Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 12:58 PM EDT

PDB ID	:	7KJ2
EMDB ID	:	EMD-22891
Title	:	SARS-CoV-2 Spike Glycoprotein with one ACE2 Bound
Authors	:	Zhang, J.; Xiao, T.S.; Cai, Y.F.; Chen, B.
Deposited on	:	2020-10-25
Resolution	:	3.60 Å(reported)
Based on initial models	:	6M17, 6VYB

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

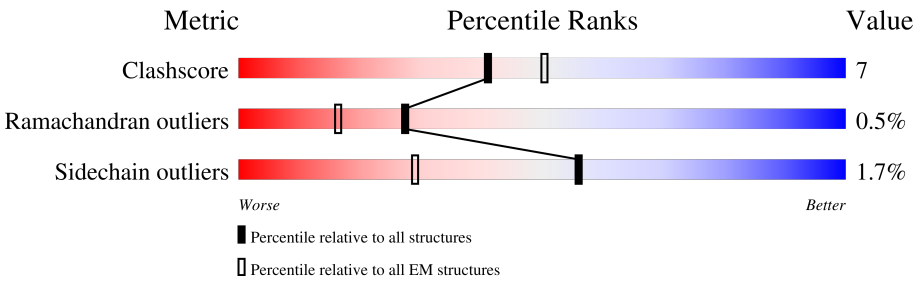
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1234	72% 6% • 22%
1	B	1234	71% 8% • 21%
1	C	1234	70% 7% • 22%
2	D	615	87% 8% • •
3	E	2	50% 50%
3	F	2	50% 50%
3	G	2	100%
3	H	2	100%

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Mol	Chain	Length	Quality of chain
3	I	2	100%
3	J	2	100%
3	K	2	100%
3	L	2	100%
3	M	2	50% 50%
3	N	2	100%
3	O	2	50% 50%
3	P	2	100%
3	Q	2	50% 50% 50%
3	R	2	50% 50%
3	S	2	50% 100%
3	T	2	100% 100%
3	U	2	100% 50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28560 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
			Total	C	N	O	S		
1	A	967	7566	4840	1255	1438	33	0	0
1	B	981	7661	4891	1270	1465	35	0	0
1	C	961	7509	4795	1246	1435	33	0	0

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	GLY	ARG	conflict	UNP P0DTC2
A	684	SER	ALA	conflict	UNP P0DTC2
A	685	GLY	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	TYR	-	expression tag	UNP P0DTC2
A	1214	ILE	-	expression tag	UNP P0DTC2
A	1215	PRO	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ALA	-	expression tag	UNP P0DTC2
A	1218	PRO	-	expression tag	UNP P0DTC2
A	1219	ARG	-	expression tag	UNP P0DTC2
A	1220	ASP	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	GLN	-	expression tag	UNP P0DTC2
A	1223	ALA	-	expression tag	UNP P0DTC2
A	1224	TYR	-	expression tag	UNP P0DTC2
A	1225	VAL	-	expression tag	UNP P0DTC2
A	1226	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	LYS	-	expression tag	UNP P0DTC2
A	1228	ASP	-	expression tag	UNP P0DTC2
A	1229	GLY	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	TRP	-	expression tag	UNP P0DTC2
A	1232	VAL	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	LEU	-	expression tag	UNP P0DTC2
A	1235	SER	-	expression tag	UNP P0DTC2
A	1236	THR	-	expression tag	UNP P0DTC2
A	1237	PHE	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	SER	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	GLY	ARG	conflict	UNP P0DTC2
B	684	SER	ALA	conflict	UNP P0DTC2
B	685	GLY	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	TYR	-	expression tag	UNP P0DTC2
B	1214	ILE	-	expression tag	UNP P0DTC2
B	1215	PRO	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ALA	-	expression tag	UNP P0DTC2
B	1218	PRO	-	expression tag	UNP P0DTC2
B	1219	ARG	-	expression tag	UNP P0DTC2
B	1220	ASP	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	GLN	-	expression tag	UNP P0DTC2
B	1223	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1224	TYR	-	expression tag	UNP P0DTC2
B	1225	VAL	-	expression tag	UNP P0DTC2
B	1226	ARG	-	expression tag	UNP P0DTC2
B	1227	LYS	-	expression tag	UNP P0DTC2
B	1228	ASP	-	expression tag	UNP P0DTC2
B	1229	GLY	-	expression tag	UNP P0DTC2
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	TRP	-	expression tag	UNP P0DTC2
B	1232	VAL	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	SER	-	expression tag	UNP P0DTC2
B	1236	THR	-	expression tag	UNP P0DTC2
B	1237	PHE	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	SER	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	GLY	ARG	conflict	UNP P0DTC2
C	684	SER	ALA	conflict	UNP P0DTC2
C	685	GLY	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	TYR	-	expression tag	UNP P0DTC2
C	1214	ILE	-	expression tag	UNP P0DTC2
C	1215	PRO	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ALA	-	expression tag	UNP P0DTC2
C	1218	PRO	-	expression tag	UNP P0DTC2
C	1219	ARG	-	expression tag	UNP P0DTC2
C	1220	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	GLN	-	expression tag	UNP P0DTC2
C	1223	ALA	-	expression tag	UNP P0DTC2
C	1224	TYR	-	expression tag	UNP P0DTC2
C	1225	VAL	-	expression tag	UNP P0DTC2
C	1226	ARG	-	expression tag	UNP P0DTC2
C	1227	LYS	-	expression tag	UNP P0DTC2
C	1228	ASP	-	expression tag	UNP P0DTC2
C	1229	GLY	-	expression tag	UNP P0DTC2
C	1230	GLU	-	expression tag	UNP P0DTC2
C	1231	TRP	-	expression tag	UNP P0DTC2
C	1232	VAL	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	SER	-	expression tag	UNP P0DTC2
C	1236	THR	-	expression tag	UNP P0DTC2
C	1237	PHE	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	SER	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2
C	1245	HIS	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	593	4844	3101	802	912	29	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	616	SER	-	expression tag	UNP Q9BYF1
D	617	GLY	-	expression tag	UNP Q9BYF1
D	618	GLY	-	expression tag	UNP Q9BYF1
D	619	SER	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	621	HIS	-	expression tag	UNP Q9BYF1
D	622	HIS	-	expression tag	UNP Q9BYF1
D	623	HIS	-	expression tag	UNP Q9BYF1
D	624	HIS	-	expression tag	UNP Q9BYF1
D	625	HIS	-	expression tag	UNP Q9BYF1

- 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
			Total	C	N	O		
3	E	2	28	16	2	10	0	0
3	F	2	28	16	2	10	0	0
3	G	2	28	16	2	10	0	0
3	H	2	28	16	2	10	0	0
3	I	2	28	16	2	10	0	0
3	J	2	28	16	2	10	0	0
3	K	2	28	16	2	10	0	0
3	L	2	28	16	2	10	0	0
3	M	2	28	16	2	10	0	0
3	N	2	28	16	2	10	0	0
3	O	2	28	16	2	10	0	0
3	P	2	28	16	2	10	0	0
3	Q	2	28	16	2	10	0	0
3	R	2	28	16	2	10	0	0

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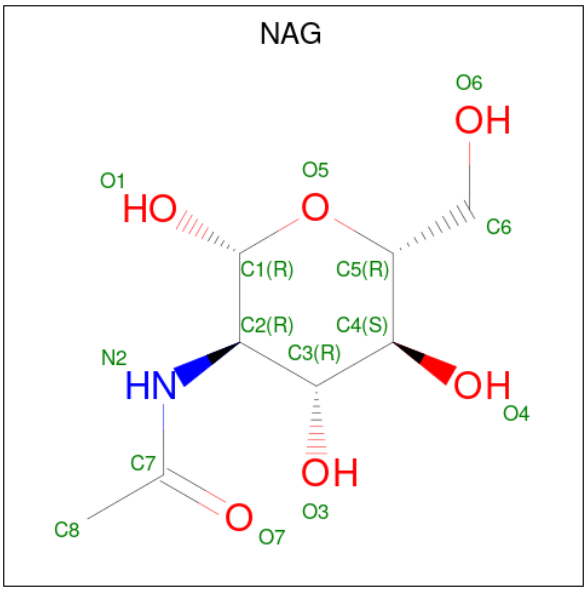
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	S	2	28	16	2	10	0	0
			Total	C	N	O		
3	T	2	28	16	2	10	0	0
			Total	C	N	O		
3	U	2	28	16	2	10	0	0

- Molecule 4 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
			Total	C	N	O	
4	A	1	14	8	1	5	0
			Total	C	N	O	
4	A	1	14	8	1	5	0
			Total	C	N	O	
4	A	1	14	8	1	5	0
			Total	C	N	O	
4	A	1	14	8	1	5	0
			Total	C	N	O	
4	A	1	14	8	1	5	0
			Total	C	N	O	
4	A	1	14	8	1	5	0
			Total	C	N	O	
4	A	1	14	8	1	5	0
			Total	C	N	O	
4	A	1	14	8	1	5	0

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

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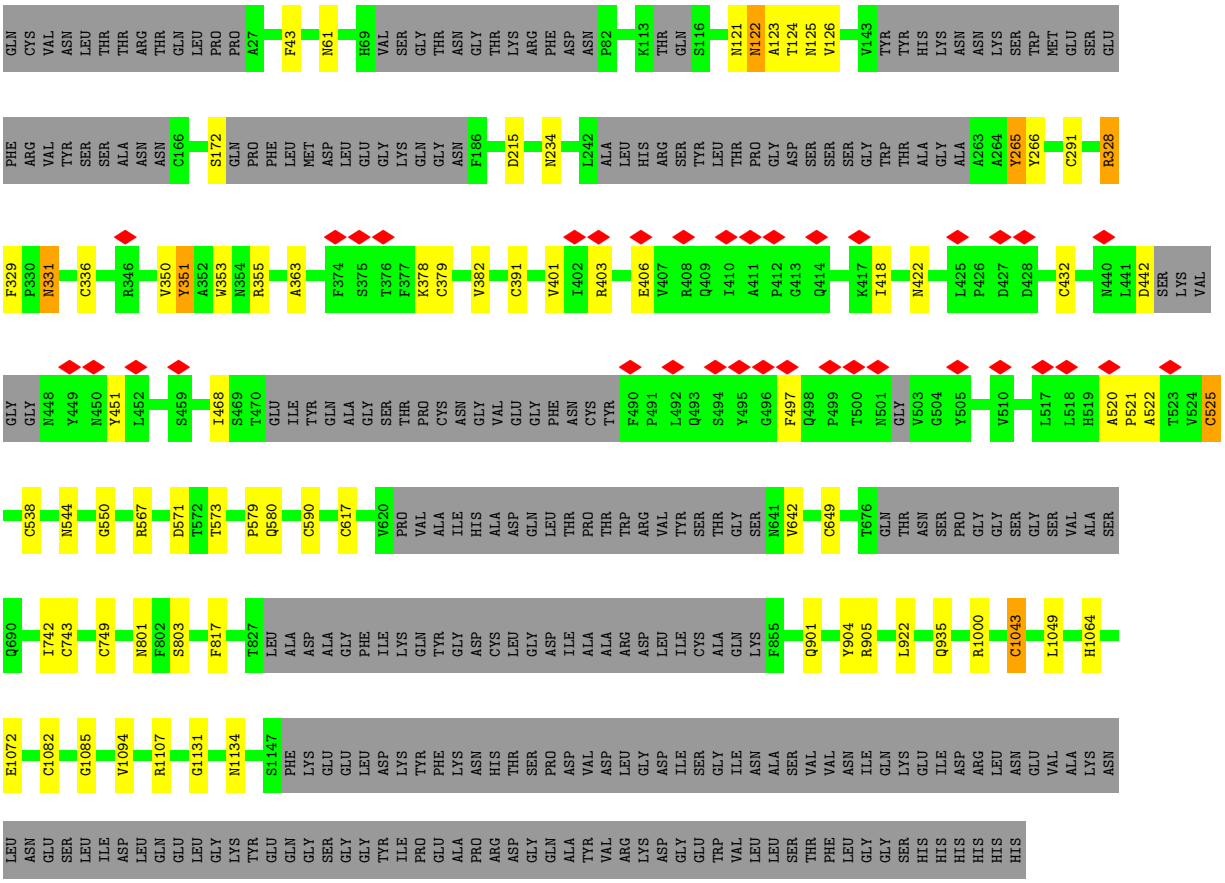
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	C	1	14	8	1	5	0
			Total	C	N	O	
4	C	1	14	8	1	5	0
			Total	C	N	O	
4	C	1	14	8	1	5	0
			Total	C	N	O	
4	C	1	14	8	1	5	0
			Total	C	N	O	
4	C	1	14	8	1	5	0
			Total	C	N	O	
4	C	1	14	8	1	5	0
			Total	C	N	O	
4	D	1	14	8	1	5	0

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.

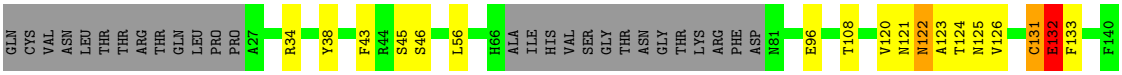
- Molecule 1: Spike glycoprotein

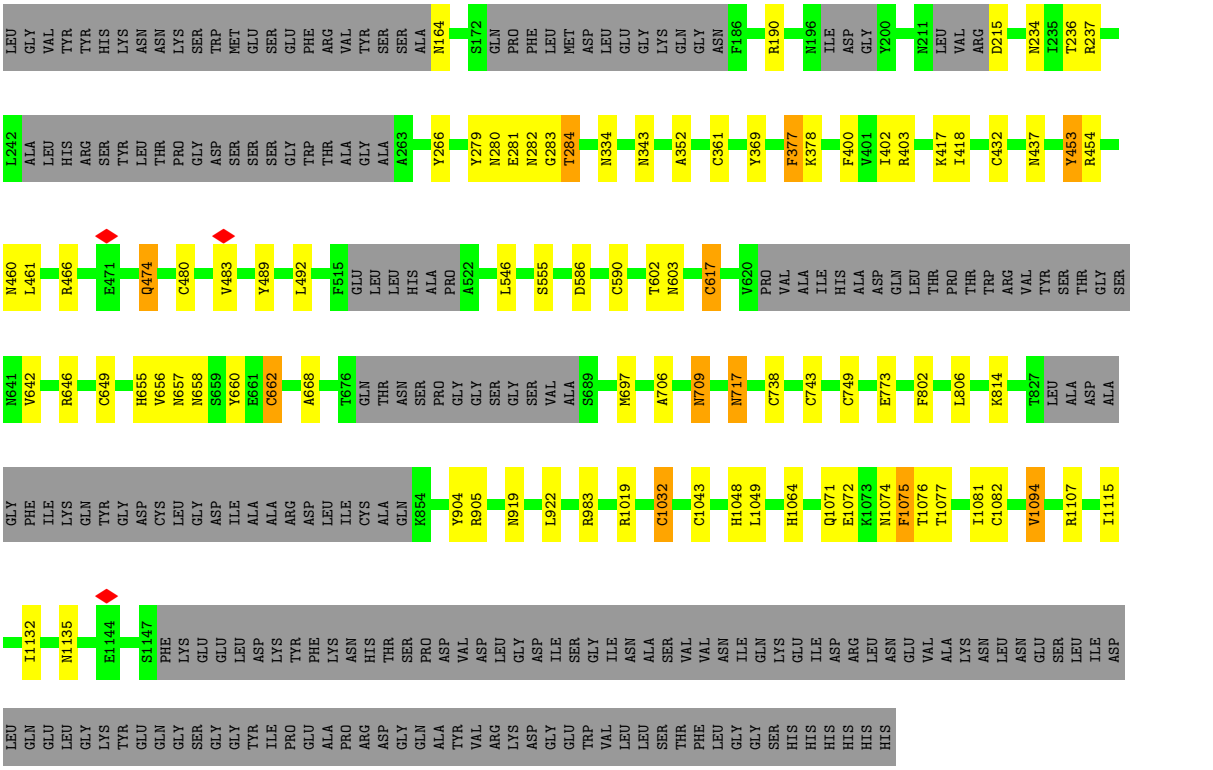
Chain A:



- Molecule 1: Spike glycoprotein

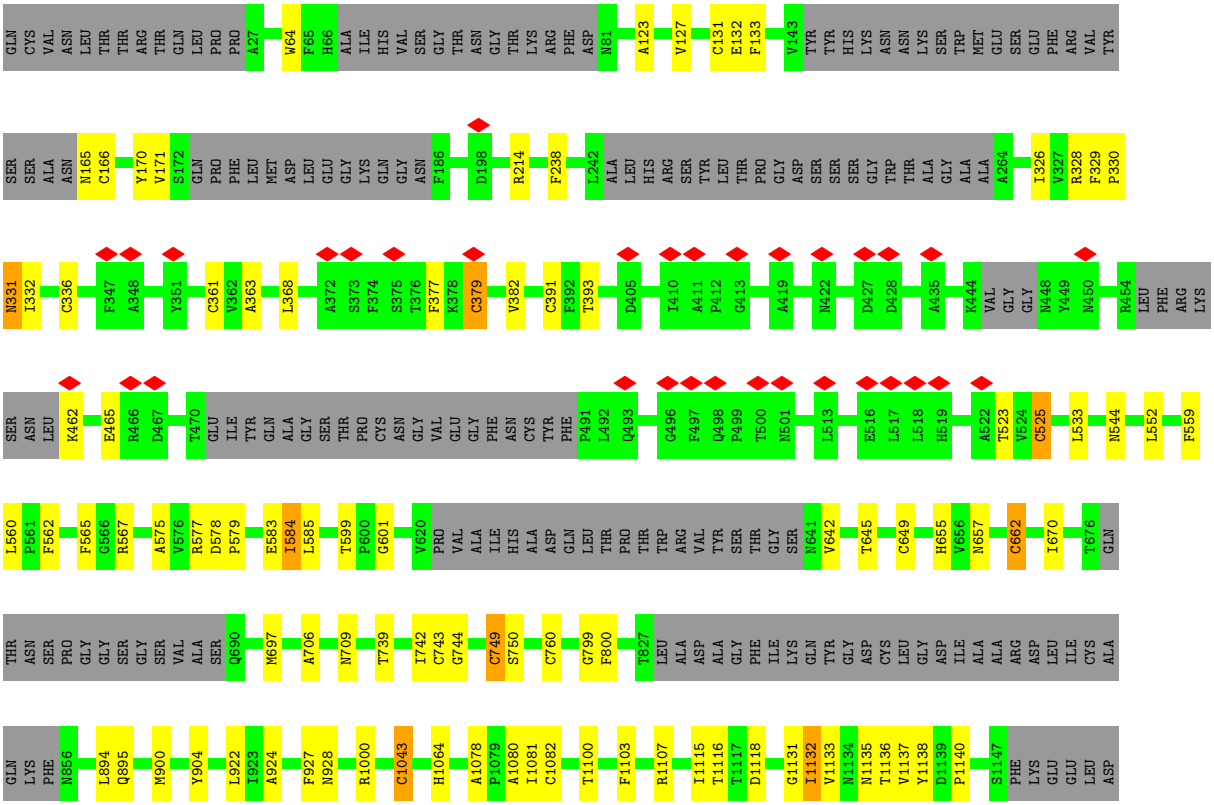
Chain B:

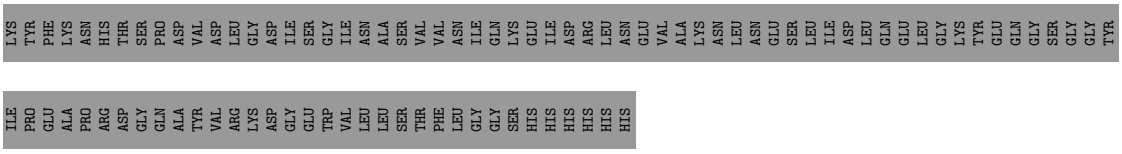




• Molecule 1: Spike glycoprotein

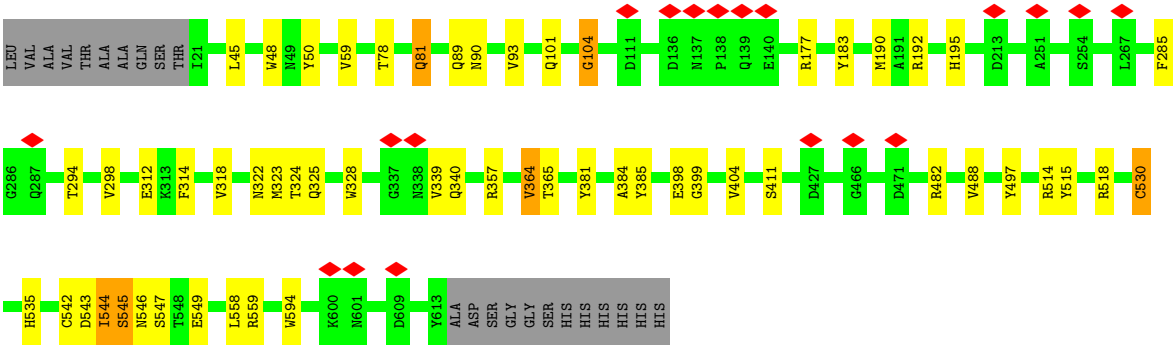
Chain C:





• Molecule 2: Angiotensin-converting enzyme 2

Chain D:



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

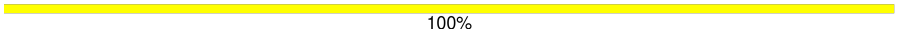
Chain E:

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

Chain F:

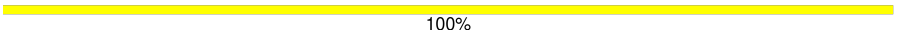
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



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

Chain I: 100%

NAG1
NAG2

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

Chain J: 100%

NAG1
NAG2

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

Chain K: 100%

NAG1
NAG2

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

Chain L: 100%

NAG1
NAG2

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

Chain M: 50% 50%

NAG1
NAG2

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

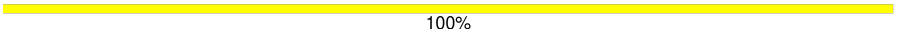
Chain N: 100%

NAG1
NAG2

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

Chain O: 50% 50%

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

Chain P: 

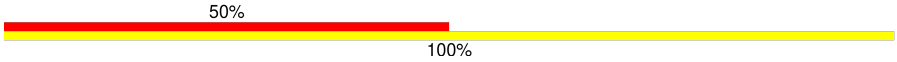
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

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

Chain R:

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

Chain S: 

• 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:
NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15964	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 ($e^-/Å^2$)	50.05	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.63	0/7733	0.92	0/10518
1	B	0.62	0/7830	0.91	0/10649
1	C	0.61	0/7673	0.91	0/10439
2	D	0.66	0/4981	0.93	0/6767
All	All	0.63	0/28217	0.92	0/38373

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	7566	0	7379	89	0
1	B	7661	0	7449	112	0
1	C	7509	0	7334	127	0
2	D	4844	0	4614	56	0
3	E	28	0	25	4	0
3	F	28	0	25	1	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	1	0
3	N	28	0	25	0	0
3	O	28	0	25	3	0
3	P	28	0	25	0	0
3	Q	28	0	25	1	0
3	R	28	0	25	0	0
3	S	28	0	25	6	0
3	T	28	0	25	6	0
3	U	28	0	25	0	0
4	A	140	0	130	14	0
4	B	182	0	169	15	0
4	C	168	0	156	22	0
4	D	14	0	13	3	0
All	All	28560	0	27669	367	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 7.

All (367) 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:B:709:ASN:HD21	4:B:1310:NAG:C1	0.89	1.50
1:C:165:ASN:ND2	4:C:1312:NAG:C1	1.70	1.50
2:D:322:ASN:HD22	4:D:701:NAG:C1	1.32	1.41
1:B:709:ASN:ND2	4:B:1310:NAG:C1	1.73	1.40
1:A:234:ASN:ND2	3:E:1:NAG:C1	1.90	1.33
2:D:322:ASN:ND2	4:D:701:NAG:C1	1.95	1.27
1:B:38:TYR:OH	1:B:284:THR:HG22	1.38	1.23
1:A:579:PRO:O	4:A:1304:NAG:H82	1.35	1.22
1:C:1081:ILE:HD12	1:C:1135:ASN:HB3	1.24	1.14
1:B:164:ASN:HD22	4:B:1313:NAG:H83	0.95	1.11
1:C:1043:CYS:SG	1:C:1064:HIS:CE1	2.43	1.11
1:A:121:ASN:OD1	1:A:125:ASN:O	1.72	1.07
1:B:279:TYR:HA	1:B:284:THR:O	1.57	1.05
1:A:1131:GLY:HA3	4:A:1309:NAG:H81	1.36	1.04
1:A:234:ASN:HD21	3:E:1:NAG:C1	1.57	1.04
1:A:1131:GLY:HA3	4:A:1309:NAG:C8	1.88	1.04
1:A:331:ASN:HB3	1:A:580:GLN:NE2	1.73	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:VAL:HG13	1:A:422:ASN:HD21	1.23	1.02
1:B:617:CYS:SG	1:B:642:VAL:HG11	1.99	1.02
1:C:1115:ILE:HD12	1:C:1135:ASN:HD21	1.23	1.02
1:B:656:VAL:HG12	1:B:657:ASN:N	1.75	1.00
1:B:1107:ARG:HD3	1:C:904:TYR:HE1	1.24	1.00
1:C:655:HIS:HD2	4:C:1309:NAG:H82	1.26	0.99
1:B:164:ASN:ND2	4:B:1313:NAG:H83	1.78	0.98
1:C:1116:THR:HG23	1:C:1140:PRO:HD3	1.43	0.97
1:C:1115:ILE:HD12	1:C:1135:ASN:ND2	1.80	0.96
1:C:329:PHE:CD2	1:C:525:CYS:SG	2.59	0.96
1:A:1131:GLY:HA2	4:A:1309:NAG:H83	1.46	0.95
1:B:617:CYS:SG	1:B:642:VAL:CG1	2.55	0.94
1:A:329:PHE:CD2	1:A:525:CYS:SG	2.61	0.93
1:B:656:VAL:HG12	1:B:657:ASN:H	1.30	0.93
1:A:1131:GLY:CA	4:A:1309:NAG:C8	2.47	0.92
1:B:662:CYS:SG	1:B:697:MET:SD	2.67	0.92
1:B:706:ALA:HB1	4:B:1312:NAG:O7	1.69	0.92
1:B:656:VAL:CG1	1:B:657:ASN:H	1.81	0.91
1:B:802:PHE:O	1:B:806:LEU:HD12	1.70	0.91
1:B:1107:ARG:HD3	1:C:904:TYR:CE1	2.04	0.91
1:A:234:ASN:HD22	3:E:1:NAG:C1	1.78	0.91
1:B:1074:ASN:HB3	1:C:895:GLN:HE22	1.36	0.90
1:A:43:PHE:HB3	1:C:559:PHE:CE1	2.07	0.90
1:B:164:ASN:HD22	4:B:1313:NAG:C8	1.82	0.90
1:A:329:PHE:HD2	1:A:525:CYS:SG	1.95	0.89
2:D:314:PHE:CE1	2:D:544:ILE:O	2.26	0.89
1:A:1131:GLY:CA	4:A:1309:NAG:H83	2.03	0.89
1:A:522:ALA:HB2	1:A:544:ASN:ND2	1.91	0.86
1:C:1081:ILE:CD1	1:C:1135:ASN:HB3	2.04	0.86
2:D:45:LEU:HD12	2:D:357:ARG:HH22	1.40	0.86
1:B:1082:CYS:SG	1:B:1132:ILE:HD13	2.15	0.86
1:A:43:PHE:HB2	1:C:559:PHE:CD1	2.10	0.85
1:C:655:HIS:CD2	4:C:1309:NAG:H82	2.12	0.85
1:B:1074:ASN:CB	1:C:895:GLN:HE22	1.88	0.85
1:B:1032:CYS:SG	1:B:1048:HIS:CE1	2.70	0.84
1:A:567:ARG:HG2	1:A:573:THR:HA	1.59	0.83
1:B:773:GLU:OE2	1:B:1019:ARG:NH1	2.11	0.83
2:D:314:PHE:HE1	2:D:544:ILE:O	1.60	0.82
1:C:1116:THR:HG23	1:C:1140:PRO:CD	2.11	0.81
1:C:1103:PHE:HZ	3:O:1:NAG:H62	1.46	0.80
1:C:331:ASN:OD1	4:C:1305:NAG:N2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:CYS:SG	1:B:1132:ILE:CD1	2.70	0.79
1:B:1074:ASN:CB	1:C:895:GLN:NE2	2.45	0.79
1:B:656:VAL:CG1	1:B:657:ASN:N	2.40	0.79
3:S:1:NAG:C3	3:S:2:NAG:HN2	1.95	0.78
1:B:45:SER:HB2	1:B:281:GLU:O	1.83	0.78
1:B:378:LYS:O	1:B:432:CYS:HB3	1.84	0.78
2:D:104:GLY:O	2:D:190:MET:SD	2.42	0.78
1:A:43:PHE:CB	1:C:559:PHE:CD1	2.67	0.77
1:C:1116:THR:CG2	1:C:1140:PRO:CD	2.63	0.77
2:D:318:VAL:HG11	2:D:544:ILE:HG22	1.65	0.76
1:A:43:PHE:HB3	1:C:559:PHE:HE1	1.51	0.76
1:C:560:LEU:HD12	1:C:562:PHE:CE2	2.21	0.76
1:A:43:PHE:HB2	1:C:559:PHE:HD1	1.51	0.76
1:B:1107:ARG:CD	1:C:904:TYR:HE1	1.98	0.76
1:C:326:ILE:HD13	1:C:533:LEU:HD12	1.68	0.75
1:A:442:ASP:CG	1:A:451:TYR:OH	2.24	0.75
1:A:522:ALA:CB	1:A:544:ASN:ND2	2.50	0.75
1:C:1081:ILE:HD13	1:C:1135:ASN:HD22	1.51	0.74
1:A:350:VAL:CG1	1:A:422:ASN:HD21	1.99	0.74
1:A:1043:CYS:SG	1:A:1064:HIS:CE1	2.80	0.74
1:A:43:PHE:CB	1:C:559:PHE:CE1	2.71	0.73
1:C:742:ILE:HA	1:C:1000:ARG:HD3	1.71	0.73
2:D:90:ASN:HB3	2:D:93:VAL:HG12	1.70	0.73
1:C:1116:THR:HG21	1:C:1140:PRO:CG	2.18	0.73
1:B:418:ILE:HG13	1:B:453:TYR:HE1	1.53	0.72
2:D:381:TYR:CD1	2:D:404:VAL:HG21	2.25	0.72
1:C:131:CYS:O	1:C:133:PHE:N	2.23	0.71
1:C:462:LYS:O	1:C:465:GLU:HG3	1.90	0.71
1:C:559:PHE:HZ	1:C:575:ALA:HB3	1.55	0.71
1:B:131:CYS:O	1:B:133:PHE:N	2.23	0.71
1:C:799:GLY:O	1:C:924:ALA:HB1	1.90	0.71
1:C:336:CYS:SG	1:C:363:ALA:HB2	2.30	0.71
1:B:343:ASN:OD1	4:B:1306:NAG:C7	2.39	0.71
1:A:817:PHE:HE2	1:A:935:GLN:HG3	1.56	0.70
1:A:817:PHE:CE2	1:A:935:GLN:HG3	2.25	0.70
2:D:101:GLN:O	2:D:101:GLN:HG2	1.91	0.70
1:B:1107:ARG:CD	1:C:904:TYR:CE1	2.73	0.70
1:C:329:PHE:HD2	1:C:525:CYS:SG	2.13	0.70
1:C:662:CYS:SG	1:C:697:MET:SD	2.89	0.70
1:C:165:ASN:ND2	4:C:1312:NAG:O5	2.23	0.69
1:C:331:ASN:CG	4:C:1305:NAG:N2	2.42	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1081:ILE:HD11	1:C:1137:VAL:HG22	1.73	0.69
1:A:126:VAL:H	1:A:172:SER:HB3	1.57	0.69
1:A:418:ILE:HD12	1:A:422:ASN:HD22	1.58	0.69
1:B:1074:ASN:HB3	1:C:895:GLN:NE2	2.04	0.69
1:C:1080:ALA:HB3	1:C:1132:ILE:HG13	1.75	0.68
2:D:381:TYR:CD2	2:D:385:TYR:HE2	2.12	0.68
1:A:418:ILE:CD1	1:A:422:ASN:HD22	2.07	0.68
1:A:329:PHE:HA	1:A:544:ASN:OD1	1.94	0.67
1:C:1081:ILE:HG22	1:C:1133:VAL:HG23	1.75	0.67
1:B:38:TYR:OH	1:B:284:THR:CG2	2.29	0.67
1:B:369:TYR:HA	1:B:377:PHE:CZ	2.30	0.67
2:D:411:SER:HB2	2:D:544:ILE:HG13	1.77	0.67
1:B:1072:GLU:N	1:B:1072:GLU:OE1	2.28	0.67
1:C:127:VAL:HG22	1:C:171:VAL:HG22	1.75	0.67
2:D:559:ARG:O	2:D:559:ARG:HG2	1.96	0.66
2:D:285:PHE:CZ	3:T:1:NAG:H82	2.30	0.66
1:B:709:ASN:CG	4:B:1310:NAG:C1	2.62	0.66
1:C:1081:ILE:HD11	1:C:1137:VAL:CG2	2.26	0.66
1:C:328:ARG:O	1:C:579:PRO:CG	2.45	0.65
1:C:1081:ILE:HD12	1:C:1135:ASN:CB	2.14	0.65
1:B:352:ALA:HA	1:B:466:ARG:HG3	1.79	0.64
1:B:1072:GLU:HG3	1:C:894:LEU:CD2	2.27	0.64
1:A:1131:GLY:CA	4:A:1309:NAG:H81	2.17	0.64
2:D:594:TRP:CD1	3:T:1:NAG:H81	2.32	0.64
1:B:922:LEU:CD2	4:B:1311:NAG:HN2	2.11	0.64
1:B:1074:ASN:HB2	1:C:895:GLN:NE2	2.12	0.64
1:C:560:LEU:HD12	1:C:562:PHE:CZ	2.33	0.64
1:C:1043:CYS:SG	1:C:1064:HIS:HE1	2.19	0.64
1:A:567:ARG:CG	1:A:573:THR:HA	2.27	0.64
1:B:1074:ASN:OD1	1:B:1074:ASN:O	2.16	0.64
1:C:368:LEU:HD21	4:C:1306:NAG:H83	1.80	0.63
1:C:379:CYS:SG	1:C:382:VAL:O	2.56	0.63
3:S:1:NAG:H3	3:S:2:NAG:HN2	1.64	0.63
1:C:655:HIS:HD2	4:C:1309:NAG:C8	2.04	0.63
2:D:322:ASN:HD21	4:D:701:NAG:C1	2.09	0.63
1:B:352:ALA:HB1	1:B:466:ARG:HE	1.62	0.62
1:C:1081:ILE:HA	1:C:1133:VAL:O	1.98	0.62
1:A:379:CYS:HB3	1:A:382:VAL:O	1.99	0.62
1:A:442:ASP:CG	1:A:451:TYR:HH	2.02	0.62
1:C:1131:GLY:HA3	4:C:1310:NAG:C8	2.29	0.62
2:D:340:GLN:HE22	3:Q:1:NAG:H82	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:NE	1:A:580:GLN:OE1	2.32	0.62
2:D:398:GLU:HG3	2:D:514:ARG:HB3	1.82	0.62
2:D:323:MET:HG3	2:D:328:TRP:CZ2	2.34	0.62
1:C:1115:ILE:CD1	1:C:1135:ASN:ND2	2.62	0.61
2:D:339:VAL:HG13	2:D:339:VAL:O	2.00	0.61
1:C:1116:THR:CG2	1:C:1140:PRO:HD3	2.19	0.61
1:C:560:LEU:CD1	1:C:562:PHE:CE2	2.83	0.61
2:D:285:PHE:HZ	3:T:1:NAG:C8	2.13	0.61
1:C:800:PHE:CE1	1:C:924:ALA:HA	2.36	0.61
1:B:215:ASP:N	1:B:266:TYR:HH	1.99	0.60
1:A:215:ASP:HA	1:A:266:TYR:OH	2.00	0.60
1:A:391:CYS:HB3	1:A:544:ASN:O	2.00	0.60
1:A:817:PHE:HE2	1:A:935:GLN:CG	2.14	0.60
1:B:466:ARG:O	1:B:466:ARG:HG2	2.01	0.60
2:D:384:ALA:O	2:D:559:ARG:HG3	2.01	0.60
1:A:442:ASP:HB3	1:A:451:TYR:OH	2.01	0.60
1:C:1131:GLY:CA	4:C:1310:NAG:C8	2.79	0.60
1:B:402:ILE:HG22	1:B:403:ARG:N	2.16	0.60
1:C:171:VAL:HG12	1:C:171:VAL:O	2.01	0.60
1:C:328:ARG:O	1:C:579:PRO:HG3	2.02	0.60
1:C:800:PHE:HD1	1:C:927:PHE:HD2	1.48	0.60
1:C:800:PHE:CD1	1:C:927:PHE:CD2	2.89	0.60
1:B:1107:ARG:NE	1:C:904:TYR:CE1	2.70	0.59
2:D:285:PHE:CZ	3:T:1:NAG:C8	2.86	0.59
1:A:442:ASP:CB	1:A:451:TYR:OH	2.51	0.59
2:D:381:TYR:HD1	2:D:404:VAL:HG21	1.67	0.59
1:C:1116:THR:HG21	1:C:1140:PRO:HG2	1.83	0.58
1:B:369:TYR:HA	1:B:377:PHE:CE2	2.38	0.58
1:B:96:GLU:OE1	1:B:190:ARG:NH1	2.35	0.58
1:B:717:ASN:HB2	1:B:1071:GLN:HB2	1.84	0.58
1:B:400:PHE:CE1	1:B:402:ILE:HD12	2.39	0.58
1:C:393:THR:O	1:C:523:THR:OG1	2.20	0.58
1:C:800:PHE:HD1	1:C:927:PHE:CD2	2.22	0.58
2:D:89:GLN:OE1	2:D:89:GLN:HA	2.04	0.57
1:A:801:ASN:OD1	1:A:803:SER:OG	2.15	0.57
1:B:922:LEU:HD21	4:B:1311:NAG:HN2	1.69	0.57
1:A:642:VAL:CG1	1:A:649:CYS:SG	2.93	0.57
2:D:381:TYR:CD1	2:D:558:LEU:HG	2.40	0.57
1:B:1094:VAL:CG2	1:C:904:TYR:OH	2.54	0.56
1:B:46:SER:OG	1:B:281:GLU:HG3	2.05	0.56
1:C:329:PHE:HB3	1:C:525:CYS:SG	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:THR:HA	2:D:81:GLN:OE1	2.05	0.56
1:B:236:THR:HG22	1:B:236:THR:O	2.05	0.56
1:B:402:ILE:CG2	1:B:403:ARG:N	2.69	0.56
2:D:482:ARG:NE	2:D:488:VAL:HG23	2.21	0.56
1:C:1136:THR:HG22	1:C:1136:THR:O	2.06	0.56
1:A:642:VAL:HG13	1:A:649:CYS:SG	2.46	0.56
1:A:922:LEU:HD12	3:F:2:NAG:H81	1.88	0.56
1:A:61:ASN:OD1	4:A:1301:NAG:N2	2.39	0.56
1:B:802:PHE:O	1:B:806:LEU:CD1	2.50	0.55
1:A:579:PRO:O	4:A:1304:NAG:C8	2.31	0.55
1:A:1043:CYS:SG	1:A:1064:HIS:ND1	2.79	0.55
1:C:330:PRO:HB2	4:C:1305:NAG:H82	1.87	0.55
1:B:131:CYS:O	1:B:133:PHE:CD1	2.59	0.55
1:C:331:ASN:N	4:C:1305:NAG:H82	2.22	0.55
1:A:351:TYR:CE1	1:A:468:ILE:HG23	2.42	0.55
1:C:1043:CYS:SG	1:C:1064:HIS:ND1	2.77	0.55
1:C:165:ASN:CG	4:C:1312:NAG:C1	2.64	0.55
2:D:192:ARG:O	2:D:195:HIS:N	2.30	0.55
1:A:401:VAL:HG11	1:A:451:TYR:CZ	2.42	0.55
1:A:1094:VAL:HB	1:B:904:TYR:OH	2.06	0.55
1:A:1072:GLU:HG3	4:A:1310:NAG:H82	1.89	0.54
1:C:577:ARG:HB2	1:C:584:ILE:HG23	1.88	0.54
1:A:567:ARG:HD3	1:A:571:ASP:O	2.07	0.54
1:A:1082:CYS:SG	1:A:1085:GLY:HA2	2.48	0.54
1:B:454:ARG:HG2	1:B:492:LEU:CD2	2.37	0.54
1:C:1116:THR:CG2	1:C:1140:PRO:CG	2.84	0.54
1:B:546:LEU:C	1:B:546:LEU:HD12	2.28	0.54
1:C:391:CYS:HB3	1:C:544:ASN:O	2.08	0.54
1:B:120:VAL:HG12	1:B:122:ASN:HB3	1.90	0.54
1:B:1076:THR:HG22	1:B:1077:THR:N	2.22	0.54
2:D:530:CYS:SG	2:D:535:HIS:CD2	3.01	0.54
1:B:1075:PHE:CD1	1:B:1075:PHE:N	2.73	0.54
1:B:1082:CYS:SG	1:B:1132:ILE:HD11	2.48	0.53
2:D:545:SER:O	2:D:547:SER:N	2.41	0.53
1:A:401:VAL:HG11	1:A:451:TYR:CE2	2.43	0.53
1:C:560:LEU:CD1	1:C:562:PHE:HE2	2.21	0.53
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.91	0.53
1:B:555:SER:HB3	1:B:586:ASP:HB2	1.91	0.53
3:I:1:NAG:C6	3:I:2:NAG:H82	2.39	0.53
1:A:567:ARG:HG2	1:A:573:THR:CA	2.33	0.53
1:C:1078:ALA:HB1	1:C:1133:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ASN:ND2	4:C:1312:NAG:C2	2.68	0.53
1:C:330:PRO:HB2	4:C:1305:NAG:C8	2.39	0.53
1:B:132:GLU:HB2	4:B:1313:NAG:H82	1.91	0.52
1:A:451:TYR:HD2	1:A:497:PHE:CD1	2.28	0.52
1:A:336:CYS:SG	1:A:363:ALA:HB2	2.49	0.52
1:B:279:TYR:CA	1:B:284:THR:O	2.46	0.52
2:D:381:TYR:CE2	2:D:385:TYR:HE2	2.27	0.52
1:C:1131:GLY:HA2	4:C:1310:NAG:H83	1.92	0.52
1:B:43:PHE:CZ	1:B:283:GLY:HA3	2.45	0.52
2:D:298:VAL:HG12	2:D:364:VAL:HG21	1.91	0.52
2:D:364:VAL:HG23	2:D:364:VAL:O	2.10	0.51
1:B:418:ILE:HG13	1:B:453:TYR:CE1	2.42	0.51
1:B:120:VAL:CG1	1:B:122:ASN:HB3	2.41	0.51
1:C:743:CYS:SG	1:C:750:SER:N	2.82	0.51
2:D:312:GLU:OE2	2:D:322:ASN:HB2	2.10	0.51
1:A:382:VAL:HA	1:B:983:ARG:O	2.10	0.51
1:B:132:GLU:HG3	1:B:164:ASN:O	2.11	0.51
3:S:1:NAG:H3	3:S:2:NAG:N2	2.25	0.50
1:A:1107:ARG:NH2	1:B:904:TYR:CE1	2.79	0.50
1:B:646:ARG:HD2	1:B:668:ALA:HB1	1.93	0.50
1:B:1094:VAL:HG22	1:C:904:TYR:OH	2.11	0.50
1:C:1116:THR:HG23	1:C:1138:TYR:O	2.11	0.50
2:D:545:SER:C	2:D:547:SER:H	2.13	0.50
3:I:1:NAG:H62	3:I:2:NAG:H82	1.92	0.50
1:A:817:PHE:HE2	1:A:935:GLN:HE21	1.58	0.50
1:C:368:LEU:CD2	4:C:1306:NAG:H83	2.42	0.50
1:C:922:LEU:HD11	3:M:1:NAG:H5	1.94	0.50
1:B:400:PHE:HE1	1:B:402:ILE:HD12	1.76	0.50
1:C:565:PHE:HE1	1:C:567:ARG:HE	1.60	0.50
1:B:919:ASN:OD1	4:B:1311:NAG:H83	2.12	0.49
1:C:583:GLU:HG3	1:C:583:GLU:O	2.11	0.49
1:C:800:PHE:HA	1:C:928:ASN:HD21	1.76	0.49
2:D:285:PHE:HZ	3:T:1:NAG:H83	1.74	0.49
1:C:645:THR:OG1	1:C:670:ILE:HG13	2.12	0.49
1:C:1081:ILE:HD13	1:C:1135:ASN:ND2	2.25	0.49
1:B:45:SER:CB	1:B:281:GLU:O	2.58	0.49
1:A:378:LYS:O	1:A:432:CYS:HB3	2.13	0.49
1:A:125:ASN:HB2	4:A:1302:NAG:H82	1.93	0.49
1:B:120:VAL:HG12	1:B:122:ASN:H	1.76	0.49
1:B:417:LYS:HB3	1:B:453:TYR:OH	2.13	0.49
1:C:1103:PHE:CZ	3:O:1:NAG:H62	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:LEU:HD11	1:C:552:LEU:HD13	1.95	0.48
1:B:369:TYR:OH	1:B:432:CYS:SG	2.71	0.48
1:C:64:TRP:CZ2	1:C:214:ARG:O	2.67	0.48
2:D:45:LEU:CD1	2:D:357:ARG:HH22	2.18	0.48
1:C:900:MET:O	1:C:904:TYR:HD2	1.97	0.48
1:C:1082:CYS:N	1:C:1133:VAL:O	2.43	0.48
2:D:411:SER:OG	2:D:543:ASP:OD1	2.30	0.48
1:A:742:ILE:HA	1:A:1000:ARG:HD3	1.96	0.48
1:C:328:ARG:O	1:C:579:PRO:HG2	2.14	0.48
1:C:1131:GLY:CA	4:C:1310:NAG:H83	2.42	0.48
1:A:522:ALA:HB2	1:A:544:ASN:CG	2.31	0.47
1:A:901:GLN:O	1:A:904:TYR:HB2	2.14	0.47
1:B:123:ALA:C	1:B:125:ASN:H	2.18	0.47
1:C:657:ASN:ND2	4:C:1309:NAG:C7	2.77	0.47
1:A:1072:GLU:HG3	4:A:1310:NAG:C8	2.44	0.47
1:C:1116:THR:HG22	1:C:1118:ASP:H	1.79	0.47
3:S:2:NAG:H83	3:S:2:NAG:C3	2.45	0.47
2:D:482:ARG:HE	2:D:488:VAL:HG23	1.78	0.47
1:C:749:CYS:SG	1:C:750:SER:N	2.87	0.47
2:D:381:TYR:CD1	2:D:404:VAL:HG11	2.50	0.47
2:D:381:TYR:CD2	2:D:385:TYR:CE2	2.99	0.47
1:B:38:TYR:HH	1:B:284:THR:HG22	1.67	0.47
1:C:1100:THR:OG1	3:O:1:NAG:N2	2.42	0.47
2:D:324:THR:HG23	2:D:324:THR:O	2.14	0.47
2:D:515:TYR:O	2:D:518:ARG:HG3	2.15	0.47
1:A:403:ARG:HD3	1:A:406:GLU:CD	2.36	0.47
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.55	0.47
1:C:577:ARG:HB2	1:C:584:ILE:CG2	2.44	0.47
1:A:265:TYR:CD2	1:A:265:TYR:N	2.83	0.46
1:B:280:ASN:OD1	1:B:284:THR:N	2.48	0.46
1:B:418:ILE:CG1	1:B:453:TYR:HE1	2.27	0.46
1:C:465:GLU:HG2	3:E:1:NAG:H81	1.97	0.46
1:B:34:ARG:O	1:B:56:LEU:HD23	2.16	0.46
1:B:121:ASN:OD1	1:B:126:VAL:HG23	2.15	0.46
1:B:454:ARG:HH21	1:B:461:LEU:HD11	1.79	0.46
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.56	0.46
1:B:46:SER:OG	1:B:281:GLU:HA	2.15	0.46
1:A:1107:ARG:HD3	1:B:904:TYR:CE2	2.51	0.45
2:D:177:ARG:HD3	2:D:497:TYR:O	2.15	0.45
2:D:294:THR:HG23	2:D:365:THR:HA	1.99	0.45
1:A:1082:CYS:HB3	1:A:1134:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:THR:HG22	1:C:601:GLY:H	1.82	0.45
1:C:706:ALA:HB1	4:C:1311:NAG:H5	1.98	0.45
1:B:43:PHE:CE1	1:B:283:GLY:HA3	2.52	0.45
3:S:1:NAG:C3	3:S:2:NAG:N2	2.74	0.45
1:A:122:ASN:OD1	1:A:122:ASN:N	2.48	0.44
1:C:559:PHE:CD2	1:C:584:ILE:HG21	2.52	0.44
1:B:281:GLU:C	1:B:283:GLY:H	2.21	0.44
1:B:1115:ILE:HD12	1:B:1135:ASN:ND2	2.31	0.44
1:C:739:THR:O	1:C:743:CYS:HB3	2.16	0.44
1:B:474:GLN:O	1:B:474:GLN:HG2	2.17	0.44
1:B:108:THR:HG21	1:B:234:ASN:HD22	1.83	0.44
1:B:1043:CYS:SG	1:B:1064:HIS:CE1	3.11	0.44
1:C:328:ARG:NH1	1:C:578:ASP:OD2	2.51	0.44
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.18	0.44
2:D:515:TYR:HA	2:D:518:ARG:CG	2.47	0.44
1:A:331:ASN:HB3	1:A:580:GLN:HE21	1.75	0.43
1:B:658:ASN:HB2	1:B:660:TYR:CZ	2.54	0.43
1:C:214:ARG:O	1:C:214:ARG:HG2	2.19	0.43
1:B:1107:ARG:H	1:B:1107:ARG:HG2	1.65	0.43
2:D:399:GLY:CA	2:D:518:ARG:HB3	2.49	0.43
1:A:122:ASN:O	1:A:124:THR:N	2.52	0.43
1:C:332:ILE:HG21	1:C:361:CYS:HA	2.01	0.43
1:B:1081:ILE:HD12	1:B:1135:ASN:HB3	2.01	0.43
1:B:919:ASN:OD1	4:B:1311:NAG:C8	2.67	0.43
2:D:50:TYR:CE1	2:D:59:VAL:HG22	2.54	0.43
1:A:550:GLY:HA2	1:A:590:CYS:SG	2.59	0.42
1:B:121:ASN:OD1	1:B:126:VAL:CG2	2.67	0.42
1:B:655:HIS:O	4:B:1309:NAG:H81	2.19	0.42
2:D:545:SER:C	2:D:547:SER:N	2.72	0.42
1:A:451:TYR:CD2	1:A:497:PHE:CE1	3.07	0.42
1:B:334:ASN:O	1:B:361:CYS:HB2	2.19	0.42
2:D:515:TYR:HA	2:D:518:ARG:HG3	2.01	0.42
1:B:1076:THR:CG2	1:B:1077:THR:N	2.81	0.42
1:A:904:TYR:CE1	1:C:1107:ARG:HD3	2.53	0.42
1:A:522:ALA:HB3	1:A:544:ASN:ND2	2.34	0.42
1:B:45:SER:HB3	1:B:283:GLY:CA	2.50	0.42
3:S:2:NAG:H83	3:S:2:NAG:H3	2.02	0.42
1:B:1094:VAL:CG1	1:C:904:TYR:OH	2.68	0.42
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.20	0.42
1:A:350:VAL:HG13	1:A:422:ASN:ND2	2.09	0.41
1:B:132:GLU:CB	4:B:1313:NAG:H82	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASN:HA	4:A:1301:NAG:H82	2.02	0.41
1:A:418:ILE:HD13	1:A:422:ASN:HD22	1.85	0.41
1:C:559:PHE:CZ	1:C:575:ALA:HB3	2.45	0.41
1:B:717:ASN:CG	1:B:1071:GLN:OE1	2.58	0.41
1:C:331:ASN:OD1	1:C:331:ASN:N	2.51	0.41
1:A:742:ILE:HG22	1:A:743:CYS:SG	2.59	0.41
1:C:329:PHE:CG	1:C:525:CYS:SG	3.05	0.41
1:C:1131:GLY:HA3	4:C:1310:NAG:H81	2.02	0.41
2:D:285:PHE:CE2	3:T:1:NAG:H82	2.55	0.41
2:D:318:VAL:CG1	2:D:544:ILE:HG22	2.44	0.41
1:A:331:ASN:CB	1:A:580:GLN:NE2	2.64	0.41
1:B:717:ASN:CB	1:B:1071:GLN:OE1	2.69	0.41
1:C:64:TRP:HH2	1:C:214:ARG:HG3	1.86	0.41
1:C:368:LEU:HD21	4:C:1306:NAG:C8	2.50	0.41
1:C:642:VAL:CG1	1:C:649:CYS:SG	3.09	0.41
1:C:1081:ILE:CD1	1:C:1135:ASN:HD22	2.29	0.41
1:A:125:ASN:HB2	4:A:1302:NAG:C8	2.50	0.41
1:C:64:TRP:CH2	1:C:214:ARG:HG3	2.55	0.41
2:D:549:GLU:OE2	2:D:549:GLU:HA	2.21	0.41
1:A:353:TRP:CZ3	1:A:355:ARG:HD3	2.56	0.40
2:D:530:CYS:SG	2:D:535:HIS:CG	3.15	0.40
2:D:48:TRP:CE3	2:D:357:ARG:HD2	2.57	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	943/1234 (76%)	881 (93%)	58 (6%)	4 (0%)	30	63
1	B	959/1234 (78%)	879 (92%)	75 (8%)	5 (0%)	25	59
1	C	939/1234 (76%)	868 (92%)	67 (7%)	4 (0%)	30	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	591/615 (96%)	568 (96%)	19 (3%)	4 (1%)	19	53
All	All	3432/4317 (80%)	3196 (93%)	219 (6%)	17 (0%)	27	59

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ALA
1	A	331	ASN
1	B	132	GLU
2	D	364	VAL
2	D	546	ASN
1	A	617	CYS
1	B	124	THR
1	C	132	GLU
2	D	104	GLY
2	D	325	GLN
1	A	291	CYS
1	B	814	LYS
1	B	282	ASN
1	C	709	ASN
1	C	123	ALA
1	B	483	VAL
1	C	744	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	848/1069 (79%)	841 (99%)	7 (1%)	79	88
1	B	859/1069 (80%)	835 (97%)	24 (3%)	38	64
1	C	844/1069 (79%)	830 (98%)	14 (2%)	56	75
2	D	524/540 (97%)	518 (99%)	6 (1%)	70	83
All	All	3075/3747 (82%)	3024 (98%)	51 (2%)	56	75

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	265	TYR
1	A	328	ARG
1	A	351	TYR
1	A	525	CYS
1	A	538	CYS
1	A	1043	CYS
1	B	122	ASN
1	B	131	CYS
1	B	132	GLU
1	B	237	ARG
1	B	284	THR
1	B	377	PHE
1	B	437	ASN
1	B	453	TYR
1	B	460	ASN
1	B	474	GLN
1	B	480	CYS
1	B	489	TYR
1	B	590	CYS
1	B	602	THR
1	B	603	ASN
1	B	617	CYS
1	B	649	CYS
1	B	662	CYS
1	B	709	ASN
1	B	717	ASN
1	B	738	CYS
1	B	1032	CYS
1	B	1075	PHE
1	B	1094	VAL
1	C	166	CYS
1	C	170	TYR
1	C	238	PHE
1	C	331	ASN
1	C	377	PHE
1	C	379	CYS
1	C	525	CYS
1	C	584	ILE
1	C	585	LEU
1	C	662	CYS
1	C	749	CYS

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Mol	Chain	Res	Type
1	C	760	CYS
1	C	1043	CYS
1	C	1132	ILE
2	D	81	GLN
2	D	183	TYR
2	D	530	CYS
2	D	542	CYS
2	D	544	ILE
2	D	545	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	125	ASN
1	A	234	ASN
1	A	422	ASN
1	B	164	ASN
1	B	709	ASN
1	B	1048	HIS
1	C	655	HIS
1	C	895	GLN
1	C	1135	ASN
2	D	322	ASN
2	D	340	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)

34 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3	14,14,15	1.71	2 (14%)	17,19,21	0.70	0
3	NAG	E	2	3	14,14,15	1.33	2 (14%)	17,19,21	0.67	0
3	NAG	F	1	3	14,14,15	1.49	2 (14%)	17,19,21	0.66	0
3	NAG	F	2	3	14,14,15	1.43	2 (14%)	17,19,21	0.73	0
3	NAG	G	1	1,3	14,14,15	1.60	2 (14%)	17,19,21	0.68	0
3	NAG	G	2	3	14,14,15	1.44	2 (14%)	17,19,21	0.64	0
3	NAG	H	1	1,3	14,14,15	1.60	2 (14%)	17,19,21	0.77	0
3	NAG	H	2	3	14,14,15	1.47	2 (14%)	17,19,21	0.62	0
3	NAG	I	1	3	14,14,15	1.64	2 (14%)	17,19,21	0.74	0
3	NAG	I	2	3	14,14,15	1.55	2 (14%)	17,19,21	0.72	0
3	NAG	J	1	1,3	14,14,15	1.57	2 (14%)	17,19,21	0.62	0
3	NAG	J	2	3	14,14,15	1.46	2 (14%)	17,19,21	0.88	0
3	NAG	K	1	3	14,14,15	1.52	2 (14%)	17,19,21	0.76	0
3	NAG	K	2	3	14,14,15	1.52	2 (14%)	17,19,21	1.09	1 (5%)
3	NAG	L	1	1,3	14,14,15	1.51	2 (14%)	17,19,21	0.71	0
3	NAG	L	2	3	14,14,15	1.49	2 (14%)	17,19,21	0.90	1 (5%)
3	NAG	M	1	1,3	14,14,15	1.49	2 (14%)	17,19,21	0.78	0
3	NAG	M	2	3	14,14,15	1.47	2 (14%)	17,19,21	0.71	0
3	NAG	N	1	1,3	14,14,15	1.56	2 (14%)	17,19,21	0.71	0
3	NAG	N	2	3	14,14,15	1.58	2 (14%)	17,19,21	0.76	0
3	NAG	O	1	3	14,14,15	1.53	2 (14%)	17,19,21	0.86	0
3	NAG	O	2	3	14,14,15	1.40	2 (14%)	17,19,21	0.74	0
3	NAG	P	1	1,3	14,14,15	1.53	2 (14%)	17,19,21	0.69	0
3	NAG	P	2	3	14,14,15	1.52	2 (14%)	17,19,21	0.63	0
3	NAG	Q	1	3	14,14,15	0.59	1 (7%)	17,19,21	0.74	0
3	NAG	Q	2	3	14,14,15	0.55	0	17,19,21	0.38	0
3	NAG	R	1	3,2	14,14,15	0.36	0	17,19,21	0.67	0
3	NAG	R	2	3	14,14,15	1.09	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	S	1	3,2	14,14,15	0.30	0	17,19,21	0.59	0
3	NAG	S	2	3	14,14,15	0.30	0	17,19,21	0.56	0
3	NAG	T	1	3,2	14,14,15	0.31	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	T	2	3	14,14,15	1.14	1 (7%)	17,19,21	1.37	1 (5%)
3	NAG	U	1	3,2	14,14,15	0.24	0	17,19,21	0.63	0
3	NAG	U	2	3	14,14,15	0.41	0	17,19,21	0.62	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
3	NAG	E	1	3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	NAG	F	1	3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
3	NAG	T	1	3,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	NAG	U	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	C1-C2	4.90	1.59	1.52
3	I	1	NAG	C1-C2	4.49	1.58	1.52
3	N	1	NAG	C1-C2	4.47	1.58	1.52
3	G	1	NAG	C1-C2	4.39	1.58	1.52
3	J	1	NAG	C1-C2	4.28	1.58	1.52
3	O	1	NAG	C1-C2	4.27	1.58	1.52
3	F	1	NAG	C1-C2	4.16	1.58	1.52
3	H	1	NAG	C1-C2	4.16	1.58	1.52
3	M	1	NAG	C1-C2	4.11	1.57	1.52
3	P	2	NAG	C1-C2	4.06	1.57	1.52
3	K	1	NAG	C1-C2	4.02	1.57	1.52
3	P	1	NAG	C1-C2	4.01	1.57	1.52
3	L	1	NAG	C1-C2	3.97	1.57	1.52
3	I	2	NAG	C1-C2	3.92	1.57	1.52
3	J	2	NAG	C1-C2	3.81	1.57	1.52
3	N	2	NAG	C1-C2	3.79	1.57	1.52
3	G	2	NAG	C1-C2	3.73	1.57	1.52
3	H	2	NAG	C1-C2	3.71	1.57	1.52
3	L	2	NAG	C1-C2	3.65	1.57	1.52
3	F	2	NAG	C1-C2	3.65	1.57	1.52
3	M	2	NAG	C1-C2	3.63	1.57	1.52
3	K	2	NAG	C1-C2	3.54	1.57	1.52
3	N	2	NAG	O5-C5	3.38	1.50	1.43
3	K	2	NAG	O5-C5	3.24	1.49	1.43
3	R	2	NAG	O5-C5	3.14	1.49	1.43
3	T	2	NAG	O5-C5	3.14	1.49	1.43
3	O	2	NAG	C1-C2	3.14	1.56	1.52
3	I	2	NAG	O5-C5	3.08	1.49	1.43
3	E	2	NAG	C1-C2	3.08	1.56	1.52
3	O	2	NAG	O5-C5	3.06	1.49	1.43
3	L	2	NAG	O5-C5	2.81	1.48	1.43
3	F	2	NAG	O5-C5	2.76	1.48	1.43
3	M	2	NAG	O5-C5	2.75	1.48	1.43
3	H	1	NAG	O5-C5	2.71	1.48	1.43
3	H	2	NAG	O5-C5	2.58	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1	NAG	O5-C5	2.55	1.48	1.43
3	I	1	NAG	O5-C5	2.44	1.48	1.43
3	J	2	NAG	O5-C5	2.43	1.48	1.43
3	P	2	NAG	O5-C5	2.42	1.48	1.43
3	G	2	NAG	O5-C5	2.39	1.48	1.43
3	E	2	NAG	O5-C5	2.39	1.48	1.43
3	L	1	NAG	O5-C5	2.39	1.48	1.43
3	O	1	NAG	O5-C5	2.37	1.48	1.43
3	G	1	NAG	O5-C5	2.35	1.48	1.43
3	E	1	NAG	O5-C5	2.33	1.48	1.43
3	M	1	NAG	O5-C5	2.32	1.47	1.43
3	P	1	NAG	O5-C5	2.29	1.47	1.43
3	F	1	NAG	O5-C5	2.19	1.47	1.43
3	J	1	NAG	O5-C5	2.18	1.47	1.43
3	N	1	NAG	O5-C5	2.16	1.47	1.43
3	Q	1	NAG	O5-C1	-2.04	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	2	NAG	C1-O5-C5	4.90	118.75	112.19
3	K	2	NAG	C1-O5-C5	3.58	116.98	112.19
3	L	2	NAG	C1-O5-C5	2.88	116.04	112.19
3	R	2	NAG	C1-O5-C5	2.69	115.80	112.19
3	U	2	NAG	C1-O5-C5	2.11	115.02	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	1	NAG	O7-C7-N2-C2
3	S	2	NAG	C3-C2-N2-C7
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	U	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	R	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	L	1	NAG	C1-C2-N2-C7
3	L	2	NAG	C1-C2-N2-C7
3	M	2	NAG	C1-C2-N2-C7

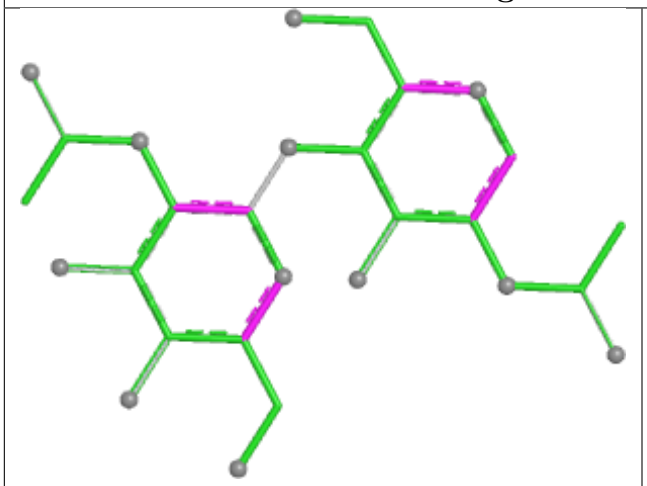
There are no ring outliers.

10 monomers are involved in 24 short contacts:

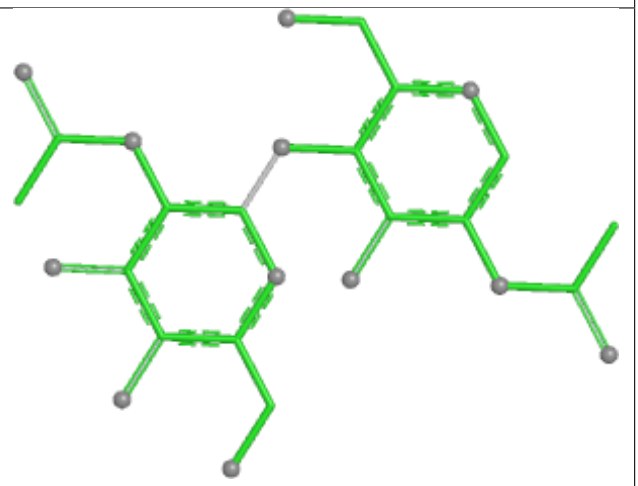
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	2	0
3	Q	1	NAG	1	0
3	S	1	NAG	4	0
3	F	2	NAG	1	0
3	O	1	NAG	3	0
3	I	2	NAG	2	0
3	T	1	NAG	6	0
3	S	2	NAG	6	0
3	M	1	NAG	1	0
3	E	1	NAG	4	0

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

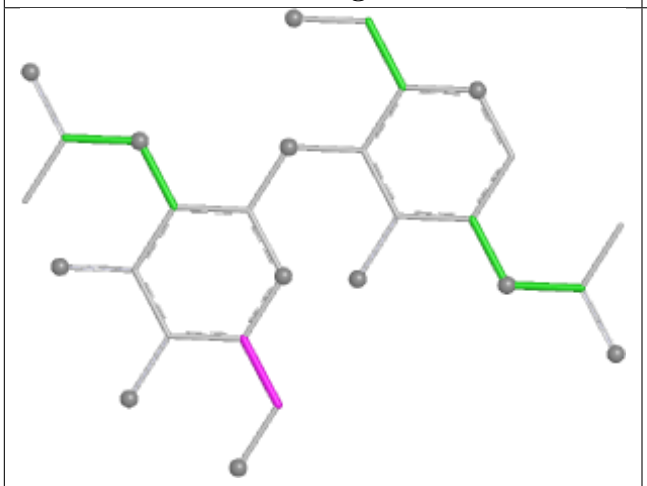
Oligosaccharide Chain E



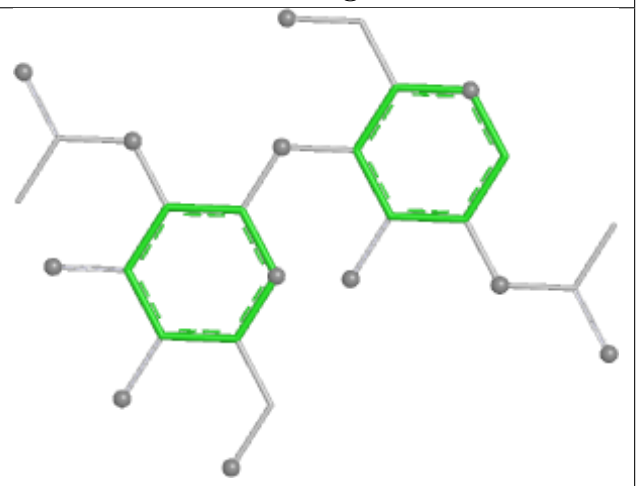
Bond lengths



Bond angles

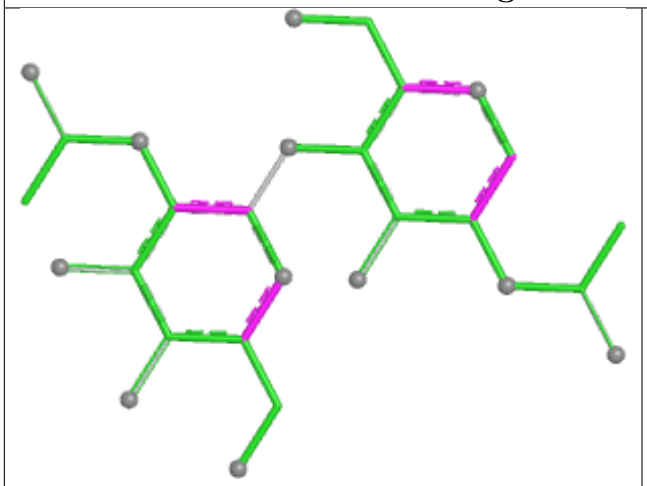


Torsions

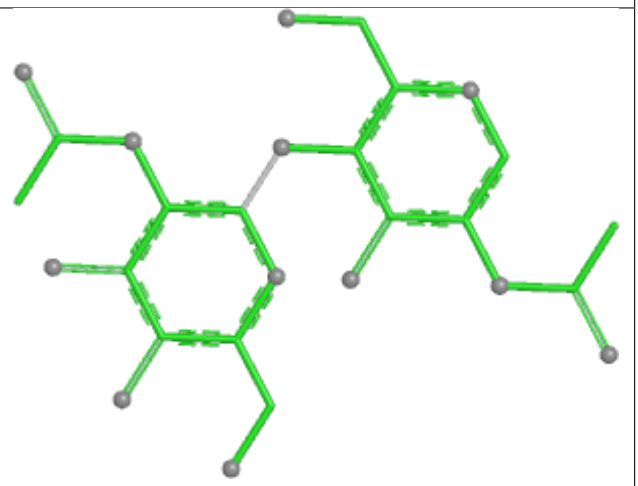


Rings

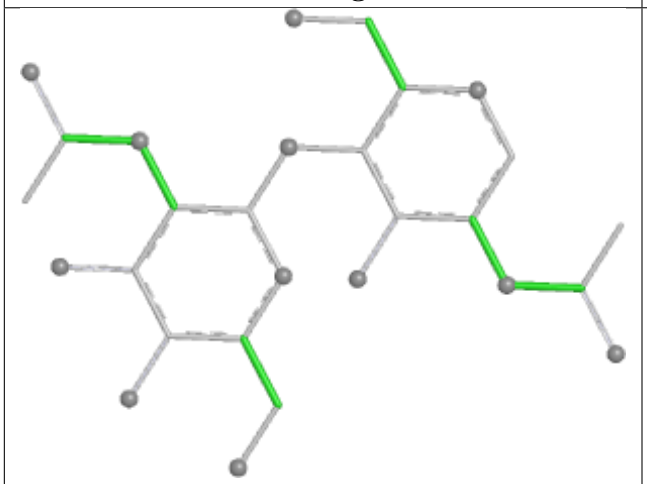
Oligosaccharide Chain F



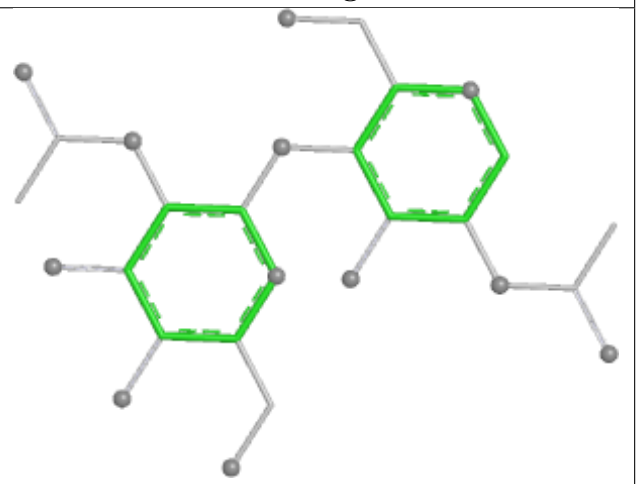
Bond lengths



Bond angles

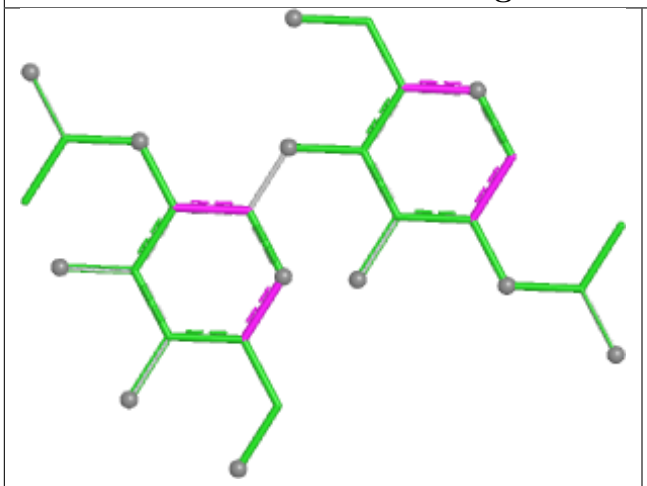


Torsions

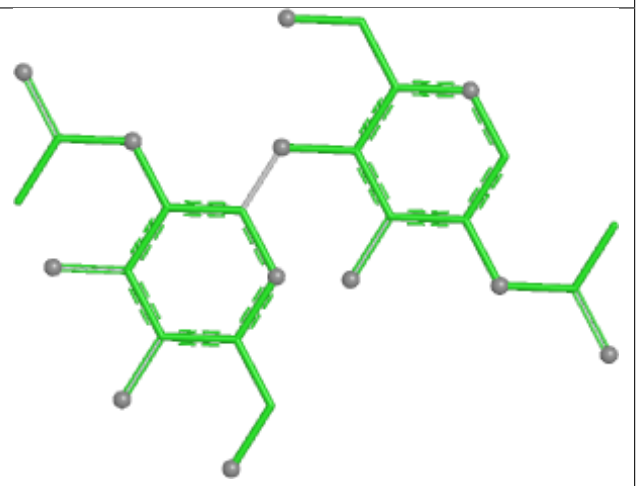


Rings

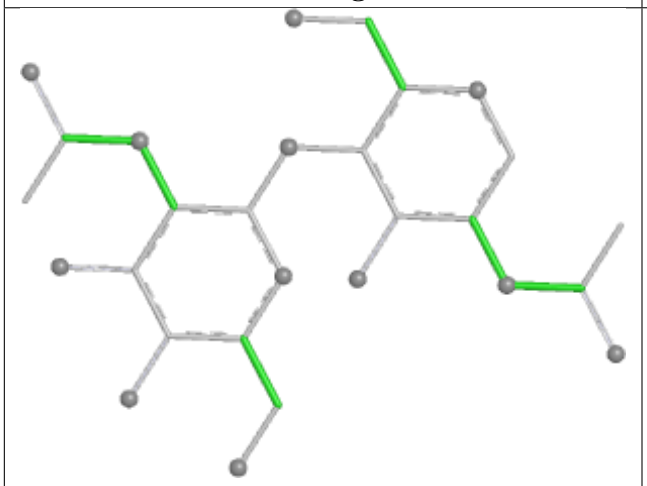
Oligosaccharide Chain G



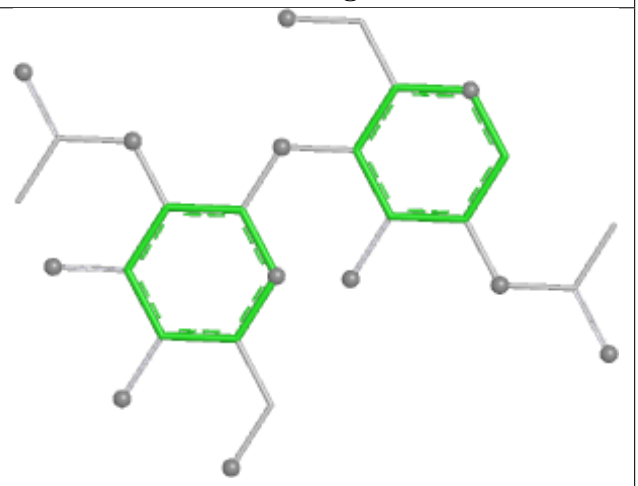
Bond lengths



Bond angles

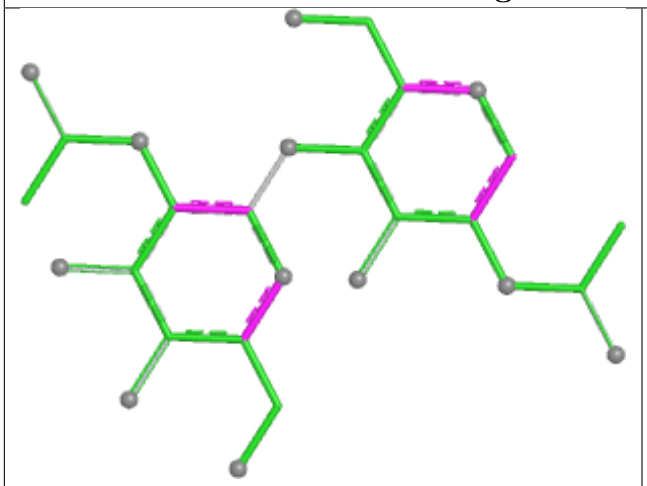


Torsions

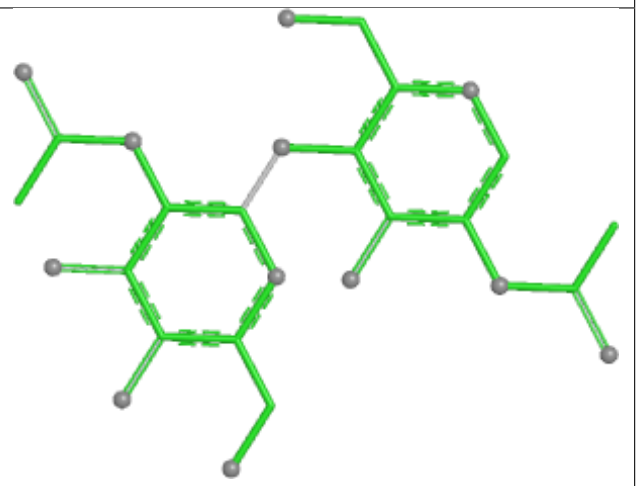


Rings

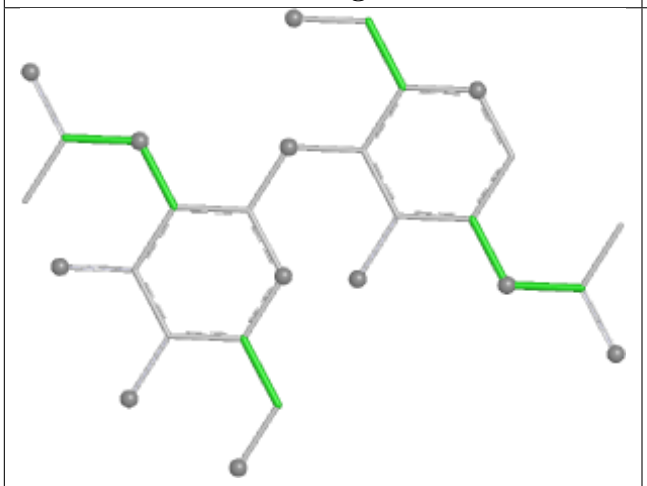
Oligosaccharide Chain H



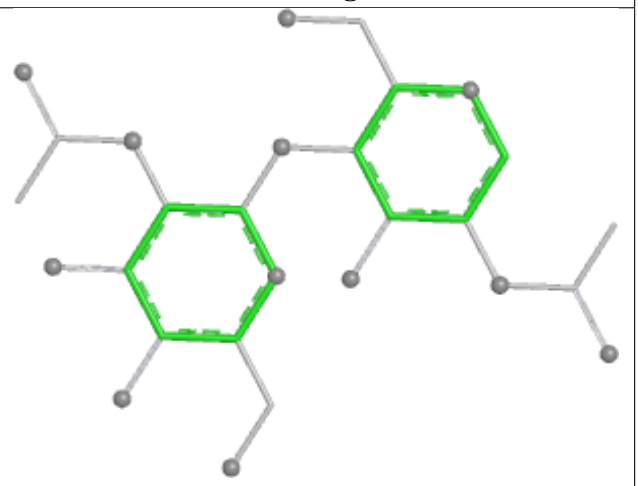
Bond lengths



Bond angles

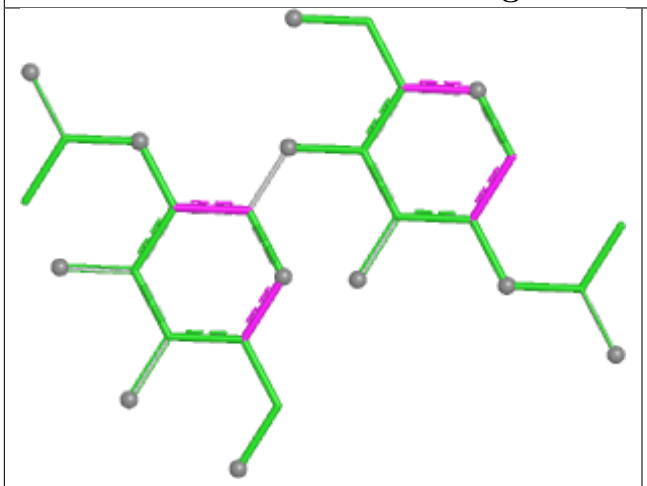


Torsions

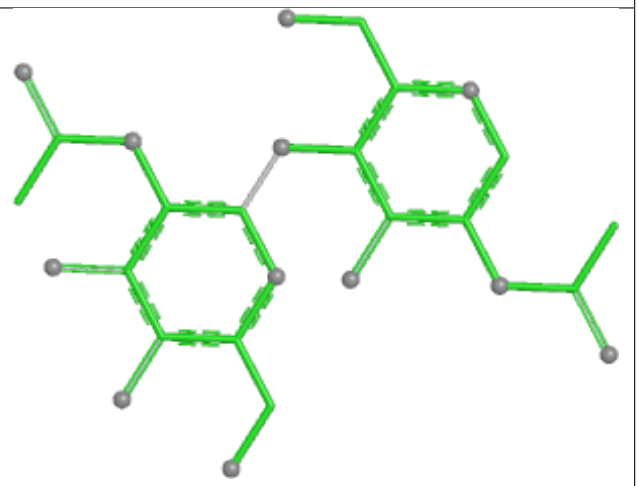


Rings

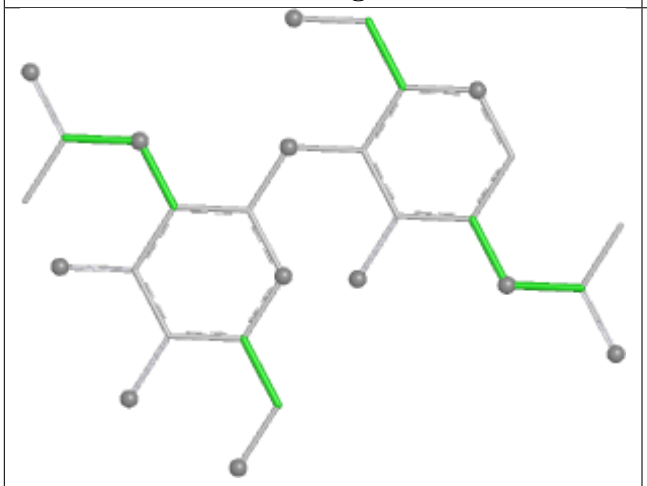
Oligosaccharide Chain I



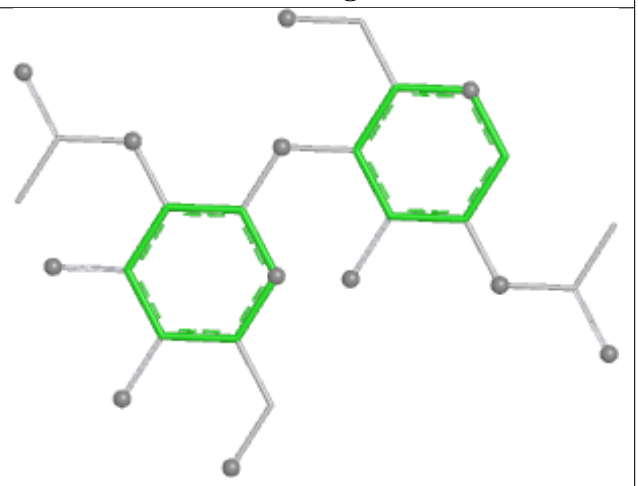
Bond lengths



Bond angles

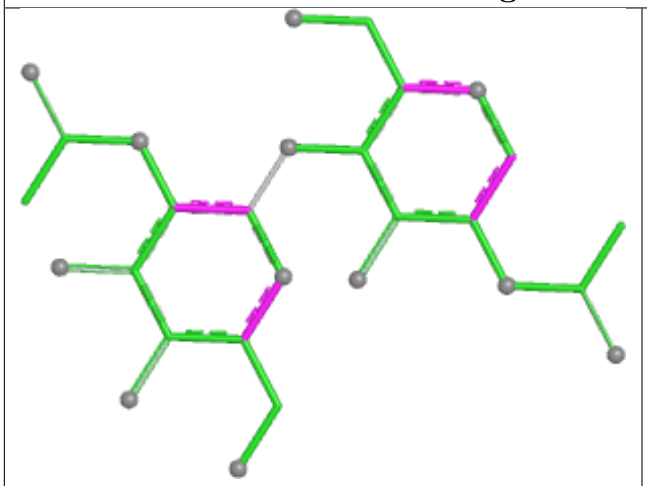


Torsions

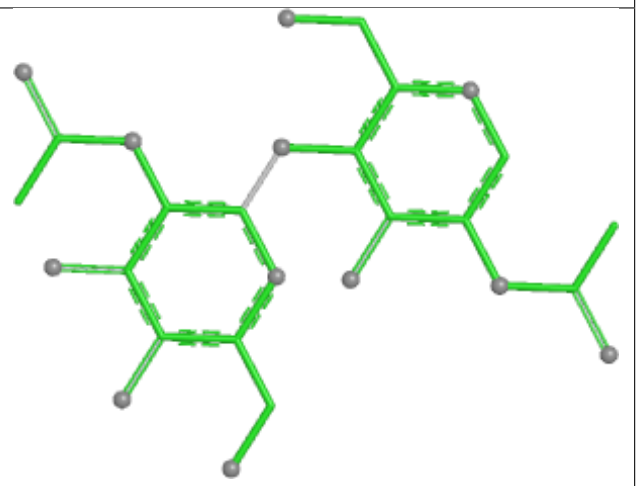


Rings

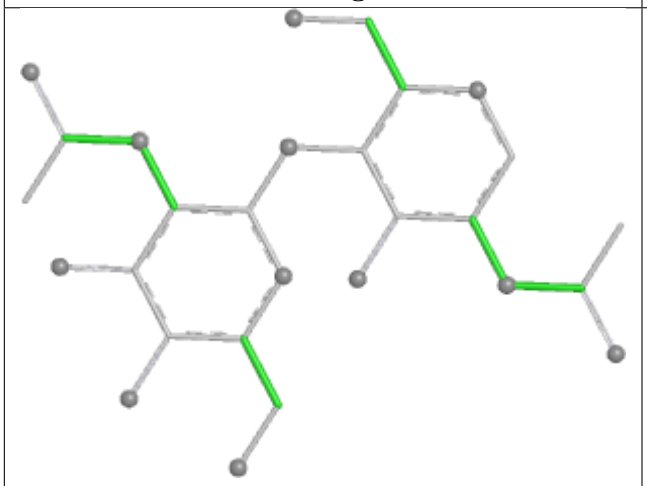
Oligosaccharide Chain J



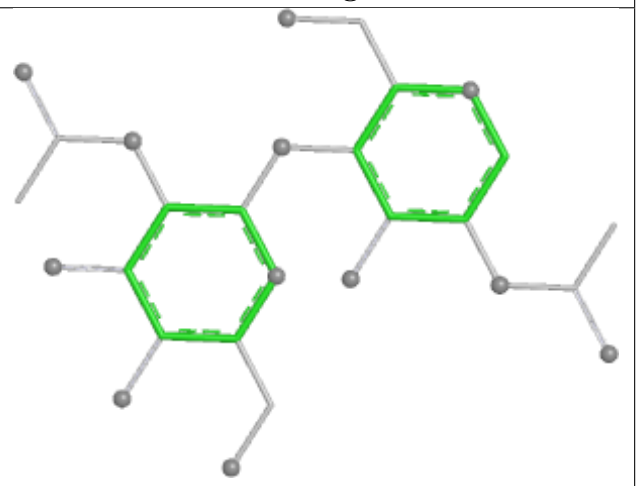
Bond lengths



Bond angles

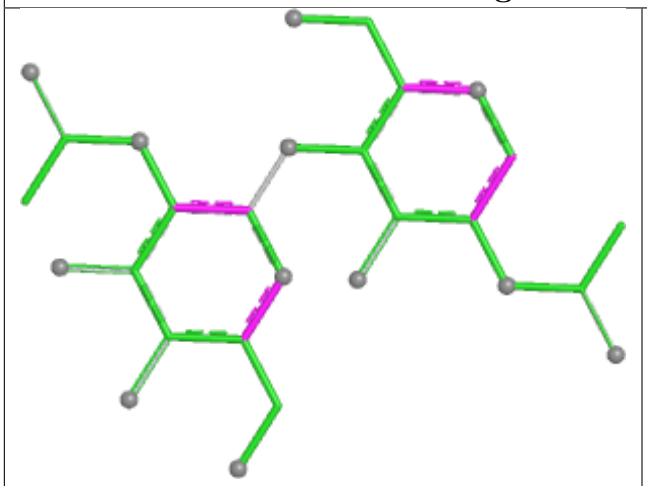


Torsions



Rings

Oligosaccharide Chain K



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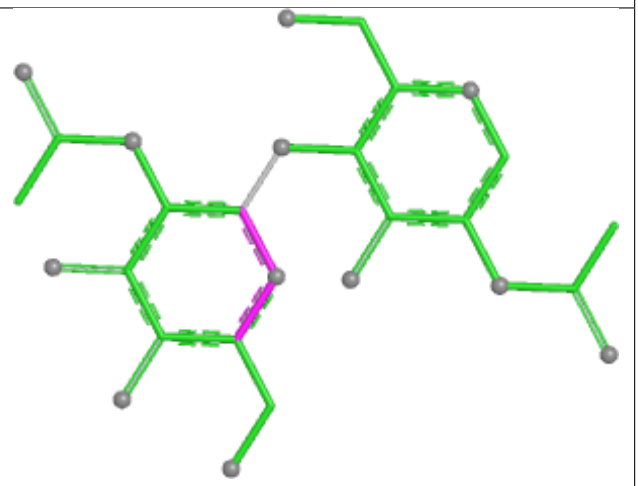
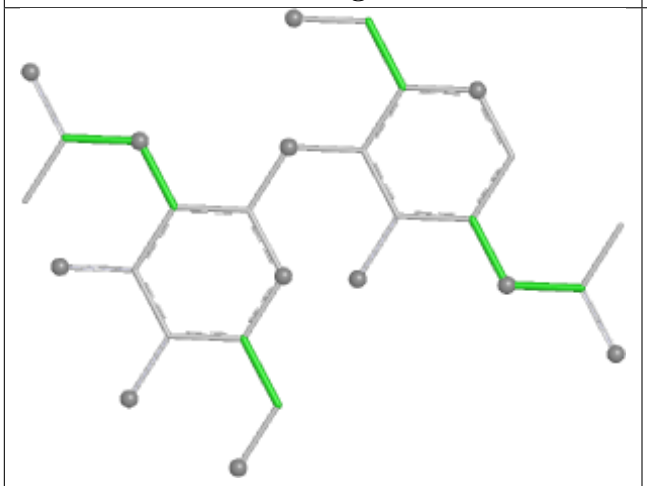


Bond angles



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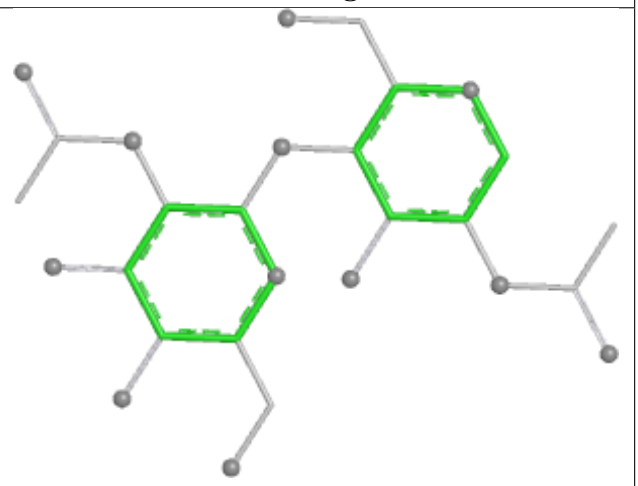
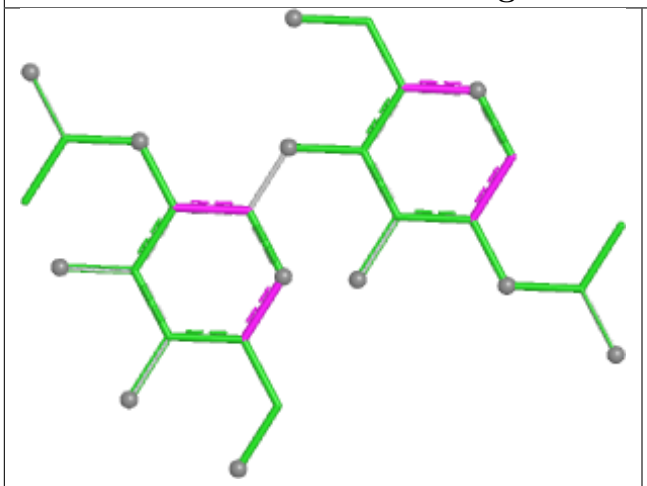


Rings

Oligosaccharide Chain L



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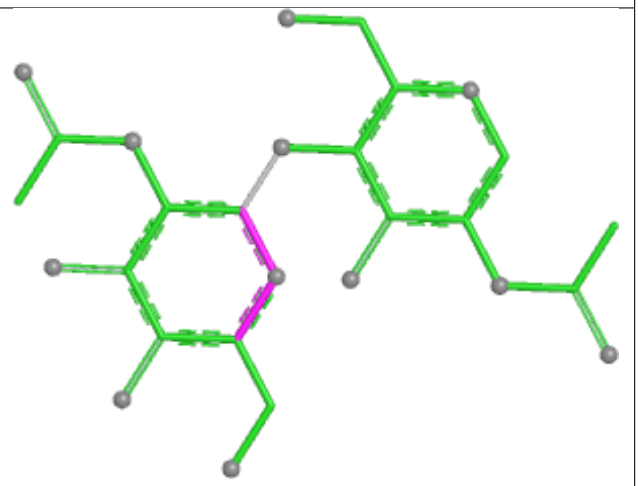
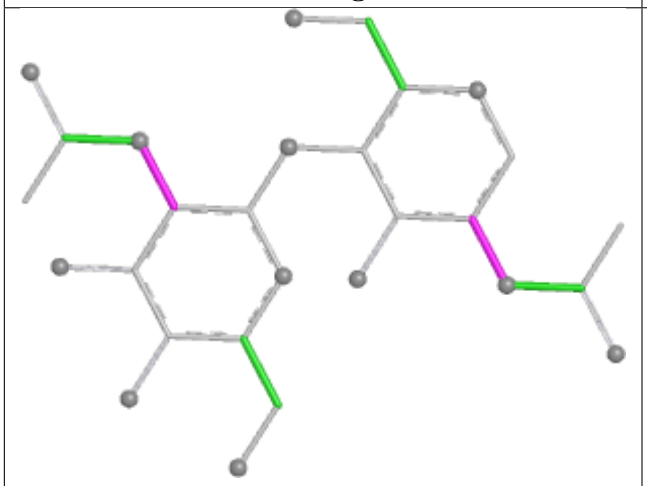
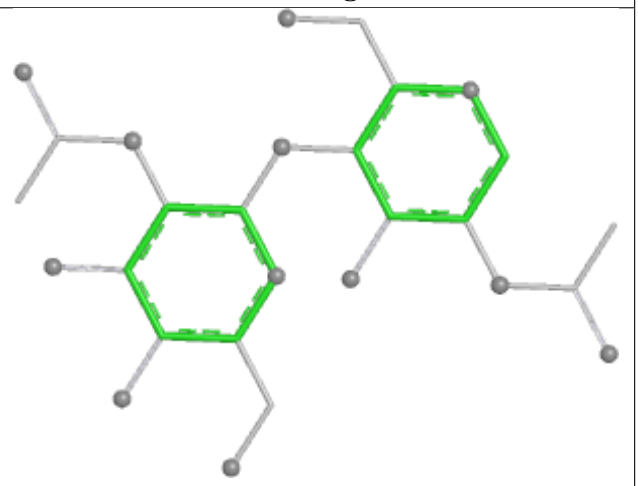


Bond angles

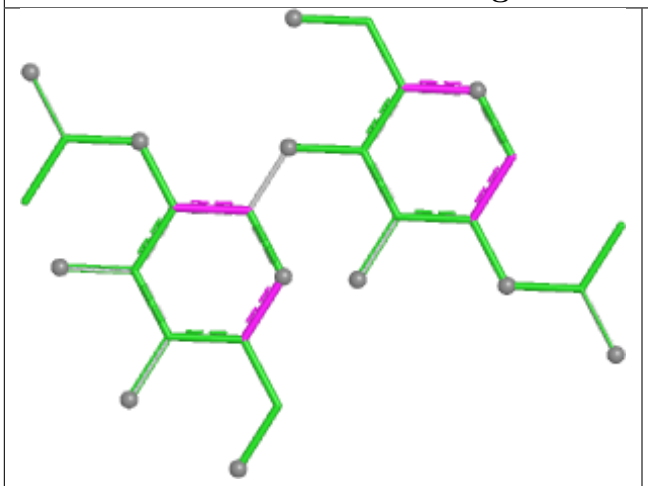


Torsions



Rings

Oligosaccharide Chain M



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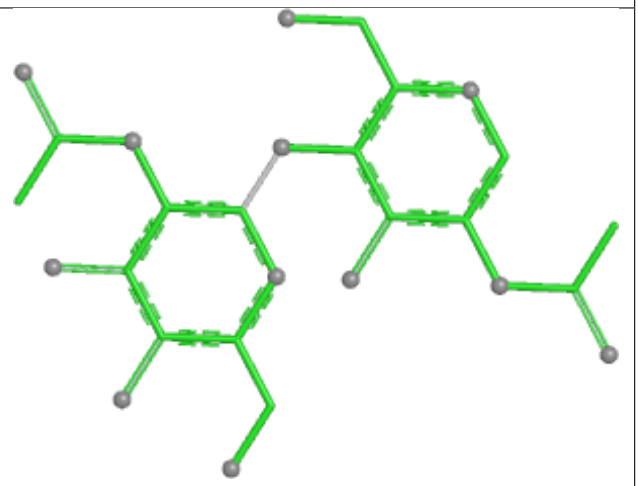
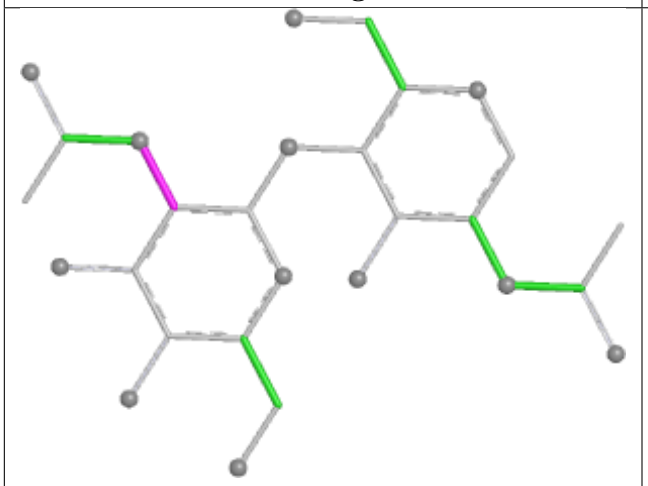
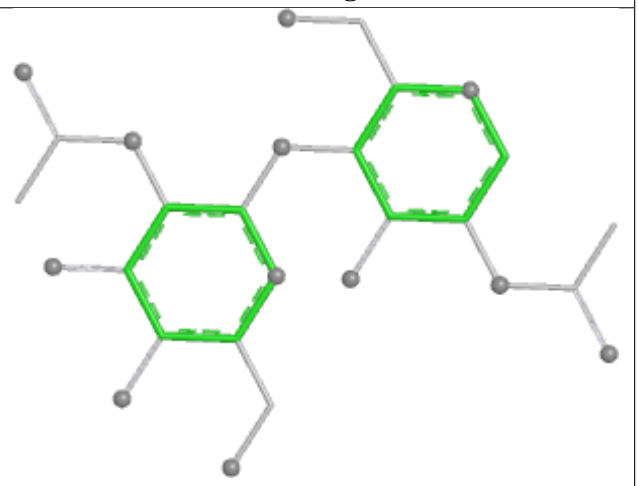


Bond angles

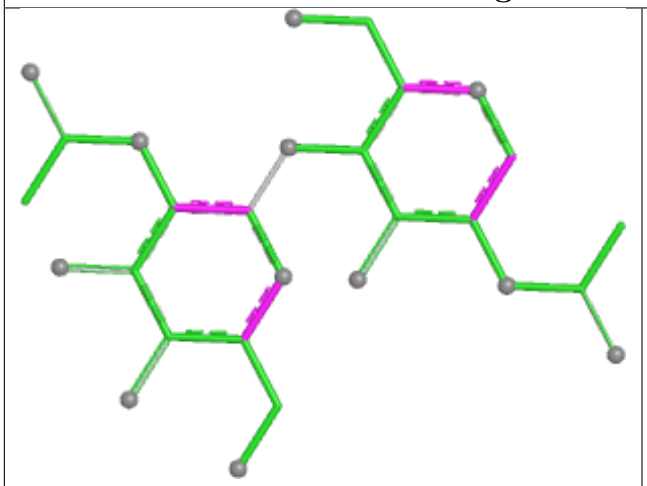


Torsions

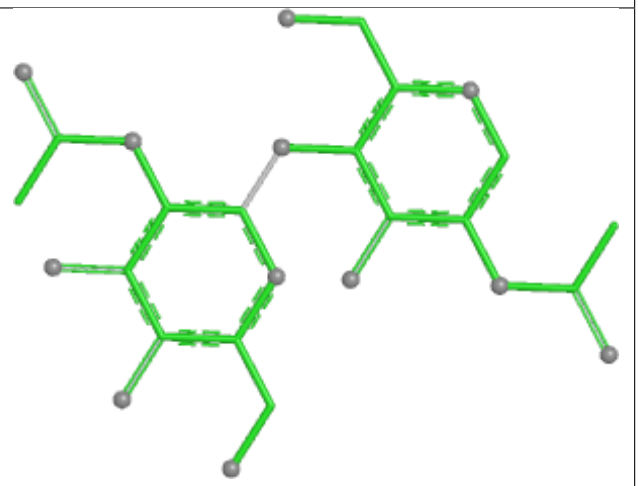


Rings

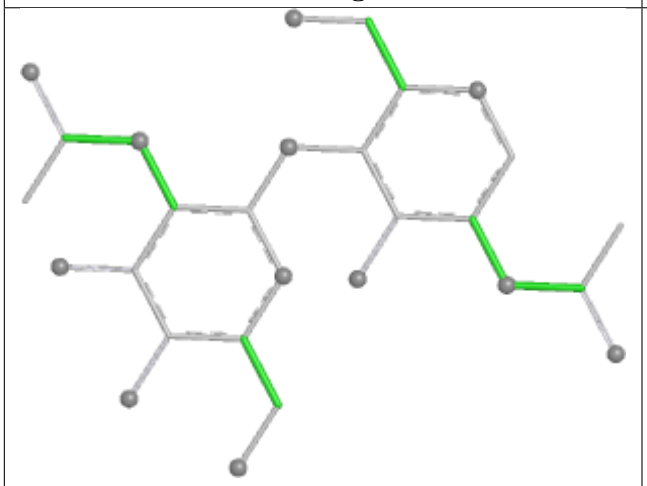
Oligosaccharide Chain N



Bond lengths



Bond angles



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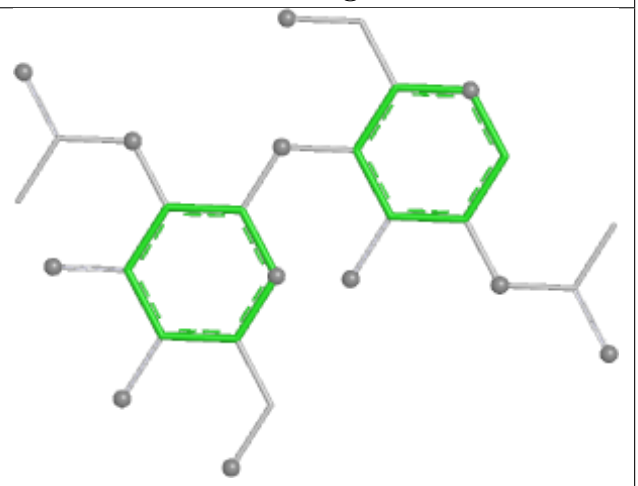
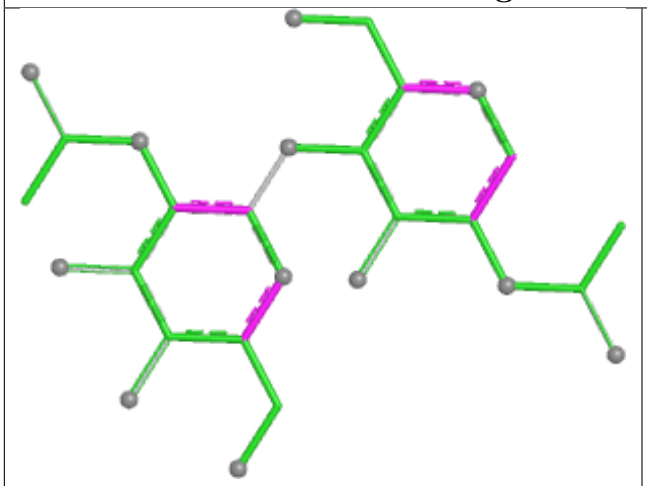


Rings

Oligosaccharide Chain O



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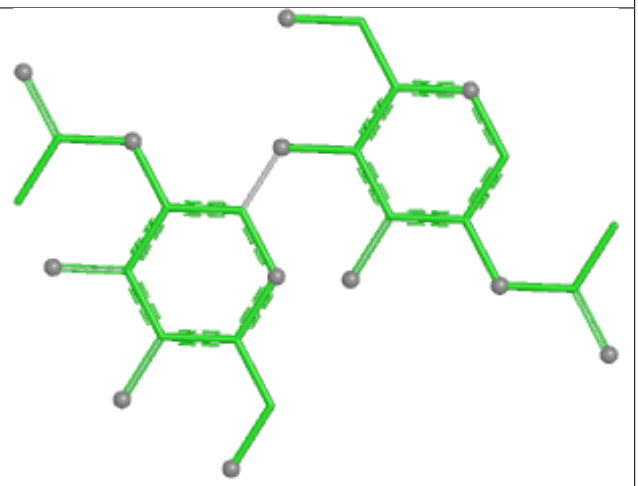
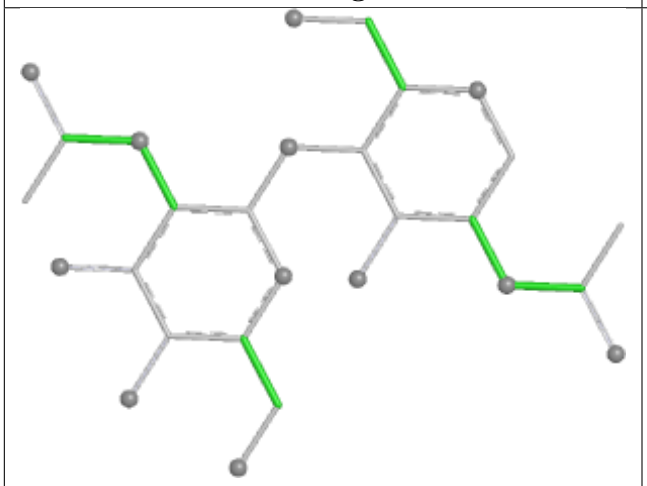


Bond angles



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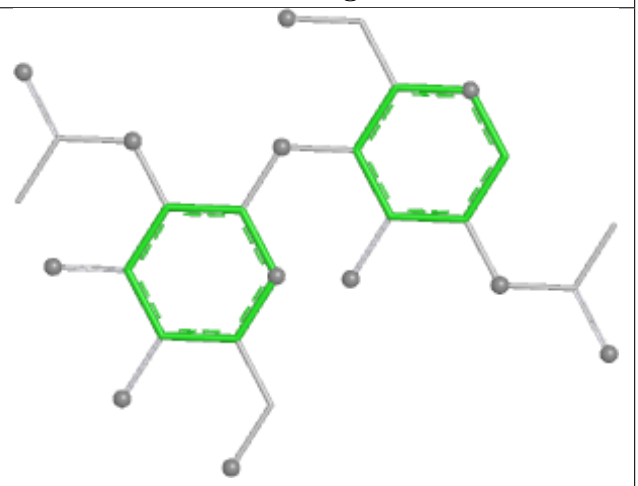
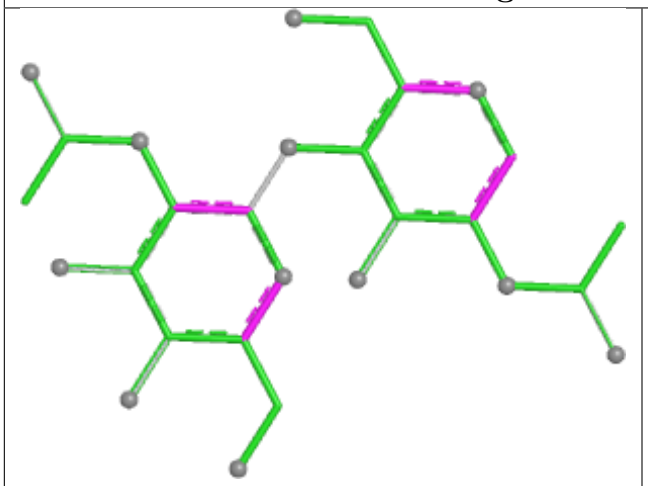


Rings

Oligosaccharide Chain P



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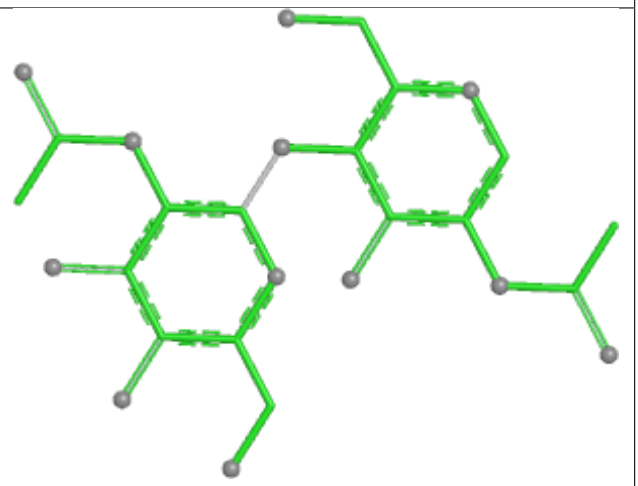
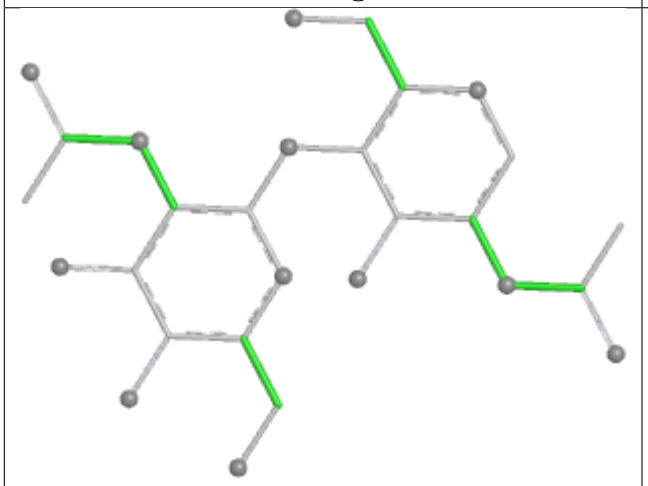


Bond angles



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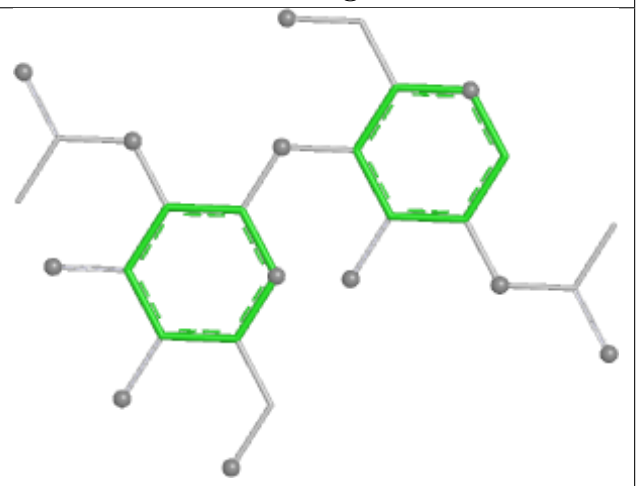
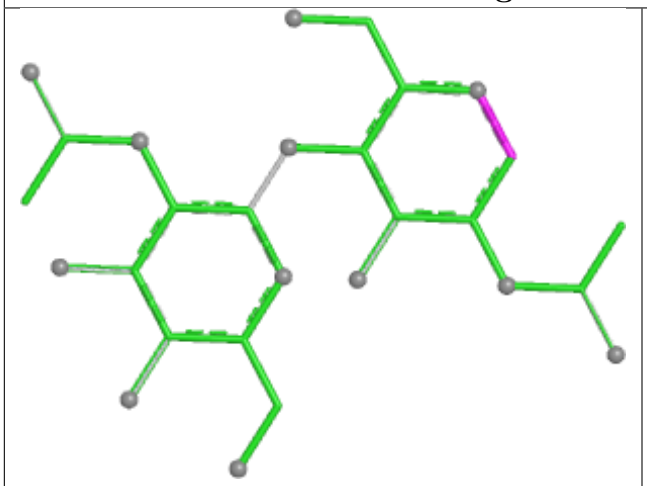


Rings

Oligosaccharide Chain Q



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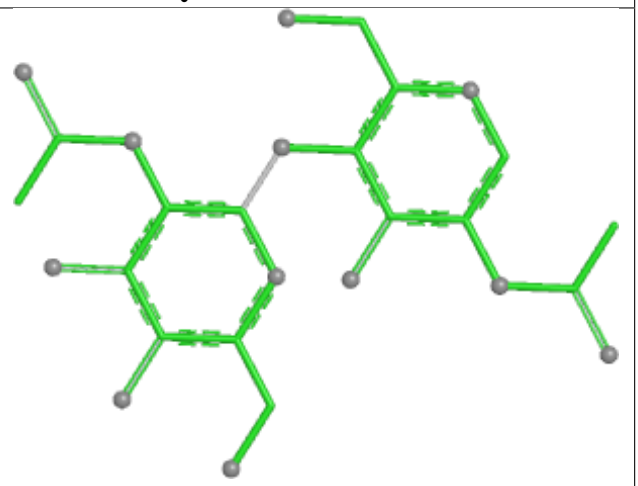

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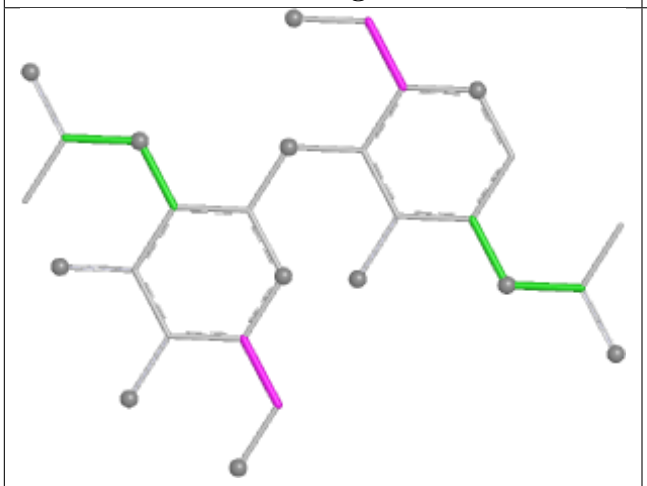

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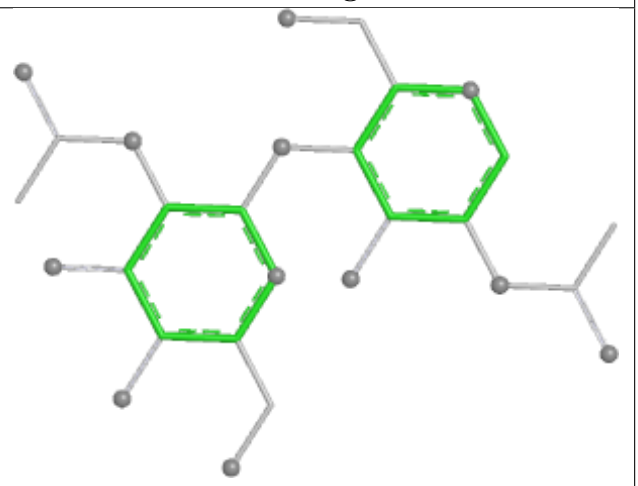
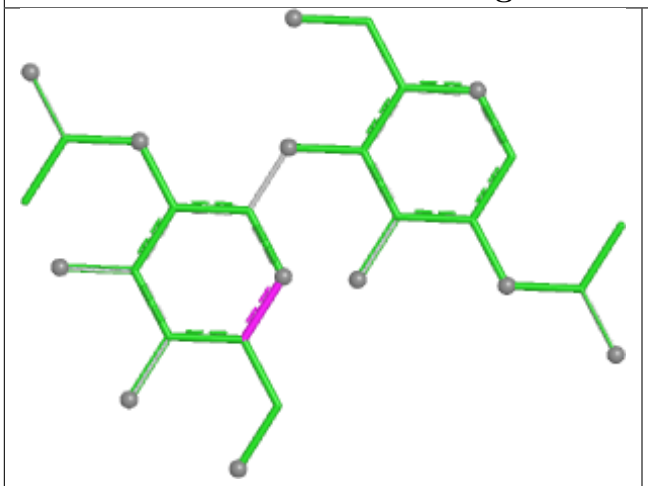
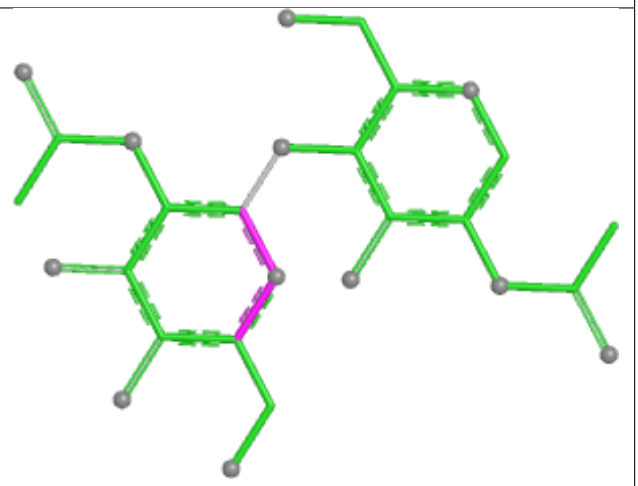


Rings

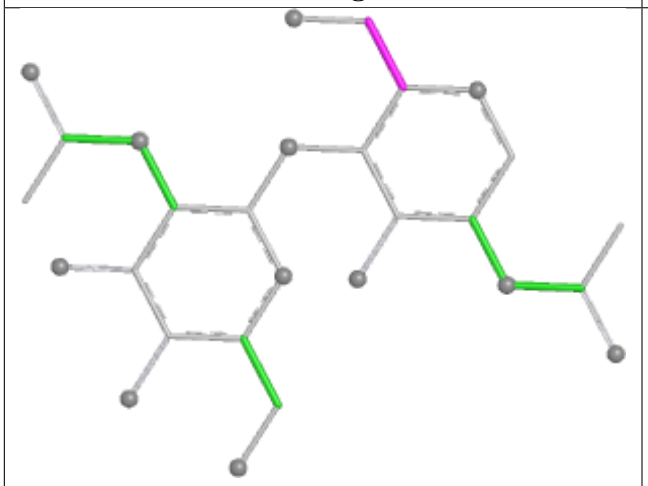
Oligosaccharide Chain R



Bond lengths



Bond angles



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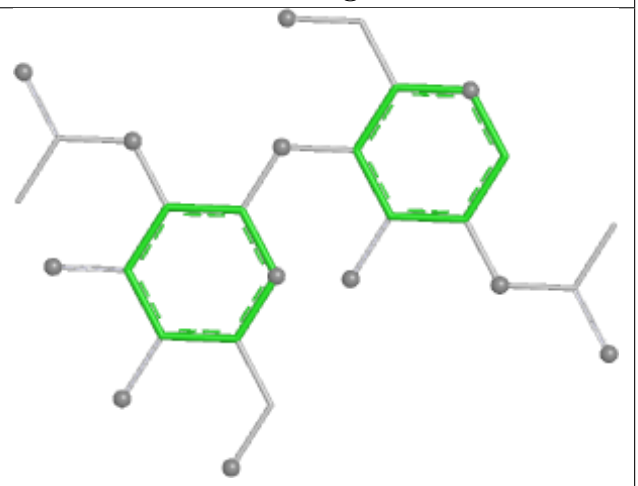
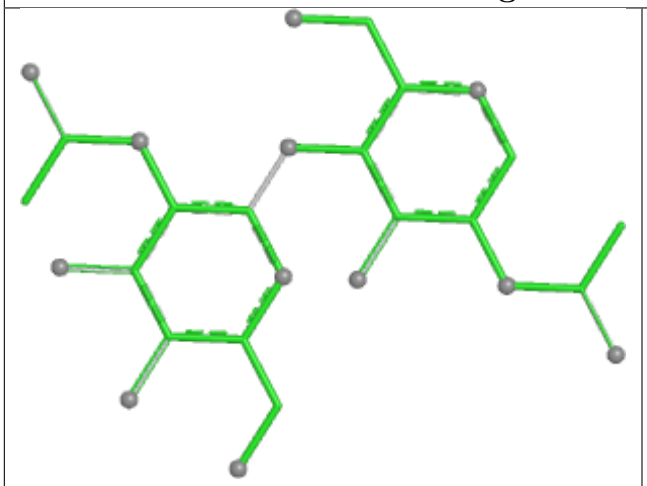


Rings

Oligosaccharide Chain S



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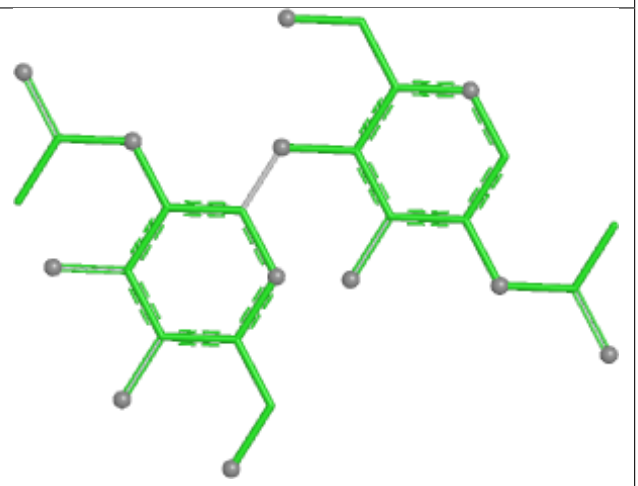
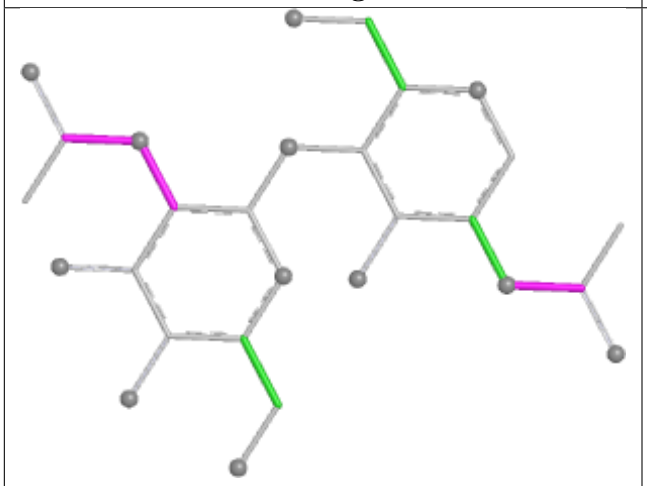


Bond angles



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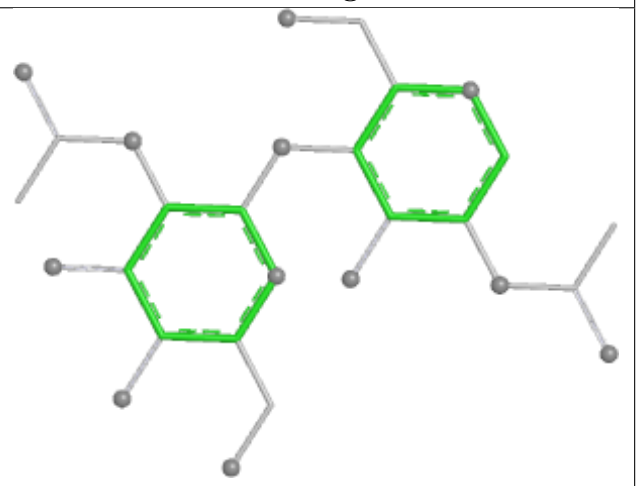
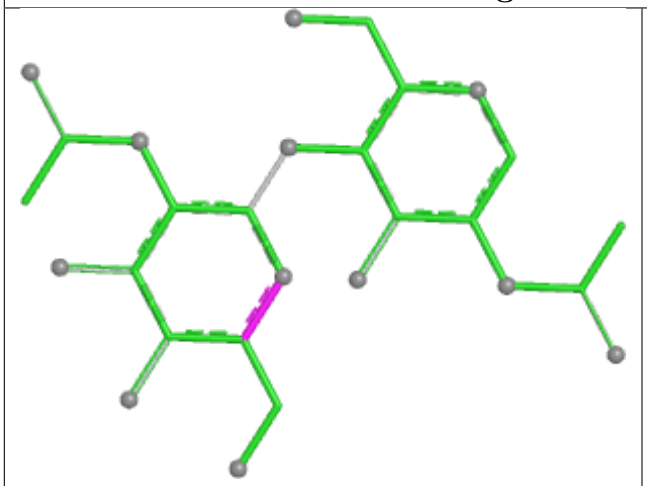
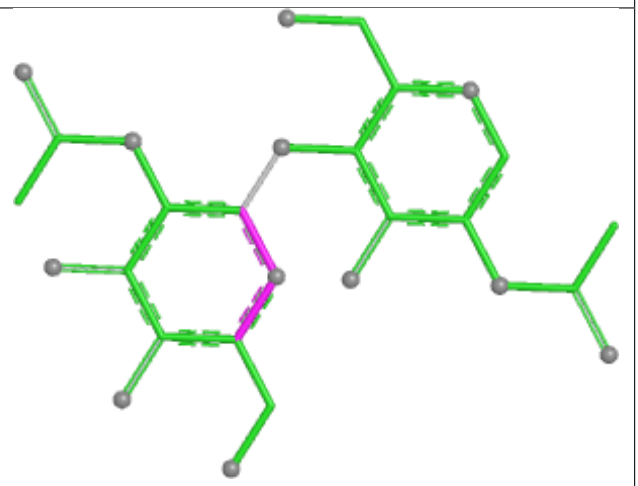


Rings

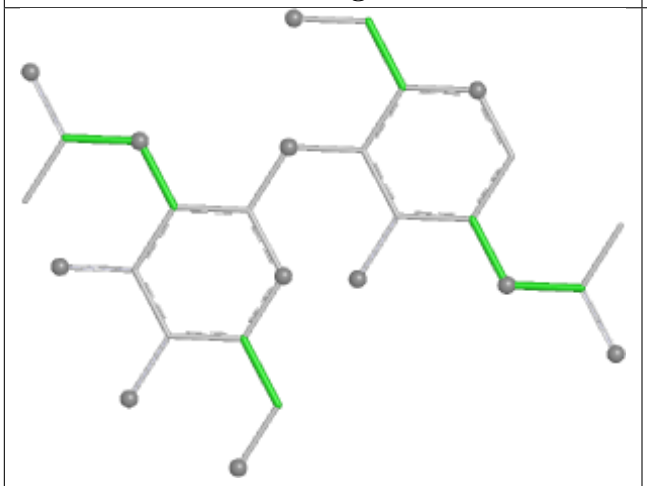
Oligosaccharide Chain T



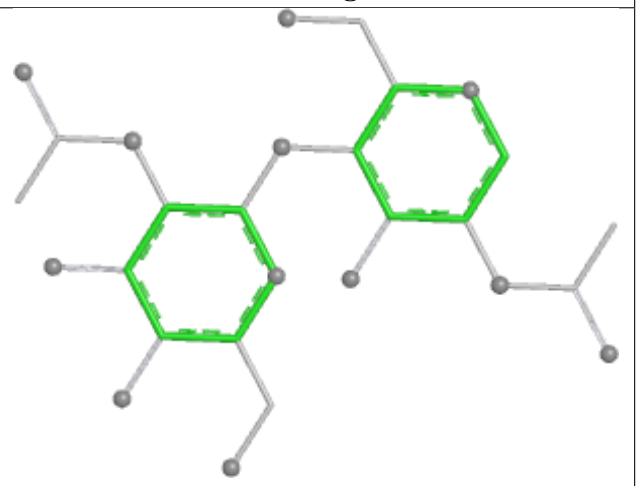
Bond lengths



Bond angles

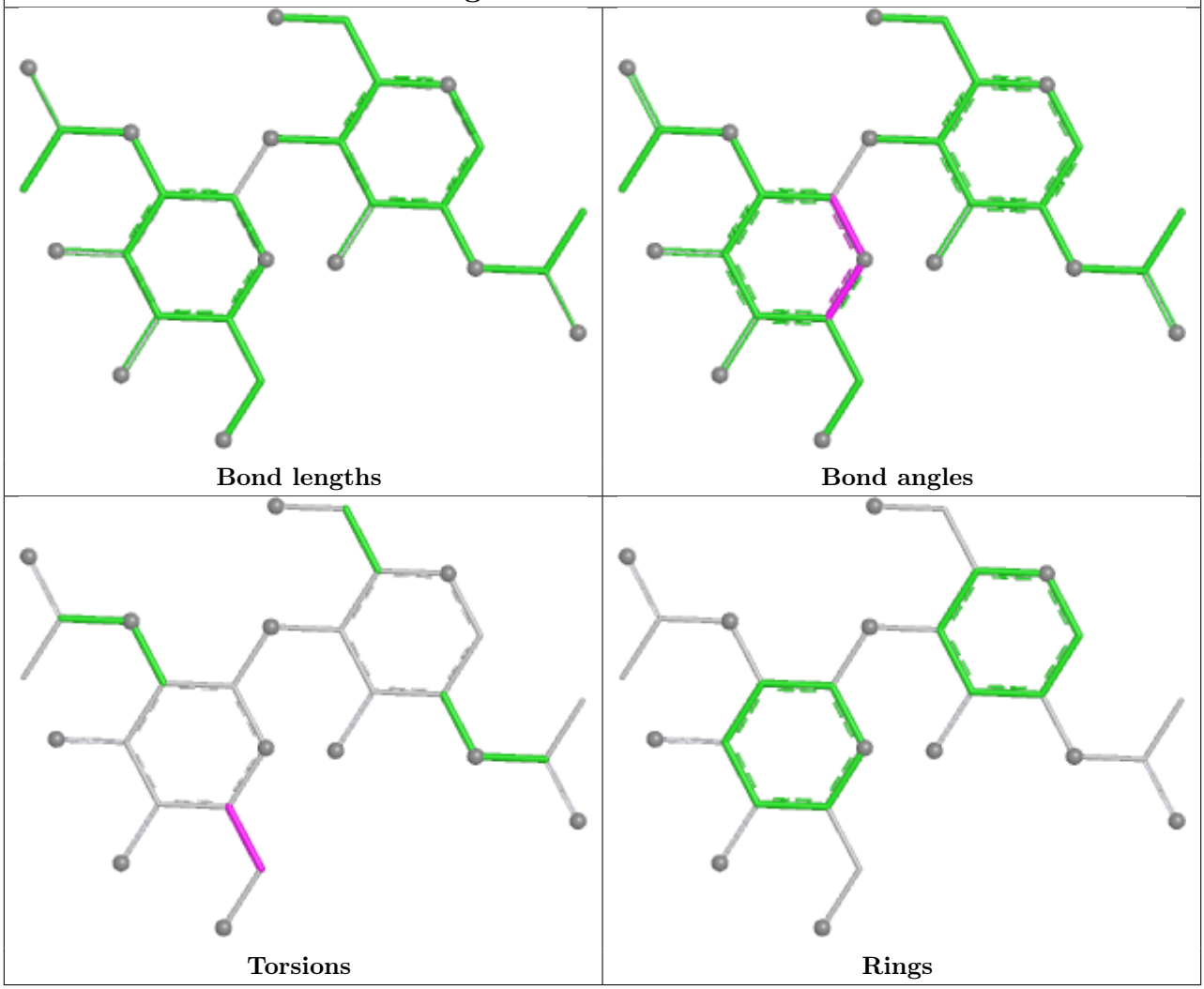


Torsions



Rings

Oligosaccharide Chain U



5.6 Ligand geometry (i)

36 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	$\#\|Z\| > 2$
4	NAG	A	1304	1	14,14,15	1.72	2 (14%)	17,19,21	0.69	0
4	NAG	A	1309	1	14,14,15	1.54	2 (14%)	17,19,21	0.69	0
4	NAG	B	1305	1	14,14,15	1.64	2 (14%)	17,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	1309	1	14,14,15	1.72	2 (14%)	17,19,21	0.66	0
4	NAG	A	1305	1	14,14,15	1.61	2 (14%)	17,19,21	0.66	0
4	NAG	B	1303	1	14,14,15	1.71	2 (14%)	17,19,21	0.67	0
4	NAG	B	1311	1	14,14,15	1.58	2 (14%)	17,19,21	0.79	0
4	NAG	A	1308	1	14,14,15	1.69	2 (14%)	17,19,21	0.71	0
4	NAG	B	1309	-	14,14,15	1.68	2 (14%)	17,19,21	0.72	0
4	NAG	C	1306	1	14,14,15	1.63	2 (14%)	17,19,21	0.68	0
4	NAG	B	1310	-	14,14,15	1.51	3 (21%)	17,19,21	0.64	0
4	NAG	C	1304	1	14,14,15	1.63	2 (14%)	17,19,21	0.72	0
4	NAG	B	1302	1	14,14,15	1.95	3 (21%)	17,19,21	0.92	1 (5%)
4	NAG	B	1306	1	14,14,15	1.72	3 (21%)	17,19,21	0.92	1 (5%)
4	NAG	A	1302	1	14,14,15	1.66	2 (14%)	17,19,21	0.73	0
4	NAG	B	1312	1	14,14,15	1.58	2 (14%)	17,19,21	0.70	0
4	NAG	A	1310	1	14,14,15	1.57	2 (14%)	17,19,21	0.74	0
4	NAG	C	1308	1	14,14,15	1.55	2 (14%)	17,19,21	0.69	0
4	NAG	C	1301	1	14,14,15	1.62	2 (14%)	17,19,21	0.64	0
4	NAG	A	1301	1	14,14,15	1.63	2 (14%)	17,19,21	0.66	0
4	NAG	B	1308	-	14,14,15	1.61	2 (14%)	17,19,21	0.63	0
4	NAG	A	1306	1	14,14,15	1.61	2 (14%)	17,19,21	0.65	0
4	NAG	C	1307	1	14,14,15	1.62	2 (14%)	17,19,21	0.70	0
4	NAG	B	1313	1	14,14,15	1.66	3 (21%)	17,19,21	0.73	0
4	NAG	C	1303	-	14,14,15	1.65	2 (14%)	17,19,21	0.69	0
4	NAG	C	1312	-	14,14,15	1.55	2 (14%)	17,19,21	0.70	0
4	NAG	B	1307	1	14,14,15	1.62	2 (14%)	17,19,21	0.67	0
4	NAG	A	1307	1	14,14,15	1.63	2 (14%)	17,19,21	0.67	0
4	NAG	B	1304	1	14,14,15	1.61	2 (14%)	17,19,21	0.71	0
4	NAG	C	1302	1	14,14,15	1.59	2 (14%)	17,19,21	0.72	0
4	NAG	C	1310	-	14,14,15	1.59	2 (14%)	17,19,21	0.68	0
4	NAG	A	1303	1	14,14,15	1.58	2 (14%)	17,19,21	0.71	0
4	NAG	B	1301	-	14,14,15	1.63	2 (14%)	17,19,21	0.68	0
4	NAG	C	1305	1	14,14,15	1.66	2 (14%)	17,19,21	0.65	0
4	NAG	C	1311	-	14,14,15	1.62	2 (14%)	17,19,21	0.67	0
4	NAG	D	701	-	14,14,15	0.39	0	17,19,21	0.61	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
4	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1309	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1310	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1303	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1312	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1310	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1311	-	-	0/6/23/26	0/1/1/1
4	NAG	D	701	-	-	2/6/23/26	0/1/1/1

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1302	NAG	C1-C2	5.67	1.60	1.52
4	A	1304	NAG	C1-C2	5.11	1.59	1.52
4	B	1309	NAG	C1-C2	4.93	1.59	1.52
4	C	1309	NAG	C1-C2	4.91	1.59	1.52
4	B	1303	NAG	C1-C2	4.78	1.58	1.52
4	A	1308	NAG	C1-C2	4.76	1.58	1.52
4	A	1302	NAG	C1-C2	4.71	1.58	1.52
4	A	1301	NAG	C1-C2	4.66	1.58	1.52
4	B	1305	NAG	C1-C2	4.64	1.58	1.52
4	C	1306	NAG	C1-C2	4.61	1.58	1.52
4	C	1311	NAG	C1-C2	4.61	1.58	1.52
4	B	1308	NAG	C1-C2	4.59	1.58	1.52
4	B	1306	NAG	C1-C2	4.59	1.58	1.52
4	C	1304	NAG	C1-C2	4.55	1.58	1.52
4	B	1301	NAG	C1-C2	4.52	1.58	1.52
4	B	1313	NAG	C1-C2	4.51	1.58	1.52
4	C	1301	NAG	C1-C2	4.50	1.58	1.52
4	B	1312	NAG	C1-C2	4.50	1.58	1.52
4	A	1307	NAG	C1-C2	4.49	1.58	1.52
4	B	1307	NAG	C1-C2	4.49	1.58	1.52
4	C	1307	NAG	C1-C2	4.48	1.58	1.52
4	C	1305	NAG	C1-C2	4.47	1.58	1.52
4	C	1302	NAG	C1-C2	4.46	1.58	1.52
4	C	1303	NAG	C1-C2	4.44	1.58	1.52
4	C	1310	NAG	C1-C2	4.44	1.58	1.52
4	B	1311	NAG	C1-C2	4.43	1.58	1.52
4	B	1304	NAG	C1-C2	4.43	1.58	1.52
4	A	1305	NAG	C1-C2	4.40	1.58	1.52
4	A	1306	NAG	C1-C2	4.36	1.58	1.52
4	A	1303	NAG	C1-C2	4.36	1.58	1.52
4	A	1310	NAG	C1-C2	4.34	1.58	1.52
4	C	1308	NAG	C1-C2	4.20	1.58	1.52
4	A	1309	NAG	C1-C2	4.18	1.58	1.52
4	C	1312	NAG	C1-C2	4.08	1.57	1.52
4	B	1310	NAG	C1-C2	3.46	1.57	1.52
4	B	1302	NAG	O5-C5	2.85	1.49	1.43
4	B	1306	NAG	O5-C5	2.81	1.48	1.43
4	C	1305	NAG	O5-C5	2.79	1.48	1.43
4	B	1303	NAG	O5-C5	2.75	1.48	1.43
4	C	1303	NAG	O5-C5	2.69	1.48	1.43
4	A	1308	NAG	O5-C5	2.69	1.48	1.43
4	C	1309	NAG	O5-C5	2.64	1.48	1.43
4	A	1306	NAG	O5-C5	2.61	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1304	NAG	O5-C5	2.58	1.48	1.43
4	B	1311	NAG	O5-C5	2.58	1.48	1.43
4	C	1312	NAG	O5-C5	2.56	1.48	1.43
4	C	1310	NAG	O5-C5	2.55	1.48	1.43
4	C	1301	NAG	O5-C5	2.52	1.48	1.43
4	A	1309	NAG	O5-C5	2.52	1.48	1.43
4	B	1307	NAG	O5-C5	2.48	1.48	1.43
4	B	1305	NAG	O5-C5	2.47	1.48	1.43
4	C	1308	NAG	O5-C5	2.46	1.48	1.43
4	B	1310	NAG	O5-C5	2.45	1.48	1.43
4	A	1303	NAG	O5-C5	2.45	1.48	1.43
4	B	1313	NAG	O5-C5	2.45	1.48	1.43
4	C	1302	NAG	O5-C5	2.44	1.48	1.43
4	C	1304	NAG	O5-C5	2.44	1.48	1.43
4	A	1307	NAG	O5-C5	2.44	1.48	1.43
4	A	1301	NAG	O5-C5	2.43	1.48	1.43
4	C	1307	NAG	O5-C5	2.42	1.48	1.43
4	B	1301	NAG	O5-C5	2.41	1.48	1.43
4	A	1305	NAG	O5-C5	2.41	1.48	1.43
4	B	1308	NAG	O5-C5	2.41	1.48	1.43
4	B	1309	NAG	O5-C5	2.41	1.48	1.43
4	A	1302	NAG	O5-C5	2.39	1.48	1.43
4	C	1306	NAG	O5-C5	2.36	1.48	1.43
4	B	1312	NAG	O5-C5	2.35	1.48	1.43
4	A	1310	NAG	O5-C5	2.33	1.48	1.43
4	B	1310	NAG	O5-C1	2.33	1.47	1.43
4	A	1304	NAG	O5-C5	2.29	1.47	1.43
4	C	1311	NAG	O5-C5	2.25	1.47	1.43
4	B	1302	NAG	O5-C1	2.22	1.47	1.43
4	B	1313	NAG	C3-C2	2.10	1.56	1.52
4	B	1306	NAG	C4-C5	2.00	1.57	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1306	NAG	O5-C1-C2	-2.39	107.59	111.29
4	D	701	NAG	C1-O5-C5	2.08	114.97	112.19
4	B	1302	NAG	C2-N2-C7	2.05	125.65	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1306	NAG	O5-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	D	701	NAG	O5-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	A	1310	NAG	O5-C5-C6-O6
4	D	701	NAG	C4-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	C	1310	NAG	C1-C2-N2-C7
4	B	1311	NAG	C4-C5-C6-O6

There are no ring outliers.

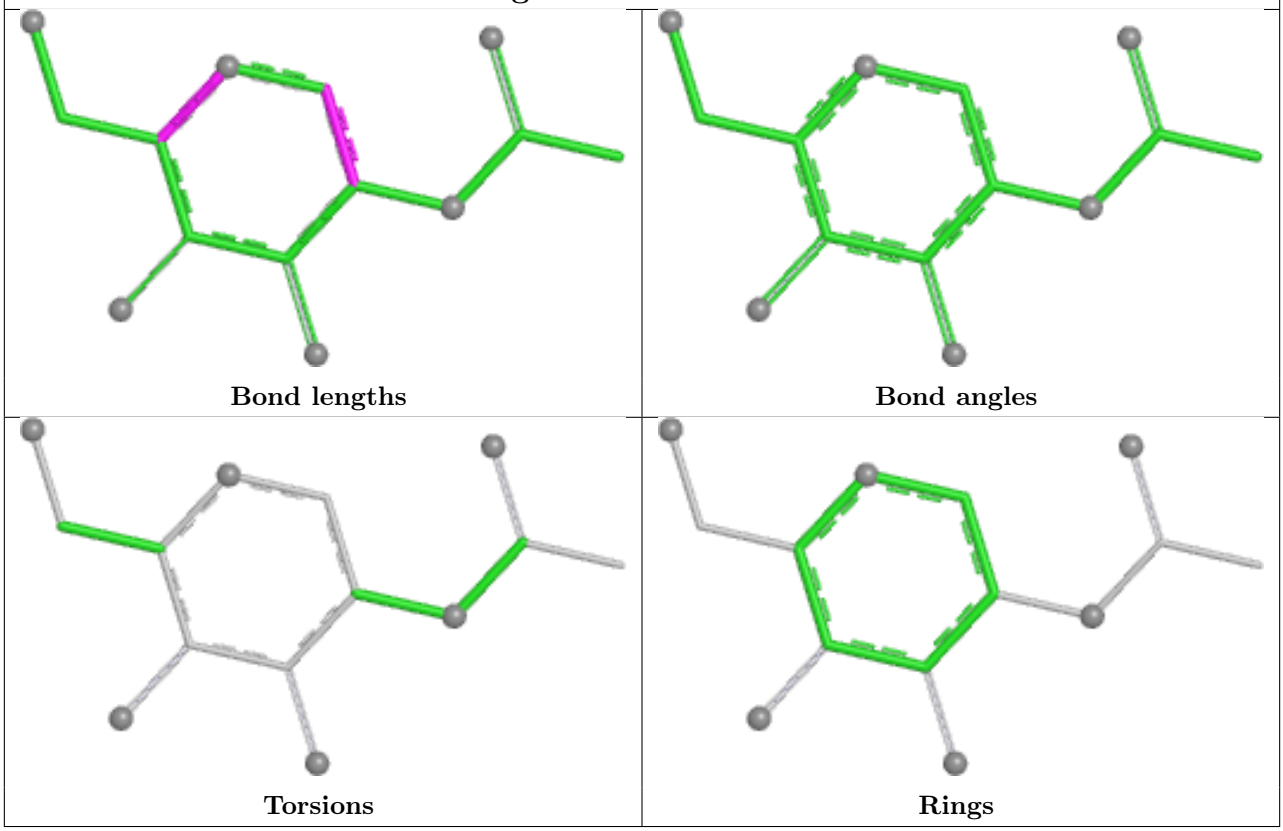
18 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1304	NAG	2	0
4	A	1309	NAG	6	0
4	C	1309	NAG	4	0
4	B	1311	NAG	4	0
4	B	1309	NAG	1	0
4	C	1306	NAG	3	0
4	B	1310	NAG	3	0
4	B	1306	NAG	1	0
4	A	1302	NAG	2	0
4	B	1312	NAG	1	0
4	A	1310	NAG	2	0
4	A	1301	NAG	2	0
4	B	1313	NAG	5	0
4	C	1312	NAG	4	0
4	C	1310	NAG	5	0
4	C	1305	NAG	5	0
4	C	1311	NAG	1	0
4	D	701	NAG	3	0

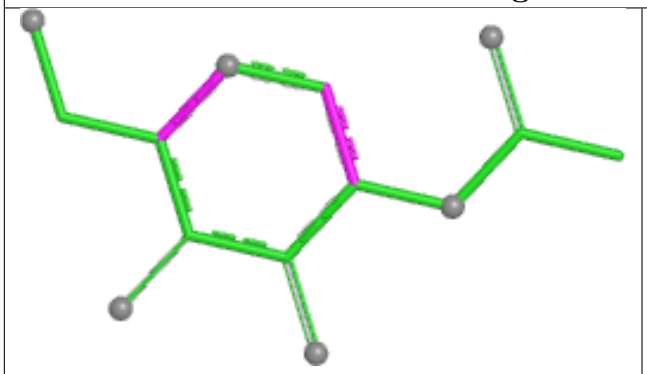
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

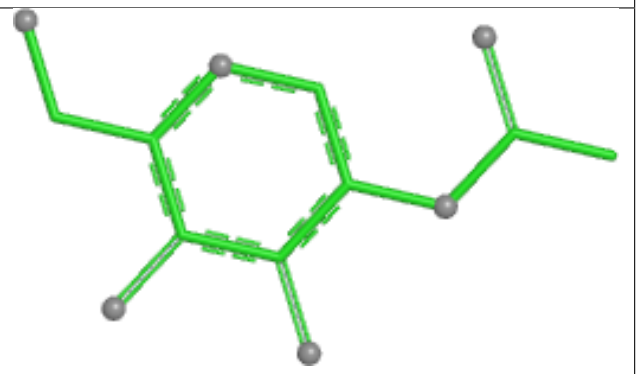
Ligand NAG A 1304



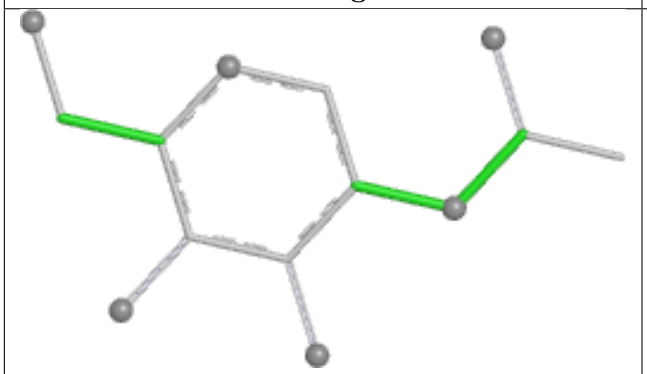
Ligand NAG A 1309



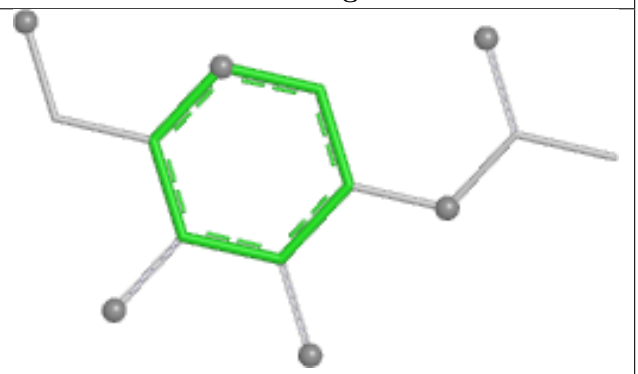
Bond lengths



Bond angles

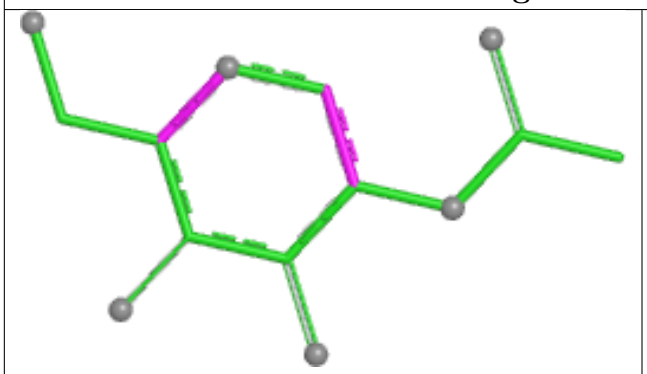


Torsions

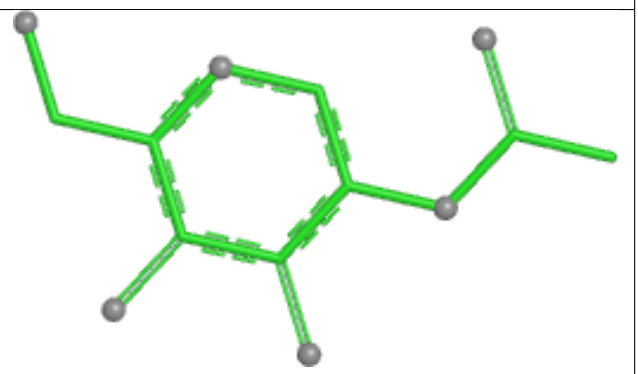


Rings

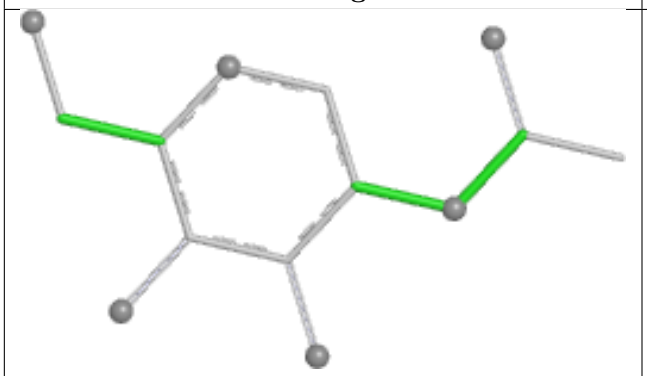
Ligand NAG B 1305



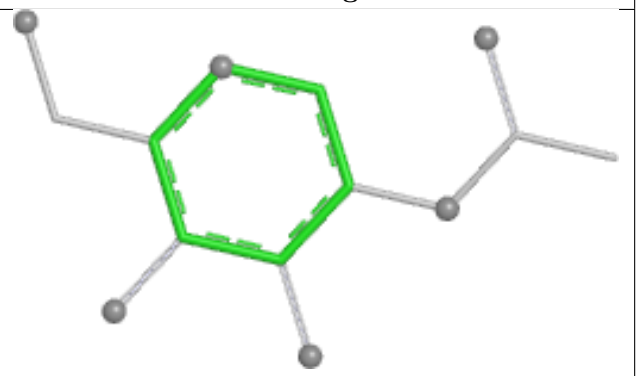
Bond lengths



Bond angles

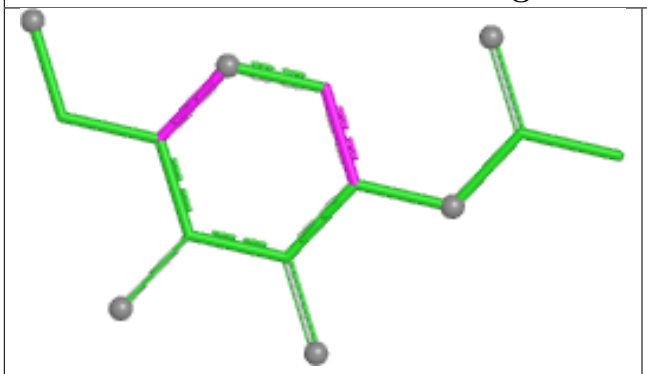


Torsions

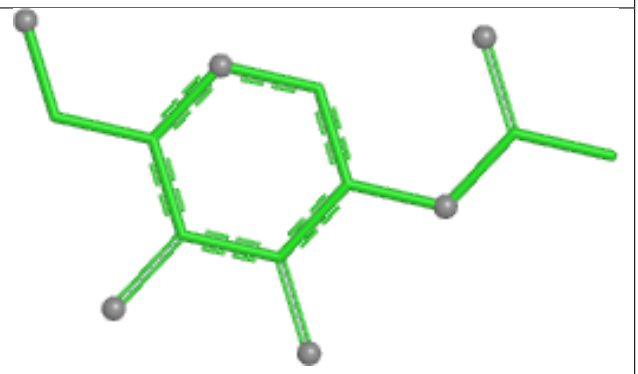


Rings

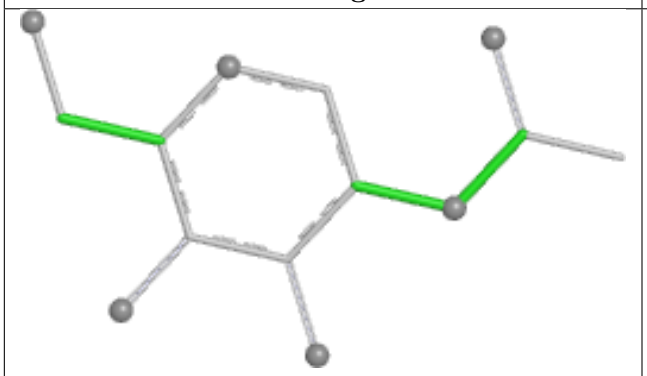
Ligand NAG C 1309



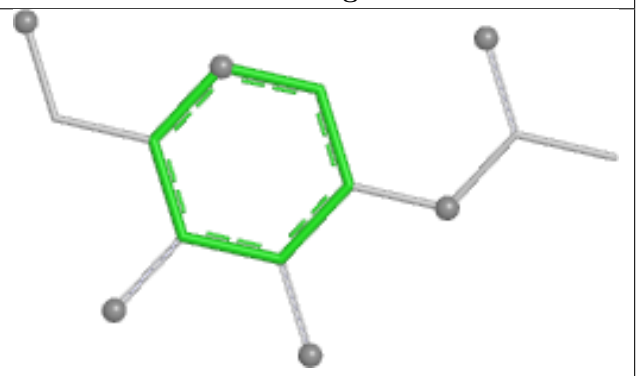
Bond lengths



Bond angles

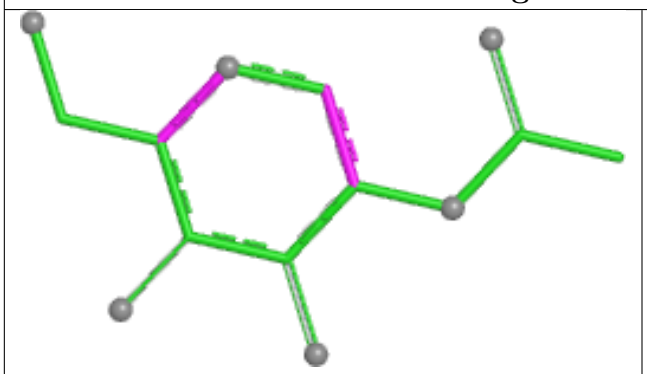


Torsions

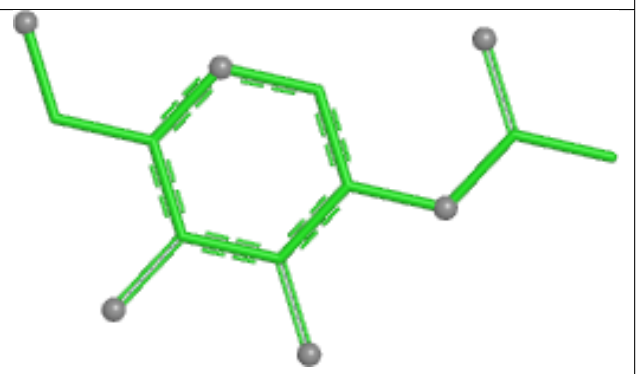


Rings

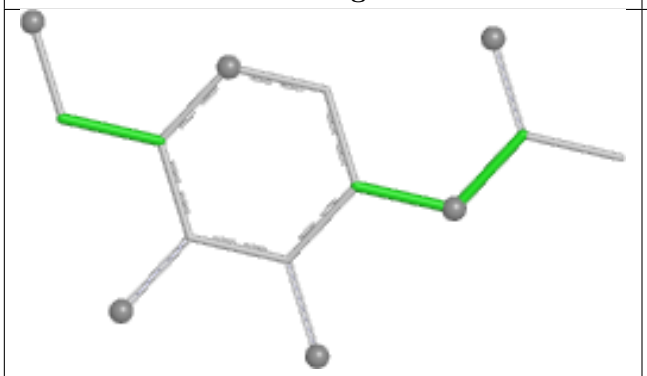
Ligand NAG A 1305



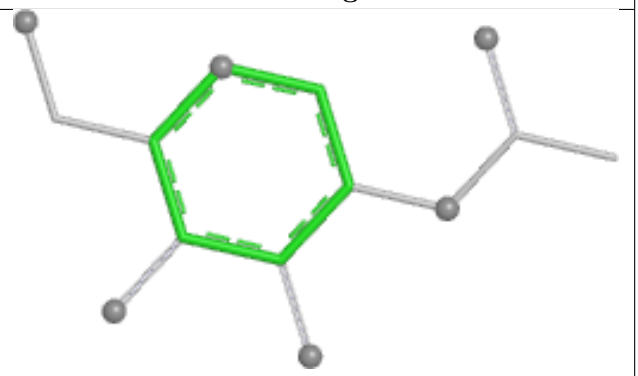
Bond lengths



Bond angles

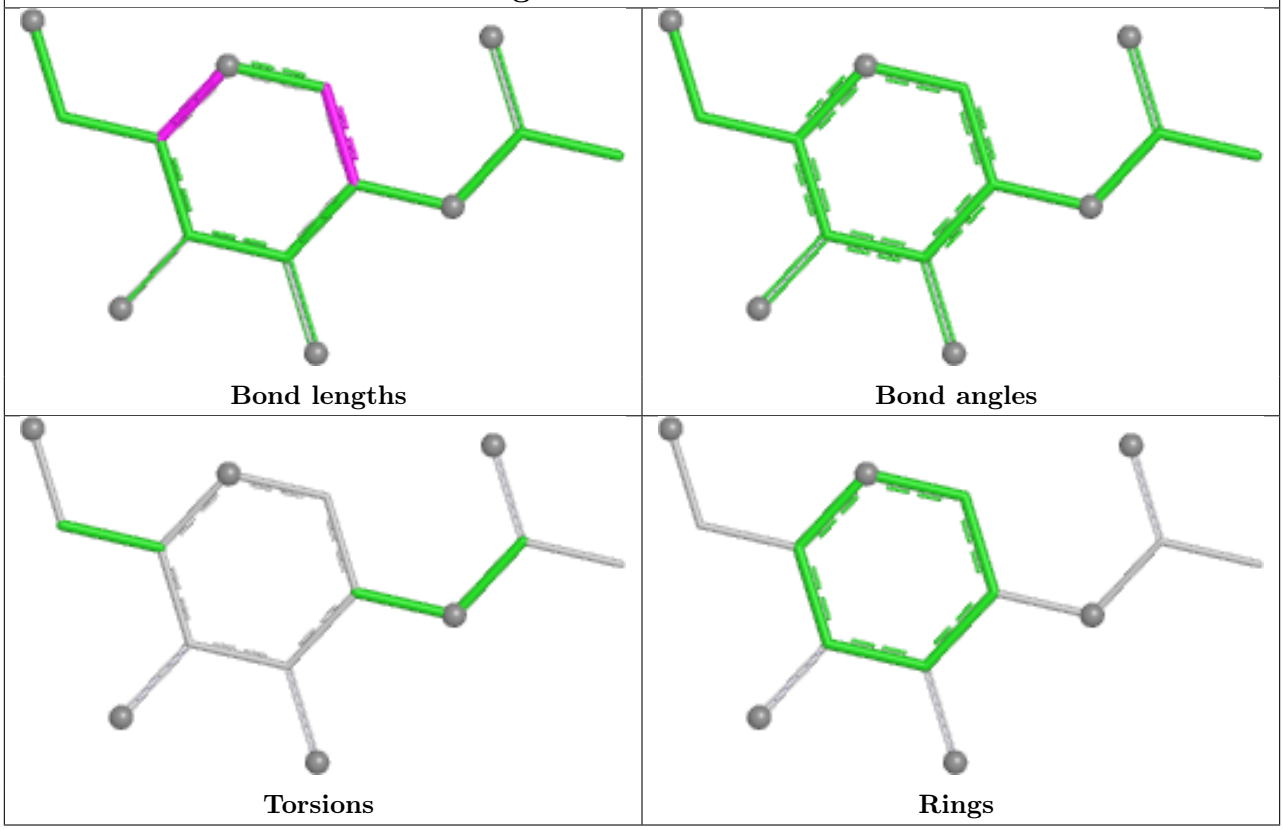


Torsions

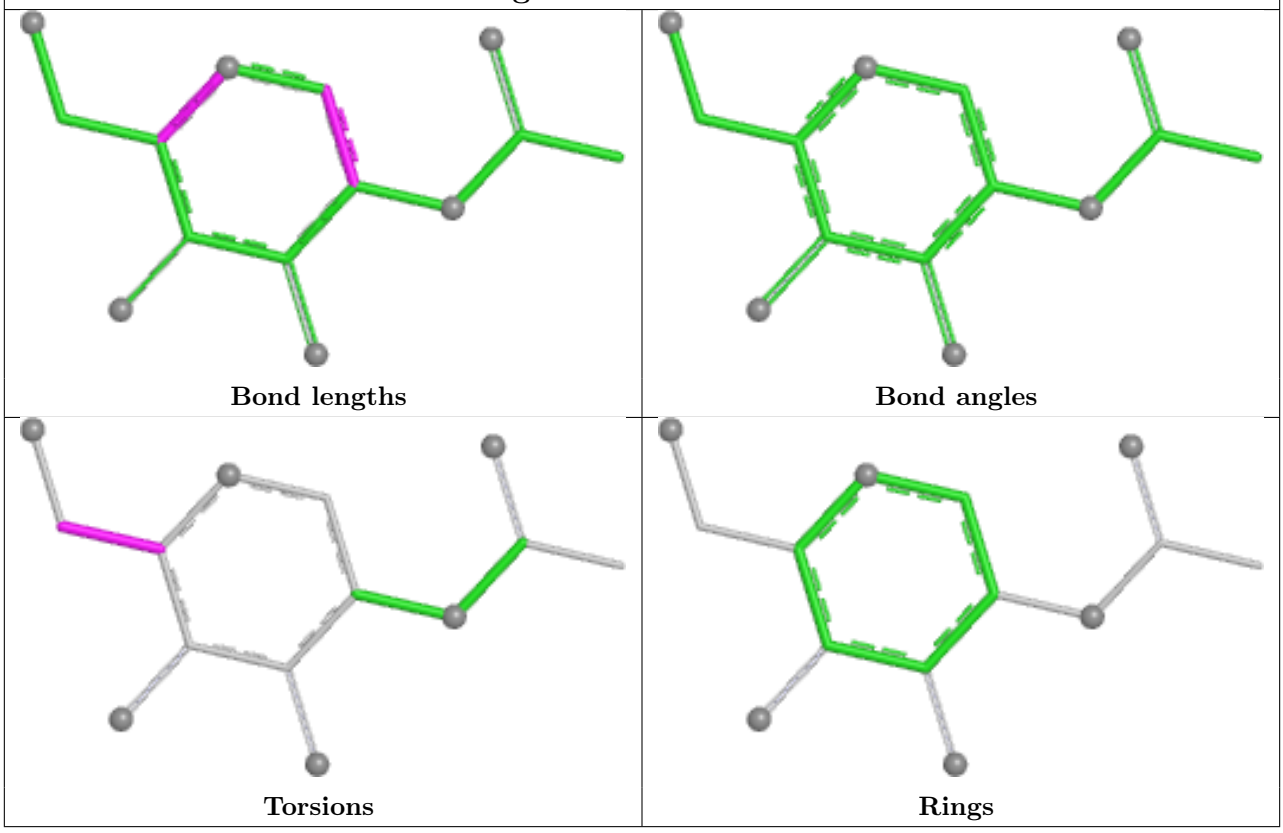


Rings

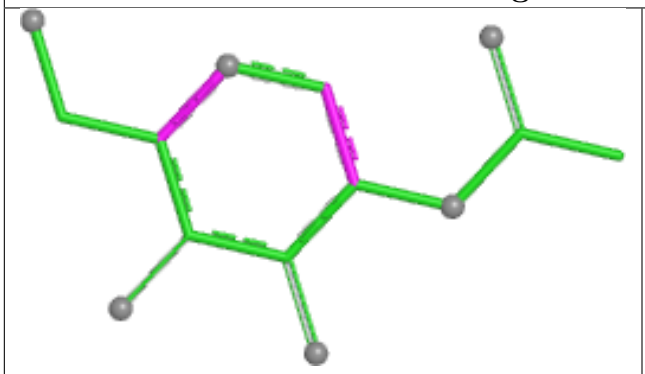
Ligand NAG B 1303



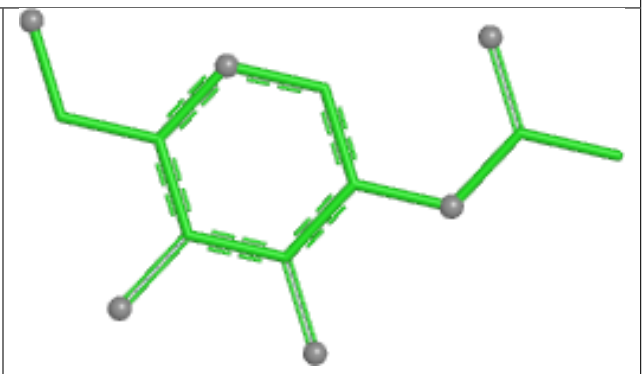
Ligand NAG B 1311



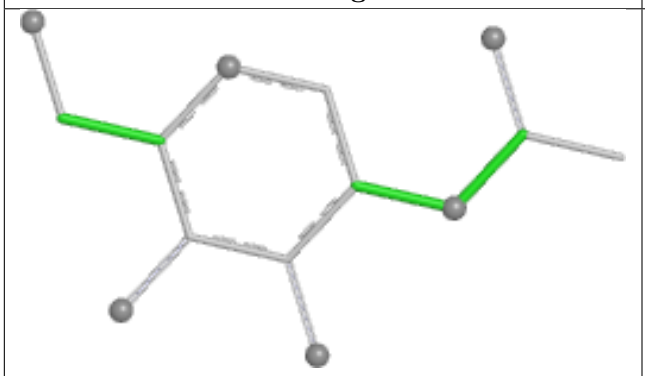
Ligand NAG A 1308



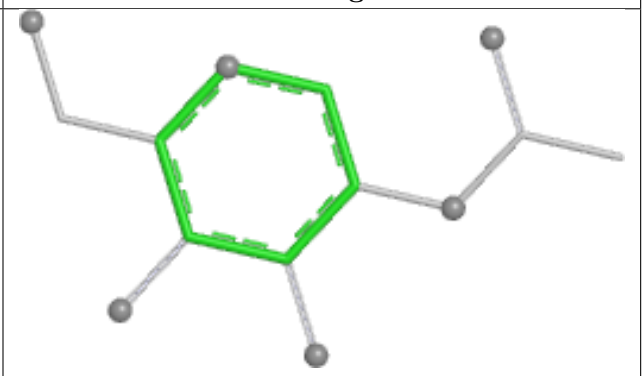
Bond lengths



Bond angles

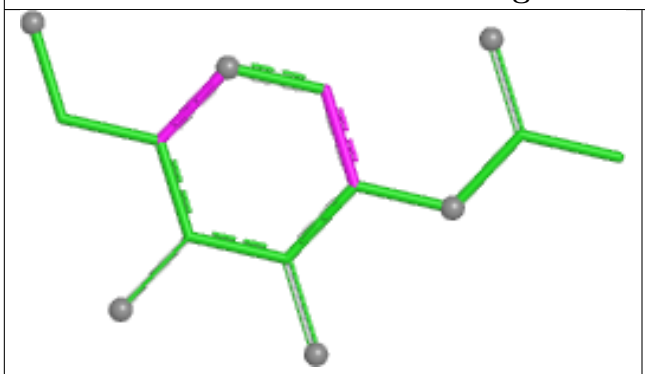


Torsions

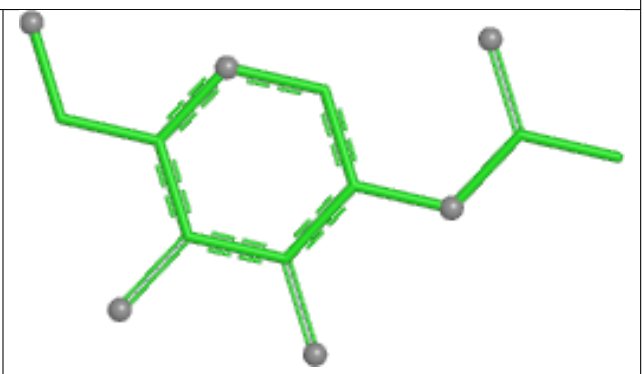


Rings

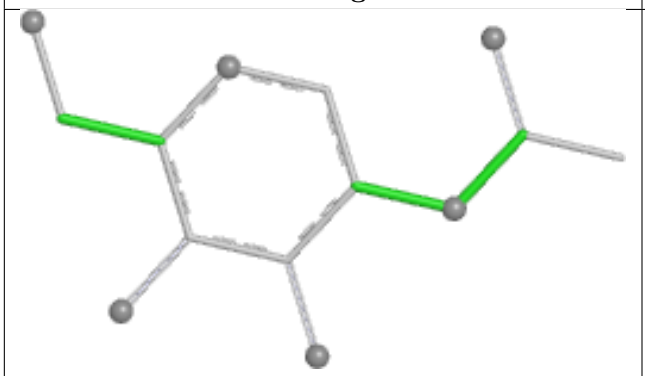
Ligand NAG B 1309



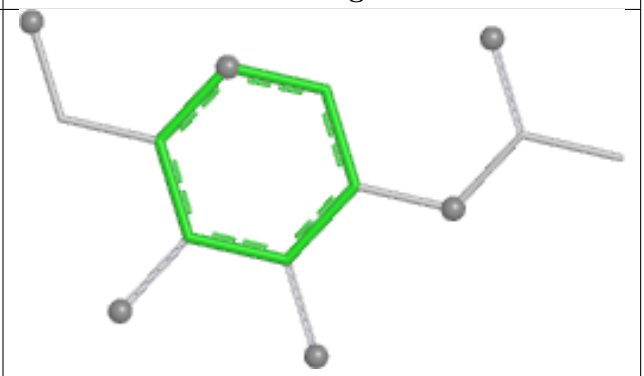
Bond lengths



Bond angles

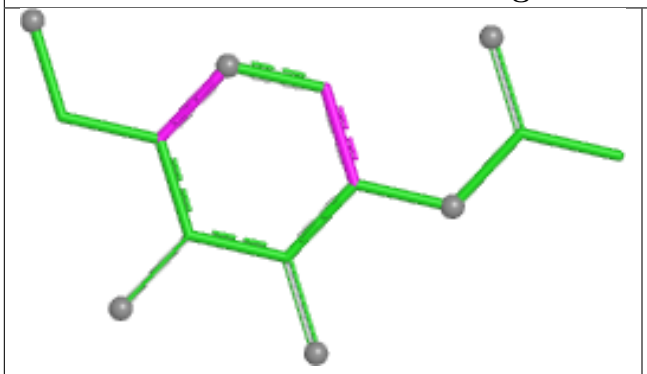


Torsions



Rings

Ligand NAG C 1306



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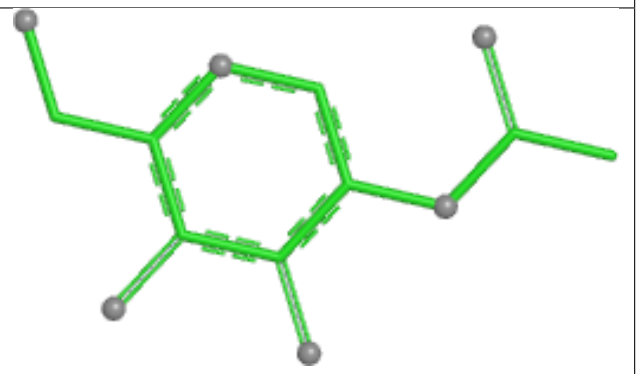
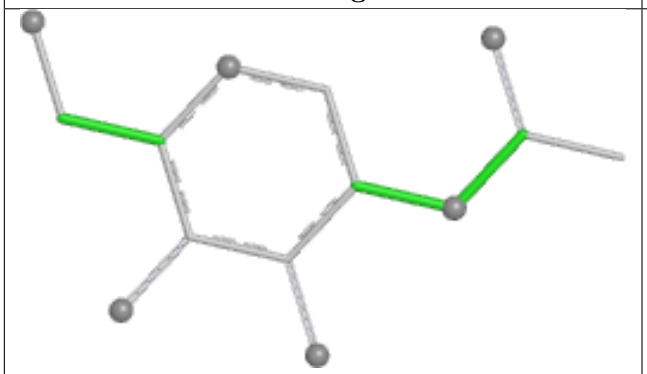
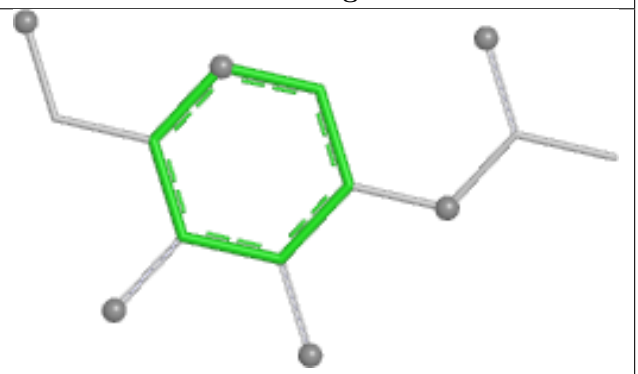


Bond angles

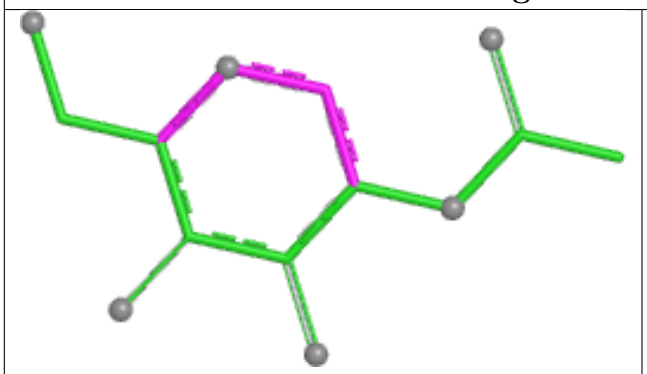


Torsions



Rings

Ligand NAG B 1310



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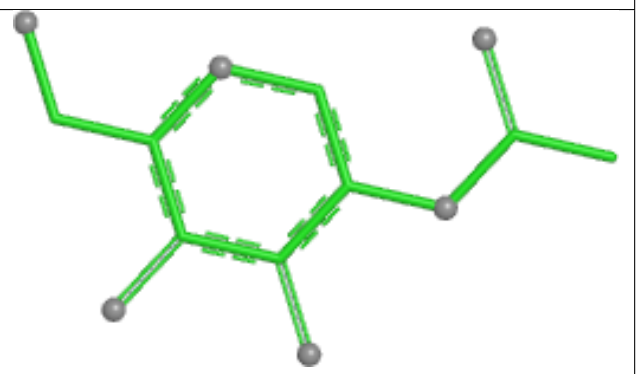
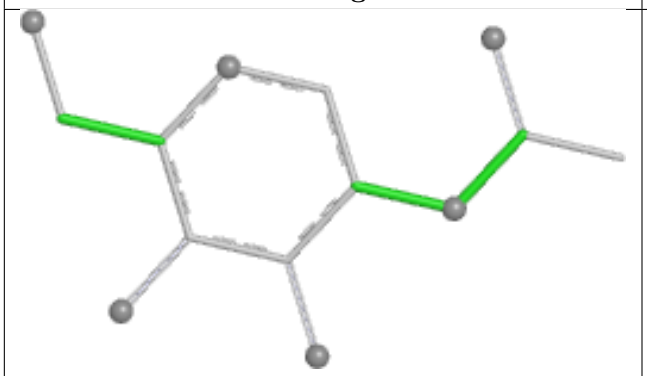
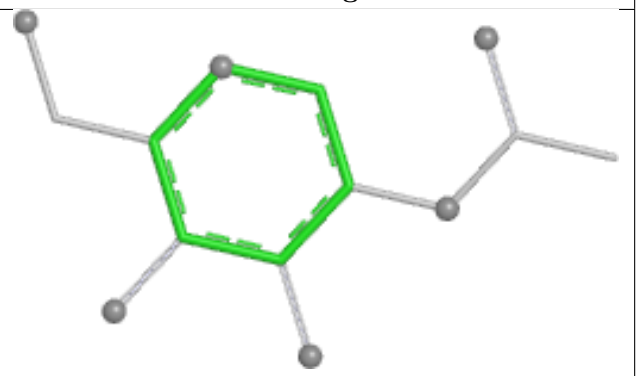


Bond angles

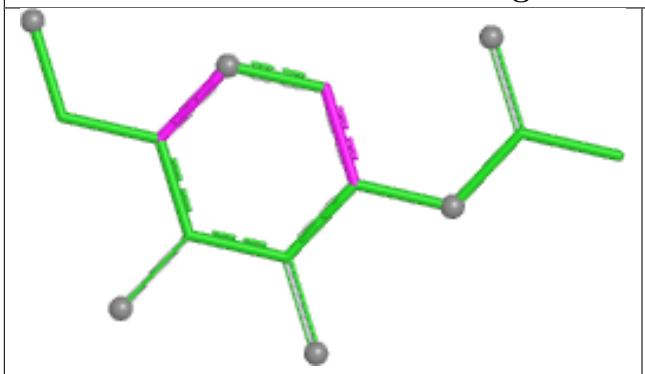


Torsions



Rings

Ligand NAG C 1304



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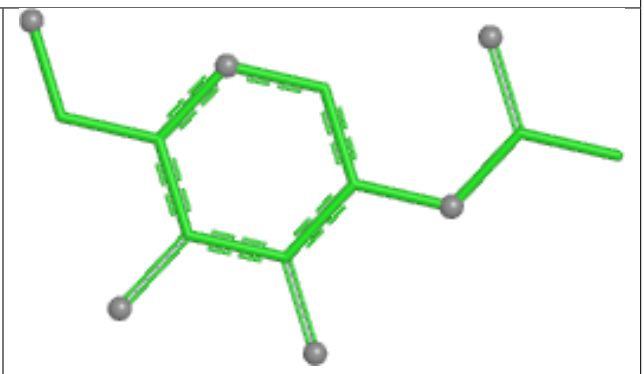
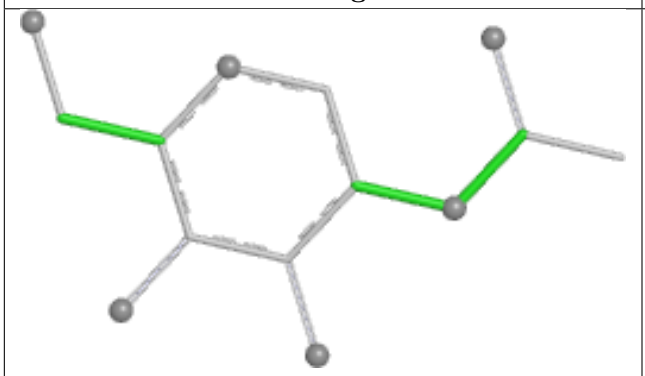


Bond angles



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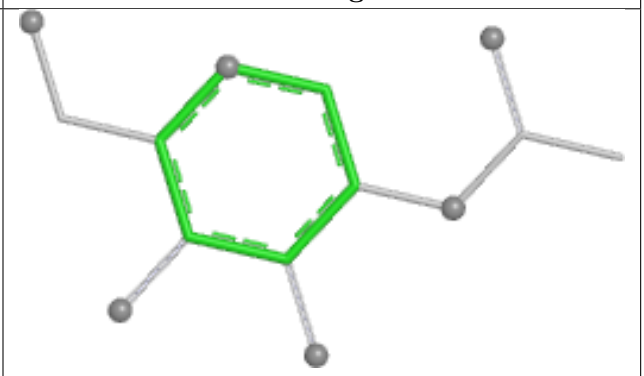
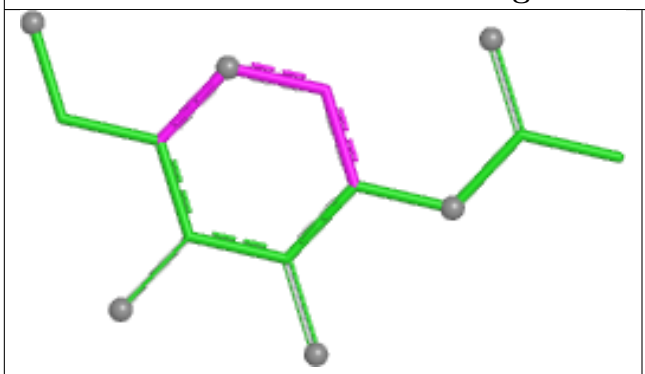


Rings

Ligand NAG B 1302



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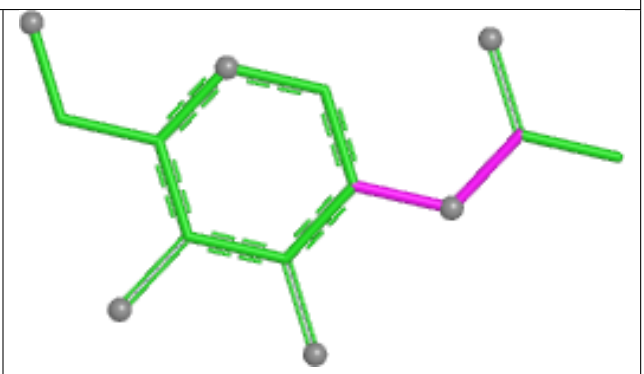
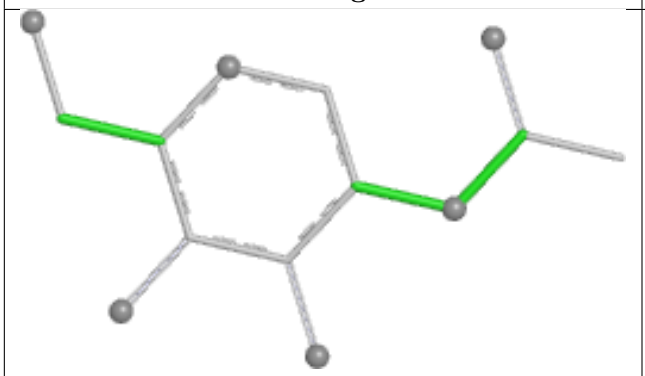


Bond angles



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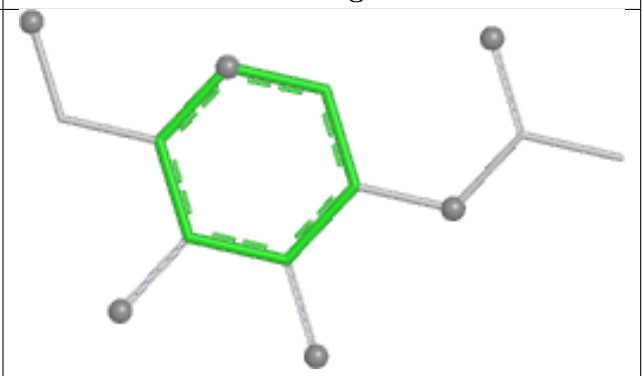
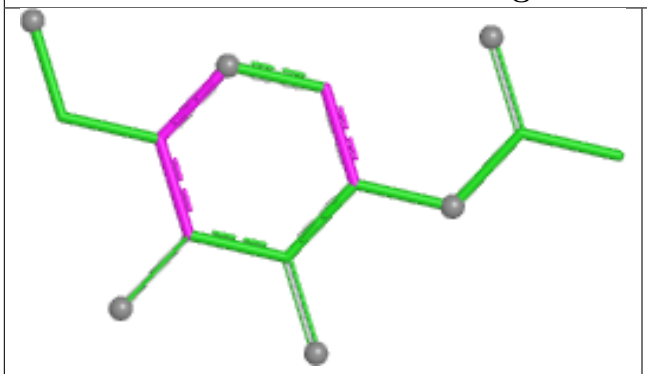


Rings

Ligand NAG B 1306



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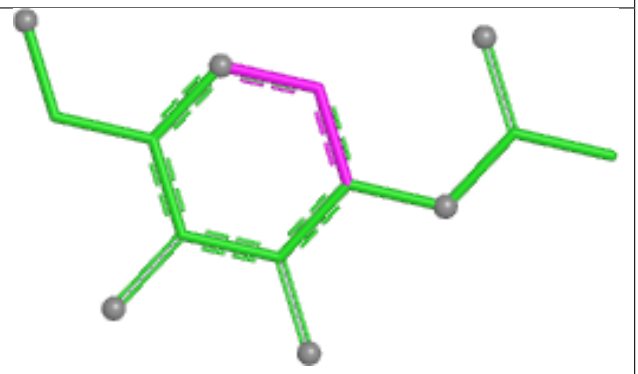
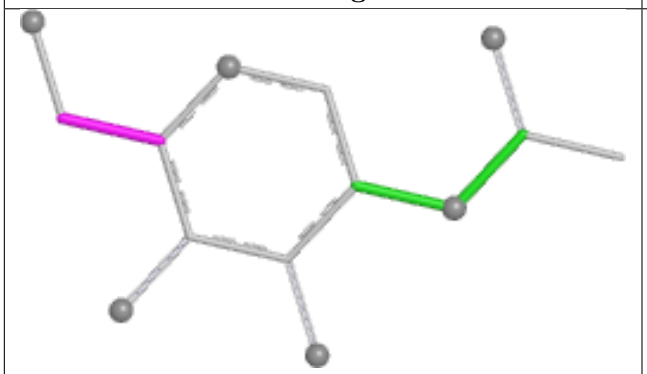


Bond angles



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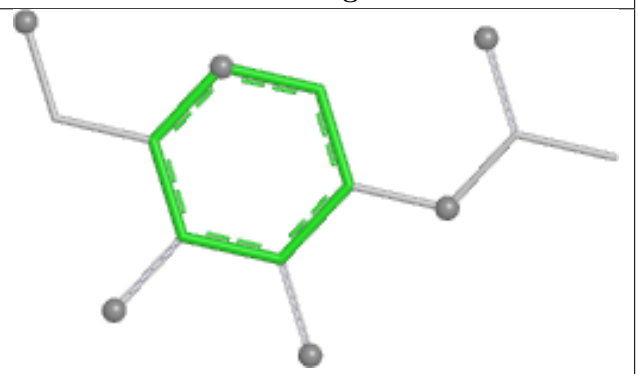
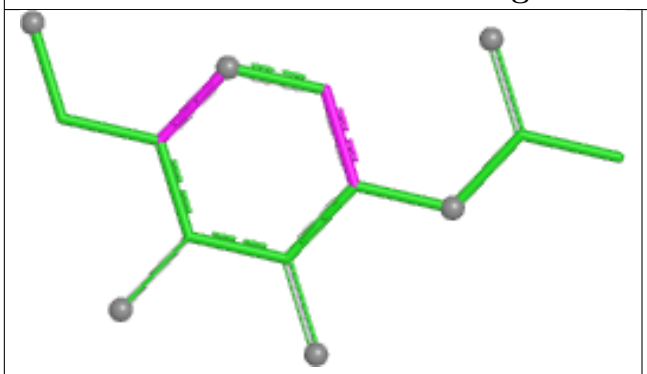


Rings

Ligand NAG A 1302



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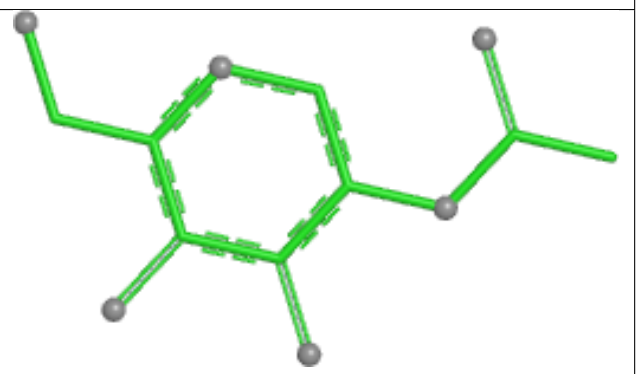

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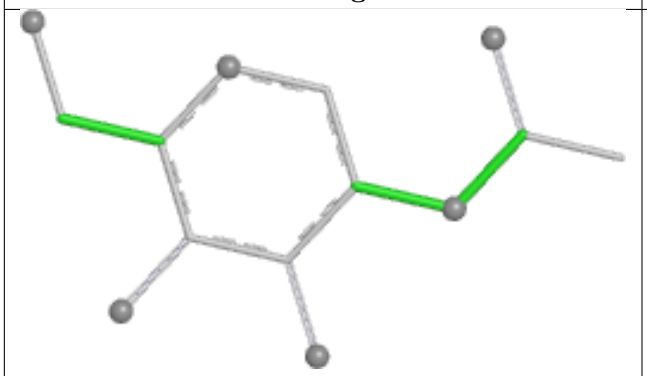

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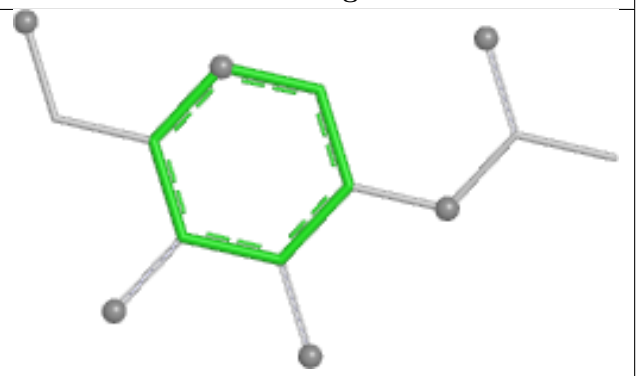
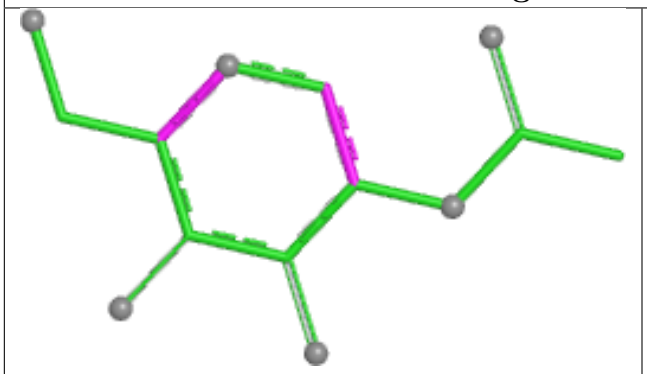


Rings

Ligand NAG B 1312



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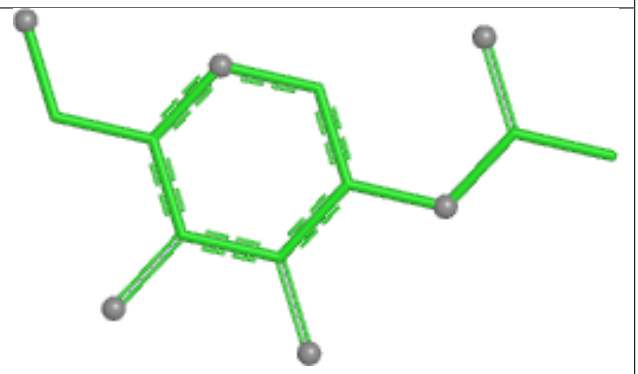
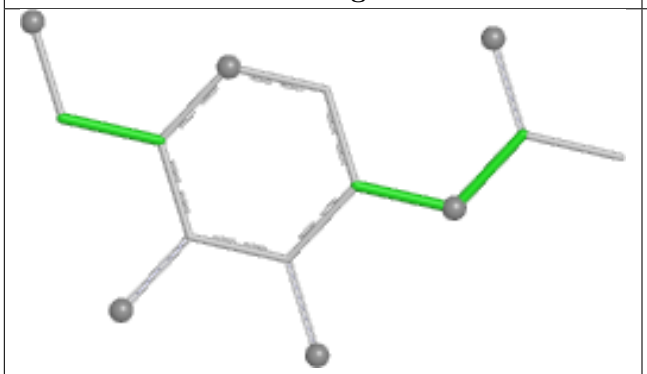


Bond angles



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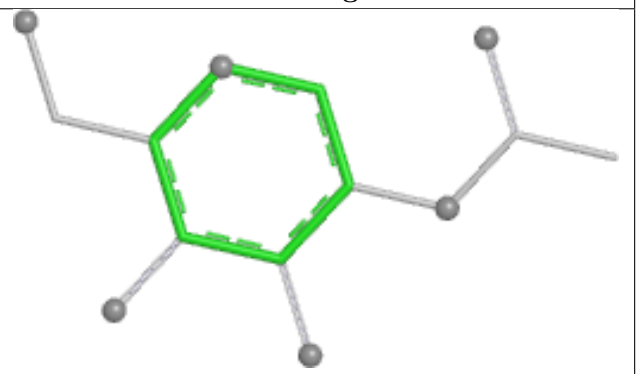
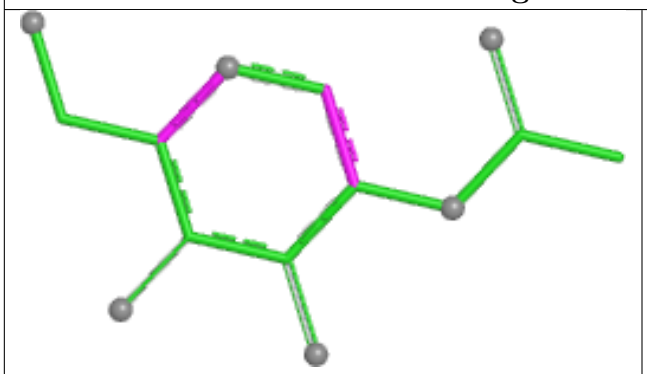


Rings

Ligand NAG A 1310



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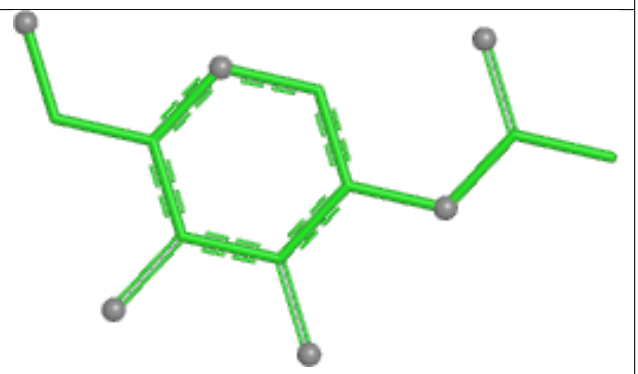
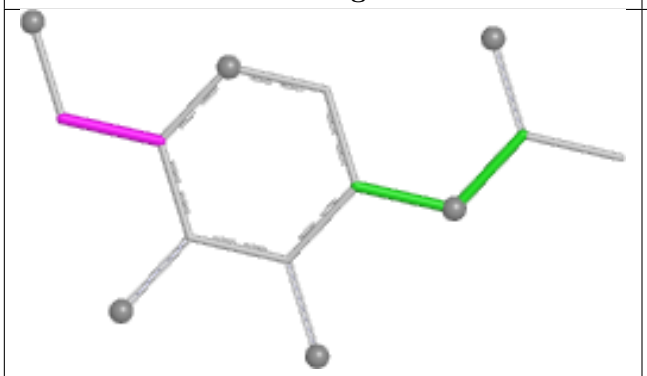


Bond angles



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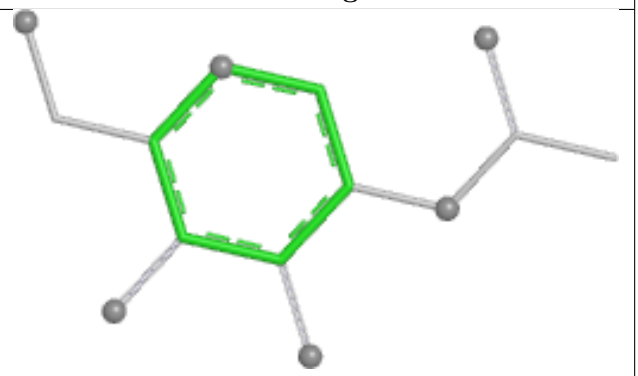
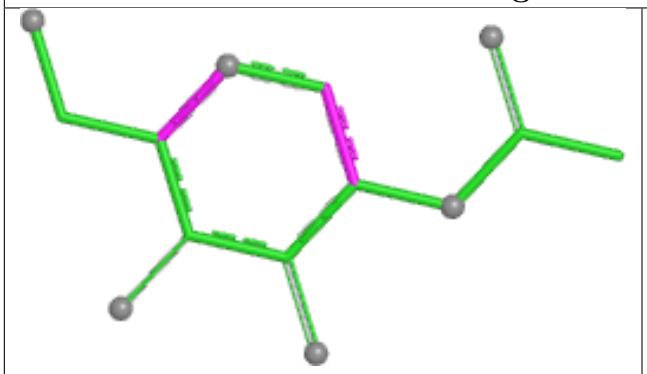


Rings

Ligand NAG C 1308



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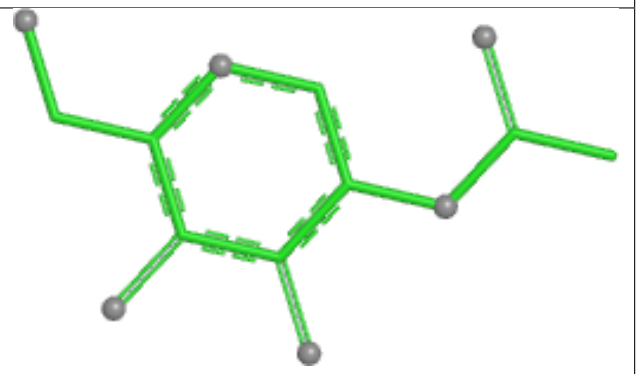

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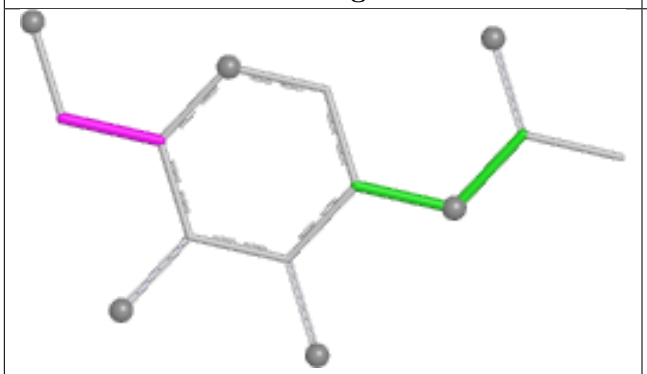

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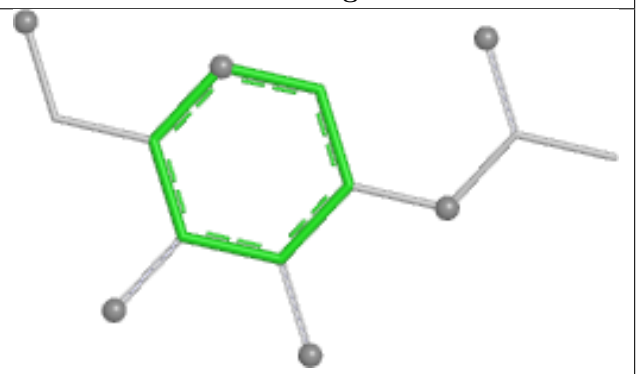
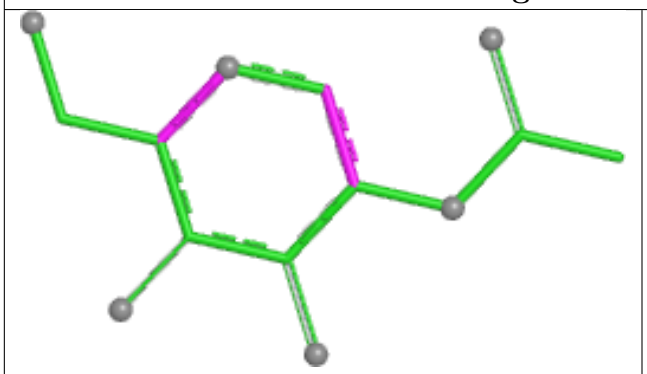


Rings

Ligand NAG C 1301



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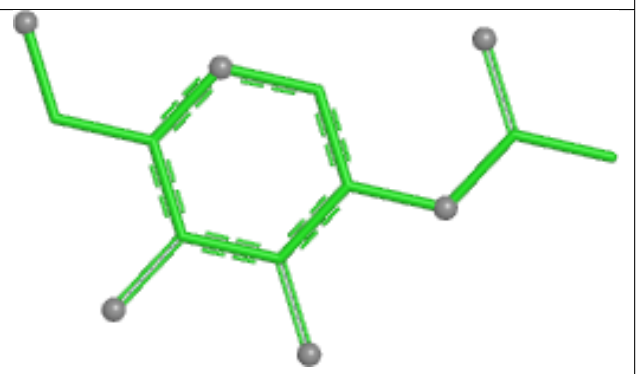
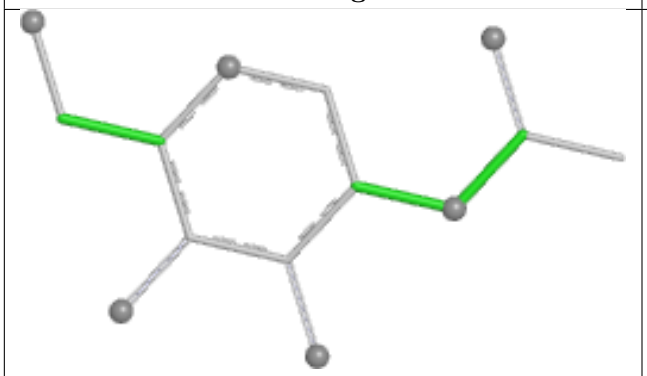


Bond angles



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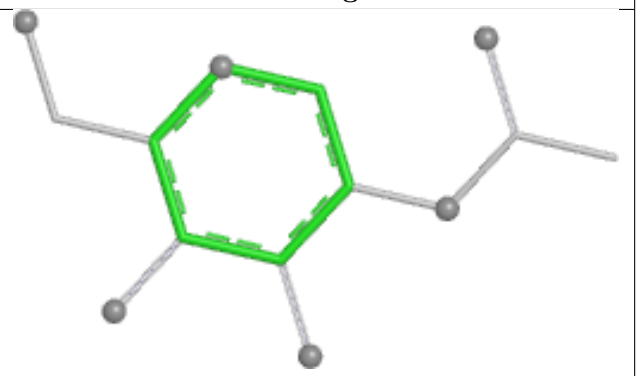
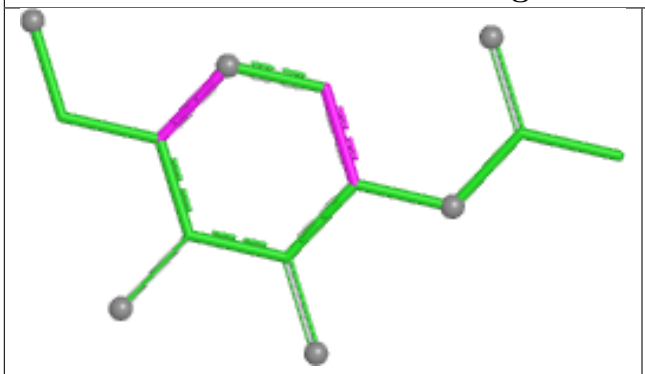


Rings

Ligand NAG A 1301



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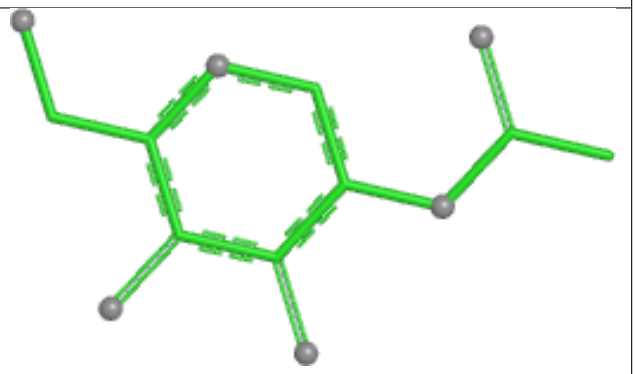
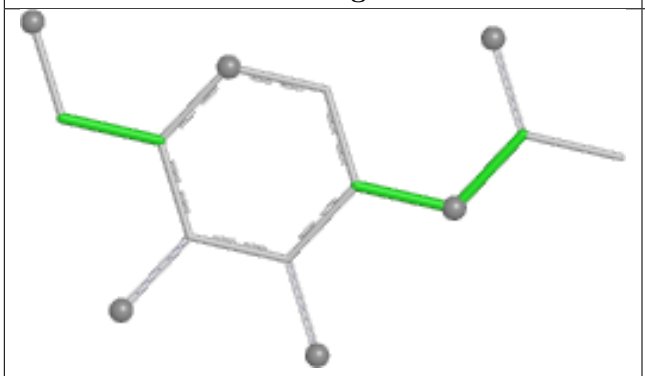


Bond angles



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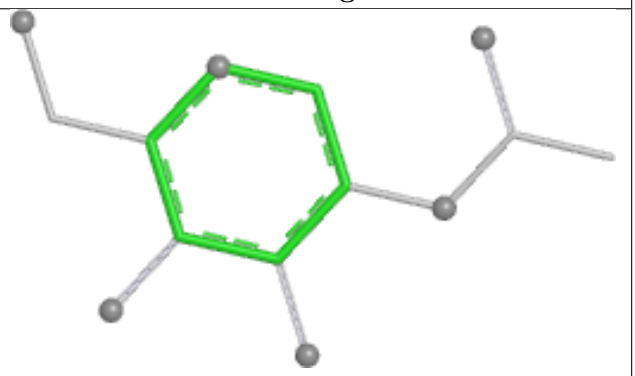
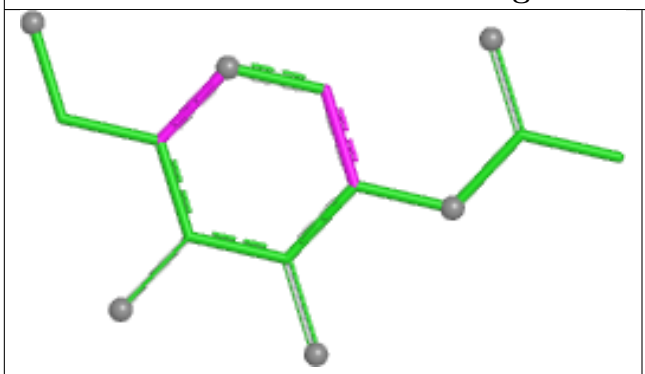


Rings

Ligand NAG B 1308



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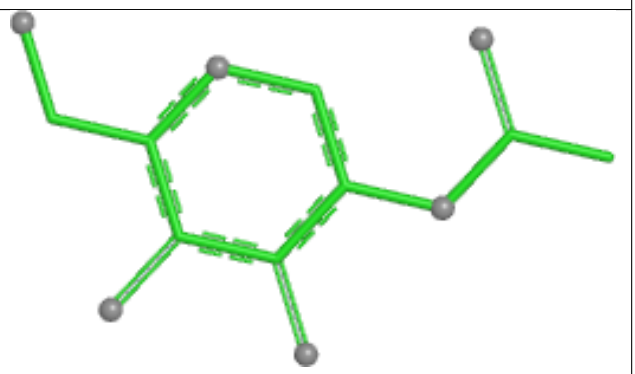
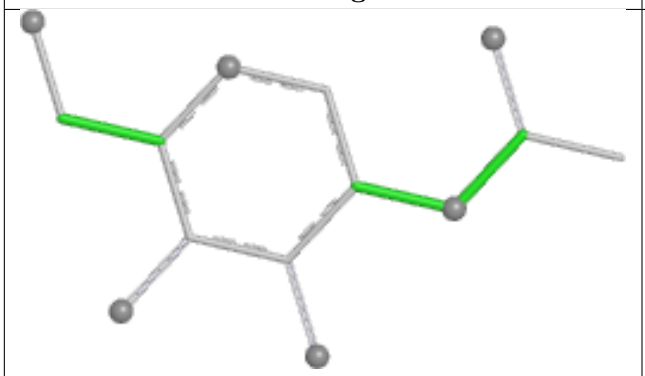


Bond angles



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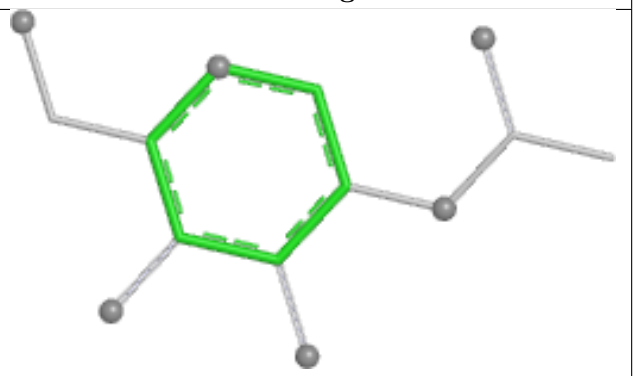
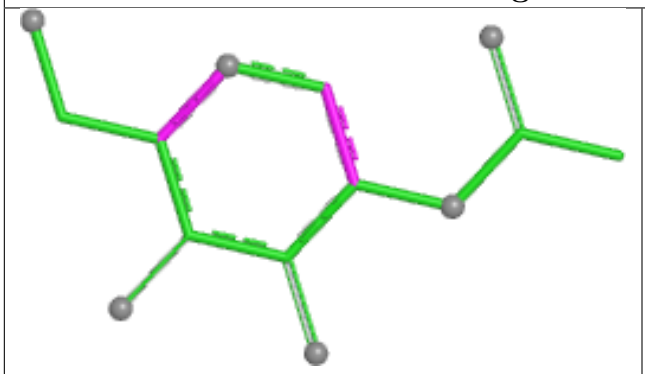
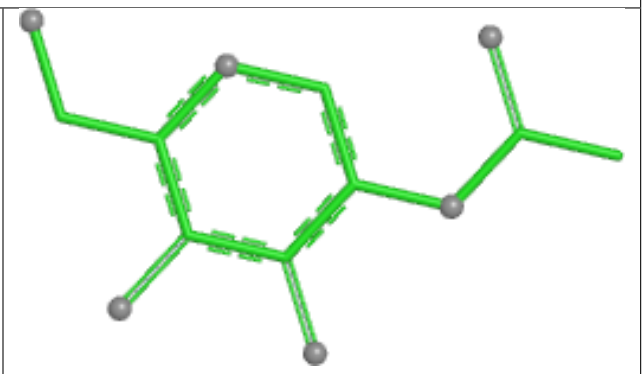


Rings

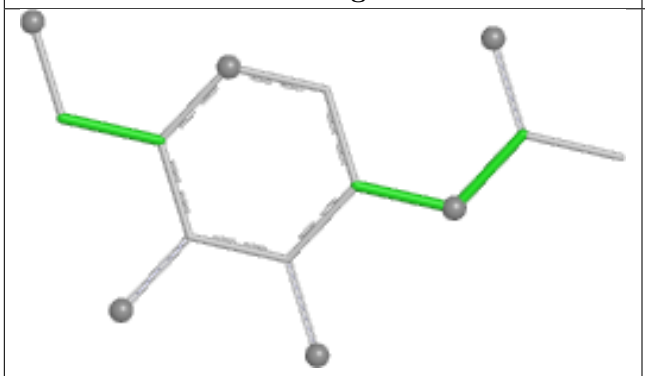
Ligand NAG A 1306



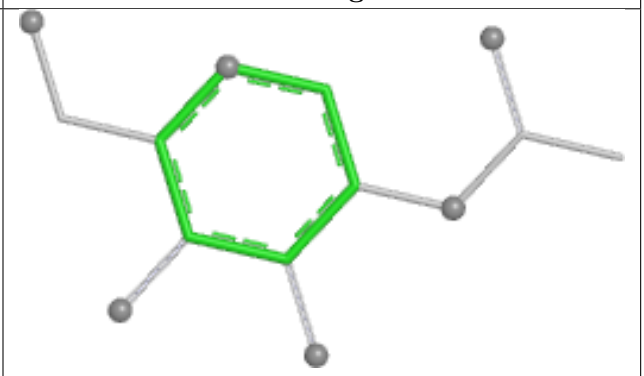
Bond lengths



Bond angles

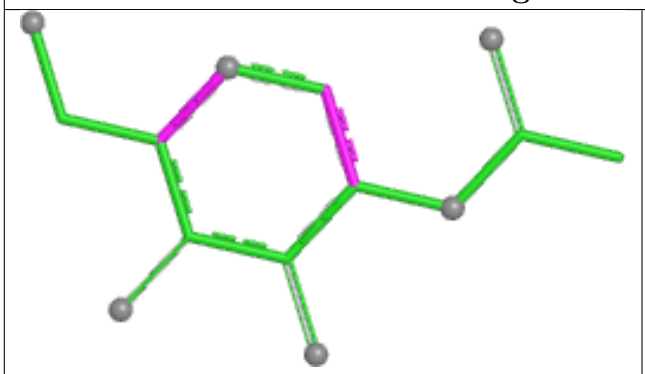


Torsions



Rings

Ligand NAG C 1307



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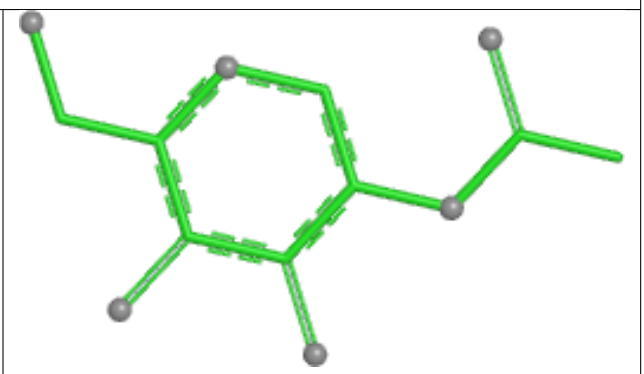

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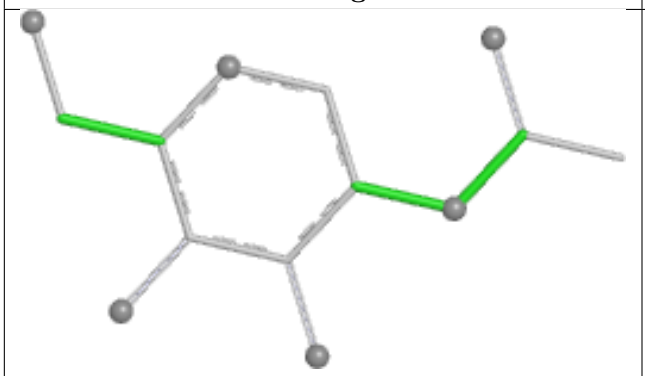

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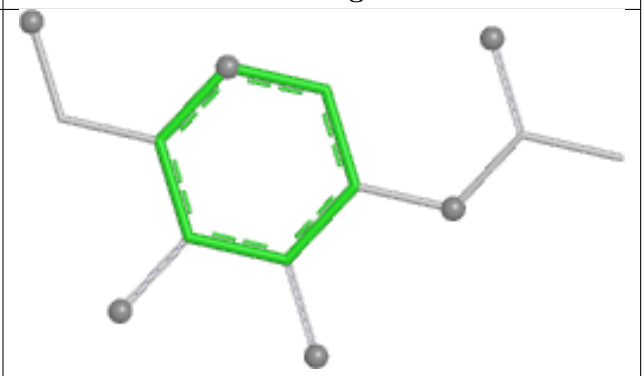
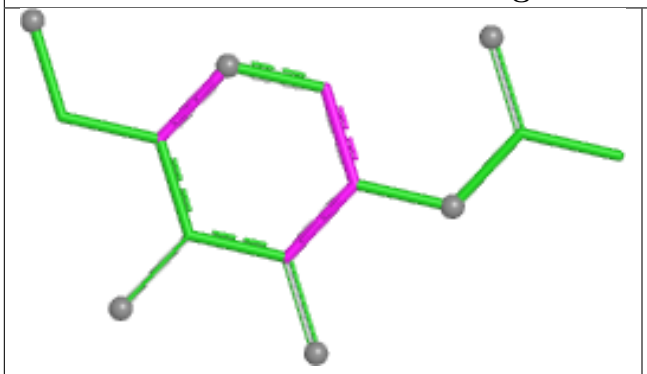


Rings

Ligand NAG B 1313



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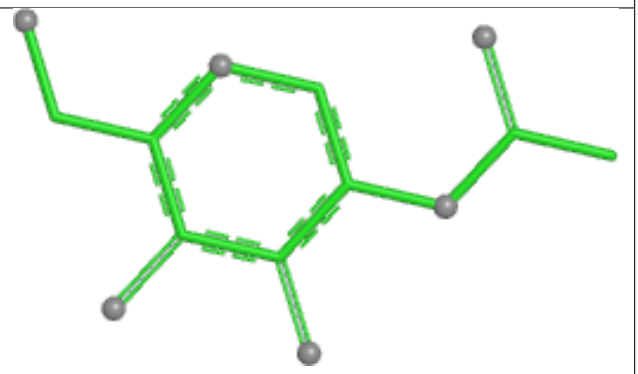
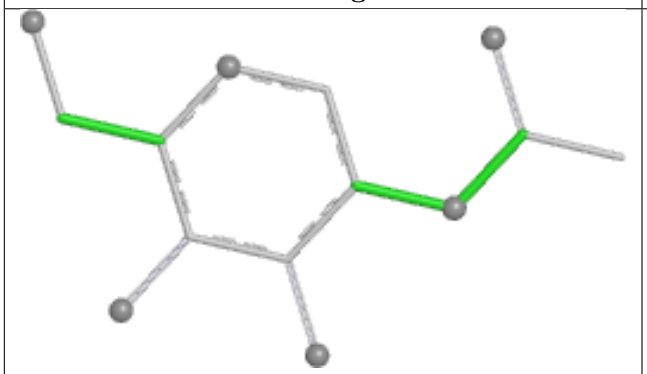


Bond angles



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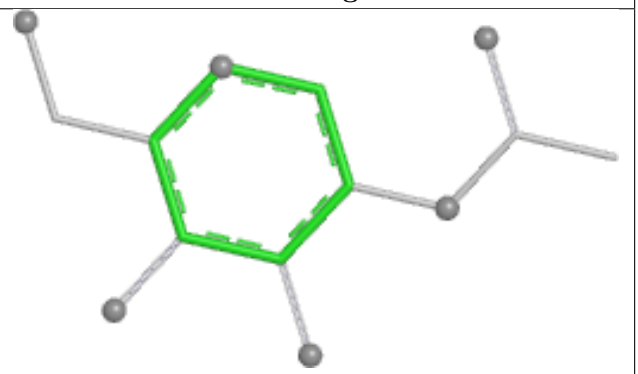
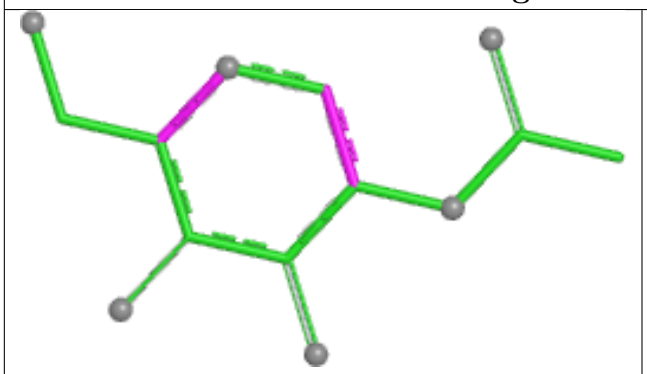


Rings

Ligand NAG C 1303



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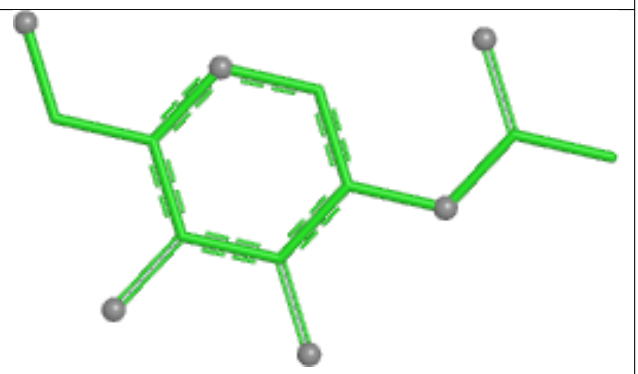

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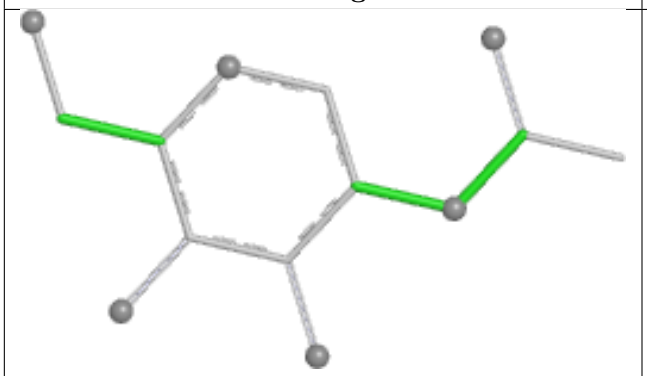

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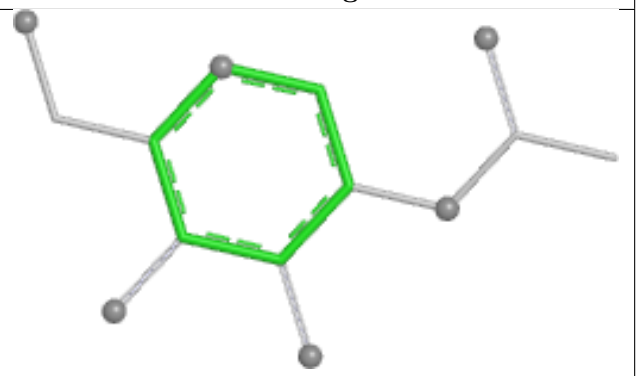
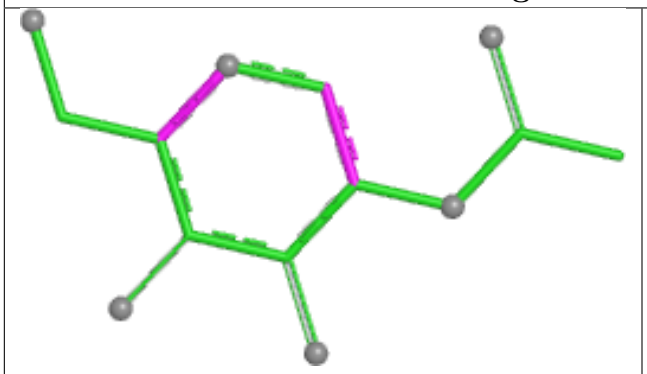


Rings

Ligand NAG C 1312



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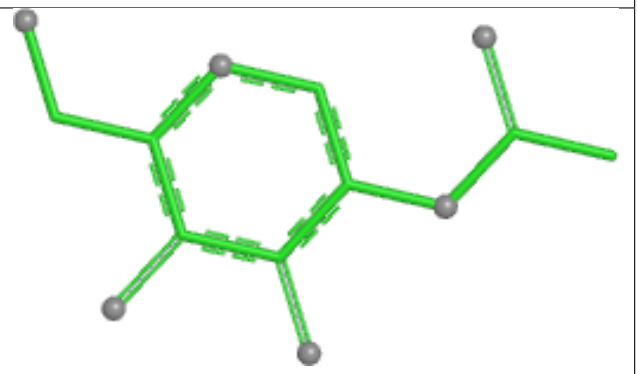
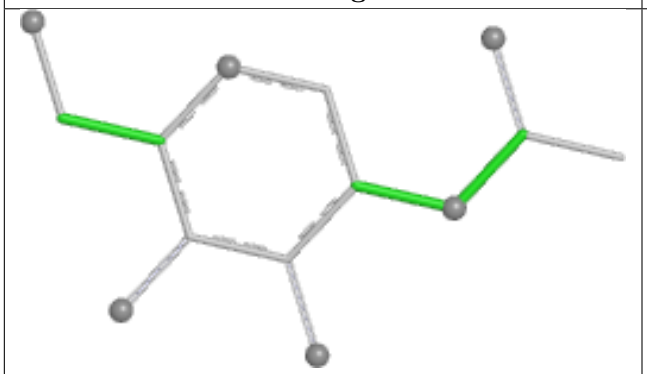


Bond angles



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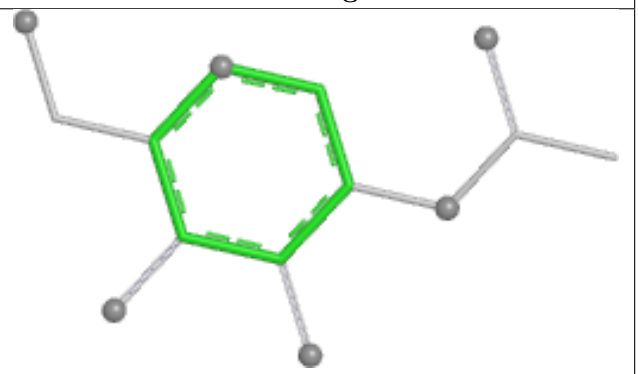
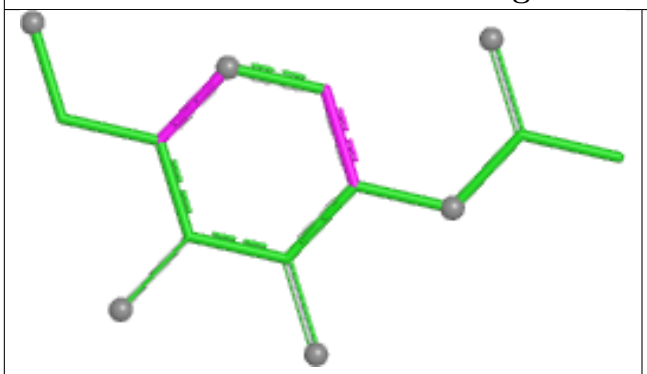


Rings

Ligand NAG B 1307



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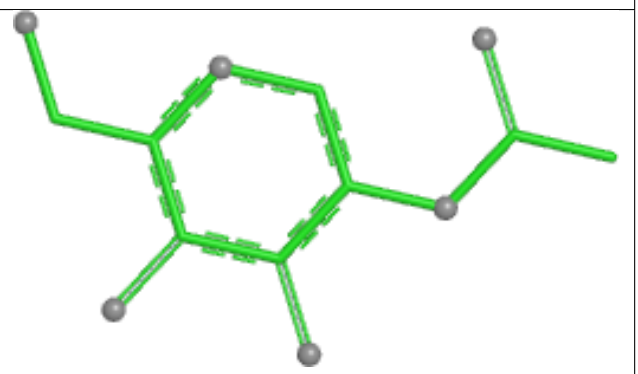
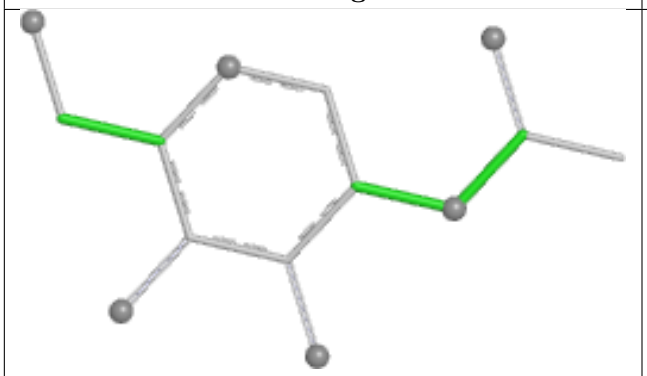


Bond angles



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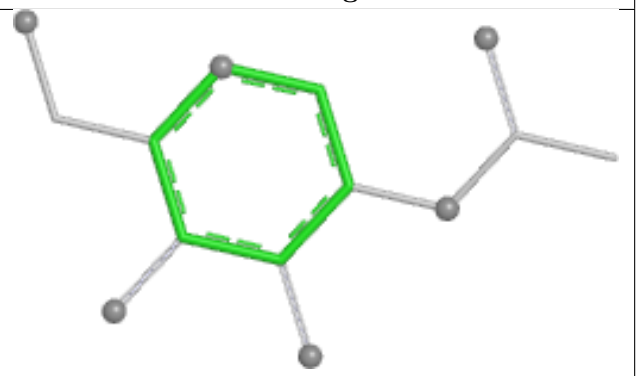

Rings

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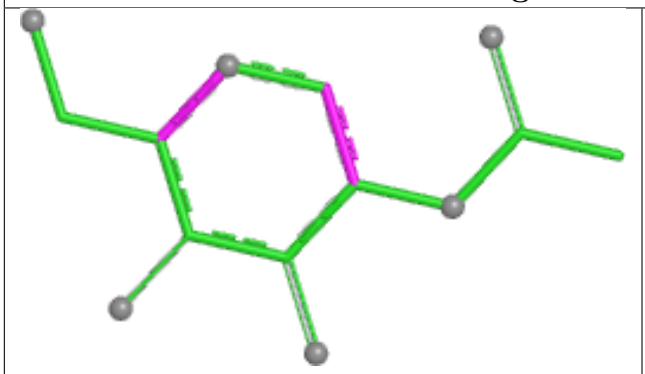

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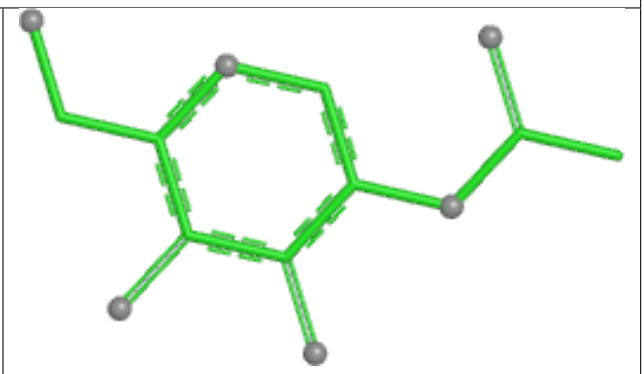
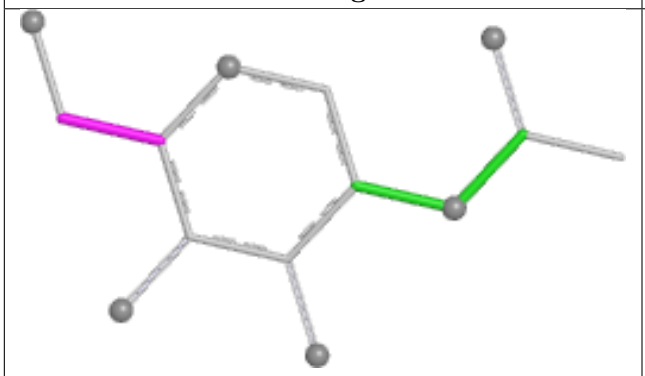


Bond angles



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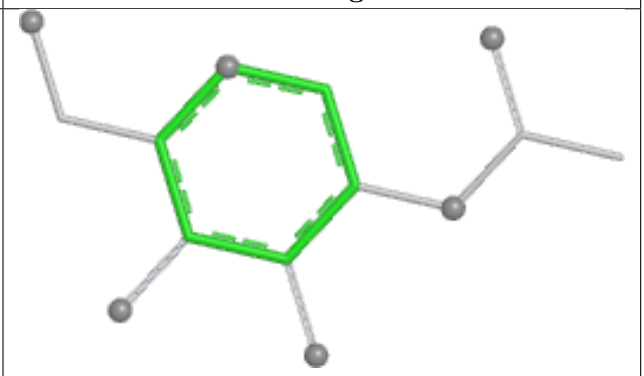
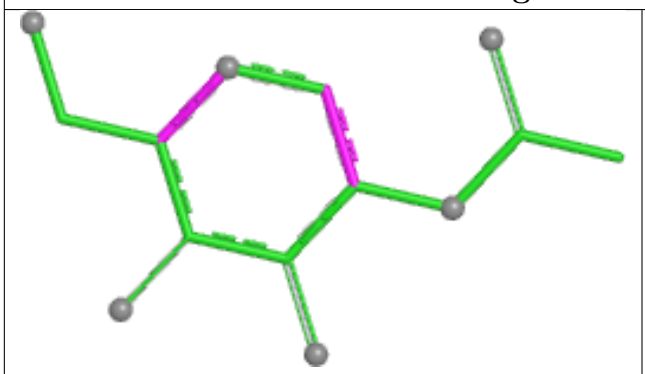


Rings

Ligand NAG B 1304



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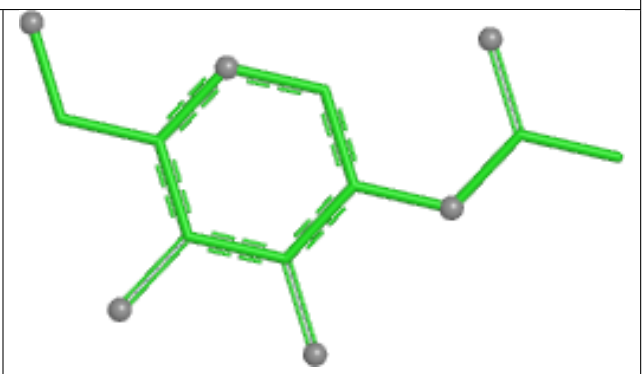
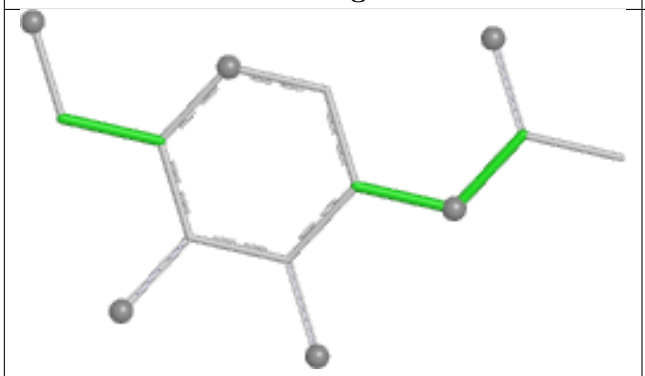


Bond angles



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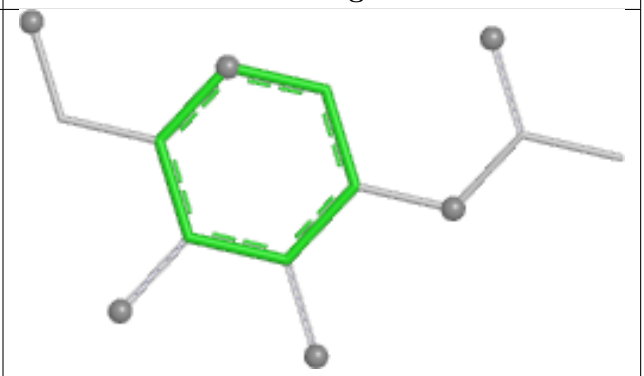
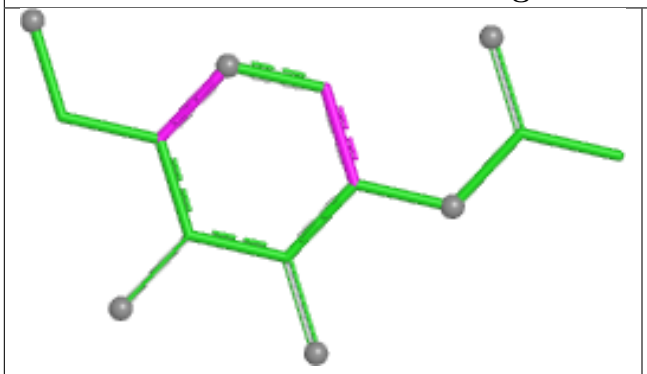


Rings

Ligand NAG C 1302



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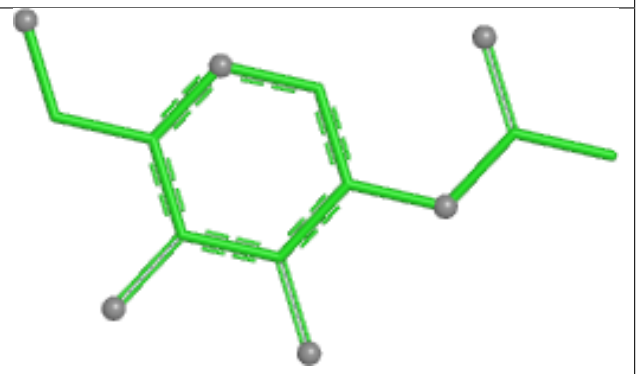
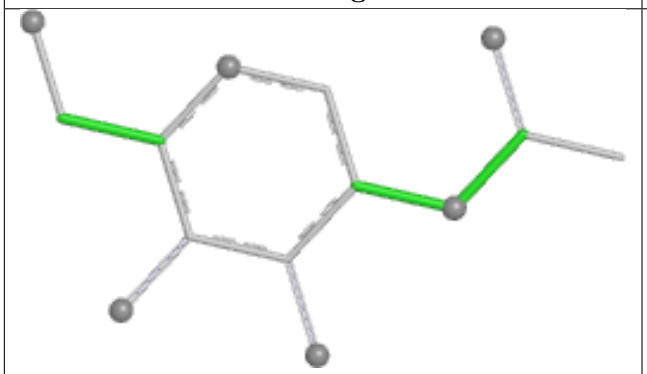


Bond angles



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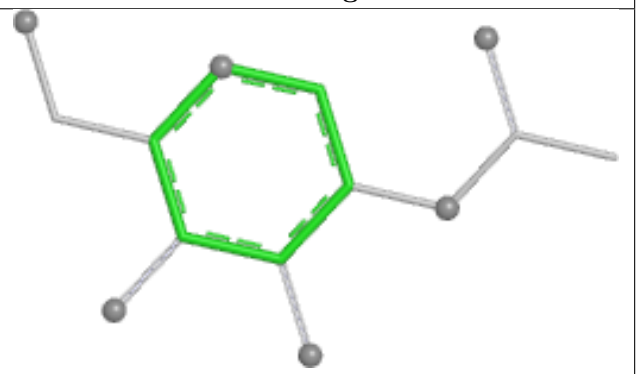

Rings

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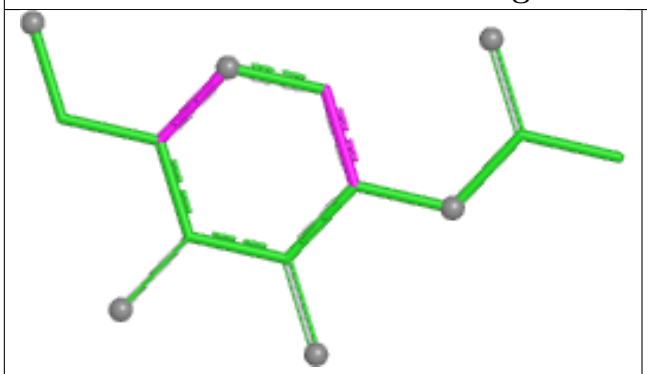

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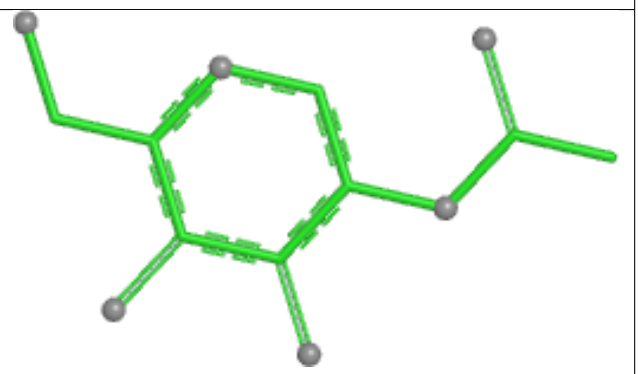
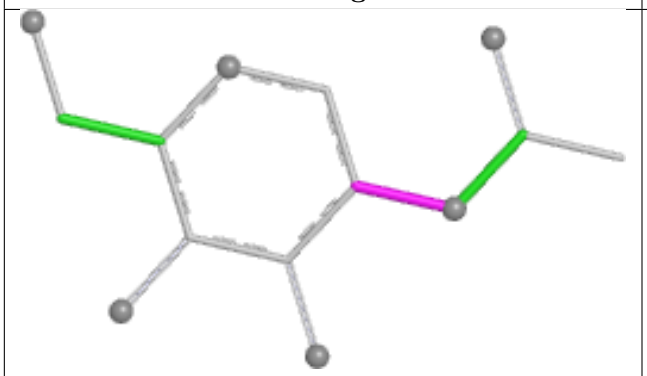


Bond angles



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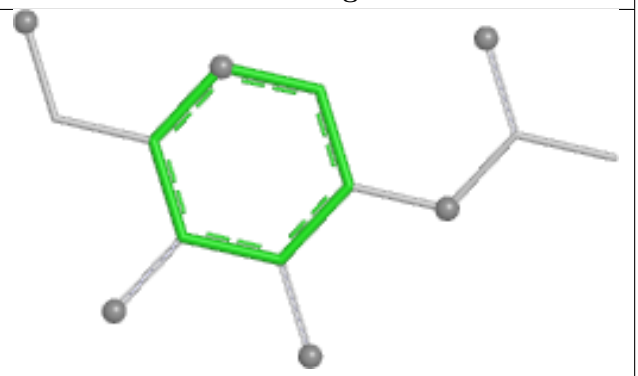
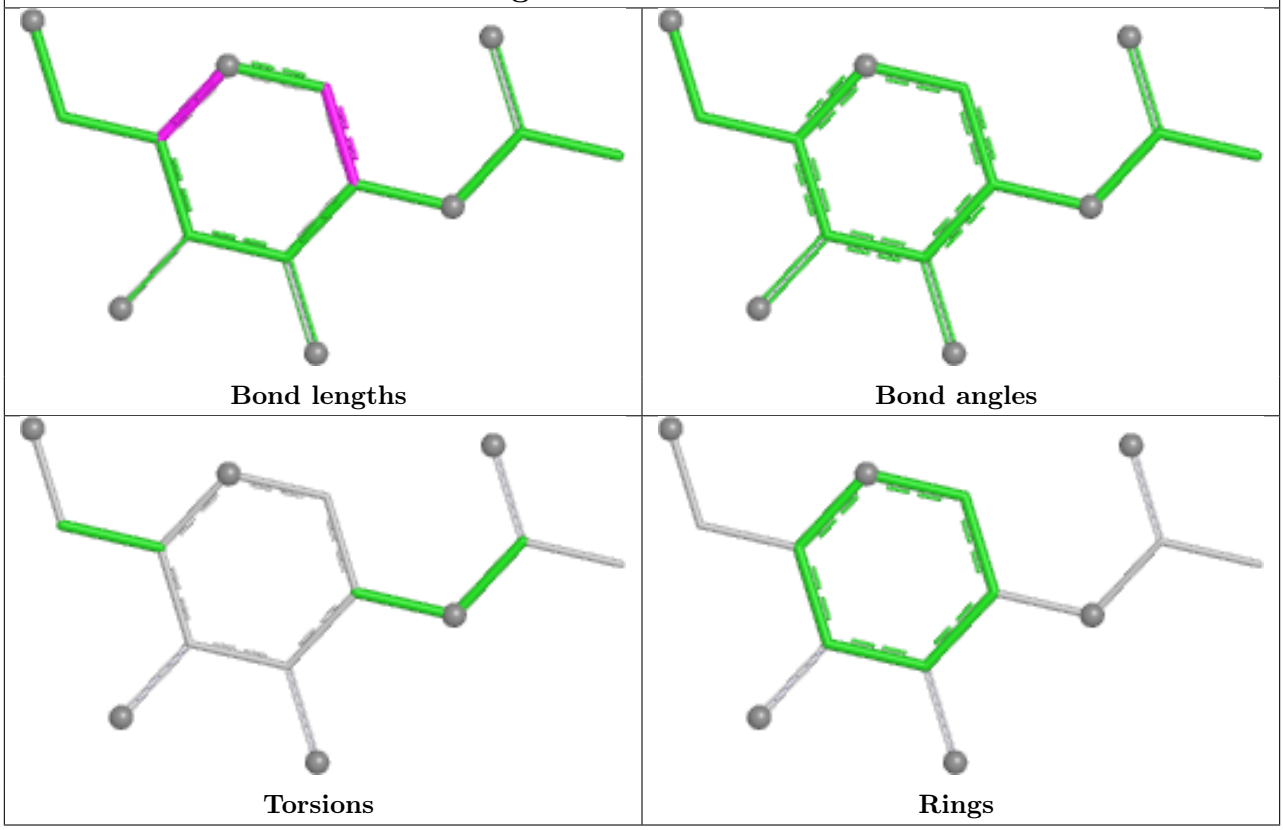
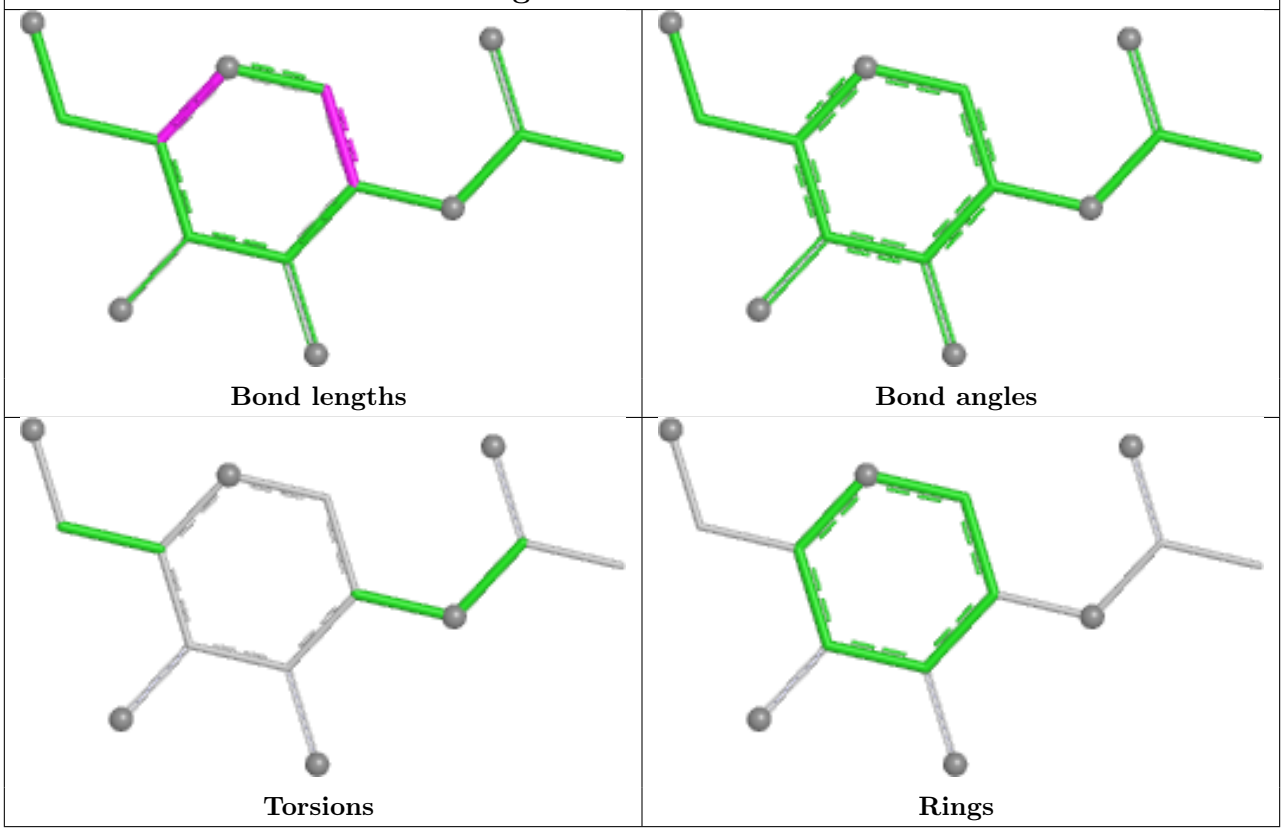


Rings

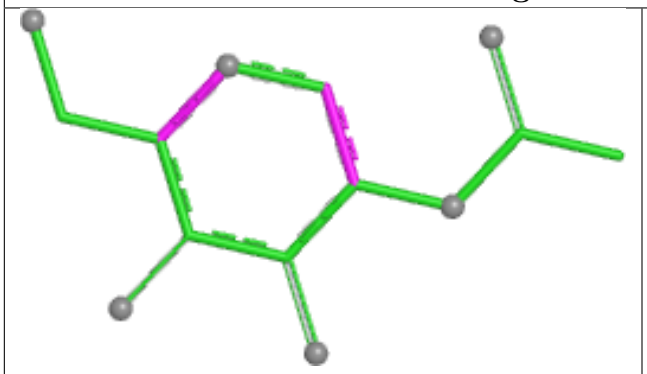
Ligand NAG A 1303



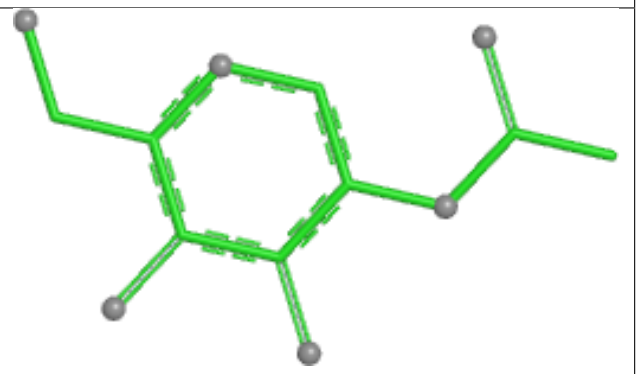
Ligand NAG B 1301



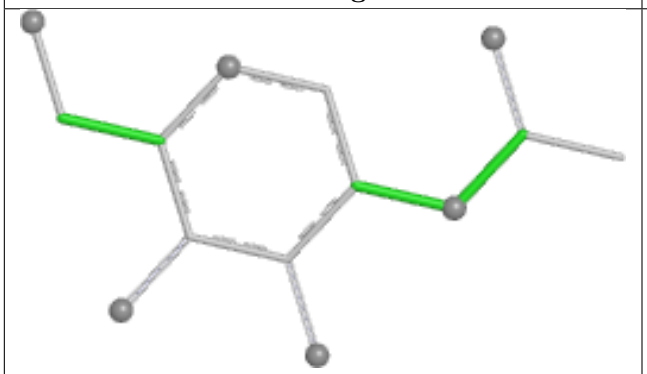
Ligand NAG C 1305



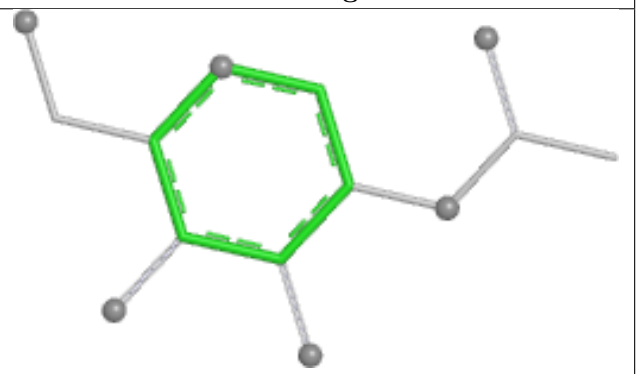
Bond lengths



Bond angles

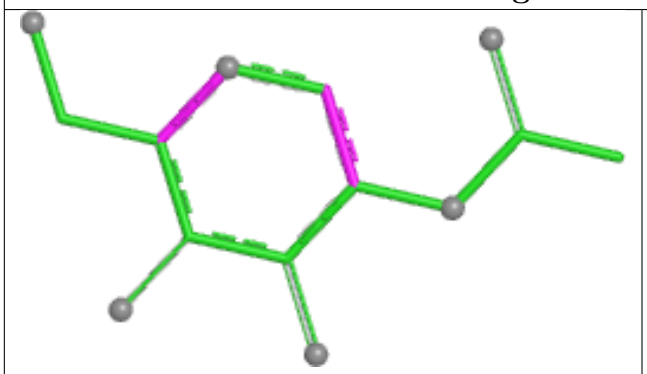


Torsions



Rings

Ligand NAG C 1311



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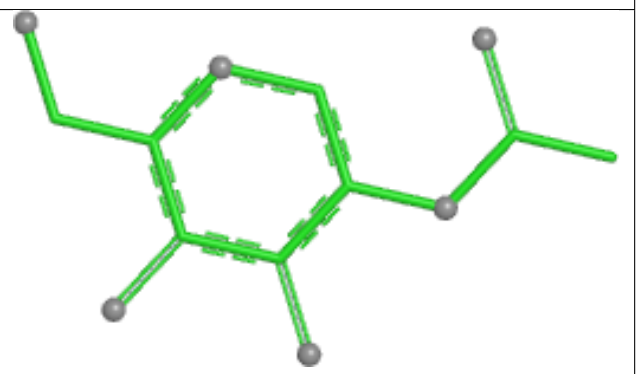
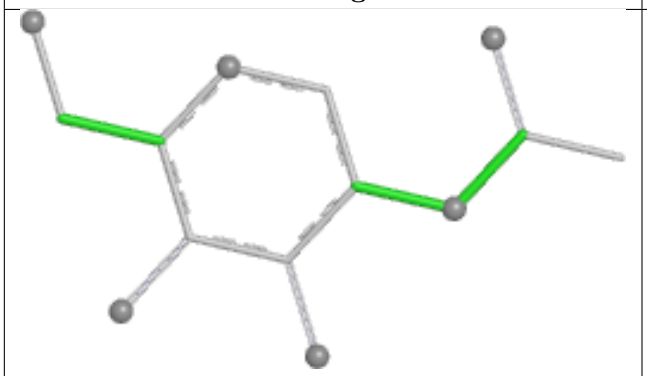
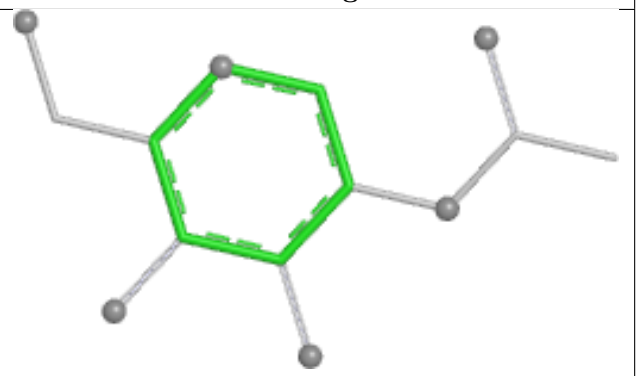


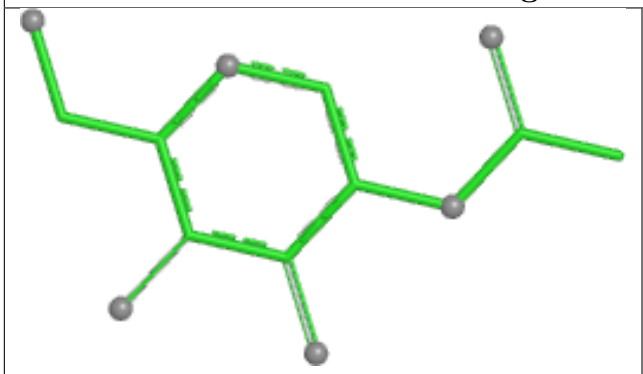
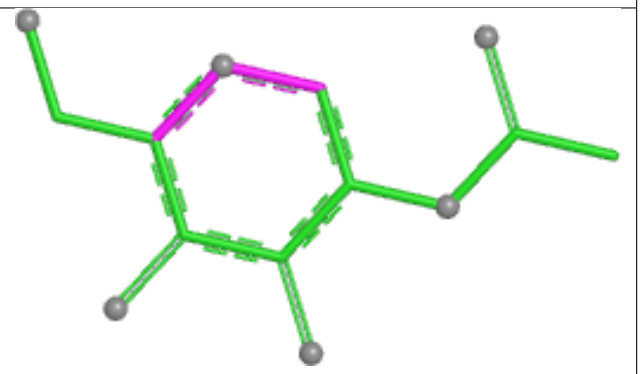
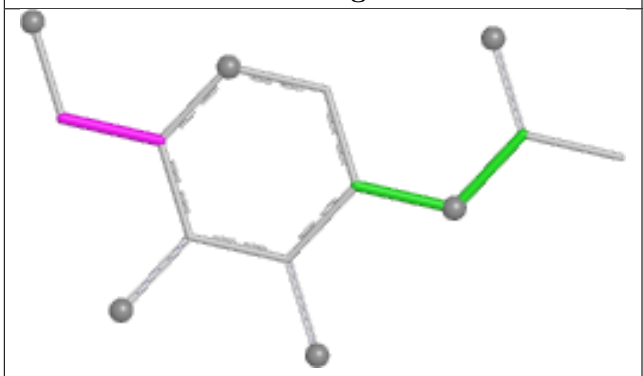
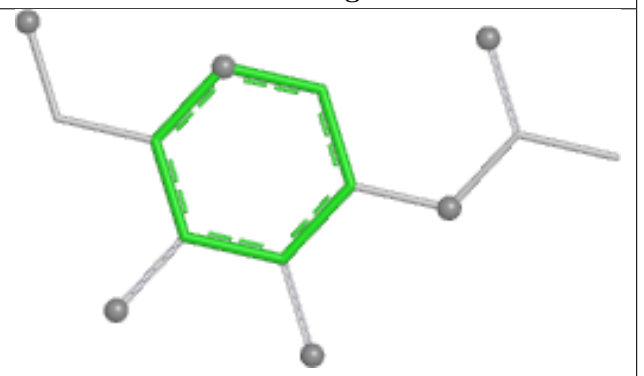
Bond angles



Torsions



Rings

Ligand NAG D 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

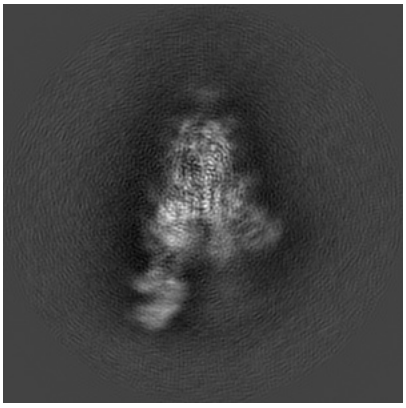
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22891. These allow visual inspection of the internal detail of the map and identification of artifacts.

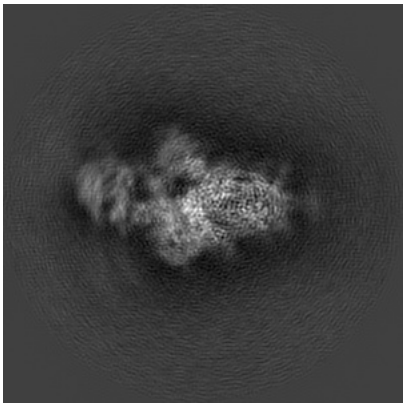
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

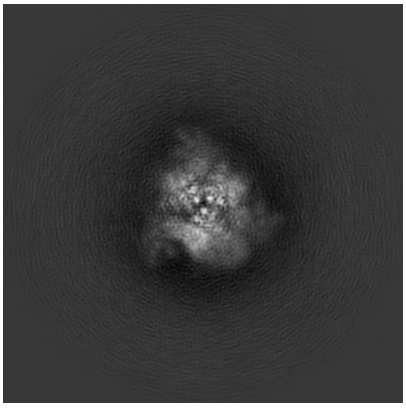
6.1.1 Primary map



X



Y

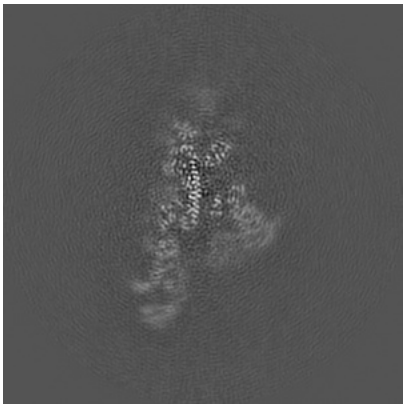


Z

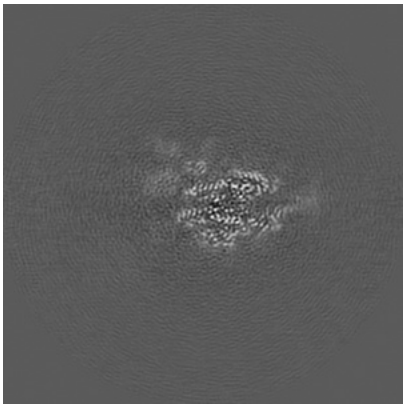
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

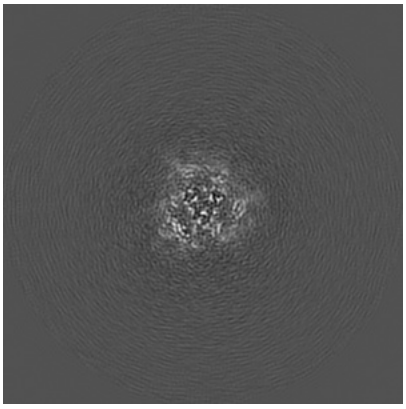
6.2.1 Primary map



X Index: 240



Y Index: 240

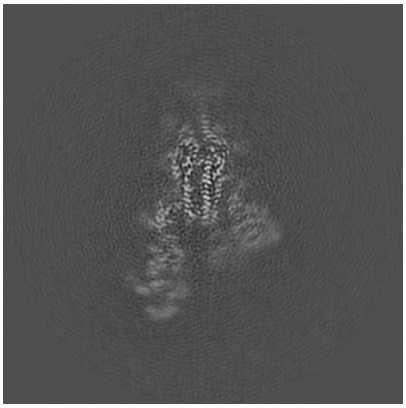


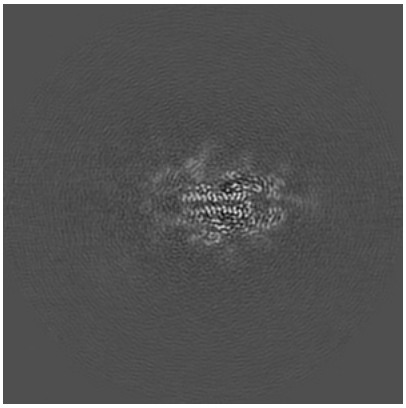
Z Index: 240

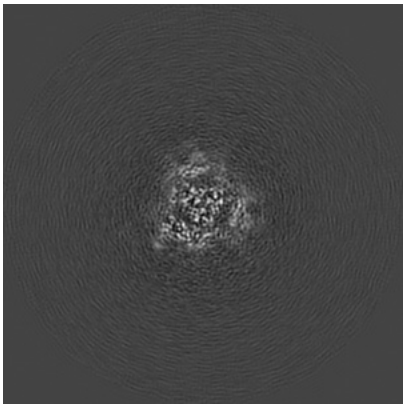
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 231

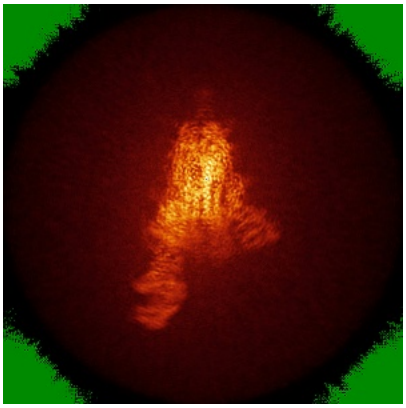

Y Index: 246

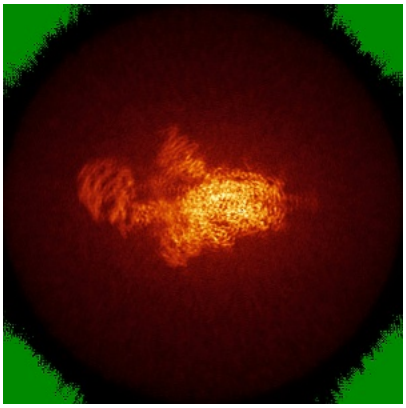

Z Index: 237

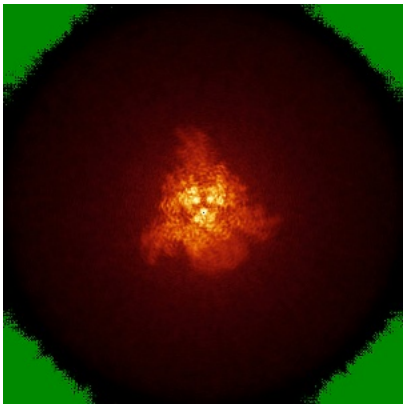
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

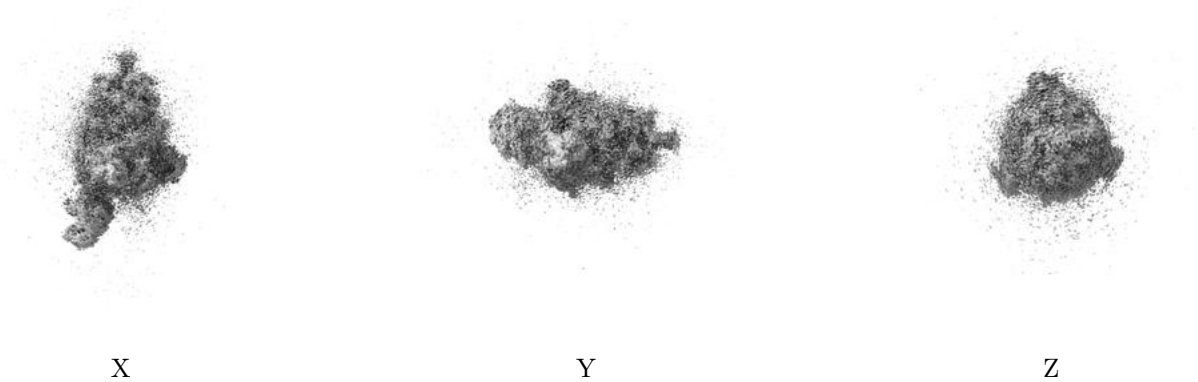

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

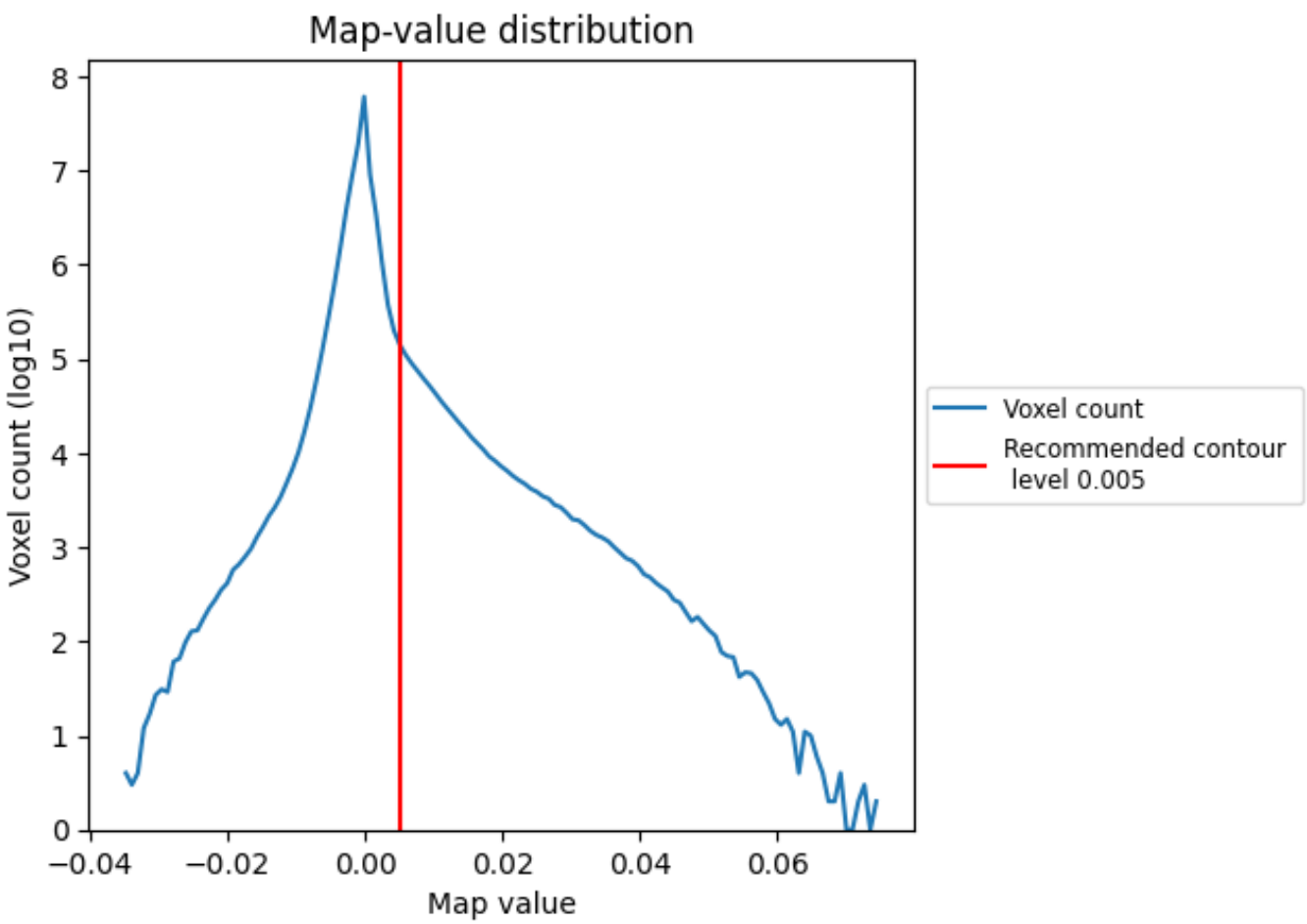
6.6 Mask visualisation (i)

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

7 Map analysis (i)

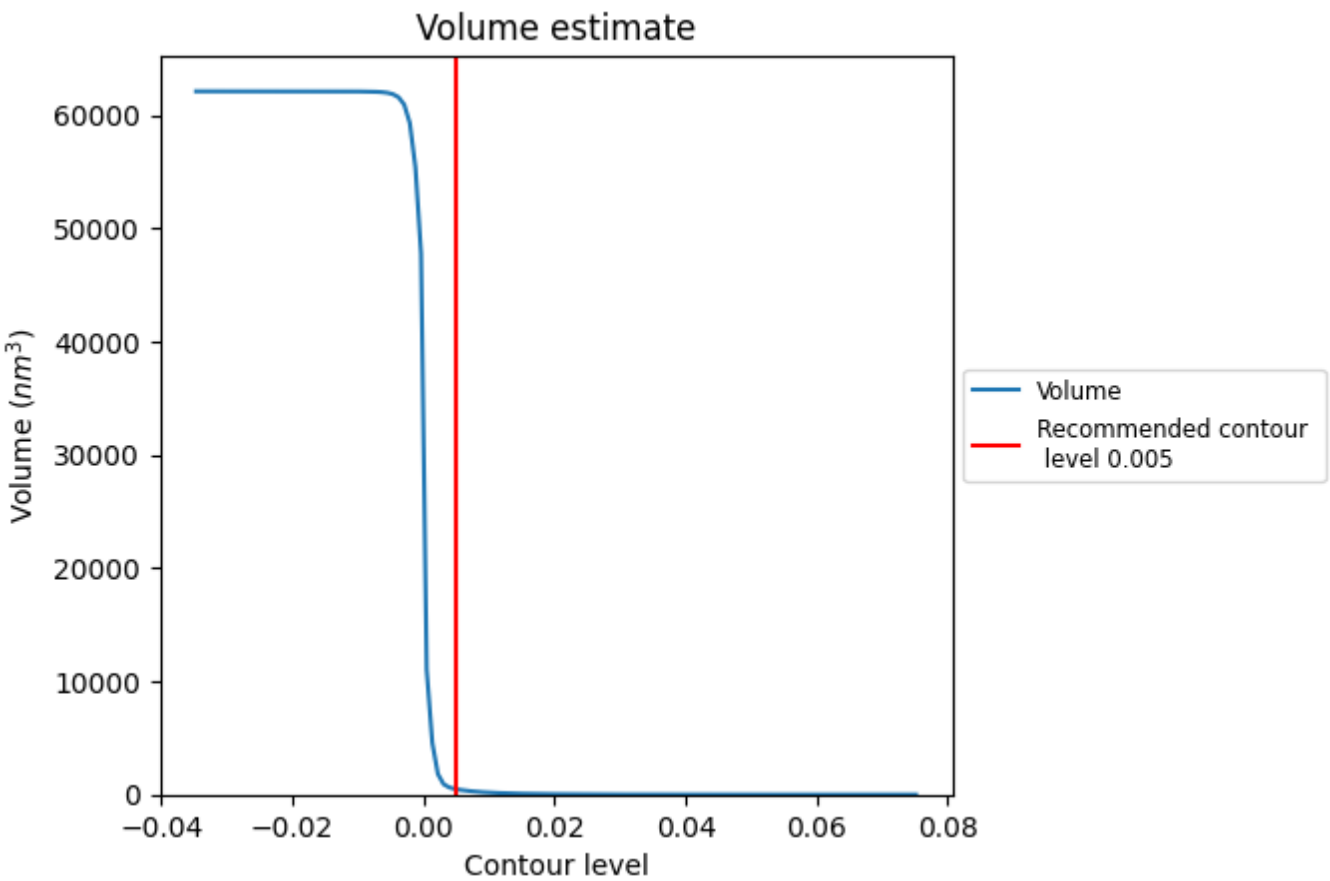
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

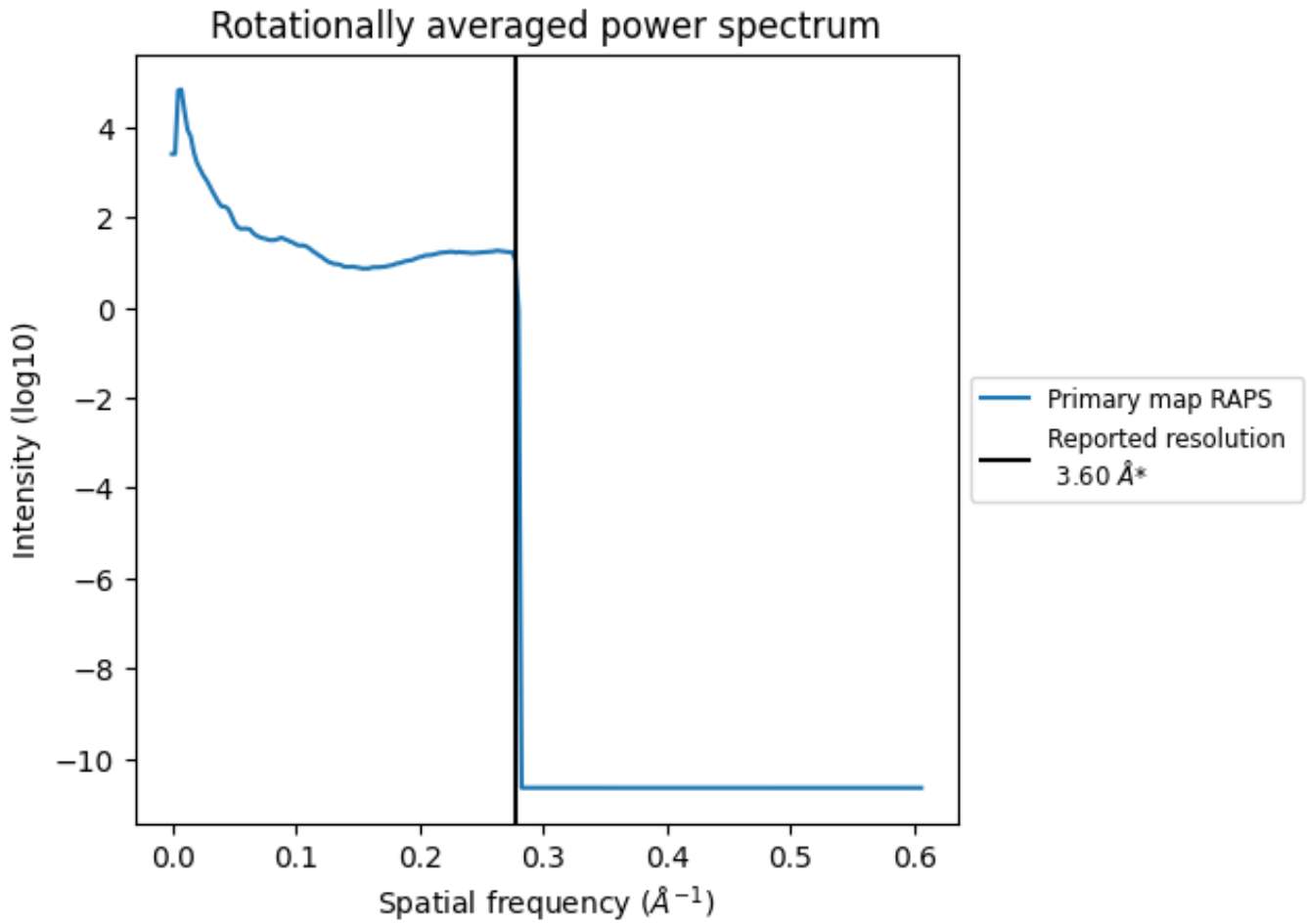
7.2 Volume estimate (i)



The volume at the recommended contour level is 478 nm^3; this corresponds to an approximate mass of 431 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 0.278 Å^{-1}

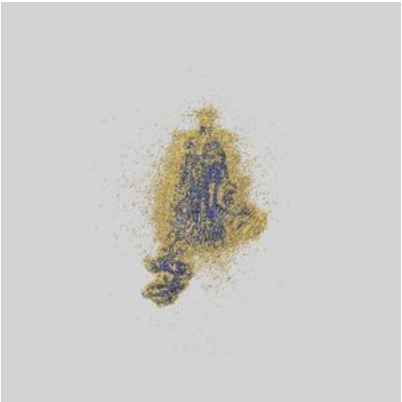
8 Fourier-Shell correlation (i)

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

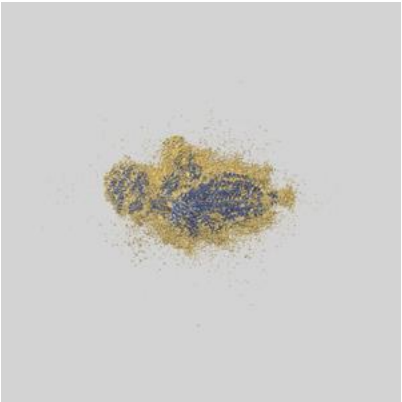
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22891 and PDB model 7KJ2. Per-residue inclusion information can be found in section 3 on page 12.

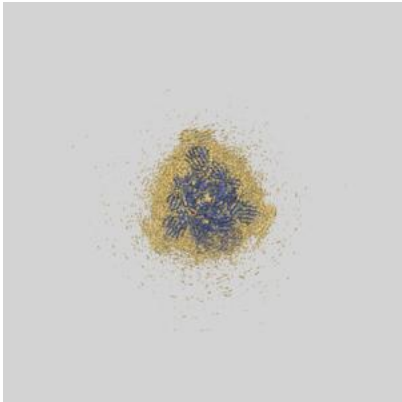
9.1 Map-model overlay (i)



X



Y



Z

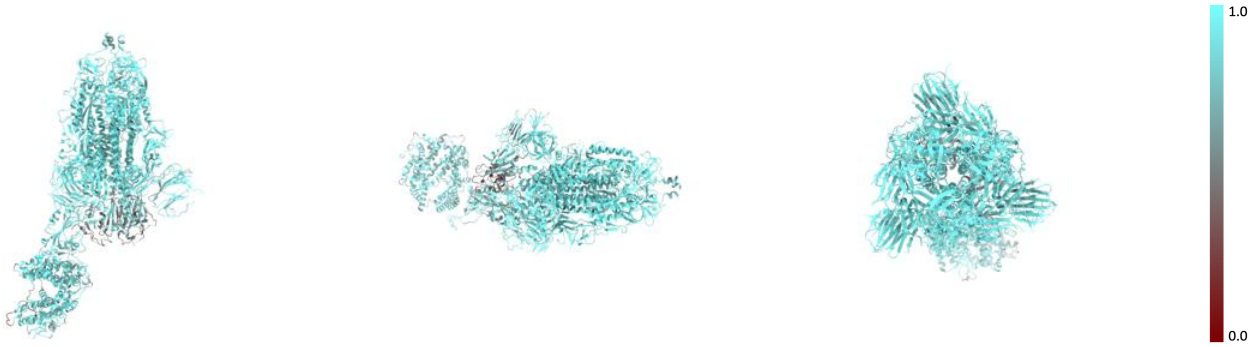
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

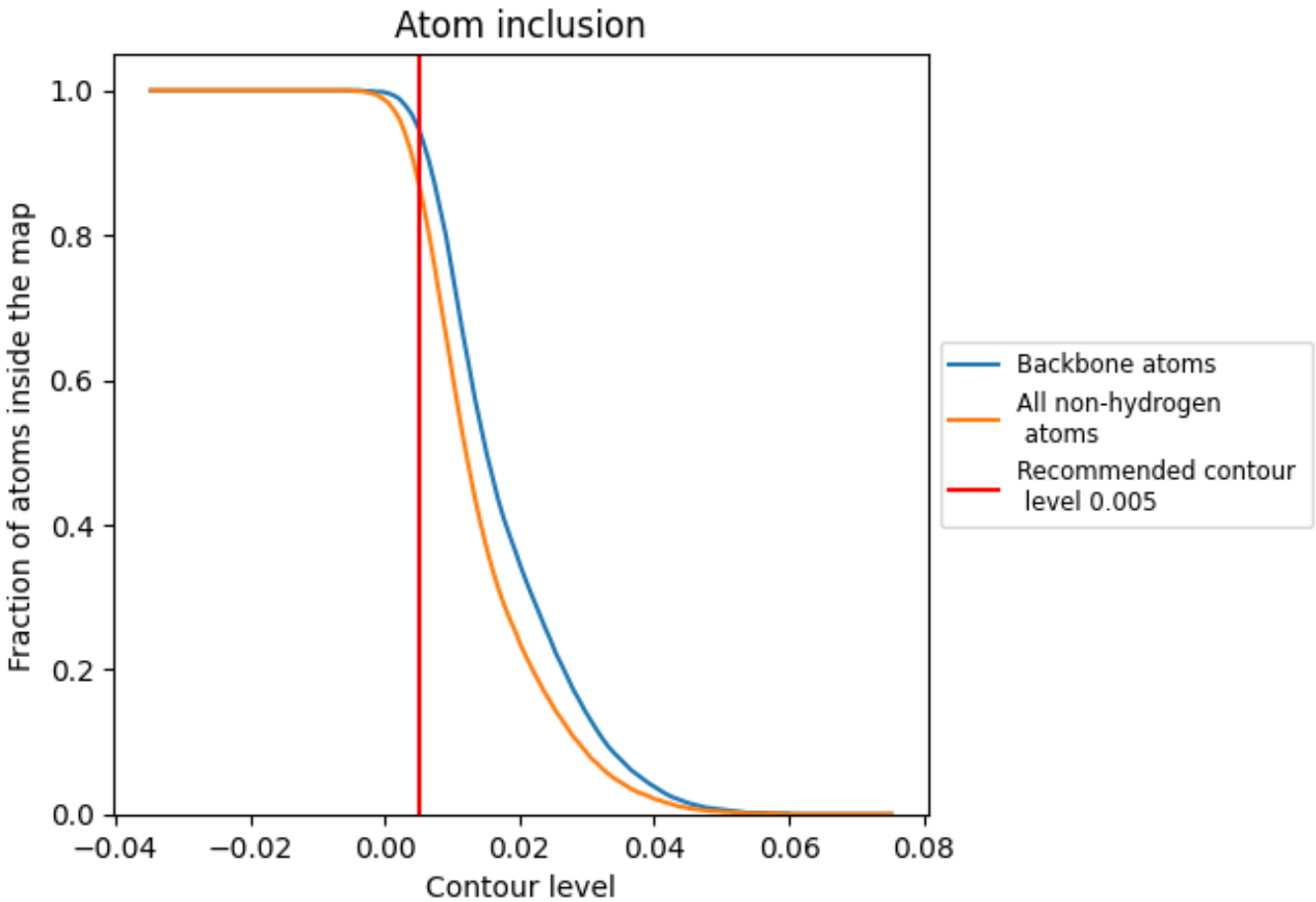
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.3550
A	0.8640	0.3700
B	0.9200	0.4070
C	0.8760	0.4020
D	0.8300	0.1840
E	0.5360	0.2600
F	0.8210	0.2340
G	0.8210	0.2770
H	0.8930	0.2800
I	0.7860	0.2320
J	0.8570	0.3320
K	0.7860	0.3300
L	0.6790	0.1360
M	0.8930	0.3600
N	0.6790	0.1680
O	0.8570	0.2990
P	0.7140	0.2700
Q	0.3930	0.0710
R	0.5360	0.0820
S	0.5360	0.1610
T	0.1430	0.0340
U	0.2860	0.0100