



Full wwPDB EM Validation Report ⓘ

Jun 13, 2022 – 01:59 pm BST

PDB ID : 7ZRC
EMDB ID : EMD-14910
Title : OMI-38 FAB IN COMPLEX WITH SARS-COV-2 BETA SPIKE
Authors : Duyvesteyn, H.M.E.; Ren, J.; Stuart, D.I.
Deposited on : 2022-05-04
Resolution : 3.50 Å (reported)
Based on initial model : 7Q9G

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

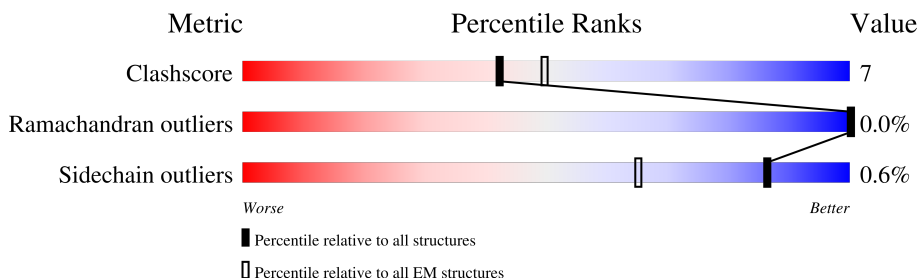
EMDB validation analysis : 0.0.1.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

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 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1285	
1	B	1285	
1	C	1285	
2	F	118	
2	H	118	
2	J	118	
3	G	108	
3	K	108	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	108	 53% 81% 19%
4	D	2	 50% 50%
4	E	2	 100%
4	I	2	 50% 50%
4	M	2	 100%
4	N	2	 100%
4	O	2	 100%
4	P	2	 100%
4	Q	2	 100%
4	R	2	 100%
4	S	2	 100%
4	T	2	 100%
4	U	2	 100%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 30724 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
			Total	C	N	O	S		
1	B	1059	8272	5286	1377	1571	38	0	0
1	C	1059	8273	5285	1378	1572	38	0	0
1	A	1056	8249	5270	1375	1567	37	0	0

There are 213 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	PHE	LEU	variant	UNP P0DTC2
B	80	ALA	ASP	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	243	ILE	ARG	engineered mutation	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	481	LYS	GLU	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	679	GLY	ARG	engineered mutation	UNP P0DTC2
B	680	SER	ARG	engineered mutation	UNP P0DTC2
B	682	SER	ARG	engineered mutation	UNP P0DTC2
B	698	VAL	ALA	variant	UNP P0DTC2
B	983	PRO	LYS	engineered mutation	UNP P0DTC2
B	984	PRO	VAL	engineered mutation	UNP P0DTC2
B	1206	GLY	-	linker	UNP P0DTC2
B	1207	SER	-	linker	UNP P0DTC2
B	1229	LEU	PHE	engineered mutation	UNP P10104
B	1235	GLY	-	expression tag	UNP P10104
B	1236	ARG	-	expression tag	UNP P10104
B	1237	SER	-	expression tag	UNP P10104
B	1238	LEU	-	expression tag	UNP P10104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	GLU	-	expression tag	UNP P10104
B	1240	VAL	-	expression tag	UNP P10104
B	1241	LEU	-	expression tag	UNP P10104
B	1242	PHE	-	expression tag	UNP P10104
B	1243	GLN	-	expression tag	UNP P10104
B	1244	GLY	-	expression tag	UNP P10104
B	1245	PRO	-	expression tag	UNP P10104
B	1246	GLY	-	expression tag	UNP P10104
B	1247	HIS	-	expression tag	UNP P10104
B	1248	HIS	-	expression tag	UNP P10104
B	1249	HIS	-	expression tag	UNP P10104
B	1250	HIS	-	expression tag	UNP P10104
B	1251	HIS	-	expression tag	UNP P10104
B	1252	HIS	-	expression tag	UNP P10104
B	1253	HIS	-	expression tag	UNP P10104
B	1254	HIS	-	expression tag	UNP P10104
B	1255	GLY	-	expression tag	UNP P10104
B	1256	SER	-	expression tag	UNP P10104
B	1257	ALA	-	expression tag	UNP P10104
B	1258	TRP	-	expression tag	UNP P10104
B	1259	SER	-	expression tag	UNP P10104
B	1260	HIS	-	expression tag	UNP P10104
B	1261	PRO	-	expression tag	UNP P10104
B	1262	GLN	-	expression tag	UNP P10104
B	1263	PHE	-	expression tag	UNP P10104
B	1264	GLU	-	expression tag	UNP P10104
B	1265	LYS	-	expression tag	UNP P10104
B	1266	GLY	-	expression tag	UNP P10104
B	1267	GLY	-	expression tag	UNP P10104
B	1268	GLY	-	expression tag	UNP P10104
B	1269	SER	-	expression tag	UNP P10104
B	1270	GLY	-	expression tag	UNP P10104
B	1271	GLY	-	expression tag	UNP P10104
B	1272	GLY	-	expression tag	UNP P10104
B	1273	SER	-	expression tag	UNP P10104
B	1274	GLY	-	expression tag	UNP P10104
B	1275	GLY	-	expression tag	UNP P10104
B	1276	SER	-	expression tag	UNP P10104
B	1277	ALA	-	expression tag	UNP P10104
B	1278	TRP	-	expression tag	UNP P10104
B	1279	SER	-	expression tag	UNP P10104
B	1280	HIS	-	expression tag	UNP P10104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1281	PRO	-	expression tag	UNP P10104
B	1282	GLN	-	expression tag	UNP P10104
B	1283	PHE	-	expression tag	UNP P10104
B	1284	GLU	-	expression tag	UNP P10104
B	1285	LYS	-	expression tag	UNP P10104
C	18	PHE	LEU	variant	UNP P0DTC2
C	80	ALA	ASP	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	243	ILE	ARG	engineered mutation	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2
C	481	LYS	GLU	variant	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	679	GLY	ARG	engineered mutation	UNP P0DTC2
C	680	SER	ARG	engineered mutation	UNP P0DTC2
C	682	SER	ARG	engineered mutation	UNP P0DTC2
C	698	VAL	ALA	variant	UNP P0DTC2
C	983	PRO	LYS	engineered mutation	UNP P0DTC2
C	984	PRO	VAL	engineered mutation	UNP P0DTC2
C	1206	GLY	-	linker	UNP P0DTC2
C	1207	SER	-	linker	UNP P0DTC2
C	1229	LEU	PHE	engineered mutation	UNP P10104
C	1235	GLY	-	expression tag	UNP P10104
C	1236	ARG	-	expression tag	UNP P10104
C	1237	SER	-	expression tag	UNP P10104
C	1238	LEU	-	expression tag	UNP P10104
C	1239	GLU	-	expression tag	UNP P10104
C	1240	VAL	-	expression tag	UNP P10104
C	1241	LEU	-	expression tag	UNP P10104
C	1242	PHE	-	expression tag	UNP P10104
C	1243	GLN	-	expression tag	UNP P10104
C	1244	GLY	-	expression tag	UNP P10104
C	1245	PRO	-	expression tag	UNP P10104
C	1246	GLY	-	expression tag	UNP P10104
C	1247	HIS	-	expression tag	UNP P10104
C	1248	HIS	-	expression tag	UNP P10104
C	1249	HIS	-	expression tag	UNP P10104
C	1250	HIS	-	expression tag	UNP P10104
C	1251	HIS	-	expression tag	UNP P10104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1252	HIS	-	expression tag	UNP P10104
C	1253	HIS	-	expression tag	UNP P10104
C	1254	HIS	-	expression tag	UNP P10104
C	1255	GLY	-	expression tag	UNP P10104
C	1256	SER	-	expression tag	UNP P10104
C	1257	ALA	-	expression tag	UNP P10104
C	1258	TRP	-	expression tag	UNP P10104
C	1259	SER	-	expression tag	UNP P10104
C	1260	HIS	-	expression tag	UNP P10104
C	1261	PRO	-	expression tag	UNP P10104
C	1262	GLN	-	expression tag	UNP P10104
C	1263	PHE	-	expression tag	UNP P10104
C	1264	GLU	-	expression tag	UNP P10104
C	1265	LYS	-	expression tag	UNP P10104
C	1266	GLY	-	expression tag	UNP P10104
C	1267	GLY	-	expression tag	UNP P10104
C	1268	GLY	-	expression tag	UNP P10104
C	1269	SER	-	expression tag	UNP P10104
C	1270	GLY	-	expression tag	UNP P10104
C	1271	GLY	-	expression tag	UNP P10104
C	1272	GLY	-	expression tag	UNP P10104
C	1273	SER	-	expression tag	UNP P10104
C	1274	GLY	-	expression tag	UNP P10104
C	1275	GLY	-	expression tag	UNP P10104
C	1276	SER	-	expression tag	UNP P10104
C	1277	ALA	-	expression tag	UNP P10104
C	1278	TRP	-	expression tag	UNP P10104
C	1279	SER	-	expression tag	UNP P10104
C	1280	HIS	-	expression tag	UNP P10104
C	1281	PRO	-	expression tag	UNP P10104
C	1282	GLN	-	expression tag	UNP P10104
C	1283	PHE	-	expression tag	UNP P10104
C	1284	GLU	-	expression tag	UNP P10104
C	1285	LYS	-	expression tag	UNP P10104
A	18	PHE	LEU	variant	UNP P0DTC2
A	80	ALA	ASP	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	243	ILE	ARG	engineered mutation	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	LYS	GLU	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	679	GLY	ARG	engineered mutation	UNP P0DTC2
A	680	SER	ARG	engineered mutation	UNP P0DTC2
A	682	SER	ARG	engineered mutation	UNP P0DTC2
A	698	VAL	ALA	variant	UNP P0DTC2
A	983	PRO	LYS	engineered mutation	UNP P0DTC2
A	984	PRO	VAL	engineered mutation	UNP P0DTC2
A	1206	GLY	-	linker	UNP P0DTC2
A	1207	SER	-	linker	UNP P0DTC2
A	1229	LEU	PHE	engineered mutation	UNP P10104
A	1235	GLY	-	expression tag	UNP P10104
A	1236	ARG	-	expression tag	UNP P10104
A	1237	SER	-	expression tag	UNP P10104
A	1238	LEU	-	expression tag	UNP P10104
A	1239	GLU	-	expression tag	UNP P10104
A	1240	VAL	-	expression tag	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	PHE	-	expression tag	UNP P10104
A	1243	GLN	-	expression tag	UNP P10104
A	1244	GLY	-	expression tag	UNP P10104
A	1245	PRO	-	expression tag	UNP P10104
A	1246	GLY	-	expression tag	UNP P10104
A	1247	HIS	-	expression tag	UNP P10104
A	1248	HIS	-	expression tag	UNP P10104
A	1249	HIS	-	expression tag	UNP P10104
A	1250	HIS	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	HIS	-	expression tag	UNP P10104
A	1254	HIS	-	expression tag	UNP P10104
A	1255	GLY	-	expression tag	UNP P10104
A	1256	SER	-	expression tag	UNP P10104
A	1257	ALA	-	expression tag	UNP P10104
A	1258	TRP	-	expression tag	UNP P10104
A	1259	SER	-	expression tag	UNP P10104
A	1260	HIS	-	expression tag	UNP P10104
A	1261	PRO	-	expression tag	UNP P10104
A	1262	GLN	-	expression tag	UNP P10104
A	1263	PHE	-	expression tag	UNP P10104
A	1264	GLU	-	expression tag	UNP P10104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1265	LYS	-	expression tag	UNP P10104
A	1266	GLY	-	expression tag	UNP P10104
A	1267	GLY	-	expression tag	UNP P10104
A	1268	GLY	-	expression tag	UNP P10104
A	1269	SER	-	expression tag	UNP P10104
A	1270	GLY	-	expression tag	UNP P10104
A	1271	GLY	-	expression tag	UNP P10104
A	1272	GLY	-	expression tag	UNP P10104
A	1273	SER	-	expression tag	UNP P10104
A	1274	GLY	-	expression tag	UNP P10104
A	1275	GLY	-	expression tag	UNP P10104
A	1276	SER	-	expression tag	UNP P10104
A	1277	ALA	-	expression tag	UNP P10104
A	1278	TRP	-	expression tag	UNP P10104
A	1279	SER	-	expression tag	UNP P10104
A	1280	HIS	-	expression tag	UNP P10104
A	1281	PRO	-	expression tag	UNP P10104
A	1282	GLN	-	expression tag	UNP P10104
A	1283	PHE	-	expression tag	UNP P10104
A	1284	GLU	-	expression tag	UNP P10104
A	1285	LYS	-	expression tag	UNP P10104

- Molecule 2 is a protein called Omi-38 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	118	Total	C	N	O	S	0	0
			900	564	155	175	6		
2	F	118	Total	C	N	O	S	0	0
			900	564	155	175	6		
2	J	118	Total	C	N	O	S	0	0
			900	564	155	175	6		

- Molecule 3 is a protein called Omi-38 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	108	Total	C	N	O	S	0	0
			834	525	139	167	3		
3	G	108	Total	C	N	O	S	0	0
			834	525	139	167	3		
3	K	108	Total	C	N	O	S	0	0
			834	525	139	167	3		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
4	E	2	28	16	2	10	0	0
4	I	2	28	16	2	10	0	0
4	M	2	28	16	2	10	0	0
4	N	2	28	16	2	10	0	0
4	O	2	28	16	2	10	0	0
4	P	2	28	16	2	10	0	0
4	Q	2	28	16	2	10	0	0
4	R	2	28	16	2	10	0	0
4	S	2	28	16	2	10	0	0
4	T	2	28	16	2	10	0	0
4	U	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



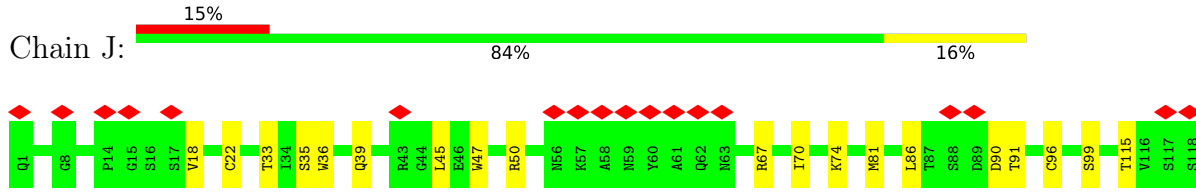
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	C	1	126	72	9	45	0
5	C	1	126	72	9	45	0
5	C	1	126	72	9	45	0
5	C	1	126	72	9	45	0
5	C	1	126	72	9	45	0

Continued on next page...

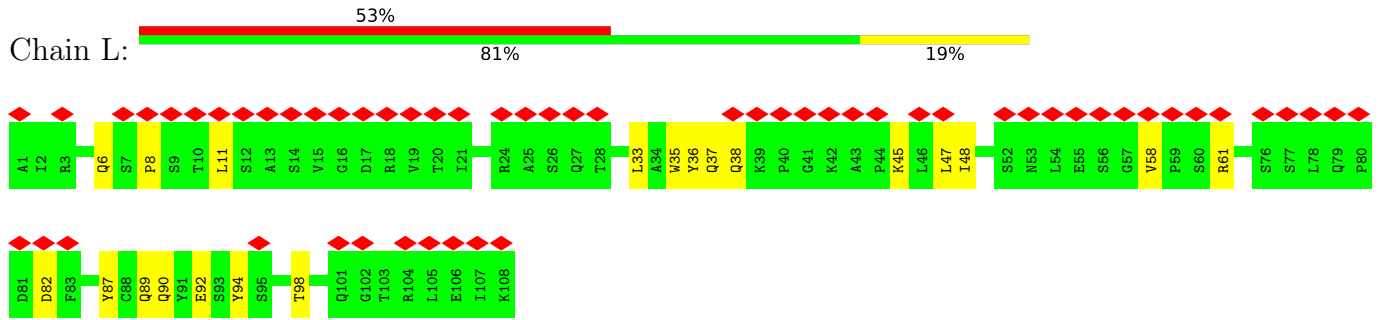
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	C	1	Total 126	C 72	N 9	O 45	0
5	C	1	Total 126	C 72	N 9	O 45	0
5	C	1	Total 126	C 72	N 9	O 45	0
5	C	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1	Total 140	C 80	N 10	O 50	0

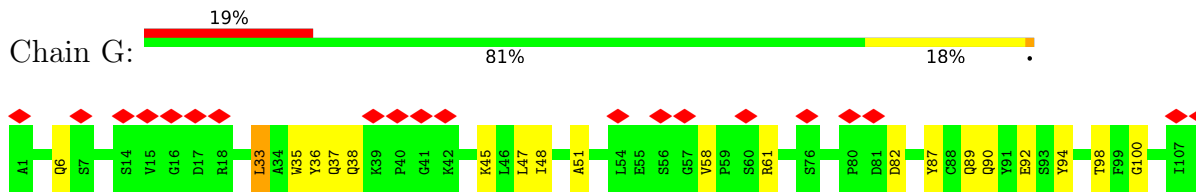
• Molecule 2: Omi-38 Fab Heavy Chain



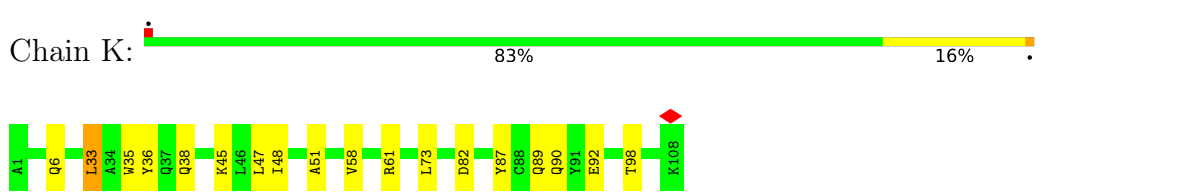
• Molecule 3: Omi-38 Fab Light Chain



• Molecule 3: Omi-38 Fab Light Chain



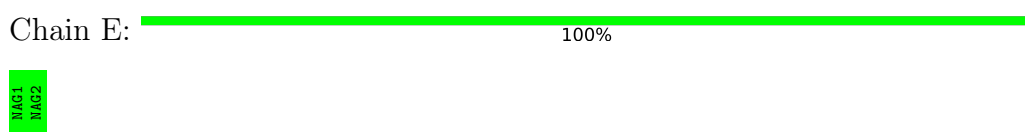
• Molecule 3: Omi-38 Fab Light Chain



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



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



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

Chain I:  50% 50%



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

Chain M:  100%



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

Chain N:  100%



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

Chain O:  100%



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

Chain P:  100%



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

Chain Q:  100%



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

Chain R:  100%

MAG1
MAG2

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

Chain S:  100%MAG1
MAG2

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

Chain T:  100%MAG1
MAG2

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

Chain U:  100%MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	201474	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF correction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.834	Depositor
Minimum map value	-1.354	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.0673	Depositor
Map size (Å)	348.6, 348.6, 348.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	0/8442	0.50	0/11489
1	B	0.37	0/8465	0.50	0/11521
1	C	0.37	0/8466	0.49	0/11521
2	F	0.25	0/919	0.49	0/1245
2	H	0.25	0/919	0.49	0/1245
2	J	0.25	0/919	0.49	0/1245
3	G	0.24	0/853	0.47	0/1159
3	K	0.25	0/853	0.47	0/1159
3	L	0.24	0/853	0.47	0/1159
All	All	0.35	0/30689	0.50	0/41743

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

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	8249	0	8033	140	0
1	B	8272	0	8055	137	0
1	C	8273	0	8058	123	0
2	F	900	0	876	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	900	0	876	13	0
2	J	900	0	876	14	0
3	G	834	0	812	14	0
3	K	834	0	812	12	0
3	L	834	0	812	13	0
4	D	28	0	25	1	0
4	E	28	0	25	0	0
4	I	28	0	25	2	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
5	A	140	0	130	7	0
5	B	126	0	117	5	0
5	C	126	0	117	0	0
All	All	30724	0	29874	439	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 (439) 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:A:596:THR:HG22	1:A:605:VAL:HG22	1.44	0.97
1:A:28:TYR:CE2	5:A:1301:NAG:O6	2.33	0.81
1:A:902:ARG:NH1	1:A:1046:LEU:O	2.17	0.75
1:A:594:VAL:HG13	1:A:605:VAL:HG13	1.69	0.73
1:C:65:PHE:HB2	1:C:262:TYR:CZ	2.23	0.73
1:C:962:GLN:HE22	1:A:755:SER:H	1.36	0.72
1:C:788:THR:HG23	1:C:789:PRO:HD2	1.70	0.72
1:C:1025:LYS:NZ	1:C:1039:PHE:O	2.24	0.70
1:B:216:LEU:HD12	1:B:217:PRO:HD2	1.74	0.69
1:A:28:TYR:HE2	5:A:1301:NAG:HO6	1.26	0.69
1:C:1113:THR:HG22	1:C:1135:TYR:HB3	1.74	0.68
1:A:294:SER:O	1:A:298:CYS:SG	2.52	0.68
1:C:326:PHE:HB3	1:C:525:LYS:HD3	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:THR:O	1:B:431:ILE:HA	1.93	0.67
1:B:164:ASN:HD22	5:B:1307:NAG:H83	1.59	0.67
1:B:1025:LYS:NZ	1:B:1039:PHE:O	2.27	0.67
1:A:1021:LEU:HG	1:A:1025:LYS:HE2	1.76	0.66
1:C:26:PRO:HB3	1:C:65:PHE:CE2	2.31	0.66
1:B:983:PRO:O	1:B:987:GLU:HG2	1.96	0.66
1:A:562:PHE:HE2	1:A:564:ARG:HE	1.42	0.66
1:A:876:ALA:O	1:A:880:THR:OG1	2.12	0.66
1:C:900:ALA:HB1	1:C:910:GLN:HB2	1.79	0.65
1:C:723:ILE:HG22	1:C:945:LEU:HD13	1.80	0.64
1:C:876:ALA:O	1:C:880:THR:OG1	2.14	0.64
1:B:31:SER:HB3	1:B:62:VAL:CG2	2.27	0.64
3:K:90:GLN:HE21	3:K:98:THR:H	1.44	0.63
1:B:722:GLU:OE1	1:B:1061:HIS:NE2	2.27	0.63
1:B:704:TYR:HB3	1:C:789:PRO:HG3	1.81	0.63
1:A:350:TRP:O	1:A:463:ARG:NH2	2.28	0.63
1:A:1113:THR:HG22	1:A:1135:TYR:HB3	1.81	0.62
1:C:1086:PHE:CE1	1:C:1120:SER:HB2	2.35	0.62
1:A:597:PRO:HB3	1:A:671:TYR:HB2	1.82	0.62
1:A:354:ARG:NH2	1:A:391:ASN:OD1	2.33	0.62
1:B:728:MET:HB2	1:B:952:ASN:HD21	1.65	0.61
1:A:596:THR:HG22	1:A:605:VAL:CG2	2.26	0.61
1:A:816:GLU:OE2	1:A:1052:SER:OG	2.18	0.61
1:C:733:VAL:HG11	1:C:1001:LEU:HD21	1.82	0.61
1:B:808:LYS:HG3	1:B:810:SER:H	1.66	0.61
2:F:35:SER:HB3	2:F:47:TRP:HE1	1.64	0.61
1:A:445:ASN:OD1	1:A:447:ASN:ND2	2.30	0.60
1:C:1087:PRO:HD2	1:A:910:GLN:HE22	1.66	0.60
1:A:216:LEU:HD12	1:A:217:PRO:HD2	1.83	0.60
1:C:902:ARG:HD2	1:C:1046:LEU:O	2.02	0.60
1:C:723:ILE:HD13	1:C:942:LEU:HD13	1.84	0.59
2:H:35:SER:HB3	2:H:47:TRP:HE1	1.65	0.59
1:C:26:PRO:HB3	1:C:65:PHE:HE2	1.66	0.59
1:C:788:THR:CG2	1:C:789:PRO:HD2	2.32	0.59
3:L:90:GLN:HE21	3:L:98:THR:H	1.51	0.59
1:C:717:ILE:HG13	1:C:920:ILE:HG23	1.84	0.59
1:B:372:SER:N	1:B:432:ALA:O	2.36	0.59
1:A:436:ASN:O	1:A:440:SER:OG	2.21	0.58
1:A:339:PHE:HB2	5:A:1310:NAG:H82	1.85	0.58
1:A:29:THR:O	1:A:61:ASN:HA	2.03	0.58
1:B:904:ASN:HD22	1:A:1104:ARG:HH22	1.50	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.86	0.58
1:A:62:VAL:HG13	1:A:264:VAL:O	2.03	0.58
1:A:81:ASN:O	1:A:239:GLN:NE2	2.37	0.58
1:B:906:ILE:HG13	1:B:908:VAL:HG23	1.86	0.58
1:B:732:SER:OG	1:B:856:THR:OG1	2.20	0.57
1:B:316:ARG:NH1	1:C:734:ASP:OD2	2.37	0.57
1:B:823:VAL:HG23	1:B:942:LEU:HD13	1.85	0.57
2:J:18:VAL:HB	2:J:86:LEU:HD11	1.86	0.57
1:A:1078:ILE:HD13	1:A:1132:ASN:HB3	1.85	0.57
3:G:90:GLN:HE21	3:G:98:THR:H	1.51	0.57
2:J:35:SER:HB3	2:J:47:TRP:HE1	1.69	0.57
1:A:482:GLY:H	1:A:485:CYS:HB2	1.69	0.57
1:B:436:ASN:O	1:B:440:SER:OG	2.21	0.57
1:B:1111:ILE:O	1:B:1116:ASN:ND2	2.37	0.57
1:C:1086:PHE:HE1	1:C:1120:SER:HB2	1.69	0.57
1:A:554:LYS:HB2	1:A:581:ILE:HG21	1.87	0.57
1:A:450:TYR:HE2	1:A:452:LEU:HD13	1.70	0.57
2:H:91:THR:HG23	2:H:115:THR:HA	1.86	0.57
2:F:39:GLN:OE1	3:G:38:GLN:NE2	2.31	0.56
2:F:18:VAL:HB	2:F:86:LEU:HD11	1.87	0.56
1:B:482:GLY:H	1:B:485:CYS:HB2	1.70	0.56
2:F:91:THR:HG23	2:F:115:THR:HA	1.86	0.56
1:C:875:LEU:HD21	1:C:1049:PHE:HB3	1.88	0.56
1:C:1078:ILE:HD13	1:C:1132:ASN:HB3	1.88	0.56
2:J:91:THR:HG23	2:J:115:THR:HA	1.87	0.56
1:B:34:ARG:HH12	1:B:221:SER:HB3	1.71	0.56
1:A:324:VAL:HG11	1:A:525:LYS:HG3	1.87	0.56
2:H:18:VAL:HB	2:H:86:LEU:HD11	1.87	0.56
1:B:663:ILE:HD11	1:B:669:ALA:HB2	1.87	0.55
1:A:723:ILE:HD13	1:A:942:LEU:HD13	1.88	0.55
1:A:517:ALA:HB3	1:A:518:PRO:HD3	1.87	0.55
1:A:26:PRO:HB3	1:A:65:PHE:HE2	1.71	0.55
1:C:482:GLY:H	1:C:485:CYS:HB2	1.71	0.55
1:B:43:PHE:HD1	1:A:560:GLN:HE22	1.54	0.55
1:B:200:TYR:OH	1:A:391:ASN:ND2	2.40	0.55
1:B:1078:ILE:HD13	1:B:1132:ASN:HB3	1.88	0.55
1:C:653:VAL:HG12	1:C:655:ASN:H	1.70	0.55
3:K:61:ARG:NE	3:K:82:ASP:OD2	2.40	0.55
3:L:61:ARG:NE	3:L:82:ASP:OD2	2.41	0.54
1:B:132:GLU:HB2	5:B:1307:NAG:H82	1.89	0.54
2:F:47:TRP:HZ2	2:F:50:ARG:HB2	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ILE:HA	1:B:419:ASN:HD22	1.72	0.54
1:C:350:TRP:O	1:C:463:ARG:NH2	2.36	0.54
1:C:517:ALA:HB3	1:C:518:PRO:HD3	1.90	0.54
1:C:712:PRO:HA	1:C:1069:GLU:HA	1.89	0.54
1:A:119:ILE:HG23	1:A:128:ILE:HG12	1.90	0.54
1:B:808:LYS:HD2	1:B:809:PRO:HD2	1.88	0.54
1:B:31:SER:HB3	1:B:62:VAL:HG21	1.90	0.54
1:B:189:LEU:HD22	1:B:217:PRO:HG3	1.90	0.54
1:C:436:ASN:O	1:C:440:SER:OG	2.25	0.54
1:A:900:ALA:HB1	1:A:910:GLN:HB2	1.90	0.53
1:B:575:ASP:HB2	1:B:578:THR:O	2.09	0.53
1:C:415:ILE:HA	1:C:419:ASN:HD22	1.74	0.53
1:A:906:ILE:HG13	1:A:908:VAL:HG23	1.90	0.53
1:A:347:VAL:HG22	1:A:419:ASN:HB3	1.90	0.53
1:A:594:VAL:HG13	1:A:605:VAL:CG1	2.36	0.53
1:B:799:PHE:HD1	1:B:802:ILE:HD11	1.73	0.53
1:A:29:THR:HG22	1:A:30:ASN:H	1.73	0.53
1:A:291:ASP:OD1	1:A:291:ASP:N	2.42	0.53
3:K:6:GLN:HE22	3:K:87:TYR:HA	1.73	0.53
1:A:801:GLN:HG2	1:A:932:GLN:NE2	2.24	0.52
1:B:1112:ILE:HG22	1:B:1134:VAL:HG12	1.91	0.52
1:A:357:ASN:OD1	1:A:520:THR:OG1	2.27	0.52
1:B:945:LEU:HD21	1:B:1056:GLY:HA3	1.91	0.52
2:H:47:TRP:HZ2	2:H:50:ARG:HB2	1.74	0.52
1:B:31:SER:HB3	1:B:62:VAL:HG23	1.92	0.52
1:A:390:THR:HG23	1:A:518:PRO:HG2	1.91	0.52
3:G:61:ARG:NE	3:G:82:ASP:OD2	2.40	0.52
1:B:877:GLY:O	1:B:881:SER:OG	2.16	0.52
1:C:562:PHE:O	1:A:43:PHE:N	2.41	0.52
2:J:33:THR:OG1	2:J:99:SER:OG	2.27	0.52
1:C:451:ARG:NH2	1:C:464:ASP:O	2.43	0.52
1:B:1083:LYS:HD3	1:B:1119:VAL:HG11	1.91	0.52
1:A:562:PHE:HE2	1:A:564:ARG:NE	2.09	0.51
3:G:6:GLN:HE22	3:G:87:TYR:HA	1.74	0.51
1:B:980:ARG:HD3	1:A:514:LEU:HD21	1.92	0.51
1:C:390:THR:HG23	1:C:518:PRO:HG2	1.91	0.51
1:C:823:VAL:HB	1:C:1054:PRO:HG2	1.91	0.51
1:C:735:CYS:SG	1:C:736:THR:N	2.84	0.51
1:A:415:ILE:HA	1:A:419:ASN:HD22	1.76	0.51
1:B:927:ALA:O	1:B:931:ILE:HG12	2.11	0.51
1:C:210:ILE:HG13	1:C:212:LEU:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1087:PRO:HD2	1:A:910:GLN:NE2	2.24	0.51
1:A:28:TYR:CD2	5:A:1301:NAG:H5	2.45	0.51
3:K:90:GLN:O	3:K:92:GLU:N	2.40	0.51
1:B:1008:GLN:OE1	1:B:1011:ARG:NH1	2.44	0.50
1:C:30:ASN:HD21	1:C:59:PHE:HB3	1.76	0.50
3:G:90:GLN:O	3:G:92:GLU:N	2.41	0.50
1:B:715:PHE:CE1	1:B:920:ILE:HG12	2.46	0.50
1:C:715:PHE:HE1	1:C:920:ILE:HG12	1.75	0.50
1:A:557:LEU:H	1:A:560:GLN:NE2	2.09	0.50
3:L:6:GLN:HE22	3:L:87:TYR:HA	1.76	0.50
3:L:90:GLN:O	3:L:92:GLU:N	2.42	0.50
2:J:39:GLN:HB2	2:J:45:LEU:HD23	1.93	0.50
1:A:593:SER:OG	1:A:610:GLN:NE2	2.45	0.50
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.93	0.50
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.93	0.50
1:B:347:VAL:HG22	1:B:419:ASN:HB3	1.94	0.50
1:A:733:VAL:HG13	1:A:855:LEU:HD12	1.94	0.50
3:L:45:LYS:HE3	3:L:47:LEU:HD21	1.94	0.50
1:B:904:ASN:ND2	1:A:1104:ARG:HH22	2.10	0.50
1:C:335:PHE:HE2	1:C:360:ALA:HB1	1.77	0.50
1:B:445:ASN:OD1	1:B:447:ASN:ND2	2.33	0.49
2:H:39:GLN:OE1	3:L:38:GLN:NE2	2.32	0.49
1:A:60:SER:O	1:A:61:ASN:C	2.50	0.49
1:B:92:PHE:HE2	1:B:240:THR:HG1	1.58	0.49
1:B:789:PRO:HG3	1:A:704:TYR:HB3	1.94	0.49
1:C:109:THR:OG1	1:C:114:THR:OG1	2.27	0.49
1:A:613:ASN:HB3	1:A:616:GLU:HG2	1.94	0.49
1:B:552:SER:HB2	1:B:583:ASP:HB2	1.95	0.49
1:B:723:ILE:CG2	1:B:945:LEU:HD13	2.42	0.49
1:A:673:THR:HG22	1:A:687:GLN:HG2	1.94	0.49
1:B:326:PHE:CD2	1:B:525:LYS:HB3	2.48	0.49
1:B:1037:VAL:HG21	1:C:1032:GLY:HA3	1.94	0.49
1:A:292:PRO:O	1:A:296:THR:HG23	2.13	0.49
1:B:46:SER:HA	1:B:276:TYR:O	2.13	0.49
1:B:816:GLU:HG3	1:B:1051:GLN:NE2	2.28	0.49
1:A:1083:LYS:HB3	1:A:1119:VAL:HG13	1.95	0.49
3:G:45:LYS:HE3	3:G:47:LEU:HD21	1.93	0.49
1:B:733:VAL:HG11	1:B:1001:LEU:HD21	1.95	0.49
1:C:419:ASN:OD1	1:C:451:ARG:N	2.40	0.49
2:J:47:TRP:HZ2	2:J:50:ARG:HB2	1.78	0.49
1:B:350:TRP:O	1:B:463:ARG:NH2	2.35	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:719:VAL:HG22	1:C:1062:VAL:HG22	1.95	0.49
1:B:451:ARG:NH2	1:B:464:ASP:O	2.43	0.49
2:F:33:THR:OG1	2:F:99:SER:OG	2.31	0.48
2:J:39:GLN:OE1	3:K:38:GLN:NE2	2.33	0.48
1:B:723:ILE:HG22	1:B:945:LEU:HD13	1.94	0.48
1:B:916:ASN:O	1:B:920:ILE:HG13	2.13	0.48
2:J:22:CYS:HB2	2:J:36:TRP:CH2	2.49	0.48
1:B:723:ILE:O	1:B:944:LYS:HD3	2.13	0.48
3:K:90:GLN:HE21	3:K:98:THR:N	2.12	0.48
1:B:700:ASN:O	1:C:786:TYR:HA	2.14	0.48
1:A:495:GLN:HB2	1:A:498:TYR:HD1	1.77	0.48
3:G:47:LEU:HA	3:G:58:VAL:HG21	1.96	0.48
2:J:70:ILE:HG12	2:J:81:MET:HG2	1.96	0.48
1:B:419:ASN:OD1	1:B:451:ARG:N	2.40	0.48
1:B:1085:HIS:CE1	1:B:1134:VAL:HG21	2.49	0.48
1:C:498:TYR:HD2	1:C:502:TYR:HB3	1.79	0.48
1:B:390:THR:O	1:B:520:THR:OG1	2.32	0.48
1:B:915:GLU:OE2	1:A:1120:SER:OG	2.16	0.48
1:C:292:PRO:O	1:C:296:THR:HG23	2.14	0.48
1:C:347:VAL:HG22	1:C:419:ASN:HB3	1.96	0.48
1:C:1050:PRO:O	1:C:1051:GLN:NE2	2.31	0.48
1:A:970:ILE:HD11	1:A:977:ILE:HG23	1.96	0.48
1:C:715:PHE:CE1	1:C:920:ILE:HG12	2.48	0.47
1:B:164:ASN:HB2	5:B:1307:NAG:H83	1.95	0.47
1:B:450:TYR:HE2	1:B:452:LEU:HD13	1.79	0.47
1:A:877:GLY:O	1:A:881:SER:OG	2.28	0.47
1:A:1050:PRO:O	1:A:1051:GLN:NE2	2.42	0.47
1:C:1086:PHE:HB3	1:A:910:GLN:HE21	1.79	0.47
1:B:1080:HIS:O	1:B:1083:LYS:HG2	2.14	0.47
1:C:911:ASN:ND2	1:C:1108:GLU:OE2	2.46	0.47
2:J:36:TRP:NE1	2:J:81:MET:HB2	2.30	0.47
3:K:45:LYS:HE3	3:K:47:LEU:HD21	1.96	0.47
2:H:33:THR:OG1	2:H:99:SER:OG	2.32	0.47
1:B:719:VAL:O	1:B:931:ILE:HD11	2.14	0.47
1:C:65:PHE:HB2	1:C:262:TYR:CE2	2.50	0.47
1:C:733:VAL:HG22	1:C:855:LEU:HD22	1.97	0.47
1:C:1084:ALA:O	1:C:1119:VAL:HA	2.14	0.47
1:A:96:GLU:OE2	1:A:190:ARG:NH1	2.47	0.47
1:B:317:VAL:HG12	1:B:588:SER:O	2.14	0.47
1:C:291:ASP:N	1:C:291:ASP:OD1	2.46	0.47
1:A:1135:TYR:OH	1:A:1140:PRO:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:760:LEU:HD22	1:C:1005:VAL:HG21	1.97	0.47
1:A:926:SER:O	1:A:930:LYS:HG3	2.15	0.47
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.47	0.47
1:B:719:VAL:HG22	1:B:1062:VAL:HG22	1.97	0.46
1:A:717:ILE:HG13	1:A:920:ILE:HG23	1.97	0.46
1:C:100:ILE:HA	1:C:243:ILE:HG22	1.96	0.46
1:C:875:LEU:HD11	1:C:1051:GLN:HE22	1.80	0.46
3:L:90:GLN:HE21	3:L:98:THR:N	2.14	0.46
2:F:67:ARG:NH2	2:F:90:ASP:OD2	2.48	0.46
1:B:498:TYR:HD2	1:B:502:TYR:HB3	1.79	0.46
1:B:822:LYS:HE2	1:B:942:LEU:HD12	1.97	0.46
1:C:119:ILE:HG23	1:C:128:ILE:HG12	1.97	0.46
1:C:1135:TYR:OH	1:C:1140:PRO:HG3	2.14	0.46
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.49	0.46
1:B:801:GLN:NE2	4:D:1:NAG:H62	2.30	0.46
1:B:823:VAL:HB	1:B:1054:PRO:HG2	1.97	0.46
1:C:388:CYS:HB3	1:C:519:ALA:HB1	1.97	0.46
1:C:1083:LYS:HE2	1:C:1119:VAL:HG11	1.96	0.46
1:C:1085:HIS:CD2	1:C:1119:VAL:HG12	2.50	0.46
1:B:371:PHE:HA	1:B:433:TRP:HB3	1.98	0.46
2:J:36:TRP:CZ3	2:J:96:CYS:HB3	2.50	0.46
3:K:47:LEU:HA	3:K:58:VAL:HG21	1.97	0.46
1:B:712:PRO:HA	1:B:1069:GLU:HA	1.97	0.46
1:B:713:THR:HG21	1:B:1070:LYS:HD2	1.98	0.46
1:B:731:THR:HG21	1:B:956:LEU:HD11	1.98	0.46
1:C:1103:GLN:NE2	1:C:1108:GLU:OE1	2.46	0.46
1:C:560:GLN:O	1:C:574:ARG:NH2	2.44	0.46
1:B:1064:TYR:HE1	1:B:1066:PRO:HG3	1.82	0.45
1:A:328:ASN:HD22	5:A:1303:NAG:C7	2.29	0.45
2:H:47:TRP:CZ2	2:H:50:ARG:HB2	2.51	0.45
1:C:450:TYR:HE2	1:C:452:LEU:HD13	1.80	0.45
2:J:36:TRP:CE2	2:J:81:MET:HB2	2.51	0.45
1:C:39:PRO:HG3	1:C:51:THR:HG21	1.98	0.45
1:C:557:LEU:HD11	1:A:281:THR:HB	1.98	0.45
1:A:730:LYS:HE3	1:A:768:ALA:HB1	1.97	0.45
1:B:291:ASP:HB2	1:B:292:PRO:HD2	1.99	0.45
1:B:867:ILE:O	1:B:871:THR:HG23	2.16	0.45
1:C:983:PRO:N	1:C:984:PRO:HD2	2.32	0.45
1:A:286:VAL:HG23	1:A:303:PHE:CE2	2.51	0.45
1:B:28:TYR:HB3	1:B:61:ASN:OD1	2.16	0.45
1:C:710:ALA:HB3	1:A:891:LEU:HB3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:GLU:HG3	1:C:787:LYS:HE3	1.99	0.45
1:B:755:SER:H	1:A:962:GLN:HE22	1.64	0.45
1:C:563:GLY:HA2	1:A:43:PHE:O	2.16	0.45
1:A:170:TYR:HE1	1:A:172:SER:HB3	1.81	0.45
1:B:715:PHE:HE1	1:B:920:ILE:HG12	1.81	0.45
1:B:1100:PHE:HZ	4:I:1:NAG:H62	1.82	0.45
1:A:34:ARG:NH1	1:A:191:GLU:OE2	2.50	0.45
1:B:1032:GLY:HA3	1:A:1037:VAL:HG21	1.98	0.45
1:A:517:ALA:O	1:A:561:GLN:HG3	2.17	0.45
1:A:577:GLN:O	5:A:1303:NAG:H4	2.16	0.45
1:A:706:ASN:N	1:A:706:ASN:OD1	2.48	0.45
1:B:347:VAL:HG21	1:B:415:ILE:HD12	1.99	0.44
1:B:875:LEU:HD21	1:B:1049:PHE:HB3	1.99	0.44
1:C:125:ASN:HB3	1:C:174:PRO:HA	1.98	0.44
1:C:376:CYS:HA	1:C:429:CYS:HA	1.99	0.44
1:C:956:LEU:O	1:C:960:VAL:HG23	2.17	0.44
1:A:210:ILE:HG13	1:A:212:LEU:H	1.82	0.44
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.99	0.44
3:L:47:LEU:HA	3:L:58:VAL:HG21	1.99	0.44
1:C:445:ASN:OD1	1:C:447:ASN:ND2	2.37	0.44
1:C:711:ILE:HD12	1:C:1102:THR:HG21	1.99	0.44
1:A:1021:LEU:CG	1:A:1025:LYS:HE2	2.46	0.44
1:B:327:PRO:CA	1:B:576:PRO:HB2	2.47	0.44
1:A:190:ARG:HB3	1:A:192:PHE:CE1	2.52	0.44
3:G:90:GLN:HE21	3:G:98:THR:N	2.15	0.44
2:J:67:ARG:NH2	2:J:90:ASP:OD2	2.50	0.44
1:A:1083:LYS:HB3	1:A:1119:VAL:CG1	2.47	0.44
1:B:1120:SER:OG	1:C:911:ASN:OD1	2.26	0.44
2:F:47:TRP:CZ2	2:F:50:ARG:HB2	2.50	0.44
1:A:21:ARG:NH1	1:A:137:ASN:HB3	2.32	0.44
1:C:723:ILE:CG2	1:C:945:LEU:HD13	2.48	0.44
1:C:1033:GLN:HA	1:C:1045:HIS:CE1	2.53	0.44
1:C:355:ILE:HB	1:C:392:VAL:HB	1.98	0.44
1:A:100:ILE:HA	1:A:243:ILE:HG22	1.99	0.44
1:A:428:GLY:HA2	1:A:512:PHE:CD2	2.52	0.44
1:B:449:LEU:HD22	2:F:54:ILE:HG12	1.99	0.43
1:C:325:ARG:HD3	1:C:575:ASP:OD1	2.18	0.43
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.52	0.43
1:A:355:ILE:HB	1:A:392:VAL:HB	1.99	0.43
1:C:1081:ASP:HB2	1:C:1083:LYS:NZ	2.33	0.43
1:B:210:ILE:HG13	1:B:212:LEU:H	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:HD21	1:C:119:ILE:HD11	2.01	0.43
1:C:329:ILE:HG23	1:C:329:ILE:O	2.19	0.43
1:A:801:GLN:HB3	1:A:932:GLN:HE21	1.82	0.43
1:B:799:PHE:CD1	1:B:802:ILE:HD11	2.53	0.43
1:C:347:VAL:HG21	1:C:415:ILE:HD12	1.99	0.43
1:A:62:VAL:HG22	1:A:265:GLY:HA3	2.00	0.43
1:C:96:GLU:OE1	1:C:96:GLU:N	2.52	0.43
1:C:793:ASP:OD1	1:C:793:ASP:N	2.52	0.43
1:C:799:PHE:HZ	1:C:895:PHE:CZ	2.37	0.43
1:A:143:VAL:HG12	1:A:154:GLU:HA	2.01	0.43
2:F:97:ALA:HB1	2:F:105:PHE:HB3	2.01	0.43
3:K:36:TYR:HE2	3:K:89:GLN:HB2	1.84	0.43
1:B:481:LYS:HZ2	2:F:74:LYS:HD3	1.84	0.43
1:B:728:MET:HB2	1:B:952:ASN:ND2	2.33	0.43
1:B:880:THR:O	1:B:892:GLN:HA	2.18	0.43
1:B:1120:SER:OG	1:B:1120:SER:O	2.36	0.43
3:G:37:GLN:HB2	3:G:47:LEU:HD11	2.00	0.43
1:B:100:ILE:HA	1:B:243:ILE:HG22	2.01	0.43
1:C:21:ARG:NH1	1:C:137:ASN:HB3	2.34	0.43
1:C:495:GLN:HB2	1:C:498:TYR:HD1	1.84	0.43
1:C:1088:ARG:HD2	1:C:1115:ASP:O	2.19	0.43
1:A:525:LYS:HD2	1:A:525:LYS:HA	1.80	0.43
3:G:36:TYR:HE2	3:G:89:GLN:HB2	1.84	0.43
1:C:575:ASP:HB3	1:C:578:THR:O	2.18	0.43
1:A:106:PHE:HB3	1:A:235:ILE:HD13	2.01	0.43
1:A:376:CYS:HA	1:A:429:CYS:HA	2.01	0.43
1:A:802:ILE:HG13	1:A:875:LEU:HD21	2.01	0.43
1:A:812:ARG:HG2	1:A:816:GLU:HB3	2.00	0.43
2:F:36:TRP:CE2	2:F:81:MET:HB2	2.54	0.43
1:C:1104:ARG:NH2	1:A:883:TRP:HZ2	2.17	0.43
1:A:499:GLY:O	1:A:503:GLN:HG3	2.19	0.43
1:A:1076:PRO:HD2	1:A:1128:GLY:O	2.18	0.43
1:B:125:ASN:HB3	1:B:174:PRO:HA	2.01	0.42
1:B:373:THR:HG23	1:B:375:LYS:HG2	2.01	0.42
1:C:117:LEU:HD13	1:C:130:VAL:HG22	2.01	0.42
1:C:819:LEU:HD22	1:C:942:LEU:HD11	2.01	0.42
1:A:399:ILE:HG22	1:A:400:ARG:O	2.19	0.42
1:A:673:THR:HA	1:A:687:GLN:HA	2.01	0.42
1:C:898:GLN:O	1:C:902:ARG:HG2	2.18	0.42
1:A:565:ASP:CG	1:A:571:ASP:HB2	2.39	0.42
1:A:594:VAL:HG12	1:A:596:THR:HG23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:ALA:HB1	2:H:105:PHE:HB3	2.01	0.42
1:B:21:ARG:NH1	1:B:137:ASN:HB3	2.34	0.42
1:C:808:LYS:HE3	1:C:810:SER:HB3	2.02	0.42
1:A:13:SER:OG	1:A:14:GLN:N	2.52	0.42
1:A:376:CYS:SG	1:A:381:PRO:HG3	2.58	0.42
1:B:164:ASN:ND2	5:B:1307:NAG:H83	2.30	0.42
1:B:228:ASP:OD1	1:B:228:ASP:N	2.51	0.42
1:C:449:LEU:HD22	2:H:54:ILE:HG12	2.01	0.42
1:C:712:PRO:HD3	1:A:891:LEU:HD13	2.01	0.42
1:C:1037:VAL:HG21	1:A:1032:GLY:HA3	2.00	0.42
1:A:71:SER:OG	1:A:75:GLY:O	2.33	0.42
1:A:415:ILE:HA	1:A:419:ASN:ND2	2.34	0.42
1:A:823:VAL:HB	1:A:1054:PRO:HG2	2.00	0.42
1:B:698:VAL:O	1:C:785:ILE:N	2.47	0.42
1:C:1104:ARG:HD2	1:A:901:TYR:CZ	2.55	0.42
1:A:514:LEU:HD12	1:A:514:LEU:HA	1.82	0.42
1:A:538:PHE:CZ	1:A:584:ILE:HD13	2.55	0.42
1:A:1033:GLN:HA	1:A:1045:HIS:CE1	2.55	0.42
1:B:1100:PHE:CZ	4:I:1:NAG:H62	2.54	0.42
1:B:49:HIS:HB3	1:B:276:TYR:HE1	1.84	0.42
1:B:495:GLN:HB2	1:B:498:TYR:HD1	1.82	0.42
1:B:980:ARG:HH11	1:A:514:LEU:HD23	1.85	0.42
1:C:945:LEU:HD21	1:C:1056:GLY:HA3	2.02	0.42
1:A:1111:ILE:O	1:A:1116:ASN:ND2	2.52	0.42
3:L:36:TYR:HE2	3:L:89:GLN:HB2	1.84	0.42
1:B:578:THR:O	1:B:580:GLU:N	2.52	0.42
1:B:717:ILE:HG13	1:B:920:ILE:HG23	2.01	0.42
1:B:819:LEU:HD22	1:B:942:LEU:HD21	2.02	0.42
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.54	0.42
3:K:33:LEU:HB3	3:K:51:ALA:HB2	2.02	0.42
1:B:785:ILE:HD11	1:A:696:LEU:HB2	2.01	0.42
1:C:291:ASP:HB2	1:C:292:PRO:HD2	2.01	0.42
1:C:750:LEU:HD21	1:C:756:PHE:HZ	1.85	0.42
1:A:192:PHE:HA	1:A:204:TYR:O	2.20	0.41
1:B:119:ILE:HG12	1:B:128:ILE:HG23	2.02	0.41
1:B:292:PRO:O	1:B:296:THR:HG23	2.20	0.41
1:B:327:PRO:HA	1:B:576:PRO:HB2	2.01	0.41
2:H:22:CYS:HB2	2:H:36:TRP:CH2	2.55	0.41
1:B:323:ILE:HG13	1:B:538:PHE:HA	2.01	0.41
1:B:724:LEU:HD11	1:B:1025:LYS:HD2	2.02	0.41
1:B:774:ASN:O	1:B:778:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:LYS:HE3	1:B:939:ALA:HA	2.03	0.41
1:C:555:LYS:NZ	5:A:1302:NAG:O6	2.53	0.41
1:A:778:VAL:O	1:A:781:GLN:HG3	2.21	0.41
2:F:22:CYS:HB2	2:F:36:TRP:CH2	2.55	0.41
1:B:499:GLY:O	1:B:503:GLN:HG3	2.20	0.41
1:C:653:VAL:HG12	1:C:655:ASN:N	2.35	0.41
1:A:128:ILE:HB	1:A:170:TYR:HB3	2.01	0.41
1:A:347:VAL:HG21	1:A:415:ILE:HD12	2.02	0.41
1:A:481:LYS:HZ2	2:J:74:LYS:HD3	1.85	0.41
1:A:575:ASP:HB3	1:A:578:THR:O	2.20	0.41
3:L:35:TRP:HB2	3:L:48:ILE:HB	2.02	0.41
1:B:443:GLY:HA3	3:G:94:TYR:HB2	2.03	0.41
1:C:44:ARG:O	1:C:280:GLY:HA2	2.20	0.41
1:C:499:GLY:O	1:C:503:GLN:HG3	2.20	0.41
1:C:863:THR:O	1:C:867:ILE:HG12	2.19	0.41
1:C:1080:HIS:HB3	1:C:1085:HIS:CE1	2.56	0.41
1:A:425:ASP:OD1	1:A:425:ASP:N	2.52	0.41
1:B:773:LYS:HE2	1:B:777:GLU:OE2	2.20	0.41
1:B:712:PRO:HG3	1:B:1066:PRO:HB3	2.02	0.41
1:A:200:TYR:CZ	1:A:230:PRO:HB3	2.56	0.41
1:A:473:GLY:HA3	1:A:484:ASN:HD22	1.86	0.41
1:B:165:ASN:OD1	1:B:165:ASN:N	2.54	0.41
1:B:1085:HIS:CE1	1:B:1119:VAL:HG22	2.55	0.41
1:B:1101:VAL:HG11	1:B:1116:ASN:HB3	2.03	0.41
1:C:336:GLY:O	1:C:340:ASN:HB2	2.21	0.41
1:C:443:GLY:HA3	3:L:94:TYR:HB2	2.03	0.41
1:A:315:PHE:O	1:A:589:PHE:HA	2.20	0.41
3:L:8:PRO:HG2	3:L:11:LEU:HB2	2.03	0.41
3:G:6:GLN:NE2	3:G:100:GLY:HA3	2.36	0.41
1:B:1083:LYS:HE2	1:B:1083:LYS:HB3	1.95	0.41
1:C:46:SER:HA	1:C:276:TYR:O	2.20	0.41
1:C:814:PHE:HE2	1:C:932:GLN:HG3	1.86	0.41
1:A:764:LEU:HD23	1:A:764:LEU:HA	1.93	0.41
1:B:891:LEU:HB3	1:A:710:ALA:HB3	2.03	0.40
1:B:971:SER:HB2	1:B:980:ARG:NH2	2.36	0.40
1:C:945:LEU:O	1:C:949:VAL:HG23	2.21	0.40
1:A:146:HIS:O	1:A:150:LYS:N	2.54	0.40
1:A:434:ASN:HB2	1:A:505:TYR:CE2	2.56	0.40
3:G:35:TRP:HB2	3:G:48:ILE:HB	2.03	0.40
1:B:428:GLY:HA2	1:B:512:PHE:CD2	2.56	0.40
1:C:95:THR:HG23	1:C:263:TYR:HE1	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:35:TRP:CE2	3:K:73:LEU:HB2	2.56	0.40
1:B:376:CYS:HA	1:B:429:CYS:HA	2.04	0.40
1:B:801:GLN:HG3	1:B:932:GLN:OE1	2.21	0.40
1:B:1045:HIS:HA	1:B:1063:THR:HG22	2.03	0.40
1:B:1080:HIS:CD2	1:B:1134:VAL:HG22	2.56	0.40
1:C:916:ASN:O	1:C:920:ILE:HG13	2.21	0.40
1:A:970:ILE:HG23	1:A:989:GLN:CD	2.42	0.40
3:G:33:LEU:HB3	3:G:51:ALA:HB2	2.03	0.40
1:B:67:ALA:N	1:B:260:ALA:O	2.54	0.40
1:A:820:PHE:CD2	1:A:1054:PRO:HG3	2.55	0.40
3:K:35:TRP:HB2	3:K:48:ILE:HB	2.04	0.40
1:B:71:SER:OG	1:B:75:GLY:O	2.38	0.40
1:B:164:ASN:HB2	5:B:1307:NAG:C8	2.51	0.40
1:C:728:MET:HB2	1:C:952:ASN:HD21	1.86	0.40
1:C:1120:SER:OG	1:A:911:ASN:ND2	2.49	0.40
1:A:28:TYR:HD2	1:A:61:ASN:OD1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1042/1285 (81%)	1000 (96%)	41 (4%)	1 (0%)	51	84
1	B	1044/1285 (81%)	1011 (97%)	33 (3%)	0	100	100
1	C	1045/1285 (81%)	1013 (97%)	32 (3%)	0	100	100
2	F	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	H	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	J	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
3	G	106/108 (98%)	102 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	106/108 (98%)	101 (95%)	5 (5%)	0	100	100
3	L	106/108 (98%)	102 (96%)	4 (4%)	0	100	100
All	All	3797/4533 (84%)	3671 (97%)	125 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	922/1109 (83%)	913 (99%)	9 (1%)	76	88
1	B	925/1109 (83%)	922 (100%)	3 (0%)	92	97
1	C	925/1109 (83%)	921 (100%)	4 (0%)	91	96
2	F	97/97 (100%)	96 (99%)	1 (1%)	76	88
2	H	97/97 (100%)	97 (100%)	0	100	100
2	J	97/97 (100%)	97 (100%)	0	100	100
3	G	93/93 (100%)	92 (99%)	1 (1%)	73	88
3	K	93/93 (100%)	92 (99%)	1 (1%)	73	88
3	L	93/93 (100%)	92 (99%)	1 (1%)	73	88
All	All	3342/3897 (86%)	3322 (99%)	20 (1%)	86	94

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	165	ASN
1	B	596	THR
1	B	903	PHE
1	C	65	PHE
1	C	612	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	721	THR
1	C	1078	ILE
1	A	29	THR
1	A	65	PHE
1	A	164	ASN
1	A	298	CYS
1	A	540	PHE
1	A	605	VAL
1	A	788	THR
1	A	1078	ILE
1	A	1103	GLN
3	L	33	LEU
2	F	106	ASP
3	G	33	LEU
3	K	33	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	ASN
1	B	904	ASN
1	B	952	ASN
1	B	962	GLN
1	B	1105	ASN
1	B	1116	ASN
1	C	49	HIS
1	C	529	ASN
1	C	561	GLN
1	C	610	GLN
1	C	952	ASN
1	C	962	GLN
1	A	49	HIS
1	A	391	ASN
1	A	560	GLN
1	A	577	GLN
1	A	610	GLN
1	A	910	GLN
1	A	932	GLN
1	A	962	GLN
1	A	999	GLN
1	A	1008	GLN
3	L	101	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	101	GLN
3	K	101	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](#)

24 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	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	D	2	4	14,14,15	0.20	0	17,19,21	0.47	0
4	NAG	E	1	1,4	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	E	2	4	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	I	1	1,4	14,14,15	0.29	0	17,19,21	0.37	0
4	NAG	I	2	4	14,14,15	0.18	0	17,19,21	0.40	0
4	NAG	M	1	1,4	14,14,15	0.32	0	17,19,21	0.41	0
4	NAG	M	2	4	14,14,15	0.19	0	17,19,21	0.42	0
4	NAG	N	1	1,4	14,14,15	0.22	0	17,19,21	0.57	0
4	NAG	N	2	4	14,14,15	0.19	0	17,19,21	0.38	0
4	NAG	O	1	1,4	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	O	2	4	14,14,15	0.19	0	17,19,21	0.47	0
4	NAG	P	1	1,4	14,14,15	0.19	0	17,19,21	0.39	0
4	NAG	P	2	4	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	Q	1	1,4	14,14,15	0.20	0	17,19,21	0.47	0
4	NAG	Q	2	4	14,14,15	0.18	0	17,19,21	0.39	0
4	NAG	R	1	1,4	14,14,15	0.29	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	R	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	S	1	1,4	14,14,15	0.36	0	17,19,21	0.48	0
4	NAG	S	2	4	14,14,15	0.22	0	17,19,21	0.39	0
4	NAG	T	1	1,4	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	T	2	4	14,14,15	0.18	0	17,19,21	0.39	0
4	NAG	U	1	1,4	14,14,15	0.22	0	17,19,21	0.49	0
4	NAG	U	2	4	14,14,15	0.20	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	1/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

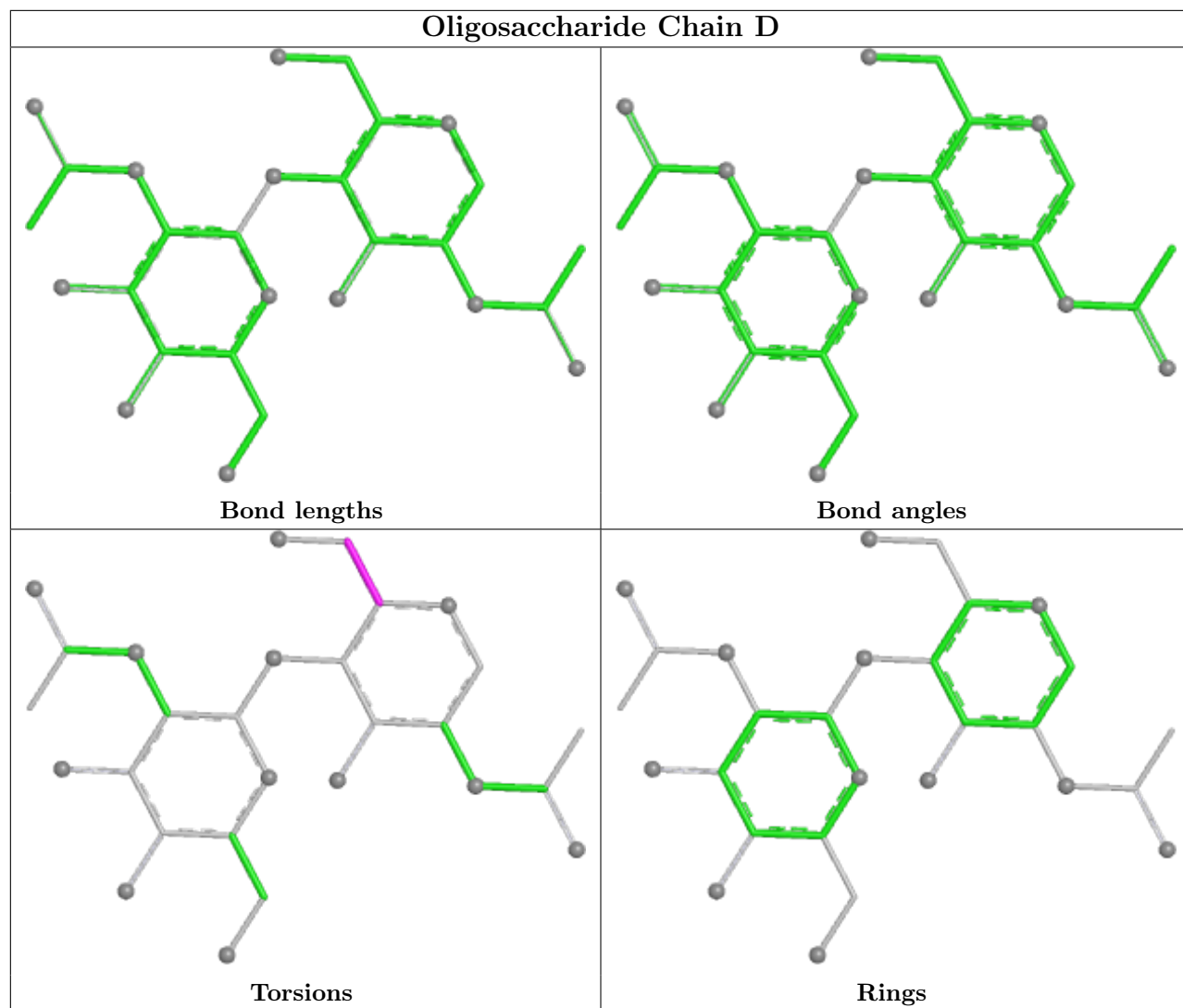
Mol	Chain	Res	Type	Atoms
4	Q	1	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6

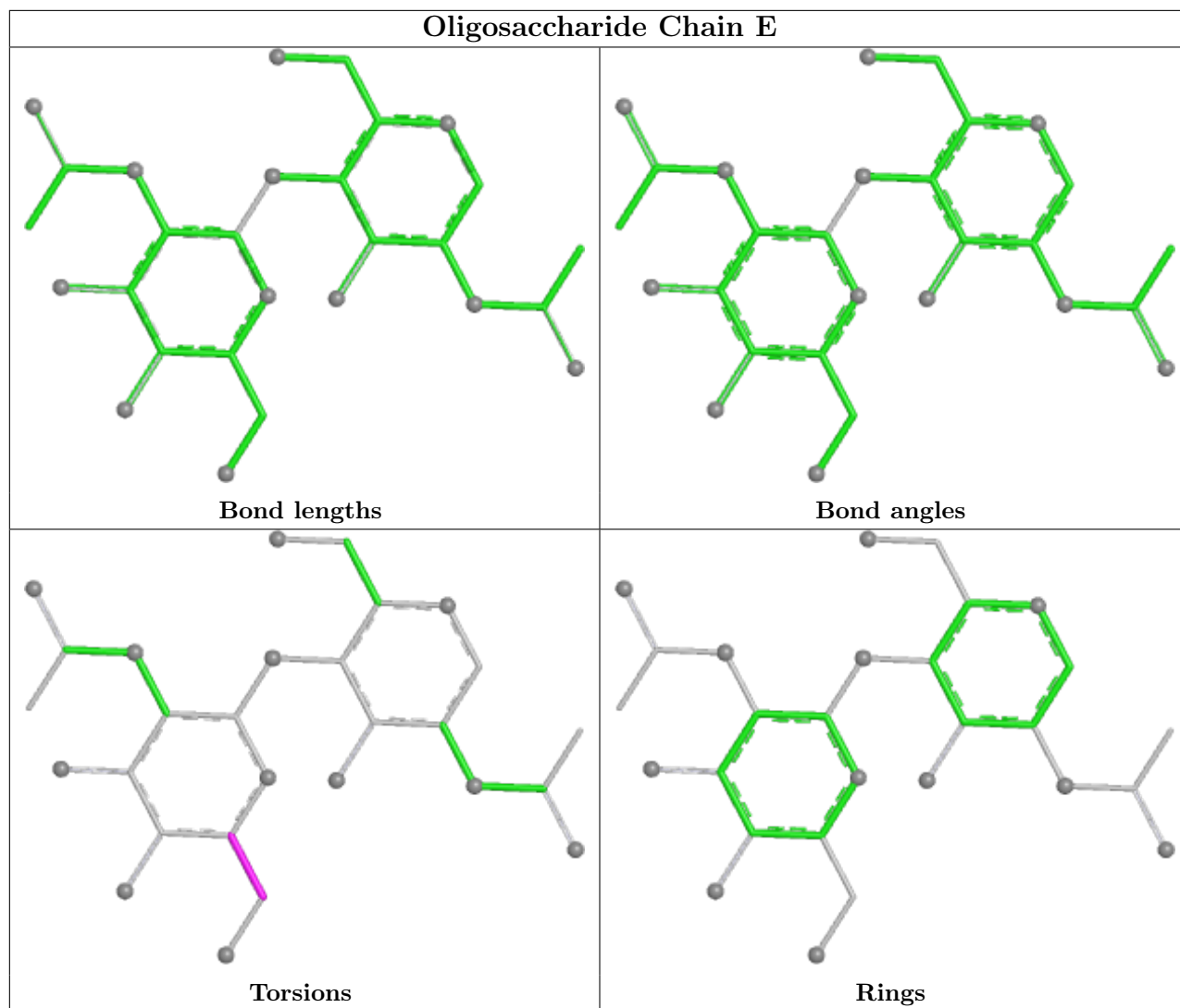
There are no ring outliers.

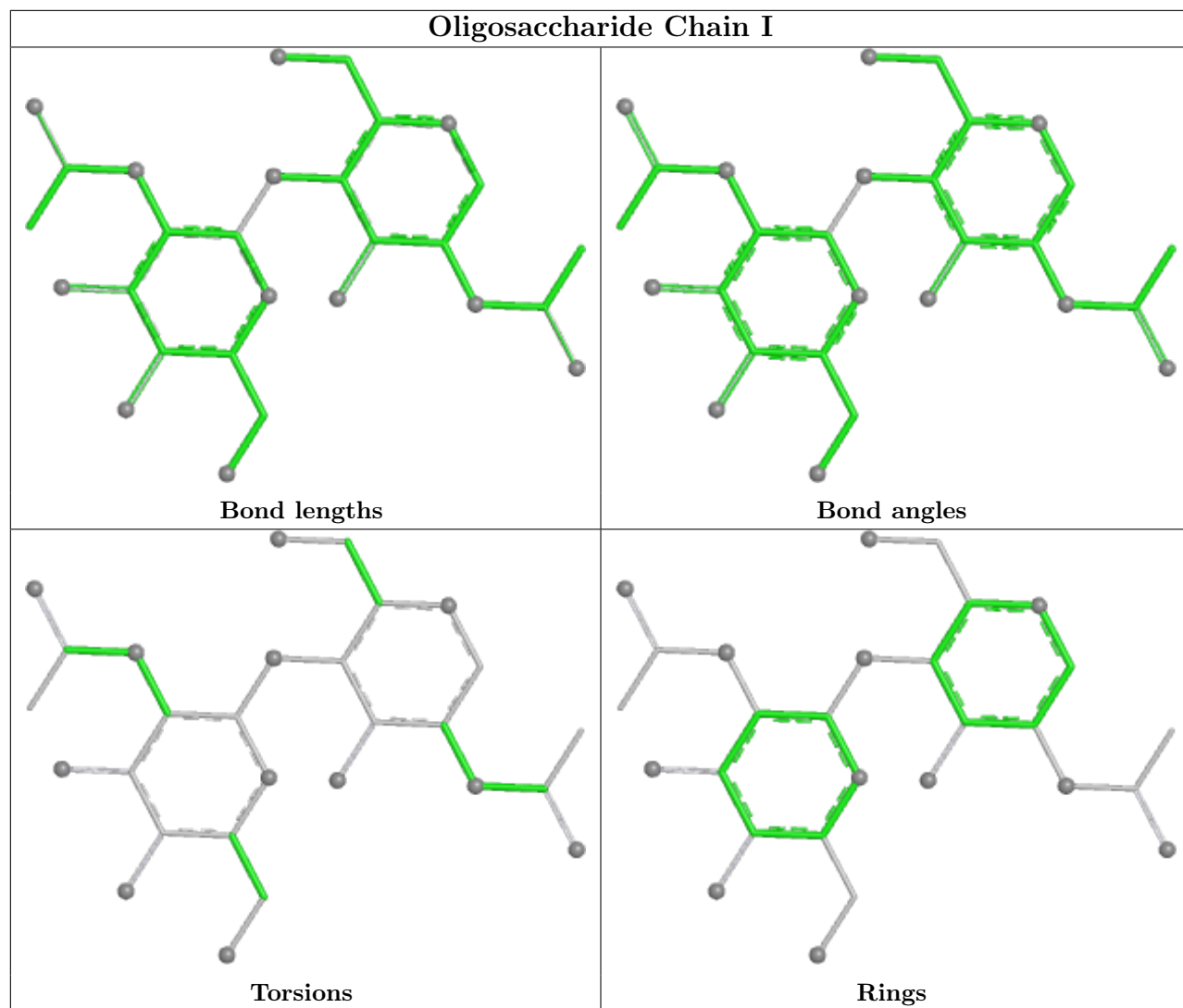
2 monomers are involved in 3 short contacts:

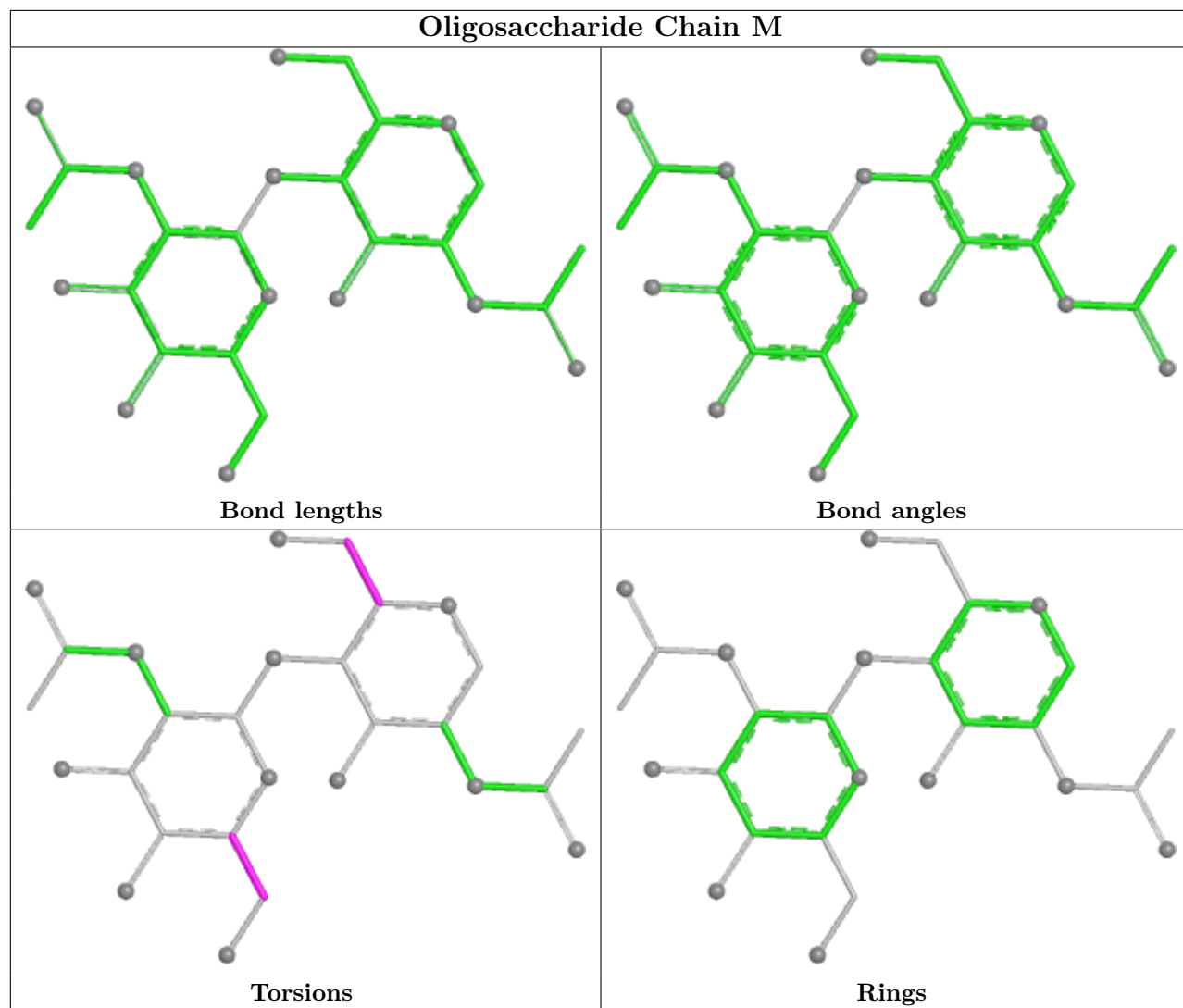
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	2	0
4	D	1	NAG	1	0

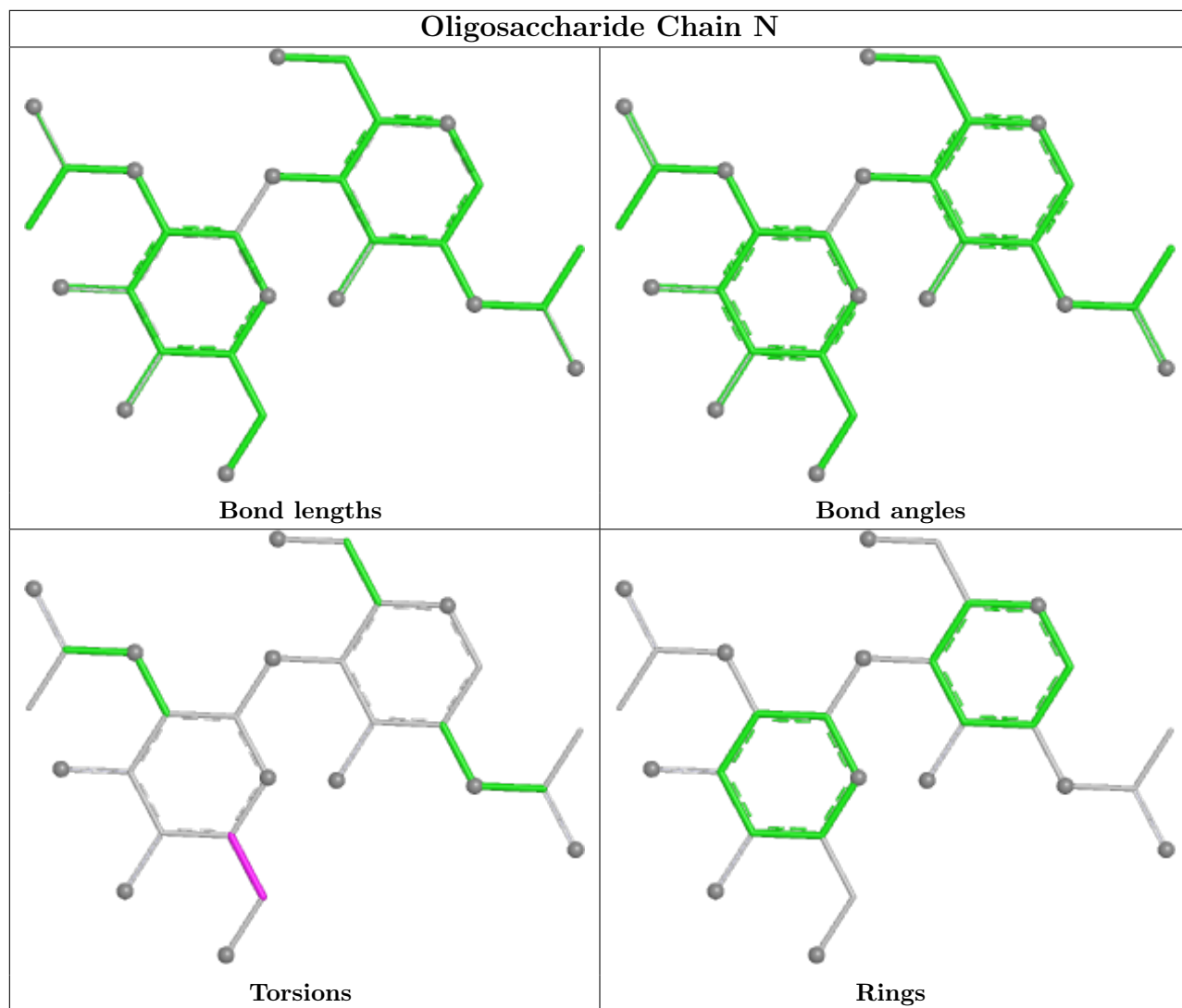
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

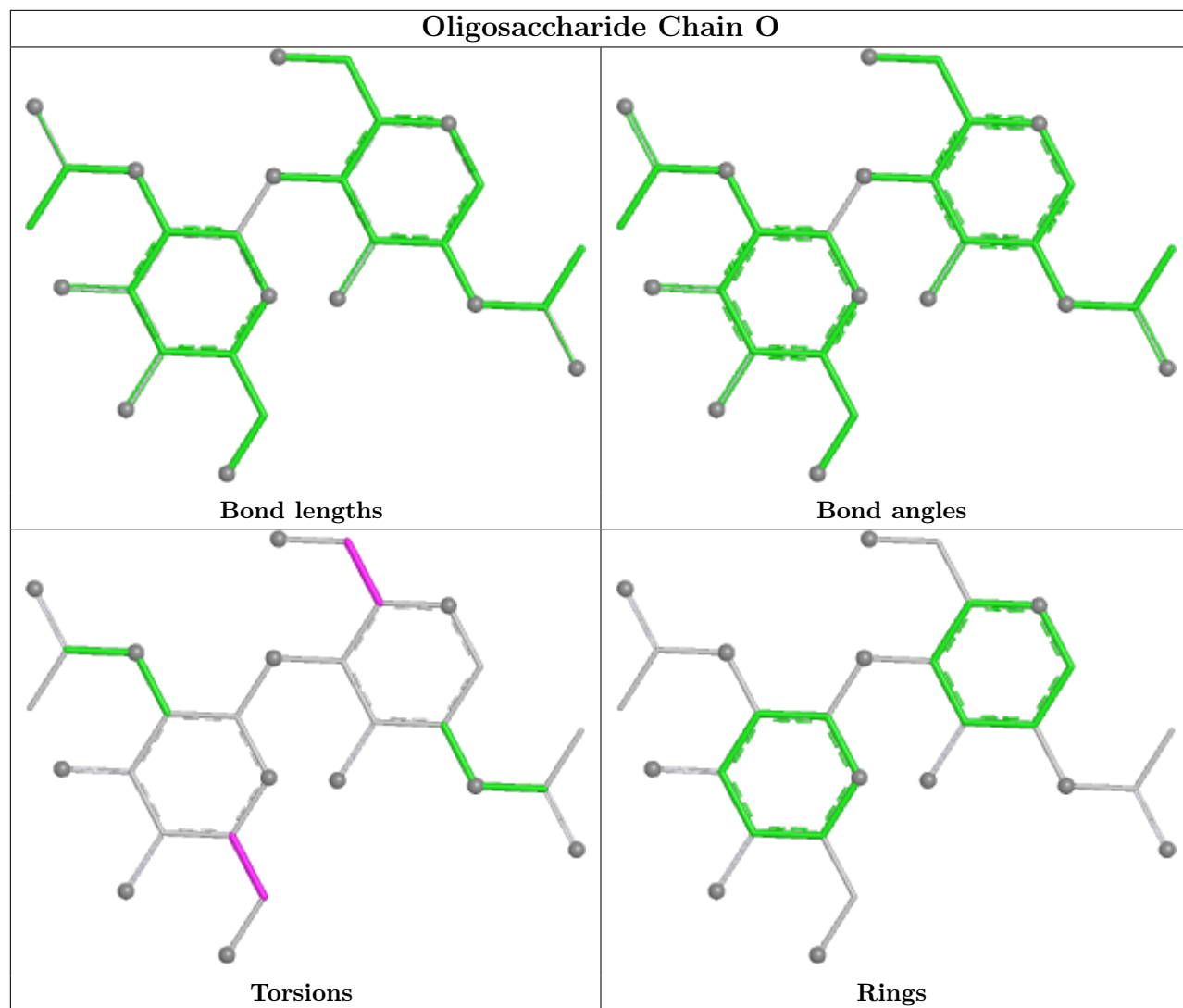


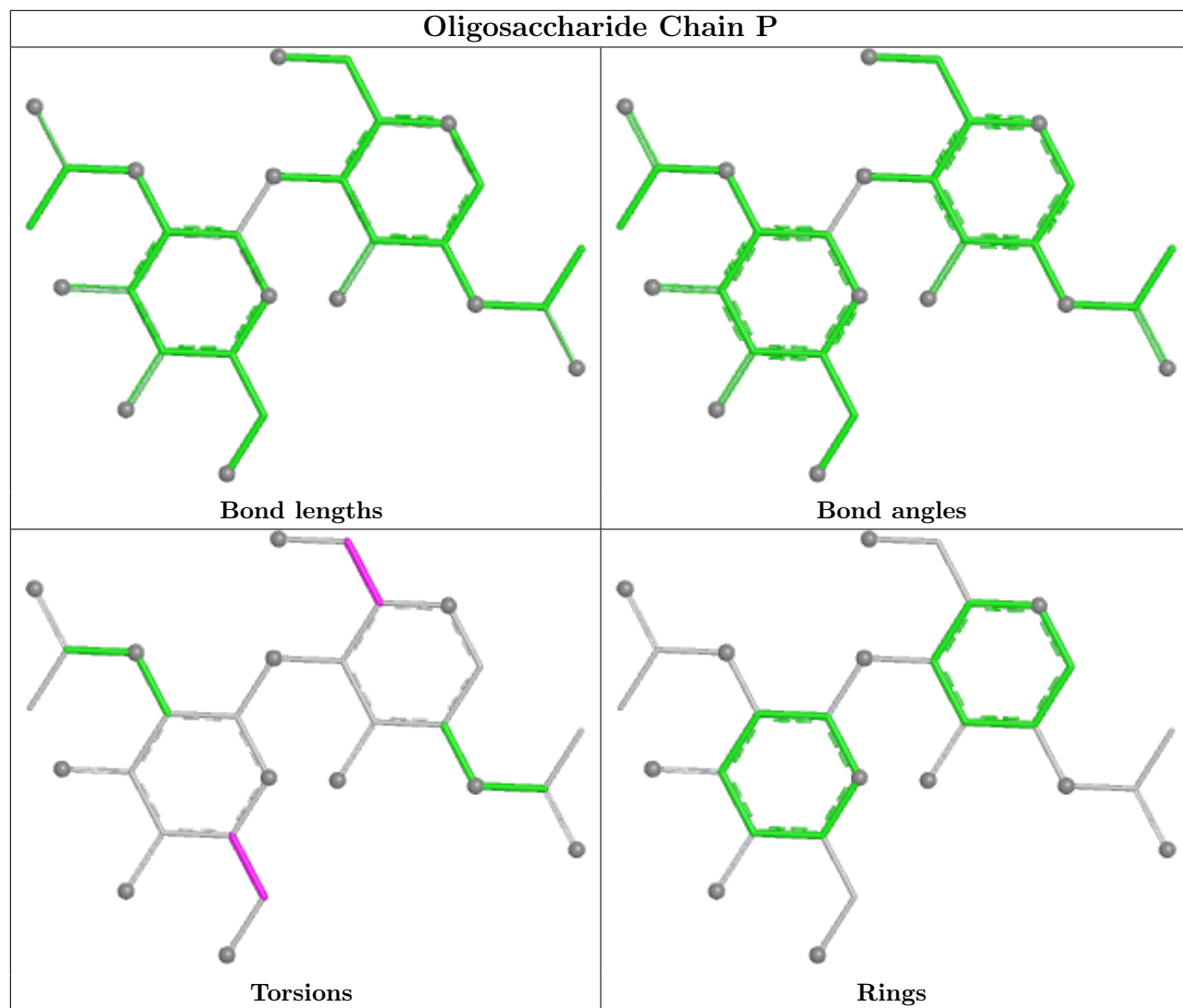


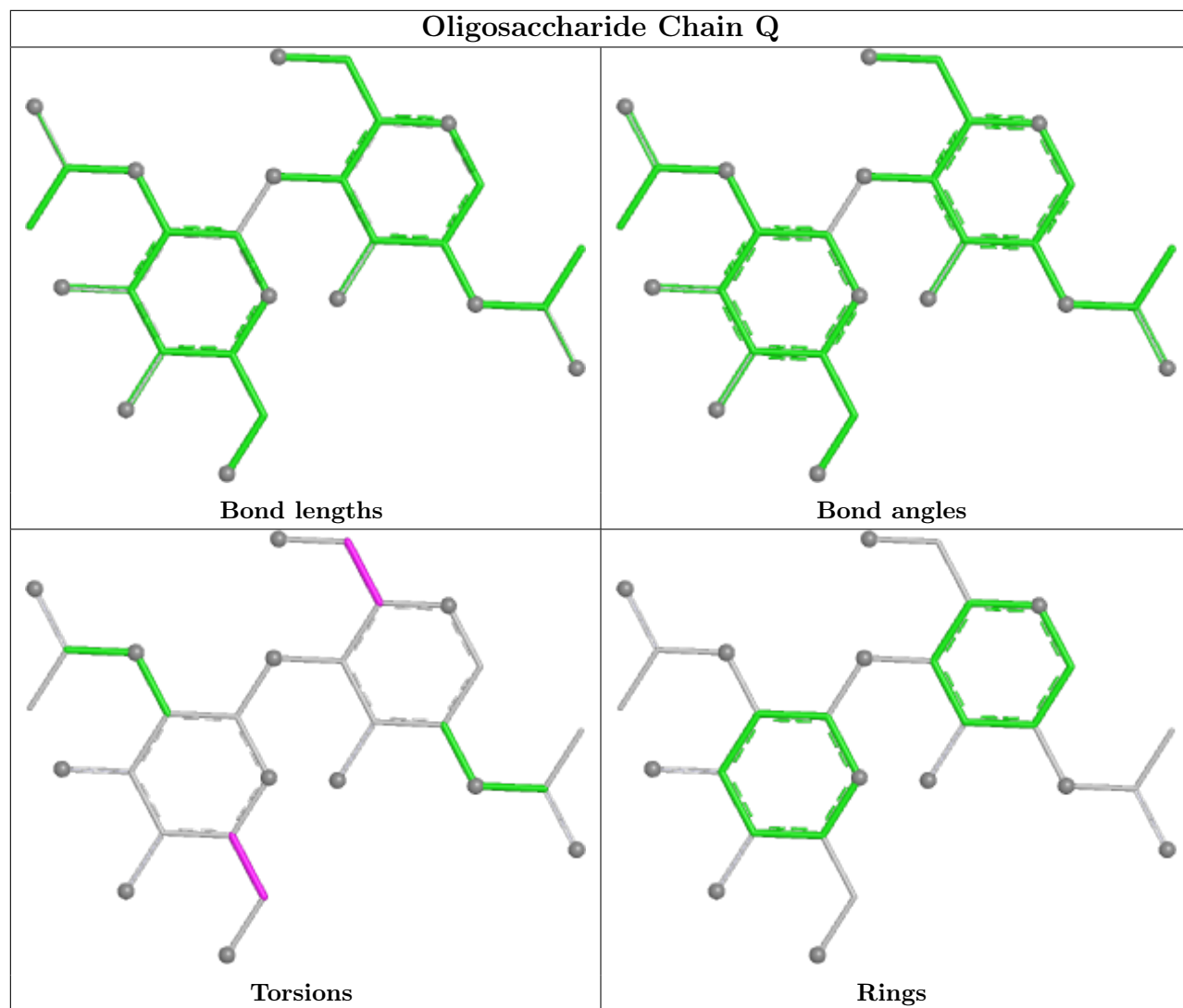


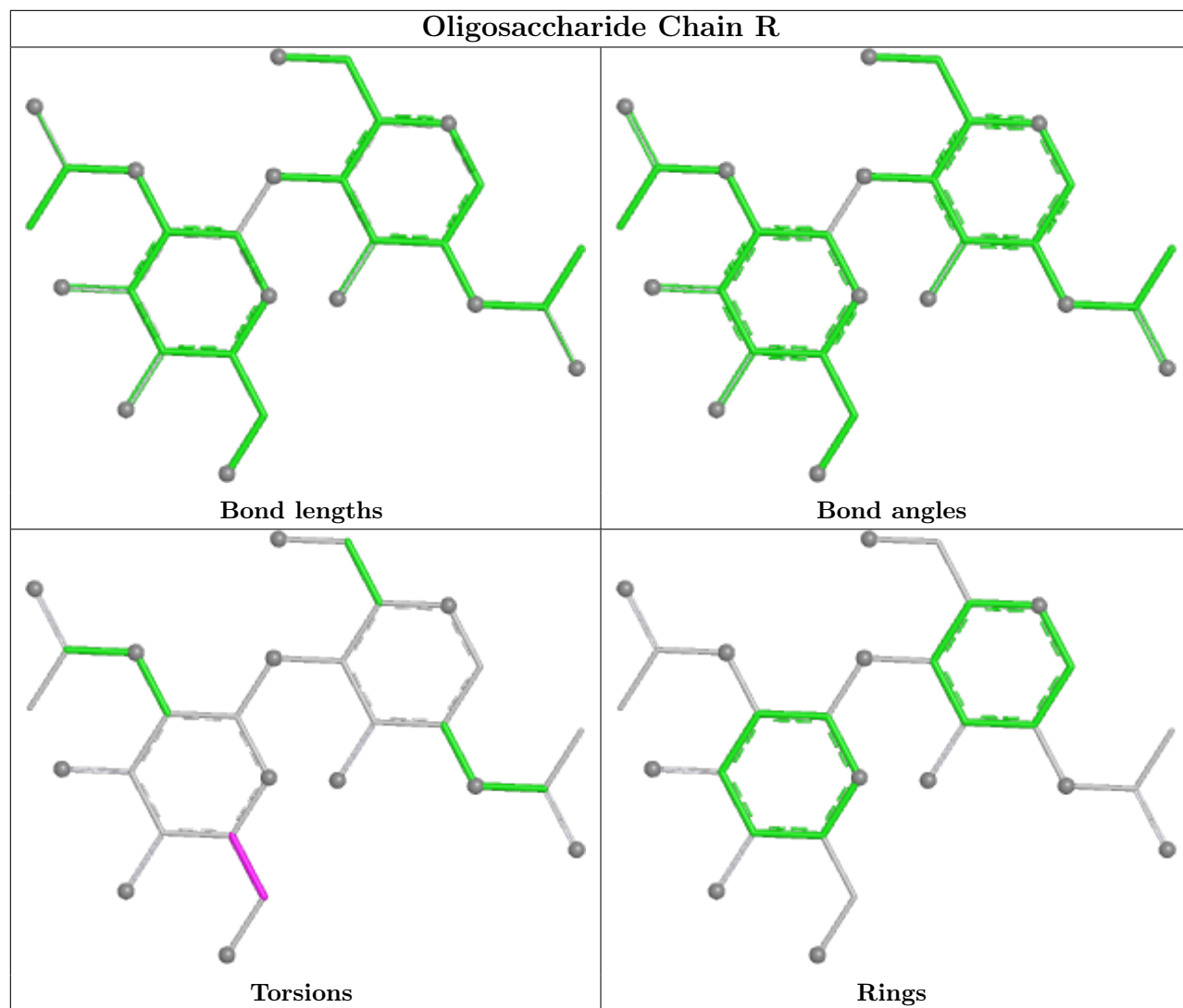


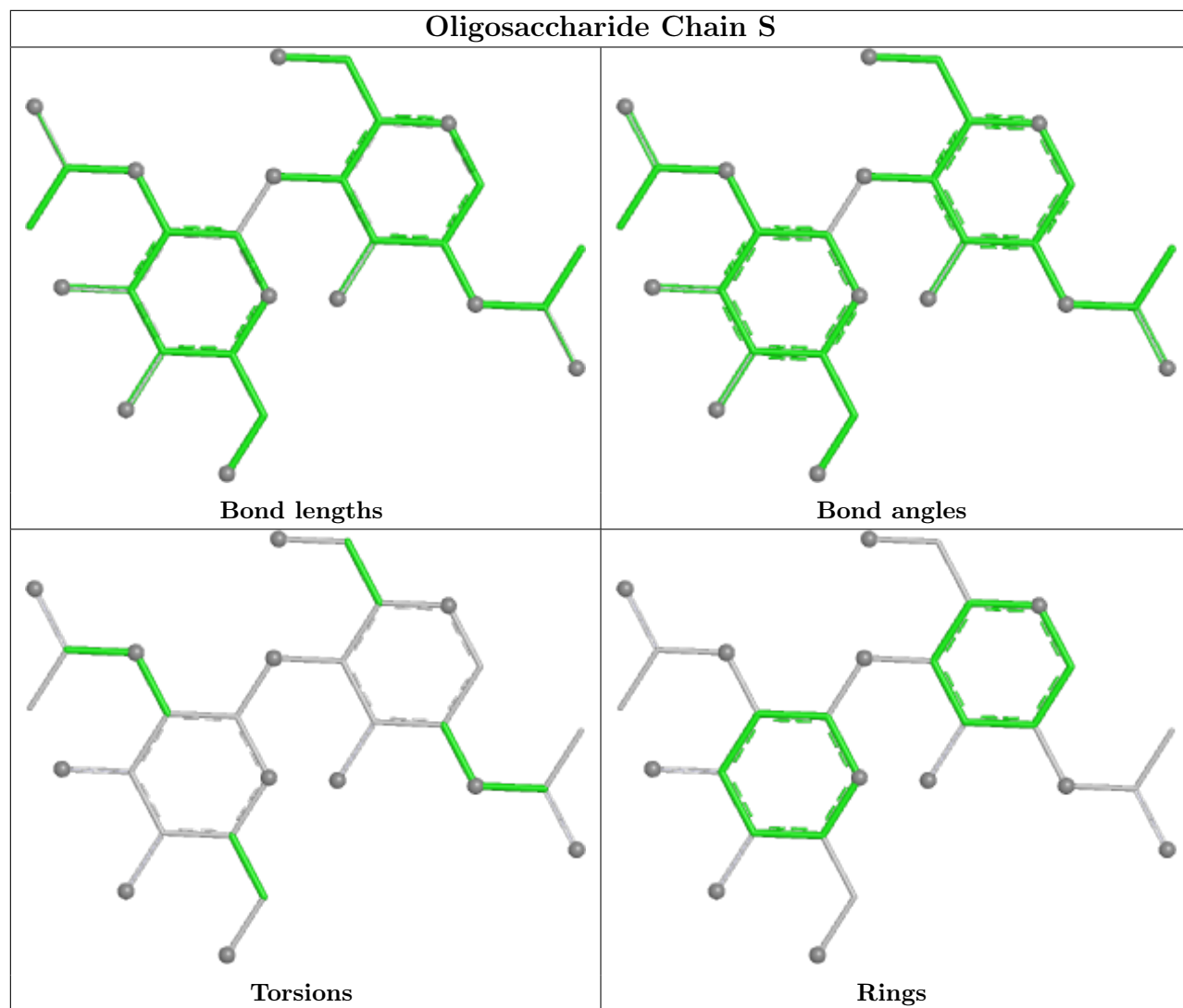


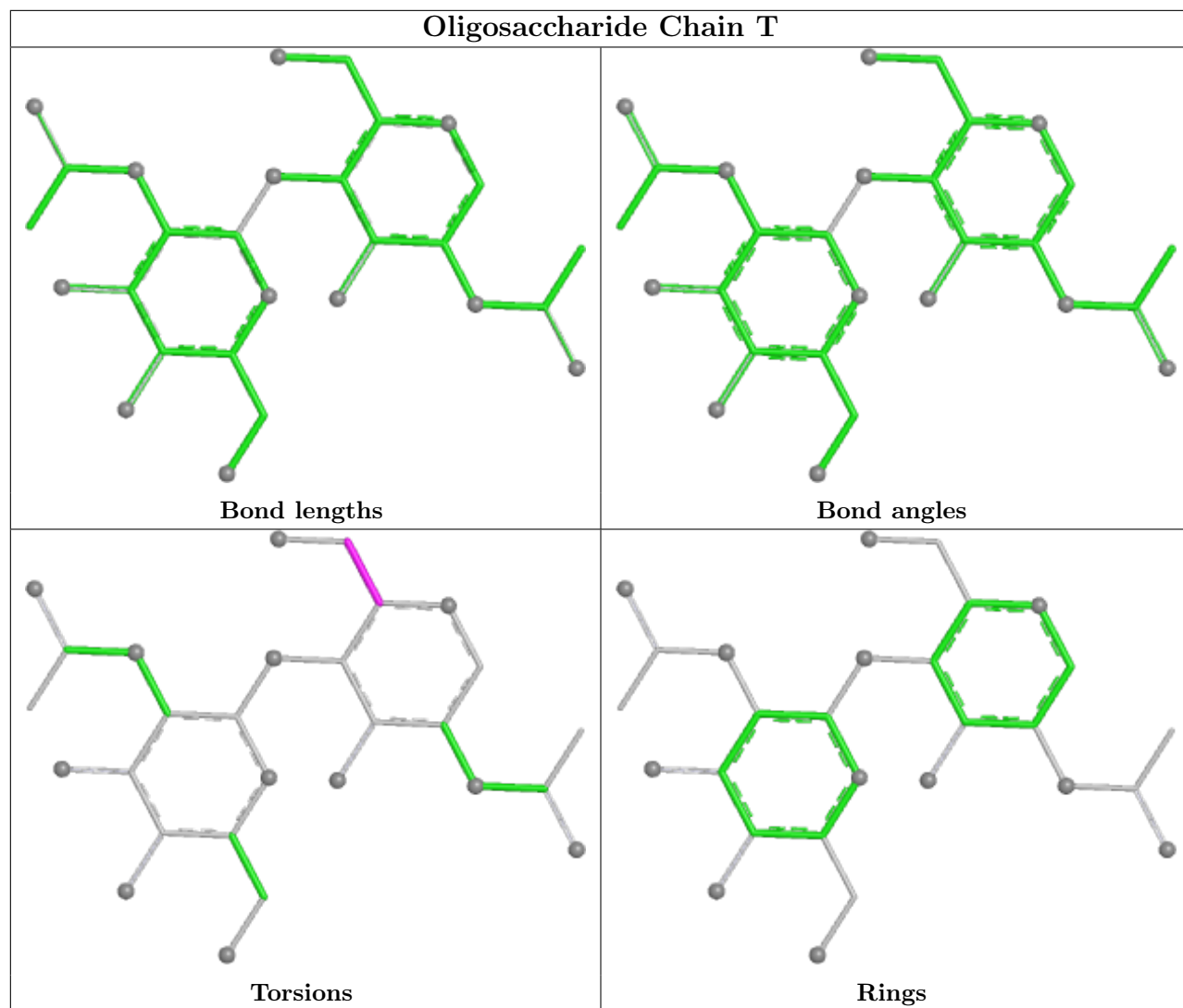


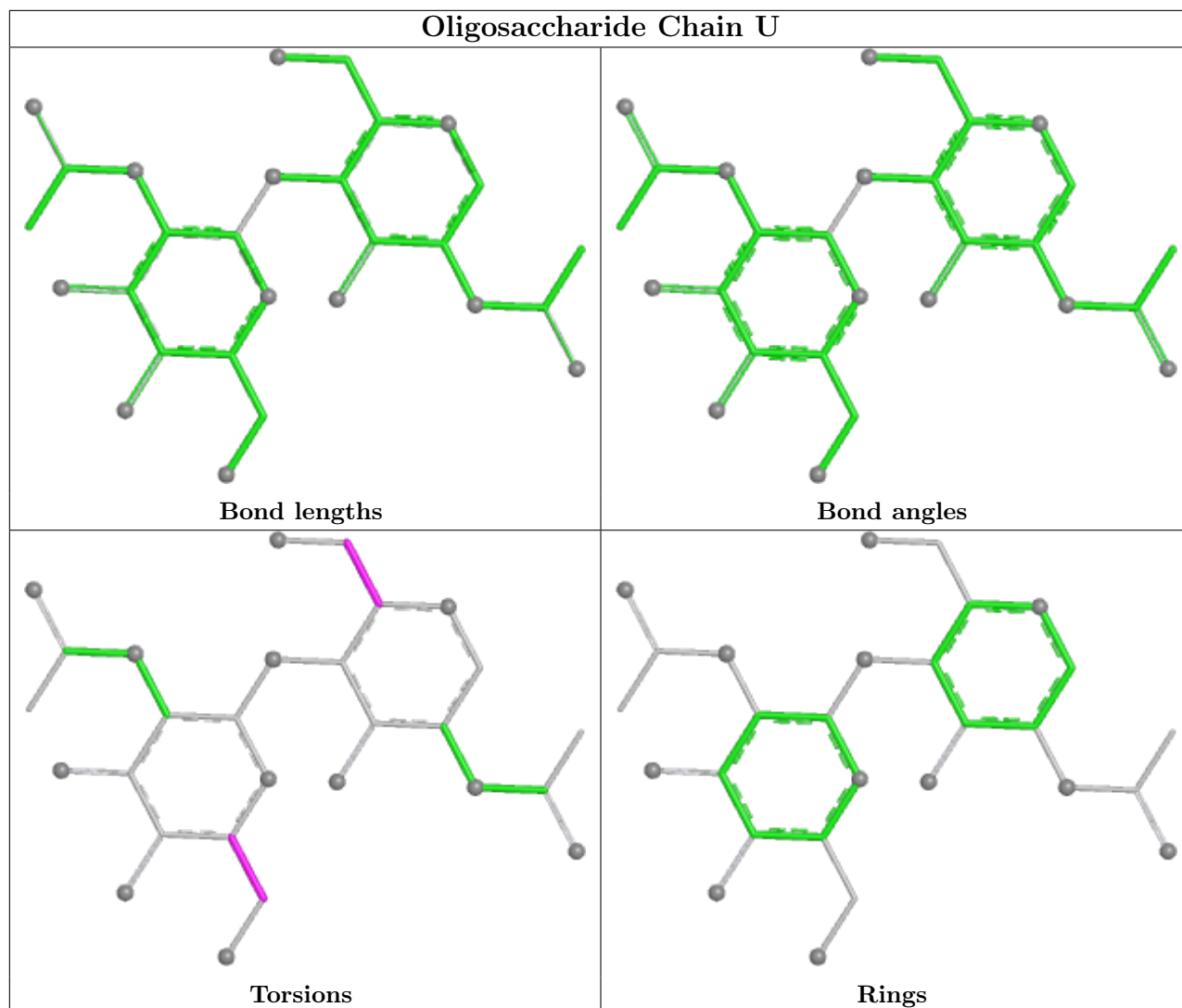












5.6 Ligand geometry [i](#)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	1309	1	14,14,15	0.20	0	17,19,21	0.38	0
5	NAG	C	1309	1	14,14,15	0.23	0	17,19,21	0.38	0
5	NAG	C	1306	1	14,14,15	0.17	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1302	1	14,14,15	0.42	0	17,19,21	1.05	1 (5%)
5	NAG	C	1302	1	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	B	1308	1	14,14,15	0.36	0	17,19,21	0.42	0
5	NAG	C	1301	1	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	B	1304	1	14,14,15	0.25	0	17,19,21	0.37	0
5	NAG	B	1307	1	14,14,15	0.31	0	17,19,21	0.83	0
5	NAG	C	1305	1	14,14,15	0.18	0	17,19,21	0.50	0
5	NAG	C	1308	1	14,14,15	0.17	0	17,19,21	0.42	0
5	NAG	C	1304	1	14,14,15	0.19	0	17,19,21	0.46	0
5	NAG	A	1303	1	14,14,15	0.29	0	17,19,21	0.71	0
5	NAG	A	1306	1	14,14,15	0.19	0	17,19,21	0.42	0
5	NAG	A	1309	1	14,14,15	0.26	0	17,19,21	0.37	0
5	NAG	C	1307	1	14,14,15	0.17	0	17,19,21	0.64	1 (5%)
5	NAG	A	1305	1	14,14,15	0.17	0	17,19,21	0.49	0
5	NAG	A	1301	1	14,14,15	0.33	0	17,19,21	0.64	0
5	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.40	0
5	NAG	B	1305	1	14,14,15	0.36	0	17,19,21	0.37	0
5	NAG	B	1306	1	14,14,15	0.19	0	17,19,21	0.57	0
5	NAG	C	1303	1	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	B	1301	1	14,14,15	0.18	0	17,19,21	0.46	0
5	NAG	A	1307	1	14,14,15	0.32	0	17,19,21	0.41	0
5	NAG	A	1308	1	14,14,15	0.21	0	17,19,21	0.61	1 (5%)
5	NAG	A	1302	1	14,14,15	0.29	0	17,19,21	0.43	0
5	NAG	A	1310	1	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	A	1304	1	14,14,15	0.19	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1302	NAG	C1-O5-C5	-3.16	107.91	112.19
5	C	1307	NAG	C1-O5-C5	2.13	115.08	112.19
5	A	1308	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1303	NAG	O5-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6
5	C	1307	NAG	C4-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
5	B	1302	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1309	NAG	C8-C7-N2-C2
5	C	1302	NAG	O5-C5-C6-O6
5	C	1306	NAG	O5-C5-C6-O6
5	A	1309	NAG	O7-C7-N2-C2
5	C	1307	NAG	O5-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	A	1306	NAG	C4-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	B	1302	NAG	O7-C7-N2-C2
5	C	1308	NAG	C8-C7-N2-C2
5	C	1308	NAG	O7-C7-N2-C2
5	C	1306	NAG	C4-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	C	1309	NAG	C4-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	A	1309	NAG	C4-C5-C6-O6
5	B	1306	NAG	O5-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	B	1305	NAG	C4-C5-C6-O6
5	A	1303	NAG	C8-C7-N2-C2
5	A	1303	NAG	O7-C7-N2-C2
5	B	1308	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 12 short contacts:

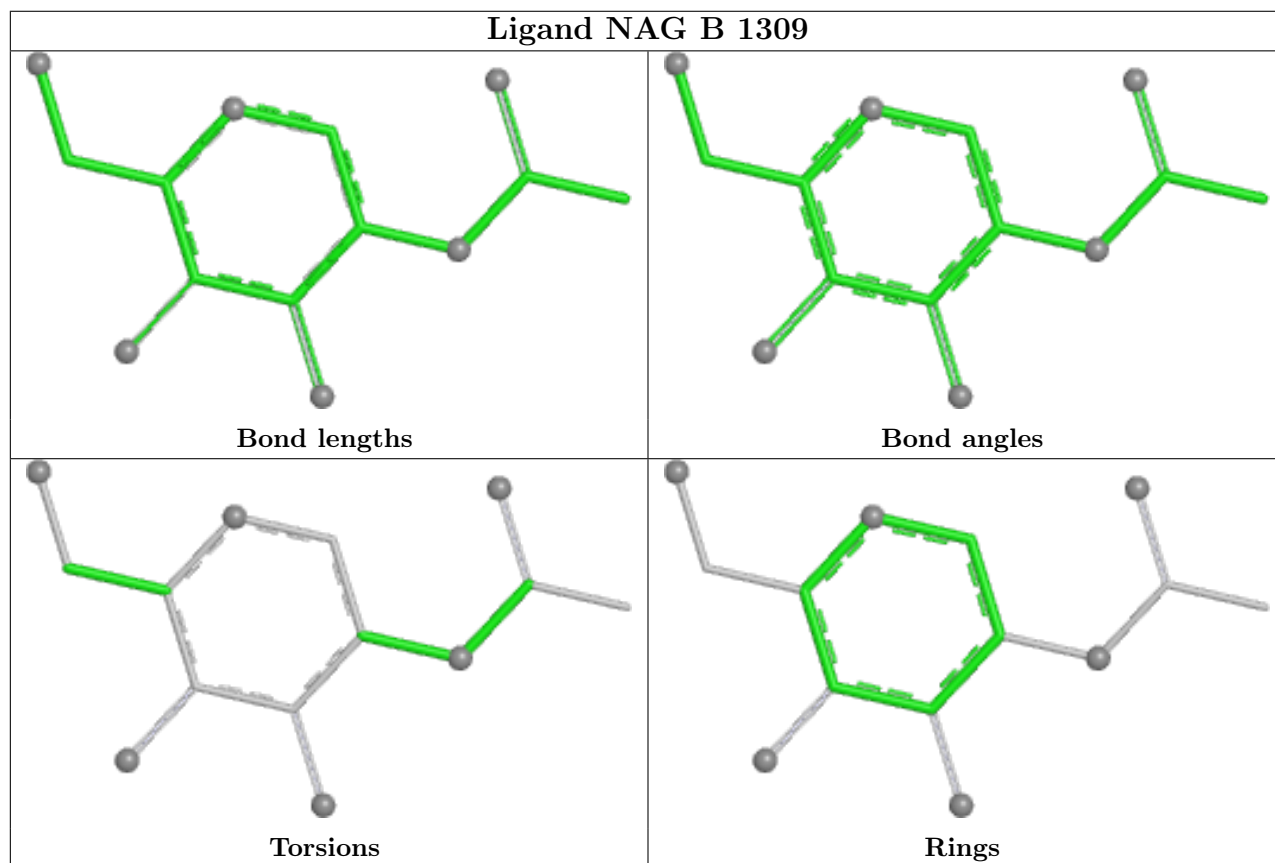
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1307	NAG	5	0
5	A	1303	NAG	2	0
5	A	1301	NAG	3	0

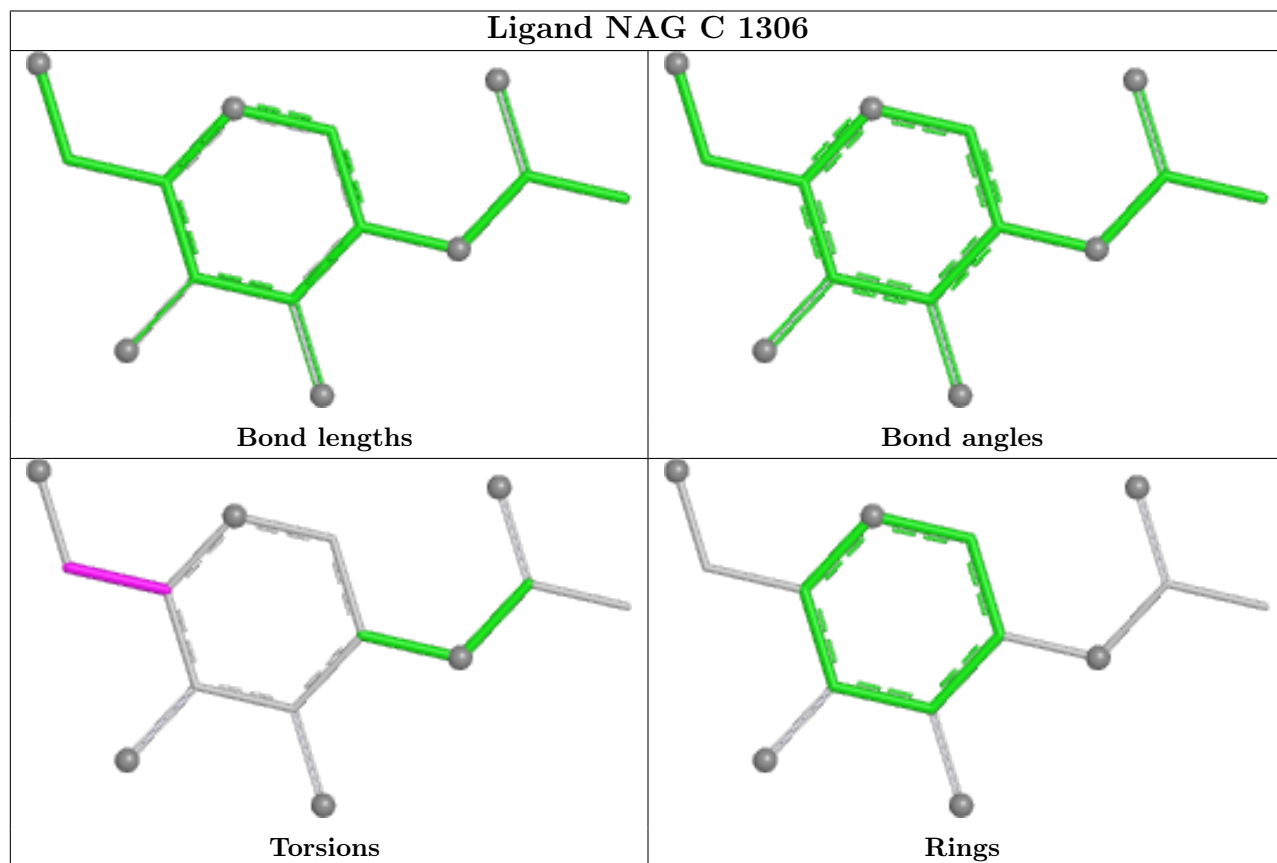
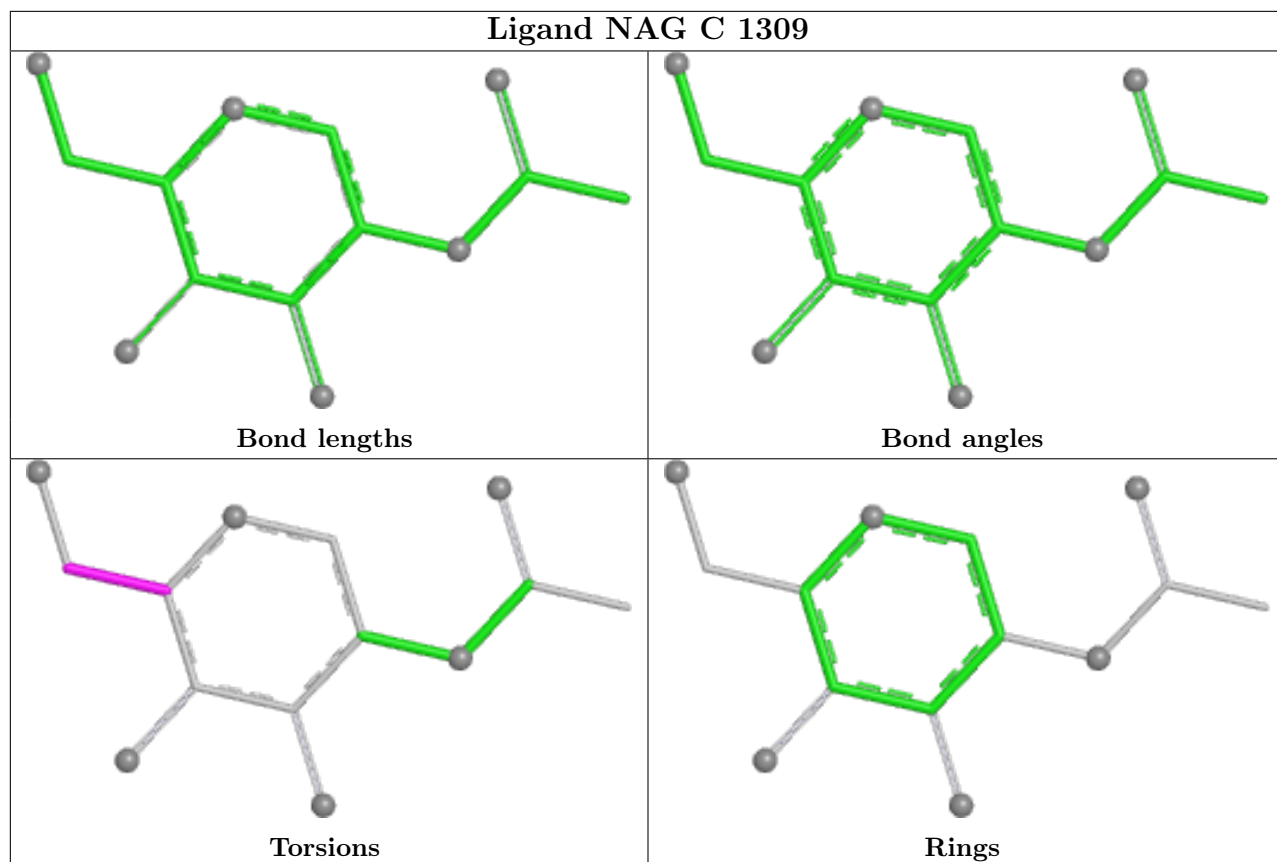
Continued on next page...

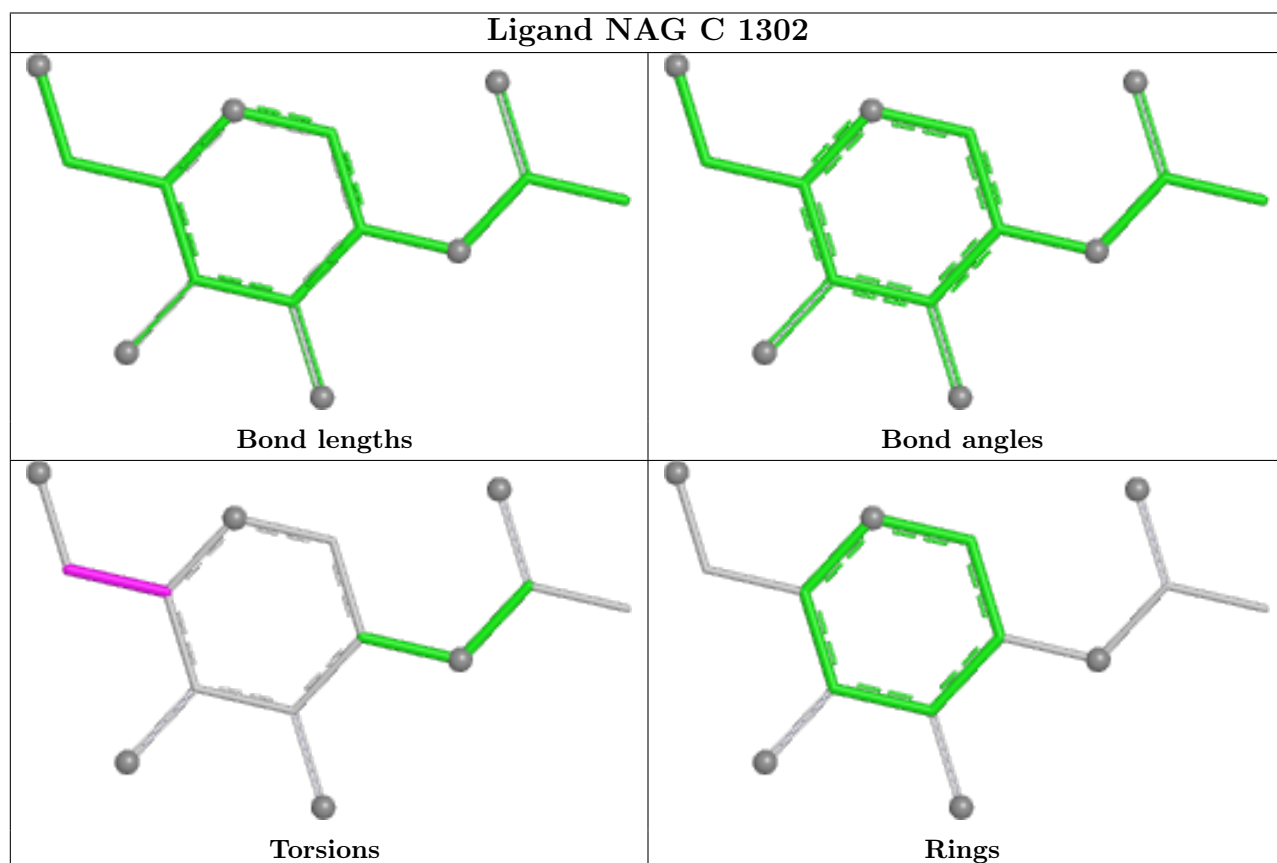
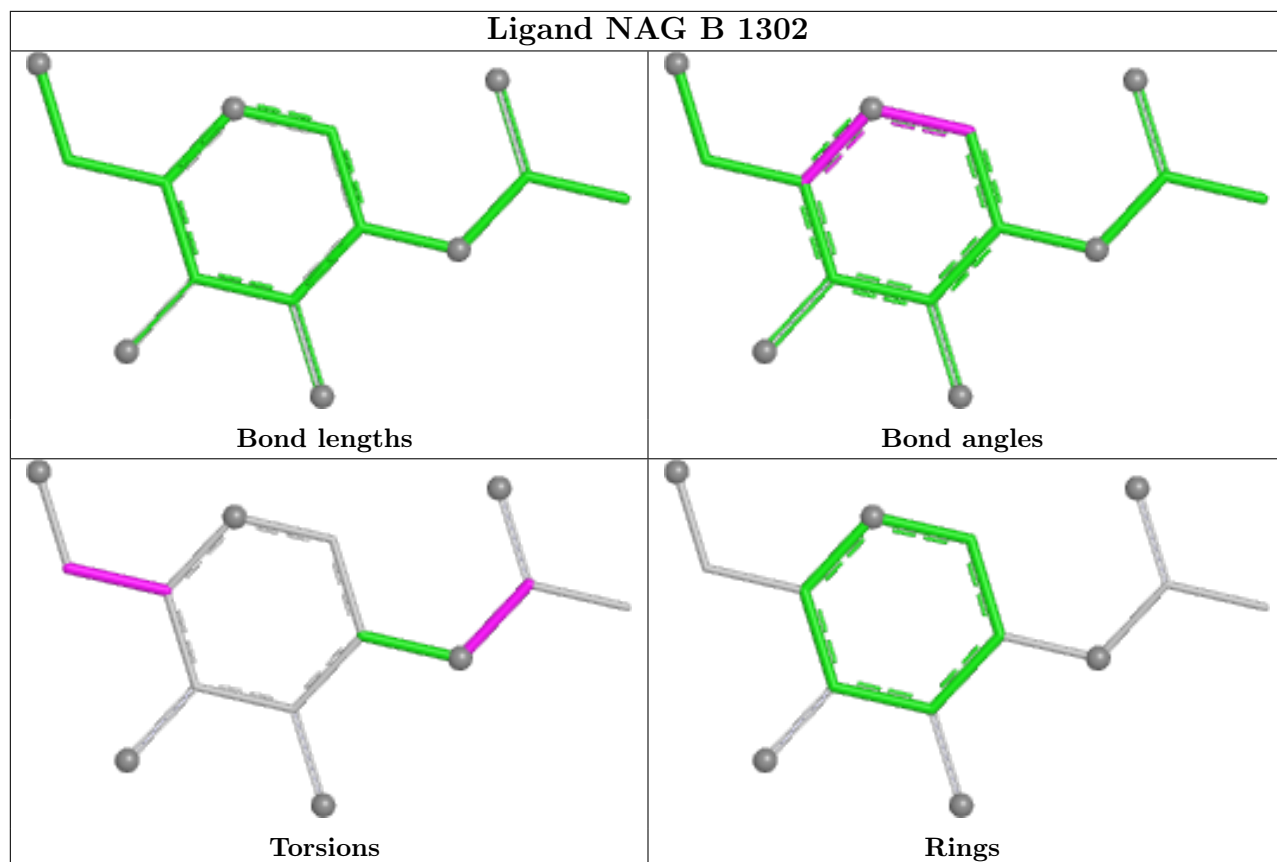
Continued from previous page...

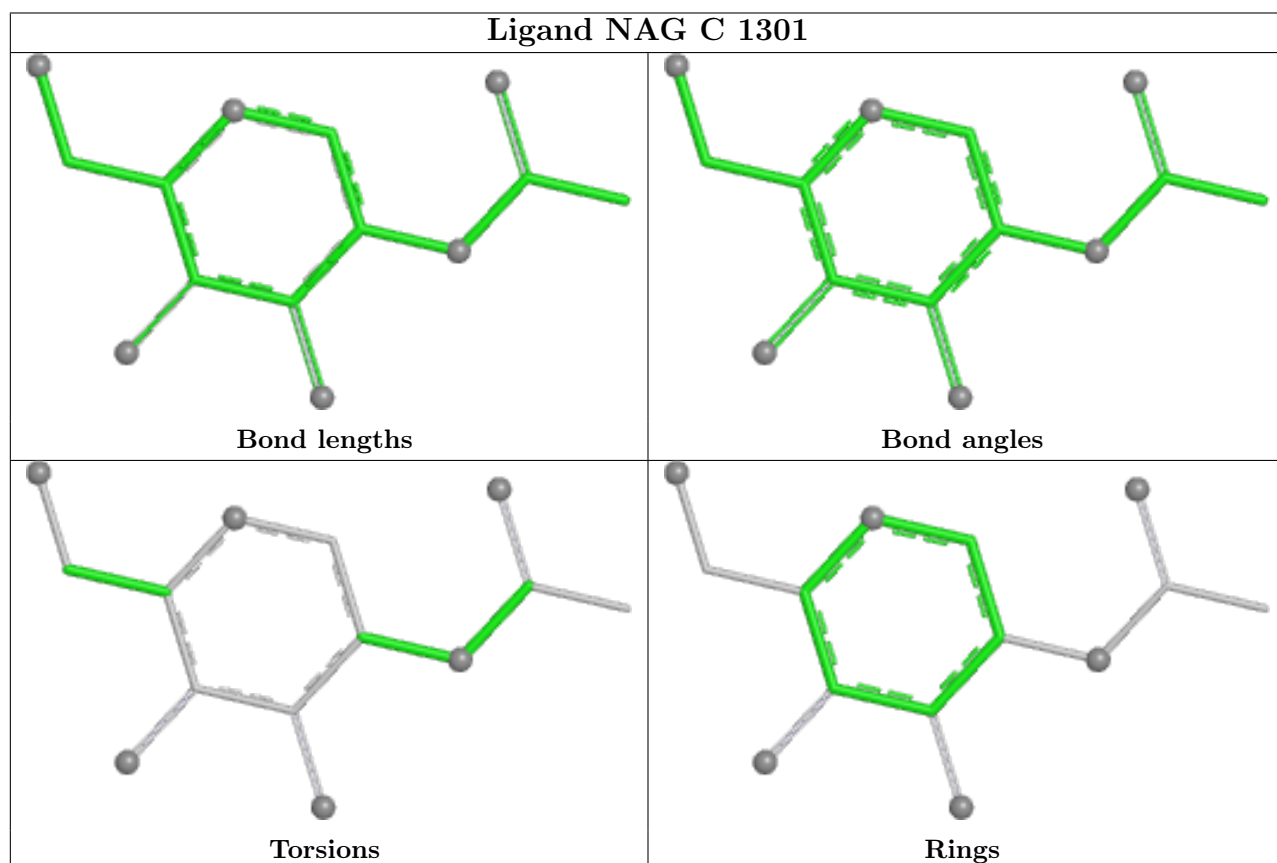
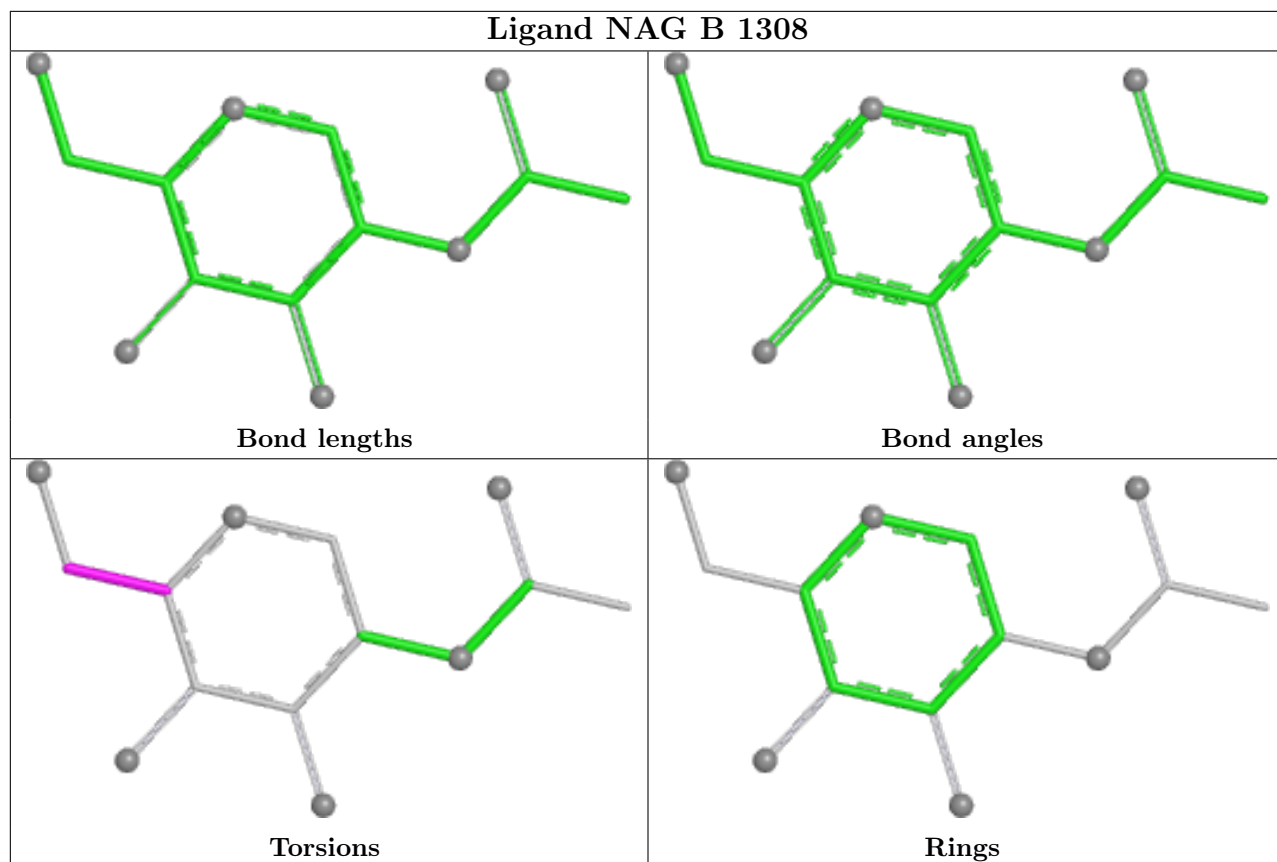
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1302	NAG	1	0
5	A	1310	NAG	1	0

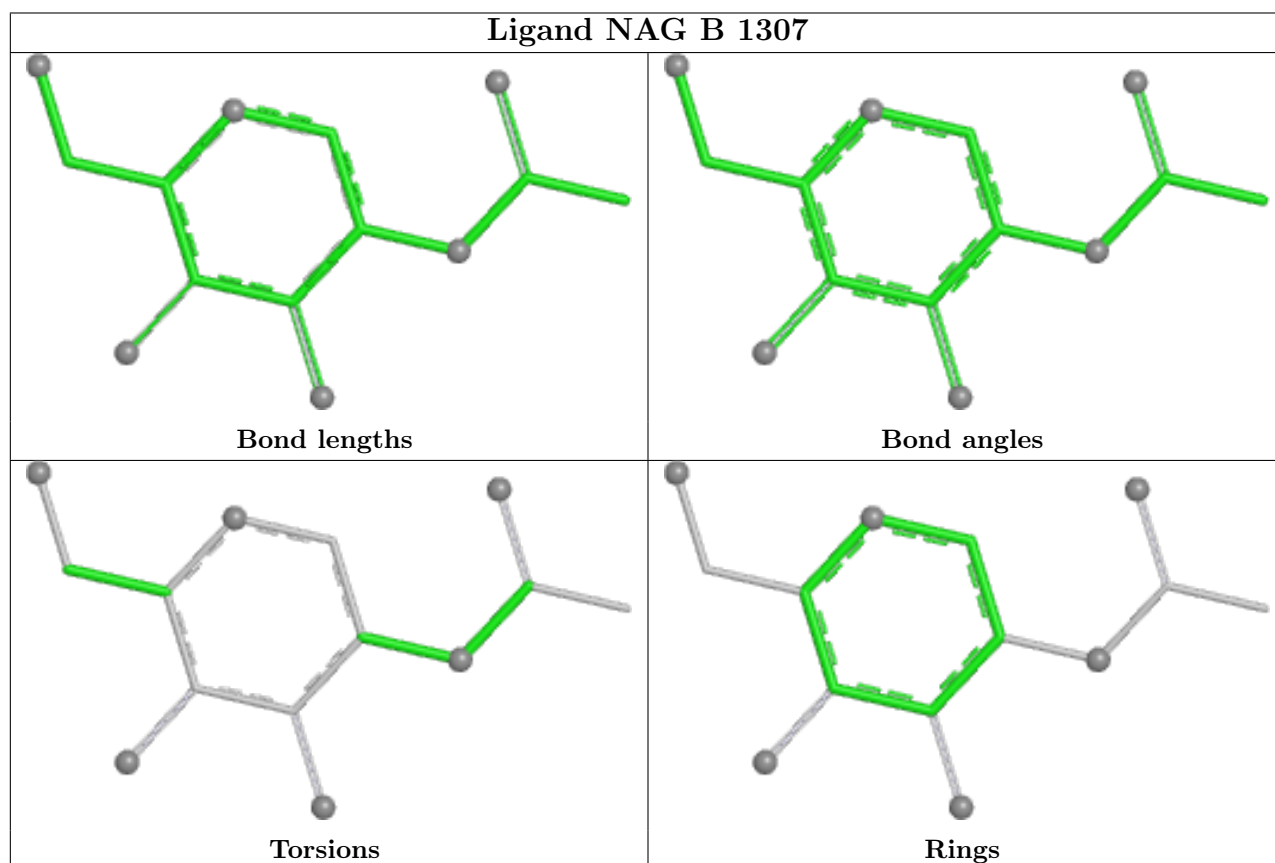
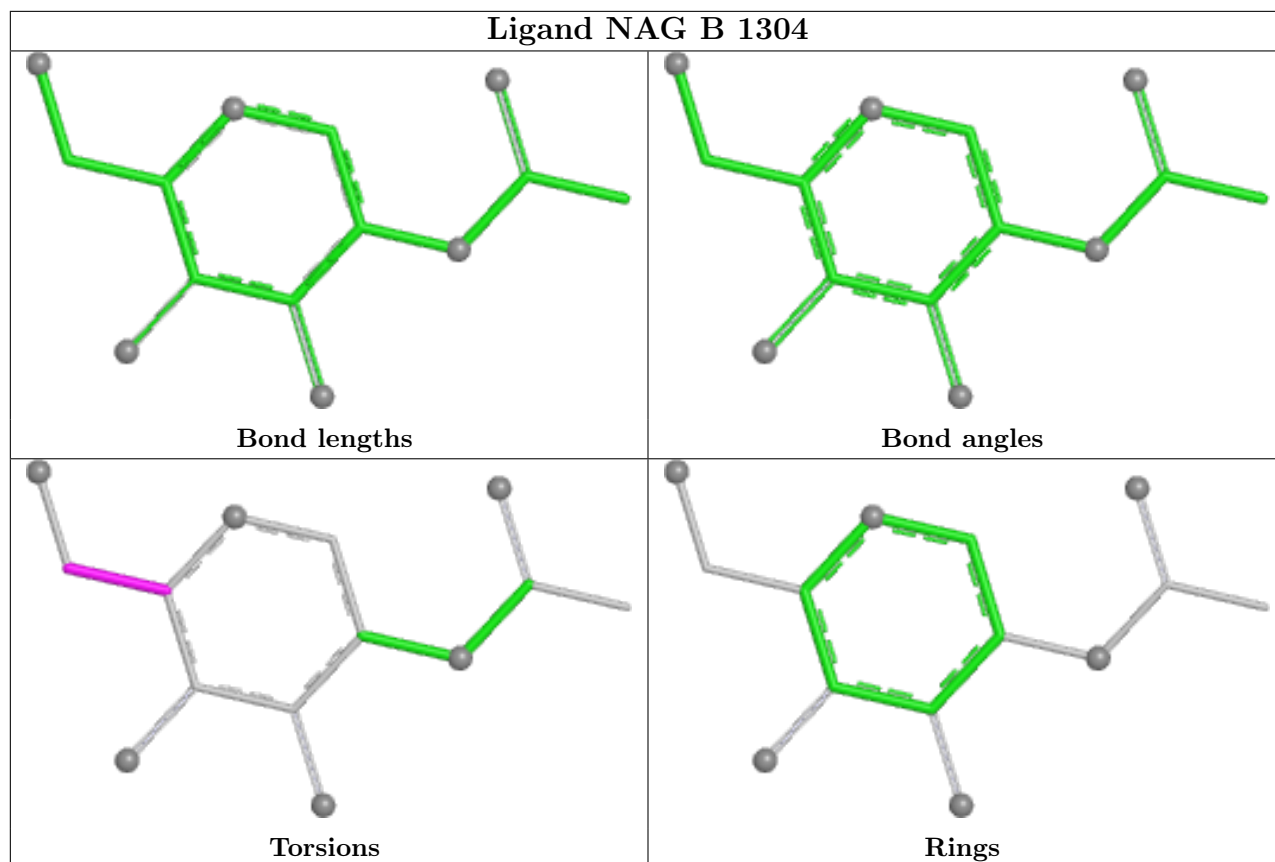
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

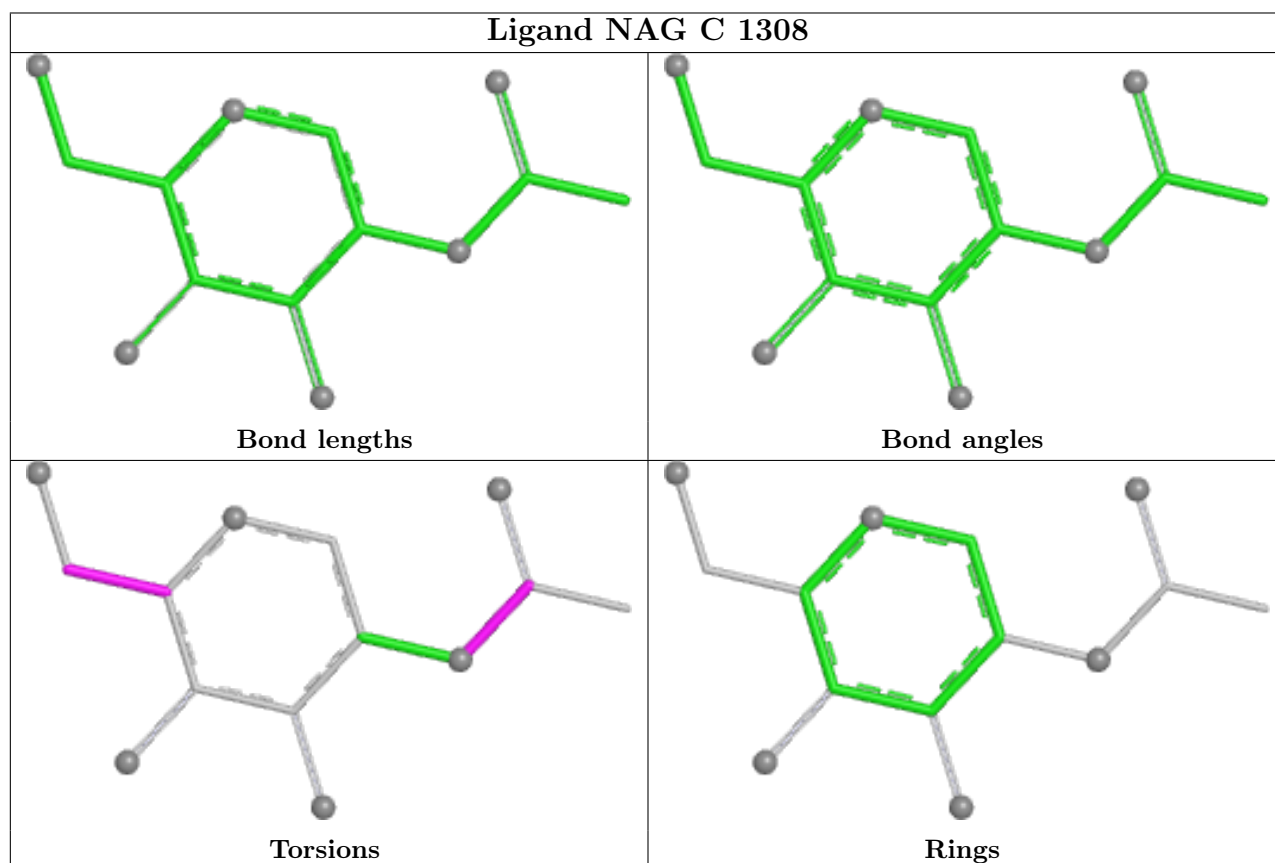
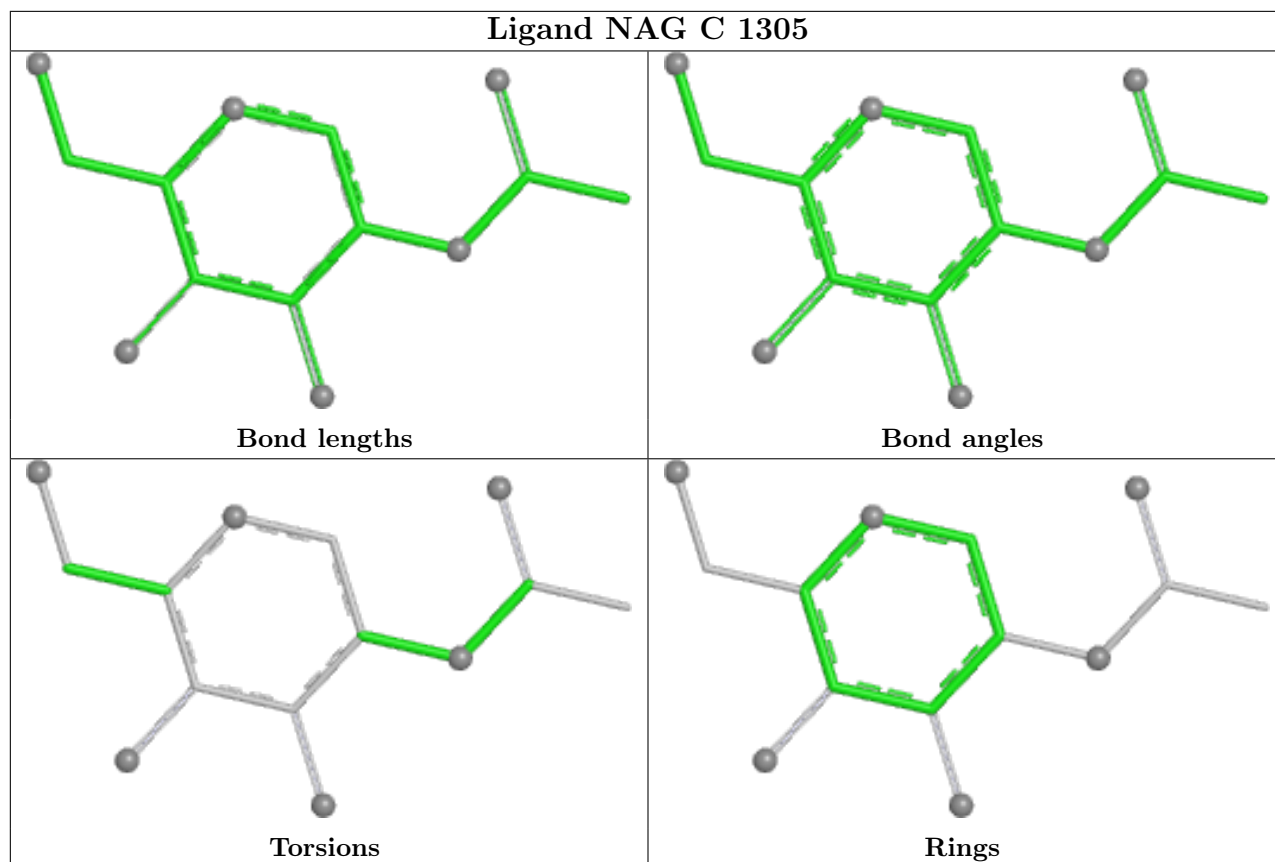


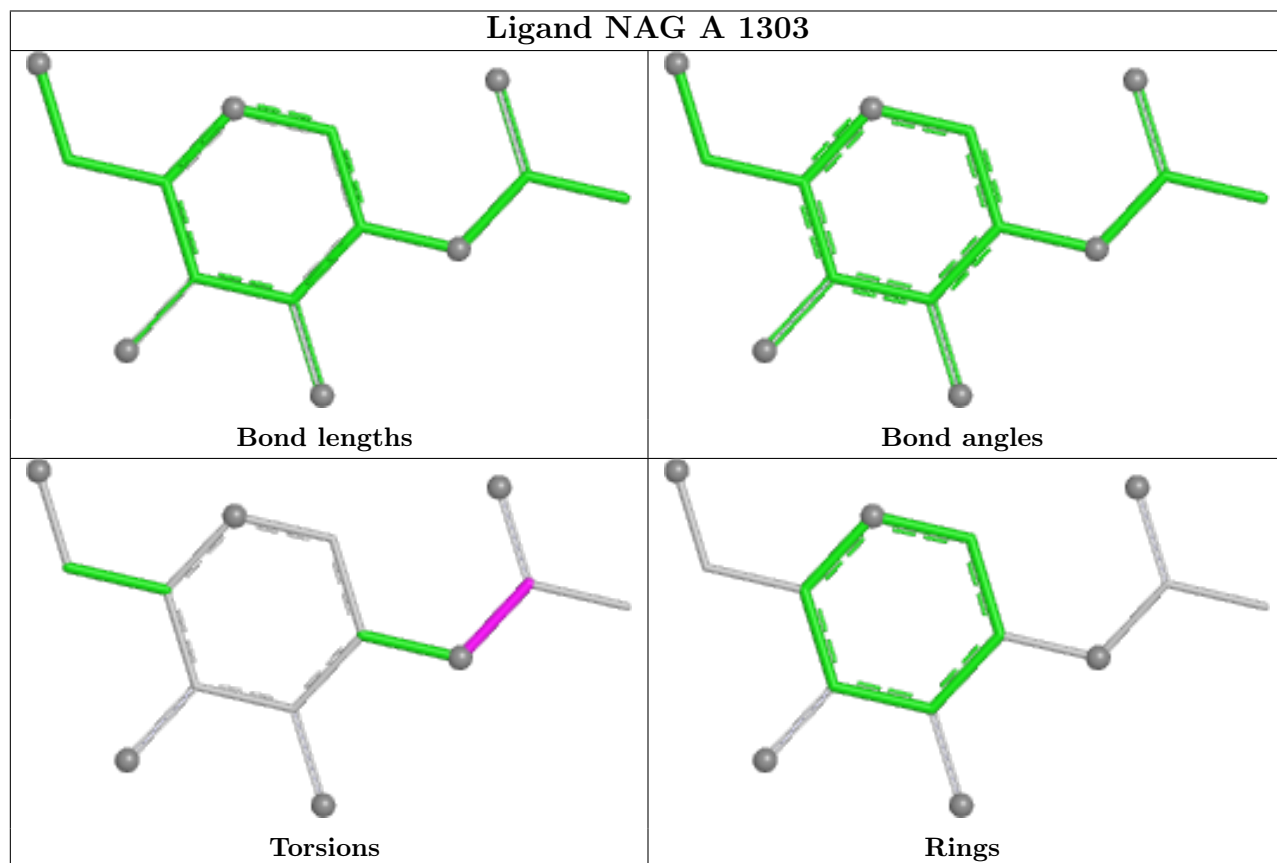
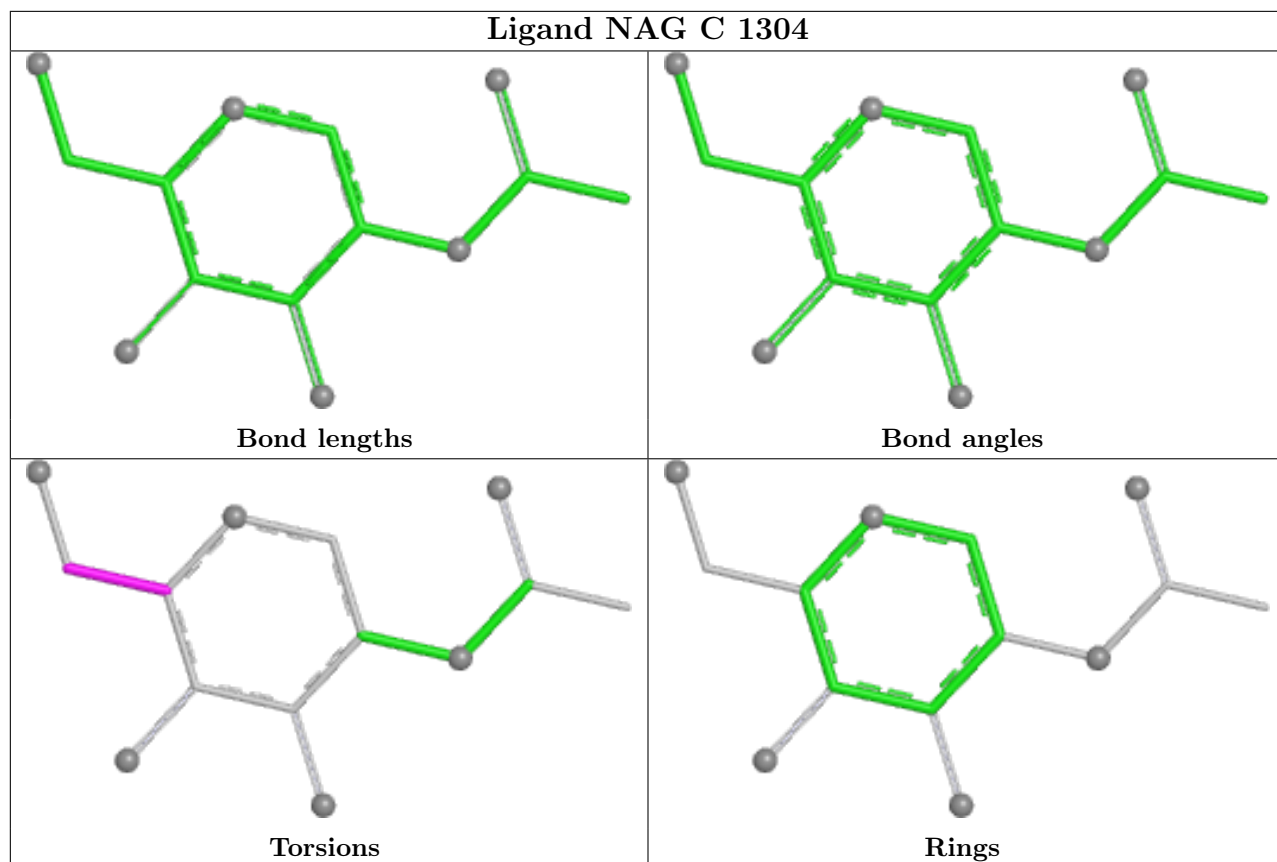


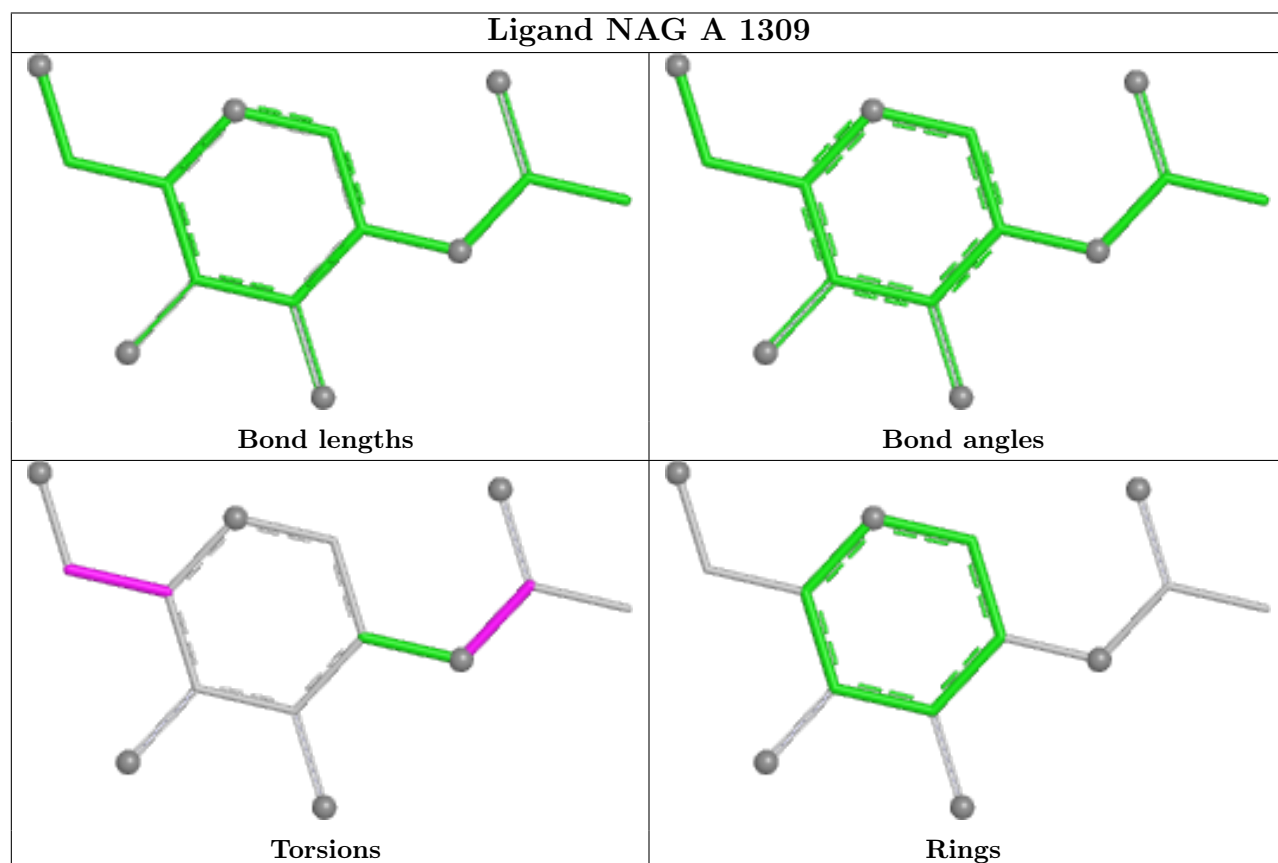
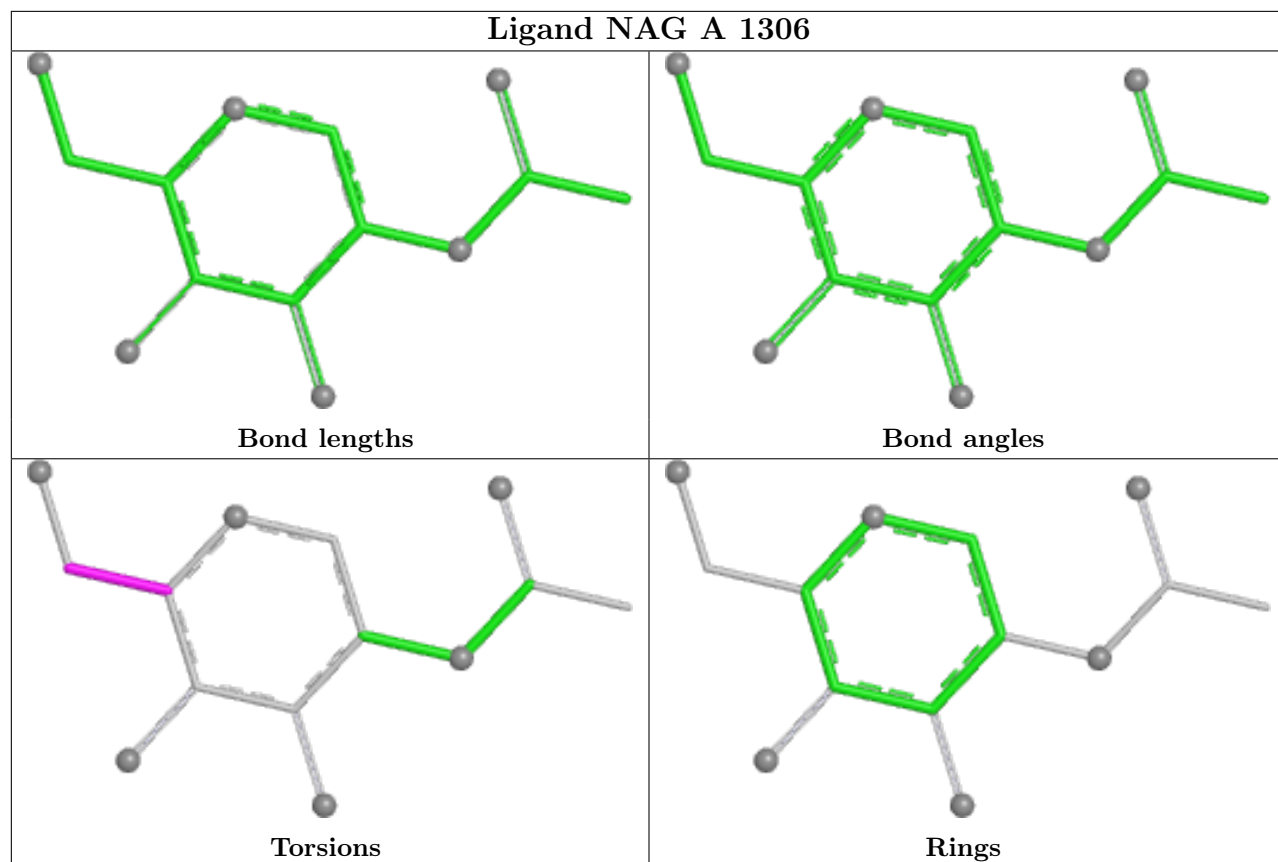


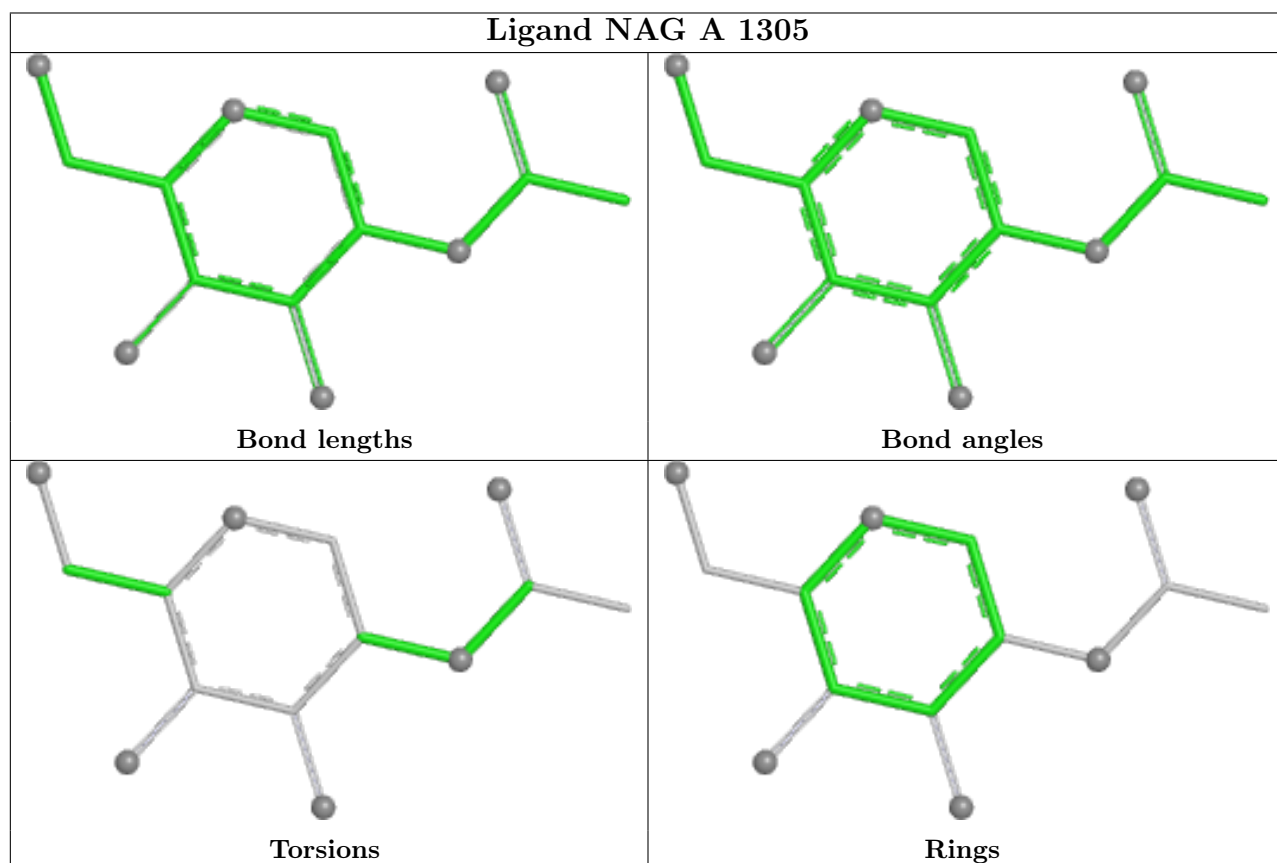
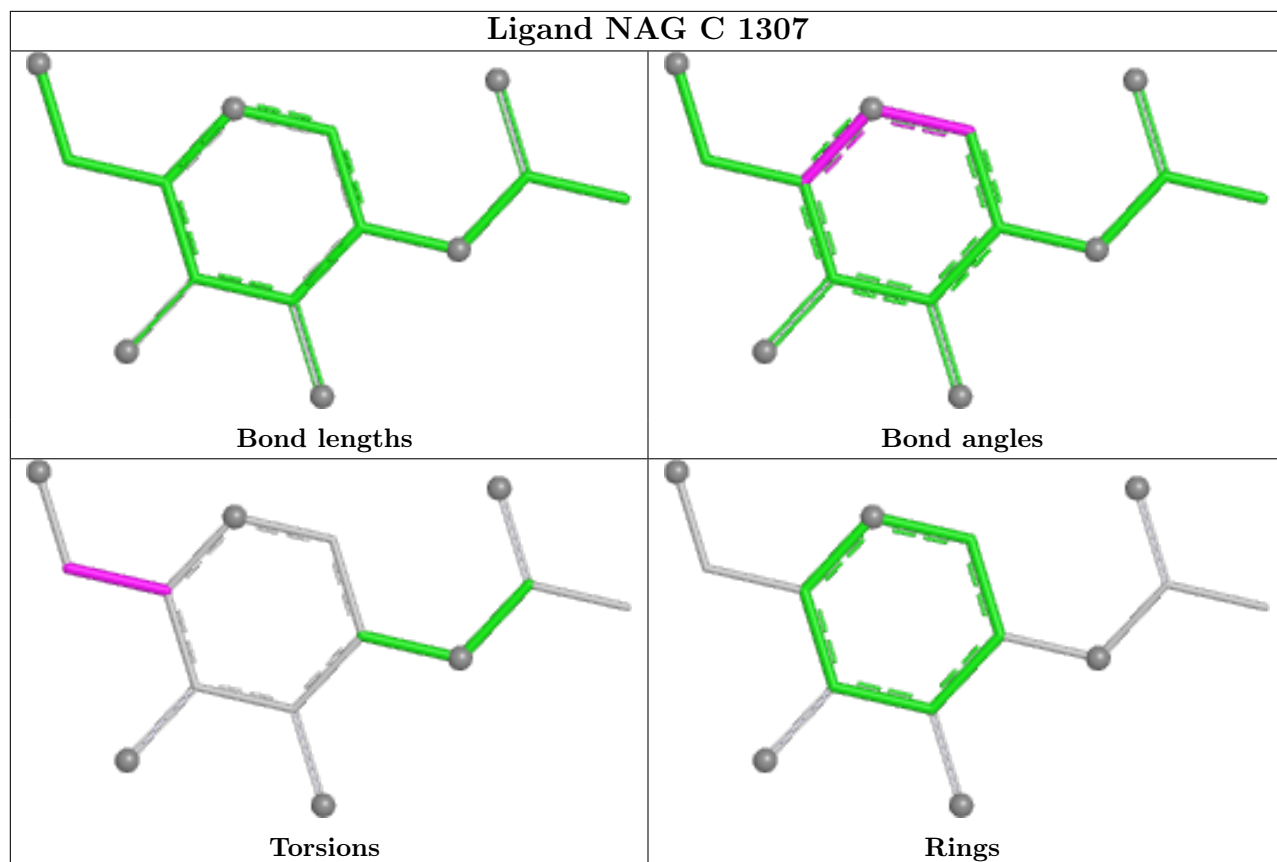


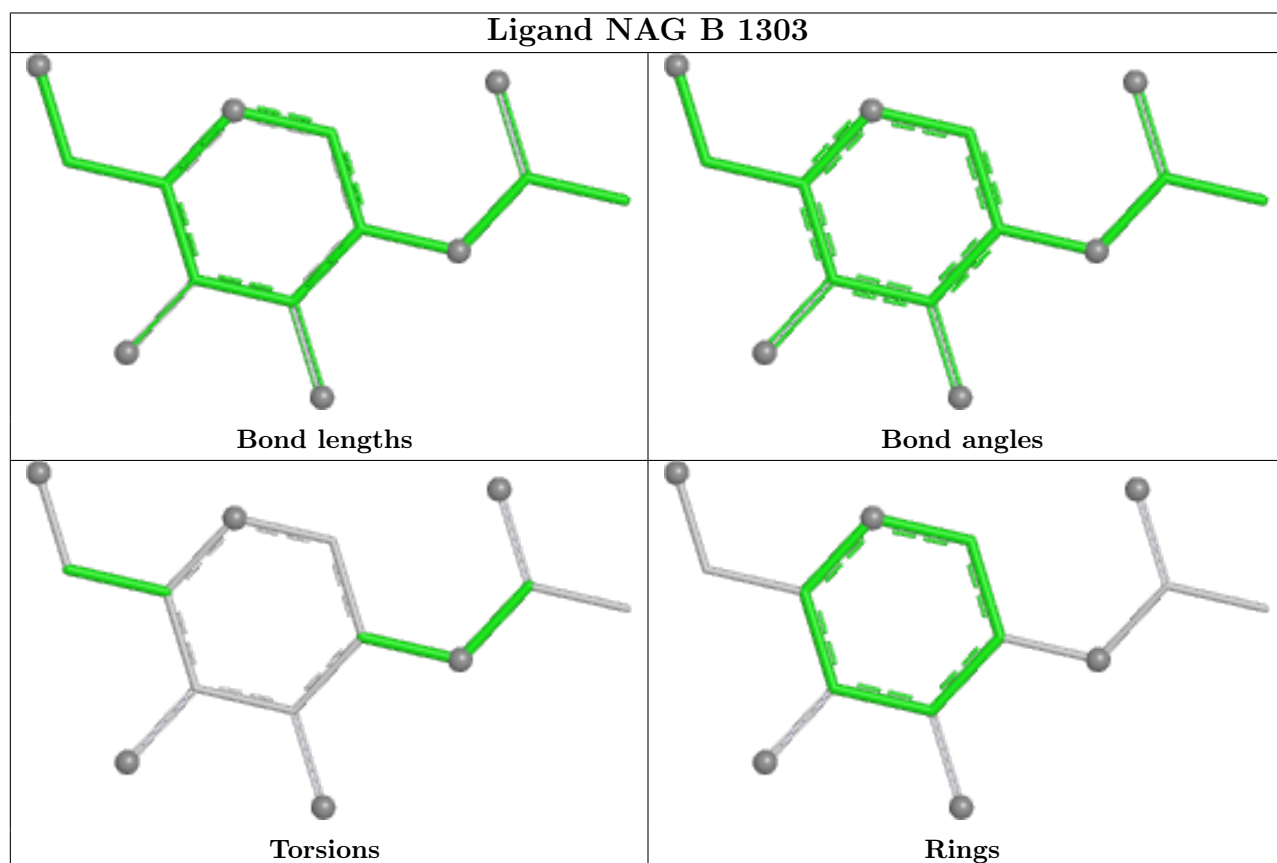
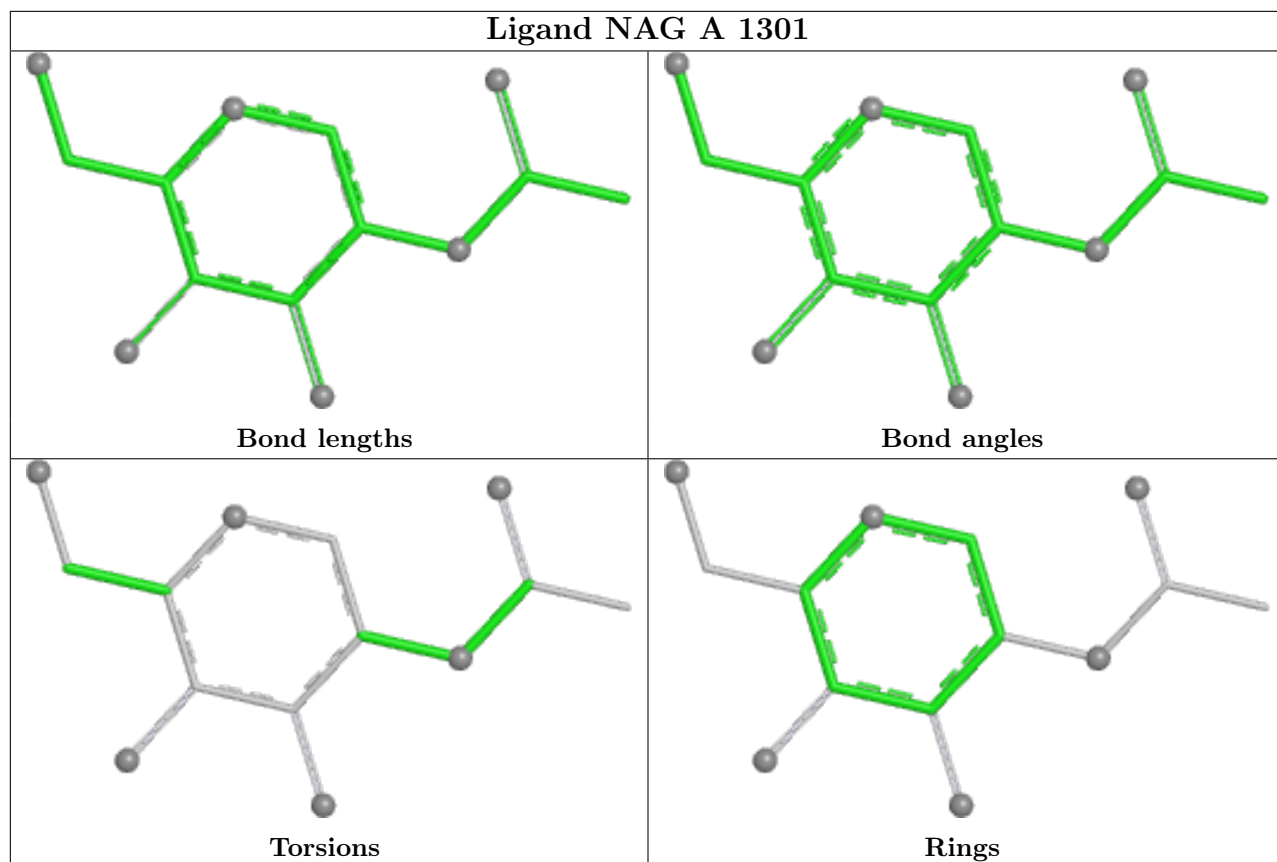


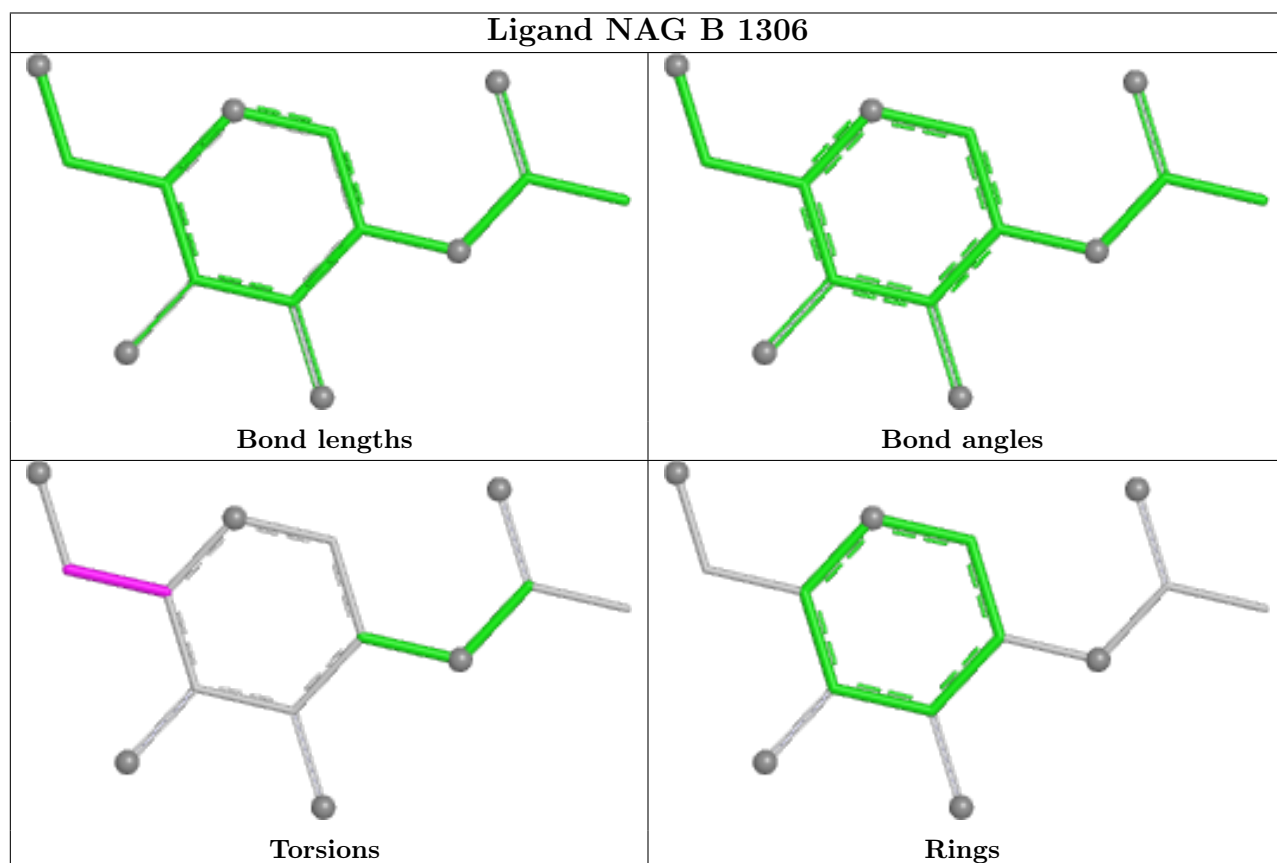
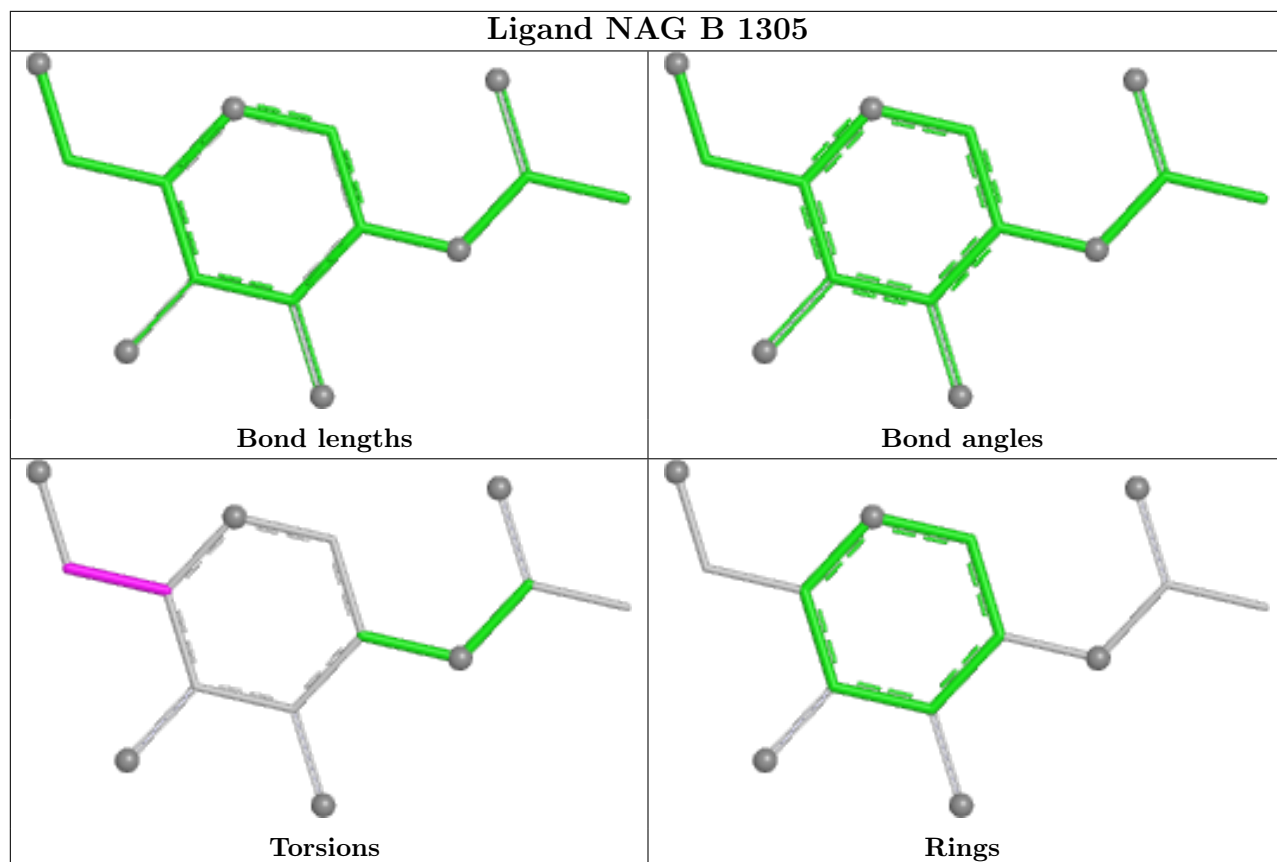


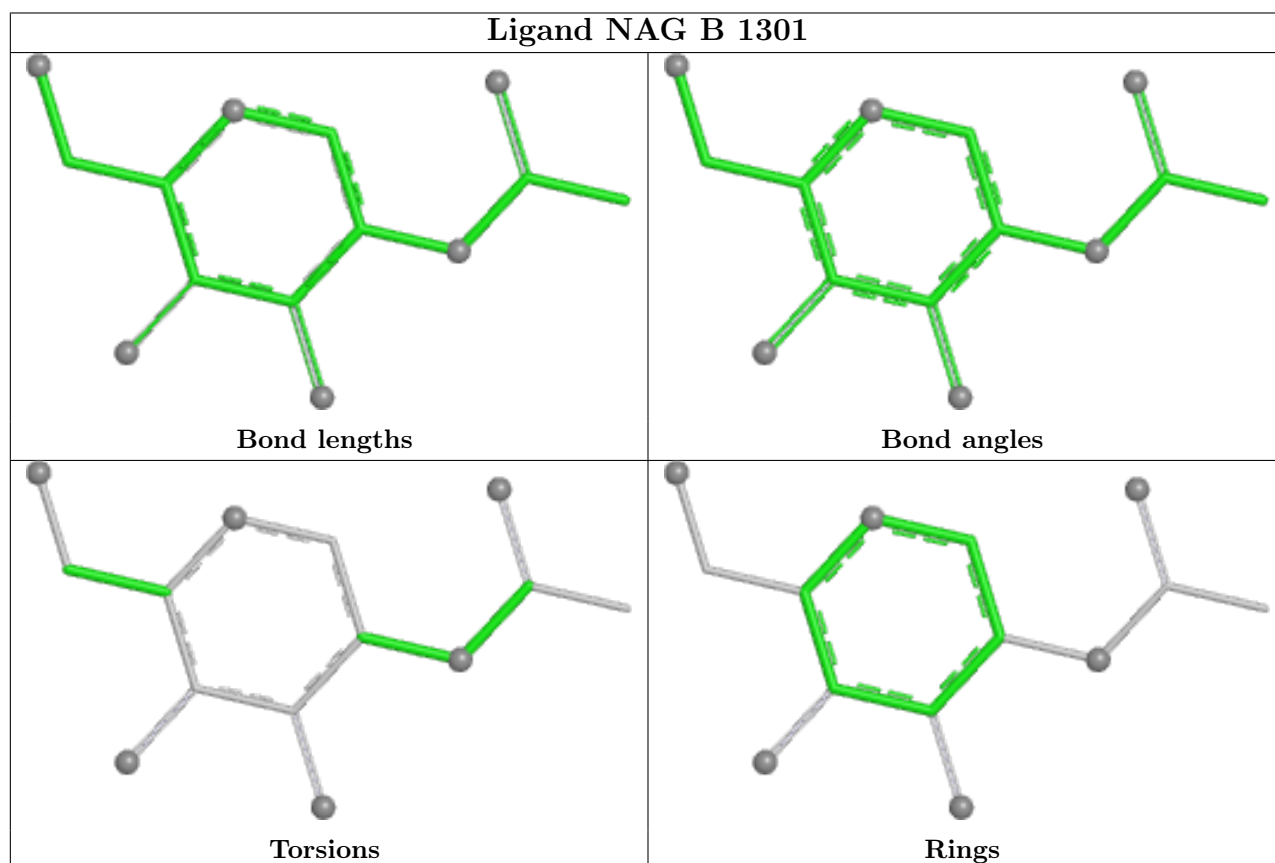
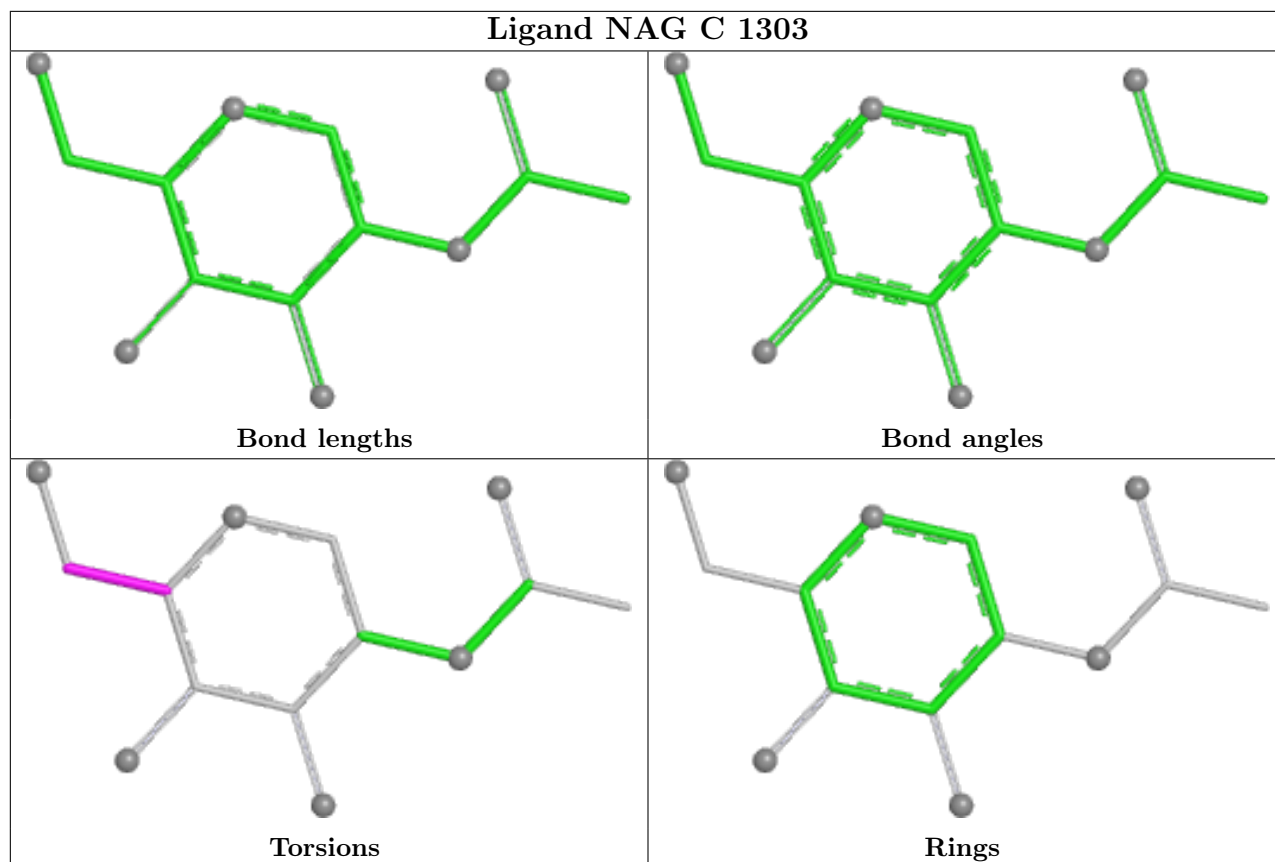


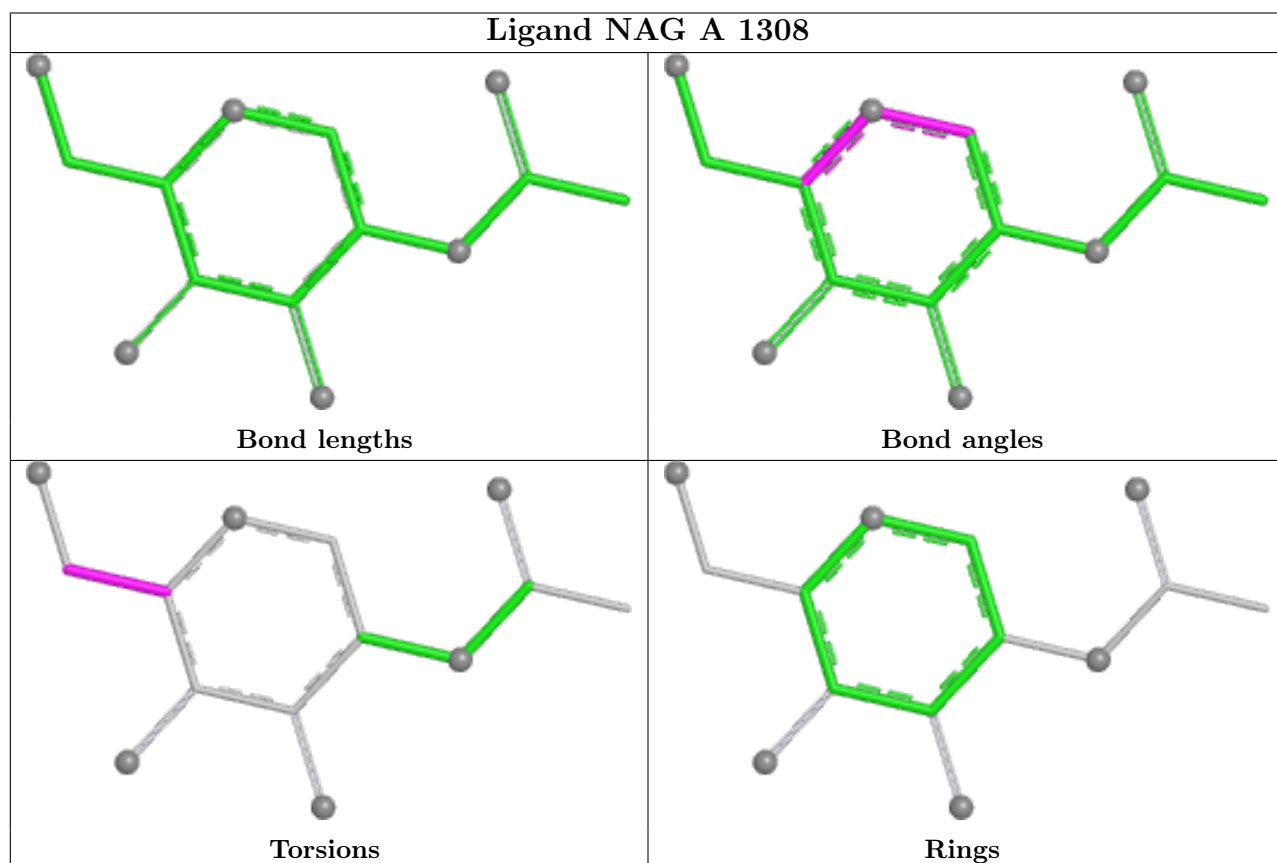
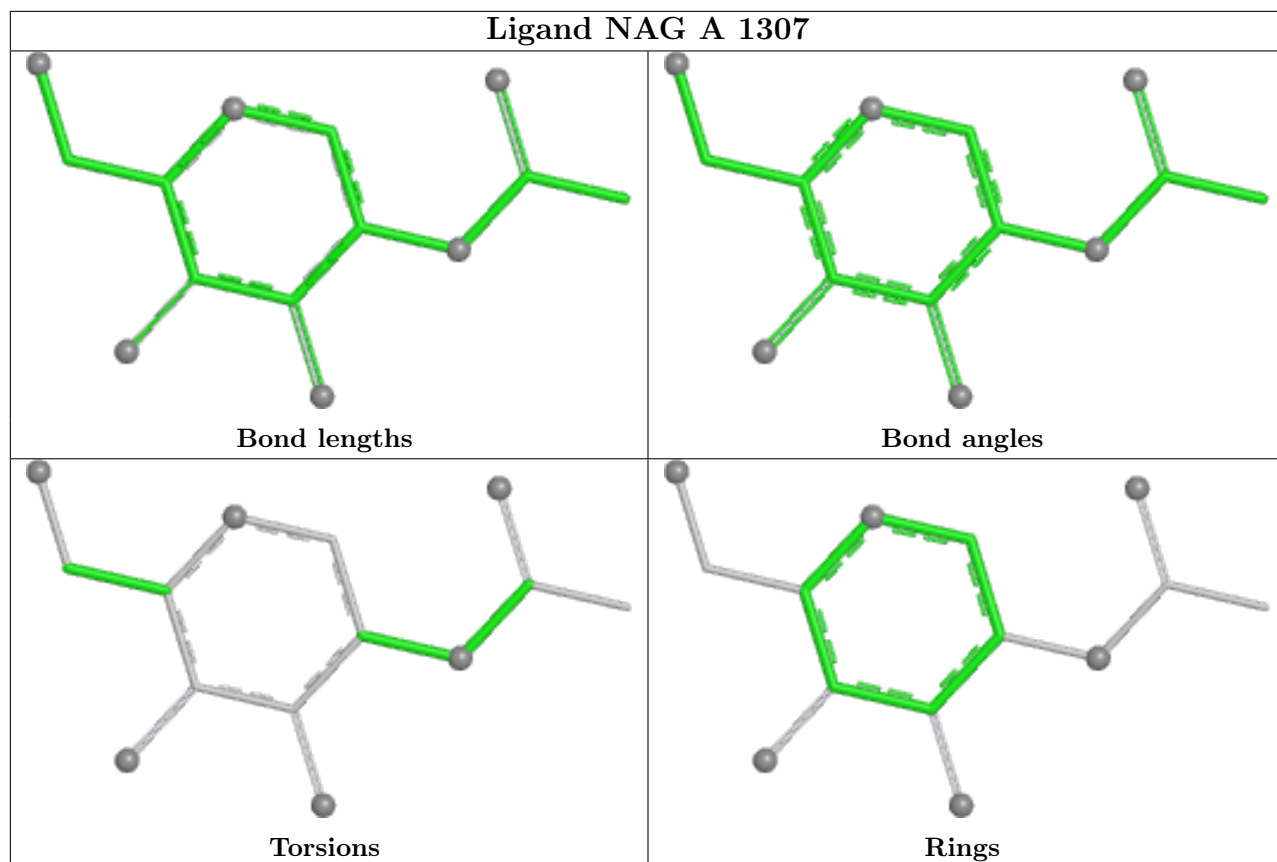


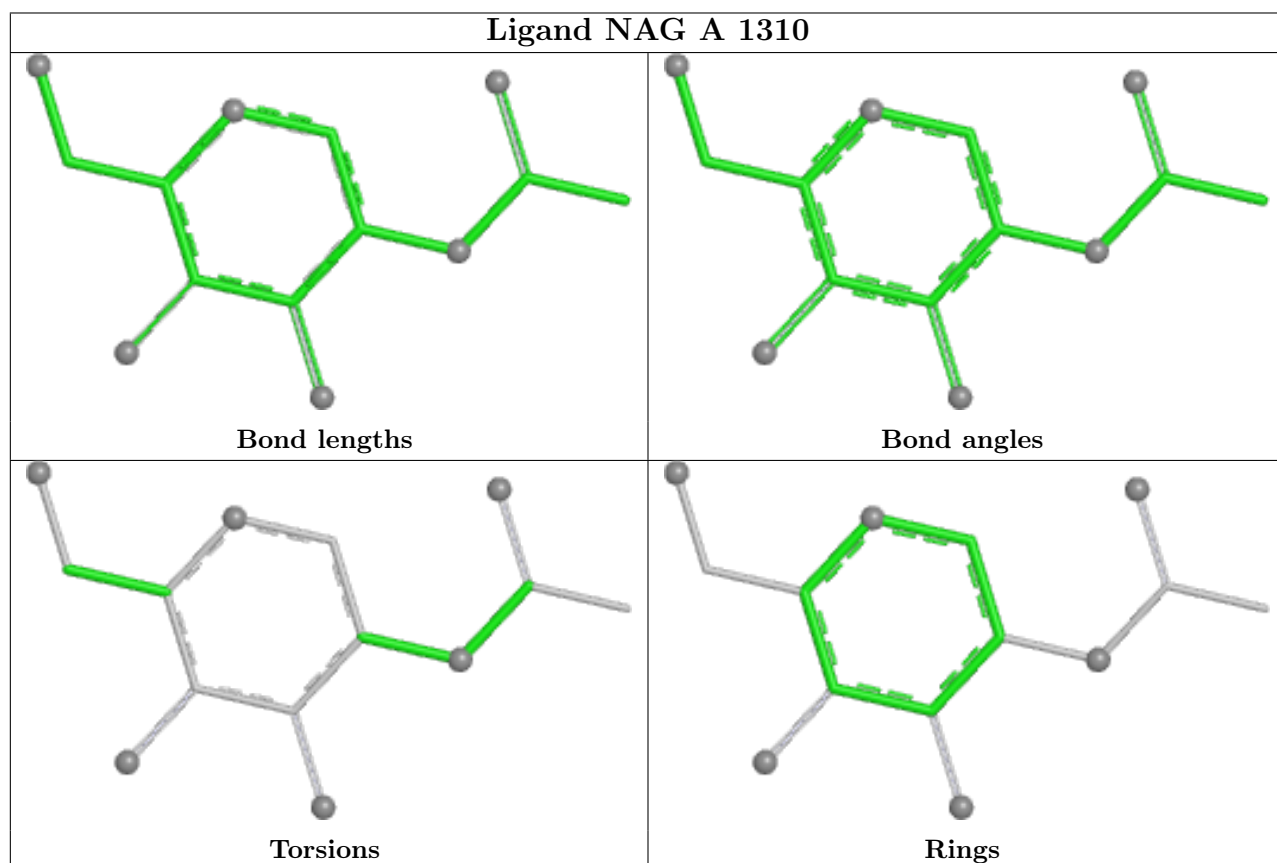
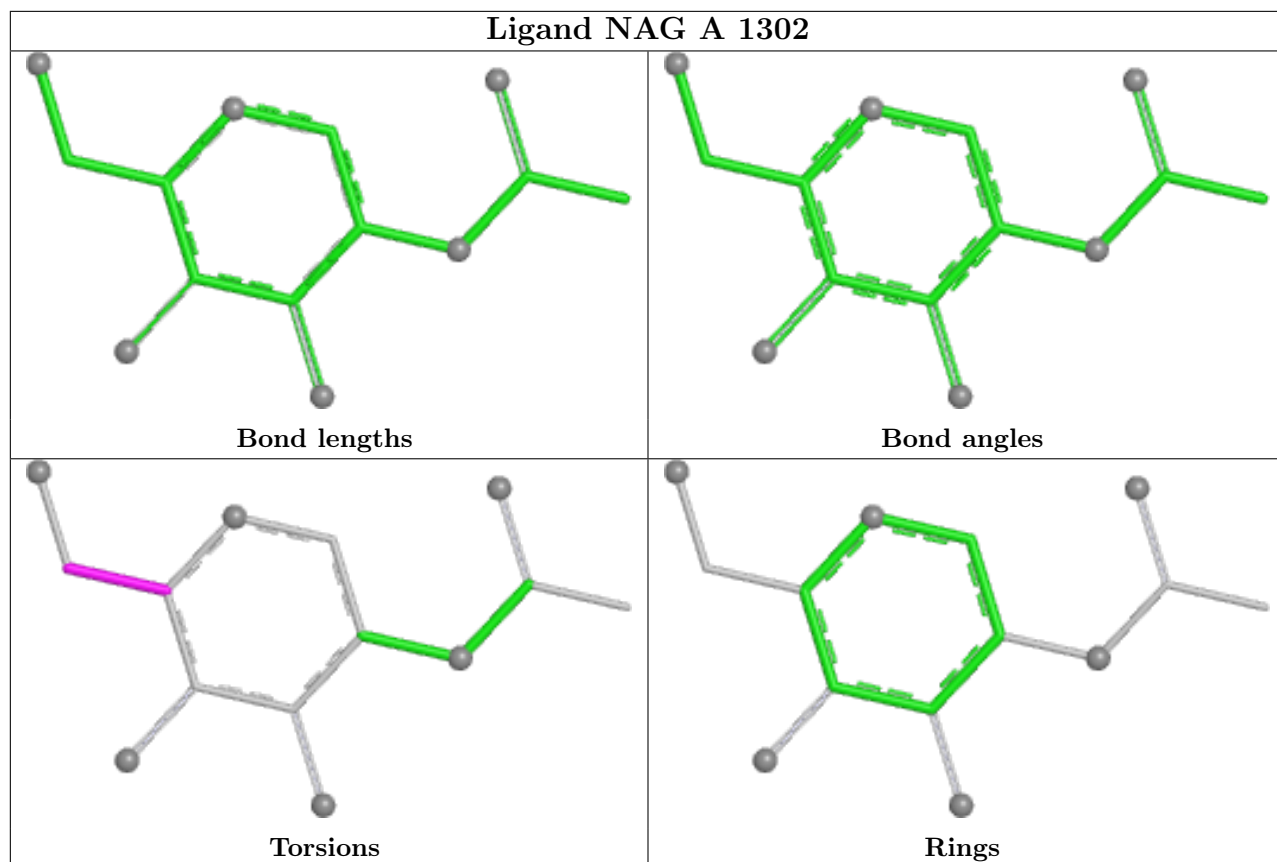


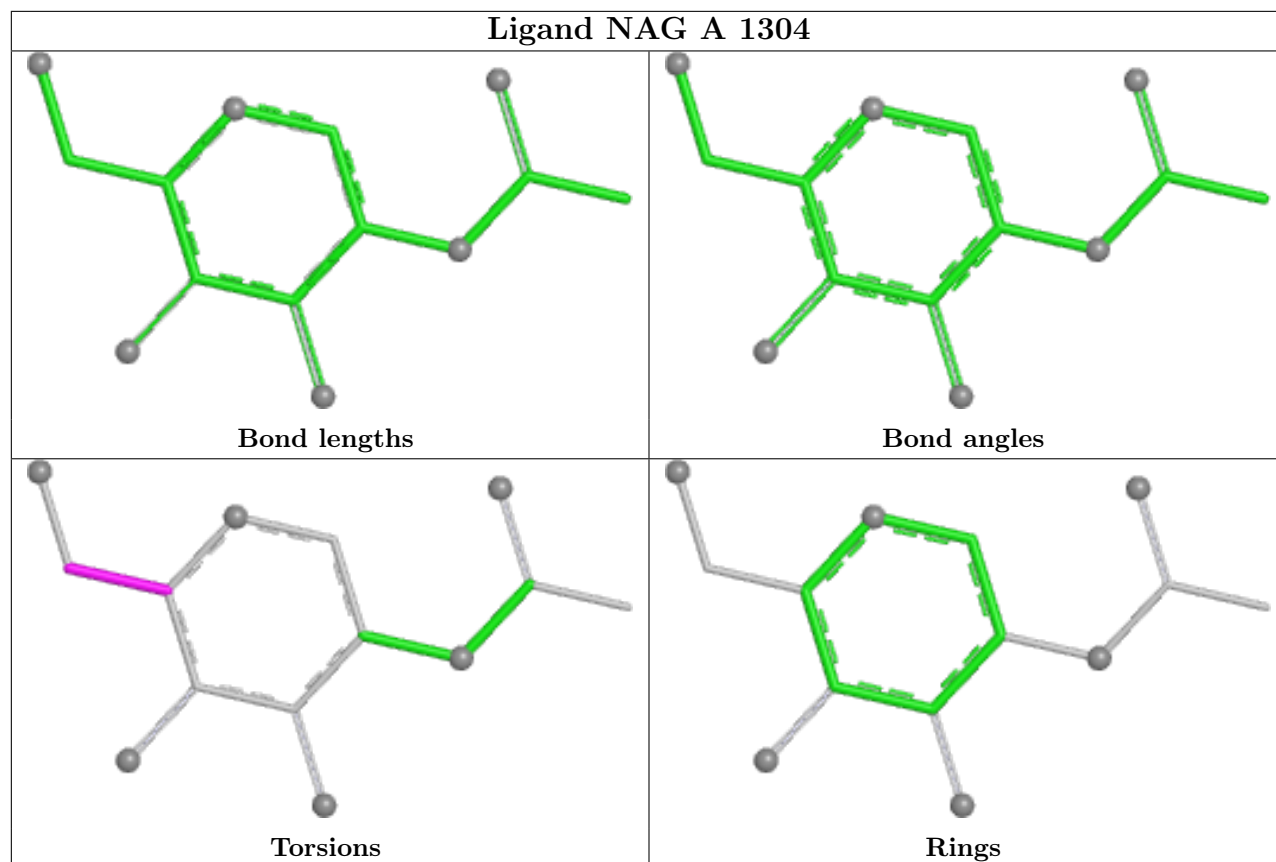












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

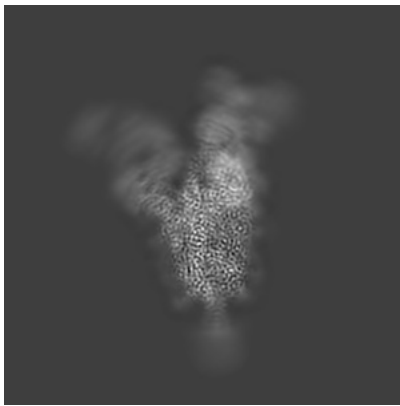
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14910. These allow visual inspection of the internal detail of the map and identification of artifacts.

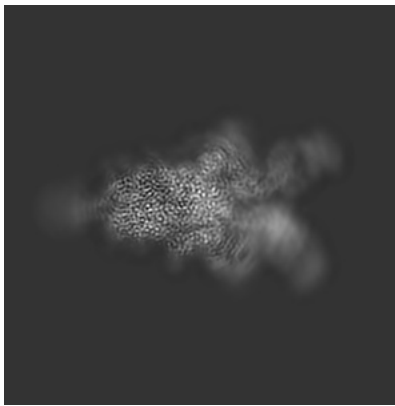
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

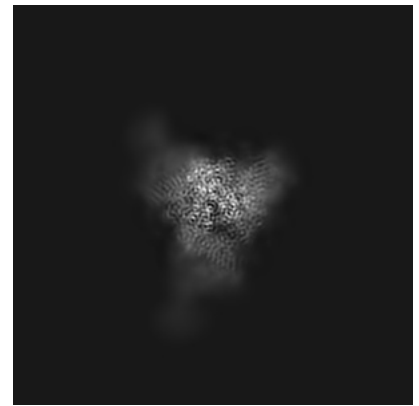
6.1.1 Primary map



X

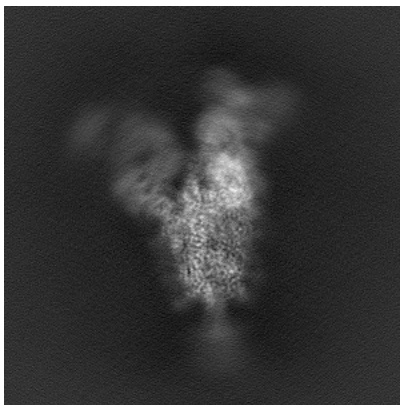


Y

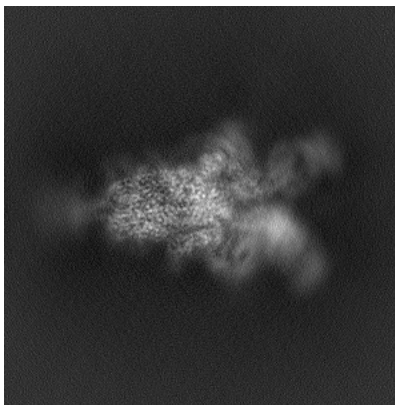


Z

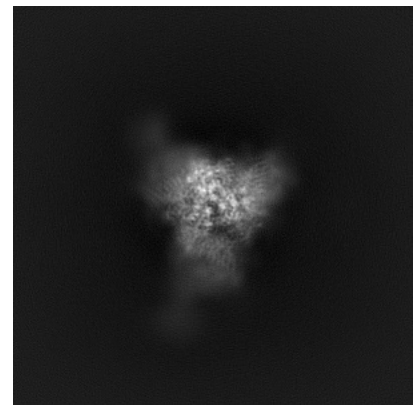
6.1.2 Raw map



X



Y

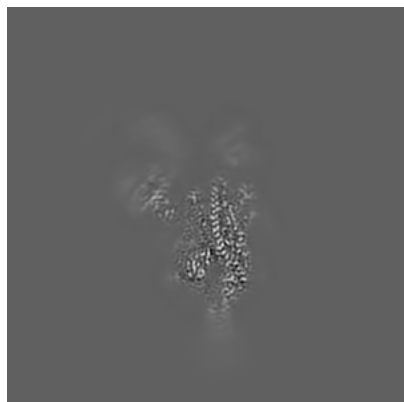


Z

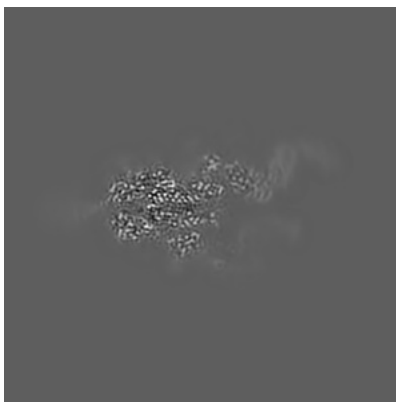
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

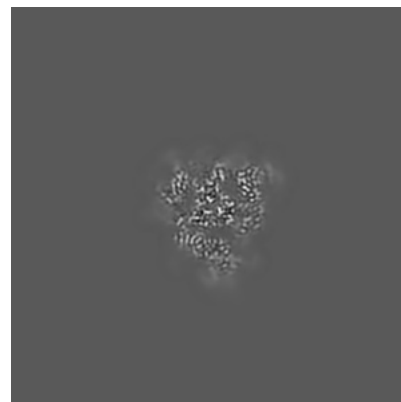
6.2.1 Primary map



X Index: 210

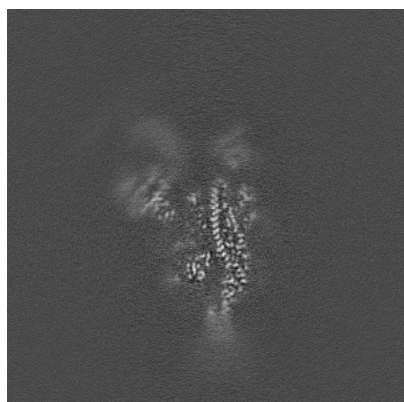


Y Index: 210

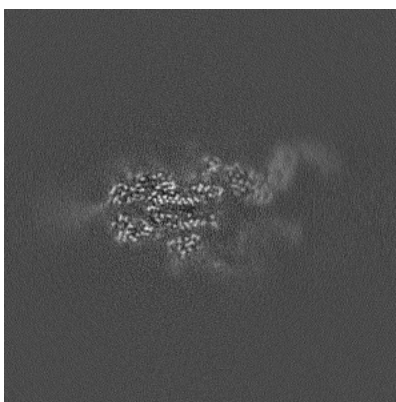


Z Index: 210

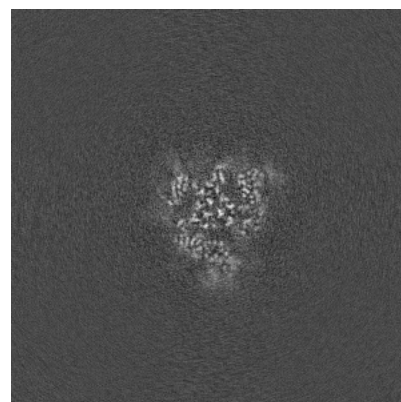
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

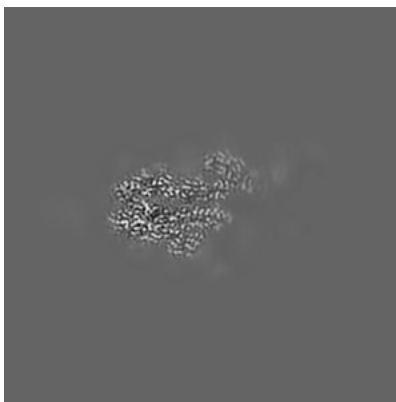
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

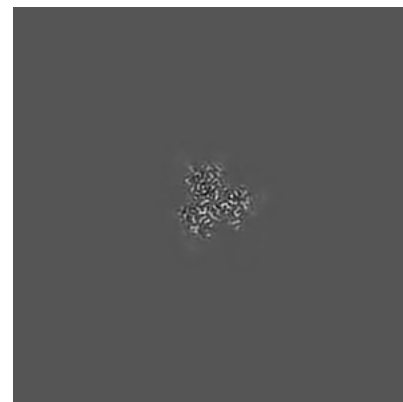
6.3.1 Primary map



X Index: 205

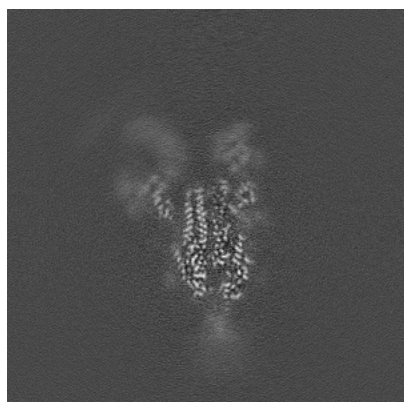


Y Index: 201

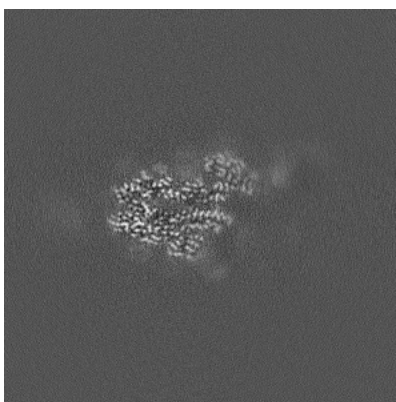


Z Index: 157

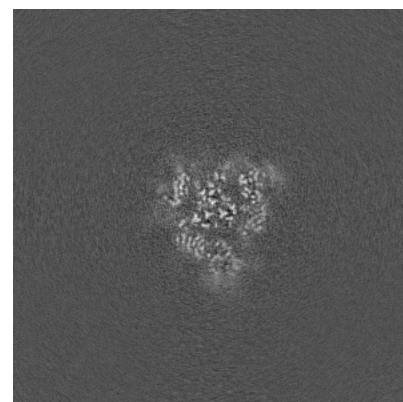
6.3.2 Raw map



X Index: 205



Y Index: 201

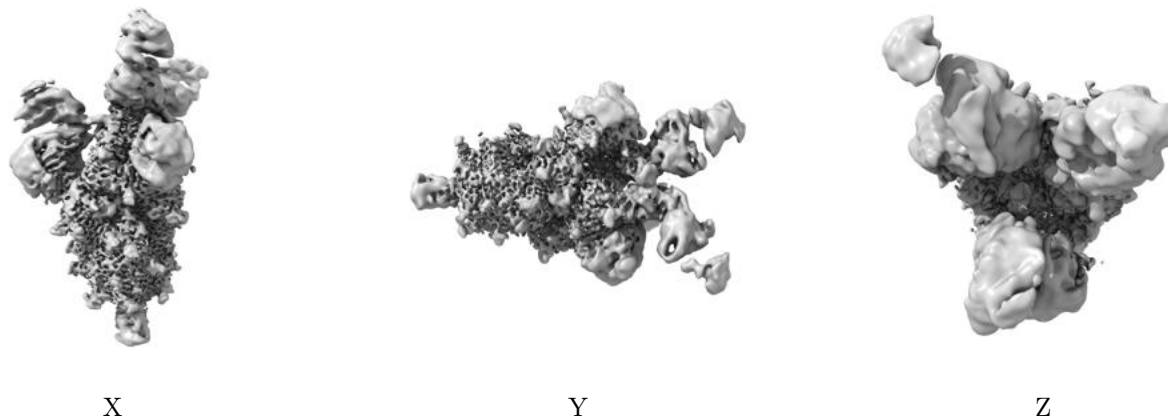


Z Index: 211

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

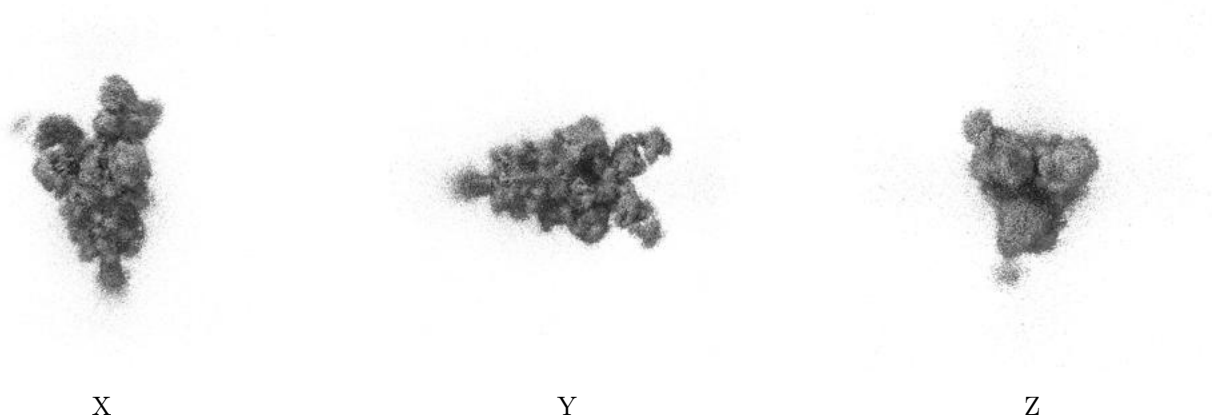
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0673. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

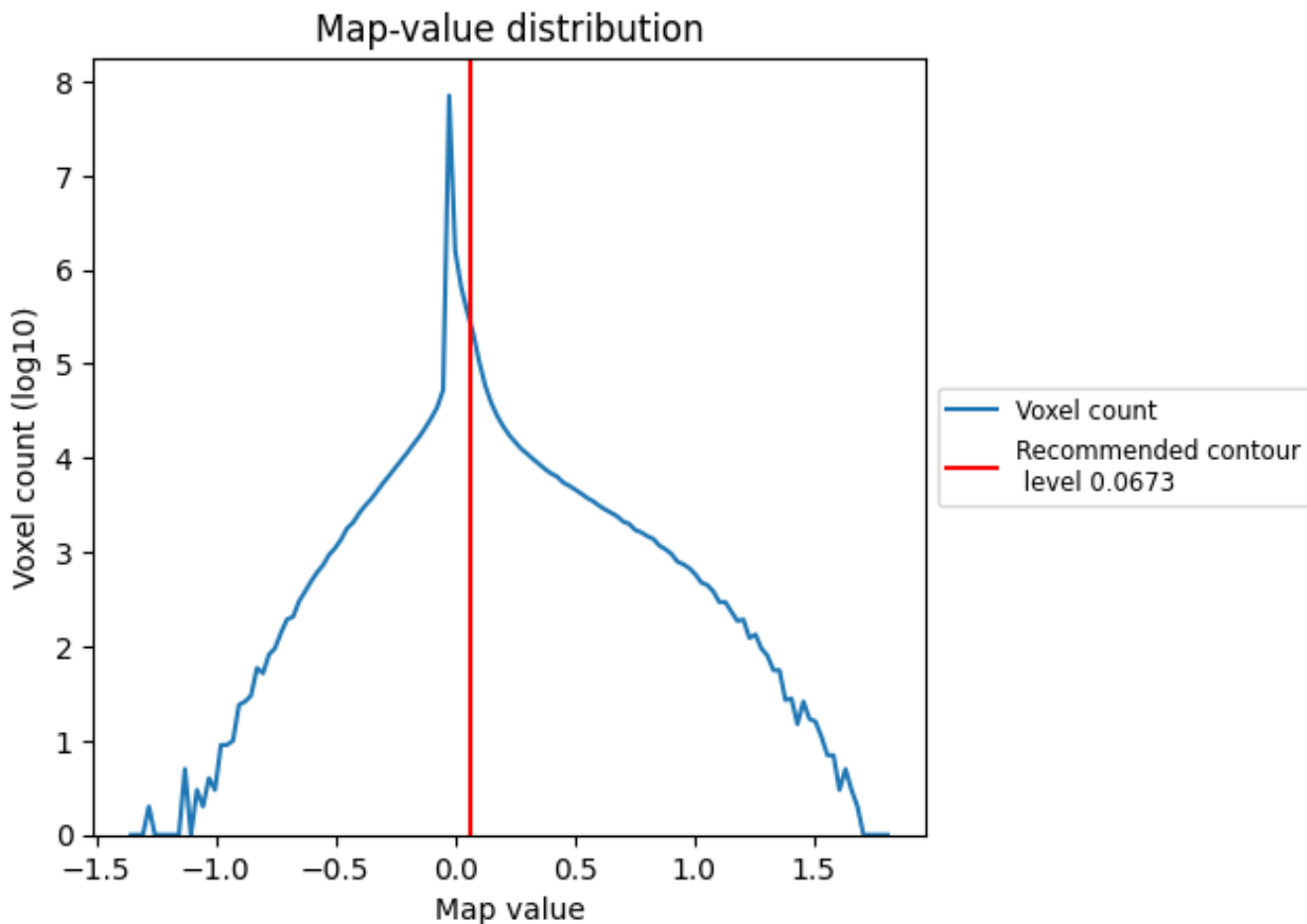
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

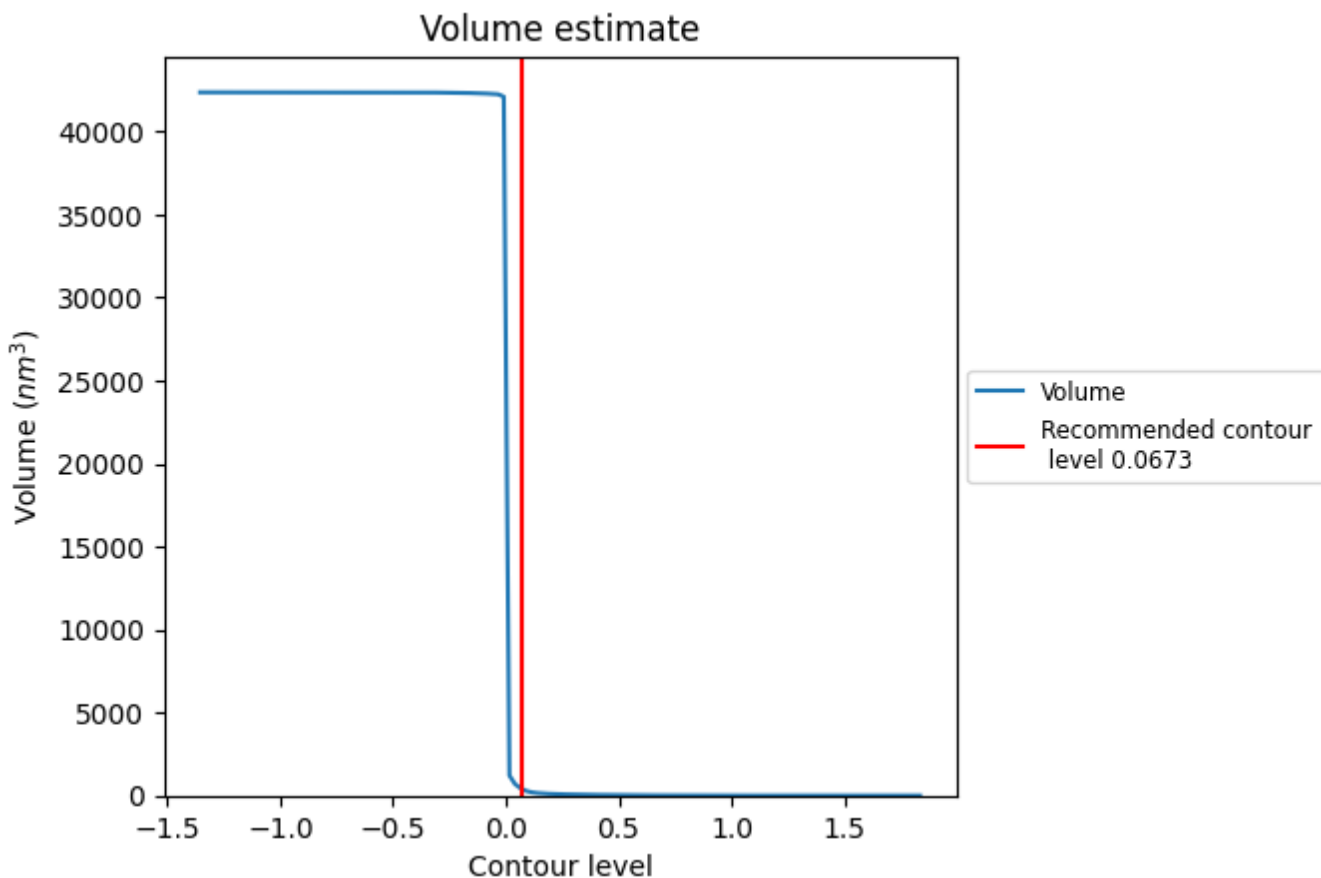
This section contains the results of statistical analysis of the map.

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.

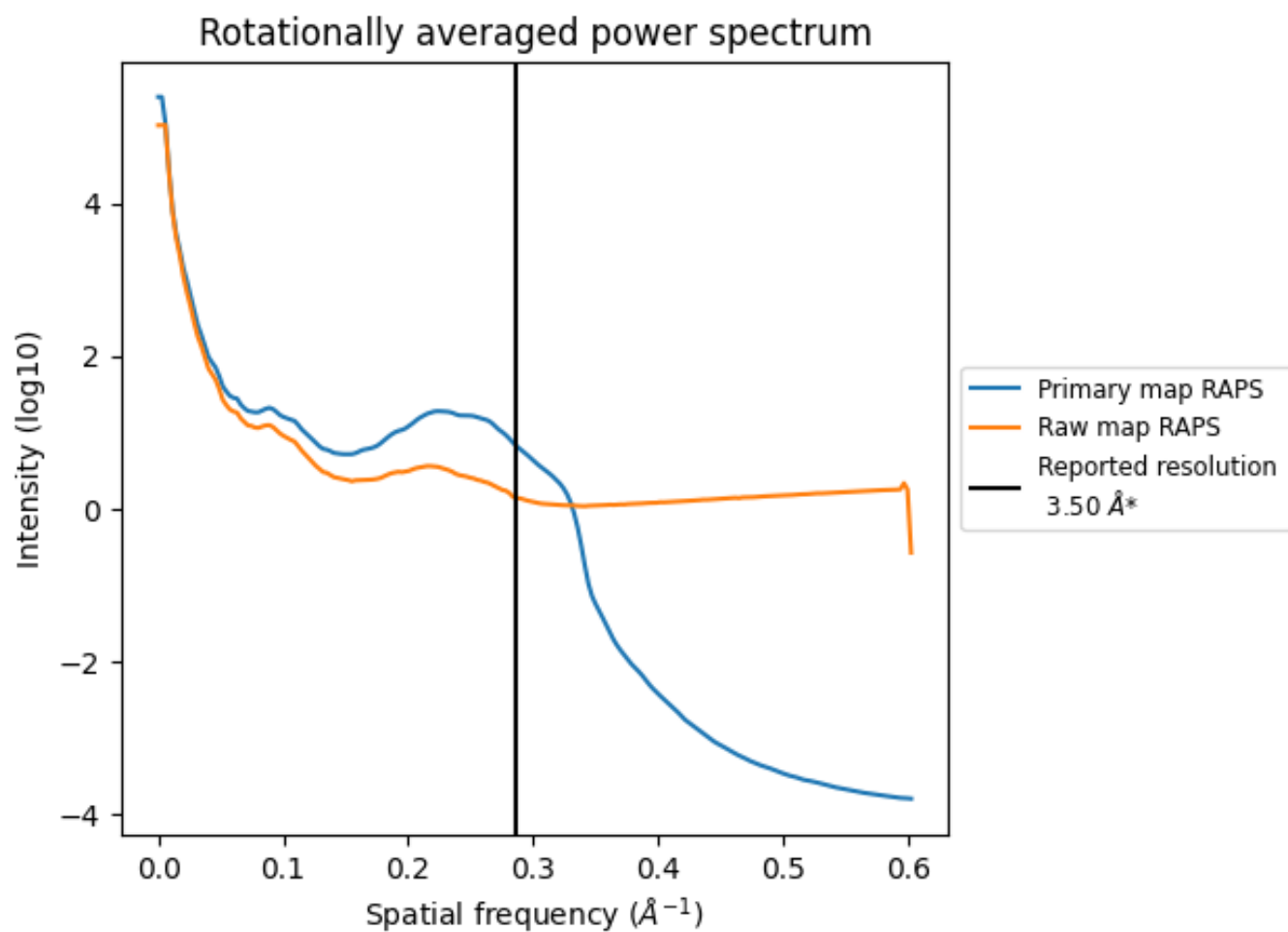
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 426 nm³; this corresponds to an approximate mass of 385 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](#)

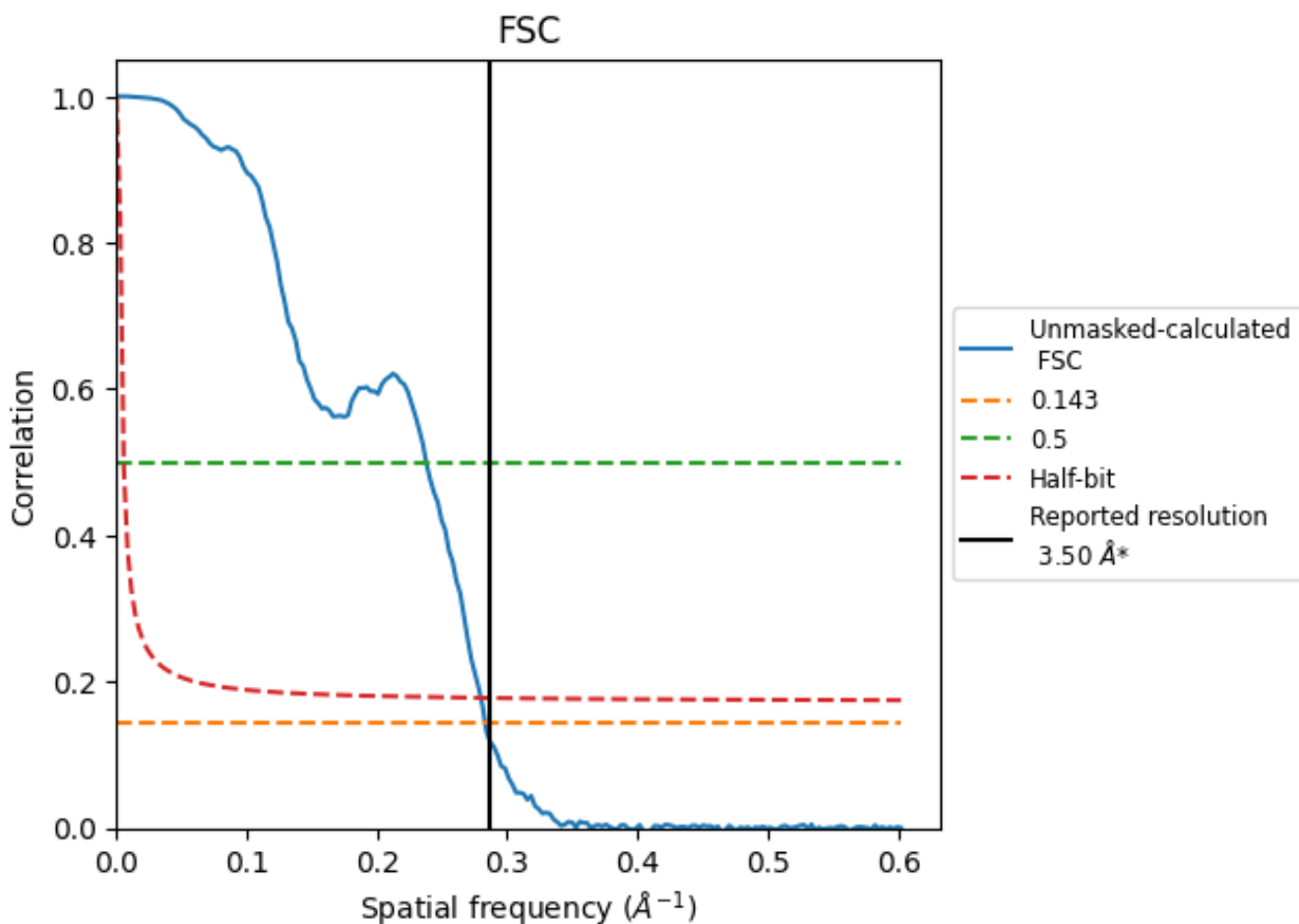


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

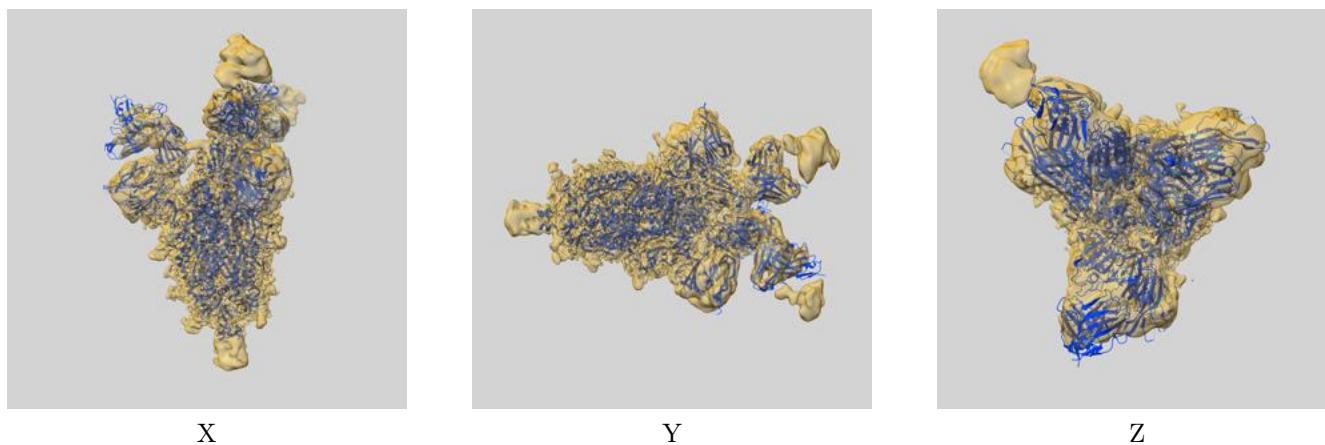
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.53	4.21	3.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

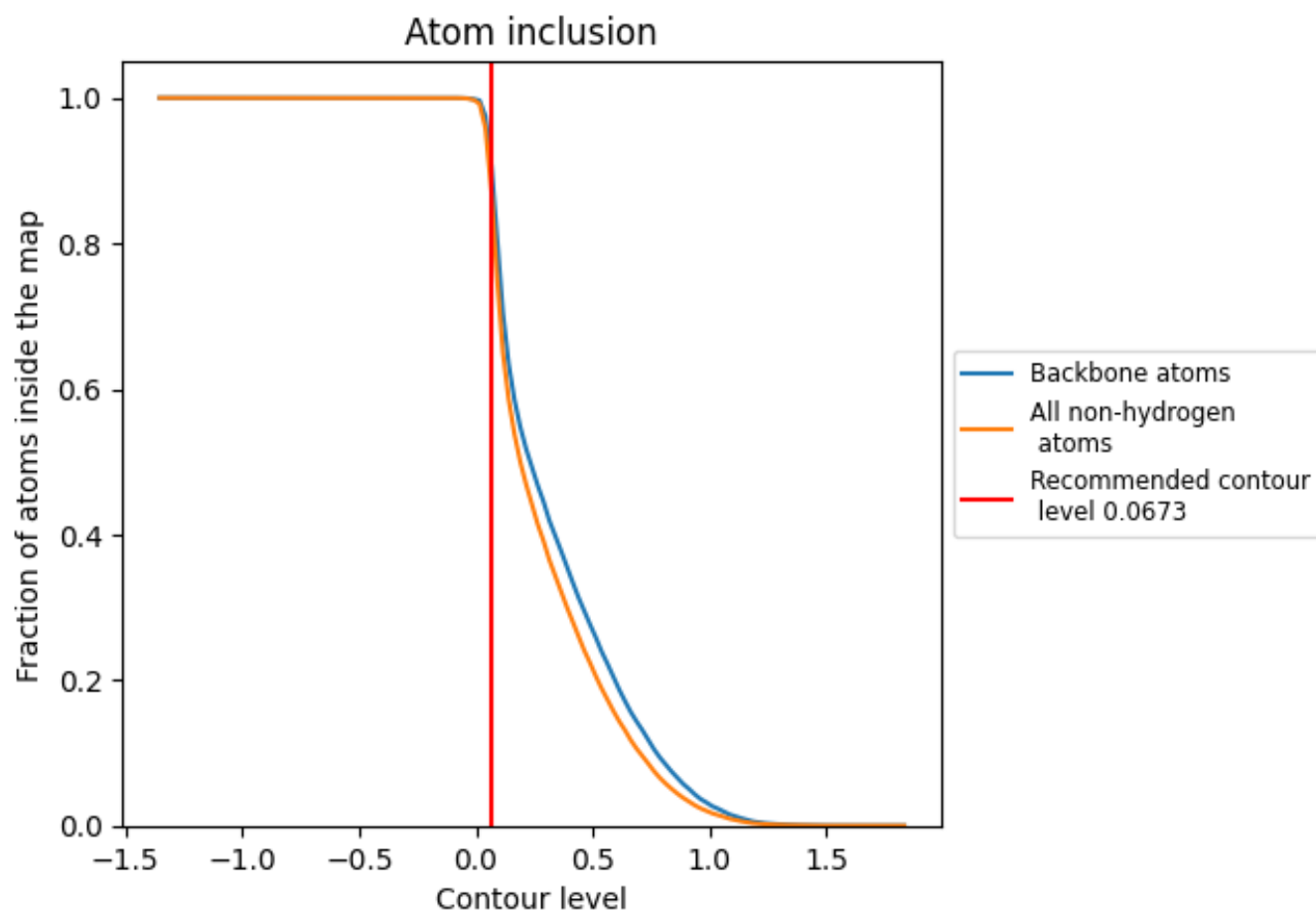
This section contains information regarding the fit between EMDB map EMD-14910 and PDB model 7ZRC. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0673 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 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.