



wwPDB EM Validation Summary Report ⓘ

Oct 15, 2024 – 05:30 AM JST

PDB ID : 8Y16
EMDB ID : EMD-38826
Title : Cryo-EM structure of SARS-CoV-2 Omicron JN.1 spike protein in complex with human ACE2
Authors : Li, L.J.; Gu, Y.H.; Qi, J.X.; Gao, G.F.
Deposited on : 2024-01-23
Resolution : 2.98 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

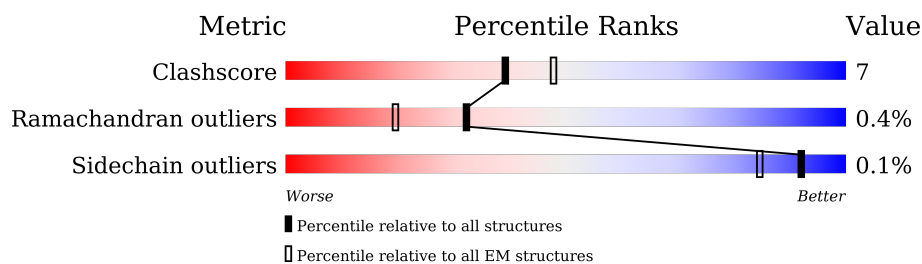
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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.




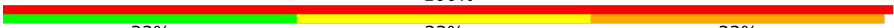

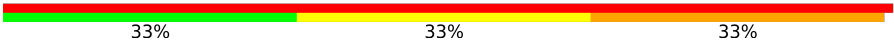

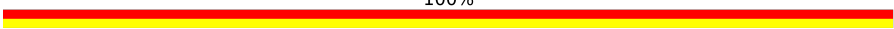
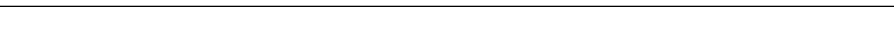
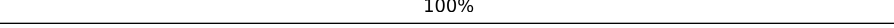
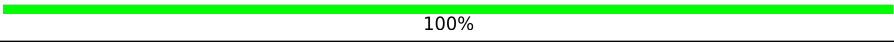


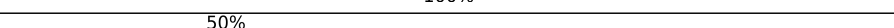
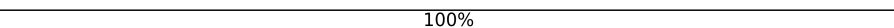
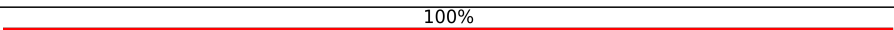

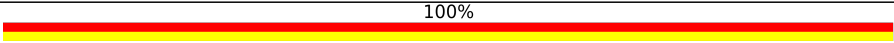
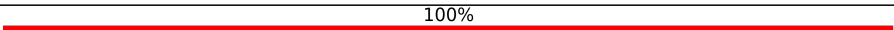
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	603	
1	E	603	
1	F	603	
2	B	1248	
2	C	1248	
2	D	1248	
3	G	3	
3	H	3	

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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 39510 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	596	Total	C	N	O	S	1	0
			4869	3116	807	917	29		
1	E	596	Total	C	N	O	S	1	0
			4869	3116	807	917	29		
1	F	596	Total	C	N	O	S	1	0
			4869	3116	807	917	29		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	HIS	-	expression tag	UNP Q9BYF1
A	617	HIS	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
E	616	HIS	-	expression tag	UNP Q9BYF1
E	617	HIS	-	expression tag	UNP Q9BYF1
E	618	HIS	-	expression tag	UNP Q9BYF1
E	619	HIS	-	expression tag	UNP Q9BYF1
E	620	HIS	-	expression tag	UNP Q9BYF1
E	621	HIS	-	expression tag	UNP Q9BYF1
F	616	HIS	-	expression tag	UNP Q9BYF1
F	617	HIS	-	expression tag	UNP Q9BYF1
F	618	HIS	-	expression tag	UNP Q9BYF1
F	619	HIS	-	expression tag	UNP Q9BYF1
F	620	HIS	-	expression tag	UNP Q9BYF1
F	621	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1001	Total 7851	C 5034	N 1302	O 1481	S 34	0	0
2	C	1015	Total 7963	C 5104	N 1318	O 1505	S 36	0	0
2	D	1016	Total 7970	C 5108	N 1319	O 1507	S 36	0	0

There are 348 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	insertion	UNP P0DTC2
B	17	PRO	ASN	variant	UNP P0DTC2
B	19	PHE	THR	variant	UNP P0DTC2
B	20	ASN	THR	variant	UNP P0DTC2
B	21	LEU	ARG	variant	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	23	THR	GLN	variant	UNP P0DTC2
B	24	THR	LEU	variant	UNP P0DTC2
B	25	THR	PRO	variant	UNP P0DTC2
B	26	GLN	PRO	variant	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	50	LEU	SER	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	variant	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	variant	UNP P0DTC2
B	158	GLY	ARG	variant	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	variant	UNP P0DTC2
B	245	ASN	HIS	variant	UNP P0DTC2
B	264	ASP	ALA	variant	UNP P0DTC2
B	332	VAL	ILE	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	356	THR	LYS	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	403	LYS	ARG	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	HIS	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	450	ASP	ASN	variant	UNP P0DTC2
B	452	TRP	LEU	variant	UNP P0DTC2
B	455	SER	LEU	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	481	LYS	ASN	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	554	LYS	GLU	variant	UNP P0DTC2
B	570	VAL	ALA	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	621	SER	PRO	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	670	VAL	ILE	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	ARG	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	939	PHE	SER	variant	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1143	LEU	PRO	variant	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	GLY	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	TYR	-	expression tag	UNP P0DTC2
B	1215	ILE	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	GLU	-	expression tag	UNP P0DTC2
B	1218	ALA	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	ASP	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLN	-	expression tag	UNP P0DTC2
B	1224	ALA	-	expression tag	UNP P0DTC2
B	1225	TYR	-	expression tag	UNP P0DTC2
B	1226	VAL	-	expression tag	UNP P0DTC2
B	1227	ARG	-	expression tag	UNP P0DTC2
B	1228	LYS	-	expression tag	UNP P0DTC2
B	1229	ASP	-	expression tag	UNP P0DTC2
B	1230	GLY	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	TRP	-	expression tag	UNP P0DTC2
B	1233	VAL	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	SER	-	expression tag	UNP P0DTC2
B	1237	THR	-	expression tag	UNP P0DTC2
B	1238	PHE	-	expression tag	UNP P0DTC2
B	1239	LEU	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	GLY	-	expression tag	UNP P0DTC2
B	1242	GLY	-	expression tag	UNP P0DTC2
B	1243	SER	-	expression tag	UNP P0DTC2
B	1244	ALA	-	expression tag	UNP P0DTC2
B	1245	TRP	-	expression tag	UNP P0DTC2
B	1246	SER	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLN	-	expression tag	UNP P0DTC2
B	1250	PHE	-	expression tag	UNP P0DTC2
B	1251	GLU	-	expression tag	UNP P0DTC2
B	1252	LYS	-	expression tag	UNP P0DTC2
C	16	MET	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	17	PRO	ASN	variant	UNP P0DTC2
C	19	PHE	THR	variant	UNP P0DTC2
C	20	ASN	THR	variant	UNP P0DTC2
C	21	LEU	ARG	variant	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	23	THR	GLN	variant	UNP P0DTC2
C	24	THR	LEU	variant	UNP P0DTC2
C	25	THR	PRO	variant	UNP P0DTC2
C	26	GLN	PRO	variant	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	50	LEU	SER	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	variant	UNP P0DTC2
C	158	GLY	ARG	variant	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	variant	UNP P0DTC2
C	245	ASN	HIS	variant	UNP P0DTC2
C	264	ASP	ALA	variant	UNP P0DTC2
C	332	VAL	ILE	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	356	THR	LYS	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	HIS	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	450	ASP	ASN	variant	UNP P0DTC2
C	452	TRP	LEU	variant	UNP P0DTC2
C	455	SER	LEU	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	481	LYS	ASN	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	554	LYS	GLU	variant	UNP P0DTC2
C	570	VAL	ALA	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	621	SER	PRO	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	670	VAL	ILE	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	939	PHE	SER	variant	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1143	LEU	PRO	variant	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	GLY	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	TYR	-	expression tag	UNP P0DTC2
C	1215	ILE	-	expression tag	UNP P0DTC2
C	1216	PRO	-	expression tag	UNP P0DTC2
C	1217	GLU	-	expression tag	UNP P0DTC2
C	1218	ALA	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLN	-	expression tag	UNP P0DTC2
C	1224	ALA	-	expression tag	UNP P0DTC2
C	1225	TYR	-	expression tag	UNP P0DTC2
C	1226	VAL	-	expression tag	UNP P0DTC2
C	1227	ARG	-	expression tag	UNP P0DTC2
C	1228	LYS	-	expression tag	UNP P0DTC2
C	1229	ASP	-	expression tag	UNP P0DTC2
C	1230	GLY	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	TRP	-	expression tag	UNP P0DTC2
C	1233	VAL	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	SER	-	expression tag	UNP P0DTC2
C	1237	THR	-	expression tag	UNP P0DTC2
C	1238	PHE	-	expression tag	UNP P0DTC2
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	GLY	-	expression tag	UNP P0DTC2
C	1242	GLY	-	expression tag	UNP P0DTC2
C	1243	SER	-	expression tag	UNP P0DTC2
C	1244	ALA	-	expression tag	UNP P0DTC2
C	1245	TRP	-	expression tag	UNP P0DTC2
C	1246	SER	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLN	-	expression tag	UNP P0DTC2
C	1250	PHE	-	expression tag	UNP P0DTC2
C	1251	GLU	-	expression tag	UNP P0DTC2
C	1252	LYS	-	expression tag	UNP P0DTC2
D	16	MET	-	insertion	UNP P0DTC2
D	17	PRO	ASN	variant	UNP P0DTC2
D	19	PHE	THR	variant	UNP P0DTC2
D	20	ASN	THR	variant	UNP P0DTC2
D	21	LEU	ARG	variant	UNP P0DTC2
D	22	ILE	THR	variant	UNP P0DTC2
D	23	THR	GLN	variant	UNP P0DTC2
D	24	THR	LEU	acetylation	UNP P0DTC2
D	25	THR	PRO	variant	UNP P0DTC2
D	26	GLN	PRO	variant	UNP P0DTC2
D	27	SER	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	50	LEU	SER	variant	UNP P0DTC2
D	?	-	HIS	deletion	UNP P0DTC2
D	?	-	VAL	deletion	UNP P0DTC2
D	127	PHE	VAL	variant	UNP P0DTC2
D	142	ASP	GLY	variant	UNP P0DTC2
D	?	-	TYR	deletion	UNP P0DTC2
D	157	SER	PHE	variant	UNP P0DTC2
D	158	GLY	ARG	variant	UNP P0DTC2
D	?	-	ASN	deletion	UNP P0DTC2
D	212	ILE	LEU	variant	UNP P0DTC2
D	213	GLY	VAL	variant	UNP P0DTC2
D	216	PHE	LEU	variant	UNP P0DTC2
D	245	ASN	HIS	variant	UNP P0DTC2
D	264	ASP	ALA	variant	UNP P0DTC2
D	332	VAL	ILE	variant	UNP P0DTC2
D	339	HIS	GLY	variant	UNP P0DTC2
D	356	THR	LYS	variant	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	376	ALA	THR	variant	UNP P0DTC2
D	403	LYS	ARG	variant	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	445	HIS	VAL	variant	UNP P0DTC2
D	446	SER	GLY	variant	UNP P0DTC2
D	450	ASP	ASN	variant	UNP P0DTC2
D	452	TRP	LEU	variant	UNP P0DTC2
D	455	SER	LEU	variant	UNP P0DTC2
D	460	LYS	ASN	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	481	LYS	ASN	variant	UNP P0DTC2
D	?	-	VAL	deletion	UNP P0DTC2
D	484	LYS	GLU	variant	UNP P0DTC2
D	486	PRO	PHE	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2
D	554	LYS	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	570	VAL	ALA	variant	UNP P0DTC2
D	614	GLY	ASP	variant	UNP P0DTC2
D	621	SER	PRO	variant	UNP P0DTC2
D	655	TYR	HIS	variant	UNP P0DTC2
D	670	VAL	ILE	variant	UNP P0DTC2
D	679	LYS	ASN	variant	UNP P0DTC2
D	681	ARG	PRO	variant	UNP P0DTC2
D	764	LYS	ASN	variant	UNP P0DTC2
D	796	TYR	ASP	variant	UNP P0DTC2
D	817	PRO	PHE	engineered mutation	UNP P0DTC2
D	892	PRO	ALA	engineered mutation	UNP P0DTC2
D	899	PRO	ALA	engineered mutation	UNP P0DTC2
D	939	PHE	SER	variant	UNP P0DTC2
D	942	PRO	ALA	engineered mutation	UNP P0DTC2
D	954	HIS	GLN	variant	UNP P0DTC2
D	969	LYS	ASN	variant	UNP P0DTC2
D	986	PRO	LYS	engineered mutation	UNP P0DTC2
D	987	PRO	VAL	engineered mutation	UNP P0DTC2
D	1143	LEU	PRO	variant	UNP P0DTC2
D	1209	GLY	-	expression tag	UNP P0DTC2
D	1210	GLY	-	expression tag	UNP P0DTC2
D	1211	GLY	-	expression tag	UNP P0DTC2
D	1212	SER	-	expression tag	UNP P0DTC2
D	1213	GLY	-	expression tag	UNP P0DTC2
D	1214	TYR	-	expression tag	UNP P0DTC2
D	1215	ILE	-	expression tag	UNP P0DTC2
D	1216	PRO	-	expression tag	UNP P0DTC2
D	1217	GLU	-	expression tag	UNP P0DTC2
D	1218	ALA	-	expression tag	UNP P0DTC2
D	1219	PRO	-	expression tag	UNP P0DTC2
D	1220	ARG	-	expression tag	UNP P0DTC2
D	1221	ASP	-	expression tag	UNP P0DTC2
D	1222	GLY	-	expression tag	UNP P0DTC2
D	1223	GLN	-	expression tag	UNP P0DTC2
D	1224	ALA	-	expression tag	UNP P0DTC2
D	1225	TYR	-	expression tag	UNP P0DTC2
D	1226	VAL	-	expression tag	UNP P0DTC2
D	1227	ARG	-	expression tag	UNP P0DTC2
D	1228	LYS	-	expression tag	UNP P0DTC2
D	1229	ASP	-	expression tag	UNP P0DTC2
D	1230	GLY	-	expression tag	UNP P0DTC2
D	1231	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1232	TRP	-	expression tag	UNP P0DTC2
D	1233	VAL	-	expression tag	UNP P0DTC2
D	1234	LEU	-	expression tag	UNP P0DTC2
D	1235	LEU	-	expression tag	UNP P0DTC2
D	1236	SER	-	expression tag	UNP P0DTC2
D	1237	THR	-	expression tag	UNP P0DTC2
D	1238	PHE	-	expression tag	UNP P0DTC2
D	1239	LEU	-	expression tag	UNP P0DTC2
D	1240	GLY	-	expression tag	UNP P0DTC2
D	1241	GLY	-	expression tag	UNP P0DTC2
D	1242	GLY	-	expression tag	UNP P0DTC2
D	1243	SER	-	expression tag	UNP P0DTC2
D	1244	ALA	-	expression tag	UNP P0DTC2
D	1245	TRP	-	expression tag	UNP P0DTC2
D	1246	SER	-	expression tag	UNP P0DTC2
D	1247	HIS	-	expression tag	UNP P0DTC2
D	1248	PRO	-	expression tag	UNP P0DTC2
D	1249	GLN	-	expression tag	UNP P0DTC2
D	1250	PHE	-	expression tag	UNP P0DTC2
D	1251	GLU	-	expression tag	UNP P0DTC2
D	1252	LYS	-	expression tag	UNP P0DTC2

- Molecule 3 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
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	R	3	Total	C	N	O	0	0
			39	22	2	15		
3	S	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	W	3	Total	C	N	O	0	0
			39	22	2	15		

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

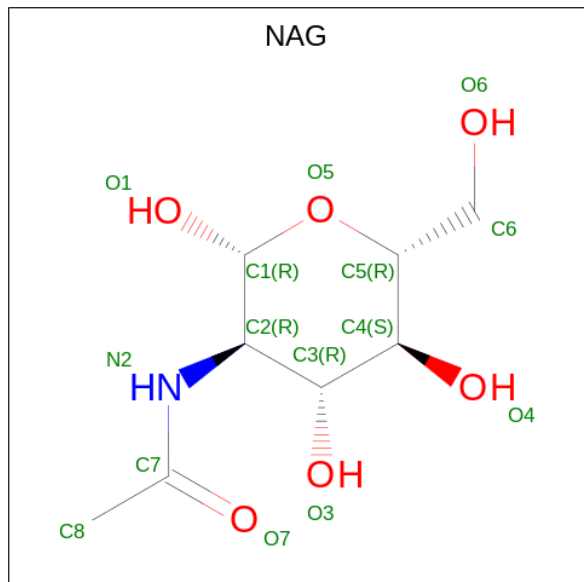


Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	F	1	Total	Zn	0
			1	1	

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

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

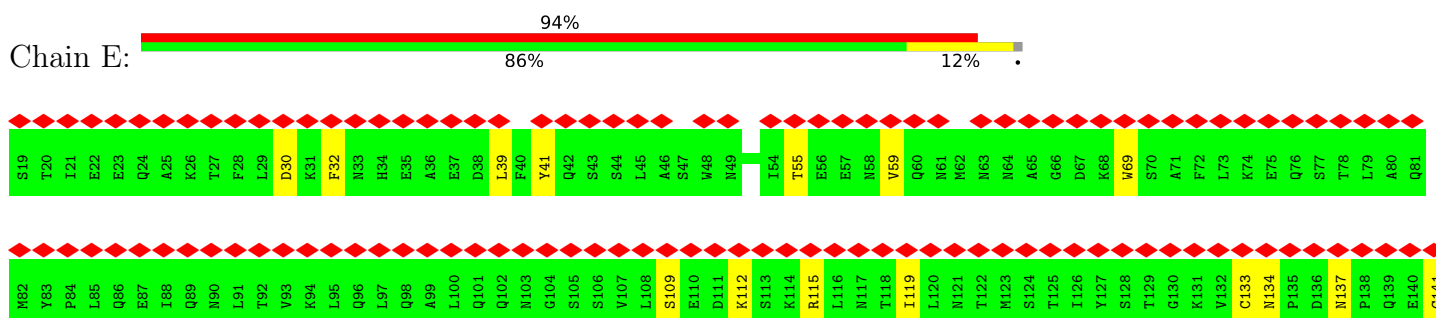
3 Residue-property plots

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: Angiotensin-converting enzyme 2




• Molecule 1: Angiotensin-converting enzyme 2



A569	L570	E571	N572	V573	W574	G575	A576	E577	N578	W579	N580	W581	R582	P583	L584	L585	N586	Y587	F588	E589	P590	L591	F592	T593	W594	L595	K596	D597	Q598	N599	K600	N601	S602	F603	V604	G605	W606	S607	T608	D609	W610	S611	P612	W613	A614	ASP	HIS	HIS	HIS	HIS	HIS	HIS										
D509	Y510	S511	F512	L513	R514	Y515	Y516	T517	R518	T519	L520	Y521	Q522	F523	Q524	F525	K465	Q526	E527	A528	L529	C530	Q531	D471	Q472	W473	W474	H535	E536	G537	P538	L539	H540	K541	C542	D543	I544	S545	N546	S547	T548	E549	A550	G551	Q552	K553	L554	F555	N556	M557	L558	R559	L560	G561	S562	S563	E564	P565	W566	T567	L568	
T449	L450	P451	F452	T453	V454	M455	L456	E457	K458	W459	R460	W461	M462	V463	F464	K465	G466	E467	I468	P469	K470	D471	Q472	W473	W474	K475	K476	W477	W478	E479	M480	K481	R482	E483	I484	V485	G486	W487	V488	E489	P490	V491	P492	H493	D494	E495	T496	Y497	C498	D499	P500	A501	S502	L503	F504	H505	W506	S507	N508			
P389	F390	L391	L392	R393	N394	G395	A396	N397	E398	G399	F400	H401	E402	A403	V404	G405	E406	I407	M408	S409	L410	S411	A412	A413	T414	P415	K416	H417	L418	K419	S420	I421	G422	L423	L424	S425	P426	D427	F428	Q429	E430	D431	N432	E433	T434	E435	N437	F438	L439	L440	K441	Q442	A443	L444	T445	I446	V447	G448				
N322	K323	T324	Q325	G326	F327	W328	E329	N330	S331	M332	L333	T334	D335	P336	G337	N338	V339	Q340	K341	A342	V343	C344	H345	L351	G352	K353	G354	D355	F356	R357	T362	K363	V364	T365	K366	D367	D368	F369	L370	A372	A373	H375	H374	E375	K376	G377	H378	L379	Q380	Y381	D382	K383	A384	Y385	A386	A387	Q388					
L262	P263	A264	H265	L266	L267	G268	D269	M270	W271	G272	R273	F274	W275	T276	N277	L278	Y279	S280	L281	L282	V283	P284	F285	G286	Q287	K288	P289	N290	I291	D292	V293	T294	A296	M297	V298	D299	Q300	A301	W302	D303	A304	Q305	R306	I307	F308	K309	E310	A311	E312	K313	F314	F315	V316	S317	V318	G319	L320	P321				
Y202	W203	R204	G205	D206	Y207	E208	V209	N210	G211	V212	D213	G214	Y215	D216	Y217	S218	R219	G220	Q221	L222	I223	E224	D225	V226	E227	H228	T229	F230	E231	E232	I233	K234	P235	L236	Y237	E238	H239	L240	H241	A242	Y243	V244	R245	A246	K247	M249	N250	A251	Y252	P253	S254	Y255	I256	S257	P258	I259	G260	C261				
L142	L143	L144	E145	E146	G147	L148	N149	E150	I151	M152	A153	N154	S155	L156	D157	Y158	N159	E160	R161	L162	W163	A164	W165	E166	S167	W168	R169	S170	E171	V172	G173	K174	Q175	L176	R177	P178	L179	Y180	E181	E182	Y183	V184	V185	L186	K187	N188	E189	M190	A191	R192	A193	N194	H195	Y196	E197	D198	Y199	D200				

• Molecule 1: Angiotensin-converting enzyme 2

Chain F:  88% 11%

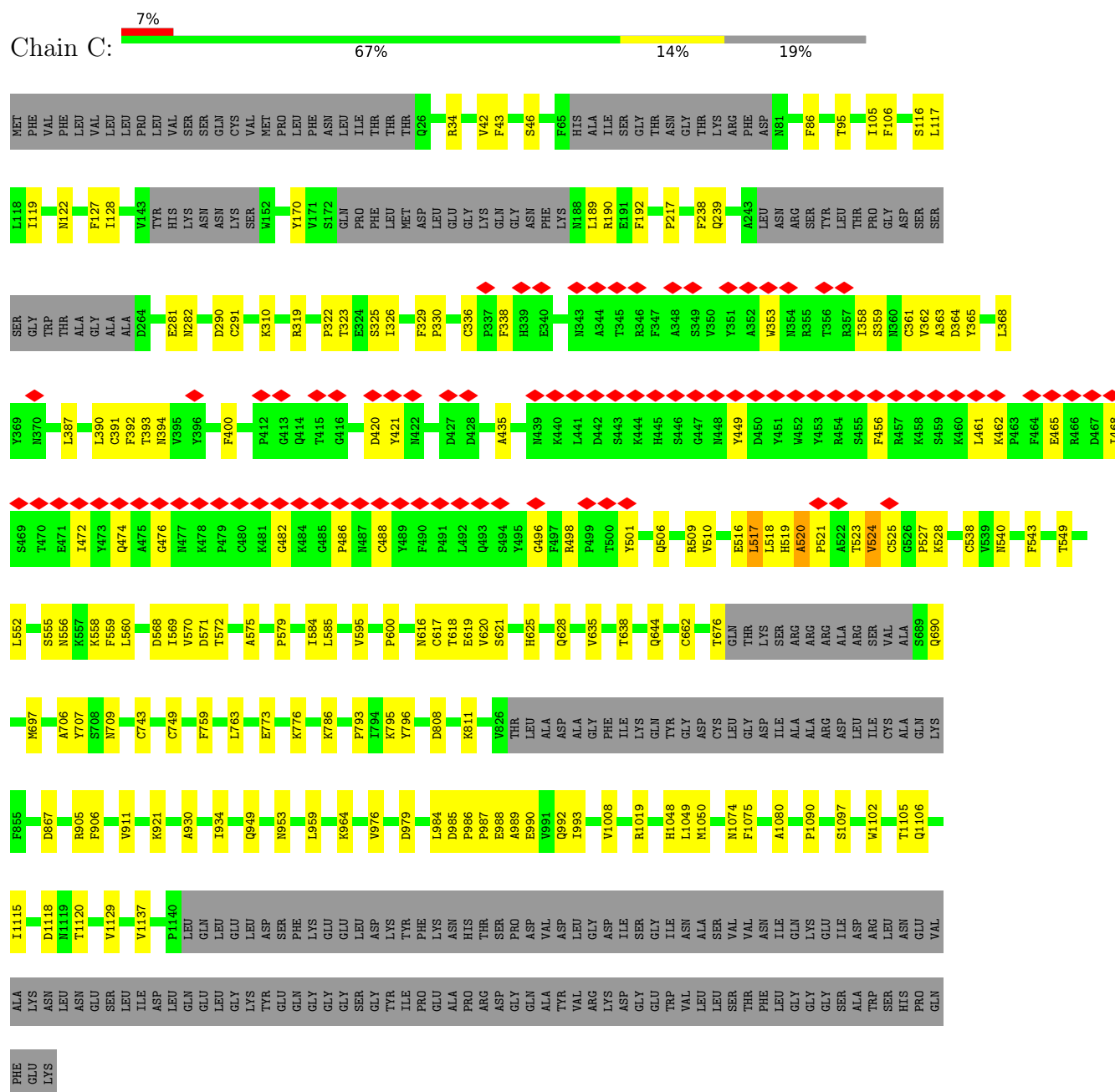
S19	T20	I21	E22	E23	Q24	A25	K26	T27	F28	L29	D30	K31	F32	N33	H34	E35	A36	E37	D38	L39	F40	Y41	Q42	L45	Y50	N53	I54	T55	E56	E57	N58	V59	Q60	M61	M62	N63	N64	A65	G66	T67	K68	W69	S70	A71	F72	L73	K74	E75	Q76	S77	T78	L79	A80	Q81	M82	Y83				
P84	L85	Q86	E87	I88	Q89	N90	A25	L91	T92	V93	K94	L95	Q96	L97	Q98	A99	L100	Q101	Q102	N103	G104	S105	S106	V107	L108	S109	E110	D111	K112	S113	K114	R115	L116	N117	T118	I119	L120	N121	M122	M123	S124	T125	I126	Y127	S128	T129	G130	K131	V132	C133	N134	P135	D136	N137	P138	Q139	E140	C141	L142	L143
L144	E145	P146	G147	N148	N149	E150	I151	G152	A153	N154	S155	L156	D157	Y158	N159	S280	R161	L162	V163	A164	W165	E166	S167	W168	R169	S170	E171	V172	K173	Q175	L176	R177	P178	L179	Y180	E181	E182	Y183	V184	V185	L186	K187	N188	E189	M190	A191	R192	A193	N194	H195	Y196	E197	D198	Y199	G200	Y201	Y202	W203		
R204	G205	D206	Y207	E208	V209	M210	G211	V212	D213	G214	Y215	D216	Y217	S218	R219	G220	Q221	L222	I223	E224	D225	V226	E227	H228	T229	F230	E231	E232	I233	K234	P235	L236	Y237	E238	H239	L240	H241	A242	Y243	V244	R245	A246	K247	L248	M249	N250	A251	Y252	P253	S254	Y255	I256	S257	P258	T259	G260	C261	L262	L263	
A264	H265	L266	L267	G268	D269	W270	W271	G272	R273	F274	W275	T276	W277	L278	Y279	S280	L281	T282	V283	P284	F285	G286	Q287	K288	P289	N290	L291	D292	V293	T294	D295	A296	W297	V298	Q300	A301	W302	D303	A304	Q305	R306	F308	K309	E310	A311	E312	F313	F314	F315	V316	S317	G319	L320	P321	N322	W323				



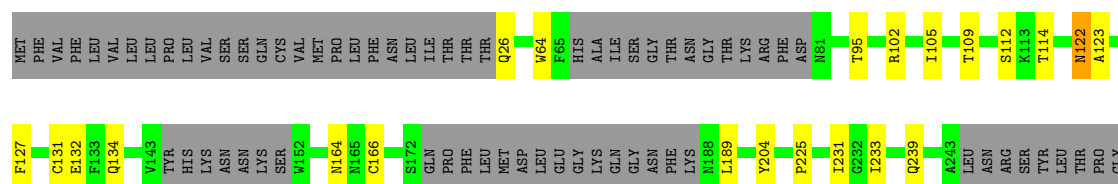
Frequency	Percentage
Daily	68%
Weekly	12%
Monthly	20%



- Molecule 2: Spike glycoprotein



- Molecule 2: Spike glycoprotein





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



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



- Molecule 3: beta-D-mannopyranose-(1-4)-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



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

Chain K:  100%



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

Chain L:  100%



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

Chain M:  50%
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%
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:  50%
100%



- 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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	593997	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.709	Depositor
Minimum map value	-0.227	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	414.0, 414.0, 414.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.69, 0.69, 0.69	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.27	0/5010	0.44	0/6807
1	E	0.27	0/5010	0.45	0/6807
1	F	0.27	0/5010	0.44	0/6807
2	B	0.29	0/8043	0.49	0/10949
2	C	0.30	0/8159	0.48	0/11107
2	D	0.30	0/8166	0.48	0/11117
All	All	0.29	0/39398	0.47	0/53594

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4869	0	4640	49	0
1	E	4869	0	4640	51	0
1	F	4869	0	4640	44	0
2	B	7851	0	7671	128	0
2	C	7963	0	7761	179	0
2	D	7970	0	7765	135	0
3	G	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	39	0	34	1	0
3	R	39	0	34	0	0
3	S	39	0	34	1	0
3	V	39	0	34	0	0
3	W	39	0	34	1	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	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	T	28	0	25	0	0
4	U	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	28	0	26	0	0
6	B	112	0	104	0	0
6	C	126	0	117	3	0
6	D	196	0	182	9	0
6	E	28	0	26	0	0
6	F	28	0	26	0	0
All	All	39510	0	38127	539	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.

The worst 5 of 539 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)
2:C:338:PHE:CE1	2:C:358:ILE:HD13	1.45	1.49
2:D:362:VAL:HG13	2:D:391:CYS:SG	1.60	1.38
2:B:390:LEU:CD1	2:B:517:LEU:HD23	1.60	1.30
2:B:390:LEU:HD12	2:B:517:LEU:CD2	1.60	1.29
2:C:338:PHE:HE1	2:C:358:ILE:CD1	1.51	1.24

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	595/603 (99%)	576 (97%)	18 (3%)	1 (0%)	44	74
1	E	595/603 (99%)	575 (97%)	20 (3%)	0	100	100
1	F	595/603 (99%)	579 (97%)	16 (3%)	0	100	100
2	B	987/1248 (79%)	914 (93%)	67 (7%)	6 (1%)	22	55
2	C	1001/1248 (80%)	910 (91%)	85 (8%)	6 (1%)	22	55
2	D	1002/1248 (80%)	928 (93%)	69 (7%)	5 (0%)	25	59
All	All	4775/5553 (86%)	4482 (94%)	275 (6%)	18 (0%)	32	63

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	520	ALA
2	C	282	ASN
2	C	520	ALA
2	D	520	ALA
2	B	1074	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	527/533 (99%)	527 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	527/533 (99%)	527 (100%)	0	100	100
1	F	527/533 (99%)	527 (100%)	0	100	100
2	B	879/1087 (81%)	879 (100%)	0	100	100
2	C	892/1087 (82%)	892 (100%)	0	100	100
2	D	893/1087 (82%)	890 (100%)	3 (0%)	91	96
All	All	4245/4860 (87%)	4242 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	122	ASN
2	D	331	ASN
2	D	332	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	487	ASN
1	E	149	ASN
1	F	524	GLN
1	F	134	ASN
1	F	137	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 ⓘ

44 monosaccharides are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	1	3,1	14,14,15	0.40	0	17,19,21	0.59	0
3	NAG	G	2	3	14,14,15	0.40	0	17,19,21	0.45	0
3	BMA	G	3	3	11,11,12	0.27	0	15,15,17	0.60	0
3	NAG	H	1	3,1	14,14,15	0.36	0	17,19,21	1.09	2 (11%)
3	NAG	H	2	3	14,14,15	0.40	0	17,19,21	1.07	2 (11%)
3	BMA	H	3	3	11,11,12	0.36	0	15,15,17	0.47	0
4	NAG	I	1	1,4	14,14,15	0.39	0	17,19,21	0.91	0
4	NAG	I	2	4	14,14,15	0.37	0	17,19,21	0.73	1 (5%)
4	NAG	J	1	1,4	14,14,15	0.42	0	17,19,21	0.74	1 (5%)
4	NAG	J	2	4	14,14,15	0.49	0	17,19,21	1.16	2 (11%)
4	NAG	K	1	4,2	14,14,15	0.26	0	17,19,21	0.41	0
4	NAG	K	2	4	14,14,15	0.22	0	17,19,21	0.37	0
4	NAG	L	1	4,2	14,14,15	0.41	0	17,19,21	0.38	0
4	NAG	L	2	4	14,14,15	0.38	0	17,19,21	0.40	0
4	NAG	M	1	4,2	14,14,15	0.39	0	17,19,21	1.02	2 (11%)
4	NAG	M	2	4	14,14,15	0.36	0	17,19,21	1.01	1 (5%)
4	NAG	N	1	4,2	14,14,15	0.41	0	17,19,21	0.72	0
4	NAG	N	2	4	14,14,15	0.38	0	17,19,21	0.71	0
4	NAG	O	1	4,2	14,14,15	0.39	0	17,19,21	1.03	2 (11%)
4	NAG	O	2	4	14,14,15	0.35	0	17,19,21	1.01	1 (5%)
4	NAG	P	1	4,2	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	P	2	4	14,14,15	0.26	0	17,19,21	0.38	0
4	NAG	Q	1	4,2	14,14,15	0.40	0	17,19,21	1.03	2 (11%)
4	NAG	Q	2	4	14,14,15	0.37	0	17,19,21	1.01	1 (5%)
3	NAG	R	1	3,1	14,14,15	0.40	0	17,19,21	0.58	0
3	NAG	R	2	3	14,14,15	0.41	0	17,19,21	0.45	0
3	BMA	R	3	3	11,11,12	0.26	0	15,15,17	0.60	0
3	NAG	S	1	3,1	14,14,15	0.36	0	17,19,21	1.09	2 (11%)
3	NAG	S	2	3	14,14,15	0.39	0	17,19,21	1.08	2 (11%)
3	BMA	S	3	3	11,11,12	0.36	0	15,15,17	0.47	0
4	NAG	T	1	1,4	14,14,15	0.40	0	17,19,21	0.91	1 (5%)
4	NAG	T	2	4	14,14,15	0.36	0	17,19,21	0.73	1 (5%)
4	NAG	U	1	1,4	14,14,15	0.43	0	17,19,21	0.74	1 (5%)
4	NAG	U	2	4	14,14,15	0.49	0	17,19,21	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	V	1	3,1	14,14,15	0.39	0	17,19,21	0.58	0
3	NAG	V	2	3	14,14,15	0.38	0	17,19,21	0.45	0
3	BMA	V	3	3	11,11,12	0.27	0	15,15,17	0.59	0
3	NAG	W	1	3,1	14,14,15	0.36	0	17,19,21	1.08	2 (11%)
3	NAG	W	2	3	14,14,15	0.40	0	17,19,21	1.07	2 (11%)
3	BMA	W	3	3	11,11,12	0.35	0	15,15,17	0.47	0
4	NAG	X	1	1,4	14,14,15	0.41	0	17,19,21	0.90	0
4	NAG	X	2	4	14,14,15	0.37	0	17,19,21	0.74	1 (5%)
4	NAG	Y	1	1,4	14,14,15	0.41	0	17,19,21	0.74	1 (5%)
4	NAG	Y	2	4	14,14,15	0.47	0	17,19,21	1.15	2 (11%)

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

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

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

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	2	NAG	C2-N2-C7	3.33	127.64	122.90
4	M	2	NAG	C2-N2-C7	3.31	127.62	122.90
4	O	2	NAG	C2-N2-C7	3.30	127.60	122.90
4	Q	1	NAG	C1-C2-N2	3.15	115.86	110.49
4	M	1	NAG	C1-C2-N2	3.12	115.81	110.49

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

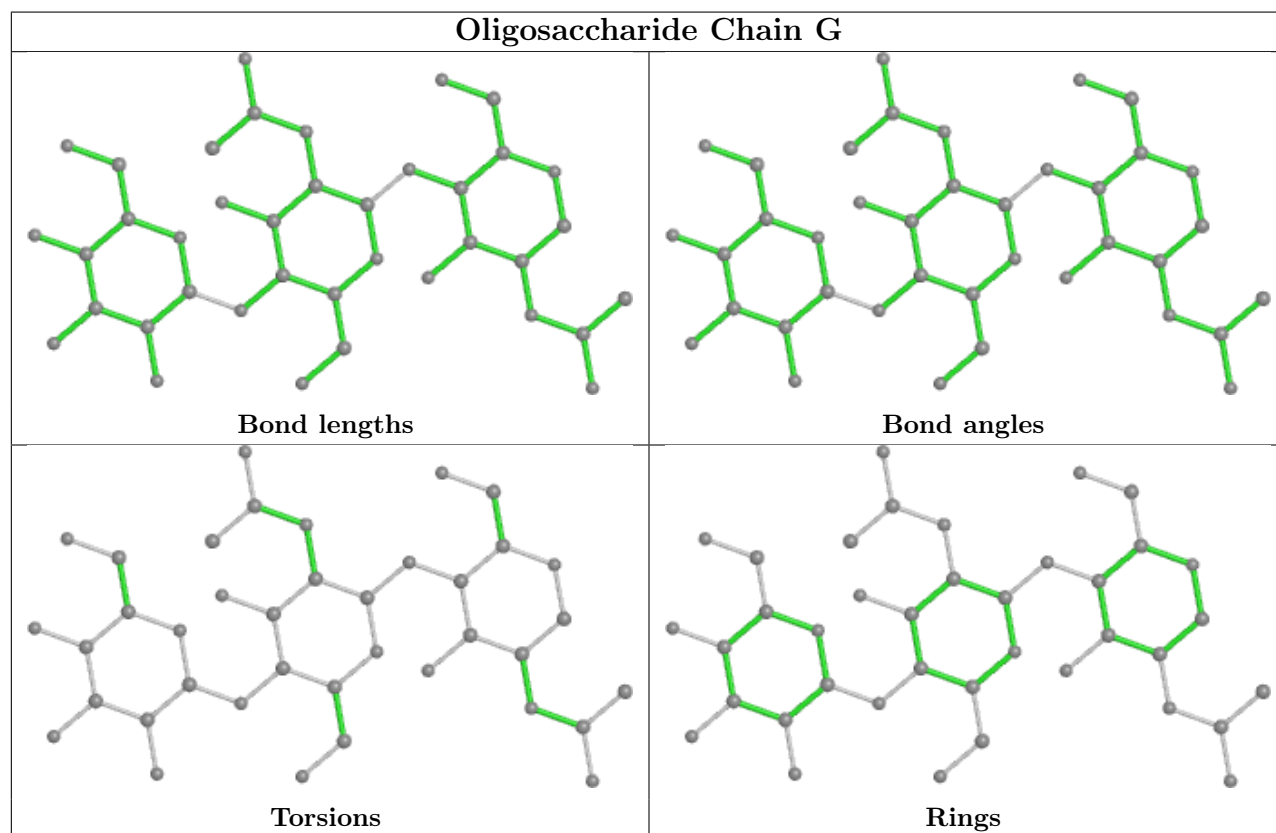
Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C3-C2-N2-C7
3	S	1	NAG	C3-C2-N2-C7
3	W	1	NAG	C3-C2-N2-C7
4	M	1	NAG	C3-C2-N2-C7
4	M	2	NAG	C3-C2-N2-C7

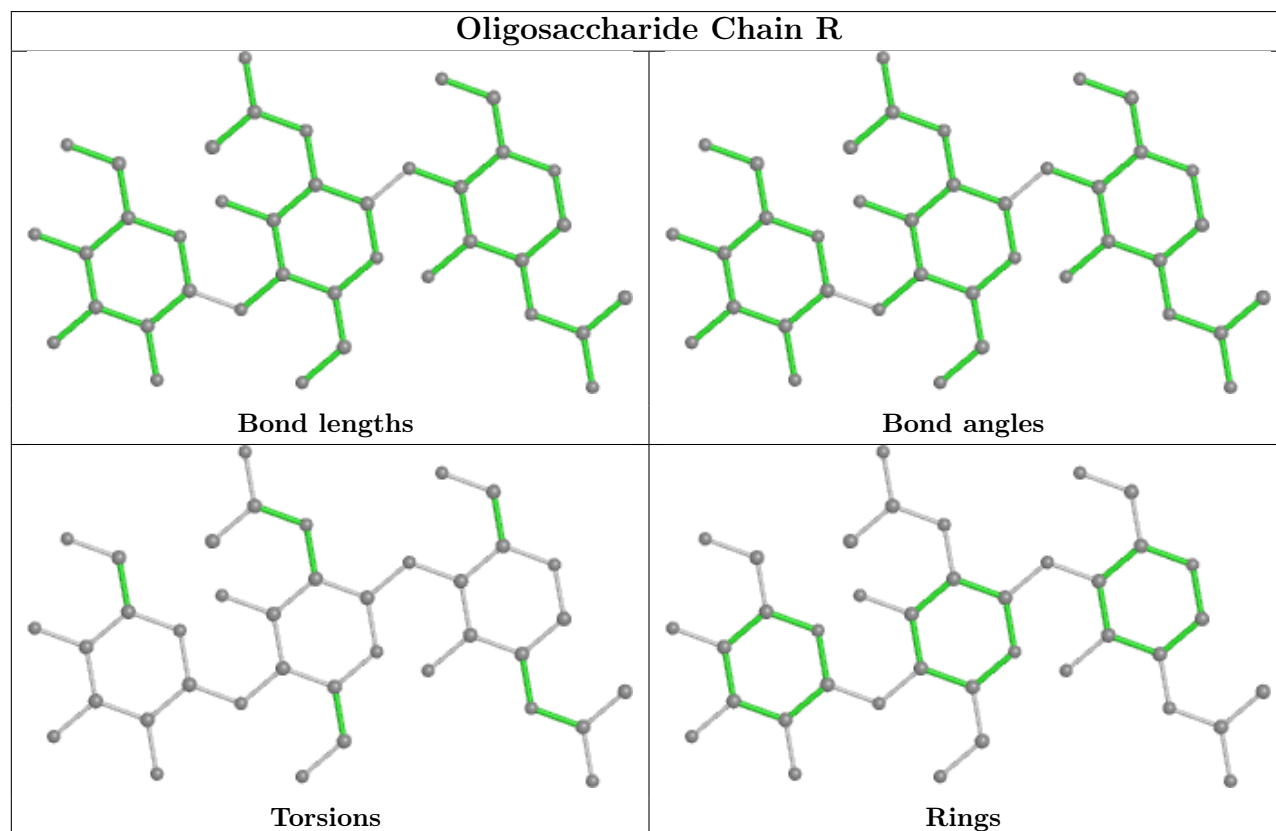
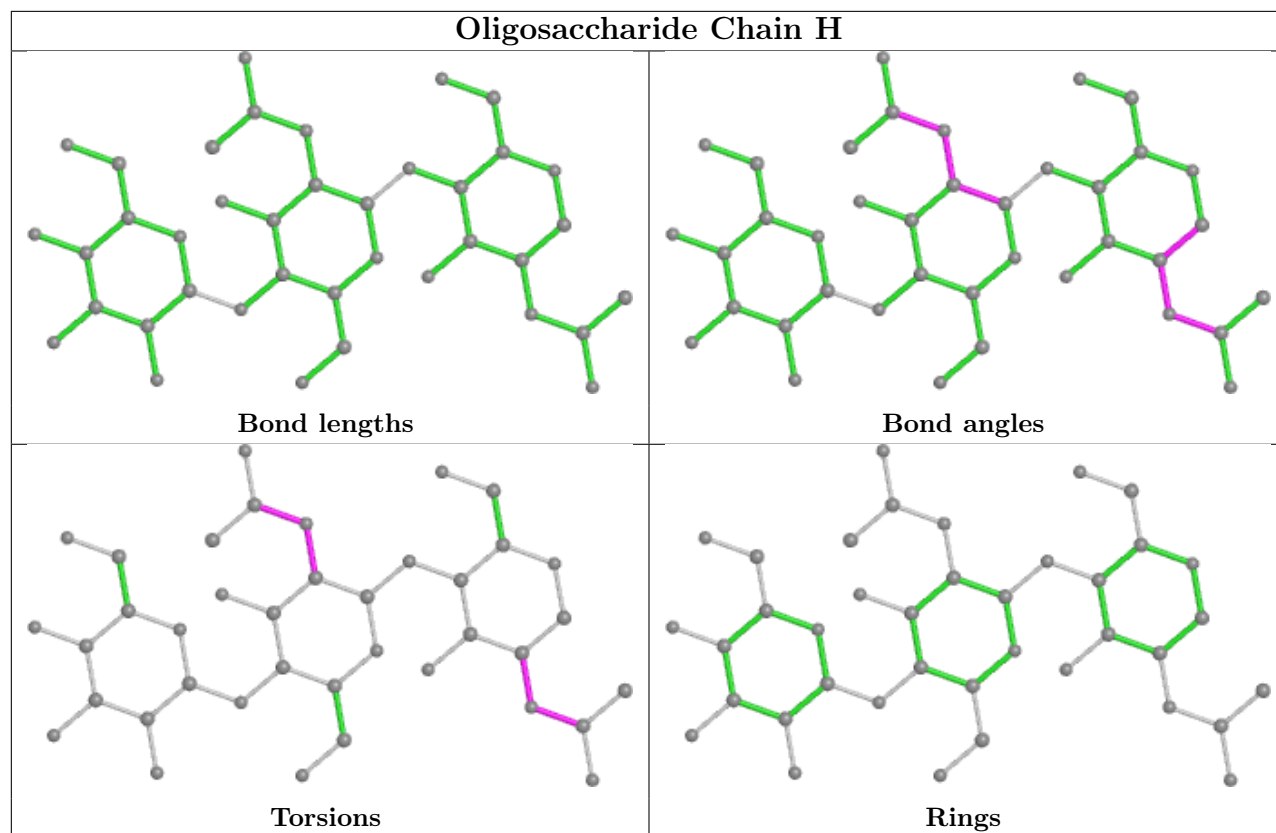
There are no ring outliers.

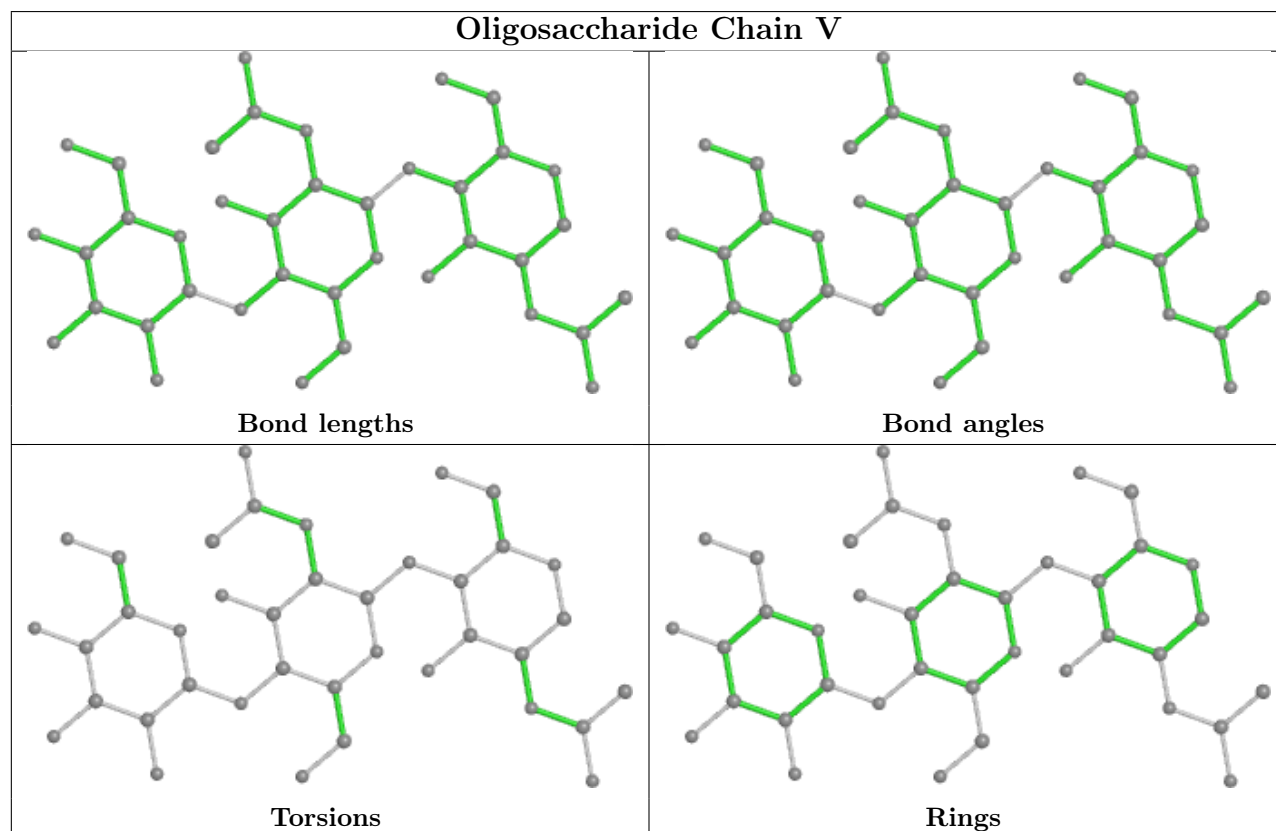
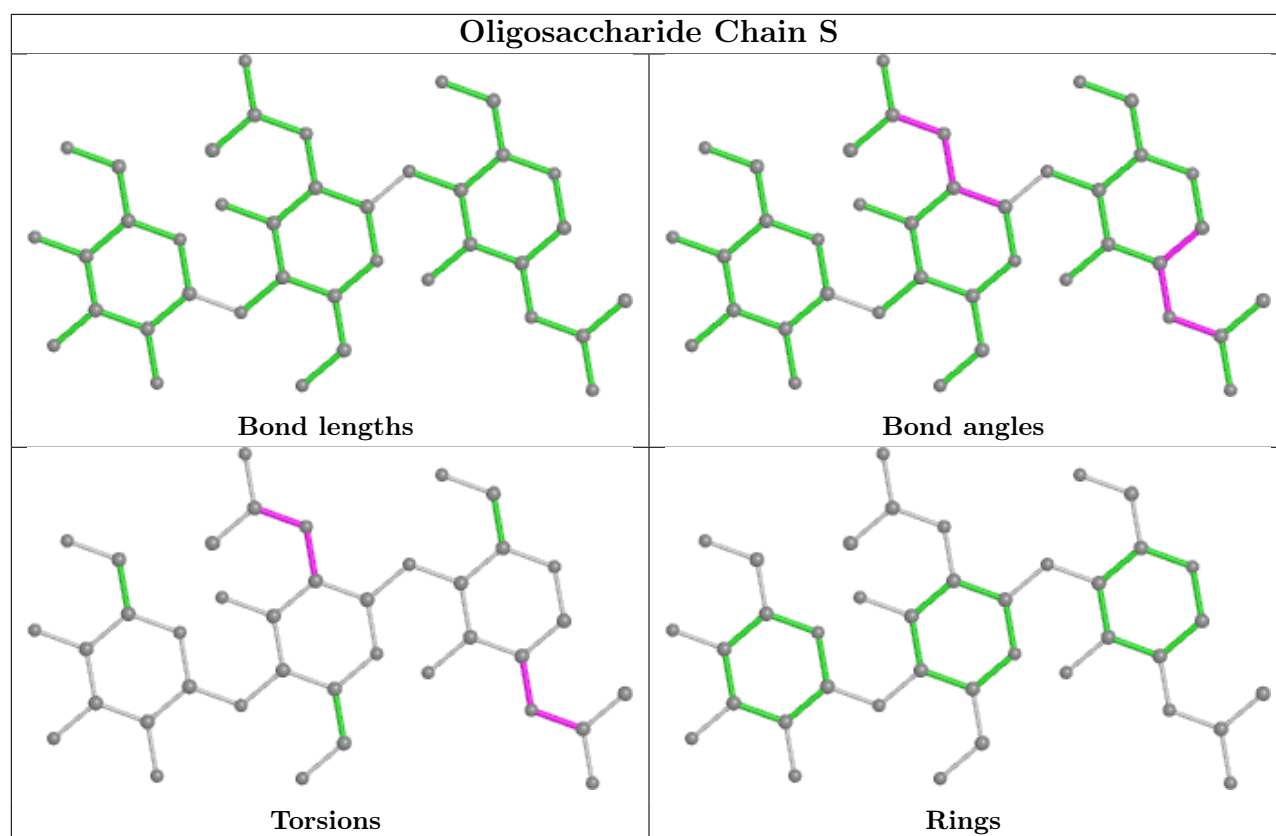
3 monomers are involved in 3 short contacts:

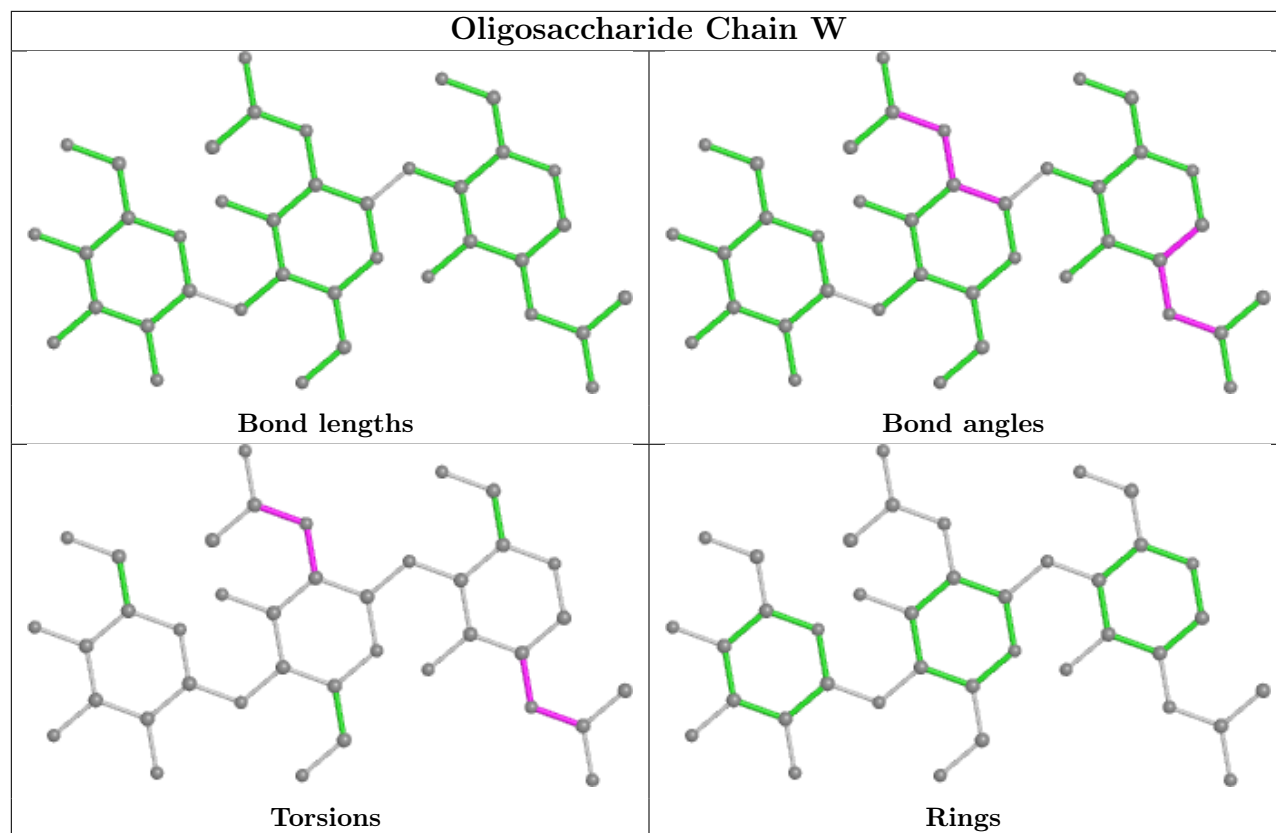
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	1	NAG	1	0
3	W	1	NAG	1	0
3	H	1	NAG	1	0

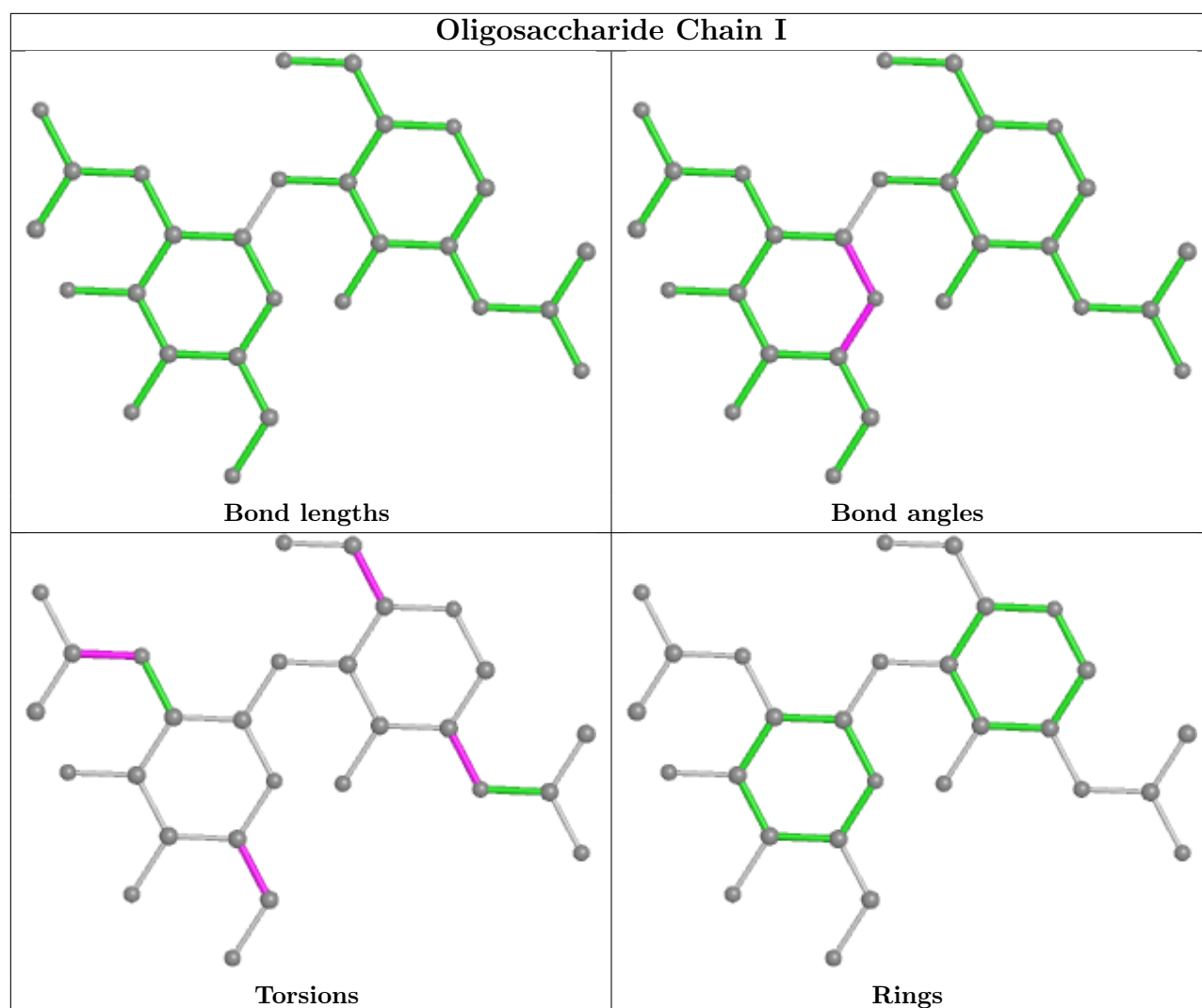
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

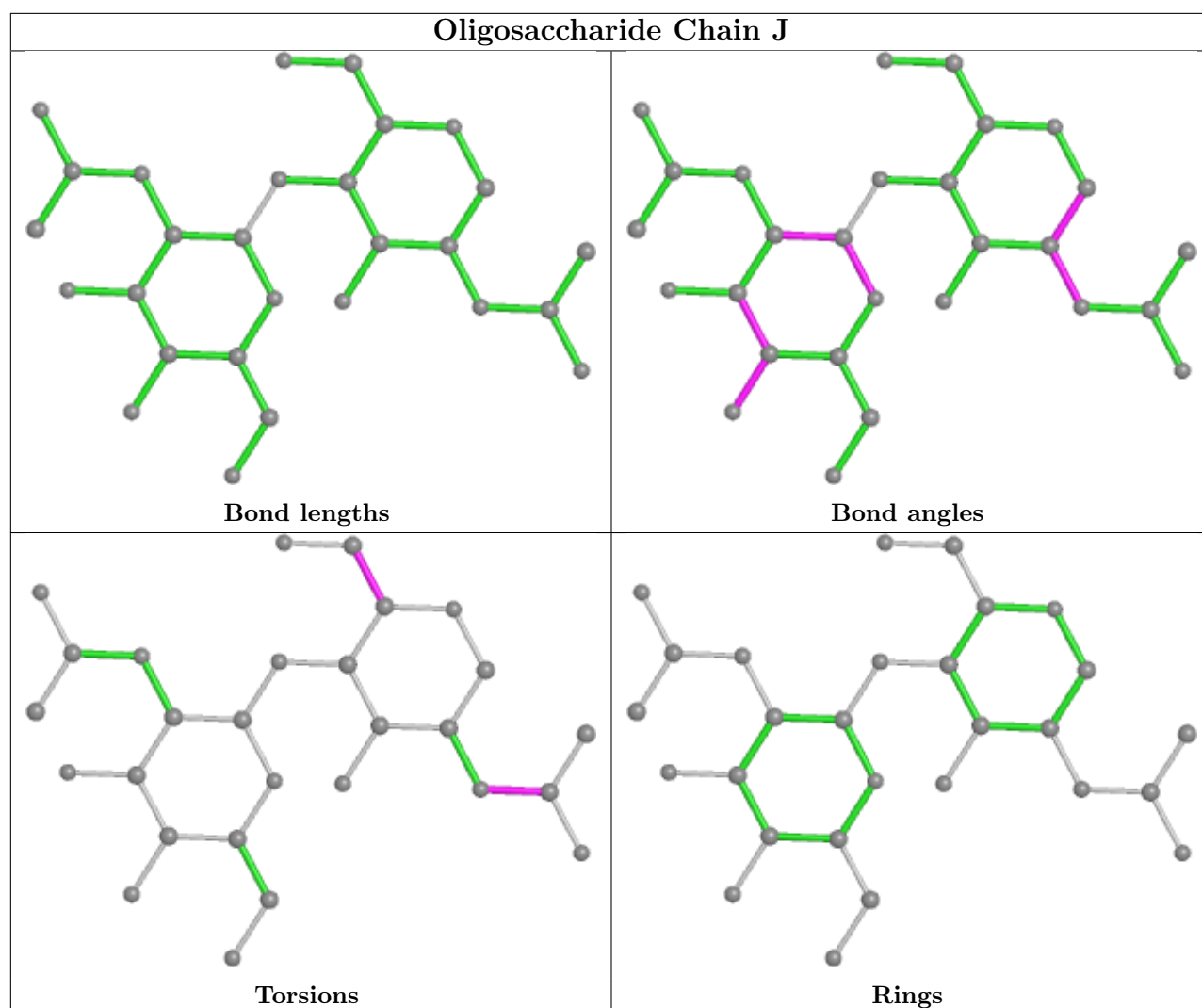


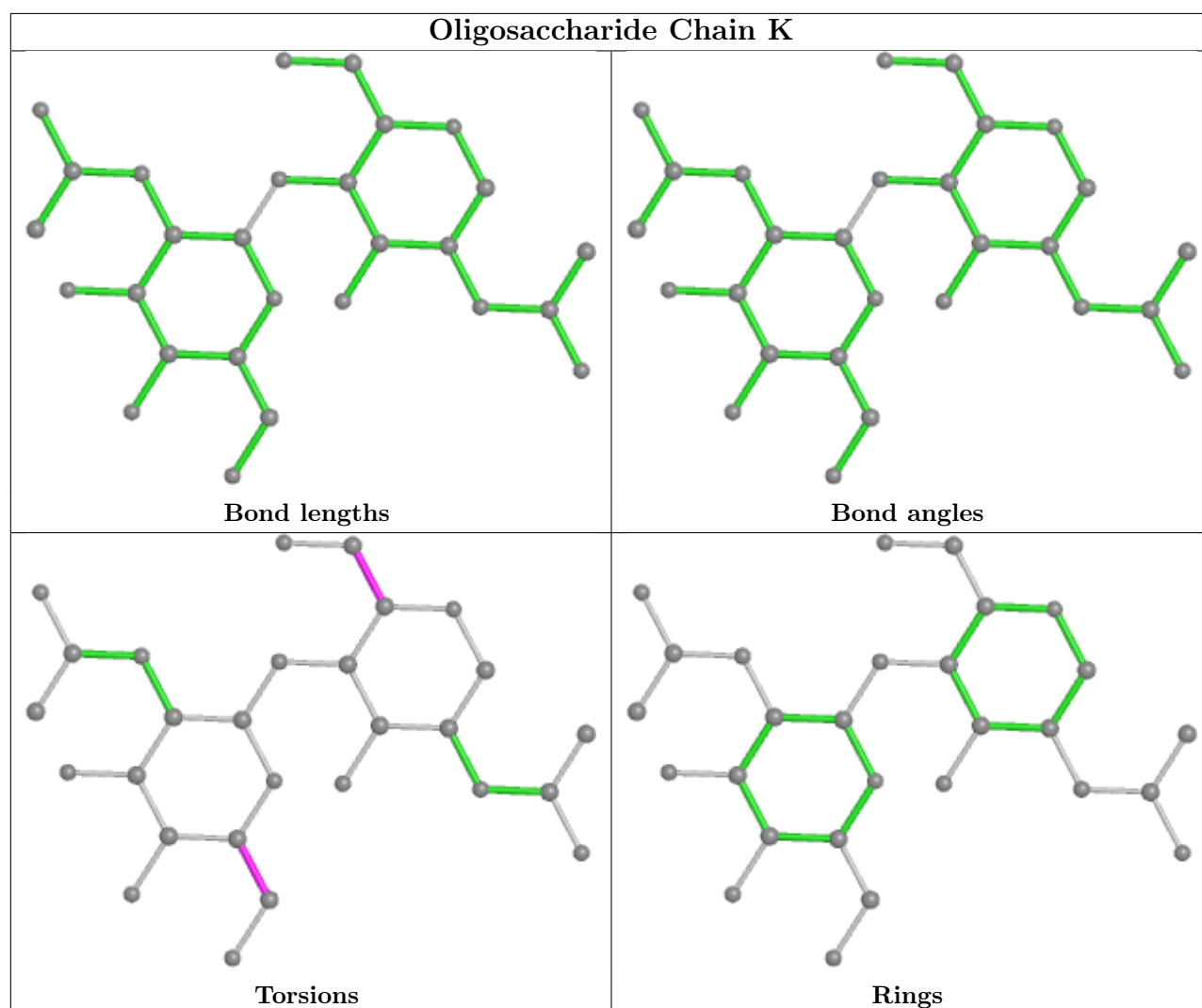


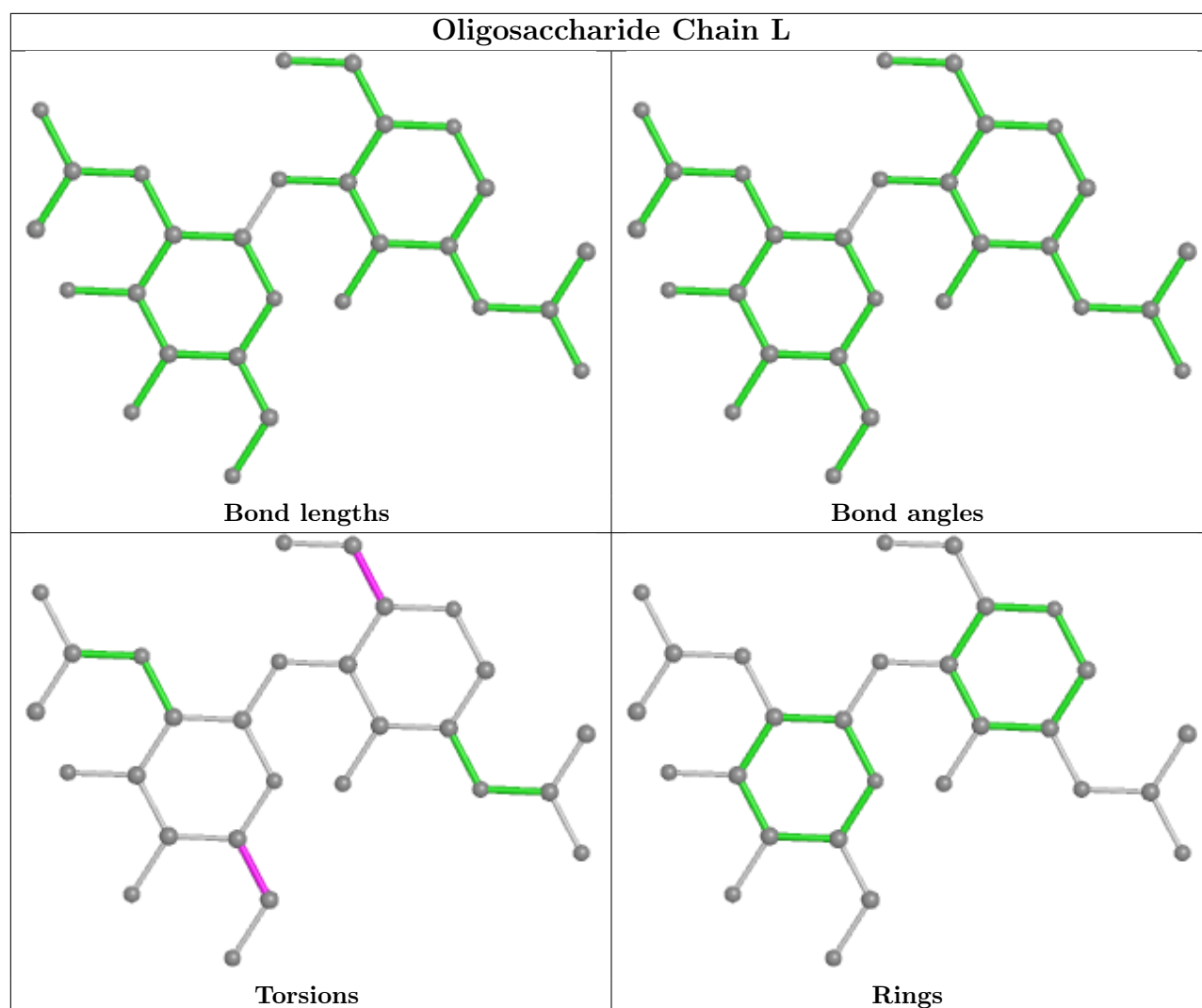


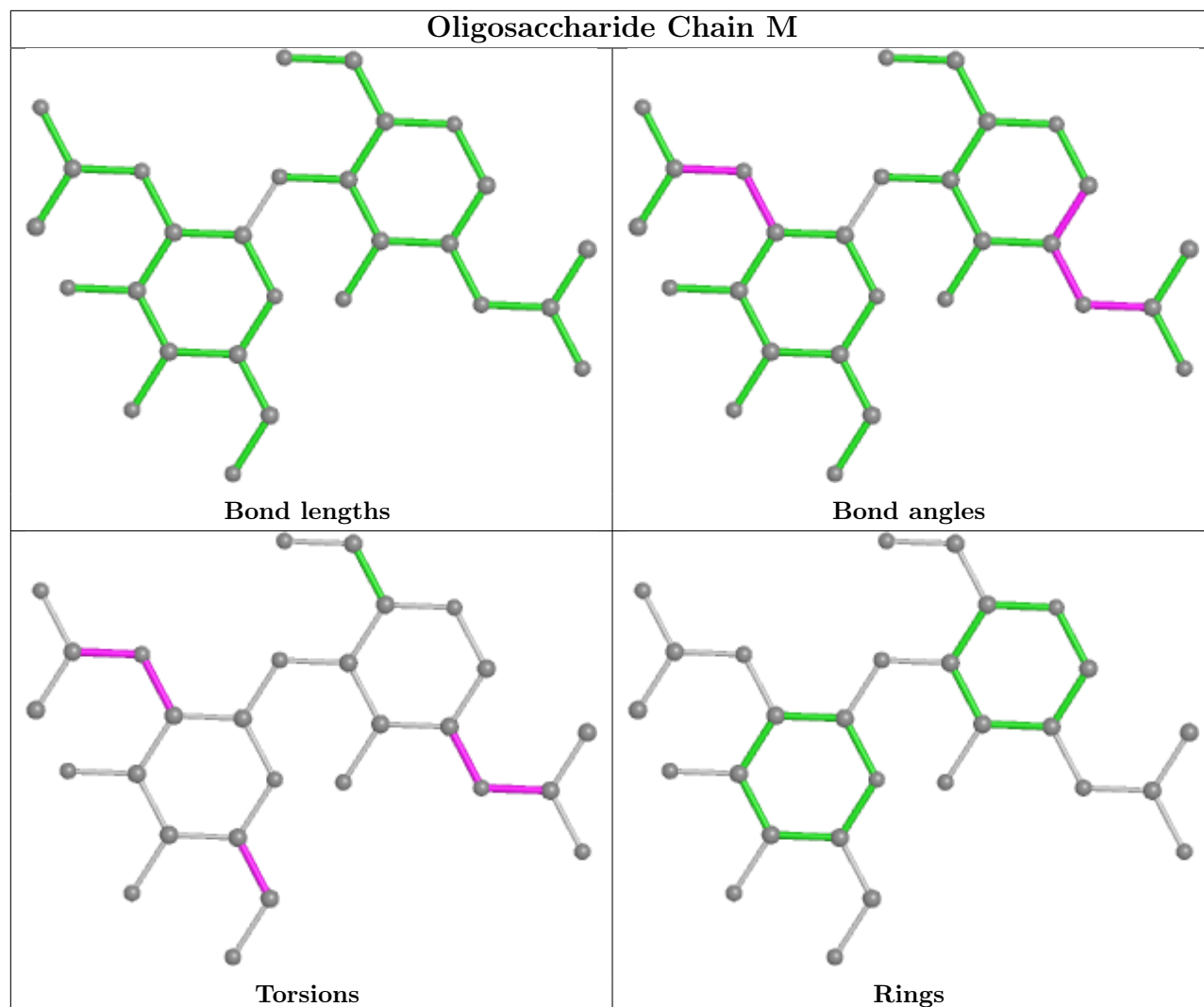


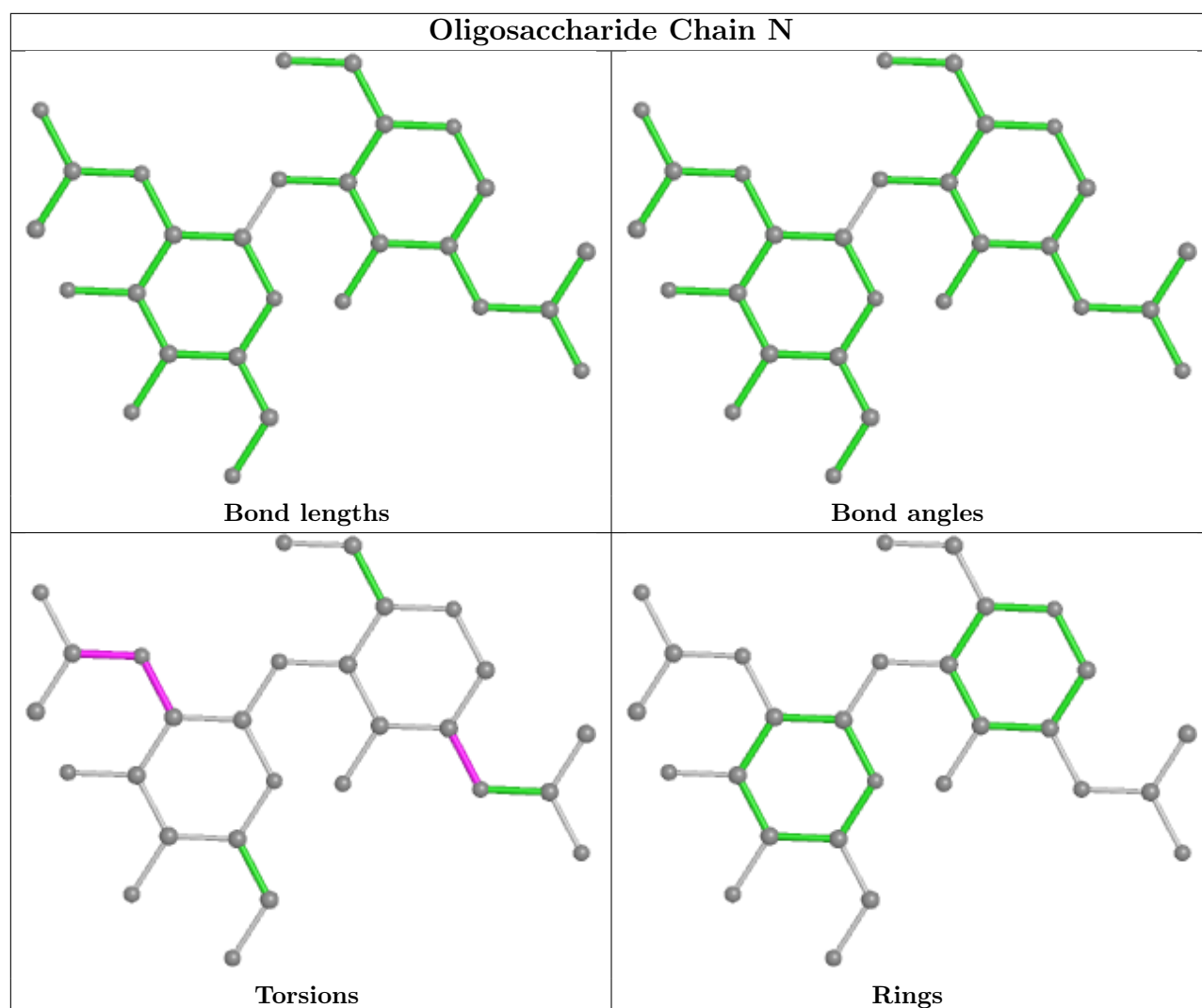


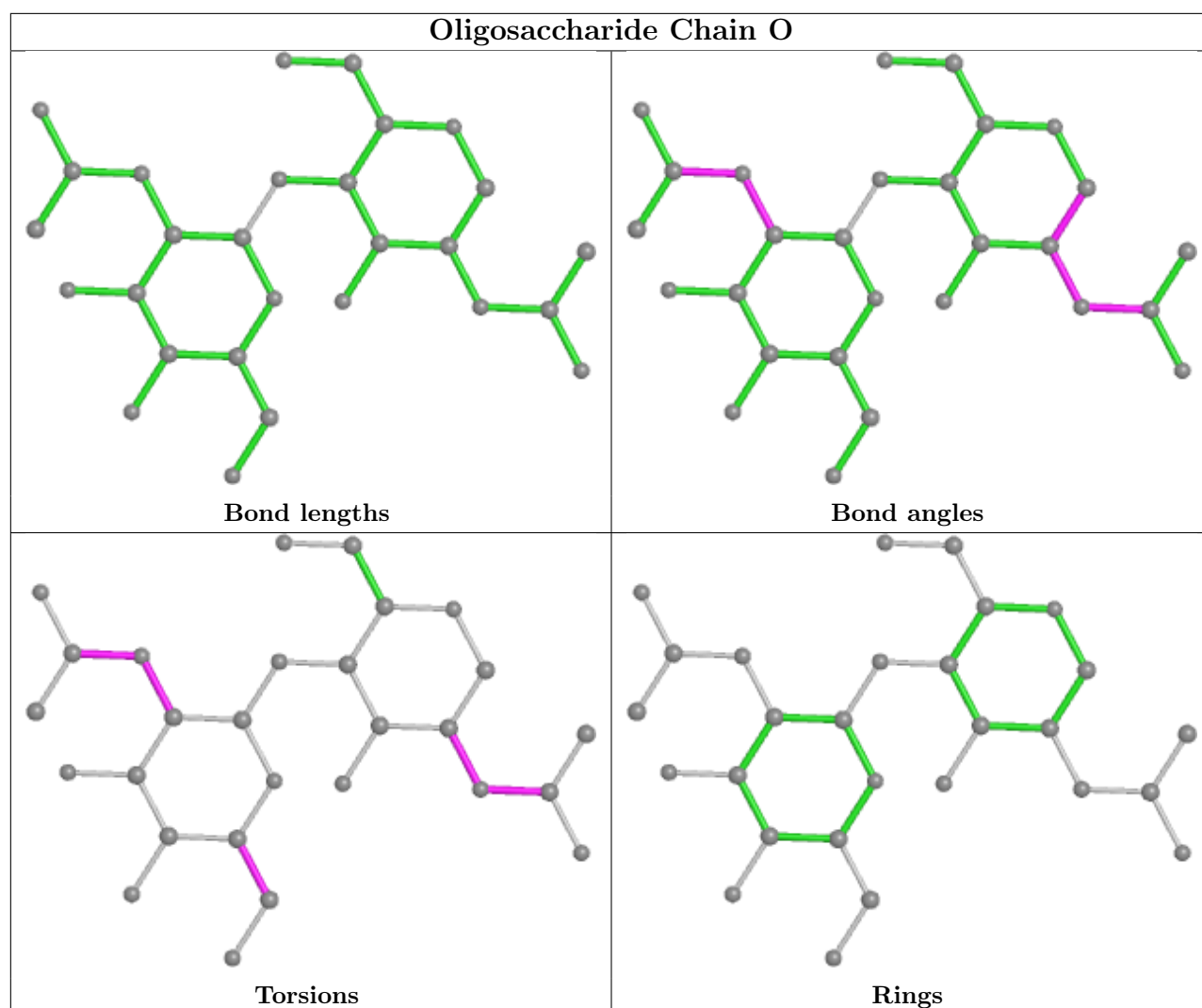


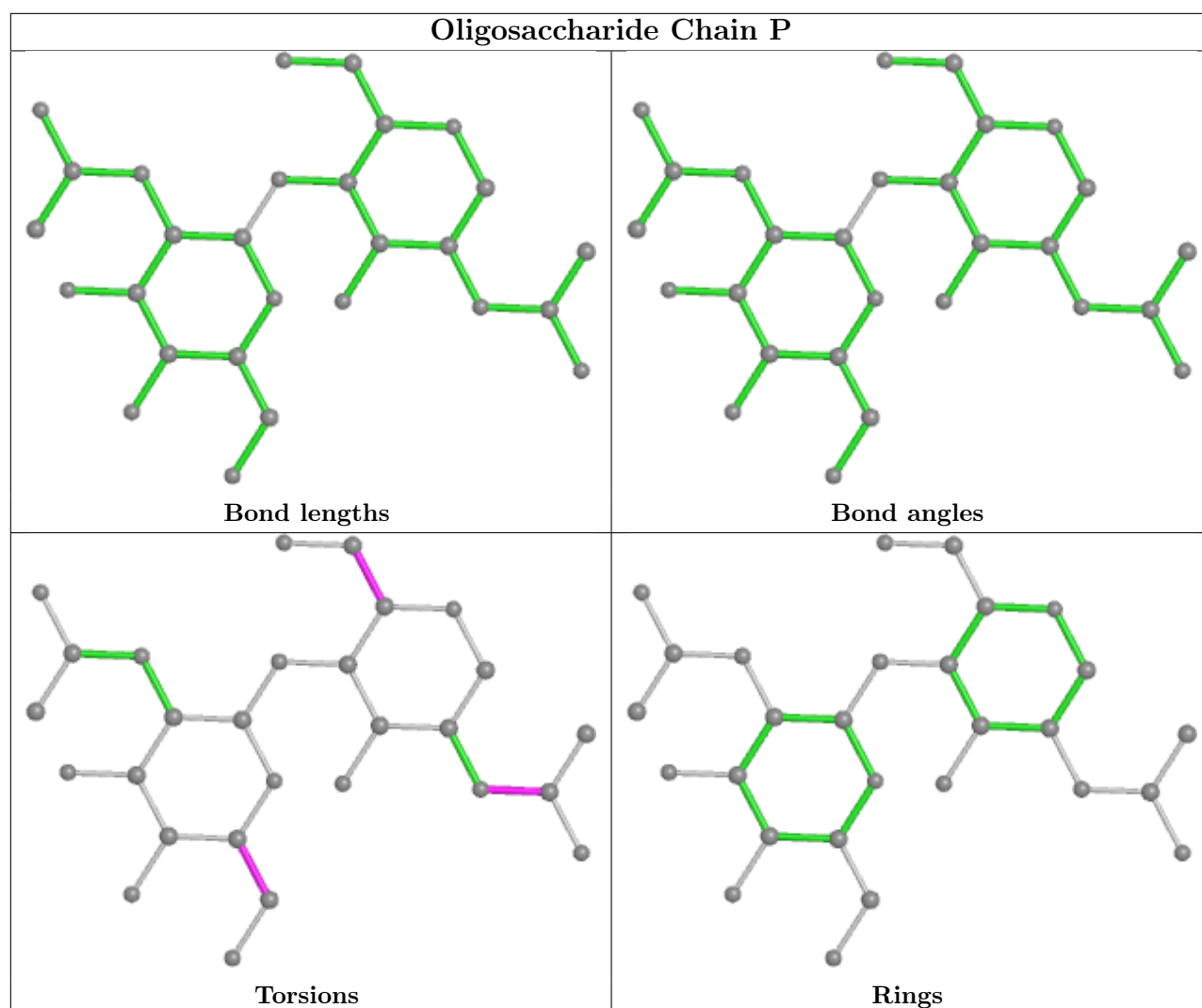


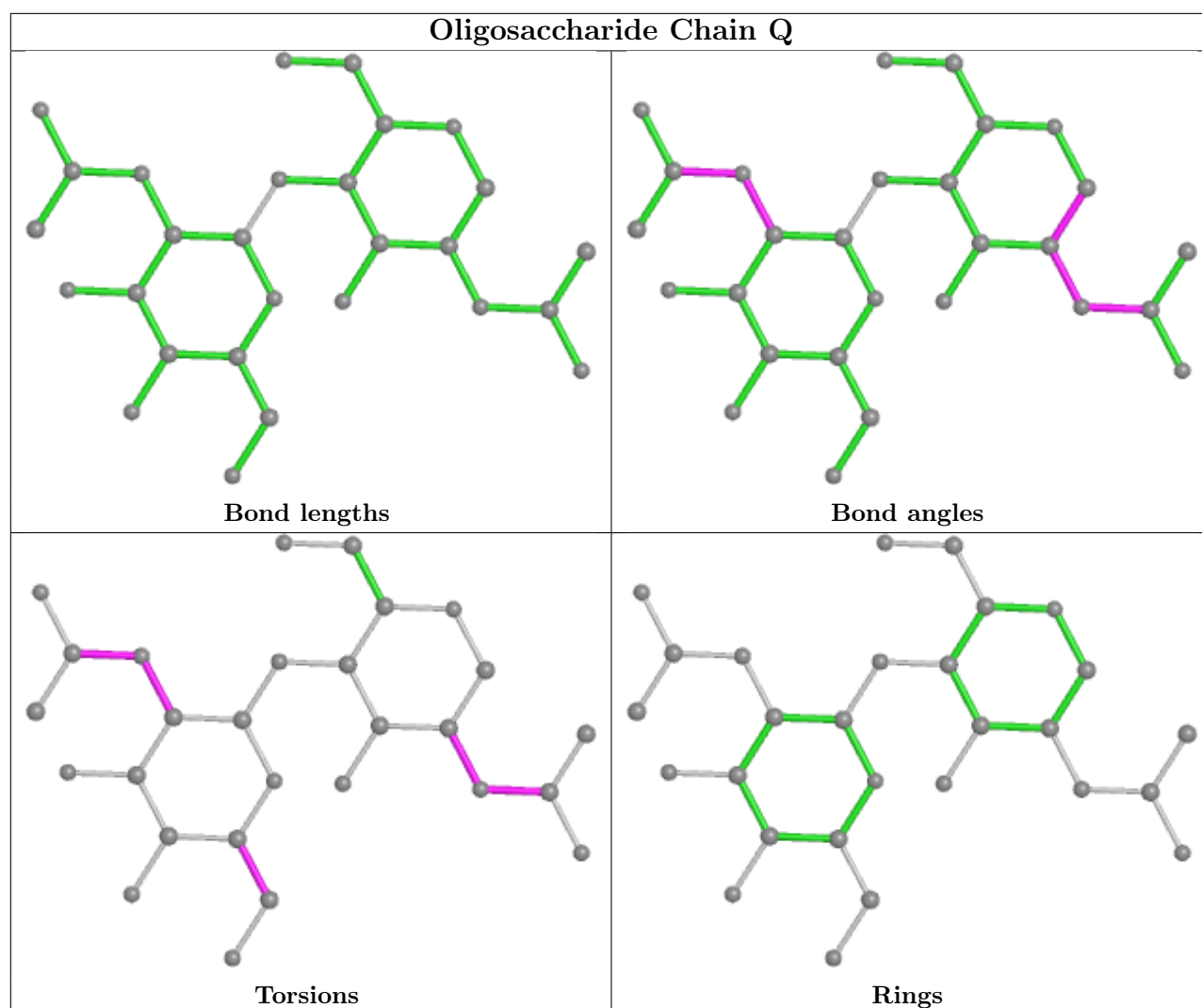


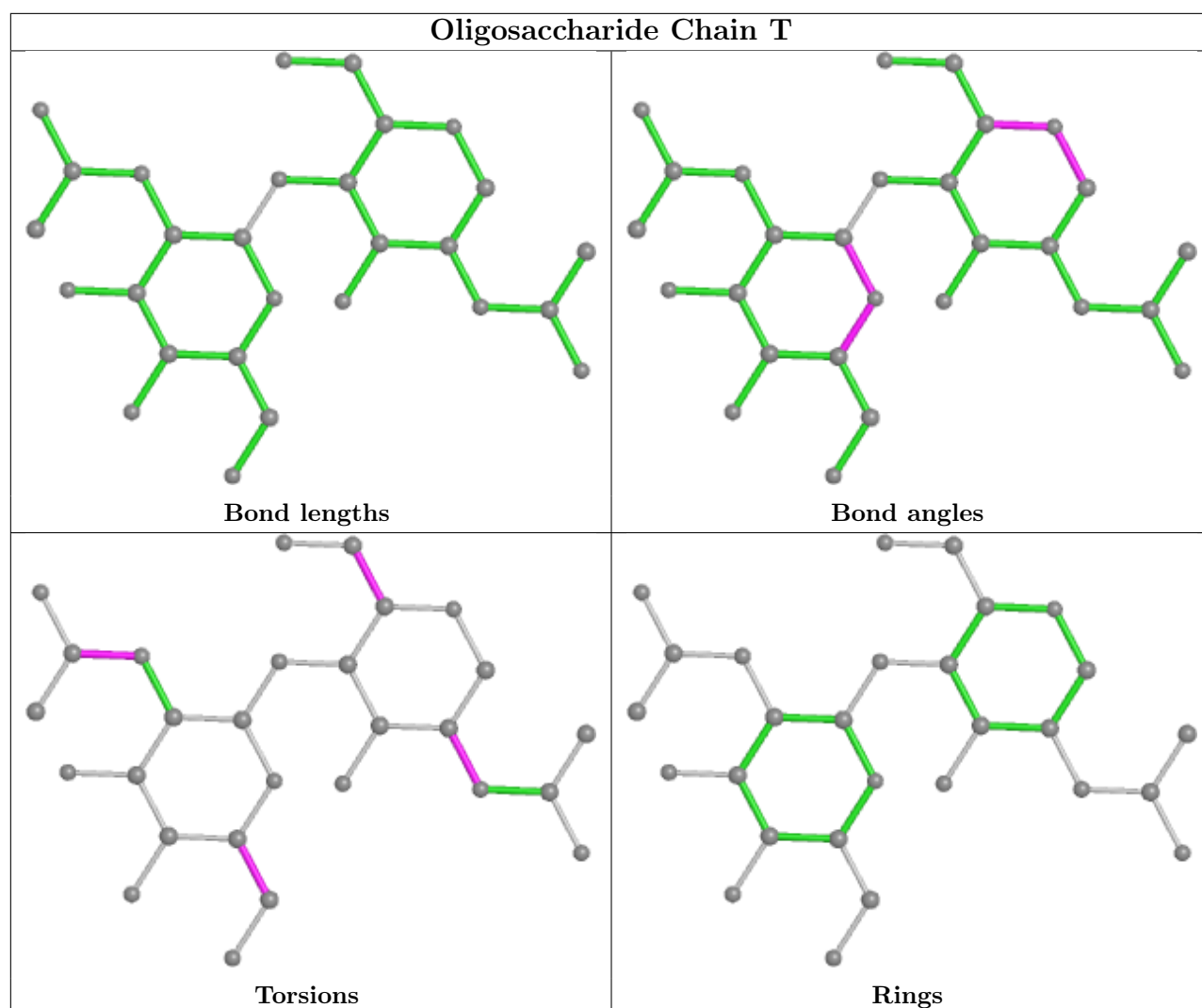


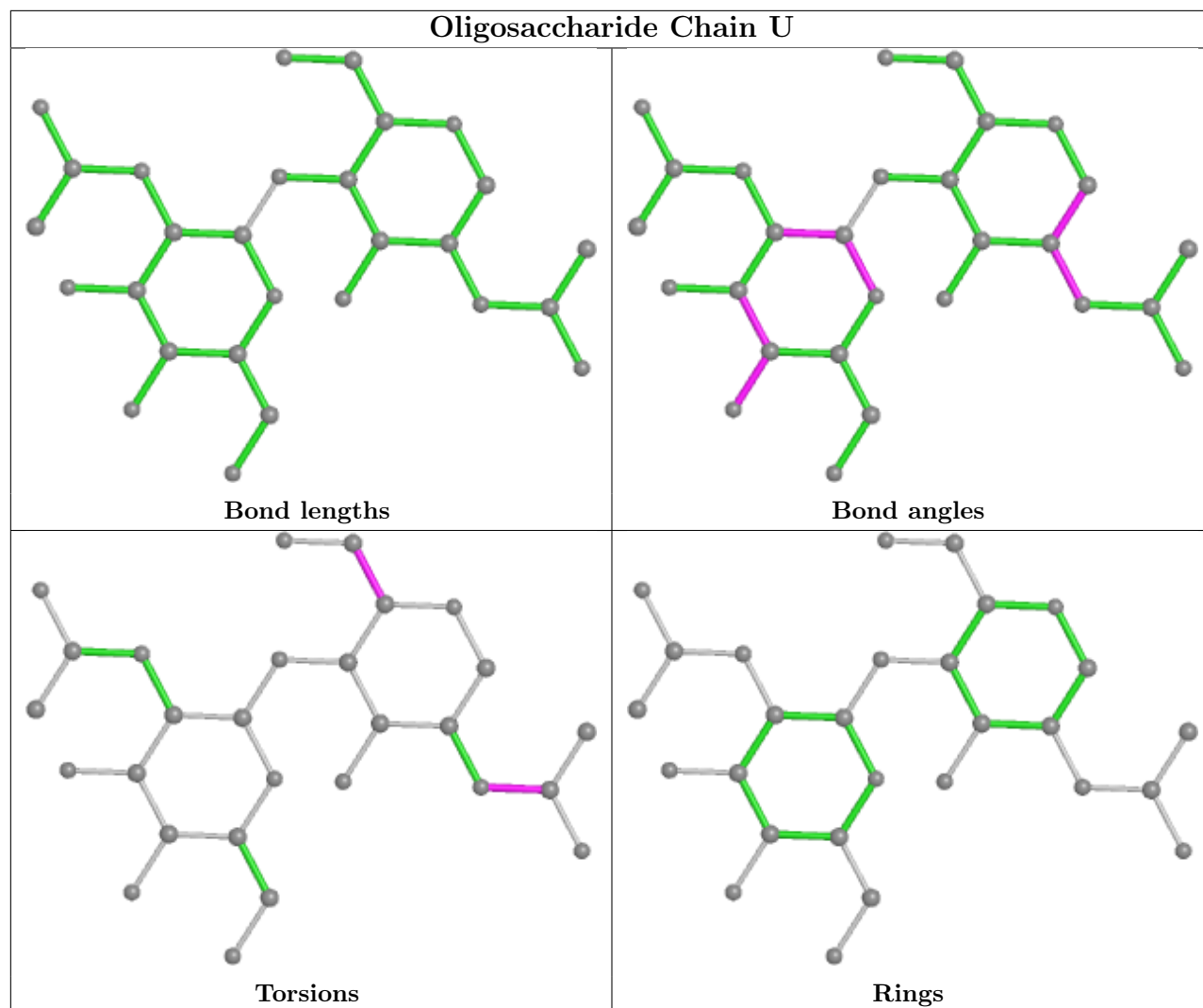


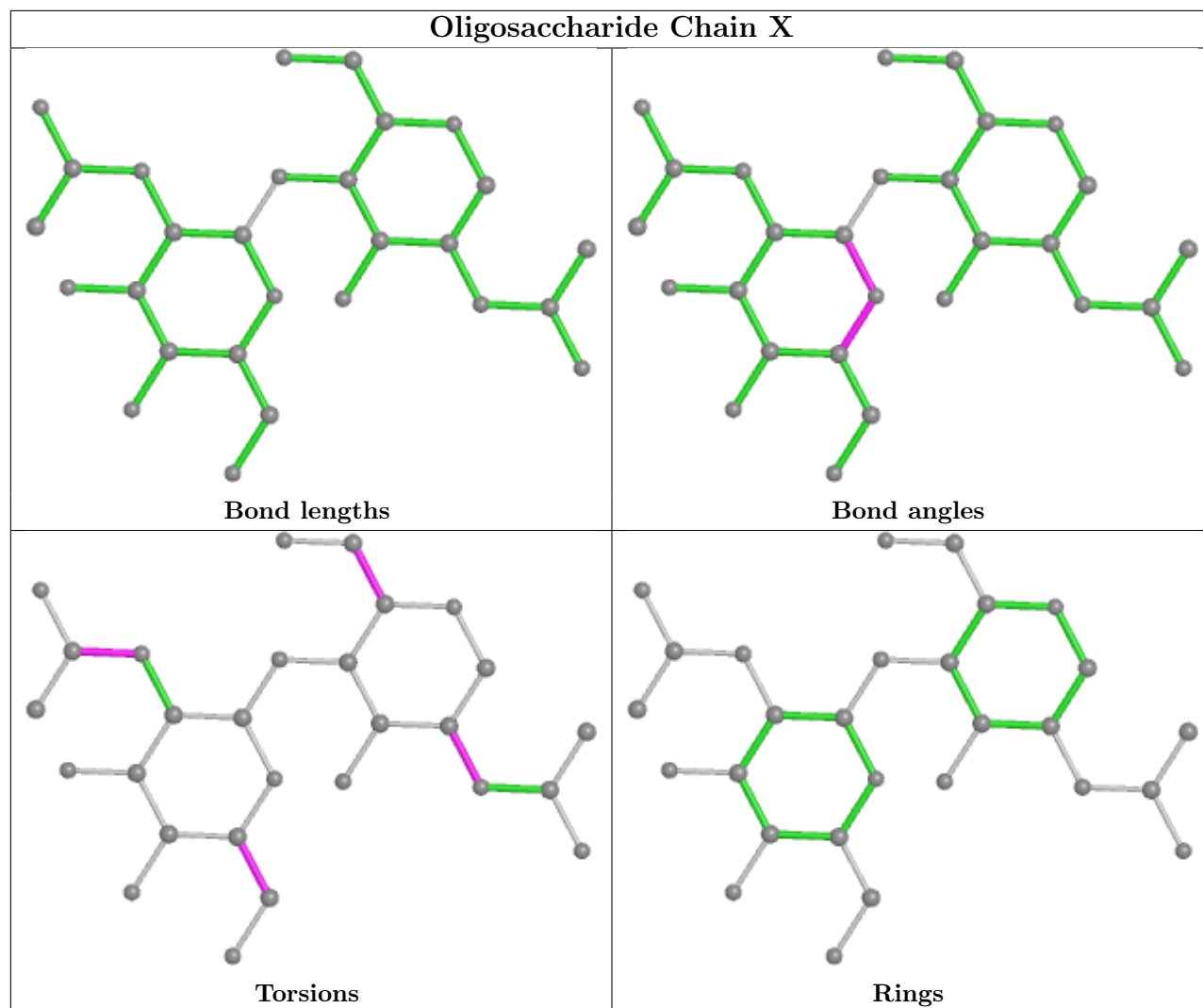


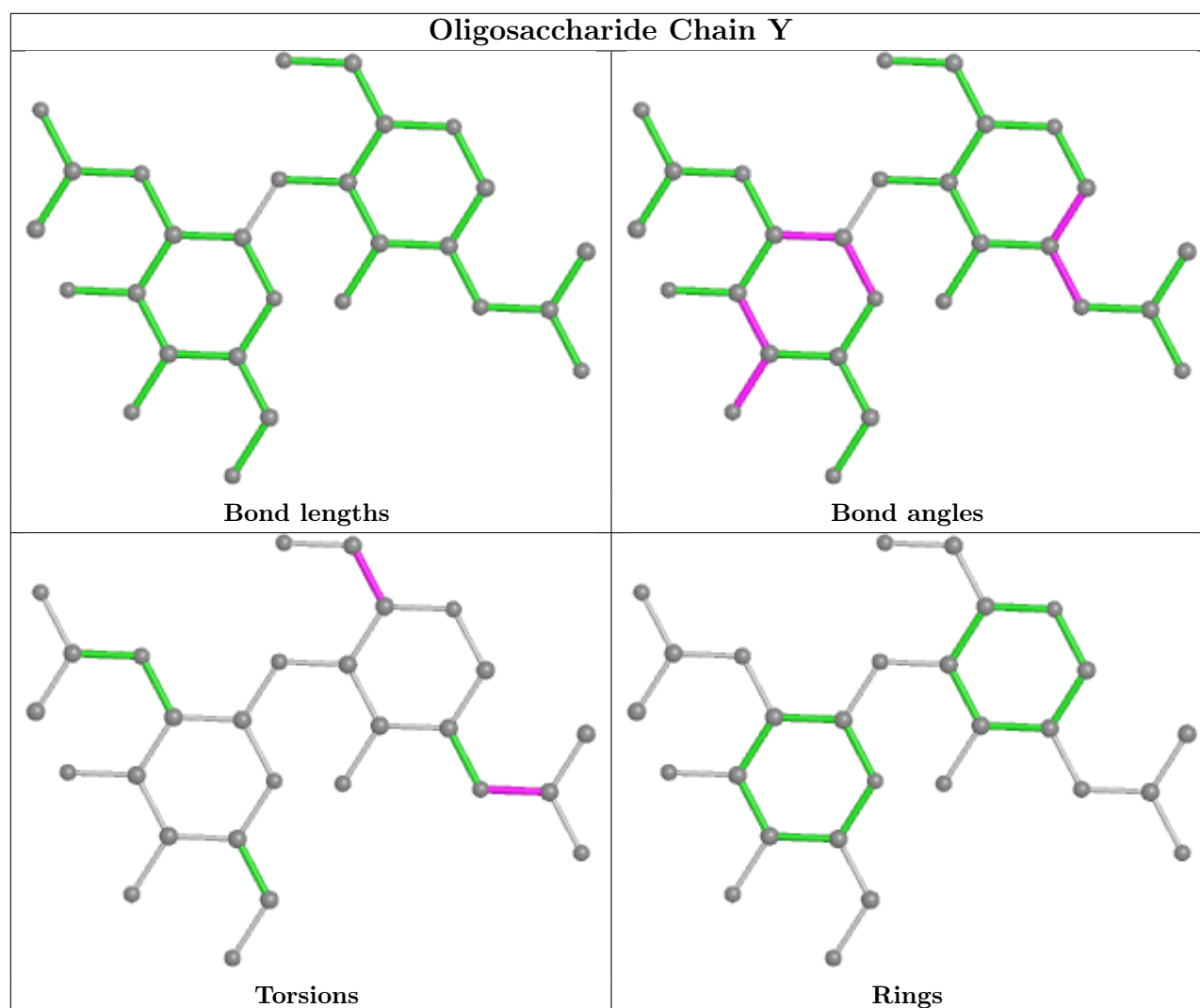












5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 3 are monoatomic - leaving 37 for Mogul analysis.

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	$\# Z > 2$
6	NAG	F	703	1	14,14,15	0.39	0	17,19,21	1.13	1 (5%)
6	NAG	D	1313	2	14,14,15	0.37	0	17,19,21	0.60	0
6	NAG	C	1303	2	14,14,15	0.22	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	1301	2	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	D	1305	2	14,14,15	0.20	0	17,19,21	0.59	0
6	NAG	E	702	1	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	B	1302	2	14,14,15	0.55	0	17,19,21	0.48	0
6	NAG	C	1304	2	14,14,15	0.26	0	17,19,21	0.52	0
6	NAG	B	1306	2	14,14,15	0.22	0	17,19,21	0.60	0
6	NAG	D	1303	2	14,14,15	0.21	0	17,19,21	0.40	0
6	NAG	D	1307	2	14,14,15	0.25	0	17,19,21	0.52	0
6	NAG	C	1309	2	14,14,15	0.40	0	17,19,21	0.99	1 (5%)
6	NAG	B	1301	2	14,14,15	0.38	0	17,19,21	0.41	0
6	NAG	D	1309	2	14,14,15	0.26	0	17,19,21	0.42	0
6	NAG	B	1304	2	14,14,15	0.19	0	17,19,21	0.40	0
6	NAG	D	1314	2	14,14,15	0.43	0	17,19,21	2.11	2 (11%)
6	NAG	A	703	1	14,14,15	0.39	0	17,19,21	1.13	1 (5%)
6	NAG	C	1307	2	14,14,15	0.38	0	17,19,21	0.54	0
6	NAG	C	1301	2	14,14,15	0.31	0	17,19,21	0.47	0
6	NAG	C	1308	2	14,14,15	0.39	0	17,19,21	0.38	0
6	NAG	B	1305	2	14,14,15	0.19	0	17,19,21	0.55	0
6	NAG	B	1303	2	14,14,15	0.24	0	17,19,21	0.51	0
6	NAG	C	1305	2	14,14,15	0.22	0	17,19,21	0.46	0
6	NAG	B	1308	2	14,14,15	0.39	0	17,19,21	0.42	0
6	NAG	D	1311	2	14,14,15	0.38	0	17,19,21	1.05	2 (11%)
6	NAG	D	1312	2	14,14,15	0.41	0	17,19,21	1.05	2 (11%)
6	NAG	F	702	1	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	C	1302	2	14,14,15	0.22	0	17,19,21	0.39	0
6	NAG	A	702	1	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	C	1306	2	14,14,15	0.40	0	17,19,21	1.01	2 (11%)
6	NAG	D	1310	2	14,14,15	0.41	0	17,19,21	1.01	2 (11%)
6	NAG	B	1307	2	14,14,15	0.40	0	17,19,21	1.01	2 (11%)
6	NAG	E	703	1	14,14,15	0.40	0	17,19,21	1.13	1 (5%)
6	NAG	D	1302	2	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	D	1308	2	14,14,15	0.21	0	17,19,21	0.36	0
6	NAG	D	1306	2	14,14,15	0.41	0	17,19,21	0.42	0
6	NAG	D	1304	2	14,14,15	0.64	0	17,19,21	0.46	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
6	NAG	F	703	1	-	2/6/23/26	0/1/1/1
6	NAG	D	1313	2	-	1/6/23/26	0/1/1/1
6	NAG	C	1303	2	-	3/6/23/26	0/1/1/1
6	NAG	D	1301	2	-	4/6/23/26	0/1/1/1
6	NAG	D	1305	2	-	3/6/23/26	0/1/1/1
6	NAG	E	702	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	2	-	1/6/23/26	0/1/1/1
6	NAG	C	1304	2	-	3/6/23/26	0/1/1/1
6	NAG	B	1306	2	-	1/6/23/26	0/1/1/1
6	NAG	D	1303	2	-	1/6/23/26	0/1/1/1
6	NAG	D	1307	2	-	3/6/23/26	0/1/1/1
6	NAG	C	1309	2	-	3/6/23/26	0/1/1/1
6	NAG	B	1301	2	-	3/6/23/26	0/1/1/1
6	NAG	D	1309	2	-	0/6/23/26	0/1/1/1
6	NAG	B	1304	2	-	1/6/23/26	0/1/1/1
6	NAG	D	1314	2	-	4/6/23/26	0/1/1/1
6	NAG	A	703	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1307	2	-	2/6/23/26	0/1/1/1
6	NAG	C	1301	2	-	3/6/23/26	0/1/1/1
6	NAG	C	1308	2	-	3/6/23/26	0/1/1/1
6	NAG	B	1305	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1303	2	-	3/6/23/26	0/1/1/1
6	NAG	C	1305	2	-	0/6/23/26	0/1/1/1
6	NAG	B	1308	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1311	2	-	5/6/23/26	0/1/1/1
6	NAG	D	1312	2	-	4/6/23/26	0/1/1/1
6	NAG	F	702	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1302	2	-	4/6/23/26	0/1/1/1
6	NAG	A	702	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1306	2	-	5/6/23/26	0/1/1/1
6	NAG	D	1310	2	-	5/6/23/26	0/1/1/1
6	NAG	B	1307	2	-	5/6/23/26	0/1/1/1
6	NAG	E	703	1	-	2/6/23/26	0/1/1/1
6	NAG	D	1302	2	-	0/6/23/26	0/1/1/1
6	NAG	D	1308	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1306	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	1304	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1314	NAG	C1-C2-N2	6.05	120.82	110.49
6	D	1314	NAG	C2-N2-C7	5.56	130.81	122.90
6	F	703	NAG	C2-N2-C7	3.77	128.28	122.90
6	A	703	NAG	C2-N2-C7	3.77	128.26	122.90
6	E	703	NAG	C2-N2-C7	3.76	128.26	122.90

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1307	NAG	C3-C2-N2-C7
6	C	1306	NAG	C3-C2-N2-C7
6	C	1309	NAG	C3-C2-N2-C7
6	C	1309	NAG	C8-C7-N2-C2
6	C	1309	NAG	O7-C7-N2-C2

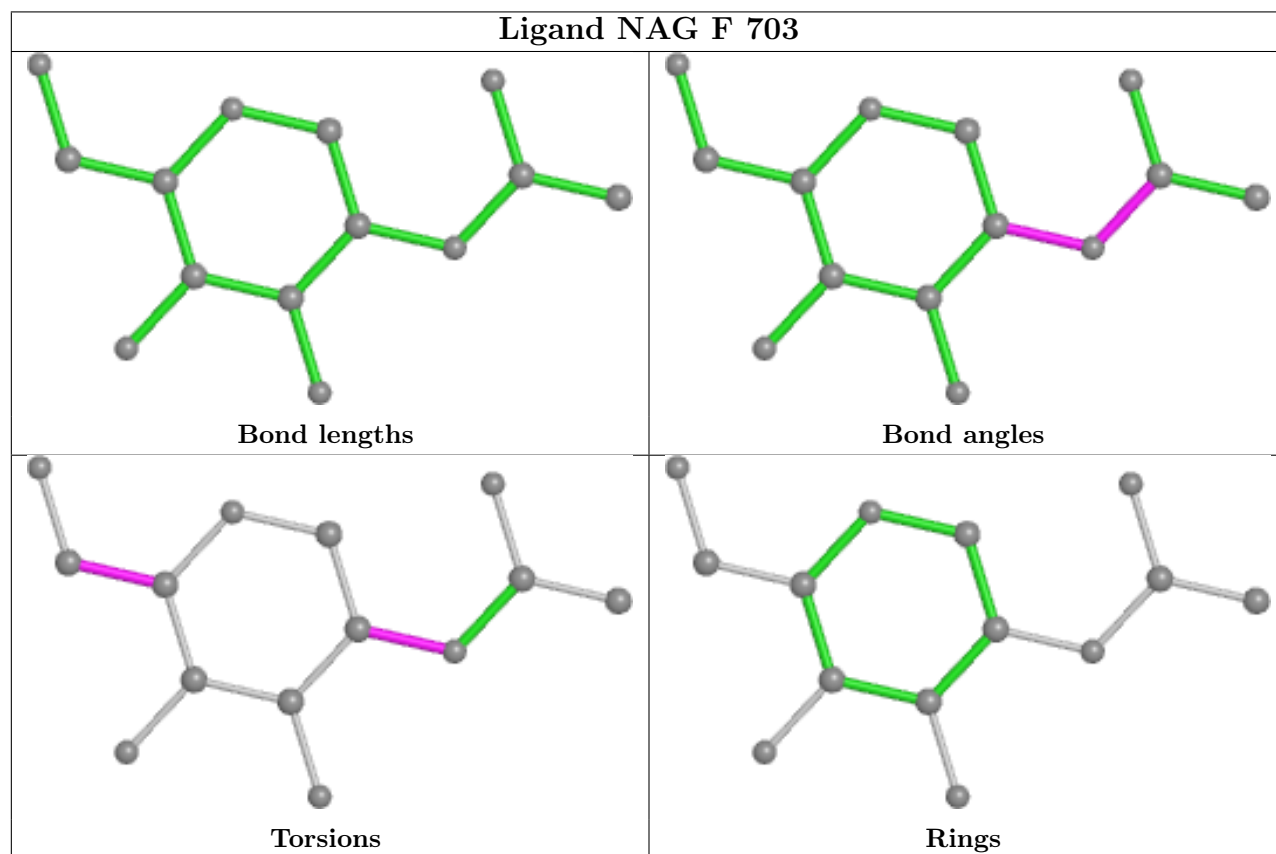
There are no ring outliers.

6 monomers are involved in 12 short contacts:

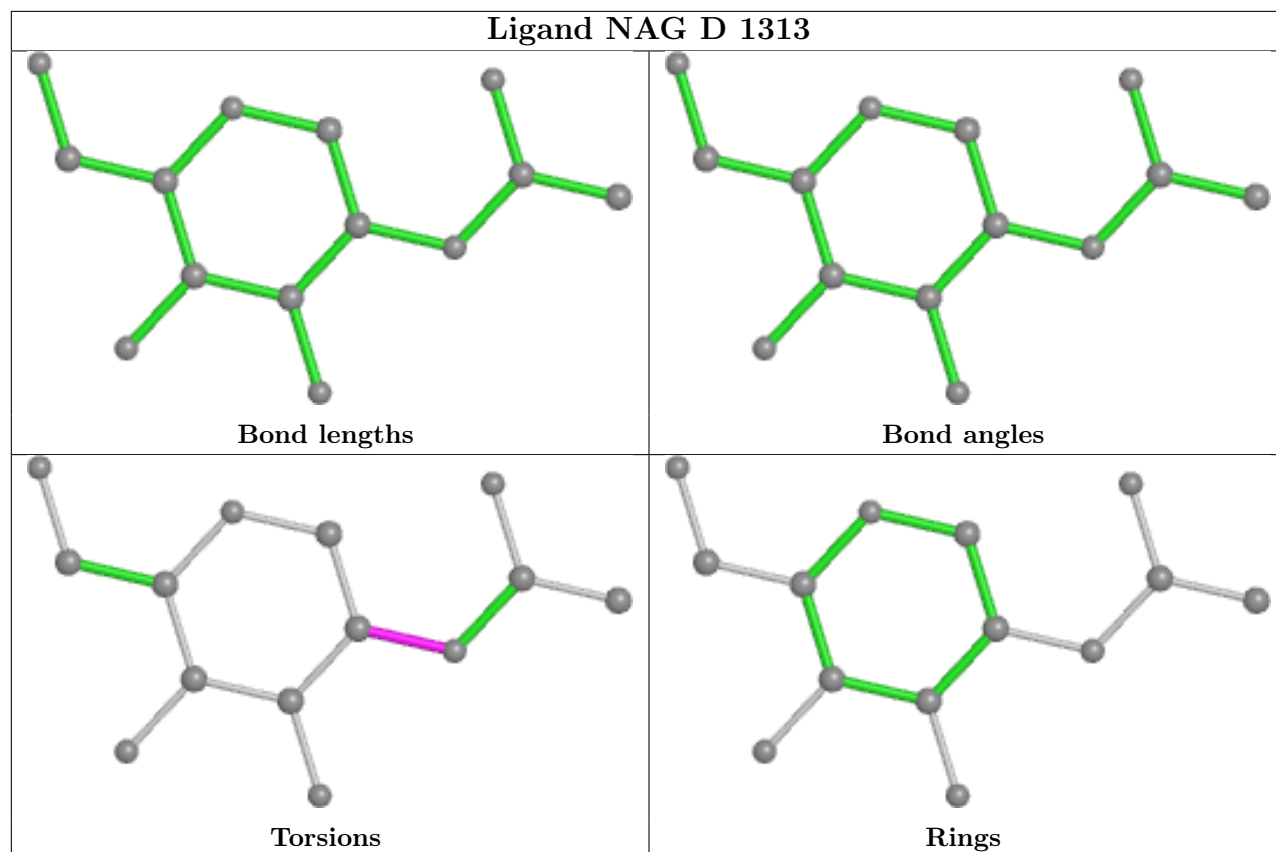
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1309	NAG	1	0
6	D	1309	NAG	1	0
6	D	1314	NAG	5	0
6	C	1308	NAG	1	0
6	C	1302	NAG	1	0
6	D	1304	NAG	3	0

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

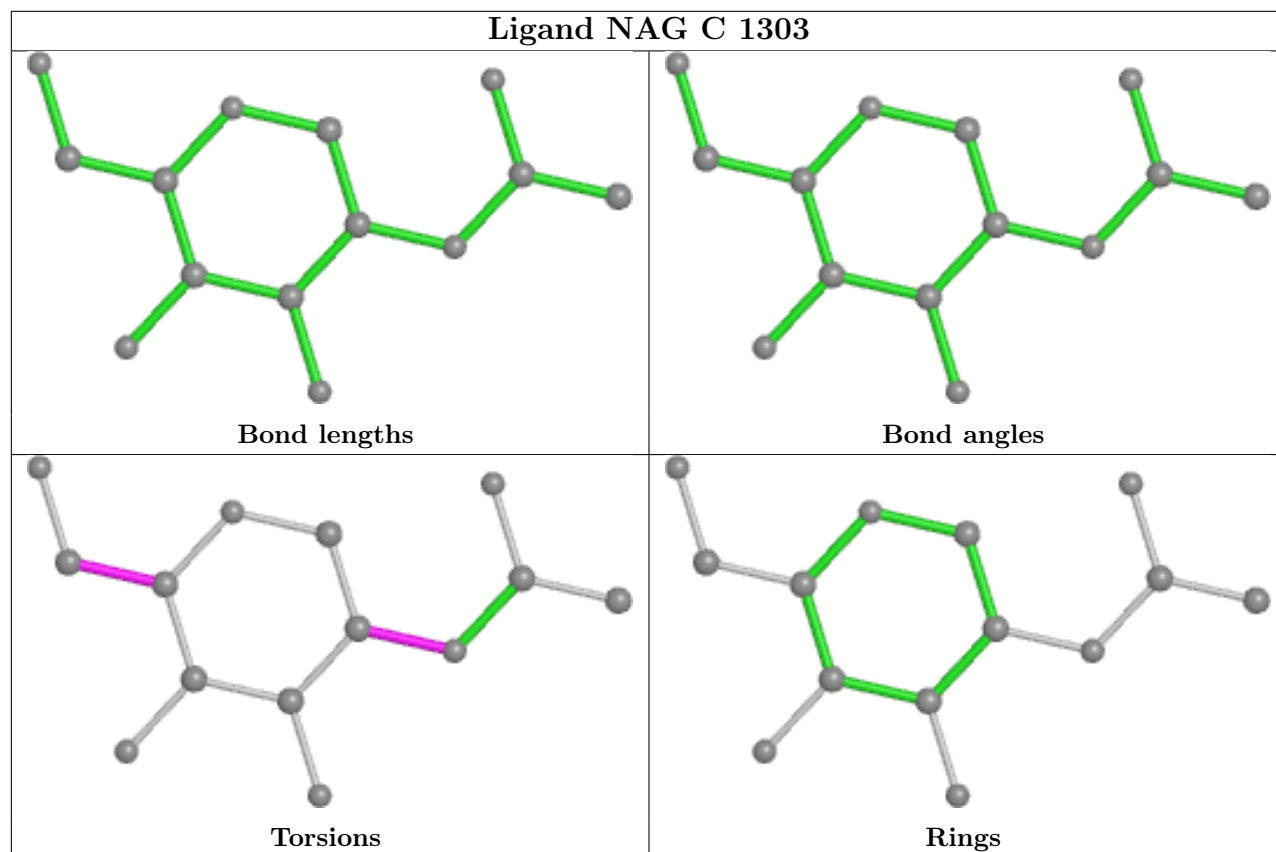
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



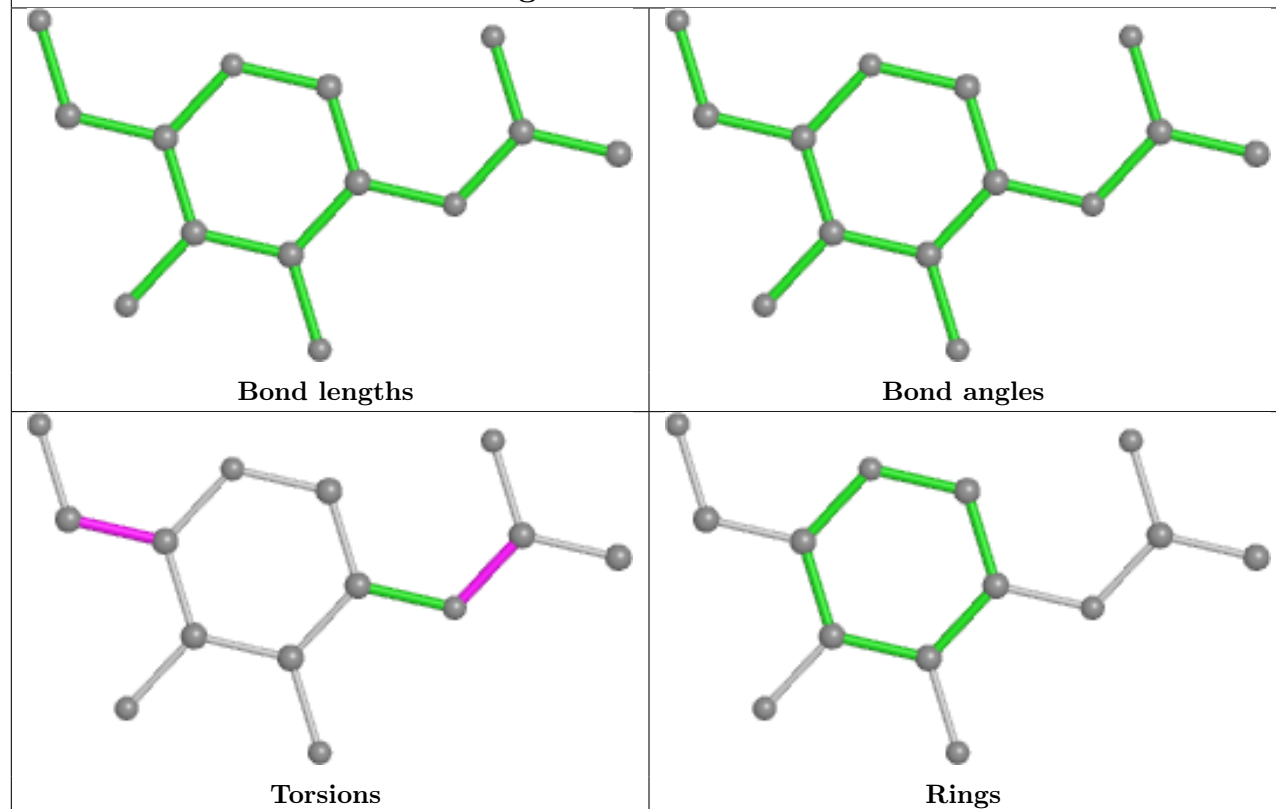
Ligand NAG D 1313



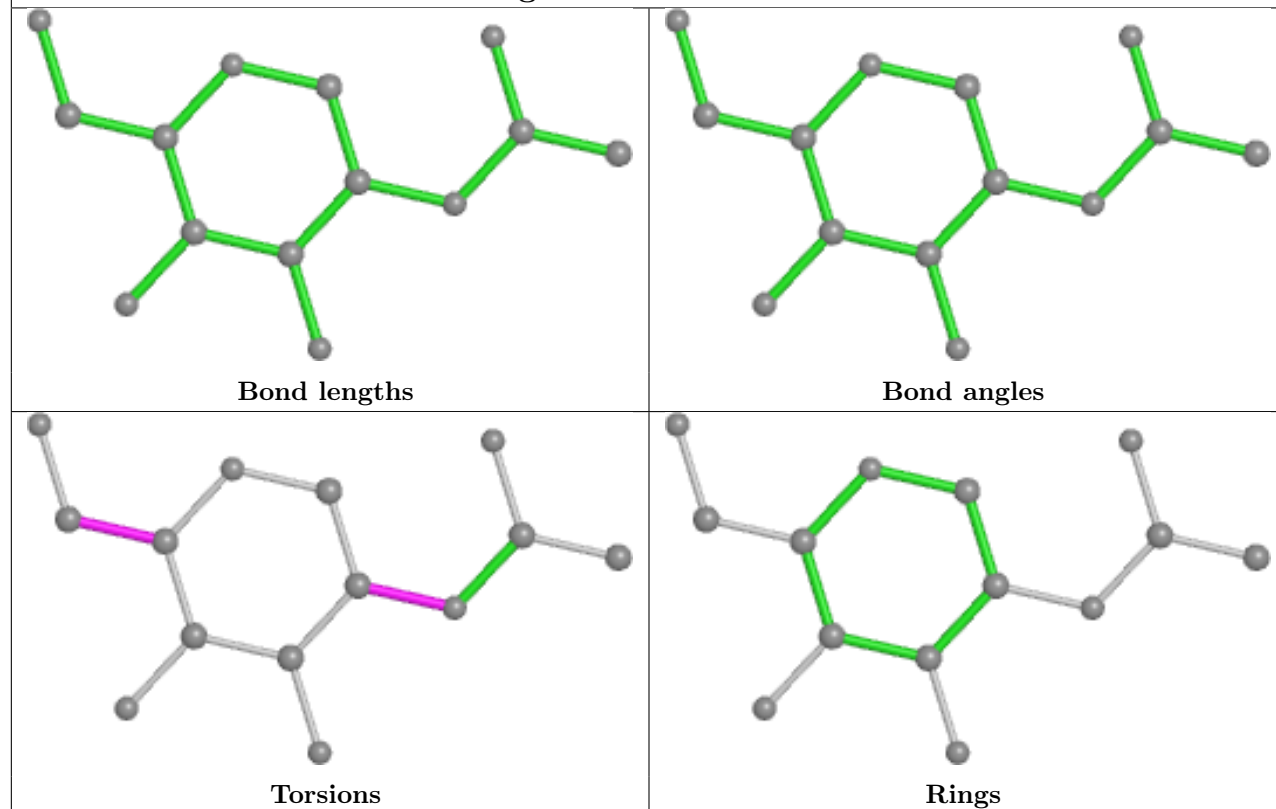
Ligand NAG C 1303

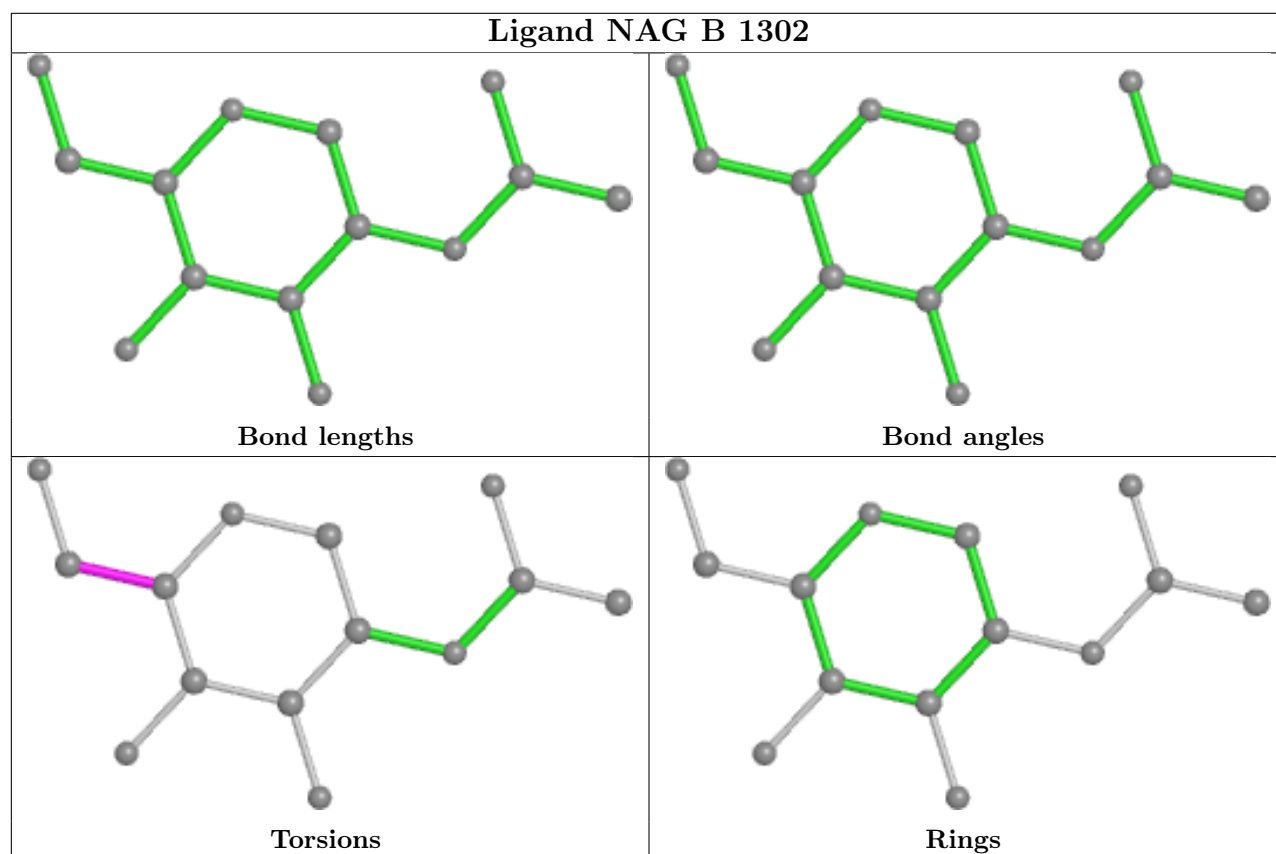
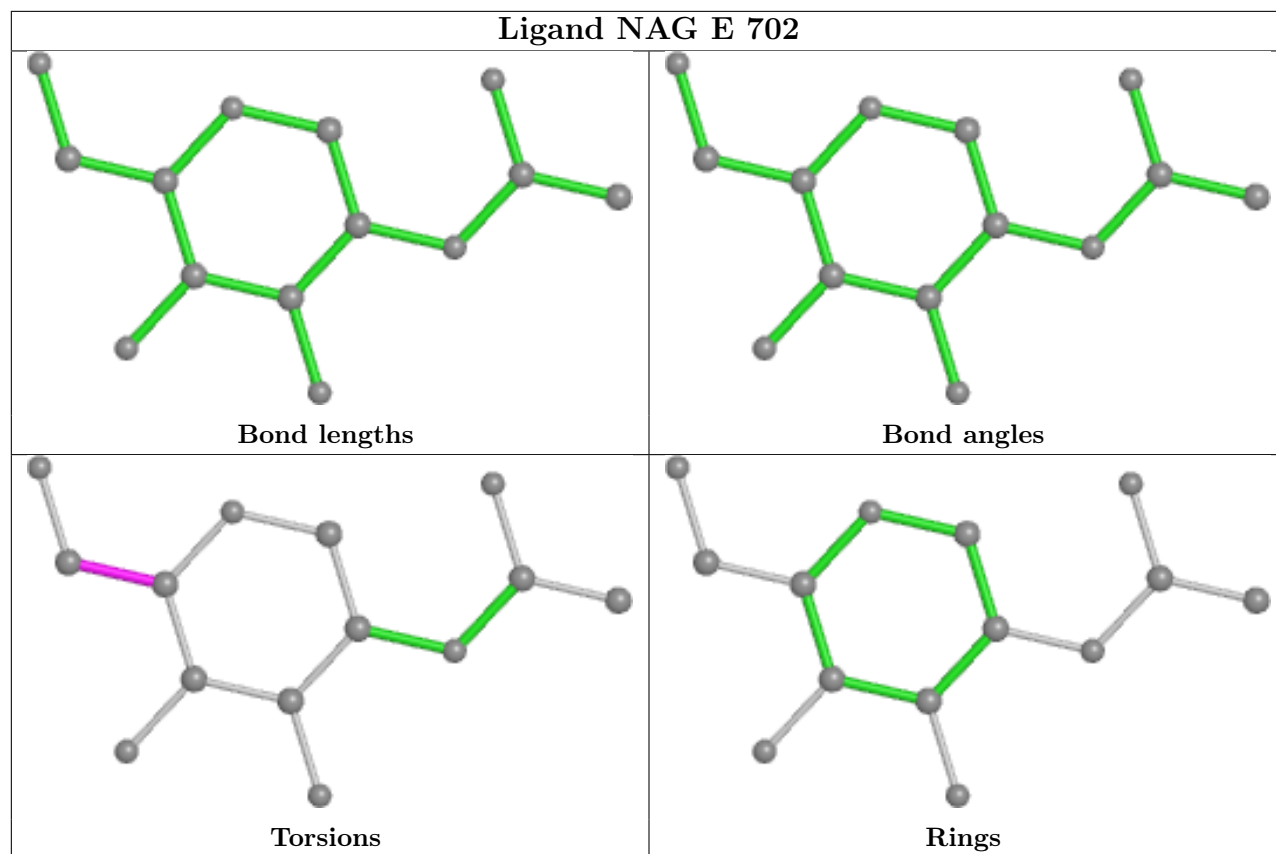


Ligand NAG D 1301

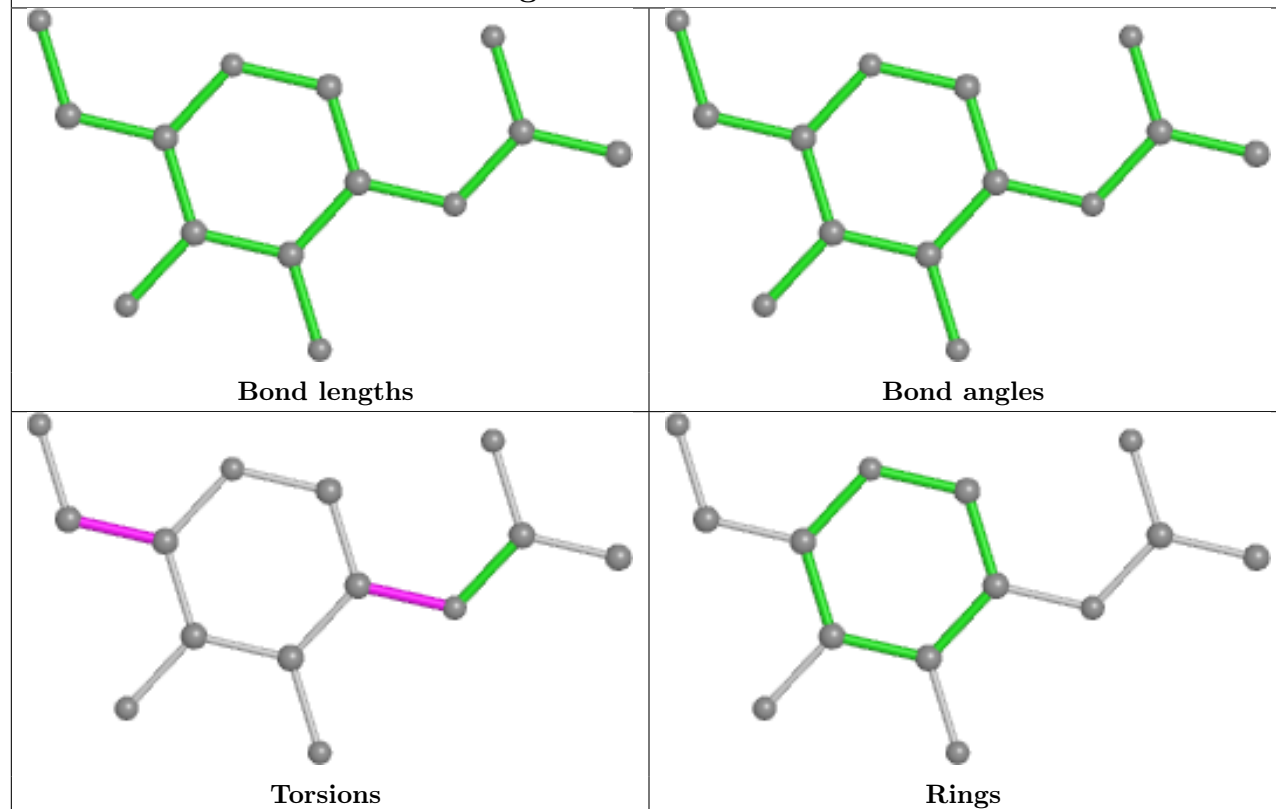


Ligand NAG D 1305

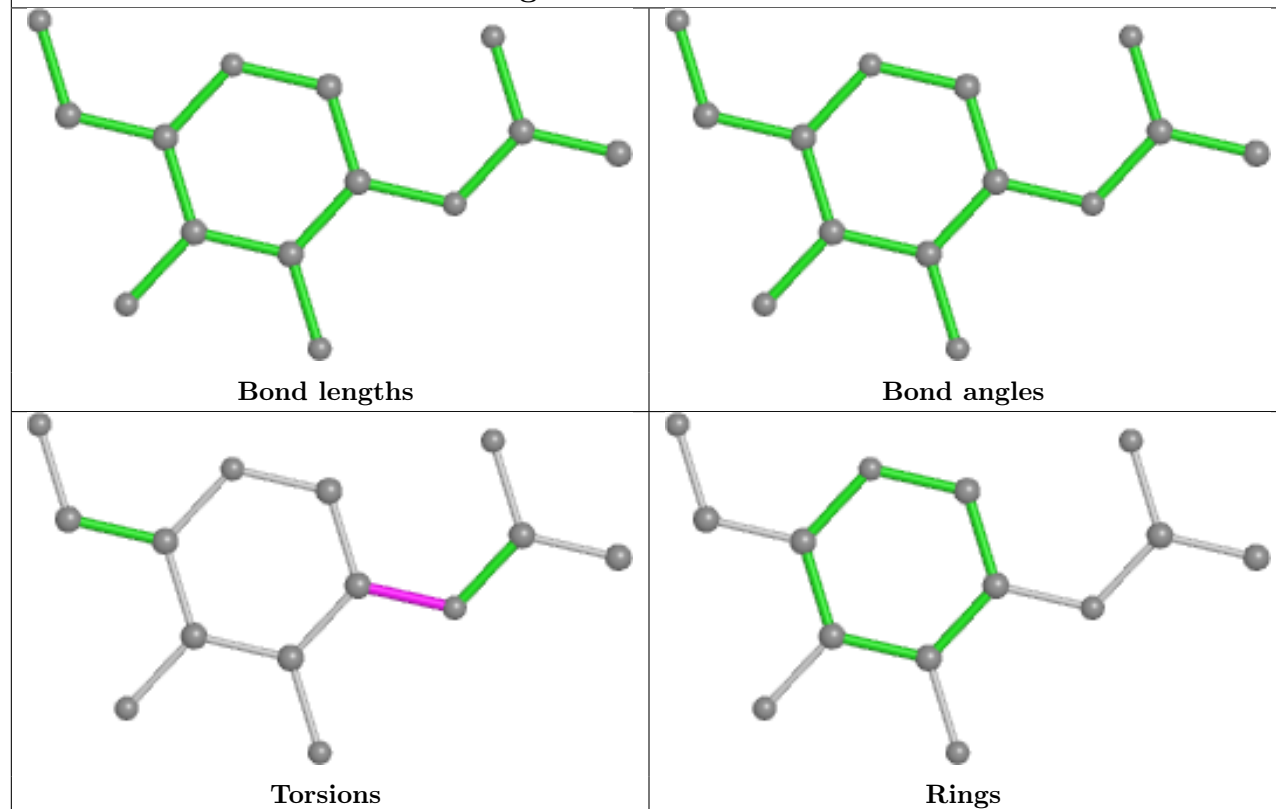


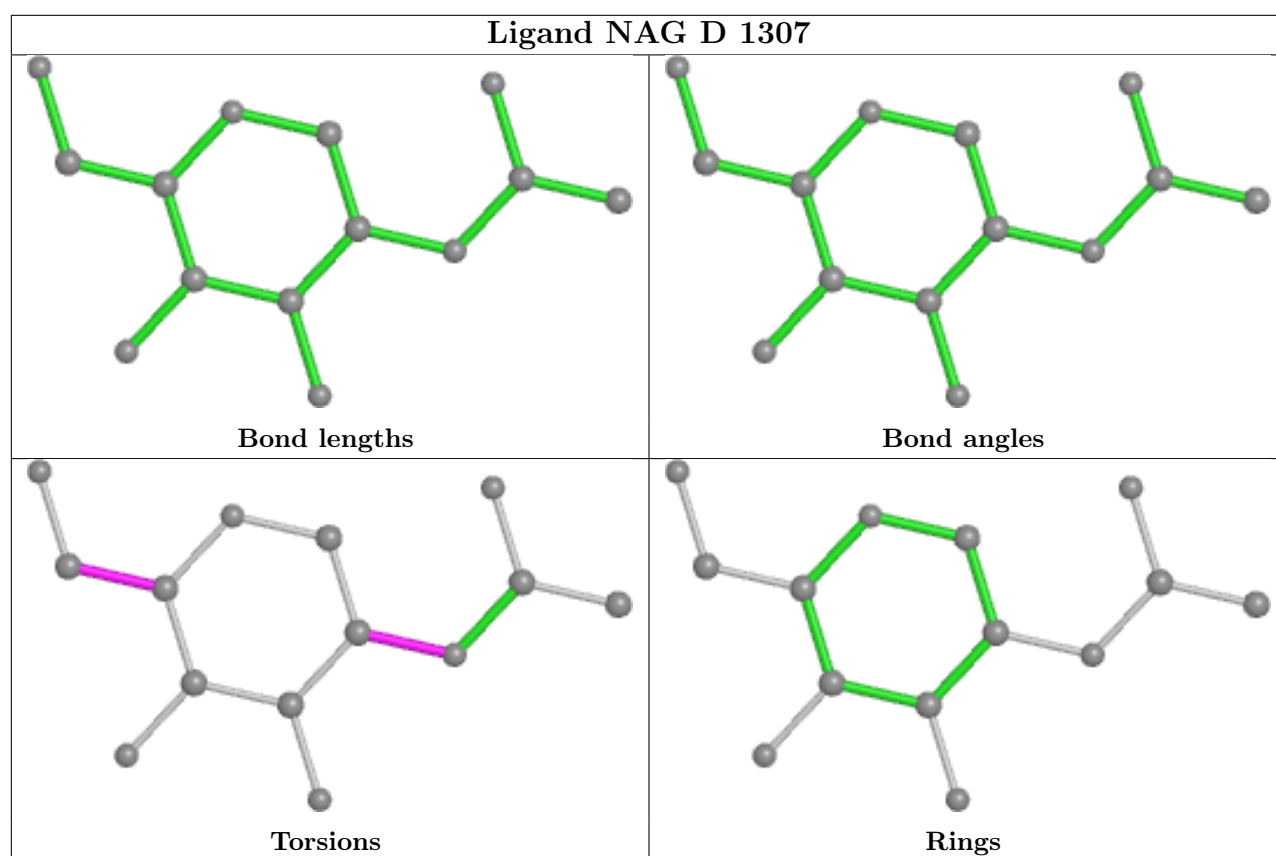
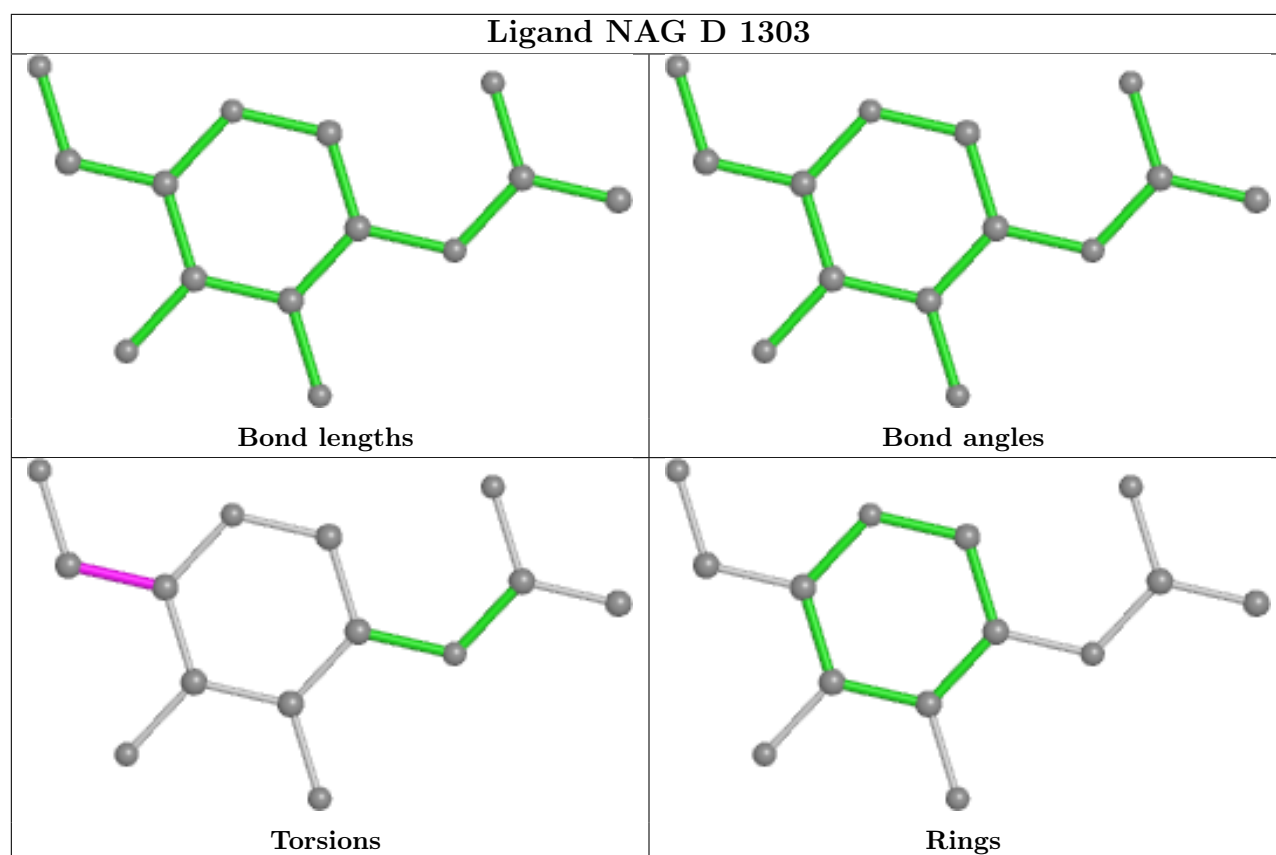


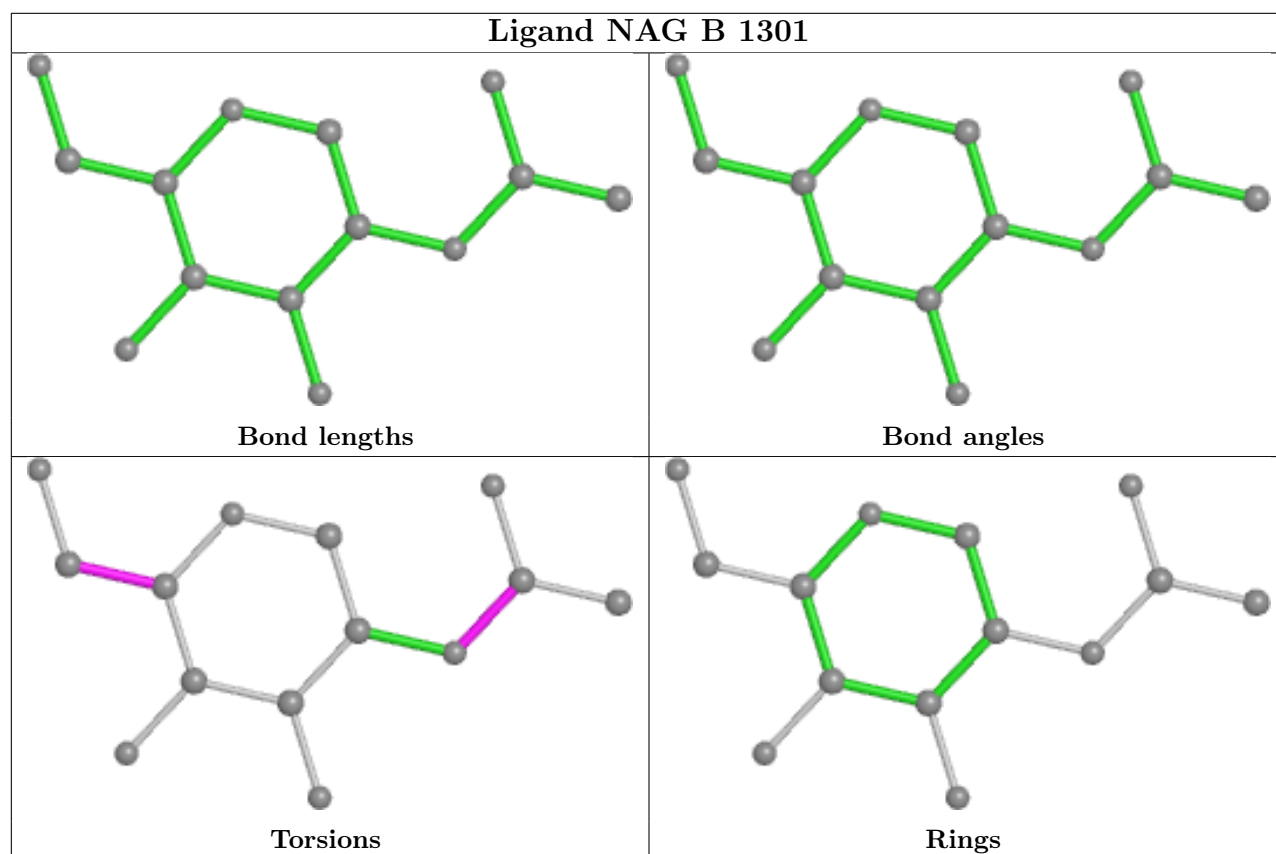
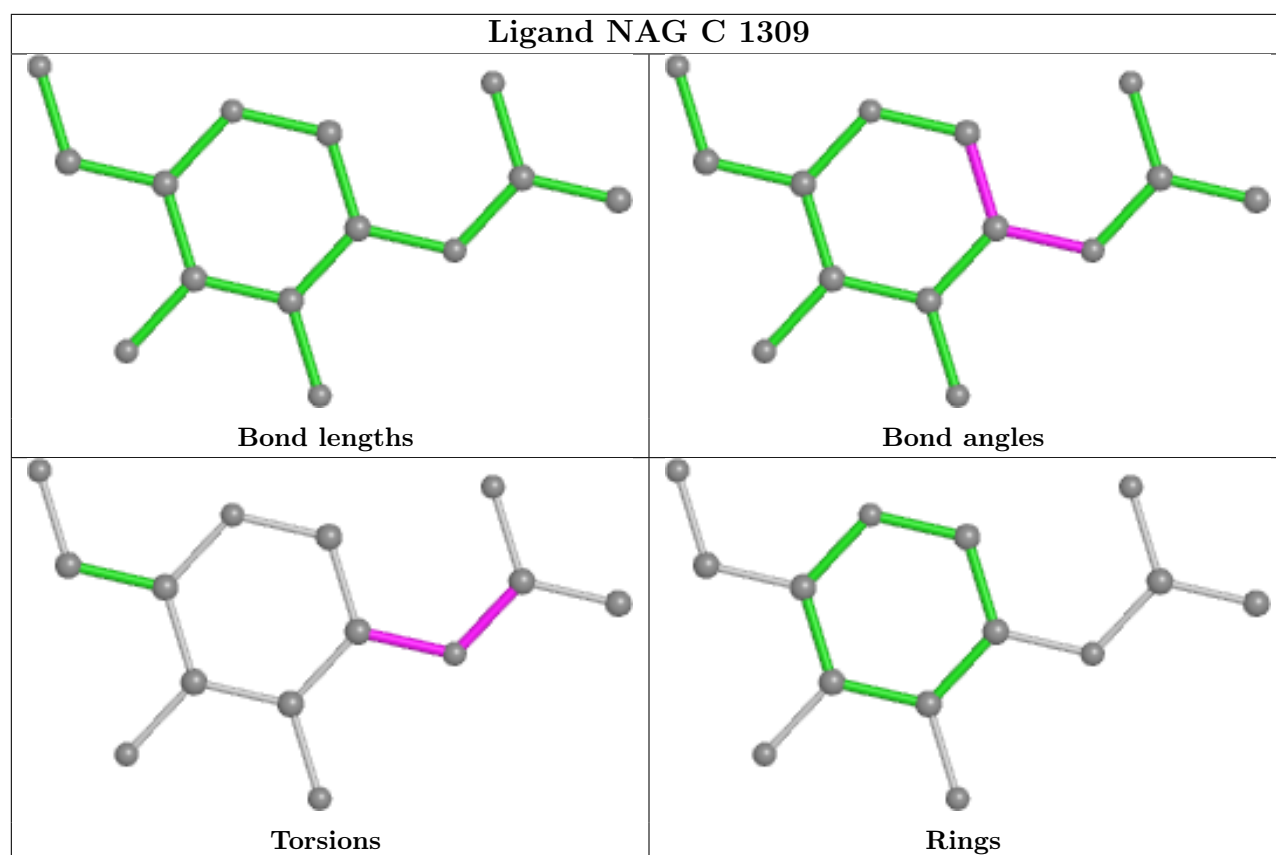
Ligand NAG C 1304

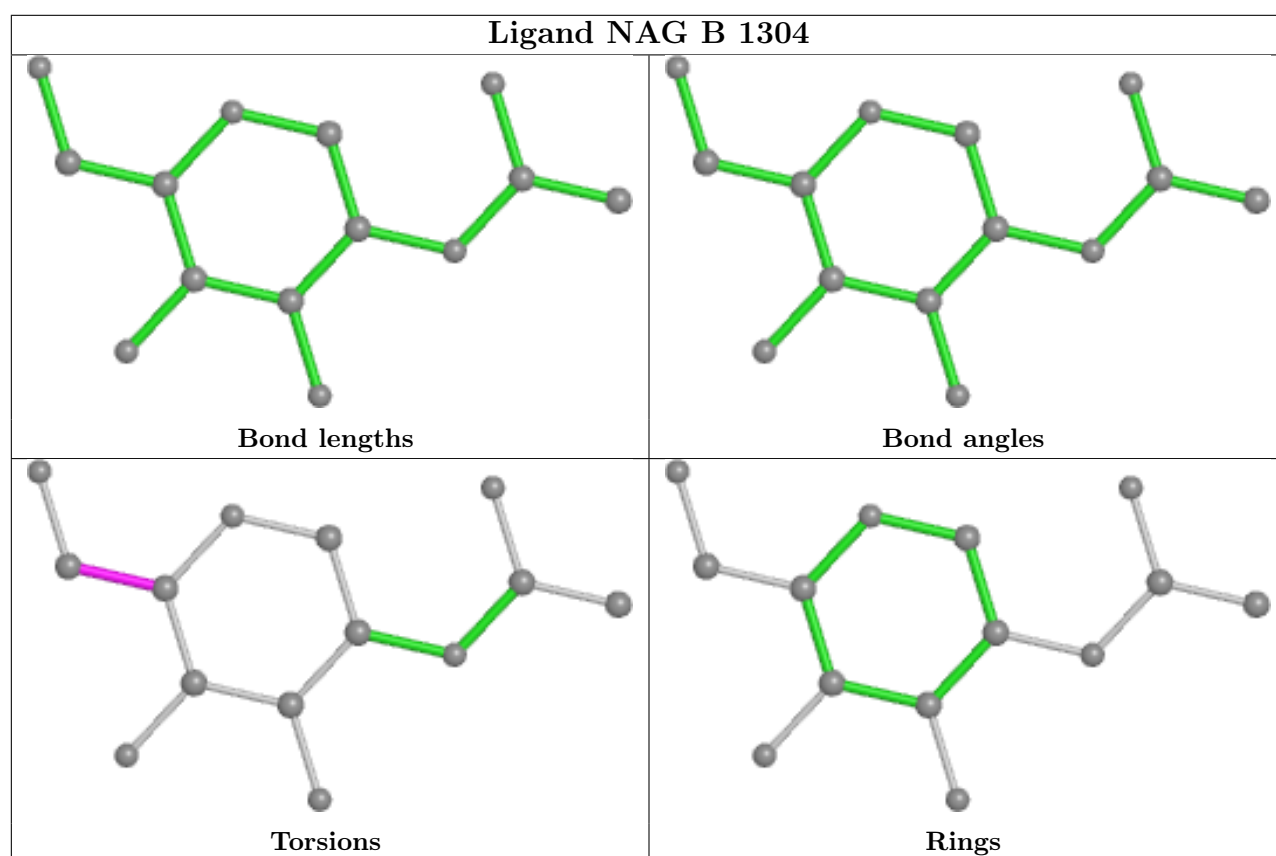
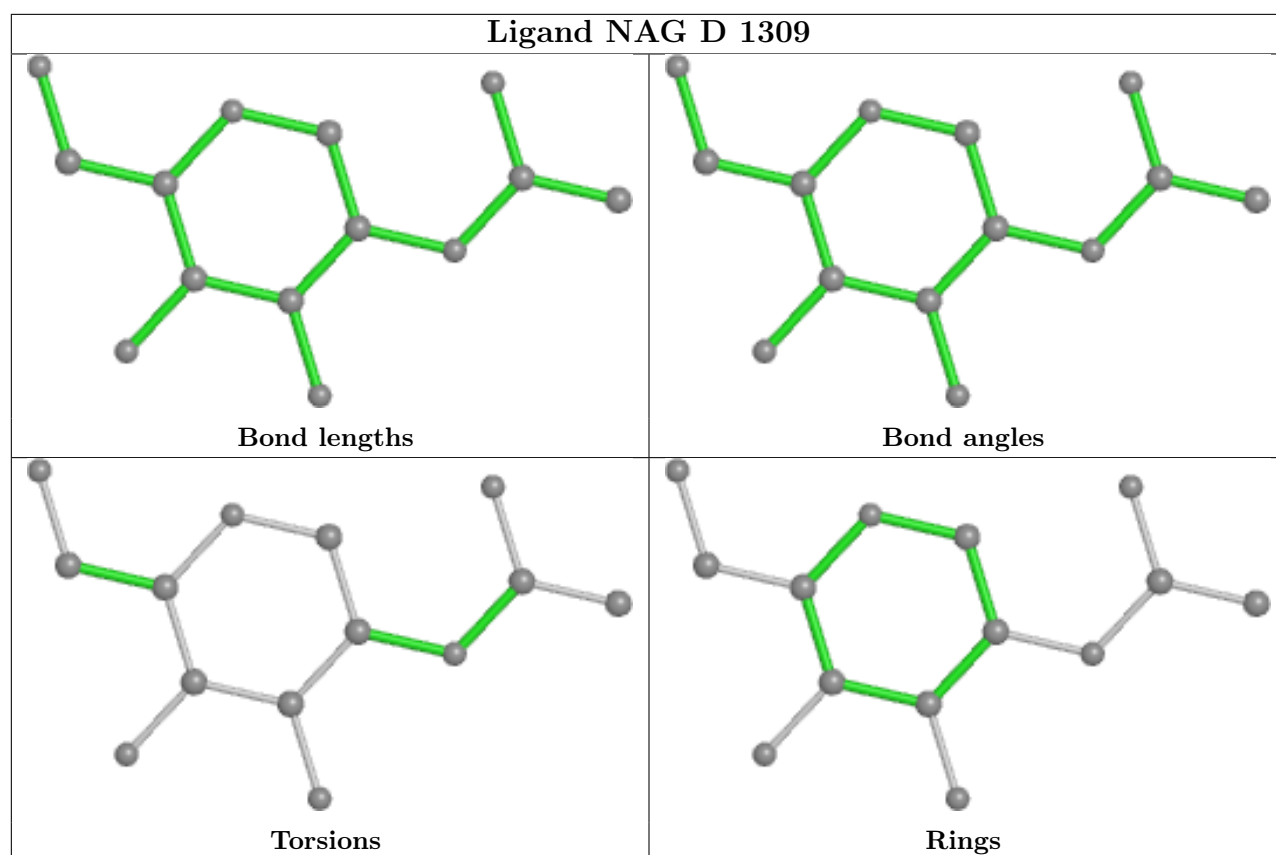


Ligand NAG B 1306

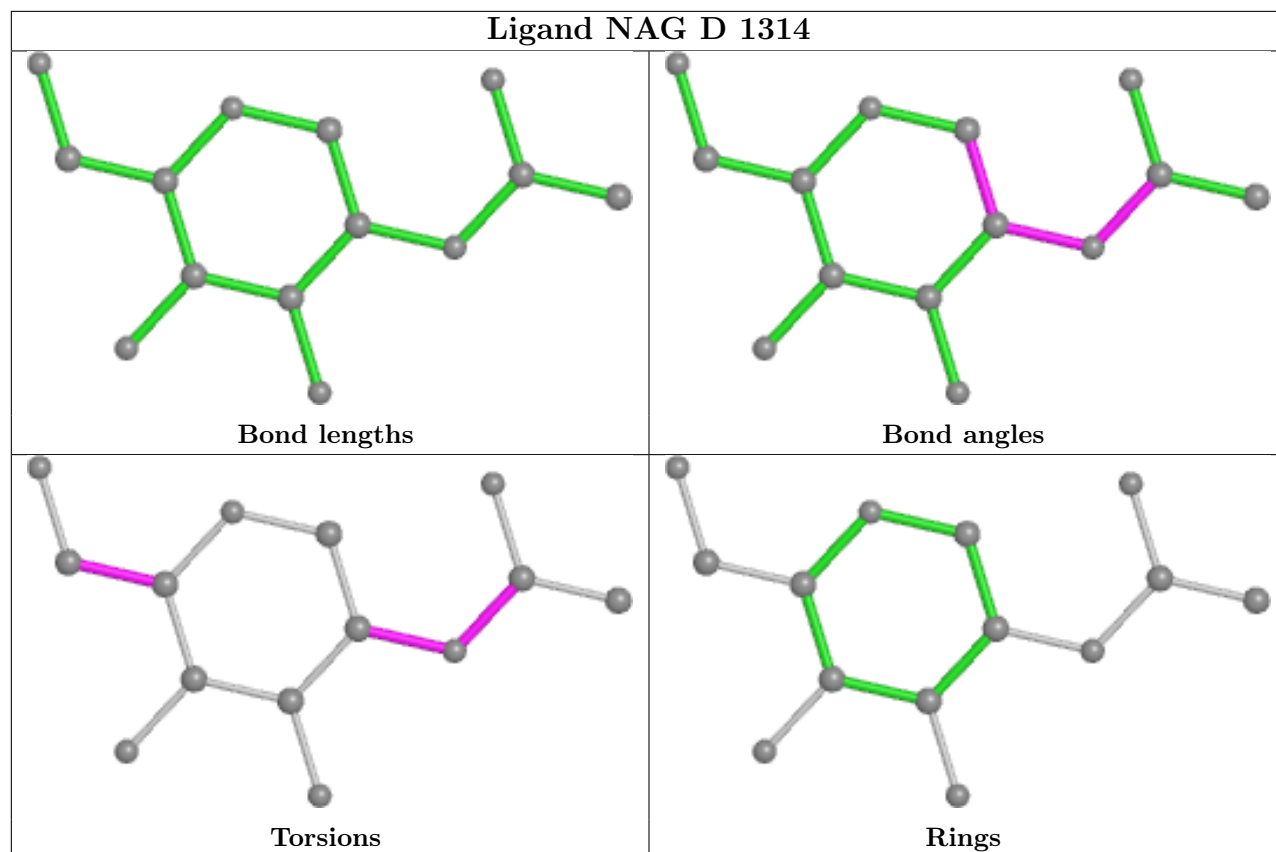




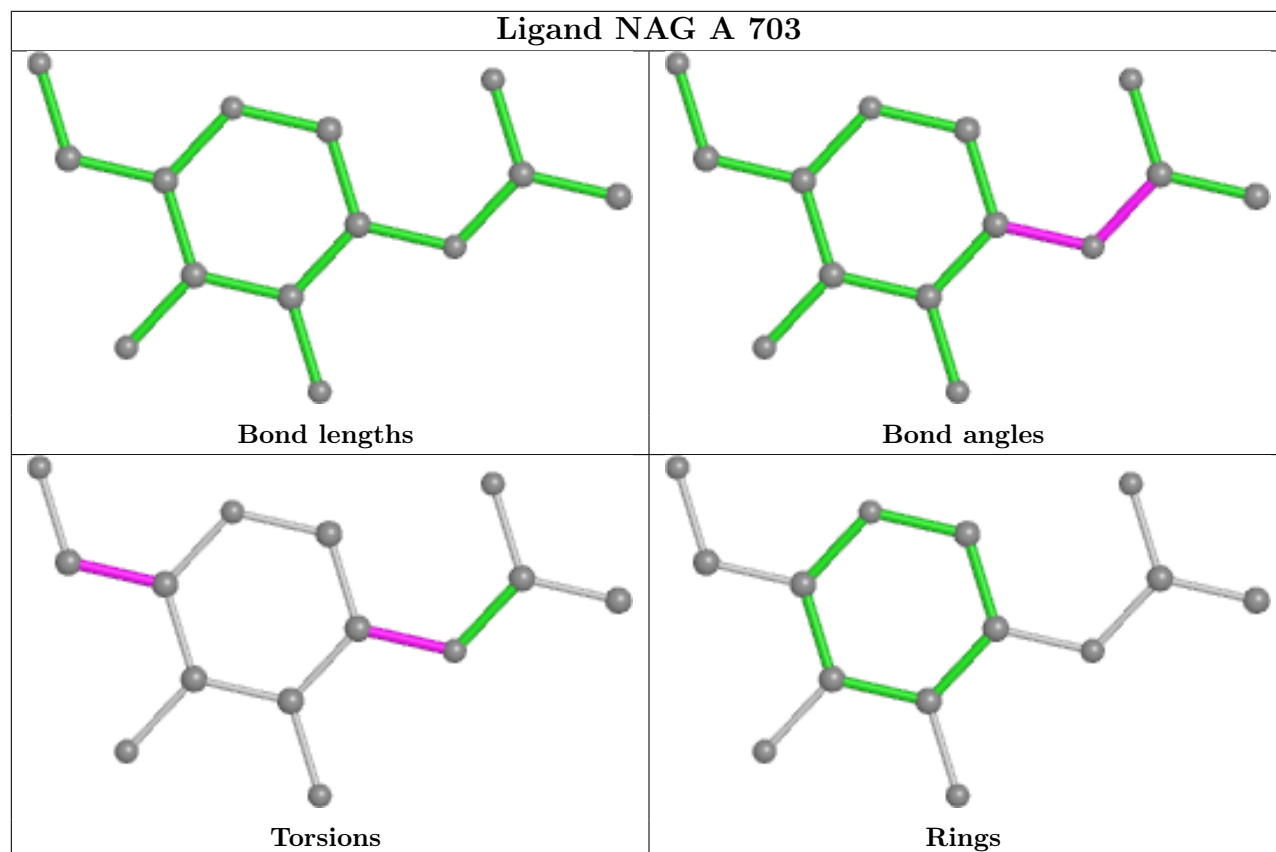


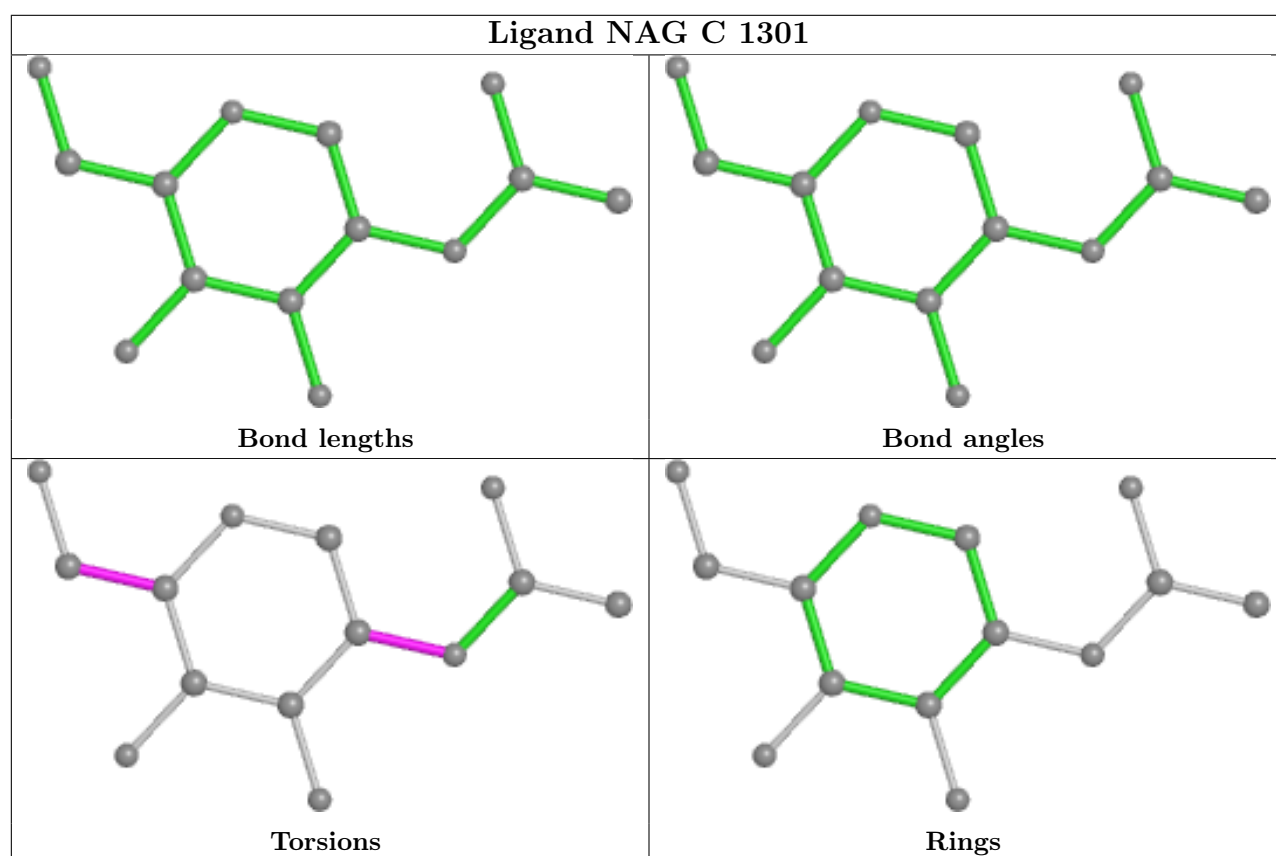
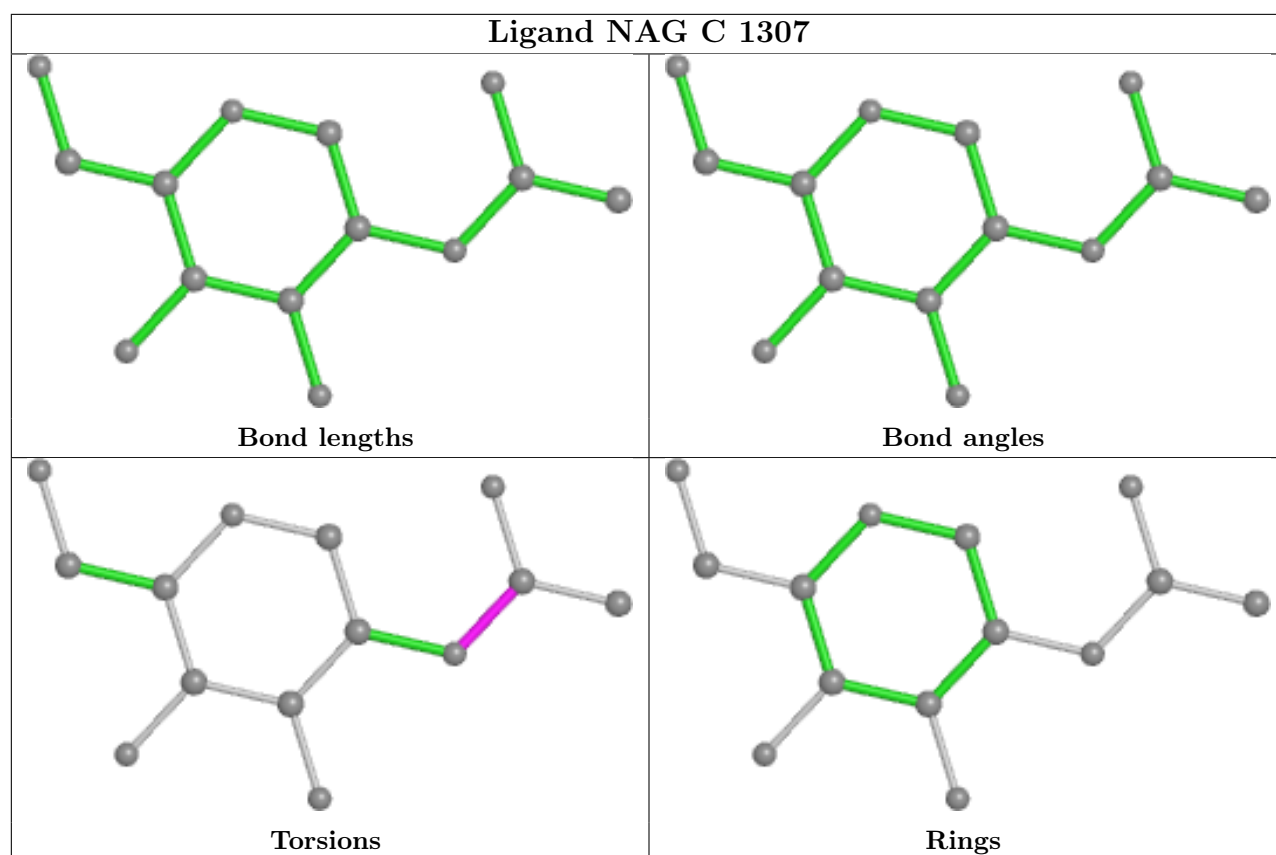


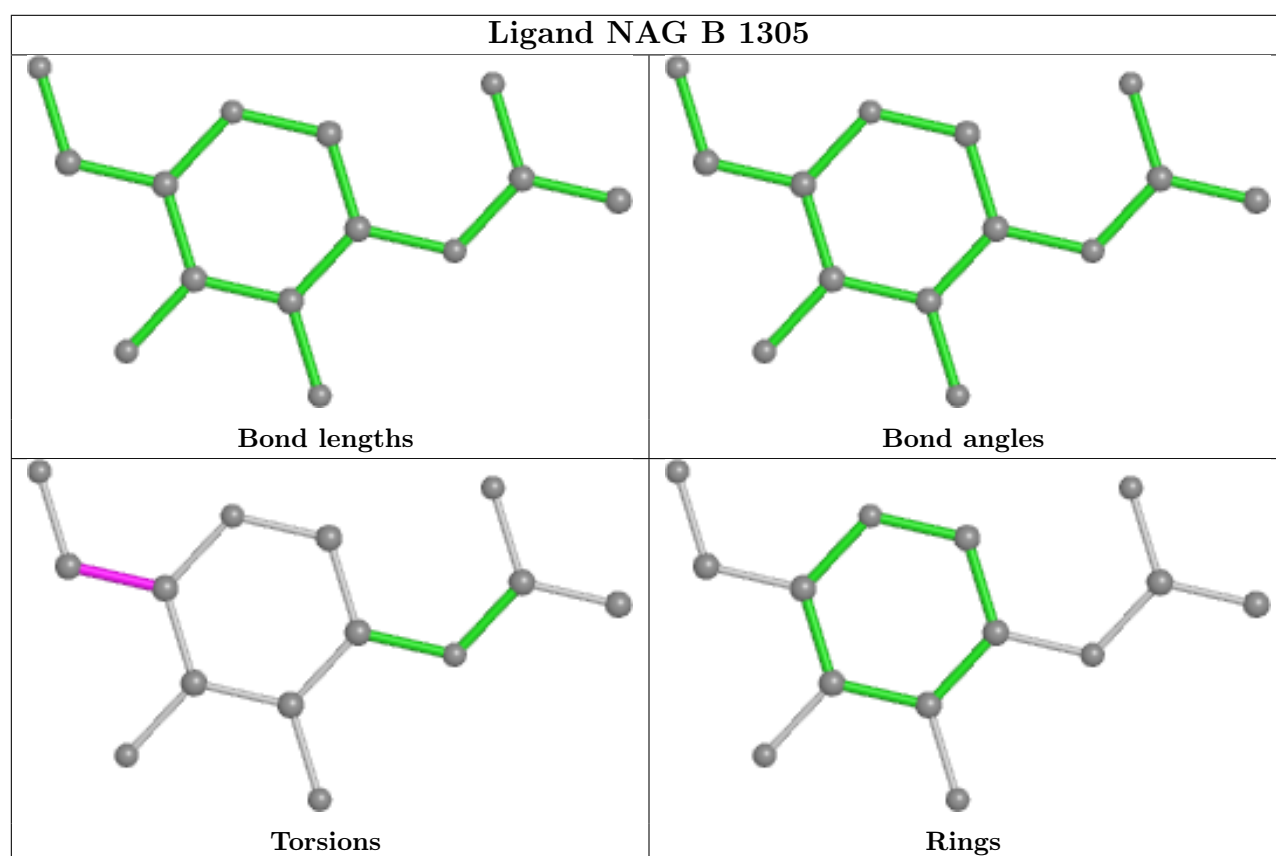
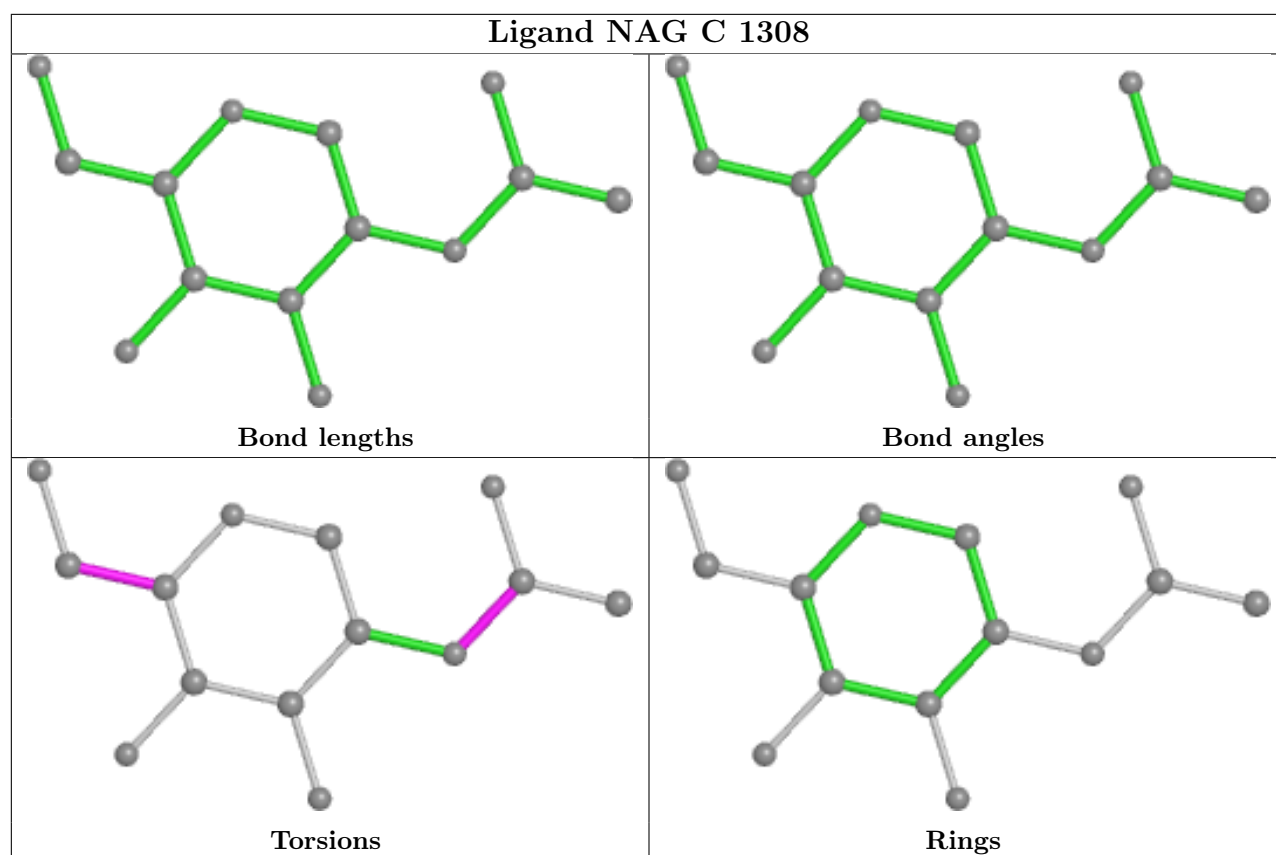
Ligand NAG D 1314



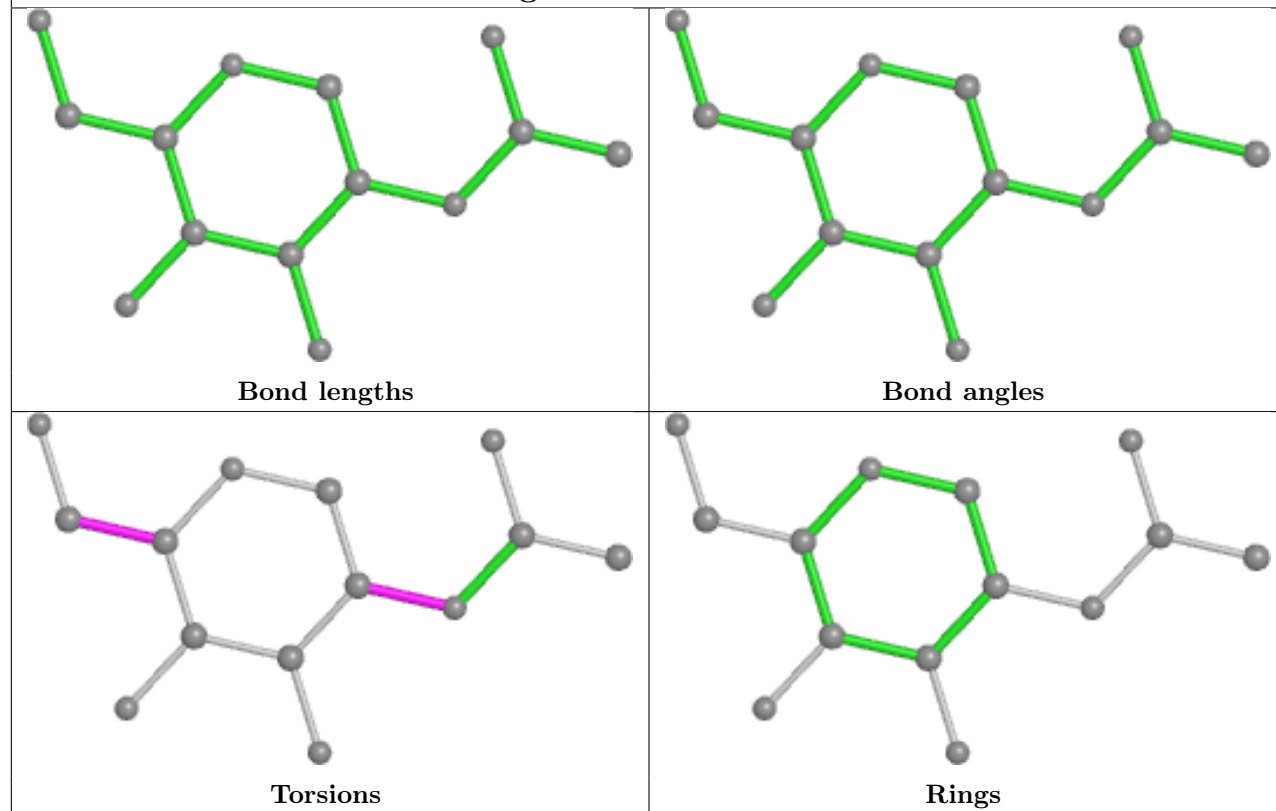
Ligand NAG A 703



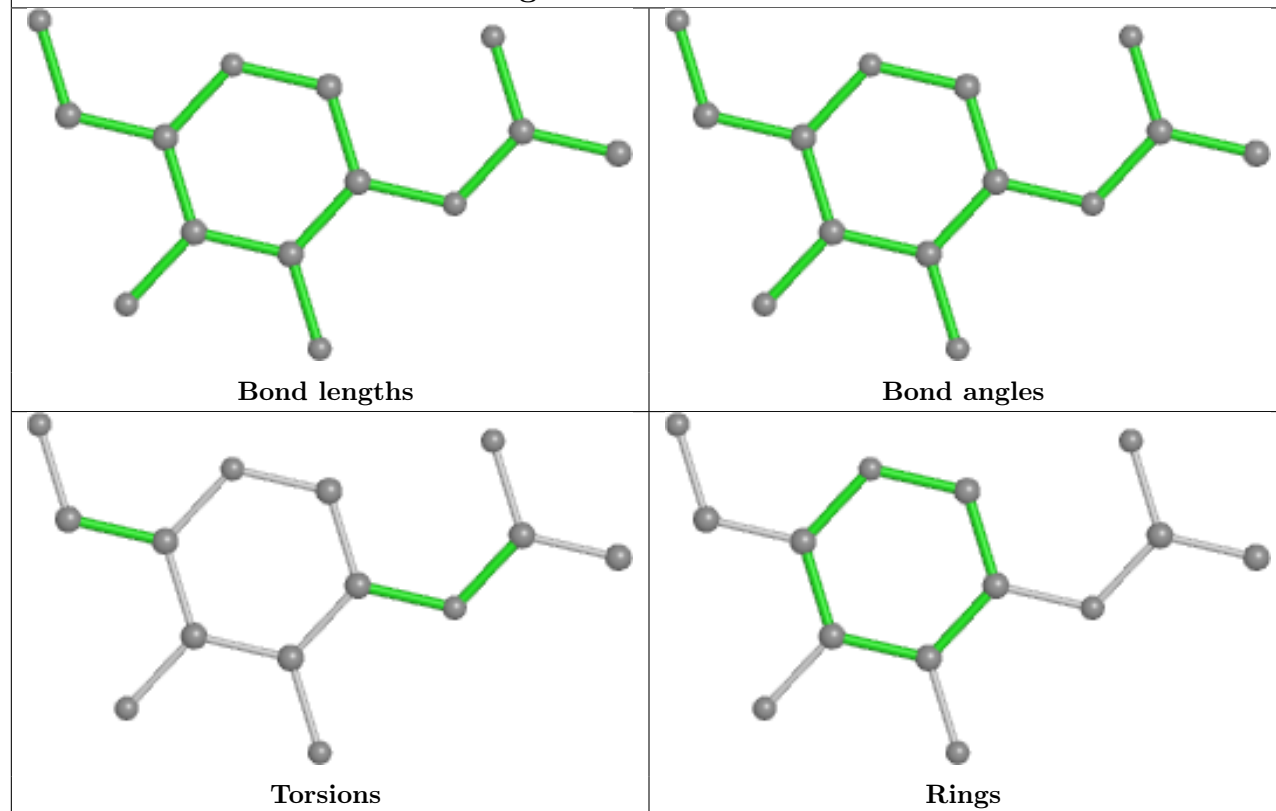


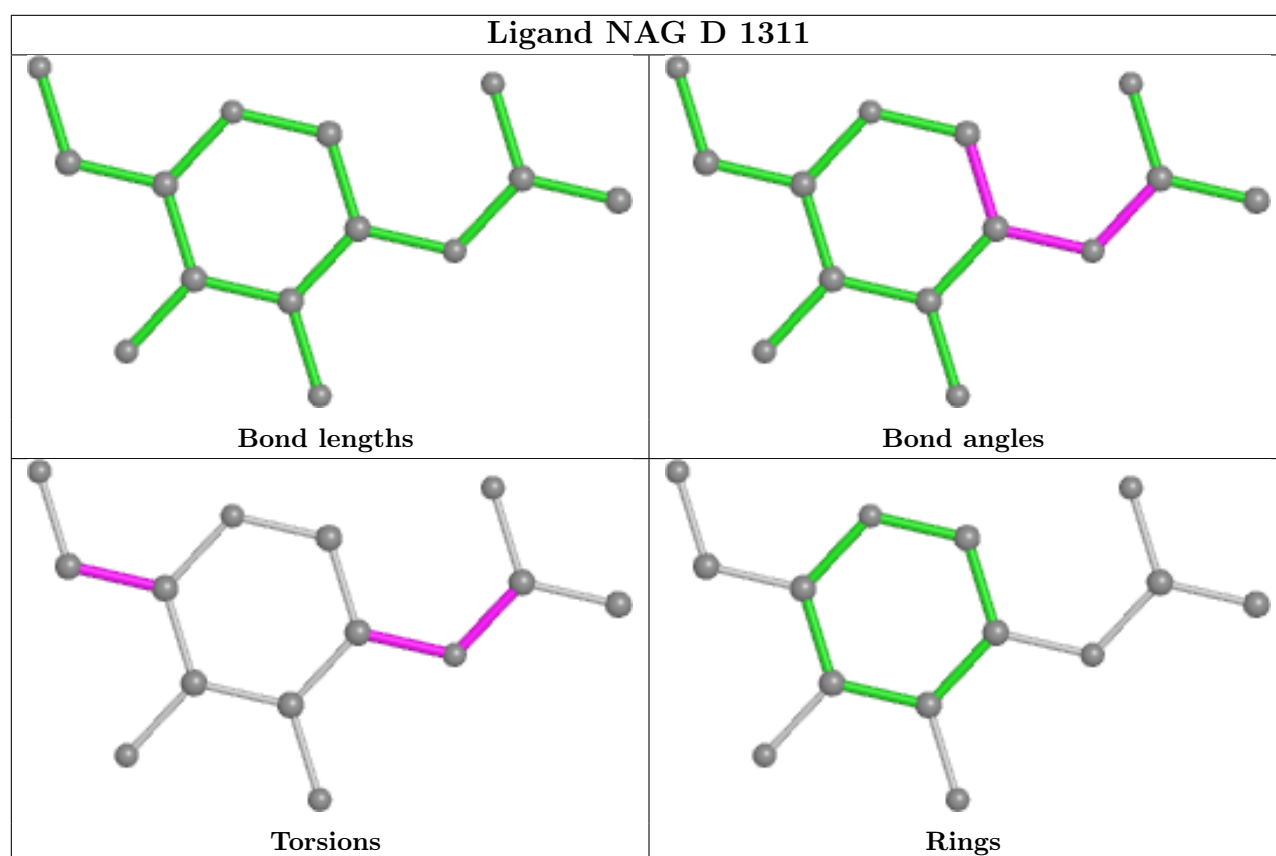
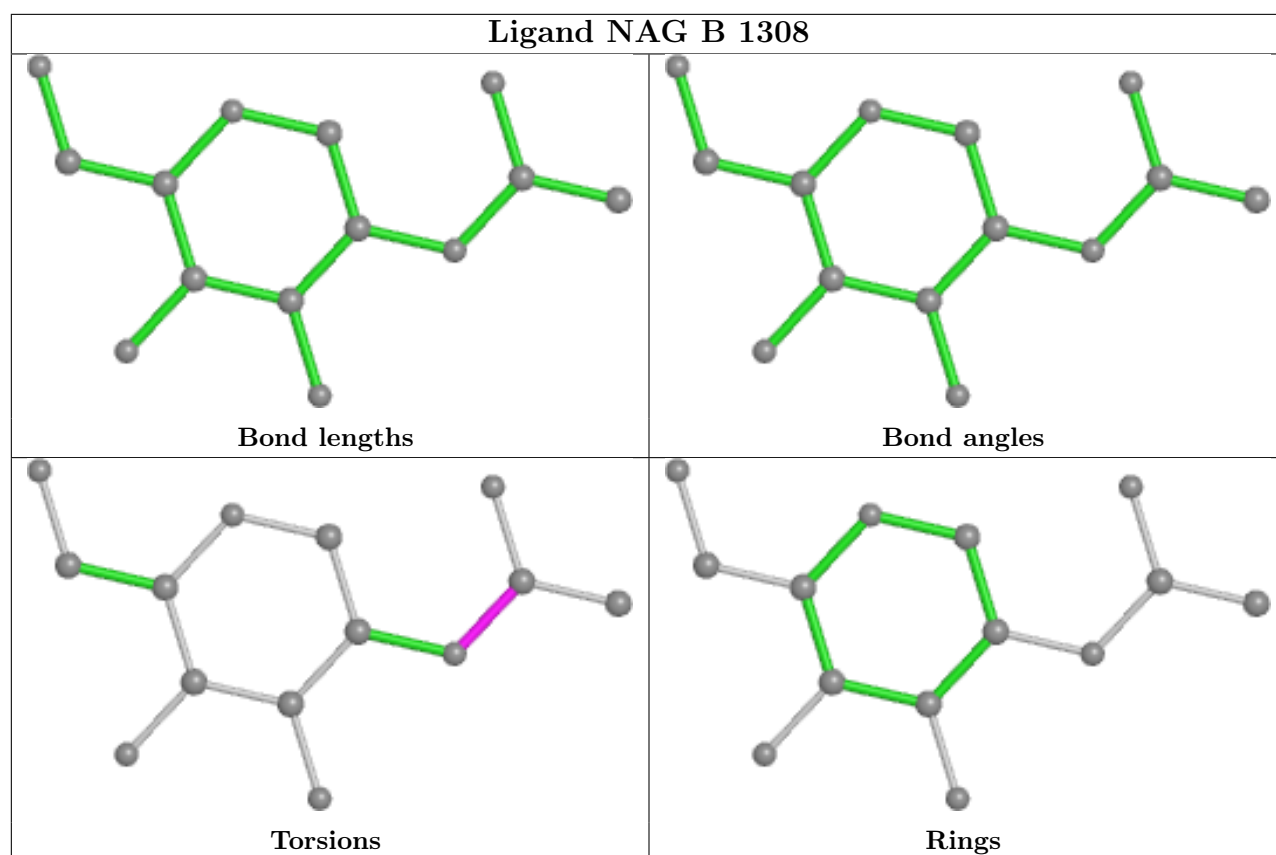


Ligand NAG B 1303

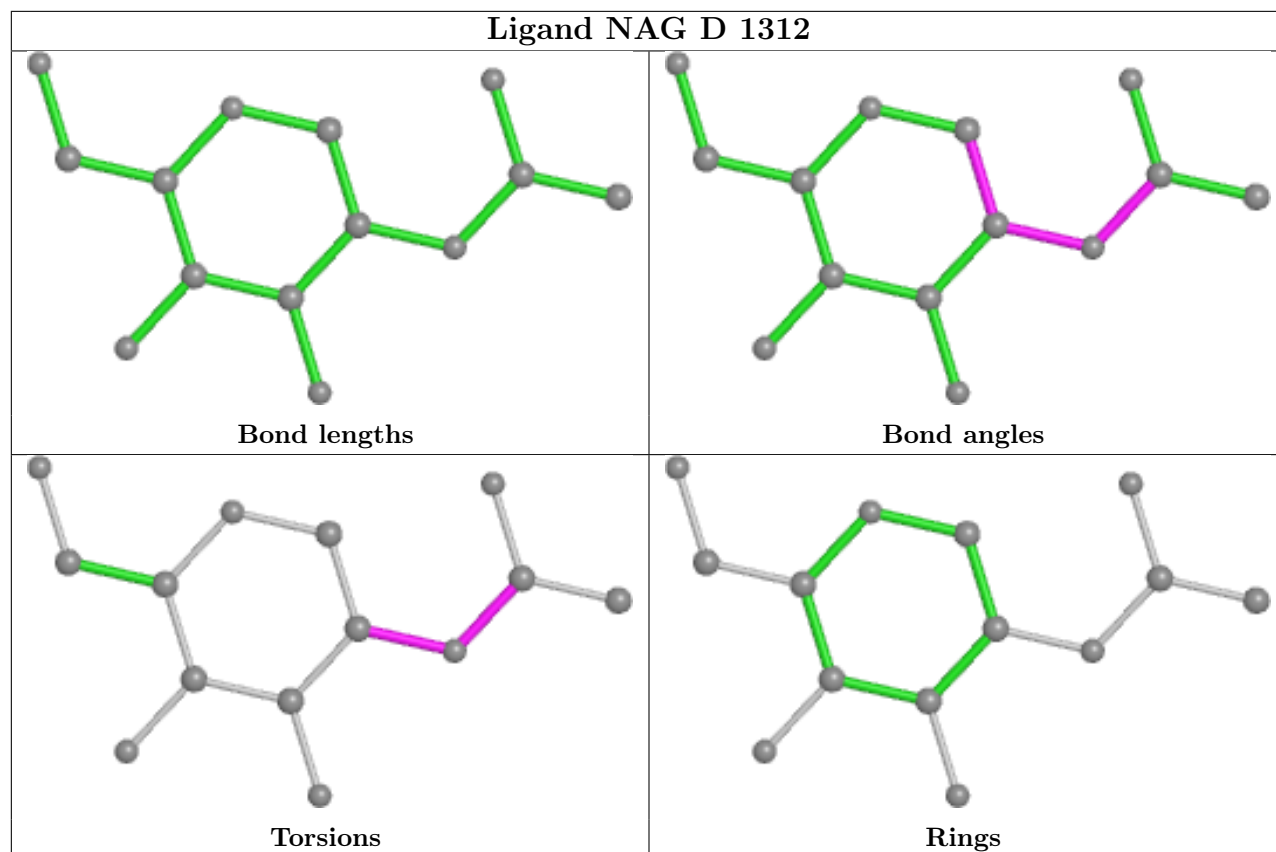


Ligand NAG C 1305

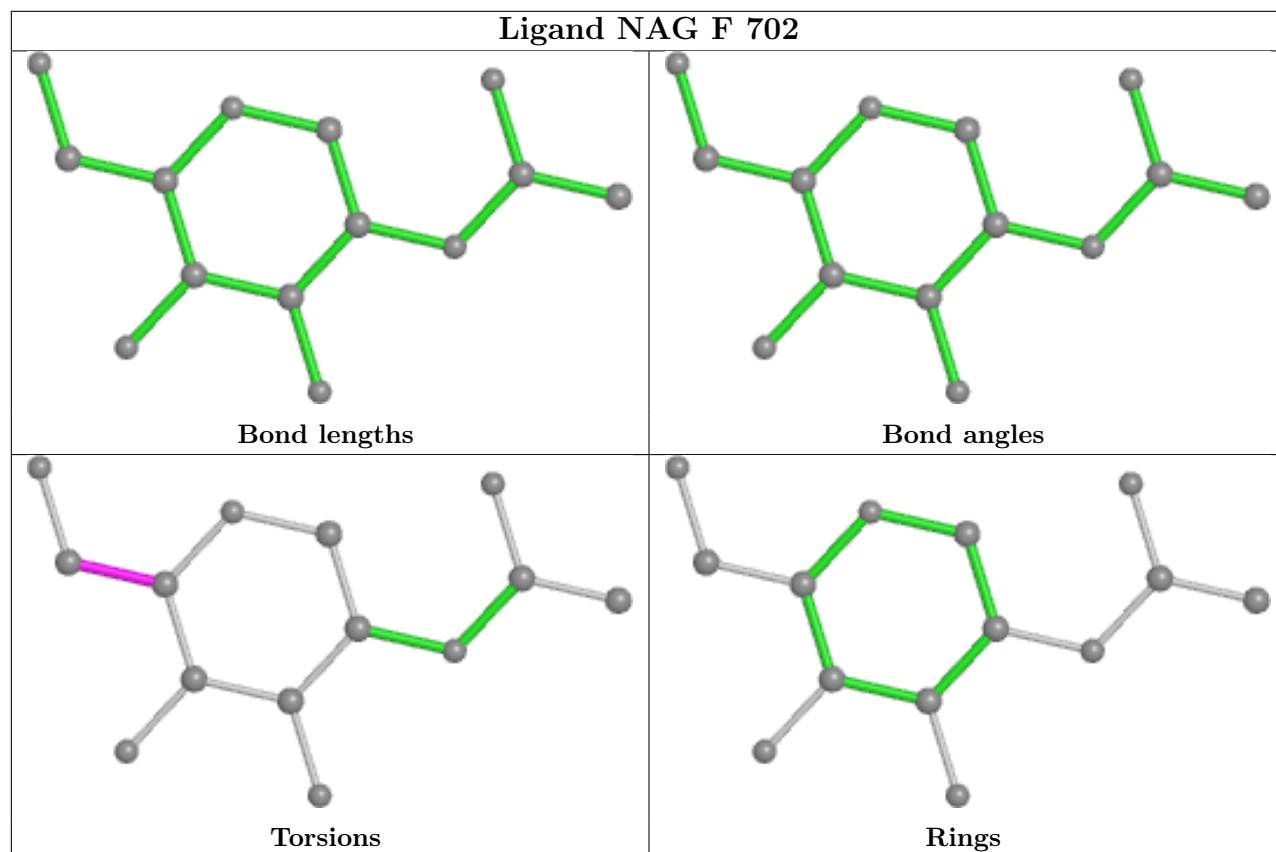


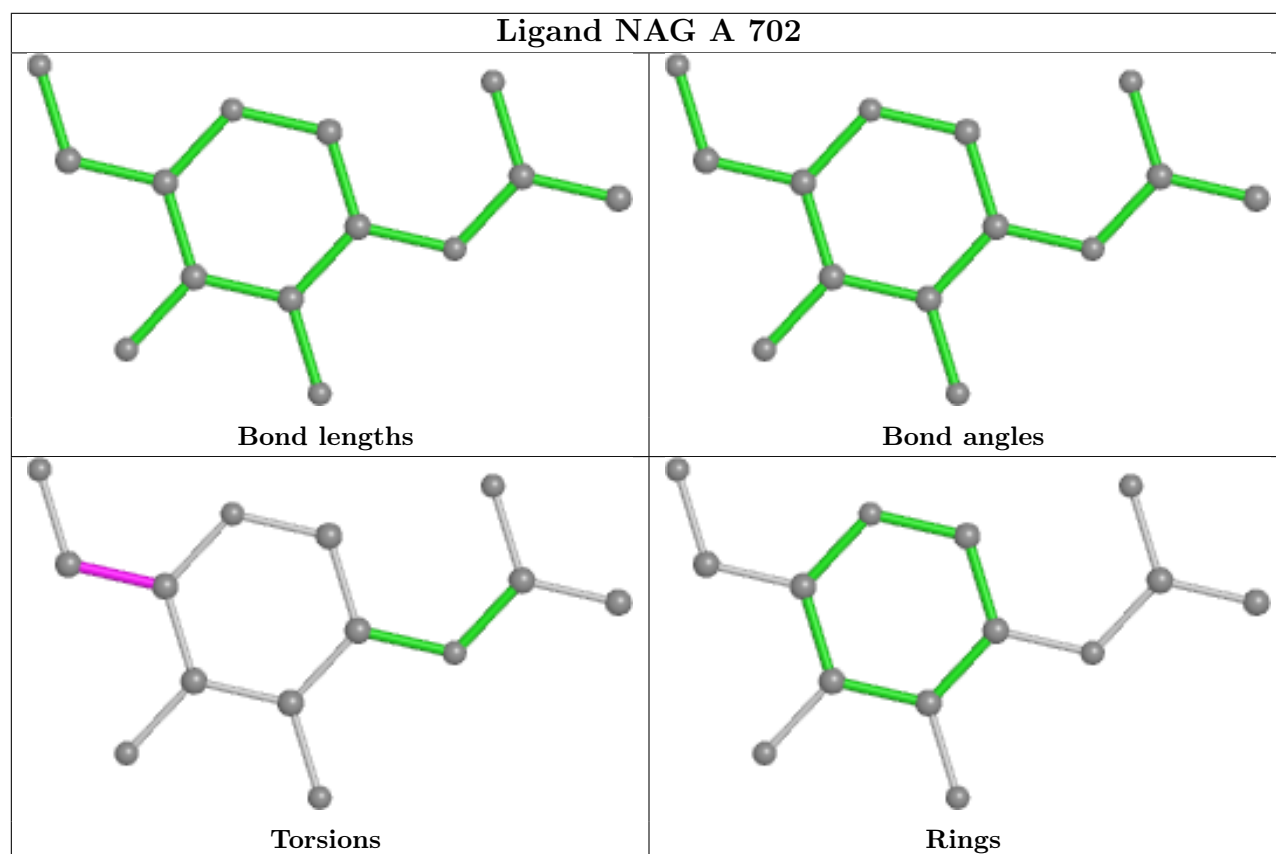
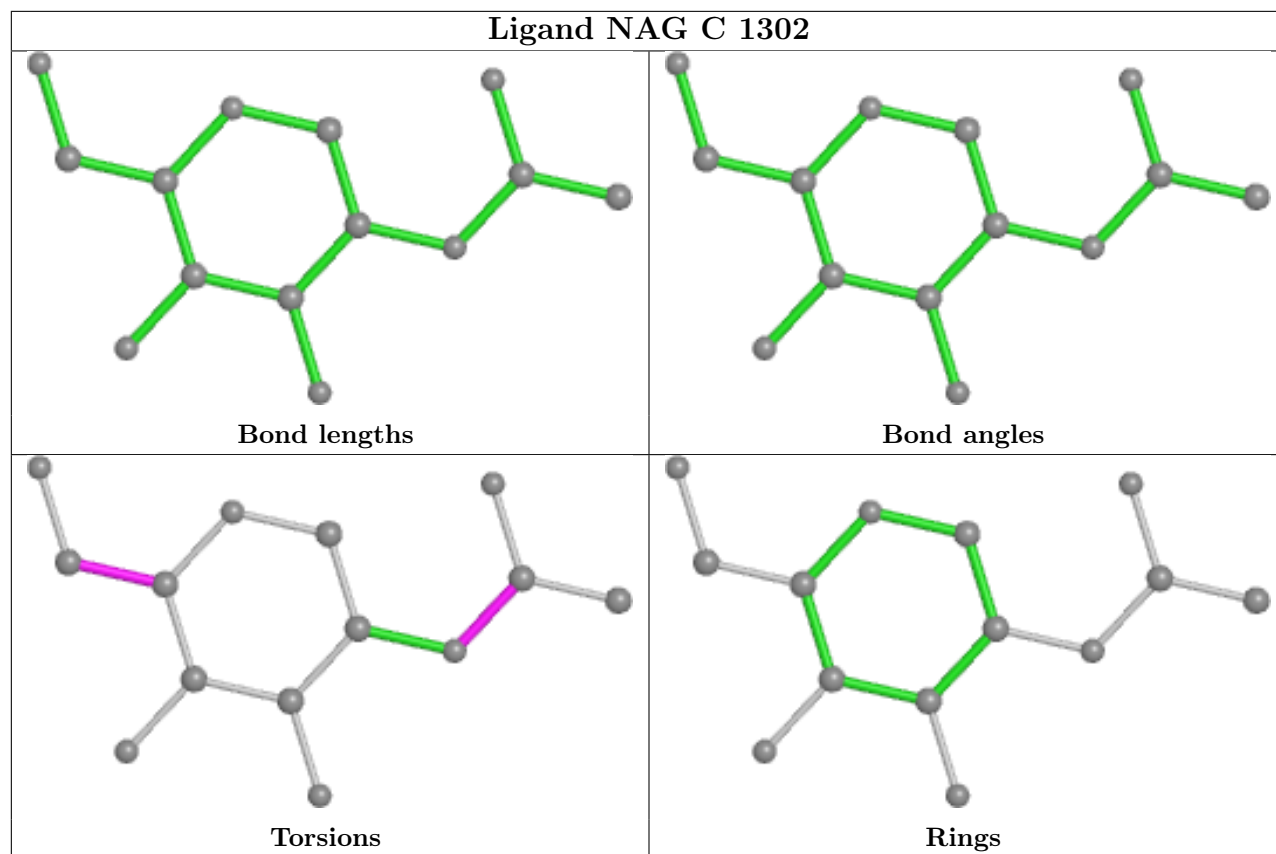


Ligand NAG D 1312

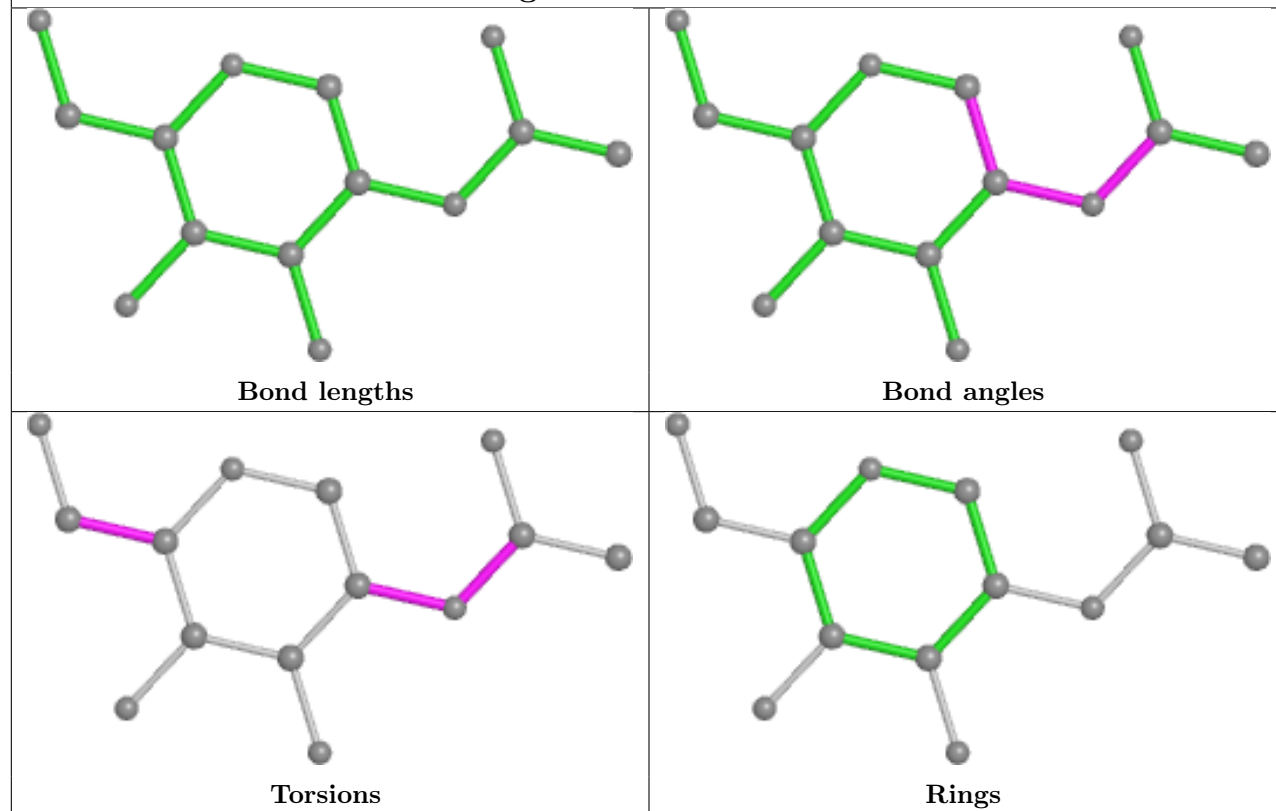


Ligand NAG F 702

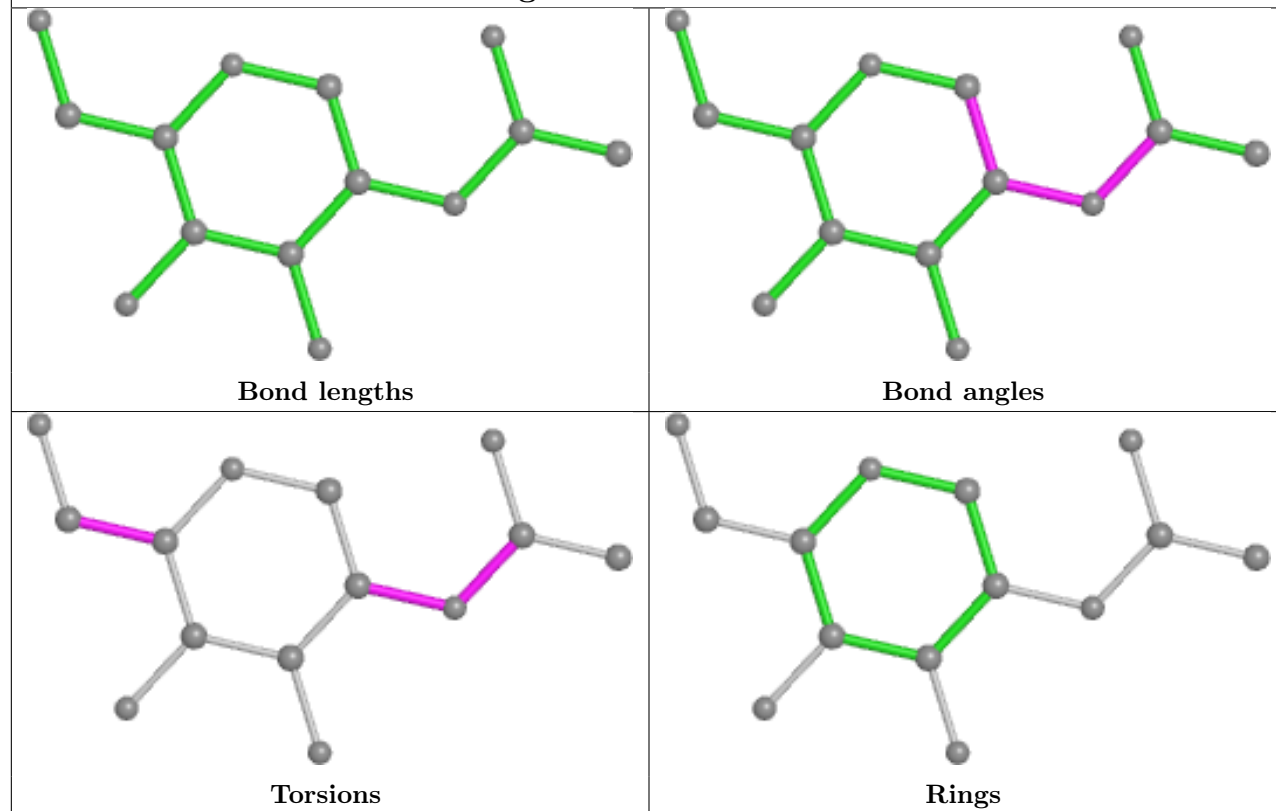


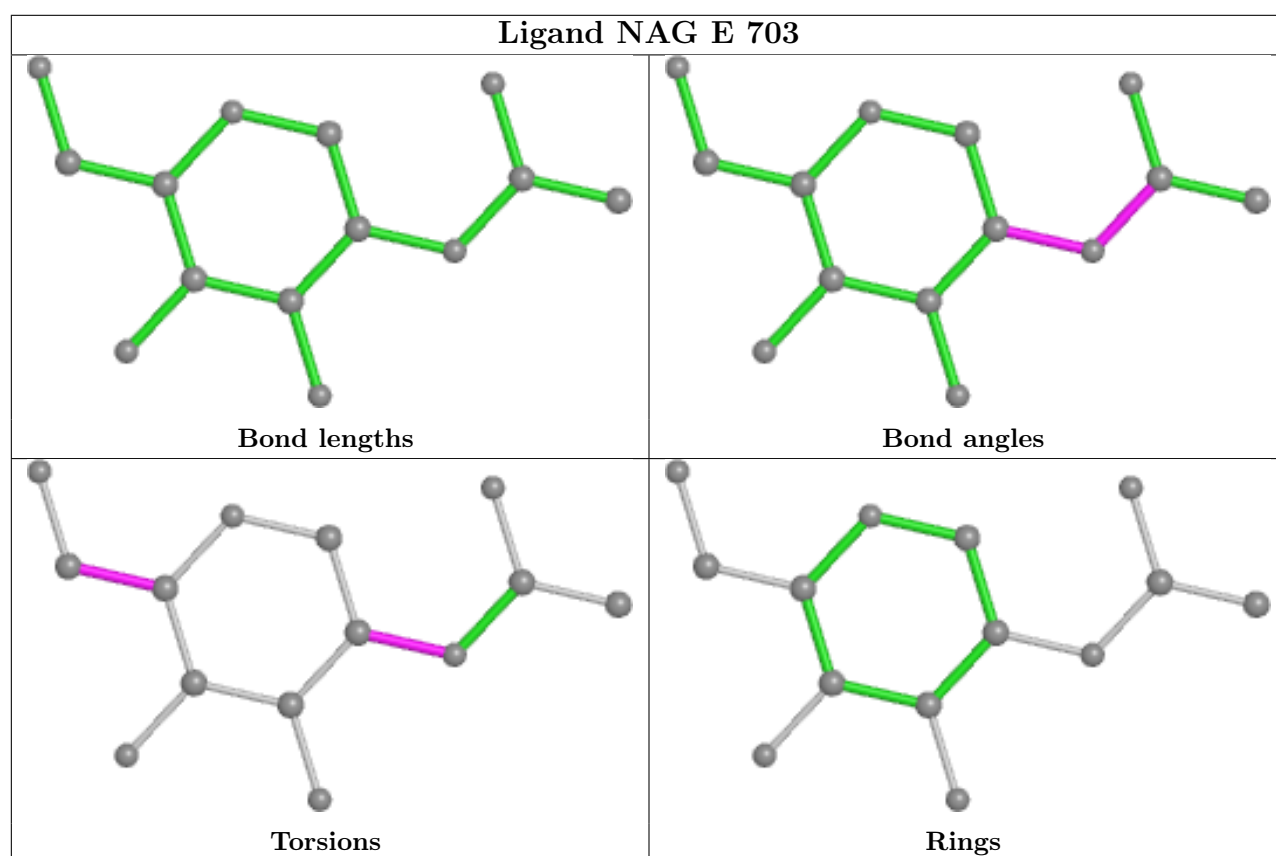
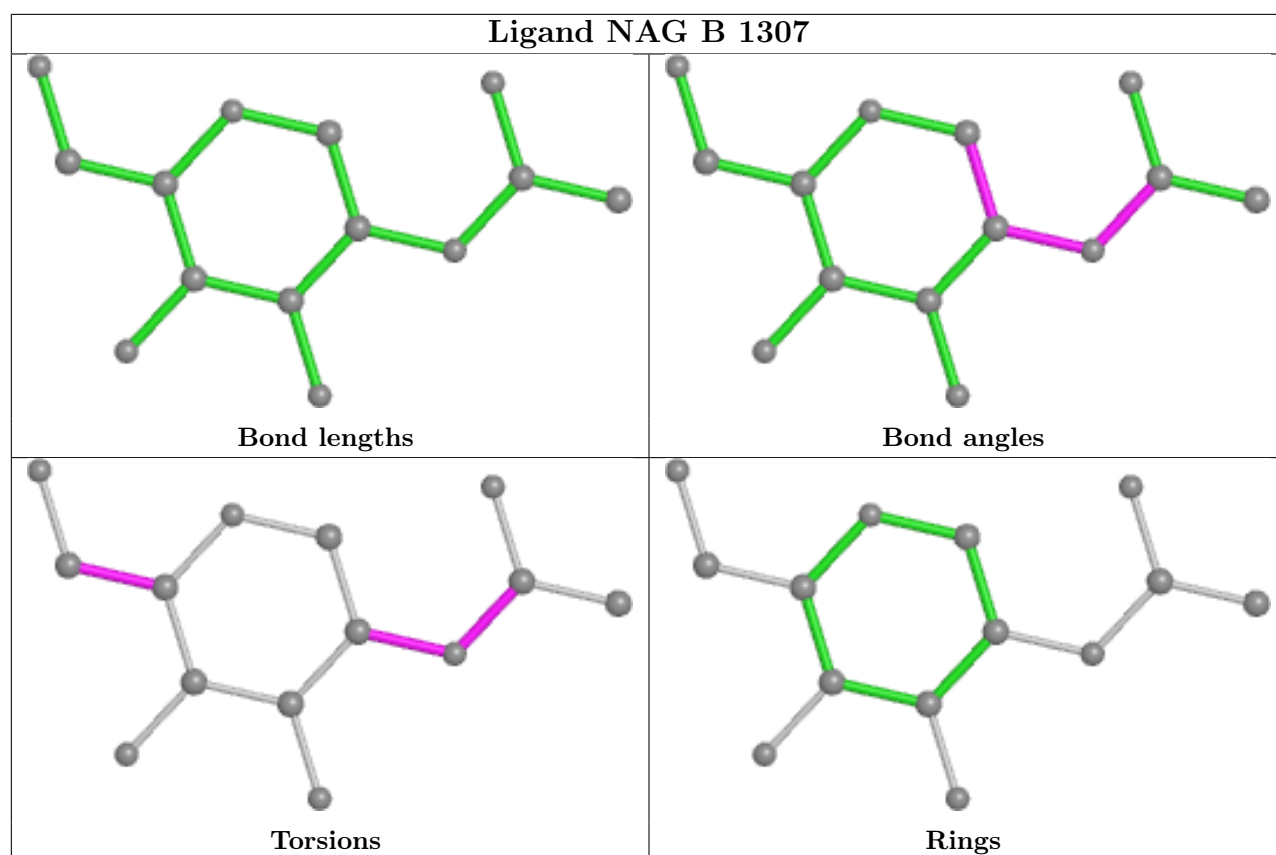


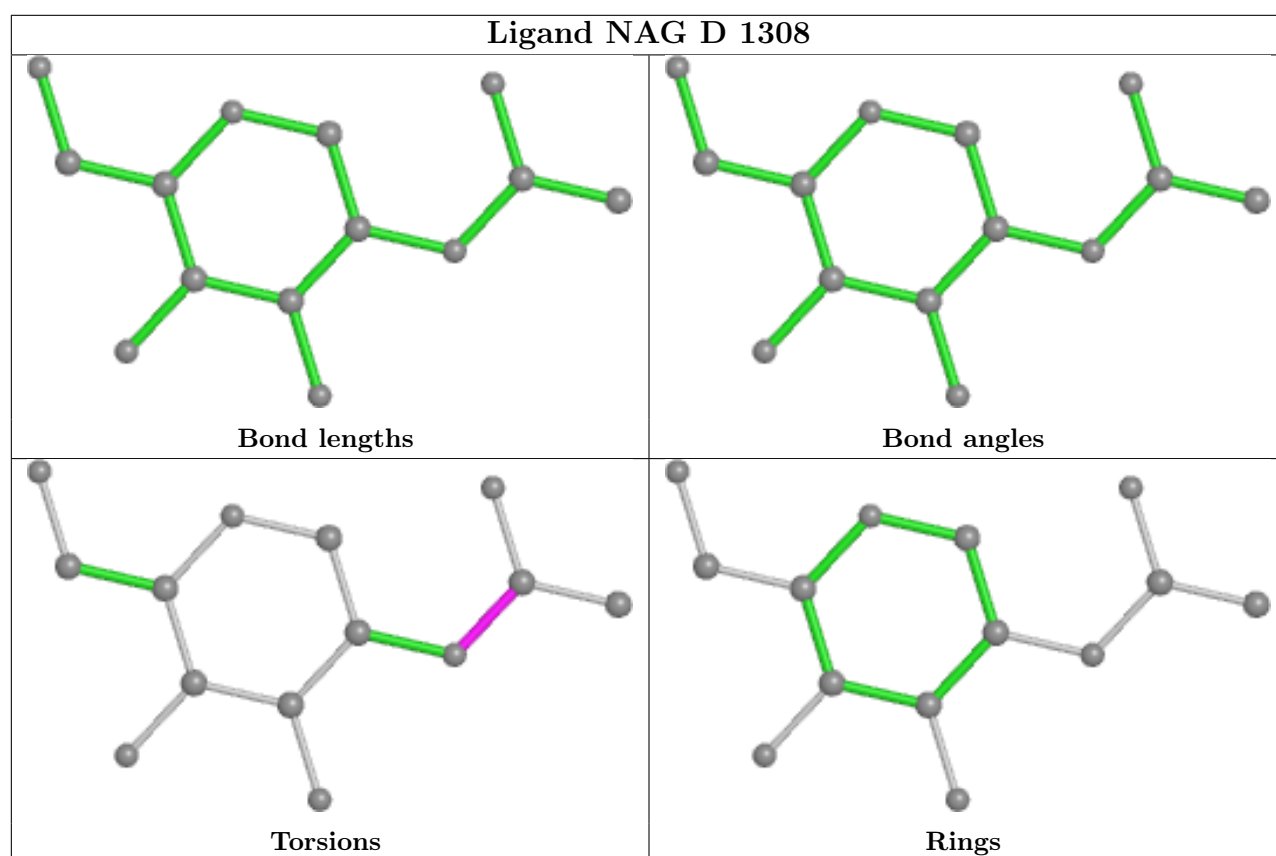
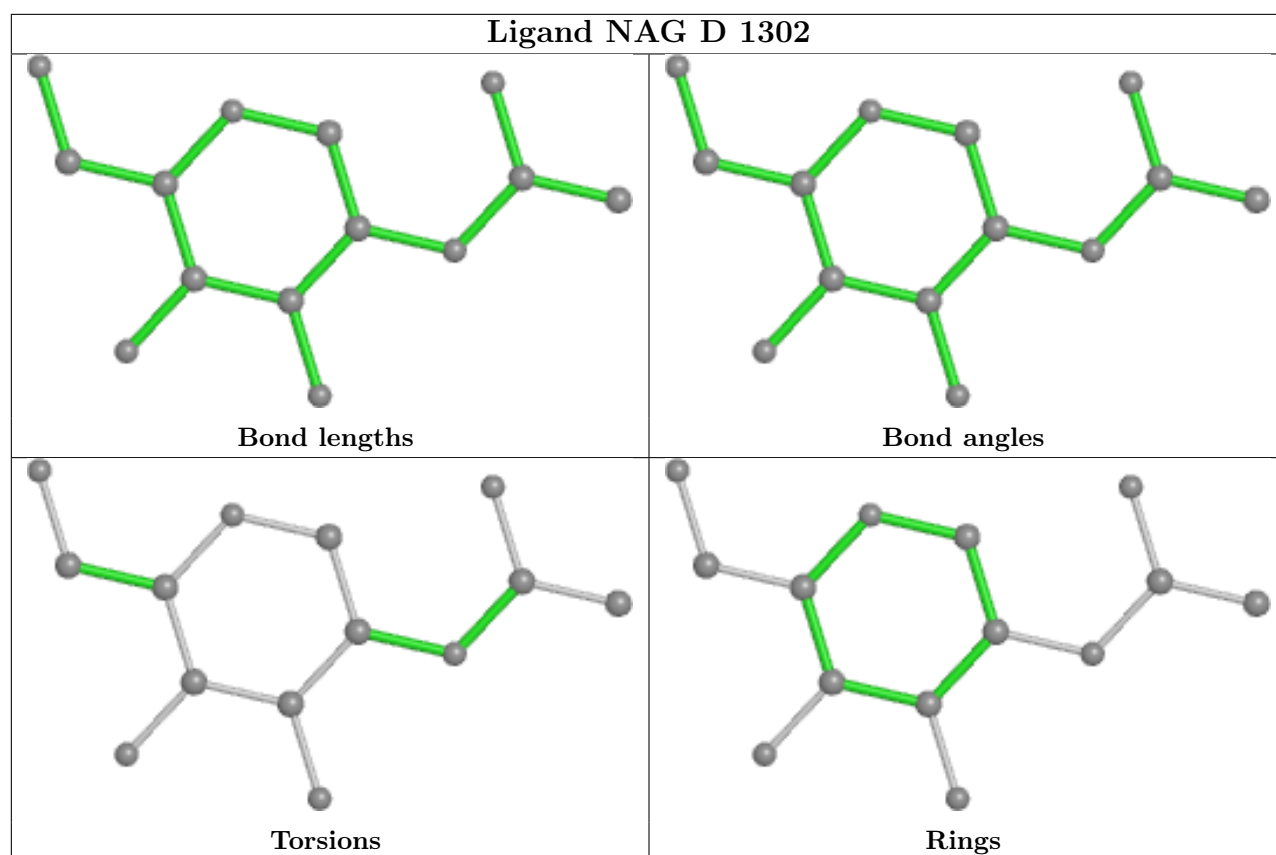
Ligand NAG C 1306

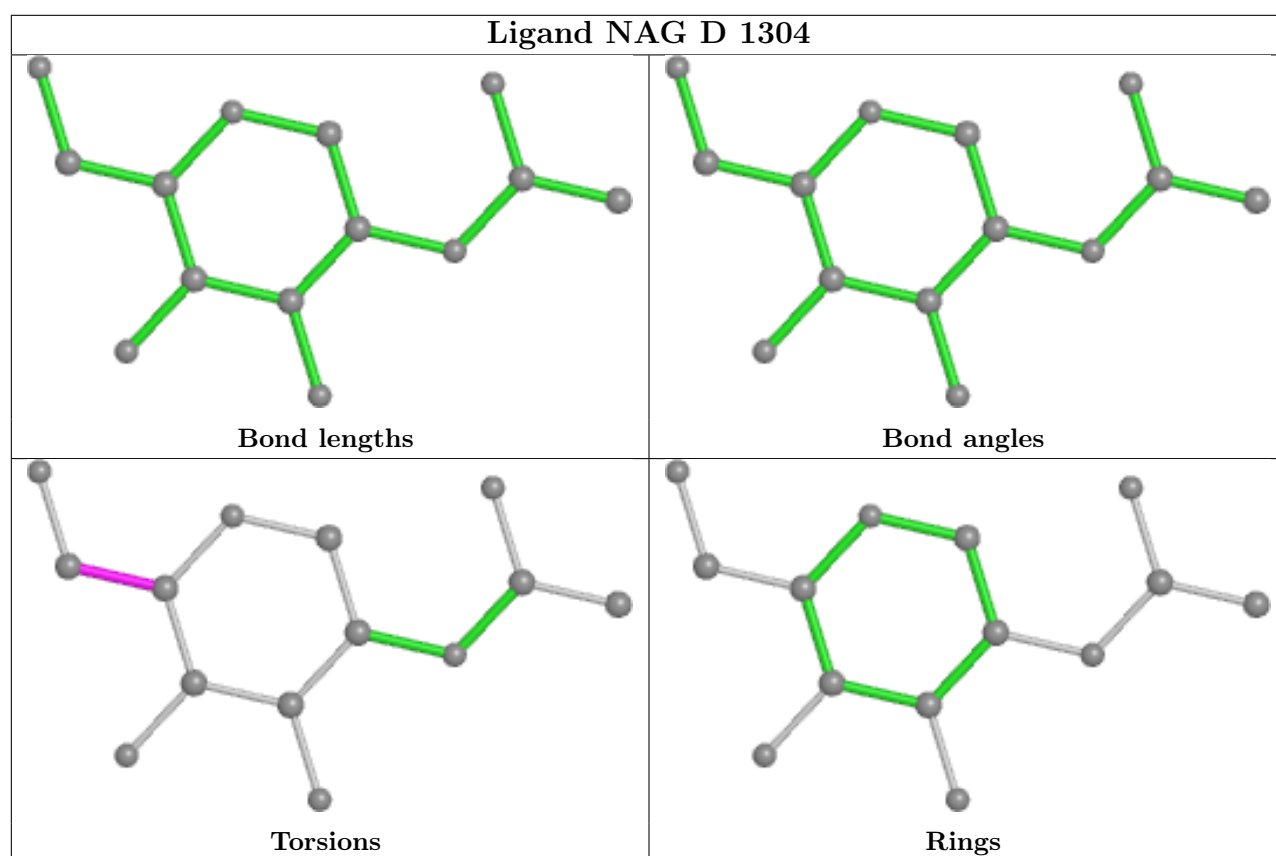
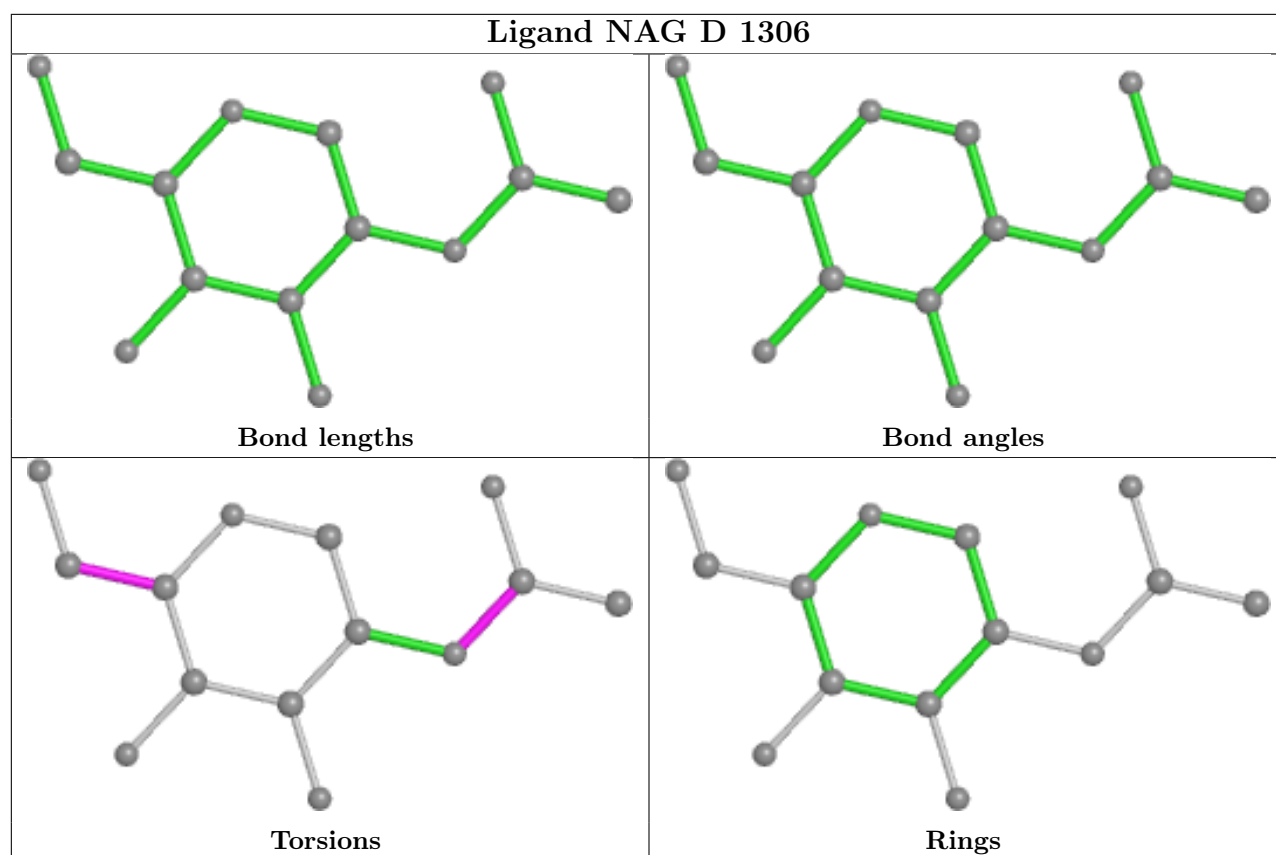


Ligand NAG D 1310









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.

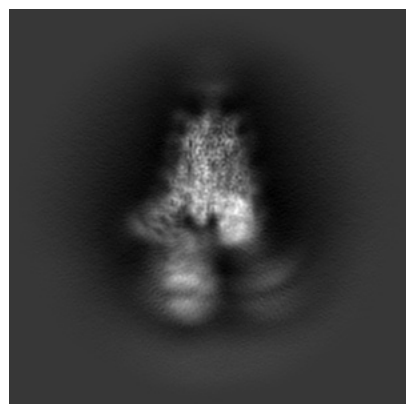
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38826. These allow visual inspection of the internal detail of the map and identification of artifacts.

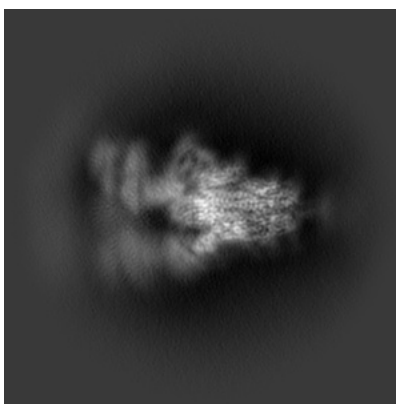
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

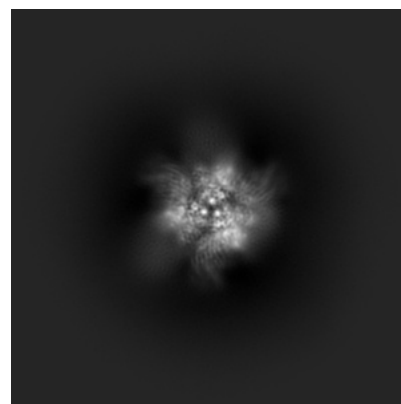
6.1.1 Primary map



X

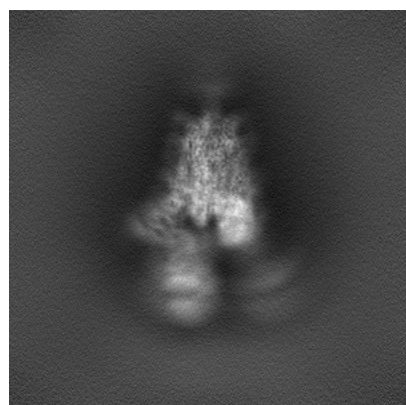


Y

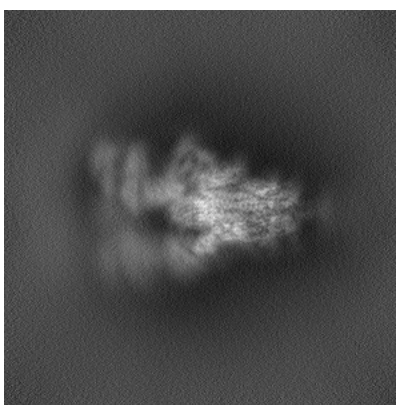


Z

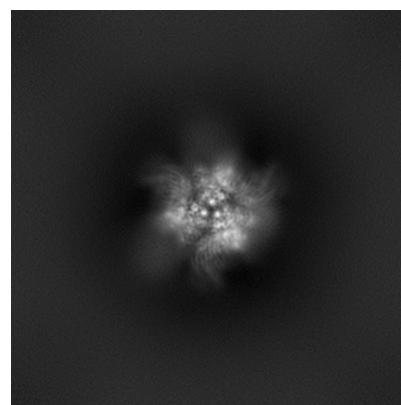
6.1.2 Raw map



X



Y

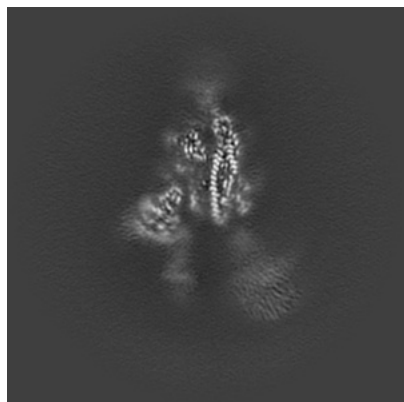


Z

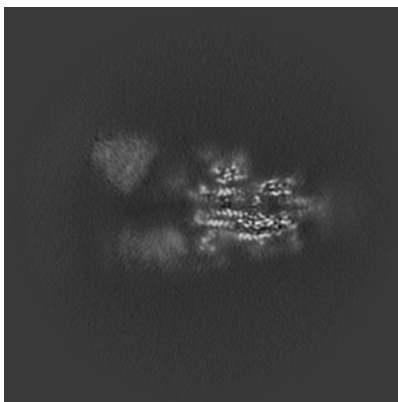
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

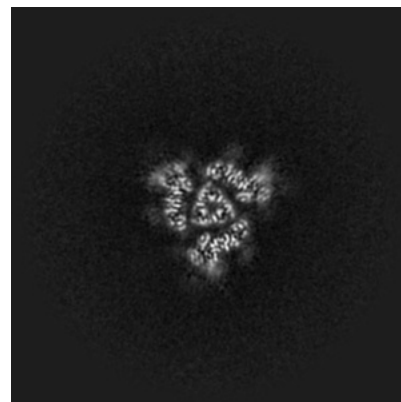
6.2.1 Primary map



X Index: 300

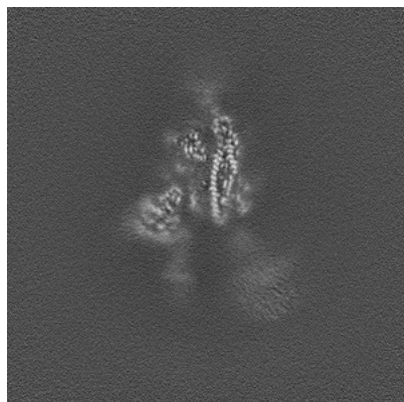


Y Index: 300

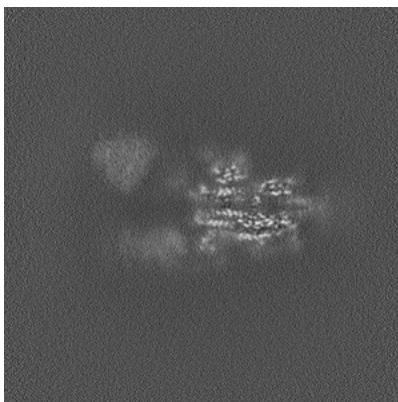


Z Index: 300

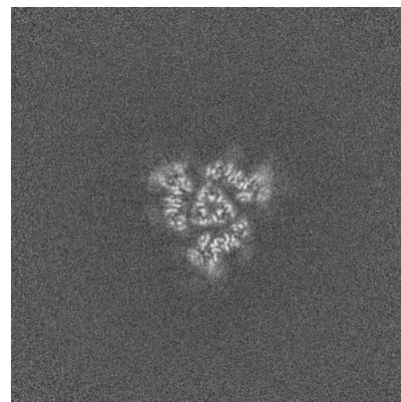
6.2.2 Raw map



X Index: 300



Y Index: 300

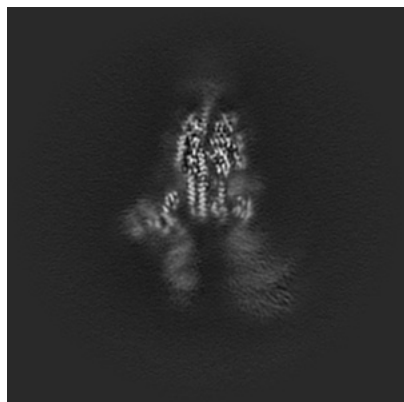


Z Index: 300

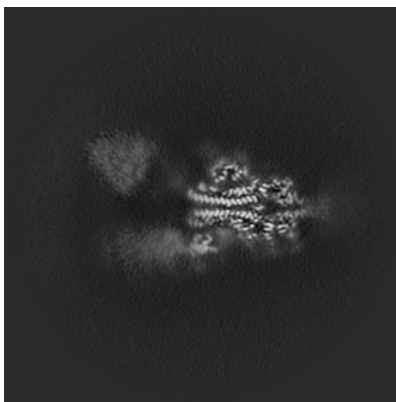
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

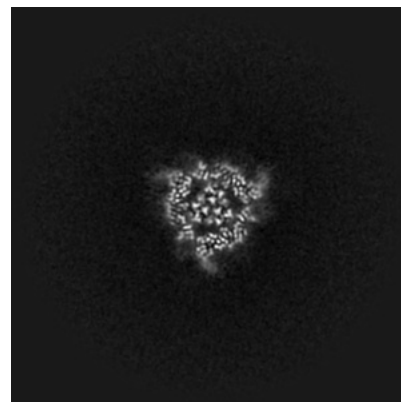
6.3.1 Primary map



X Index: 311

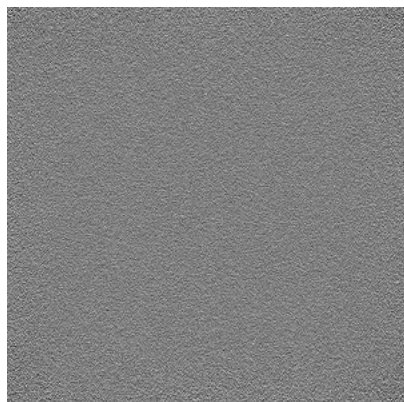


Y Index: 294

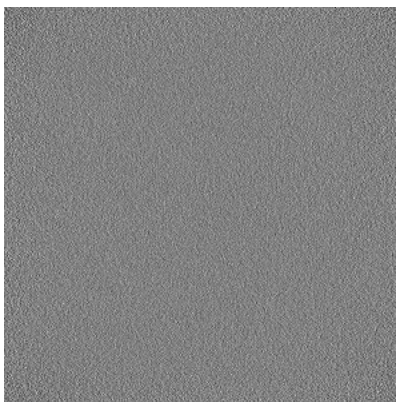


Z Index: 312

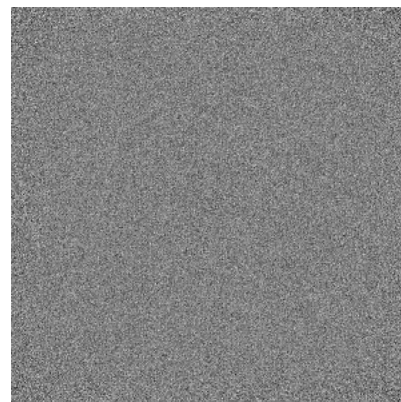
6.3.2 Raw map



X Index: 0



Y Index: 0

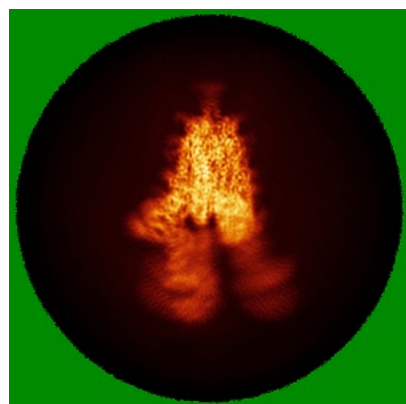


Z Index: 0

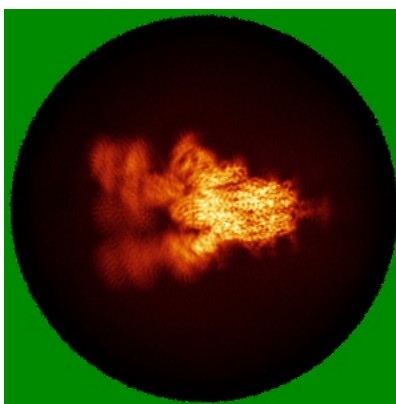
The images above show the largest variance slices of the map in three orthogonal directions.

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

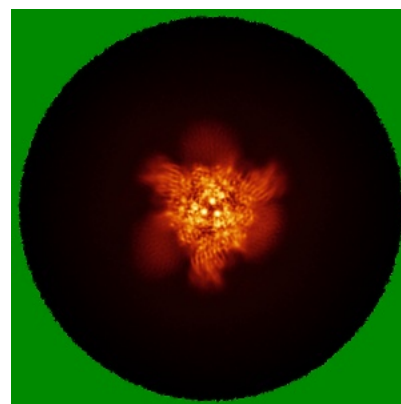
6.4.1 Primary map



X

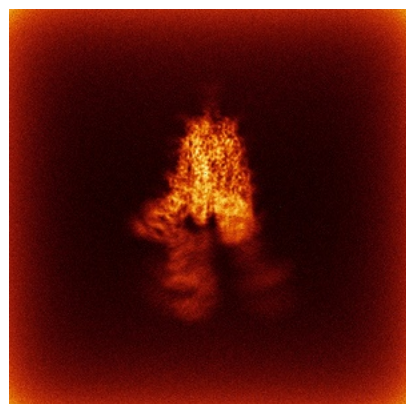


Y

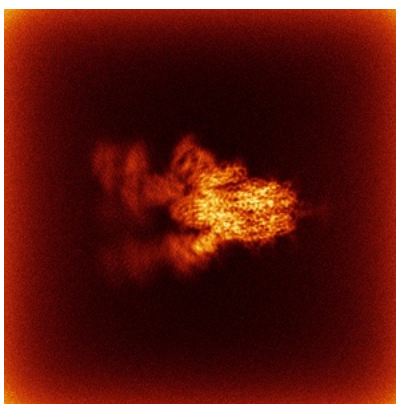


Z

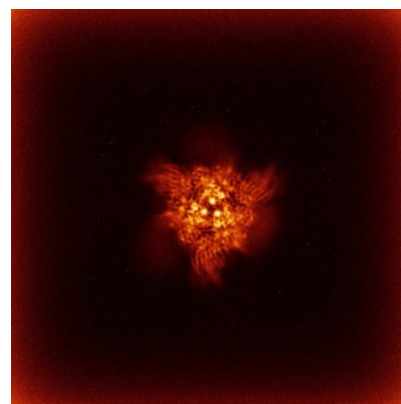
6.4.2 Raw map



X



Y

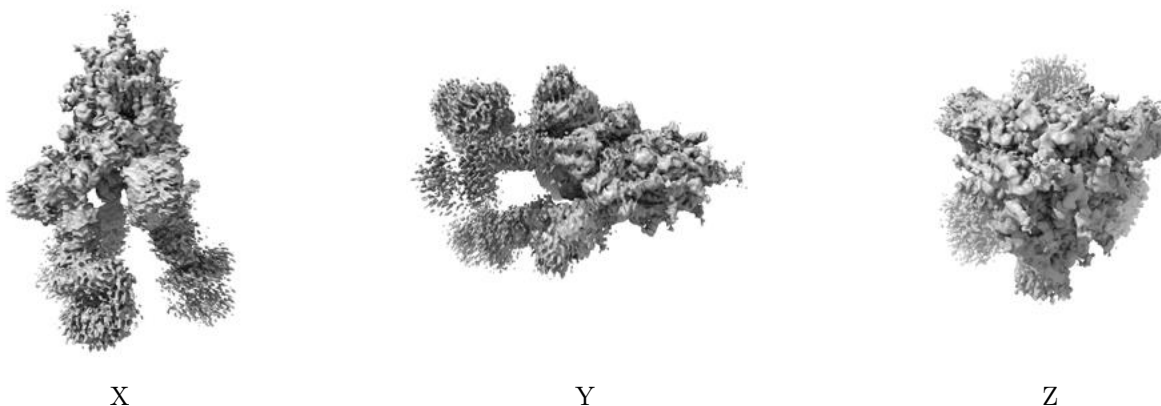


Z

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.

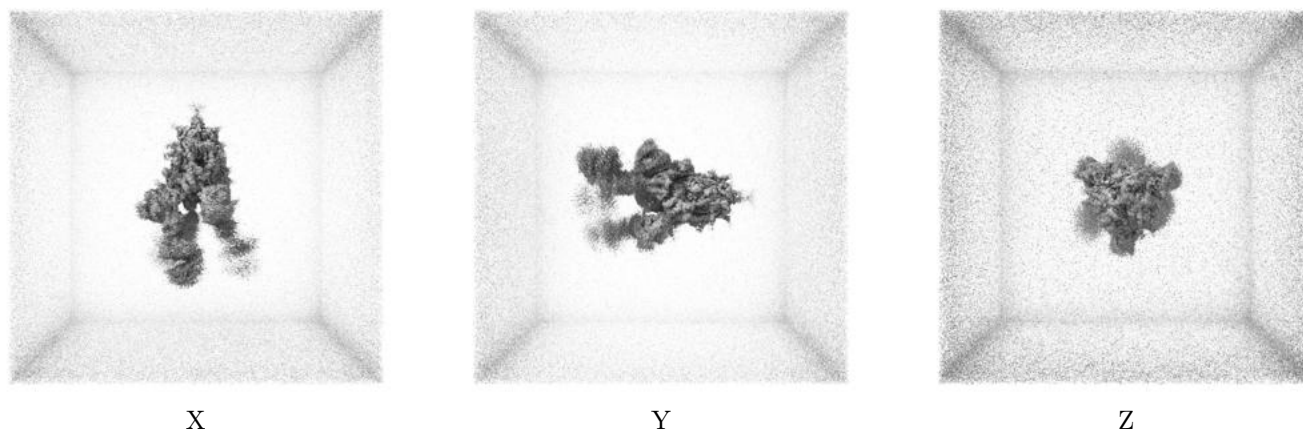
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

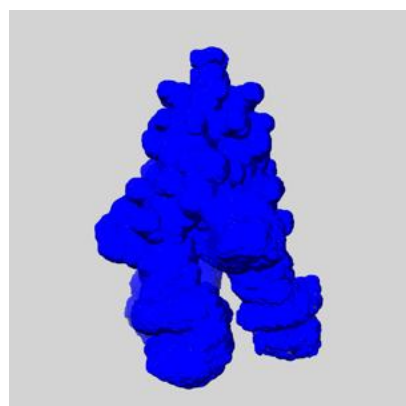
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

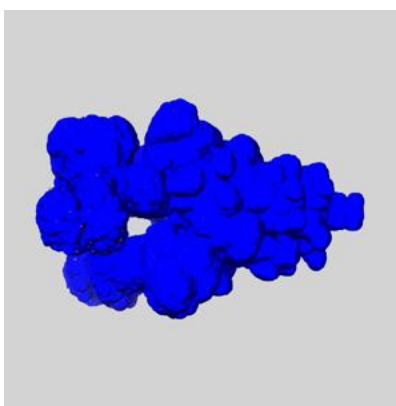
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

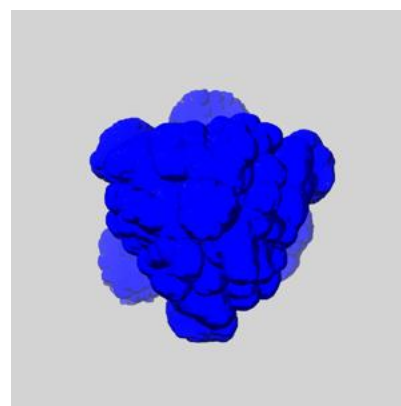
6.6.1 emd_38826_msk_1.map [i](#)



X



Y

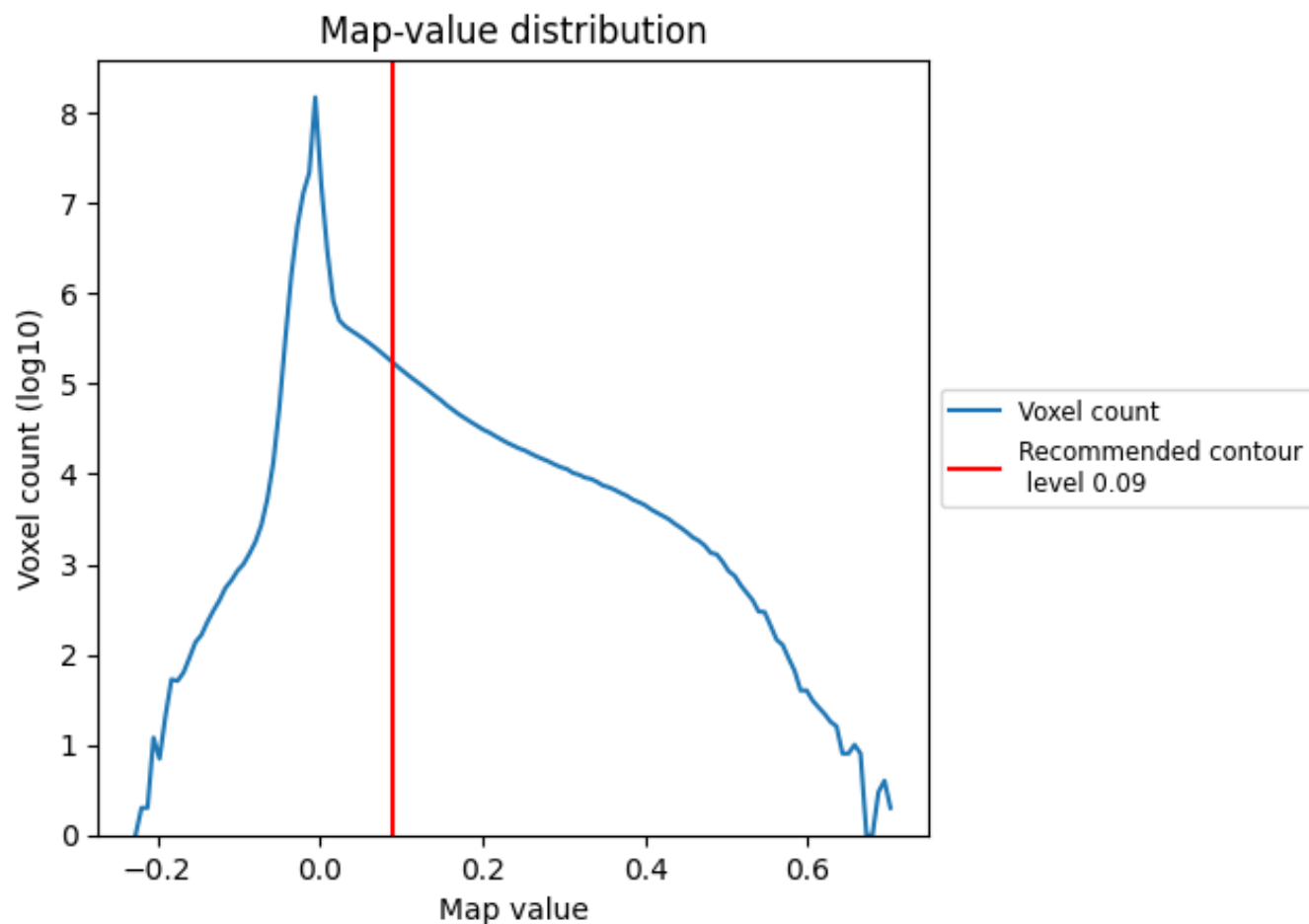


Z

7 Map analysis [i](#)

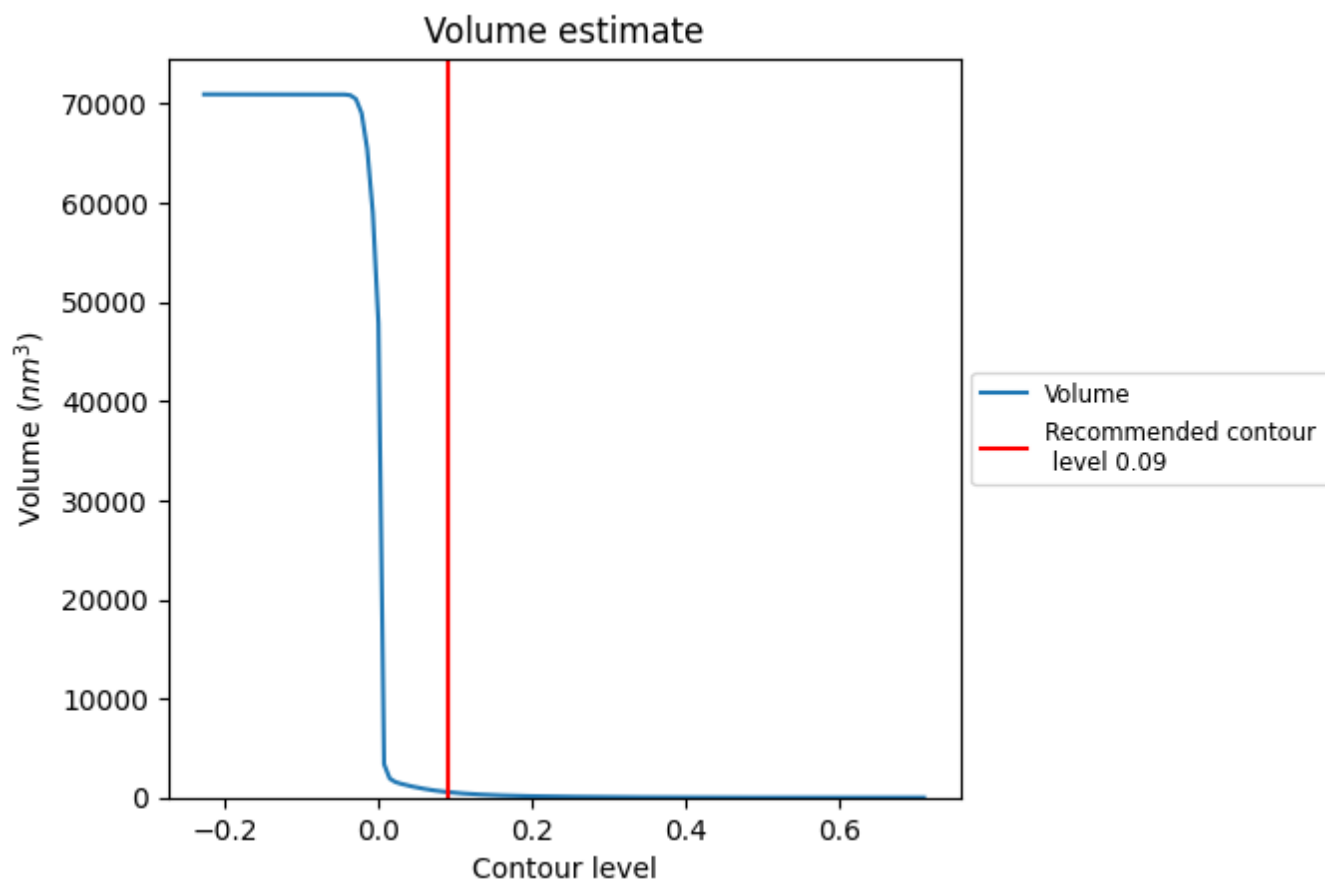
This section contains the results of statistical analysis of the map.

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.

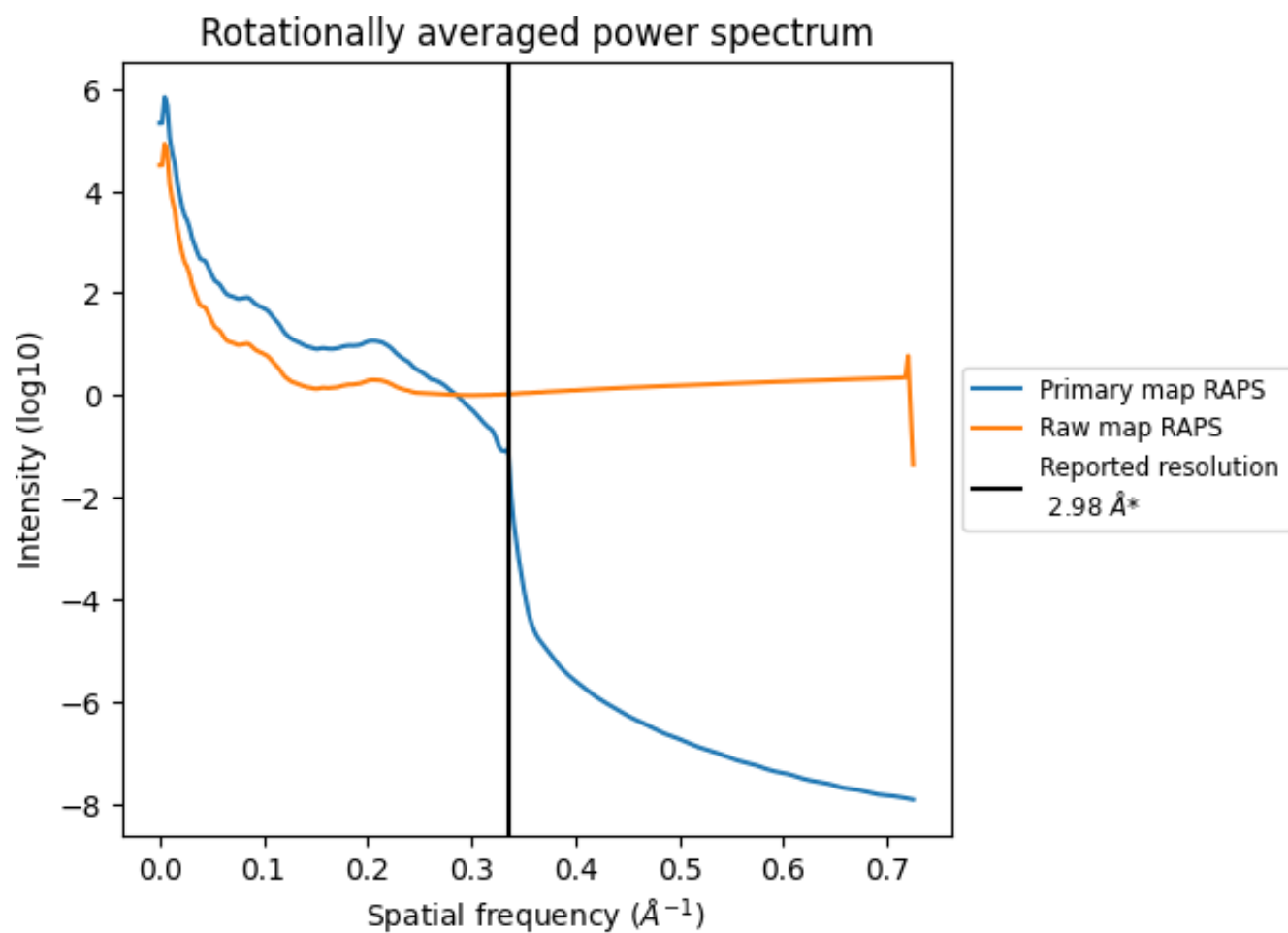
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 551 nm³; this corresponds to an approximate mass of 498 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 ⓘ

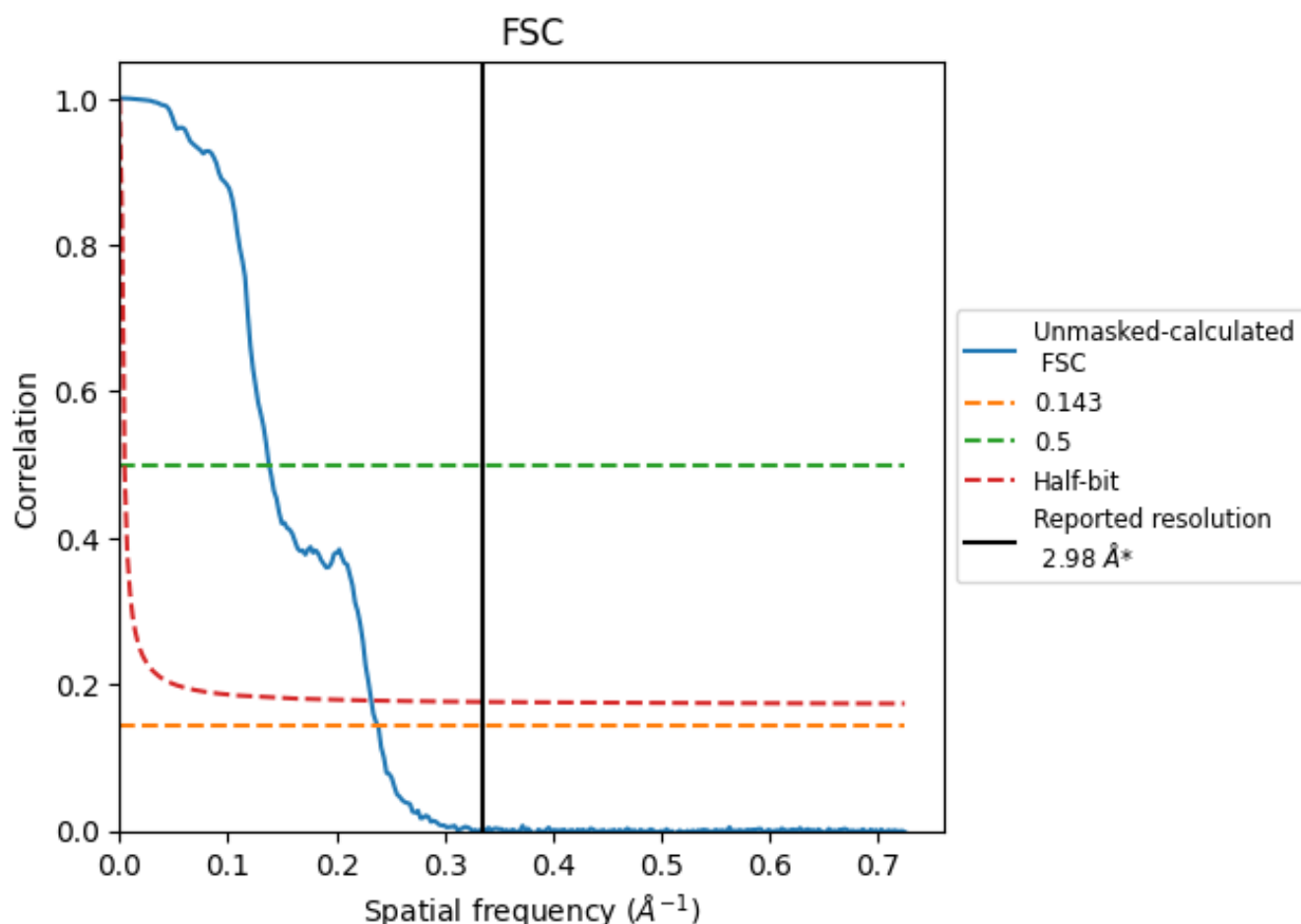


*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

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 0.336 \AA^{-1}

8.2 Resolution estimates [i](#)

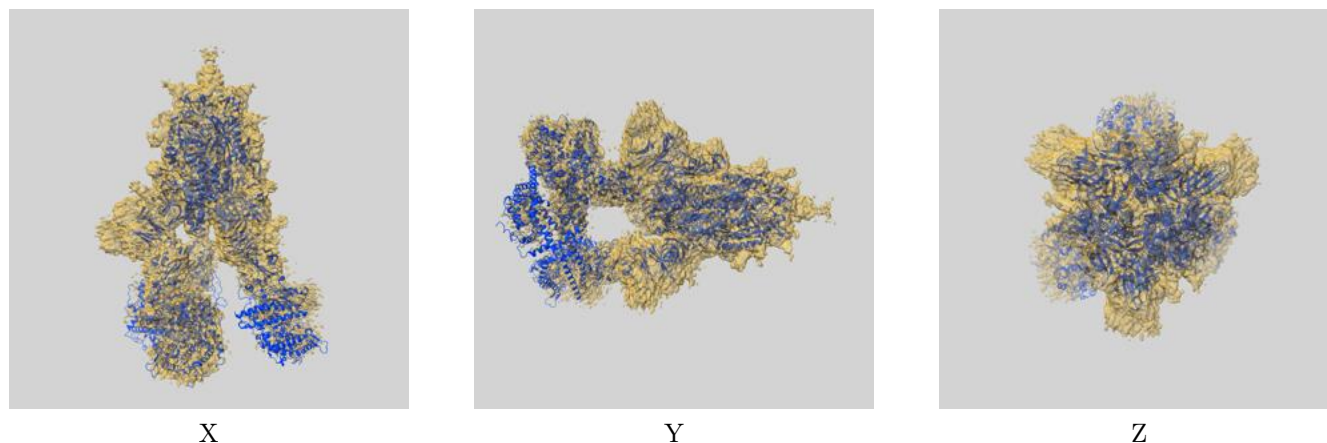
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	7.25	4.30

*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 4.20 differs from the reported value 2.98 by more than 10 %

9 Map-model fit [i](#)

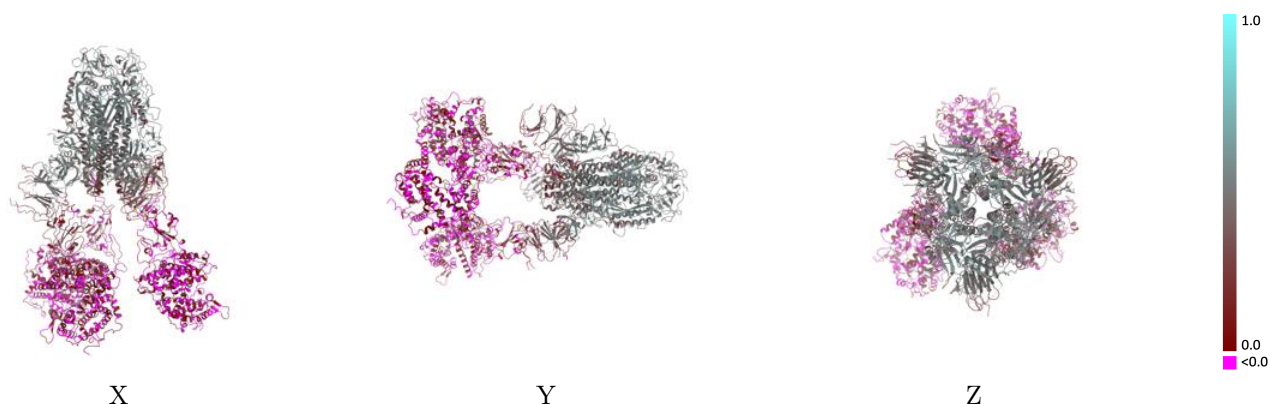
This section contains information regarding the fit between EMDB map EMD-38826 and PDB model 8Y16. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



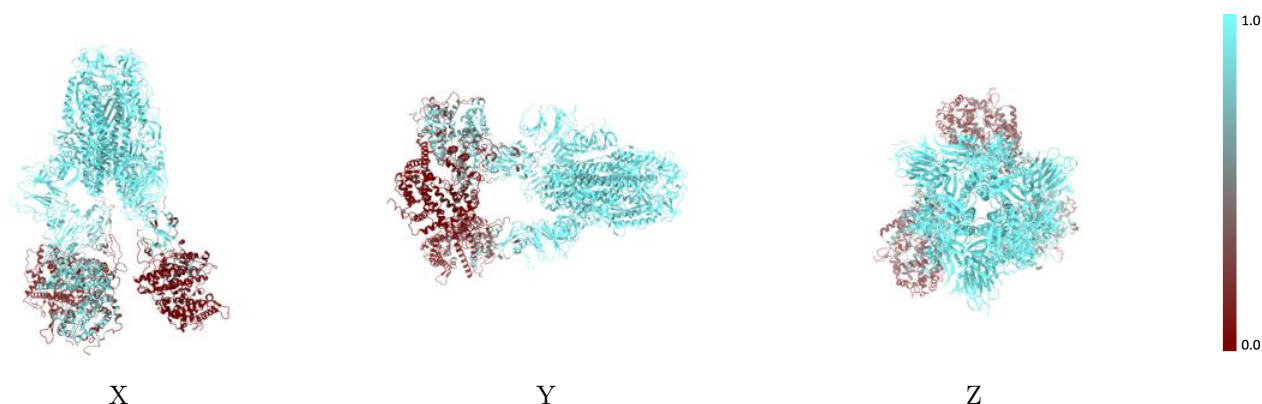
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



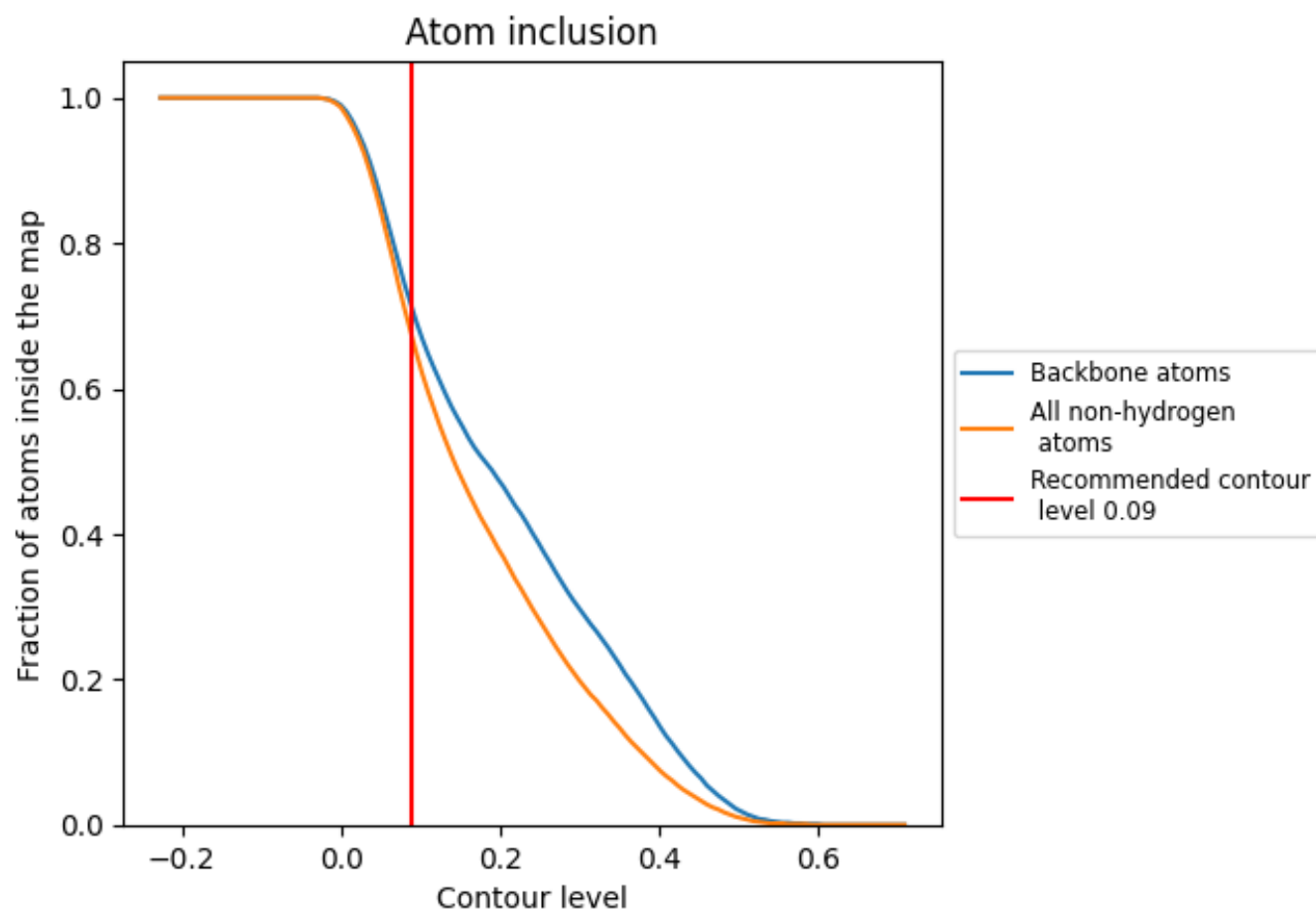
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 67% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6680	 0.2460
A	 0.6440	 0.0830
B	 0.9560	 0.3960
C	 0.8840	 0.3500
D	 0.8980	 0.3670
E	 0.0800	 0.0210
F	 0.1250	 0.0280
G	 0.0510	 0.0650
H	 0.0510	 0.0280
I	 0.2500	 -0.0540
J	 0.0360	 0.0580
K	 0.9640	 0.4130
L	 0.9290	 0.4030
M	 0.3570	 0.2510
N	 1.0000	 0.4180
O	 0.0360	 0.1060
P	 0.8570	 0.3520
Q	 0.2140	 0.1450
R	 0.0000	 -0.0830
S	 0.0000	 0.0870
T	 0.0000	 0.1250
U	 0.0000	 0.0100
V	 0.0000	 0.0200
W	 0.0000	 0.0470
X	 0.0000	 0.0710
Y	 0.0000	 -0.1050

