
B	1300	ASN	-	expression tag	UNP K0BRG7
B	1301	LEU	-	expression tag	UNP K0BRG7
B	1302	TYR	-	expression tag	UNP K0BRG7
B	1303	PHE	-	expression tag	UNP K0BRG7
B	1304	GLN	-	expression tag	UNP K0BRG7
B	1305	GLY	-	expression tag	UNP K0BRG7
B	1306	GLY	-	expression tag	UNP K0BRG7
B	1307	GLY	-	expression tag	UNP K0BRG7
B	1308	GLY	-	expression tag	UNP K0BRG7
B	1309	SER	-	expression tag	UNP K0BRG7
B	1310	GLY	-	expression tag	UNP K0BRG7
B	1311	TYR	-	expression tag	UNP K0BRG7
B	1312	ILE	-	expression tag	UNP K0BRG7
B	1313	PRO	-	expression tag	UNP K0BRG7
B	1314	GLU	-	expression tag	UNP K0BRG7
B	1315	ALA	-	expression tag	UNP K0BRG7
B	1316	PRO	-	expression tag	UNP K0BRG7
B	1317	ARG	-	expression tag	UNP K0BRG7
B	1318	ASP	-	expression tag	UNP K0BRG7
B	1319	GLY	-	expression tag	UNP K0BRG7
B	1320	GLN	-	expression tag	UNP K0BRG7
B	1321	ALA	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1322	TYR	-	expression tag	UNP K0BRG7
B	1323	VAL	-	expression tag	UNP K0BRG7
B	1324	ARG	-	expression tag	UNP K0BRG7
B	1325	LYS	-	expression tag	UNP K0BRG7
B	1326	ASP	-	expression tag	UNP K0BRG7
B	1327	GLY	-	expression tag	UNP K0BRG7
B	1328	GLU	-	expression tag	UNP K0BRG7
B	1329	TRP	-	expression tag	UNP K0BRG7
B	1330	VAL	-	expression tag	UNP K0BRG7
B	1331	LEU	-	expression tag	UNP K0BRG7
B	1332	LEU	-	expression tag	UNP K0BRG7
B	1333	SER	-	expression tag	UNP K0BRG7
B	1334	THR	-	expression tag	UNP K0BRG7
B	1335	PHE	-	expression tag	UNP K0BRG7
B	1336	LEU	-	expression tag	UNP K0BRG7
B	1337	GLY	-	expression tag	UNP K0BRG7
B	1338	HIS	-	expression tag	UNP K0BRG7
B	1339	HIS	-	expression tag	UNP K0BRG7
B	1340	HIS	-	expression tag	UNP K0BRG7
B	1341	HIS	-	expression tag	UNP K0BRG7
B	1342	HIS	-	expression tag	UNP K0BRG7
B	1343	HIS	-	expression tag	UNP K0BRG7
B	1344	HIS	-	expression tag	UNP K0BRG7
B	1345	HIS	-	expression tag	UNP K0BRG7
C	-13	MET	-	initiating methionine	UNP K0BRG7
C	-12	GLY	-	expression tag	UNP K0BRG7
C	-11	ILE	-	expression tag	UNP K0BRG7
C	-10	LEU	-	expression tag	UNP K0BRG7
C	-9	PRO	-	expression tag	UNP K0BRG7
C	-8	SER	-	expression tag	UNP K0BRG7
C	-7	PRO	-	expression tag	UNP K0BRG7
C	-6	GLY	-	expression tag	UNP K0BRG7
C	-5	MET	-	expression tag	UNP K0BRG7
C	-4	PRO	-	expression tag	UNP K0BRG7
C	-3	ALA	-	expression tag	UNP K0BRG7
C	-2	LEU	-	expression tag	UNP K0BRG7
C	-1	LEU	-	expression tag	UNP K0BRG7
C	0	SER	-	expression tag	UNP K0BRG7
C	1	LEU	-	expression tag	UNP K0BRG7
C	2	VAL	-	expression tag	UNP K0BRG7
C	3	SER	-	expression tag	UNP K0BRG7
C	4	LEU	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	5	LEU	-	expression tag	UNP K0BRG7
C	6	SER	-	expression tag	UNP K0BRG7
C	7	VAL	-	expression tag	UNP K0BRG7
C	8	LEU	-	expression tag	UNP K0BRG7
C	9	LEU	-	expression tag	UNP K0BRG7
C	10	MET	-	expression tag	UNP K0BRG7
C	11	GLY	-	expression tag	UNP K0BRG7
C	12	CYS	-	expression tag	UNP K0BRG7
C	13	VAL	-	expression tag	UNP K0BRG7
C	14	ALA	-	expression tag	UNP K0BRG7
C	15	GLU	-	expression tag	UNP K0BRG7
C	16	THR	-	expression tag	UNP K0BRG7
C	17	GLY	-	expression tag	UNP K0BRG7
C	18	THR	-	expression tag	UNP K0BRG7
C	748	ALA	ARG	engineered mutation	UNP K0BRG7
C	751	GLY	ARG	engineered mutation	UNP K0BRG7
C	1060	PRO	VAL	engineered mutation	UNP K0BRG7
C	1061	PRO	LEU	engineered mutation	UNP K0BRG7
C	1295	GLY	-	expression tag	UNP K0BRG7
C	1296	SER	-	expression tag	UNP K0BRG7
C	1297	GLY	-	expression tag	UNP K0BRG7
C	1298	ARG	-	expression tag	UNP K0BRG7
C	1299	GLU	-	expression tag	UNP K0BRG7
C	1300	ASN	-	expression tag	UNP K0BRG7
C	1301	LEU	-	expression tag	UNP K0BRG7
C	1302	TYR	-	expression tag	UNP K0BRG7
C	1303	PHE	-	expression tag	UNP K0BRG7
C	1304	GLN	-	expression tag	UNP K0BRG7
C	1305	GLY	-	expression tag	UNP K0BRG7
C	1306	GLY	-	expression tag	UNP K0BRG7
C	1307	GLY	-	expression tag	UNP K0BRG7
C	1308	GLY	-	expression tag	UNP K0BRG7
C	1309	SER	-	expression tag	UNP K0BRG7
C	1310	GLY	-	expression tag	UNP K0BRG7
C	1311	TYR	-	expression tag	UNP K0BRG7
C	1312	ILE	-	expression tag	UNP K0BRG7
C	1313	PRO	-	expression tag	UNP K0BRG7
C	1314	GLU	-	expression tag	UNP K0BRG7
C	1315	ALA	-	expression tag	UNP K0BRG7
C	1316	PRO	-	expression tag	UNP K0BRG7
C	1317	ARG	-	expression tag	UNP K0BRG7
C	1318	ASP	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1319	GLY	-	expression tag	UNP K0BRG7
C	1320	GLN	-	expression tag	UNP K0BRG7
C	1321	ALA	-	expression tag	UNP K0BRG7
C	1322	TYR	-	expression tag	UNP K0BRG7
C	1323	VAL	-	expression tag	UNP K0BRG7
C	1324	ARG	-	expression tag	UNP K0BRG7
C	1325	LYS	-	expression tag	UNP K0BRG7
C	1326	ASP	-	expression tag	UNP K0BRG7
C	1327	GLY	-	expression tag	UNP K0BRG7
C	1328	GLU	-	expression tag	UNP K0BRG7
C	1329	TRP	-	expression tag	UNP K0BRG7
C	1330	VAL	-	expression tag	UNP K0BRG7
C	1331	LEU	-	expression tag	UNP K0BRG7
C	1332	LEU	-	expression tag	UNP K0BRG7
C	1333	SER	-	expression tag	UNP K0BRG7
C	1334	THR	-	expression tag	UNP K0BRG7
C	1335	PHE	-	expression tag	UNP K0BRG7
C	1336	LEU	-	expression tag	UNP K0BRG7
C	1337	GLY	-	expression tag	UNP K0BRG7
C	1338	HIS	-	expression tag	UNP K0BRG7
C	1339	HIS	-	expression tag	UNP K0BRG7
C	1340	HIS	-	expression tag	UNP K0BRG7
C	1341	HIS	-	expression tag	UNP K0BRG7
C	1342	HIS	-	expression tag	UNP K0BRG7
C	1343	HIS	-	expression tag	UNP K0BRG7
C	1344	HIS	-	expression tag	UNP K0BRG7
C	1345	HIS	-	expression tag	UNP K0BRG7

- Molecule 2 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
2	D	4	Total	C	N	O	0	0
			50	28	2	20		
2	H	4	Total	C	N	O	0	0
			50	28	2	20		

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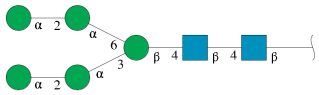
Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	4	Total	C	N	O	0	0
			50	28	2	20		
2	S	4	Total	C	N	O	0	0
			50	28	2	20		
2	Z	4	Total	C	N	O	0	0
			50	28	2	20		
2	d	4	Total	C	N	O	0	0
			50	28	2	20		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		
3	e	2	Total	C	N	O	0	0
			28	16	2	10		
3	f	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		

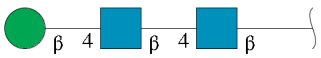
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran

ose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glu copyranose.



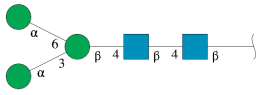
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	7	Total	C	N	O	0	0
			83	46	2	35		
4	Q	7	Total	C	N	O	0	0
			83	46	2	35		
4	b	7	Total	C	N	O	0	0
			83	46	2	35		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	R	3	Total	C	N	O	0	0
			39	22	2	15		
5	c	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	5	Total	C	N	O	0	0
			61	34	2	25		
6	L	5	Total	C	N	O	0	0
			61	34	2	25		

Continued on next page...

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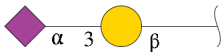
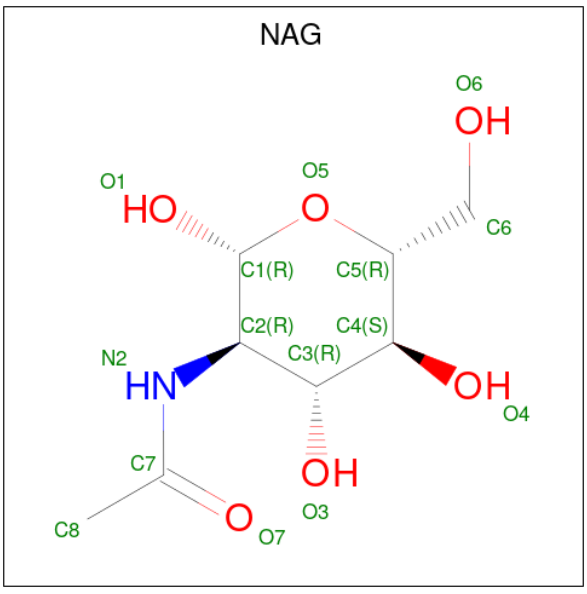
Mol	Chain	Residues	Atoms				AltConf	Trace
6	V	5	Total	C	N	O	0	0
			61	34	2	25		
6	W	5	Total	C	N	O	0	0
			61	34	2	25		
6	g	5	Total	C	N	O	0	0
			61	34	2	25		
6	h	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	2	Total	C	N	O	0	0
			32	17	1	14		
7	Y	2	Total	C	N	O	0	0
			32	17	1	14		
7	j	2	Total	C	N	O	0	0
			32	17	1	14		

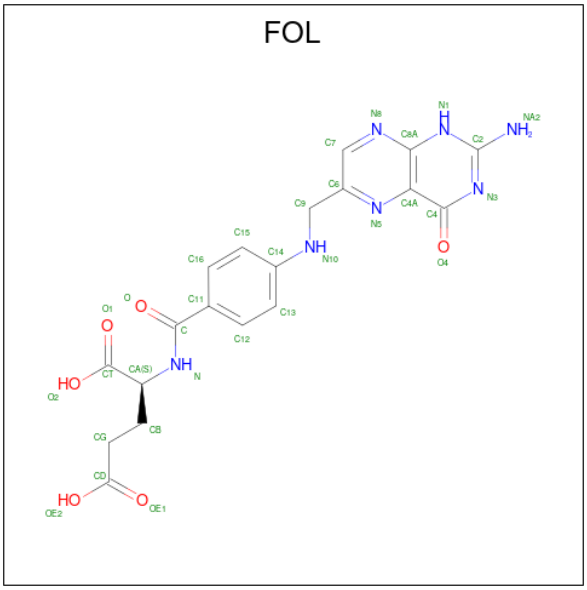
- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total 98	C 56	N 7	O 35	0
8	A	1	Total 98	C 56	N 7	O 35	0
8	A	1	Total 98	C 56	N 7	O 35	0
8	A	1	Total 98	C 56	N 7	O 35	0
8	A	1	Total 98	C 56	N 7	O 35	0
8	A	1	Total 98	C 56	N 7	O 35	0
8	A	1	Total 98	C 56	N 7	O 35	0
8	B	1	Total 98	C 56	N 7	O 35	0
8	B	1	Total 98	C 56	N 7	O 35	0
8	B	1	Total 98	C 56	N 7	O 35	0
8	B	1	Total 98	C 56	N 7	O 35	0
8	B	1	Total 98	C 56	N 7	O 35	0
8	B	1	Total 98	C 56	N 7	O 35	0
8	B	1	Total 98	C 56	N 7	O 35	0
8	C	1	Total 98	C 56	N 7	O 35	0
8	C	1	Total 98	C 56	N 7	O 35	0
8	C	1	Total 98	C 56	N 7	O 35	0
8	C	1	Total 98	C 56	N 7	O 35	0
8	C	1	Total 98	C 56	N 7	O 35	0
8	C	1	Total 98	C 56	N 7	O 35	0
8	C	1	Total 98	C 56	N 7	O 35	0

- Molecule 9 is FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C N O 32 19 7 6	0
9	B	1	Total C N O 32 19 7 6	0
9	C	1	Total C N O 32 19 7 6	0

- Molecule 10 is water.

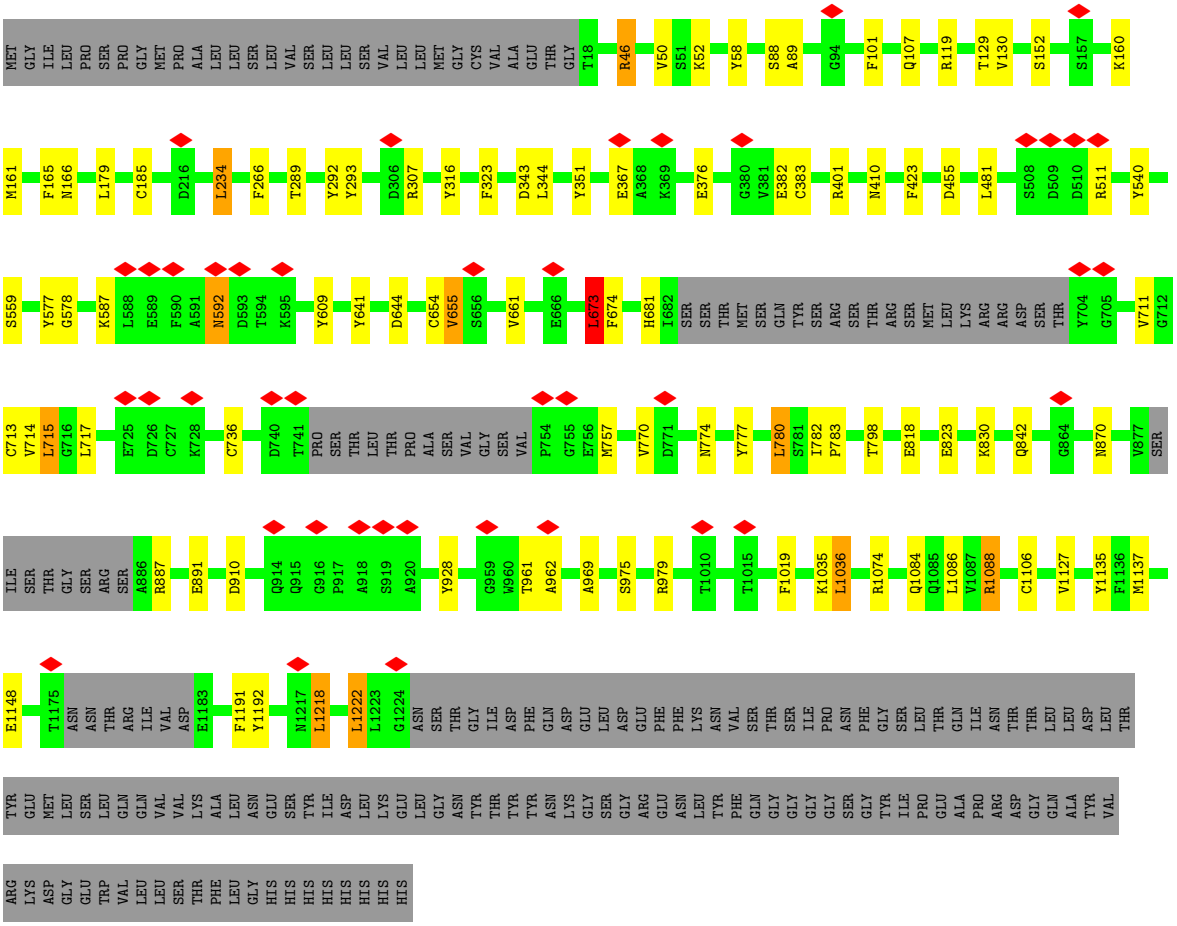
Mol	Chain	Residues	Atoms	AltConf
10	A	72	Total O 72 72	0
10	B	72	Total O 72 72	0
10	C	72	Total O 72 72	0

3 Residue-property plots (i)

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

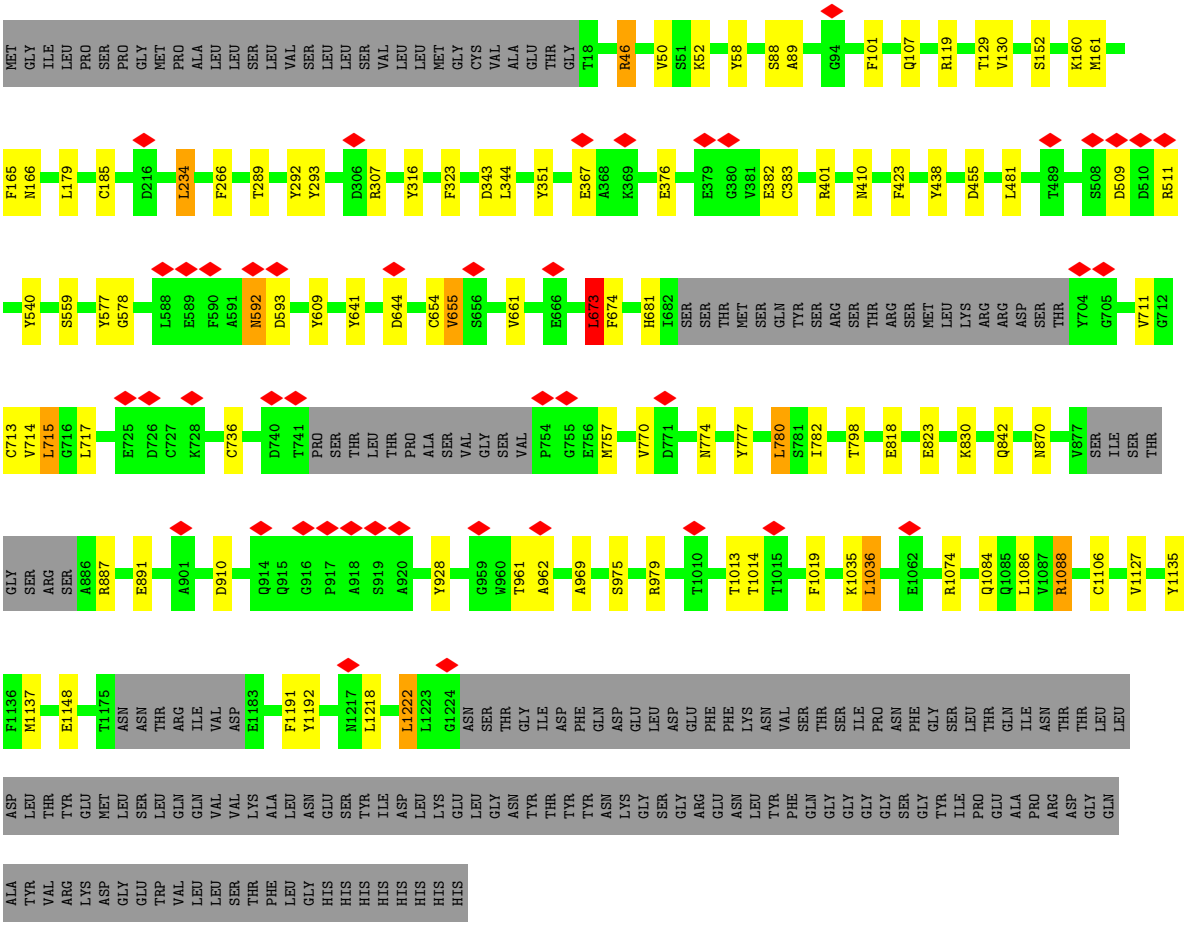
• Molecule 1: Spike glycoprotein

Chain A:



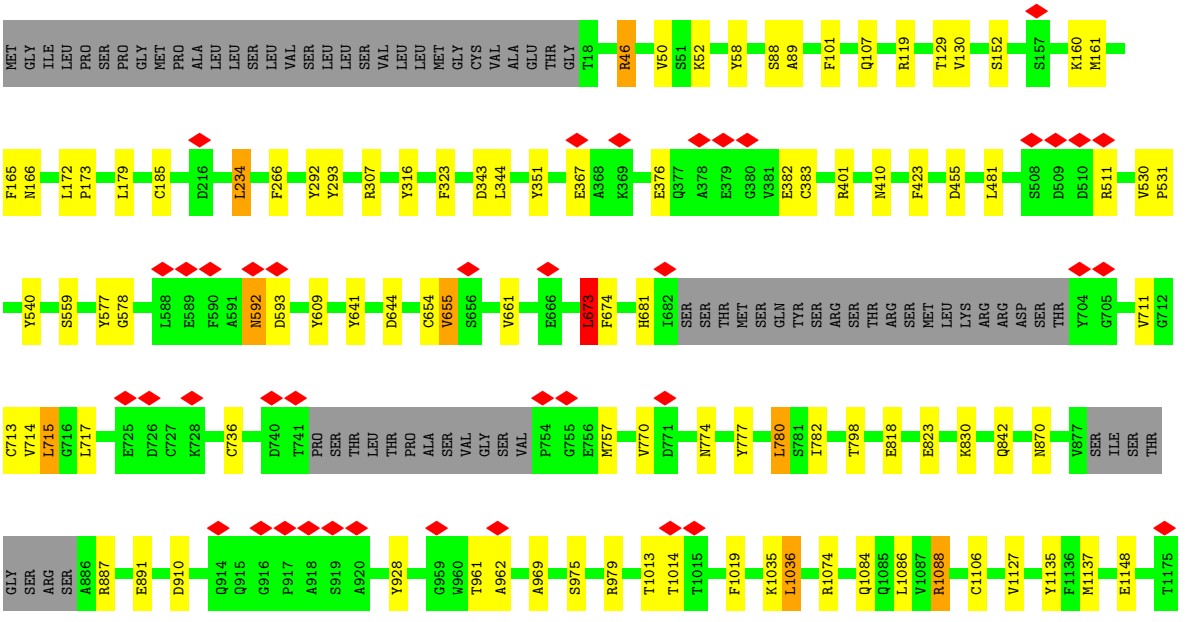
• Molecule 1: Spike glycoprotein

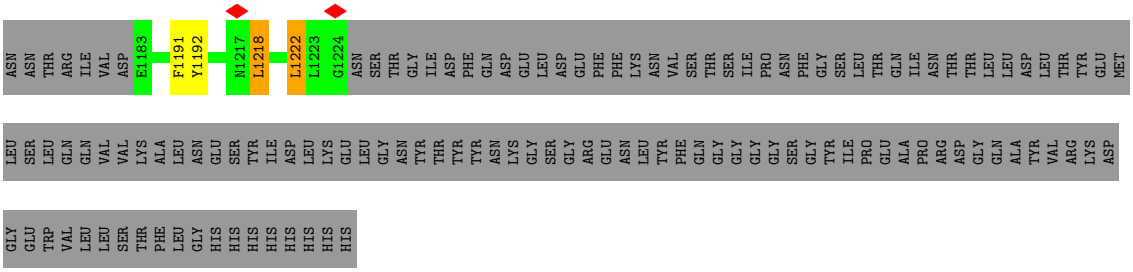
Chain B:



• Molecule 1: Spike glycoprotein

Chain C:



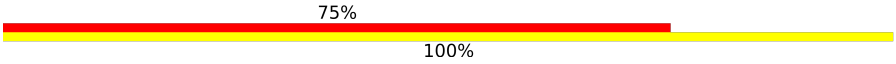


• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

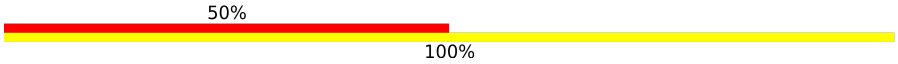
• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain O:

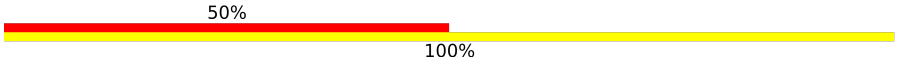


• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

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

Chain Z:

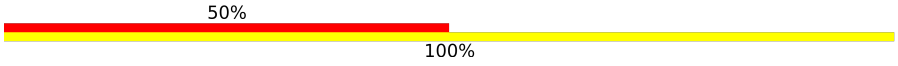


• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

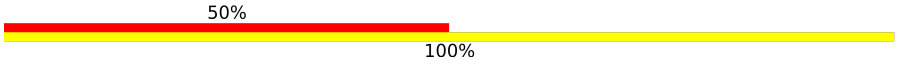
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain I:

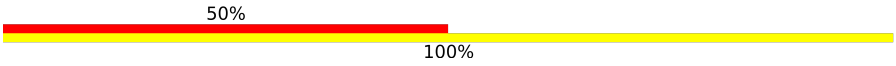


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

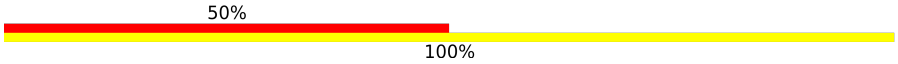
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



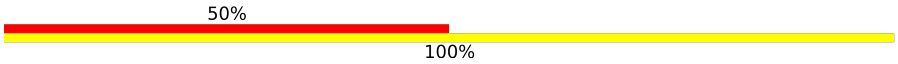
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



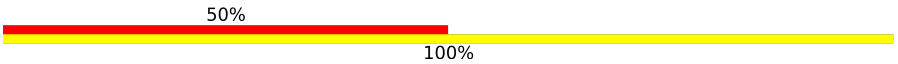
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



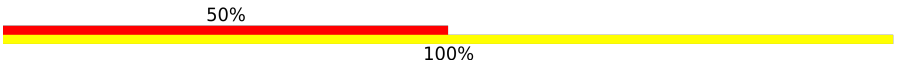
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



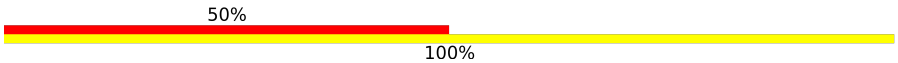
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



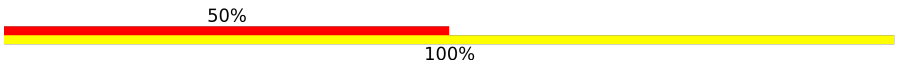
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



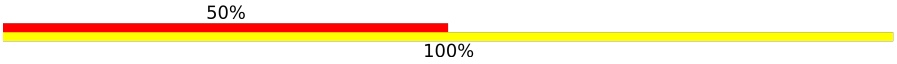
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



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

Chain f:

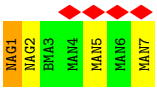


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

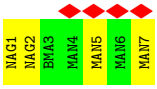
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



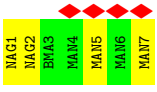
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



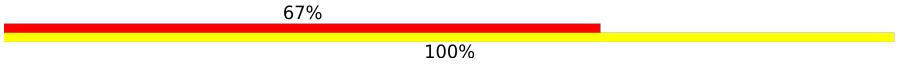
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



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

Chain G:



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

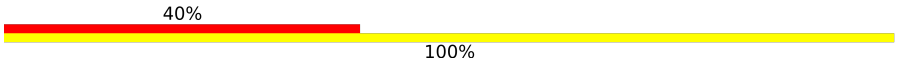
Chain R:

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

Chain c:

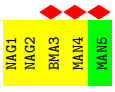
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



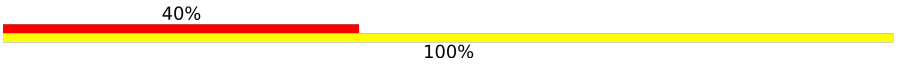
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



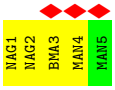
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



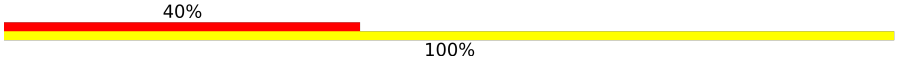
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



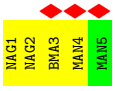
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



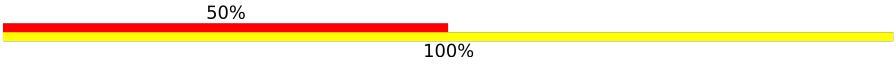
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



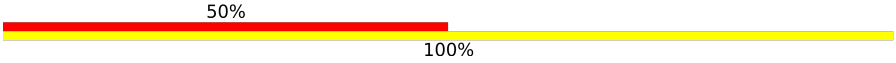
• Molecule 7: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain N:



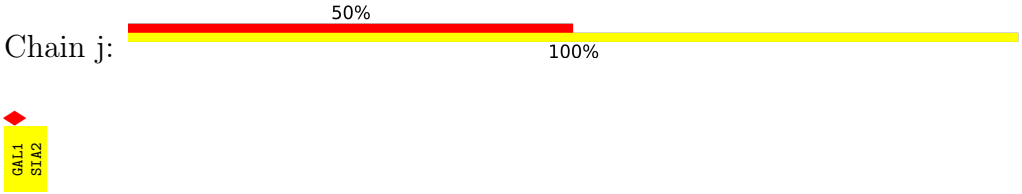
• Molecule 7: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain Y:



• Molecule 7: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain j:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	34458	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	6.963	Depositor
Minimum map value	-4.174	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.9	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 (i)

5.1 Standard geometry (i)

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

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	1.29	41/9163 (0.4%)	1.02	44/12471 (0.4%)
1	B	1.29	41/9163 (0.4%)	1.02	46/12471 (0.4%)
1	C	1.29	41/9163 (0.4%)	1.02	44/12471 (0.4%)
All	All	1.29	123/27489 (0.4%)	1.02	134/37413 (0.4%)

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	383	CYS	C-O	-19.08	0.87	1.23
1	C	383	CYS	C-O	-19.07	0.87	1.23
1	A	383	CYS	C-O	-19.04	0.87	1.23
1	A	383	CYS	N-CA	10.30	1.67	1.46
1	B	383	CYS	N-CA	10.30	1.67	1.46
1	C	383	CYS	N-CA	10.27	1.66	1.46
1	B	383	CYS	C-N	9.59	1.56	1.34
1	A	383	CYS	C-N	9.56	1.56	1.34
1	C	383	CYS	C-N	9.54	1.56	1.34
1	C	870	ASN	C-O	9.24	1.41	1.23
1	B	870	ASN	C-O	9.24	1.41	1.23
1	A	870	ASN	C-O	9.23	1.40	1.23
1	C	292	TYR	CB-CG	-7.57	1.40	1.51
1	A	292	TYR	CB-CG	-7.55	1.40	1.51
1	B	292	TYR	CB-CG	-7.54	1.40	1.51
1	B	1127	VAL	CB-CG2	-7.14	1.37	1.52
1	A	1127	VAL	CB-CG2	-7.11	1.38	1.52
1	C	1127	VAL	CB-CG2	-7.08	1.38	1.52
1	B	774	ASN	C-O	6.90	1.36	1.23
1	C	774	ASN	C-O	6.90	1.36	1.23
1	A	774	ASN	C-O	6.89	1.36	1.23
1	C	58	TYR	CB-CG	-6.85	1.41	1.51
1	A	58	TYR	CB-CG	-6.83	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	58	TYR	CB-CG	-6.82	1.41	1.51
1	B	101	PHE	CB-CG	-6.82	1.39	1.51
1	C	293	TYR	CD1-CE1	-6.81	1.29	1.39
1	B	293	TYR	CD1-CE1	-6.80	1.29	1.39
1	A	101	PHE	CB-CG	-6.80	1.39	1.51
1	C	101	PHE	CB-CG	-6.79	1.39	1.51
1	A	293	TYR	CD1-CE1	-6.79	1.29	1.39
1	B	777	TYR	CB-CG	-6.74	1.41	1.51
1	A	777	TYR	CB-CG	-6.73	1.41	1.51
1	C	777	TYR	CB-CG	-6.72	1.41	1.51
1	C	681	HIS	CB-CG	-6.70	1.38	1.50
1	A	681	HIS	CB-CG	-6.67	1.38	1.50
1	B	681	HIS	CB-CG	-6.66	1.38	1.50
1	C	655	VAL	CB-CG1	6.58	1.66	1.52
1	B	655	VAL	CB-CG1	6.56	1.66	1.52
1	A	655	VAL	CB-CG1	6.56	1.66	1.52
1	C	166	ASN	C-O	-6.52	1.10	1.23
1	A	166	ASN	C-O	-6.52	1.10	1.23
1	B	166	ASN	C-O	-6.51	1.10	1.23
1	A	1106	CYS	C-O	-6.42	1.11	1.23
1	B	1106	CYS	C-O	-6.42	1.11	1.23
1	C	1106	CYS	C-O	-6.42	1.11	1.23
1	B	410	ASN	C-O	-6.25	1.11	1.23
1	C	410	ASN	C-O	-6.24	1.11	1.23
1	A	410	ASN	C-O	-6.23	1.11	1.23
1	C	383	CYS	CA-CB	6.18	1.67	1.53
1	A	383	CYS	CA-CB	6.17	1.67	1.53
1	B	383	CYS	CA-CB	6.17	1.67	1.53
1	A	376	GLU	CD-OE2	-6.15	1.18	1.25
1	B	376	GLU	CD-OE2	-6.15	1.18	1.25
1	B	1192	TYR	CB-CG	-6.15	1.42	1.51
1	C	376	GLU	CD-OE2	-6.14	1.18	1.25
1	A	293	TYR	CG-CD1	-6.14	1.31	1.39
1	C	1192	TYR	CB-CG	-6.13	1.42	1.51
1	A	1192	TYR	CB-CG	-6.12	1.42	1.51
1	C	293	TYR	CG-CD1	-6.11	1.31	1.39
1	B	293	TYR	CG-CD1	-6.07	1.31	1.39
1	B	1019	PHE	CB-CG	-6.05	1.41	1.51
1	A	1019	PHE	CB-CG	-6.04	1.41	1.51
1	C	1019	PHE	CB-CG	-6.04	1.41	1.51
1	C	1106	CYS	N-CA	-6.04	1.34	1.46
1	A	1106	CYS	N-CA	-6.02	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1106	CYS	N-CA	-6.01	1.34	1.46
1	C	1191	PHE	CB-CG	-6.01	1.41	1.51
1	A	1191	PHE	CB-CG	-6.00	1.41	1.51
1	B	1191	PHE	CB-CG	-5.98	1.41	1.51
1	B	661	VAL	CB-CG2	-5.86	1.40	1.52
1	A	661	VAL	CB-CG2	-5.85	1.40	1.52
1	C	661	VAL	CB-CG2	-5.84	1.40	1.52
1	C	713	CYS	CB-SG	-5.82	1.72	1.81
1	A	655	VAL	CB-CG2	-5.80	1.40	1.52
1	A	713	CYS	CB-SG	-5.79	1.72	1.81
1	C	655	VAL	CB-CG2	-5.79	1.40	1.52
1	B	655	VAL	CB-CG2	-5.78	1.40	1.52
1	B	713	CYS	CB-SG	-5.78	1.72	1.81
1	A	185	CYS	CB-SG	-5.75	1.72	1.81
1	B	185	CYS	CB-SG	-5.74	1.72	1.81
1	C	185	CYS	CB-SG	-5.73	1.72	1.81
1	C	823	GLU	CD-OE1	-5.57	1.19	1.25
1	A	823	GLU	CD-OE1	-5.53	1.19	1.25
1	B	823	GLU	CD-OE1	-5.47	1.19	1.25
1	C	1137	MET	CB-CG	-5.46	1.33	1.51
1	C	367	GLU	CD-OE2	-5.46	1.19	1.25
1	B	1137	MET	CB-CG	-5.45	1.33	1.51
1	A	1137	MET	CB-CG	-5.45	1.33	1.51
1	A	367	GLU	CD-OE2	-5.42	1.19	1.25
1	B	367	GLU	CD-OE2	-5.41	1.19	1.25
1	B	736	CYS	CB-SG	-5.39	1.73	1.81
1	C	1148	GLU	CD-OE1	-5.38	1.19	1.25
1	A	1086	LEU	CB-CG	5.37	1.68	1.52
1	A	736	CYS	CB-SG	-5.37	1.73	1.81
1	C	1086	LEU	CB-CG	5.37	1.68	1.52
1	B	1086	LEU	CB-CG	5.36	1.68	1.52
1	C	736	CYS	CB-SG	-5.34	1.73	1.81
1	A	818	GLU	CD-OE1	-5.34	1.19	1.25
1	A	1148	GLU	CD-OE1	-5.33	1.19	1.25
1	B	1148	GLU	CD-OE1	-5.33	1.19	1.25
1	B	818	GLU	CD-OE1	-5.31	1.19	1.25
1	C	559	SER	CB-OG	-5.31	1.35	1.42
1	B	559	SER	CB-OG	-5.31	1.35	1.42
1	A	559	SER	CB-OG	-5.30	1.35	1.42
1	C	818	GLU	CD-OE1	-5.29	1.19	1.25
1	B	50	VAL	CB-CG1	-5.24	1.41	1.52
1	A	50	VAL	CB-CG1	-5.23	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	PHE	CB-CG	-5.23	1.42	1.51
1	C	50	VAL	CB-CG1	-5.23	1.41	1.52
1	B	266	PHE	CB-CG	-5.23	1.42	1.51
1	C	266	PHE	CB-CG	-5.22	1.42	1.51
1	B	870	ASN	C-N	-5.21	1.22	1.34
1	C	870	ASN	C-N	-5.19	1.22	1.34
1	A	870	ASN	C-N	-5.18	1.22	1.34
1	C	641	TYR	CB-CG	-5.18	1.43	1.51
1	A	641	TYR	CB-CG	-5.18	1.43	1.51
1	B	641	TYR	CB-CG	-5.17	1.43	1.51
1	A	58	TYR	CD2-CE2	-5.13	1.31	1.39
1	B	58	TYR	CD2-CE2	-5.13	1.31	1.39
1	C	58	TYR	CD2-CE2	-5.12	1.31	1.39
1	C	891	GLU	CB-CG	-5.05	1.42	1.52
1	A	891	GLU	CB-CG	-5.05	1.42	1.52
1	B	891	GLU	CB-CG	-5.01	1.42	1.52

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	655	VAL	CG1-CB-CG2	12.18	130.38	110.90
1	A	655	VAL	CG1-CB-CG2	12.17	130.37	110.90
1	B	655	VAL	CG1-CB-CG2	12.14	130.32	110.90
1	A	383	CYS	CA-C-O	10.53	142.21	120.10
1	B	383	CYS	CA-C-O	10.51	142.17	120.10
1	C	383	CYS	CA-C-O	10.49	142.13	120.10
1	B	383	CYS	CA-C-N	-10.34	94.46	117.20
1	A	383	CYS	CA-C-N	-10.33	94.47	117.20
1	C	383	CYS	CA-C-N	-10.32	94.49	117.20
1	A	673	LEU	CB-CG-CD2	9.87	127.78	111.00
1	B	673	LEU	CB-CG-CD2	9.87	127.77	111.00
1	C	673	LEU	CB-CG-CD2	9.86	127.77	111.00
1	A	344	LEU	CB-CG-CD2	8.98	126.26	111.00
1	C	344	LEU	CB-CG-CD2	8.96	126.24	111.00
1	B	344	LEU	CB-CG-CD2	8.96	126.23	111.00
1	A	1086	LEU	CB-CG-CD2	8.60	125.62	111.00
1	B	1086	LEU	CB-CG-CD2	8.59	125.60	111.00
1	C	1086	LEU	CB-CG-CD2	8.58	125.59	111.00
1	A	383	CYS	N-CA-CB	-8.42	95.44	110.60
1	B	383	CYS	N-CA-CB	-8.42	95.45	110.60
1	C	383	CYS	N-CA-CB	-8.41	95.45	110.60
1	C	1074	ARG	NE-CZ-NH2	-8.36	116.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1074	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	B	1074	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	B	655	VAL	CA-CB-CG1	-7.74	99.29	110.90
1	A	655	VAL	CA-CB-CG1	-7.74	99.29	110.90
1	C	655	VAL	CA-CB-CG1	-7.73	99.31	110.90
1	A	382	GLU	C-N-CA	-7.50	102.95	121.70
1	C	382	GLU	C-N-CA	-7.50	102.95	121.70
1	B	382	GLU	C-N-CA	-7.49	102.97	121.70
1	C	577	TYR	CB-CG-CD2	-7.46	116.53	121.00
1	A	577	TYR	CB-CG-CD2	-7.43	116.54	121.00
1	B	577	TYR	CB-CG-CD2	-7.43	116.54	121.00
1	C	1135	TYR	CB-CG-CD1	-7.39	116.57	121.00
1	C	1222	LEU	CD1-CG-CD2	7.38	132.65	110.50
1	A	1222	LEU	CD1-CG-CD2	7.38	132.63	110.50
1	B	1222	LEU	CD1-CG-CD2	7.37	132.62	110.50
1	A	1135	TYR	CB-CG-CD1	-7.34	116.59	121.00
1	B	1135	TYR	CB-CG-CD1	-7.33	116.60	121.00
1	B	481	LEU	CB-CG-CD1	-7.13	98.88	111.00
1	A	481	LEU	CB-CG-CD1	-7.12	98.90	111.00
1	C	481	LEU	CB-CG-CD1	-7.11	98.91	111.00
1	B	1218	LEU	CD1-CG-CD2	6.92	131.25	110.50
1	A	1218	LEU	CD1-CG-CD2	6.90	131.19	110.50
1	C	1218	LEU	CD1-CG-CD2	6.88	131.14	110.50
1	C	1218	LEU	CB-CG-CD1	-6.84	99.37	111.00
1	B	1218	LEU	CB-CG-CD1	-6.84	99.38	111.00
1	A	1218	LEU	CB-CG-CD1	-6.83	99.38	111.00
1	B	715	LEU	CD1-CG-CD2	6.83	131.00	110.50
1	B	1106	CYS	CA-C-O	6.83	134.44	120.10
1	C	1106	CYS	CA-C-O	6.83	134.44	120.10
1	A	1106	CYS	CA-C-O	6.82	134.43	120.10
1	A	715	LEU	CD1-CG-CD2	6.82	130.96	110.50
1	C	715	LEU	CD1-CG-CD2	6.81	130.94	110.50
1	A	401	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	C	401	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	1036	LEU	CD1-CG-CD2	6.73	130.70	110.50
1	A	1036	LEU	CD1-CG-CD2	6.73	130.68	110.50
1	B	1036	LEU	CD1-CG-CD2	6.72	130.67	110.50
1	B	401	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	C	307	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	307	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	307	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	234	LEU	CD1-CG-CD2	6.29	129.38	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	LEU	CD1-CG-CD2	6.29	129.38	110.50
1	C	234	LEU	CD1-CG-CD2	6.29	129.37	110.50
1	B	46	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	C	46	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	383	CYS	N-CA-C	-6.27	94.07	111.00
1	B	119	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	383	CYS	N-CA-C	-6.26	94.10	111.00
1	C	383	CYS	N-CA-C	-6.26	94.10	111.00
1	A	46	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	119	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	887	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	887	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	119	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	887	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	780	LEU	CD1-CG-CD2	6.16	128.99	110.50
1	B	780	LEU	CD1-CG-CD2	6.16	128.98	110.50
1	C	780	LEU	CD1-CG-CD2	6.16	128.97	110.50
1	C	511	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	511	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	511	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	481	LEU	CD1-CG-CD2	6.05	128.65	110.50
1	C	481	LEU	CD1-CG-CD2	6.04	128.62	110.50
1	A	481	LEU	CD1-CG-CD2	6.04	128.60	110.50
1	A	910	ASP	CB-CG-OD1	-5.96	112.93	118.30
1	B	910	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	C	910	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	B	58	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	A	58	TYR	CB-CG-CD2	-5.84	117.50	121.00
1	C	58	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	C	540	TYR	CB-CG-CD1	-5.74	117.56	121.00
1	B	540	TYR	CB-CG-CD1	-5.69	117.59	121.00
1	A	928	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	C	928	TYR	CB-CG-CD2	-5.66	117.61	121.00
1	B	928	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	383	CYS	CB-CA-C	-5.64	99.12	110.40
1	A	540	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	C	383	CYS	CB-CA-C	-5.62	99.16	110.40
1	B	383	CYS	CB-CA-C	-5.62	99.16	110.40
1	C	351	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	B	351	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	A	351	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	B	323	PHE	CB-CG-CD1	5.54	124.68	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1088	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	1088	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	1088	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	323	PHE	CB-CG-CD1	5.52	124.67	120.80
1	C	323	PHE	CB-CG-CD1	5.48	124.64	120.80
1	A	1106	CYS	CA-C-N	-5.47	105.16	117.20
1	B	293	TYR	CD1-CE1-CZ	5.47	124.73	119.80
1	B	1106	CYS	CA-C-N	-5.47	105.16	117.20
1	C	293	TYR	CD1-CE1-CZ	5.47	124.72	119.80
1	C	1106	CYS	CA-C-N	-5.47	105.17	117.20
1	A	293	TYR	CD1-CE1-CZ	5.45	124.70	119.80
1	A	423	PHE	CB-CG-CD2	5.41	124.58	120.80
1	C	423	PHE	CB-CG-CD2	5.39	124.57	120.80
1	B	910	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	910	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	910	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	423	PHE	CB-CG-CD2	5.36	124.55	120.80
1	A	323	PHE	CB-CG-CD2	-5.31	117.08	120.80
1	B	323	PHE	CB-CG-CD2	-5.29	117.10	120.80
1	C	323	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	C	316	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	316	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	B	316	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	B	654	CYS	N-CA-C	-5.02	97.44	111.00
1	B	438	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	B	509	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	C	654	CYS	N-CA-C	-5.02	97.45	111.00
1	A	654	CYS	N-CA-C	-5.01	97.46	111.00

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	8952	0	8631	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8952	0	8631	33	0
1	C	8952	0	8631	34	0
2	D	50	0	43	0	0
2	H	50	0	43	0	0
2	O	50	0	43	0	0
2	S	50	0	43	0	0
2	Z	50	0	43	0	0
2	d	50	0	43	0	0
3	E	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	M	28	0	25	0	0
3	P	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	X	28	0	25	0	0
3	a	28	0	25	0	0
3	e	28	0	25	0	0
3	f	28	0	25	0	0
3	i	28	0	25	0	0
4	F	83	0	70	1	0
4	Q	83	0	70	0	0
4	b	83	0	70	0	0
5	G	39	0	34	0	0
5	R	39	0	34	0	0
5	c	39	0	34	0	0
6	K	61	0	52	0	0
6	L	61	0	52	0	0
6	V	61	0	52	0	0
6	W	61	0	52	0	0
6	g	61	0	52	0	0
6	h	61	0	52	0	0
7	N	32	0	28	0	0
7	Y	32	0	28	0	0
7	j	32	0	28	0	0
8	A	98	0	91	0	0
8	B	98	0	91	0	0
8	C	98	0	91	0	0
9	A	32	0	17	1	0
9	B	32	0	17	1	0
9	C	32	0	17	1	0
10	A	72	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	72	0	0	3	0
10	C	72	0	0	2	0
All	All	28926	0	27483	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (91) 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:673:LEU:HD13	1:C:714:VAL:HG22	1.57	0.87
1:B:673:LEU:HD13	1:B:714:VAL:HG22	1.57	0.86
1:A:673:LEU:HD13	1:A:714:VAL:HG22	1.57	0.85
1:B:107:GLN:HE21	1:B:160:LYS:HB3	1.42	0.85
1:A:673:LEU:HD21	1:A:711:VAL:HG23	1.59	0.82
1:C:673:LEU:HD21	1:C:711:VAL:HG23	1.59	0.82
1:B:673:LEU:HD21	1:B:711:VAL:HG23	1.59	0.82
1:A:107:GLN:HE21	1:A:160:LYS:HB3	1.42	0.81
1:C:107:GLN:HE21	1:C:160:LYS:HB3	1.42	0.81
1:C:673:LEU:HD13	1:C:714:VAL:CG2	2.21	0.71
1:A:107:GLN:NE2	1:A:160:LYS:HB3	2.06	0.71
1:B:673:LEU:HD13	1:B:714:VAL:CG2	2.21	0.71
1:A:673:LEU:HD13	1:A:714:VAL:CG2	2.21	0.70
1:C:107:GLN:NE2	1:C:160:LYS:HB3	2.06	0.70
1:B:107:GLN:NE2	1:B:160:LYS:HB3	2.06	0.69
1:B:673:LEU:HD21	1:B:711:VAL:CG2	2.28	0.63
1:C:673:LEU:HD21	1:C:711:VAL:CG2	2.28	0.63
1:A:673:LEU:HD21	1:A:711:VAL:CG2	2.28	0.63
1:A:107:GLN:NE2	1:A:160:LYS:HD3	2.17	0.60
1:B:107:GLN:NE2	1:B:160:LYS:HD3	2.17	0.60
1:C:107:GLN:NE2	1:C:160:LYS:HD3	2.17	0.59
1:A:107:GLN:HE22	1:A:160:LYS:HD3	1.68	0.58
1:C:107:GLN:HE22	1:C:160:LYS:HD3	1.69	0.58
1:C:343:ASP:N	1:C:343:ASP:OD1	2.35	0.58
1:C:46:ARG:HD3	10:C:8028:HOH:O	2.03	0.57
1:A:46:ARG:HD3	10:A:8028:HOH:O	2.03	0.57
1:B:46:ARG:HD3	10:B:8028:HOH:O	2.03	0.57
1:B:107:GLN:HE22	1:B:160:LYS:HD3	1.68	0.57
1:A:1035:LYS:HE3	1:B:830:LYS:HD2	1.87	0.57
1:A:830:LYS:HD2	1:C:1035:LYS:HE3	1.87	0.57
1:B:343:ASP:N	1:B:343:ASP:OD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1035:LYS:HE3	1:C:830:LYS:HD2	1.87	0.56
1:A:343:ASP:OD1	1:A:343:ASP:N	2.35	0.56
1:A:798:THR:HA	1:A:842:GLN:OE1	2.07	0.54
1:B:798:THR:HA	1:B:842:GLN:OE1	2.07	0.54
1:C:798:THR:HA	1:C:842:GLN:OE1	2.07	0.53
1:C:130:VAL:HG13	10:C:8045:HOH:O	2.09	0.52
1:A:129:THR:H	9:A:1444:FOL:HN1	1.58	0.52
1:B:129:THR:H	9:B:1444:FOL:HN1	1.58	0.52
1:C:129:THR:H	9:C:1444:FOL:HN1	1.58	0.52
1:A:130:VAL:HG13	10:A:8045:HOH:O	2.09	0.52
1:A:830:LYS:CD	1:C:1035:LYS:HE3	2.41	0.51
1:A:1035:LYS:HE3	1:B:830:LYS:CD	2.41	0.51
1:B:130:VAL:HG13	10:B:8045:HOH:O	2.09	0.51
1:B:1035:LYS:HE3	1:C:830:LYS:CD	2.41	0.51
1:A:107:GLN:HG2	1:A:161:MET:O	2.11	0.50
1:B:107:GLN:HG2	1:B:161:MET:O	2.11	0.50
1:C:107:GLN:HG2	1:C:161:MET:O	2.11	0.49
1:B:592:ASN:OD1	1:B:592:ASN:N	2.45	0.49
1:B:961:THR:OG1	1:B:962:ALA:N	2.46	0.48
1:A:592:ASN:OD1	1:A:592:ASN:N	2.45	0.48
1:B:780:LEU:HG	1:B:782:ILE:HB	1.95	0.48
1:A:780:LEU:HG	1:A:782:ILE:HB	1.95	0.48
1:C:592:ASN:OD1	1:C:592:ASN:N	2.45	0.48
1:C:780:LEU:HG	1:C:782:ILE:HB	1.95	0.47
1:A:88:SER:OG	1:A:89:ALA:N	2.48	0.47
1:A:961:THR:OG1	1:A:962:ALA:N	2.46	0.47
1:C:975:SER:OG	1:C:979:ARG:NH1	2.48	0.47
1:C:88:SER:OG	1:C:89:ALA:N	2.48	0.46
1:B:88:SER:OG	1:B:89:ALA:N	2.48	0.46
1:B:975:SER:OG	1:B:979:ARG:NH1	2.48	0.46
1:C:673:LEU:HD12	1:C:674:PHE:N	2.31	0.46
1:A:673:LEU:HD12	1:A:674:PHE:N	2.31	0.46
1:B:673:LEU:HD12	1:B:674:PHE:N	2.31	0.46
1:A:770:VAL:HG12	1:B:969:ALA:HB2	1.98	0.46
1:A:975:SER:OG	1:A:979:ARG:NH1	2.48	0.45
1:B:770:VAL:HG12	1:C:969:ALA:HB2	1.98	0.45
1:A:969:ALA:HB2	1:C:770:VAL:HG12	1.98	0.45
1:B:152:SER:OG	1:B:165:PHE:HB2	2.18	0.44
1:C:961:THR:OG1	1:C:962:ALA:N	2.46	0.44
1:A:152:SER:OG	1:A:165:PHE:HB2	2.18	0.44
1:C:152:SER:OG	1:C:165:PHE:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:GLN:HE21	1:A:1088:ARG:HD2	1.83	0.44
1:C:1084:GLN:HE21	1:C:1088:ARG:HD2	1.83	0.43
1:B:717:LEU:HD23	1:B:757:MET:HB2	2.01	0.43
1:B:1084:GLN:HE21	1:B:1088:ARG:HD2	1.83	0.43
1:A:782:ILE:HA	1:A:783:PRO:HD3	1.91	0.42
1:C:609:TYR:OH	1:C:644:ASP:OD2	2.38	0.42
1:C:717:LEU:HD23	1:C:757:MET:HB2	2.01	0.42
1:B:609:TYR:OH	1:B:644:ASP:OD2	2.38	0.42
1:C:530:VAL:HA	1:C:531:PRO:HD3	1.90	0.42
1:C:172:LEU:HA	1:C:173:PRO:HD2	1.95	0.41
1:B:1013:THR:OG1	1:B:1014:THR:N	2.51	0.41
1:A:717:LEU:HD23	1:A:757:MET:HB2	2.01	0.41
1:B:593:ASP:N	1:B:593:ASP:OD1	2.51	0.41
1:A:609:TYR:OH	1:A:644:ASP:OD2	2.38	0.41
1:A:289:THR:HG23	10:A:8024:HOH:O	2.21	0.40
1:C:1013:THR:OG1	1:C:1014:THR:N	2.51	0.40
1:A:587:LYS:CG	4:F:1:NAG:H81	2.52	0.40
1:B:289:THR:HG23	10:B:8024:HOH:O	2.21	0.40
1:C:593:ASP:N	1:C:593:ASP:OD1	2.51	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	1149/1359 (84%)	1130 (98%)	18 (2%)	1 (0%)	51	78
1	B	1149/1359 (84%)	1130 (98%)	18 (2%)	1 (0%)	51	78
1	C	1149/1359 (84%)	1130 (98%)	18 (2%)	1 (0%)	51	78
All	All	3447/4077 (84%)	3390 (98%)	54 (2%)	3 (0%)	54	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	GLY
1	B	578	GLY
1	C	578	GLY

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	992/1167 (85%)	981 (99%)	11 (1%)	73	90
1	B	992/1167 (85%)	982 (99%)	10 (1%)	76	91
1	C	992/1167 (85%)	981 (99%)	11 (1%)	73	90
All	All	2976/3501 (85%)	2944 (99%)	32 (1%)	74	90

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	179	LEU
1	A	234	LEU
1	A	455	ASP
1	A	592	ASN
1	A	655	VAL
1	A	673	LEU
1	A	715	LEU
1	A	1036	LEU
1	A	1218	LEU
1	A	1222	LEU
1	B	52	LYS
1	B	179	LEU
1	B	234	LEU
1	B	455	ASP
1	B	592	ASN
1	B	655	VAL
1	B	673	LEU
1	B	715	LEU
1	B	1036	LEU

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Mol	Chain	Res	Type
1	B	1222	LEU
1	C	52	LYS
1	C	179	LEU
1	C	234	LEU
1	C	455	ASP
1	C	592	ASN
1	C	655	VAL
1	C	673	LEU
1	C	715	LEU
1	C	1036	LEU
1	C	1218	LEU
1	C	1222	LEU

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	107	GLN
1	A	280	GLN
1	A	1208	GLN
1	B	107	GLN
1	B	280	GLN
1	B	1208	GLN
1	C	107	GLN
1	C	280	GLN
1	C	1208	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

114 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	1.40	4 (28%)	17,19,21	1.89	6 (35%)
2	NAG	D	2	2	14,14,15	1.23	2 (14%)	17,19,21	1.65	3 (17%)
2	BMA	D	3	2	11,11,12	1.56	2 (18%)	15,15,17	1.69	1 (6%)
2	MAN	D	4	2	11,11,12	1.14	1 (9%)	15,15,17	1.33	3 (20%)
3	NAG	E	1	3,1	14,14,15	1.47	3 (21%)	17,19,21	1.80	5 (29%)
3	NAG	E	2	3	14,14,15	1.06	1 (7%)	17,19,21	0.87	1 (5%)
4	NAG	F	1	4,1	14,14,15	1.27	1 (7%)	17,19,21	0.83	0
4	NAG	F	2	4	14,14,15	1.34	1 (7%)	17,19,21	0.74	0
4	BMA	F	3	4	11,11,12	1.03	0	15,15,17	0.65	0
4	MAN	F	4	4	11,11,12	0.70	0	15,15,17	0.66	0
4	MAN	F	5	4	11,11,12	1.43	3 (27%)	15,15,17	0.64	0
4	MAN	F	6	4	11,11,12	0.64	0	15,15,17	0.64	0
4	MAN	F	7	4	11,11,12	1.43	3 (27%)	15,15,17	0.61	0
5	NAG	G	1	5,1	14,14,15	1.54	5 (35%)	17,19,21	1.76	3 (17%)
5	NAG	G	2	5	14,14,15	1.51	3 (21%)	17,19,21	1.28	1 (5%)
5	BMA	G	3	5	11,11,12	0.75	1 (9%)	15,15,17	0.90	1 (6%)
2	NAG	H	1	2,1	14,14,15	1.73	5 (35%)	17,19,21	2.19	4 (23%)
2	NAG	H	2	2	14,14,15	1.63	3 (21%)	17,19,21	1.93	3 (17%)
2	BMA	H	3	2	11,11,12	1.50	2 (18%)	15,15,17	1.90	2 (13%)
2	MAN	H	4	2	11,11,12	1.18	1 (9%)	15,15,17	1.32	4 (26%)
3	NAG	I	1	3,1	14,14,15	1.50	4 (28%)	17,19,21	1.83	3 (17%)
3	NAG	I	2	3	14,14,15	1.07	1 (7%)	17,19,21	0.68	0
3	NAG	J	1	3,1	14,14,15	1.72	5 (35%)	17,19,21	1.76	2 (11%)
3	NAG	J	2	3	14,14,15	1.17	1 (7%)	17,19,21	0.77	0
6	NAG	K	1	6,1	14,14,15	1.45	4 (28%)	17,19,21	1.84	2 (11%)
6	NAG	K	2	6	14,14,15	1.37	2 (14%)	17,19,21	1.31	1 (5%)
6	BMA	K	3	6	11,11,12	2.15	3 (27%)	15,15,17	1.71	3 (20%)
6	MAN	K	4	6	11,11,12	1.09	1 (9%)	15,15,17	1.37	3 (20%)
6	MAN	K	5	6	11,11,12	1.07	1 (9%)	15,15,17	1.32	3 (20%)
6	NAG	L	1	6,1	14,14,15	0.81	0	17,19,21	1.12	1 (5%)
6	NAG	L	2	6	14,14,15	0.75	1 (7%)	17,19,21	1.35	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BMA	L	3	6	11,11,12	0.68	0	15,15,17	1.01	1 (6%)
6	MAN	L	4	6	11,11,12	0.70	0	15,15,17	0.82	1 (6%)
6	MAN	L	5	6	11,11,12	0.71	0	15,15,17	0.81	0
3	NAG	M	1	3,1	14,14,15	1.57	5 (35%)	17,19,21	1.66	2 (11%)
3	NAG	M	2	3	14,14,15	1.13	1 (7%)	17,19,21	0.79	1 (5%)
7	GAL	N	1	7	12,12,12	0.82	0	17,17,17	1.91	4 (23%)
7	SIA	N	2	7	20,20,21	1.71	4 (20%)	24,28,31	1.24	4 (16%)
2	NAG	O	1	2,1	14,14,15	1.40	4 (28%)	17,19,21	1.89	6 (35%)
2	NAG	O	2	2	14,14,15	1.23	2 (14%)	17,19,21	1.64	3 (17%)
2	BMA	O	3	2	11,11,12	1.57	2 (18%)	15,15,17	1.69	1 (6%)
2	MAN	O	4	2	11,11,12	1.14	1 (9%)	15,15,17	1.32	3 (20%)
3	NAG	P	1	3,1	14,14,15	1.47	3 (21%)	17,19,21	1.80	5 (29%)
3	NAG	P	2	3	14,14,15	1.06	1 (7%)	17,19,21	0.86	1 (5%)
4	NAG	Q	1	4,1	14,14,15	1.27	1 (7%)	17,19,21	0.83	0
4	NAG	Q	2	4	14,14,15	1.34	1 (7%)	17,19,21	0.73	0
4	BMA	Q	3	4	11,11,12	1.03	0	15,15,17	0.66	0
4	MAN	Q	4	4	11,11,12	0.70	0	15,15,17	0.66	0
4	MAN	Q	5	4	11,11,12	1.42	3 (27%)	15,15,17	0.65	0
4	MAN	Q	6	4	11,11,12	0.64	0	15,15,17	0.64	0
4	MAN	Q	7	4	11,11,12	1.43	3 (27%)	15,15,17	0.61	0
5	NAG	R	1	5,1	14,14,15	1.54	5 (35%)	17,19,21	1.77	3 (17%)
5	NAG	R	2	5	14,14,15	1.51	3 (21%)	17,19,21	1.28	1 (5%)
5	BMA	R	3	5	11,11,12	0.75	1 (9%)	15,15,17	0.89	1 (6%)
2	NAG	S	1	2,1	14,14,15	1.73	5 (35%)	17,19,21	2.19	4 (23%)
2	NAG	S	2	2	14,14,15	1.63	3 (21%)	17,19,21	1.93	3 (17%)
2	BMA	S	3	2	11,11,12	1.49	2 (18%)	15,15,17	1.90	2 (13%)
2	MAN	S	4	2	11,11,12	1.17	1 (9%)	15,15,17	1.33	4 (26%)
3	NAG	T	1	3,1	14,14,15	1.49	4 (28%)	17,19,21	1.83	3 (17%)
3	NAG	T	2	3	14,14,15	1.07	1 (7%)	17,19,21	0.68	0
3	NAG	U	1	3,1	14,14,15	1.73	5 (35%)	17,19,21	1.76	2 (11%)
3	NAG	U	2	3	14,14,15	1.16	1 (7%)	17,19,21	0.78	0
6	NAG	V	1	6,1	14,14,15	1.44	4 (28%)	17,19,21	1.84	2 (11%)
6	NAG	V	2	6	14,14,15	1.37	2 (14%)	17,19,21	1.31	1 (5%)
6	BMA	V	3	6	11,11,12	2.15	3 (27%)	15,15,17	1.71	3 (20%)
6	MAN	V	4	6	11,11,12	1.10	1 (9%)	15,15,17	1.37	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	V	5	6	11,11,12	1.06	1 (9%)	15,15,17	1.32	3 (20%)
6	NAG	W	1	6,1	14,14,15	0.81	0	17,19,21	1.12	1 (5%)
6	NAG	W	2	6	14,14,15	0.75	1 (7%)	17,19,21	1.35	3 (17%)
6	BMA	W	3	6	11,11,12	0.68	0	15,15,17	1.01	1 (6%)
6	MAN	W	4	6	11,11,12	0.70	0	15,15,17	0.82	1 (6%)
6	MAN	W	5	6	11,11,12	0.71	0	15,15,17	0.81	0
3	NAG	X	1	3,1	14,14,15	1.57	5 (35%)	17,19,21	1.66	2 (11%)
3	NAG	X	2	3	14,14,15	1.13	1 (7%)	17,19,21	0.79	1 (5%)
7	GAL	Y	1	7	12,12,12	0.82	0	17,17,17	1.91	4 (23%)
7	SIA	Y	2	7	20,20,21	1.71	4 (20%)	24,28,31	1.24	4 (16%)
2	NAG	Z	1	2,1	14,14,15	1.41	4 (28%)	17,19,21	1.89	6 (35%)
2	NAG	Z	2	2	14,14,15	1.24	2 (14%)	17,19,21	1.65	3 (17%)
2	BMA	Z	3	2	11,11,12	1.55	2 (18%)	15,15,17	1.69	1 (6%)
2	MAN	Z	4	2	11,11,12	1.14	1 (9%)	15,15,17	1.33	3 (20%)
3	NAG	a	1	3,1	14,14,15	1.49	3 (21%)	17,19,21	1.80	5 (29%)
3	NAG	a	2	3	14,14,15	1.06	1 (7%)	17,19,21	0.87	1 (5%)
4	NAG	b	1	4,1	14,14,15	1.27	1 (7%)	17,19,21	0.82	0
4	NAG	b	2	4	14,14,15	1.34	1 (7%)	17,19,21	0.73	0
4	BMA	b	3	4	11,11,12	1.03	0	15,15,17	0.65	0
4	MAN	b	4	4	11,11,12	0.70	0	15,15,17	0.65	0
4	MAN	b	5	4	11,11,12	1.43	3 (27%)	15,15,17	0.64	0
4	MAN	b	6	4	11,11,12	0.63	0	15,15,17	0.65	0
4	MAN	b	7	4	11,11,12	1.43	3 (27%)	15,15,17	0.60	0
5	NAG	c	1	5,1	14,14,15	1.55	5 (35%)	17,19,21	1.77	3 (17%)
5	NAG	c	2	5	14,14,15	1.52	3 (21%)	17,19,21	1.28	1 (5%)
5	BMA	c	3	5	11,11,12	0.75	1 (9%)	15,15,17	0.90	1 (6%)
2	NAG	d	1	2,1	14,14,15	1.71	4 (28%)	17,19,21	2.18	4 (23%)
2	NAG	d	2	2	14,14,15	1.64	3 (21%)	17,19,21	1.93	3 (17%)
2	BMA	d	3	2	11,11,12	1.50	2 (18%)	15,15,17	1.91	2 (13%)
2	MAN	d	4	2	11,11,12	1.18	1 (9%)	15,15,17	1.32	4 (26%)
3	NAG	e	1	3,1	14,14,15	1.49	4 (28%)	17,19,21	1.83	3 (17%)
3	NAG	e	2	3	14,14,15	1.07	1 (7%)	17,19,21	0.67	0
3	NAG	f	1	3,1	14,14,15	1.72	5 (35%)	17,19,21	1.75	2 (11%)
3	NAG	f	2	3	14,14,15	1.16	1 (7%)	17,19,21	0.78	0
6	NAG	g	1	6,1	14,14,15	1.45	4 (28%)	17,19,21	1.85	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	g	2	6	14,14,15	1.37	2 (14%)	17,19,21	1.31	1 (5%)
6	BMA	g	3	6	11,11,12	2.16	3 (27%)	15,15,17	1.71	3 (20%)
6	MAN	g	4	6	11,11,12	1.10	1 (9%)	15,15,17	1.36	3 (20%)
6	MAN	g	5	6	11,11,12	1.07	1 (9%)	15,15,17	1.32	3 (20%)
6	NAG	h	1	6,1	14,14,15	0.81	0	17,19,21	1.11	1 (5%)
6	NAG	h	2	6	14,14,15	0.76	1 (7%)	17,19,21	1.35	3 (17%)
6	BMA	h	3	6	11,11,12	0.67	0	15,15,17	1.00	1 (6%)
6	MAN	h	4	6	11,11,12	0.70	0	15,15,17	0.82	1 (6%)
6	MAN	h	5	6	11,11,12	0.71	0	15,15,17	0.81	0
3	NAG	i	1	3,1	14,14,15	1.57	5 (35%)	17,19,21	1.66	2 (11%)
3	NAG	i	2	3	14,14,15	1.13	1 (7%)	17,19,21	0.79	1 (5%)
7	GAL	j	1	7	12,12,12	0.81	0	17,17,17	1.92	4 (23%)
7	SIA	j	2	7	20,20,21	1.70	4 (20%)	24,28,31	1.25	4 (16%)

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	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1
2	MAN	D	4	2	-	1/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	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	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	1/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	1/2/19/22	0/1/1/1
4	MAN	F	7	4	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	H	4	2	-	2/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
6	NAG	K	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
6	MAN	K	5	6	-	0/2/19/22	0/1/1/1
6	NAG	L	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	BMA	L	3	6	-	1/2/19/22	0/1/1/1
6	MAN	L	4	6	-	1/2/19/22	0/1/1/1
6	MAN	L	5	6	-	1/2/19/22	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
7	GAL	N	1	7	-	0/2/22/22	0/1/1/1
7	SIA	N	2	7	-	3/18/34/38	0/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	BMA	O	3	2	-	1/2/19/22	0/1/1/1
2	MAN	O	4	2	-	1/2/19/22	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	2/2/19/22	0/1/1/1
4	MAN	Q	4	4	-	1/2/19/22	0/1/1/1
4	MAN	Q	5	4	-	0/2/19/22	0/1/1/1
4	MAN	Q	6	4	-	1/2/19/22	0/1/1/1
4	MAN	Q	7	4	-	0/2/19/22	0/1/1/1
5	NAG	R	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	BMA	R	3	5	-	1/2/19/22	0/1/1/1
2	NAG	S	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	1/6/23/26	0/1/1/1
2	BMA	S	3	2	-	1/2/19/22	0/1/1/1
2	MAN	S	4	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	1/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	1/6/23/26	0/1/1/1
6	NAG	V	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	0/6/23/26	0/1/1/1
6	BMA	V	3	6	-	2/2/19/22	0/1/1/1
6	MAN	V	4	6	-	0/2/19/22	0/1/1/1
6	MAN	V	5	6	-	0/2/19/22	0/1/1/1
6	NAG	W	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	BMA	W	3	6	-	1/2/19/22	0/1/1/1
6	MAN	W	4	6	-	1/2/19/22	0/1/1/1
6	MAN	W	5	6	-	1/2/19/22	0/1/1/1
3	NAG	X	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	1/6/23/26	0/1/1/1
7	GAL	Y	1	7	-	0/2/22/22	0/1/1/1
7	SIA	Y	2	7	-	3/18/34/38	0/1/1/1
2	NAG	Z	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	0/6/23/26	0/1/1/1
2	BMA	Z	3	2	-	1/2/19/22	0/1/1/1
2	MAN	Z	4	2	-	1/2/19/22	0/1/1/1
3	NAG	a	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	1/6/23/26	0/1/1/1
4	NAG	b	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	BMA	b	3	4	-	2/2/19/22	0/1/1/1
4	MAN	b	4	4	-	1/2/19/22	0/1/1/1
4	MAN	b	5	4	-	0/2/19/22	0/1/1/1
4	MAN	b	6	4	-	1/2/19/22	0/1/1/1
4	MAN	b	7	4	-	0/2/19/22	0/1/1/1
5	NAG	c	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	BMA	c	3	5	-	1/2/19/22	0/1/1/1
2	NAG	d	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	1/6/23/26	0/1/1/1
2	BMA	d	3	2	-	1/2/19/22	0/1/1/1
2	MAN	d	4	2	-	2/2/19/22	0/1/1/1
3	NAG	e	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	e	2	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	f	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	f	2	3	-	1/6/23/26	0/1/1/1
6	NAG	g	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	g	2	6	-	0/6/23/26	0/1/1/1
6	BMA	g	3	6	-	2/2/19/22	0/1/1/1
6	MAN	g	4	6	-	0/2/19/22	0/1/1/1
6	MAN	g	5	6	-	0/2/19/22	0/1/1/1
6	NAG	h	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	h	2	6	-	2/6/23/26	0/1/1/1
6	BMA	h	3	6	-	1/2/19/22	0/1/1/1
6	MAN	h	4	6	-	1/2/19/22	0/1/1/1
6	MAN	h	5	6	-	1/2/19/22	0/1/1/1
3	NAG	i	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	i	2	3	-	1/6/23/26	0/1/1/1
7	GAL	j	1	7	-	0/2/22/22	0/1/1/1
7	SIA	j	2	7	-	3/18/34/38	0/1/1/1

All (221) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	2	SIA	C6-C5	5.20	1.61	1.53
7	j	2	SIA	C6-C5	5.20	1.61	1.53
7	N	2	SIA	C6-C5	5.19	1.61	1.53
6	g	3	BMA	O3-C3	-4.59	1.32	1.43
6	K	3	BMA	O3-C3	-4.58	1.32	1.43
6	V	3	BMA	O3-C3	-4.57	1.32	1.43
3	J	2	NAG	C1-C2	4.22	1.58	1.52
3	U	2	NAG	C1-C2	4.20	1.58	1.52
3	f	2	NAG	C1-C2	4.19	1.58	1.52
3	X	2	NAG	C1-C2	4.08	1.58	1.52
3	M	2	NAG	C1-C2	4.07	1.58	1.52
3	i	2	NAG	C1-C2	4.07	1.58	1.52
2	S	2	NAG	C1-C2	3.87	1.58	1.52
2	d	2	NAG	C1-C2	3.86	1.58	1.52
2	H	2	NAG	C1-C2	3.84	1.58	1.52
3	a	2	NAG	C1-C2	3.74	1.57	1.52
3	E	2	NAG	C1-C2	3.73	1.57	1.52
3	e	2	NAG	C1-C2	3.73	1.57	1.52
3	P	2	NAG	C1-C2	3.73	1.57	1.52
3	I	2	NAG	C1-C2	3.71	1.57	1.52
3	T	2	NAG	C1-C2	3.71	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	2	NAG	C1-C2	3.71	1.57	1.52
5	R	2	NAG	C1-C2	3.69	1.57	1.52
5	G	2	NAG	C1-C2	3.69	1.57	1.52
4	F	1	NAG	C1-C2	3.54	1.57	1.52
4	b	1	NAG	C1-C2	3.54	1.57	1.52
4	Q	1	NAG	C1-C2	3.53	1.57	1.52
2	S	1	NAG	C1-C2	3.52	1.57	1.52
2	H	1	NAG	C1-C2	3.50	1.57	1.52
3	a	1	NAG	C1-C2	3.49	1.57	1.52
4	b	2	NAG	C1-C2	3.46	1.57	1.52
3	U	1	NAG	C1-C2	3.45	1.57	1.52
2	d	1	NAG	C1-C2	3.45	1.57	1.52
4	F	2	NAG	C1-C2	3.43	1.57	1.52
3	J	1	NAG	C1-C2	3.43	1.57	1.52
3	f	1	NAG	C1-C2	3.43	1.57	1.52
4	Q	2	NAG	C1-C2	3.42	1.57	1.52
3	P	1	NAG	C1-C2	3.42	1.57	1.52
3	E	1	NAG	C1-C2	3.41	1.57	1.52
2	D	3	BMA	C1-C2	3.28	1.59	1.52
2	O	3	BMA	C1-C2	3.28	1.59	1.52
2	Z	3	BMA	C1-C2	3.28	1.59	1.52
6	g	2	NAG	C1-C2	3.25	1.57	1.52
6	V	2	NAG	C1-C2	3.24	1.57	1.52
6	K	2	NAG	C1-C2	3.23	1.57	1.52
7	Y	2	SIA	C3-C2	3.20	1.57	1.52
7	N	2	SIA	C3-C2	3.20	1.57	1.52
7	j	2	SIA	C3-C2	3.18	1.57	1.52
5	R	1	NAG	O4-C4	-2.96	1.36	1.43
2	H	4	MAN	C1-C2	2.96	1.58	1.52
5	c	1	NAG	O4-C4	-2.96	1.36	1.43
2	S	4	MAN	C1-C2	2.95	1.58	1.52
2	d	4	MAN	C1-C2	2.94	1.58	1.52
5	G	1	NAG	O4-C4	-2.93	1.36	1.43
6	g	4	MAN	C1-C2	2.91	1.58	1.52
6	V	4	MAN	C1-C2	2.90	1.58	1.52
6	K	4	MAN	C1-C2	2.89	1.58	1.52
3	i	1	NAG	C1-C2	2.88	1.56	1.52
2	d	3	BMA	C1-C2	2.88	1.58	1.52
3	U	1	NAG	C3-C2	2.86	1.58	1.52
3	J	1	NAG	C3-C2	2.86	1.58	1.52
2	H	3	BMA	C1-C2	2.86	1.58	1.52
3	M	1	NAG	C1-C2	2.86	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	f	1	NAG	C3-C2	2.85	1.58	1.52
6	g	3	BMA	O6-C6	-2.85	1.30	1.42
6	K	3	BMA	O6-C6	-2.85	1.30	1.42
6	V	3	BMA	O6-C6	-2.85	1.30	1.42
2	S	3	BMA	C1-C2	2.84	1.58	1.52
3	X	1	NAG	C1-C2	2.84	1.56	1.52
2	O	4	MAN	C1-C2	2.83	1.58	1.52
2	O	2	NAG	O4-C4	-2.82	1.36	1.43
2	Z	4	MAN	C1-C2	2.82	1.58	1.52
2	D	4	MAN	C1-C2	2.82	1.58	1.52
2	Z	2	NAG	O4-C4	-2.81	1.36	1.43
2	D	2	NAG	O4-C4	-2.81	1.36	1.43
6	K	5	MAN	C1-C2	2.76	1.58	1.52
2	H	1	NAG	O5-C5	2.76	1.49	1.43
2	S	1	NAG	O5-C5	2.75	1.49	1.43
2	d	1	NAG	O5-C5	2.74	1.49	1.43
6	g	5	MAN	C1-C2	2.74	1.58	1.52
6	g	1	NAG	O4-C4	-2.73	1.36	1.43
6	V	5	MAN	C1-C2	2.73	1.58	1.52
6	K	1	NAG	O4-C4	-2.72	1.36	1.43
6	V	1	NAG	O4-C4	-2.71	1.36	1.43
2	Z	1	NAG	O4-C4	-2.70	1.36	1.43
2	O	1	NAG	O4-C4	-2.69	1.36	1.43
2	D	1	NAG	O4-C4	-2.69	1.36	1.43
2	H	2	NAG	O4-C4	-2.68	1.36	1.43
5	c	1	NAG	C1-C2	2.68	1.56	1.52
3	E	1	NAG	O5-C5	2.67	1.48	1.43
3	P	1	NAG	O5-C5	2.67	1.48	1.43
3	a	1	NAG	O5-C5	2.67	1.48	1.43
3	U	1	NAG	O5-C5	2.67	1.48	1.43
3	M	1	NAG	O4-C4	-2.67	1.36	1.43
2	d	2	NAG	O4-C4	-2.66	1.36	1.43
3	i	1	NAG	O4-C4	-2.66	1.36	1.43
3	X	1	NAG	O4-C4	-2.66	1.36	1.43
2	S	2	NAG	O4-C4	-2.66	1.36	1.43
3	J	1	NAG	O5-C5	2.65	1.48	1.43
3	f	1	NAG	O5-C5	2.65	1.48	1.43
2	S	1	NAG	O4-C4	-2.65	1.36	1.43
2	H	1	NAG	O4-C4	-2.63	1.36	1.43
5	c	2	NAG	C4-C5	2.62	1.58	1.53
7	N	2	SIA	O6-C2	-2.62	1.40	1.43
5	G	2	NAG	C4-C5	2.62	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	2	SIA	O6-C2	-2.61	1.40	1.43
5	R	2	NAG	C4-C5	2.61	1.58	1.53
5	G	1	NAG	C1-C2	2.61	1.56	1.52
7	j	2	SIA	O6-C2	-2.61	1.40	1.43
3	I	1	NAG	C1-C2	2.60	1.56	1.52
5	R	1	NAG	C1-C2	2.60	1.56	1.52
2	d	1	NAG	O4-C4	-2.60	1.36	1.43
3	e	1	NAG	C1-C2	2.59	1.56	1.52
3	T	1	NAG	C1-C2	2.59	1.56	1.52
6	g	2	NAG	O4-C4	-2.57	1.36	1.43
6	V	2	NAG	O4-C4	-2.56	1.36	1.43
6	K	2	NAG	O4-C4	-2.56	1.36	1.43
4	b	5	MAN	O5-C5	2.53	1.48	1.43
4	F	5	MAN	O5-C5	2.53	1.48	1.43
6	K	3	BMA	C1-C2	2.51	1.57	1.52
6	V	3	BMA	C1-C2	2.51	1.57	1.52
6	g	3	BMA	C1-C2	2.51	1.57	1.52
3	I	1	NAG	O4-C4	-2.50	1.37	1.43
3	e	1	NAG	O4-C4	-2.50	1.37	1.43
4	Q	5	MAN	O5-C5	2.49	1.48	1.43
2	D	1	NAG	C1-C2	2.49	1.56	1.52
2	O	1	NAG	C1-C2	2.49	1.56	1.52
2	Z	1	NAG	C1-C2	2.49	1.56	1.52
2	H	1	NAG	C3-C2	2.49	1.57	1.52
2	d	1	NAG	C3-C2	2.48	1.57	1.52
3	T	1	NAG	O4-C4	-2.47	1.37	1.43
2	S	1	NAG	C3-C2	2.46	1.57	1.52
4	Q	7	MAN	C1-C2	2.46	1.57	1.52
3	X	1	NAG	C3-C2	2.44	1.57	1.52
3	i	1	NAG	C3-C2	2.44	1.57	1.52
6	K	1	NAG	O5-C5	2.44	1.48	1.43
3	M	1	NAG	C3-C2	2.43	1.57	1.52
4	F	7	MAN	C1-C2	2.43	1.57	1.52
6	V	1	NAG	O5-C5	2.43	1.48	1.43
5	c	2	NAG	O4-C4	-2.43	1.37	1.43
6	g	1	NAG	O5-C5	2.43	1.48	1.43
4	b	7	MAN	O5-C5	2.41	1.48	1.43
5	G	2	NAG	O4-C4	-2.41	1.37	1.43
4	F	7	MAN	O5-C5	2.41	1.48	1.43
4	Q	7	MAN	O5-C5	2.40	1.48	1.43
4	b	7	MAN	C1-C2	2.40	1.57	1.52
5	R	2	NAG	O4-C4	-2.39	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	2	NAG	C1-C2	2.36	1.55	1.52
2	O	2	NAG	C1-C2	2.36	1.55	1.52
2	D	2	NAG	C1-C2	2.35	1.55	1.52
2	H	3	BMA	O3-C3	-2.35	1.37	1.43
3	I	1	NAG	O5-C5	2.35	1.48	1.43
2	d	3	BMA	O3-C3	-2.35	1.37	1.43
3	T	1	NAG	O5-C5	2.35	1.48	1.43
3	e	1	NAG	O5-C5	2.35	1.48	1.43
6	K	1	NAG	C1-C2	2.34	1.55	1.52
6	g	1	NAG	C1-C2	2.34	1.55	1.52
2	S	3	BMA	O3-C3	-2.32	1.37	1.43
2	O	3	BMA	O3-C3	-2.31	1.37	1.43
2	D	1	NAG	C4-C5	2.31	1.57	1.53
2	O	1	NAG	C4-C5	2.31	1.57	1.53
2	D	3	BMA	O3-C3	-2.31	1.37	1.43
2	Z	1	NAG	C4-C5	2.31	1.57	1.53
6	V	1	NAG	C1-C2	2.31	1.55	1.52
3	P	1	NAG	O4-C4	-2.29	1.37	1.43
3	E	1	NAG	O4-C4	-2.29	1.37	1.43
3	a	1	NAG	O4-C4	-2.28	1.37	1.43
3	f	1	NAG	O4-C4	-2.28	1.37	1.43
5	R	3	BMA	C1-C2	2.27	1.57	1.52
3	T	1	NAG	C3-C2	2.27	1.57	1.52
3	J	1	NAG	O4-C4	-2.27	1.37	1.43
2	Z	3	BMA	O3-C3	-2.27	1.37	1.43
3	I	1	NAG	C3-C2	2.27	1.57	1.52
3	U	1	NAG	O4-C4	-2.27	1.37	1.43
5	c	3	BMA	C1-C2	2.27	1.57	1.52
3	e	1	NAG	C3-C2	2.27	1.57	1.52
5	G	3	BMA	C1-C2	2.27	1.57	1.52
2	d	2	NAG	C4-C5	2.26	1.57	1.53
4	Q	5	MAN	C1-C2	2.26	1.57	1.52
6	V	1	NAG	C3-C2	2.26	1.57	1.52
2	S	2	NAG	C4-C5	2.26	1.57	1.53
2	H	2	NAG	C4-C5	2.25	1.57	1.53
5	G	1	NAG	O5-C5	2.25	1.48	1.43
6	g	1	NAG	C3-C2	2.25	1.57	1.52
5	R	1	NAG	O5-C5	2.25	1.48	1.43
6	K	1	NAG	C3-C2	2.25	1.57	1.52
5	c	1	NAG	O5-C5	2.25	1.48	1.43
4	b	5	MAN	C1-C2	2.23	1.57	1.52
4	F	5	MAN	C1-C2	2.23	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	h	2	NAG	C1-C2	2.22	1.55	1.52
6	W	2	NAG	C1-C2	2.21	1.55	1.52
5	R	1	NAG	C3-C2	2.19	1.57	1.52
6	L	2	NAG	C1-C2	2.19	1.55	1.52
5	G	1	NAG	C3-C2	2.19	1.57	1.52
3	i	1	NAG	O5-C5	2.18	1.47	1.43
3	X	1	NAG	O5-C5	2.17	1.47	1.43
3	M	1	NAG	O5-C5	2.17	1.47	1.43
5	c	1	NAG	C3-C2	2.15	1.57	1.52
7	N	2	SIA	O1A-C1	2.13	1.28	1.22
7	j	2	SIA	O1A-C1	2.13	1.28	1.22
7	Y	2	SIA	O1A-C1	2.12	1.28	1.22
2	Z	1	NAG	O5-C5	2.11	1.47	1.43
3	X	1	NAG	C4-C3	2.11	1.57	1.52
4	b	5	MAN	C2-C3	2.11	1.55	1.52
4	F	5	MAN	C2-C3	2.10	1.55	1.52
3	M	1	NAG	C4-C3	2.10	1.57	1.52
3	U	1	NAG	C4-C5	2.09	1.57	1.53
3	J	1	NAG	C4-C5	2.09	1.57	1.53
3	f	1	NAG	C4-C5	2.08	1.57	1.53
2	D	1	NAG	O5-C5	2.08	1.47	1.43
2	O	1	NAG	O5-C5	2.06	1.47	1.43
3	i	1	NAG	C4-C3	2.06	1.57	1.52
5	c	1	NAG	C4-C3	2.06	1.57	1.52
4	Q	5	MAN	C2-C3	2.04	1.55	1.52
2	S	1	NAG	C4-C5	2.02	1.57	1.53
4	b	7	MAN	C2-C3	2.02	1.55	1.52
5	R	1	NAG	C4-C3	2.01	1.57	1.52
4	F	7	MAN	C2-C3	2.01	1.55	1.52
2	H	1	NAG	C4-C5	2.01	1.57	1.53
5	G	1	NAG	C4-C3	2.01	1.57	1.52
4	Q	7	MAN	C2-C3	2.01	1.55	1.52

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	1	NAG	C3-C4-C5	-6.53	98.59	110.24
2	H	1	NAG	C3-C4-C5	-6.53	98.59	110.24
2	d	3	BMA	C2-C3-C4	-6.51	99.63	110.89
2	S	3	BMA	C2-C3-C4	-6.51	99.63	110.89
2	d	1	NAG	C3-C4-C5	-6.51	98.63	110.24
2	H	3	BMA	C2-C3-C4	-6.50	99.65	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	1	NAG	C3-C4-C5	-6.22	99.15	110.24
3	J	1	NAG	C3-C4-C5	-6.21	99.16	110.24
3	f	1	NAG	C3-C4-C5	-6.19	99.20	110.24
2	O	3	BMA	C2-C3-C4	-5.95	100.59	110.89
2	D	3	BMA	C2-C3-C4	-5.94	100.62	110.89
2	Z	3	BMA	C2-C3-C4	-5.93	100.63	110.89
6	g	1	NAG	C3-C4-C5	-5.85	99.81	110.24
6	V	1	NAG	C3-C4-C5	-5.84	99.83	110.24
6	K	1	NAG	C3-C4-C5	-5.83	99.84	110.24
2	S	2	NAG	C3-C4-C5	-5.69	100.10	110.24
2	H	2	NAG	C3-C4-C5	-5.68	100.11	110.24
2	d	2	NAG	C3-C4-C5	-5.68	100.11	110.24
2	D	1	NAG	C3-C4-C5	-5.52	100.39	110.24
2	O	1	NAG	C3-C4-C5	-5.51	100.40	110.24
2	Z	1	NAG	C3-C4-C5	-5.50	100.42	110.24
3	X	1	NAG	C3-C4-C5	-5.37	100.66	110.24
3	M	1	NAG	C3-C4-C5	-5.35	100.69	110.24
3	i	1	NAG	C3-C4-C5	-5.34	100.72	110.24
5	R	1	NAG	C3-C4-C5	-5.31	100.77	110.24
5	c	1	NAG	C3-C4-C5	-5.30	100.78	110.24
5	G	1	NAG	C3-C4-C5	-5.29	100.80	110.24
2	D	2	NAG	C3-C4-C5	-5.26	100.86	110.24
2	Z	2	NAG	C3-C4-C5	-5.25	100.87	110.24
2	O	2	NAG	C3-C4-C5	-5.24	100.89	110.24
3	I	1	NAG	C3-C4-C5	-4.93	101.45	110.24
3	T	1	NAG	C3-C4-C5	-4.93	101.45	110.24
3	e	1	NAG	C3-C4-C5	-4.92	101.46	110.24
7	N	1	GAL	C4-C3-C2	-4.27	103.38	110.82
7	j	1	GAL	C4-C3-C2	-4.25	103.40	110.82
7	Y	1	GAL	C4-C3-C2	-4.25	103.40	110.82
5	G	2	NAG	C3-C4-C5	-4.24	102.67	110.24
5	R	2	NAG	C3-C4-C5	-4.23	102.69	110.24
5	c	2	NAG	C3-C4-C5	-4.23	102.70	110.24
6	W	2	NAG	C3-C4-C5	-3.95	103.19	110.24
6	L	2	NAG	C3-C4-C5	-3.94	103.21	110.24
6	h	2	NAG	C3-C4-C5	-3.94	103.22	110.24
6	V	2	NAG	C3-C4-C5	-3.92	103.24	110.24
6	g	2	NAG	C3-C4-C5	-3.91	103.26	110.24
6	K	2	NAG	C3-C4-C5	-3.91	103.27	110.24
7	Y	1	GAL	C3-C4-C5	-3.89	103.31	110.24
7	j	1	GAL	C3-C4-C5	-3.89	103.31	110.24
7	N	1	GAL	C3-C4-C5	-3.88	103.32	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	3	BMA	O6-C6-C5	-3.77	98.35	111.29
6	g	3	BMA	O6-C6-C5	-3.77	98.36	111.29
6	V	3	BMA	O6-C6-C5	-3.77	98.37	111.29
3	a	1	NAG	O4-C4-C5	3.73	118.56	109.30
3	E	1	NAG	O4-C4-C5	3.72	118.54	109.30
3	P	1	NAG	O4-C4-C3	3.72	118.95	110.35
3	E	1	NAG	O4-C4-C3	3.71	118.92	110.35
3	P	1	NAG	O4-C4-C5	3.71	118.50	109.30
3	a	1	NAG	O4-C4-C3	3.70	118.90	110.35
3	I	1	NAG	C1-O5-C5	3.56	117.01	112.19
3	e	1	NAG	C1-O5-C5	3.55	117.00	112.19
3	T	1	NAG	C1-O5-C5	3.54	116.99	112.19
6	W	1	NAG	C3-C4-C5	-3.54	103.92	110.24
6	L	1	NAG	C3-C4-C5	-3.54	103.92	110.24
6	h	1	NAG	C3-C4-C5	-3.53	103.94	110.24
2	H	1	NAG	C4-C3-C2	3.52	116.17	111.02
2	S	1	NAG	C4-C3-C2	3.51	116.17	111.02
2	d	1	NAG	C4-C3-C2	3.51	116.17	111.02
6	K	3	BMA	C2-C3-C4	-3.50	104.84	110.89
6	g	3	BMA	C2-C3-C4	-3.49	104.85	110.89
6	V	3	BMA	C2-C3-C4	-3.49	104.86	110.89
3	I	1	NAG	O5-C1-C2	-3.49	105.78	111.29
3	e	1	NAG	O5-C1-C2	-3.48	105.80	111.29
3	T	1	NAG	O5-C1-C2	-3.46	105.82	111.29
2	Z	4	MAN	O5-C1-C2	-3.15	105.90	110.77
2	S	2	NAG	O5-C5-C4	3.15	118.50	110.83
2	D	4	MAN	O5-C1-C2	-3.14	105.92	110.77
2	H	2	NAG	O5-C5-C4	3.14	118.47	110.83
2	d	2	NAG	O5-C5-C4	3.13	118.45	110.83
2	O	4	MAN	O5-C1-C2	-3.13	105.94	110.77
3	P	1	NAG	C1-O5-C5	3.03	116.30	112.19
2	d	1	NAG	O4-C4-C3	-3.03	103.36	110.35
3	E	1	NAG	C1-O5-C5	3.02	116.29	112.19
3	a	1	NAG	C1-O5-C5	3.02	116.29	112.19
2	S	1	NAG	O4-C4-C3	-3.02	103.38	110.35
2	H	1	NAG	O4-C4-C3	-3.02	103.38	110.35
3	P	1	NAG	O5-C1-C2	-2.99	106.56	111.29
3	a	1	NAG	O5-C1-C2	-2.99	106.57	111.29
3	E	1	NAG	O5-C1-C2	-2.98	106.58	111.29
2	S	4	MAN	O5-C1-C2	-2.96	106.20	110.77
2	H	4	MAN	O5-C1-C2	-2.94	106.23	110.77
2	d	4	MAN	O5-C1-C2	-2.92	106.26	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	4	MAN	O5-C1-C2	-2.90	106.30	110.77
6	V	4	MAN	O5-C1-C2	-2.90	106.30	110.77
6	g	4	MAN	O5-C1-C2	-2.89	106.32	110.77
7	j	1	GAL	O1-C1-C2	-2.83	101.07	109.03
7	N	1	GAL	O1-C1-C2	-2.82	101.08	109.03
7	Y	1	GAL	O1-C1-C2	-2.81	101.11	109.03
6	g	5	MAN	O5-C1-C2	-2.72	106.57	110.77
6	K	5	MAN	O5-C1-C2	-2.72	106.58	110.77
6	V	5	MAN	O5-C1-C2	-2.70	106.60	110.77
6	g	5	MAN	C1-O5-C5	2.69	115.84	112.19
3	E	2	NAG	C4-C3-C2	-2.69	107.08	111.02
6	V	5	MAN	C1-O5-C5	2.69	115.83	112.19
6	K	5	MAN	C1-O5-C5	2.68	115.83	112.19
3	a	2	NAG	C4-C3-C2	-2.68	107.09	111.02
3	P	2	NAG	C4-C3-C2	-2.65	107.13	111.02
6	g	4	MAN	C1-O5-C5	2.65	115.79	112.19
6	V	4	MAN	C1-O5-C5	2.65	115.78	112.19
6	K	4	MAN	C1-O5-C5	2.65	115.78	112.19
2	d	4	MAN	C2-C3-C4	-2.58	106.44	110.89
2	S	4	MAN	C2-C3-C4	-2.57	106.45	110.89
2	H	4	MAN	C2-C3-C4	-2.56	106.46	110.89
2	O	1	NAG	O5-C1-C2	-2.54	107.27	111.29
2	D	1	NAG	O5-C1-C2	-2.52	107.31	111.29
2	Z	1	NAG	O5-C1-C2	-2.51	107.32	111.29
7	j	2	SIA	C6-O6-C2	2.51	116.71	111.34
7	Y	2	SIA	C6-O6-C2	2.50	116.70	111.34
7	N	2	SIA	C6-O6-C2	2.50	116.68	111.34
2	O	1	NAG	O5-C5-C6	-2.48	103.32	107.20
2	D	1	NAG	O5-C5-C6	-2.47	103.33	107.20
5	c	1	NAG	O5-C1-C2	-2.47	107.39	111.29
5	R	1	NAG	O5-C1-C2	-2.45	107.42	111.29
2	Z	1	NAG	O5-C5-C6	-2.45	103.37	107.20
5	G	1	NAG	O5-C1-C2	-2.44	107.44	111.29
6	K	4	MAN	C1-C2-C3	2.43	112.65	109.67
6	V	4	MAN	C1-C2-C3	2.41	112.63	109.67
6	g	4	MAN	C1-C2-C3	2.40	112.62	109.67
2	O	2	NAG	C4-C3-C2	2.38	114.51	111.02
2	D	2	NAG	C4-C3-C2	2.38	114.51	111.02
6	L	3	BMA	C2-C3-C4	-2.38	106.78	110.89
6	W	3	BMA	C2-C3-C4	-2.37	106.80	110.89
2	Z	2	NAG	C4-C3-C2	2.37	114.49	111.02
2	D	1	NAG	O4-C4-C5	-2.36	103.44	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	1	NAG	O4-C4-C5	-2.36	103.44	109.30
6	h	3	BMA	C2-C3-C4	-2.36	106.81	110.89
2	Z	1	NAG	O4-C4-C5	-2.36	103.44	109.30
5	c	1	NAG	O4-C4-C3	-2.34	104.94	110.35
5	R	1	NAG	O4-C4-C3	-2.34	104.94	110.35
2	D	4	MAN	C2-C3-C4	-2.33	106.86	110.89
2	O	4	MAN	C2-C3-C4	-2.33	106.86	110.89
5	G	1	NAG	O4-C4-C3	-2.33	104.97	110.35
2	d	3	BMA	C1-C2-C3	2.33	112.53	109.67
7	Y	2	SIA	O1B-C1-C2	2.33	119.67	113.03
7	N	2	SIA	O1B-C1-C2	2.32	119.67	113.03
6	K	1	NAG	O5-C1-C2	-2.32	107.63	111.29
2	Z	4	MAN	C2-C3-C4	-2.32	106.89	110.89
3	i	1	NAG	O5-C1-C2	-2.32	107.63	111.29
2	S	3	BMA	C1-C2-C3	2.32	112.51	109.67
2	H	3	BMA	C1-C2-C3	2.31	112.51	109.67
7	j	2	SIA	O1B-C1-C2	2.31	119.62	113.03
6	V	1	NAG	O5-C1-C2	-2.31	107.65	111.29
6	g	1	NAG	O5-C1-C2	-2.30	107.65	111.29
3	M	1	NAG	O5-C1-C2	-2.29	107.67	111.29
3	X	1	NAG	O5-C1-C2	-2.28	107.69	111.29
7	j	2	SIA	C11-C10-N5	2.26	119.93	116.10
2	d	1	NAG	O5-C5-C4	2.25	116.31	110.83
2	H	1	NAG	O5-C5-C4	2.25	116.30	110.83
2	S	1	NAG	O5-C5-C4	2.25	116.30	110.83
7	N	2	SIA	C11-C10-N5	2.25	119.91	116.10
7	Y	2	SIA	C11-C10-N5	2.24	119.89	116.10
5	R	3	BMA	C1-C2-C3	-2.23	106.92	109.67
5	G	3	BMA	C1-C2-C3	-2.23	106.93	109.67
5	c	3	BMA	C1-C2-C3	-2.22	106.94	109.67
7	N	2	SIA	C4-C5-N5	-2.20	106.01	110.38
7	j	2	SIA	C4-C5-N5	-2.20	106.01	110.38
3	a	1	NAG	C3-C4-C5	-2.20	106.31	110.24
3	E	1	NAG	C3-C4-C5	-2.20	106.32	110.24
7	Y	2	SIA	C4-C5-N5	-2.19	106.03	110.38
3	P	1	NAG	C3-C4-C5	-2.19	106.33	110.24
6	W	2	NAG	O4-C4-C3	-2.19	105.29	110.35
7	N	1	GAL	O3-C3-C4	2.19	115.40	110.35
3	U	1	NAG	O5-C1-C2	-2.18	107.84	111.29
6	W	4	MAN	C2-C3-C4	-2.18	107.12	110.89
6	L	2	NAG	O4-C4-C3	-2.18	105.30	110.35
3	J	1	NAG	O5-C1-C2	-2.18	107.84	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	h	2	NAG	O4-C4-C3	-2.18	105.31	110.35
7	Y	1	GAL	O3-C3-C4	2.18	115.38	110.35
7	j	1	GAL	O3-C3-C4	2.18	115.38	110.35
6	L	4	MAN	C2-C3-C4	-2.17	107.15	110.89
6	h	4	MAN	C2-C3-C4	-2.17	107.15	110.89
2	S	2	NAG	C6-C5-C4	-2.16	107.94	113.00
2	H	2	NAG	C6-C5-C4	-2.16	107.94	113.00
6	g	3	BMA	O3-C3-C2	-2.16	105.86	109.99
2	d	2	NAG	C6-C5-C4	-2.16	107.95	113.00
3	f	1	NAG	O5-C1-C2	-2.15	107.89	111.29
6	K	3	BMA	O3-C3-C2	-2.15	105.88	109.99
2	S	4	MAN	C1-C2-C3	2.15	112.30	109.67
6	V	3	BMA	O3-C3-C2	-2.14	105.89	109.99
2	O	1	NAG	O5-C5-C4	2.14	116.04	110.83
2	D	1	NAG	O5-C5-C4	2.14	116.04	110.83
2	Z	1	NAG	O5-C5-C4	2.14	116.03	110.83
2	H	4	MAN	C1-C2-C3	2.13	112.29	109.67
2	D	1	NAG	C4-C3-C2	2.13	114.14	111.02
2	d	4	MAN	C1-C2-C3	2.13	112.28	109.67
3	X	2	NAG	C4-C3-C2	-2.12	107.91	111.02
2	O	1	NAG	C4-C3-C2	2.12	114.12	111.02
2	Z	1	NAG	C4-C3-C2	2.11	114.10	111.02
3	M	2	NAG	C4-C3-C2	-2.10	107.95	111.02
2	S	4	MAN	C1-O5-C5	2.09	115.02	112.19
2	D	4	MAN	C1-O5-C5	2.09	115.02	112.19
2	O	4	MAN	C1-O5-C5	2.09	115.02	112.19
2	H	4	MAN	C1-O5-C5	2.08	115.01	112.19
3	i	2	NAG	C4-C3-C2	-2.08	107.97	111.02
6	K	5	MAN	C1-C2-C3	2.07	112.21	109.67
2	Z	4	MAN	C1-O5-C5	2.07	114.99	112.19
6	g	5	MAN	C1-C2-C3	2.07	112.21	109.67
2	d	4	MAN	C1-O5-C5	2.07	114.99	112.19
6	W	2	NAG	C4-C3-C2	2.06	114.04	111.02
6	V	5	MAN	C1-C2-C3	2.06	112.19	109.67
6	L	2	NAG	C4-C3-C2	2.05	114.02	111.02
6	h	2	NAG	C4-C3-C2	2.05	114.02	111.02
2	Z	2	NAG	C1-C2-N2	-2.05	106.99	110.49
2	O	2	NAG	C1-C2-N2	-2.03	107.02	110.49
2	D	2	NAG	C1-C2-N2	-2.02	107.03	110.49

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	3	BMA	C4-C5-C6-O6
4	Q	3	BMA	C4-C5-C6-O6
4	b	3	BMA	C4-C5-C6-O6
6	K	3	BMA	O5-C5-C6-O6
6	V	3	BMA	O5-C5-C6-O6
6	g	3	BMA	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	Z	1	NAG	C4-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6
6	h	2	NAG	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	Q	3	BMA	O5-C5-C6-O6
4	b	3	BMA	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6
6	K	3	BMA	C4-C5-C6-O6
6	V	3	BMA	C4-C5-C6-O6
6	g	3	BMA	C4-C5-C6-O6
2	H	4	MAN	O5-C5-C6-O6
2	S	4	MAN	O5-C5-C6-O6
2	d	4	MAN	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
6	g	1	NAG	O5-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
6	W	2	NAG	C4-C5-C6-O6
6	h	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	Z	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
7	N	2	SIA	O8-C8-C9-O9

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Mol	Chain	Res	Type	Atoms
7	Y	2	SIA	O8-C8-C9-O9
7	j	2	SIA	O8-C8-C9-O9
4	F	4	MAN	O5-C5-C6-O6
4	Q	4	MAN	O5-C5-C6-O6
4	b	4	MAN	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
2	Z	4	MAN	O5-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	O	4	MAN	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
4	F	6	MAN	O5-C5-C6-O6
4	Q	6	MAN	O5-C5-C6-O6
4	b	6	MAN	O5-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6
6	W	4	MAN	O5-C5-C6-O6
6	h	4	MAN	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
2	S	3	BMA	O5-C5-C6-O6
2	Z	3	BMA	O5-C5-C6-O6
2	d	3	BMA	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	e	2	NAG	O5-C5-C6-O6
3	i	2	NAG	O5-C5-C6-O6
6	L	5	MAN	O5-C5-C6-O6
6	W	5	MAN	O5-C5-C6-O6
6	h	5	MAN	O5-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
6	W	3	BMA	O5-C5-C6-O6
6	h	3	BMA	O5-C5-C6-O6
3	e	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C4-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
6	g	1	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
7	N	2	SIA	C7-C8-C9-O9
7	Y	2	SIA	C7-C8-C9-O9
7	j	2	SIA	C7-C8-C9-O9
3	e	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
2	H	4	MAN	C4-C5-C6-O6
2	S	4	MAN	C4-C5-C6-O6
2	d	4	MAN	C4-C5-C6-O6
7	N	2	SIA	O1A-C1-C2-O6
7	Y	2	SIA	O1A-C1-C2-O6
7	j	2	SIA	O1A-C1-C2-O6

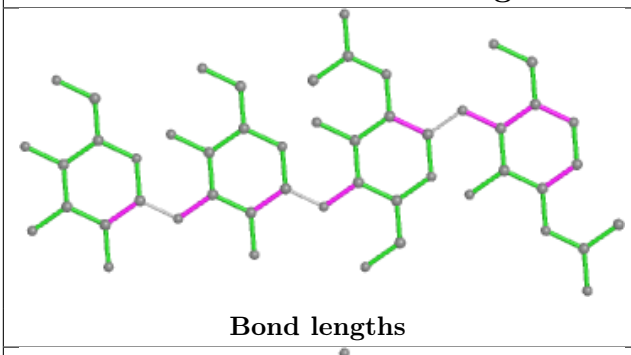
There are no ring outliers.

1 monomer is involved in 1 short contact:

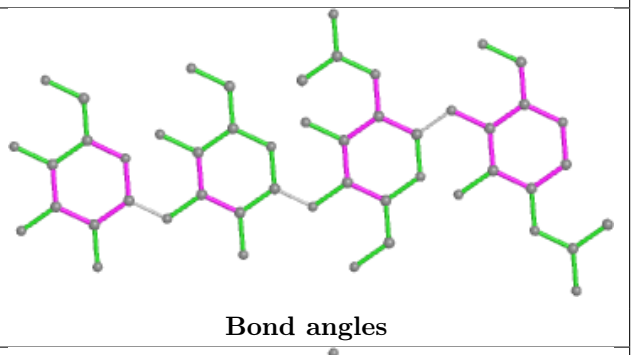
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	1	0

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

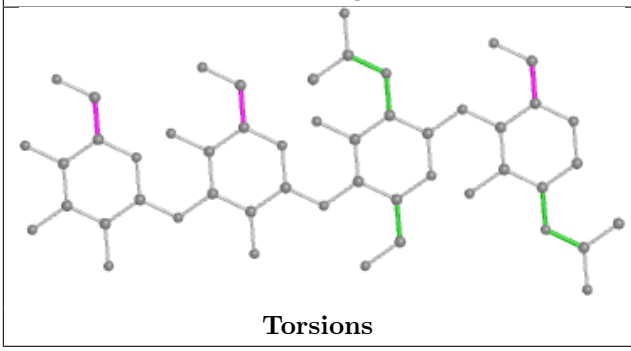
Oligosaccharide Chain D



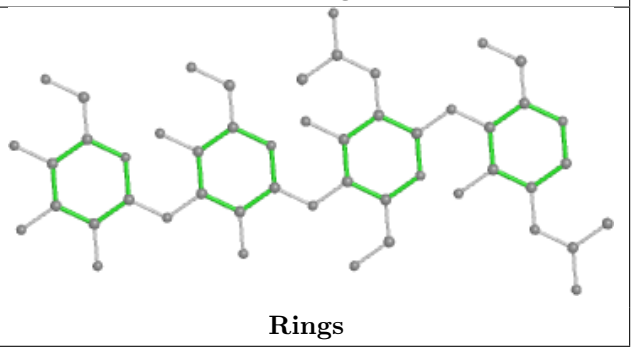
Bond lengths



Bond angles

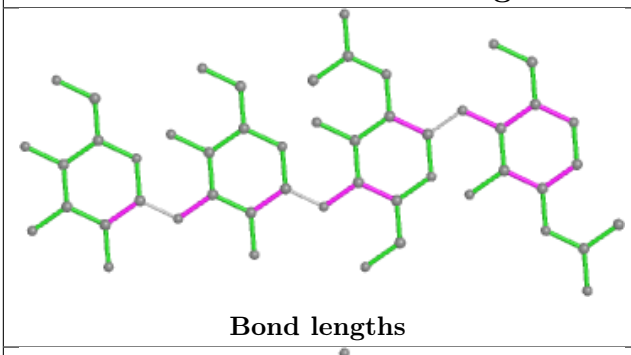


Torsions

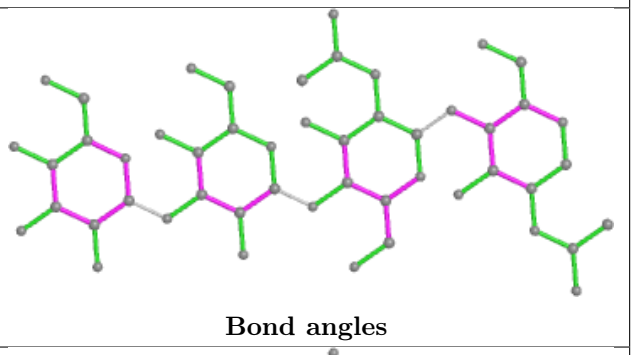


Rings

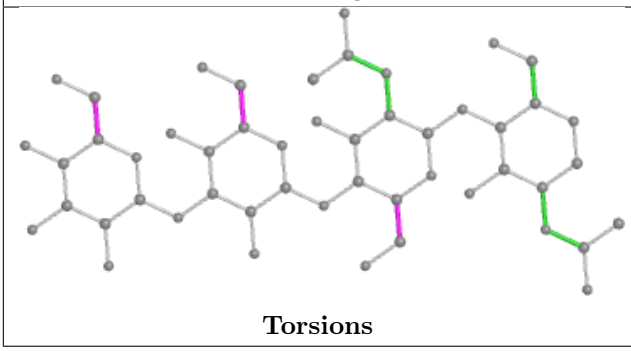
Oligosaccharide Chain H



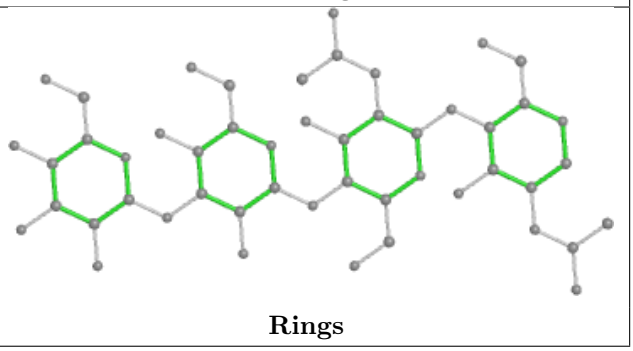
Bond lengths



Bond angles

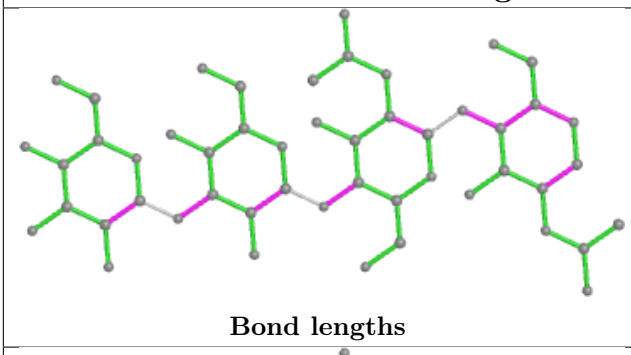


Torsions

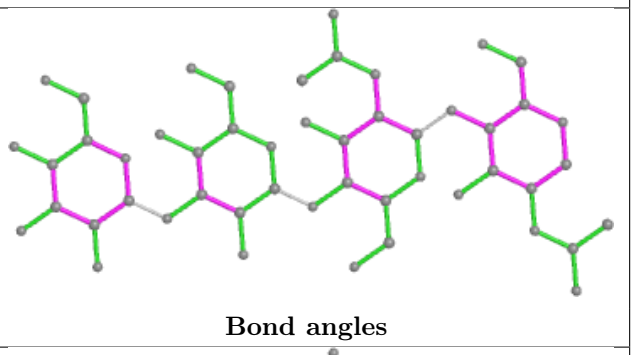


Rings

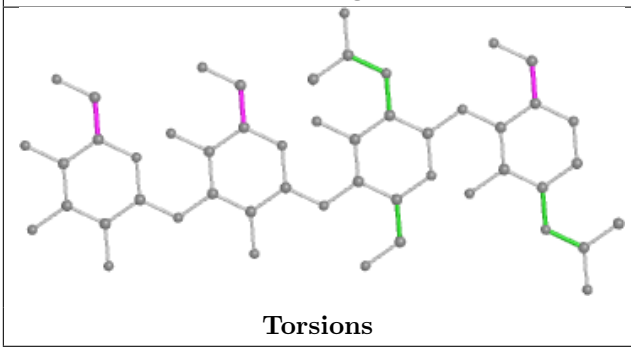
Oligosaccharide Chain O



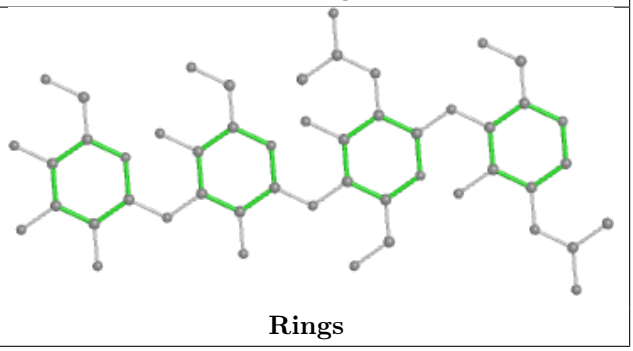
Bond lengths



Bond angles

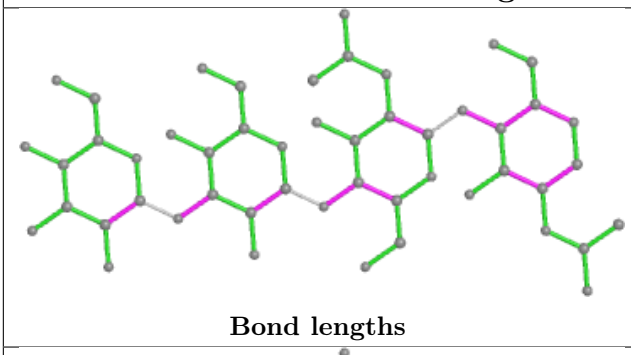


Torsions



Rings

Oligosaccharide Chain S



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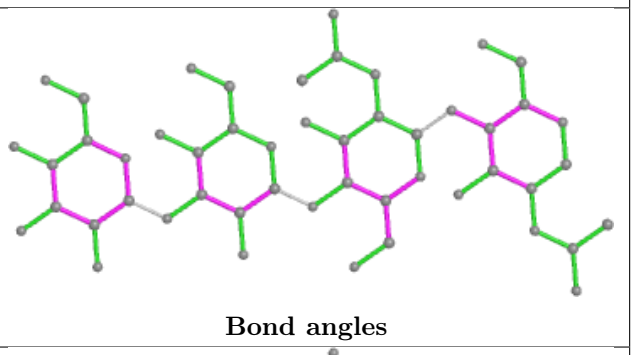
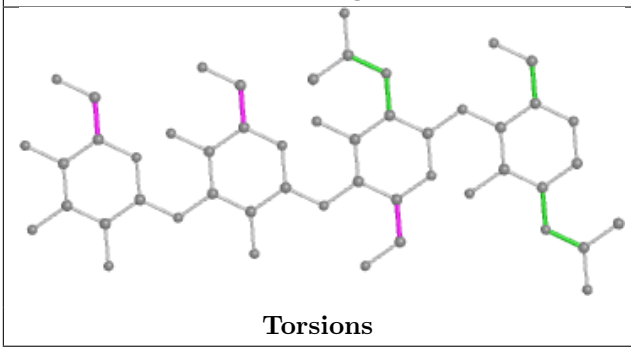


Bond angles



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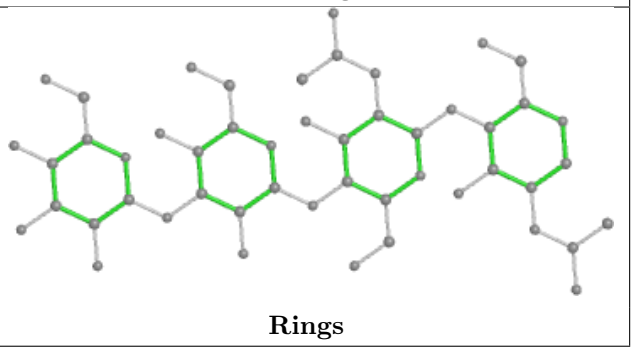
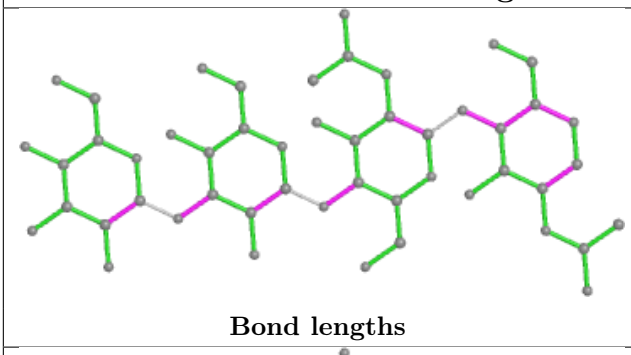


Rings

Oligosaccharide Chain Z



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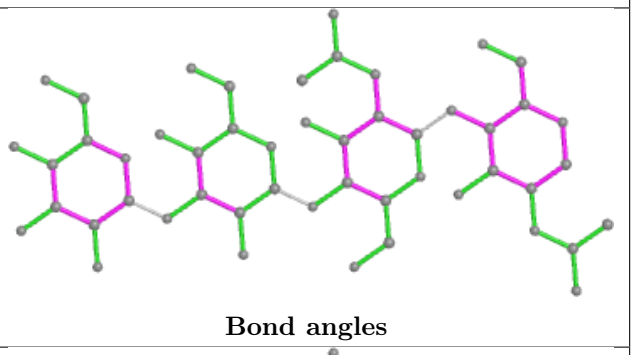
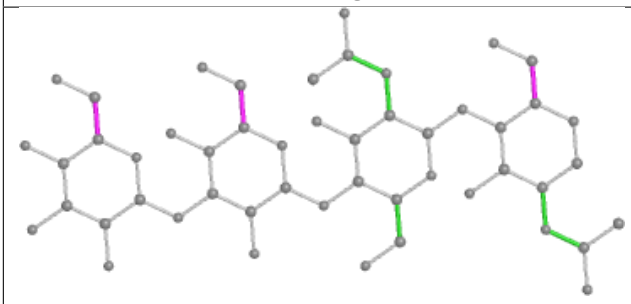


Bond angles



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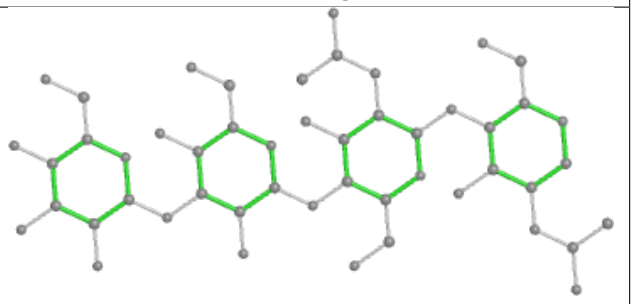
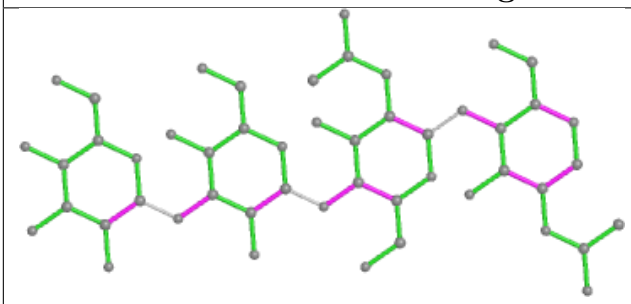


Rings

Oligosaccharide Chain d



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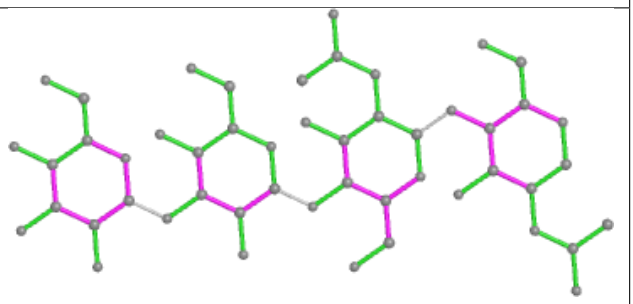
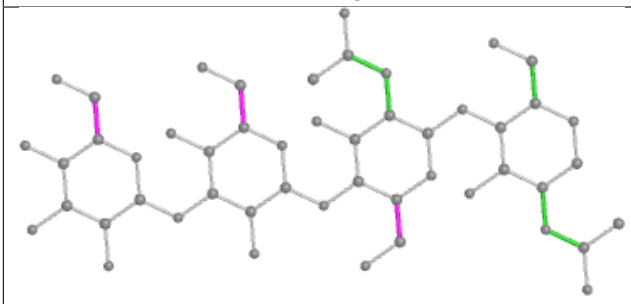


Bond angles



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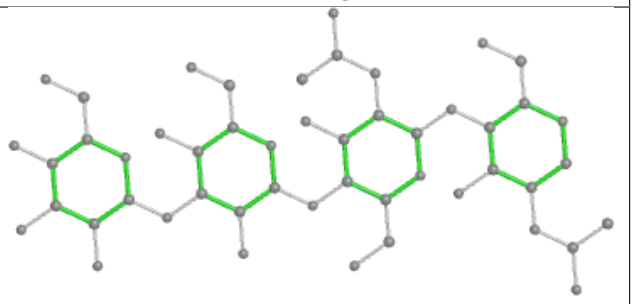
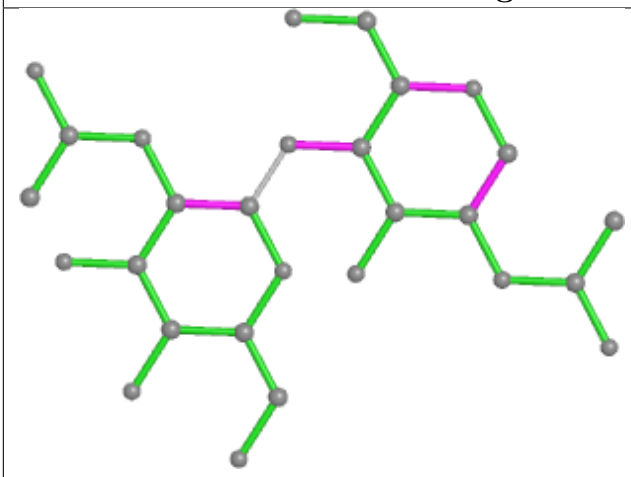


Rings

Oligosaccharide Chain E



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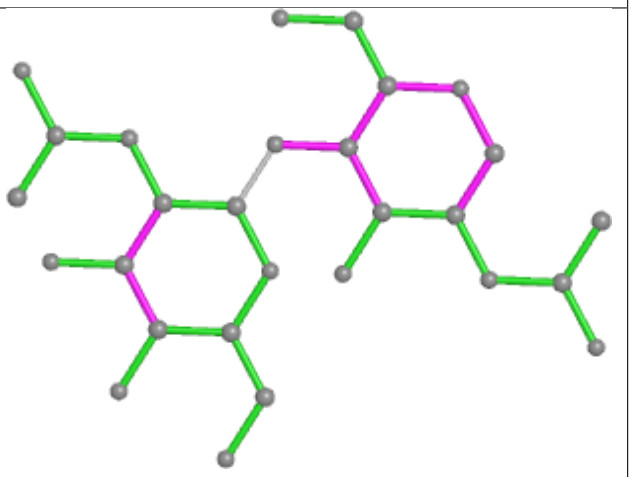
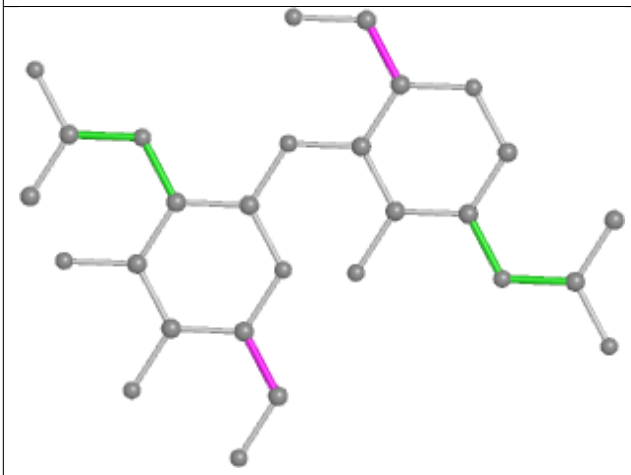


Bond angles



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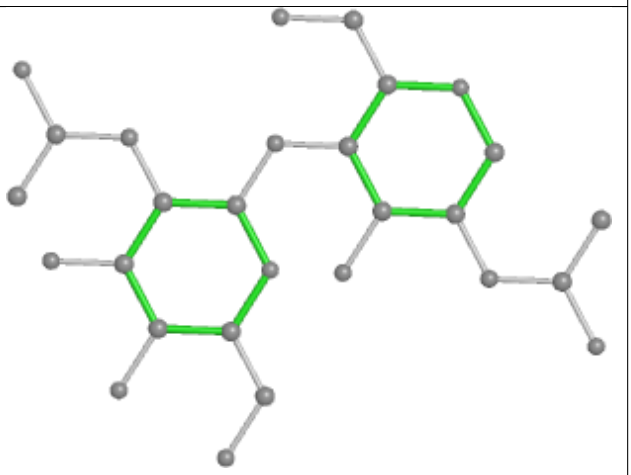
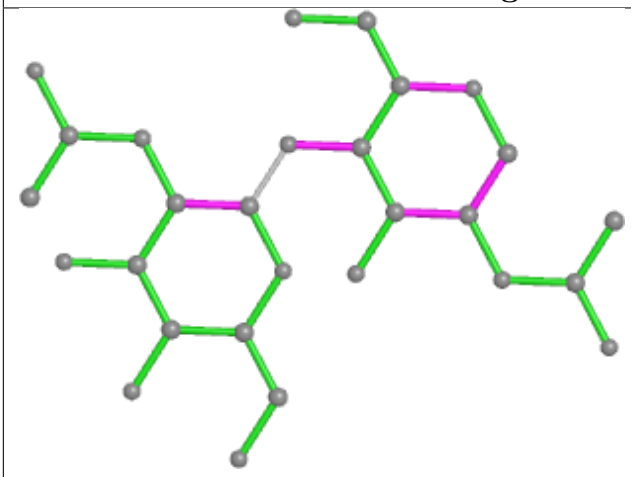


Rings

Oligosaccharide Chain I



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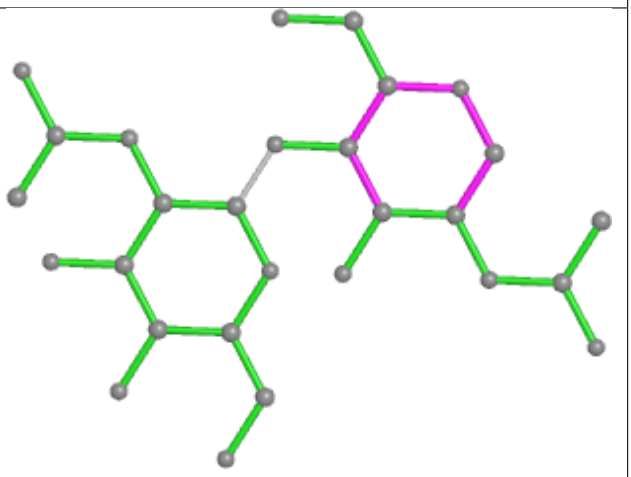
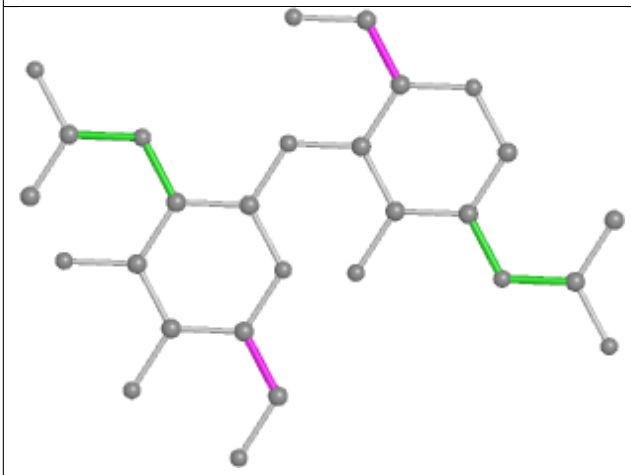


Bond angles



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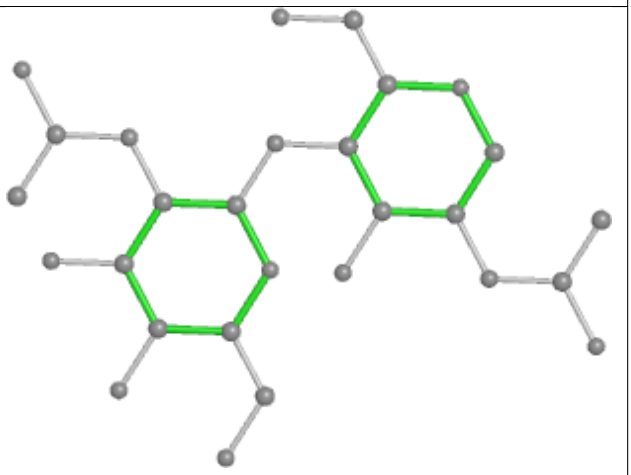
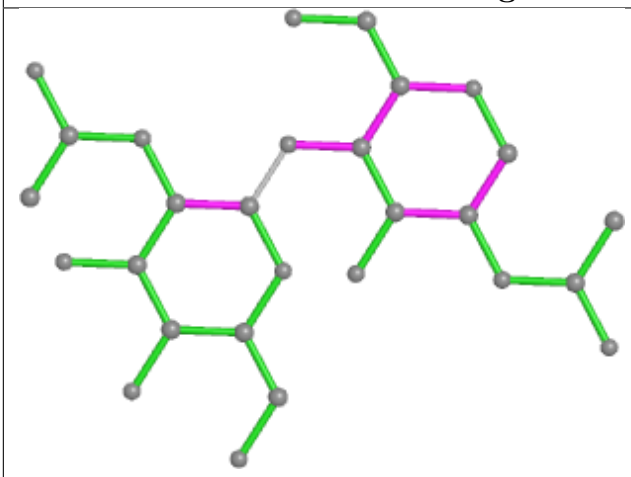


Rings

Oligosaccharide Chain J



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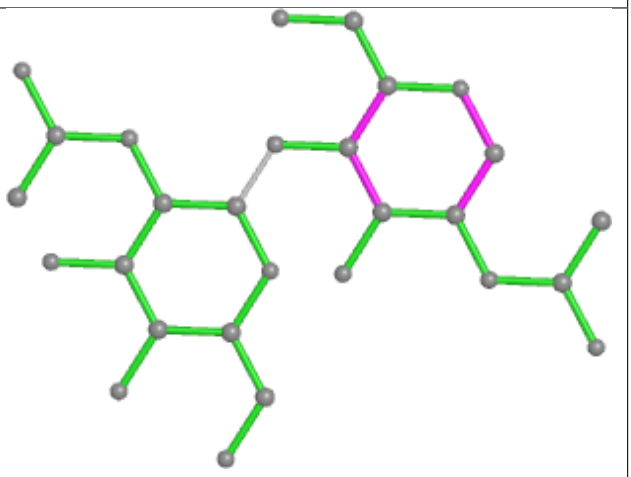
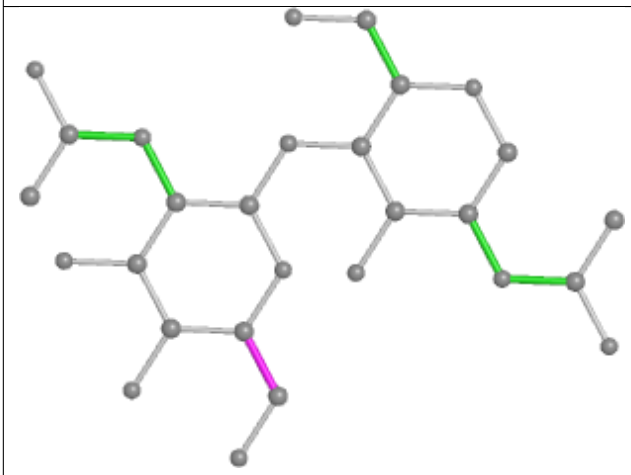
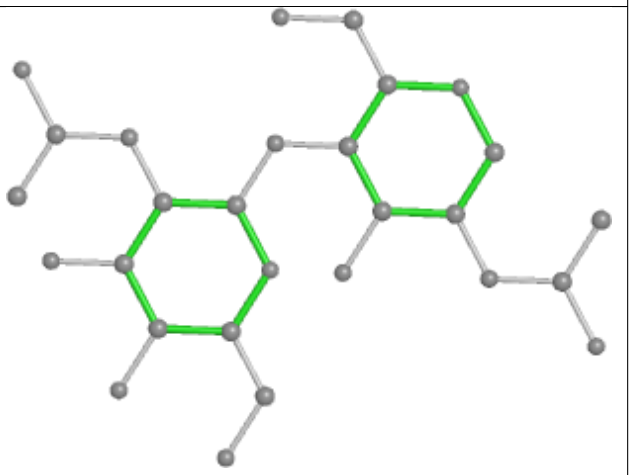


Bond angles

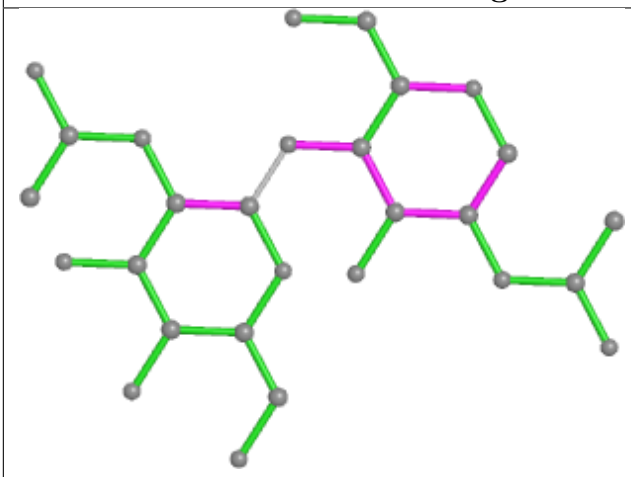


Torsions



Rings

Oligosaccharide Chain M



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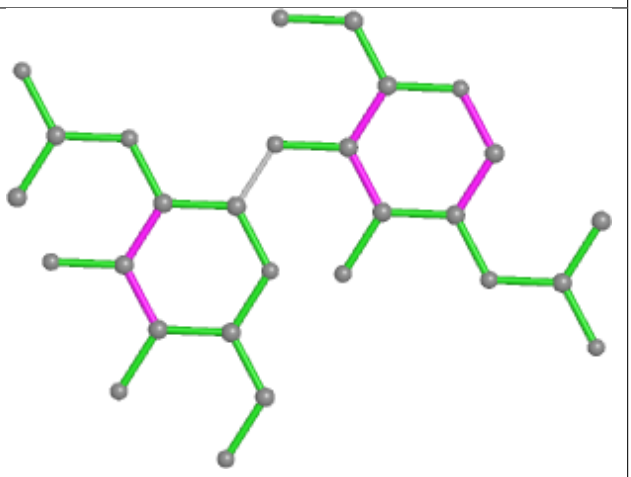
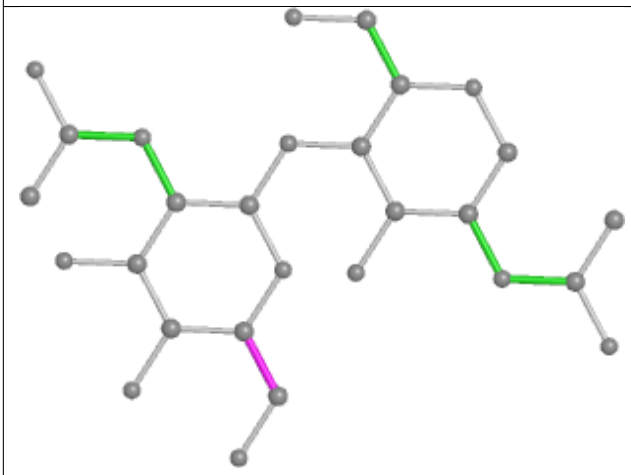


Bond angles



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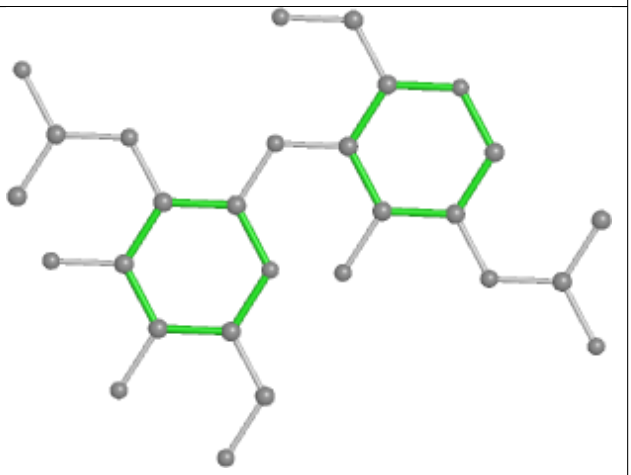
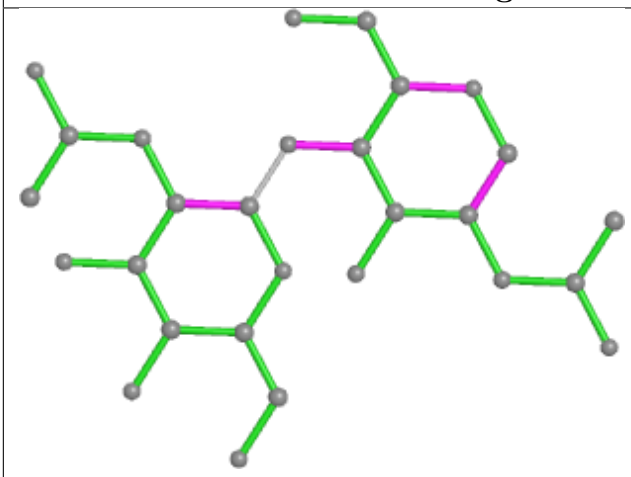


Rings

Oligosaccharide Chain P



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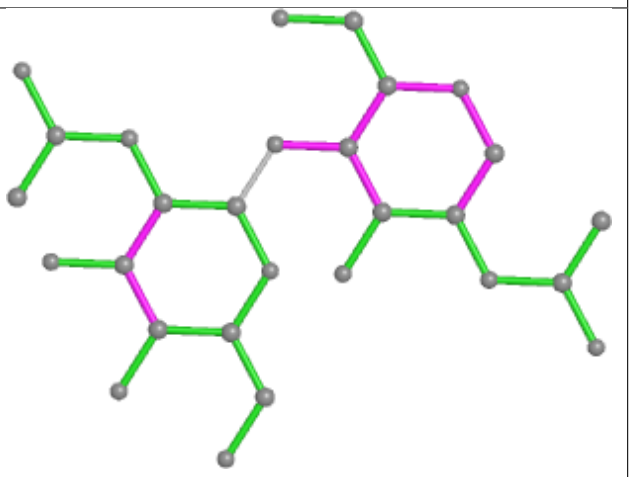
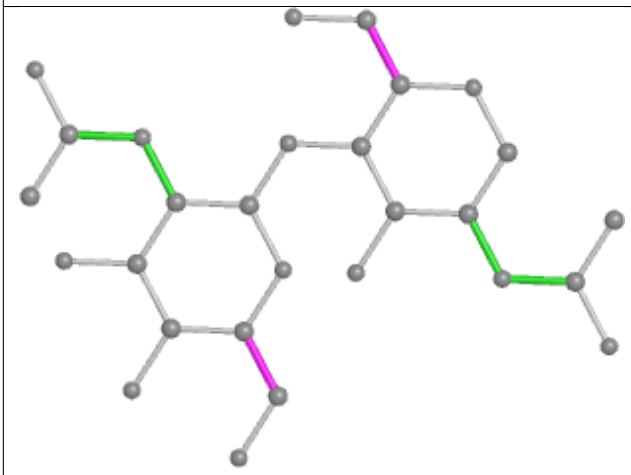
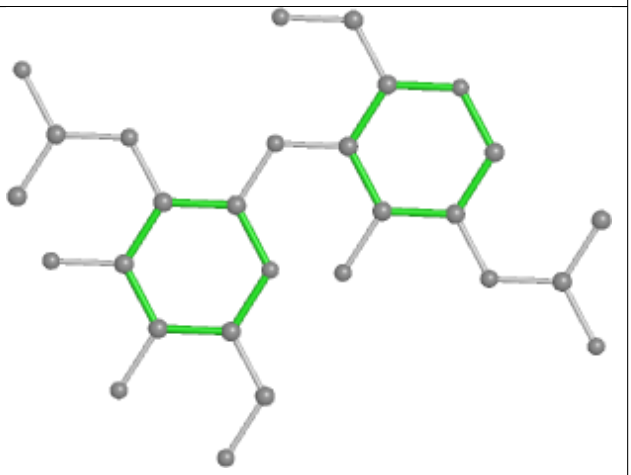


Bond angles

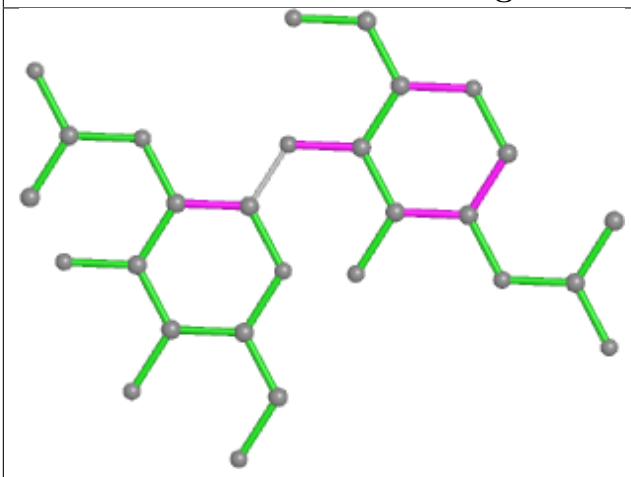


Torsions



Rings

Oligosaccharide Chain T



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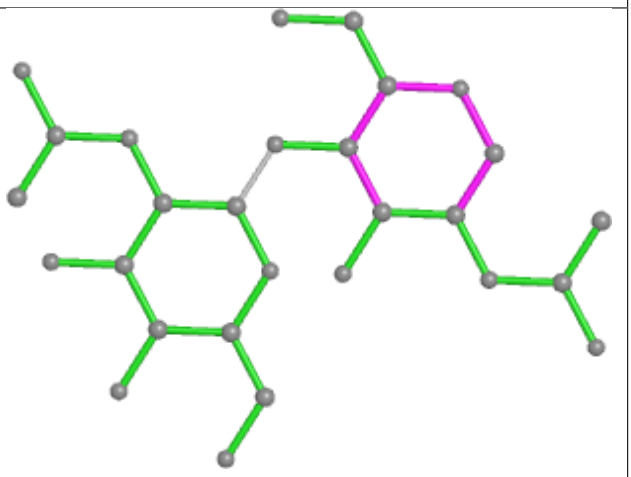
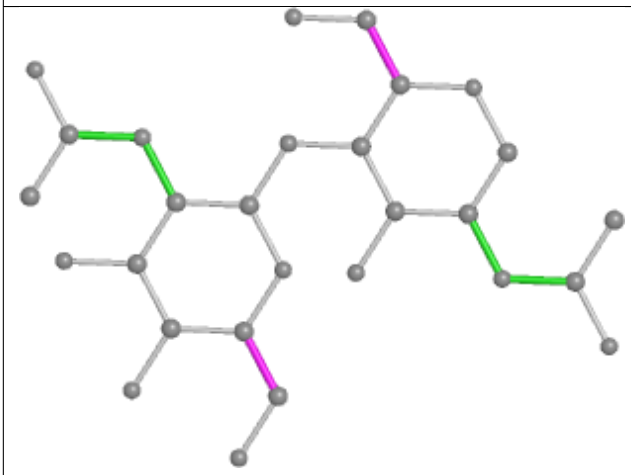
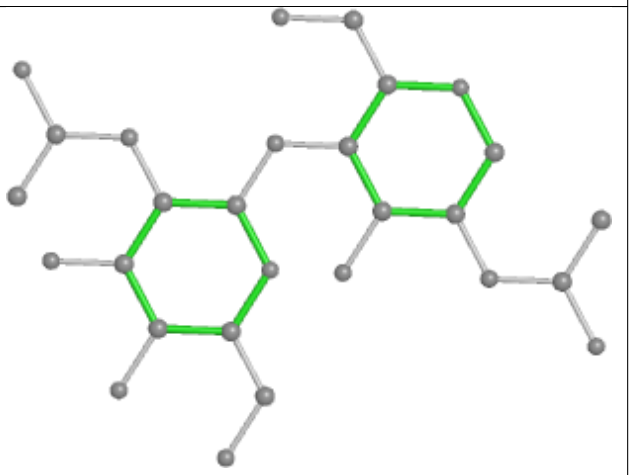


Bond angles

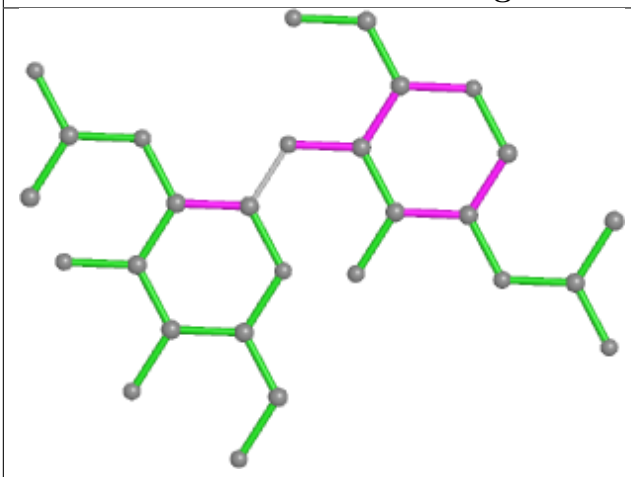


Torsions



Rings

Oligosaccharide Chain U



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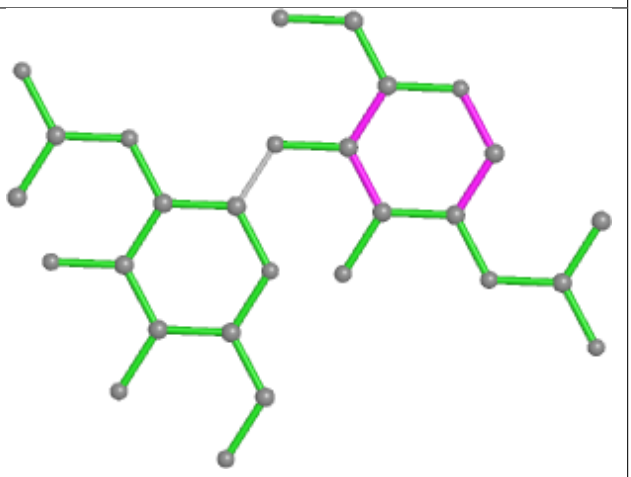
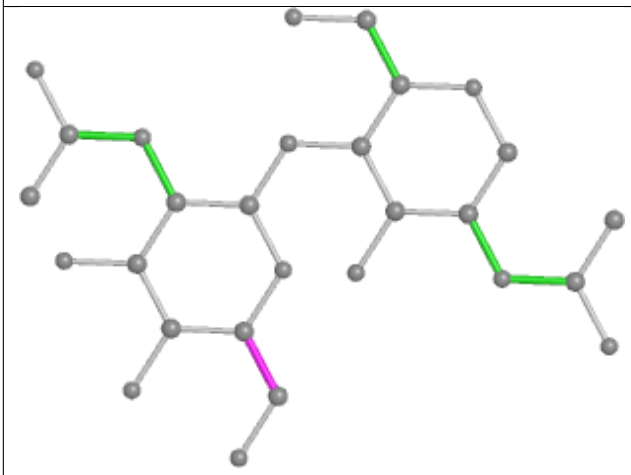


Bond angles



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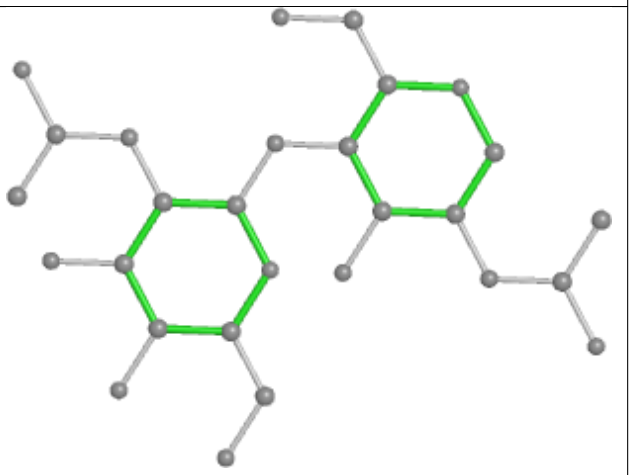
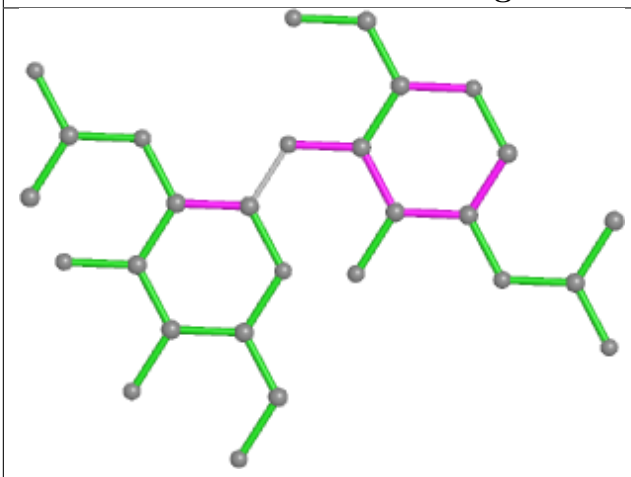


Rings

Oligosaccharide Chain X



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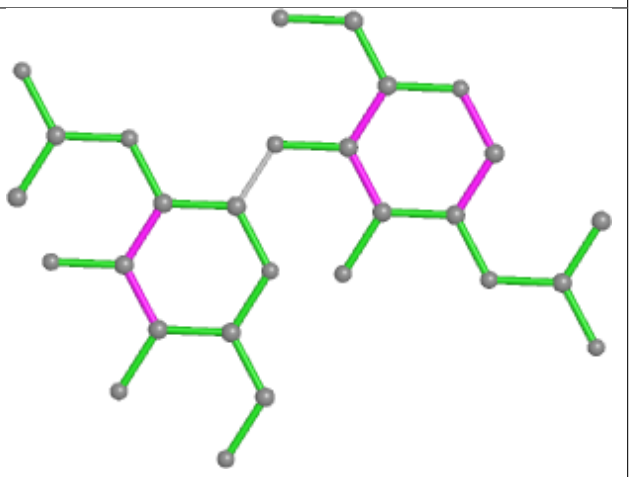
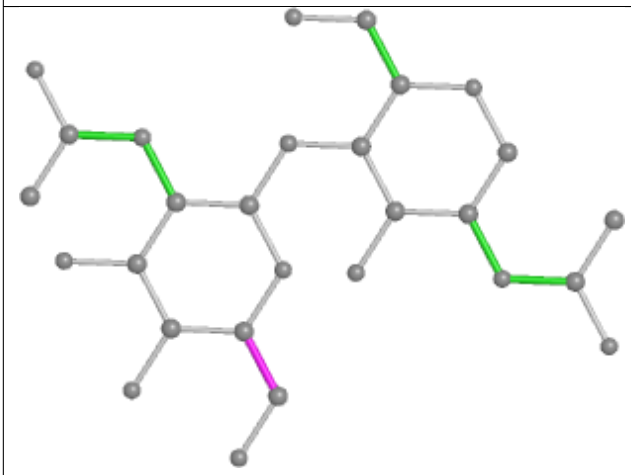


Bond angles



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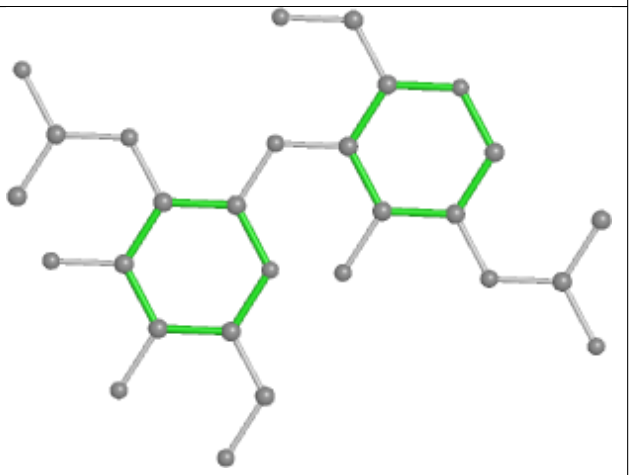
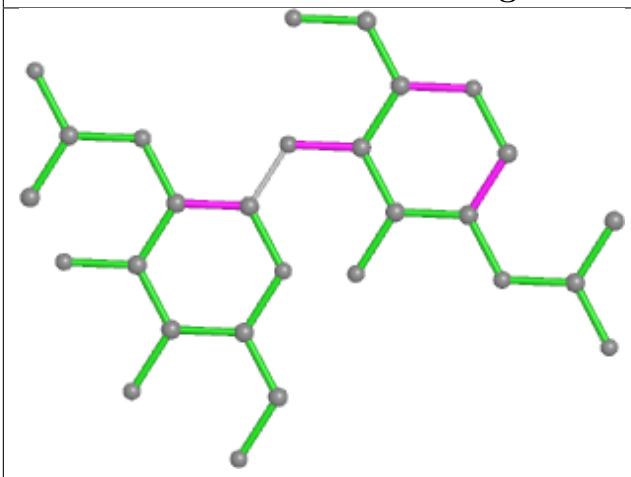


Rings

Oligosaccharide Chain a



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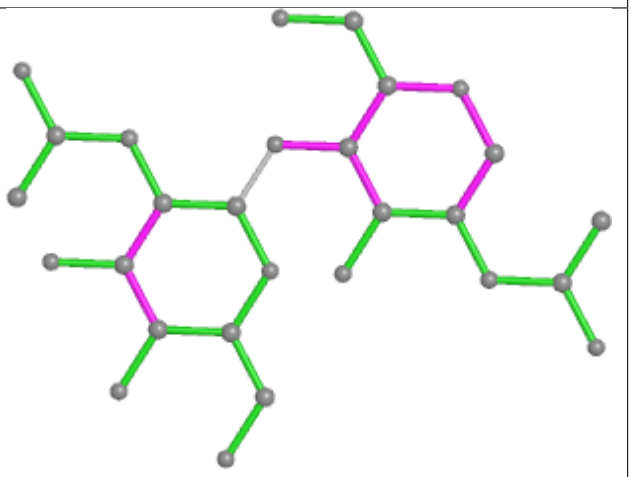
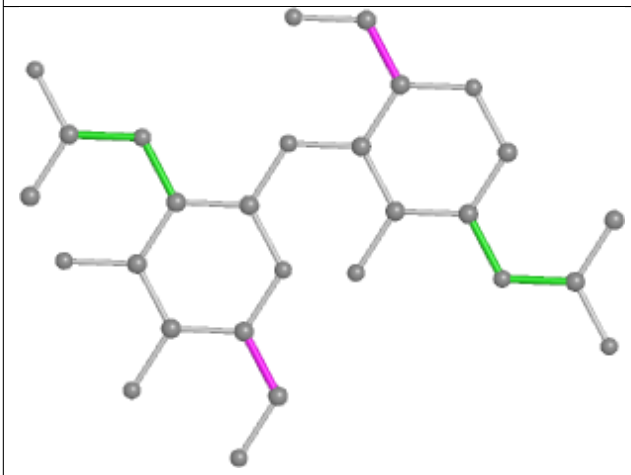


Bond angles



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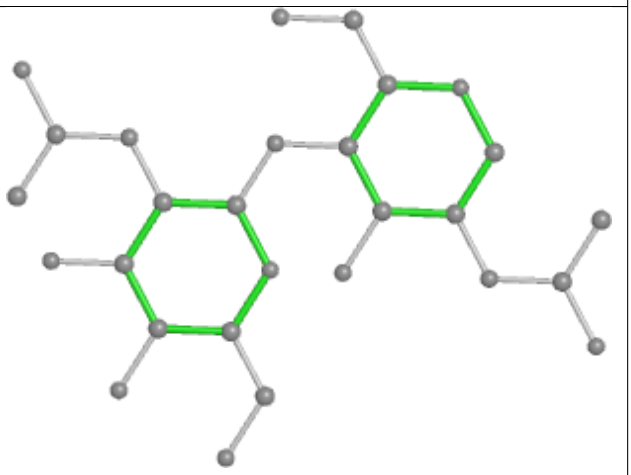
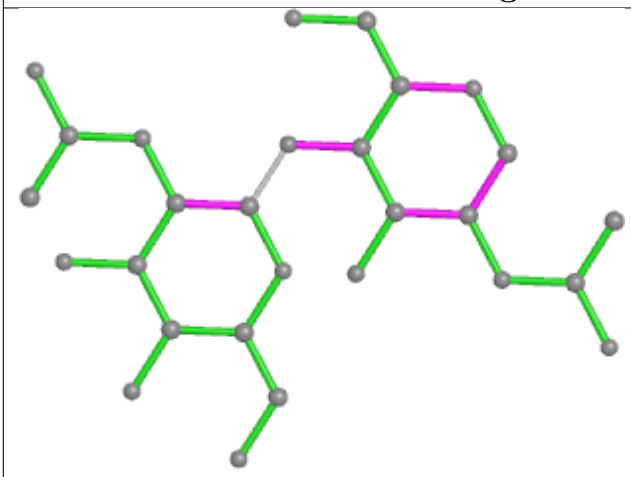


Rings

Oligosaccharide Chain e



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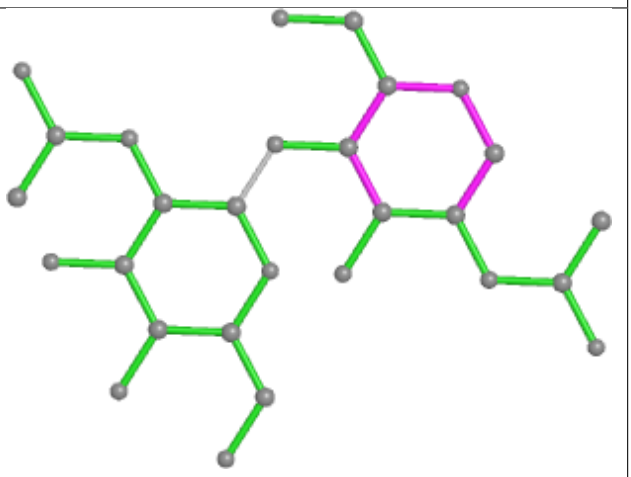
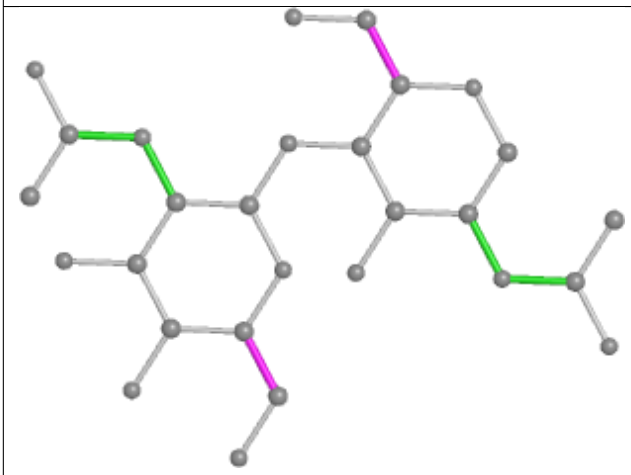


Bond angles



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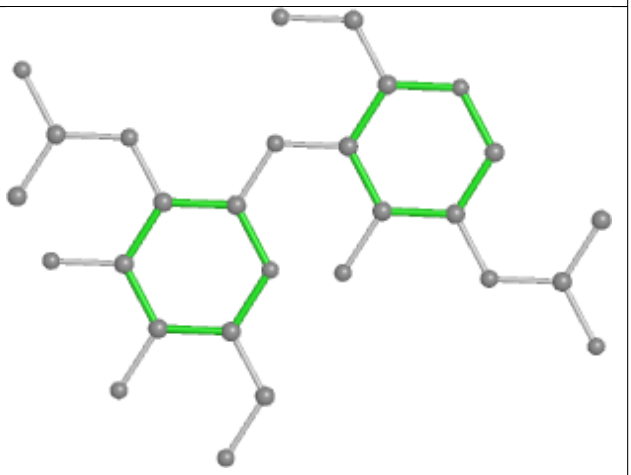
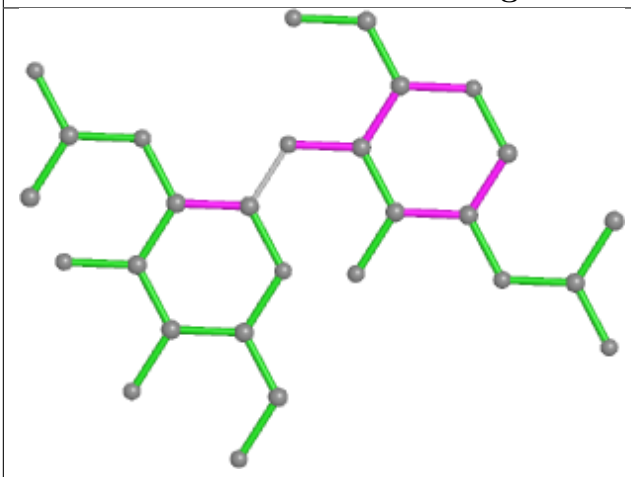
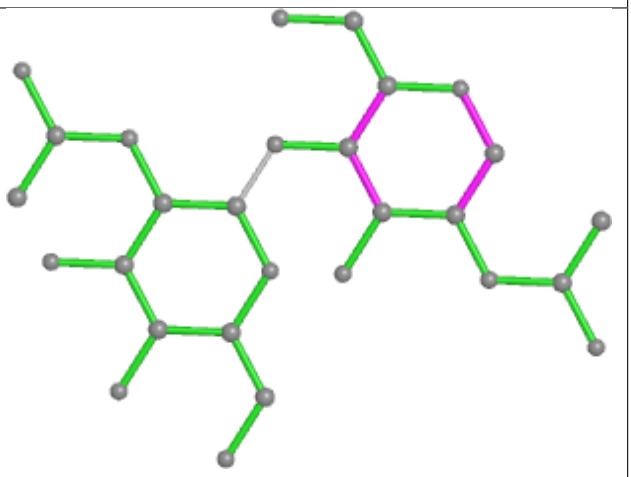


Rings

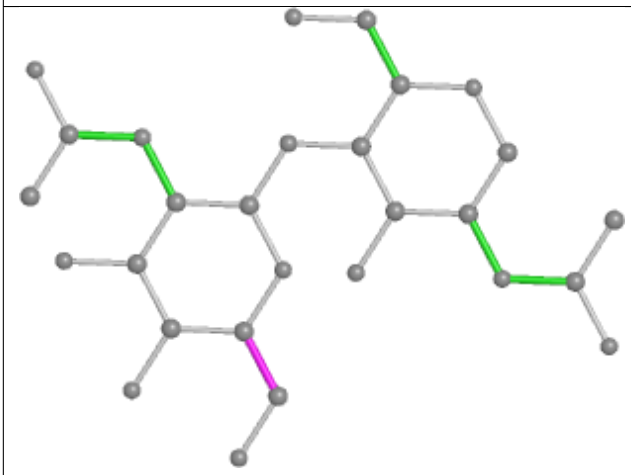
Oligosaccharide Chain f



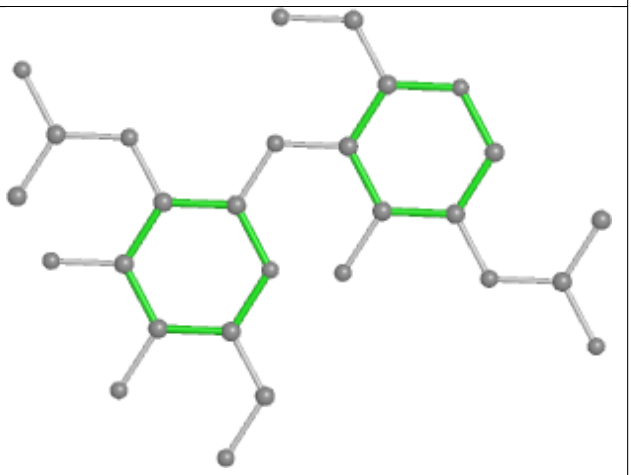
Bond lengths



Bond angles

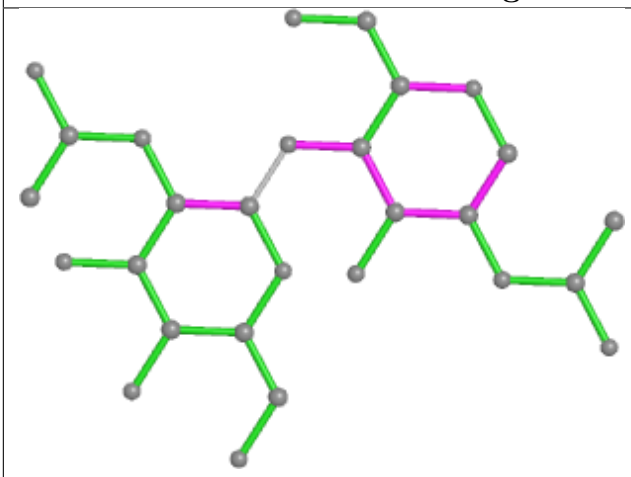


Torsions



Rings

Oligosaccharide Chain i



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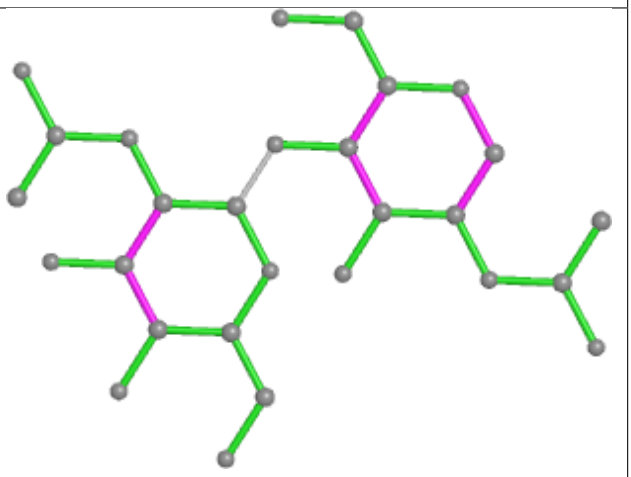
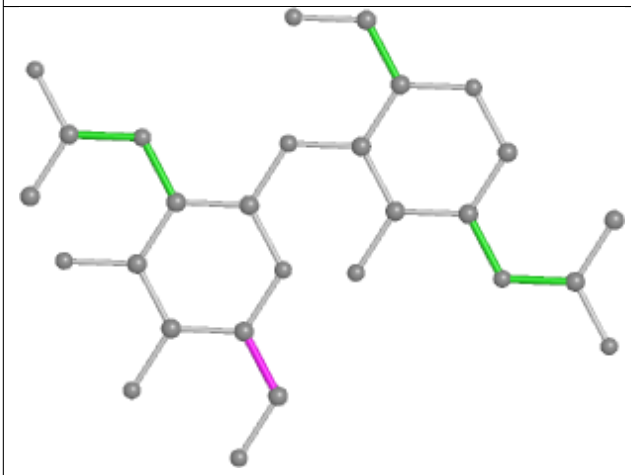
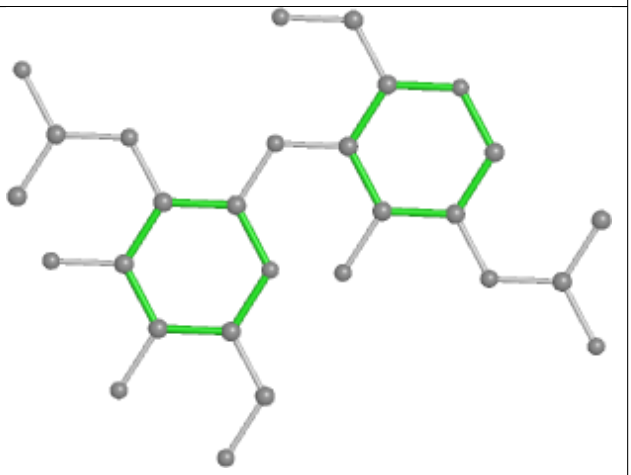


Bond angles

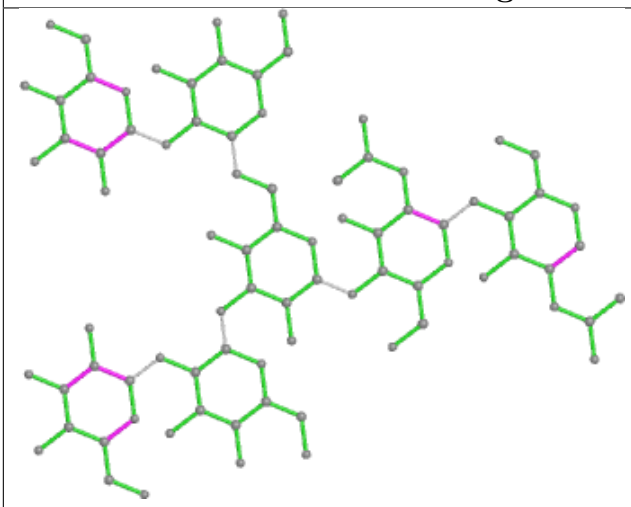


Torsions



Rings

Oligosaccharide Chain F



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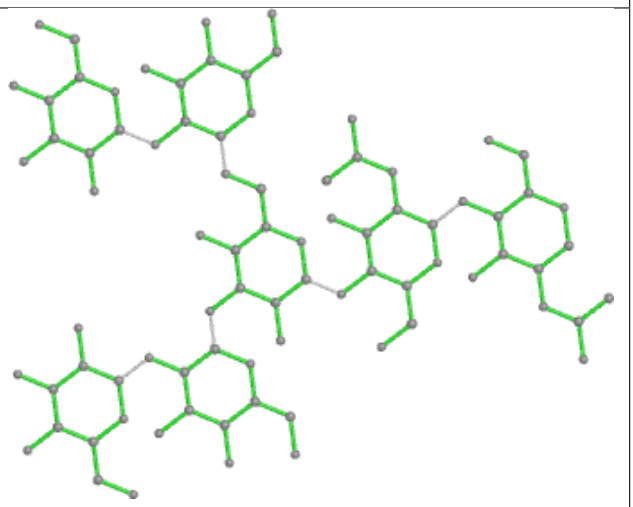
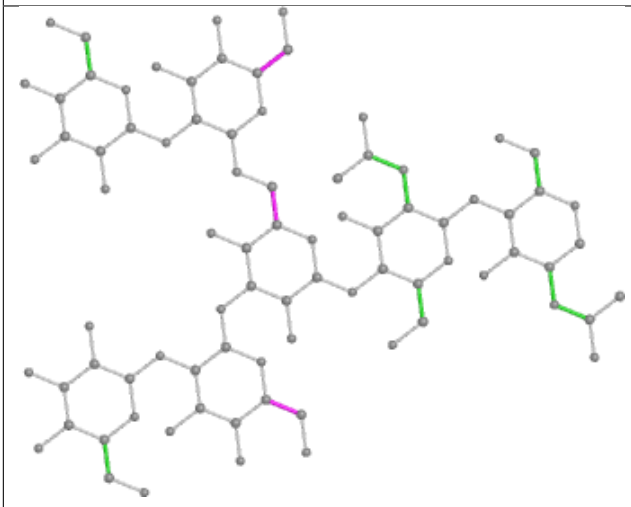


Bond angles



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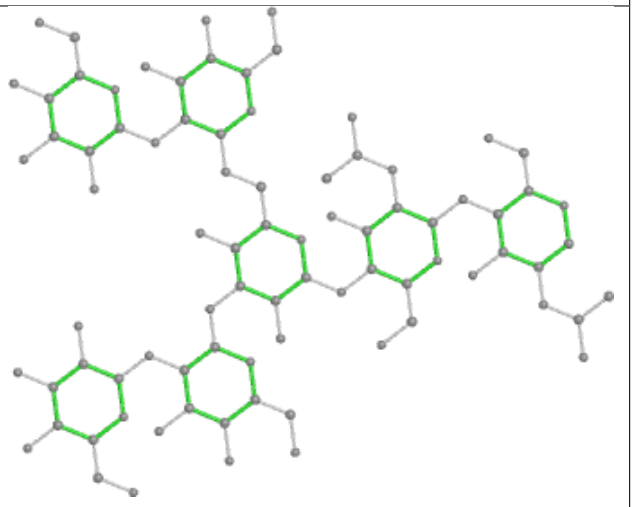
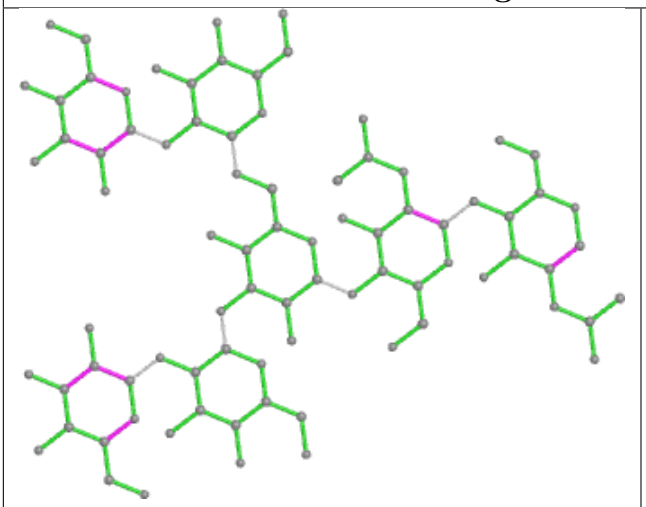


Rings

Oligosaccharide Chain Q



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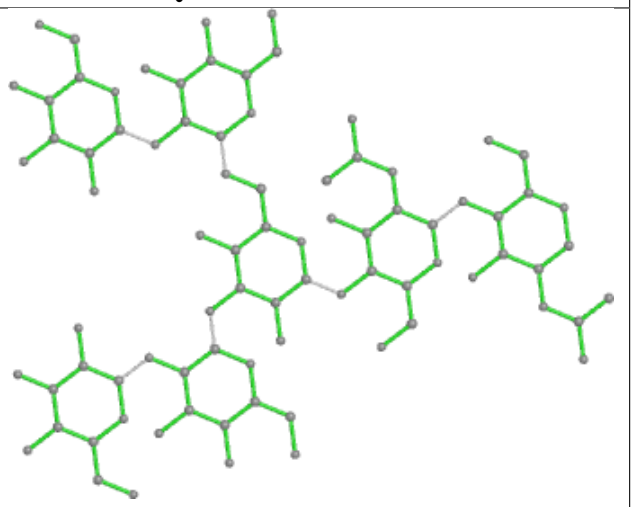
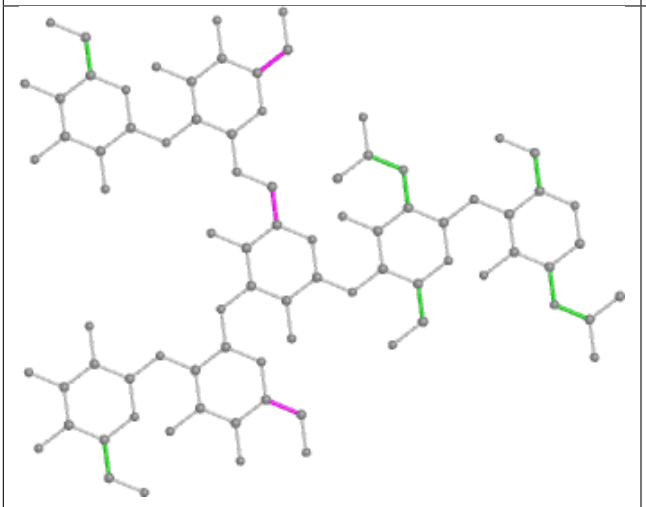


Bond angles



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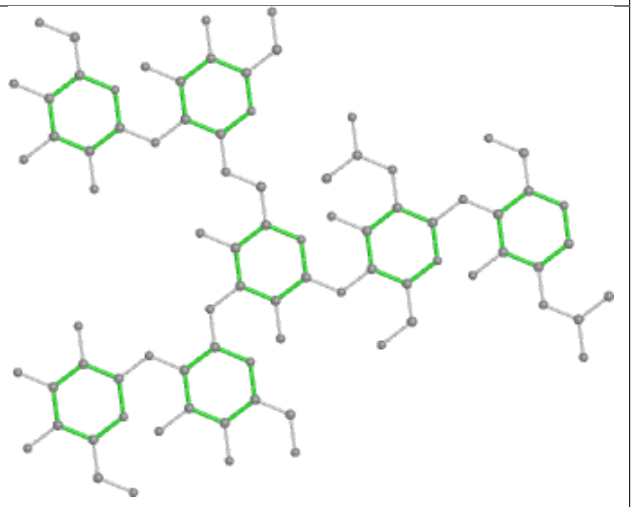
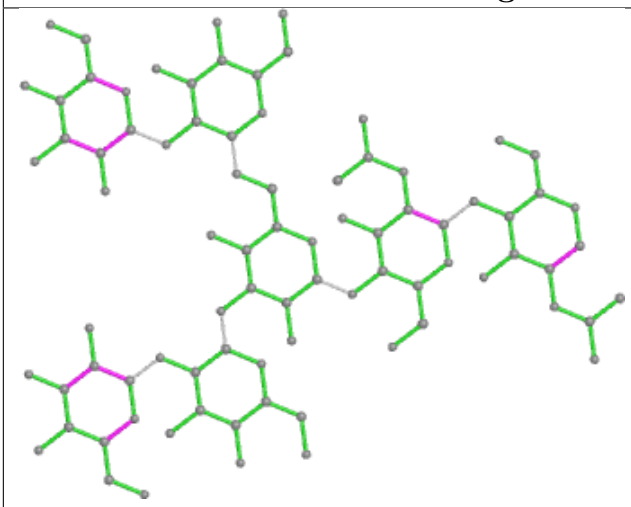


Rings

Oligosaccharide Chain b



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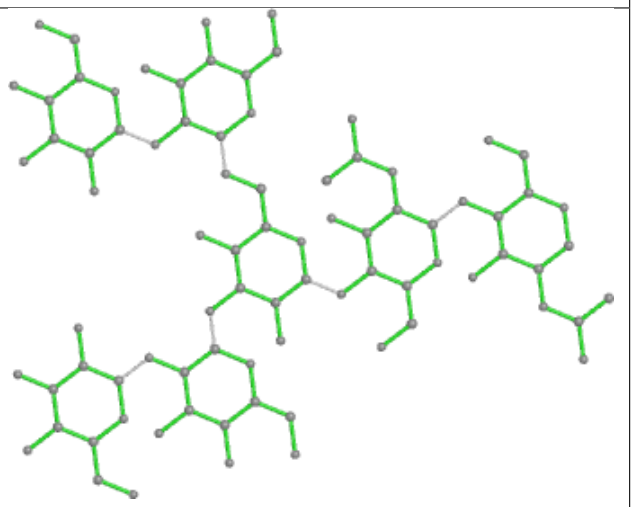
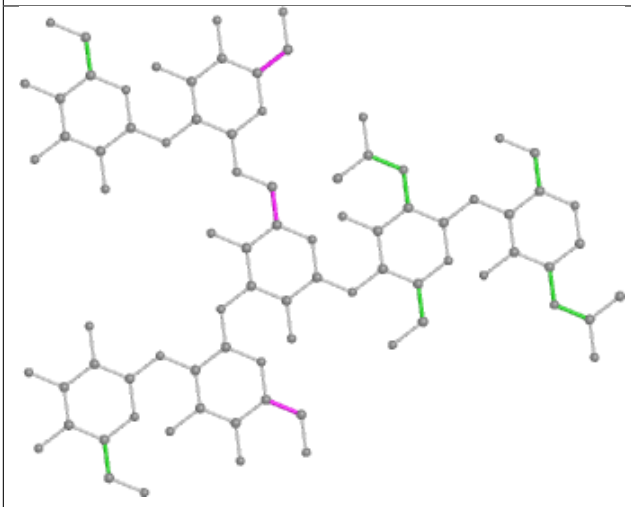


Bond angles



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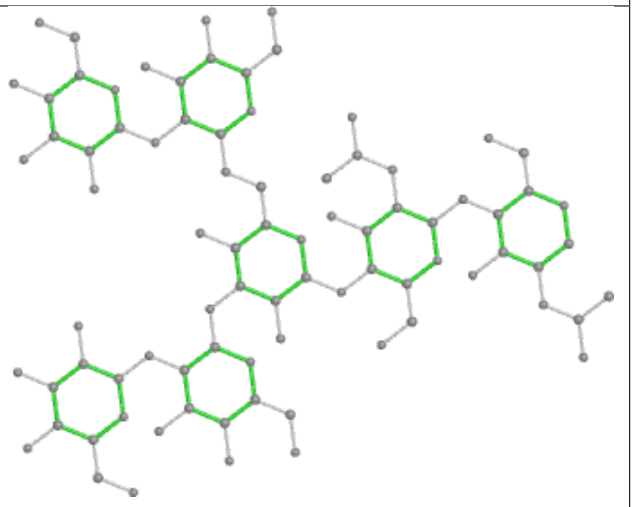
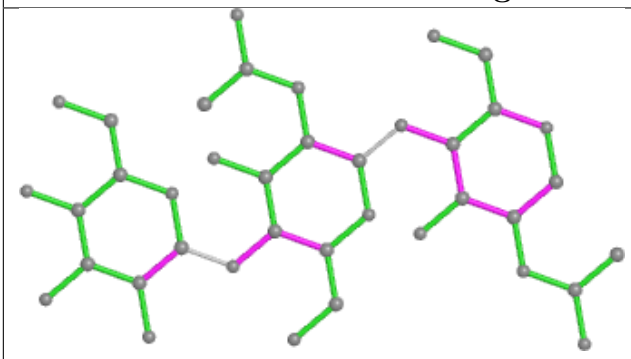


Rings

Oligosaccharide Chain G



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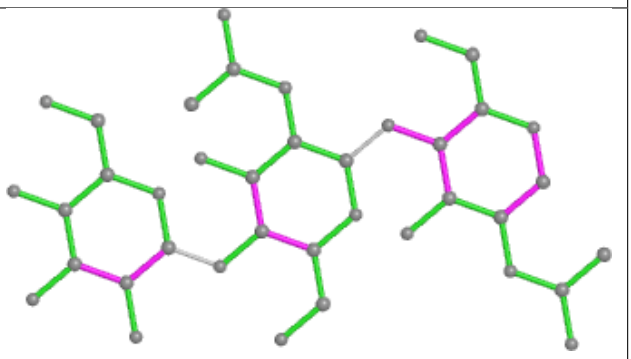
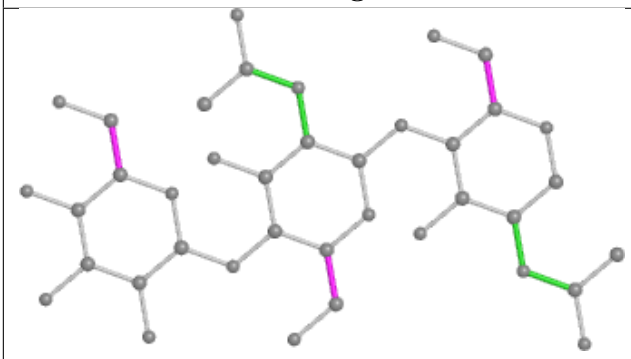


Bond angles



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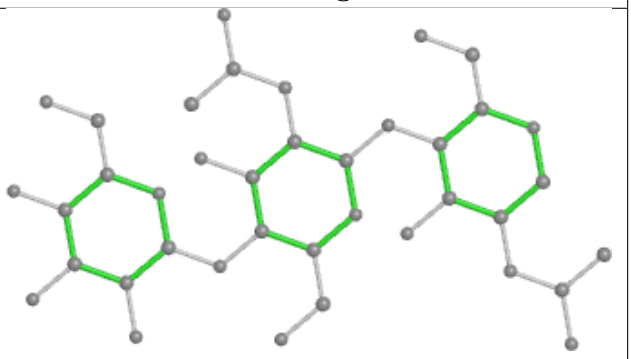
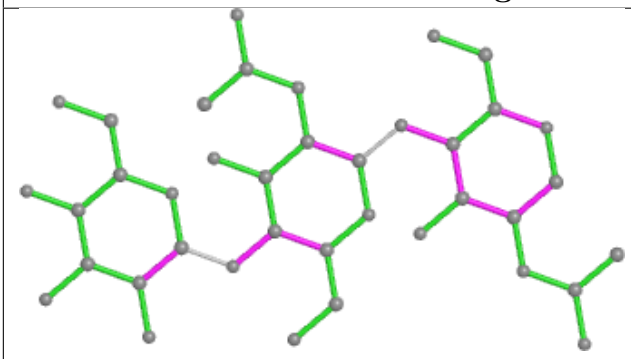


Rings

Oligosaccharide Chain R



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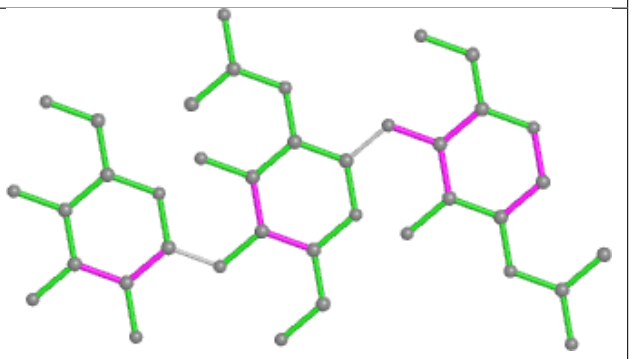
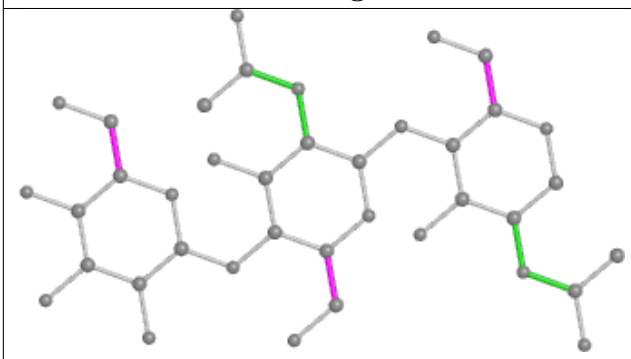


Bond angles



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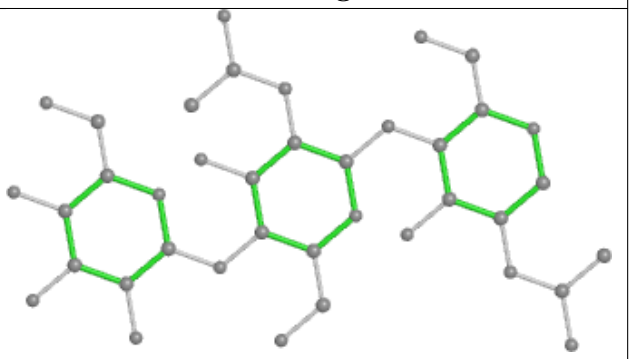
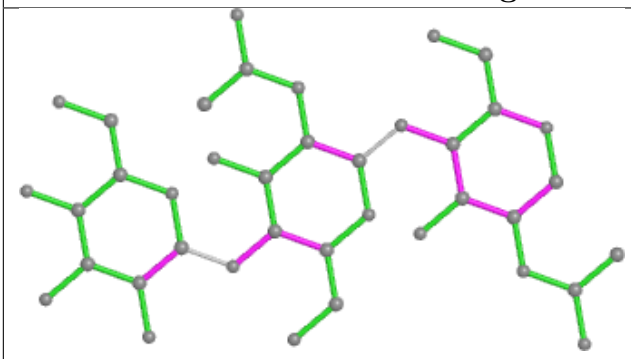


Rings

Oligosaccharide Chain c



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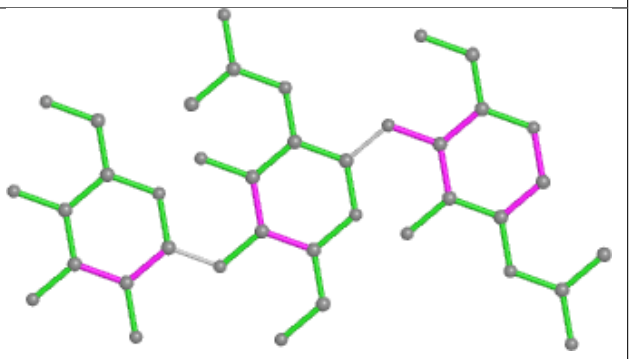
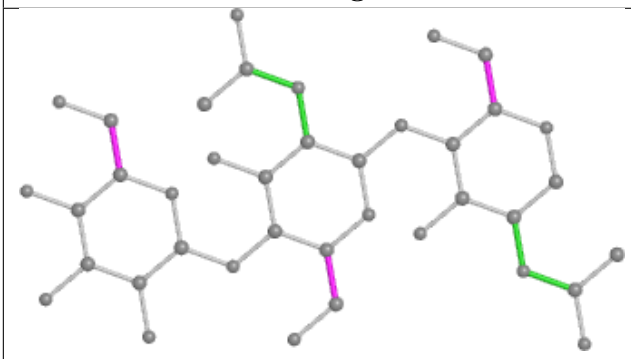


Bond angles



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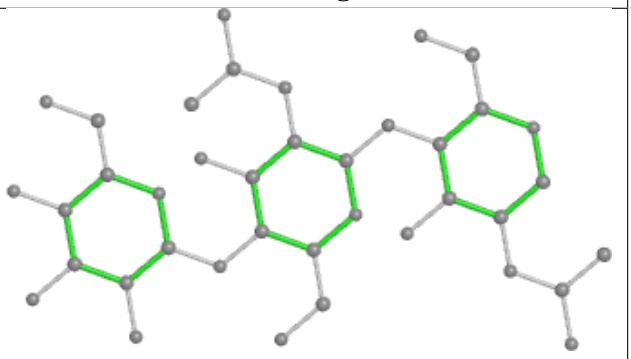
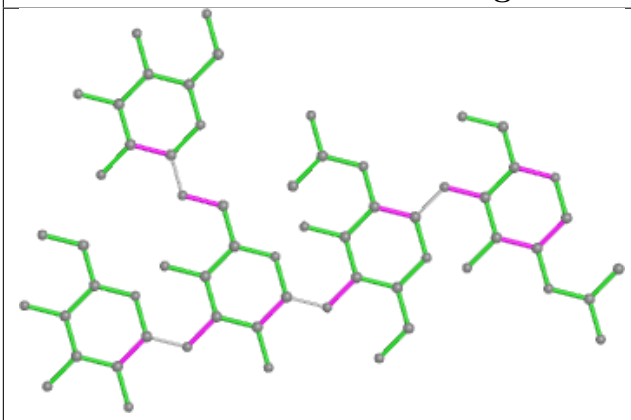


Rings

Oligosaccharide Chain K



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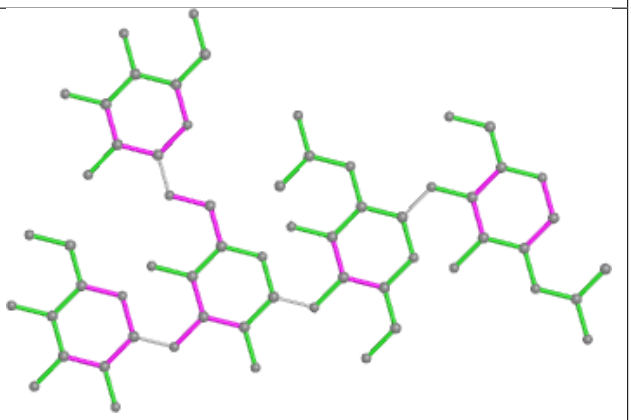
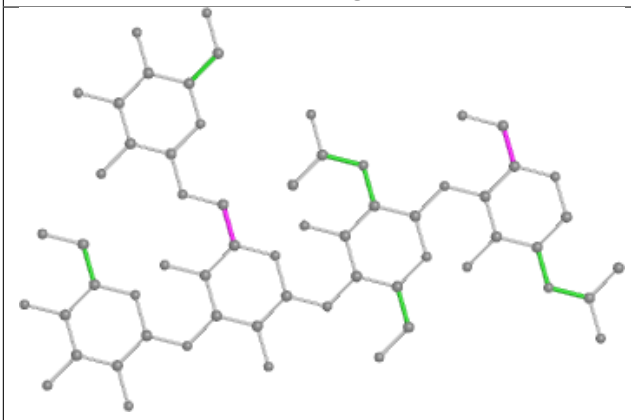


Bond angles



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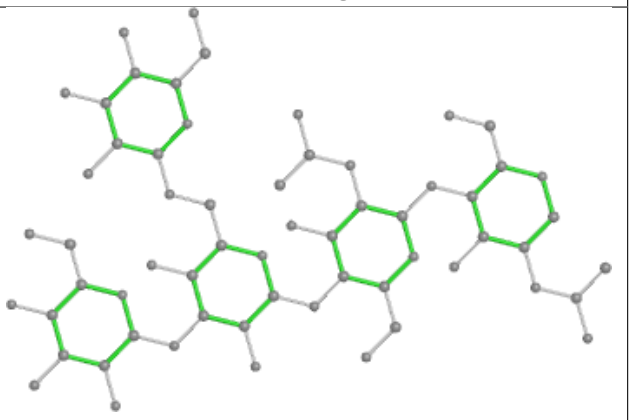
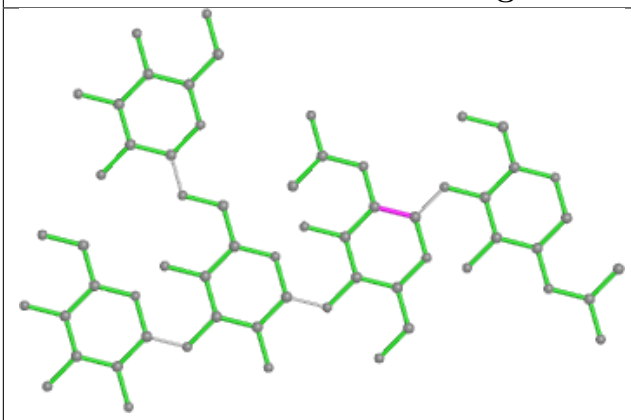


Rings

Oligosaccharide Chain L



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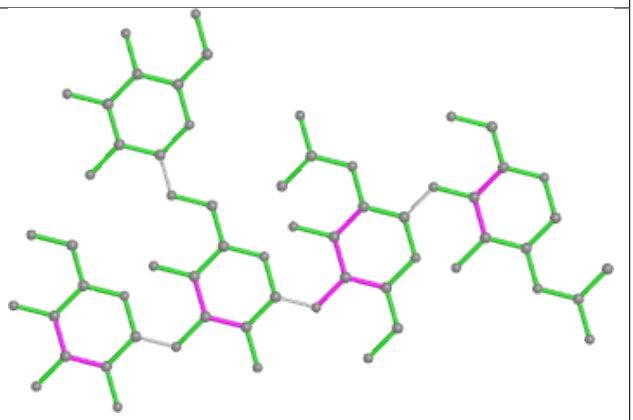
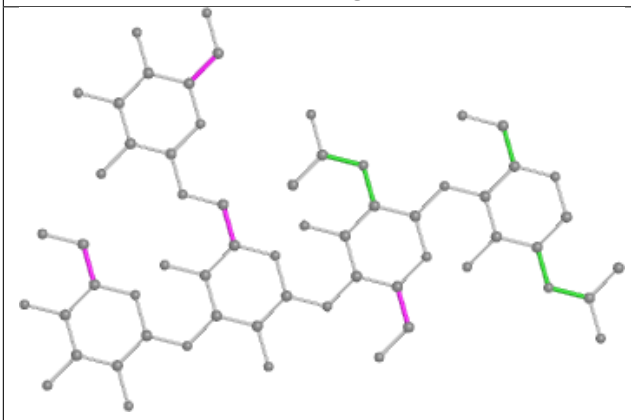
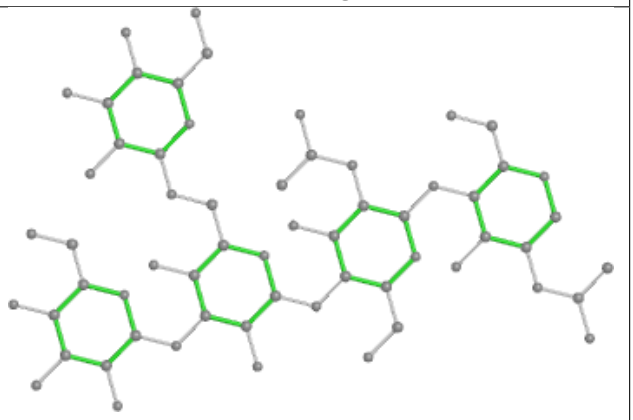


Bond angles

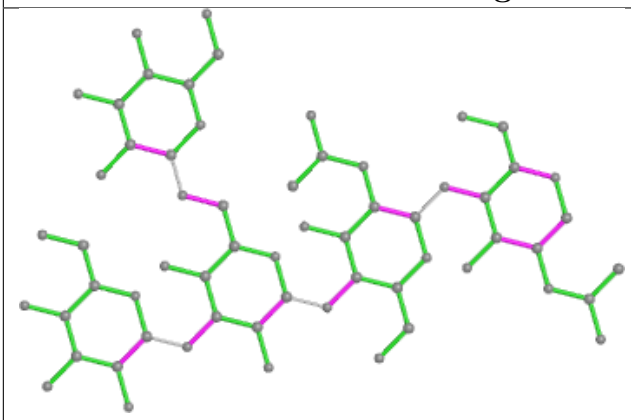


Torsions



Rings

Oligosaccharide Chain V



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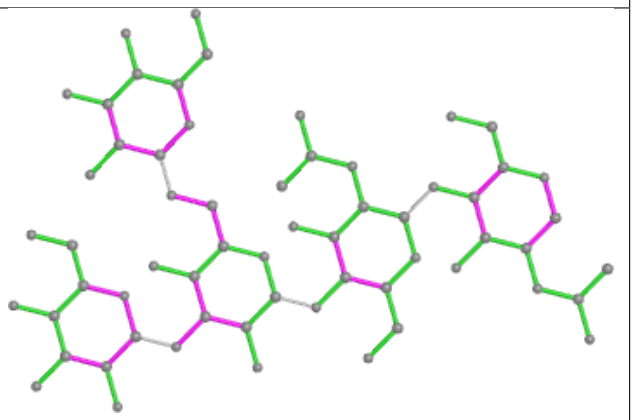
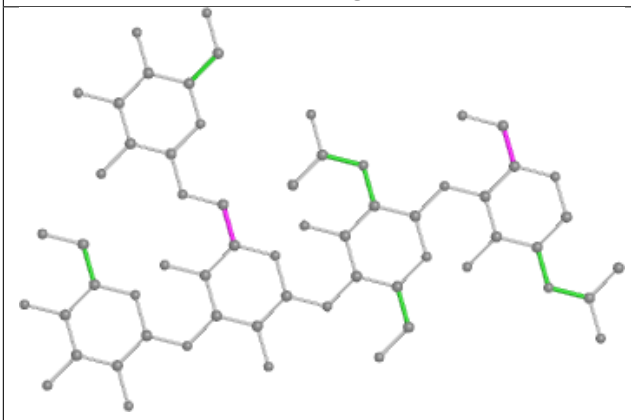
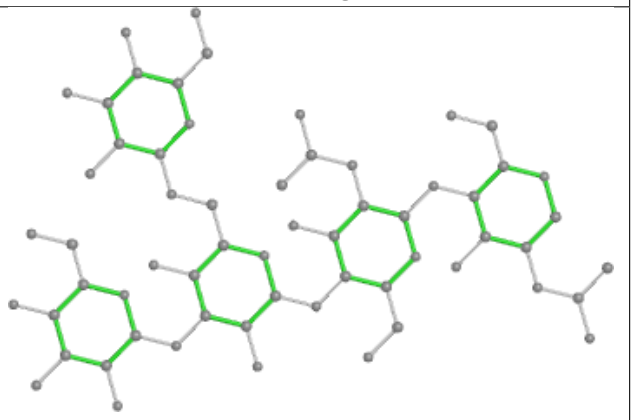


Bond angles

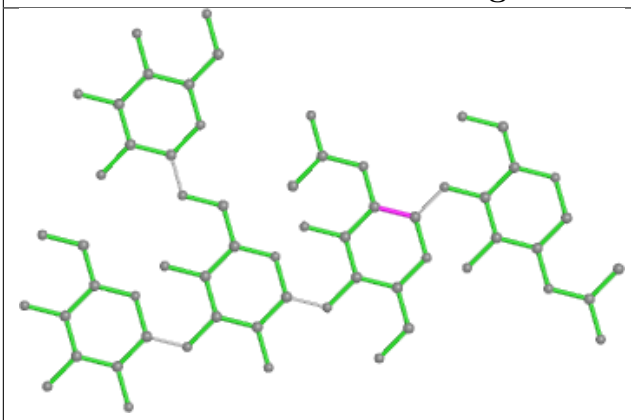


Torsions



Rings

Oligosaccharide Chain W



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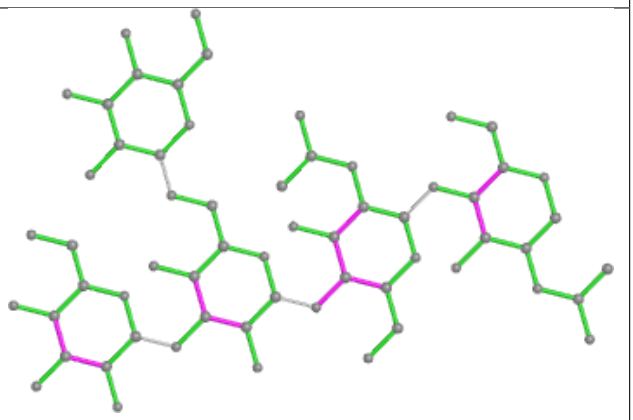
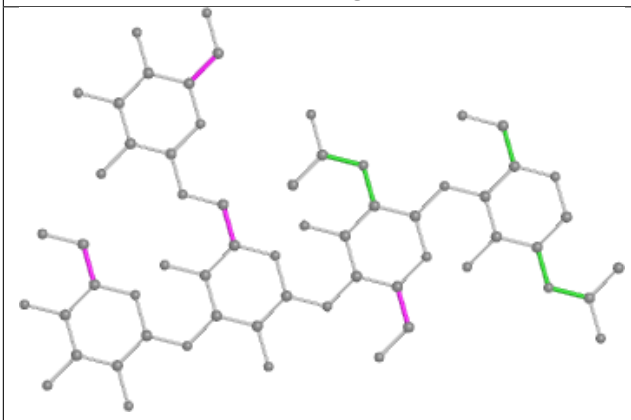


Bond angles



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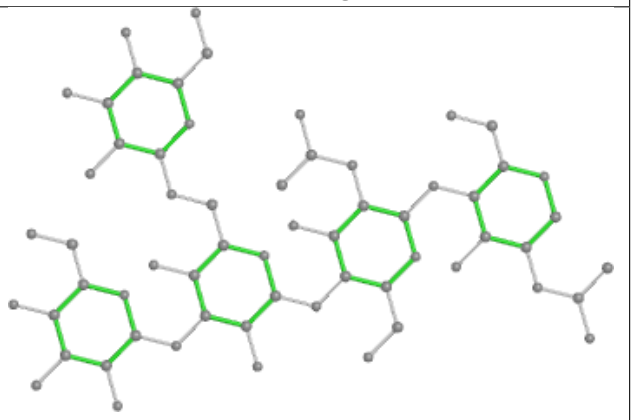
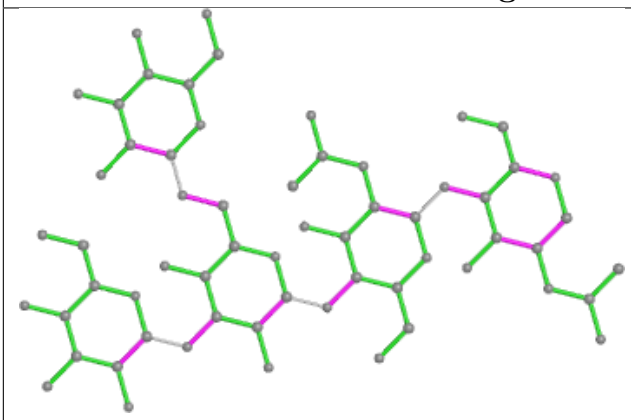


Rings

Oligosaccharide Chain g



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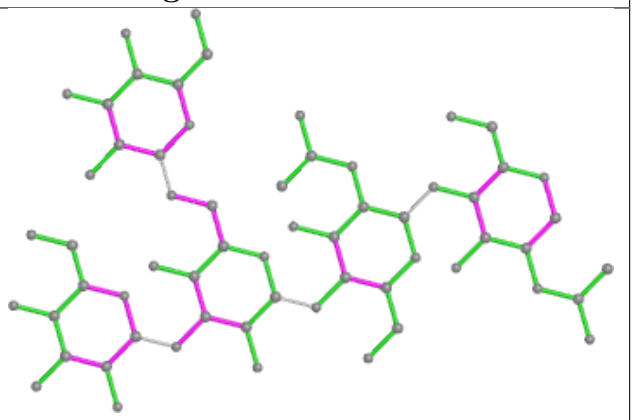
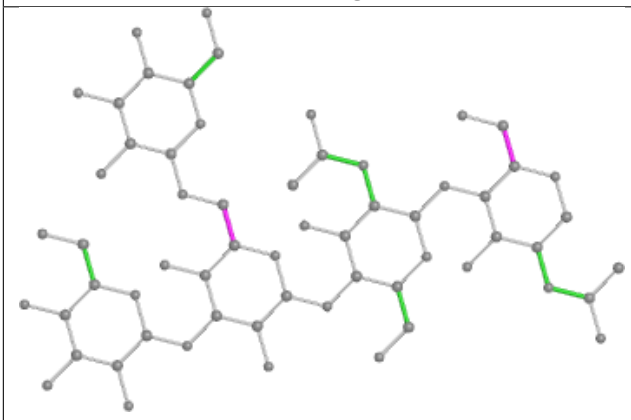


Bond angles



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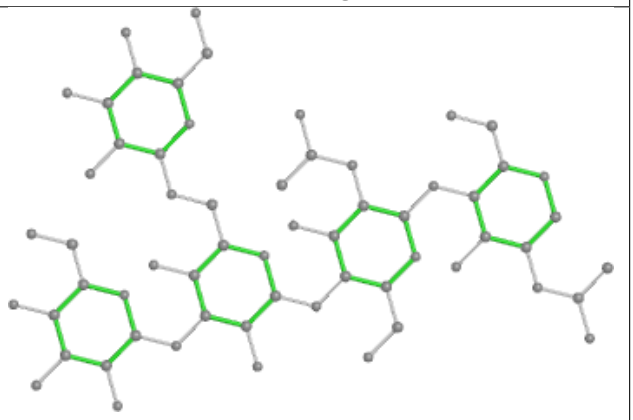
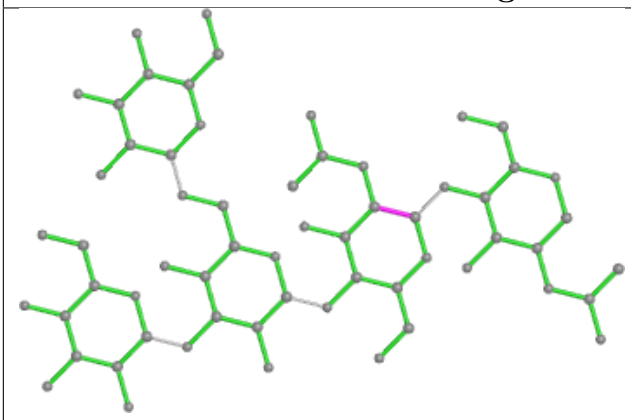
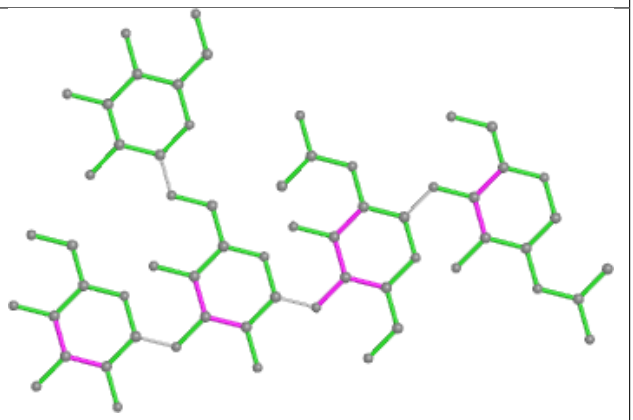


Rings

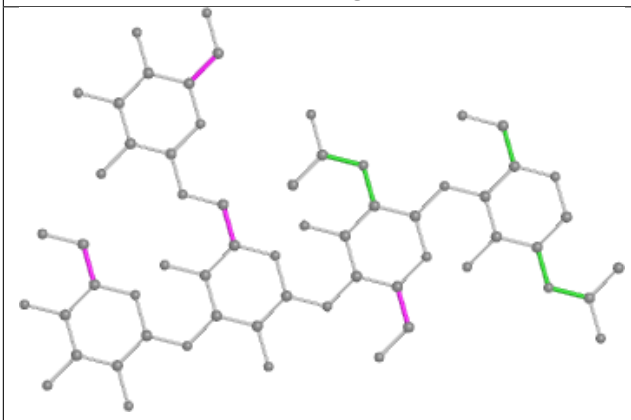
Oligosaccharide Chain h



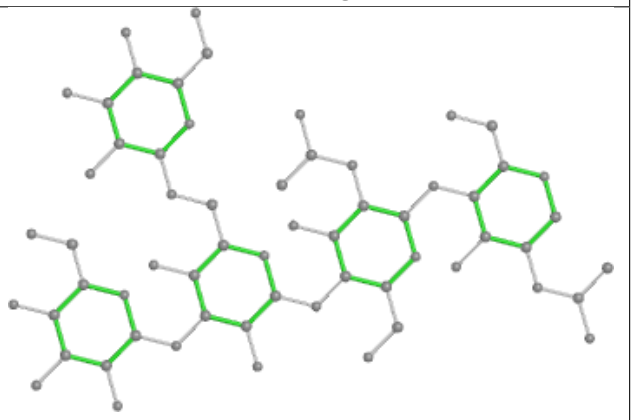
Bond lengths



Bond angles

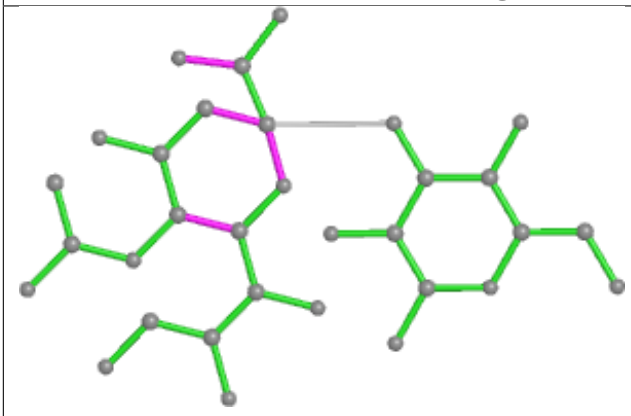


Torsions

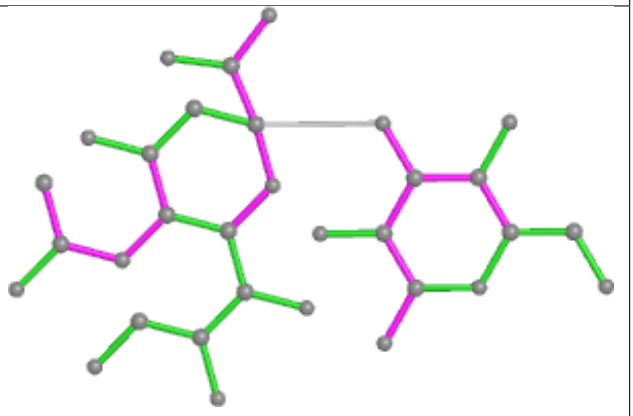


Rings

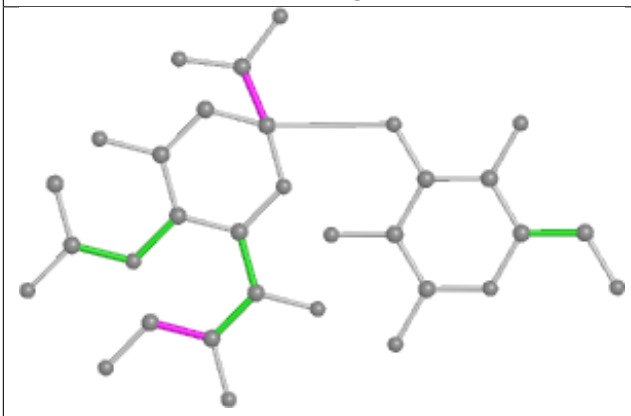
Oligosaccharide Chain N



Bond lengths



Bond angles



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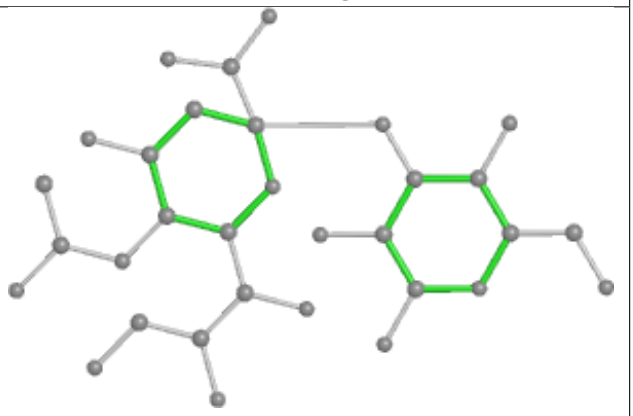
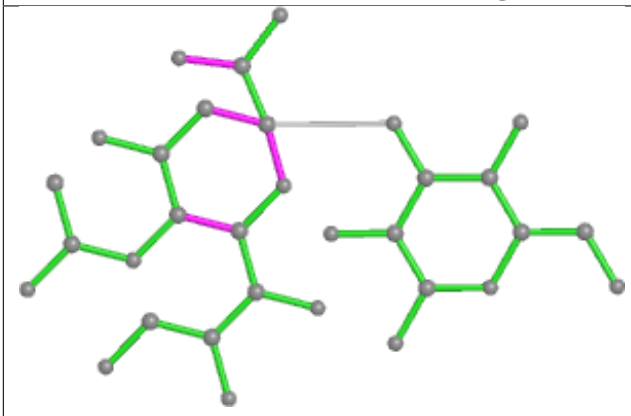
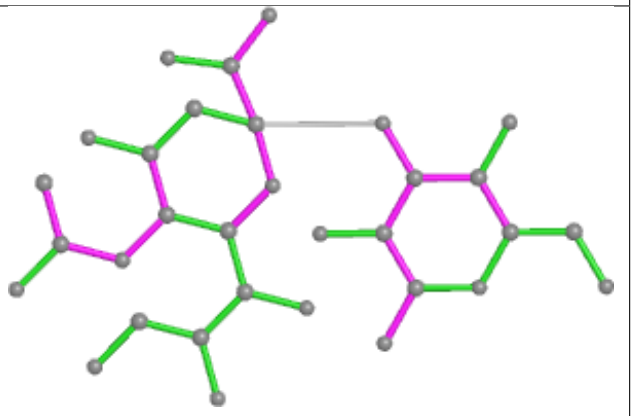


Rings

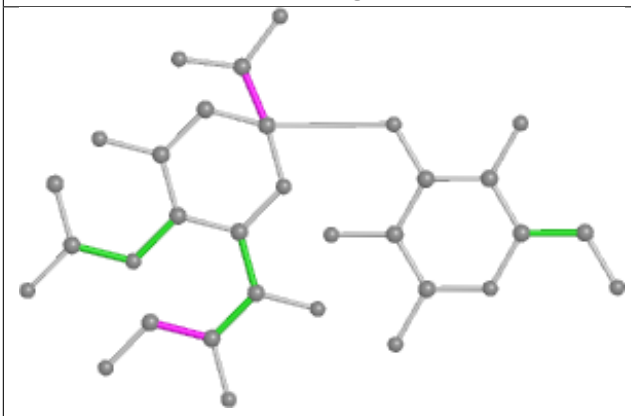
Oligosaccharide Chain Y



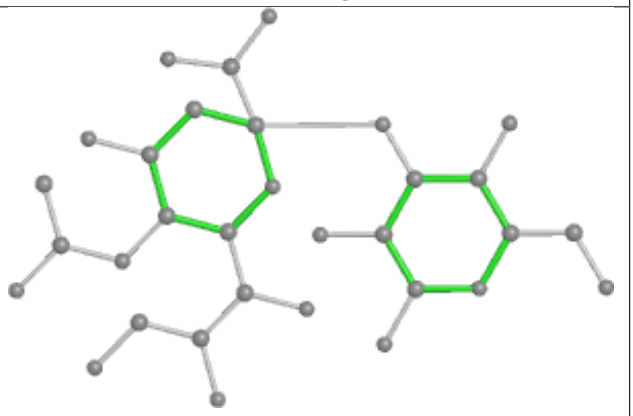
Bond lengths



Bond angles

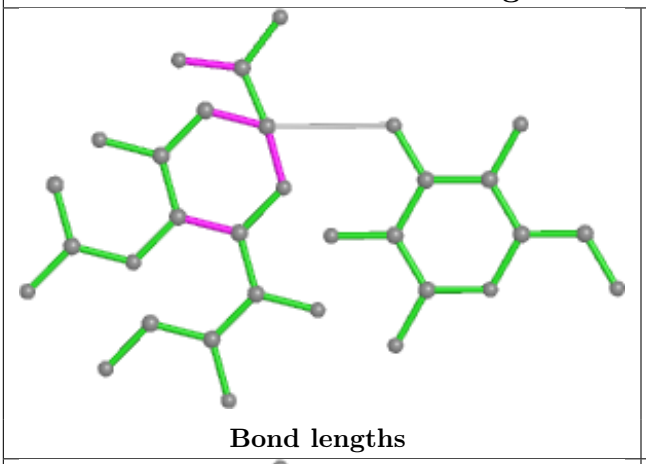


Torsions

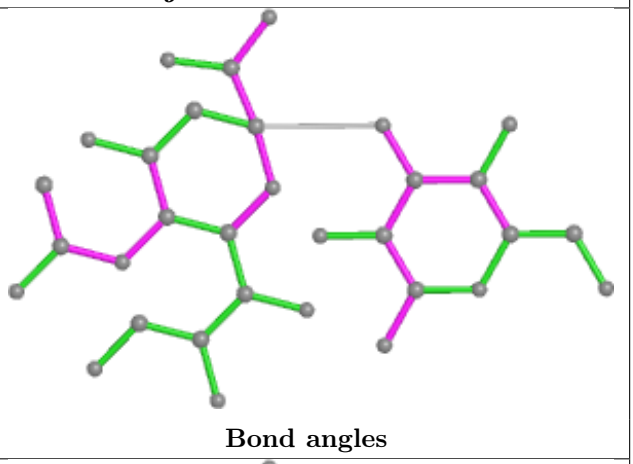


Rings

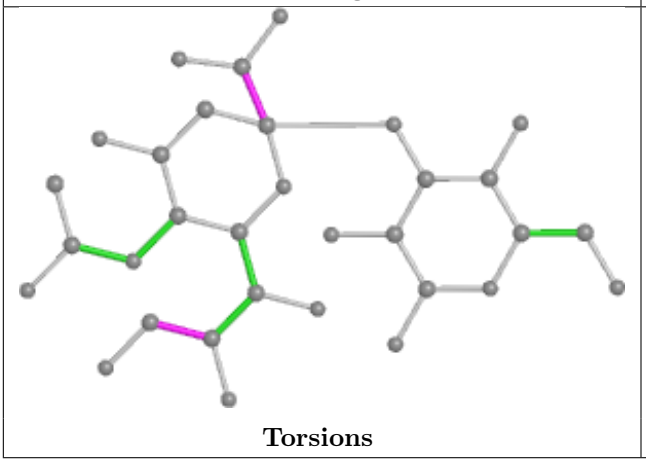
Oligosaccharide Chain j



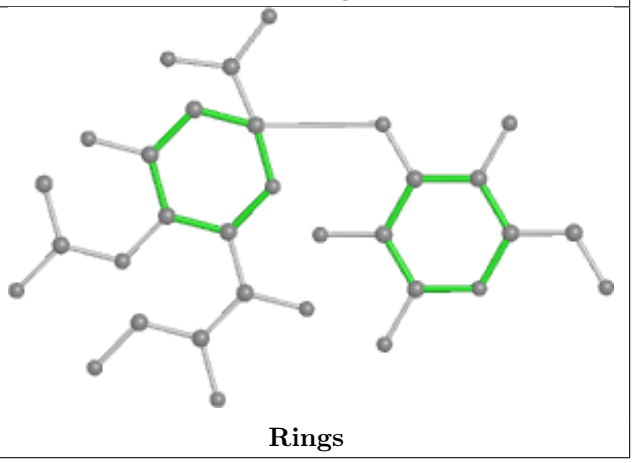
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	B	1414	1	14,14,15	1.13	1 (7%)	17,19,21	1.02	1 (5%)
8	NAG	A	1414	1	14,14,15	1.12	1 (7%)	17,19,21	1.02	1 (5%)
8	NAG	A	1415	1	14,14,15	1.15	1 (7%)	17,19,21	1.12	2 (11%)
8	NAG	B	1417	1	14,14,15	0.99	1 (7%)	17,19,21	1.09	2 (11%)
8	NAG	B	1416	1	14,14,15	1.59	4 (28%)	17,19,21	1.76	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	C	1417	1	14,14,15	0.98	1 (7%)	17,19,21	1.08	2 (11%)
8	NAG	C	1416	1	14,14,15	1.59	4 (28%)	17,19,21	1.75	5 (29%)
9	FOL	B	1444	-	34,34,34	1.29	2 (5%)	44,47,47	2.13	10 (22%)
8	NAG	A	1416	1	14,14,15	1.59	4 (28%)	17,19,21	1.76	5 (29%)
8	NAG	C	1436	1	14,14,15	1.61	5 (35%)	17,19,21	1.94	4 (23%)
9	FOL	A	1444	-	34,34,34	1.29	2 (5%)	44,47,47	2.13	10 (22%)
8	NAG	B	1415	1	14,14,15	1.15	1 (7%)	17,19,21	1.11	2 (11%)
8	NAG	C	1415	1	14,14,15	1.15	1 (7%)	17,19,21	1.12	2 (11%)
8	NAG	A	1417	1	14,14,15	0.98	1 (7%)	17,19,21	1.08	2 (11%)
8	NAG	B	1436	1	14,14,15	1.63	5 (35%)	17,19,21	1.95	4 (23%)
8	NAG	C	1419	1	14,14,15	1.08	1 (7%)	17,19,21	1.26	2 (11%)
8	NAG	C	1414	1	14,14,15	1.13	1 (7%)	17,19,21	1.02	1 (5%)
8	NAG	B	1419	1	14,14,15	1.06	1 (7%)	17,19,21	1.25	2 (11%)
8	NAG	B	1418	1	14,14,15	1.02	1 (7%)	17,19,21	1.12	1 (5%)
9	FOL	C	1444	-	34,34,34	1.29	2 (5%)	44,47,47	2.13	10 (22%)
8	NAG	A	1436	1	14,14,15	1.62	5 (35%)	17,19,21	1.95	4 (23%)
8	NAG	C	1418	1	14,14,15	1.02	1 (7%)	17,19,21	1.11	1 (5%)
8	NAG	A	1419	1	14,14,15	1.07	1 (7%)	17,19,21	1.25	2 (11%)
8	NAG	A	1418	1	14,14,15	1.02	1 (7%)	17,19,21	1.12	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
8	NAG	B	1414	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1414	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1415	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1417	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1416	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1417	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1416	1	-	2/6/23/26	0/1/1/1
9	FOL	B	1444	-	-	2/22/22/22	0/3/3/3
8	NAG	A	1416	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1436	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FOL	A	1444	-	-	2/22/22/22	0/3/3/3
8	NAG	B	1415	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1415	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1417	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1436	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1419	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1414	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1419	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1418	1	-	1/6/23/26	0/1/1/1
9	FOL	C	1444	-	-	2/22/22/22	0/3/3/3
8	NAG	A	1436	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1418	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1419	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1418	1	-	1/6/23/26	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1444	FOL	C4A-C4	4.17	1.48	1.41
9	B	1444	FOL	C4A-C4	4.16	1.48	1.41
9	A	1444	FOL	C4A-C4	4.15	1.48	1.41
9	A	1444	FOL	C4A-C8A	3.89	1.48	1.40
9	C	1444	FOL	C4A-C8A	3.86	1.48	1.40
9	B	1444	FOL	C4A-C8A	3.85	1.48	1.40
8	B	1416	NAG	C1-C2	3.69	1.57	1.52
8	C	1416	NAG	C1-C2	3.69	1.57	1.52
8	A	1416	NAG	C1-C2	3.67	1.57	1.52
8	A	1415	NAG	C1-C2	3.66	1.57	1.52
8	C	1415	NAG	C1-C2	3.66	1.57	1.52
8	B	1415	NAG	C1-C2	3.65	1.57	1.52
8	B	1414	NAG	C1-C2	3.28	1.57	1.52
8	C	1414	NAG	C1-C2	3.24	1.57	1.52
8	A	1414	NAG	C1-C2	3.23	1.57	1.52
8	C	1419	NAG	C1-C2	3.20	1.57	1.52
8	A	1419	NAG	C1-C2	3.18	1.57	1.52
8	B	1419	NAG	C1-C2	3.14	1.57	1.52
8	A	1418	NAG	C1-C2	3.13	1.57	1.52
8	B	1418	NAG	C1-C2	3.13	1.57	1.52
8	C	1418	NAG	C1-C2	3.13	1.57	1.52
8	B	1416	NAG	O5-C5	3.02	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1416	NAG	O5-C5	3.00	1.49	1.43
8	C	1416	NAG	O5-C5	2.99	1.49	1.43
8	B	1436	NAG	C1-C2	2.84	1.56	1.52
8	C	1436	NAG	C1-C2	2.84	1.56	1.52
8	A	1436	NAG	C1-C2	2.83	1.56	1.52
8	C	1417	NAG	C1-C2	2.81	1.56	1.52
8	B	1417	NAG	C1-C2	2.81	1.56	1.52
8	A	1417	NAG	C1-C2	2.81	1.56	1.52
8	B	1436	NAG	O4-C4	-2.60	1.36	1.43
8	A	1436	NAG	O4-C4	-2.59	1.36	1.43
8	C	1436	NAG	O4-C4	-2.54	1.37	1.43
8	B	1436	NAG	C3-C2	2.46	1.57	1.52
8	A	1436	NAG	C3-C2	2.44	1.57	1.52
8	C	1436	NAG	C3-C2	2.42	1.57	1.52
8	B	1436	NAG	O5-C5	2.42	1.48	1.43
8	A	1436	NAG	O5-C5	2.39	1.48	1.43
8	C	1436	NAG	O5-C5	2.38	1.48	1.43
8	B	1436	NAG	C4-C3	2.25	1.58	1.52
8	A	1436	NAG	C4-C3	2.25	1.58	1.52
8	C	1436	NAG	C4-C3	2.24	1.58	1.52
8	C	1416	NAG	C3-C2	2.14	1.57	1.52
8	A	1416	NAG	C3-C2	2.14	1.57	1.52
8	B	1416	NAG	C3-C2	2.14	1.57	1.52
8	A	1416	NAG	O4-C4	-2.05	1.38	1.43
8	C	1416	NAG	O4-C4	-2.03	1.38	1.43
8	B	1416	NAG	O4-C4	-2.03	1.38	1.43

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1444	FOL	C2-N1-C8A	5.69	121.85	115.36
9	B	1444	FOL	C2-N1-C8A	5.66	121.82	115.36
9	C	1444	FOL	C2-N1-C8A	5.66	121.82	115.36
9	A	1444	FOL	N8-C8A-N1	5.21	121.77	115.82
9	C	1444	FOL	N8-C8A-N1	5.18	121.73	115.82
9	B	1444	FOL	N8-C8A-N1	5.17	121.72	115.82
8	A	1436	NAG	C3-C4-C5	-5.17	101.02	110.24
8	B	1436	NAG	C3-C4-C5	-5.17	101.02	110.24
8	C	1436	NAG	C3-C4-C5	-5.16	101.03	110.24
9	A	1444	FOL	C8A-C4A-C4	-4.76	116.80	119.95
9	B	1444	FOL	C8A-C4A-C4	-4.74	116.81	119.95
9	C	1444	FOL	C8A-C4A-C4	-4.74	116.81	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1416	NAG	O4-C4-C5	4.34	120.07	109.30
8	A	1416	NAG	O4-C4-C5	4.33	120.04	109.30
8	C	1416	NAG	O4-C4-C5	4.31	120.00	109.30
9	A	1444	FOL	C4-C4A-N5	4.28	123.49	118.60
9	C	1444	FOL	C4-C4A-N5	4.26	123.47	118.60
9	B	1444	FOL	C4-C4A-N5	4.26	123.46	118.60
9	B	1444	FOL	C4A-C4-N3	-4.25	117.62	123.43
9	C	1444	FOL	C4A-C4-N3	-4.23	117.64	123.43
9	A	1444	FOL	C4A-C4-N3	-4.23	117.65	123.43
9	B	1444	FOL	C2-N3-C4	3.95	122.20	115.93
9	A	1444	FOL	C2-N3-C4	3.94	122.19	115.93
9	C	1444	FOL	C2-N3-C4	3.93	122.18	115.93
9	A	1444	FOL	N1-C2-N3	-3.59	122.43	127.22
9	B	1444	FOL	N1-C2-N3	-3.59	122.43	127.22
9	C	1444	FOL	N1-C2-N3	-3.58	122.44	127.22
8	B	1436	NAG	C1-O5-C5	3.51	116.95	112.19
8	A	1436	NAG	C1-O5-C5	3.49	116.93	112.19
8	C	1436	NAG	C1-O5-C5	3.49	116.92	112.19
8	C	1415	NAG	C4-C3-C2	-3.39	106.05	111.02
8	A	1415	NAG	C4-C3-C2	-3.38	106.06	111.02
8	A	1436	NAG	O5-C1-C2	-3.38	105.95	111.29
8	C	1436	NAG	O5-C1-C2	-3.38	105.95	111.29
8	B	1436	NAG	O5-C1-C2	-3.38	105.96	111.29
8	B	1415	NAG	C4-C3-C2	-3.35	106.11	111.02
8	B	1418	NAG	C4-C3-C2	-3.31	106.17	111.02
8	A	1418	NAG	C4-C3-C2	-3.30	106.18	111.02
8	C	1418	NAG	C4-C3-C2	-3.28	106.21	111.02
8	C	1419	NAG	C4-C3-C2	-3.15	106.40	111.02
8	A	1419	NAG	C4-C3-C2	-3.11	106.45	111.02
8	B	1419	NAG	C4-C3-C2	-3.10	106.48	111.02
8	C	1419	NAG	O5-C1-C2	-2.88	106.73	111.29
8	A	1419	NAG	O5-C1-C2	-2.88	106.74	111.29
8	B	1419	NAG	O5-C1-C2	-2.86	106.77	111.29
8	C	1416	NAG	O4-C4-C3	2.83	116.90	110.35
8	A	1416	NAG	O4-C4-C3	2.83	116.88	110.35
8	B	1416	NAG	O4-C4-C3	2.81	116.85	110.35
8	B	1416	NAG	O5-C1-C2	-2.80	106.86	111.29
8	C	1416	NAG	O5-C1-C2	-2.80	106.87	111.29
8	A	1416	NAG	O5-C1-C2	-2.79	106.88	111.29
9	A	1444	FOL	C7-N8-C8A	2.78	119.49	116.69
9	B	1444	FOL	C7-N8-C8A	2.75	119.46	116.69
9	C	1444	FOL	C7-N8-C8A	2.75	119.45	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1436	NAG	O5-C5-C6	-2.66	103.03	107.20
8	C	1436	NAG	O5-C5-C6	-2.65	103.04	107.20
8	B	1436	NAG	O5-C5-C6	-2.65	103.05	107.20
8	B	1414	NAG	O5-C1-C2	-2.51	107.32	111.29
8	A	1414	NAG	O5-C1-C2	-2.50	107.34	111.29
8	C	1414	NAG	O5-C1-C2	-2.48	107.37	111.29
8	C	1416	NAG	C1-O5-C5	2.47	115.54	112.19
8	A	1416	NAG	C1-O5-C5	2.46	115.53	112.19
8	C	1415	NAG	O5-C1-C2	-2.46	107.40	111.29
8	B	1416	NAG	C3-C4-C5	-2.46	105.85	110.24
8	A	1415	NAG	O5-C1-C2	-2.46	107.40	111.29
8	B	1415	NAG	O5-C1-C2	-2.45	107.41	111.29
8	A	1416	NAG	C3-C4-C5	-2.45	105.87	110.24
8	B	1416	NAG	C1-O5-C5	2.44	115.49	112.19
8	C	1416	NAG	C3-C4-C5	-2.42	105.92	110.24
8	B	1417	NAG	C4-C3-C2	-2.40	107.49	111.02
8	B	1417	NAG	O5-C1-C2	-2.39	107.52	111.29
8	A	1417	NAG	C4-C3-C2	-2.38	107.53	111.02
8	C	1417	NAG	C4-C3-C2	-2.38	107.53	111.02
8	C	1417	NAG	O5-C1-C2	-2.37	107.55	111.29
8	A	1417	NAG	O5-C1-C2	-2.37	107.55	111.29
9	A	1444	FOL	C8A-C4A-N5	-2.32	119.71	122.33
9	C	1444	FOL	C8A-C4A-N5	-2.31	119.72	122.33
9	B	1444	FOL	C8A-C4A-N5	-2.30	119.72	122.33
9	C	1444	FOL	C11-C-N	2.18	121.24	117.06
9	A	1444	FOL	C11-C-N	2.16	121.21	117.06
9	B	1444	FOL	C11-C-N	2.16	121.20	117.06

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1436	NAG	O5-C5-C6-O6
8	B	1436	NAG	O5-C5-C6-O6
8	C	1436	NAG	O5-C5-C6-O6
8	A	1416	NAG	O5-C5-C6-O6
8	B	1416	NAG	O5-C5-C6-O6
8	C	1416	NAG	O5-C5-C6-O6
8	A	1419	NAG	O5-C5-C6-O6
8	B	1419	NAG	O5-C5-C6-O6
8	C	1419	NAG	O5-C5-C6-O6
8	A	1436	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	B	1436	NAG	C4-C5-C6-O6
8	C	1436	NAG	C4-C5-C6-O6
8	A	1416	NAG	C4-C5-C6-O6
8	B	1416	NAG	C4-C5-C6-O6
8	C	1416	NAG	C4-C5-C6-O6
8	A	1417	NAG	O5-C5-C6-O6
8	B	1417	NAG	O5-C5-C6-O6
8	C	1417	NAG	O5-C5-C6-O6
8	A	1415	NAG	O5-C5-C6-O6
8	B	1415	NAG	O5-C5-C6-O6
8	C	1415	NAG	O5-C5-C6-O6
8	C	1417	NAG	C4-C5-C6-O6
8	A	1417	NAG	C4-C5-C6-O6
8	B	1417	NAG	C4-C5-C6-O6
8	A	1419	NAG	C4-C5-C6-O6
8	B	1419	NAG	C4-C5-C6-O6
8	C	1419	NAG	C4-C5-C6-O6
8	A	1414	NAG	O5-C5-C6-O6
8	B	1414	NAG	O5-C5-C6-O6
8	C	1414	NAG	O5-C5-C6-O6
8	A	1418	NAG	O5-C5-C6-O6
8	B	1418	NAG	O5-C5-C6-O6
8	C	1418	NAG	O5-C5-C6-O6
8	A	1415	NAG	C4-C5-C6-O6
8	B	1415	NAG	C4-C5-C6-O6
8	C	1415	NAG	C4-C5-C6-O6
9	A	1444	FOL	OE1-CD-CG-CB
9	B	1444	FOL	OE1-CD-CG-CB
9	C	1444	FOL	OE1-CD-CG-CB
9	A	1444	FOL	OE2-CD-CG-CB
9	C	1444	FOL	OE2-CD-CG-CB
9	B	1444	FOL	OE2-CD-CG-CB

There are no ring outliers.

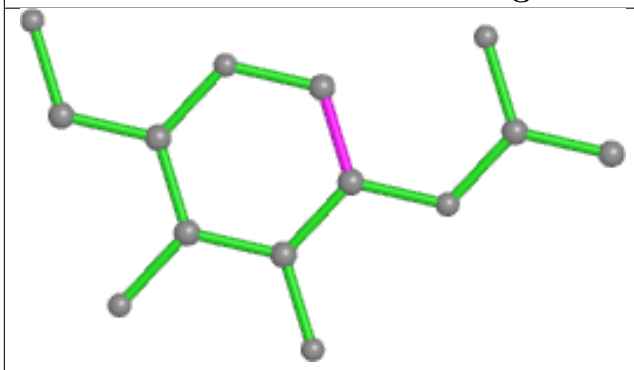
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1444	FOL	1	0
9	A	1444	FOL	1	0
9	C	1444	FOL	1	0

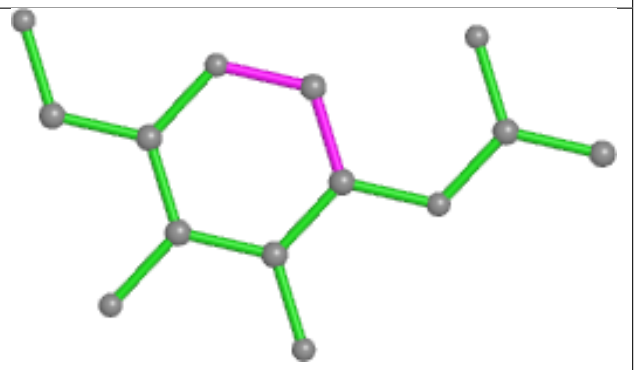
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

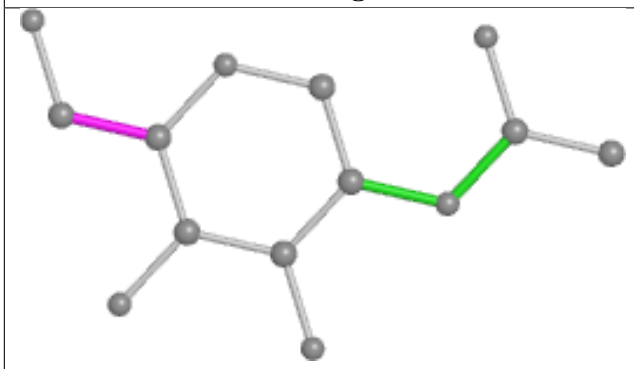
Ligand NAG B 1414



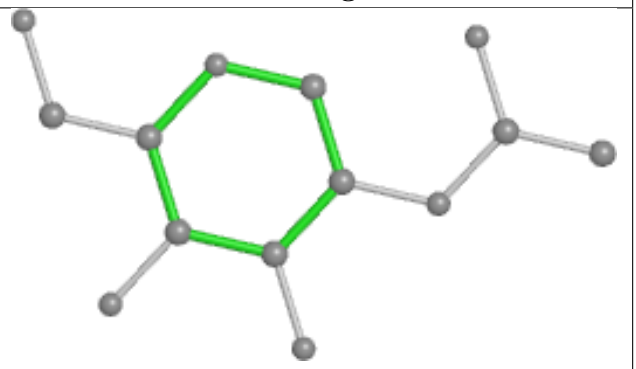
Bond lengths



Bond angles

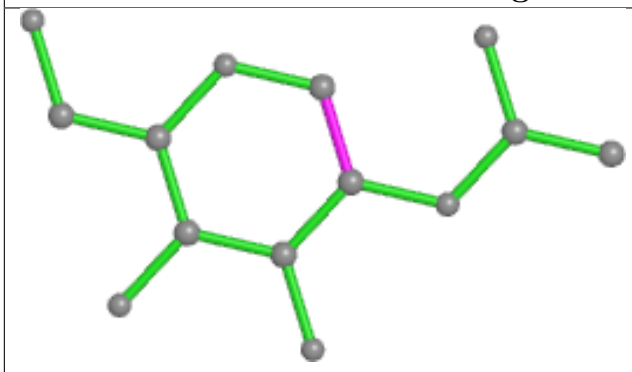


Torsions



Rings

Ligand NAG A 1414



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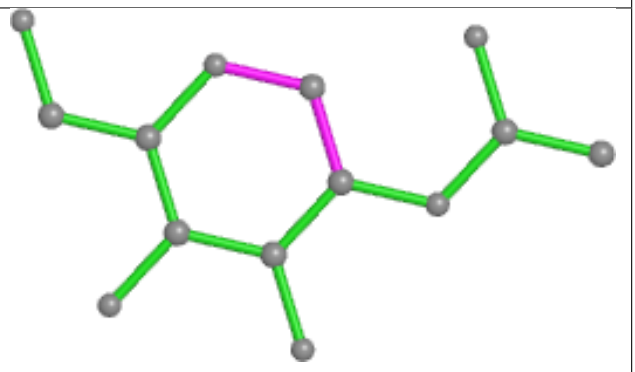

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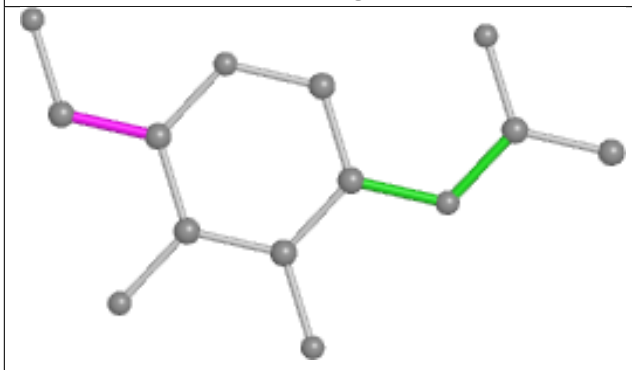
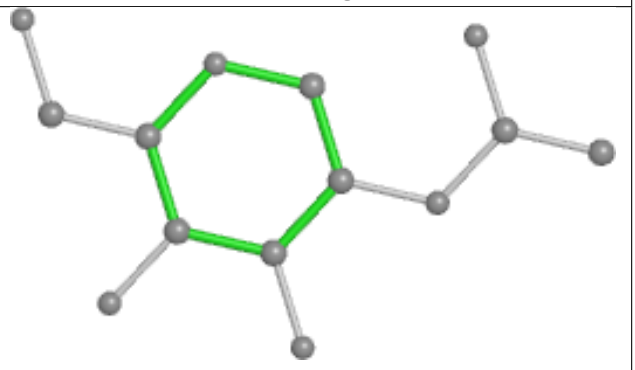
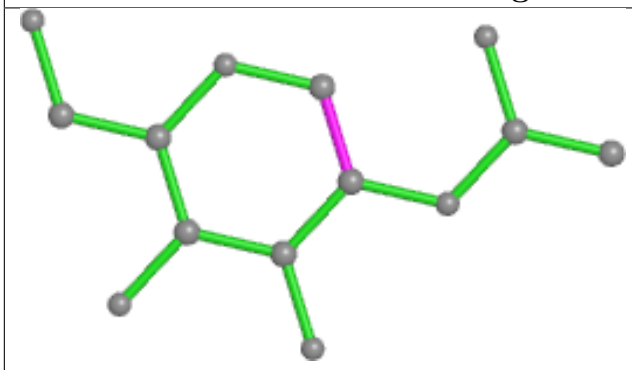


Torsions

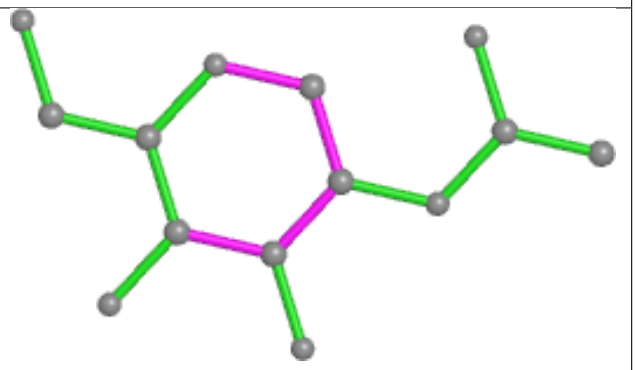


Rings

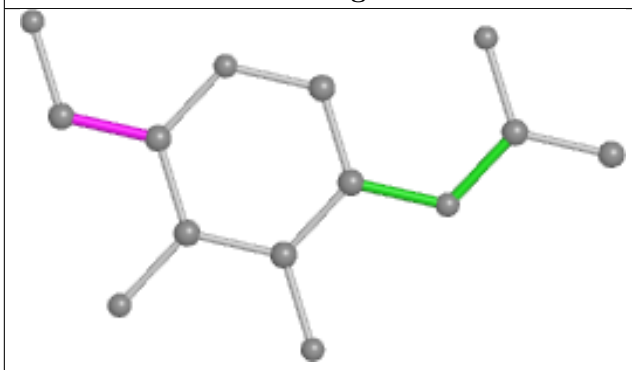
Ligand NAG A 1415



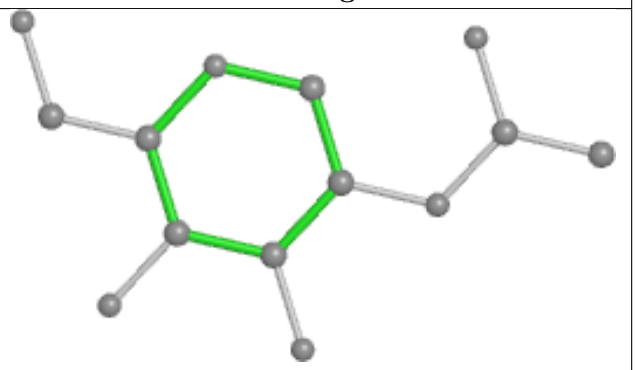
Bond lengths



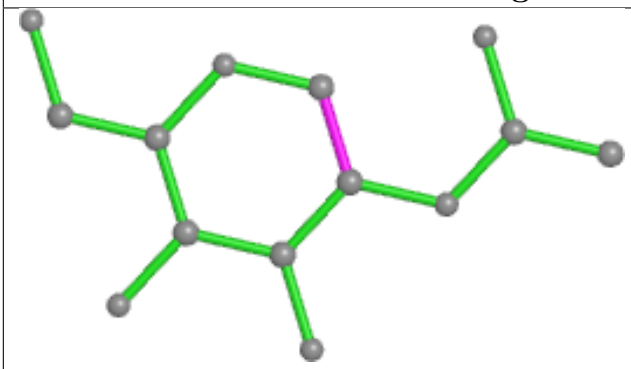
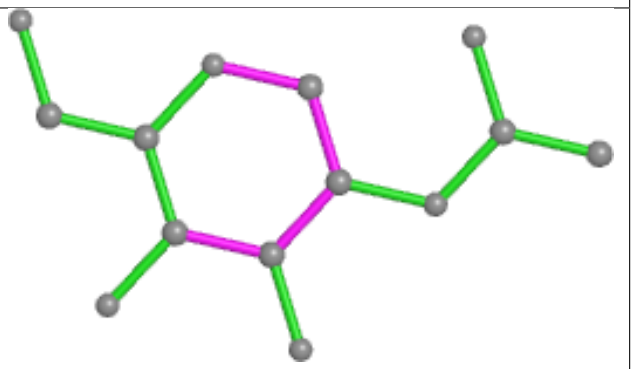
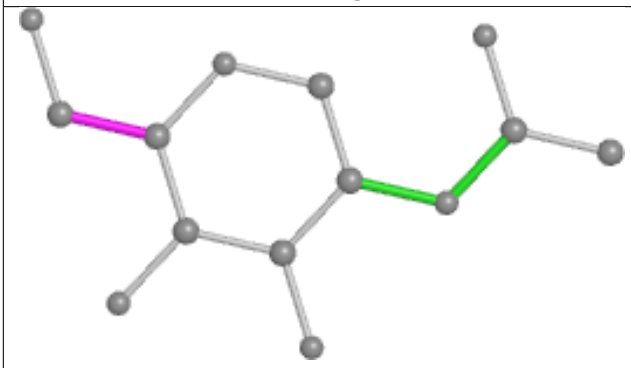
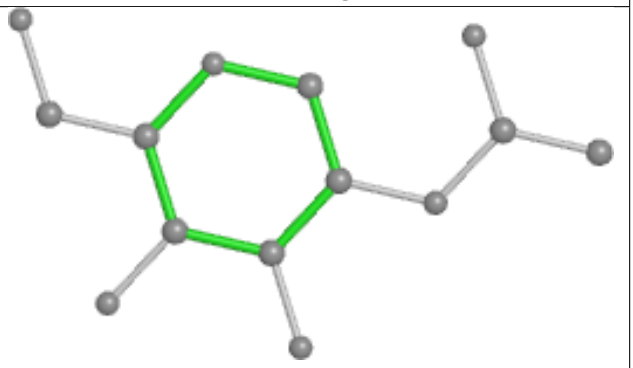
Bond angles



Torsions



Rings

Ligand NAG B 1417	
 Bond lengths	 Bond angles
 Torsions	 Rings

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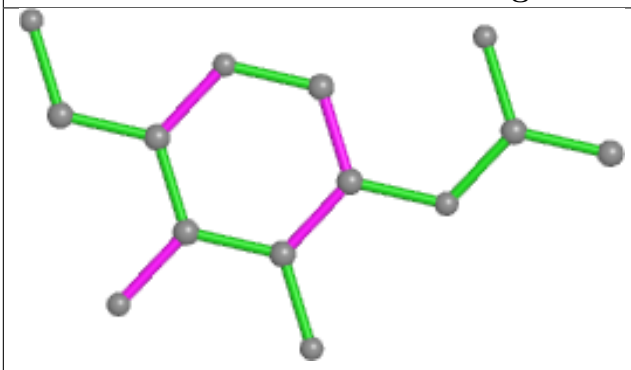
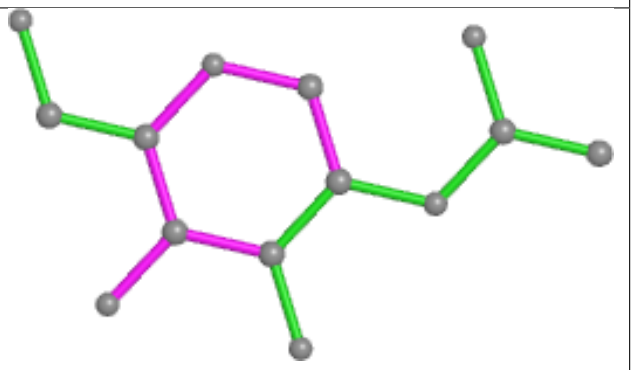
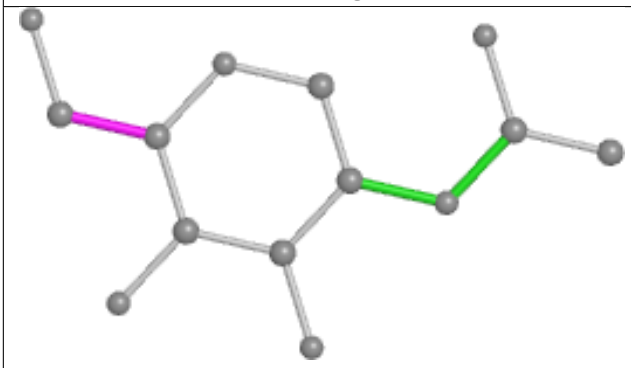
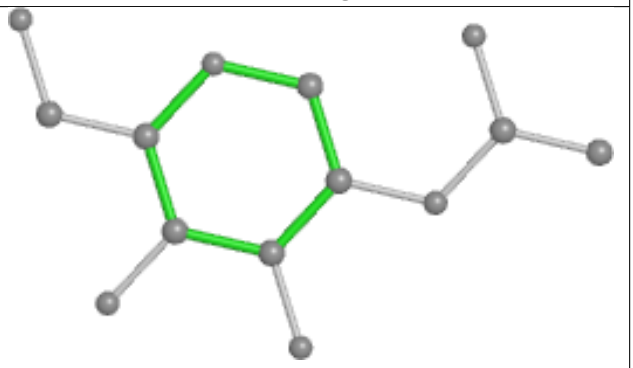
 Bond lengths	 Bond angles
 Torsions	 Rings

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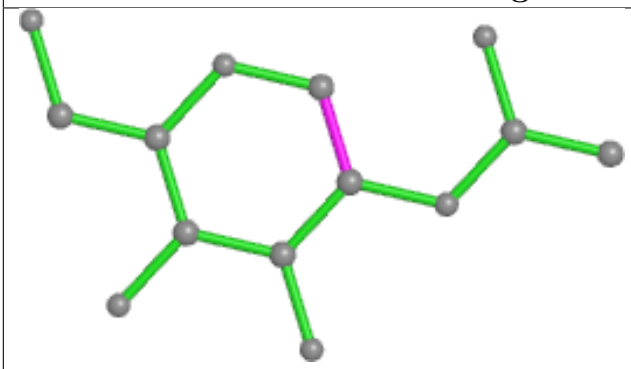
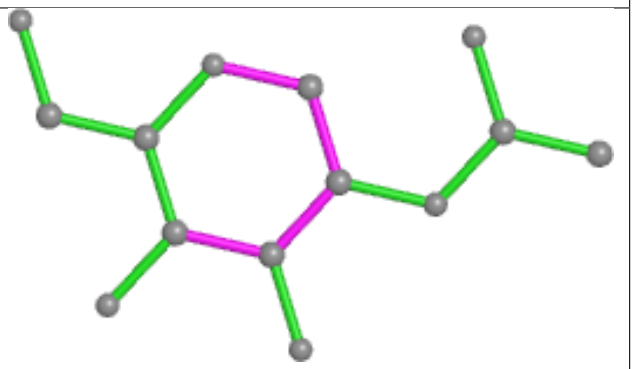
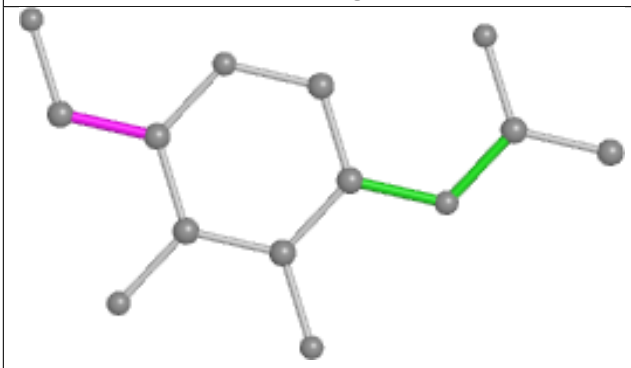
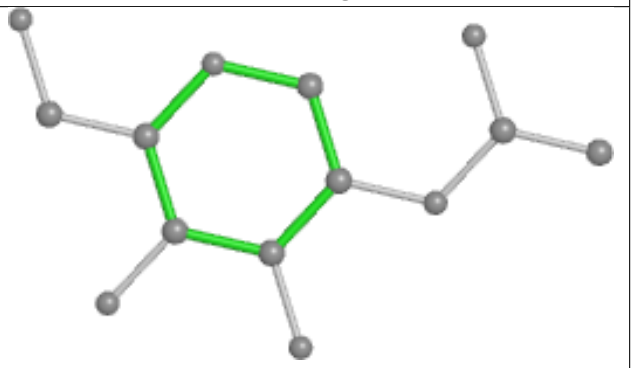
 Bond lengths	 Bond angles
 Torsions	 Rings

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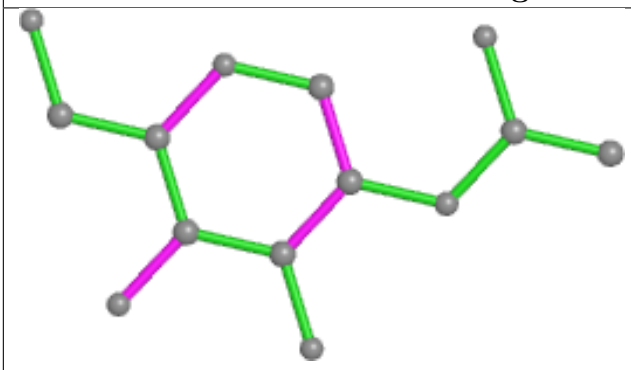
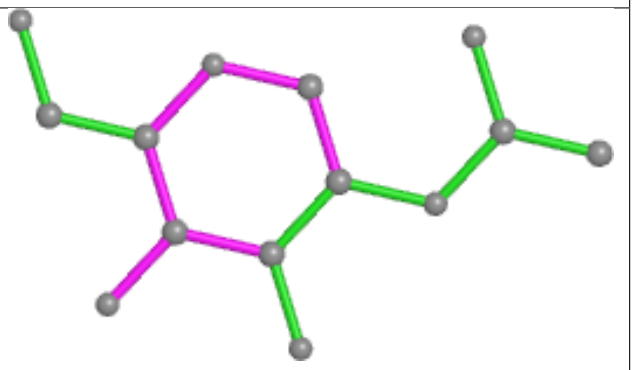
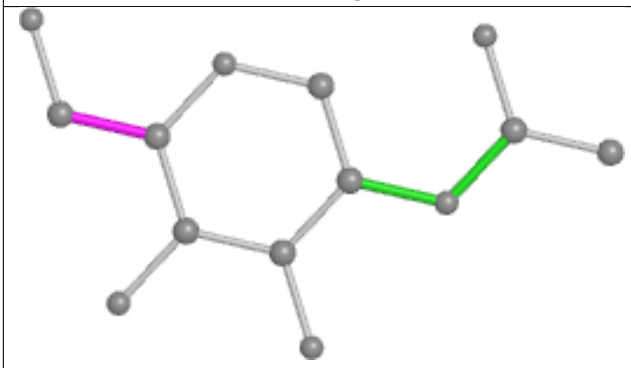
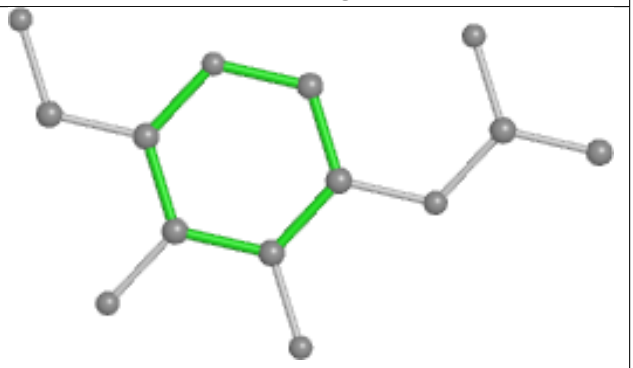
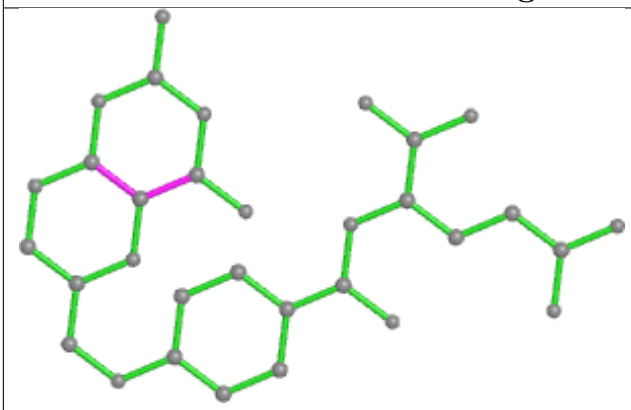
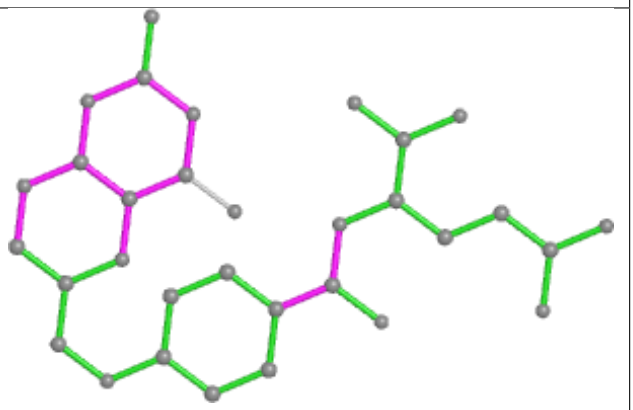
 Bond lengths	 Bond angles
 Torsions	 Rings

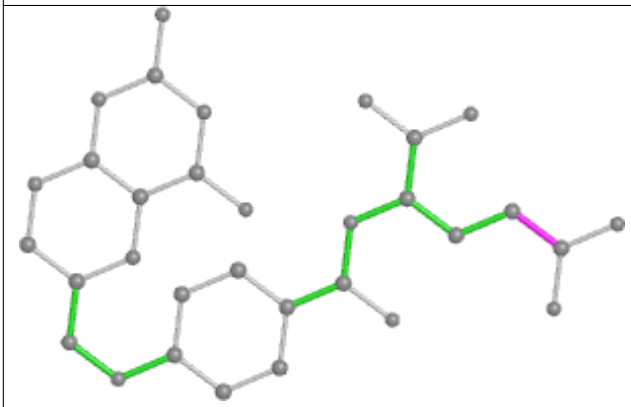
Ligand FOL B 1444



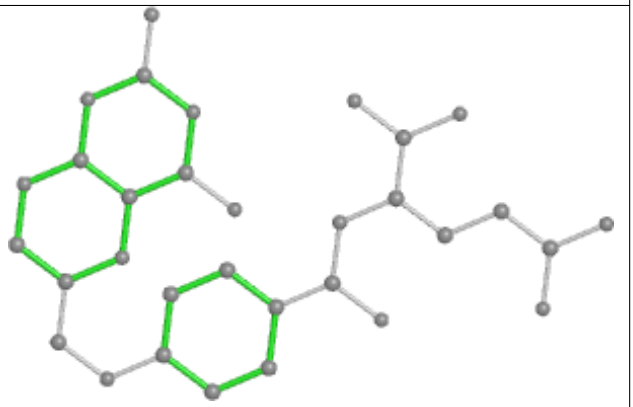
Bond lengths



Bond angles

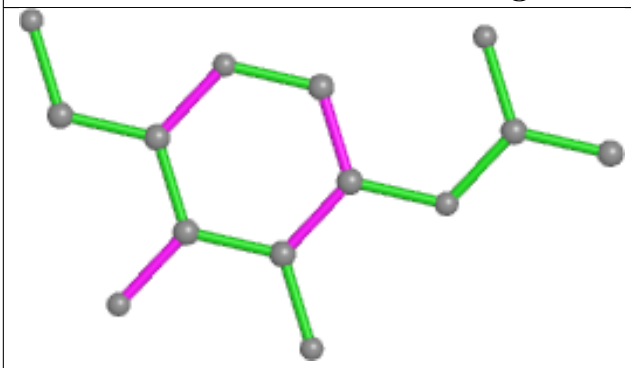


Torsions

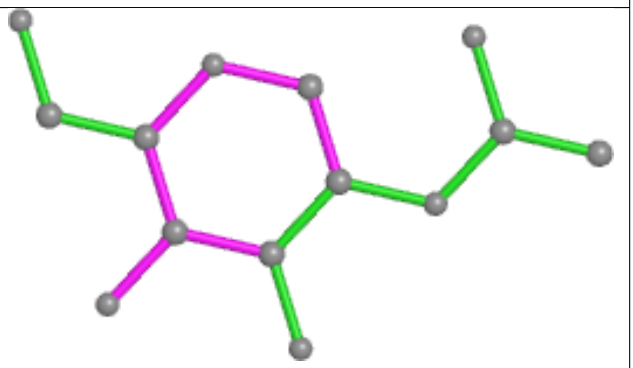


Rings

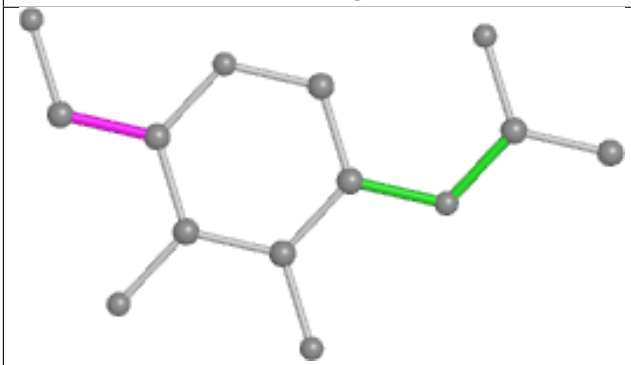
Ligand NAG A 1416



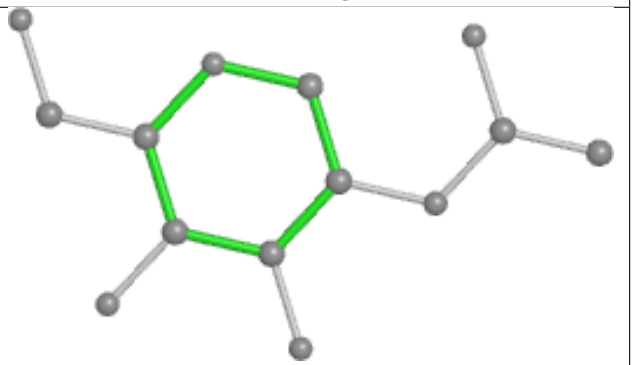
Bond lengths



Bond angles

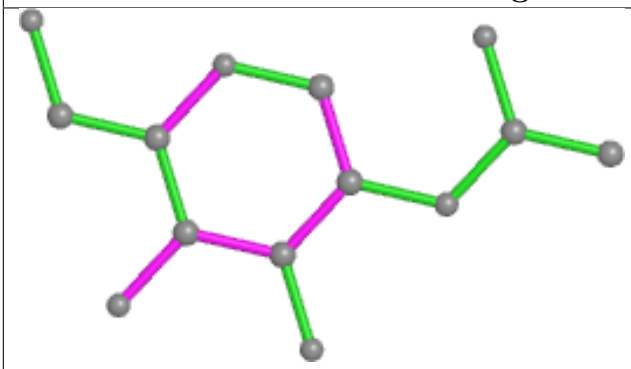


Torsions

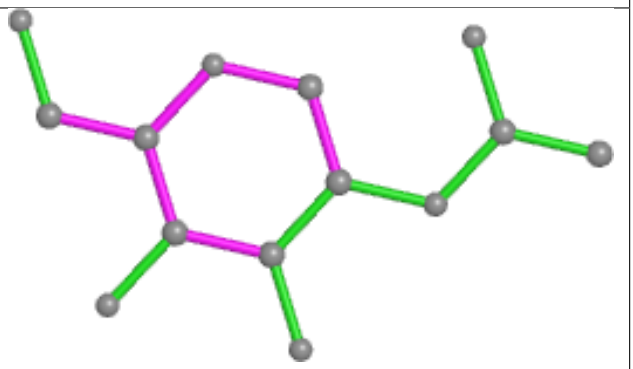


Rings

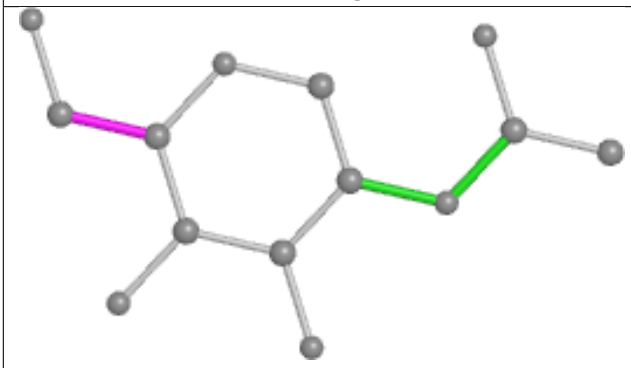
Ligand NAG C 1436



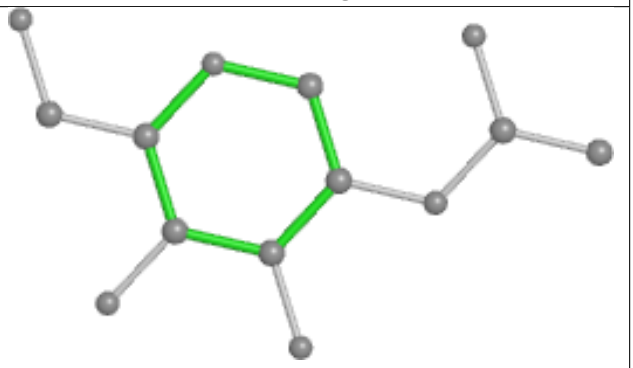
Bond lengths



Bond angles

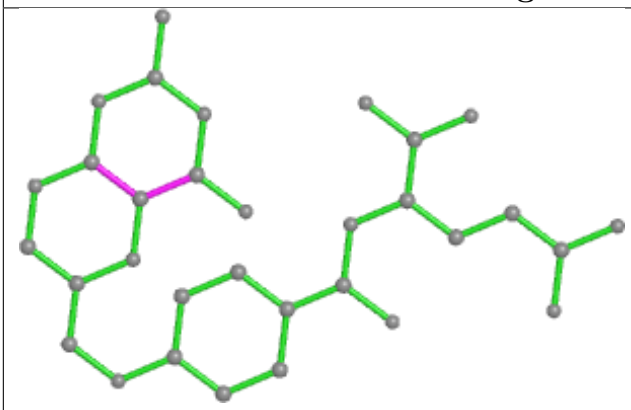


Torsions

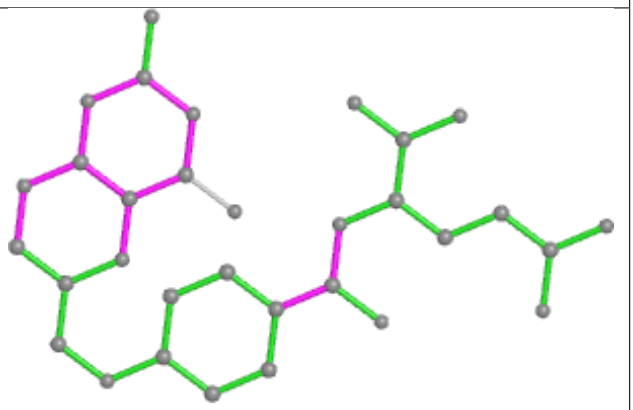


Rings

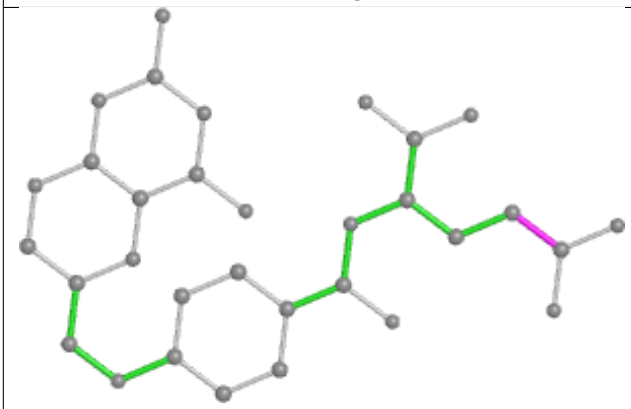
Ligand FOL A 1444



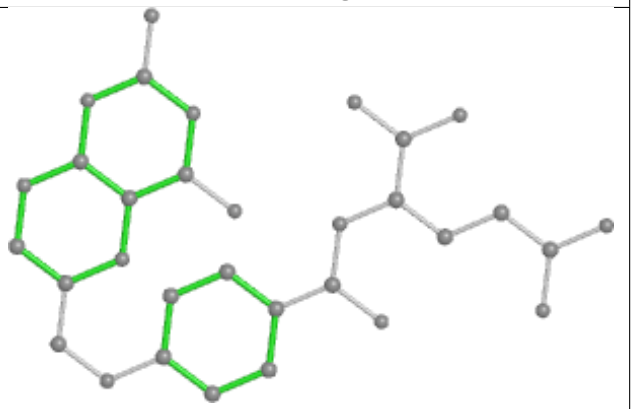
Bond lengths



Bond angles

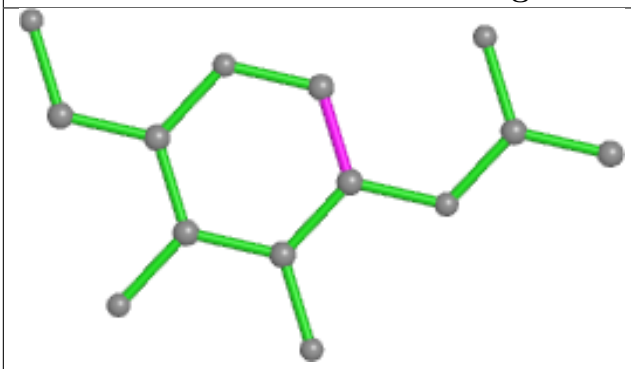


Torsions

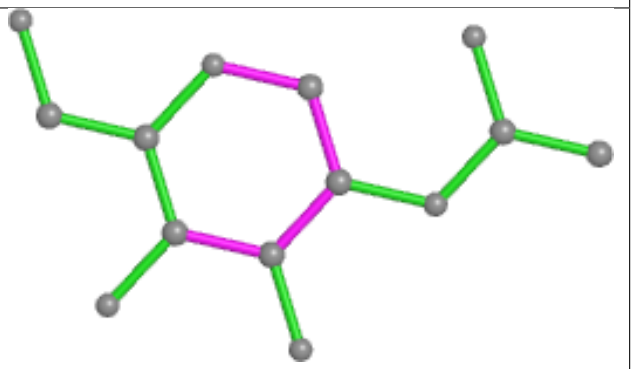


Rings

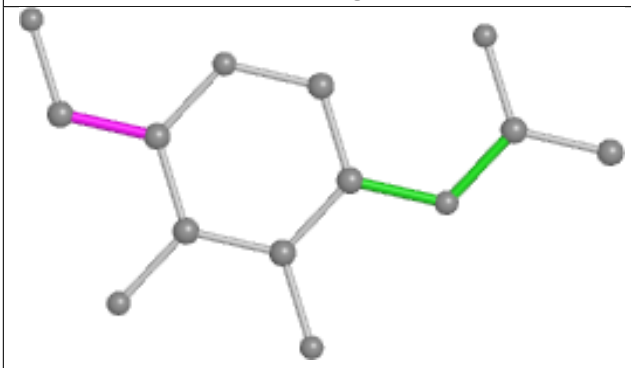
Ligand NAG B 1415



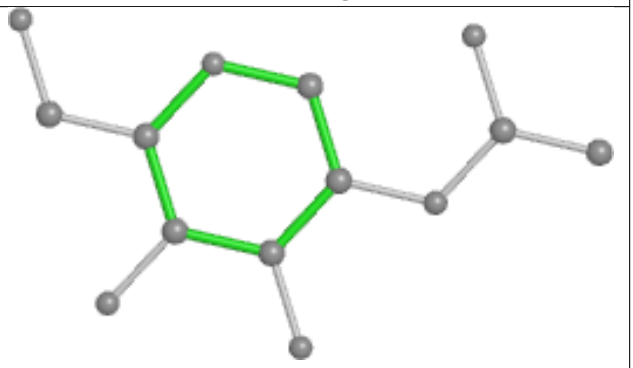
Bond lengths



Bond angles

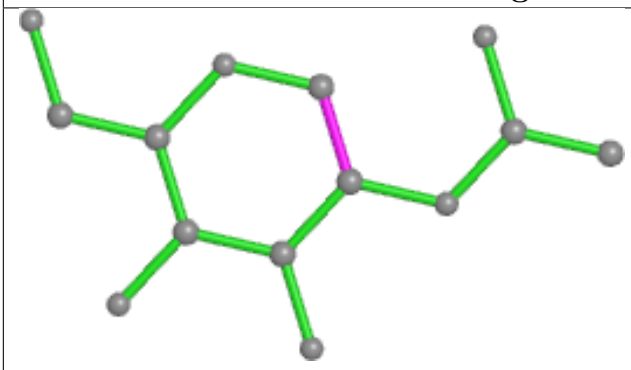


Torsions

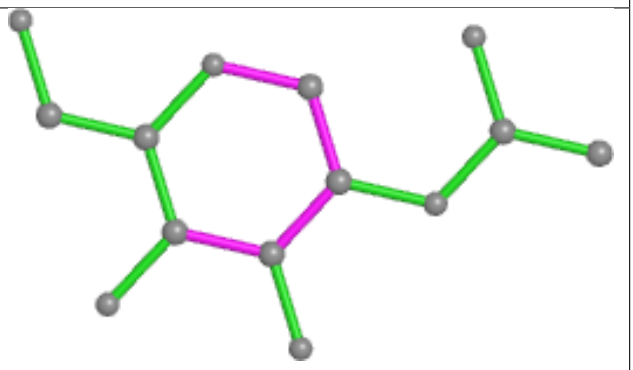


Rings

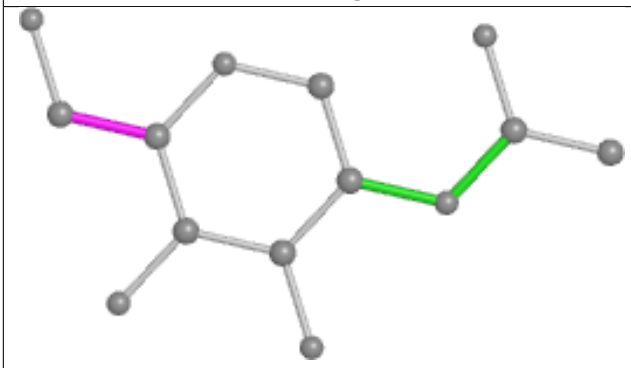
Ligand NAG C 1415



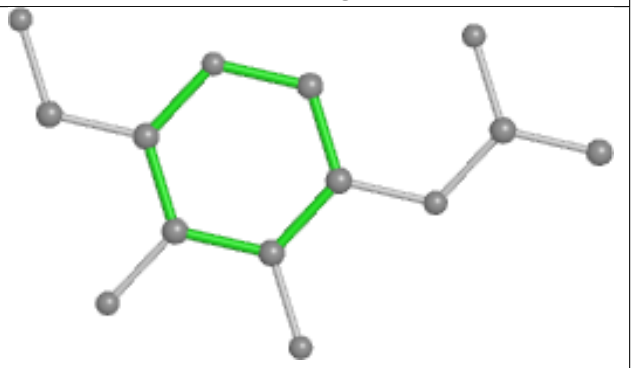
Bond lengths



Bond angles

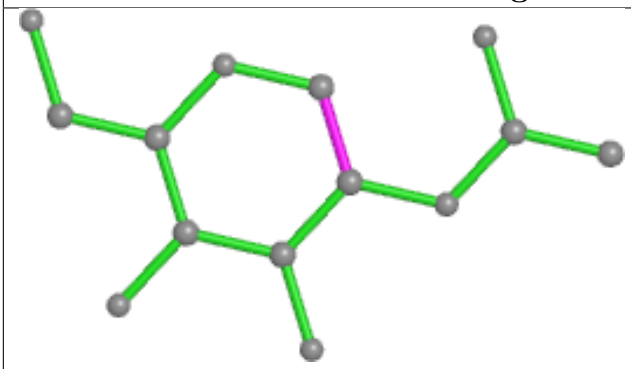


Torsions

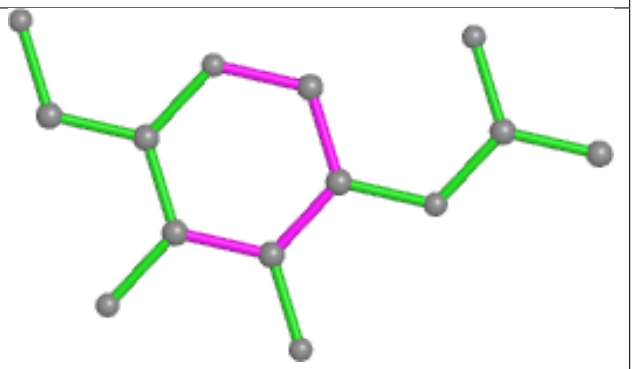


Rings

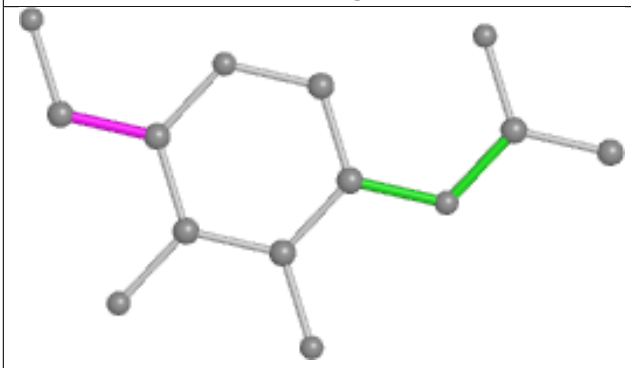
Ligand NAG A 1417



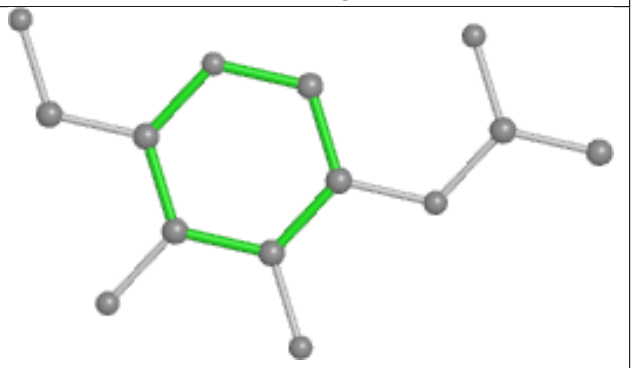
Bond lengths



Bond angles

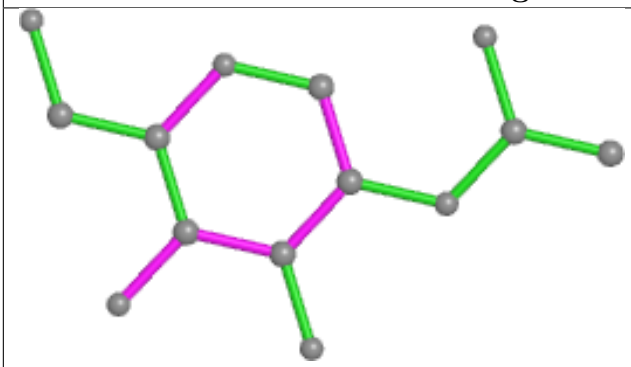


Torsions

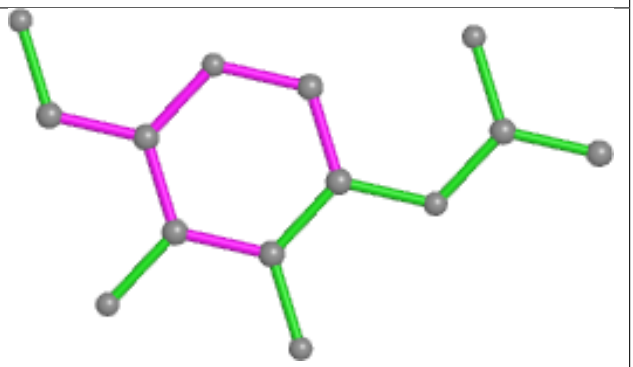


Rings

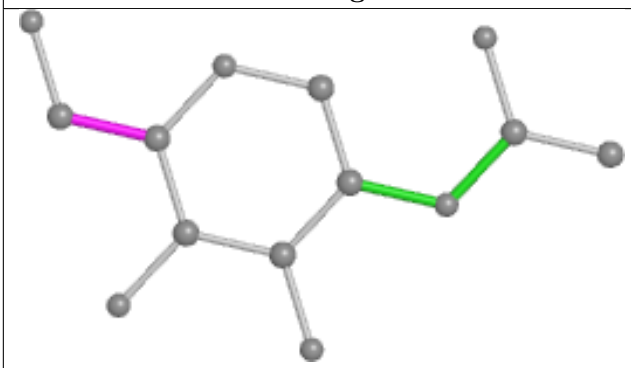
Ligand NAG B 1436



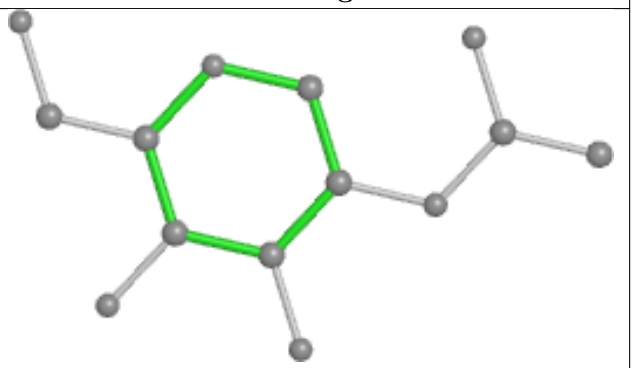
Bond lengths



Bond angles

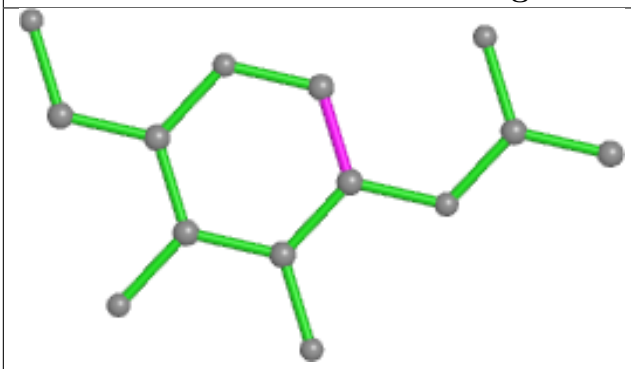


Torsions

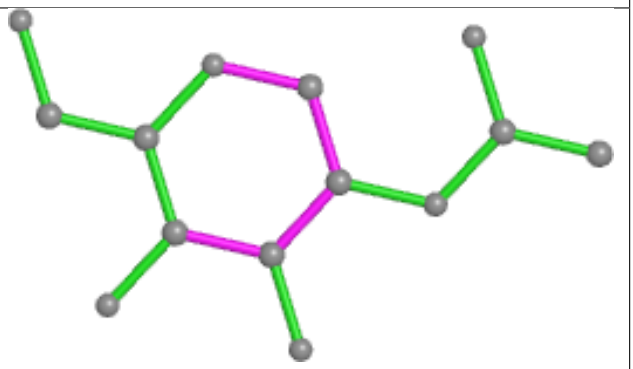


Rings

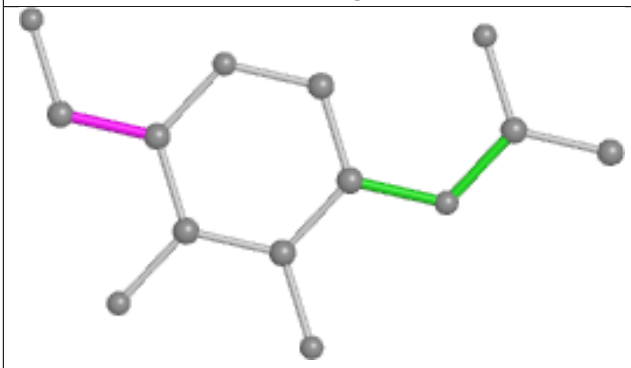
Ligand NAG C 1419



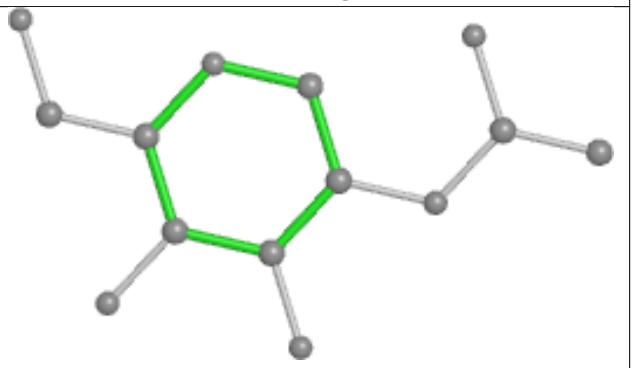
Bond lengths



Bond angles

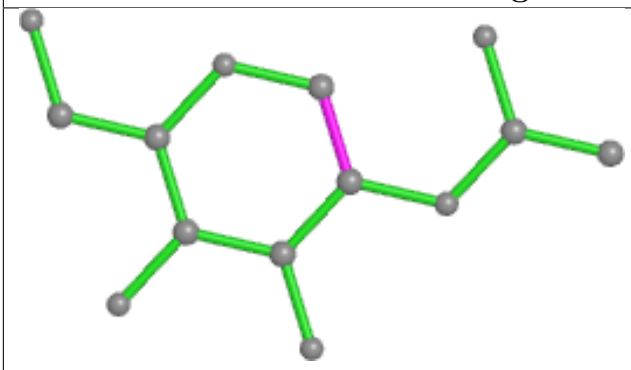


Torsions

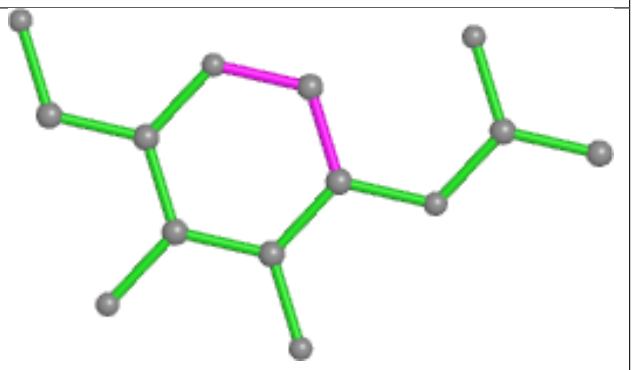


Rings

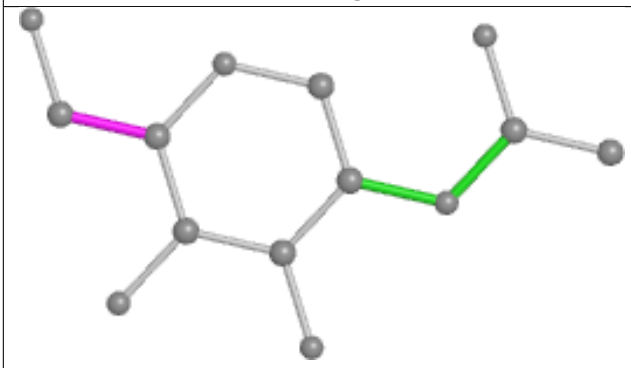
Ligand NAG C 1414



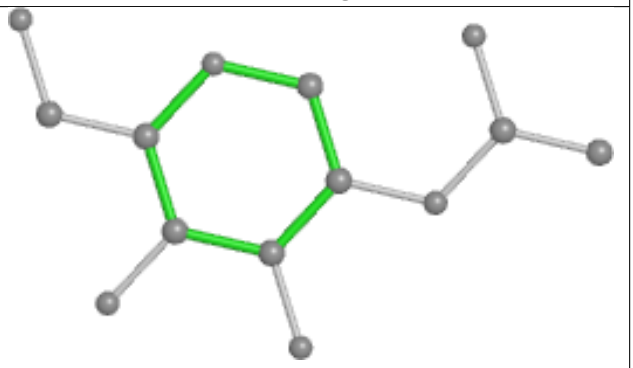
Bond lengths



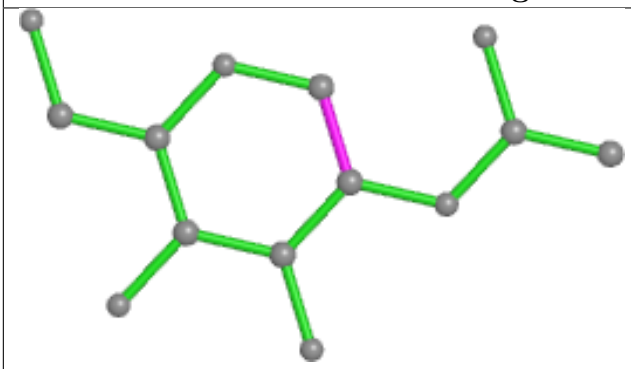
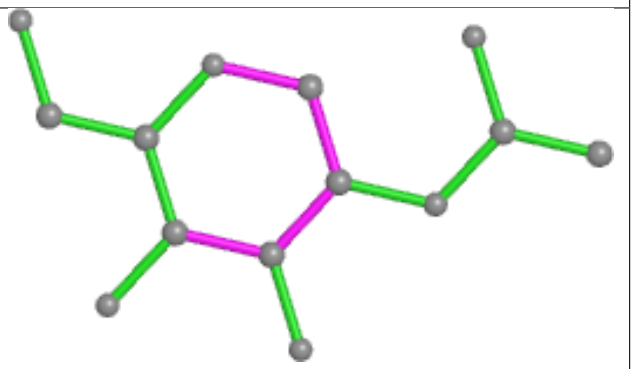
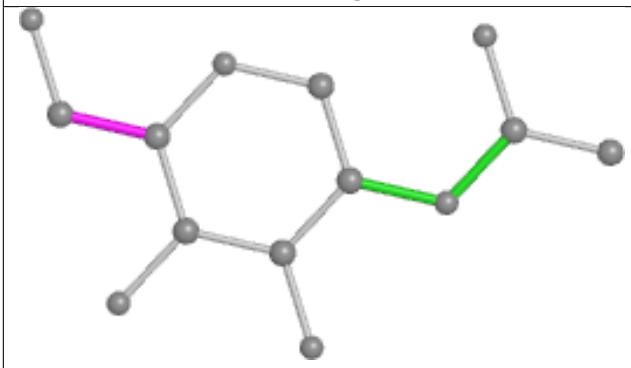
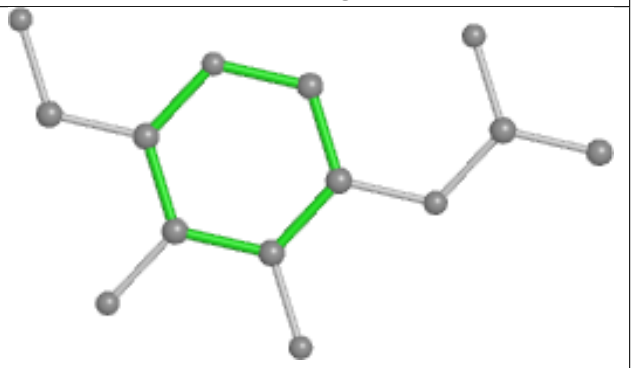
Bond angles

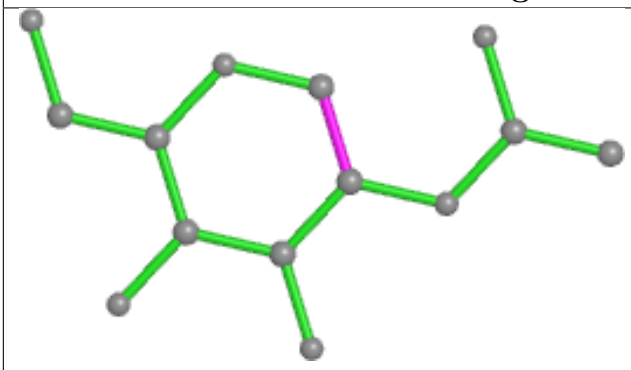
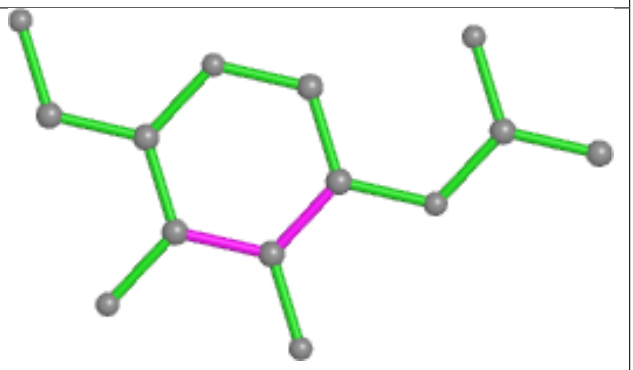
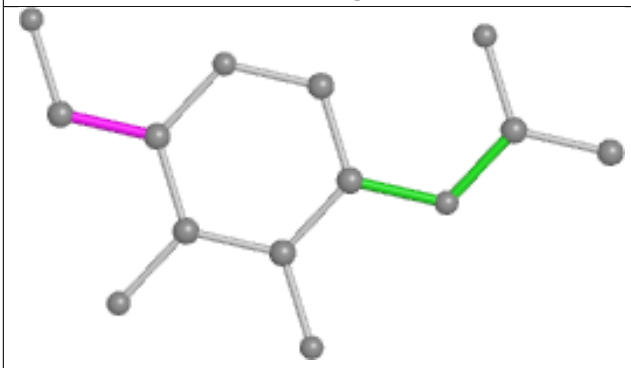
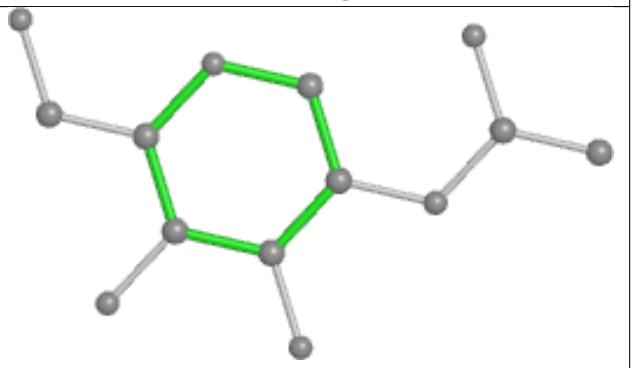


Torsions

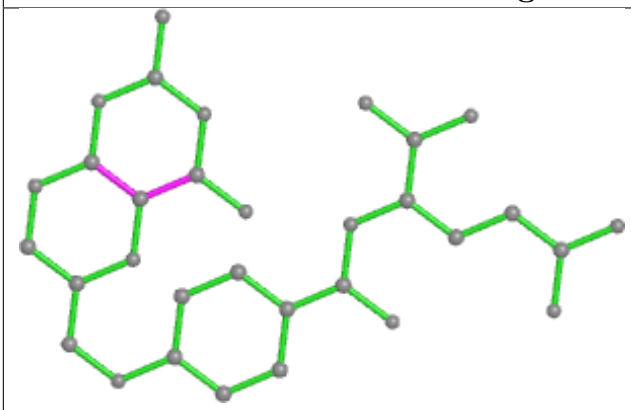


Rings

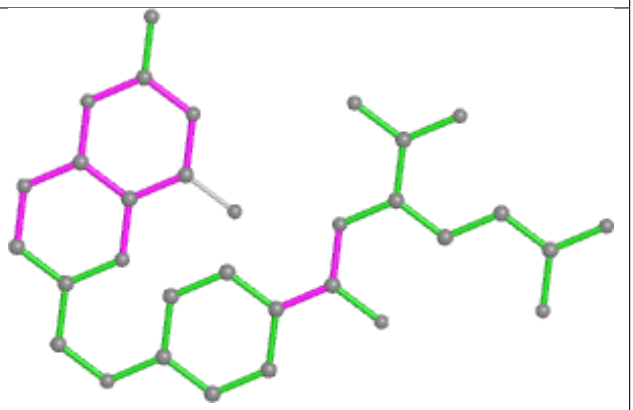
Ligand NAG B 1419	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1418	
 Bond lengths	 Bond angles
 Torsions	 Rings

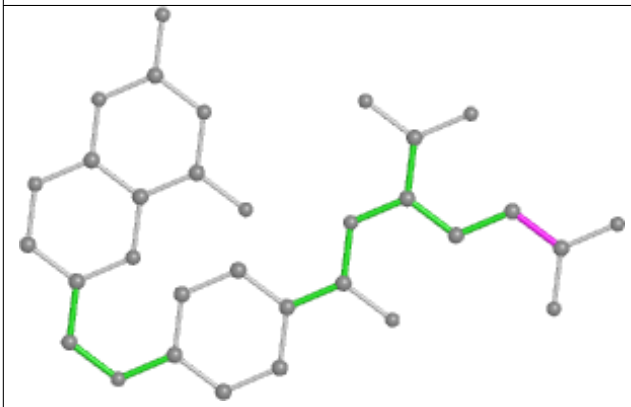
Ligand FOL C 1444



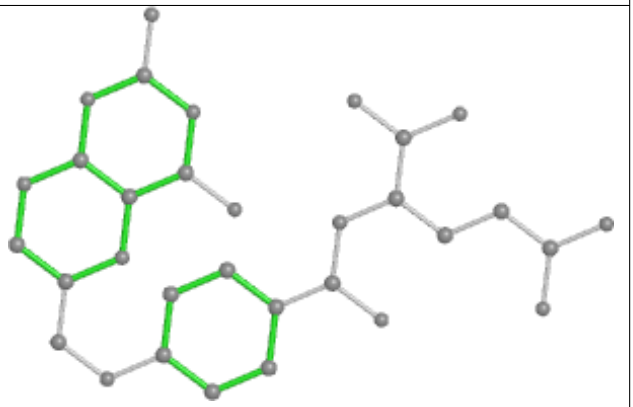
Bond lengths



Bond angles

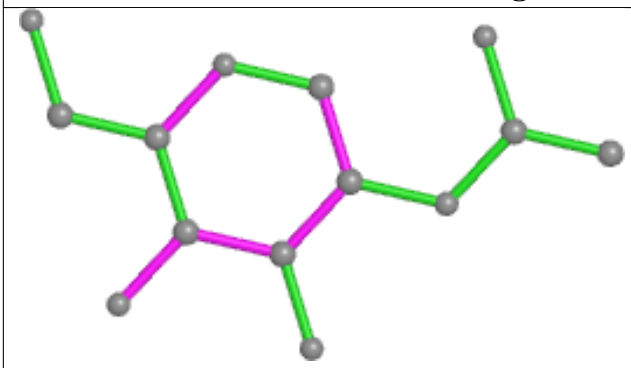


Torsions

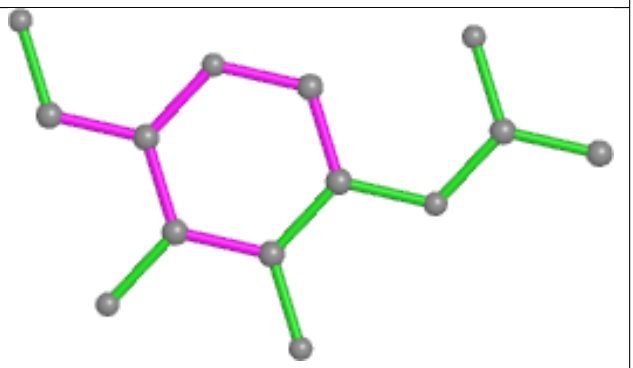


Rings

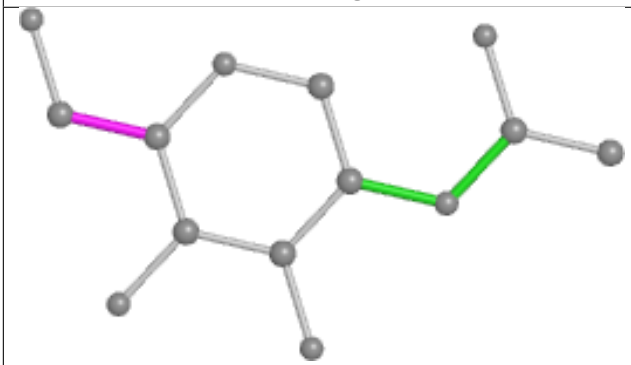
Ligand NAG A 1436



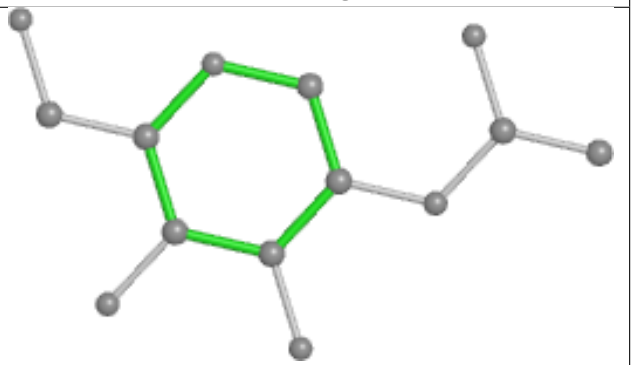
Bond lengths



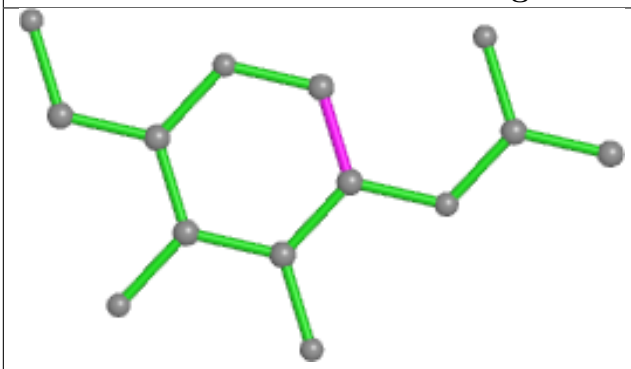
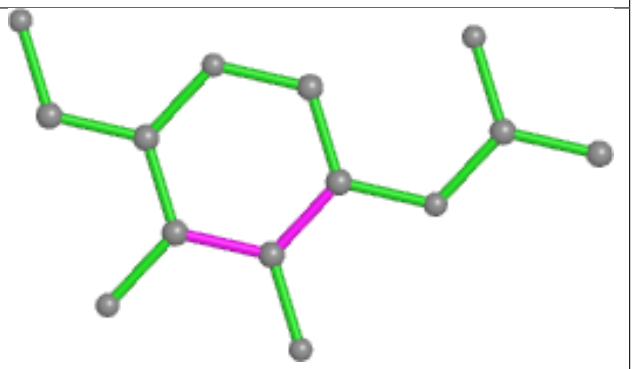
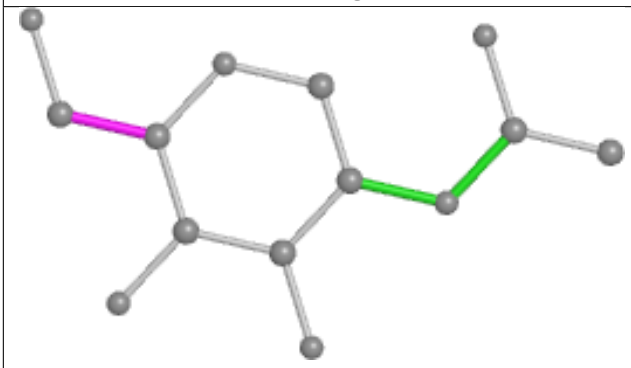
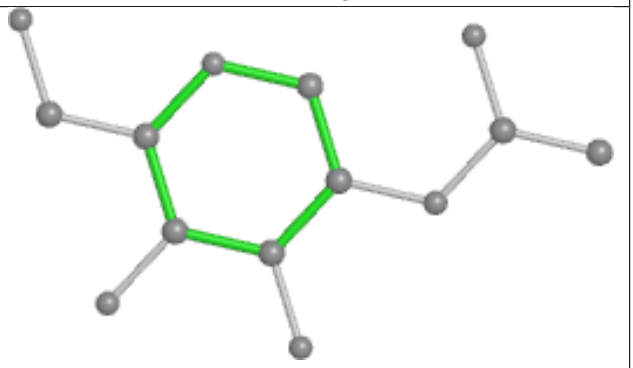
Bond angles

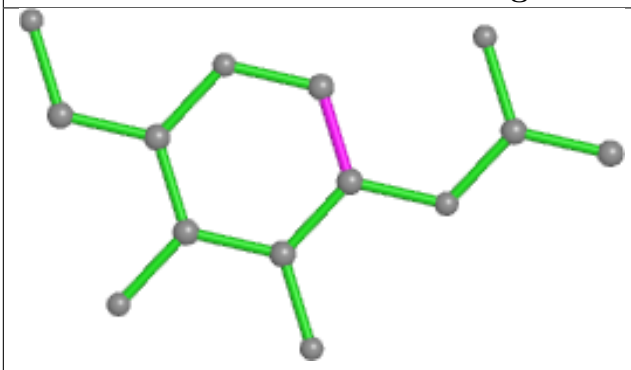
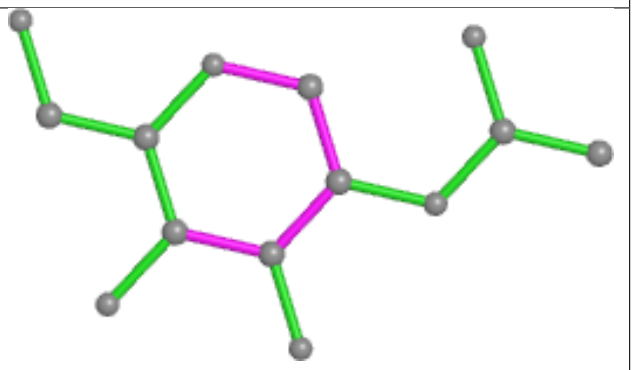
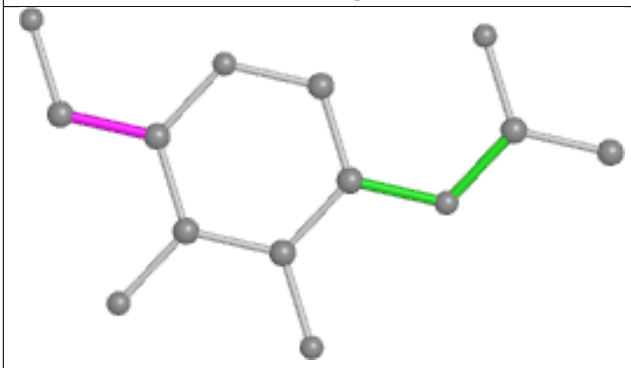
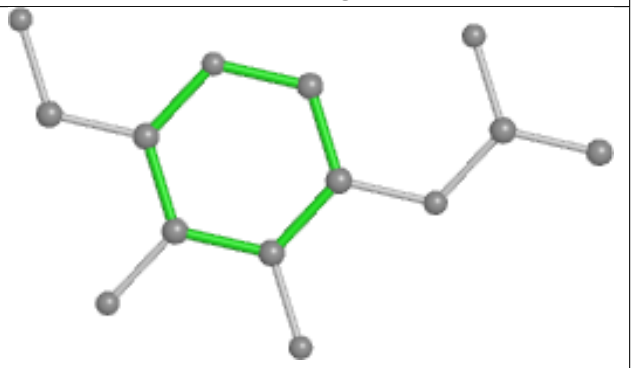


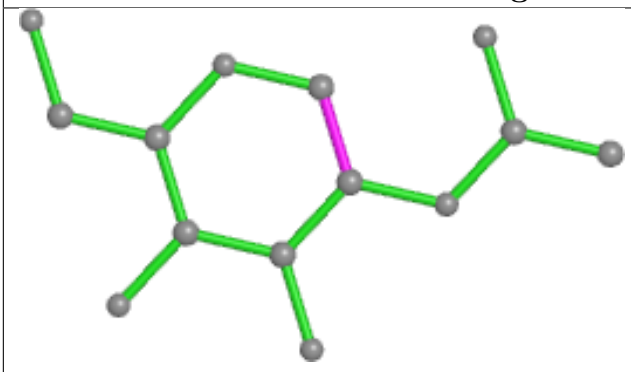
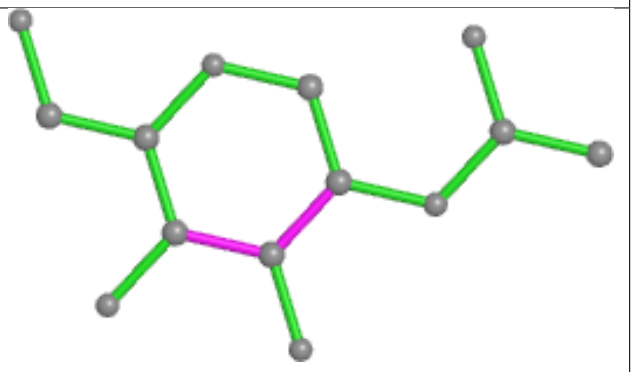
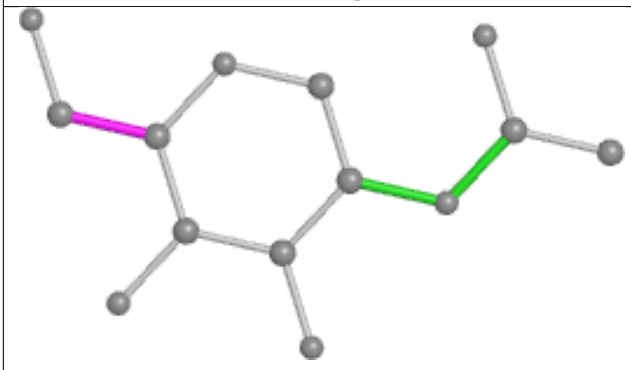
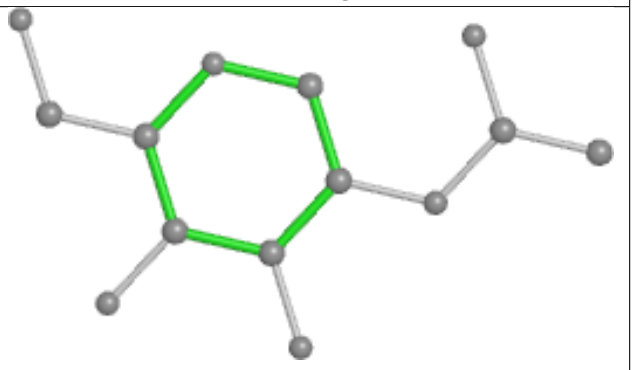
Torsions



Rings

Ligand NAG C 1418	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1419	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1418	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

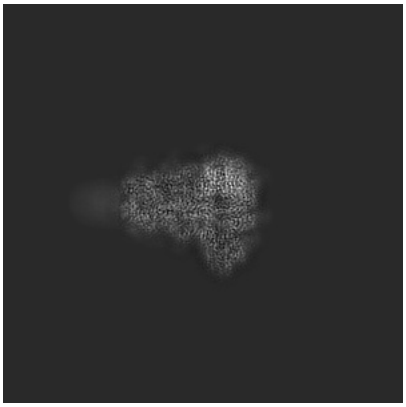
This section contains visualisations of the EMDB entry EMD-20544. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

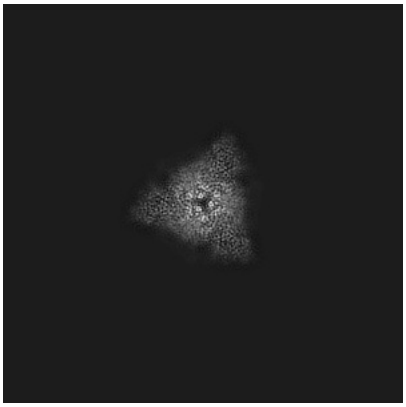
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

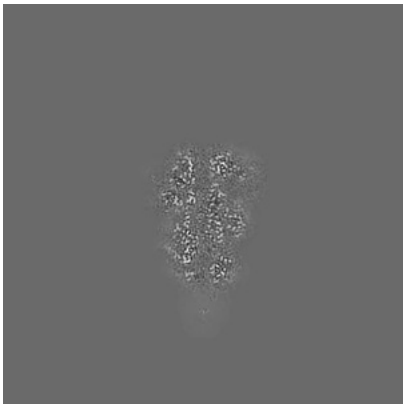


Z

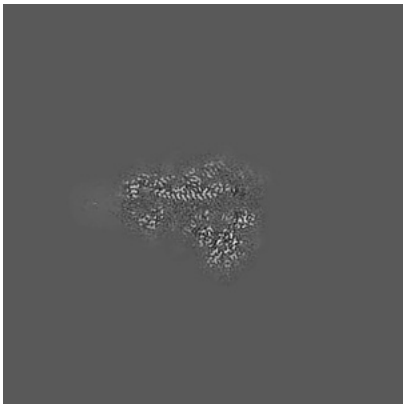
The images above show the map projected in three orthogonal directions.

6.2 Central slices

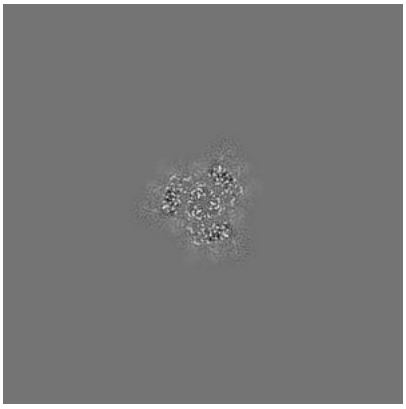
6.2.1 Primary map



X Index: 200



Y Index: 200



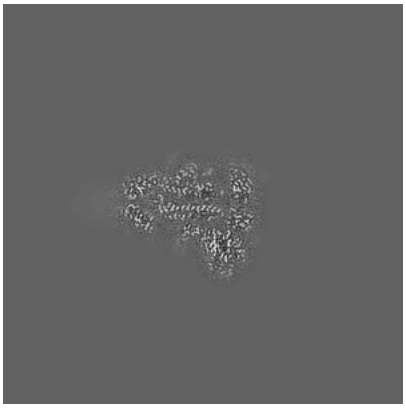
Z Index: 200

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

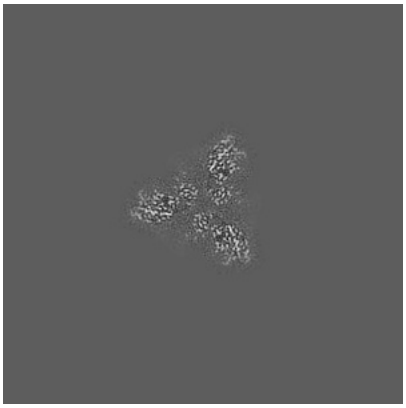
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 215



Y Index: 193

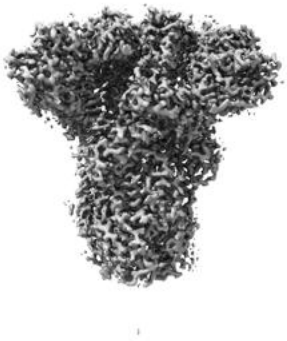


Z Index: 223

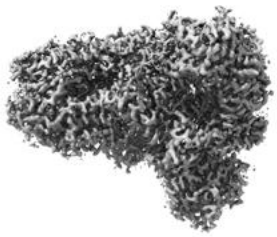
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

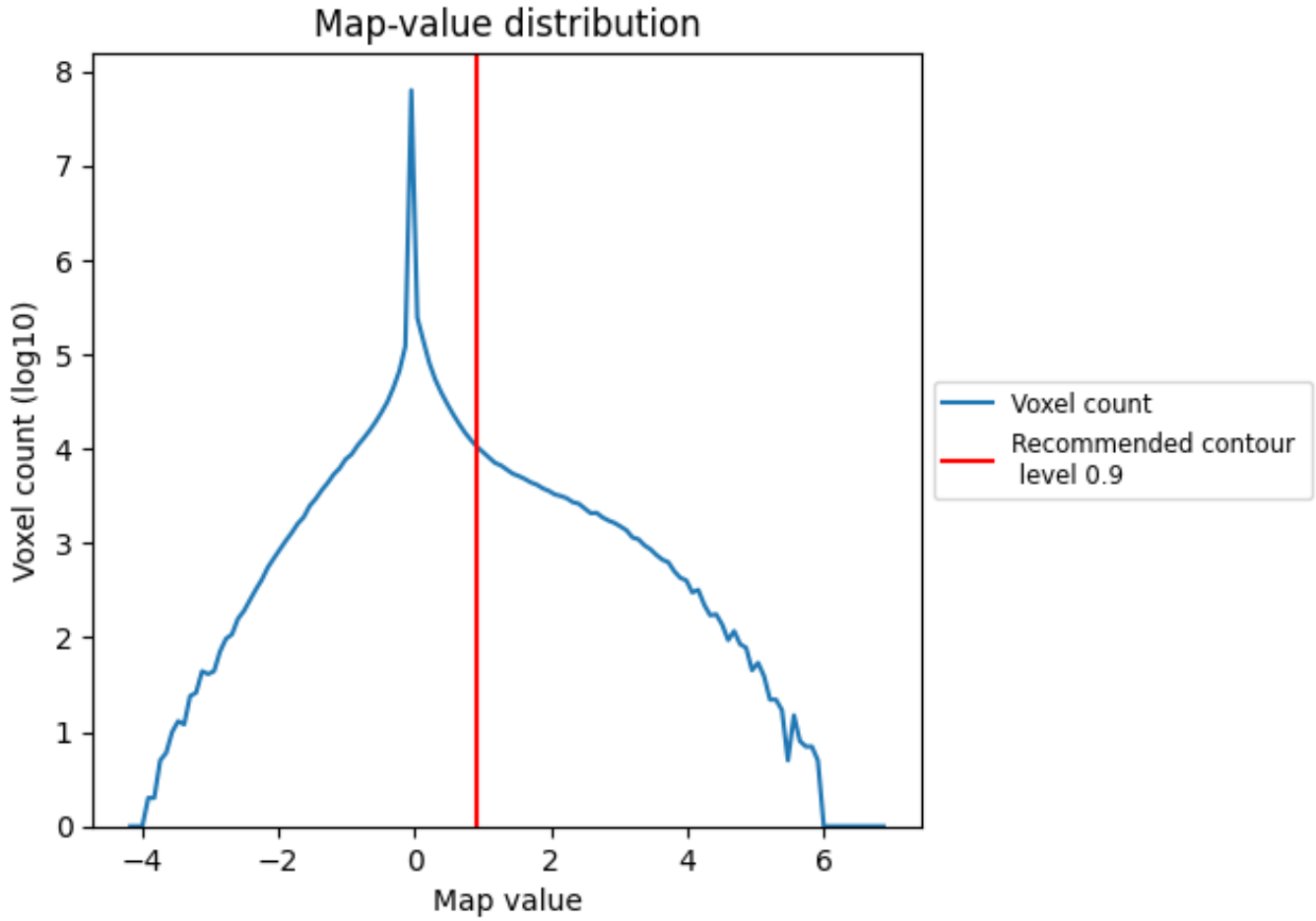
6.5 Mask visualisation (i)

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

7 Map analysis

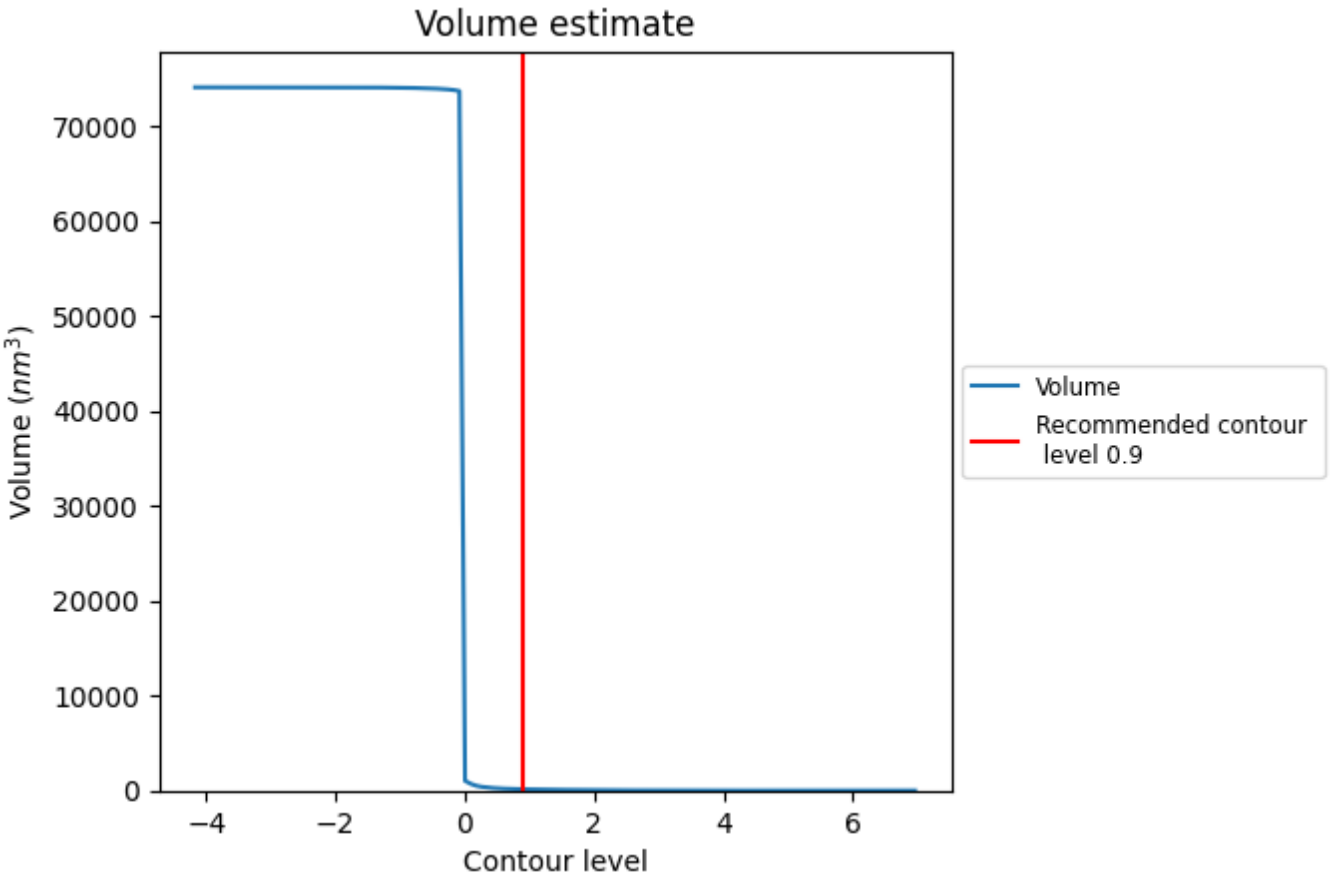
This section contains the results of statistical analysis of the map.

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.

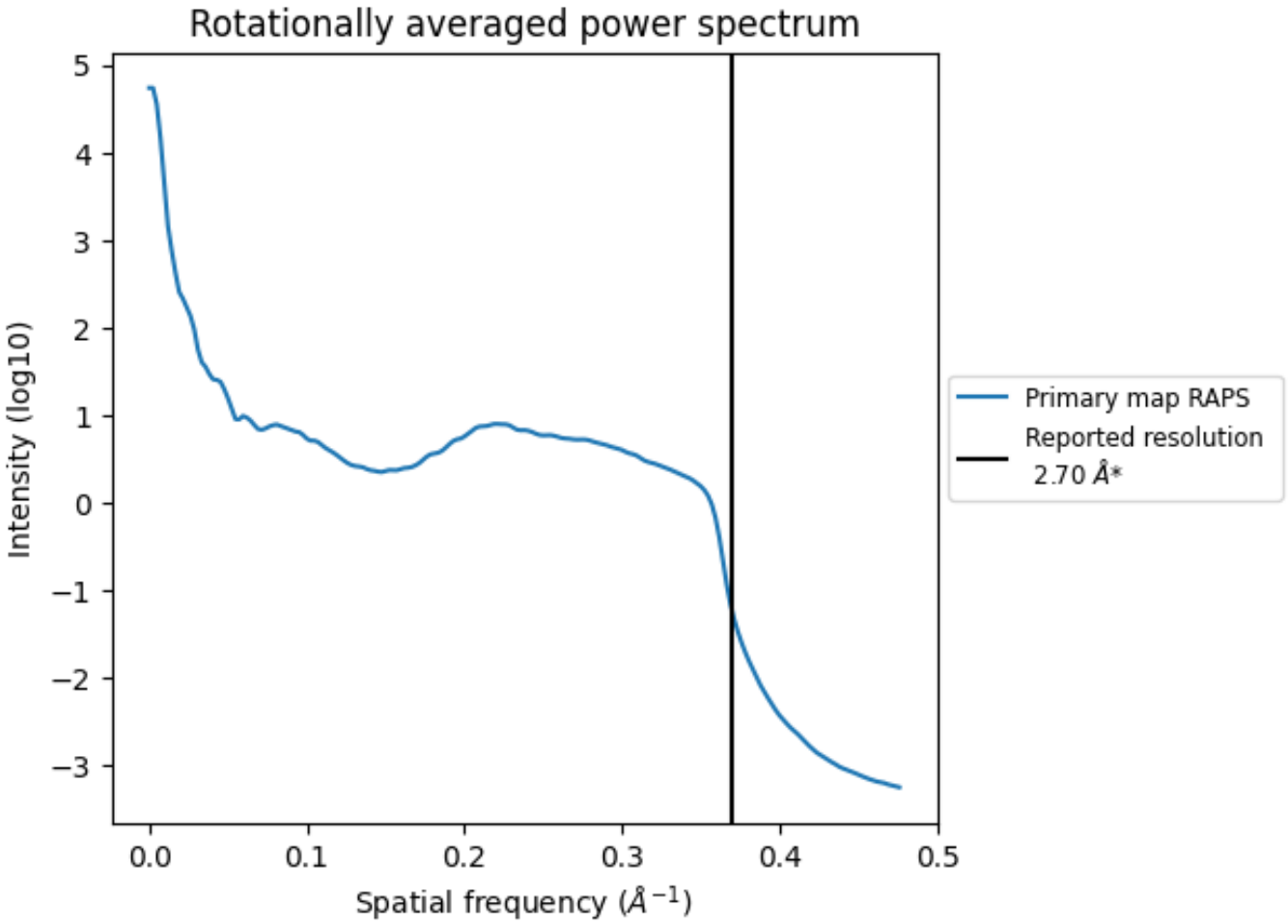
7.2 Volume estimate (i)



The volume at the recommended contour level is 138 nm^3; this corresponds to an approximate mass of 125 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 0.370 Å^{-1}

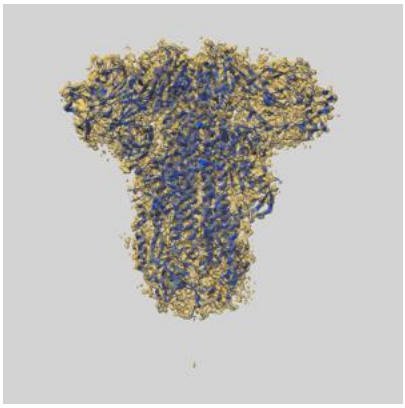
8 Fourier-Shell correlation (i)

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

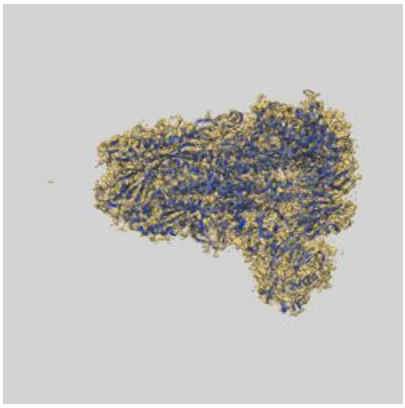
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20544 and PDB model 6Q06. Per-residue inclusion information can be found in section 3 on page 17.

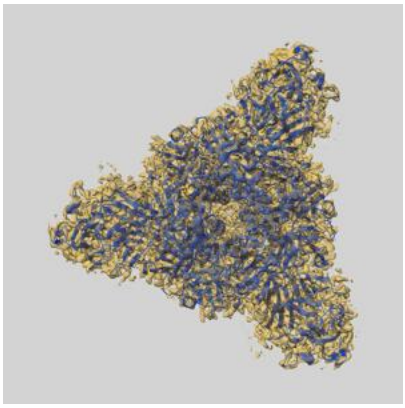
9.1 Map-model overlay



X



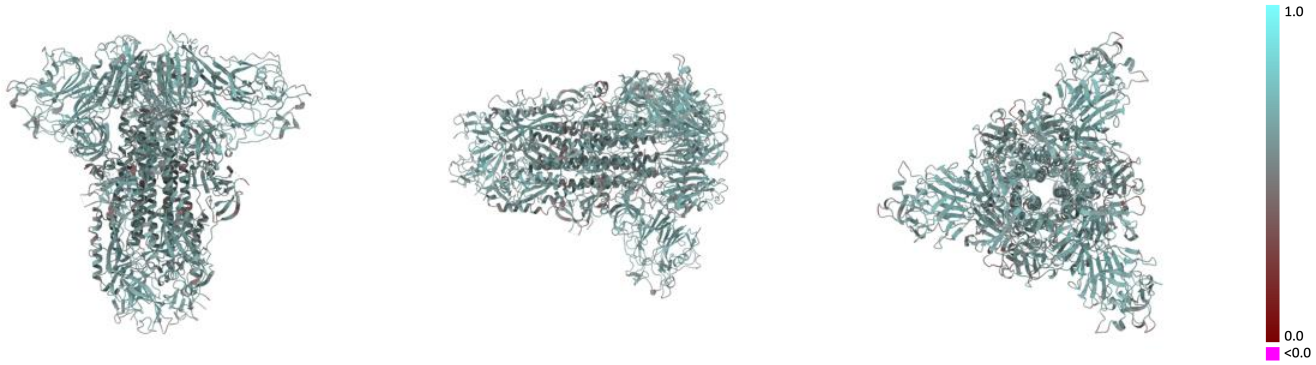
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

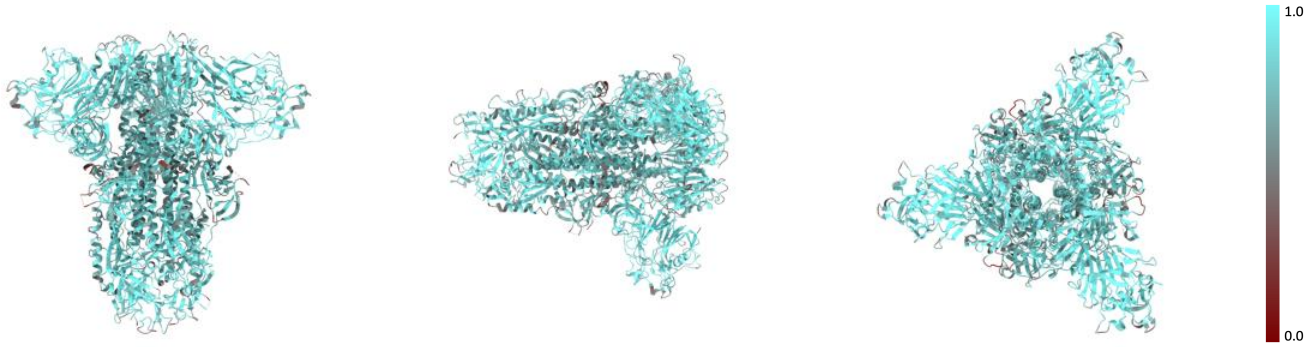
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

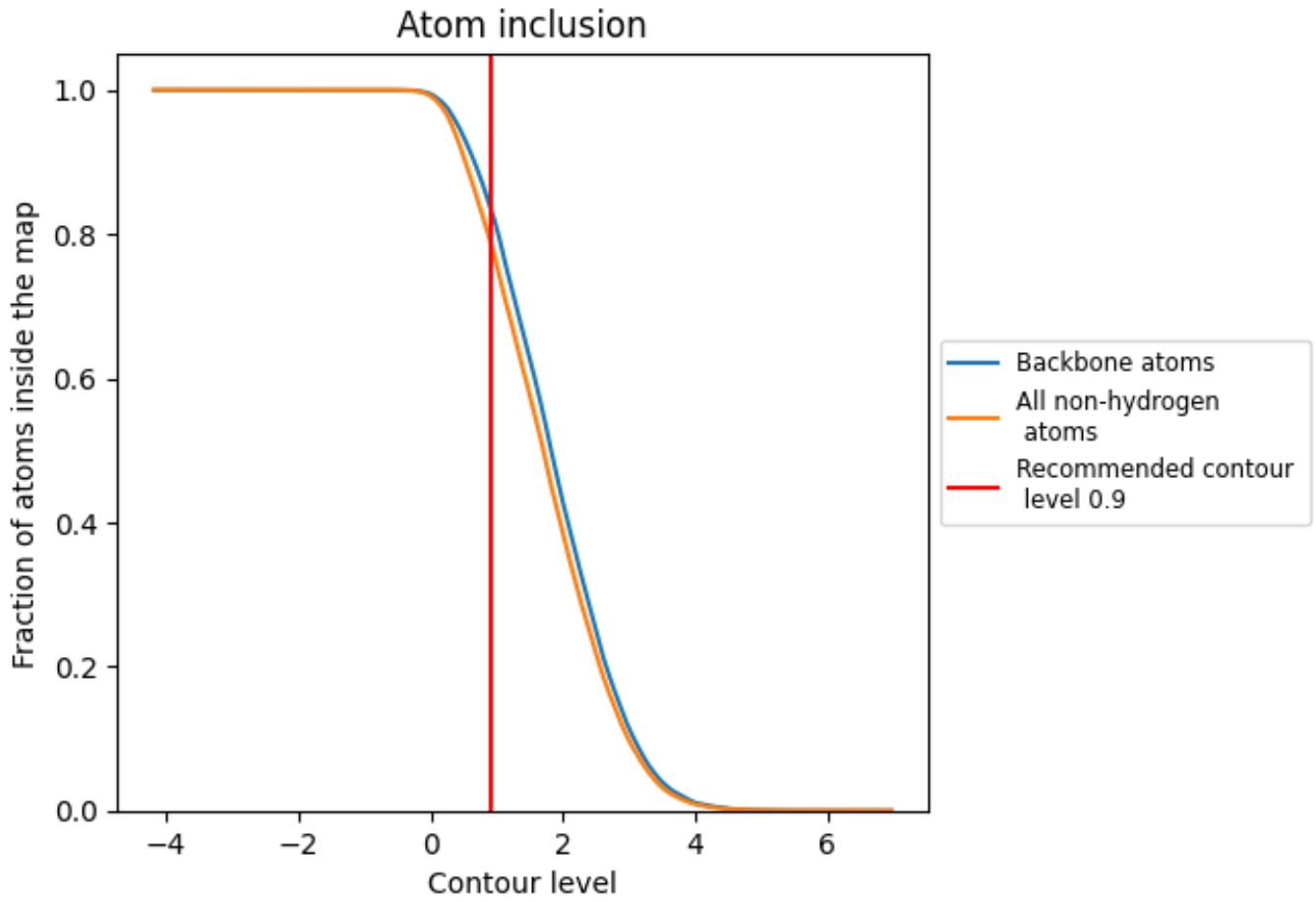
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.9).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7906	0.5740
A	0.8209	0.5840
B	0.8179	0.5840
C	0.8206	0.5850
D	0.4600	0.4190
E	0.2143	0.3020
F	0.3012	0.3650
G	0.1538	0.3000
H	0.2000	0.3570
I	0.2500	0.4920
J	0.2143	0.2810
K	0.4754	0.4650
L	0.3115	0.3700
M	0.3929	0.3670
N	0.3750	0.4810
O	0.4000	0.4250
P	0.2500	0.2860
Q	0.3133	0.3580
R	0.1282	0.2820
S	0.2200	0.3570
T	0.2857	0.4780
U	0.2500	0.2930
V	0.4590	0.4630
W	0.3279	0.3700
X	0.3214	0.3710
Y	0.3750	0.4680
Z	0.4400	0.4190
a	0.2143	0.2680
b	0.3133	0.3590
c	0.1538	0.2820
d	0.2000	0.3560
e	0.2857	0.4660
f	0.2143	0.2730
g	0.4754	0.4590
h	0.2951	0.3650

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Chain	Atom inclusion	Q-score
i	0.2857	0.3770
j	0.3125	0.4810