



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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

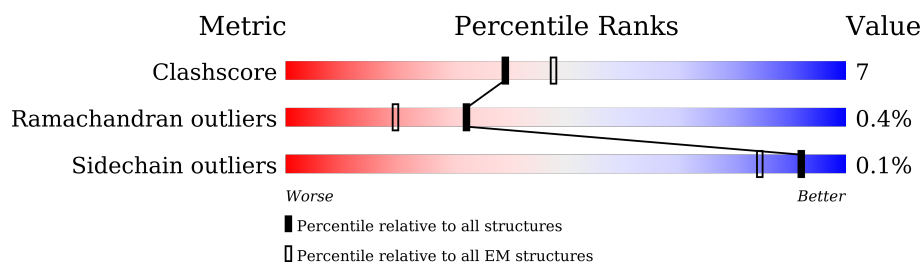
# 1 Overall quality at a glance

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.




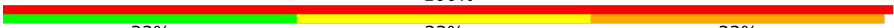

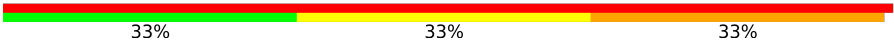

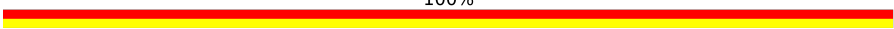
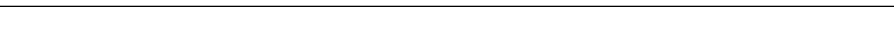
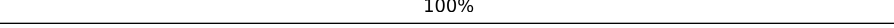
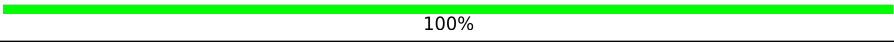


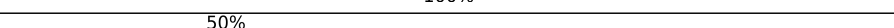
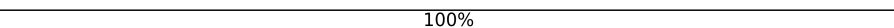
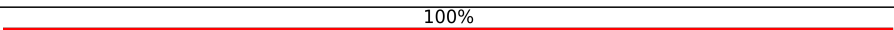

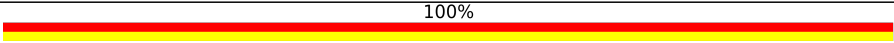
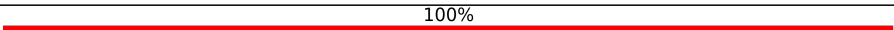
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	 25% 86% 13%
1	E	603	 94% 86% 12%
1	F	603	 88% 88% 11%
2	B	1248	 68% 12% 20%
2	C	1248	 7% 67% 14% 19%
2	D	1248	 6% 69% 12% 19%
3	G	3	 100% 100%
3	H	3	 33% 33% 33%

*Continued on next page...*

Continued from previous page...

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

Continued from previous page...

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.

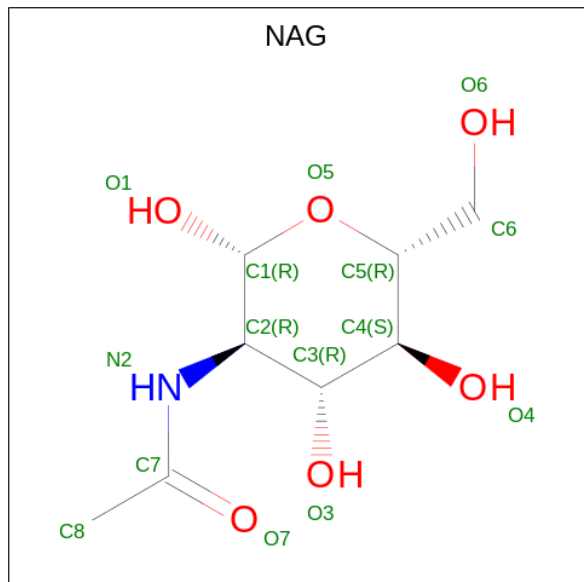


Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	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	

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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	

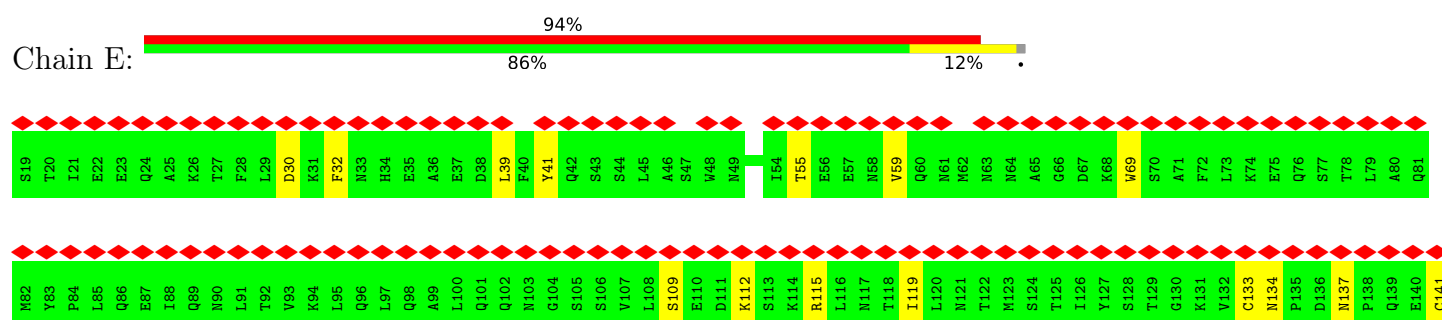
### 3 Residue-property plots

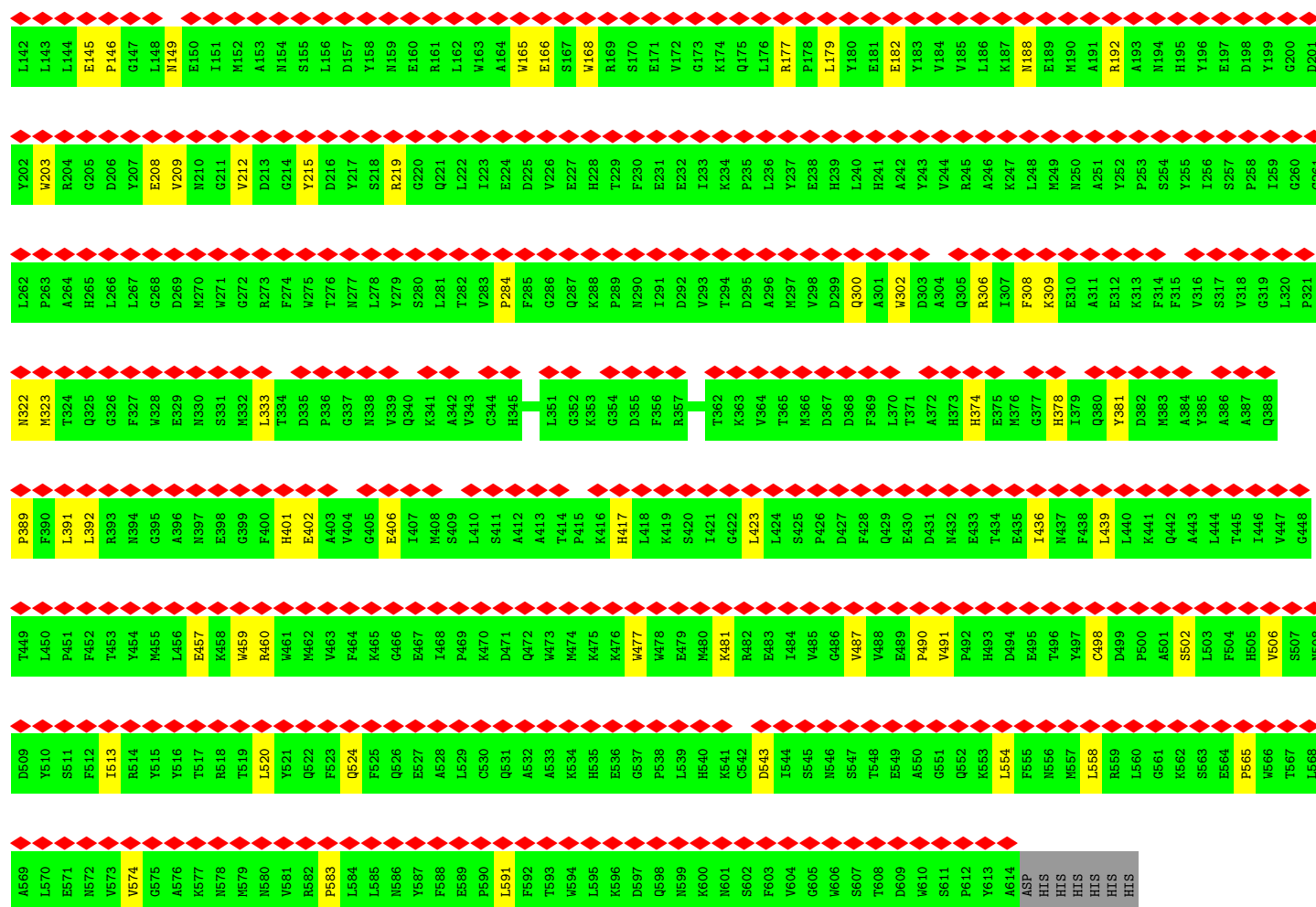
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

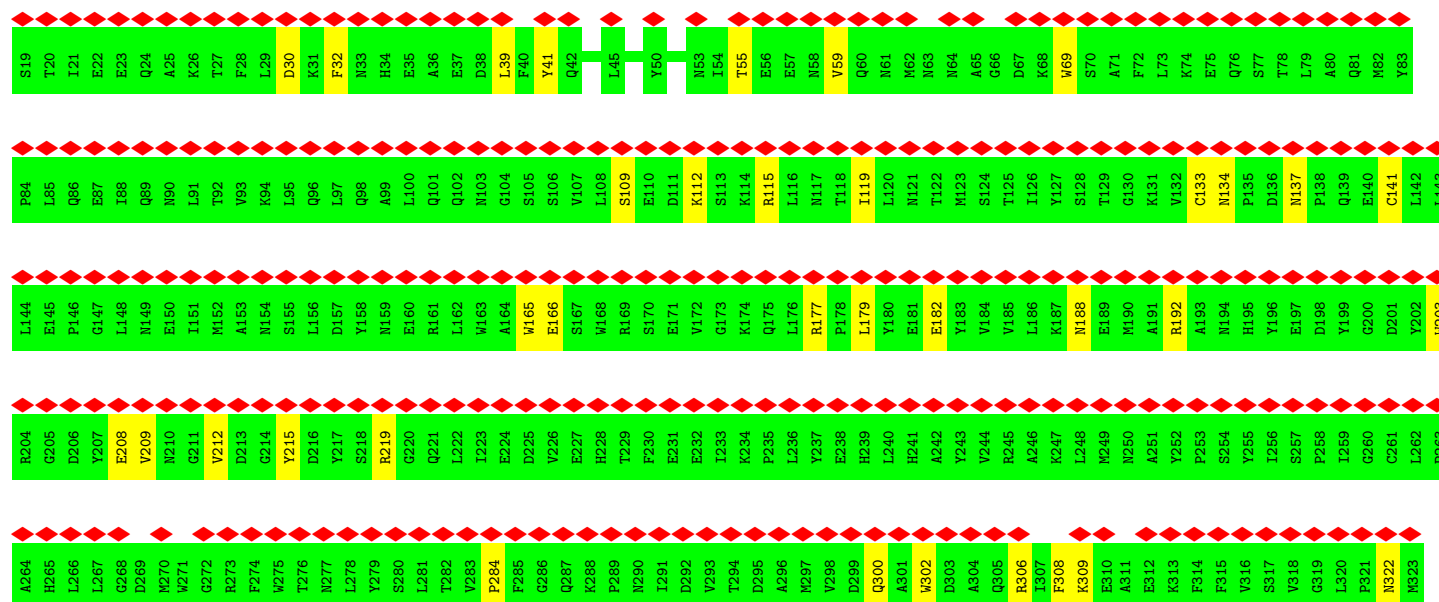
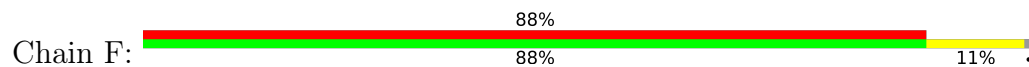


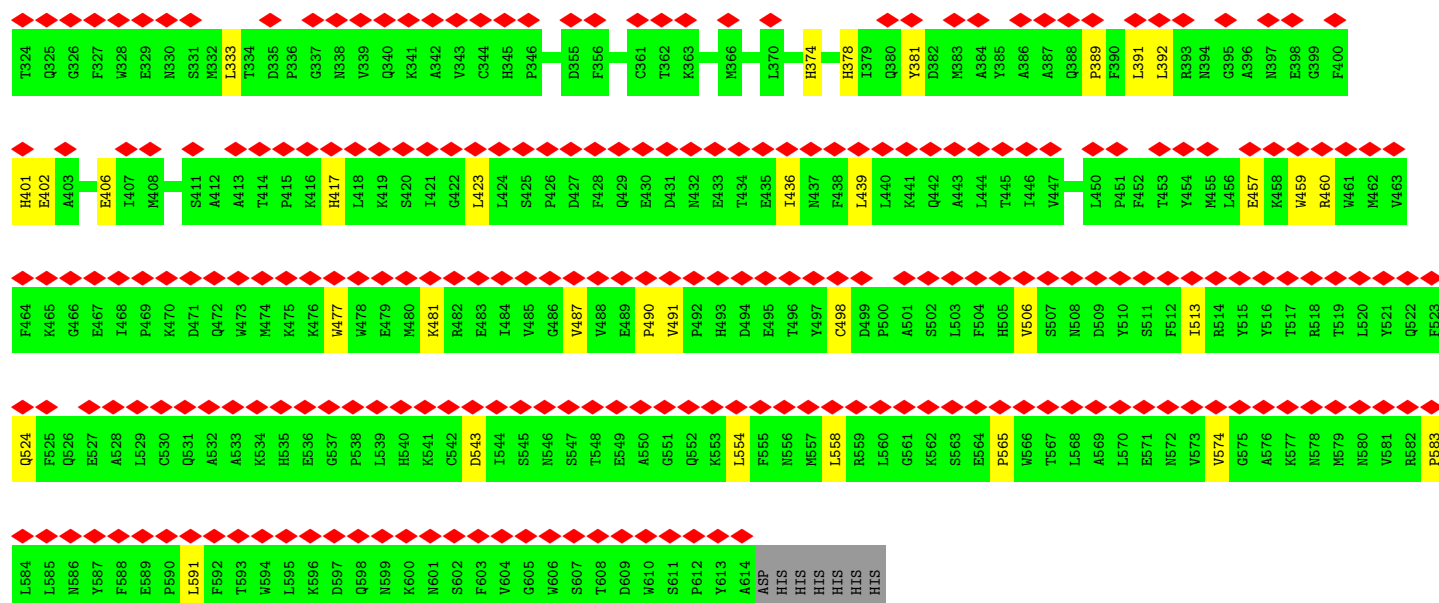
#### • Molecule 1: Angiotensin-converting enzyme 2





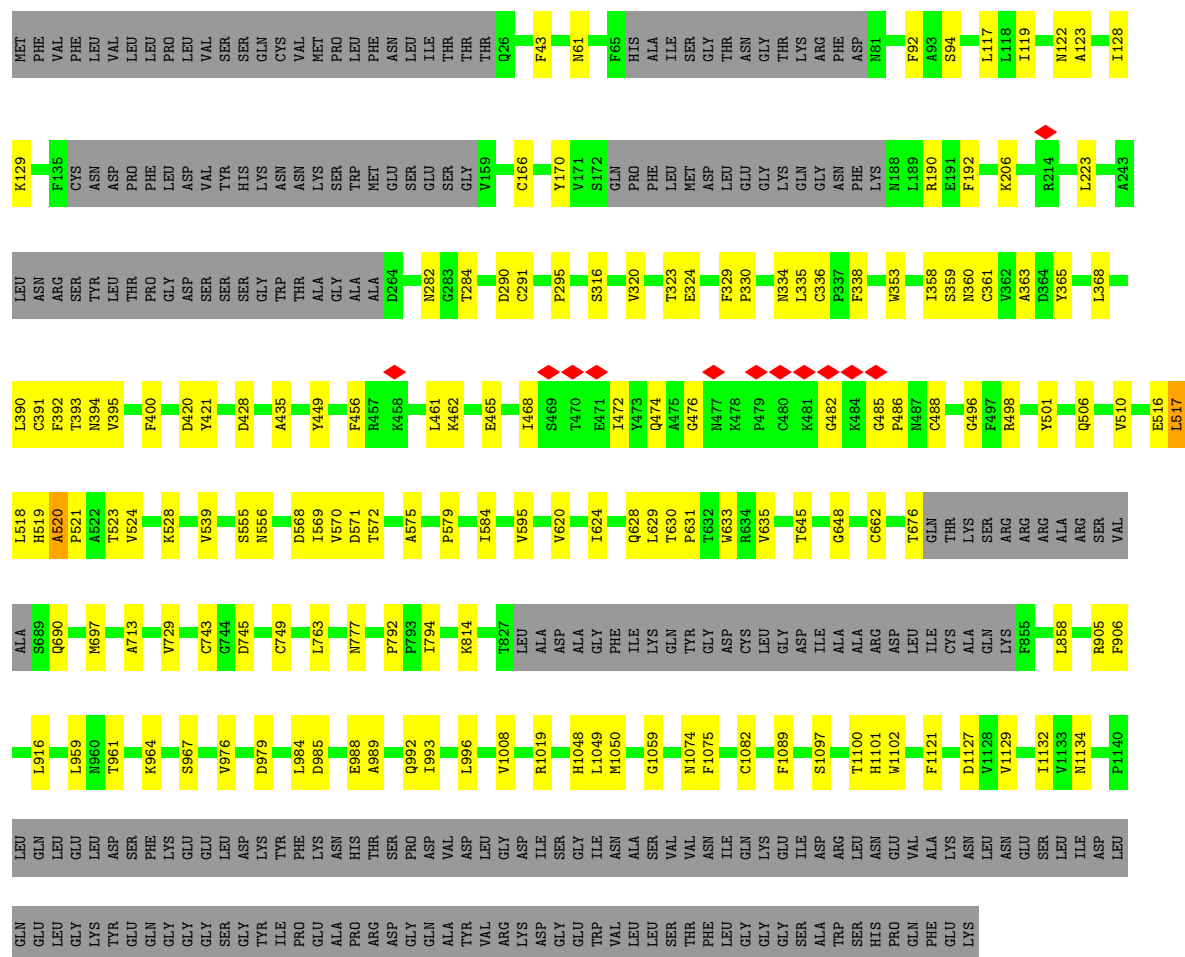
• Molecule 1: Angiotensin-converting enzyme 2



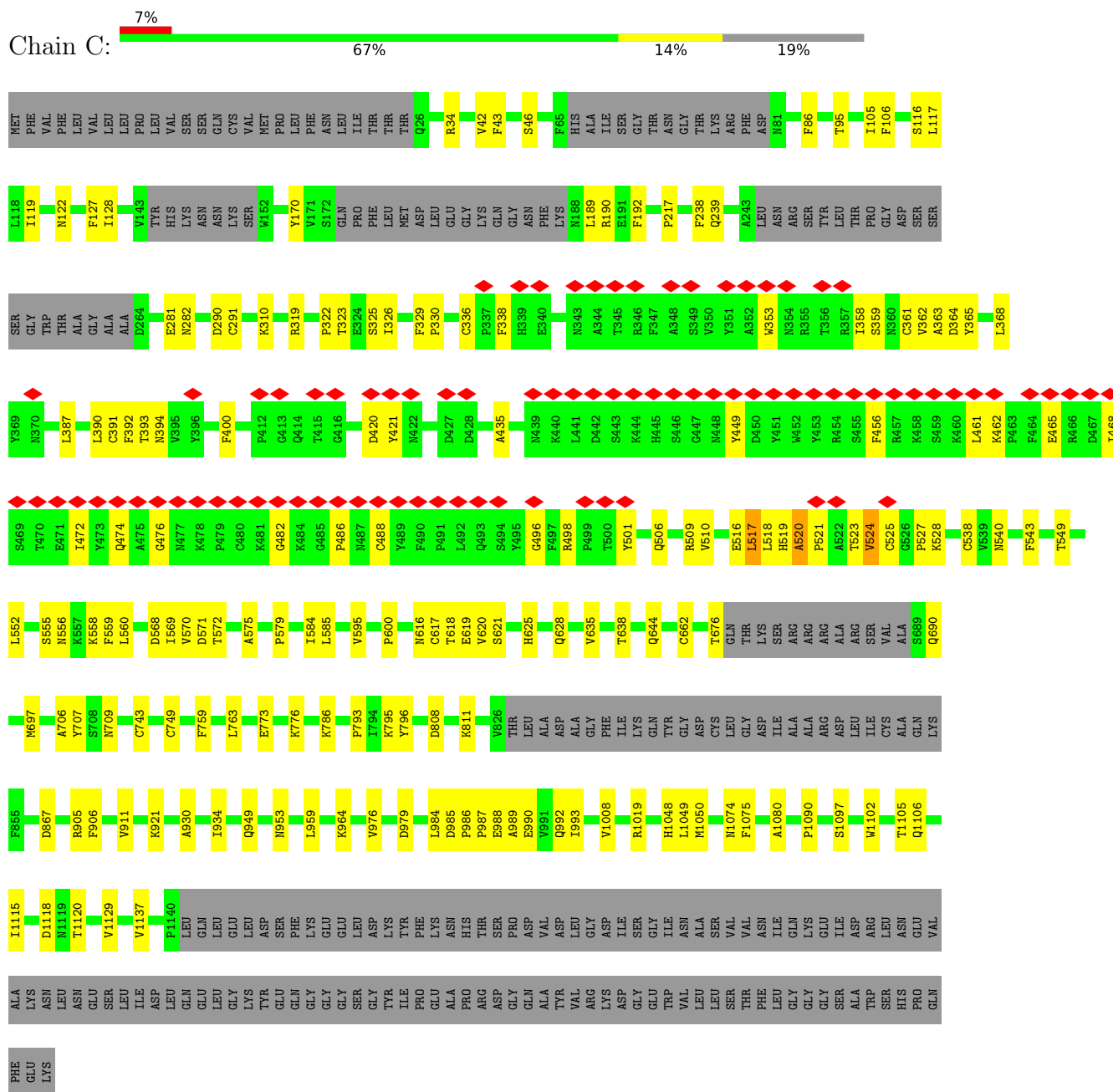


## • Molecule 2: Spike glycoprotein

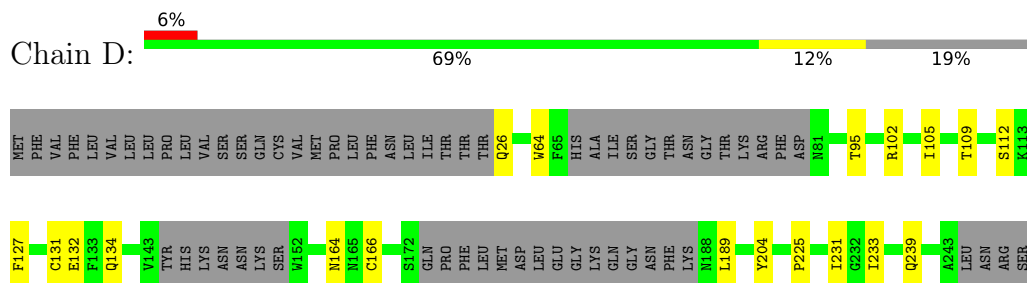
Chain B: 68% 12% 20%



## • 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

*Continued on next page...*

*Continued from previous page...*

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.

All (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
2:C:362:VAL:HB	2:C:391:CYS:SG	1.79	1.22

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:336:CYS:SG	2:D:338:PHE:CE2	2.36	1.18
2:C:336:CYS:SG	2:C:338:PHE:CE2	2.36	1.18
2:B:336:CYS:SG	2:B:338:PHE:CE2	2.36	1.17
2:D:362:VAL:CG1	2:D:391:CYS:SG	2.32	1.16
2:C:362:VAL:CG1	2:C:364:ASP:HB2	1.77	1.14
2:C:362:VAL:HG13	2:C:364:ASP:HB2	1.12	1.11
2:C:338:PHE:CE1	2:C:358:ILE:CD1	2.30	1.06
2:B:390:LEU:HD13	2:B:517:LEU:HD23	1.36	1.04
2:C:393:THR:HB	2:C:519:HIS:HB3	1.38	1.04
2:C:362:VAL:CB	2:C:391:CYS:SG	2.46	1.03
2:D:393:THR:HB	2:D:519:HIS:HB3	1.38	1.03
2:B:43:PHE:CD2	2:C:559:PHE:CE1	2.48	1.01
2:B:390:LEU:CD1	2:B:517:LEU:CD2	2.29	1.01
2:D:362:VAL:HA	2:D:391:CYS:SG	2.01	1.01
2:B:393:THR:HB	2:B:519:HIS:HB3	1.38	1.01
1:E:166:GLU:OE2	1:E:491:VAL:HG11	1.60	1.01
1:A:166:GLU:OE2	1:A:491:VAL:HG11	1.60	1.00
2:B:390:LEU:HD12	2:B:517:LEU:HD23	1.25	0.99
1:F:166:GLU:OE2	1:F:491:VAL:HG11	1.60	0.99
2:C:46:SER:OG	2:C:281:GLU:HG2	1.63	0.98
2:C:519:HIS:HB2	2:C:523:THR:OG1	1.66	0.96
2:B:43:PHE:CG	2:C:559:PHE:CD1	2.54	0.96
2:D:520:ALA:HB3	2:D:521:PRO:CD	1.96	0.95
2:C:358:ILE:CG2	2:C:361:CYS:SG	2.55	0.95
2:C:520:ALA:HB3	2:C:521:PRO:CD	1.97	0.95
2:B:519:HIS:HB2	2:B:523:THR:OG1	1.65	0.94
2:B:520:ALA:HB3	2:B:521:PRO:CD	1.97	0.94
2:D:519:HIS:HB2	2:D:523:THR:OG1	1.66	0.94
2:C:358:ILE:HG22	2:C:361:CYS:SG	2.09	0.92
2:D:520:ALA:HB3	2:D:521:PRO:HD2	1.52	0.92
2:C:520:ALA:HB3	2:C:521:PRO:HD2	1.52	0.92
2:B:520:ALA:HB3	2:B:521:PRO:HD2	1.52	0.91
2:B:964:LYS:HD2	2:C:570:VAL:HG13	1.53	0.91
2:C:338:PHE:CE2	2:C:365:TYR:HE1	1.89	0.88
2:B:43:PHE:CD2	2:C:559:PHE:HE1	1.88	0.87
2:C:43:PHE:CE1	2:D:558:LYS:O	2.28	0.86
2:C:338:PHE:HE2	2:C:365:TYR:HE1	1.24	0.85
1:E:145:GLU:OE1	1:E:146:PRO:HD3	1.77	0.84
2:C:362:VAL:CG2	2:C:391:CYS:SG	2.67	0.82
2:B:520:ALA:CB	2:B:521:PRO:CD	2.58	0.82
2:D:520:ALA:CB	2:D:521:PRO:CD	2.58	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:520:ALA:CB	2:C:521:PRO:CD	2.58	0.79
2:C:552:LEU:HB3	2:C:585:LEU:HD11	1.63	0.79
2:C:336:CYS:SG	2:C:338:PHE:CD2	2.76	0.78
2:C:362:VAL:HG23	2:C:391:CYS:SG	2.24	0.77
2:C:338:PHE:CE2	2:C:365:TYR:CE1	2.72	0.77
2:B:316:SER:O	2:B:595:VAL:HG12	1.87	0.75
2:C:43:PHE:CG	2:D:559:PHE:CD1	2.76	0.74
2:B:984:LEU:HD13	2:B:988:GLU:HB3	1.70	0.73
2:B:43:PHE:CD2	2:C:559:PHE:CD1	2.76	0.73
2:B:43:PHE:CG	2:C:559:PHE:CE1	2.77	0.73
2:C:358:ILE:HG21	2:C:361:CYS:SG	2.28	0.72
2:D:132:GLU:H	2:D:164:ASN:HD21	1.37	0.72
2:D:362:VAL:CA	2:D:391:CYS:SG	2.78	0.72
2:D:336:CYS:SG	2:D:338:PHE:CD2	2.76	0.72
2:B:390:LEU:HD12	2:B:517:LEU:HD22	1.67	0.72
2:B:336:CYS:SG	2:B:338:PHE:CD2	2.76	0.71
2:C:43:PHE:HE1	2:D:558:LYS:O	1.73	0.70
2:B:519:HIS:CB	2:B:523:THR:OG1	2.40	0.70
2:B:43:PHE:CD1	2:C:559:PHE:HA	2.28	0.68
2:C:46:SER:OG	2:C:281:GLU:CG	2.38	0.68
2:C:519:HIS:CB	2:C:523:THR:OG1	2.40	0.68
2:B:61:ASN:OD1	2:B:61:ASN:O	2.09	0.68
2:C:676:THR:HA	2:C:690:GLN:HA	1.76	0.68
2:C:365:TYR:HB3	2:C:368:LEU:HD12	1.75	0.68
1:F:134:ASN:OD1	1:F:137:ASN:ND2	2.27	0.68
2:D:474:GLN:NE2	2:D:476:GLY:O	2.27	0.67
1:E:134:ASN:OD1	1:E:137:ASN:ND2	2.27	0.67
2:D:127:PHE:CD2	6:D:1314:NAG:H83	2.30	0.67
2:C:474:GLN:NE2	2:C:476:GLY:O	2.27	0.67
2:B:905:ARG:NH1	2:B:1049:LEU:O	2.27	0.67
2:B:474:GLN:NE2	2:B:476:GLY:O	2.27	0.66
2:C:552:LEU:HD13	2:C:585:LEU:HD21	1.77	0.66
1:A:134:ASN:OD1	1:A:137:ASN:ND2	2.27	0.66
2:D:971:GLY:O	2:D:995:ARG:NH1	2.28	0.66
2:B:391:CYS:O	2:B:523:THR:HG23	1.97	0.65
2:C:362:VAL:HB	2:C:391:CYS:HG	1.58	0.65
2:C:635:VAL:HG13	2:C:638:THR:HG23	1.79	0.65
2:D:331:ASN:HB3	2:D:333:THR:HG23	1.78	0.65
2:B:334:ASN:CG	2:B:361:CYS:SG	2.75	0.65
2:D:519:HIS:CB	2:D:523:THR:OG1	2.40	0.64
2:B:745:ASP:OD1	2:C:319:ARG:NH2	2.31	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:392:PHE:HB3	2:C:519:HIS:ND1	2.12	0.63
2:D:709:ASN:OD1	6:D:1304:NAG:N2	2.31	0.63
2:C:391:CYS:O	2:C:523:THR:HG23	1.96	0.63
2:C:362:VAL:HG21	2:C:527:PRO:HD3	1.80	0.63
2:C:930:ALA:O	2:C:934:ILE:HG12	1.99	0.63
2:D:132:GLU:H	2:D:164:ASN:ND2	1.97	0.63
2:D:326:ILE:N	2:D:540:ASN:O	2.28	0.62
2:B:43:PHE:CD1	2:C:559:PHE:HD1	2.17	0.62
2:B:569:ILE:HG13	2:B:570:VAL:HG23	1.82	0.62
1:F:119:ILE:HD11	1:F:179:LEU:HB3	1.82	0.62
2:B:365:TYR:HB2	2:B:368:LEU:HD12	1.82	0.62
2:C:391:CYS:HB2	2:C:525:CYS:H	1.62	0.62
2:C:569:ILE:HG13	2:C:570:VAL:HG23	1.82	0.62
2:C:326:ILE:N	2:C:540:ASN:O	2.33	0.62
2:C:362:VAL:HA	2:C:391:CYS:HA	1.82	0.61
2:C:1080:ALA:HB3	2:C:1129:VAL:HG11	1.82	0.61
2:D:984:LEU:HD13	2:D:988:GLU:HB3	1.82	0.61
2:D:362:VAL:HA	2:D:391:CYS:CB	2.30	0.61
1:E:119:ILE:HD11	1:E:179:LEU:HB3	1.82	0.61
2:B:43:PHE:CD1	2:C:559:PHE:CD1	2.88	0.61
2:B:334:ASN:ND2	2:B:361:CYS:SG	2.73	0.61
2:D:365:TYR:HB2	2:D:368:LEU:HD12	1.82	0.61
1:A:322:ASN:HD22	3:H:1:NAG:C7	2.14	0.60
2:D:569:ILE:HG13	2:D:570:VAL:HG23	1.82	0.60
1:F:322:ASN:HD22	3:W:1:NAG:C7	2.14	0.60
1:A:109:SER:H	1:A:112:LYS:HD2	1.66	0.60
1:E:322:ASN:HD22	3:S:1:NAG:C7	2.14	0.60
1:A:119:ILE:HD11	1:A:179:LEU:HB3	1.82	0.60
2:B:360:ASN:O	2:B:361:CYS:SG	2.56	0.60
2:B:43:PHE:CE1	2:C:558:LYS:O	2.55	0.60
1:F:109:SER:H	1:F:112:LYS:HD2	1.66	0.60
2:C:43:PHE:CG	2:D:559:PHE:HD1	2.20	0.60
2:C:43:PHE:CD1	2:D:559:PHE:HA	2.35	0.60
2:B:1100:THR:OG1	2:B:1101:HIS:ND1	2.31	0.60
2:D:394:ASN:H	2:D:519:HIS:CG	2.21	0.59
2:D:1019:ARG:NH1	2:D:1023:ASN:OD1	2.35	0.59
2:B:92:PHE:HE1	2:B:94:SER:HB3	1.68	0.59
2:D:676:THR:HA	2:D:690:GLN:HA	1.85	0.59
2:B:122:ASN:OD1	2:B:123:ALA:N	2.33	0.59
2:B:394:ASN:H	2:B:519:HIS:CG	2.21	0.59
2:B:393:THR:HB	2:B:519:HIS:CB	2.25	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:PHE:HB3	2:D:559:PHE:CE1	2.38	0.59
2:C:394:ASN:H	2:C:519:HIS:CG	2.21	0.59
1:E:109:SER:H	1:E:112:LYS:HD2	1.66	0.58
2:D:26:GLN:N	2:D:64:TRP:O	2.35	0.58
2:D:520:ALA:HB3	2:D:521:PRO:HD3	1.84	0.58
2:C:520:ALA:HB3	2:C:521:PRO:HD3	1.84	0.58
2:C:330:PRO:HA	2:C:579:PRO:HB2	1.84	0.58
2:C:676:THR:HG22	2:C:690:GLN:HB3	1.85	0.58
2:B:392:PHE:HB3	2:B:519:HIS:ND1	2.19	0.58
2:B:520:ALA:HB3	2:B:521:PRO:HD3	1.84	0.58
2:D:353:TRP:HB3	2:D:400:PHE:HE1	1.70	0.57
2:C:43:PHE:CB	2:D:559:PHE:CE1	2.88	0.57
2:C:393:THR:HB	2:C:519:HIS:CB	2.25	0.57
2:D:131:CYS:HB3	2:D:166:CYS:HA	1.86	0.57
2:D:390:LEU:HD12	2:D:524:VAL:HG22	1.85	0.57
2:C:808:ASP:HB3	2:C:811:LYS:HE2	1.86	0.57
2:D:393:THR:HB	2:D:519:HIS:CB	2.24	0.57
2:D:985:ASP:HB2	2:D:987:PRO:HD2	1.86	0.57
2:B:392:PHE:HA	2:B:523:THR:HG23	1.86	0.57
2:B:571:ASP:OD2	2:D:967:SER:OG	2.23	0.57
2:C:43:PHE:CD1	2:D:559:PHE:HD1	2.23	0.57
2:B:1082:CYS:HB2	2:B:1132:ILE:HD11	1.85	0.56
2:D:109:THR:HG1	2:D:114:THR:HG1	1.51	0.56
2:C:363:ALA:HA	2:C:365:TYR:CZ	2.41	0.56
2:C:763:LEU:HD22	2:C:1008:VAL:HG21	1.87	0.56
2:D:336:CYS:SG	2:D:338:PHE:CZ	2.96	0.56
1:F:374:HIS:CE1	1:F:406:GLU:HG2	2.41	0.56
2:D:362:VAL:HA	2:D:391:CYS:HB3	1.88	0.56
1:A:374:HIS:CE1	1:A:406:GLU:HG2	2.41	0.56
2:B:763:LEU:HD22	2:B:1008:VAL:HG21	1.85	0.56
2:C:363:ALA:HB3	2:C:387:LEU:HB3	1.88	0.56
2:C:617:CYS:SG	2:C:644:GLN:NE2	2.78	0.56
2:C:964:LYS:HA	2:D:570:VAL:HG11	1.86	0.56
1:E:306:ARG:HA	1:E:309:LYS:HG2	1.88	0.56
1:E:439:LEU:HB3	1:E:591:LEU:HD12	1.88	0.56
2:B:336:CYS:SG	2:B:338:PHE:CZ	2.96	0.56
2:B:1048:HIS:NE2	2:B:1050:MET:O	2.38	0.56
2:B:43:PHE:CE1	2:C:559:PHE:HA	2.40	0.56
2:C:43:PHE:CB	2:D:559:PHE:CD1	2.89	0.56
2:C:516:GLU:O	2:C:518:LEU:N	2.39	0.56
2:D:516:GLU:O	2:D:518:LEU:N	2.39	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ARG:HA	1:A:309:LYS:HG2	1.88	0.55
2:C:362:VAL:CG1	2:C:364:ASP:CB	2.69	0.55
1:E:374:HIS:CE1	1:E:406:GLU:HG2	2.41	0.55
2:C:985:ASP:HB2	2:C:987:PRO:HD2	1.88	0.55
2:C:353:TRP:HB3	2:C:400:PHE:HE1	1.70	0.55
2:D:127:PHE:CE2	6:D:1314:NAG:H83	2.41	0.55
2:D:520:ALA:CB	2:D:521:PRO:HD3	2.36	0.55
2:D:804:GLN:NE2	2:D:935:GLN:OE1	2.30	0.55
1:F:306:ARG:HA	1:F:309:LYS:HG2	1.88	0.55
2:B:353:TRP:HB3	2:B:400:PHE:HE1	1.70	0.55
1:F:439:LEU:HB3	1:F:591:LEU:HD12	1.88	0.55
2:D:763:LEU:HD22	2:D:1008:VAL:HG21	1.88	0.55
2:D:295:PRO:HB2	2:D:608:VAL:HG11	1.88	0.55
2:B:282:ASN:O	2:C:558:LYS:O	2.25	0.54
1:A:439:LEU:HB3	1:A:591:LEU:HD12	1.88	0.54
2:C:336:CYS:SG	2:C:338:PHE:CZ	2.96	0.54
2:C:42:VAL:HG11	2:D:567:ARG:HB2	1.89	0.54
2:D:676:THR:HG22	2:D:690:GLN:HB3	1.88	0.54
2:C:325:SER:HA	2:C:540:ASN:HB2	1.87	0.54
2:C:95:THR:HG22	2:C:189:LEU:HA	1.90	0.54
1:E:524:GLN:NE2	1:E:574:VAL:HG11	2.23	0.54
2:B:964:LYS:HA	2:C:570:VAL:CG1	2.38	0.54
2:D:322:PRO:HA	2:D:538:CYS:SG	2.47	0.54
2:C:1097:SER:HB2	2:C:1102:TRP:CD2	2.43	0.53
2:C:520:ALA:CB	2:C:521:PRO:HD3	2.36	0.53
1:A:524:GLN:NE2	1:A:574:VAL:HG11	2.23	0.53
2:B:520:ALA:CB	2:B:521:PRO:HD3	2.36	0.53
2:C:390:LEU:HD22	2:C:524:VAL:HG22	1.90	0.53
1:F:524:GLN:NE2	1:F:574:VAL:HG11	2.23	0.53
2:C:362:VAL:HG22	2:C:362:VAL:O	2.08	0.53
1:A:145:GLU:HB3	1:A:146:PRO:HD3	1.89	0.53
2:D:616:ASN:HB3	2:D:619:GLU:HG2	1.90	0.53
2:B:516:GLU:O	2:B:518:LEU:N	2.39	0.53
2:C:43:PHE:CG	2:D:559:PHE:CE1	2.97	0.53
1:E:115:ARG:NH2	1:E:182:GLU:OE1	2.42	0.53
2:C:568:ASP:OD1	2:C:572:THR:N	2.42	0.53
2:B:568:ASP:OD1	2:B:572:THR:N	2.42	0.52
2:D:362:VAL:HG12	2:D:391:CYS:SG	2.43	0.52
1:F:115:ARG:NH2	1:F:182:GLU:OE1	2.42	0.52
2:B:390:LEU:HD12	2:B:517:LEU:HD21	1.78	0.52
2:C:796:TYR:CD2	6:D:1304:NAG:H61	2.45	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:568:ASP:OD1	2:D:572:THR:N	2.42	0.52
1:F:177:ARG:HB2	1:F:498:CYS:HB2	1.92	0.52
2:B:330:PRO:HA	2:B:579:PRO:HB2	1.92	0.52
2:D:123:ALA:H	6:D:1314:NAG:C7	2.22	0.52
1:A:115:ARG:NH2	1:A:182:GLU:OE1	2.42	0.52
2:C:621:SER:O	2:C:625:HIS:ND1	2.36	0.52
1:A:389:PRO:HD2	1:A:392:LEU:HD12	1.92	0.52
2:C:358:ILE:HG22	2:C:359:SER:N	2.25	0.52
2:C:988:GLU:O	2:C:992:GLN:HG2	2.10	0.51
2:D:360:ASN:O	2:D:361:CYS:C	2.49	0.51
2:D:325:SER:HA	2:D:540:ASN:HB2	1.91	0.51
1:E:389:PRO:HD2	1:E:392:LEU:HD12	1.92	0.51
1:A:177:ARG:HB2	1:A:498:CYS:HB2	1.92	0.51
1:F:389:PRO:HD2	1:F:392:LEU:HD12	1.92	0.51
2:B:324:GLU:HB2	2:B:539:VAL:HG12	1.93	0.51
2:B:620:VAL:O	2:B:624:ILE:HG12	2.11	0.51
2:B:336:CYS:HB2	2:B:363:ALA:HA	1.93	0.51
2:D:231:ILE:HD12	2:D:233:ILE:HG12	1.93	0.51
1:E:524:GLN:HE21	1:E:574:VAL:HG11	1.76	0.51
2:C:1090:PRO:HA	2:C:1120:THR:HG22	1.93	0.50
2:D:595:VAL:HG12	2:D:595:VAL:O	2.10	0.50
1:F:212:VAL:HG23	1:F:215:TYR:HB2	1.93	0.50
2:D:123:ALA:HB3	6:D:1314:NAG:H2	1.91	0.50
2:D:362:VAL:CB	2:D:391:CYS:SG	2.99	0.50
2:B:323:THR:HG23	2:B:324:GLU:OE1	2.11	0.50
2:D:930:ALA:O	2:D:934:ILE:HG12	2.11	0.50
1:E:145:GLU:OE1	1:E:146:PRO:CD	2.53	0.50
2:B:43:PHE:CG	2:C:559:PHE:HD1	2.16	0.50
2:B:329:PHE:CG	2:B:528:LYS:HB3	2.47	0.50
2:C:290:ASP:OD1	2:C:291:CYS:N	2.44	0.50
2:C:392:PHE:HE1	2:C:517:LEU:HG	1.76	0.50
1:E:177:ARG:HB2	1:E:498:CYS:HB2	1.92	0.50
2:D:102:ARG:HD2	2:D:122:ASN:HA	1.94	0.50
2:C:329:PHE:CG	2:C:528:LYS:HB3	2.47	0.49
2:C:363:ALA:HB2	2:C:392:PHE:HE2	1.77	0.49
2:D:1097:SER:HB2	2:D:1102:TRP:CD2	2.48	0.49
1:A:524:GLN:HE21	1:A:574:VAL:HG11	1.76	0.49
2:D:638:THR:HB	2:D:641:ASN:HB2	1.94	0.49
1:E:374:HIS:HE1	1:E:406:GLU:HG2	1.77	0.49
1:A:374:HIS:HE1	1:A:406:GLU:HG2	1.77	0.49
1:E:212:VAL:HG23	1:E:215:TYR:HB2	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:524:GLN:HE21	1:F:574:VAL:HG11	1.76	0.49
2:D:666:ILE:HD11	2:D:672:ALA:HB2	1.95	0.49
1:A:133:CYS:HA	1:A:141:CYS:HA	1.95	0.49
2:C:552:LEU:CB	2:C:585:LEU:HD11	2.39	0.49
1:E:481:LYS:HD3	1:E:487:VAL:HG23	1.95	0.49
2:B:662:CYS:HB2	2:B:697:MET:HG3	1.95	0.48
2:C:362:VAL:CA	2:C:391:CYS:SG	3.00	0.48
1:F:300:GLN:HB2	1:F:302:TRP:CD1	2.48	0.48
2:D:329:PHE:CG	2:D:528:LYS:HB3	2.47	0.48
1:A:457:GLU:HG2	1:A:513:ILE:HD13	1.95	0.48
1:A:212:VAL:HG23	1:A:215:TYR:HB2	1.93	0.48
1:A:300:GLN:HB2	1:A:302:TRP:CD1	2.48	0.48
2:B:1082:CYS:HB3	2:B:1134:ASN:OD1	2.14	0.48
1:E:457:GLU:HG2	1:E:513:ILE:HD13	1.95	0.48
2:C:322:PRO:HA	2:C:538:CYS:SG	2.54	0.48
1:A:481:LYS:HD3	1:A:487:VAL:HG23	1.95	0.48
2:D:421:TYR:HA	2:D:461:LEU:HD23	1.96	0.48
1:E:133:CYS:HA	1:E:141:CYS:HA	1.95	0.48
1:E:460:ARG:NH2	1:E:506:VAL:HG22	2.29	0.48
1:A:188:ASN:O	1:A:192:ARG:HG3	2.14	0.48
2:B:988:GLU:O	2:B:992:GLN:HG2	2.14	0.48
2:C:358:ILE:CG2	2:C:359:SER:N	2.76	0.48
1:F:133:CYS:HA	1:F:141:CYS:HA	1.95	0.48
2:B:421:TYR:HA	2:B:461:LEU:HD23	1.96	0.48
2:C:964:LYS:HA	2:D:570:VAL:CG1	2.43	0.48
2:D:290:ASP:OD1	2:D:291:CYS:N	2.45	0.48
1:F:457:GLU:HG2	1:F:513:ILE:HD13	1.95	0.47
1:F:460:ARG:NH2	1:F:506:VAL:HG22	2.29	0.47
2:C:391:CYS:HB2	2:C:525:CYS:N	2.28	0.47
2:C:976:VAL:HG23	2:C:979:ASP:HB2	1.96	0.47
2:D:356:THR:O	2:D:396:TYR:HA	2.14	0.47
1:E:300:GLN:HB2	1:E:302:TRP:CD1	2.48	0.47
1:F:481:LYS:HD3	1:F:487:VAL:HG23	1.95	0.47
2:C:105:ILE:HD11	2:C:116:SER:HB3	1.95	0.47
2:C:105:ILE:HG22	2:C:239:GLN:HB2	1.95	0.47
2:C:709:ASN:HB2	6:C:1302:NAG:O5	2.14	0.47
2:D:336:CYS:SG	2:D:361:CYS:HA	2.54	0.47
2:C:449:TYR:HE1	2:C:496:GLY:HA2	1.79	0.47
1:E:188:ASN:O	1:E:192:ARG:HG3	2.14	0.47
1:F:188:ASN:O	1:F:192:ARG:HG3	2.14	0.47
2:B:129:LYS:HB3	2:B:166:CYS:SG	2.54	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:743:CYS:HB3	2:B:749:CYS:HB3	1.79	0.47
2:B:449:TYR:HE1	2:B:496:GLY:HA2	1.79	0.47
1:A:460:ARG:NH2	1:A:506:VAL:HG22	2.29	0.47
2:B:284:THR:HG22	2:C:560:LEU:HD21	1.96	0.47
2:D:449:TYR:HE1	2:D:496:GLY:HA2	1.79	0.47
2:D:1081:ILE:HD12	2:D:1135:ASN:HB3	1.96	0.47
1:F:374:HIS:HE1	1:F:406:GLU:HG2	1.77	0.47
2:C:46:SER:HG	2:C:281:GLU:HG2	1.76	0.47
2:B:472:ILE:HD13	2:B:482:GLY:H	1.81	0.46
2:C:552:LEU:HB3	2:C:585:LEU:CD1	2.40	0.46
2:C:190:ARG:HB3	2:C:192:PHE:HE1	1.80	0.46
2:C:421:TYR:HA	2:C:461:LEU:HD23	1.96	0.46
2:C:34:ARG:NH2	2:C:217:PRO:O	2.48	0.46
2:C:543:PHE:HE2	2:C:585:LEU:HD23	1.80	0.46
1:E:209:VAL:HG11	1:E:565:PRO:HB3	1.98	0.46
2:B:629:LEU:HB3	2:B:631:PRO:HD3	1.98	0.46
2:B:1097:SER:HB2	2:B:1102:TRP:CD2	2.50	0.46
1:A:209:VAL:HG11	1:A:565:PRO:HB3	1.98	0.46
2:B:43:PHE:HE1	2:C:558:LYS:O	1.98	0.46
2:D:295:PRO:HG3	2:D:633:TRP:CE3	2.51	0.46
2:D:420:ASP:O	2:D:461:LEU:HD23	2.16	0.46
2:B:335:LEU:O	2:B:361:CYS:SG	2.73	0.46
2:C:472:ILE:HD13	2:C:482:GLY:H	1.81	0.46
2:B:428:ASP:OD1	2:B:428:ASP:N	2.46	0.46
2:B:1129:VAL:HG12	2:D:917:TYR:HB3	1.97	0.46
2:D:486:PRO:O	2:D:488:CYS:N	2.50	0.46
1:F:374:HIS:CE1	1:F:402:GLU:OE1	2.68	0.46
2:B:676:THR:HG22	2:B:690:GLN:HB3	1.98	0.45
2:B:989:ALA:O	2:B:993:ILE:HG12	2.17	0.45
2:B:1127:ASP:OD1	2:B:1127:ASP:N	2.49	0.45
2:C:323:THR:OG1	2:C:628:GLN:HG2	2.17	0.45
1:E:378:HIS:ND1	1:E:401:HIS:CE1	2.85	0.45
2:C:793:PRO:HB2	2:C:795:LYS:HE2	1.97	0.45
2:C:906:PHE:HB3	2:C:911:VAL:HG23	1.98	0.45
2:C:1118:ASP:OD1	2:C:1118:ASP:N	2.46	0.45
1:E:145:GLU:O	1:E:149:ASN:HB2	2.15	0.45
2:C:486:PRO:O	2:C:488:CYS:N	2.50	0.45
1:F:208:GLU:HB2	1:F:219:ARG:HG2	1.98	0.45
1:F:306:ARG:HA	1:F:309:LYS:HE3	1.99	0.45
2:B:713:ALA:HB3	2:D:894:LEU:HB3	1.98	0.45
2:C:743:CYS:HB3	2:C:749:CYS:HB3	1.78	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1115:ILE:HG22	2:C:1137:VAL:HG13	1.98	0.45
1:F:209:VAL:HG11	1:F:565:PRO:HB3	1.98	0.45
2:B:420:ASP:O	2:B:461:LEU:HD23	2.16	0.45
2:B:906:PHE:CD2	2:B:916:LEU:HB2	2.51	0.45
2:C:616:ASN:OD1	2:C:617:CYS:N	2.45	0.45
2:C:921:LYS:HA	2:C:921:LYS:HD2	1.78	0.45
2:D:743:CYS:HB3	2:D:749:CYS:HB3	1.70	0.45
1:E:460:ARG:HH21	1:E:506:VAL:HG22	1.82	0.45
2:C:46:SER:HG	2:C:281:GLU:CG	2.30	0.45
2:D:472:ILE:HD13	2:D:482:GLY:H	1.81	0.45
2:D:1048:HIS:NE2	2:D:1050:MET:O	2.47	0.45
1:F:203:TRP:HZ3	1:F:460:ARG:HH11	1.65	0.45
2:B:190:ARG:HB3	2:B:192:PHE:HE1	1.81	0.45
2:B:486:PRO:O	2:B:488:CYS:N	2.50	0.45
2:C:449:TYR:OH	2:C:498:ARG:NH2	2.49	0.45
1:F:378:HIS:ND1	1:F:401:HIS:CE1	2.85	0.45
1:F:417:HIS:ND1	1:F:543:ASP:OD2	2.46	0.45
1:A:308:PHE:CE2	1:A:333:LEU:HD22	2.52	0.45
2:C:759:PHE:O	2:C:763:LEU:HG	2.17	0.45
1:E:308:PHE:CE2	1:E:333:LEU:HD22	2.52	0.45
1:A:208:GLU:HB2	1:A:219:ARG:HG2	1.98	0.45
2:B:967:SER:OG	2:C:571:ASP:HB2	2.17	0.44
2:C:420:ASP:O	2:C:461:LEU:HD23	2.16	0.44
2:C:949:GLN:HG3	2:C:953:ASN:ND2	2.31	0.44
2:D:295:PRO:HG3	2:D:633:TRP:CZ3	2.51	0.44
2:D:662:CYS:HB2	2:D:697:MET:HG3	1.98	0.44
1:E:203:TRP:HZ3	1:E:460:ARG:HH11	1.65	0.44
1:E:208:GLU:HB2	1:E:219:ARG:HG2	1.98	0.44
2:B:1089:PHE:HE2	2:D:917:TYR:HD2	1.64	0.44
2:C:117:LEU:HG	2:C:119:ILE:HG13	1.98	0.44
1:A:419:LYS:NZ	1:A:428:PHE:O	2.31	0.44
2:B:128:ILE:HB	2:B:170:TYR:HB3	1.99	0.44
2:C:986:PRO:O	2:C:990:GLU:HG2	2.17	0.44
2:D:357:ARG:HA	2:D:396:TYR:HD1	1.82	0.44
2:D:867:ASP:OD1	2:D:867:ASP:N	2.49	0.44
1:A:306:ARG:HA	1:A:309:LYS:HE3	1.99	0.44
2:B:777:ASN:OD1	2:B:1019:ARG:NH1	2.48	0.44
2:C:776:LYS:HB3	2:C:776:LYS:HE2	1.88	0.44
2:D:906:PHE:CD2	2:D:916:LEU:HB2	2.53	0.44
1:A:19:SER:O	1:A:20:THR:C	2.56	0.44
2:C:662:CYS:HB2	2:C:697:MET:HG3	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:LEU:CD1	2:B:517:LEU:HD22	2.32	0.44
2:B:392:PHE:CE1	2:B:517:LEU:HG	2.52	0.44
2:B:729:VAL:HG23	2:B:1059:GLY:HA2	2.00	0.44
2:B:964:LYS:HA	2:C:570:VAL:HG11	1.99	0.44
2:B:1121:PHE:HE2	2:D:914:ASN:HD21	1.64	0.44
2:C:618:THR:O	2:C:621:SER:OG	2.28	0.44
2:B:206:LYS:HB2	2:B:223:LEU:HG	2.00	0.44
1:E:417:HIS:ND1	1:E:543:ASP:OD2	2.46	0.44
1:F:308:PHE:CE2	1:F:333:LEU:HD22	2.52	0.44
2:B:449:TYR:OH	2:B:498:ARG:NH2	2.49	0.44
2:B:814:LYS:HD3	2:B:814:LYS:HA	1.76	0.44
2:C:456:PHE:HE1	1:E:30:ASP:OD2	2.01	0.44
2:C:959:LEU:HD23	2:C:959:LEU:HA	1.89	0.44
2:C:984:LEU:HD13	2:C:988:GLU:HB3	1.99	0.44
2:D:95:THR:HG22	2:D:189:LEU:HA	1.99	0.44
2:D:456:PHE:HE1	1:F:30:ASP:OD2	2.01	0.44
1:A:460:ARG:HH21	1:A:506:VAL:HG22	1.82	0.44
2:C:619:GLU:O	2:C:620:VAL:HB	2.18	0.44
2:C:867:ASP:N	2:C:867:ASP:OD1	2.51	0.44
2:D:105:ILE:HD11	2:D:239:GLN:HB2	2.00	0.44
1:A:203:TRP:HZ3	1:A:460:ARG:HH11	1.65	0.43
2:B:792:PRO:HG2	2:C:707:TYR:HB3	2.00	0.43
1:E:306:ARG:HA	1:E:309:LYS:HE3	1.99	0.43
2:B:575:ALA:HB1	2:B:584:ILE:HD11	2.00	0.43
2:D:449:TYR:OH	2:D:498:ARG:NH2	2.49	0.43
2:D:776:LYS:HB3	2:D:776:LYS:HE2	1.86	0.43
1:E:374:HIS:CE1	1:E:402:GLU:OE1	2.68	0.43
1:A:30:ASP:OD2	2:B:456:PHE:HE1	2.01	0.43
1:E:145:GLU:HG2	1:E:149:ASN:HD22	1.83	0.43
1:F:460:ARG:HH21	1:F:506:VAL:HG22	1.82	0.43
2:C:128:ILE:HB	2:C:170:TYR:HB3	2.00	0.43
2:D:726:ILE:HG12	2:D:1061:VAL:HG22	2.00	0.43
2:D:921:LYS:HD2	2:D:921:LYS:HA	1.84	0.43
1:E:39:LEU:HB3	1:E:69:TRP:HE3	1.84	0.43
2:D:501:TYR:O	2:D:506:GLN:NE2	2.51	0.43
2:D:529:LYS:HE2	2:D:529:LYS:HB3	1.83	0.43
1:A:431:ASP:OD1	1:A:431:ASP:N	2.45	0.43
2:B:295:PRO:HG3	2:B:633:TRP:CE3	2.54	0.43
2:B:501:TYR:O	2:B:506:GLN:NE2	2.51	0.43
2:C:105:ILE:HD12	2:C:105:ILE:HA	1.93	0.43
2:C:989:ALA:O	2:C:993:ILE:HG12	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:554:LEU:O	1:F:558:LEU:HG	2.19	0.43
2:B:858:LEU:HD13	2:B:959:LEU:HD22	2.01	0.43
2:C:281:GLU:HB2	6:C:1309:NAG:H81	2.01	0.43
1:F:39:LEU:HB3	1:F:69:TRP:HE3	1.83	0.43
1:F:524:GLN:HA	1:F:583:PRO:HG2	2.01	0.43
2:B:359:SER:HA	2:B:393:THR:O	2.18	0.43
2:B:630:THR:N	2:B:631:PRO:HD3	2.34	0.43
2:D:599:THR:HG22	2:D:608:VAL:HG22	2.01	0.43
2:C:362:VAL:HA	2:C:391:CYS:SG	2.59	0.42
2:C:462:LYS:HG2	2:C:465:GLU:OE1	2.19	0.42
2:C:595:VAL:HG12	2:C:595:VAL:O	2.19	0.42
2:D:122:ASN:OD1	6:D:1314:NAG:H82	2.18	0.42
2:B:976:VAL:HG23	2:B:979:ASP:HB2	2.01	0.42
1:A:39:LEU:HB3	1:A:69:TRP:HE3	1.83	0.42
2:B:462:LYS:HG2	2:B:465:GLU:OE1	2.19	0.42
2:B:906:PHE:CE2	2:B:916:LEU:HB2	2.54	0.42
2:D:858:LEU:HD23	2:D:959:LEU:HD22	2.02	0.42
2:C:575:ALA:HB1	2:C:584:ILE:HD11	2.00	0.42
2:D:462:LYS:HG2	2:D:465:GLU:OE1	2.19	0.42
2:D:575:ALA:HB1	2:D:584:ILE:HD11	2.00	0.42
2:D:814:LYS:HA	2:D:814:LYS:HD3	1.74	0.42
1:E:32:PHE:HE2	1:E:391:LEU:HD21	1.84	0.42
2:C:122:ASN:HD21	2:C:127:PHE:HD2	1.67	0.42
2:C:501:TYR:HE1	1:E:41:TYR:CZ	2.37	0.42
2:C:501:TYR:O	2:C:506:GLN:NE2	2.51	0.42
2:C:905:ARG:NH1	2:C:1049:LEU:O	2.46	0.42
2:D:984:LEU:HD12	2:D:985:ASP:O	2.19	0.42
1:E:381:TYR:HD1	1:E:558:LEU:HD22	1.85	0.42
1:A:524:GLN:HA	1:A:583:PRO:HG2	2.01	0.42
2:D:501:TYR:HE1	1:F:41:TYR:CZ	2.37	0.42
2:D:612:TYR:HE2	2:D:651:ILE:HD12	1.83	0.42
1:E:459:TRP:CD1	1:E:477:TRP:HE3	2.38	0.42
1:E:524:GLN:HA	1:E:583:PRO:HG2	2.01	0.42
1:E:554:LEU:O	1:E:558:LEU:HG	2.19	0.42
2:C:86:PHE:HB2	2:C:238:PHE:HD1	1.85	0.42
2:C:435:ALA:HB2	2:C:510:VAL:HG22	2.02	0.42
2:D:114:THR:O	2:D:132:GLU:HG2	2.20	0.42
1:F:459:TRP:CD1	1:F:477:TRP:HE3	2.38	0.42
1:A:381:TYR:HD1	1:A:558:LEU:HD22	1.85	0.42
2:C:338:PHE:CZ	2:C:358:ILE:HG21	2.54	0.42
2:C:468:ILE:HG22	2:C:468:ILE:O	2.20	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TYR:CZ	2:B:501:TYR:HE1	2.37	0.42
2:B:794:ILE:HD12	2:B:794:ILE:H	1.83	0.42
1:E:32:PHE:CE2	1:E:391:LEU:HD21	2.55	0.42
1:E:302:TRP:CZ2	1:E:423:LEU:HD21	2.55	0.42
1:F:308:PHE:HD2	1:F:333:LEU:HD13	1.85	0.42
1:A:459:TRP:CD1	1:A:477:TRP:HE3	2.38	0.42
2:C:310:LYS:HG3	2:C:600:PRO:HA	2.02	0.42
2:C:773:GLU:OE2	2:C:1019:ARG:HD3	2.19	0.42
2:C:786:LYS:NZ	2:D:1045:LYS:HE3	2.34	0.42
2:C:949:GLN:HG3	2:C:953:ASN:HD21	1.85	0.42
1:F:32:PHE:HE2	1:F:391:LEU:HD21	1.84	0.42
1:A:302:TRP:CZ2	1:A:423:LEU:HD21	2.55	0.41
2:C:555:SER:OG	2:C:556:ASN:N	2.53	0.41
1:E:308:PHE:HD2	1:E:333:LEU:HD13	1.85	0.41
1:F:381:TYR:HD1	1:F:558:LEU:HD22	1.85	0.41
1:A:55:THR:O	1:A:59:VAL:HG23	2.20	0.41
1:A:554:LEU:O	1:A:558:LEU:HG	2.19	0.41
2:B:334:ASN:OD1	2:B:361:CYS:SG	2.78	0.41
2:B:392:PHE:HE1	2:B:517:LEU:HG	1.85	0.41
2:C:359:SER:O	2:C:361:CYS:SG	2.78	0.41
2:D:435:ALA:HB2	2:D:510:VAL:HG22	2.02	0.41
1:F:302:TRP:CZ2	1:F:423:LEU:HD21	2.55	0.41
2:B:435:ALA:HB2	2:B:510:VAL:HG22	2.02	0.41
2:D:112:SER:HB3	2:D:134:GLN:HA	2.03	0.41
2:D:555:SER:OG	2:D:556:ASN:N	2.53	0.41
1:E:55:THR:O	1:E:59:VAL:HG23	2.20	0.41
1:A:32:PHE:CE2	1:A:391:LEU:HD21	2.55	0.41
2:B:117:LEU:HG	2:B:119:ILE:HG13	2.02	0.41
2:B:290:ASP:OD1	2:B:291:CYS:N	2.50	0.41
2:D:391:CYS:HB2	2:D:525:CYS:SG	2.60	0.41
1:A:417:HIS:ND1	1:A:543:ASP:OD2	2.46	0.41
2:B:645:THR:HG23	2:B:648:GLY:H	1.84	0.41
2:C:106:PHE:HB2	2:C:117:LEU:HB3	2.01	0.41
2:D:204:TYR:CD1	2:D:225:PRO:HA	2.55	0.41
2:B:358:ILE:HB	2:B:395:VAL:HG13	2.03	0.41
2:B:985:ASP:N	2:B:985:ASP:OD1	2.53	0.41
2:C:322:PRO:HB3	2:C:549:THR:CG2	2.50	0.41
2:C:392:PHE:HA	2:C:523:THR:HG23	2.02	0.41
1:E:284:PRO:HG2	1:E:436:ILE:HG22	2.03	0.41
2:B:468:ILE:HG22	2:B:468:ILE:O	2.20	0.41
2:C:1105:THR:OG1	2:C:1106:GLN:N	2.54	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:435:ALA:HA	2:D:509:ARG:O	2.21	0.41
2:D:726:ILE:HD13	2:D:945:LEU:HD23	2.02	0.41
1:A:165:TRP:CH2	1:A:490:PRO:HD2	2.56	0.41
2:D:657:ASN:HB2	6:D:1309:NAG:H2	2.03	0.41
1:E:165:TRP:CH2	1:E:490:PRO:HD2	2.56	0.41
1:A:32:PHE:HE2	1:A:391:LEU:HD21	1.84	0.41
1:A:168:TRP:HE1	1:A:502:SER:HB3	1.86	0.41
1:A:374:HIS:CE1	1:A:402:GLU:OE1	2.68	0.41
2:B:320:VAL:HG13	2:B:628:GLN:HB3	2.03	0.41
2:B:555:SER:OG	2:B:556:ASN:N	2.53	0.41
2:C:392:PHE:CE1	2:C:517:LEU:HG	2.53	0.41
2:D:329:PHE:CB	2:D:528:LYS:HB3	2.51	0.41
2:D:969:LYS:HB2	2:D:969:LYS:HE2	1.92	0.41
2:D:996:LEU:HD23	2:D:996:LEU:HA	1.92	0.41
2:D:1079:PRO:HD2	2:D:1131:GLY:O	2.21	0.41
1:E:520:LEU:HD23	1:E:520:LEU:HA	1.90	0.41
1:F:32:PHE:CE2	1:F:391:LEU:HD21	2.55	0.41
1:F:55:THR:O	1:F:59:VAL:HG23	2.20	0.41
1:F:165:TRP:CH2	1:F:490:PRO:HD2	2.56	0.41
1:F:284:PRO:HG2	1:F:436:ILE:HG22	2.03	0.41
1:A:378:HIS:CE1	1:A:401:HIS:CD2	3.09	0.41
2:B:329:PHE:CB	2:B:528:LYS:HB3	2.51	0.41
2:B:961:THR:HG21	2:D:762:GLN:NE2	2.36	0.41
2:B:996:LEU:HD23	2:B:996:LEU:HA	1.93	0.41
2:B:485:GLY:HA3	2:B:486:PRO:HD3	1.95	0.40
2:D:468:ILE:O	2:D:468:ILE:HG22	2.20	0.40
1:E:322:ASN:HB3	1:E:323:MET:H	1.69	0.40
1:A:308:PHE:HD2	1:A:333:LEU:HD13	1.85	0.40
2:D:102:ARG:HD3	2:D:102:ARG:HA	1.81	0.40
2:D:318:PHE:HZ	2:D:615:VAL:HG11	1.85	0.40
1:A:284:PRO:HG2	1:A:436:ILE:HG22	2.03	0.40
2:B:964:LYS:HA	2:C:570:VAL:HG13	2.02	0.40
2:C:329:PHE:CB	2:C:528:LYS:HB3	2.52	0.40
2:C:706:ALA:HB3	6:C:1308:NAG:H4	2.04	0.40
2:D:988:GLU:O	2:D:992:GLN:HG2	2.22	0.40
2:C:796:TYR:CG	6:D:1304:NAG:H61	2.56	0.40
2:D:324:GLU:HB2	2:D:539:VAL:HG12	2.03	0.40
2:D:1049:LEU:HD23	2:D:1049:LEU:HA	1.94	0.40
2:C:435:ALA:HA	2:C:509:ARG:O	2.21	0.40
2:C:1048:HIS:NE2	2:C:1050:MET:O	2.54	0.40
1:E:168:TRP:HE1	1:E:502:SER:HB3	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

All (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
2	B	1075	PHE
2	C	1074	ASN
2	C	1075	PHE
1	A	20	THR
2	B	517	LEU
2	B	635	VAL
2	C	517	LEU
2	D	517	LEU
2	D	361	CYS
2	B	524	VAL
2	C	524	VAL
2	D	524	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	332	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	527/533 (99%)	527 (100%)	0	100	100
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. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	137	ASN
1	A	524	GLN
2	B	61	ASN
2	B	487	ASN
2	C	487	ASN
2	D	164	ASN
2	D	487	ASN
1	E	149	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	401	HIS
1	E	524	GLN
1	F	134	ASN
1	F	137	ASN
1	F	524	GLN

### 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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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
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

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

All (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
4	O	1	NAG	C1-C2-N2	3.11	115.79	110.49
4	Y	2	NAG	O4-C4-C3	-2.93	103.57	110.35
4	U	2	NAG	O4-C4-C3	-2.93	103.58	110.35
3	W	2	NAG	C2-N2-C7	2.92	127.05	122.90
4	J	2	NAG	O4-C4-C3	-2.91	103.61	110.35
3	S	2	NAG	C2-N2-C7	2.91	127.05	122.90
3	H	2	NAG	C2-N2-C7	2.91	127.05	122.90
3	S	1	NAG	C2-N2-C7	2.89	127.02	122.90
3	H	1	NAG	C2-N2-C7	2.89	127.01	122.90
3	W	1	NAG	C2-N2-C7	2.88	127.00	122.90
3	H	1	NAG	C1-C2-N2	2.49	114.73	110.49
3	W	1	NAG	C1-C2-N2	2.47	114.71	110.49
3	S	1	NAG	C1-C2-N2	2.47	114.71	110.49
3	H	2	NAG	C1-C2-N2	2.47	114.71	110.49
3	S	2	NAG	C1-C2-N2	2.47	114.71	110.49
3	W	2	NAG	C1-C2-N2	2.46	114.69	110.49
4	X	2	NAG	C1-O5-C5	2.37	115.40	112.19
4	I	2	NAG	C1-O5-C5	2.35	115.38	112.19
4	T	2	NAG	C1-O5-C5	2.33	115.35	112.19
4	J	2	NAG	O5-C1-C2	2.27	114.88	111.29
4	U	2	NAG	O5-C1-C2	2.27	114.87	111.29
4	Y	2	NAG	O5-C1-C2	2.23	114.81	111.29
4	O	1	NAG	C2-N2-C7	2.19	126.02	122.90
4	Q	1	NAG	C2-N2-C7	2.17	125.99	122.90
4	M	1	NAG	C2-N2-C7	2.17	125.99	122.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	1	NAG	C1-C2-N2	2.09	114.05	110.49
4	Y	1	NAG	C1-C2-N2	2.08	114.03	110.49
4	J	1	NAG	C1-C2-N2	2.08	114.03	110.49
4	T	1	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (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
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	O	1	NAG	C3-C2-N2-C7
4	O	2	NAG	C3-C2-N2-C7
4	O	2	NAG	C8-C7-N2-C2
4	O	2	NAG	O7-C7-N2-C2
4	Q	1	NAG	C3-C2-N2-C7
4	Q	2	NAG	C3-C2-N2-C7
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	Q	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
4	J	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	I	2	NAG	C8-C7-N2-C2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	I	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	P	1	NAG	C8-C7-N2-C2
4	P	1	NAG	O7-C7-N2-C2
4	T	2	NAG	C8-C7-N2-C2
4	T	2	NAG	O7-C7-N2-C2
4	U	1	NAG	C8-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
4	X	2	NAG	C8-C7-N2-C2
4	X	2	NAG	O7-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
4	K	2	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C8-C7-N2-C2
3	W	1	NAG	C8-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	W	2	NAG	C8-C7-N2-C2
4	N	1	NAG	C1-C2-N2-C7
4	L	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O7-C7-N2-C2
3	W	1	NAG	O7-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
3	W	2	NAG	O7-C7-N2-C2

*Continued on next page...*

*Continued from previous page...*

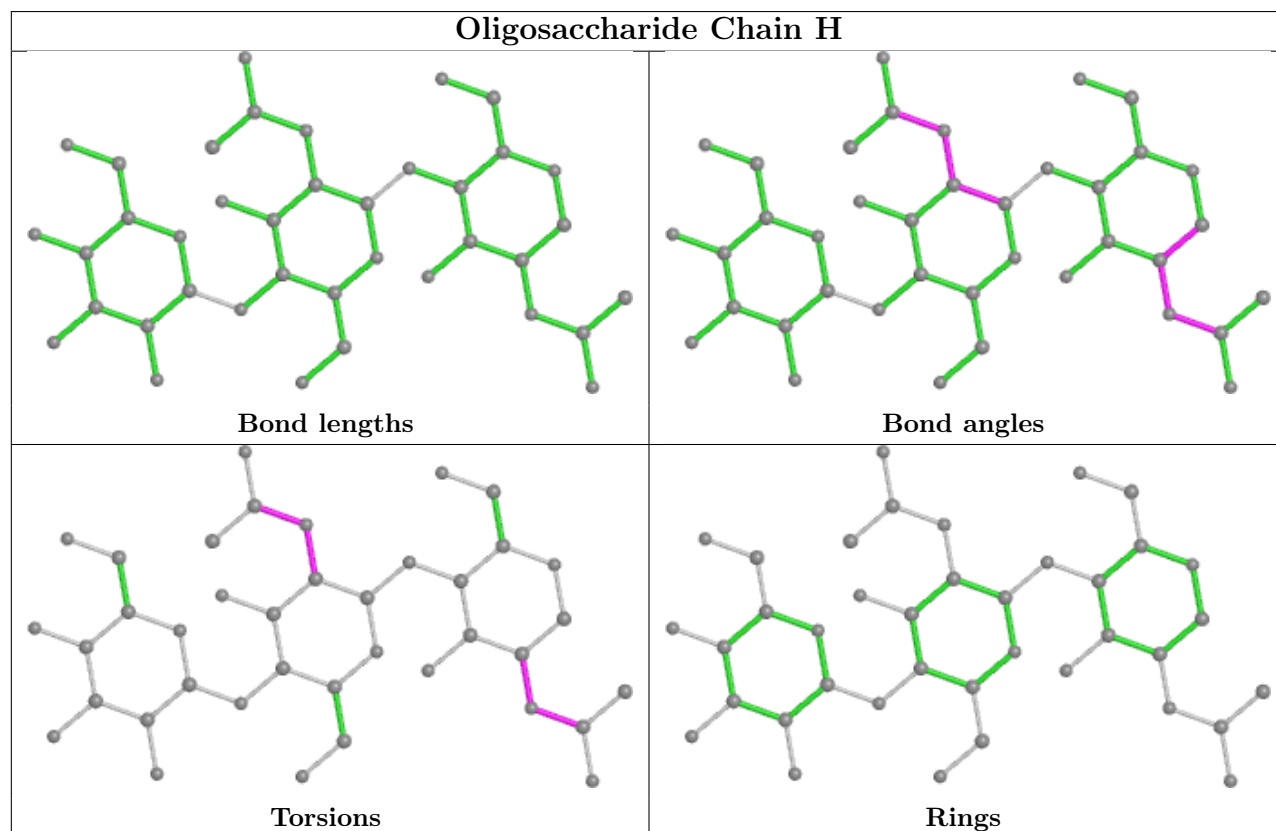
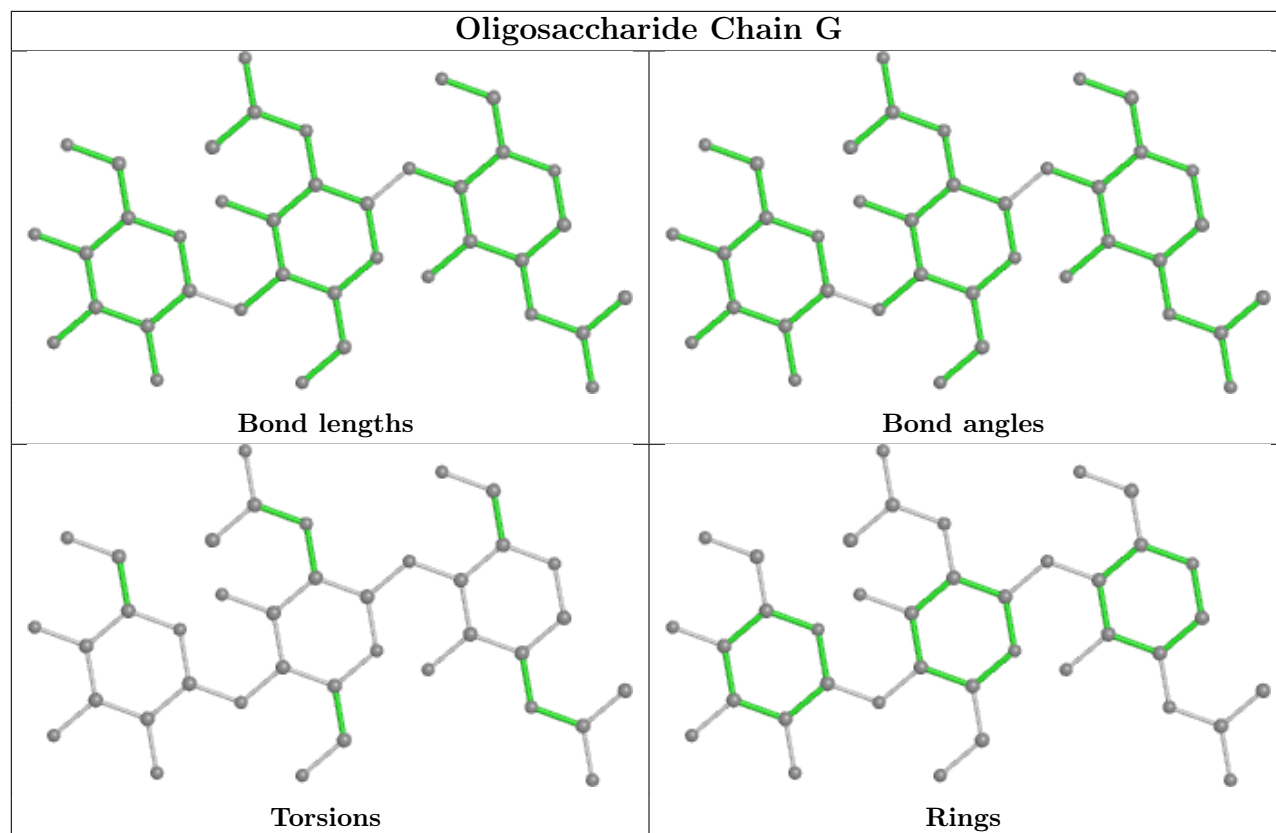
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C1-C2-N2-C7
4	T	1	NAG	C1-C2-N2-C7
4	X	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	S	2	NAG	C3-C2-N2-C7
3	W	2	NAG	C3-C2-N2-C7
4	N	2	NAG	C3-C2-N2-C7
3	H	1	NAG	C1-C2-N2-C7
3	S	1	NAG	C1-C2-N2-C7
3	W	1	NAG	C1-C2-N2-C7
4	M	1	NAG	C1-C2-N2-C7
4	O	1	NAG	C1-C2-N2-C7
4	Q	1	NAG	C1-C2-N2-C7
4	N	1	NAG	C3-C2-N2-C7

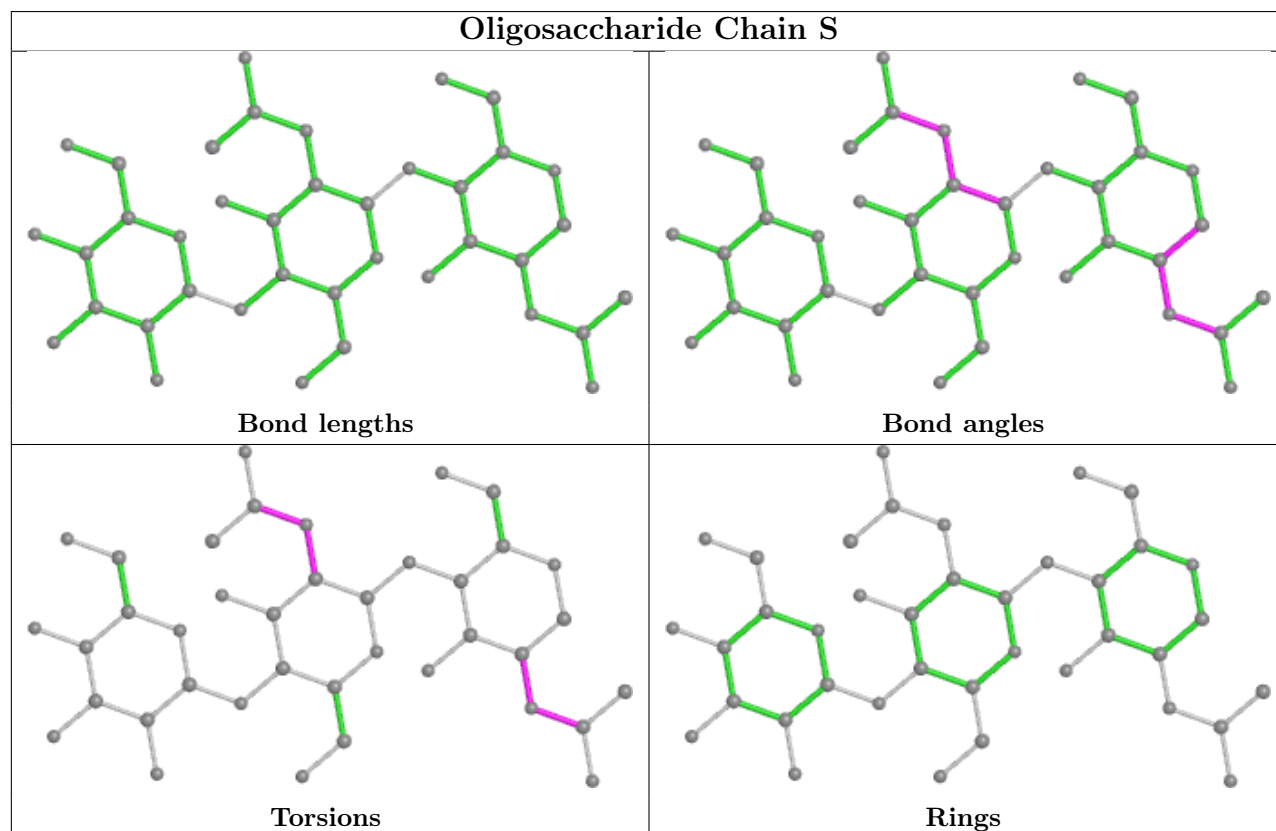
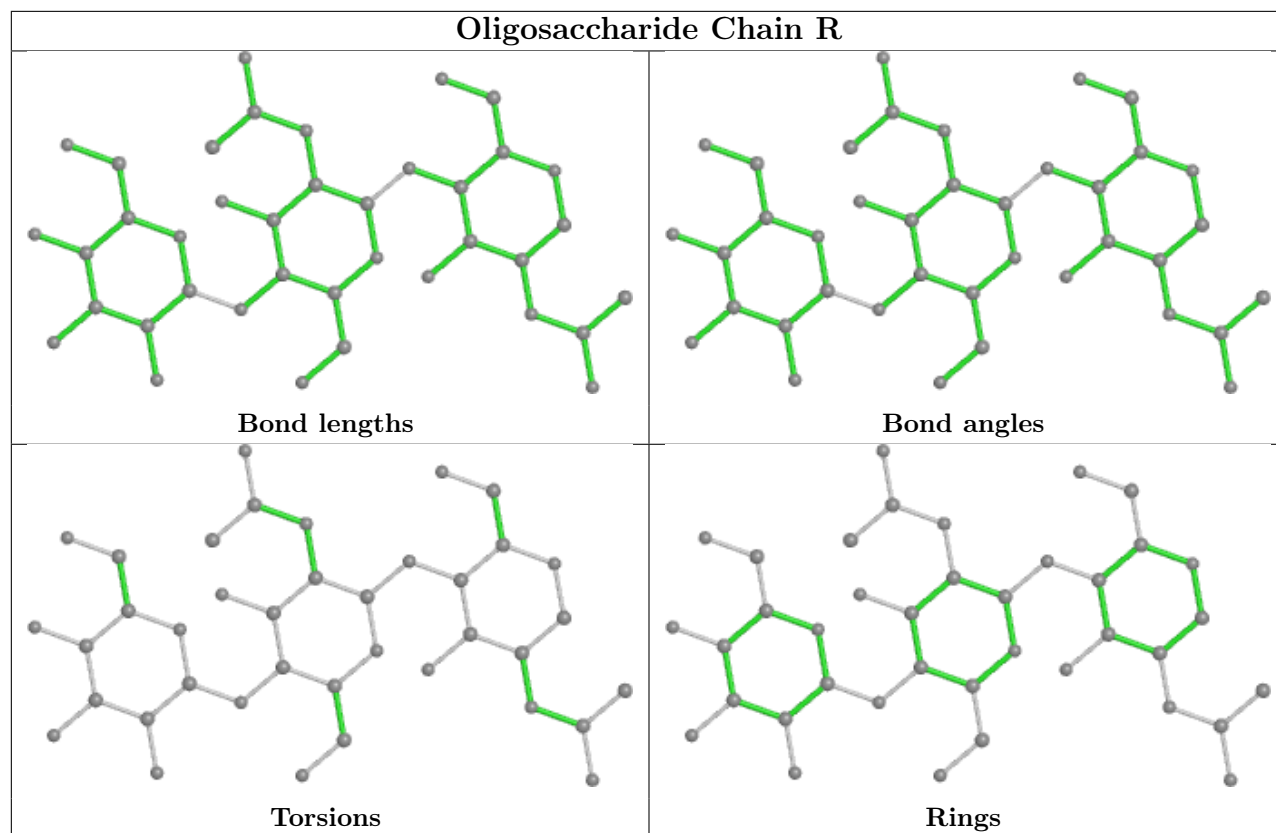
There are no ring outliers.

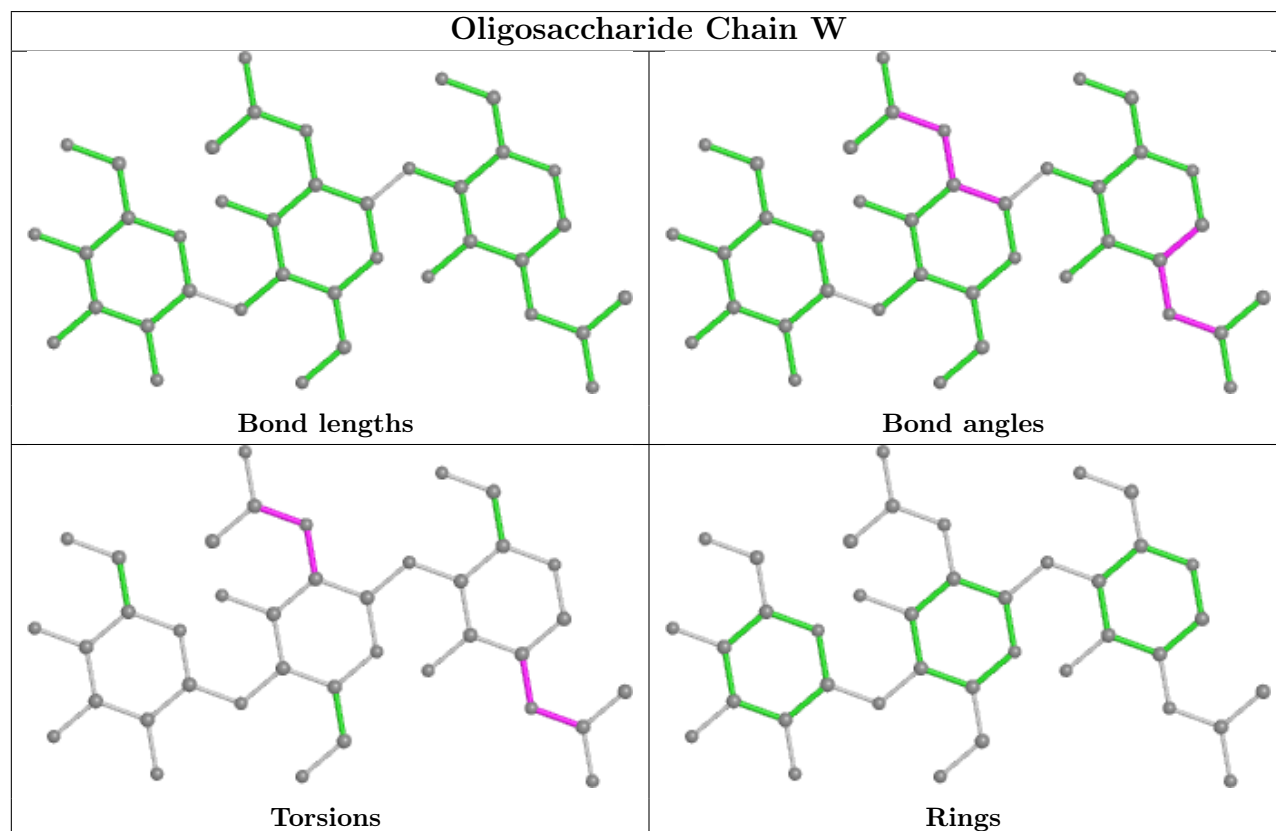
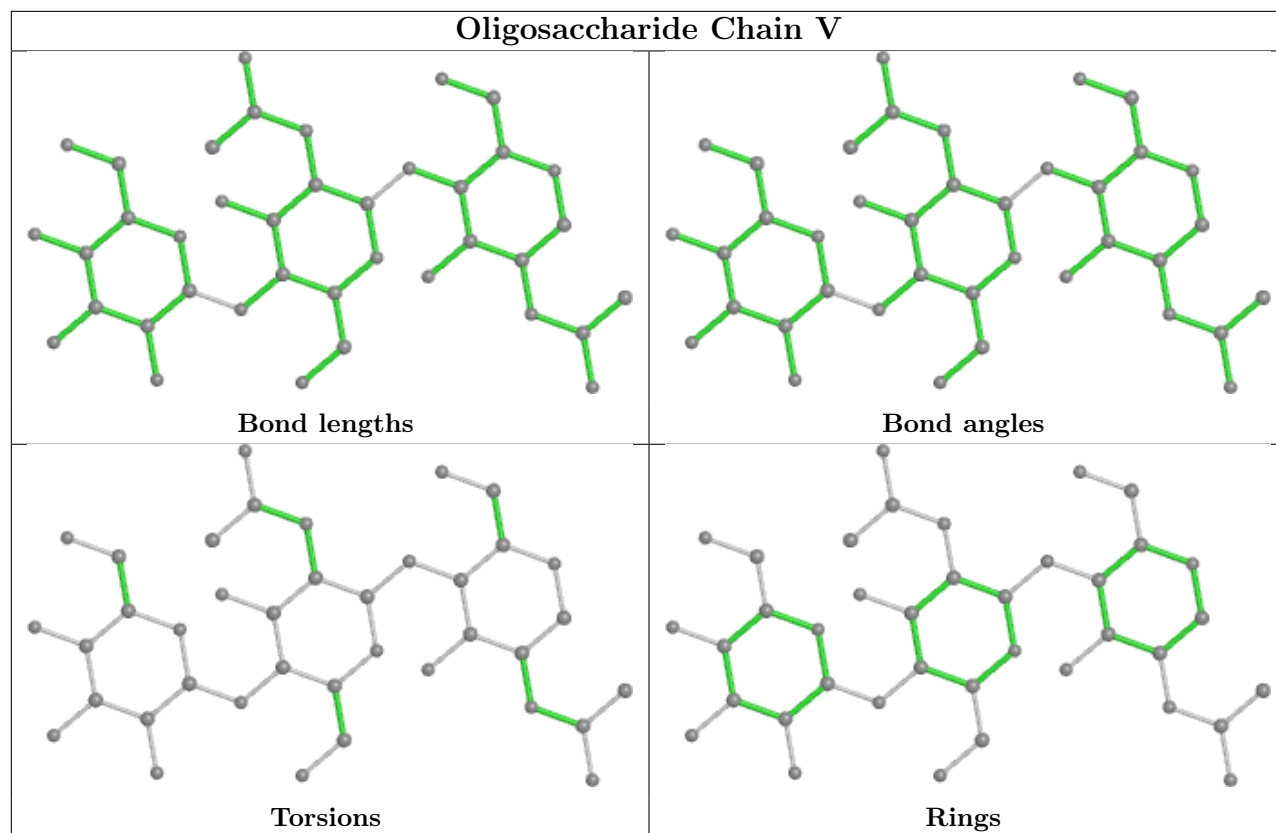
3 monomers are involved in 3 short contacts:

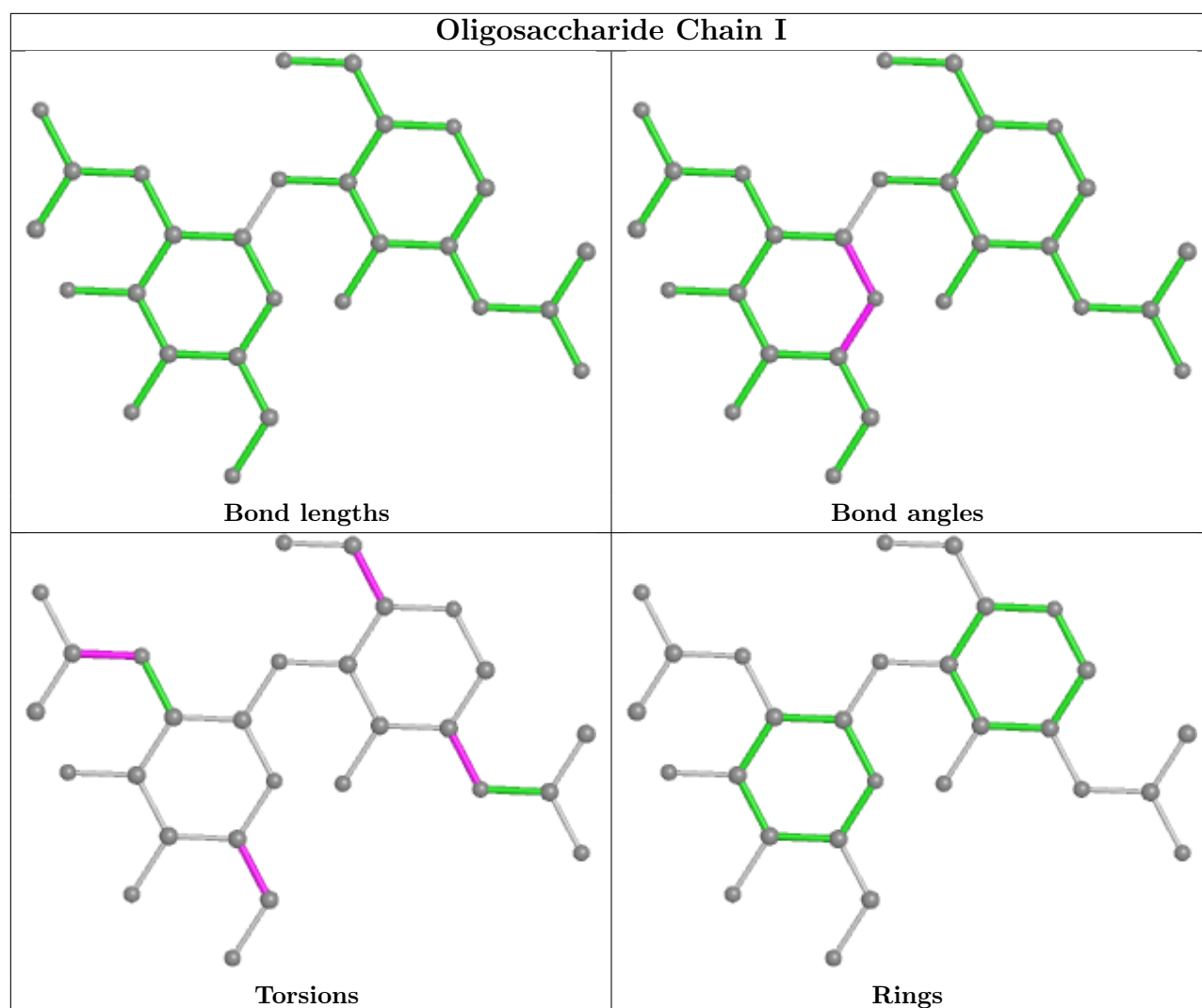
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	1	NAG	1	0
3	W	1	NAG	1	0
3	H	1	NAG	1	0

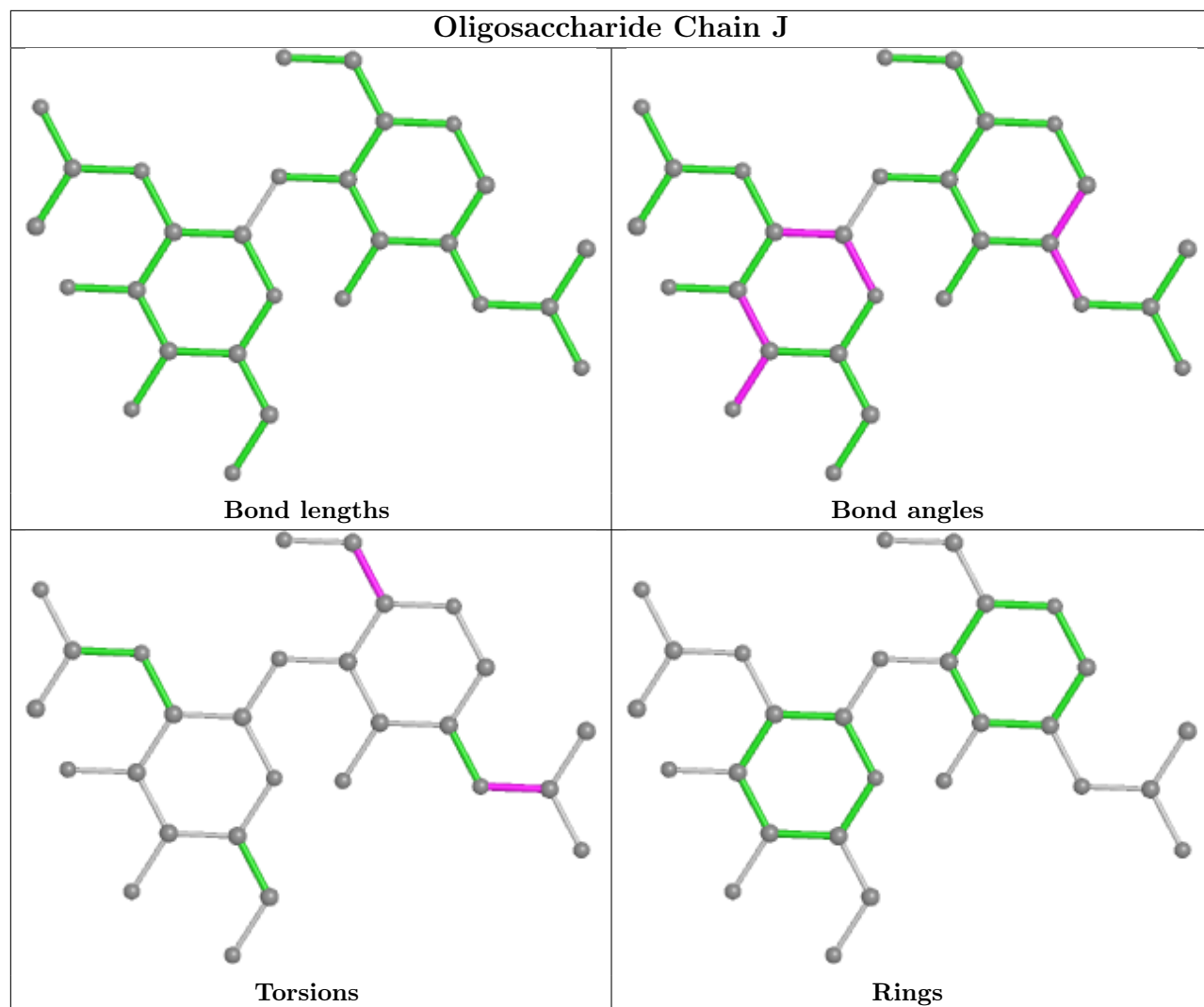
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

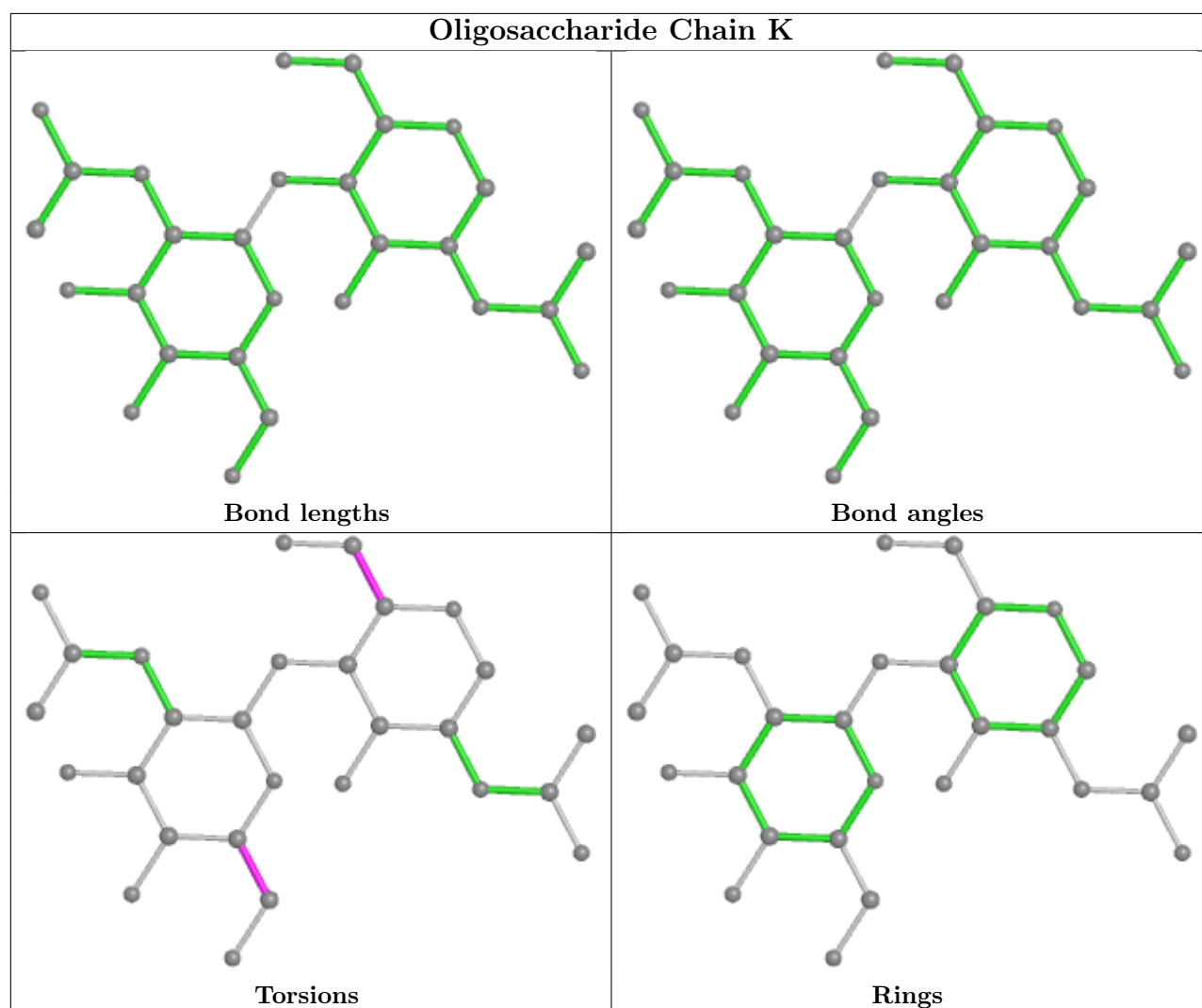




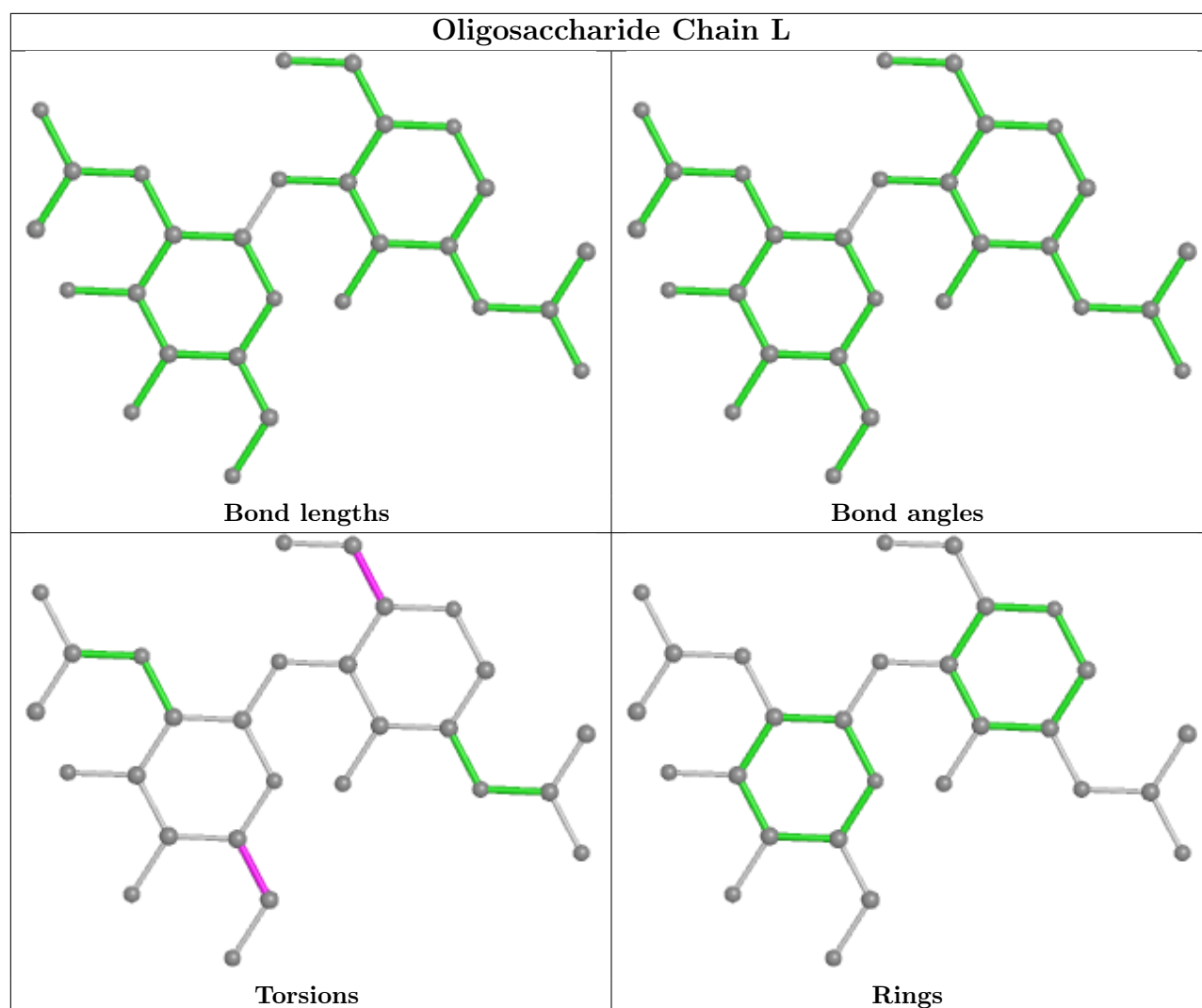


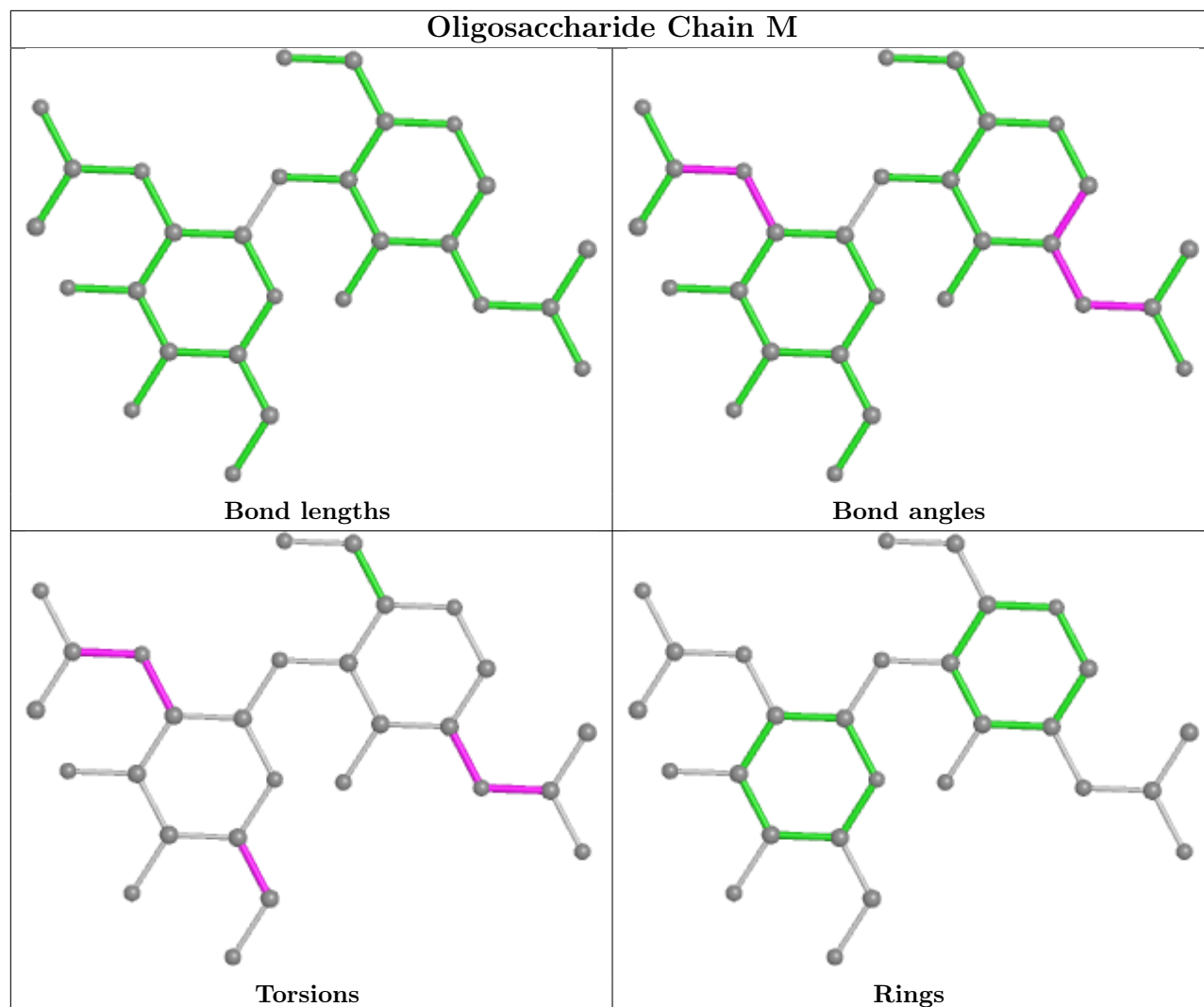


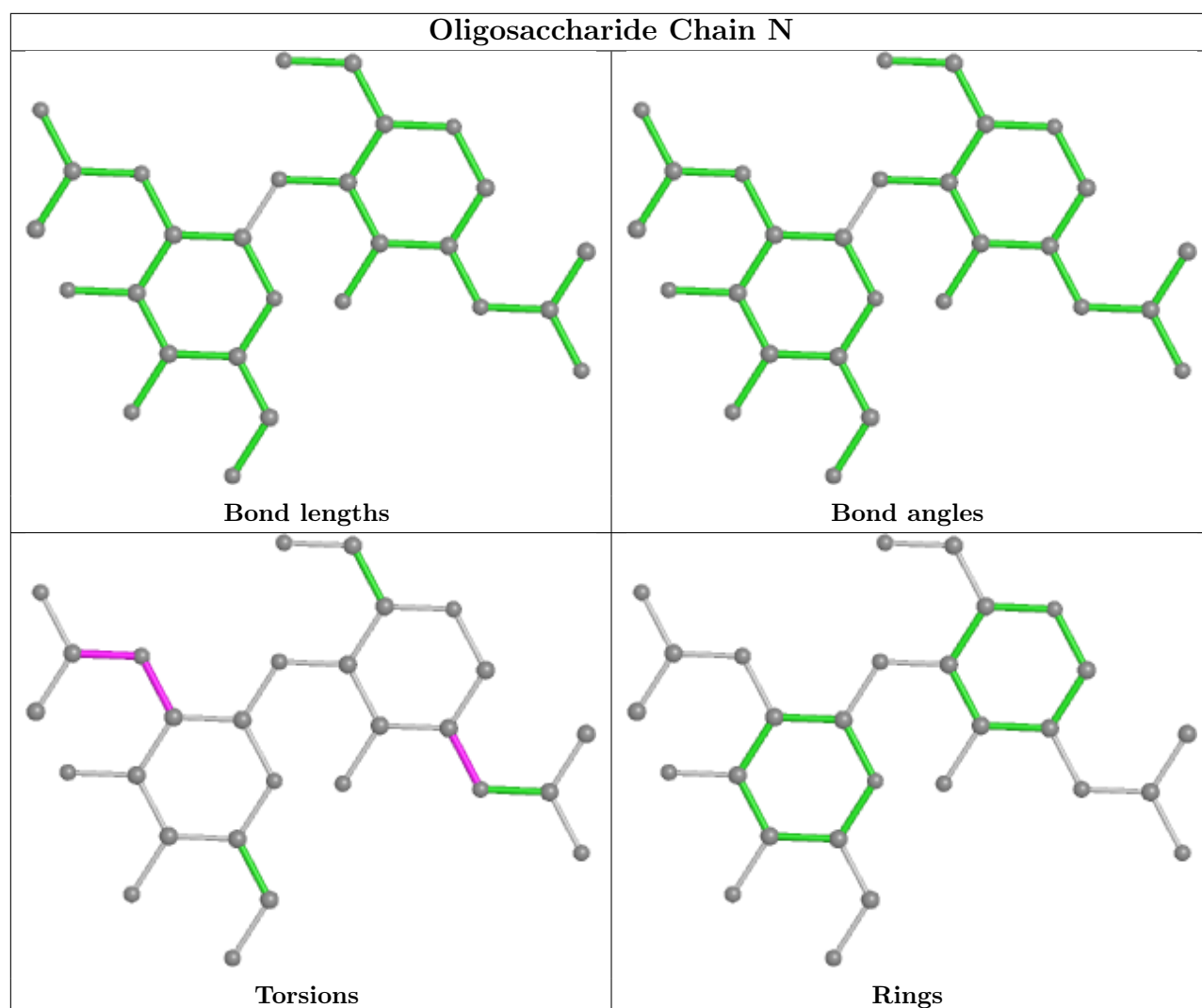


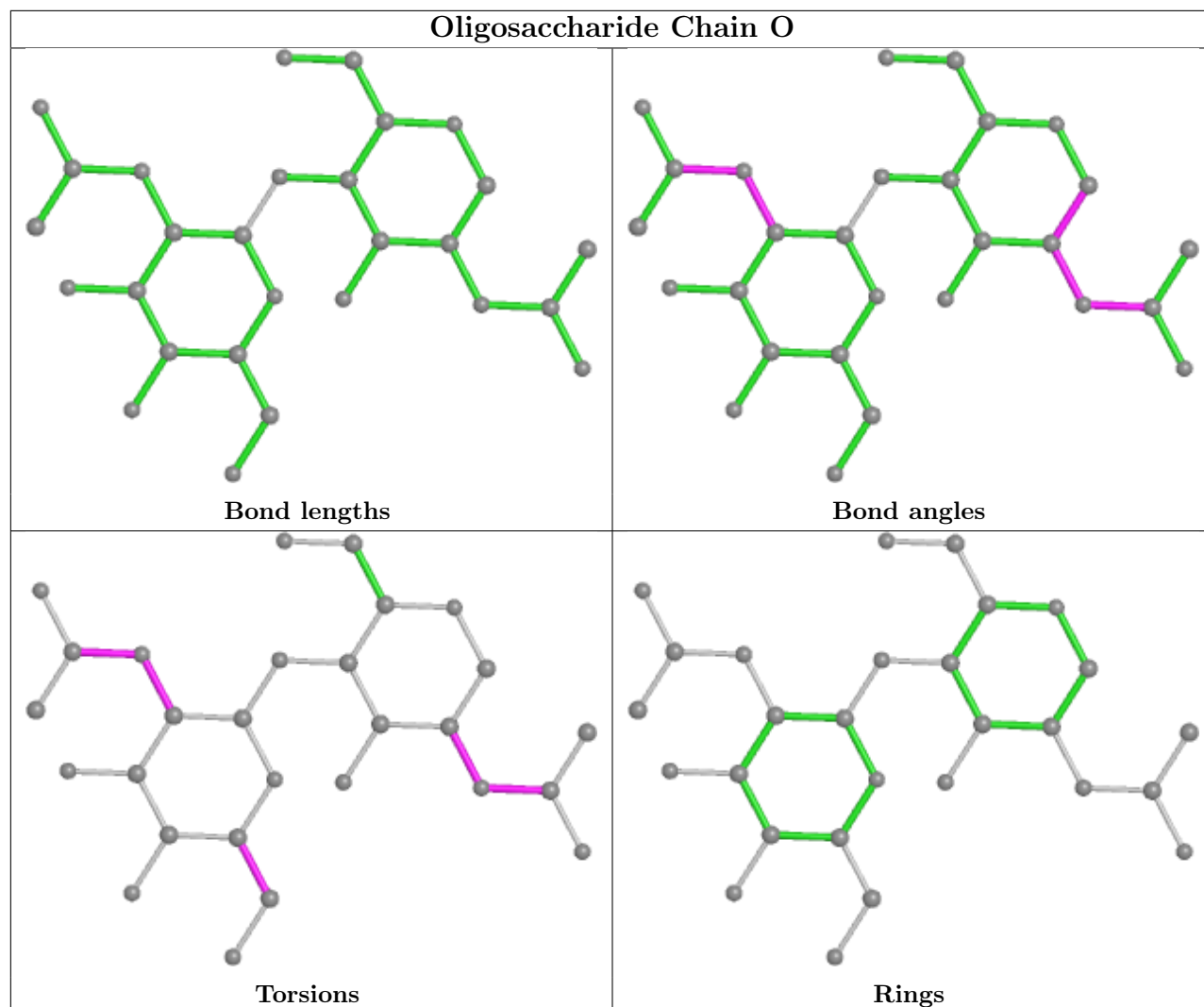


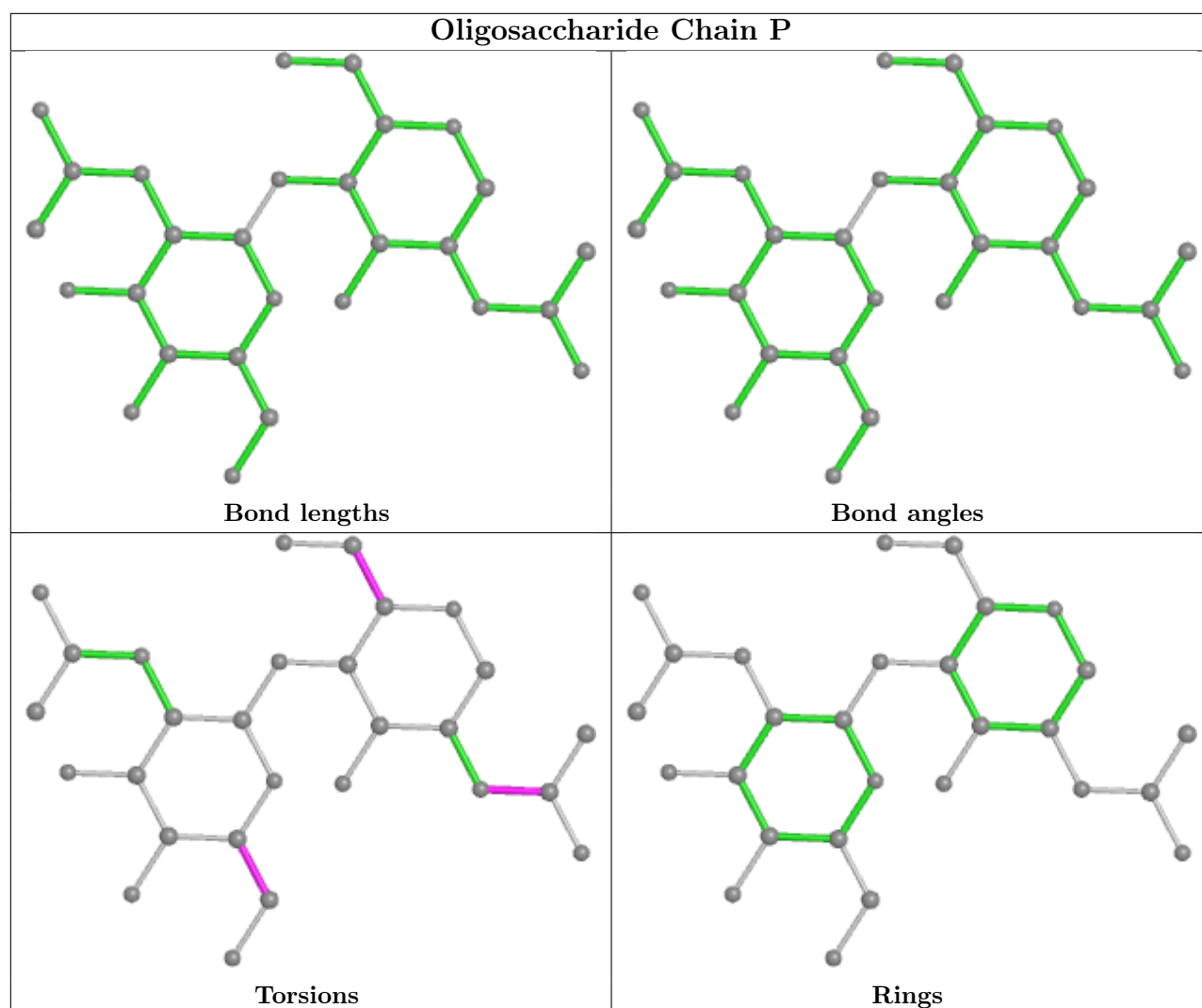


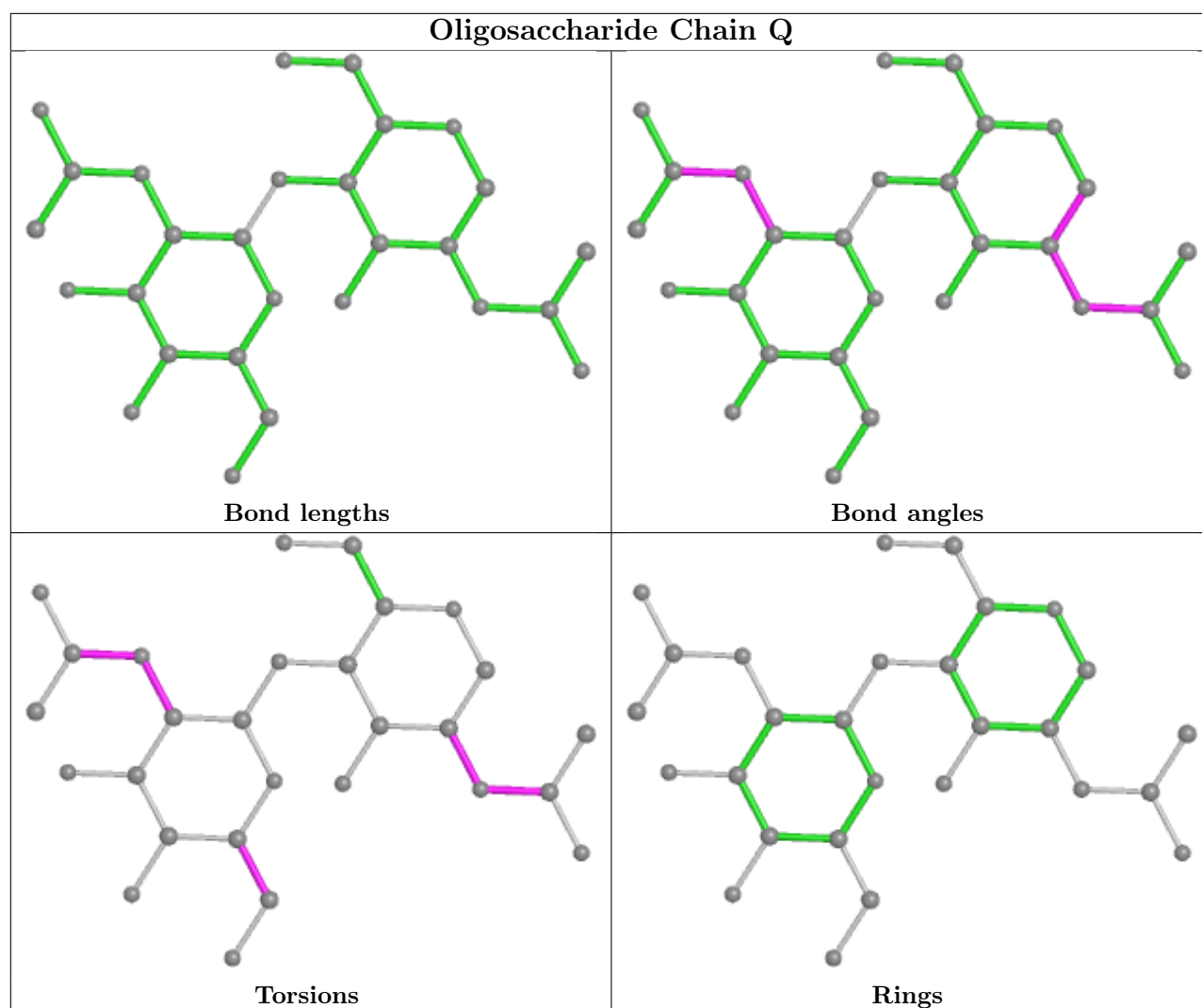


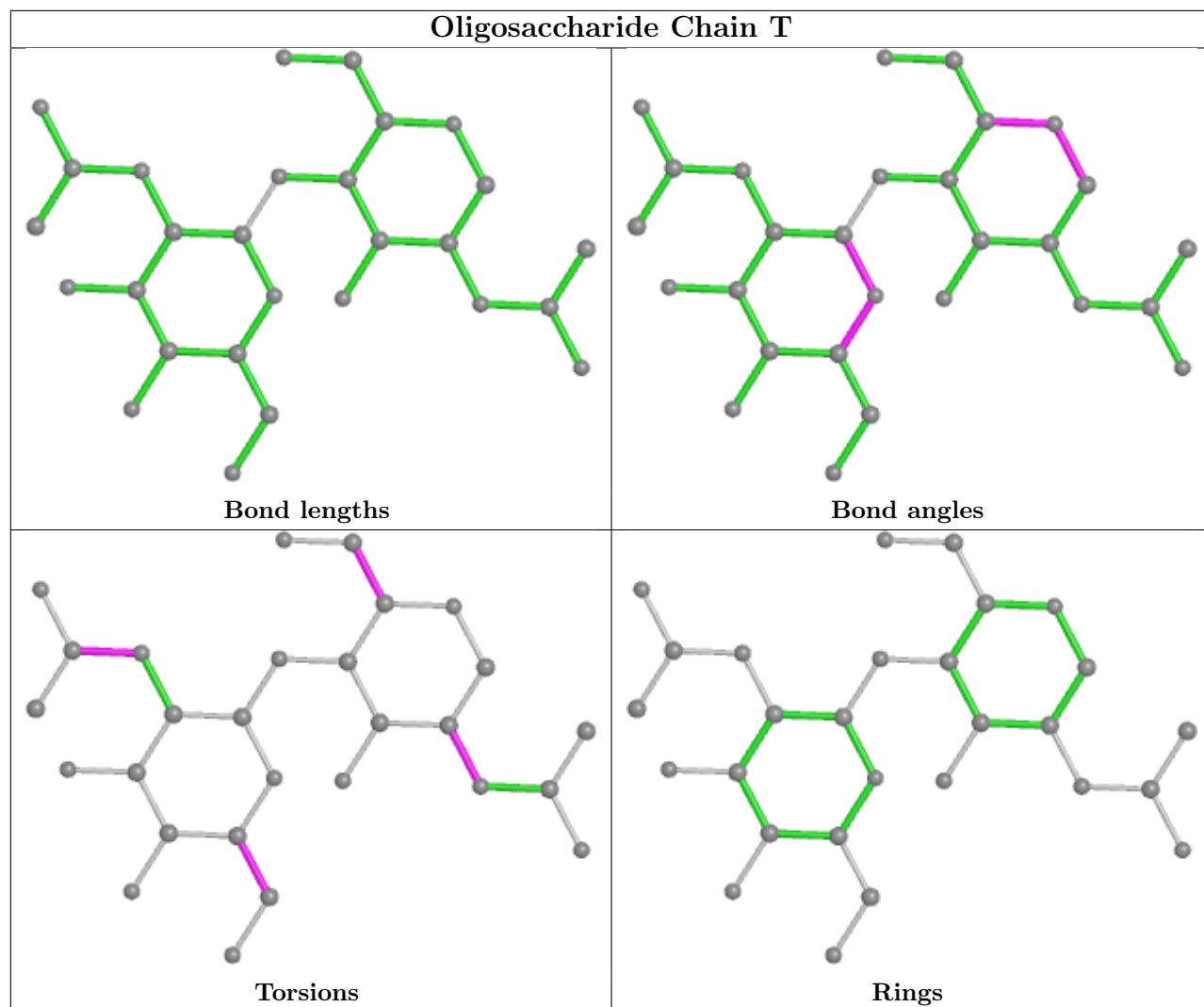


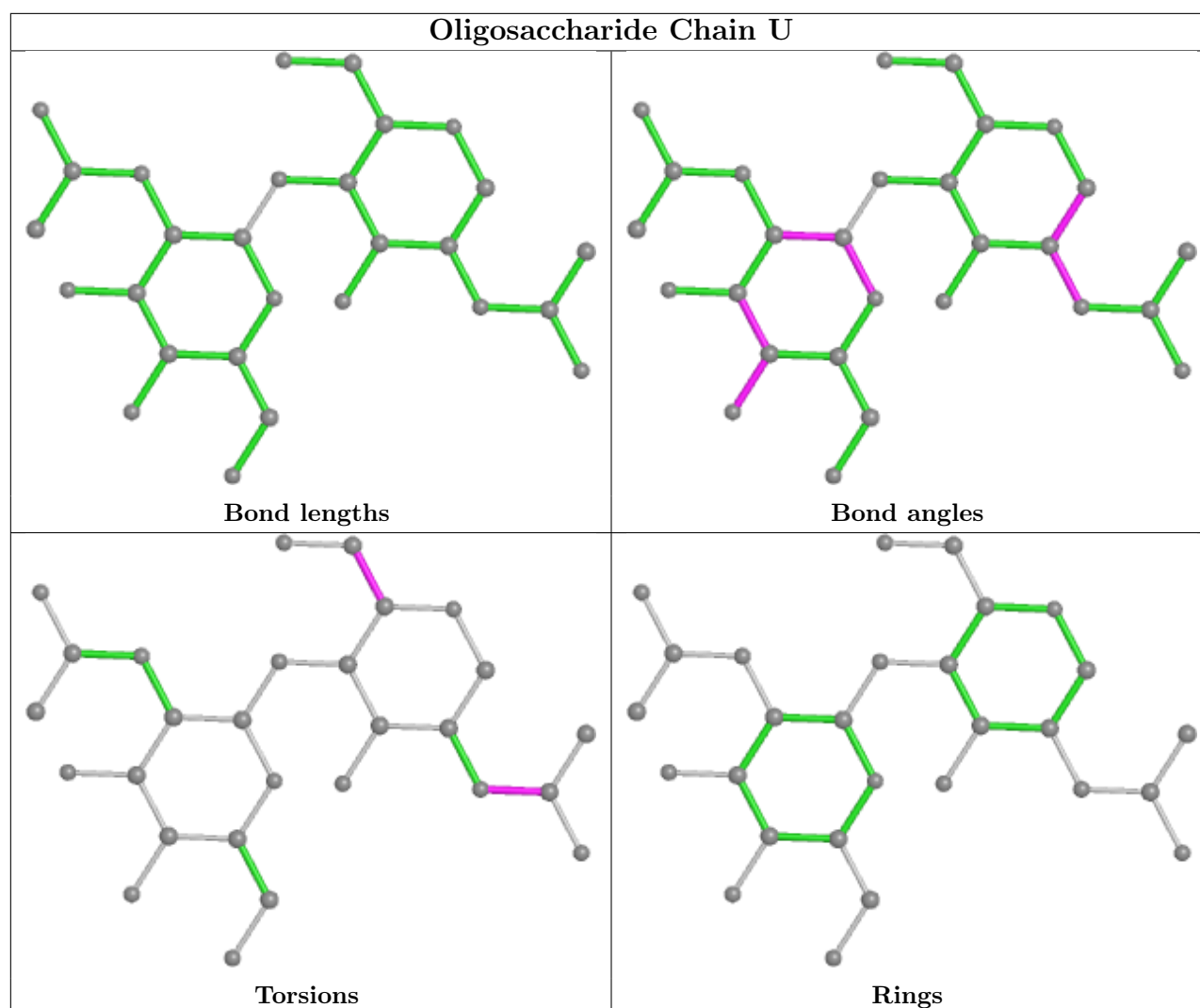




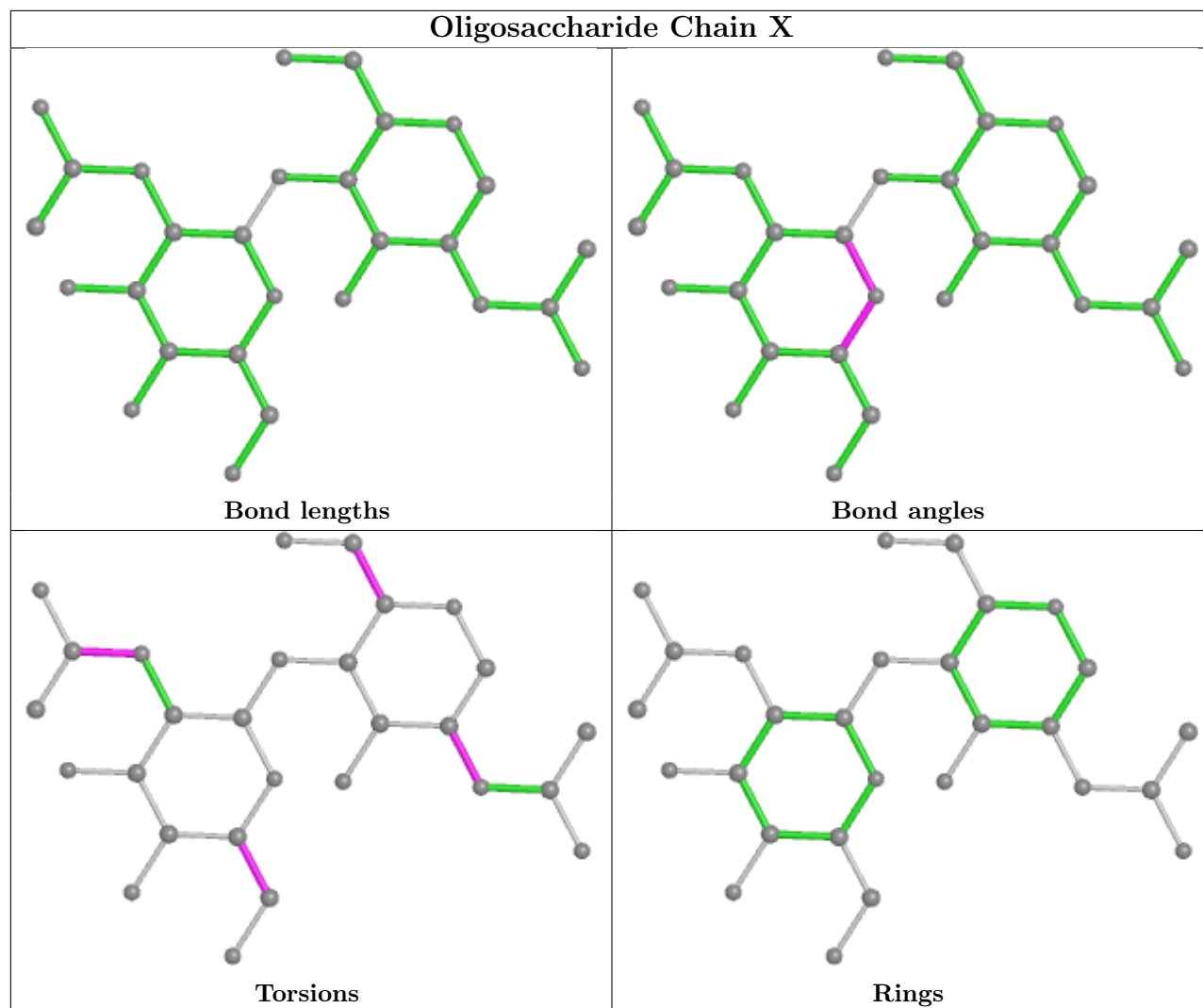


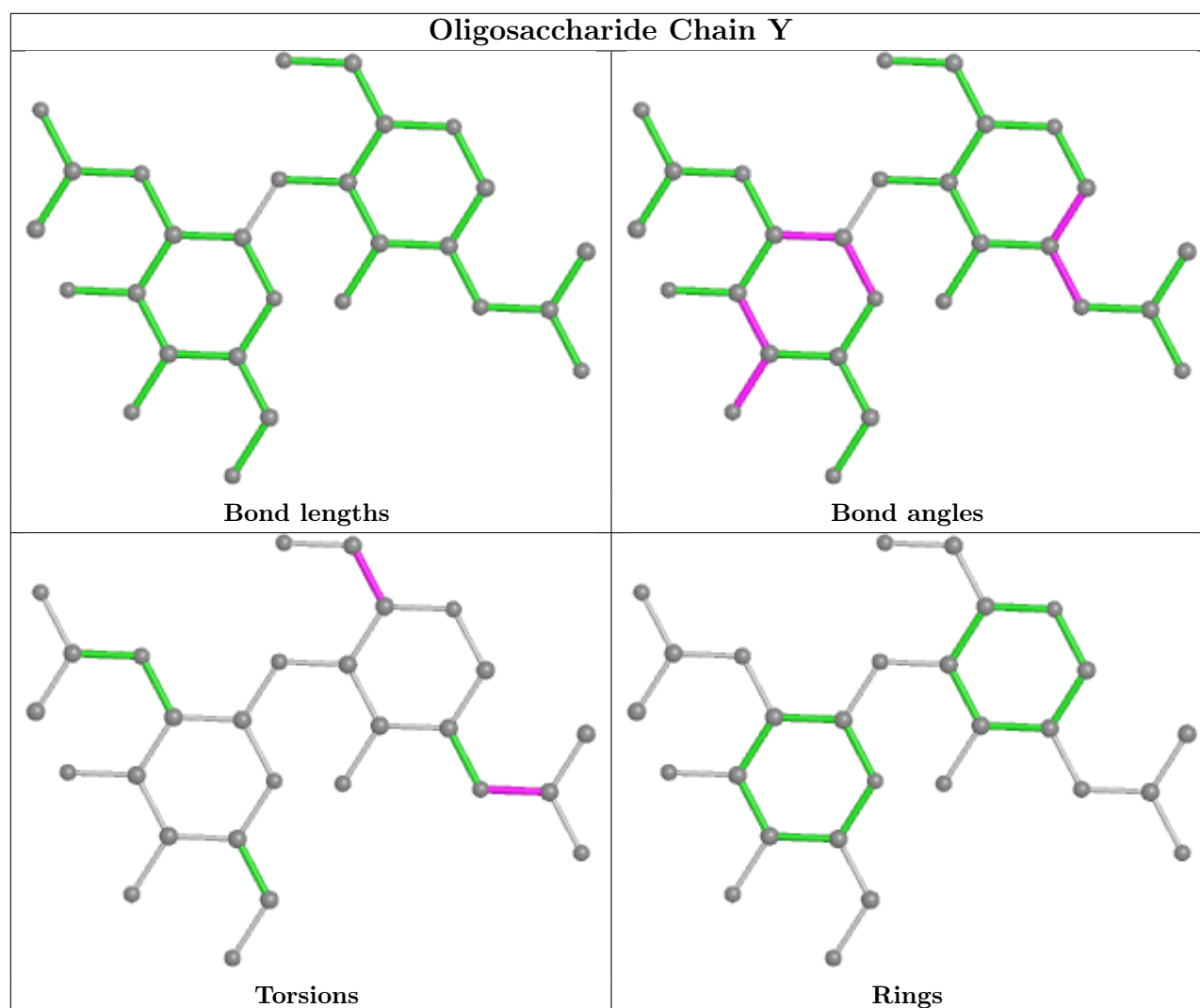












## 5.6 Ligand geometry [i](#)

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

Continued on next page...

*Continued from previous page...*

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.

All (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
6	C	1309	NAG	C1-C2-N2	3.40	116.29	110.49
6	D	1312	NAG	C1-C2-N2	2.96	115.55	110.49
6	C	1306	NAG	C1-C2-N2	2.93	115.50	110.49
6	B	1307	NAG	C1-C2-N2	2.93	115.50	110.49
6	D	1310	NAG	C1-C2-N2	2.92	115.47	110.49
6	D	1311	NAG	C1-C2-N2	2.86	115.38	110.49
6	D	1311	NAG	C2-N2-C7	2.72	126.78	122.90
6	C	1306	NAG	C2-N2-C7	2.51	126.47	122.90
6	D	1310	NAG	C2-N2-C7	2.50	126.46	122.90
6	B	1307	NAG	C2-N2-C7	2.49	126.45	122.90
6	D	1312	NAG	C2-N2-C7	2.48	126.43	122.90

There are no chirality outliers.

All (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
6	D	1310	NAG	C3-C2-N2-C7
6	D	1311	NAG	C3-C2-N2-C7
6	D	1312	NAG	C3-C2-N2-C7
6	D	1314	NAG	C1-C2-N2-C7
6	D	1314	NAG	C8-C7-N2-C2
6	D	1314	NAG	O7-C7-N2-C2
6	D	1307	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	C	1302	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	A	702	NAG	O5-C5-C6-O6
6	E	702	NAG	O5-C5-C6-O6
6	F	702	NAG	O5-C5-C6-O6
6	B	1305	NAG	O5-C5-C6-O6
6	D	1305	NAG	O5-C5-C6-O6
6	B	1303	NAG	C4-C5-C6-O6
6	D	1307	NAG	C4-C5-C6-O6
6	C	1301	NAG	O5-C5-C6-O6
6	C	1304	NAG	O5-C5-C6-O6
6	D	1304	NAG	O5-C5-C6-O6
6	B	1303	NAG	O5-C5-C6-O6
6	C	1302	NAG	C4-C5-C6-O6
6	C	1303	NAG	C4-C5-C6-O6
6	B	1305	NAG	C4-C5-C6-O6
6	D	1305	NAG	C4-C5-C6-O6
6	A	702	NAG	C4-C5-C6-O6
6	E	702	NAG	C4-C5-C6-O6
6	F	702	NAG	C4-C5-C6-O6
6	B	1301	NAG	C8-C7-N2-C2
6	B	1301	NAG	O7-C7-N2-C2
6	B	1308	NAG	C8-C7-N2-C2
6	B	1308	NAG	O7-C7-N2-C2
6	C	1302	NAG	C8-C7-N2-C2
6	C	1302	NAG	O7-C7-N2-C2
6	C	1307	NAG	C8-C7-N2-C2
6	C	1307	NAG	O7-C7-N2-C2
6	C	1308	NAG	C8-C7-N2-C2
6	C	1308	NAG	O7-C7-N2-C2
6	D	1301	NAG	C8-C7-N2-C2
6	D	1301	NAG	O7-C7-N2-C2
6	D	1306	NAG	C8-C7-N2-C2
6	D	1306	NAG	O7-C7-N2-C2
6	D	1308	NAG	C8-C7-N2-C2
6	D	1308	NAG	O7-C7-N2-C2
6	D	1311	NAG	C8-C7-N2-C2
6	D	1311	NAG	O7-C7-N2-C2
6	D	1312	NAG	C8-C7-N2-C2
6	D	1312	NAG	O7-C7-N2-C2
6	D	1301	NAG	C4-C5-C6-O6
6	B	1307	NAG	C8-C7-N2-C2
6	C	1306	NAG	C8-C7-N2-C2
6	D	1310	NAG	C8-C7-N2-C2

*Continued on next page...*

*Continued from previous page...*

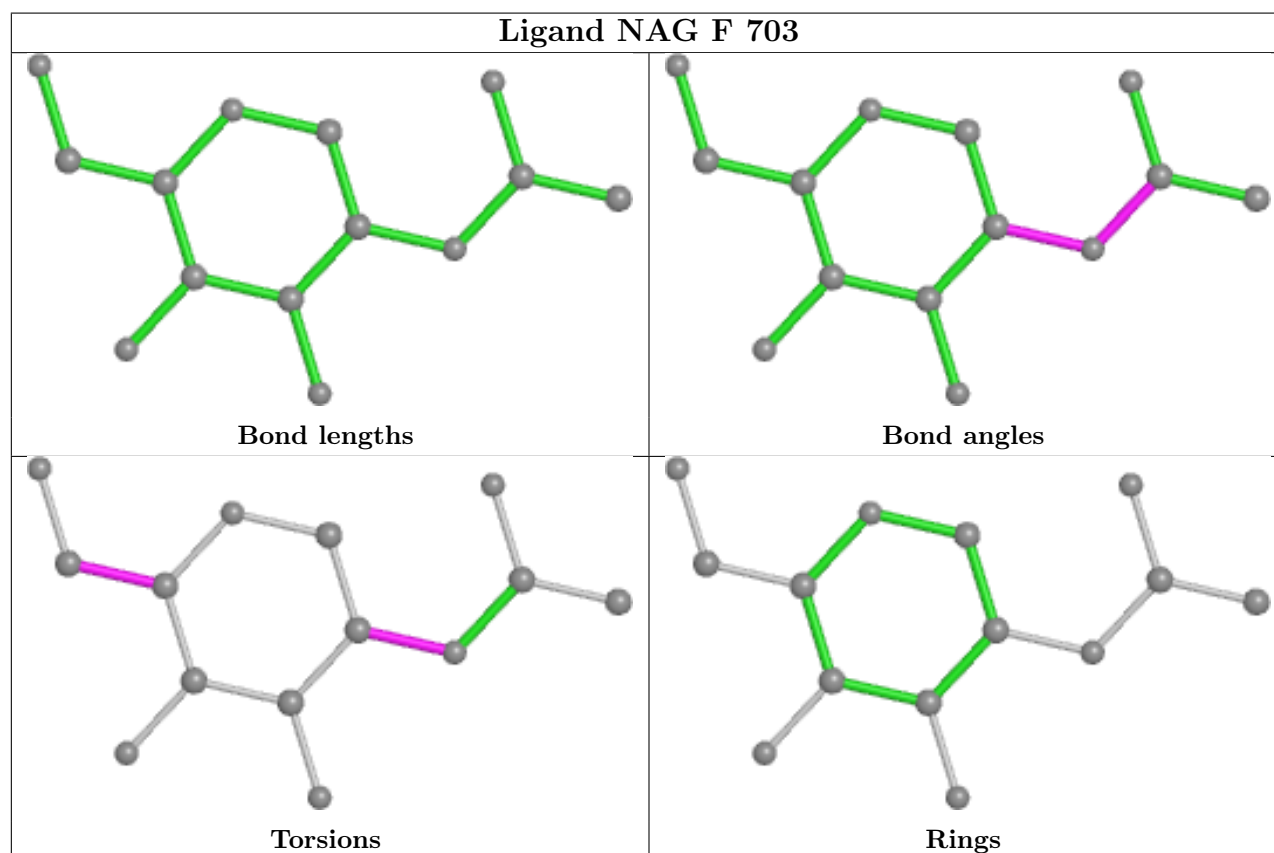
Mol	Chain	Res	Type	Atoms
6	C	1301	NAG	C4-C5-C6-O6
6	B	1307	NAG	O7-C7-N2-C2
6	C	1306	NAG	O7-C7-N2-C2
6	D	1301	NAG	O5-C5-C6-O6
6	C	1304	NAG	C4-C5-C6-O6
6	D	1310	NAG	O7-C7-N2-C2
6	B	1301	NAG	O5-C5-C6-O6
6	B	1307	NAG	O5-C5-C6-O6
6	C	1306	NAG	O5-C5-C6-O6
6	D	1310	NAG	O5-C5-C6-O6
6	D	1311	NAG	O5-C5-C6-O6
6	D	1306	NAG	O5-C5-C6-O6
6	C	1308	NAG	O5-C5-C6-O6
6	D	1314	NAG	O5-C5-C6-O6
6	E	703	NAG	O5-C5-C6-O6
6	A	703	NAG	O5-C5-C6-O6
6	F	703	NAG	O5-C5-C6-O6
6	D	1303	NAG	O5-C5-C6-O6
6	B	1302	NAG	O5-C5-C6-O6
6	D	1304	NAG	C4-C5-C6-O6
6	D	1313	NAG	C1-C2-N2-C7
6	A	703	NAG	C3-C2-N2-C7
6	B	1303	NAG	C3-C2-N2-C7
6	B	1306	NAG	C3-C2-N2-C7
6	C	1303	NAG	C3-C2-N2-C7
6	C	1304	NAG	C3-C2-N2-C7
6	D	1305	NAG	C3-C2-N2-C7
6	D	1307	NAG	C3-C2-N2-C7
6	E	703	NAG	C3-C2-N2-C7
6	F	703	NAG	C3-C2-N2-C7
6	B	1307	NAG	C1-C2-N2-C7
6	C	1306	NAG	C1-C2-N2-C7
6	D	1310	NAG	C1-C2-N2-C7
6	D	1312	NAG	C1-C2-N2-C7
6	B	1304	NAG	O5-C5-C6-O6
6	D	1311	NAG	C1-C2-N2-C7
6	C	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 12 short contacts:

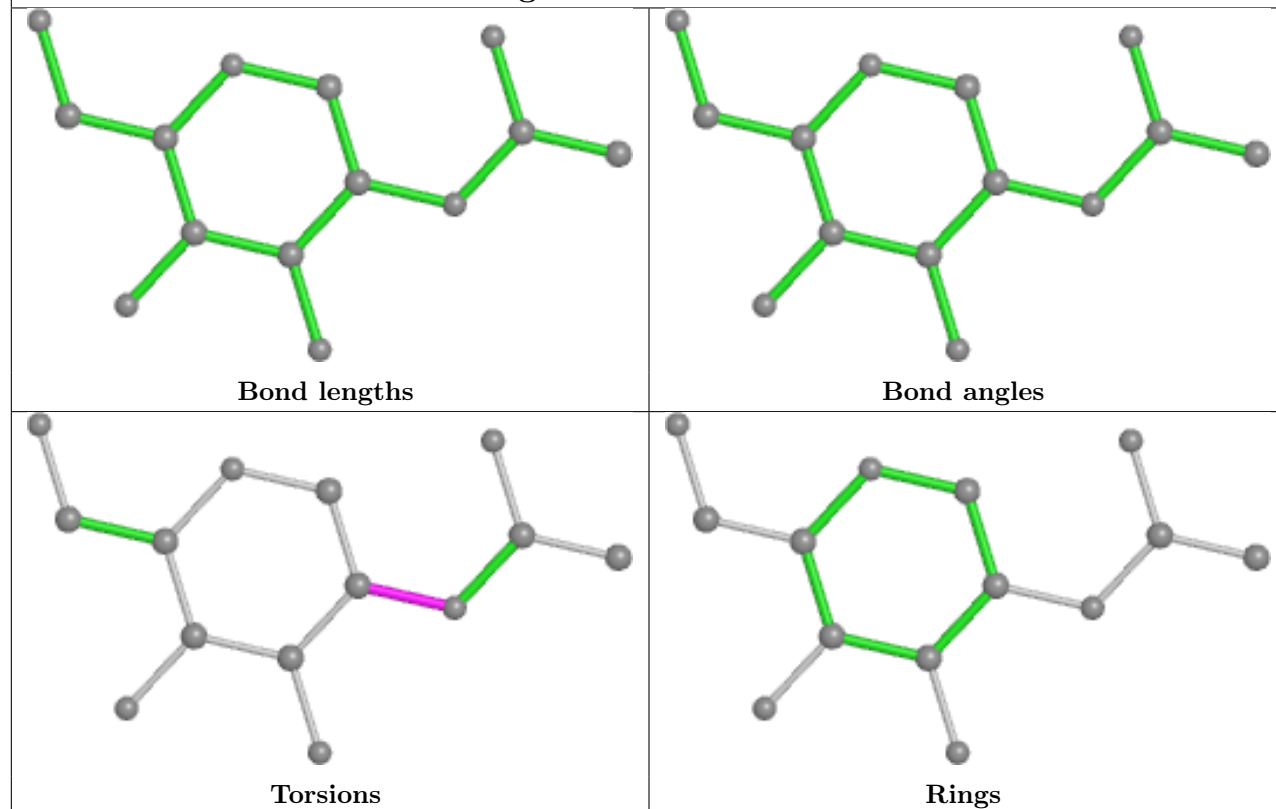
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1309	NAG	1	0
6	D	1309	NAG	1	0
6	D	1314	NAG	5	0
6	C	1308	NAG	1	0
6	C	1302	NAG	1	0
6	D	1304	NAG	3	0

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.

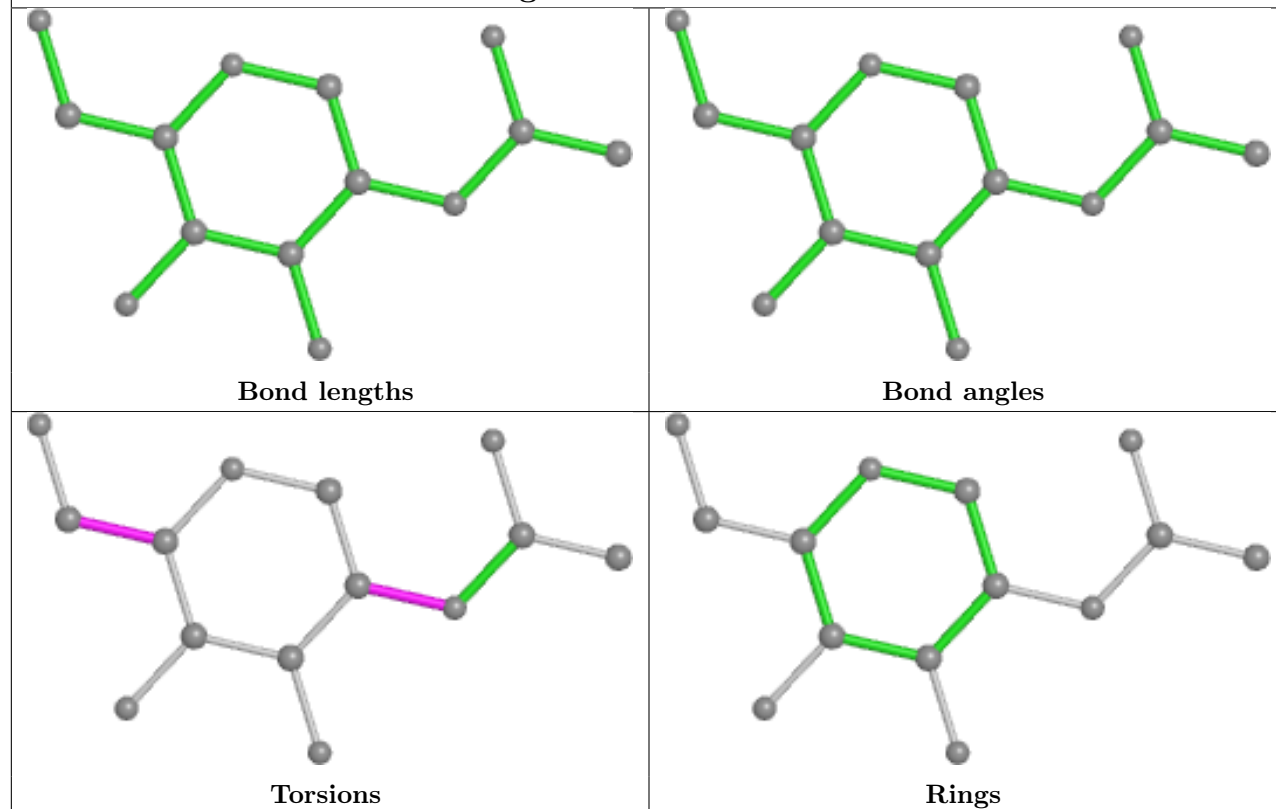




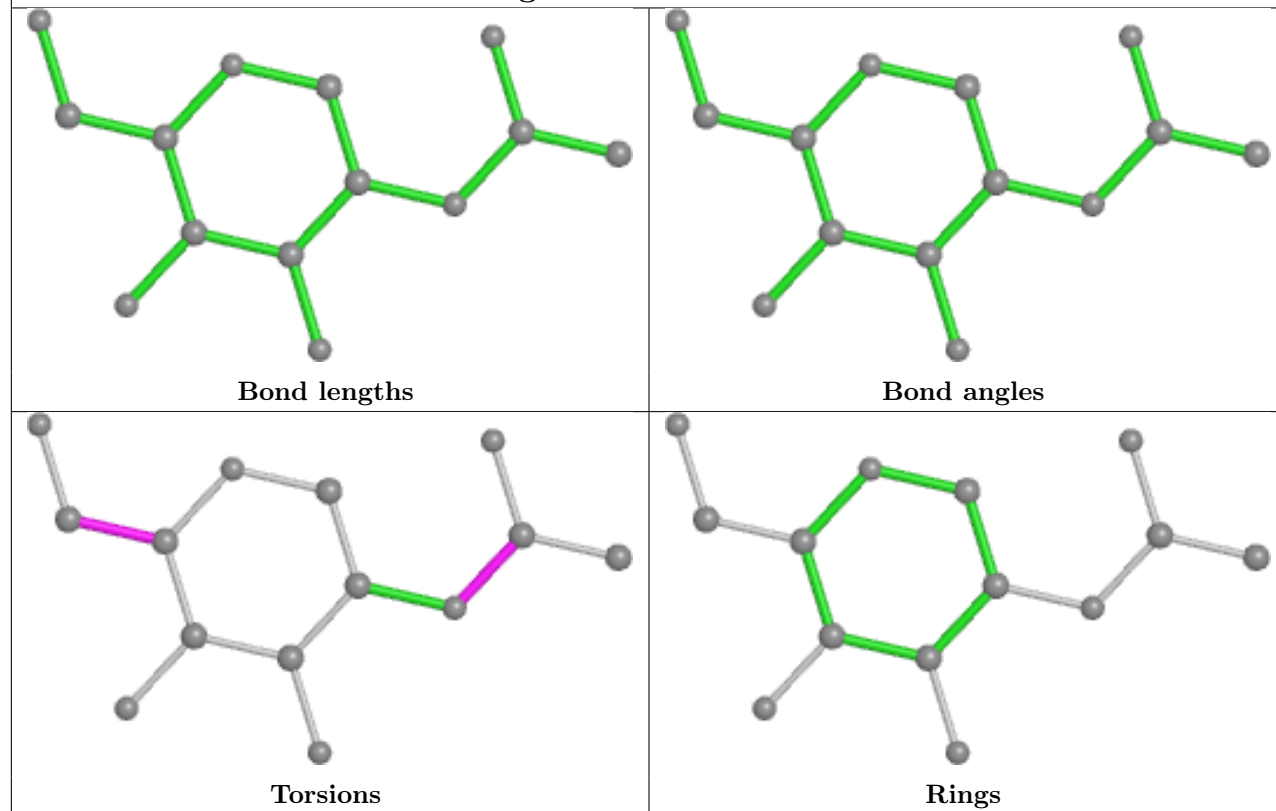
## Ligand NAG D 1313



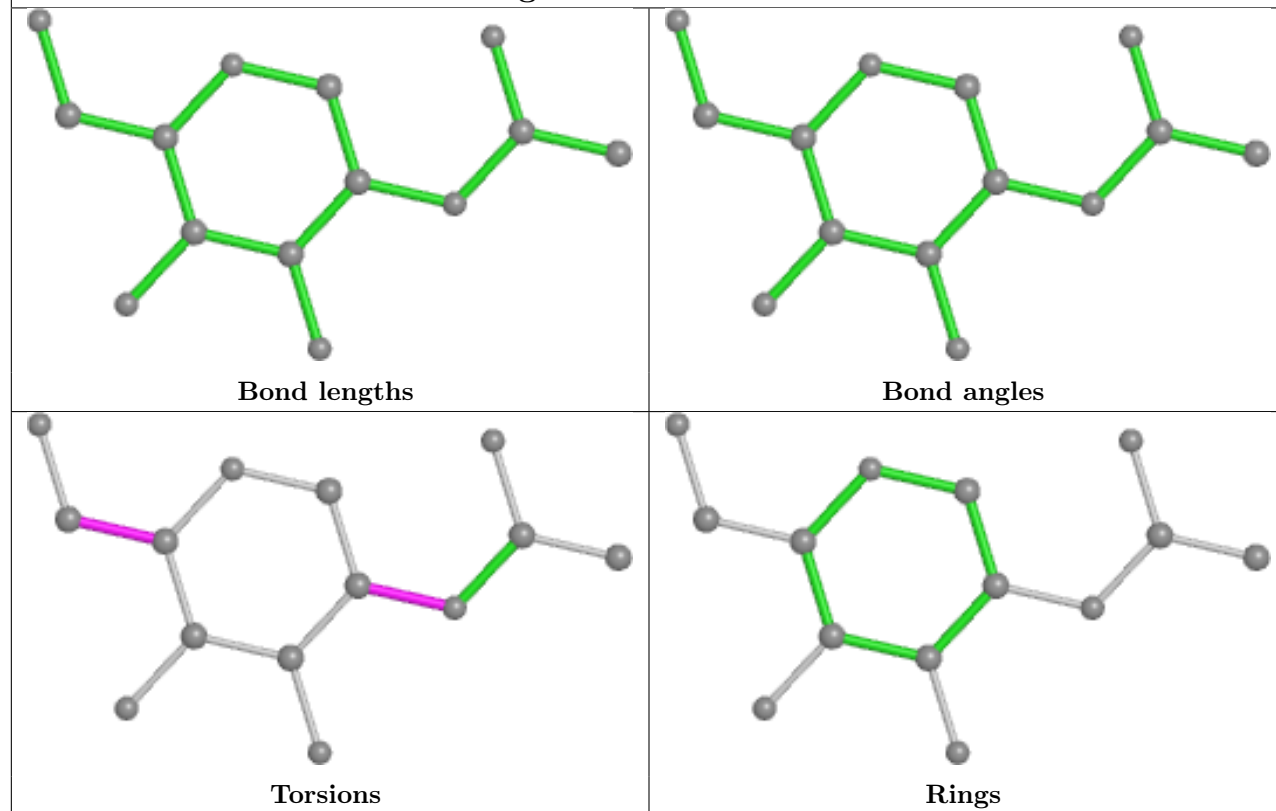
## Ligand NAG C 1303

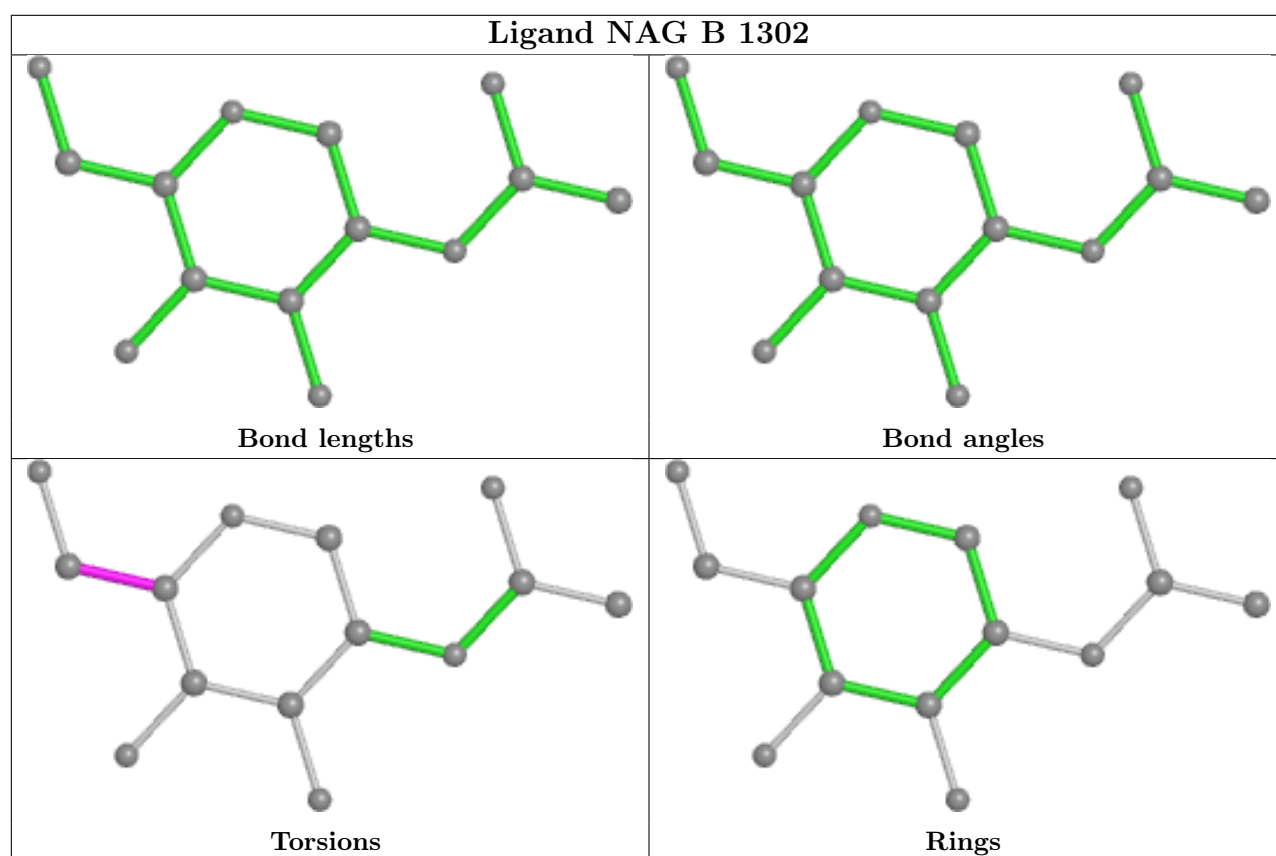
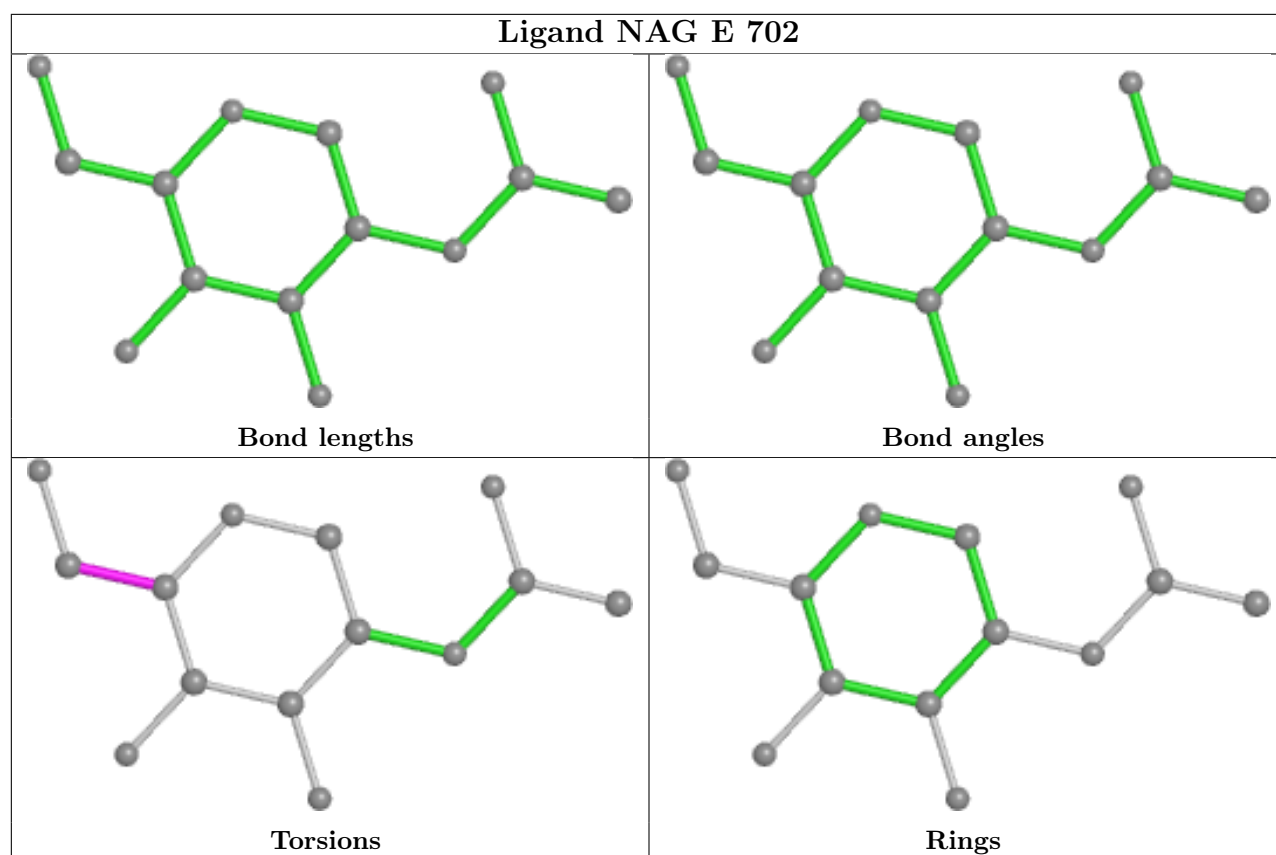


## Ligand NAG D 1301

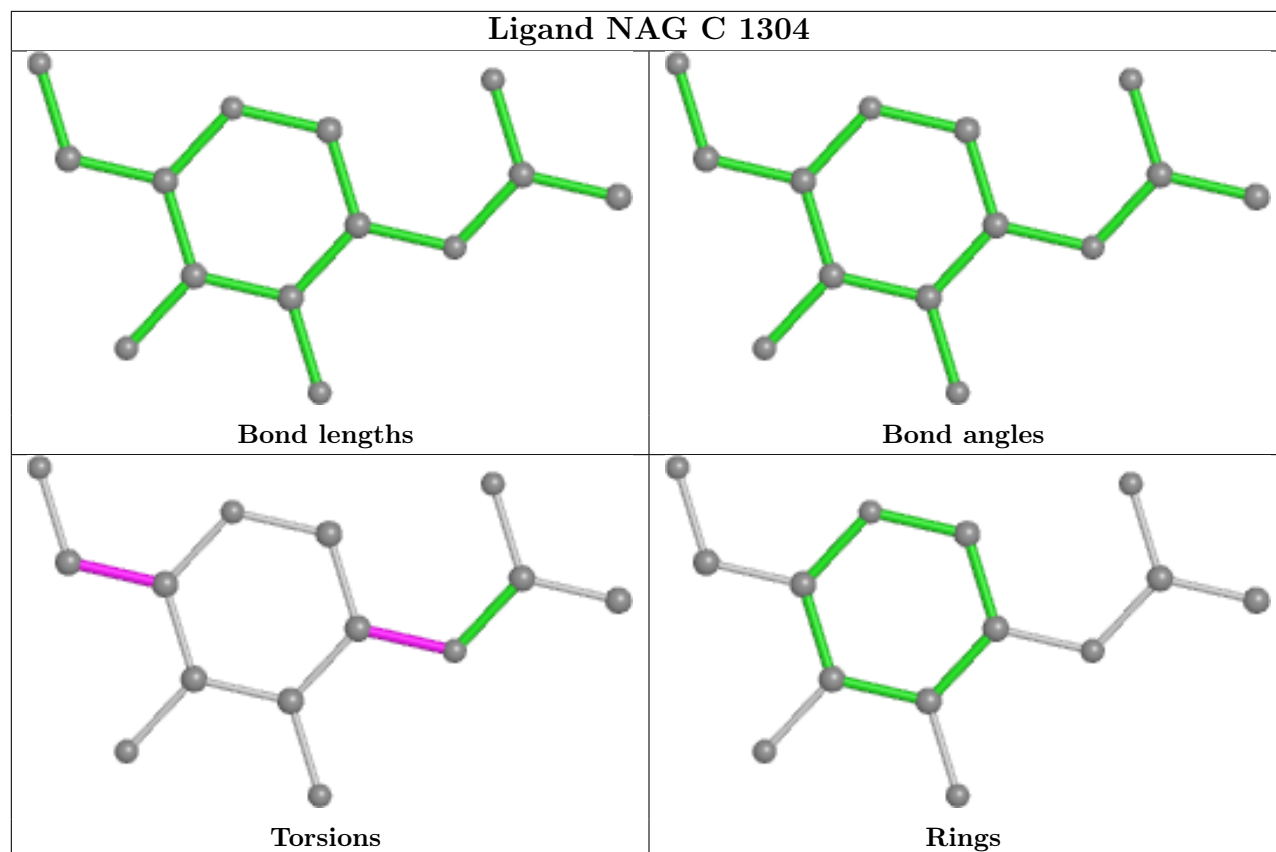


## Ligand NAG D 1305

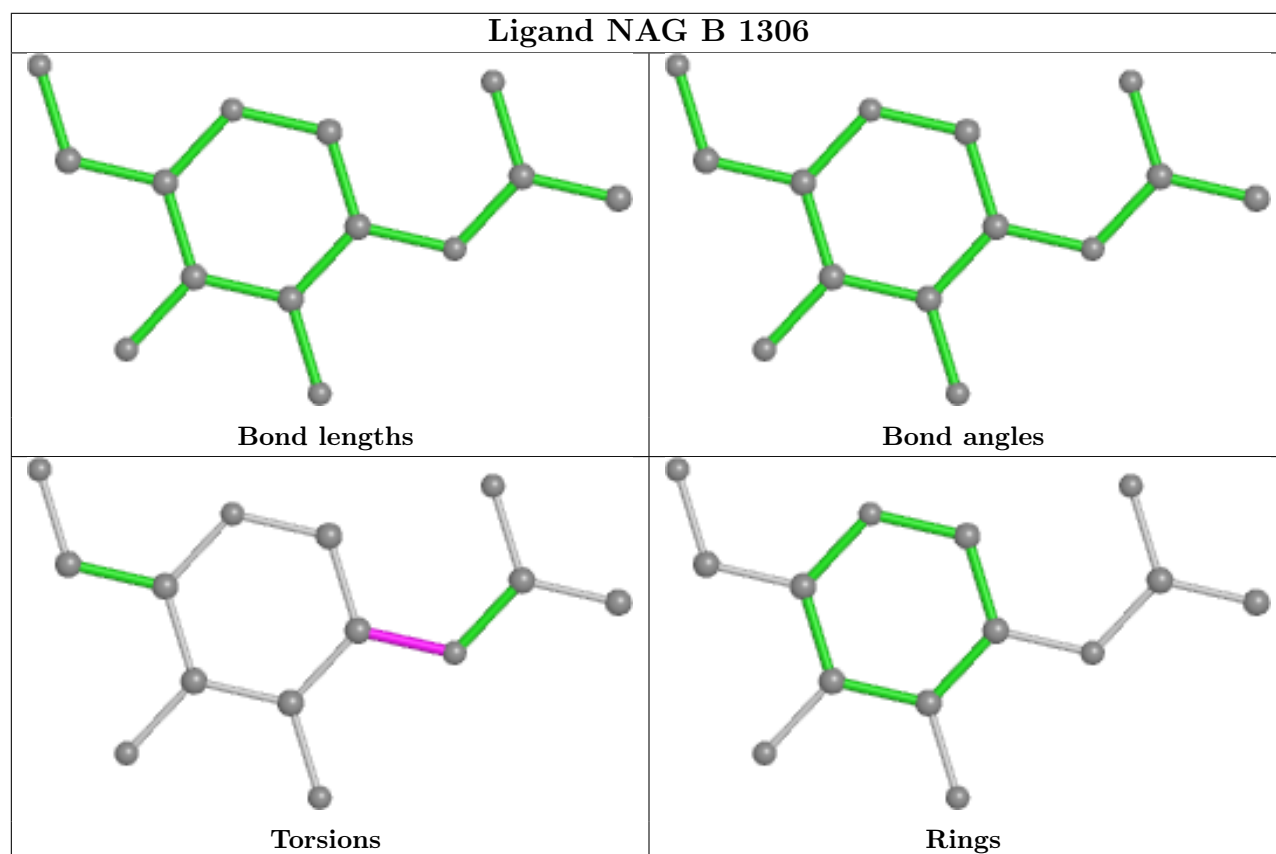


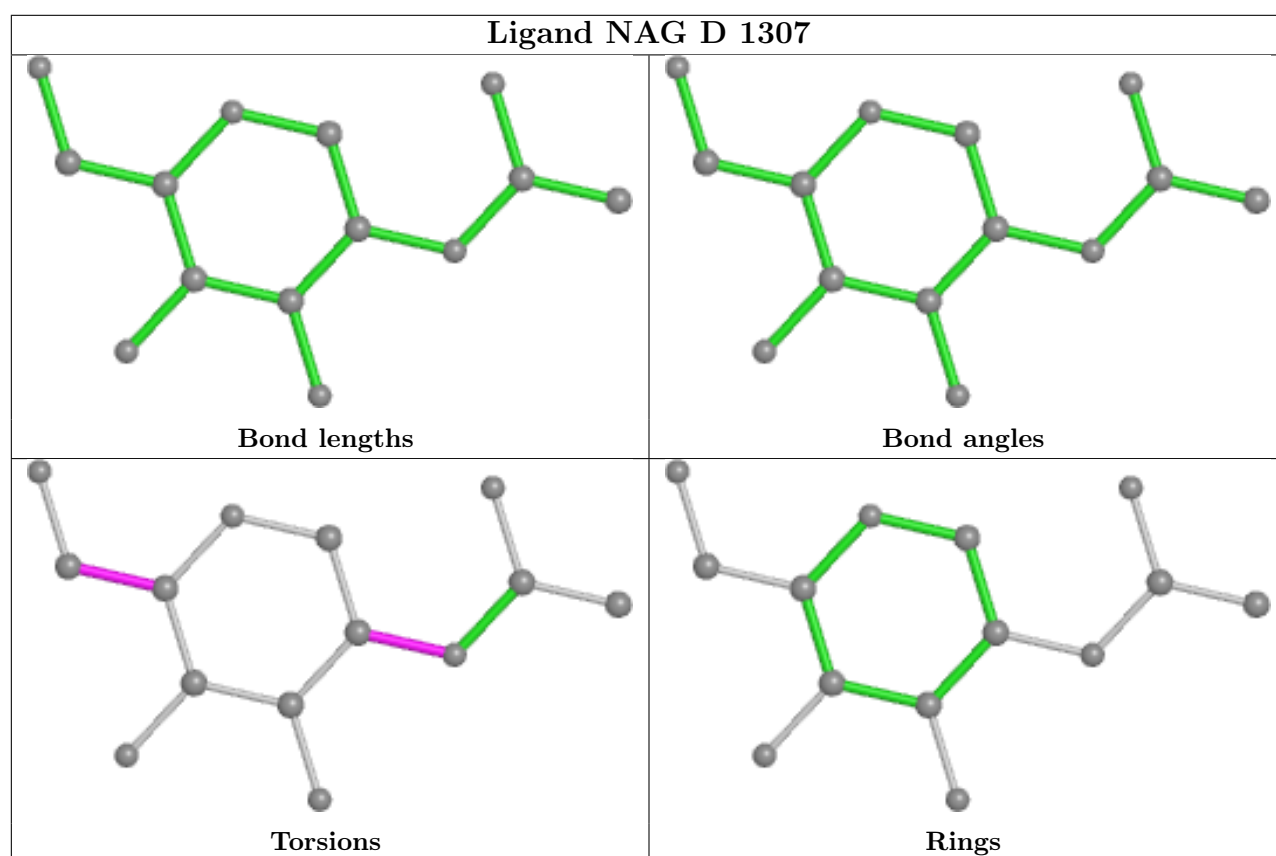
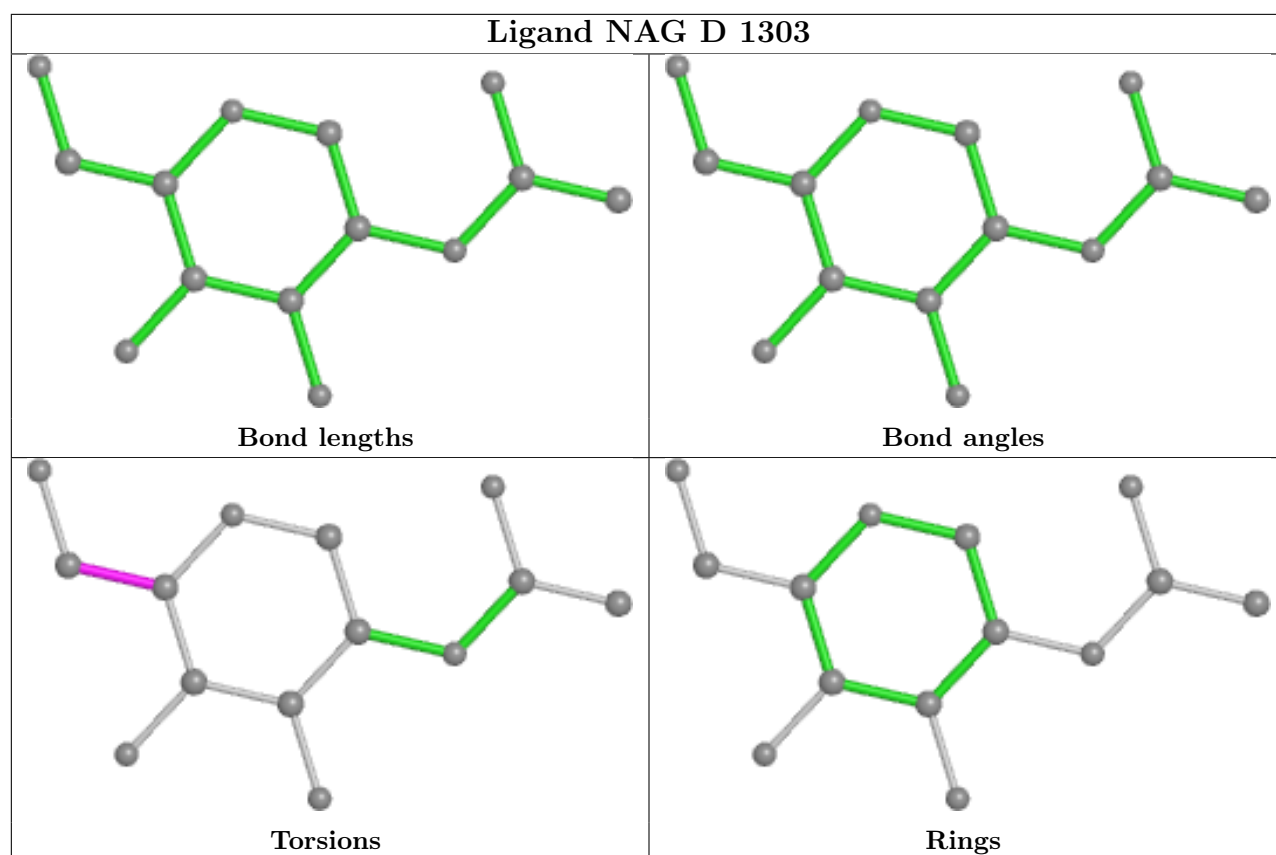


## Ligand NAG C 1304

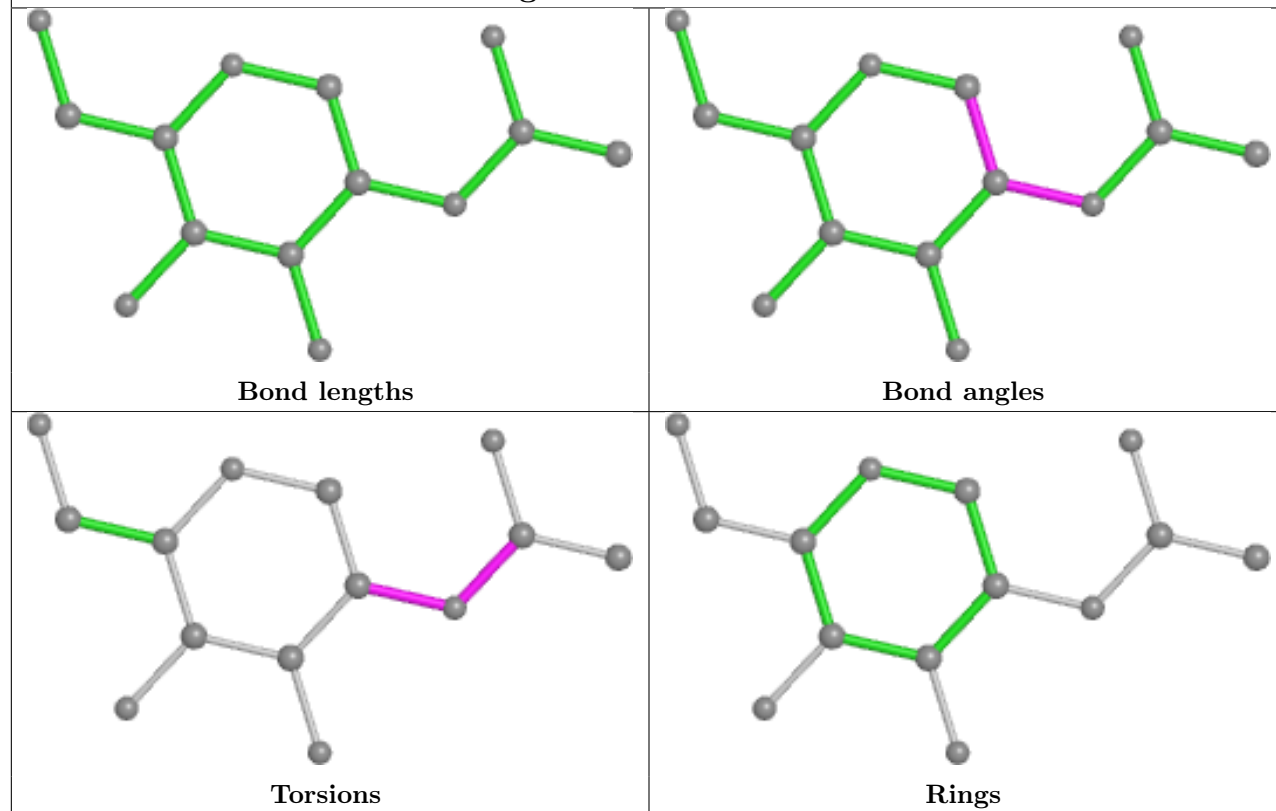


## Ligand NAG B 1306

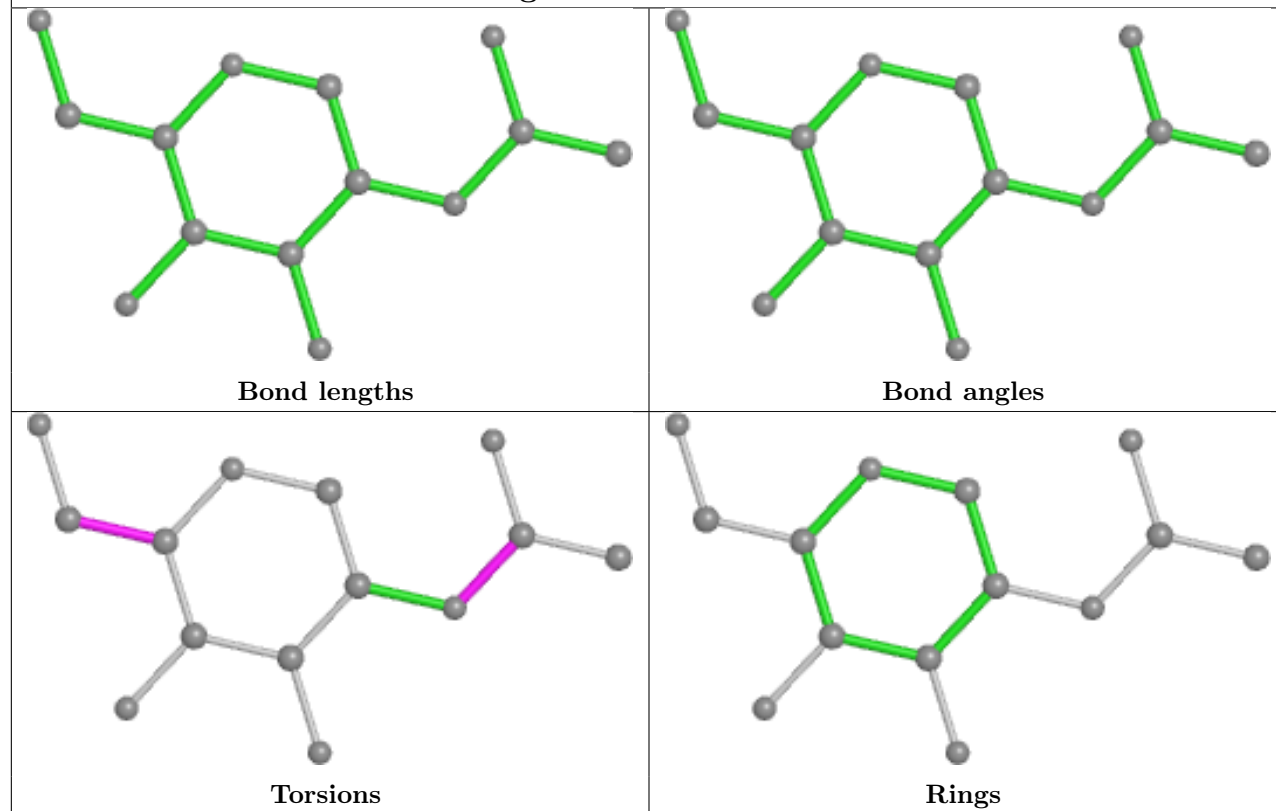




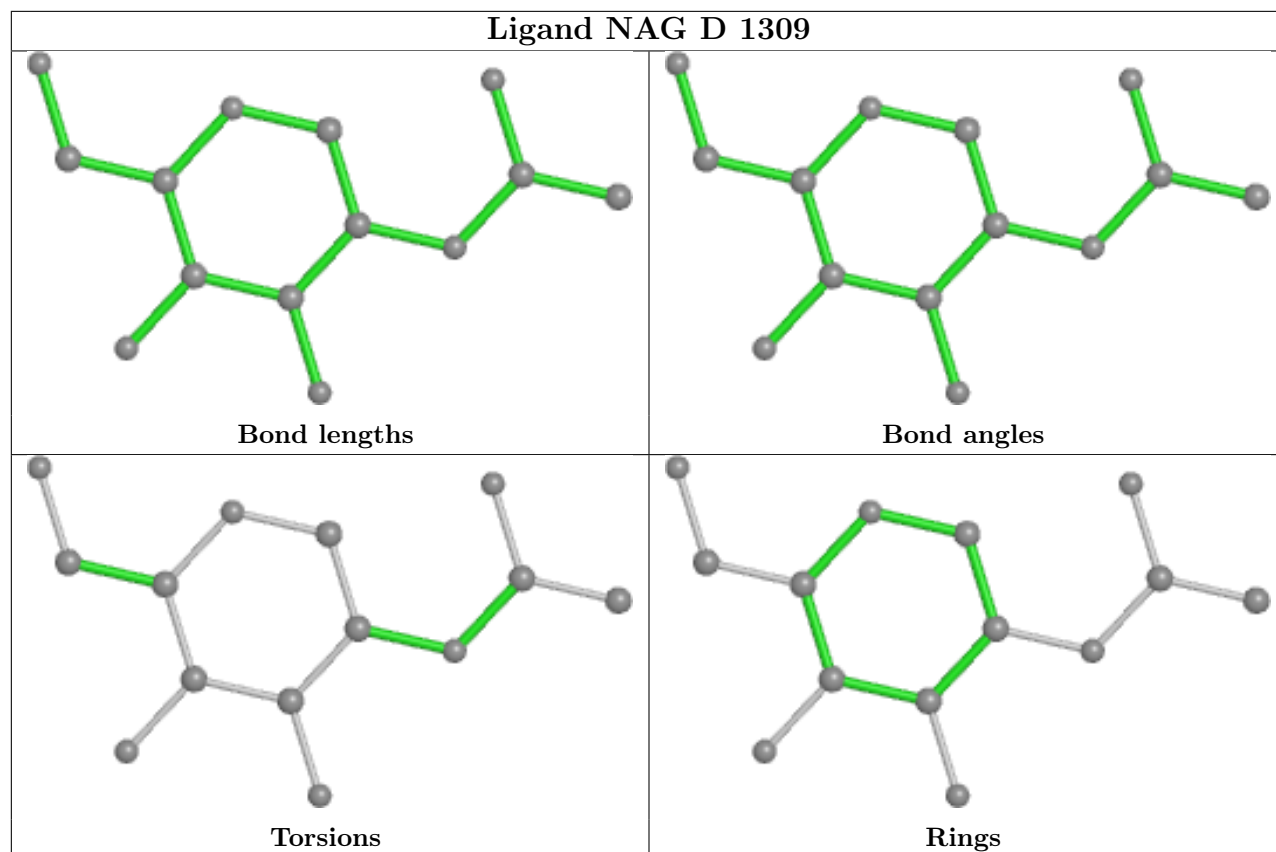
## Ligand NAG C 1309



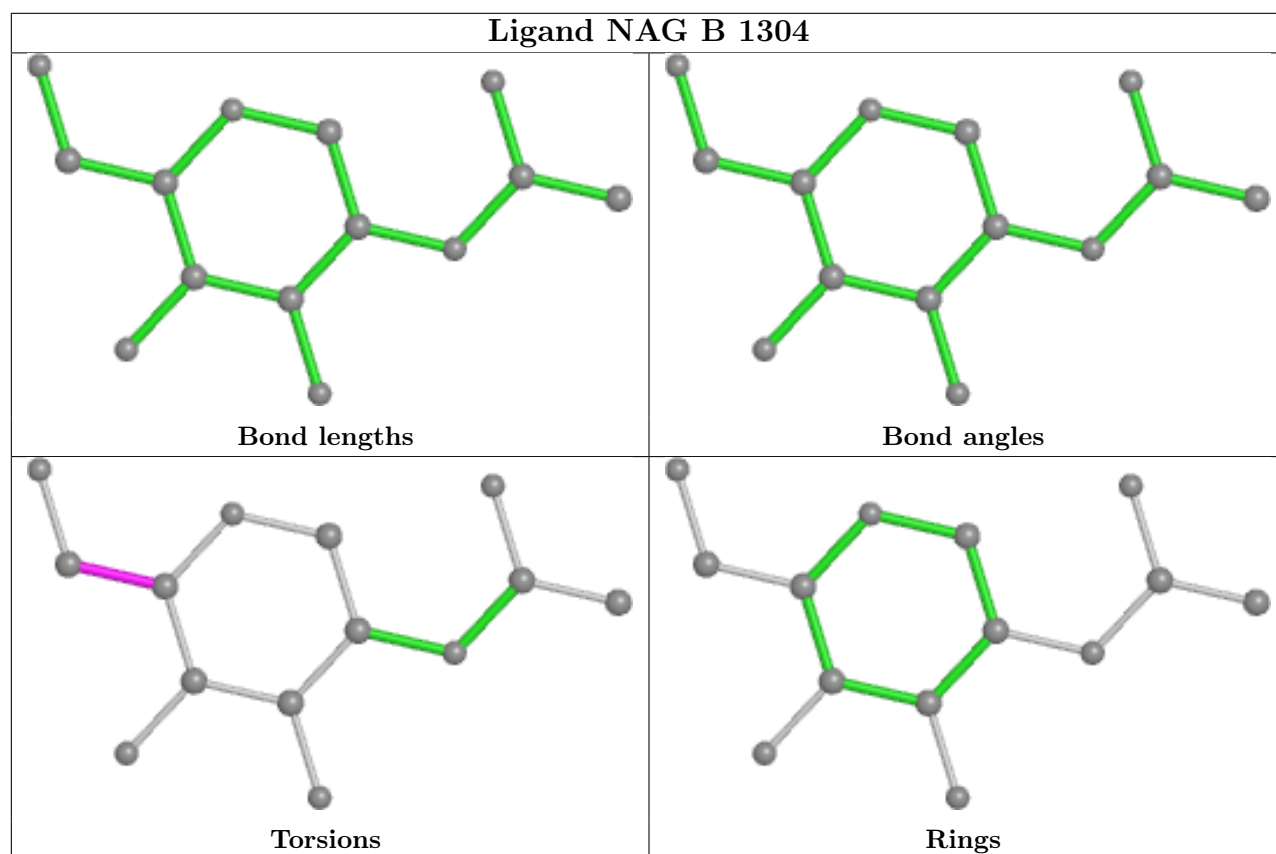
## Ligand NAG B 1301

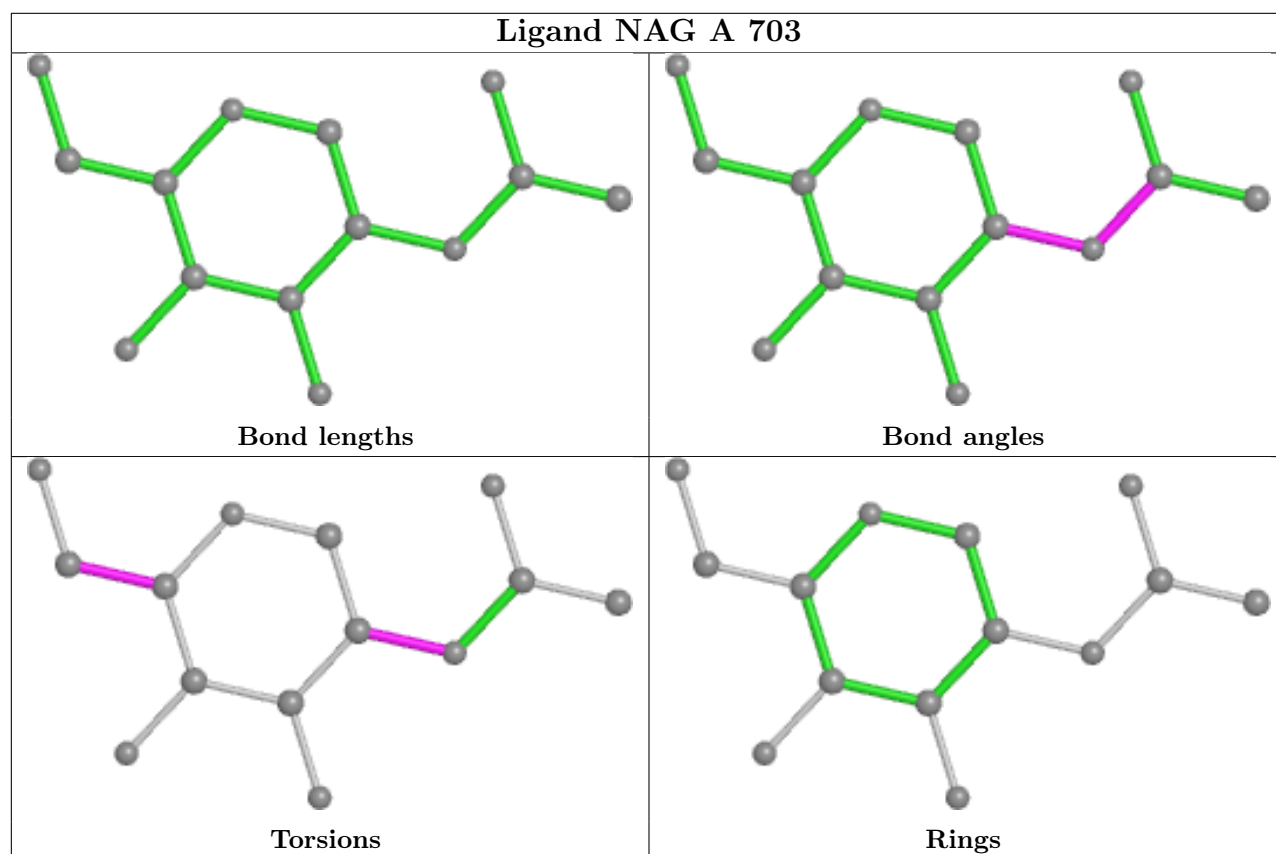
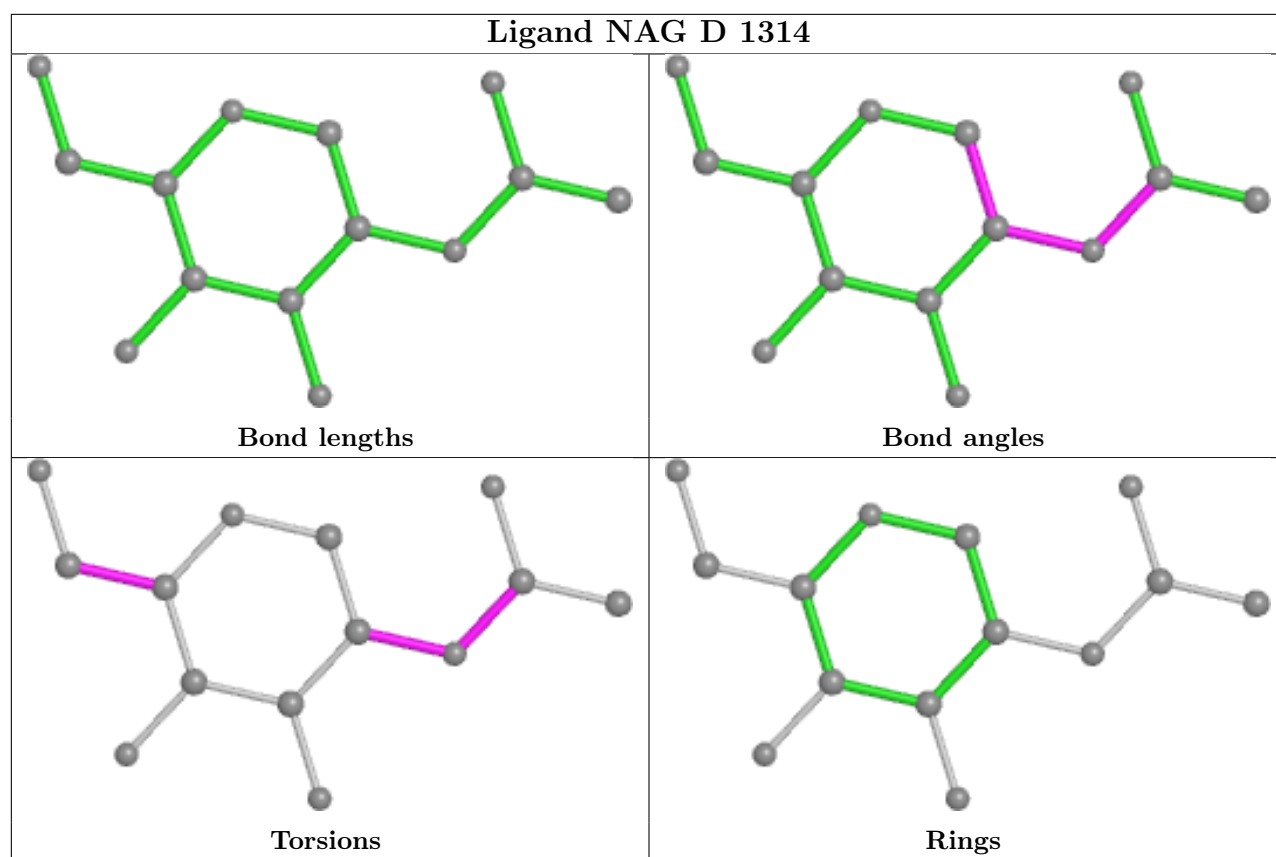


## Ligand NAG D 1309

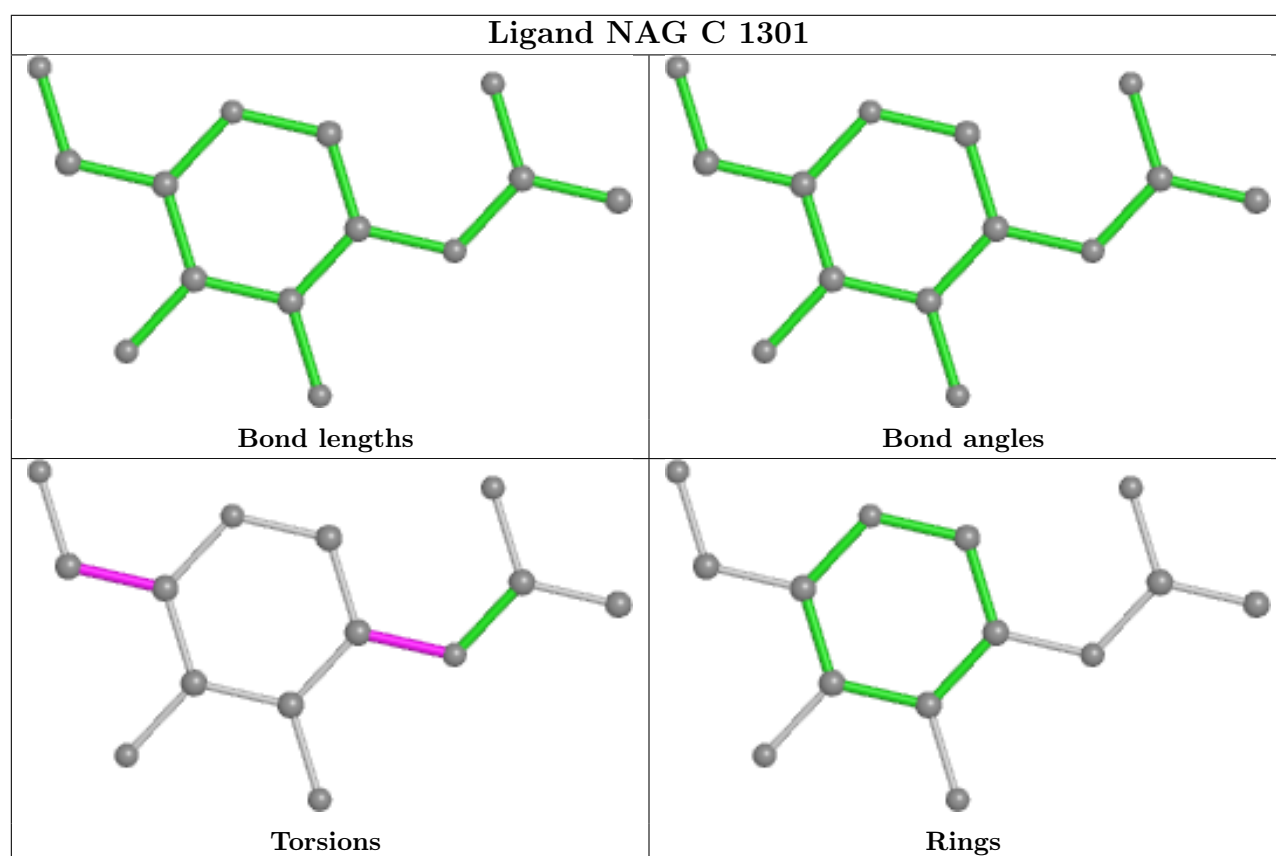
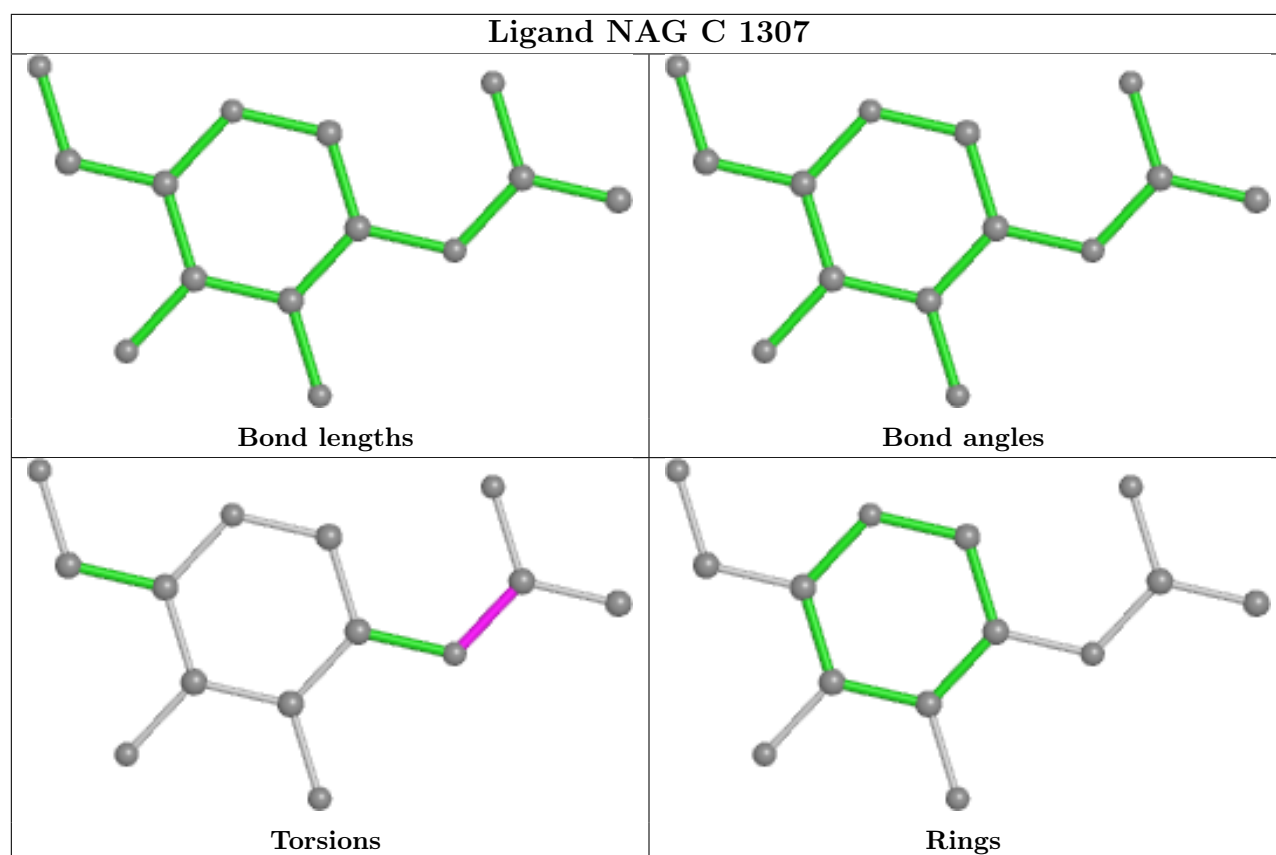


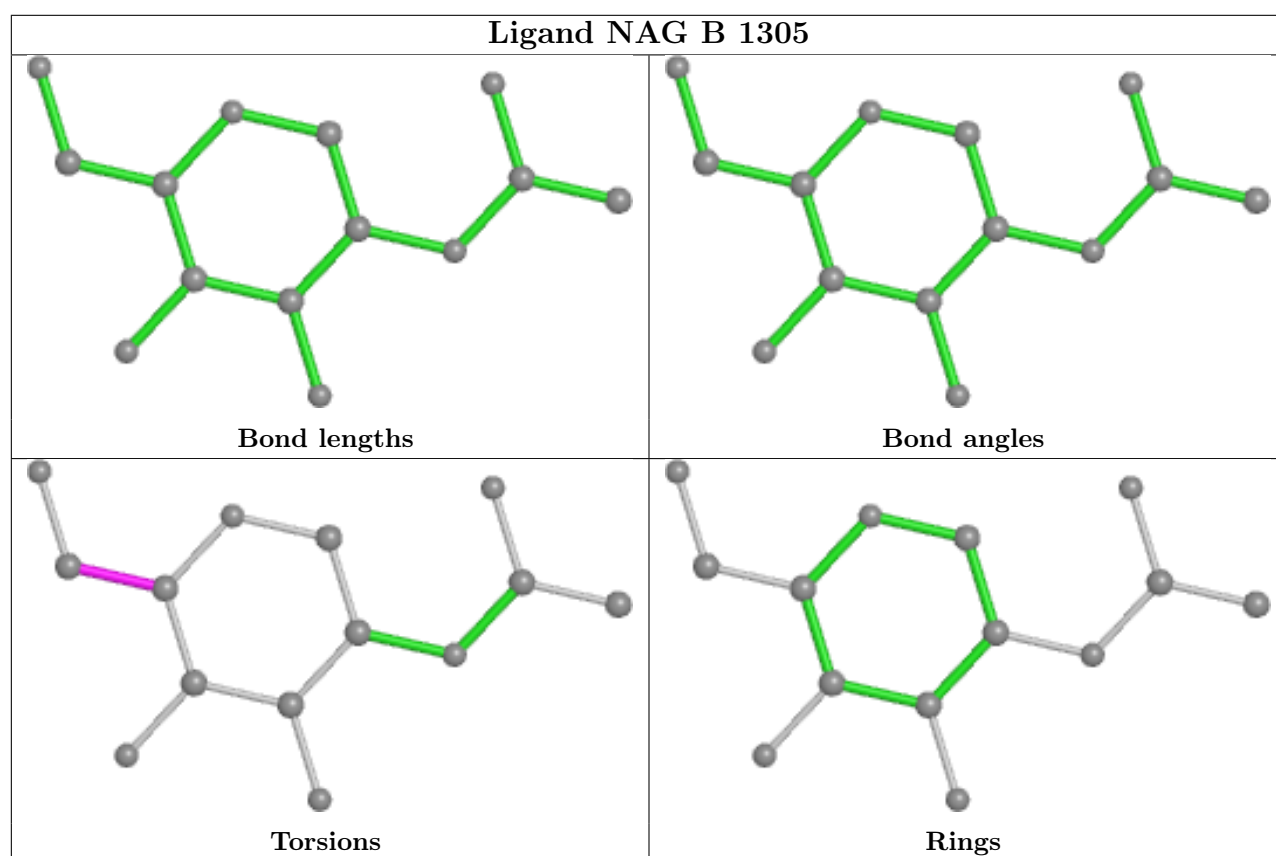
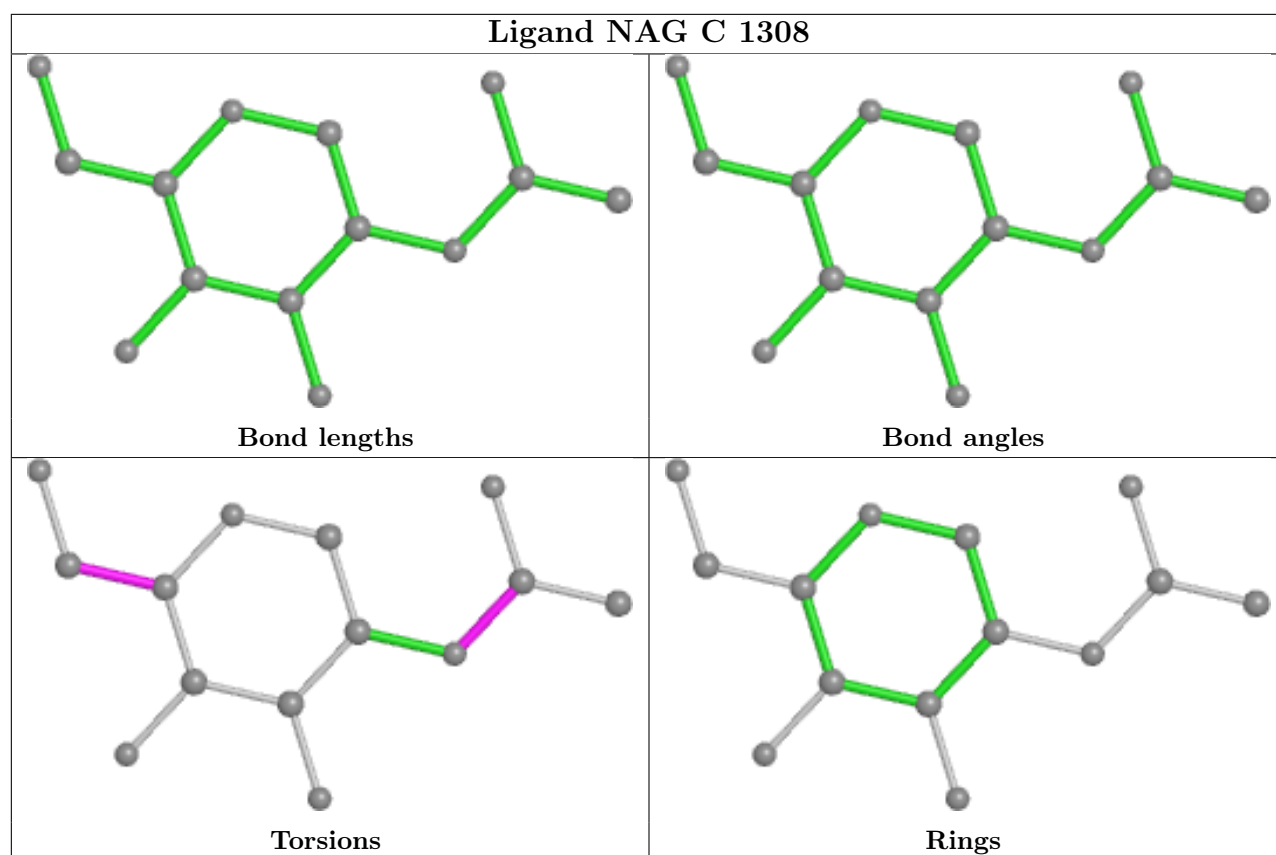
## Ligand NAG B 1304



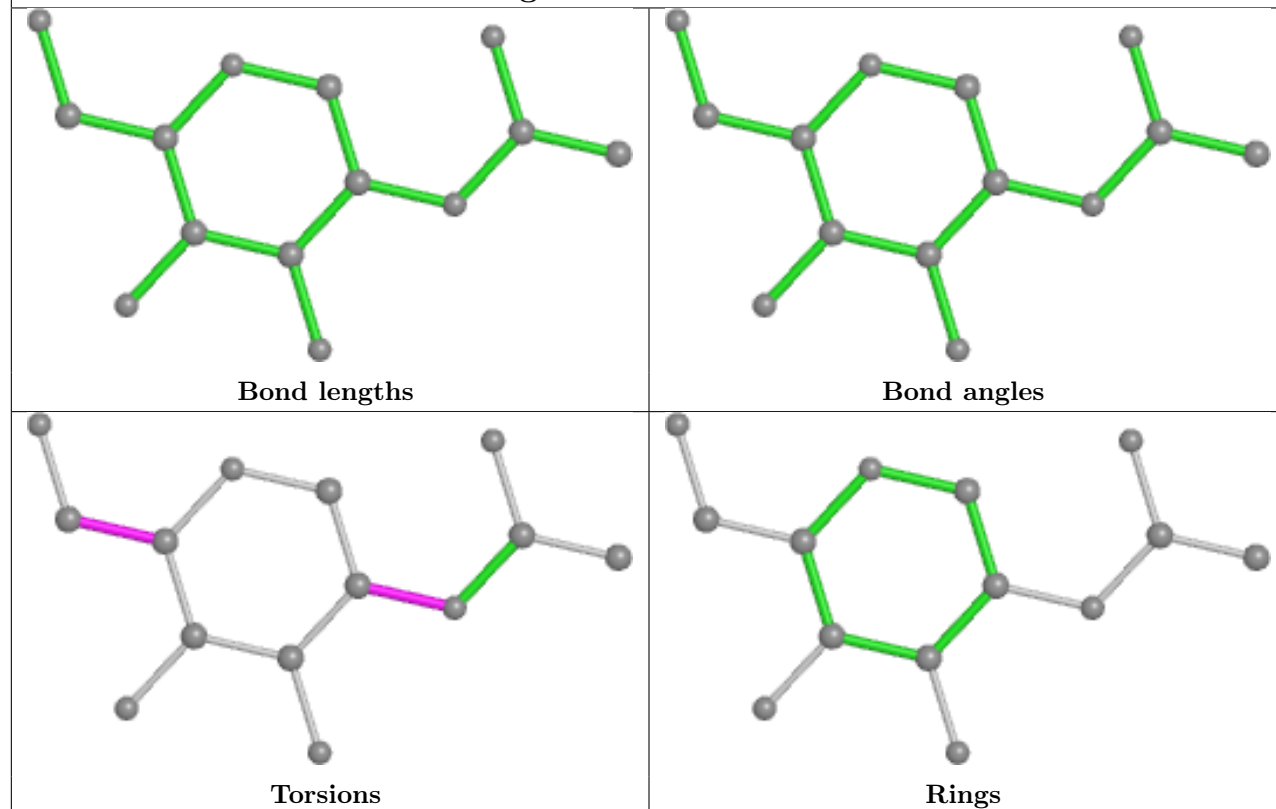




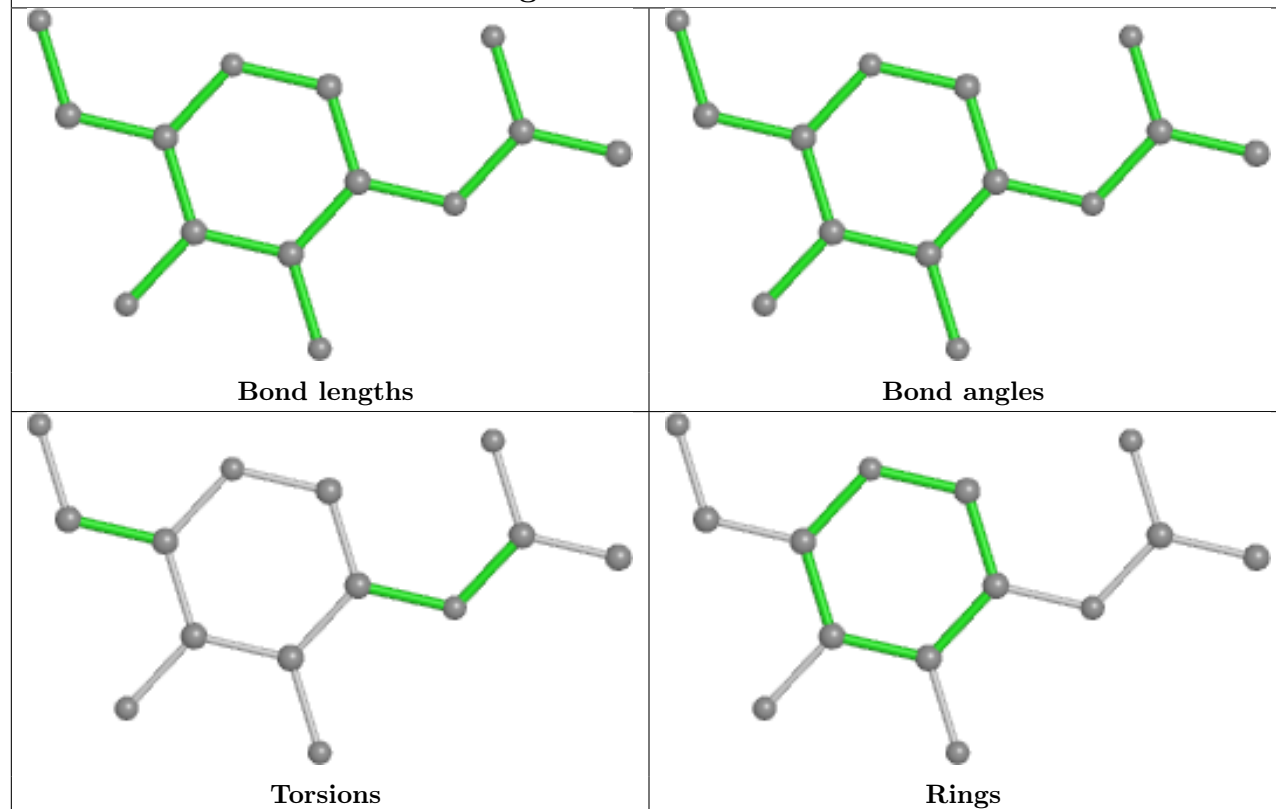


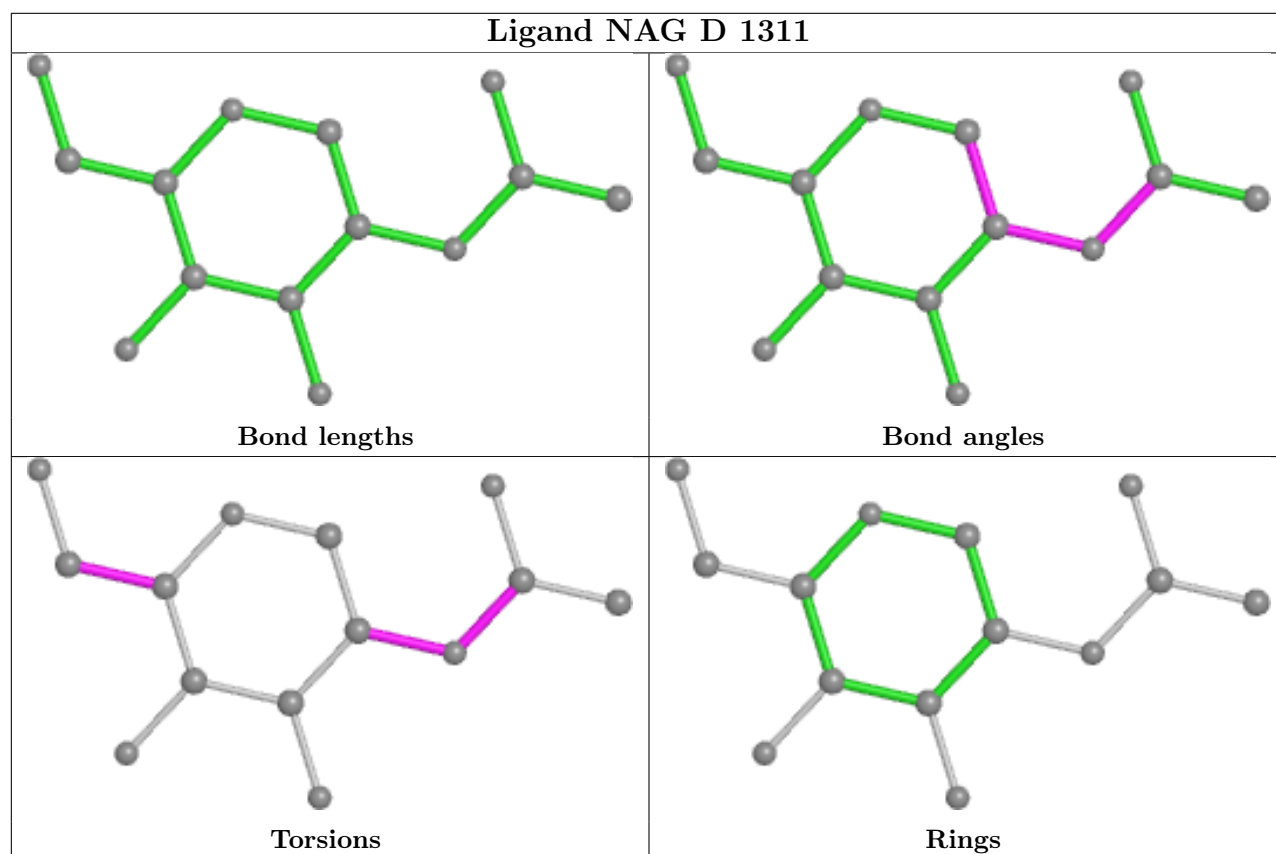
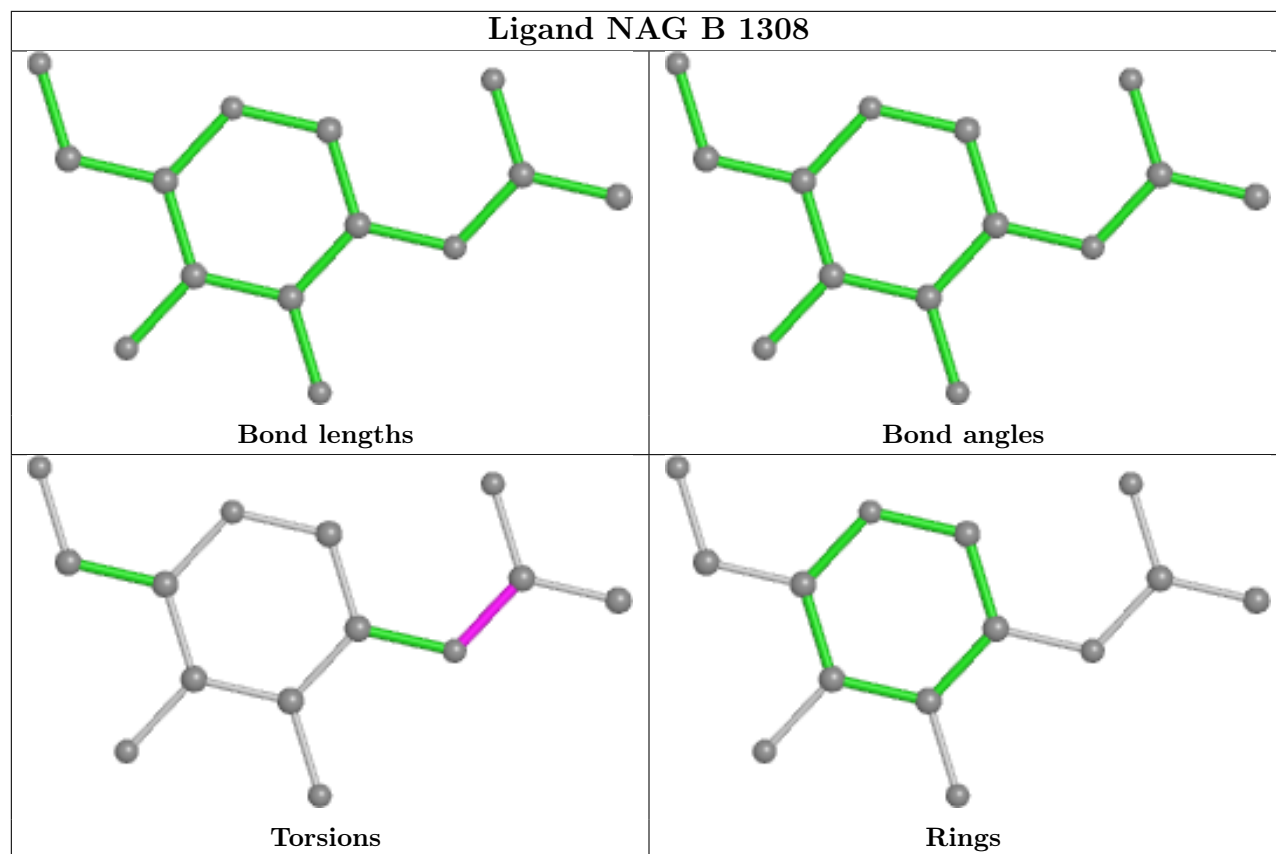


## Ligand NAG B 1303

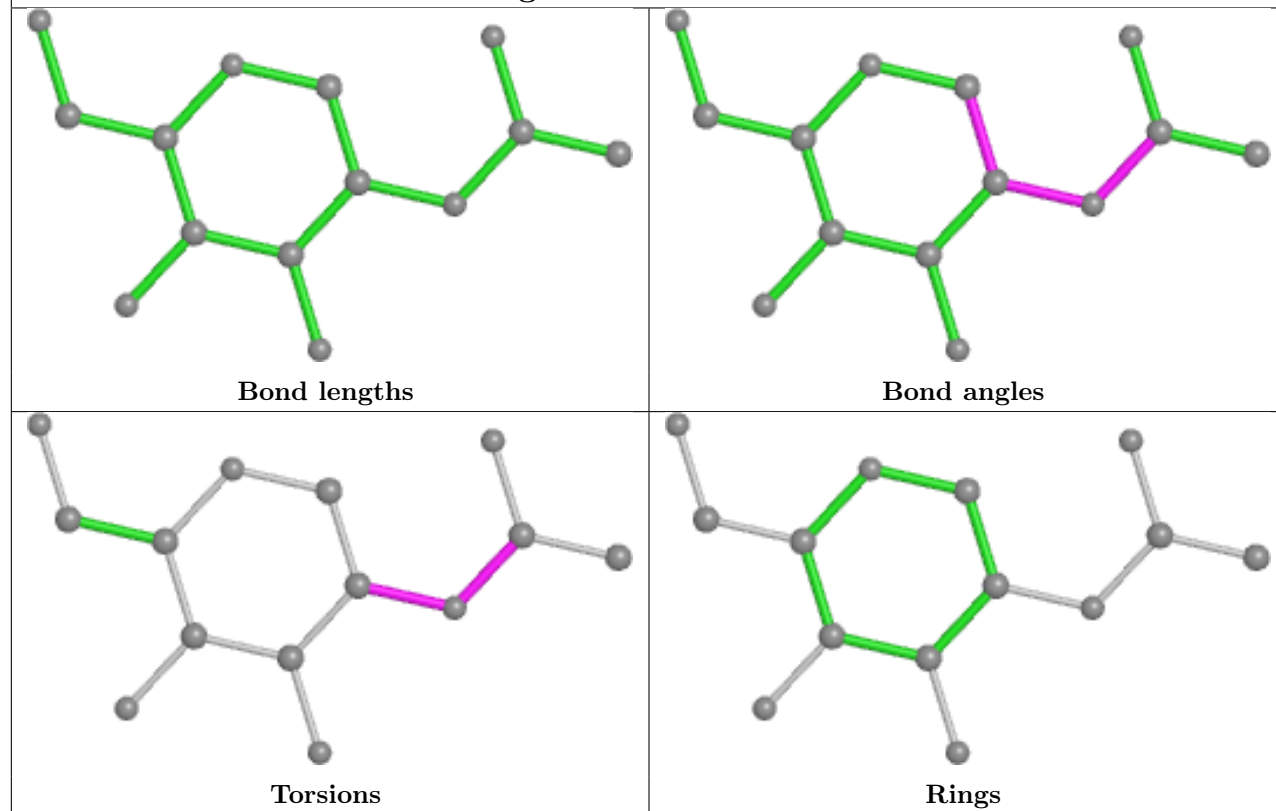


## Ligand NAG C 1305

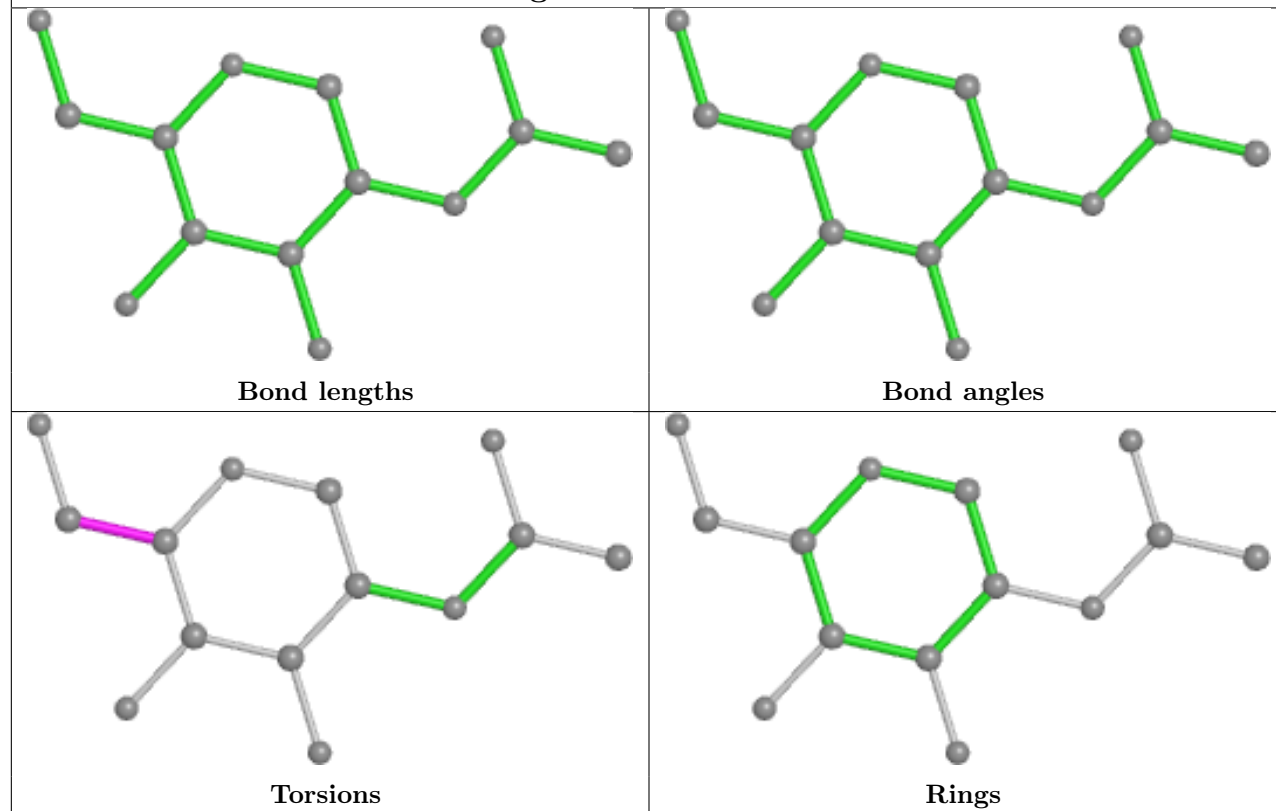




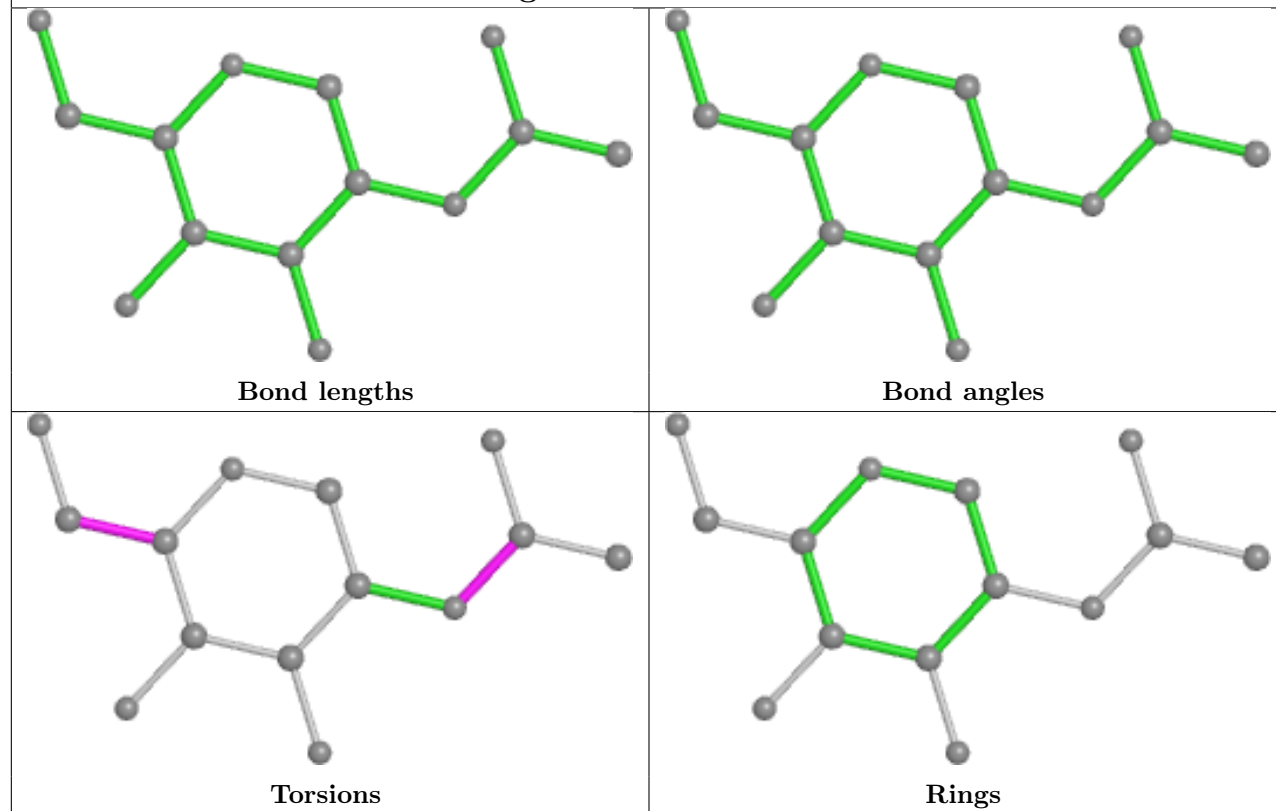
## Ligand NAG D 1312



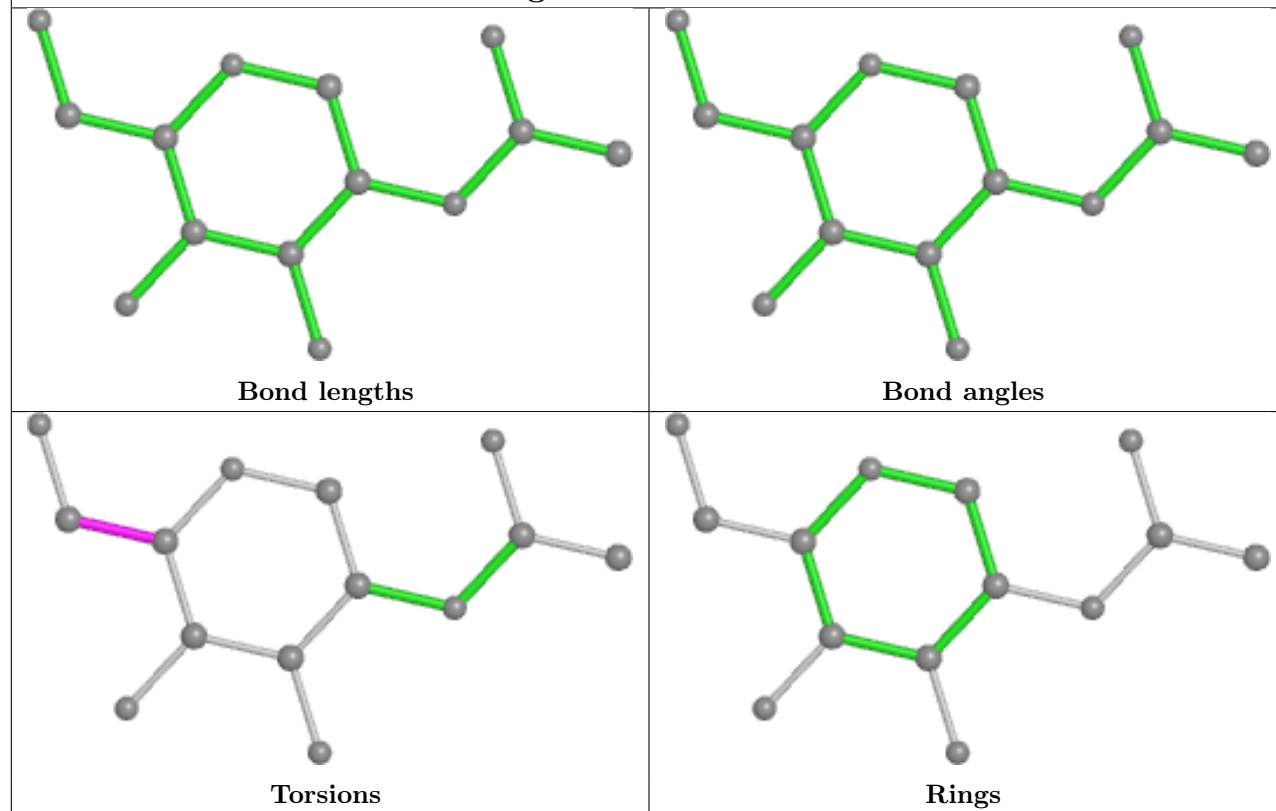
## Ligand NAG F 702



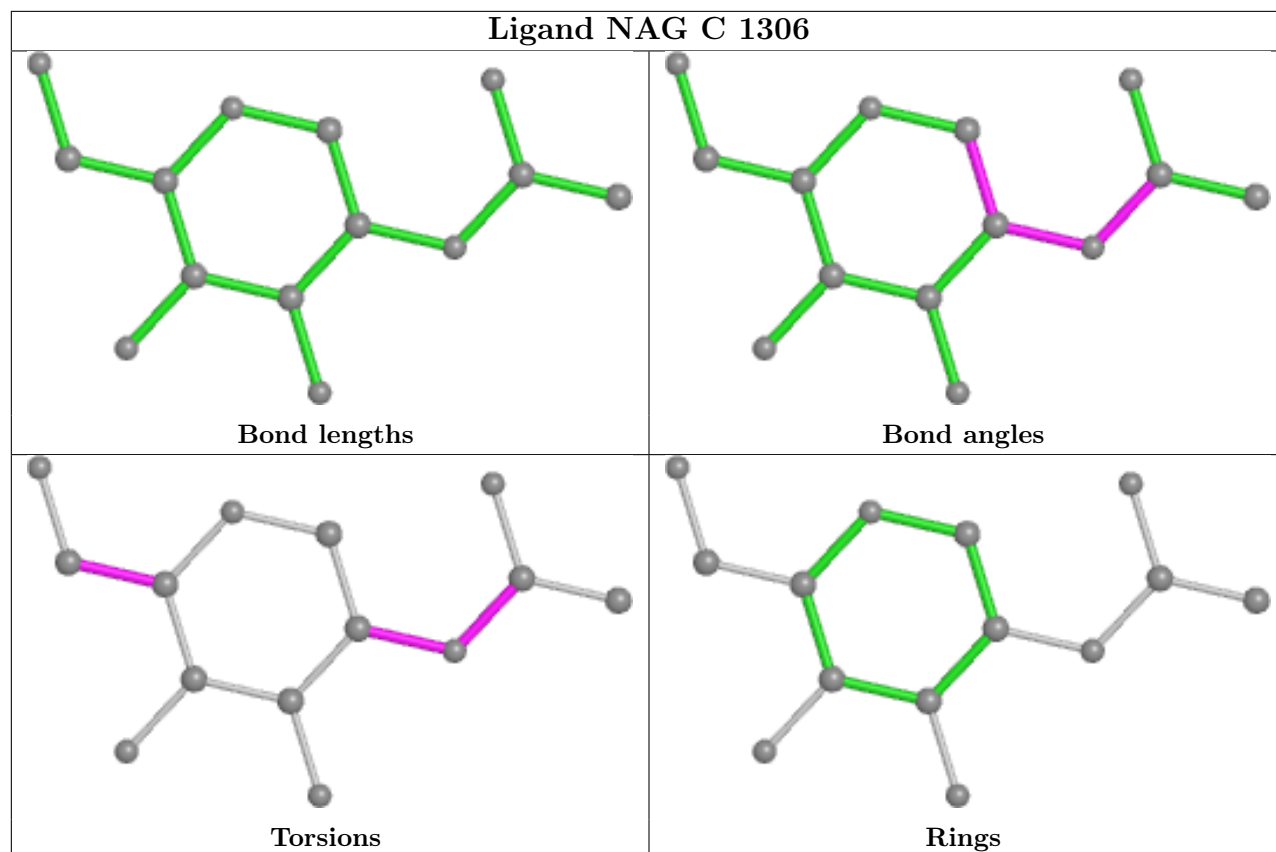
## Ligand NAG C 1302



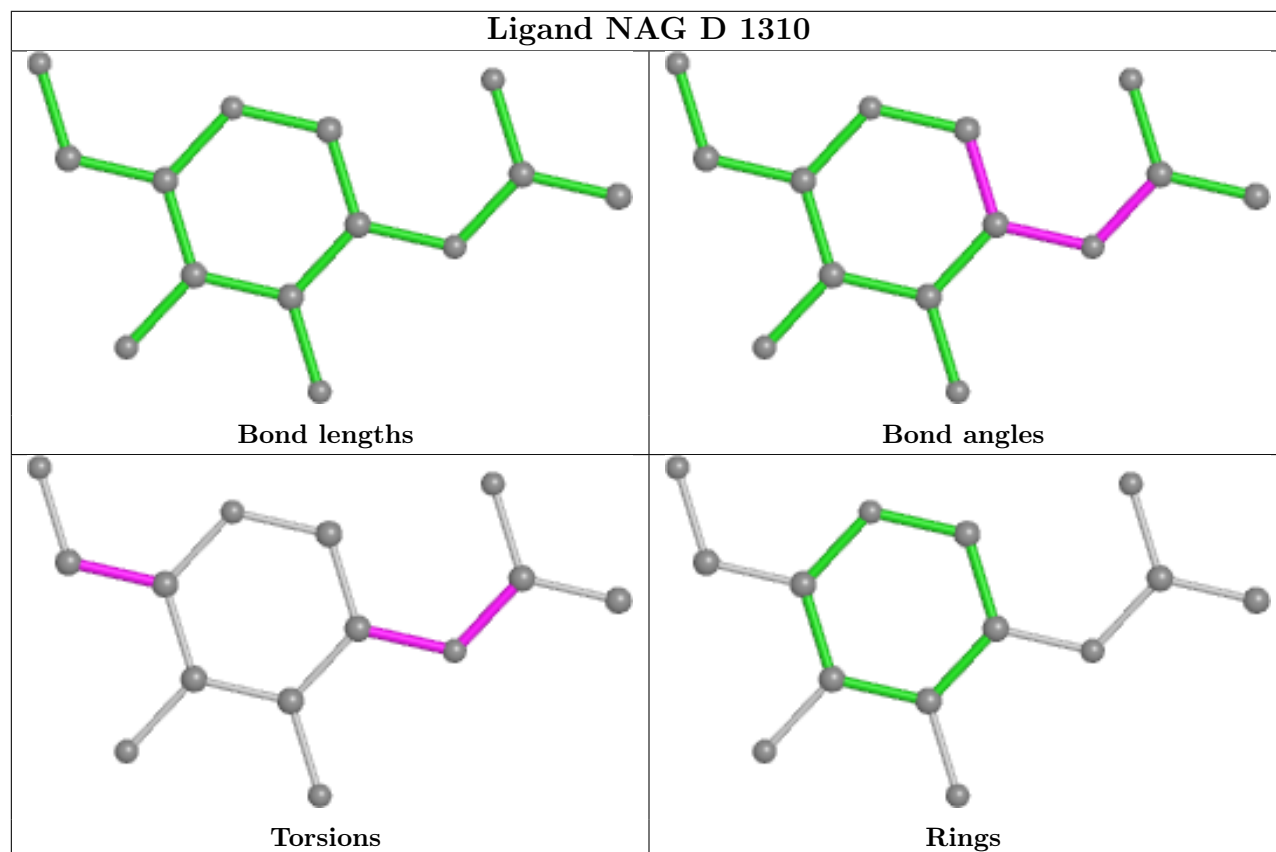
## Ligand NAG A 702



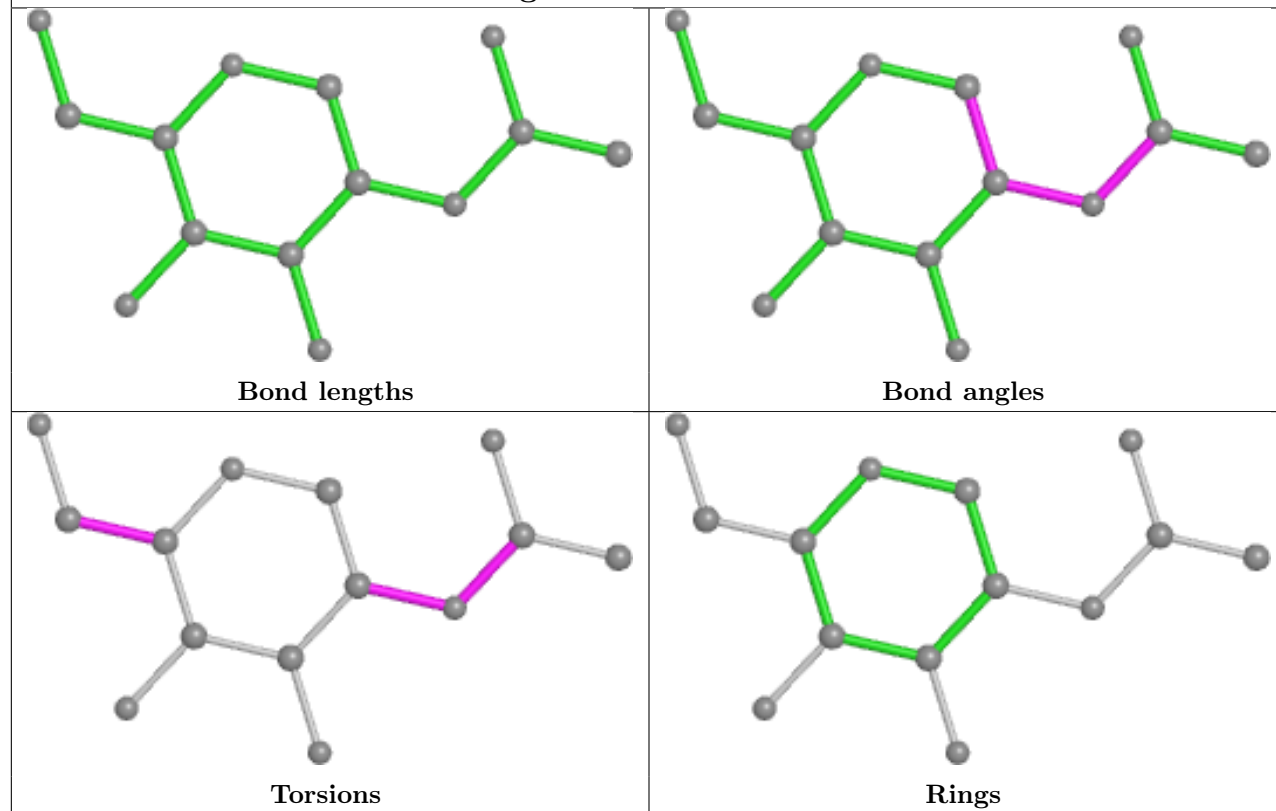
## Ligand NAG C 1306



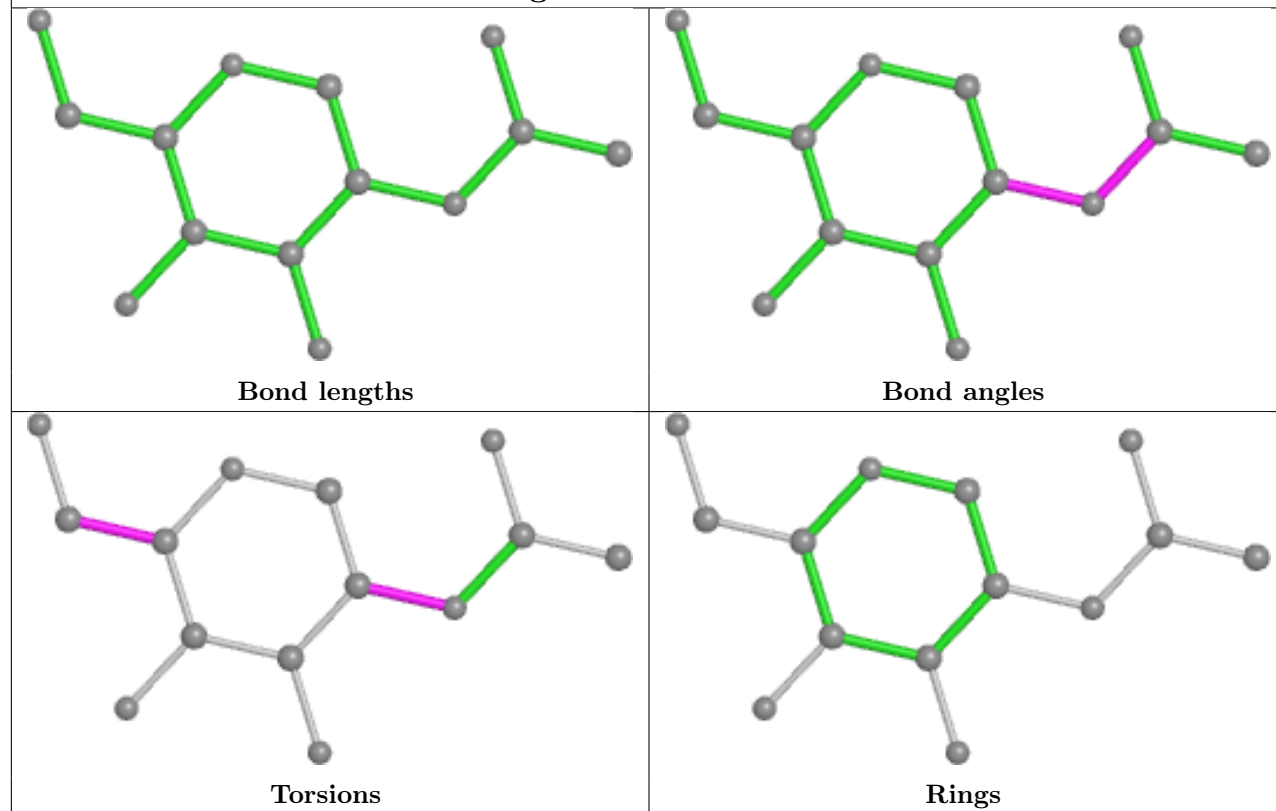
## Ligand NAG D 1310



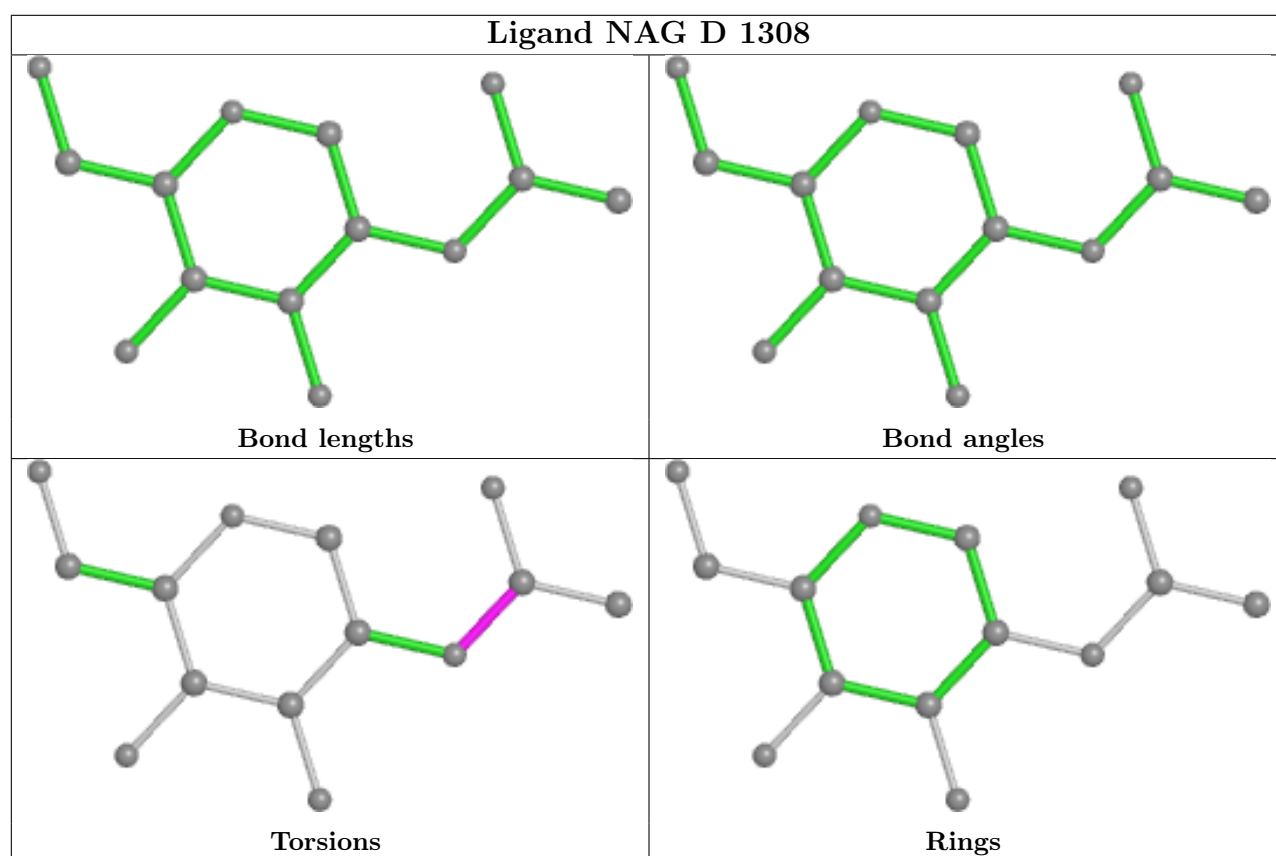
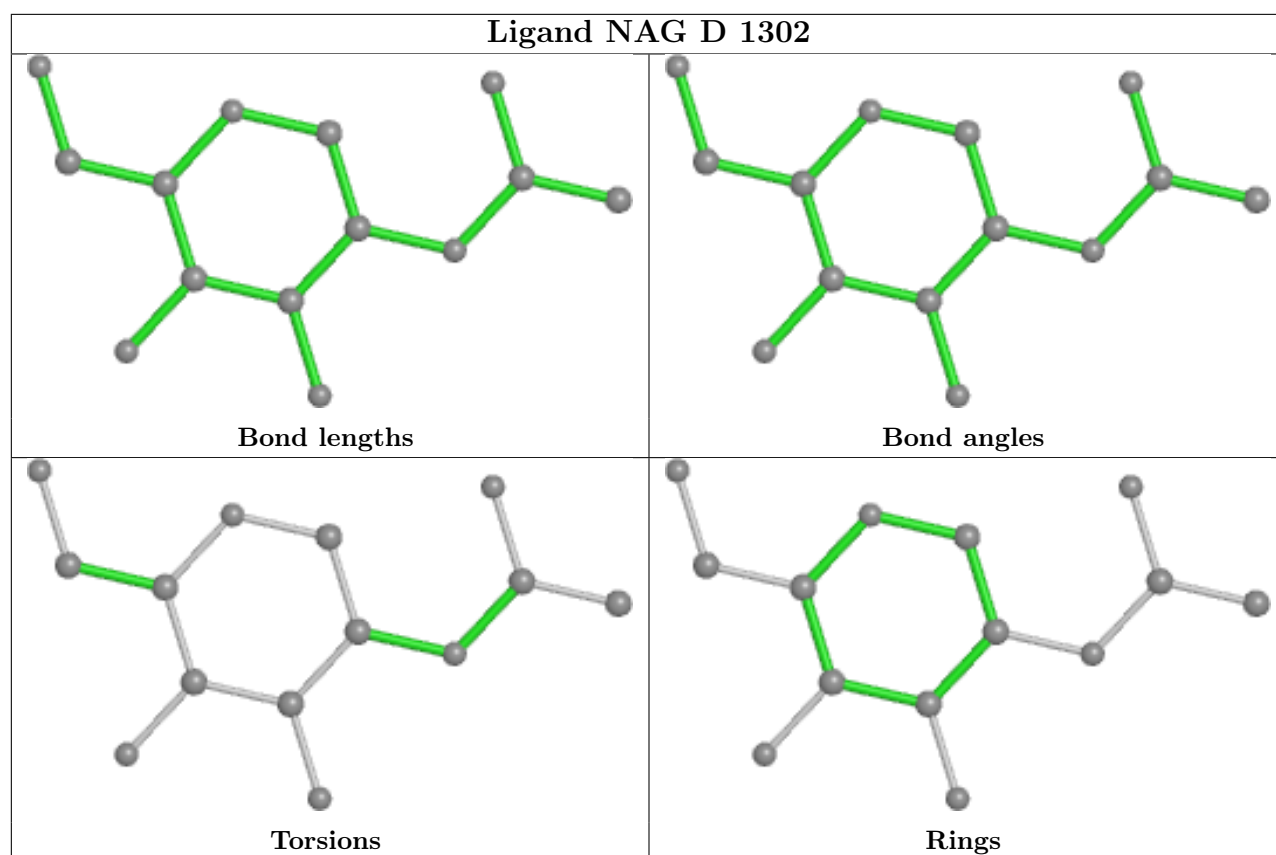
## Ligand NAG B 1307



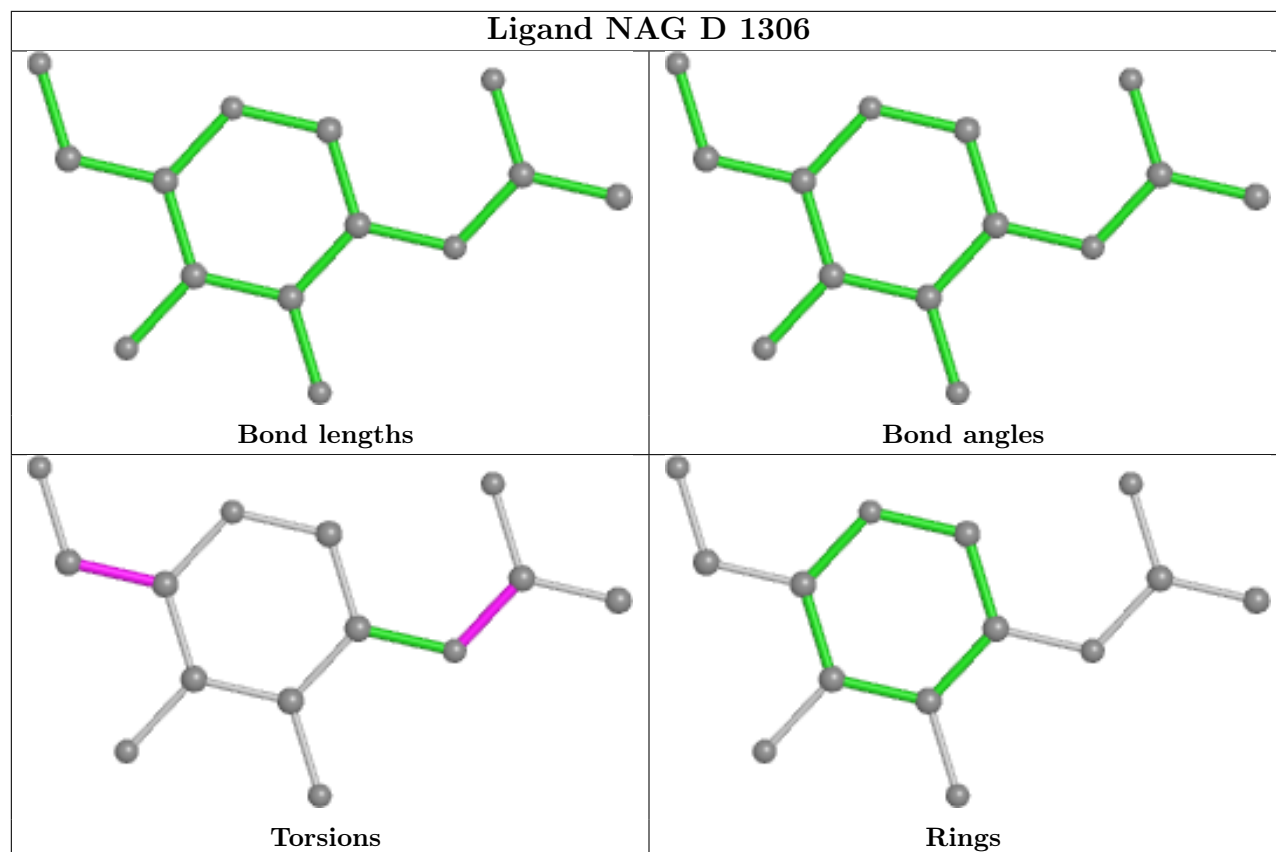
## Ligand NAG E 703



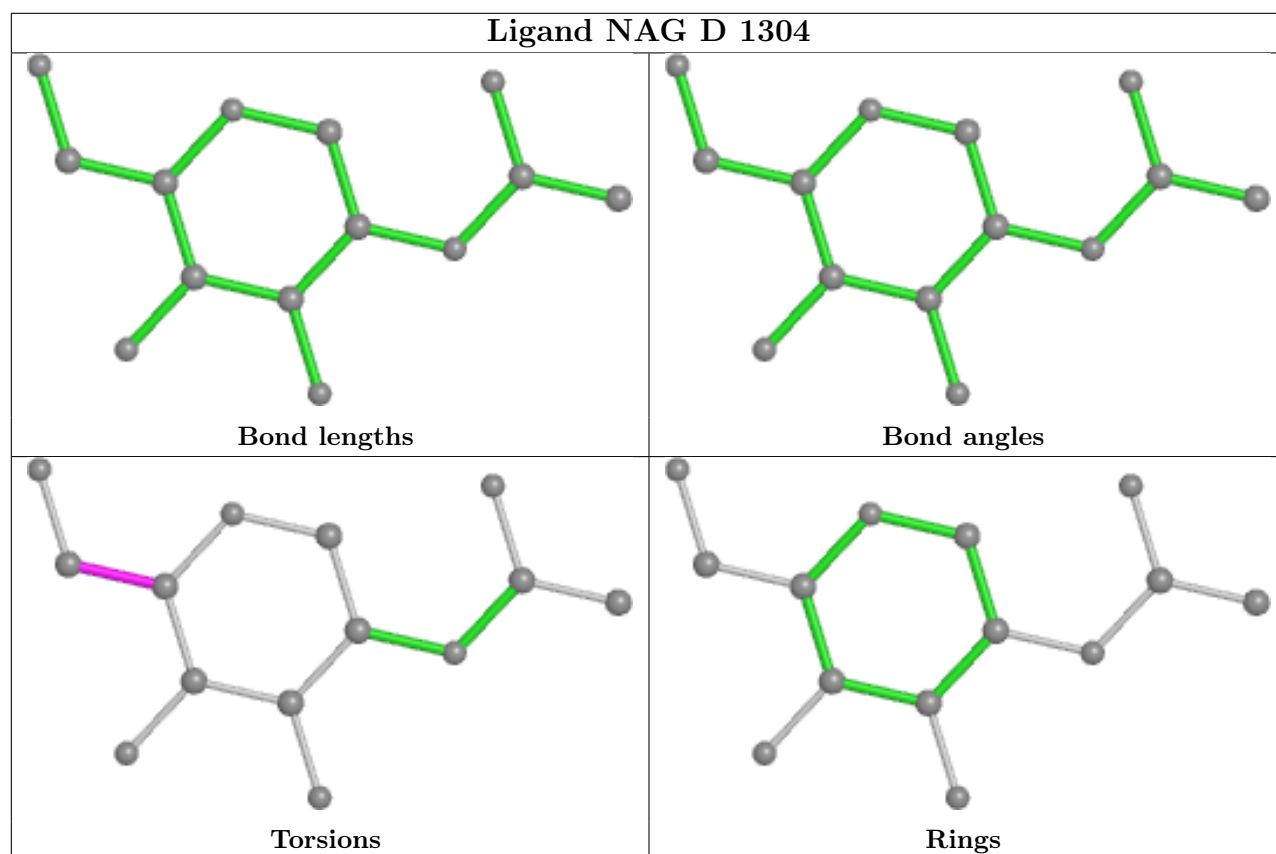




## Ligand NAG D 1306



## Ligand NAG D 1304



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

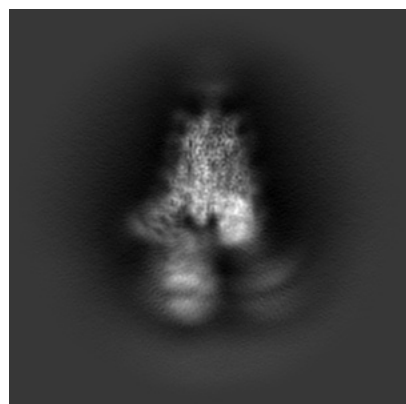
## 6 Map visualisation [i](#)

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

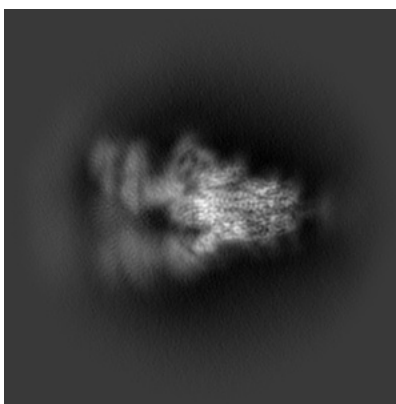
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

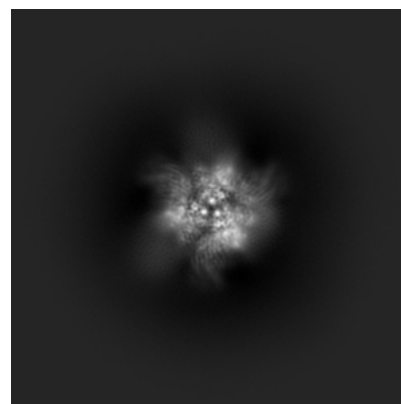
#### 6.1.1 Primary map



X

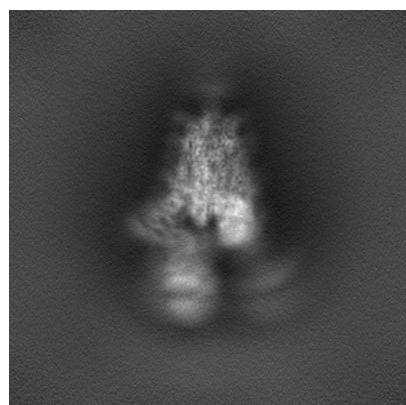


Y

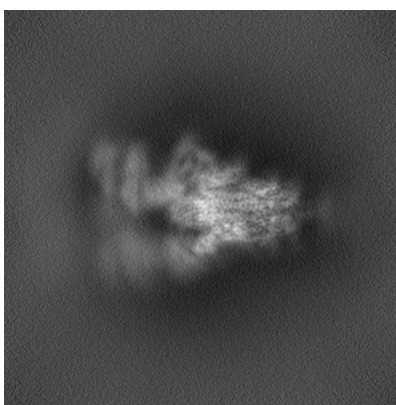


Z

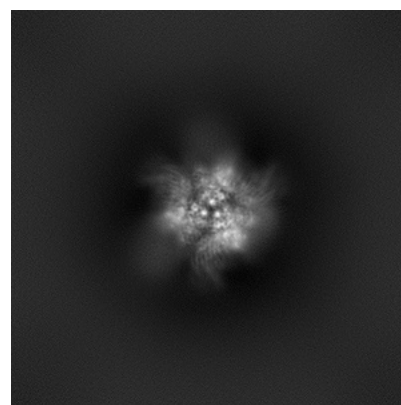
#### 6.1.2 Raw map



X



Y

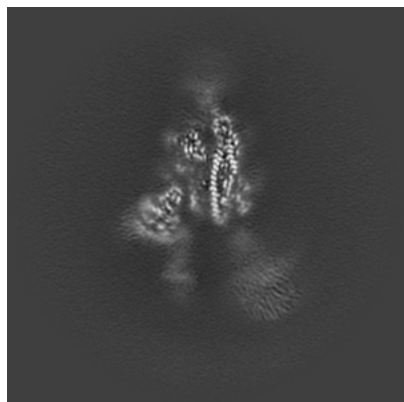


Z

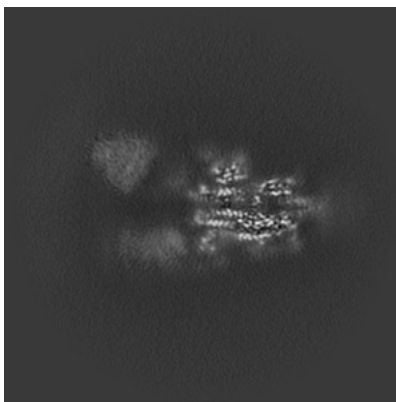
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

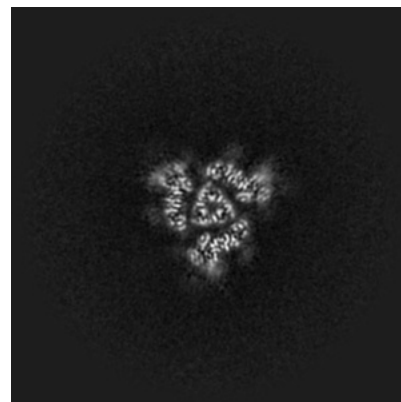
### 6.2.1 Primary map



X Index: 300

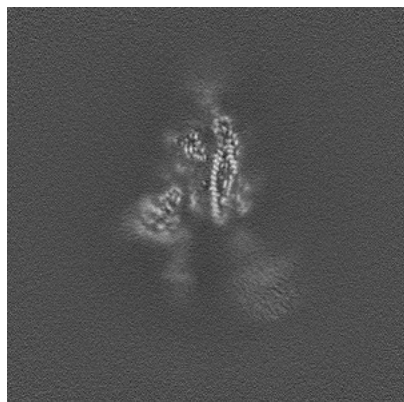


Y Index: 300

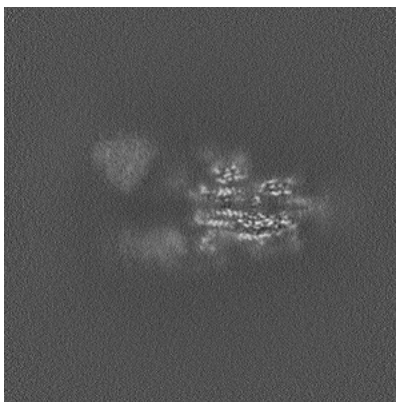


Z Index: 300

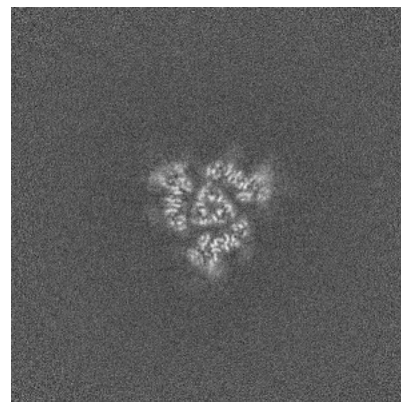
### 6.2.2 Raw map



X Index: 300



Y Index: 300

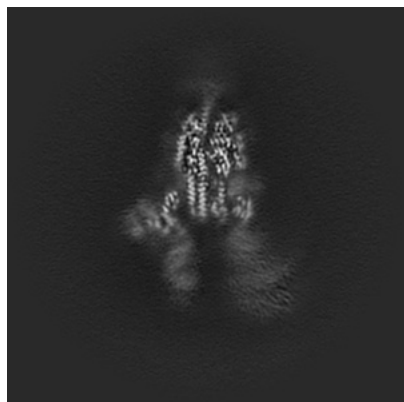


Z Index: 300

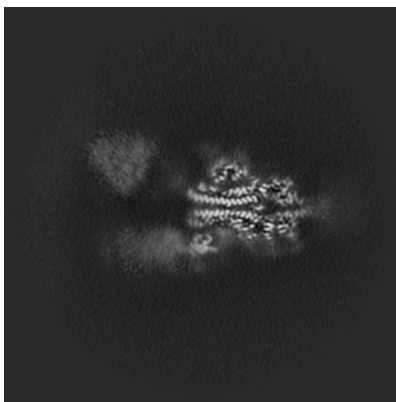
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

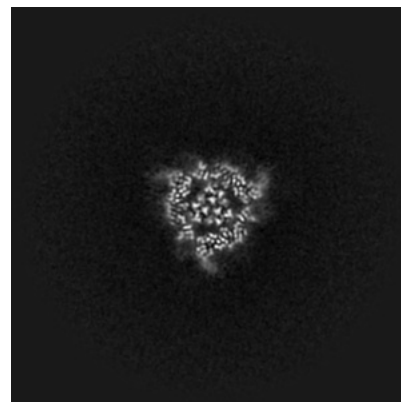
### 6.3.1 Primary map



X Index: 311

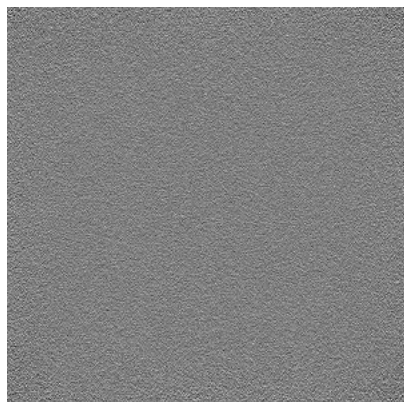


Y Index: 294

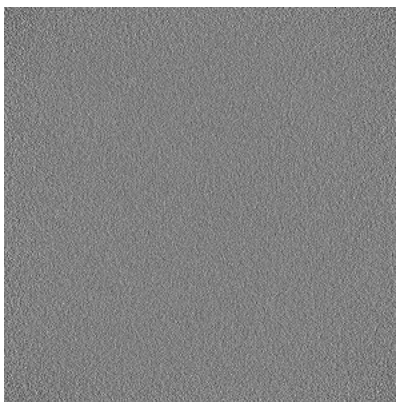


Z Index: 312

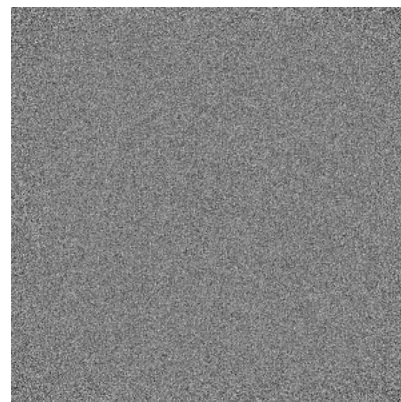
### 6.3.2 Raw map



X Index: 0



Y Index: 0



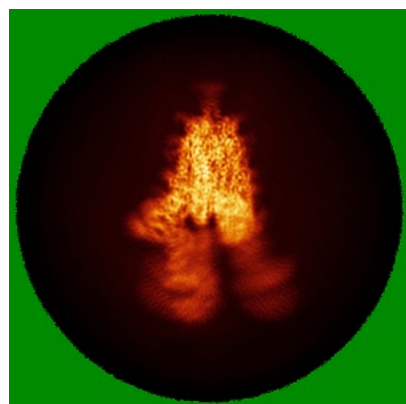
Z Index: 0

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

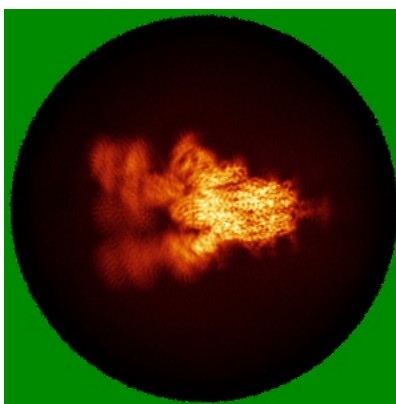


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

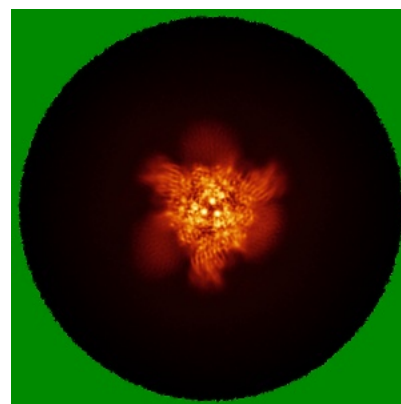
### 6.4.1 Primary map



X

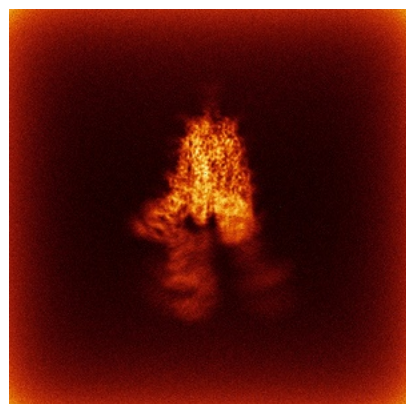


Y

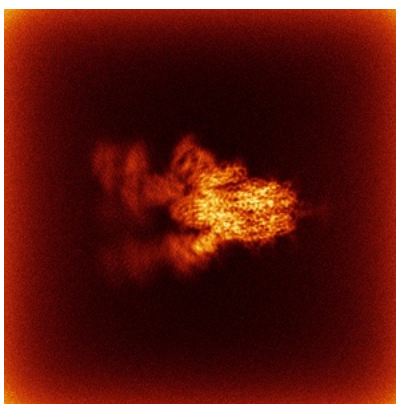


Z

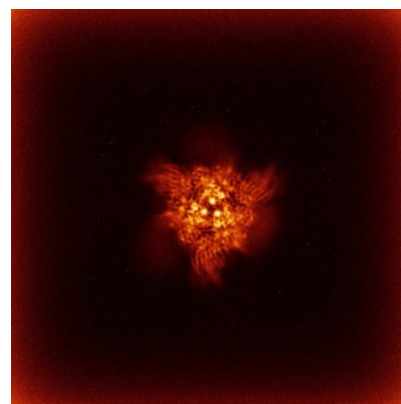
### 6.4.2 Raw map



X



Y

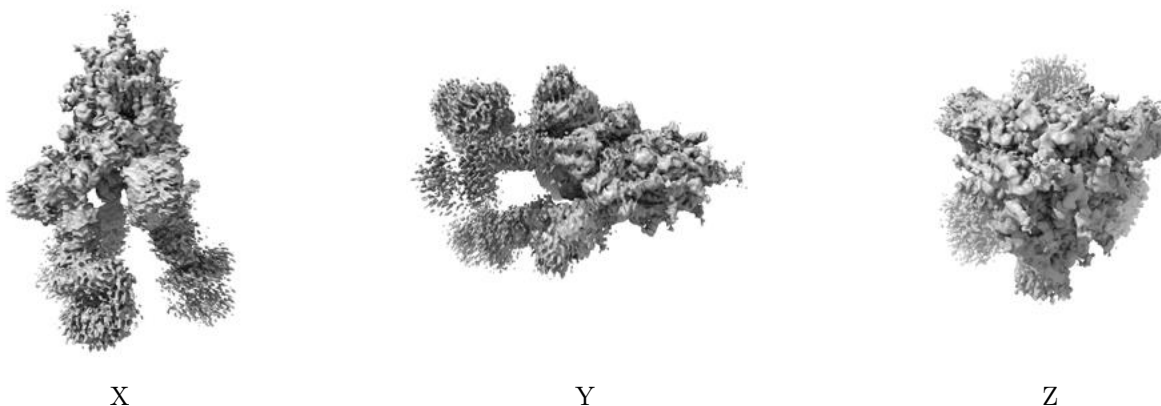


Z

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.

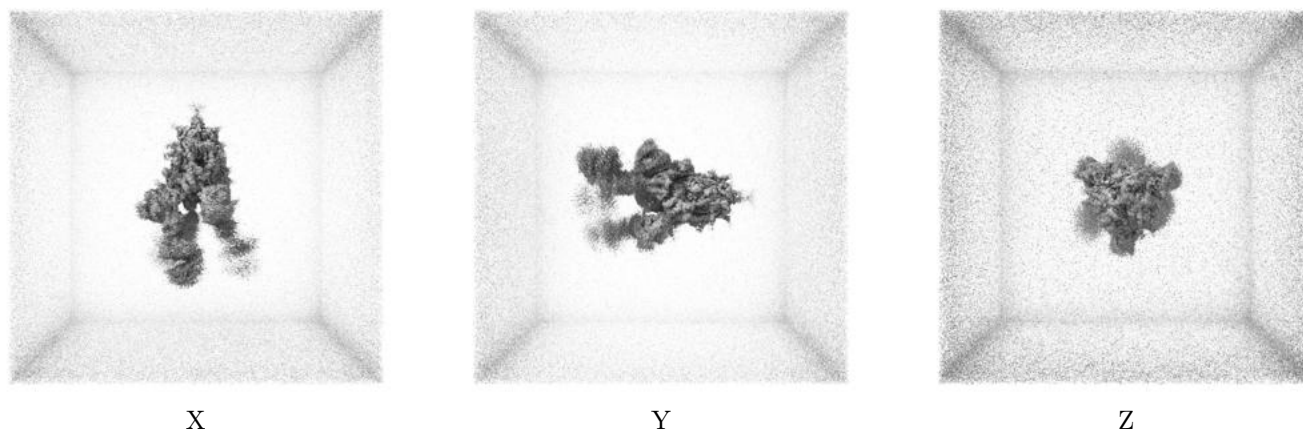
## 6.5 Orthogonal surface views [i](#)

### 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.



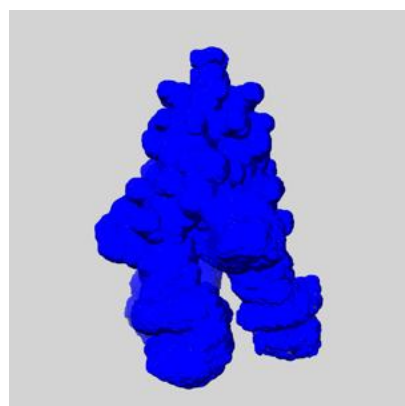
## 6.6 Mask visualisation [i](#)

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

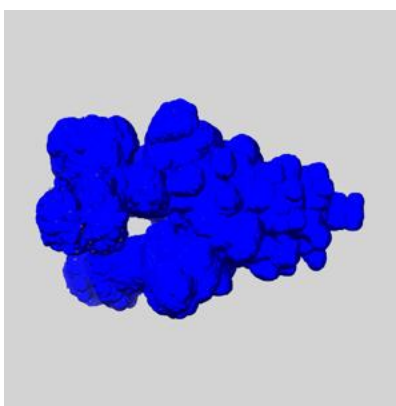
A mask typically either:

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

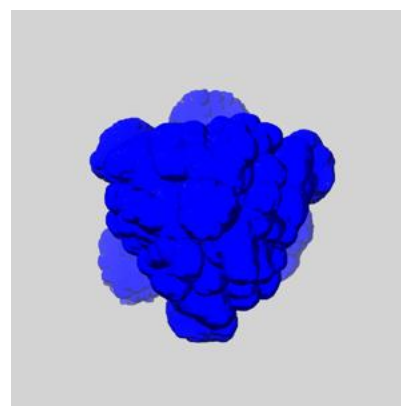
### 6.6.1 emd\_38826\_msk\_1.map [i](#)



X



Y

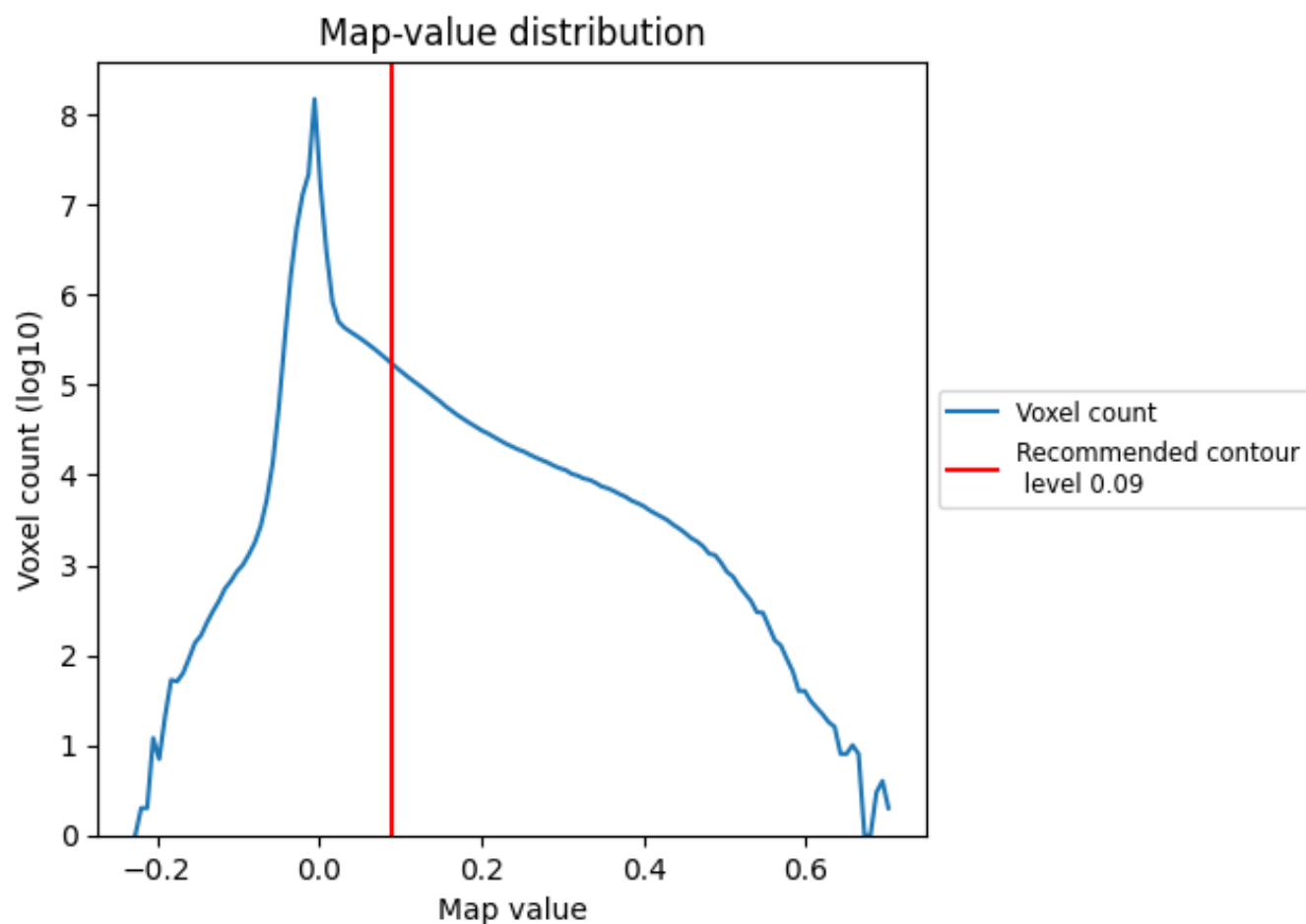


Z

## 7 Map analysis [i](#)

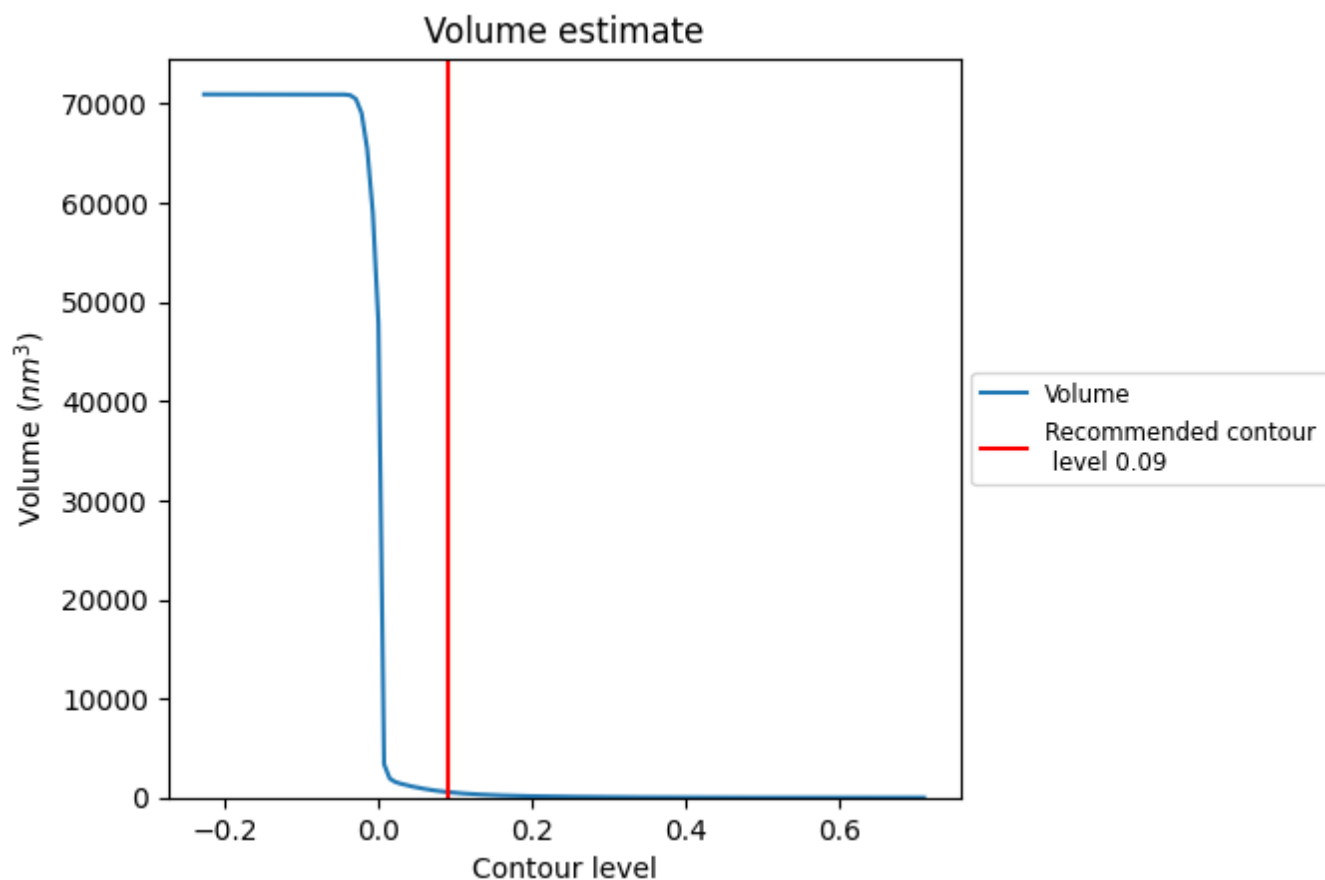
This section contains the results of statistical analysis of the map.

### 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.

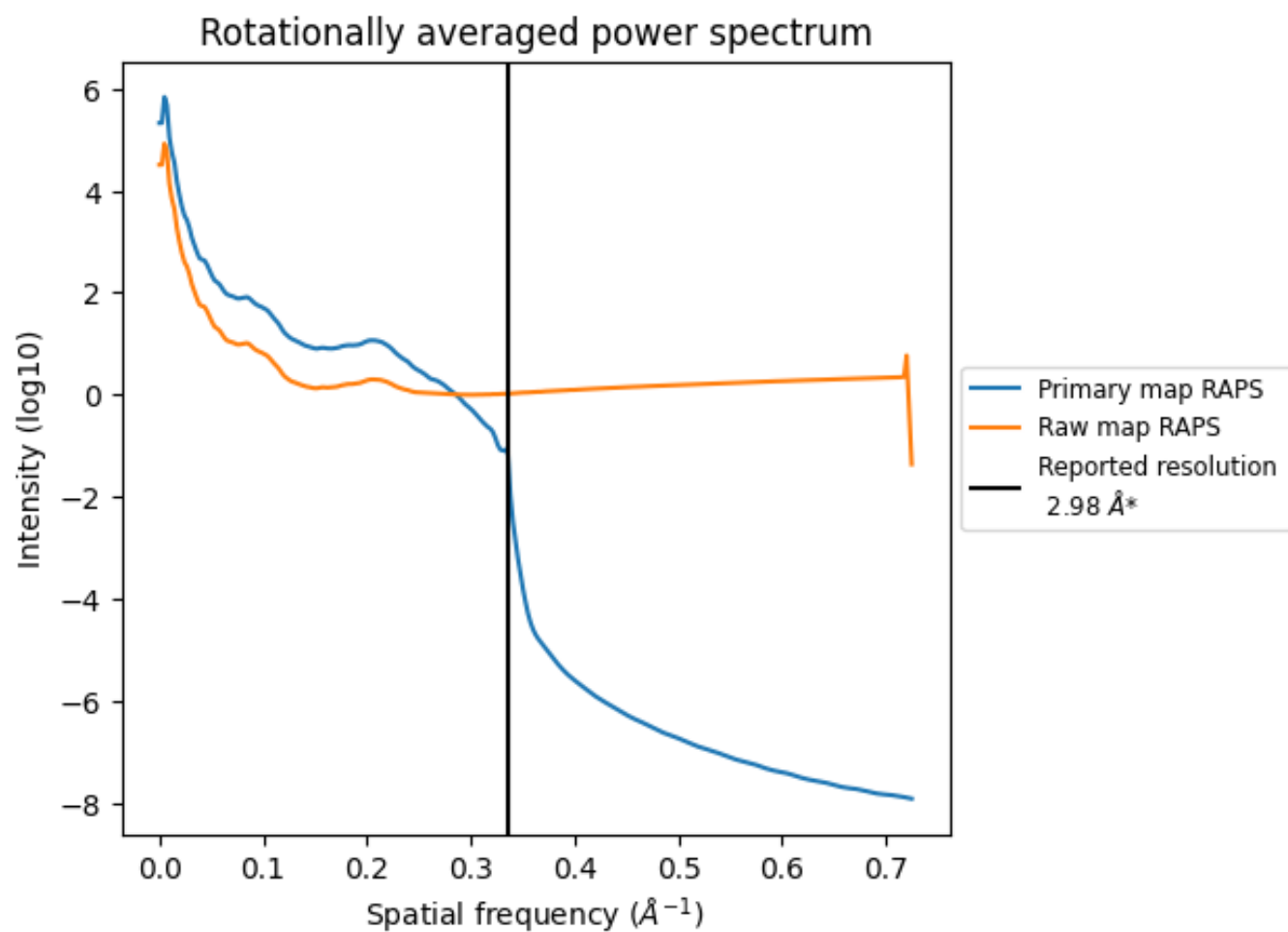
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 551  $\text{nm}^3$ ; 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 [i](#)

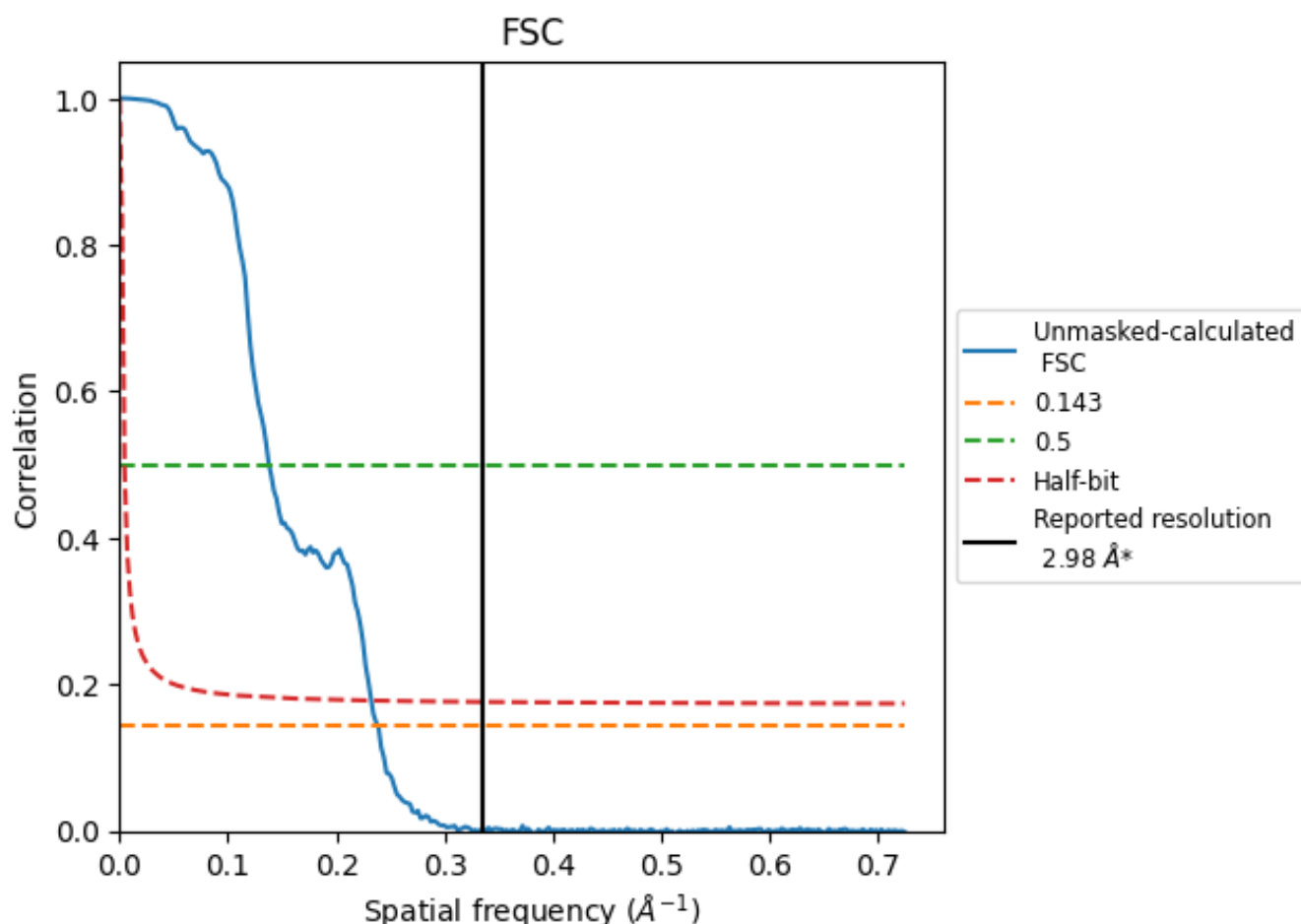


\*Reported resolution corresponds to spatial frequency of 0.336  $\text{\AA}^{-1}$

## 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  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

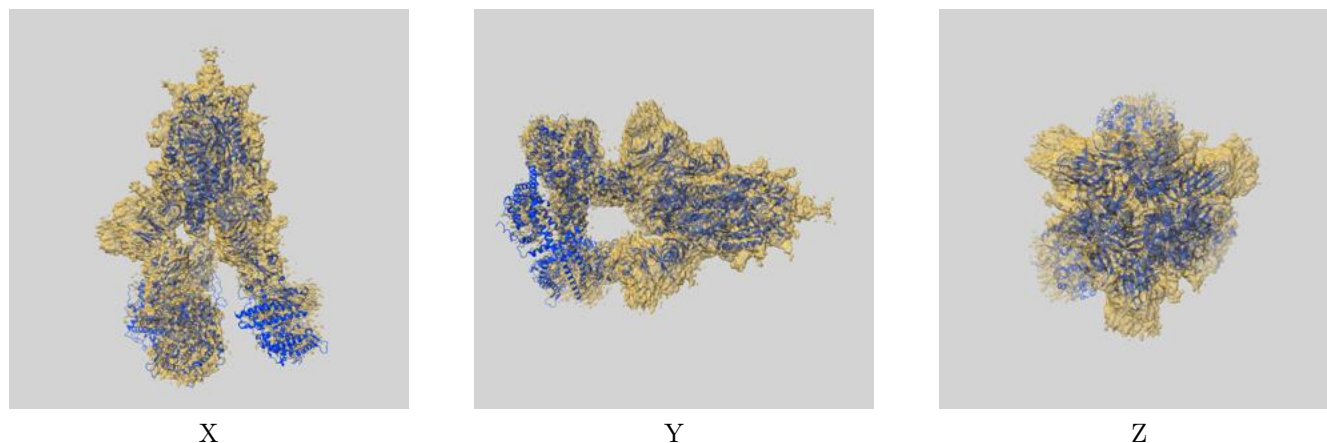
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	7.25	4.30

\*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](#)

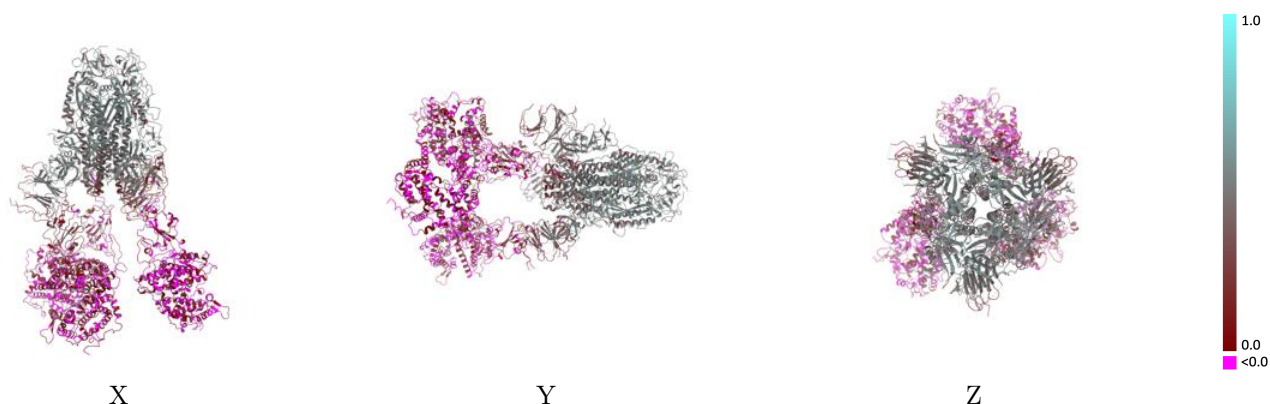
This section contains information regarding the fit between EMDB map EMD-38826 and PDB model 8Y16. Per-residue inclusion information can be found in section 3 on page 18.

### 9.1 Map-model overlay [i](#)



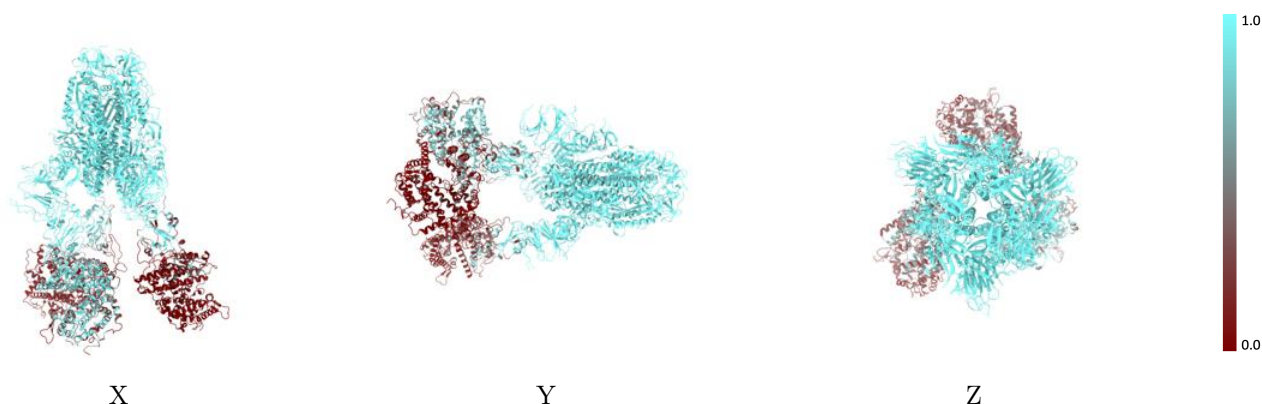
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

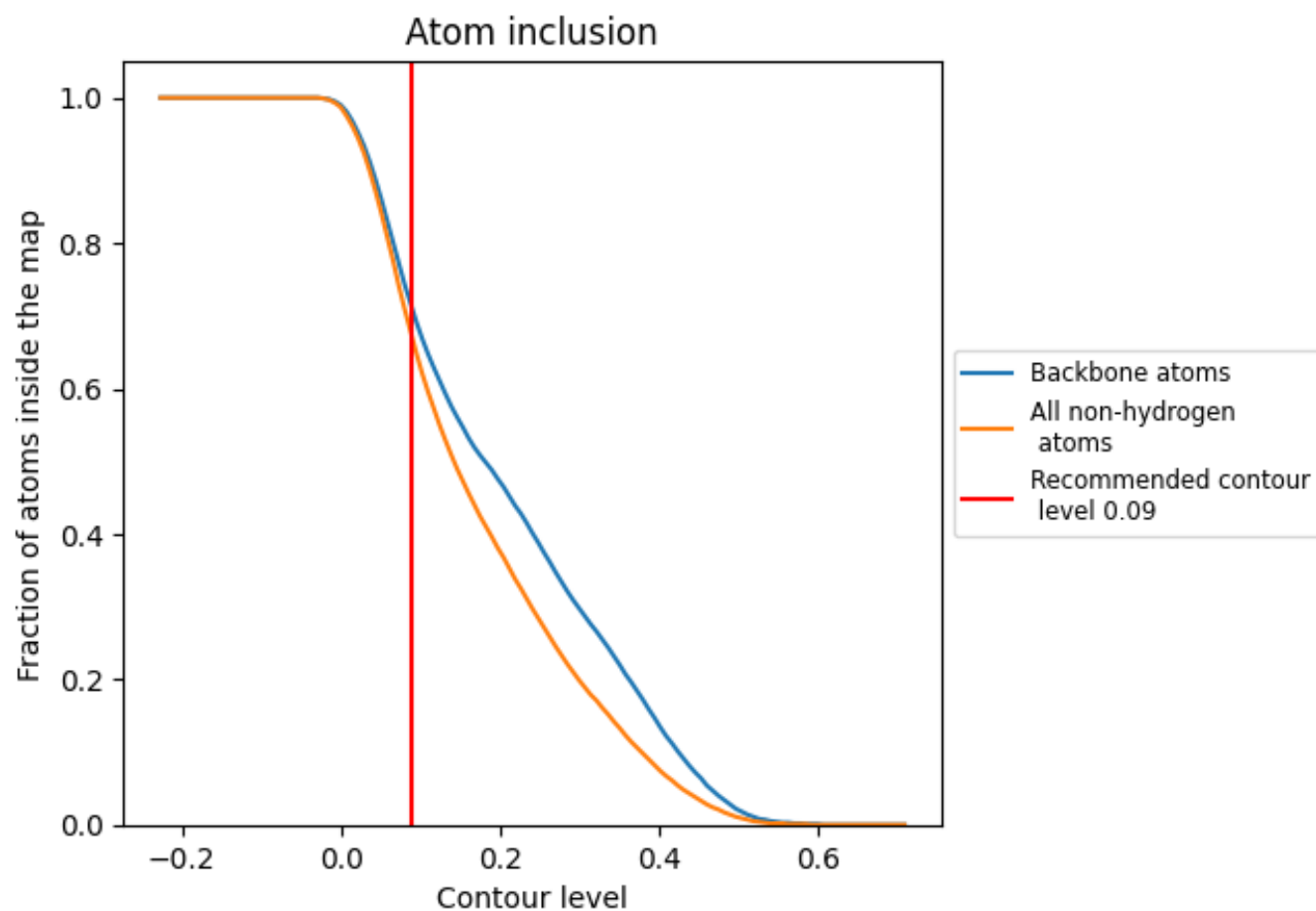
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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

