



Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 02:17 PM JST

PDB ID : 9JMN / pdb_00009jmn
EMDB ID : EMD-61607
Title : Cryo-EM structure of CN-HedgehogCoV (HKU31/Erinaceus amurensis/China/2014) S-trimer in a locked-1 conformation
Authors : Yuan, H.; Xiong, X.
Deposited on : 2024-09-20
Resolution : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

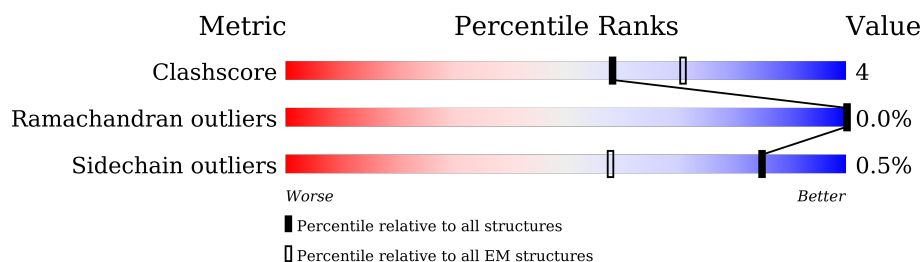
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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






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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1349	 73% 9% 18%
1	B	1349	 73% 10% 18%
1	C	1349	 72% 10% 18%
2	D	3	 67% 33%
2	E	3	 100%
2	F	3	 100%
2	H	3	 100%
2	I	3	 33% 67%

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Mol	Chain	Length	Quality of chain
2	K	3	 100%
3	G	2	 50%50%
3	J	2	 50%50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26833 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1110	Total	C	N	O	S	0	0
			8679	5501	1444	1677	57		
1	B	1110	Total	C	N	O	S	0	0
			8679	5501	1444	1677	57		
1	C	1110	Total	C	N	O	S	0	0
			8679	5501	1444	1677	57		

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1271	GLY	-	linker	UNP A0A5Q0TVR1
A	1272	SER	-	linker	UNP A0A5Q0TVR1
A	1294	LEU	PHE	conflict	UNP P10104
A	1300	LEU	-	expression tag	UNP P10104
A	1301	GLU	-	expression tag	UNP P10104
A	1302	VAL	-	expression tag	UNP P10104
A	1303	LEU	-	expression tag	UNP P10104
A	1304	PHE	-	expression tag	UNP P10104
A	1305	GLN	-	expression tag	UNP P10104
A	1306	GLY	-	expression tag	UNP P10104
A	1307	PRO	-	expression tag	UNP P10104
A	1308	GLY	-	expression tag	UNP P10104
A	1309	HIS	-	expression tag	UNP P10104
A	1310	HIS	-	expression tag	UNP P10104
A	1311	HIS	-	expression tag	UNP P10104
A	1312	HIS	-	expression tag	UNP P10104
A	1313	HIS	-	expression tag	UNP P10104
A	1314	HIS	-	expression tag	UNP P10104
A	1315	HIS	-	expression tag	UNP P10104
A	1316	HIS	-	expression tag	UNP P10104
A	1317	SER	-	expression tag	UNP P10104
A	1318	ALA	-	expression tag	UNP P10104
A	1319	TRP	-	expression tag	UNP P10104
A	1320	SER	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1321	HIS	-	expression tag	UNP P10104
A	1322	PRO	-	expression tag	UNP P10104
A	1323	GLN	-	expression tag	UNP P10104
A	1324	PHE	-	expression tag	UNP P10104
A	1325	GLU	-	expression tag	UNP P10104
A	1326	LYS	-	expression tag	UNP P10104
A	1327	GLY	-	expression tag	UNP P10104
A	1328	GLY	-	expression tag	UNP P10104
A	1329	GLY	-	expression tag	UNP P10104
A	1330	SER	-	expression tag	UNP P10104
A	1331	GLY	-	expression tag	UNP P10104
A	1332	GLY	-	expression tag	UNP P10104
A	1333	GLY	-	expression tag	UNP P10104
A	1334	GLY	-	expression tag	UNP P10104
A	1335	SER	-	expression tag	UNP P10104
A	1336	GLY	-	expression tag	UNP P10104
A	1337	GLY	-	expression tag	UNP P10104
A	1338	SER	-	expression tag	UNP P10104
A	1339	ALA	-	expression tag	UNP P10104
A	1340	TRP	-	expression tag	UNP P10104
A	1341	SER	-	expression tag	UNP P10104
A	1342	HIS	-	expression tag	UNP P10104
A	1343	PRO	-	expression tag	UNP P10104
A	1344	GLN	-	expression tag	UNP P10104
A	1345	PHE	-	expression tag	UNP P10104
A	1346	GLU	-	expression tag	UNP P10104
A	1347	LYS	-	expression tag	UNP P10104
A	1348	SER	-	expression tag	UNP P10104
A	1349	ALA	-	expression tag	UNP P10104
B	1271	GLY	-	linker	UNP A0A5Q0TVR1
B	1272	SER	-	linker	UNP A0A5Q0TVR1
B	1294	LEU	PHE	conflict	UNP P10104
B	1300	LEU	-	expression tag	UNP P10104
B	1301	GLU	-	expression tag	UNP P10104
B	1302	VAL	-	expression tag	UNP P10104
B	1303	LEU	-	expression tag	UNP P10104
B	1304	PHE	-	expression tag	UNP P10104
B	1305	GLN	-	expression tag	UNP P10104
B	1306	GLY	-	expression tag	UNP P10104
B	1307	PRO	-	expression tag	UNP P10104
B	1308	GLY	-	expression tag	UNP P10104
B	1309	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1310	HIS	-	expression tag	UNP P10104
B	1311	HIS	-	expression tag	UNP P10104
B	1312	HIS	-	expression tag	UNP P10104
B	1313	HIS	-	expression tag	UNP P10104
B	1314	HIS	-	expression tag	UNP P10104
B	1315	HIS	-	expression tag	UNP P10104
B	1316	HIS	-	expression tag	UNP P10104
B	1317	SER	-	expression tag	UNP P10104
B	1318	ALA	-	expression tag	UNP P10104
B	1319	TRP	-	expression tag	UNP P10104
B	1320	SER	-	expression tag	UNP P10104
B	1321	HIS	-	expression tag	UNP P10104
B	1322	PRO	-	expression tag	UNP P10104
B	1323	GLN	-	expression tag	UNP P10104
B	1324	PHE	-	expression tag	UNP P10104
B	1325	GLU	-	expression tag	UNP P10104
B	1326	LYS	-	expression tag	UNP P10104
B	1327	GLY	-	expression tag	UNP P10104
B	1328	GLY	-	expression tag	UNP P10104
B	1329	GLY	-	expression tag	UNP P10104
B	1330	SER	-	expression tag	UNP P10104
B	1331	GLY	-	expression tag	UNP P10104
B	1332	GLY	-	expression tag	UNP P10104
B	1333	GLY	-	expression tag	UNP P10104
B	1334	GLY	-	expression tag	UNP P10104
B	1335	SER	-	expression tag	UNP P10104
B	1336	GLY	-	expression tag	UNP P10104
B	1337	GLY	-	expression tag	UNP P10104
B	1338	SER	-	expression tag	UNP P10104
B	1339	ALA	-	expression tag	UNP P10104
B	1340	TRP	-	expression tag	UNP P10104
B	1341	SER	-	expression tag	UNP P10104
B	1342	HIS	-	expression tag	UNP P10104
B	1343	PRO	-	expression tag	UNP P10104
B	1344	GLN	-	expression tag	UNP P10104
B	1345	PHE	-	expression tag	UNP P10104
B	1346	GLU	-	expression tag	UNP P10104
B	1347	LYS	-	expression tag	UNP P10104
B	1348	SER	-	expression tag	UNP P10104
B	1349	ALA	-	expression tag	UNP P10104
C	1271	GLY	-	linker	UNP A0A5Q0TVR1
C	1272	SER	-	linker	UNP A0A5Q0TVR1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1294	LEU	PHE	conflict	UNP P10104
C	1300	LEU	-	expression tag	UNP P10104
C	1301	GLU	-	expression tag	UNP P10104
C	1302	VAL	-	expression tag	UNP P10104
C	1303	LEU	-	expression tag	UNP P10104
C	1304	PHE	-	expression tag	UNP P10104
C	1305	GLN	-	expression tag	UNP P10104
C	1306	GLY	-	expression tag	UNP P10104
C	1307	PRO	-	expression tag	UNP P10104
C	1308	GLY	-	expression tag	UNP P10104
C	1309	HIS	-	expression tag	UNP P10104
C	1310	HIS	-	expression tag	UNP P10104
C	1311	HIS	-	expression tag	UNP P10104
C	1312	HIS	-	expression tag	UNP P10104
C	1313	HIS	-	expression tag	UNP P10104
C	1314	HIS	-	expression tag	UNP P10104
C	1315	HIS	-	expression tag	UNP P10104
C	1316	HIS	-	expression tag	UNP P10104
C	1317	SER	-	expression tag	UNP P10104
C	1318	ALA	-	expression tag	UNP P10104
C	1319	TRP	-	expression tag	UNP P10104
C	1320	SER	-	expression tag	UNP P10104
C	1321	HIS	-	expression tag	UNP P10104
C	1322	PRO	-	expression tag	UNP P10104
C	1323	GLN	-	expression tag	UNP P10104
C	1324	PHE	-	expression tag	UNP P10104
C	1325	GLU	-	expression tag	UNP P10104
C	1326	LYS	-	expression tag	UNP P10104
C	1327	GLY	-	expression tag	UNP P10104
C	1328	GLY	-	expression tag	UNP P10104
C	1329	GLY	-	expression tag	UNP P10104
C	1330	SER	-	expression tag	UNP P10104
C	1331	GLY	-	expression tag	UNP P10104
C	1332	GLY	-	expression tag	UNP P10104
C	1333	GLY	-	expression tag	UNP P10104
C	1334	GLY	-	expression tag	UNP P10104
C	1335	SER	-	expression tag	UNP P10104
C	1336	GLY	-	expression tag	UNP P10104
C	1337	GLY	-	expression tag	UNP P10104
C	1338	SER	-	expression tag	UNP P10104
C	1339	ALA	-	expression tag	UNP P10104
C	1340	TRP	-	expression tag	UNP P10104

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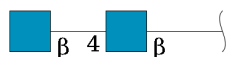
Chain	Residue	Modelled	Actual	Comment	Reference
C	1341	SER	-	expression tag	UNP P10104
C	1342	HIS	-	expression tag	UNP P10104
C	1343	PRO	-	expression tag	UNP P10104
C	1344	GLN	-	expression tag	UNP P10104
C	1345	PHE	-	expression tag	UNP P10104
C	1346	GLU	-	expression tag	UNP P10104
C	1347	LYS	-	expression tag	UNP P10104
C	1348	SER	-	expression tag	UNP P10104
C	1349	ALA	-	expression tag	UNP P10104

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	E	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	H	3	Total	C	N	O	0	0
			39	22	2	15		
2	I	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22	2	15		

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



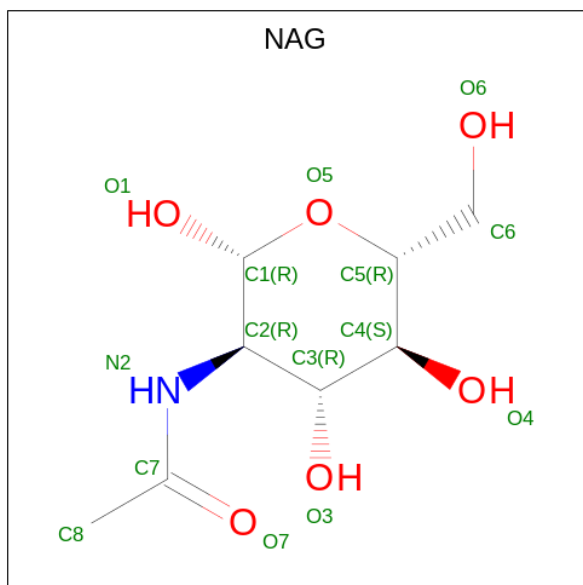
Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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	Total 14	8	1	5	0
4	A	1	Total 14	8	1	5	0
4	A	1	Total 14	8	1	5	0
4	A	1	Total 14	8	1	5	0
4	A	1	Total 14	8	1	5	0
4	A	1	Total 14	8	1	5	0
4	A	1	Total 14	8	1	5	0
4	A	1	Total 14	8	1	5	0
4	B	1	Total 14	8	1	5	0

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

- Molecule 5 is FOLIC ACID (CCD ID: FOL) (formula: C₁₉H₁₉N₇O₆) (labeled as "Ligand of Interest" by depositor).



- Molecule 6 is LINOLEIC ACID (CCD ID: EIC) (formula: $C_{18}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).

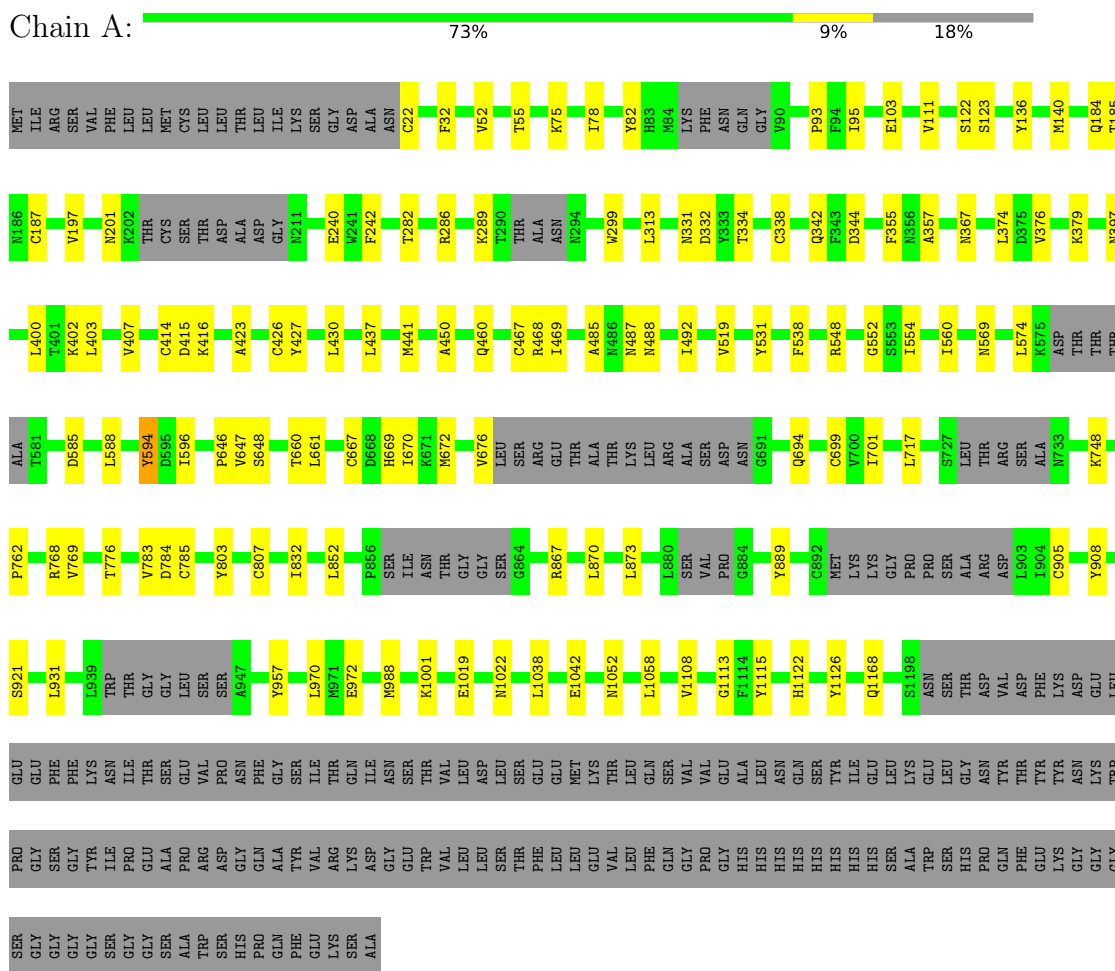


Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total 20	C 18	O 2	0
6	A	1	Total 20	C 18	O 2	0
6	B	1	Total 20	C 18	O 2	0

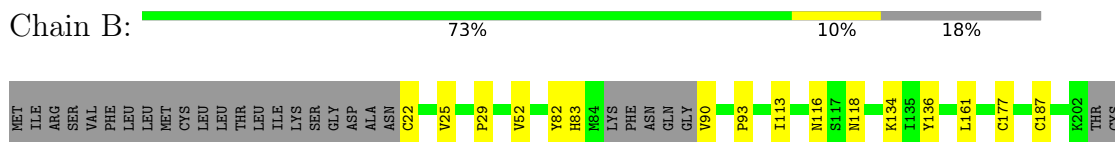
3 Residue-property plots

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,Fibritin



• Molecule 1: Spike glycoprotein,Fibritin



[illegible]

SER	VAL	VAL	GLU	ALA	LEU	ASN	GLN	SER	SER	TYR	ILE	GLU	LEU	LYS	GLU	SER	GLY	ASN	TYR	THR	TYR	TYR	LYS	ASN	LYS	TRP	PRO	GLY	SER	GLY	TYR	ILE	PRO	GLU	ALA	ALA	PRO	ARG	ASP	ASP	GLY	GLN	ALA	TYR	VAL	ARG	LYS	ASP	GLY	GLU	TRP	VAL	LEU	LEU	SER	SER	THR	PHE	LEU	LEU	GLU	VAL	VAL	LEU	PHE
GLN	GLY	PRO	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	GLY	GLY	SER	GLY	GLY	GLY	SER	GLY	SER	ALA	TRP	SER	SER	HIS	PRO	PRO	GLN	PHE	GLU	LYS	SER	SER	ALA																		

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

Chain D:  67% 33%

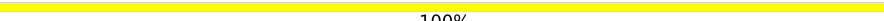
NAG1	NAG2	BMA3
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- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

NAG1	NAG2	BMA3
------	------	------

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

Chain F:  100%

NAG1	NAG2	BMA3
------	------	------

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

Chain H:  100%

NAG1	NAG2	BMA3
------	------	------

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

Chain I:  33% 67%

NAG1	NAG2	BMA3
------	------	------

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

Chain K:  100%

NAG1	NAG2	BMA3
------	------	------

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

Chain G:  50% 50%

MAG1
MAG2

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

Chain J:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23410	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	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: EIC, NAG, FOL, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/8867	0.39	0/12033
1	B	0.17	0/8867	0.37	0/12033
1	C	0.18	0/8867	0.38	1/12033 (0.0%)
All	All	0.18	0/26601	0.38	1/36099 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	TYR	N-CA-C	-6.79	103.17	113.89

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	8679	0	8363	78	0
1	B	8679	0	8362	79	0
1	C	8679	0	8362	90	0
2	D	39	0	34	1	0
2	E	39	0	34	0	0
2	F	39	0	34	0	0
2	H	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	39	0	34	1	0
2	K	39	0	34	0	0
3	G	28	0	25	1	0
3	J	28	0	25	1	0
4	A	126	0	117	0	0
4	B	112	0	104	1	0
4	C	112	0	104	1	0
5	A	32	0	17	1	0
5	B	32	0	17	1	0
5	C	32	0	17	1	0
6	A	40	0	62	7	0
6	B	20	0	31	0	0
All	All	26833	0	25810	237	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 4.

All (237) 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:1040:THR:HA	1:B:1043:GLN:HE21	1.52	0.74
1:B:82:TYR:HE1	1:B:289:LYS:HA	1.59	0.68
1:A:487:ASN:OD1	1:A:488:ASN:ND2	2.28	0.67
1:B:587:LEU:HD13	1:B:592:ILE:HG13	1.76	0.66
1:A:55:THR:HG21	1:C:613:ILE:H	1.61	0.65
1:A:414:CYS:HB3	1:A:467:CYS:HA	1.79	0.65
1:B:1173:THR:HG23	1:B:1175:PHE:H	1.64	0.63
1:A:768:ARG:HD3	1:A:1122:HIS:HB2	1.81	0.62
1:A:460:GLN:OE1	1:A:468:ARG:NH1	2.33	0.61
1:A:867:ARG:NH2	1:A:921:SER:OG	2.34	0.61
1:B:885:TYR:HE2	1:B:916:PRO:HB3	1.66	0.61
1:B:177:CYS:HA	1:B:225:CYS:HB3	1.83	0.61
1:A:667:CYS:SG	1:A:694:GLN:NE2	2.73	0.60
1:A:776:THR:HG22	1:A:1113:GLY:HA2	1.83	0.60
1:C:332:ASP:OD1	1:C:332:ASP:N	2.35	0.60
1:C:135:ILE:HG21	1:C:299:TRP:HB3	1.84	0.59
1:B:748:LYS:HD2	1:C:839:PRO:HG3	1.84	0.59
1:B:660:THR:HB	1:B:701:ILE:HG12	1.85	0.59
1:A:136:TYR:O	1:A:286:ARG:NH1	2.35	0.59
1:A:376:VAL:HA	1:A:379:LYS:HB2	1.85	0.59
1:B:399:ASN:HB2	1:B:574:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1019:GLU:OE1	1:C:1022:ASN:ND2	2.35	0.58
1:C:460:GLN:OE1	1:C:468:ARG:NH1	2.38	0.57
1:B:29:PRO:HG2	4:B:1403:NAG:H62	1.86	0.57
1:C:36:TRP:H	1:C:76:GLN:HE22	1.53	0.57
1:B:722:CYS:SG	1:B:723:ALA:N	2.78	0.57
1:C:300:SER:OG	1:C:301:ALA:N	2.38	0.57
1:C:414:CYS:HB3	1:C:467:CYS:HA	1.86	0.57
1:C:32:PHE:HD1	1:C:78:ILE:HG13	1.70	0.56
1:A:22:CYS:N	1:A:185:THR:O	2.38	0.56
1:C:662:TYR:HB3	1:C:665:VAL:HB	1.87	0.56
1:C:1187:GLN:HA	4:C:1407:NAG:H82	1.87	0.56
1:A:594:TYR:HB3	1:A:596:ILE:HD12	1.86	0.56
1:A:660:THR:HB	1:A:701:ILE:HG12	1.86	0.56
1:B:1108:VAL:HG23	1:B:1115:TYR:HB3	1.87	0.56
1:B:83:HIS:O	1:B:90:VAL:N	2.38	0.56
1:A:75:LYS:NZ	1:A:103:GLU:OE2	2.39	0.56
1:B:400:LEU:HD22	1:B:423:ALA:HB2	1.88	0.56
1:A:492:ILE:HG12	1:A:519:VAL:HG21	1.87	0.56
1:A:870:LEU:HD23	1:A:1108:VAL:HG21	1.87	0.56
1:A:299:TRP:O	5:A:1410:FOL:NA2	2.38	0.55
1:B:847:ASP:OD2	1:B:975:LYS:NZ	2.39	0.55
1:B:434:TRP:HD1	1:B:556:MET:HE1	1.71	0.55
1:C:265:ASN:HD21	1:C:322:ILE:H	1.55	0.55
1:A:769:VAL:HG11	1:A:988:MET:HG3	1.88	0.55
1:C:111:VAL:HG12	1:C:304:ILE:HG12	1.89	0.55
1:B:25:VAL:HA	1:B:93:PRO:HD2	1.89	0.55
1:C:263:SER:OG	1:C:264:ASN:N	2.40	0.54
1:A:82:TYR:HA	1:A:93:PRO:HA	1.88	0.54
1:B:460:GLN:OE1	1:B:468:ARG:NH1	2.40	0.54
1:C:337:GLN:HE21	1:C:343:PHE:HA	1.71	0.54
1:A:342:GLN:NE2	1:A:344:ASP:O	2.41	0.54
1:B:613:ILE:H	1:C:55:THR:HG21	1.73	0.54
1:C:347:SER:HB2	1:C:653:LYS:H	1.73	0.54
1:C:115:ALA:O	1:C:300:SER:OG	2.23	0.53
1:C:1136:CYS:SG	1:C:1137:ASP:N	2.80	0.53
1:B:82:TYR:HA	1:B:93:PRO:HA	1.91	0.53
1:B:116:ASN:ND2	5:B:1407:FOL:O4	2.42	0.53
1:C:777:SER:HA	1:C:821:GLN:HE22	1.74	0.53
1:A:55:THR:HB	1:C:619:VAL:HG12	1.89	0.53
1:B:783:VAL:HG11	1:B:1058:LEU:HD21	1.90	0.53
1:B:426:CYS:O	1:B:569:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:672:MET:HG3	1:C:673:ILE:HG23	1.90	0.53
1:C:56:TYR:HB3	1:C:59:ILE:HD11	1.90	0.53
1:C:1102:HIS:NE2	1:C:1105:SER:OG	2.42	0.53
1:C:1038:LEU:O	1:C:1043:GLN:NE2	2.42	0.52
1:A:832:ILE:HG23	1:A:931:LEU:HD22	1.91	0.52
1:C:238:ARG:HH11	2:I:2:NAG:H4	1.74	0.52
1:C:96:SER:OG	1:C:97:ASN:N	2.41	0.52
1:A:1038:LEU:HD13	1:A:1042:GLU:HG2	1.91	0.52
1:C:374:LEU:HD12	1:C:403:LEU:HD21	1.92	0.52
1:B:867:ARG:NH2	1:B:921:SER:OG	2.43	0.52
1:A:784:ASP:OD1	1:A:784:ASP:N	2.40	0.52
1:C:196:TYR:HE1	1:C:284:MET:HG2	1.75	0.52
1:C:226:LEU:O	1:C:227:PHE:C	2.51	0.52
1:B:662:TYR:HB3	1:B:665:VAL:HB	1.92	0.52
1:A:313:LEU:HD12	1:A:338:CYS:HA	1.92	0.52
1:B:667:CYS:N	1:B:699:CYS:SG	2.83	0.52
1:B:870:LEU:HD23	1:B:1108:VAL:HG21	1.91	0.52
1:C:100:TYR:HE1	1:C:152:LYS:HD2	1.76	0.51
1:B:1129:GLN:HG3	1:B:1167:TYR:HE2	1.74	0.51
1:A:32:PHE:HD2	1:A:78:ILE:HG13	1.75	0.51
1:C:492:ILE:HG12	1:C:519:VAL:HG21	1.93	0.51
1:C:722:CYS:SG	1:C:723:ALA:N	2.83	0.51
1:B:776:THR:HG22	1:B:1113:GLY:HA2	1.92	0.51
1:B:492:ILE:HG12	1:B:519:VAL:HG21	1.93	0.51
1:C:667:CYS:N	1:C:699:CYS:SG	2.84	0.50
1:B:313:LEU:HD12	1:B:338:CYS:HA	1.92	0.50
1:C:776:THR:HG22	1:C:1113:GLY:HA2	1.93	0.50
1:A:357:ALA:HA	1:A:676:VAL:HG21	1.92	0.50
1:C:826:LYS:HE3	1:C:918:LEU:HD21	1.94	0.50
1:C:29:PRO:HB3	1:C:97:ASN:HB2	1.92	0.50
1:B:619:VAL:HB	1:B:628:GLY:HA3	1.94	0.50
1:B:1023:THR:OG1	1:C:802:GLN:O	2.30	0.50
1:B:134:LYS:NZ	1:B:240:GLU:OE2	2.45	0.49
1:A:585:ASP:HA	1:A:588:LEU:HD13	1.94	0.49
1:A:957:TYR:HD1	1:A:970:LEU:HD22	1.77	0.49
1:C:99:SER:OG	1:C:195:SER:HB2	2.12	0.49
1:B:830:GLU:OE1	1:B:833:ARG:NH1	2.42	0.49
1:A:122:SER:OG	1:A:123:SER:N	2.45	0.49
1:A:669:HIS:HA	1:A:672:MET:SD	2.53	0.48
1:B:486:ASN:ND2	1:B:486:ASN:O	2.46	0.48
1:A:783:VAL:HG11	1:A:1058:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:VAL:HG23	1:A:1115:TYR:HB3	1.95	0.48
1:B:520:LEU:HD23	3:G:1:NAG:H82	1.96	0.48
1:B:904:ILE:HD12	1:B:904:ILE:H	1.79	0.48
1:A:407:VAL:HG11	6:A:1411:EIC:H183	1.96	0.47
1:A:908:TYR:CZ	1:C:646:PRO:HG3	2.49	0.47
1:A:184:GLN:HB2	1:A:187:CYS:HB3	1.96	0.47
1:C:62:MET:HE1	1:C:311:ASN:HB2	1.97	0.47
1:B:671:LYS:HA	1:B:671:LYS:HD2	1.74	0.47
1:B:832:ILE:HG23	1:B:931:LEU:HD22	1.96	0.47
1:B:25:VAL:HG12	1:B:93:PRO:HG2	1.95	0.47
1:A:560:ILE:HD11	6:A:1411:EIC:H142	1.95	0.46
1:C:27:MET:HE1	1:C:100:TYR:CE2	2.51	0.46
1:A:355:PHE:CE2	1:A:647:VAL:HG11	2.49	0.46
1:A:140:MET:HB3	1:A:282:THR:HG22	1.98	0.46
1:A:426:CYS:O	1:A:569:ASN:ND2	2.48	0.46
1:A:852:LEU:HD23	1:A:870:LEU:HD13	1.96	0.46
1:C:299:TRP:O	5:C:1408:FOL:NA2	2.37	0.46
1:C:996:ASN:OD1	1:C:996:ASN:N	2.47	0.46
1:A:111:VAL:HG13	1:A:242:PHE:HB3	1.98	0.46
1:A:397:ASN:HB3	1:A:574:LEU:HD13	1.97	0.46
1:C:1190:THR:OG1	1:C:1191:ASN:N	2.45	0.46
1:A:646:PRO:HG3	1:B:908:TYR:CZ	2.50	0.46
1:B:372:CYS:HB3	1:B:374:LEU:HG	1.98	0.46
1:B:993:THR:OG1	1:B:994:THR:N	2.46	0.45
1:A:402:LYS:HG3	2:D:1:NAG:H82	1.99	0.45
1:B:661:LEU:HA	1:B:700:VAL:HG12	1.99	0.45
1:A:1001:LYS:HD3	1:A:1001:LYS:HA	1.76	0.45
1:C:22:CYS:SG	1:C:23:ILE:N	2.90	0.45
1:B:258:LYS:HE2	1:B:258:LYS:HB3	1.83	0.45
1:C:167:LYS:O	1:C:170:THR:OG1	2.30	0.45
1:C:754:SER:OG	1:C:755:SER:N	2.50	0.45
1:C:769:VAL:HG11	1:C:988:MET:HG3	1.98	0.45
1:C:414:CYS:CB	1:C:467:CYS:HA	2.46	0.45
1:B:288:ILE:HB	1:B:299:TRP:HE1	1.82	0.44
1:B:799:LEU:O	1:B:803:TYR:HB2	2.17	0.44
1:C:34:ARG:HG2	1:C:36:TRP:CZ2	2.52	0.44
1:A:136:TYR:OH	1:A:240:GLU:OE2	2.32	0.44
1:A:331:ASN:O	1:A:334:THR:OG1	2.30	0.44
1:B:161:LEU:HD11	1:B:272:LEU:HD13	2.00	0.44
1:C:1142:LYS:NZ	1:C:1196:PRO:O	2.50	0.44
1:A:95:ILE:HD13	1:A:197:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LYS:HE2	1:A:289:LYS:HB2	1.87	0.44
1:B:113:ILE:HD13	1:B:113:ILE:HA	1.87	0.44
1:C:32:PHE:CG	1:C:96:SER:HB2	2.53	0.44
1:B:214:GLN:O	1:B:218:THR:HG23	2.18	0.44
1:C:159:HIS:HA	1:C:178:VAL:HB	2.00	0.44
1:B:848:TYR:HE2	1:B:953:ALA:HA	1.81	0.44
1:C:1136:CYS:HA	1:C:1143:CYS:HA	2.00	0.44
1:A:648:SER:N	1:A:661:LEU:O	2.50	0.44
1:A:785:CYS:HB3	1:A:807:CYS:HB3	1.67	0.44
1:B:22:CYS:HB2	1:B:187:CYS:HB2	1.38	0.44
1:B:852:LEU:HD23	1:B:870:LEU:HD13	2.00	0.43
1:C:520:LEU:HD13	3:J:1:NAG:H82	1.99	0.43
1:C:1110:ALA:HB2	1:C:1115:TYR:HB2	2.00	0.43
1:A:400:LEU:HD22	1:A:423:ALA:HB2	1.98	0.43
1:B:531:TYR:N	1:B:538:PHE:O	2.51	0.43
1:C:439:LEU:HD22	1:C:442:LYS:HE2	2.00	0.43
1:C:441:MET:HE2	1:C:441:MET:HB3	1.93	0.43
1:A:374:LEU:HD13	1:A:403:LEU:HD21	2.00	0.43
1:A:585:ASP:OD1	1:A:585:ASP:N	2.51	0.43
1:C:355:PHE:CE2	1:C:647:VAL:HG11	2.53	0.43
1:C:660:THR:HB	1:C:701:ILE:HG12	2.01	0.43
1:C:819:LEU:HD12	1:C:819:LEU:HA	1.87	0.43
1:A:667:CYS:N	1:A:699:CYS:SG	2.91	0.43
1:B:668:ASP:O	1:B:672:MET:HG3	2.19	0.43
1:A:485:ALA:HB2	1:A:554:ILE:HD12	1.98	0.43
1:A:548:ARG:NH1	1:A:552:GLY:O	2.52	0.43
1:B:474:ASN:HA	1:B:553:SER:HB2	2.00	0.43
1:C:707:SER:O	1:C:707:SER:OG	2.30	0.43
1:A:972:GLU:OE1	1:A:1168:GLN:NE2	2.46	0.43
1:B:415:ASP:OD1	1:B:466:THR:OG1	2.37	0.43
1:C:499:ASP:OD1	1:C:499:ASP:N	2.52	0.43
1:B:1040:THR:HA	1:B:1043:GLN:HB2	2.01	0.43
1:C:234:SER:O	1:C:257:ARG:NH2	2.52	0.43
1:C:362:TYR:OH	1:C:595:ASP:OD2	2.33	0.43
1:C:388:TYR:HE1	1:C:511:PRO:HD3	1.83	0.43
1:C:84:MET:HA	1:C:90:VAL:HG23	2.01	0.43
1:C:377:LEU:O	1:C:558:TYR:OH	2.36	0.43
1:C:284:MET:HE3	1:C:284:MET:HB2	1.90	0.43
1:A:416:LYS:O	1:B:1037:ARG:NH2	2.52	0.42
1:B:661:LEU:HD13	1:B:717:LEU:HD22	2.00	0.42
1:A:748:LYS:HE2	1:A:748:LYS:HB3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:TYR:N	1:A:538:PHE:O	2.48	0.42
1:C:543:LYS:HE3	1:C:543:LYS:HB2	1.73	0.42
1:C:781:VAL:HG21	1:C:1013:LEU:HD21	2.01	0.42
1:B:543:LYS:HB2	1:B:543:LYS:HE3	1.71	0.42
1:C:1058:LEU:HD23	1:C:1058:LEU:HA	1.91	0.42
1:A:415:ASP:OD1	1:A:415:ASP:N	2.47	0.42
1:A:803:TYR:OH	1:A:1052:ASN:OD1	2.37	0.42
1:C:313:LEU:HD13	1:C:338:CYS:HA	2.01	0.42
1:A:670:ILE:HD12	1:A:670:ILE:HA	1.88	0.42
1:A:873:LEU:HD12	1:A:873:LEU:HA	1.92	0.42
1:C:1050:LEU:HD23	1:C:1050:LEU:HA	1.89	0.42
1:A:717:LEU:HD12	1:A:717:LEU:HA	1.95	0.42
1:B:819:LEU:HD12	1:B:819:LEU:HA	1.86	0.42
1:B:1129:GLN:HB3	1:B:1152:ILE:HD11	2.01	0.42
1:B:223:LYS:HA	1:B:223:LYS:HD2	1.81	0.42
1:A:367:ASN:OD1	1:A:367:ASN:N	2.52	0.41
6:A:1412:EIC:H111	1:B:560:ILE:HD13	2.02	0.41
1:A:201:ASN:OD1	1:A:289:LYS:NZ	2.39	0.41
1:A:427:TYR:HE2	1:A:430:LEU:HB2	1.85	0.41
1:A:469:ILE:HG21	6:A:1411:EIC:H182	2.01	0.41
1:C:926:MET:HE3	1:C:926:MET:HB2	1.91	0.41
1:B:136:TYR:O	1:B:286:ARG:NH1	2.54	0.41
1:C:670:ILE:HD12	1:C:670:ILE:HA	1.84	0.41
1:C:733:ASN:HB3	1:C:734:ASN:H	1.68	0.41
1:C:788:TYR:OH	1:C:1016:LEU:O	2.30	0.41
1:A:332:ASP:OD1	1:A:332:ASP:N	2.51	0.41
1:A:889:TYR:CD2	1:C:665:VAL:HG22	2.55	0.41
1:B:1058:LEU:HD23	1:B:1058:LEU:HA	1.84	0.41
1:C:309:LYS:HB2	1:C:309:LYS:HE2	1.93	0.41
1:B:118:ASN:OD1	1:B:118:ASN:N	2.53	0.41
1:B:385:ILE:HG13	1:B:457:ASN:HD22	1.85	0.41
1:B:398:TYR:OH	1:B:422:LEU:O	2.35	0.41
1:B:754:SER:OG	1:B:755:SER:N	2.54	0.41
1:C:387:ASN:HB2	1:C:520:LEU:HD11	2.01	0.41
1:A:437:LEU:HD21	1:A:441:MET:HB2	2.03	0.41
1:A:762:PRO:HA	1:A:1126:TYR:HA	2.03	0.41
1:A:1019:GLU:OE1	1:A:1022:ASN:ND2	2.54	0.41
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.88	0.41
1:B:411:GLU:OE1	1:B:442:LYS:NZ	2.54	0.41
1:B:1004:ASP:O	1:B:1005:ALA:C	2.63	0.41
1:C:566:GLU:O	1:C:620:TYR:OH	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:890:ASP:N	1:C:890:ASP:OD1	2.54	0.41
1:B:444:THR:HG21	1:B:453:ILE:HD12	2.03	0.40
1:C:162:VAL:HG22	1:C:175:LEU:HB2	2.03	0.40
1:C:867:ARG:HH21	1:C:925:ALA:HB2	1.84	0.40
1:A:1058:LEU:HD23	1:A:1058:LEU:HA	1.90	0.40
6:A:1412:EIC:H142	1:B:403:LEU:HD13	2.04	0.40
1:B:516:ARG:NH1	1:C:276:GLU:OE2	2.45	0.40
1:C:799:LEU:HD23	1:C:799:LEU:HA	1.89	0.40
1:C:867:ARG:HG3	1:C:871:GLU:HB2	2.04	0.40
1:A:450:ALA:N	6:A:1412:EIC:O1	2.43	0.40
6:A:1412:EIC:H1O1	1:B:398:TYR:CE2	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	1088/1349 (81%)	1032 (95%)	56 (5%)	0	100	100
1	B	1088/1349 (81%)	1042 (96%)	46 (4%)	0	100	100
1	C	1088/1349 (81%)	1046 (96%)	41 (4%)	1 (0%)	48	79
All	All	3264/4047 (81%)	3120 (96%)	143 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	227	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	965/1165 (83%)	962 (100%)	3 (0%)	91	92
1	B	965/1165 (83%)	959 (99%)	6 (1%)	84	88
1	C	965/1165 (83%)	959 (99%)	6 (1%)	84	88
All	All	2895/3495 (83%)	2880 (100%)	15 (0%)	85	90

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

Mol	Chain	Res	Type
1	A	52	VAL
1	A	594	TYR
1	A	905	CYS
1	B	52	VAL
1	B	310	LEU
1	B	447	ILE
1	B	594	TYR
1	B	749	VAL
1	B	814	LEU
1	C	78	ILE
1	C	118	ASN
1	C	225	CYS
1	C	356	ASN
1	C	692	LEU
1	C	907	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	249	GLN
1	A	252	HIS
1	A	331	ASN
1	A	464	ASN
1	A	470	HIS

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Mol	Chain	Res	Type
1	A	488	ASN
1	A	532	ASN
1	A	534	ASN
1	A	821	GLN
1	A	973	ASN
1	A	1003	GLN
1	A	1084	ASN
1	A	1090	GLN
1	A	1109	ASN
1	A	1191	ASN
1	A	1192	ASN
1	B	184	GLN
1	B	246	GLN
1	B	249	GLN
1	B	296	HIS
1	B	534	ASN
1	B	630	HIS
1	B	798	GLN
1	B	821	GLN
1	B	922	ASN
1	B	1043	GLN
1	B	1046	GLN
1	B	1077	GLN
1	B	1084	ASN
1	B	1094	ASN
1	B	1109	ASN
1	B	1112	ASN
1	B	1140	ASN
1	C	70	GLN
1	C	91	ASN
1	C	159	HIS
1	C	183	ASN
1	C	337	GLN
1	C	380	ASN
1	C	384	GLN
1	C	395	ASN
1	C	583	ASN
1	C	779	GLN
1	C	815	HIS
1	C	967	GLN
1	C	1003	GLN
1	C	1043	GLN

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Mol	Chain	Res	Type
1	C	1122	HIS
1	C	1192	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

22 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.65	1 (7%)	17,19,21	0.83	0
2	NAG	D	2	2	14,14,15	0.18	0	17,19,21	0.64	1 (5%)
2	BMA	D	3	2	11,11,12	0.58	0	15,15,17	1.14	2 (13%)
2	NAG	E	1	2,1	14,14,15	0.40	0	17,19,21	0.55	0
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.62	0
2	BMA	E	3	2	11,11,12	0.80	0	15,15,17	0.86	0
2	NAG	F	1	2,1	14,14,15	0.62	0	17,19,21	1.97	2 (11%)
2	NAG	F	2	2	14,14,15	0.28	0	17,19,21	0.87	1 (5%)
2	BMA	F	3	2	11,11,12	1.01	1 (9%)	15,15,17	1.02	1 (6%)
3	NAG	G	1	3,1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	G	2	3	14,14,15	0.20	0	17,19,21	0.53	0
2	NAG	H	1	2,1	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	H	2	2	14,14,15	0.22	0	17,19,21	0.47	0
2	BMA	H	3	2	11,11,12	0.56	0	15,15,17	0.84	0
2	NAG	I	1	2,1	14,14,15	0.32	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	I	2	2	14,14,15	0.28	0	17,19,21	0.57	0
2	BMA	I	3	2	11,11,12	0.54	0	15,15,17	0.91	1 (6%)
3	NAG	J	1	3,1	14,14,15	0.21	0	17,19,21	0.50	0
3	NAG	J	2	3	14,14,15	0.21	0	17,19,21	0.52	0
2	NAG	K	1	2,1	14,14,15	0.21	0	17,19,21	0.62	0
2	NAG	K	2	2	14,14,15	0.20	0	17,19,21	0.47	0
2	BMA	K	3	2	11,11,12	0.53	0	15,15,17	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	1/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	BMA	I	3	2	-	1/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	BMA	C1-C2	2.63	1.58	1.52
2	D	1	NAG	O5-C1	-2.22	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C2-N2-C7	6.91	132.74	122.90
2	F	1	NAG	C1-C2-N2	3.23	116.01	110.49
2	D	3	BMA	C1-O5-C5	2.79	115.98	112.19
2	D	3	BMA	O2-C2-C3	-2.43	105.27	110.14
2	F	2	NAG	C2-N2-C7	2.39	126.30	122.90
2	I	3	BMA	C1-O5-C5	2.08	115.01	112.19
2	D	2	NAG	C1-O5-C5	2.05	114.97	112.19
2	F	3	BMA	O2-C2-C3	-2.05	106.03	110.14

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	I	3	BMA	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6

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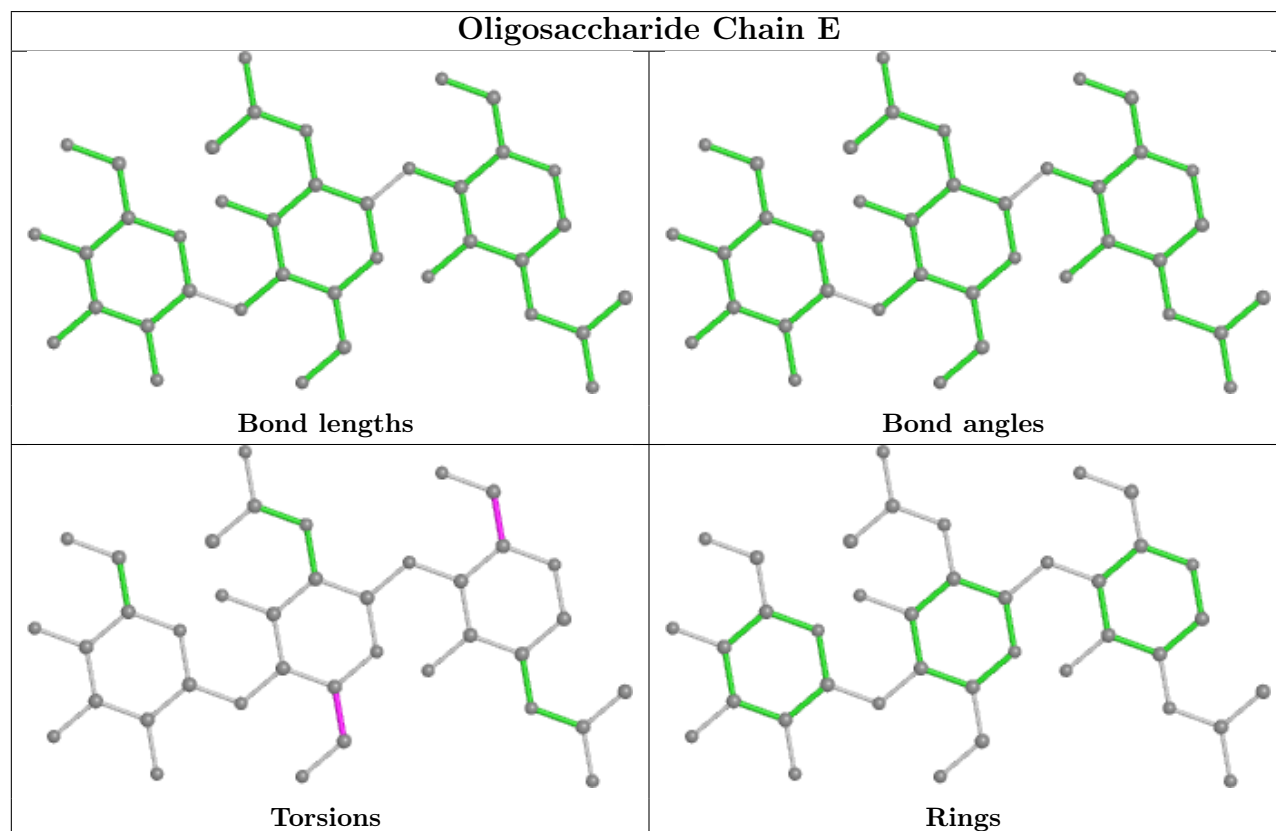
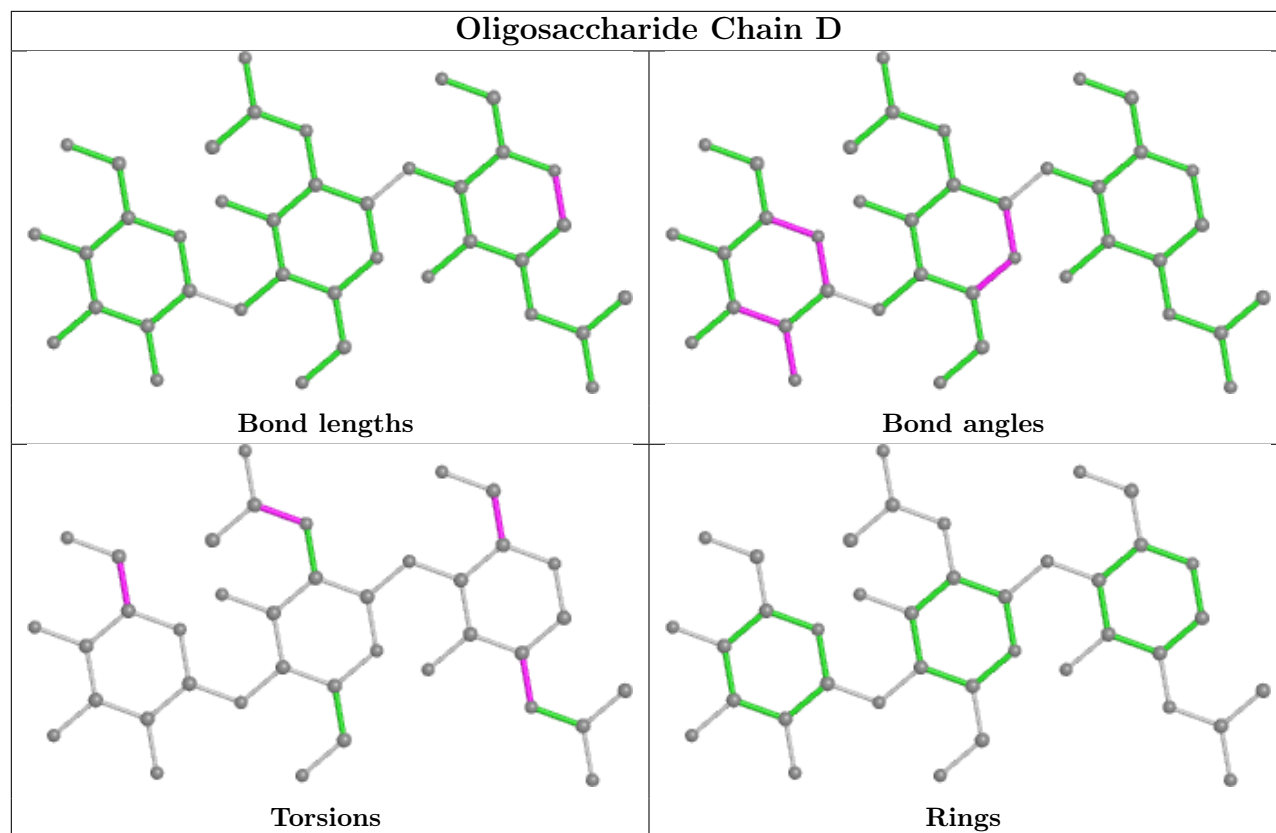
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7
2	F	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
2	F	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

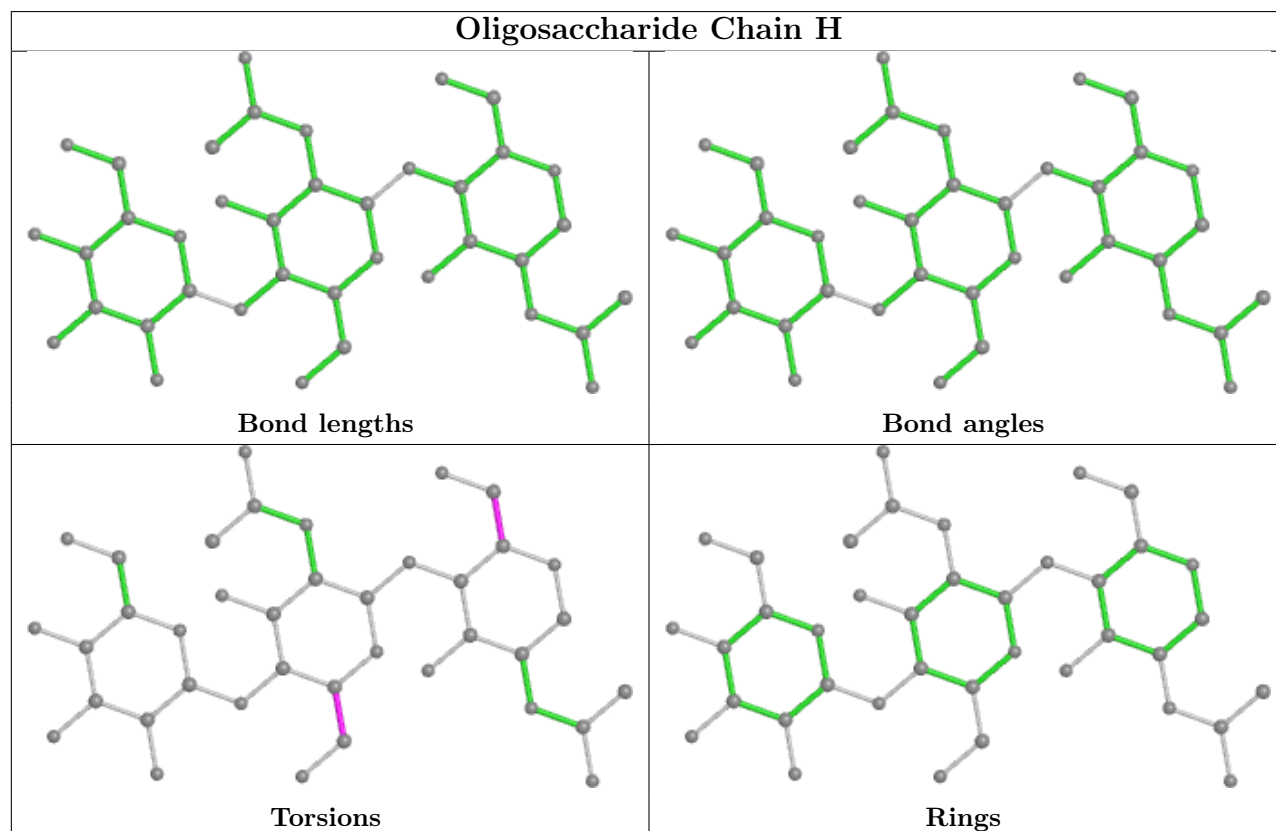
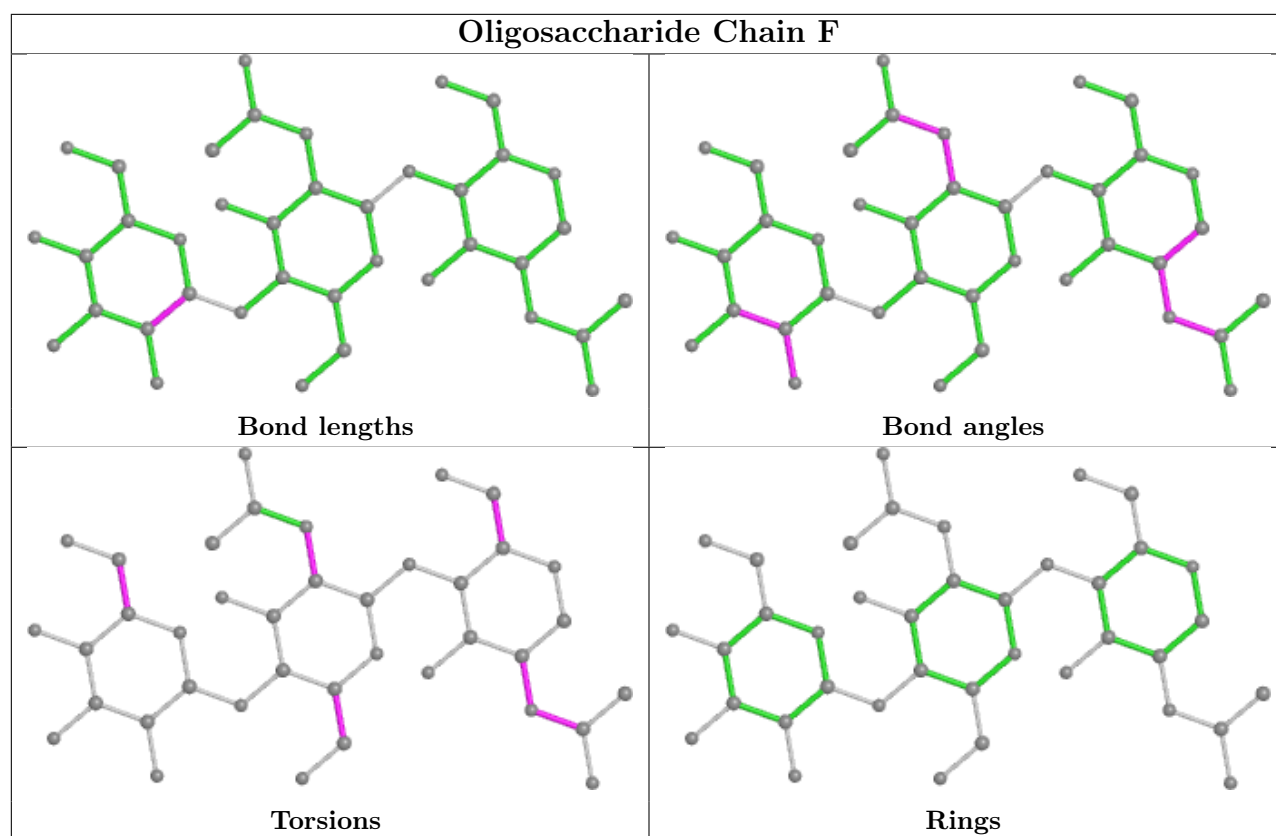
There are no ring outliers.

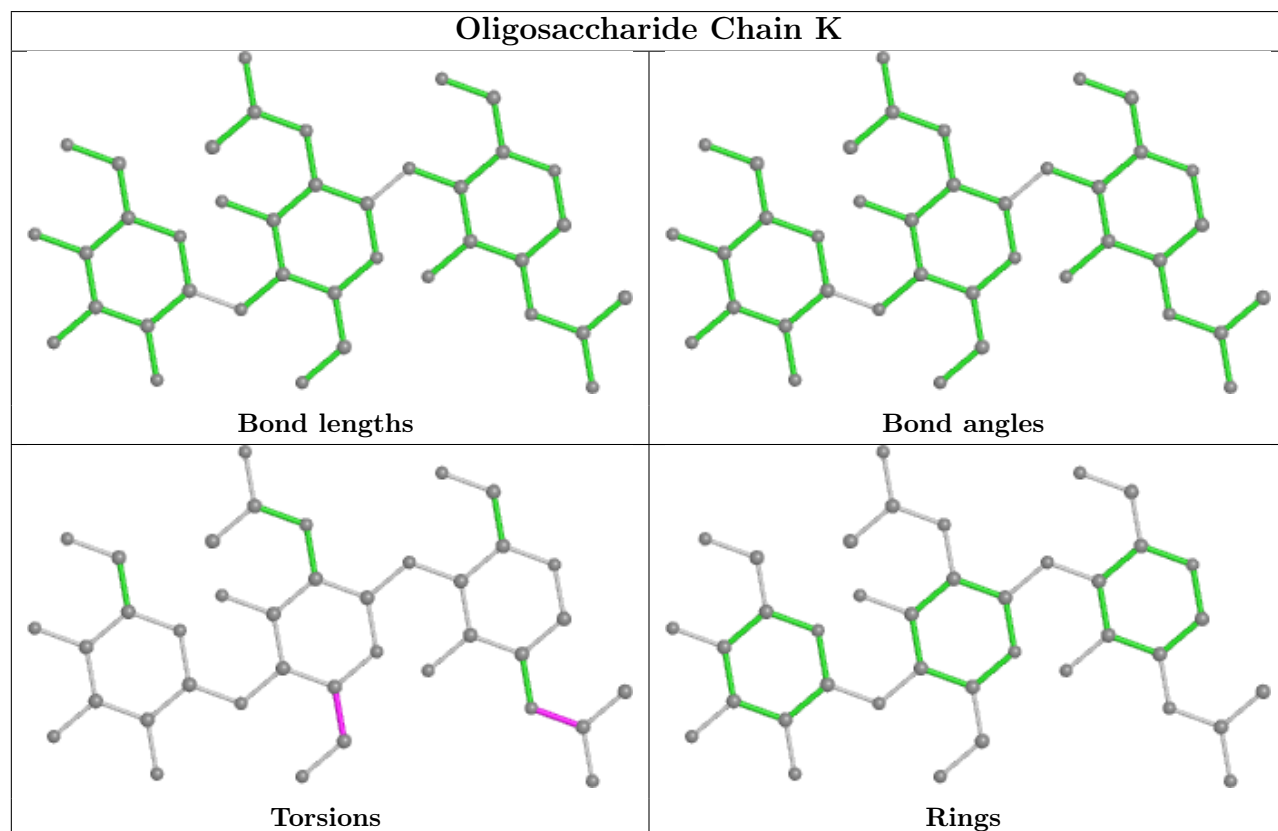
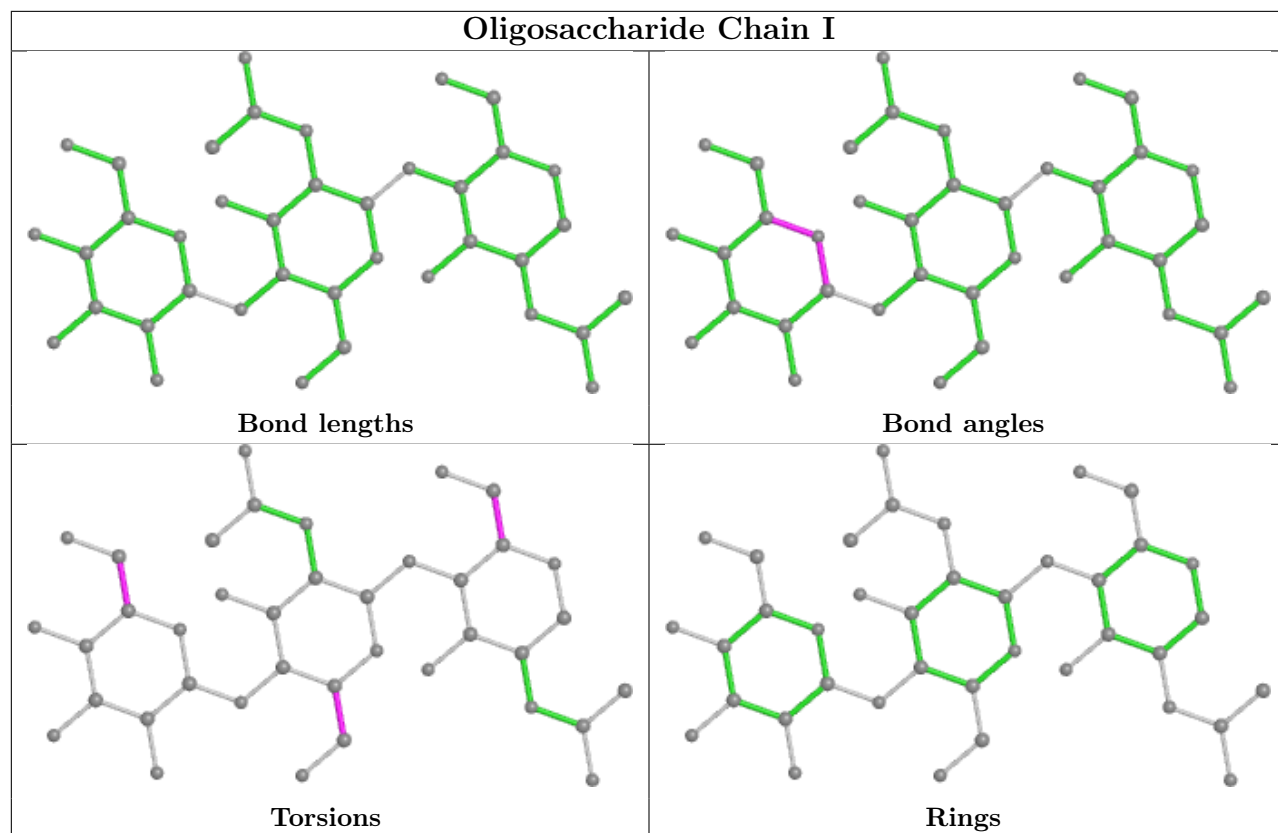
4 monomers are involved in 4 short contacts:

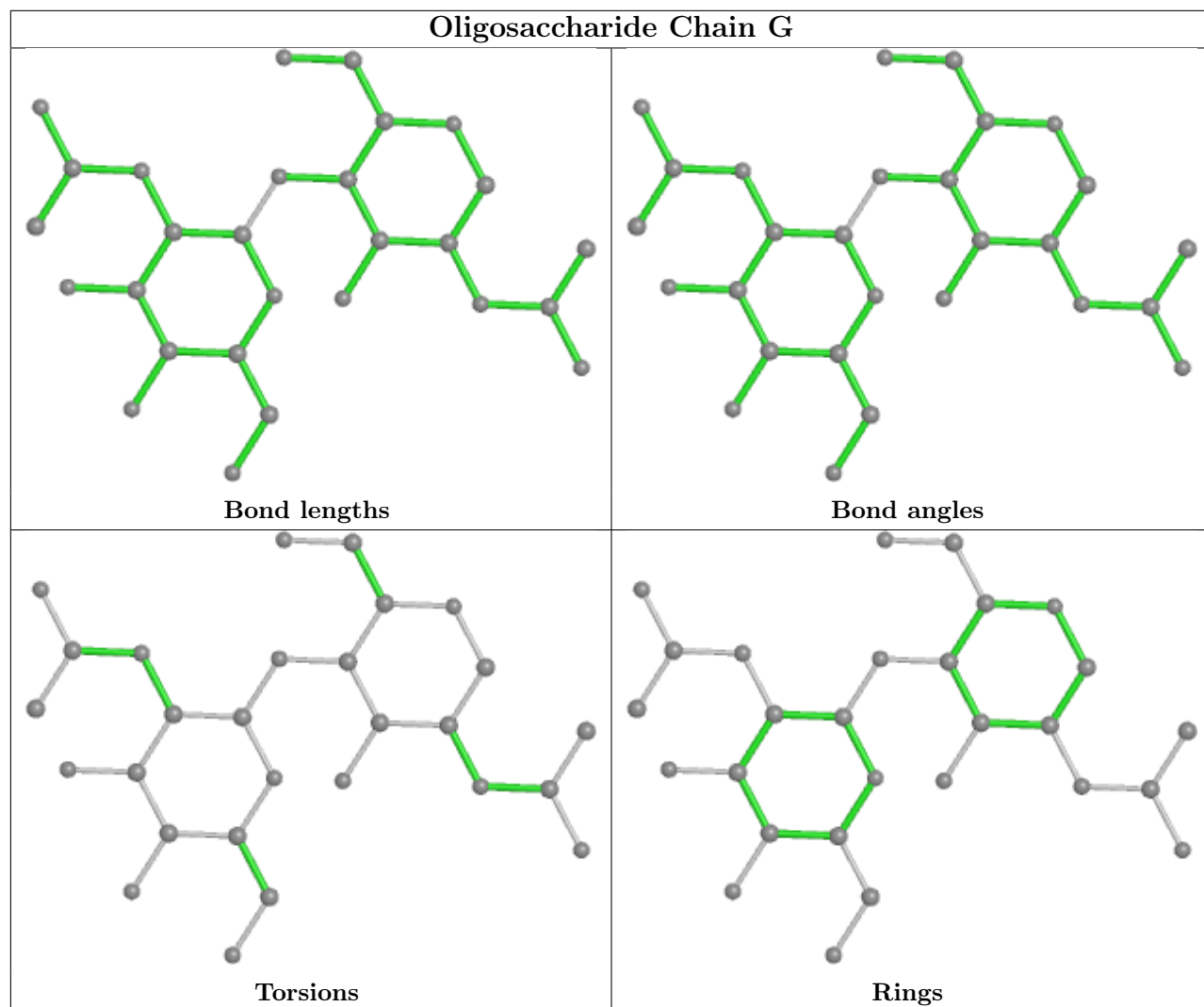
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1	NAG	1	0
2	I	2	NAG	1	0
2	D	1	NAG	1	0
3	G	1	NAG	1	0

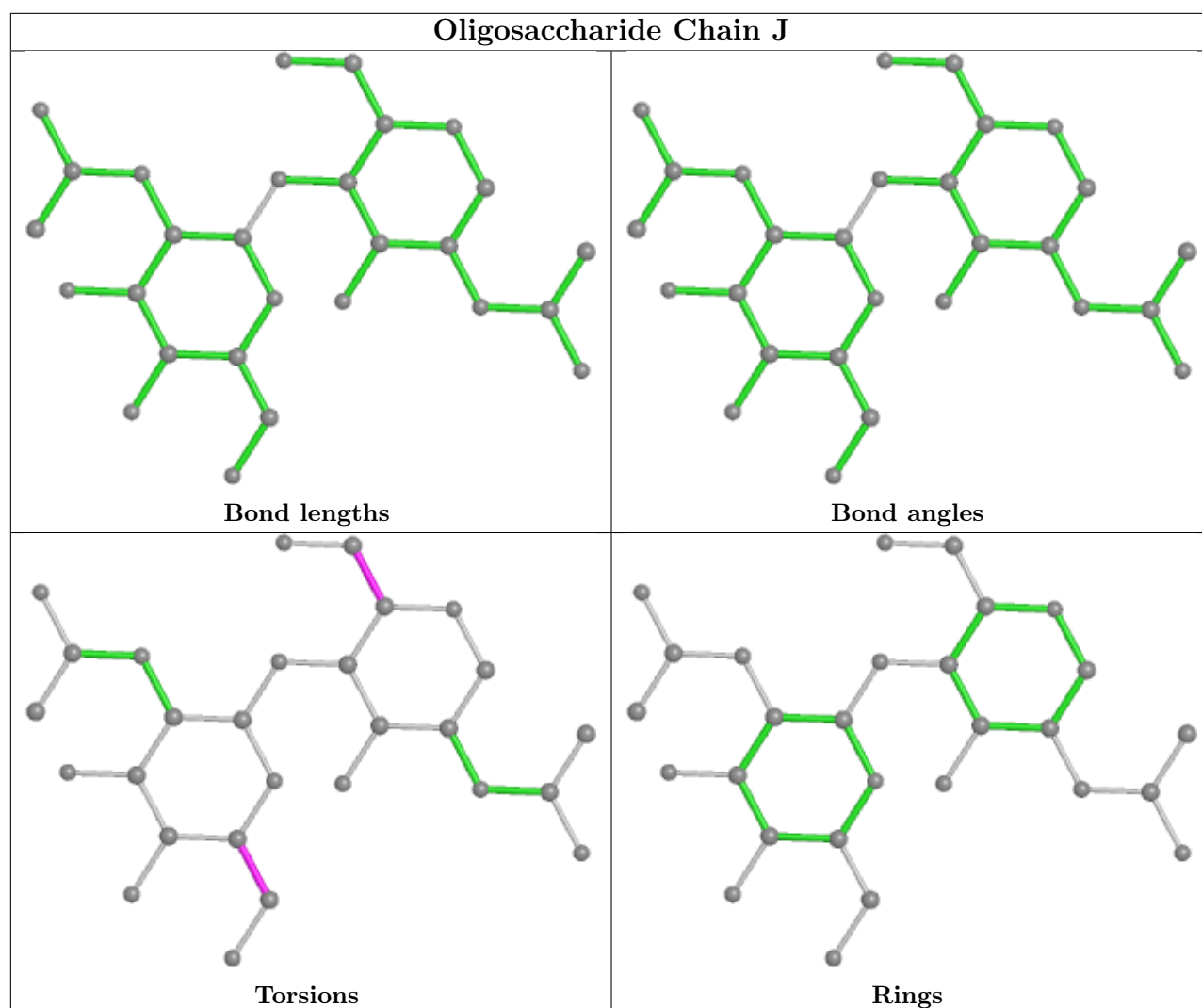
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

31 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	C	1404	1	14,14,15	0.29	0	17,19,21	0.48	0
5	FOL	A	1410	-	34,34,34	1.19	2 (5%)	44,47,47	1.98	8 (18%)
4	NAG	C	1402	1	14,14,15	0.70	1 (7%)	17,19,21	1.99	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EIC	A	1412	-	19,19,19	0.55	0	19,19,19	0.61	0
4	NAG	B	1405	1	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	C	1407	1	14,14,15	0.28	0	17,19,21	0.47	0
4	NAG	A	1408	1	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	B	1409	1	14,14,15	0.22	0	17,19,21	0.54	0
4	NAG	B	1402	1	14,14,15	0.29	0	17,19,21	0.37	0
6	EIC	A	1411	-	19,19,19	0.56	0	19,19,19	0.58	0
4	NAG	C	1409	1	14,14,15	0.23	0	17,19,21	0.46	0
5	FOL	C	1408	-	34,34,34	1.27	2 (5%)	44,47,47	2.37	12 (27%)
4	NAG	C	1405	1	14,14,15	0.21	0	17,19,21	0.53	0
4	NAG	B	1406	1	14,14,15	0.19	0	17,19,21	0.48	0
4	NAG	A	1406	1	14,14,15	0.16	0	17,19,21	0.44	0
4	NAG	C	1406	1	14,14,15	0.22	0	17,19,21	0.51	0
4	NAG	B	1408	1	14,14,15	0.26	0	17,19,21	0.39	0
4	NAG	C	1403	1	14,14,15	0.31	0	17,19,21	0.45	0
4	NAG	C	1401	1	14,14,15	0.24	0	17,19,21	0.47	0
4	NAG	A	1404	1	14,14,15	0.32	0	17,19,21	0.52	0
4	NAG	B	1403	1	14,14,15	0.33	0	17,19,21	0.35	0
4	NAG	A	1402	1	14,14,15	0.31	0	17,19,21	0.43	0
4	NAG	A	1409	1	14,14,15	0.28	0	17,19,21	0.50	0
4	NAG	A	1405	1	14,14,15	0.22	0	17,19,21	0.48	0
4	NAG	B	1404	1	14,14,15	0.33	0	17,19,21	0.51	0
4	NAG	A	1403	1	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	A	1401	1	14,14,15	0.23	0	17,19,21	0.52	0
6	EIC	B	1410	-	19,19,19	0.56	0	19,19,19	0.56	0
5	FOL	B	1407	-	34,34,34	1.23	2 (5%)	44,47,47	2.40	12 (27%)
4	NAG	A	1407	-	14,14,15	0.19	0	17,19,21	0.48	0
4	NAG	B	1401	1	14,14,15	0.31	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
5	FOL	A	1410	-	-	13/22/22/22	0/3/3/3
4	NAG	C	1402	1	-	4/6/23/26	0/1/1/1
6	EIC	A	1412	-	-	7/17/17/17	-
4	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
6	EIC	A	1411	-	-	5/17/17/17	-
4	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
5	FOL	C	1408	-	-	17/22/22/22	0/3/3/3
4	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1406	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
6	EIC	B	1410	-	-	5/17/17/17	-
5	FOL	B	1407	-	-	17/22/22/22	0/3/3/3
4	NAG	A	1407	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1408	FOL	C4A-C4	4.08	1.48	1.41
5	B	1407	FOL	C4A-C4	3.87	1.48	1.41
5	C	1408	FOL	C4A-C8A	3.77	1.47	1.40
5	B	1407	FOL	C4A-C8A	3.72	1.47	1.40
5	A	1410	FOL	C4A-C8A	3.60	1.47	1.40
5	A	1410	FOL	C4A-C4	3.57	1.47	1.41
4	C	1402	NAG	C1-C2	2.13	1.55	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1407	FOL	CB-CA-N	6.98	124.99	110.88
5	C	1408	FOL	CB-CA-N	6.92	124.87	110.88
4	C	1402	NAG	C2-N2-C7	6.90	132.72	122.90
5	A	1410	FOL	N8-C8A-N1	6.12	122.81	115.82
5	A	1410	FOL	C2-N1-C8A	5.51	121.65	115.36
5	B	1407	FOL	N8-C8A-N1	5.51	122.11	115.82
5	B	1407	FOL	C2-N1-C8A	5.50	121.64	115.36
5	C	1408	FOL	C2-N1-C8A	5.49	121.63	115.36
5	C	1408	FOL	N8-C8A-N1	5.33	121.91	115.82
5	C	1408	FOL	C8A-C4A-C4	-4.64	116.88	119.95
5	B	1407	FOL	C8A-C4A-C4	-4.49	116.98	119.95
5	C	1408	FOL	C4-C4A-N5	4.20	123.40	118.60
5	C	1408	FOL	C4A-C4-N3	-4.11	117.81	123.43
5	B	1407	FOL	C4A-C4-N3	-4.07	117.86	123.43
5	B	1407	FOL	C4-C4A-N5	3.97	123.14	118.60
5	A	1410	FOL	C4A-C4-N3	-3.88	118.13	123.43
5	A	1410	FOL	C8A-C4A-C4	-3.83	117.41	119.95
5	B	1407	FOL	C2-N3-C4	3.77	121.91	115.93
5	C	1408	FOL	C2-N3-C4	3.64	121.72	115.93
4	C	1402	NAG	C1-C2-N2	3.38	116.25	110.49
5	B	1407	FOL	N1-C2-N3	-3.37	122.72	127.22
5	A	1410	FOL	C2-N3-C4	3.37	121.28	115.93
5	C	1408	FOL	N1-C2-N3	-3.18	122.97	127.22
5	A	1410	FOL	N1-C2-N3	-3.13	123.05	127.22
5	A	1410	FOL	C4-C4A-N5	3.04	122.07	118.60
5	C	1408	FOL	C7-N8-C8A	2.81	119.51	116.69
5	B	1407	FOL	C6-C9-N10	-2.79	106.89	113.07
5	B	1407	FOL	C7-N8-C8A	2.78	119.48	116.69
5	A	1410	FOL	C7-N8-C8A	2.51	119.21	116.69
5	B	1407	FOL	O-C-C11	-2.48	116.51	120.94
5	C	1408	FOL	C6-C9-N10	-2.32	107.94	113.07
5	C	1408	FOL	C8A-C4A-N5	-2.30	119.72	122.33
5	C	1408	FOL	O-C-C11	-2.28	116.87	120.94
5	B	1407	FOL	C8A-C4A-N5	-2.16	119.89	122.33

There are no chirality outliers.

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1410	FOL	C6-C9-N10-C14
5	A	1410	FOL	O-C-N-CA

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Mol	Chain	Res	Type	Atoms
5	B	1407	FOL	N-CA-CB-CG
5	C	1408	FOL	C6-C9-N10-C14
6	A	1412	EIC	C10-C11-C12-C13
5	B	1407	FOL	O-C-C11-C12
5	B	1407	FOL	O-C-C11-C16
4	A	1409	NAG	C4-C5-C6-O6
5	A	1410	FOL	C11-C-N-CA
5	B	1407	FOL	N-C-C11-C12
5	B	1407	FOL	N-C-C11-C16
4	C	1405	NAG	O5-C5-C6-O6
4	A	1405	NAG	O5-C5-C6-O6
5	C	1408	FOL	N-C-C11-C12
4	B	1403	NAG	C4-C5-C6-O6
4	A	1409	NAG	O5-C5-C6-O6
5	C	1408	FOL	N-C-C11-C16
4	A	1404	NAG	C4-C5-C6-O6
4	B	1404	NAG	C4-C5-C6-O6
4	C	1409	NAG	O5-C5-C6-O6
4	A	1406	NAG	C4-C5-C6-O6
5	A	1410	FOL	O-C-C11-C12
5	C	1408	FOL	O-C-N-CA
5	A	1410	FOL	C15-C14-N10-C9
5	C	1408	FOL	C15-C14-N10-C9
5	A	1410	FOL	N-C-C11-C12
5	C	1408	FOL	O-C-C11-C12
4	C	1401	NAG	O5-C5-C6-O6
5	C	1408	FOL	CT-CA-N-C
4	B	1403	NAG	O5-C5-C6-O6
4	C	1404	NAG	O5-C5-C6-O6
4	C	1405	NAG	C4-C5-C6-O6
4	B	1409	NAG	O5-C5-C6-O6
4	C	1401	NAG	C4-C5-C6-O6
5	A	1410	FOL	C13-C14-N10-C9
5	C	1408	FOL	C13-C14-N10-C9
4	A	1404	NAG	O5-C5-C6-O6
4	B	1404	NAG	O5-C5-C6-O6
4	A	1403	NAG	C4-C5-C6-O6
4	C	1404	NAG	C4-C5-C6-O6
5	C	1408	FOL	C11-C-N-CA
5	B	1407	FOL	CT-CA-N-C
4	A	1405	NAG	C4-C5-C6-O6
5	A	1410	FOL	N-C-C11-C16

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Mol	Chain	Res	Type	Atoms
4	C	1406	NAG	O5-C5-C6-O6
5	A	1410	FOL	O-C-C11-C16
4	C	1403	NAG	C4-C5-C6-O6
5	C	1408	FOL	O-C-C11-C16
4	C	1406	NAG	C4-C5-C6-O6
4	A	1406	NAG	C8-C7-N2-C2
4	A	1406	NAG	O7-C7-N2-C2
4	A	1409	NAG	C8-C7-N2-C2
4	A	1409	NAG	O7-C7-N2-C2
4	B	1406	NAG	C8-C7-N2-C2
4	B	1406	NAG	O7-C7-N2-C2
4	B	1408	NAG	C8-C7-N2-C2
4	B	1408	NAG	O7-C7-N2-C2
4	C	1402	NAG	C8-C7-N2-C2
4	C	1402	NAG	O7-C7-N2-C2
4	C	1406	NAG	C8-C7-N2-C2
4	C	1406	NAG	O7-C7-N2-C2
4	C	1409	NAG	C4-C5-C6-O6
4	B	1402	NAG	O5-C5-C6-O6
4	C	1403	NAG	O5-C5-C6-O6
5	B	1407	FOL	O-C-N-CA
4	A	1407	NAG	O5-C5-C6-O6
4	C	1402	NAG	O5-C5-C6-O6
5	B	1407	FOL	C13-C14-N10-C9
4	A	1406	NAG	O5-C5-C6-O6
5	B	1407	FOL	C11-C-N-CA
4	B	1402	NAG	C4-C5-C6-O6
4	A	1407	NAG	C4-C5-C6-O6
4	A	1403	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
6	A	1411	EIC	C5-C6-C7-C8
6	A	1412	EIC	C3-C4-C5-C6
4	A	1402	NAG	O5-C5-C6-O6
4	C	1407	NAG	O5-C5-C6-O6
6	A	1411	EIC	C4-C5-C6-C7
6	B	1410	EIC	C2-C3-C4-C5
4	B	1401	NAG	C4-C5-C6-O6
5	B	1407	FOL	C15-C14-N10-C9
4	B	1406	NAG	C4-C5-C6-O6
4	B	1406	NAG	O5-C5-C6-O6
5	C	1408	FOL	N-CA-CT-O1
5	C	1408	FOL	N-CA-CT-O2

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Mol	Chain	Res	Type	Atoms
6	A	1411	EIC	C6-C7-C8-C9
4	B	1409	NAG	C4-C5-C6-O6
5	B	1407	FOL	CB-CA-CT-O1
5	B	1407	FOL	CB-CA-CT-O2
5	B	1407	FOL	CT-CA-CB-CG
4	B	1401	NAG	O5-C5-C6-O6
6	B	1410	EIC	C1-C2-C3-C4
5	B	1407	FOL	C6-C9-N10-C14
6	A	1412	EIC	C4-C5-C6-C7
6	A	1412	EIC	C2-C3-C4-C5
6	A	1411	EIC	C3-C4-C5-C6
5	C	1408	FOL	CB-CA-CT-O1
5	C	1408	FOL	CB-CA-CT-O2
6	B	1410	EIC	C14-C15-C16-C17
4	C	1402	NAG	C3-C2-N2-C7
6	B	1410	EIC	C12-C13-C14-C15
6	B	1410	EIC	C13-C14-C15-C16
5	A	1410	FOL	OE1-CD-CG-CB
5	C	1408	FOL	OE1-CD-CG-CB
4	A	1408	NAG	C4-C5-C6-O6
5	B	1407	FOL	N-CA-CT-O2
5	B	1407	FOL	OE1-CD-CG-CB
6	A	1411	EIC	C14-C15-C16-C17
5	B	1407	FOL	OE2-CD-CG-CB
5	C	1408	FOL	OE2-CD-CG-CB
5	A	1410	FOL	OE2-CD-CG-CB
6	A	1412	EIC	O2-C1-C2-C3
5	A	1410	FOL	C7-C6-C9-N10
6	A	1412	EIC	O1-C1-C2-C3
5	C	1408	FOL	N-CA-CB-CG
5	A	1410	FOL	N5-C6-C9-N10
6	A	1412	EIC	C12-C13-C14-C15
4	A	1408	NAG	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 12 short contacts:

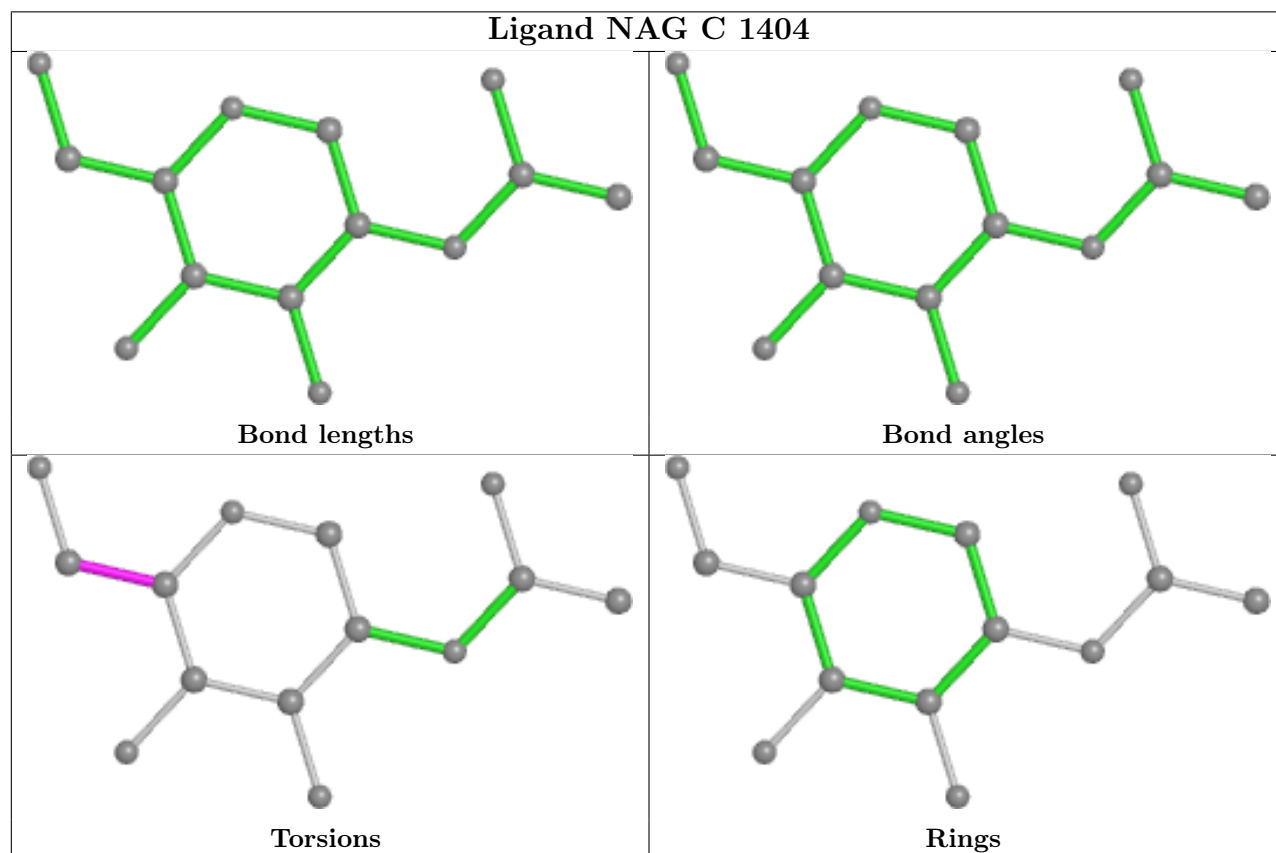
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1410	FOL	1	0
6	A	1412	EIC	4	0
4	C	1407	NAG	1	0
6	A	1411	EIC	3	0

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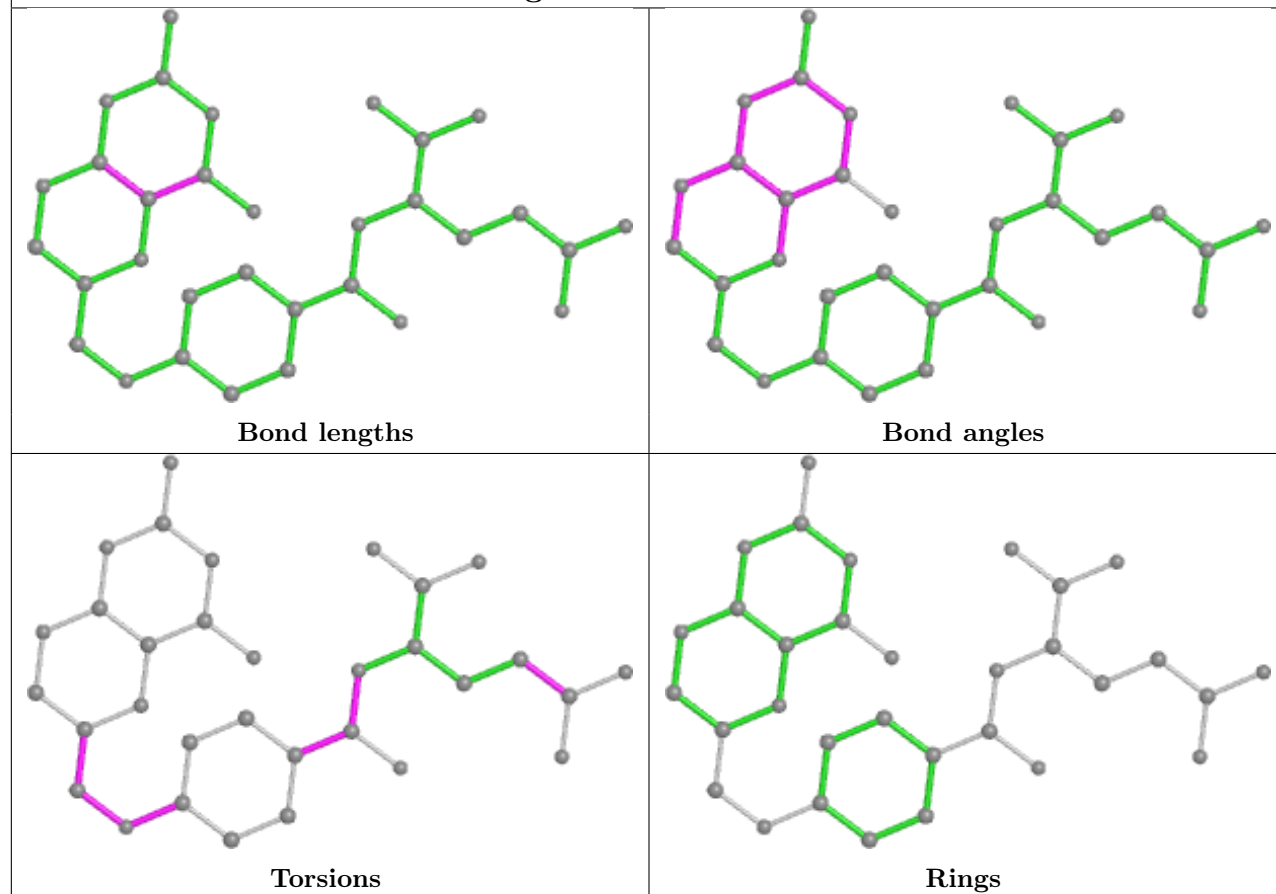
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1408	FOL	1	0
4	B	1403	NAG	1	0
5	B	1407	FOL	1	0

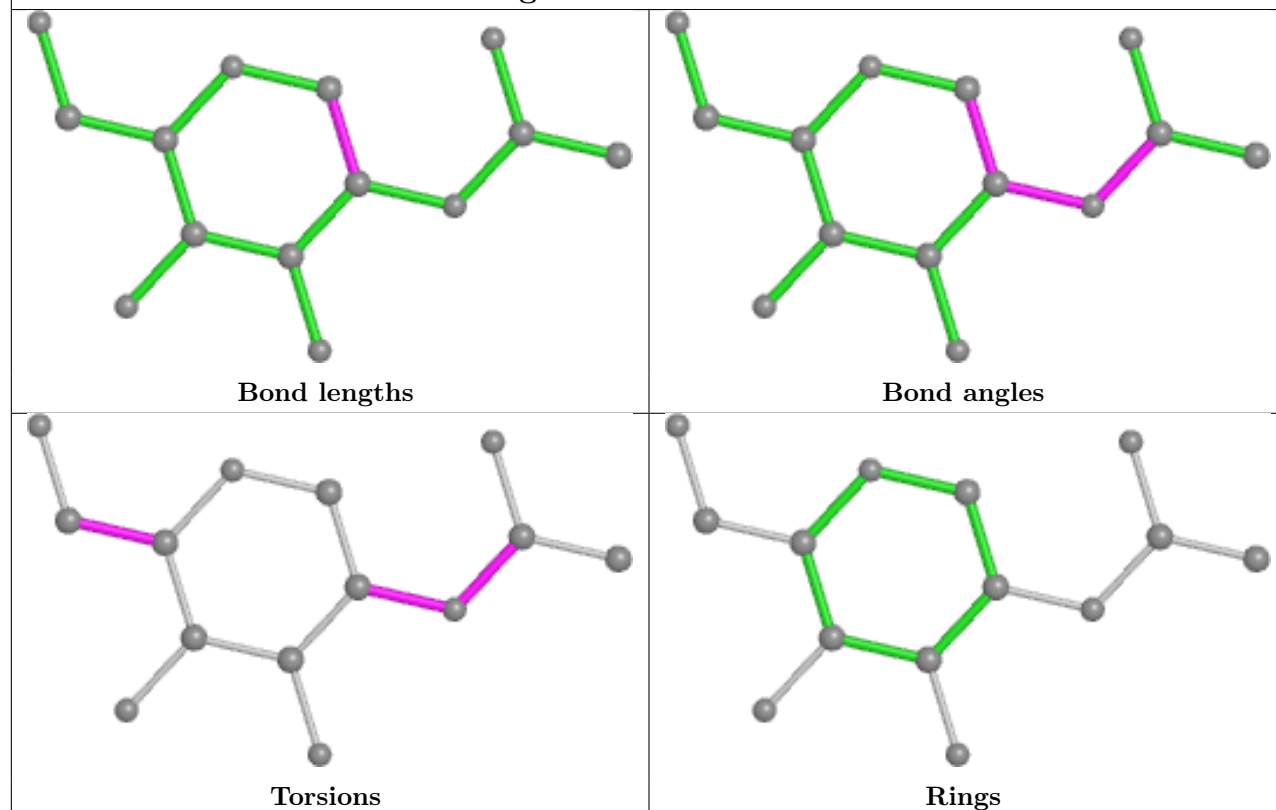
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

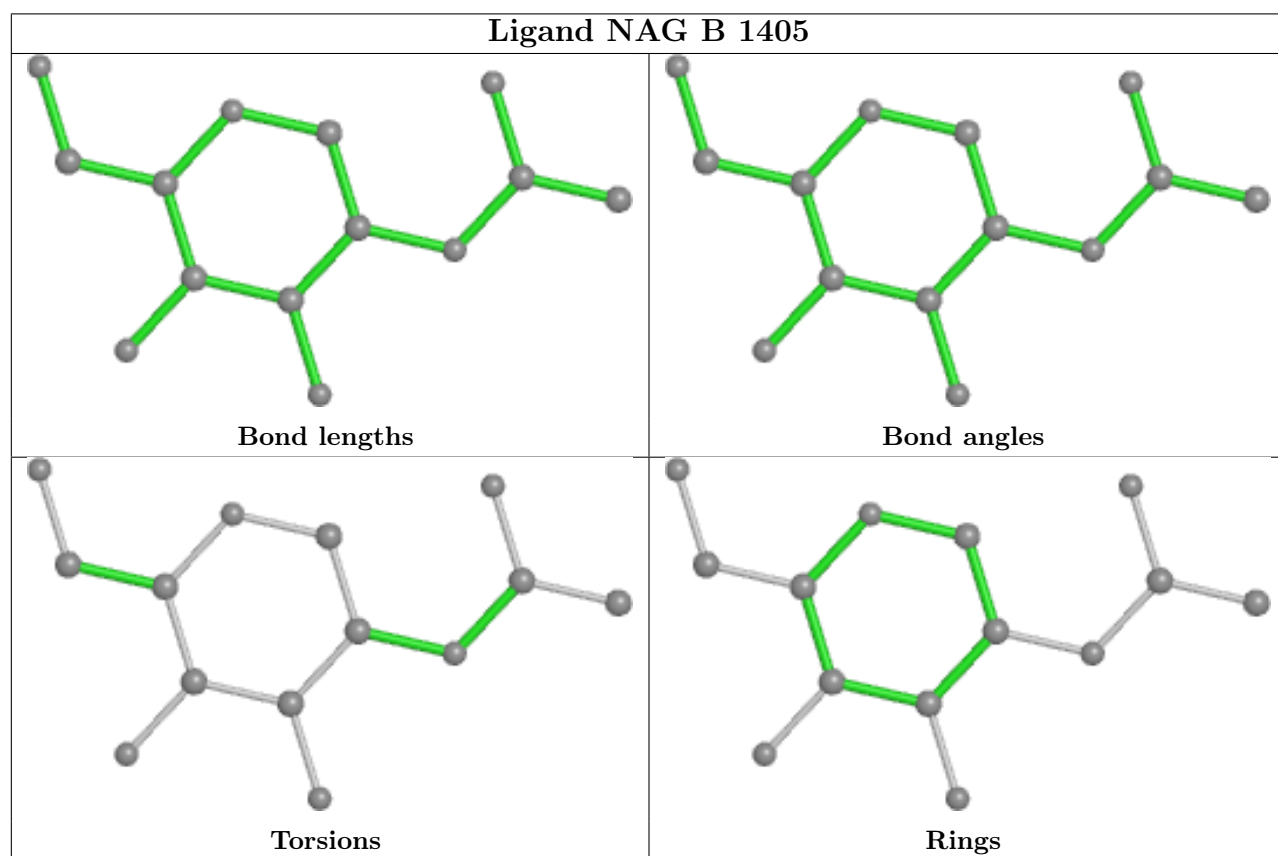
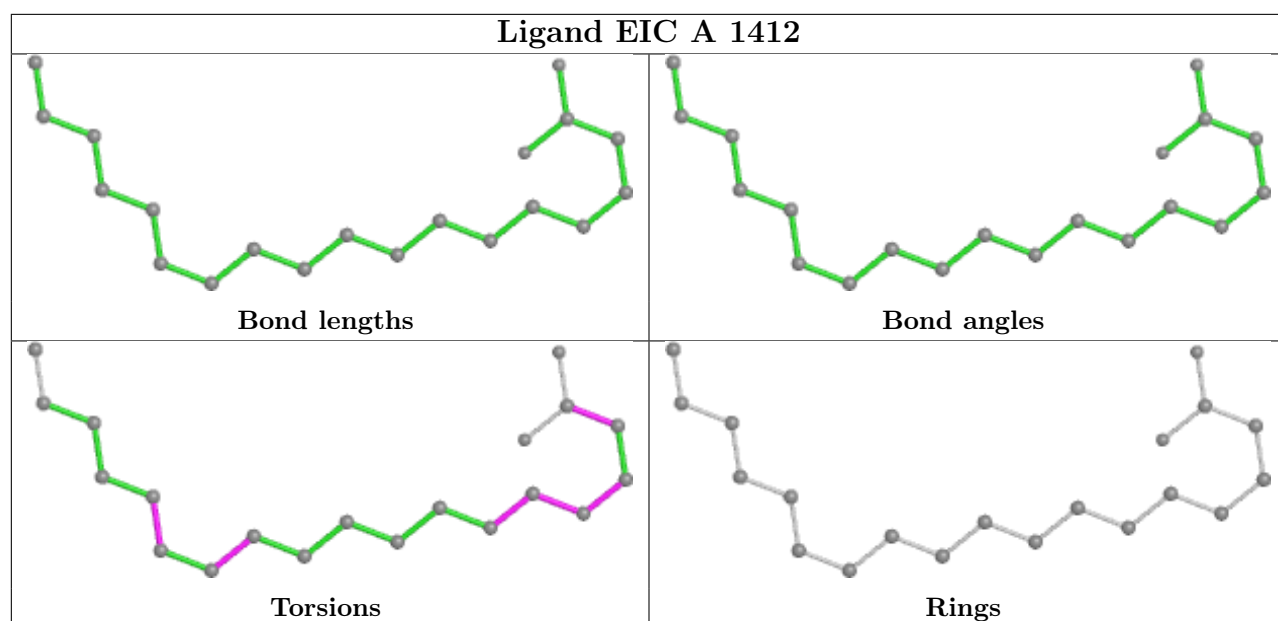


Ligand FOL A 1410

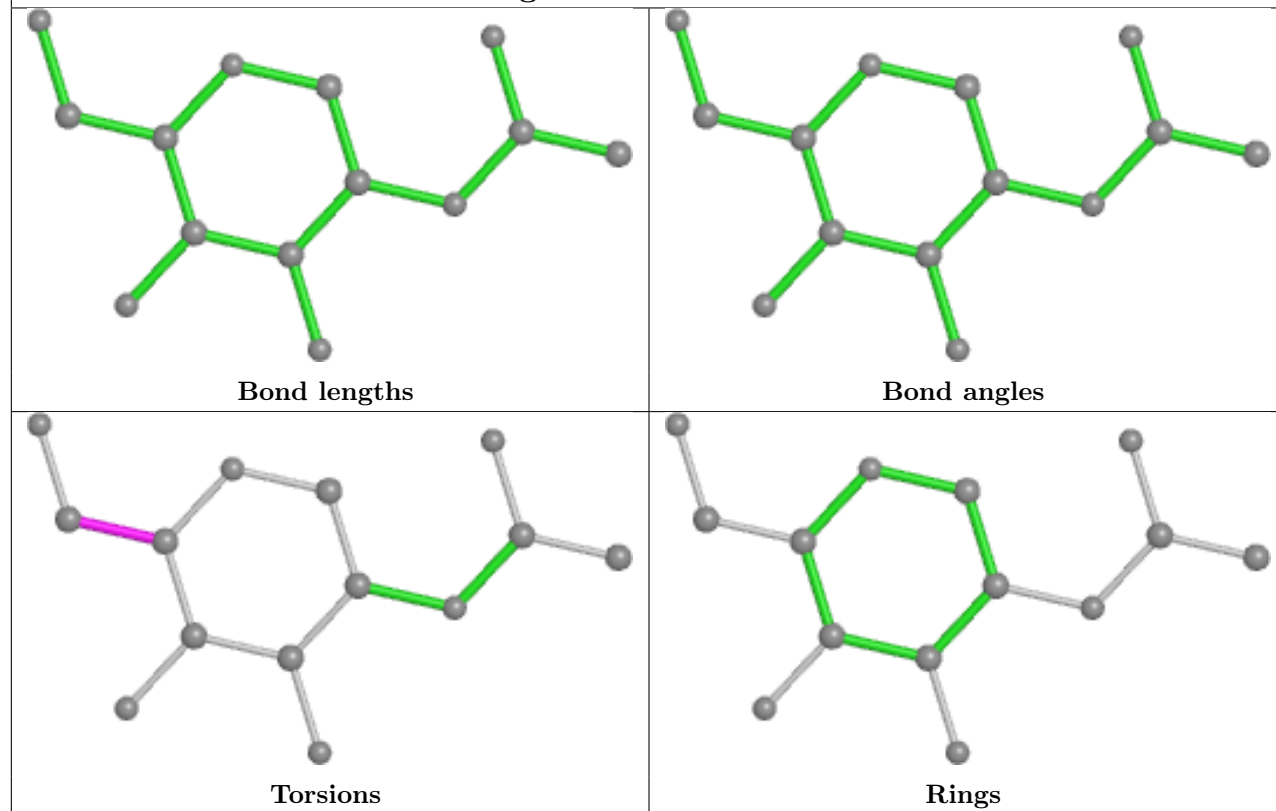


Ligand NAG C 1402

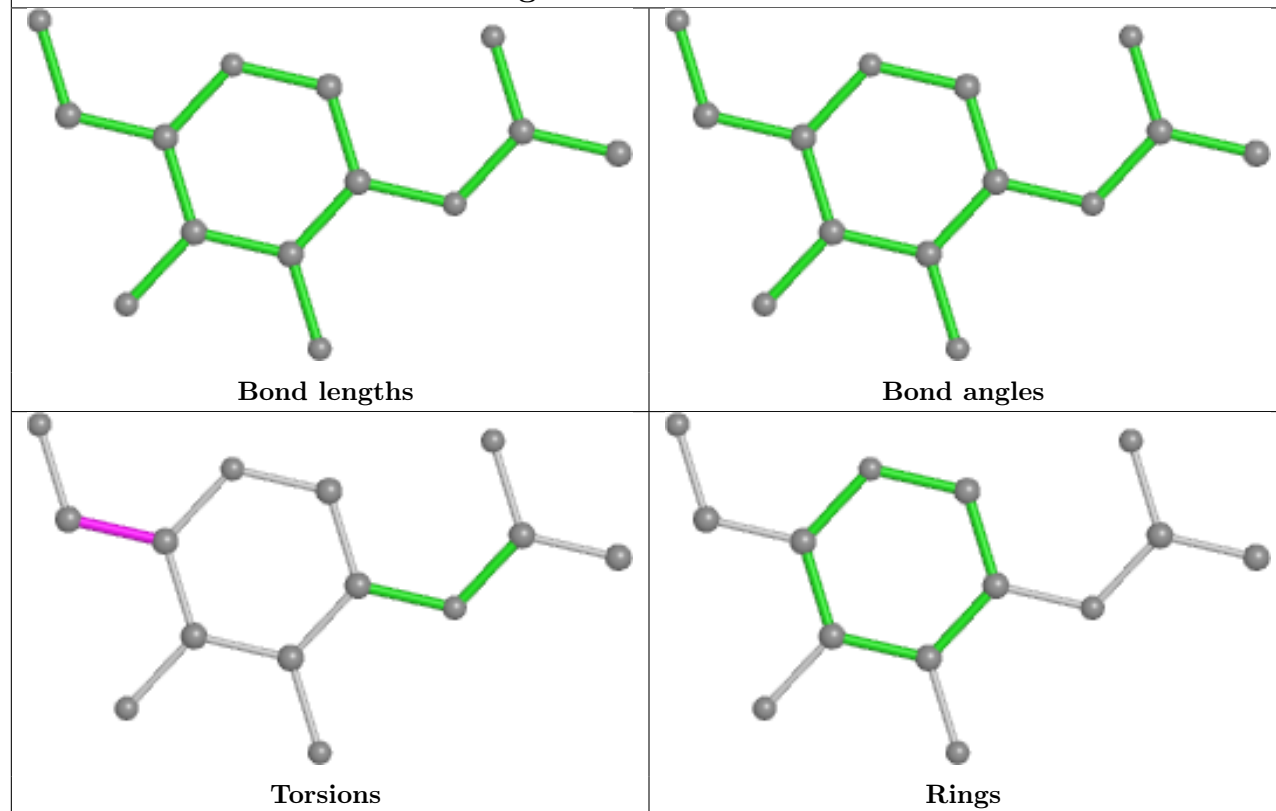




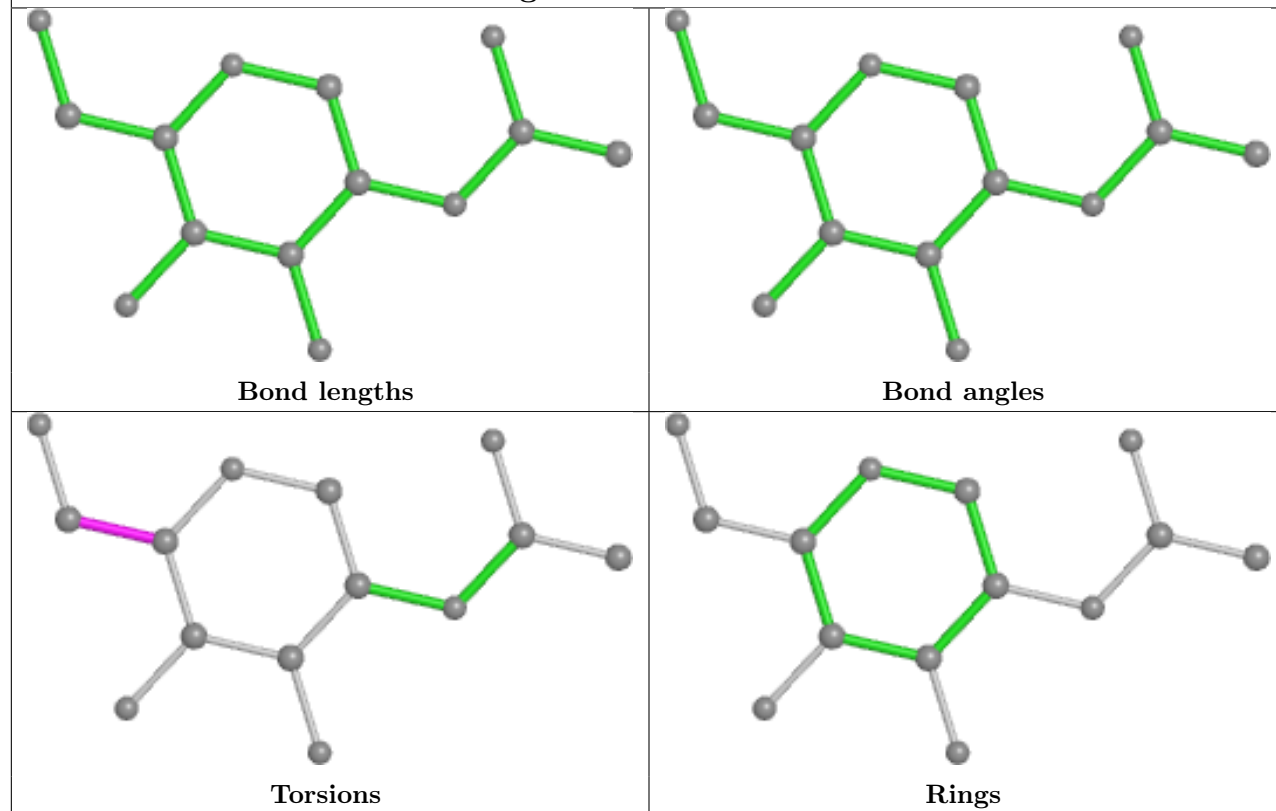
Ligand NAG C 1407



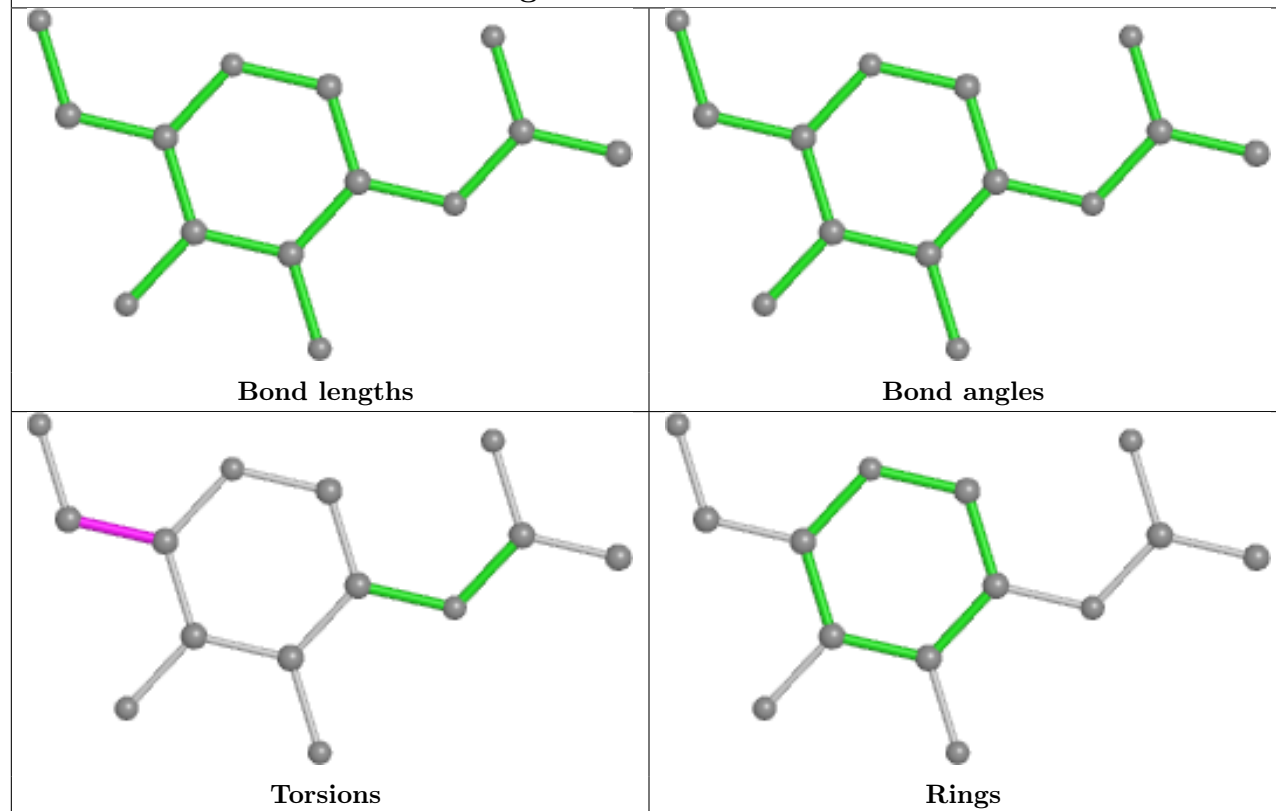
Ligand NAG A 1408

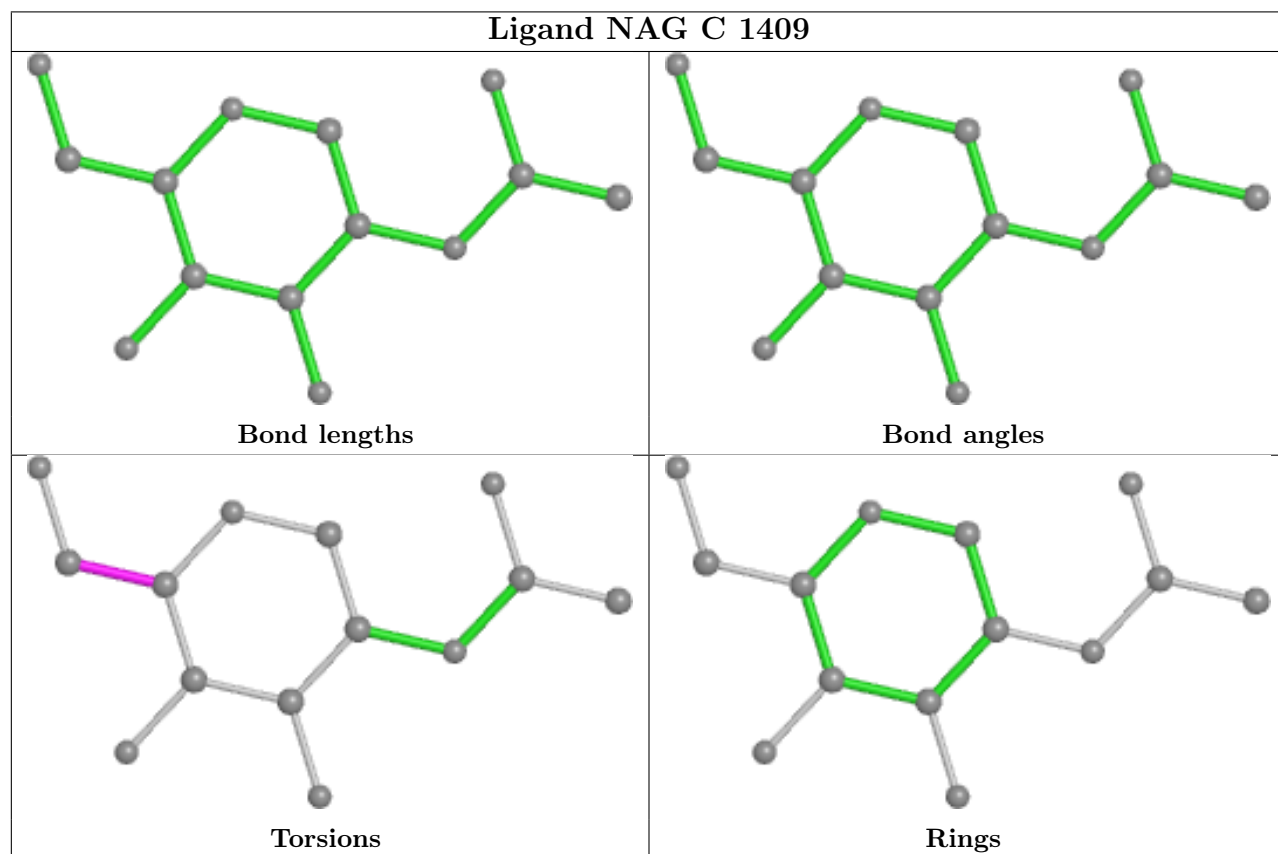
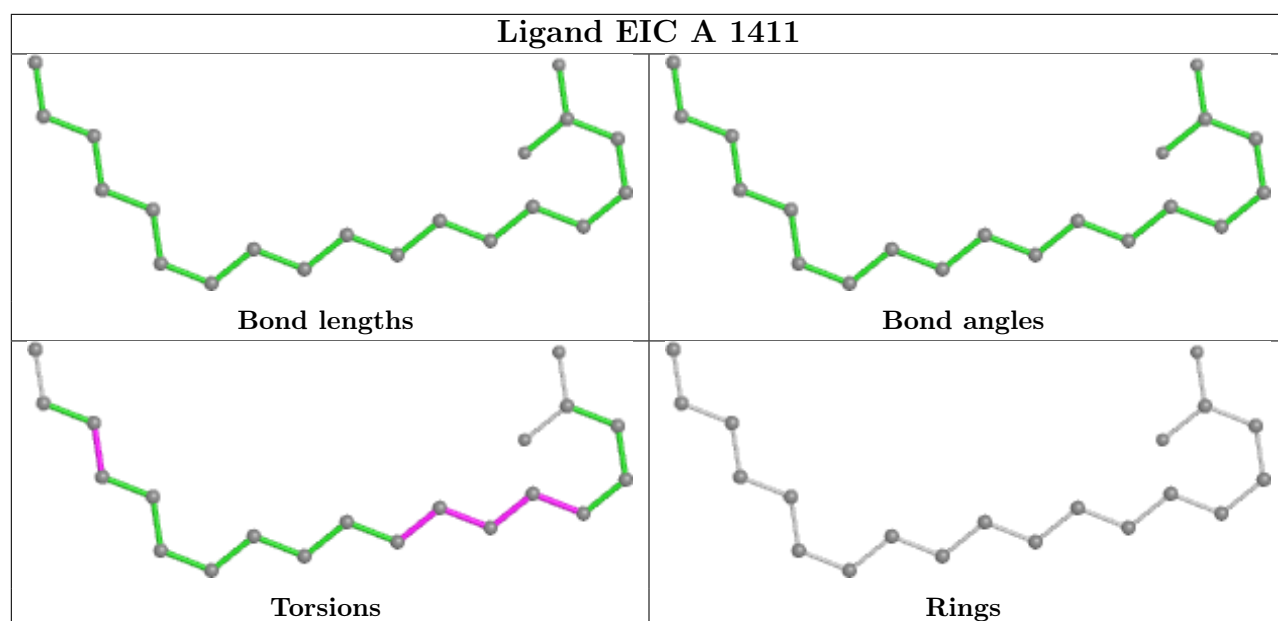


Ligand NAG B 1409

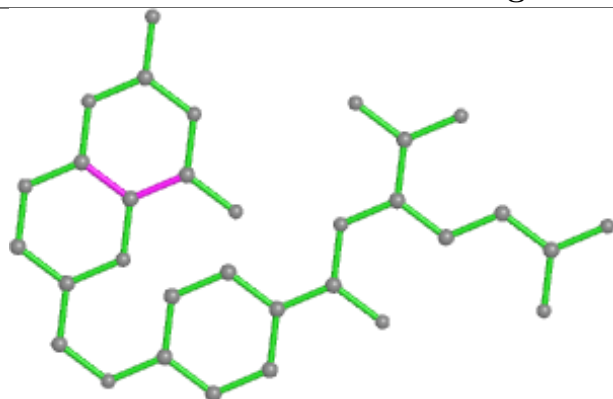


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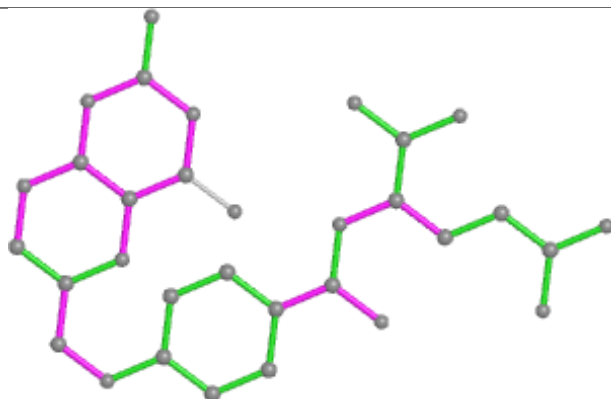




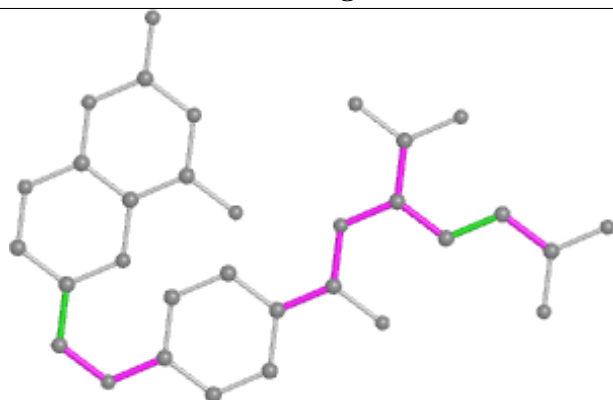
Ligand FOL C 1408



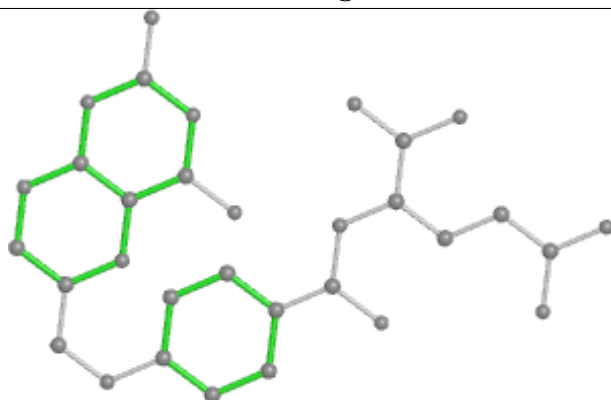
Bond lengths



Bond angles

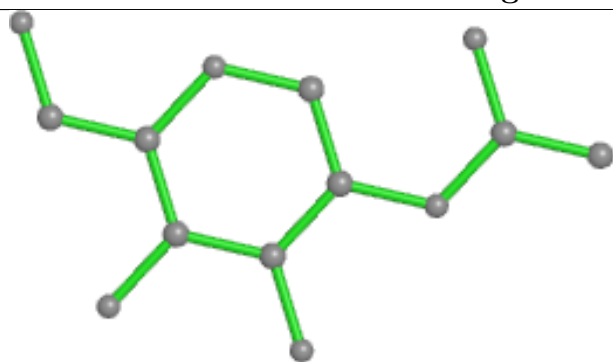


Torsions

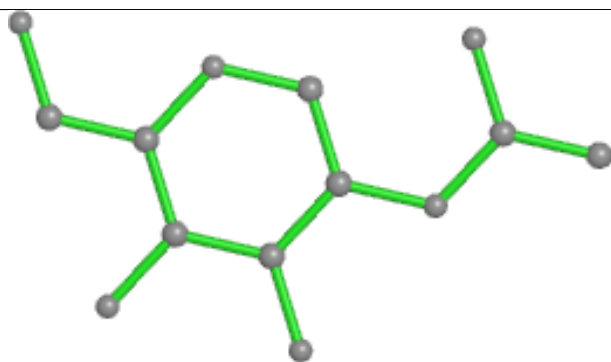


Rings

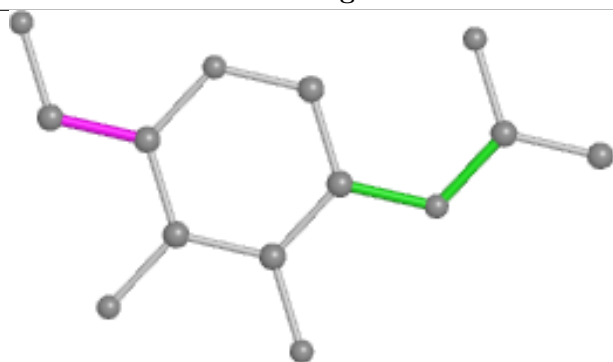
Ligand NAG C 1405



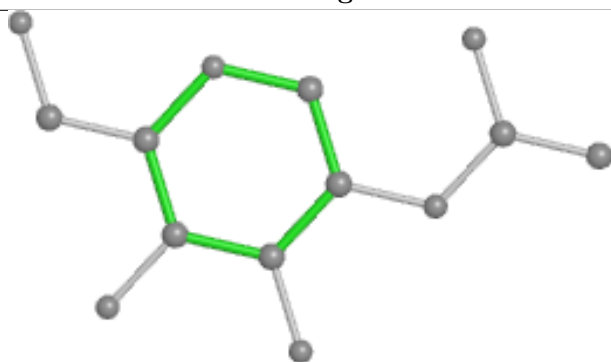
Bond lengths



Bond angles

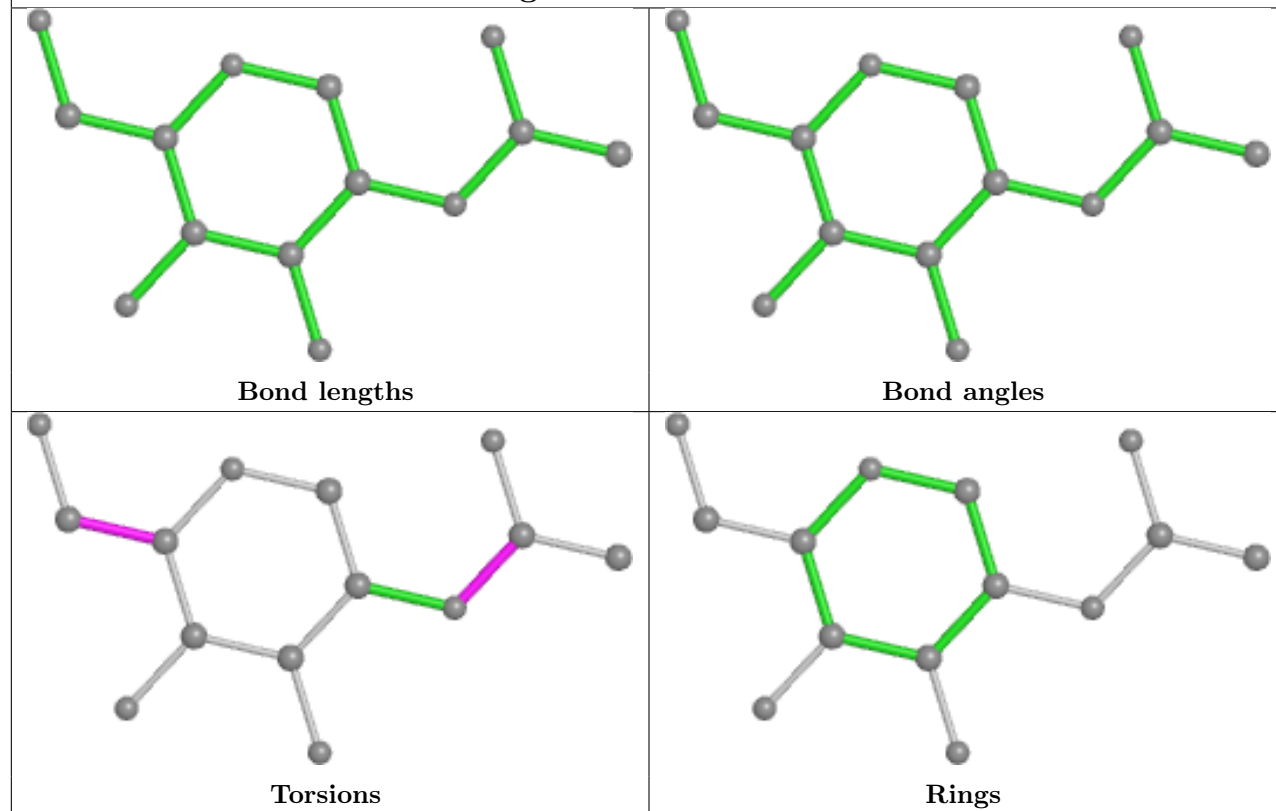


Torsions

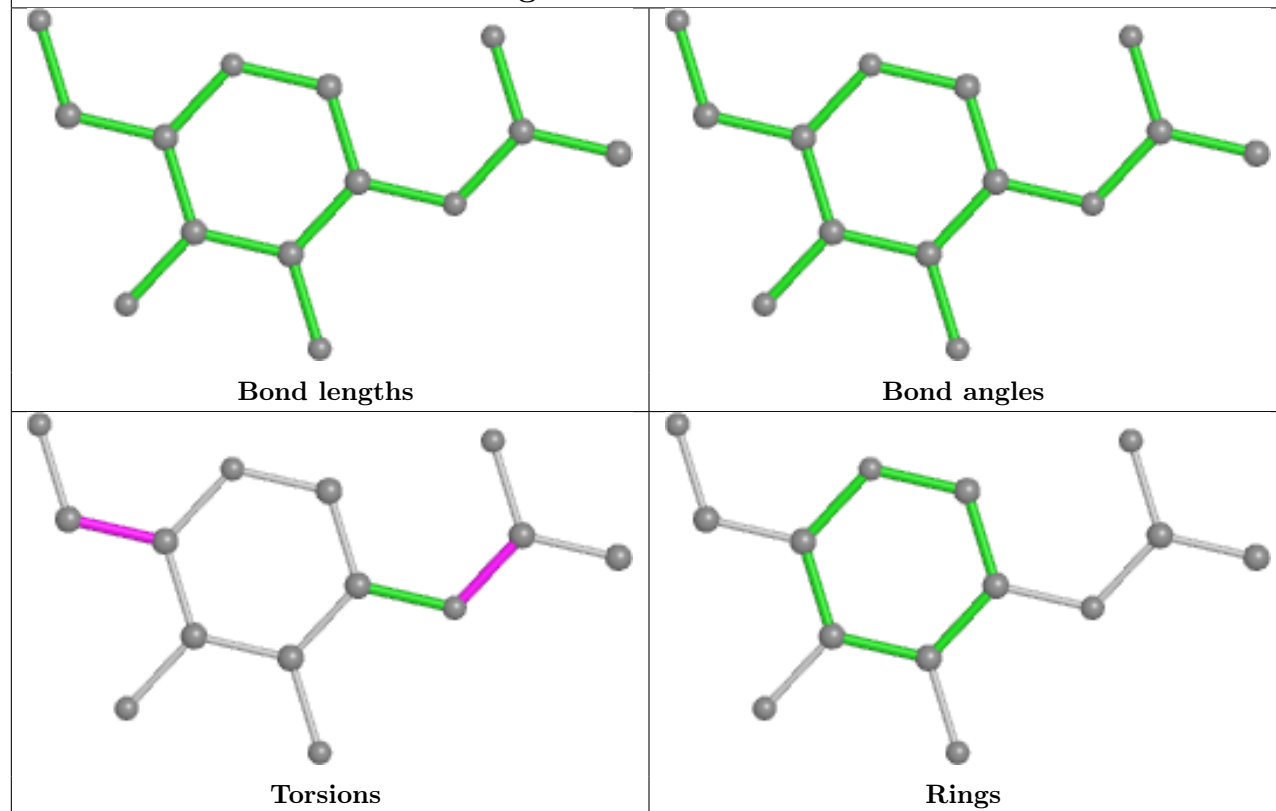


Rings

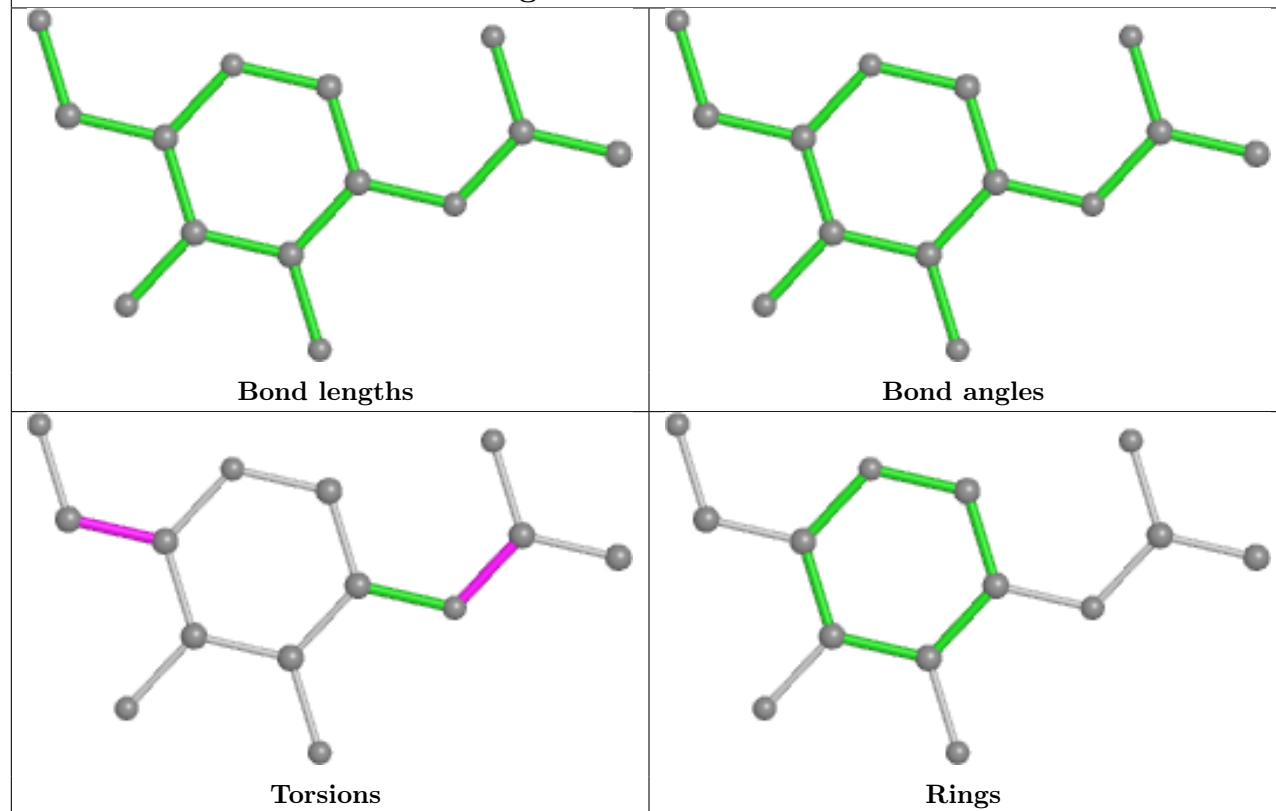
Ligand NAG B 1406



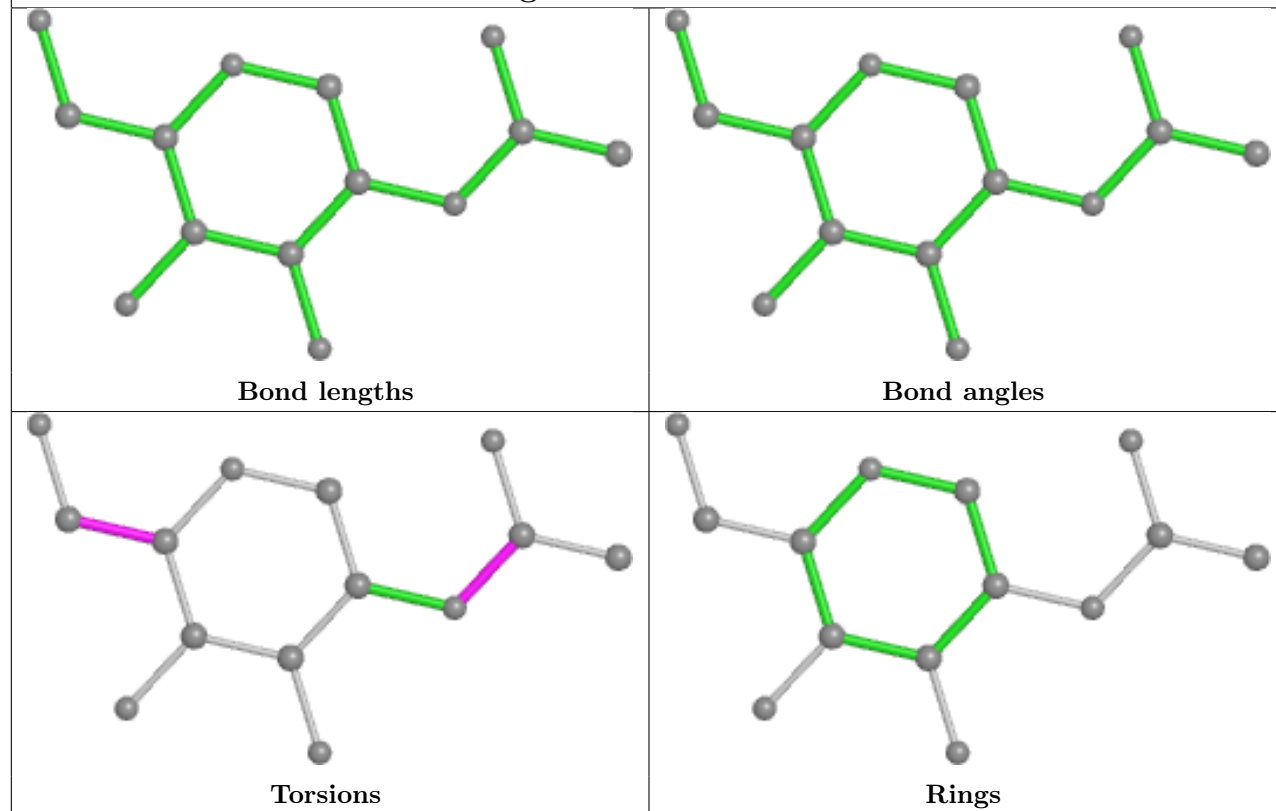
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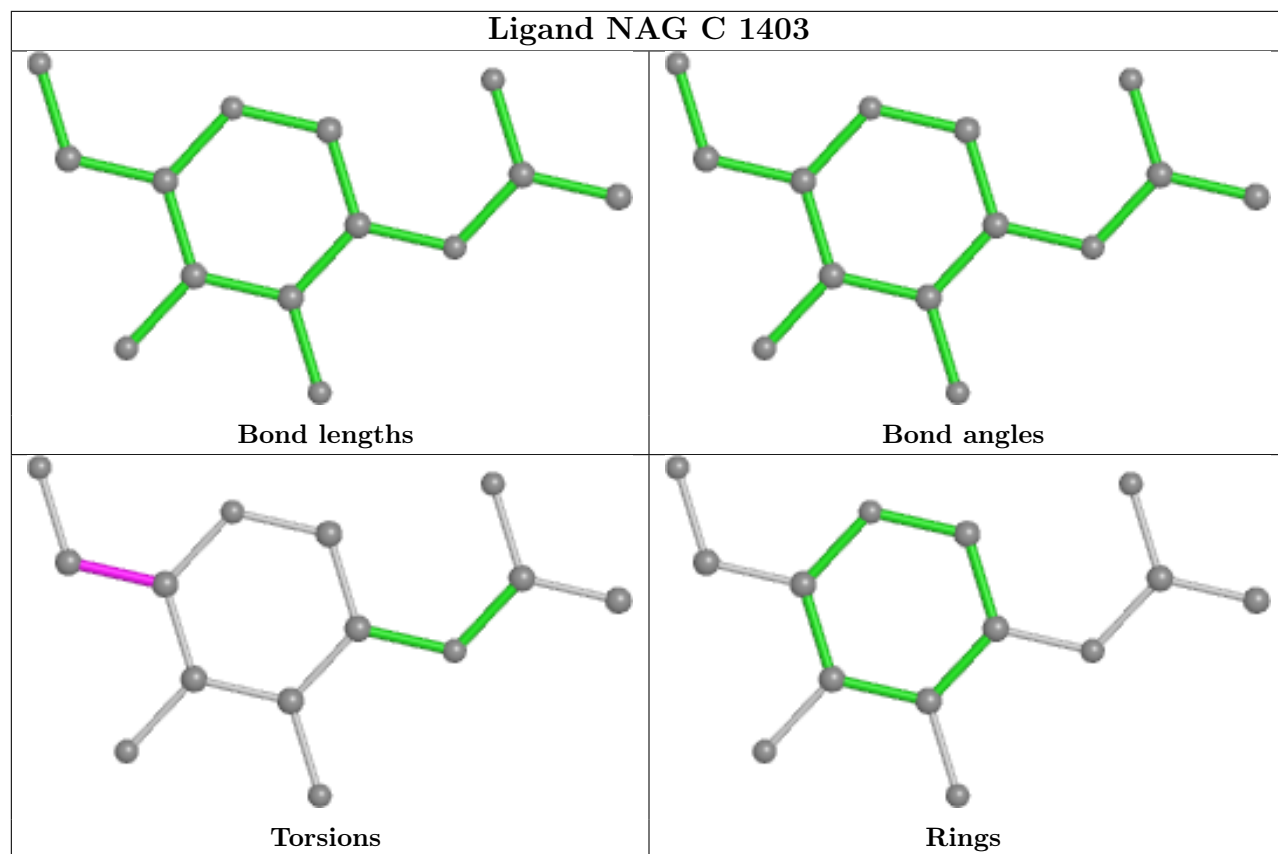
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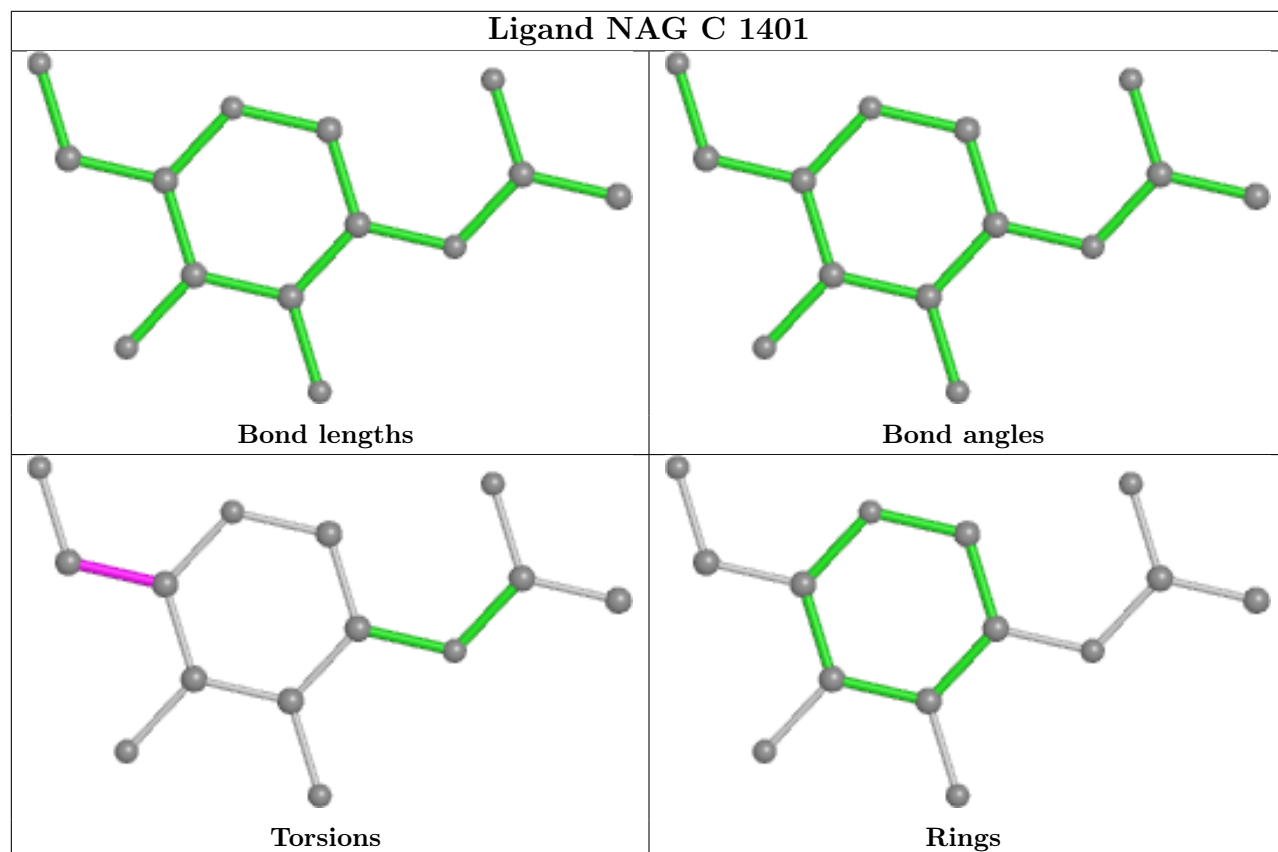
Ligand NAG B 1408



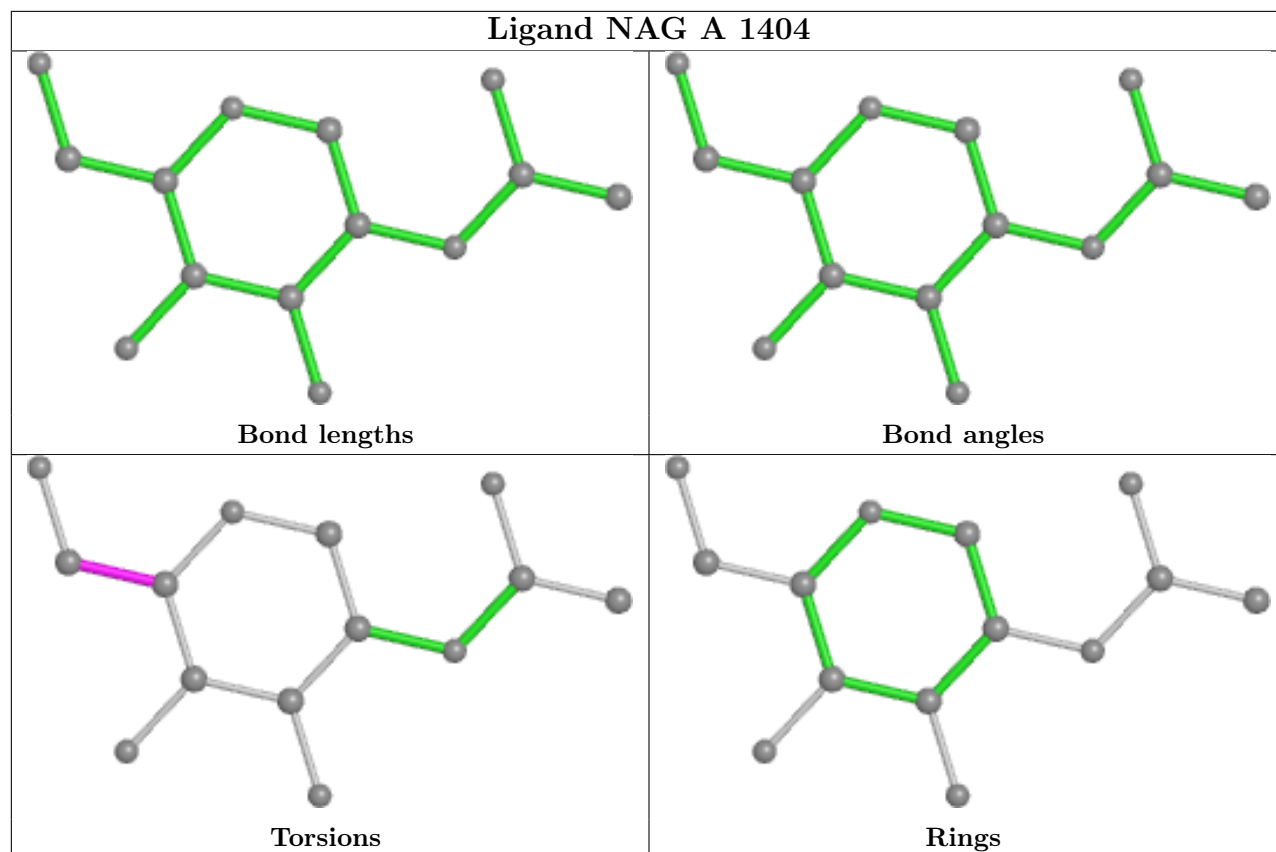
Ligand NAG C 1403



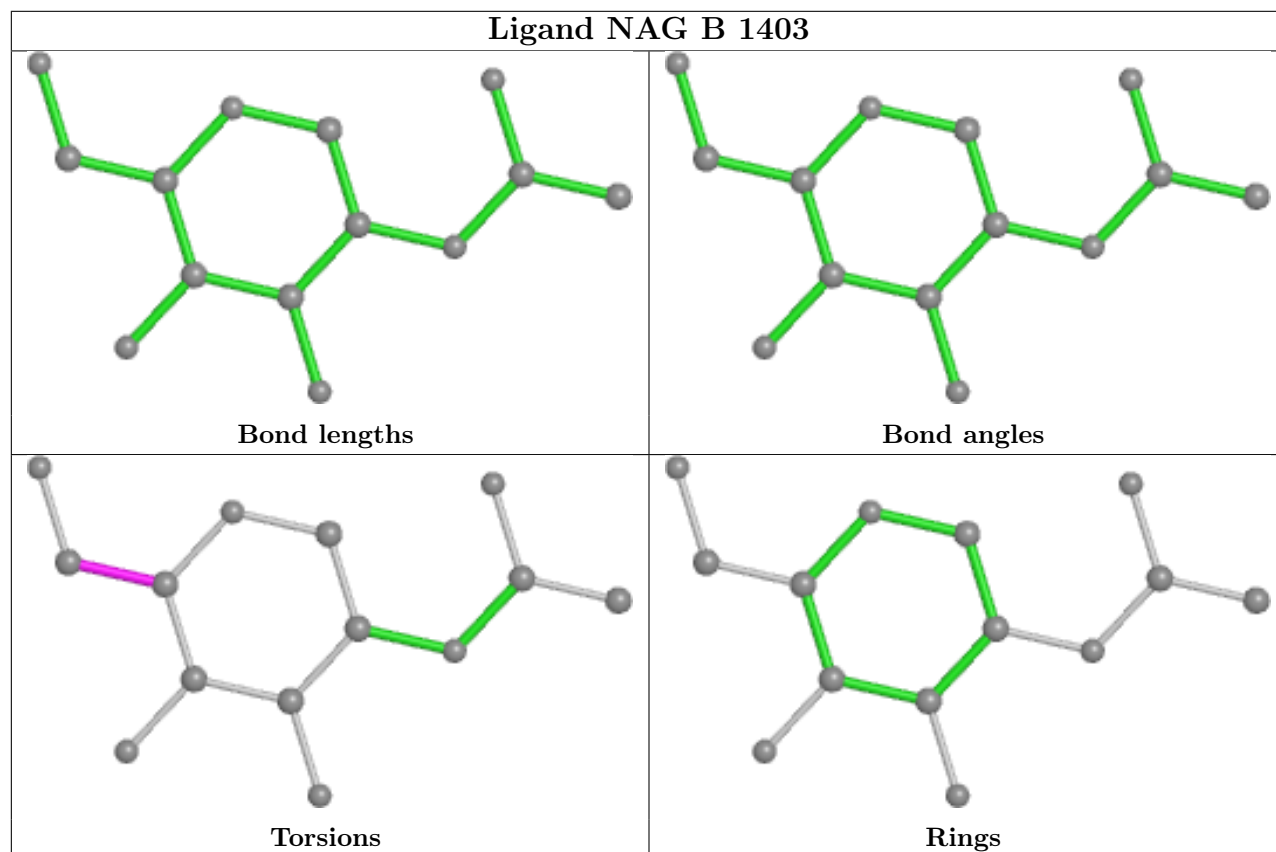
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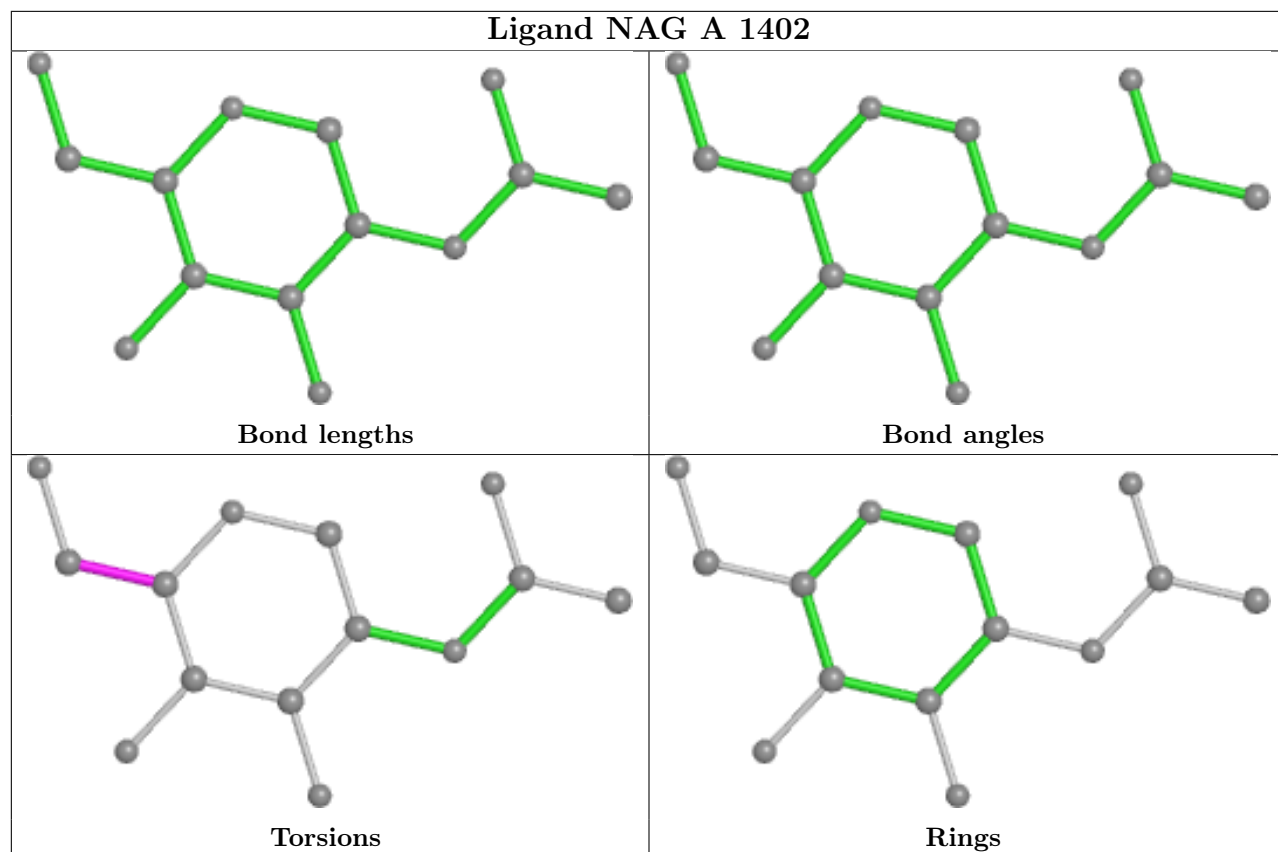
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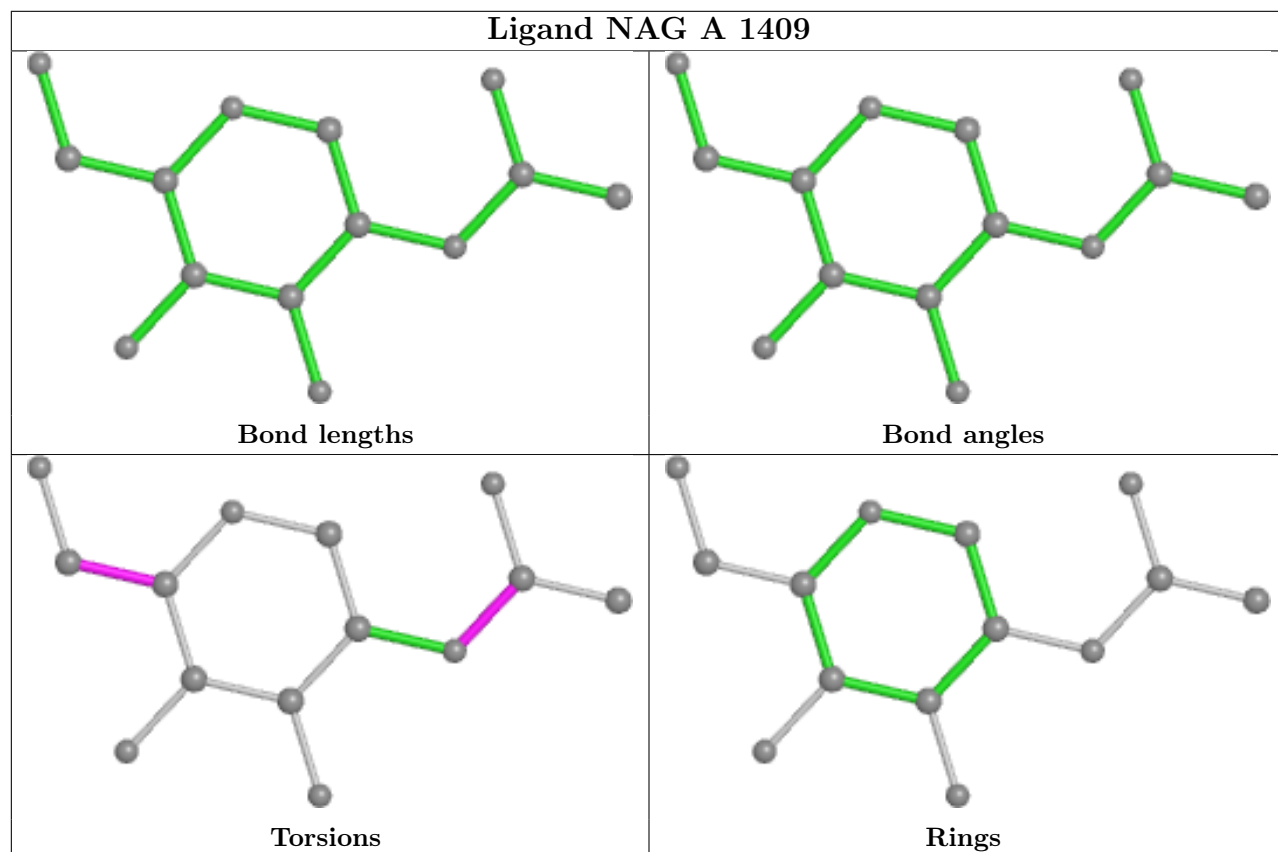
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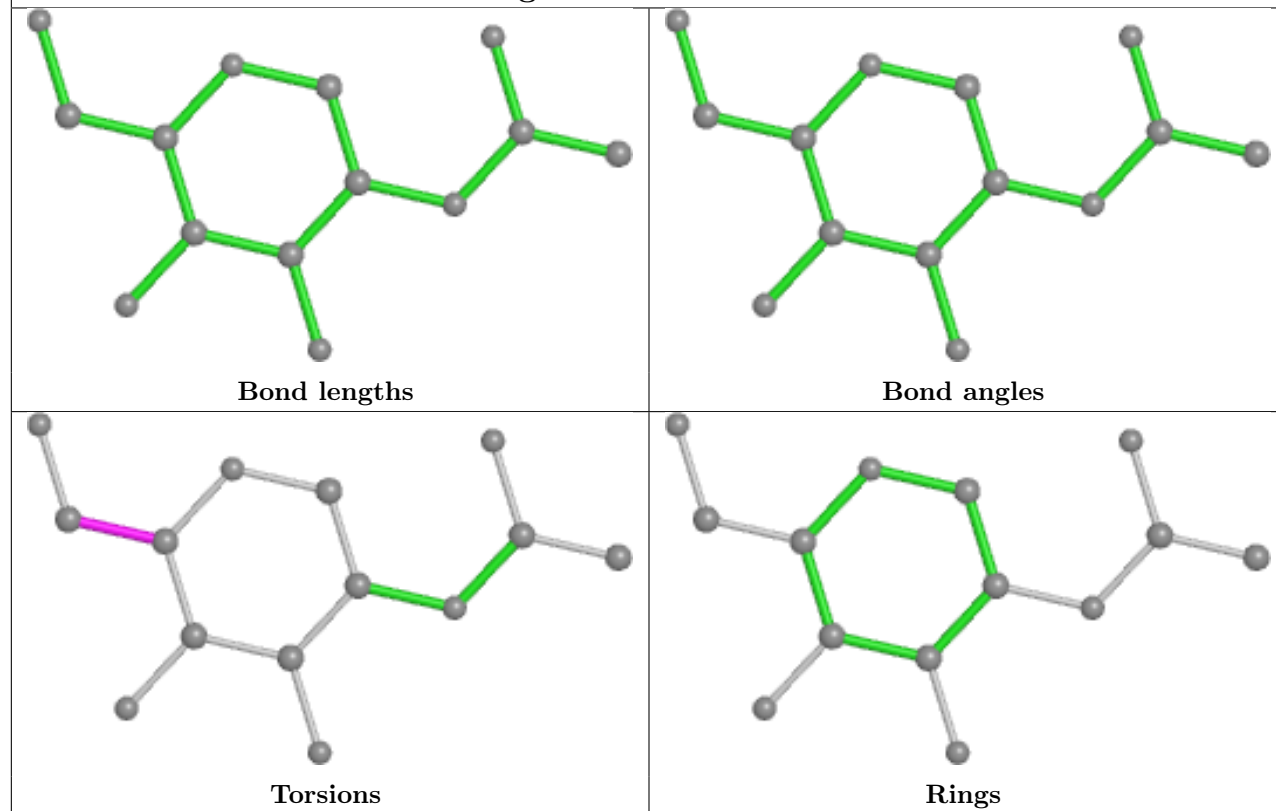
Ligand NAG A 1402



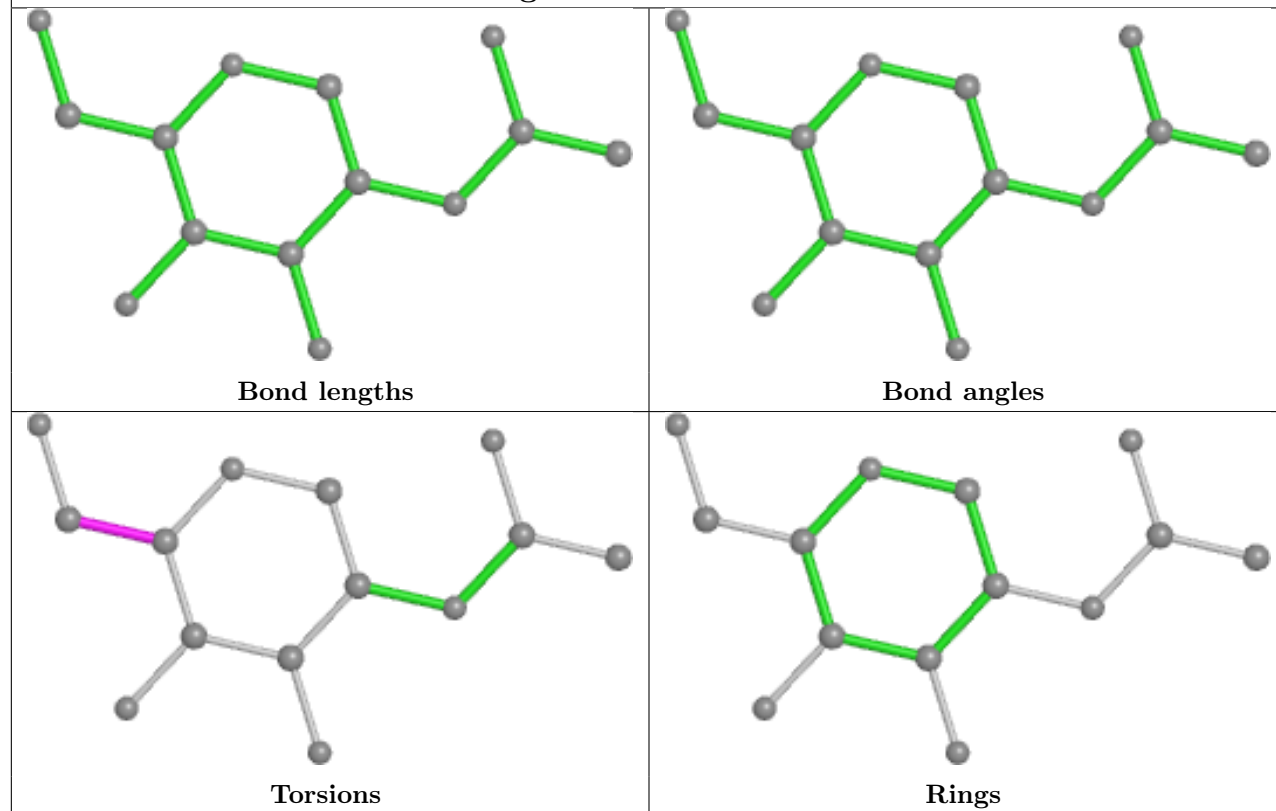
Ligand NAG A 1409



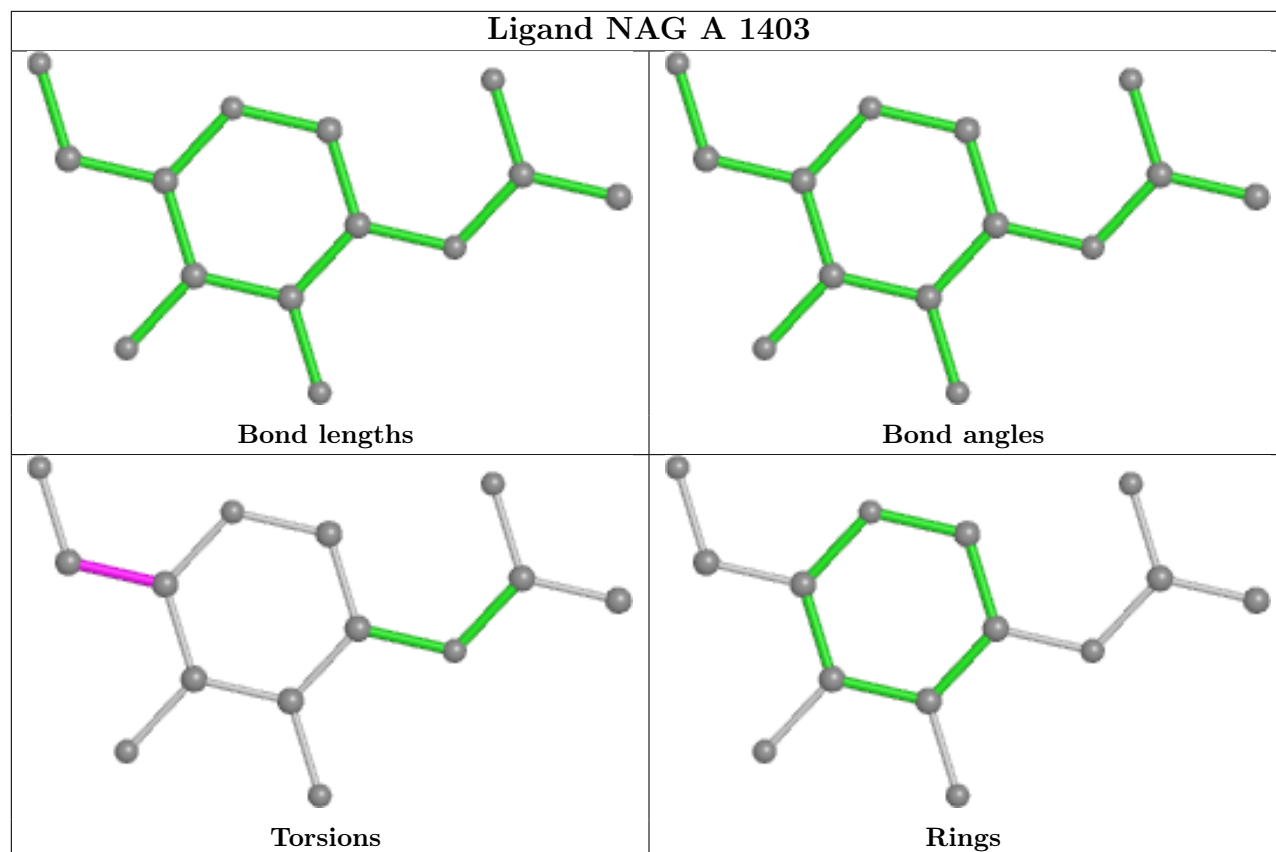
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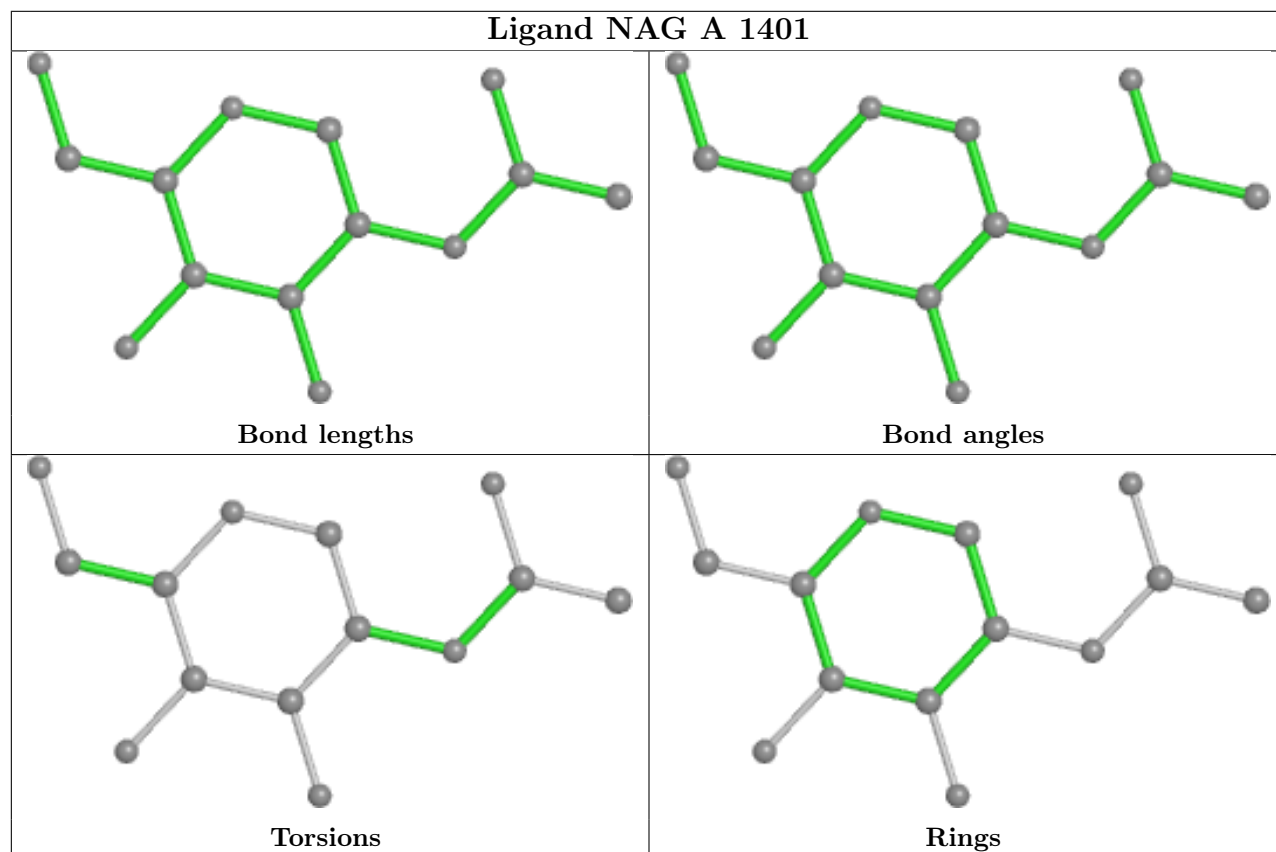
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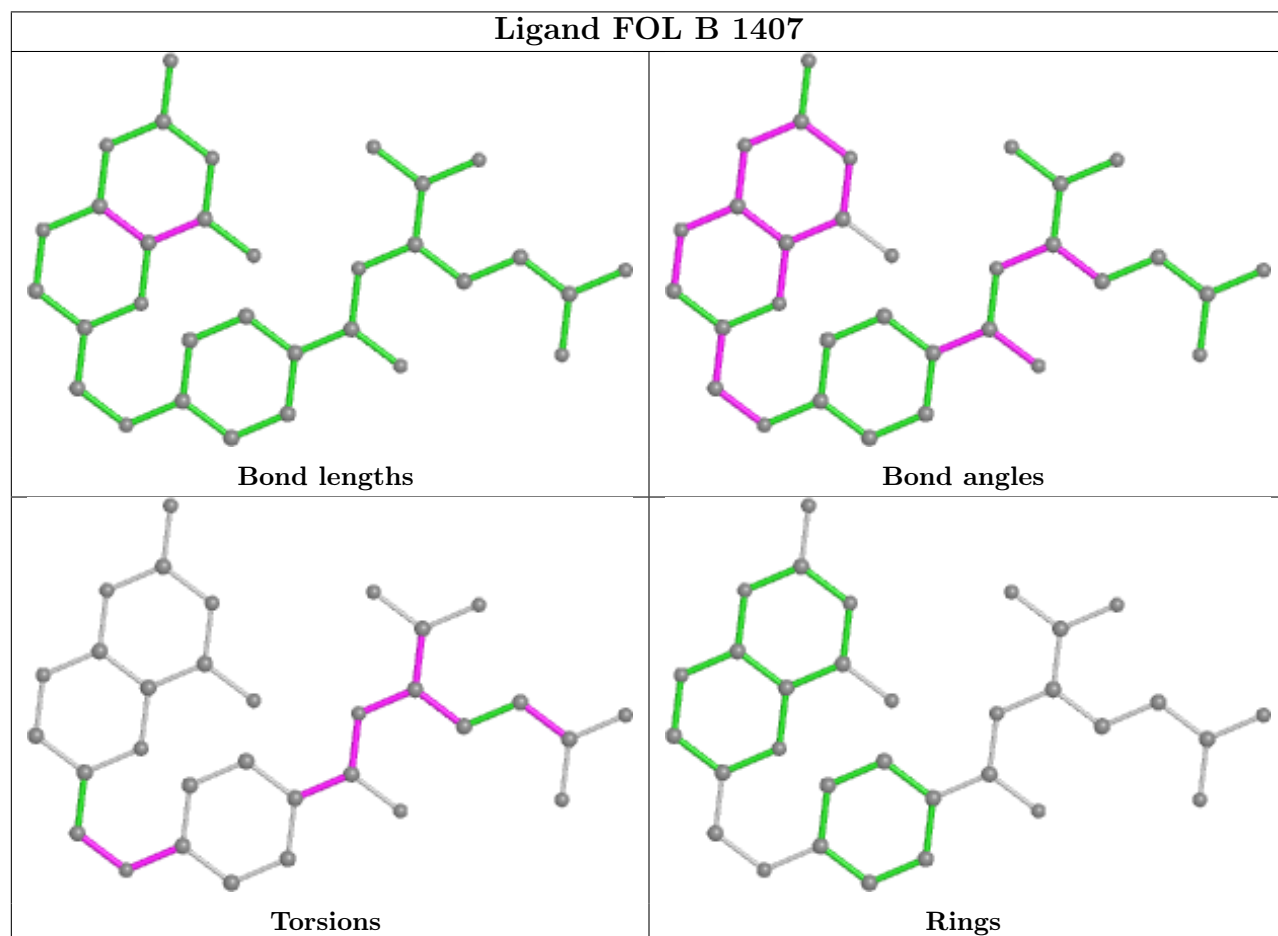
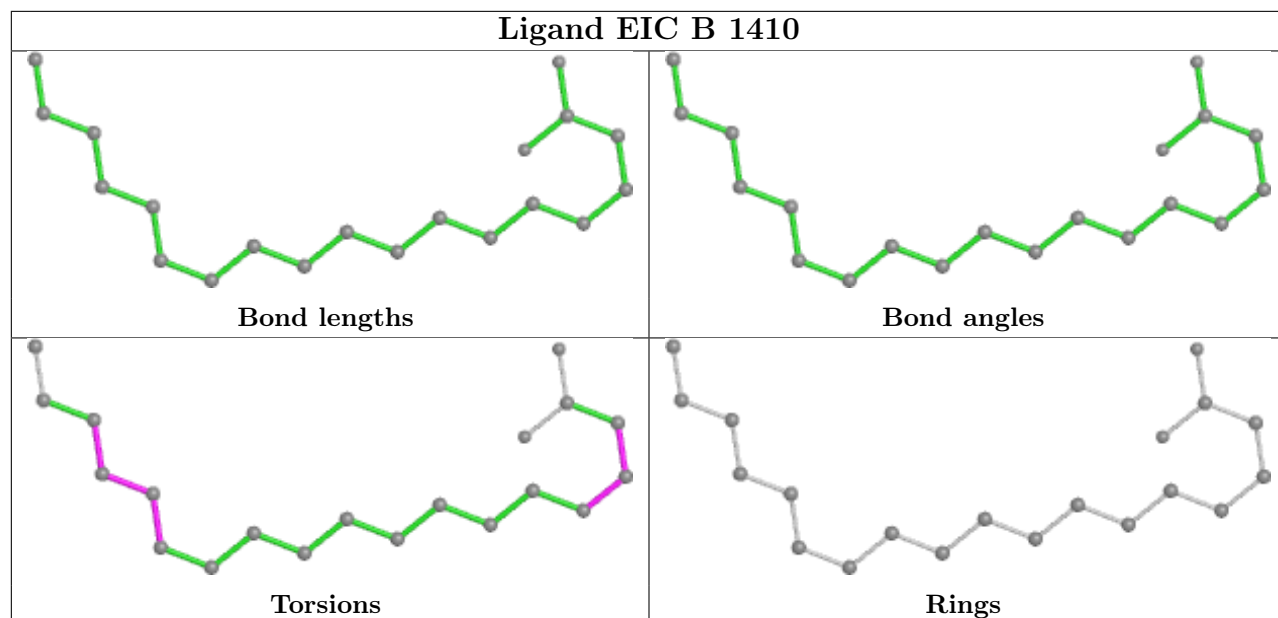


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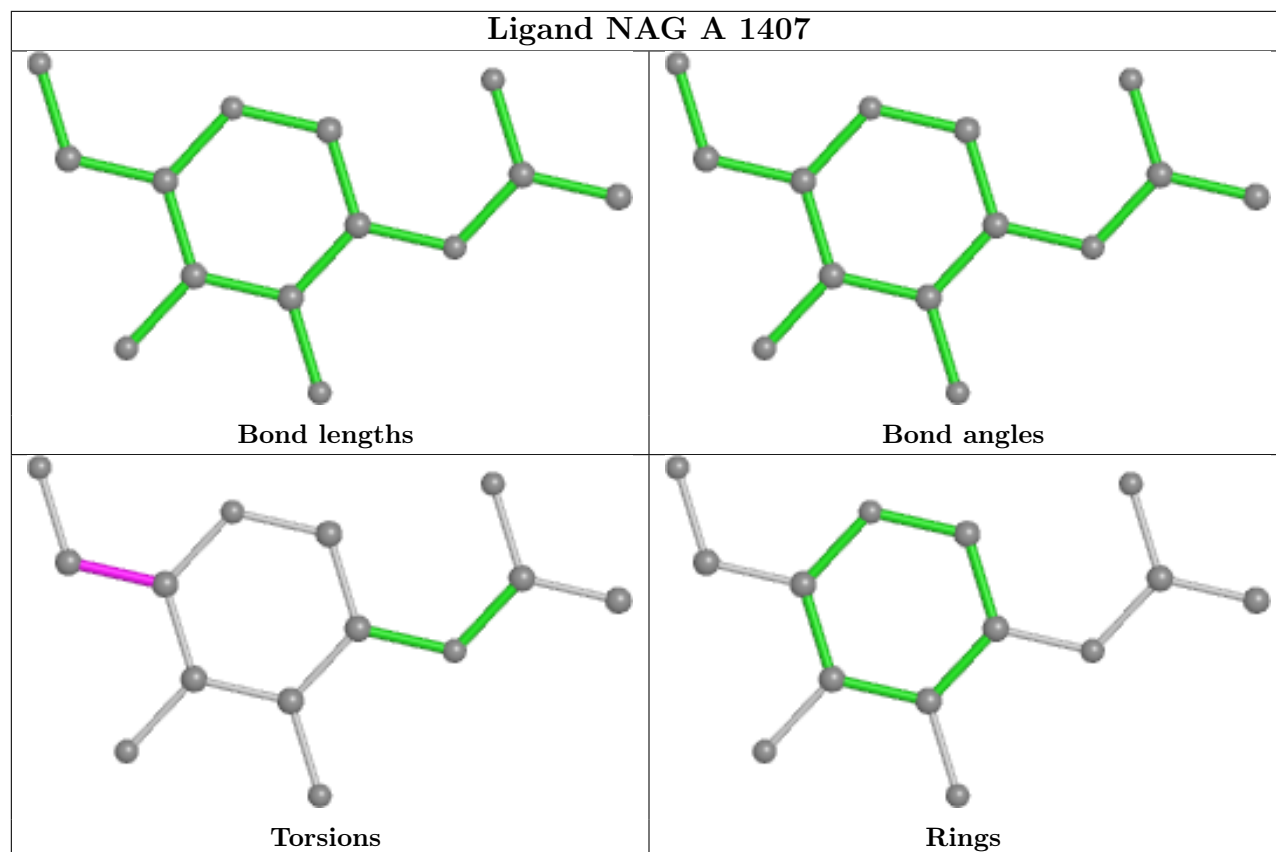


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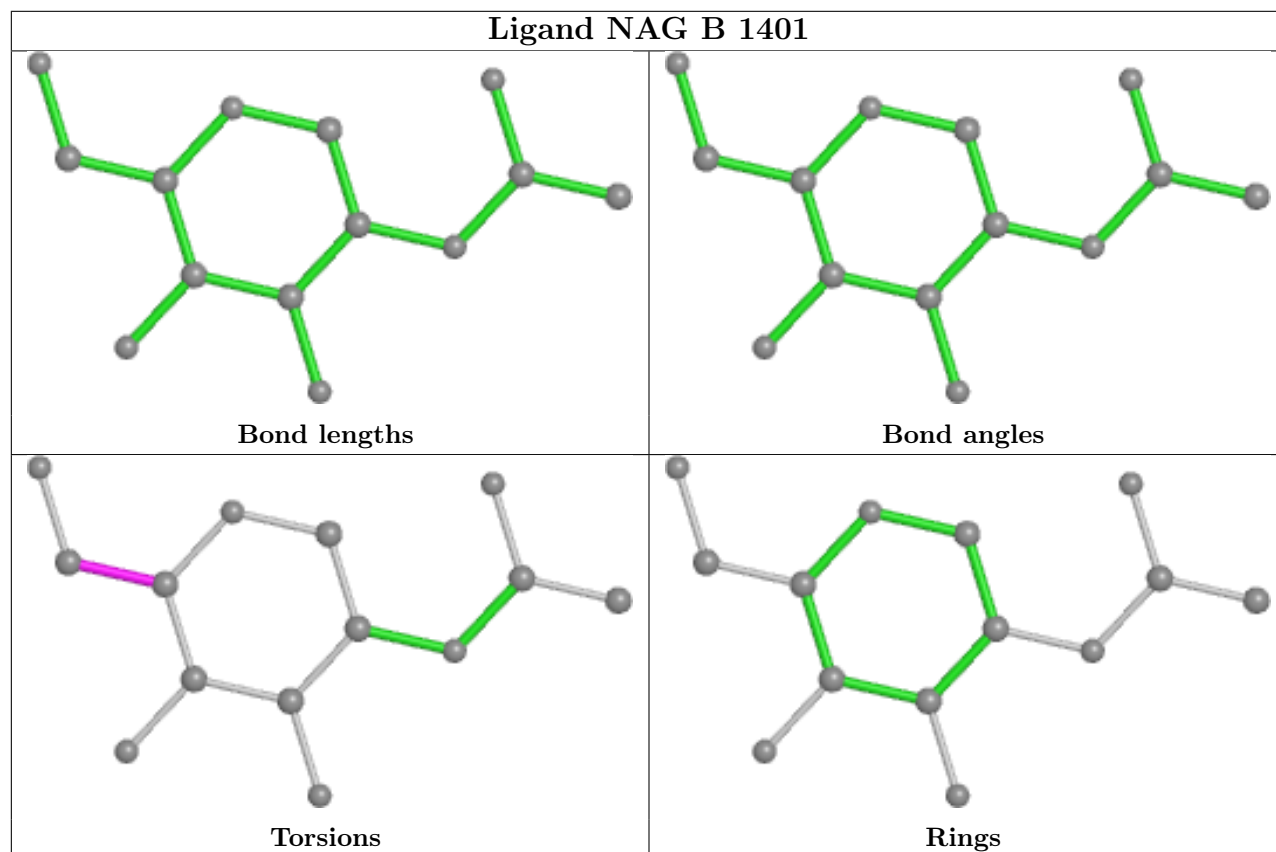




Ligand NAG A 1407



Ligand NAG B 1401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

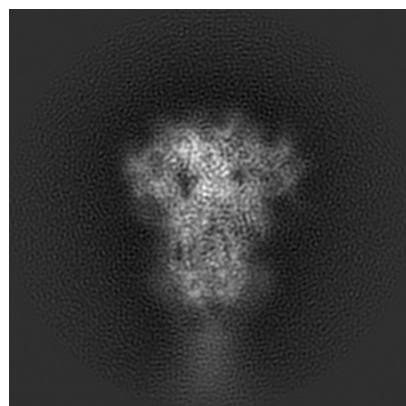
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61607. These allow visual inspection of the internal detail of the map and identification of artifacts.

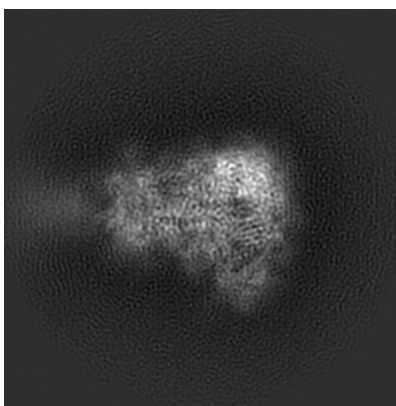
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

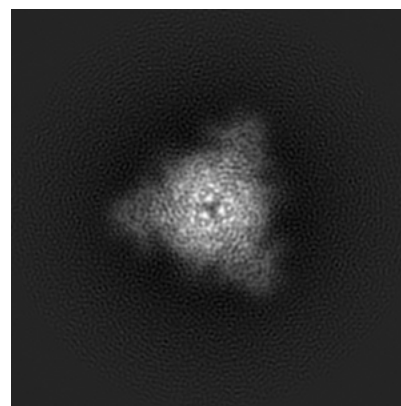
6.1.1 Primary map



X

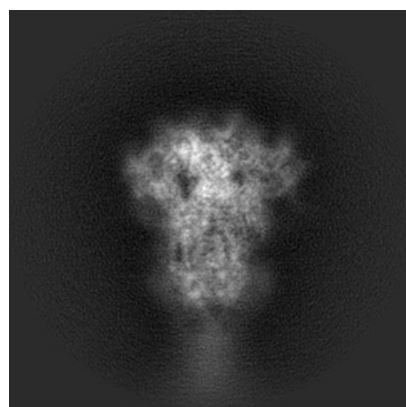


Y

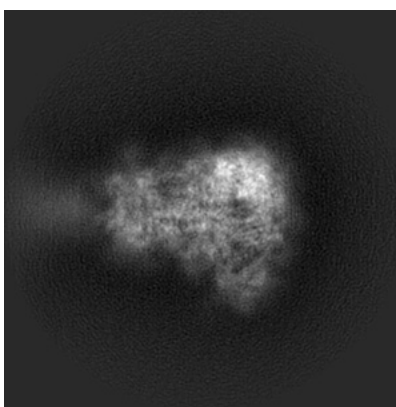


Z

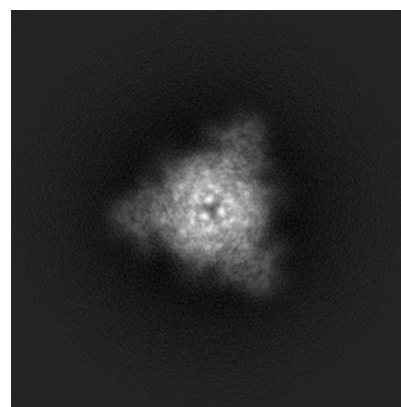
6.1.2 Raw map



X



Y

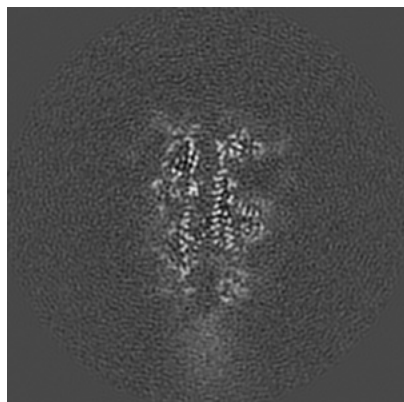


Z

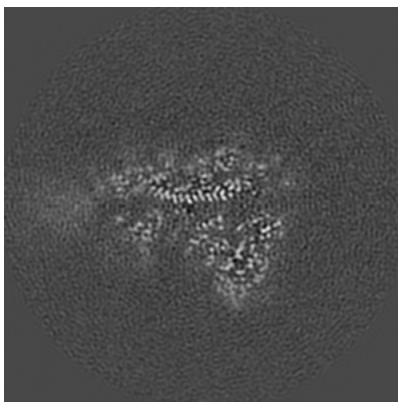
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

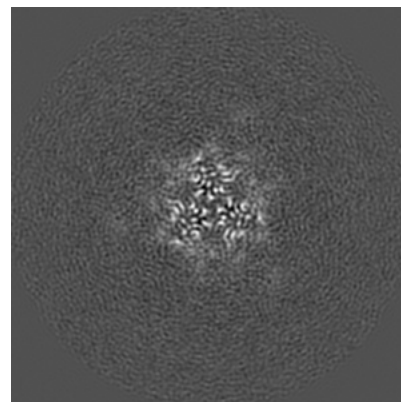
6.2.1 Primary map



X Index: 120

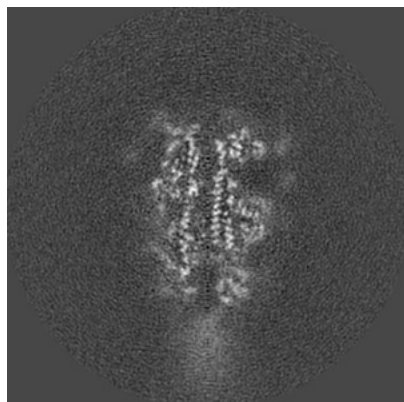


Y Index: 120

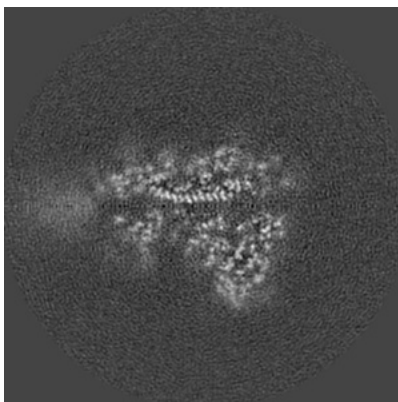


Z Index: 120

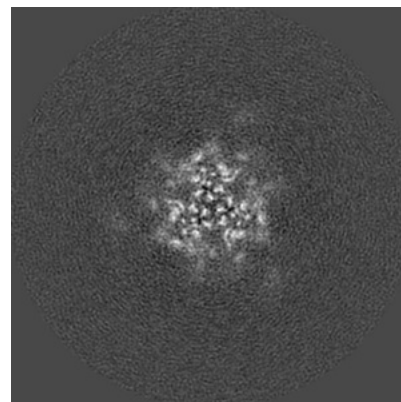
6.2.2 Raw map



X Index: 120



Y Index: 120

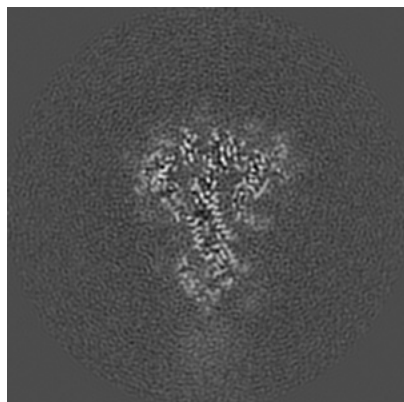


Z Index: 120

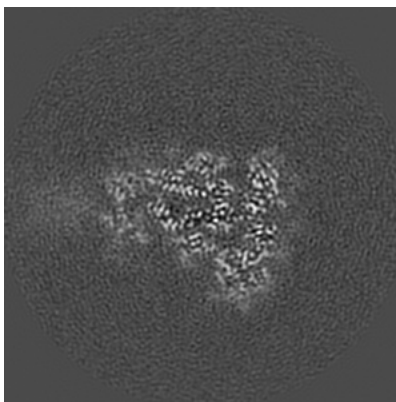
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

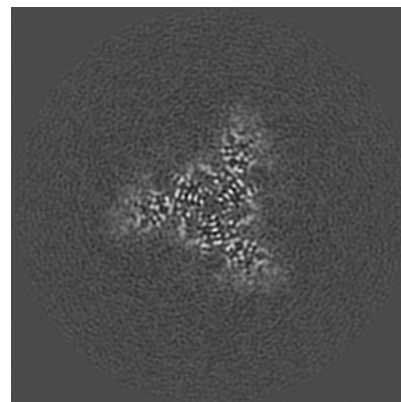
6.3.1 Primary map



X Index: 131

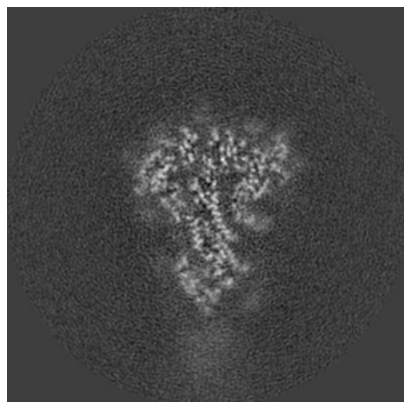


Y Index: 113

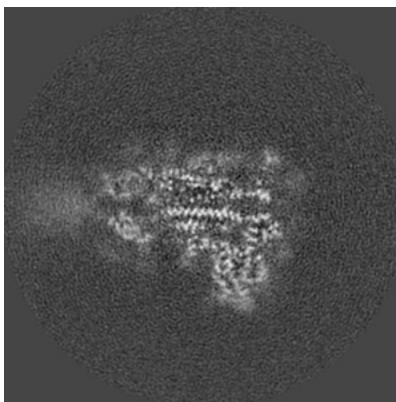


Z Index: 148

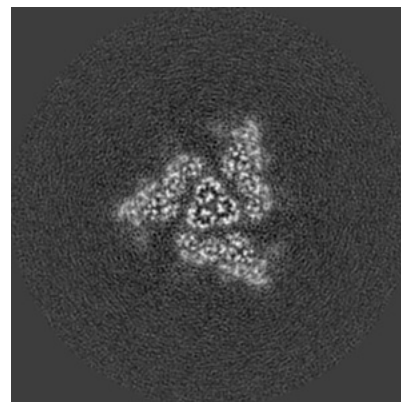
6.3.2 Raw map



X Index: 131



Y Index: 116

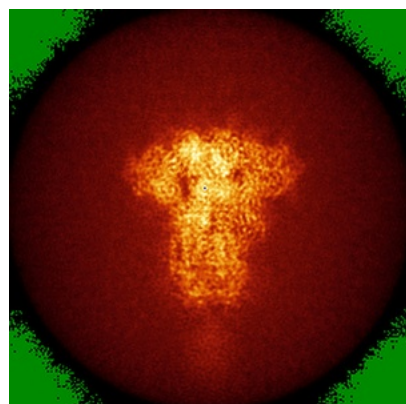


Z Index: 132

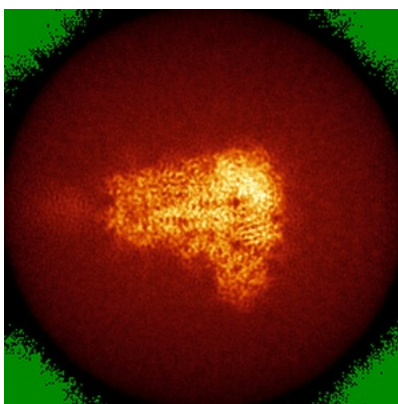
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

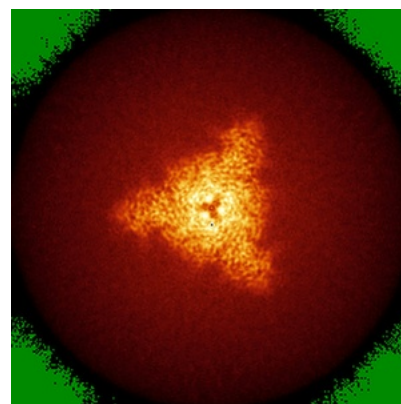
6.4.1 Primary map



X

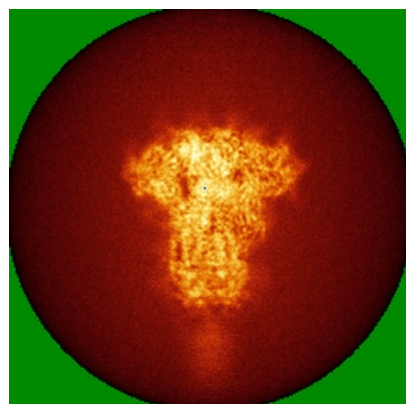


Y

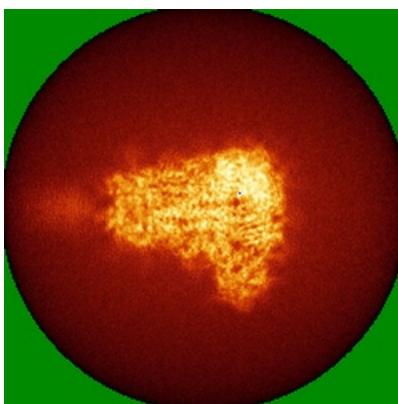


Z

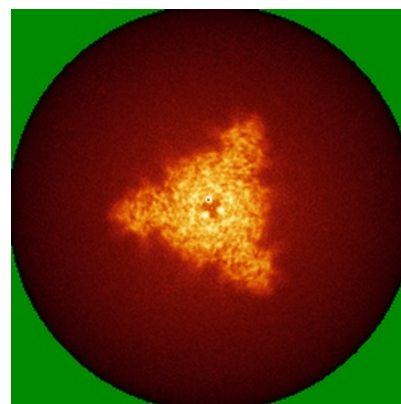
6.4.2 Raw map



X



Y

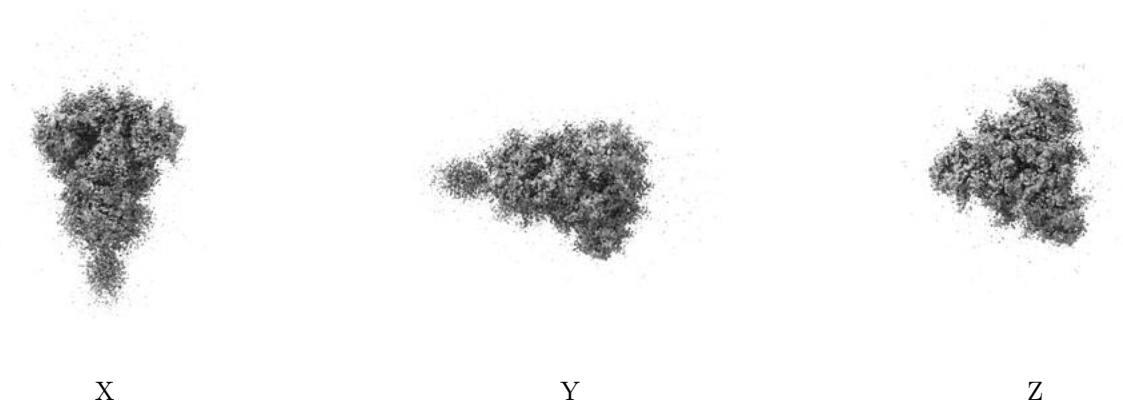


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

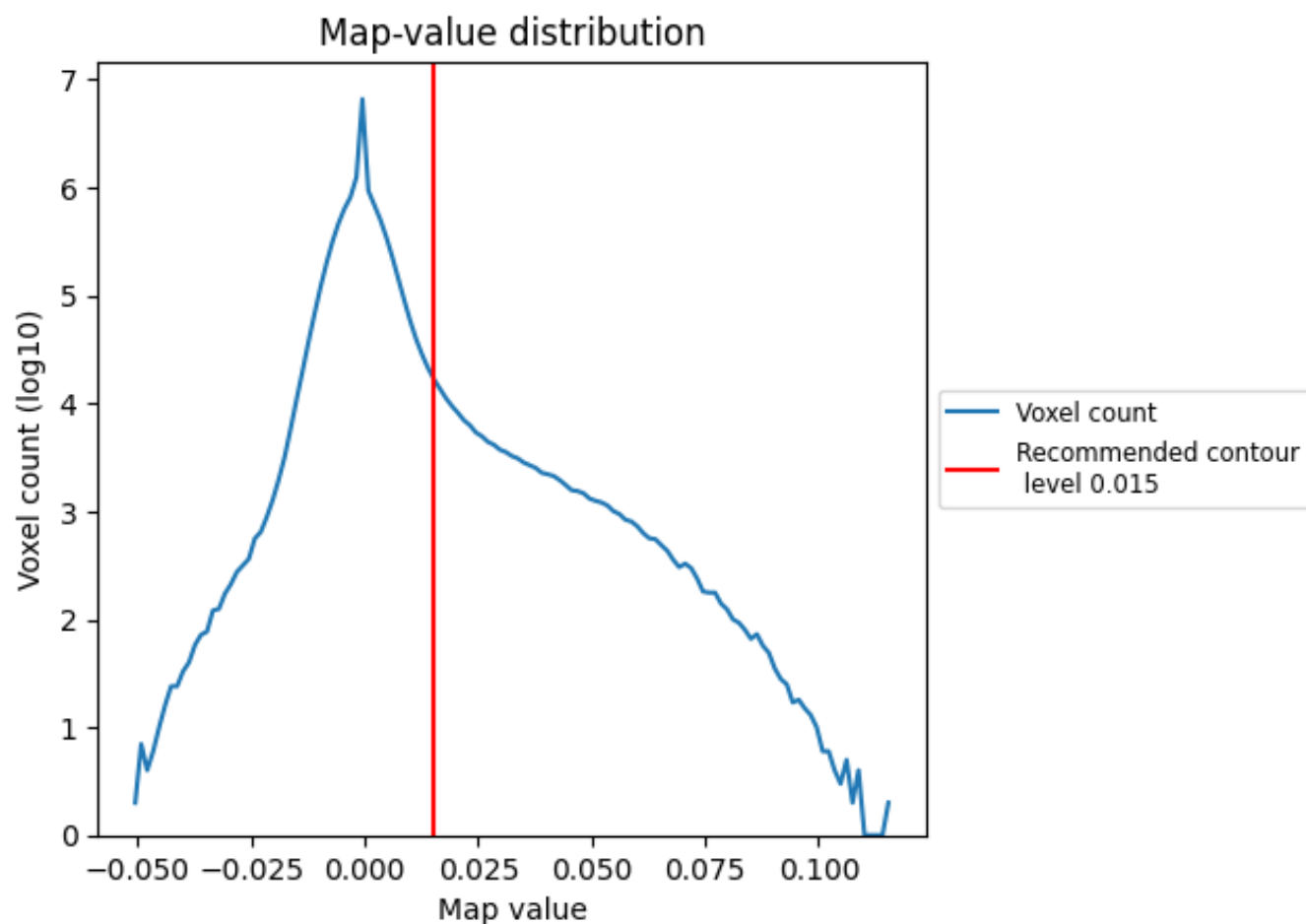
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

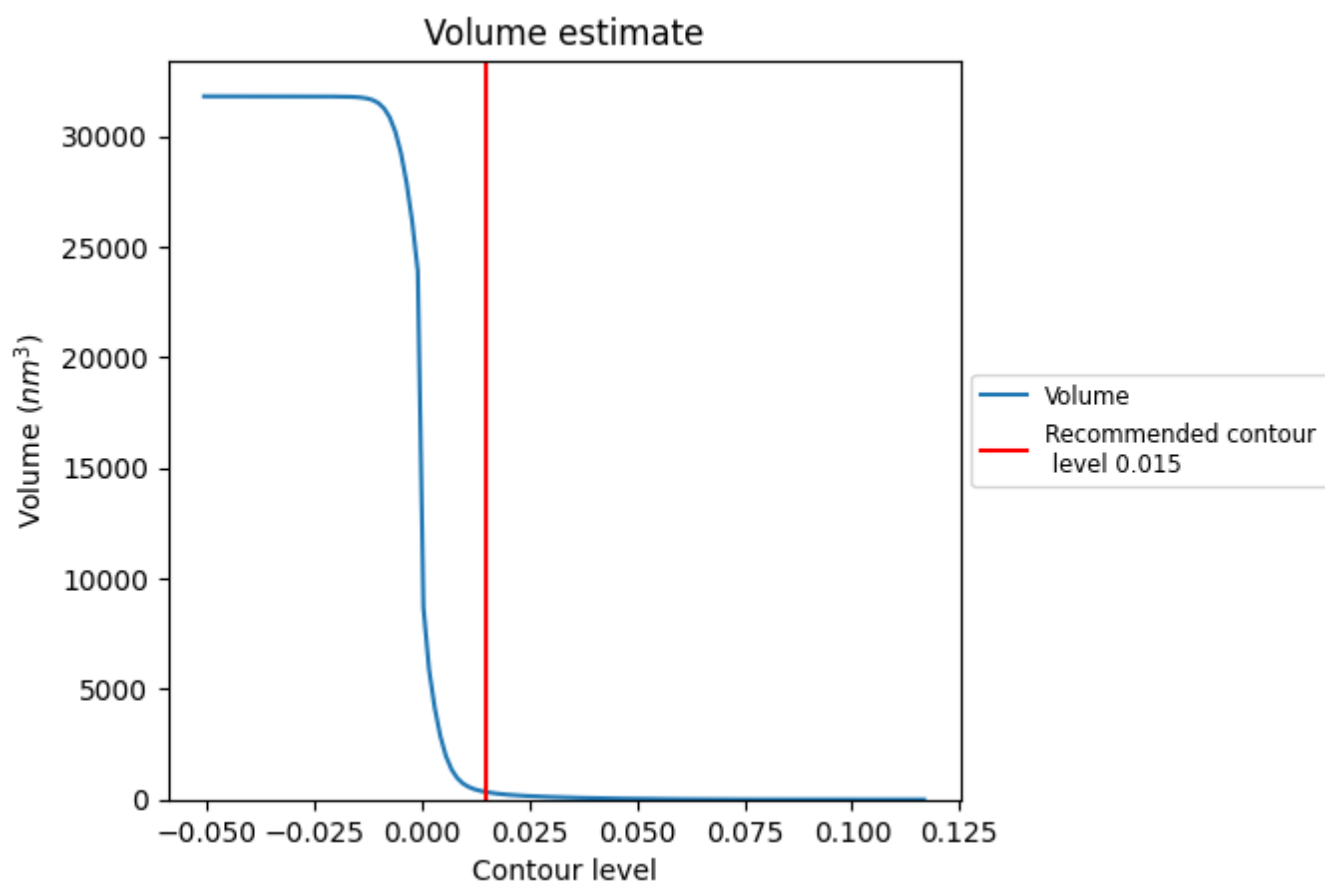
This section contains the results of statistical analysis of the map.

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.

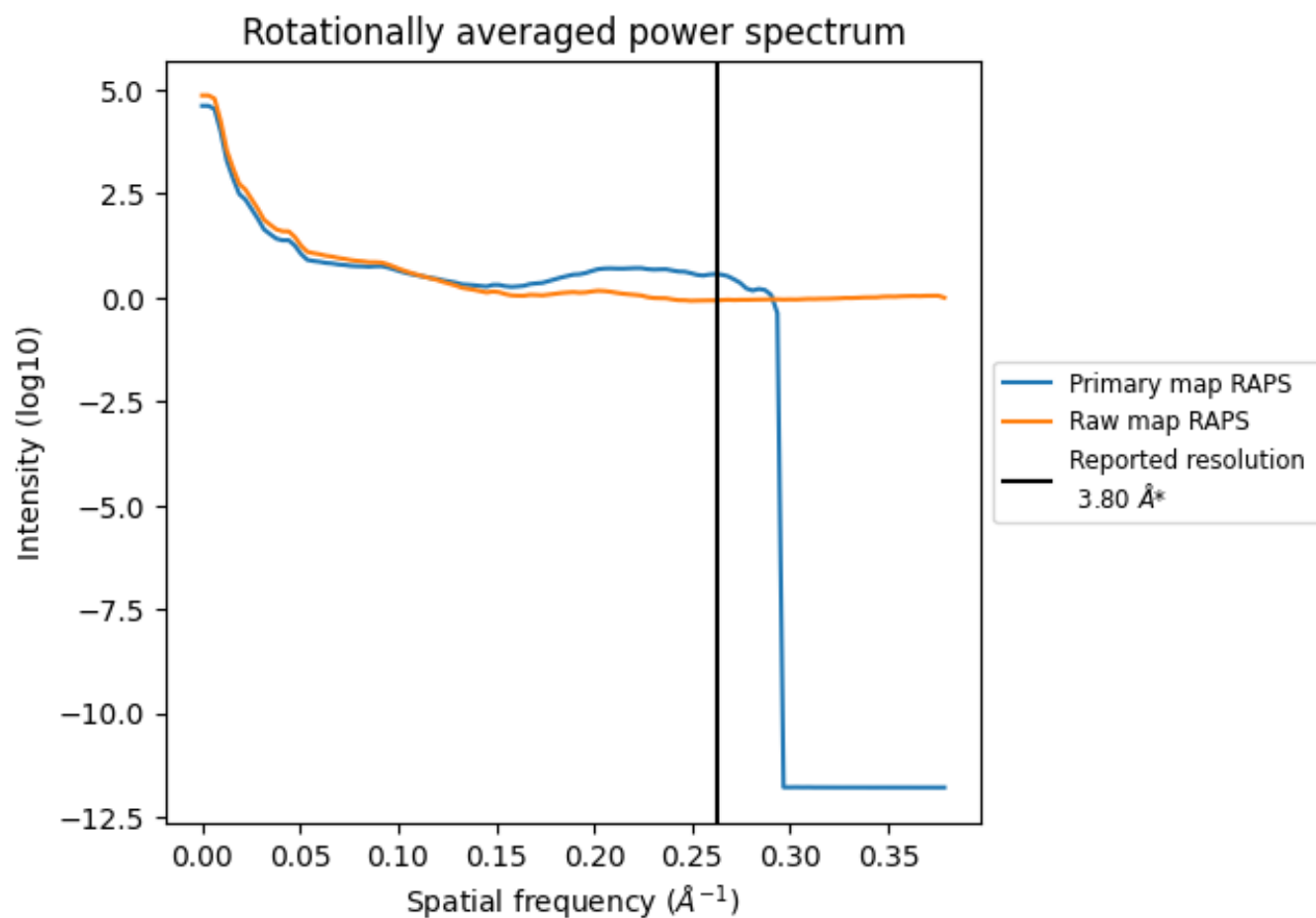
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm³; this corresponds to an approximate mass of 307 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 ⓘ

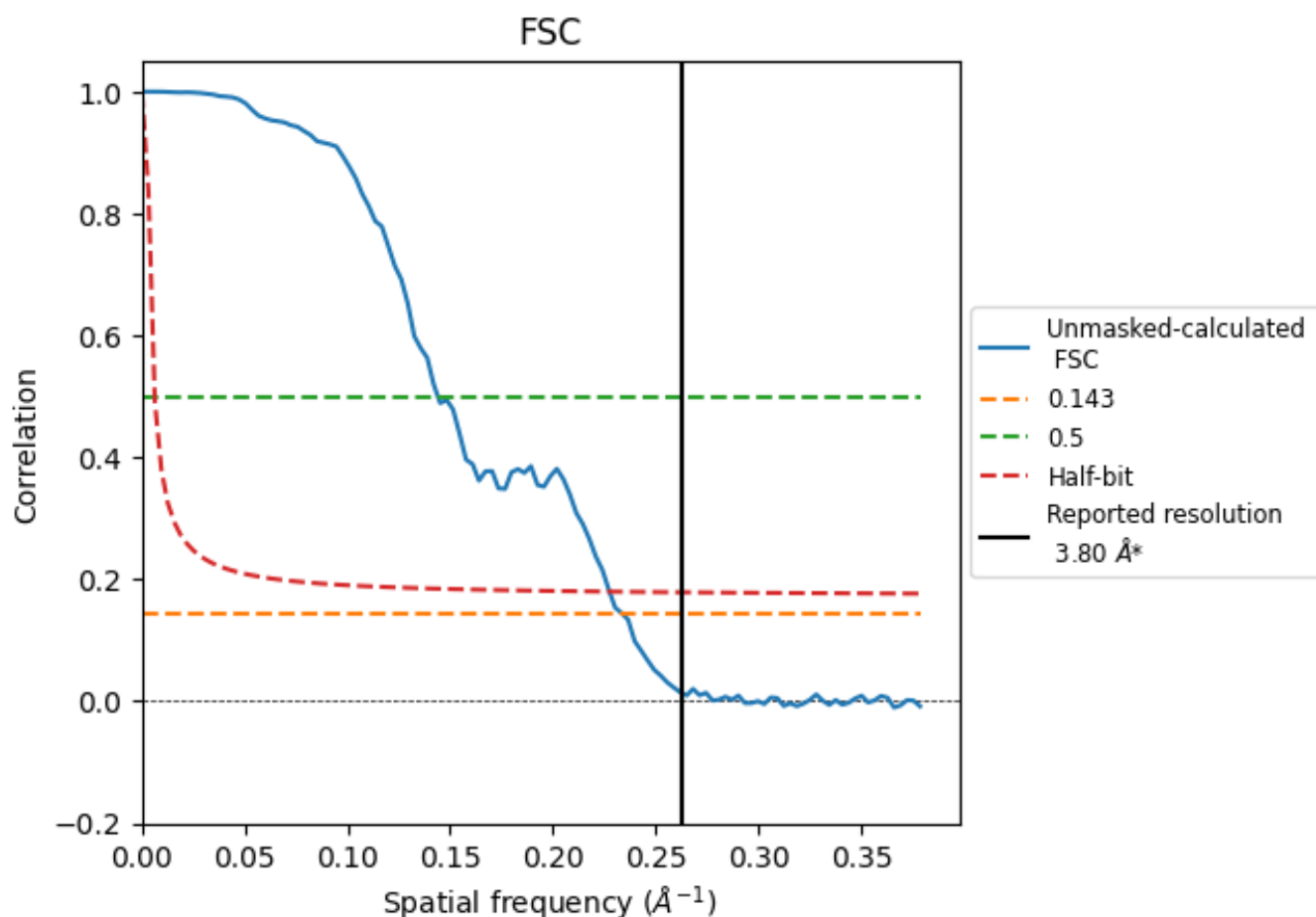


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

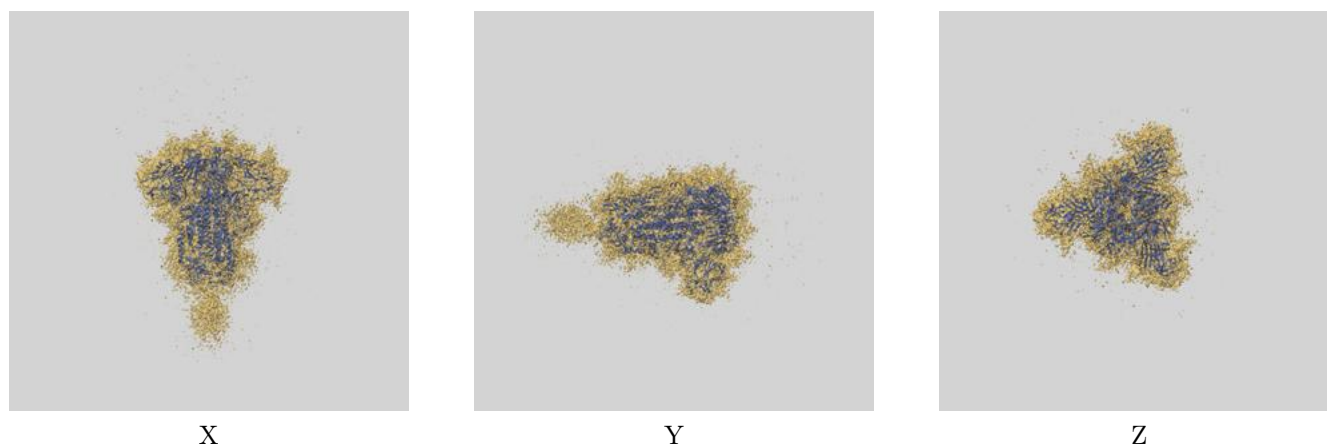
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.27	6.94	4.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

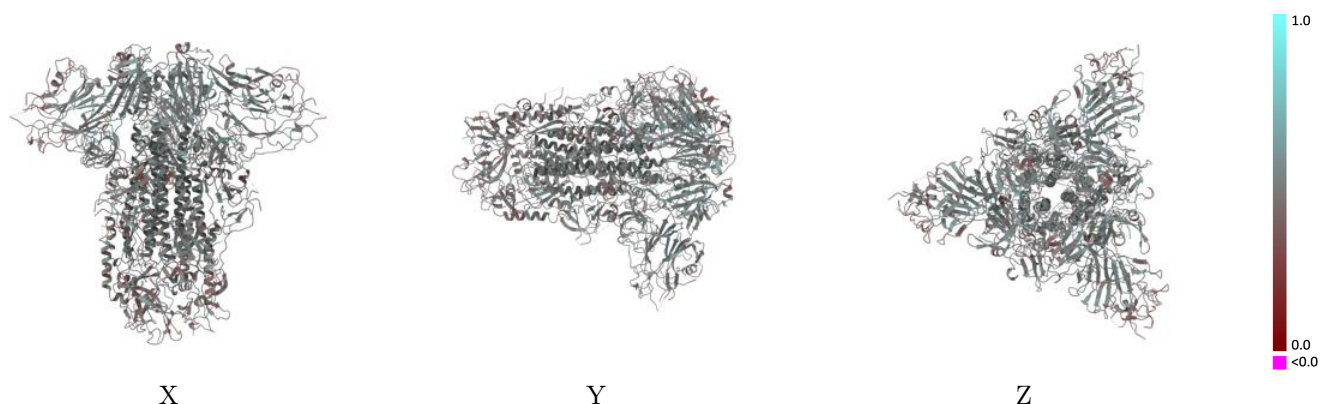
This section contains information regarding the fit between EMDB map EMD-61607 and PDB model 9JMN. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



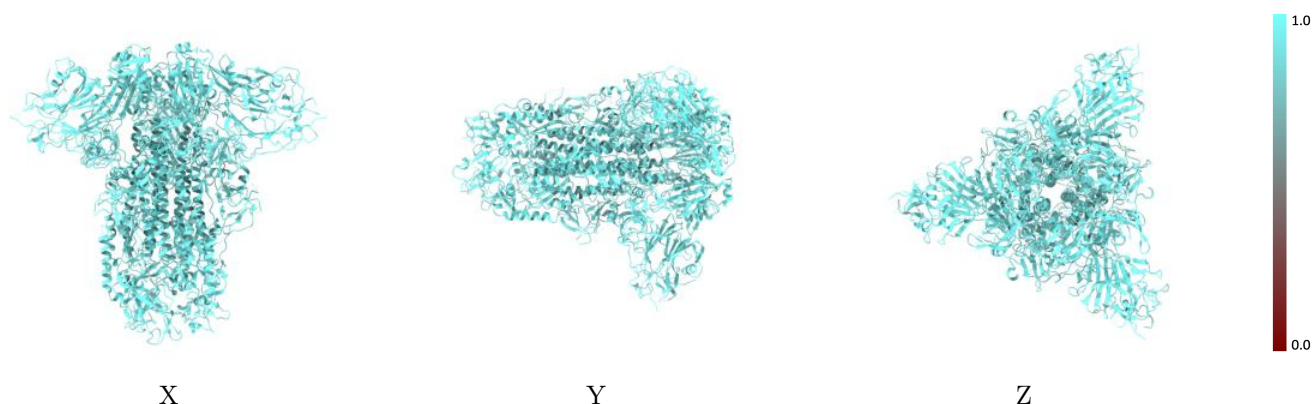
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



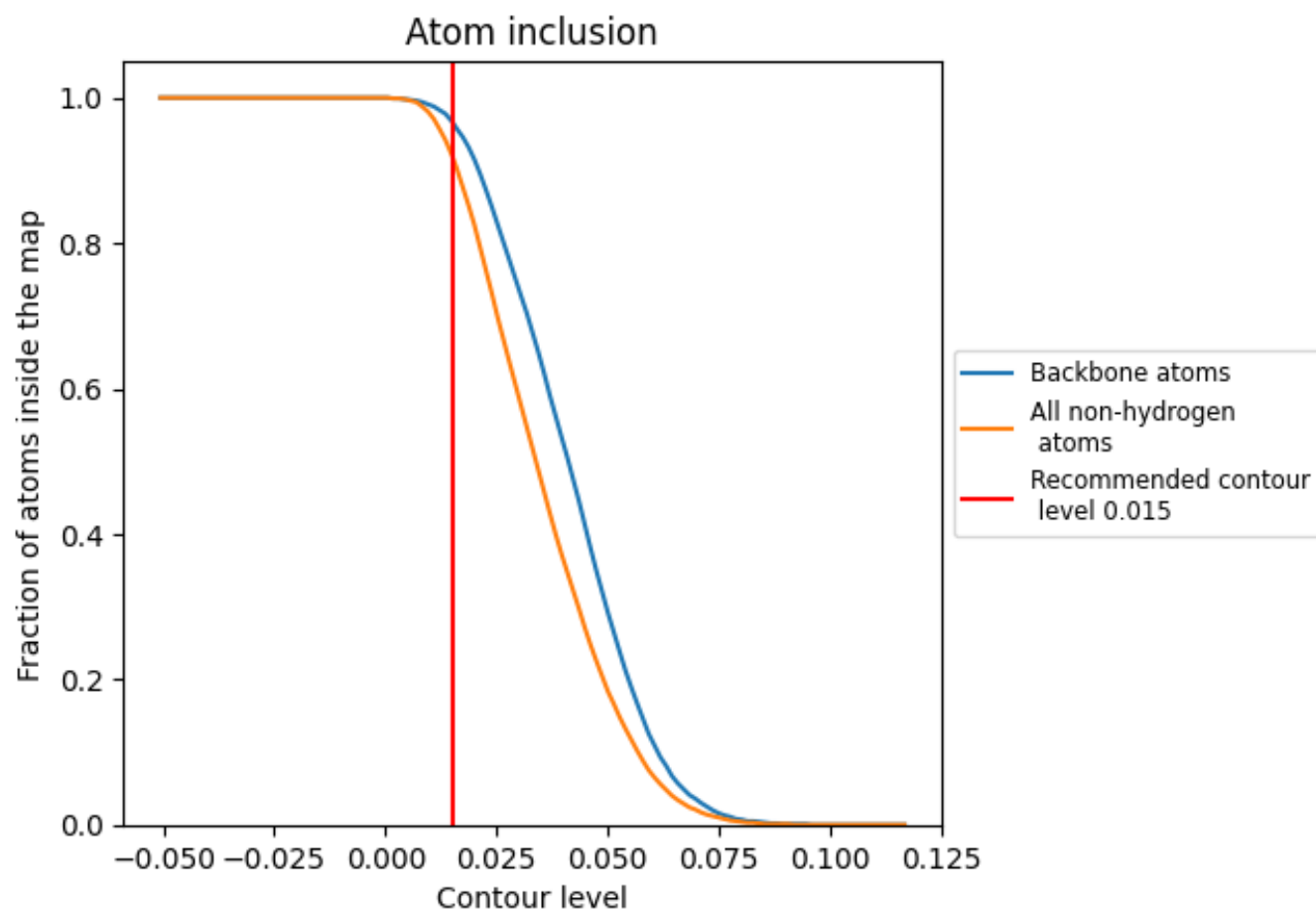
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9200	<div><div></div></div> 0.4770
A	<div><div></div></div> 0.9210	<div><div></div></div> 0.4790
B	<div><div></div></div> 0.9210	<div><div></div></div> 0.4770
C	<div><div></div></div> 0.9210	<div><div></div></div> 0.4790
D	<div><div></div></div> 0.7950	<div><div></div></div> 0.3710
E	<div><div></div></div> 0.7690	<div><div></div></div> 0.3790
F	<div><div></div></div> 0.8720	<div><div></div></div> 0.3860
G	<div><div></div></div> 0.8930	<div><div></div></div> 0.4550
H	<div><div></div></div> 0.8720	<div><div></div></div> 0.4430
I	<div><div></div></div> 0.7950	<div><div></div></div> 0.3980
J	<div><div></div></div> 0.9290	<div><div></div></div> 0.4830
K	<div><div></div></div> 0.8720	<div><div></div></div> 0.4370

1.0

0.0

<0.0