



Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 08:22 PM JST

PDB ID : 8XUX / pdb_00008xux
EMDB ID : EMD-38459
Title : Structure of the SARS-CoV-2 BA.2.86 spike protein (1-up state)
Authors : Yajima, H.; Anraku, Y.; Kita, S.; Kimura, K.; Maenaka, K.; Hashiguchi, T.
Deposited on : 2024-01-14
Resolution : 3.22 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

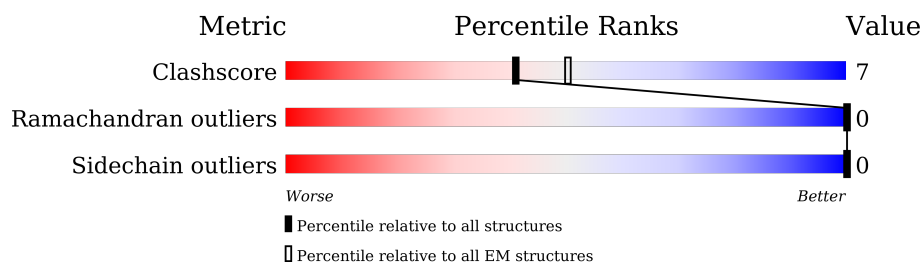
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.22 Å.

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





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

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

Mol	Chain	Length	Quality of chain
1	A	1235	<div> <div>5%</div> <div>70%</div> <div>14%</div> <div>16%</div> </div>
1	B	1235	<div> <div>68%</div> <div>15%</div> <div>18%</div> </div>
1	C	1235	<div> <div>69%</div> <div>13%</div> <div>18%</div> </div>
2	E	2	<div> <div>100%</div> </div>
2	F	2	<div> <div>100%</div> </div>
2	G	2	<div> <div>100%</div> </div>
2	H	2	<div> <div>100%</div> </div>
2	I	2	<div> <div>50%</div> <div>100%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	2	 100%
2	K	2	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24730 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1034	Total	C	N	O	S	0	0
			8104	5193	1344	1530	37		
1	B	1018	Total	C	N	O	S	0	0
			7988	5122	1322	1508	36		
1	C	1014	Total	C	N	O	S	0	0
			7952	5099	1317	1502	34		

There are 357 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	SER	-	expression tag	UNP P0DTC2
A	12	SER	-	expression tag	UNP P0DTC2
A	13	GLN	-	expression tag	UNP P0DTC2
A	14	CYS	-	expression tag	UNP P0DTC2
A	15	VAL	-	expression tag	UNP P0DTC2
A	16	MET	-	expression tag	UNP P0DTC2
A	17	PRO	-	expression tag	UNP P0DTC2
A	18	LEU	-	expression tag	UNP P0DTC2
A	19	PHE	-	expression tag	UNP P0DTC2
A	20	ASN	-	expression tag	UNP P0DTC2
A	21	LEU	-	expression tag	UNP P0DTC2
A	22	ILE	-	expression tag	UNP P0DTC2
A	23	THR	-	expression tag	UNP P0DTC2
A	24	THR	-	expression tag	UNP P0DTC2
A	25	THR	-	expression tag	UNP P0DTC2
A	26	GLN	-	expression tag	UNP P0DTC2
A	27	SER	-	expression tag	UNP P0DTC2
A	50	LEU	SER	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	GLY	ARG	variant	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	211	ILE	LEU	variant	UNP P0DTC2
A	212	GLY	VAL	variant	UNP P0DTC2
A	215	PHE	LEU	variant	UNP P0DTC2
A	244	ASN	HIS	variant	UNP P0DTC2
A	263	ASP	ALA	variant	UNP P0DTC2
A	331	VAL	ILE	variant	UNP P0DTC2
A	338	HIS	GLY	variant	UNP P0DTC2
A	355	THR	LYS	variant	UNP P0DTC2
A	370	PHE	SER	variant	UNP P0DTC2
A	372	PRO	SER	variant	UNP P0DTC2
A	374	PHE	SER	variant	UNP P0DTC2
A	375	ALA	THR	variant	UNP P0DTC2
A	402	LYS	ARG	variant	UNP P0DTC2
A	404	ASN	ASP	variant	UNP P0DTC2
A	407	SER	ARG	variant	UNP P0DTC2
A	416	ASN	LYS	variant	UNP P0DTC2
A	439	LYS	ASN	variant	UNP P0DTC2
A	444	HIS	VAL	variant	UNP P0DTC2
A	445	SER	GLY	variant	UNP P0DTC2
A	449	ASP	ASN	variant	UNP P0DTC2
A	451	TRP	LEU	variant	UNP P0DTC2
A	459	LYS	ASN	variant	UNP P0DTC2
A	476	ASN	SER	variant	UNP P0DTC2
A	477	LYS	THR	variant	UNP P0DTC2
A	480	LYS	ASN	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	482	LYS	GLU	variant	UNP P0DTC2
A	484	PRO	PHE	variant	UNP P0DTC2
A	496	ARG	GLN	variant	UNP P0DTC2
A	499	TYR	ASN	variant	UNP P0DTC2
A	503	HIS	TYR	variant	UNP P0DTC2
A	552	LYS	GLU	variant	UNP P0DTC2
A	568	VAL	ALA	variant	UNP P0DTC2
A	612	GLY	ASP	variant	UNP P0DTC2
A	619	SER	PRO	variant	UNP P0DTC2
A	653	TYR	HIS	variant	UNP P0DTC2
A	677	LYS	ASN	variant	UNP P0DTC2
A	679	ARG	PRO	variant	UNP P0DTC2
A	680	GLY	ARG	engineered mutation	UNP P0DTC2
A	681	SER	ARG	engineered mutation	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	683	GLY	ARG	engineered mutation	UNP P0DTC2
A	762	LYS	ASN	variant	UNP P0DTC2
A	794	TYR	ASP	variant	UNP P0DTC2
A	815	PRO	PHE	engineered mutation	UNP P0DTC2
A	890	PRO	ALA	engineered mutation	UNP P0DTC2
A	897	PRO	ALA	engineered mutation	UNP P0DTC2
A	937	PHE	SER	variant	UNP P0DTC2
A	940	PRO	ALA	engineered mutation	UNP P0DTC2
A	952	HIS	GLN	variant	UNP P0DTC2
A	967	LYS	ASN	variant	UNP P0DTC2
A	984	PRO	LYS	engineered mutation	UNP P0DTC2
A	985	PRO	VAL	engineered mutation	UNP P0DTC2
A	1141	LEU	PRO	variant	UNP P0DTC2
A	1209	ALA	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	SER	-	expression tag	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	TYR	-	expression tag	UNP P0DTC2
A	1214	ILE	-	expression tag	UNP P0DTC2
A	1215	PRO	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ALA	-	expression tag	UNP P0DTC2
A	1218	PRO	-	expression tag	UNP P0DTC2
A	1219	ARG	-	expression tag	UNP P0DTC2
A	1220	ASP	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	GLN	-	expression tag	UNP P0DTC2
A	1223	ALA	-	expression tag	UNP P0DTC2
A	1224	TYR	-	expression tag	UNP P0DTC2
A	1225	VAL	-	expression tag	UNP P0DTC2
A	1226	ARG	-	expression tag	UNP P0DTC2
A	1227	LYS	-	expression tag	UNP P0DTC2
A	1228	ASP	-	expression tag	UNP P0DTC2
A	1229	GLY	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	TRP	-	expression tag	UNP P0DTC2
A	1232	VAL	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	LEU	-	expression tag	UNP P0DTC2
A	1235	SER	-	expression tag	UNP P0DTC2
A	1236	THR	-	expression tag	UNP P0DTC2
A	1237	PHE	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	GLU	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	THR	-	expression tag	UNP P0DTC2
A	1242	LYS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
A	1248	HIS	-	expression tag	UNP P0DTC2
B	11	SER	-	expression tag	UNP P0DTC2
B	12	SER	-	expression tag	UNP P0DTC2
B	13	GLN	-	expression tag	UNP P0DTC2
B	14	CYS	-	expression tag	UNP P0DTC2
B	15	VAL	-	expression tag	UNP P0DTC2
B	16	MET	-	expression tag	UNP P0DTC2
B	17	PRO	-	expression tag	UNP P0DTC2
B	18	LEU	-	expression tag	UNP P0DTC2
B	19	PHE	-	expression tag	UNP P0DTC2
B	20	ASN	-	expression tag	UNP P0DTC2
B	21	LEU	-	expression tag	UNP P0DTC2
B	22	ILE	-	expression tag	UNP P0DTC2
B	23	THR	-	expression tag	UNP P0DTC2
B	24	THR	-	expression tag	UNP P0DTC2
B	25	THR	-	expression tag	UNP P0DTC2
B	26	GLN	-	expression tag	UNP P0DTC2
B	27	SER	-	expression tag	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	142	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	211	ILE	LEU	variant	UNP P0DTC2
B	212	GLY	VAL	variant	UNP P0DTC2
B	215	PHE	LEU	variant	UNP P0DTC2
B	244	ASN	HIS	variant	UNP P0DTC2
B	263	ASP	ALA	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	331	VAL	ILE	variant	UNP P0DTC2
B	338	HIS	GLY	variant	UNP P0DTC2
B	355	THR	LYS	variant	UNP P0DTC2
B	370	PHE	SER	variant	UNP P0DTC2
B	372	PRO	SER	variant	UNP P0DTC2
B	374	PHE	SER	variant	UNP P0DTC2
B	375	ALA	THR	variant	UNP P0DTC2
B	402	LYS	ARG	variant	UNP P0DTC2
B	404	ASN	ASP	variant	UNP P0DTC2
B	407	SER	ARG	variant	UNP P0DTC2
B	416	ASN	LYS	variant	UNP P0DTC2
B	439	LYS	ASN	variant	UNP P0DTC2
B	444	HIS	VAL	variant	UNP P0DTC2
B	445	SER	GLY	variant	UNP P0DTC2
B	449	ASP	ASN	variant	UNP P0DTC2
B	451	TRP	LEU	variant	UNP P0DTC2
B	459	LYS	ASN	variant	UNP P0DTC2
B	476	ASN	SER	variant	UNP P0DTC2
B	477	LYS	THR	variant	UNP P0DTC2
B	480	LYS	ASN	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	482	LYS	GLU	variant	UNP P0DTC2
B	484	PRO	PHE	variant	UNP P0DTC2
B	496	ARG	GLN	variant	UNP P0DTC2
B	499	TYR	ASN	variant	UNP P0DTC2
B	503	HIS	TYR	variant	UNP P0DTC2
B	552	LYS	GLU	variant	UNP P0DTC2
B	568	VAL	ALA	variant	UNP P0DTC2
B	612	GLY	ASP	variant	UNP P0DTC2
B	619	SER	PRO	variant	UNP P0DTC2
B	653	TYR	HIS	variant	UNP P0DTC2
B	677	LYS	ASN	variant	UNP P0DTC2
B	679	ARG	PRO	variant	UNP P0DTC2
B	680	GLY	ARG	engineered mutation	UNP P0DTC2
B	681	SER	ARG	engineered mutation	UNP P0DTC2
B	683	GLY	ARG	engineered mutation	UNP P0DTC2
B	762	LYS	ASN	variant	UNP P0DTC2
B	794	TYR	ASP	variant	UNP P0DTC2
B	815	PRO	PHE	engineered mutation	UNP P0DTC2
B	890	PRO	ALA	engineered mutation	UNP P0DTC2
B	897	PRO	ALA	engineered mutation	UNP P0DTC2
B	937	PHE	SER	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	940	PRO	ALA	engineered mutation	UNP P0DTC2
B	952	HIS	GLN	variant	UNP P0DTC2
B	967	LYS	ASN	variant	UNP P0DTC2
B	984	PRO	LYS	engineered mutation	UNP P0DTC2
B	985	PRO	VAL	engineered mutation	UNP P0DTC2
B	1141	LEU	PRO	variant	UNP P0DTC2
B	1209	ALA	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	SER	-	expression tag	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	TYR	-	expression tag	UNP P0DTC2
B	1214	ILE	-	expression tag	UNP P0DTC2
B	1215	PRO	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ALA	-	expression tag	UNP P0DTC2
B	1218	PRO	-	expression tag	UNP P0DTC2
B	1219	ARG	-	expression tag	UNP P0DTC2
B	1220	ASP	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	GLN	-	expression tag	UNP P0DTC2
B	1223	ALA	-	expression tag	UNP P0DTC2
B	1224	TYR	-	expression tag	UNP P0DTC2
B	1225	VAL	-	expression tag	UNP P0DTC2
B	1226	ARG	-	expression tag	UNP P0DTC2
B	1227	LYS	-	expression tag	UNP P0DTC2
B	1228	ASP	-	expression tag	UNP P0DTC2
B	1229	GLY	-	expression tag	UNP P0DTC2
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	TRP	-	expression tag	UNP P0DTC2
B	1232	VAL	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	SER	-	expression tag	UNP P0DTC2
B	1236	THR	-	expression tag	UNP P0DTC2
B	1237	PHE	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	GLU	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	THR	-	expression tag	UNP P0DTC2
B	1242	LYS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
C	11	SER	-	expression tag	UNP P0DTC2
C	12	SER	-	expression tag	UNP P0DTC2
C	13	GLN	-	expression tag	UNP P0DTC2
C	14	CYS	-	expression tag	UNP P0DTC2
C	15	VAL	-	expression tag	UNP P0DTC2
C	16	MET	-	expression tag	UNP P0DTC2
C	17	PRO	-	expression tag	UNP P0DTC2
C	18	LEU	-	expression tag	UNP P0DTC2
C	19	PHE	-	expression tag	UNP P0DTC2
C	20	ASN	-	expression tag	UNP P0DTC2
C	21	LEU	-	expression tag	UNP P0DTC2
C	22	ILE	-	expression tag	UNP P0DTC2
C	23	THR	-	expression tag	UNP P0DTC2
C	24	THR	-	expression tag	UNP P0DTC2
C	25	THR	-	expression tag	UNP P0DTC2
C	26	GLN	-	expression tag	UNP P0DTC2
C	27	SER	-	expression tag	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	211	ILE	LEU	variant	UNP P0DTC2
C	212	GLY	VAL	variant	UNP P0DTC2
C	215	PHE	LEU	variant	UNP P0DTC2
C	244	ASN	HIS	variant	UNP P0DTC2
C	263	ASP	ALA	variant	UNP P0DTC2
C	331	VAL	ILE	variant	UNP P0DTC2
C	338	HIS	GLY	variant	UNP P0DTC2
C	355	THR	LYS	variant	UNP P0DTC2
C	370	PHE	SER	variant	UNP P0DTC2
C	372	PRO	SER	variant	UNP P0DTC2
C	374	PHE	SER	variant	UNP P0DTC2
C	375	ALA	THR	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

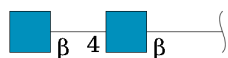
Chain	Residue	Modelled	Actual	Comment	Reference
C	402	LYS	ARG	variant	UNP P0DTC2
C	404	ASN	ASP	variant	UNP P0DTC2
C	407	SER	ARG	variant	UNP P0DTC2
C	416	ASN	LYS	variant	UNP P0DTC2
C	439	LYS	ASN	variant	UNP P0DTC2
C	444	HIS	VAL	variant	UNP P0DTC2
C	445	SER	GLY	variant	UNP P0DTC2
C	449	ASP	ASN	variant	UNP P0DTC2
C	451	TRP	LEU	variant	UNP P0DTC2
C	459	LYS	ASN	variant	UNP P0DTC2
C	476	ASN	SER	variant	UNP P0DTC2
C	477	LYS	THR	variant	UNP P0DTC2
C	480	LYS	ASN	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	482	LYS	GLU	variant	UNP P0DTC2
C	484	PRO	PHE	variant	UNP P0DTC2
C	496	ARG	GLN	variant	UNP P0DTC2
C	499	TYR	ASN	variant	UNP P0DTC2
C	503	HIS	TYR	variant	UNP P0DTC2
C	552	LYS	GLU	variant	UNP P0DTC2
C	568	VAL	ALA	variant	UNP P0DTC2
C	612	GLY	ASP	variant	UNP P0DTC2
C	619	SER	PRO	variant	UNP P0DTC2
C	653	TYR	HIS	variant	UNP P0DTC2
C	677	LYS	ASN	variant	UNP P0DTC2
C	679	ARG	PRO	variant	UNP P0DTC2
C	680	GLY	ARG	engineered mutation	UNP P0DTC2
C	681	SER	ARG	engineered mutation	UNP P0DTC2
C	683	GLY	ARG	engineered mutation	UNP P0DTC2
C	762	LYS	ASN	variant	UNP P0DTC2
C	794	TYR	ASP	variant	UNP P0DTC2
C	815	PRO	PHE	engineered mutation	UNP P0DTC2
C	890	PRO	ALA	engineered mutation	UNP P0DTC2
C	897	PRO	ALA	engineered mutation	UNP P0DTC2
C	937	PHE	SER	variant	UNP P0DTC2
C	940	PRO	ALA	engineered mutation	UNP P0DTC2
C	952	HIS	GLN	variant	UNP P0DTC2
C	967	LYS	ASN	variant	UNP P0DTC2
C	984	PRO	LYS	engineered mutation	UNP P0DTC2
C	985	PRO	VAL	engineered mutation	UNP P0DTC2
C	1141	LEU	PRO	variant	UNP P0DTC2
C	1209	ALA	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

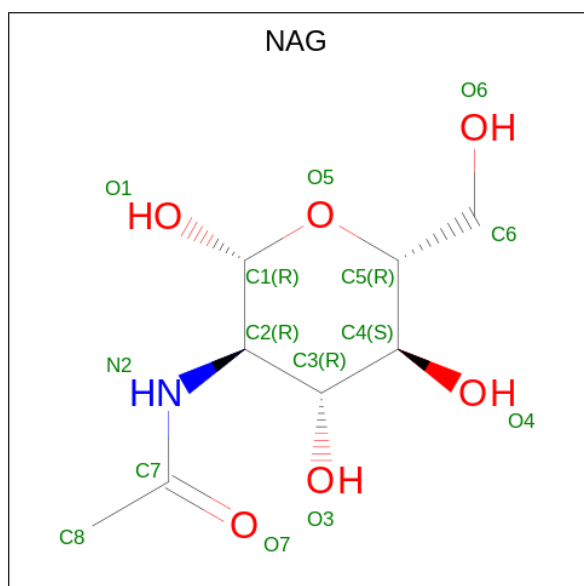
Chain	Residue	Modelled	Actual	Comment	Reference
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	SER	-	expression tag	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	TYR	-	expression tag	UNP P0DTC2
C	1214	ILE	-	expression tag	UNP P0DTC2
C	1215	PRO	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ALA	-	expression tag	UNP P0DTC2
C	1218	PRO	-	expression tag	UNP P0DTC2
C	1219	ARG	-	expression tag	UNP P0DTC2
C	1220	ASP	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	GLN	-	expression tag	UNP P0DTC2
C	1223	ALA	-	expression tag	UNP P0DTC2
C	1224	TYR	-	expression tag	UNP P0DTC2
C	1225	VAL	-	expression tag	UNP P0DTC2
C	1226	ARG	-	expression tag	UNP P0DTC2
C	1227	LYS	-	expression tag	UNP P0DTC2
C	1228	ASP	-	expression tag	UNP P0DTC2
C	1229	GLY	-	expression tag	UNP P0DTC2
C	1230	GLU	-	expression tag	UNP P0DTC2
C	1231	TRP	-	expression tag	UNP P0DTC2
C	1232	VAL	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	SER	-	expression tag	UNP P0DTC2
C	1236	THR	-	expression tag	UNP P0DTC2
C	1237	PHE	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	GLU	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	THR	-	expression tag	UNP P0DTC2
C	1242	LYS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2
C	1245	HIS	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

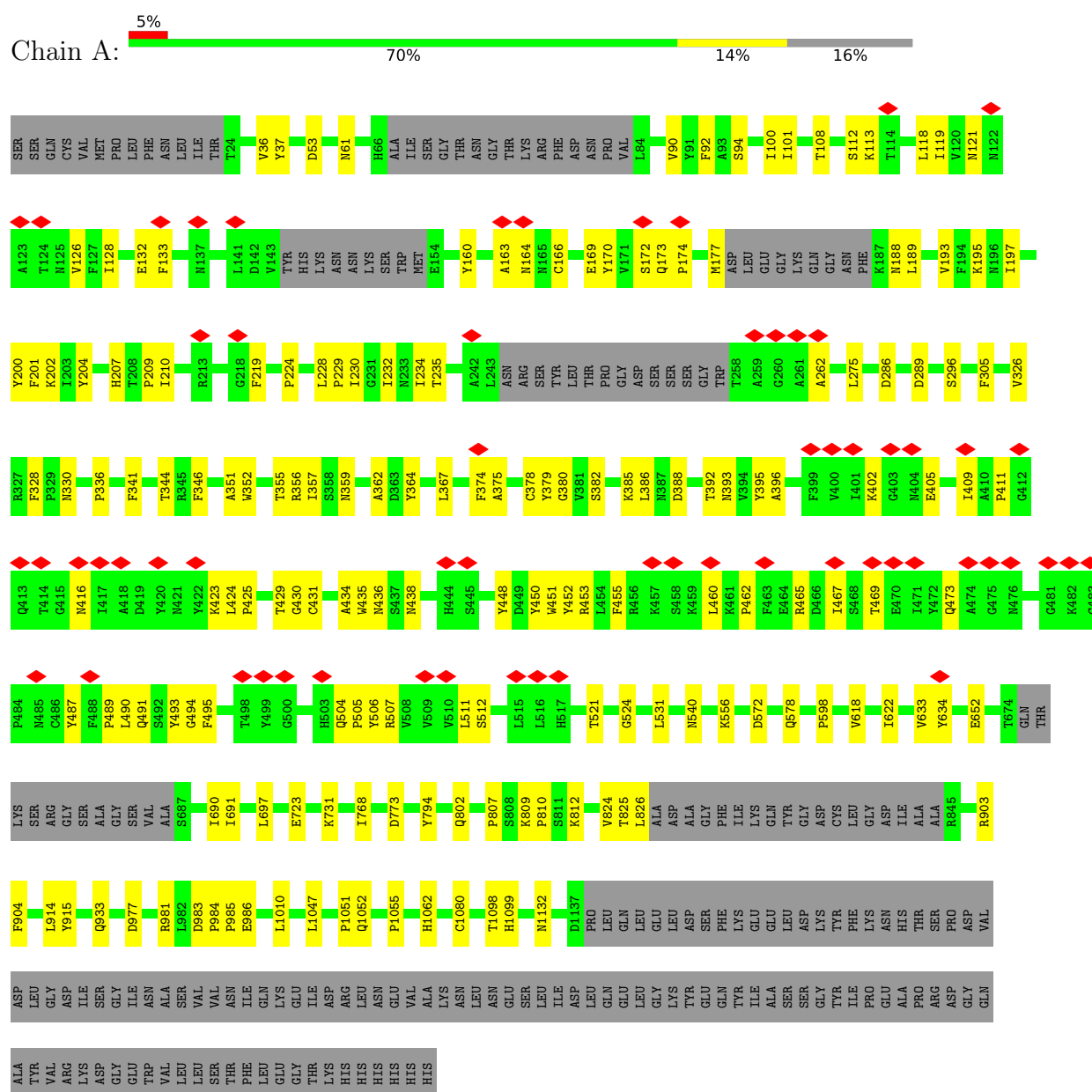
Continued from previous page...

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

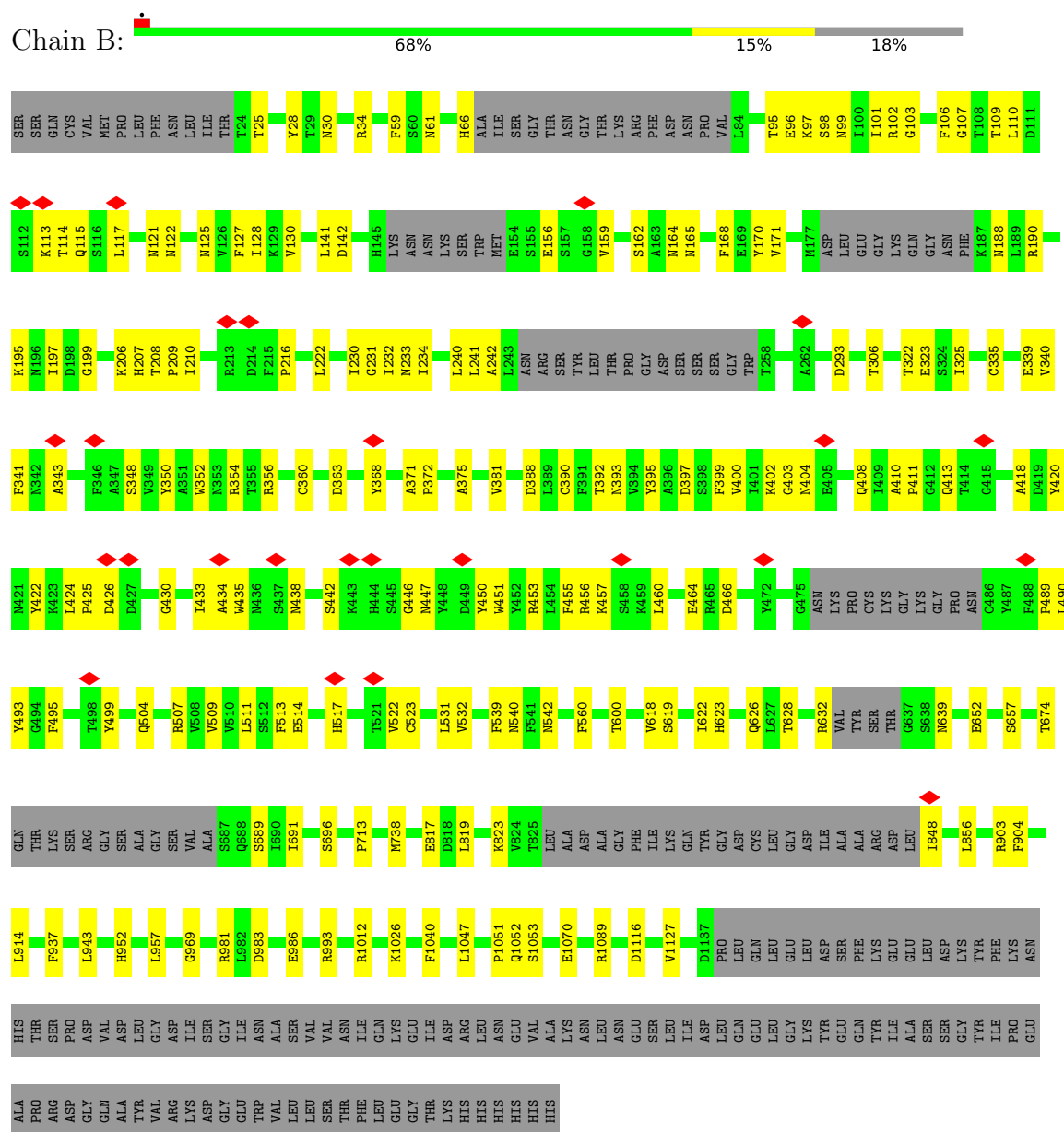
3 Residue-property plots

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.

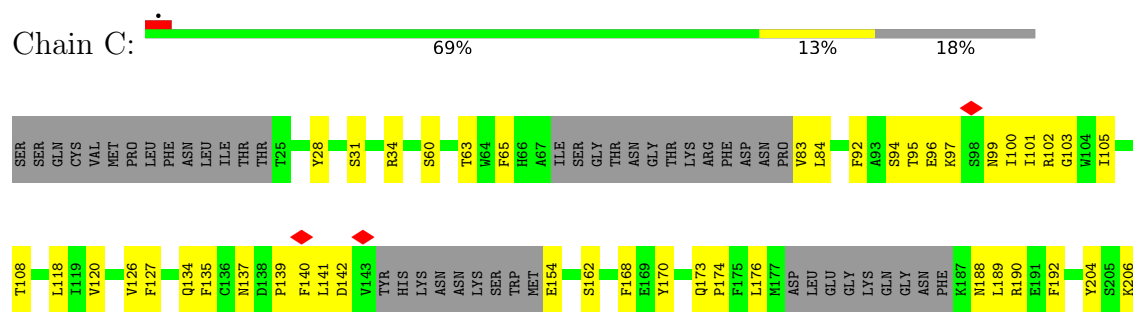
• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein



WORLDWIDE
PDB
PROTEIN DATA BANK



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



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



- Molecule 2: 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, C1	Depositor
Number of particles used	32669	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.725	Depositor
Minimum map value	-0.310	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0802	Depositor
Map size (Å)	385.91998, 385.91998, 385.91998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.005, 1.005, 1.005	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.10	0/8299	0.25	0/11293
1	B	0.12	0/8180	0.29	0/11130
1	C	0.11	0/8142	0.27	0/11080
All	All	0.11	0/24621	0.27	0/33503

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	8104	0	7914	114	0
1	B	7988	0	7788	118	0
1	C	7952	0	7772	105	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	196	0	182	3	0
3	B	154	0	143	1	0
3	C	140	0	130	1	0
All	All	24730	0	24104	328	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 (328) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ARG:HD3	1:C:398:SER:HA	1.55	0.88
1:C:344:THR:HG22	1:C:345:ARG:H	1.38	0.85
1:B:460:LEU:HD13	1:B:464:GLU:HB3	1.65	0.78
1:B:348:SER:HB3	1:B:450:TYR:HB2	1.64	0.77
1:A:132:GLU:HB2	1:A:164:ASN:HD21	1.51	0.76
1:B:442:SER:HA	1:B:447:ASN:HD21	1.52	0.74
1:B:626:GLN:NE2	1:B:628:THR:OG1	2.20	0.74
1:B:102:ARG:NH2	1:B:121:ASN:O	2.22	0.72
1:A:229:PRO:HB2	1:B:356:ARG:HH12	1.55	0.72
1:B:96:GLU:CD	1:B:97:LYS:H	1.99	0.71
1:A:188:ASN:HA	1:A:209:PRO:HA	1.73	0.70
1:B:411:PRO:HB3	1:B:426:ASP:HA	1.74	0.69
1:A:425:PRO:HA	1:A:462:PRO:HB3	1.75	0.69
1:C:99:ASN:HB2	1:C:243:LEU:HA	1.73	0.69
1:C:328:PHE:O	1:C:578:GLN:NE2	2.27	0.68
1:B:1089:ARG:NH1	1:B:1116:ASP:O	2.26	0.67
1:C:96:GLU:HG3	1:C:100:ILE:HD13	1.76	0.67
1:A:382:SER:HB3	1:A:385:LYS:HE2	1.75	0.67
1:C:344:THR:HB	1:C:507:ARG:HH11	1.60	0.67
1:B:325:ILE:HD11	1:B:531:LEU:HA	1.77	0.67
1:C:341:PHE:O	1:C:344:THR:OG1	2.14	0.65
1:A:1080:CYS:HB3	1:A:1132:ASN:HB3	1.77	0.65
1:B:113:LYS:HG2	1:B:114:THR:HG22	1.78	0.65
1:C:100:ILE:HG13	1:C:101:ILE:HG12	1.78	0.65
1:C:433:ILE:HG13	1:C:509:VAL:HB	1.79	0.64
1:B:455:PHE:H	1:B:489:PRO:HB2	1.61	0.64
1:C:415:GLY:H	1:C:418:ALA:HB3	1.63	0.64
1:C:392:THR:HG22	1:C:393:ASN:H	1.62	0.64
1:C:1120:VAL:HG13	1:C:1121:SER:H	1.63	0.64
1:C:453:ARG:NH1	1:C:466:ASP:O	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ALA:HB3	1:B:413:GLN:HE21	1.63	0.63
1:B:95:THR:OG1	1:B:188:ASN:O	2.11	0.62
1:B:142:ASP:HB2	1:B:156:GLU:HA	1.81	0.62
1:C:102:ARG:NH2	1:C:140:PHE:O	2.32	0.62
1:B:325:ILE:HD12	1:B:532:VAL:HG22	1.81	0.62
1:C:392:THR:HB	1:C:514:GLU:HG3	1.82	0.62
1:B:103:GLY:HA3	1:B:240:LEU:HB2	1.82	0.62
1:C:340:VAL:HB	1:C:345:ARG:HH22	1.64	0.62
1:B:34:ARG:NH1	1:B:216:PRO:O	2.32	0.61
1:B:354:ARG:HE	1:B:395:TYR:HE2	1.48	0.61
1:A:451:TRP:HB3	1:A:490:LEU:HB3	1.83	0.61
1:A:330:ASN:OD1	3:A:1312:NAG:N2	2.34	0.60
1:B:632:ARG:HG2	1:B:639:ASN:HB2	1.83	0.60
1:C:134:GLN:HG2	1:C:162:SER:HB3	1.82	0.60
1:C:349:VAL:HA	1:C:399:PHE:HB2	1.82	0.60
1:C:34:ARG:NH2	1:C:216:PRO:O	2.35	0.60
1:C:632:ARG:NH2	1:C:635:SER:OG	2.35	0.59
1:C:1051:PRO:O	1:C:1052:GLN:NE2	2.35	0.59
1:B:451:TRP:HB3	1:B:490:LEU:HB3	1.85	0.59
1:C:352:TRP:O	1:C:465:ARG:NH1	2.35	0.59
1:A:378:CYS:HA	1:A:431:CYS:HA	1.84	0.59
1:B:1051:PRO:O	1:B:1052:GLN:NE2	2.33	0.59
1:A:1051:PRO:O	1:A:1052:GLN:NE2	2.34	0.59
1:B:674:THR:OG1	1:B:689:SER:N	2.36	0.59
1:A:100:ILE:HG13	1:A:101:ILE:HD12	1.84	0.59
1:C:126:VAL:HG13	1:C:174:PRO:HA	1.84	0.59
1:C:120:VAL:HG22	1:C:127:PHE:HB2	1.85	0.58
1:B:322:THR:HG23	1:B:323:GLU:HG2	1.85	0.58
1:A:193:VAL:HB	1:A:204:TYR:HD2	1.67	0.58
1:B:400:VAL:HG22	1:B:507:ARG:HG3	1.85	0.57
1:A:177:MET:SD	1:A:207:HIS:ND1	2.72	0.57
1:B:1026:LYS:NZ	1:B:1040:PHE:O	2.37	0.57
1:B:393:ASN:ND2	1:B:514:GLU:OE2	2.37	0.57
1:C:92:PHE:HB2	1:C:192:PHE:HB2	1.86	0.57
1:C:1080:CYS:HB3	1:C:1132:ASN:HB3	1.86	0.57
1:A:379:TYR:CZ	1:A:411:PRO:HG2	2.39	0.57
1:C:173:GLN:HG2	1:C:174:PRO:HD2	1.87	0.57
1:C:903:ARG:NH1	1:C:1047:LEU:O	2.37	0.57
1:A:362:ALA:HB3	1:A:524:GLY:HA2	1.84	0.57
1:A:344:THR:O	1:A:507:ARG:NH2	2.38	0.56
1:A:802:GLN:OE1	1:A:933:GLN:NE2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:THR:OG1	1:A:1099:HIS:ND1	2.38	0.56
1:A:118:LEU:HD22	1:A:133:PHE:HD2	1.69	0.56
1:B:408:GLN:HE21	1:B:418:ALA:HB2	1.71	0.56
1:A:423:LYS:NZ	1:A:424:LEU:O	2.31	0.56
1:C:344:THR:HB	1:C:507:ARG:NH1	2.20	0.56
1:B:453:ARG:HD2	1:B:456:ARG:HE	1.70	0.56
1:A:473:GLN:HG3	1:A:487:TYR:CZ	2.42	0.55
1:A:915:TYR:HB3	1:B:1127:VAL:HG12	1.88	0.55
1:C:441:ASP:CG	1:C:507:ARG:HH21	2.13	0.55
1:B:446:GLY:HA2	1:B:495:PHE:H	1.72	0.55
1:A:794:TYR:HB3	3:B:1307:NAG:H83	1.89	0.55
1:B:453:ARG:NH1	1:B:466:ASP:OD2	2.30	0.55
1:B:618:VAL:HG23	1:B:619:SER:H	1.72	0.55
1:A:37:TYR:OH	1:A:195:LYS:NZ	2.40	0.55
1:A:396:ALA:HA	1:A:511:LEU:HA	1.88	0.54
1:C:102:ARG:HH22	1:C:141:LEU:HA	1.72	0.54
1:C:354:ARG:HA	1:C:397:ASP:HA	1.89	0.54
1:C:453:ARG:HA	1:C:490:LEU:HA	1.89	0.54
1:A:723:GLU:OE1	1:A:1062:HIS:NE2	2.28	0.54
1:C:94:SER:HB2	1:C:100:ILE:HG12	1.90	0.54
1:C:142:ASP:OD2	1:C:154:GLU:N	2.41	0.54
1:B:402:LYS:HA	1:B:495:PHE:HZ	1.73	0.54
1:B:438:ASN:ND2	1:B:499:TYR:O	2.38	0.54
1:C:108:THR:OG1	1:C:233:ASN:O	2.26	0.53
1:C:566:ASP:OD1	1:C:570:THR:N	2.38	0.53
1:C:118:LEU:HD21	1:C:135:PHE:HZ	1.73	0.53
1:C:523:CYS:SG	1:C:524:GLY:N	2.82	0.53
1:C:135:PHE:O	1:C:137:ASN:ND2	2.42	0.52
1:B:433:ILE:HB	1:B:509:VAL:HG23	1.92	0.52
1:B:856:LEU:HD13	1:B:957:LEU:HD22	1.91	0.52
1:A:37:TYR:OH	1:A:53:ASP:OD2	2.27	0.52
1:A:201:PHE:HZ	1:A:234:ILE:HG13	1.73	0.52
1:B:325:ILE:HG22	1:B:539:PHE:HA	1.90	0.52
1:C:344:THR:HG22	1:C:345:ARG:N	2.18	0.52
1:A:556:LYS:NZ	3:C:1303:NAG:O6	2.39	0.52
1:B:96:GLU:OE1	1:B:98:SER:N	2.42	0.52
1:B:657:SER:HB3	1:B:696:SER:HB2	1.91	0.52
1:B:981:ARG:HH11	1:C:515:LEU:HD22	1.75	0.52
1:C:983:ASP:OD2	1:C:985:PRO:HD2	2.09	0.52
1:B:390:CYS:HA	1:B:523:CYS:HA	1.92	0.52
1:A:374:PHE:H	1:A:435:TRP:HB3	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ASP:OD1	1:A:388:ASP:N	2.39	0.52
1:B:25:THR:OG1	1:B:66:HIS:ND1	2.41	0.52
1:B:622:ILE:HG22	1:B:623:HIS:CD2	2.44	0.52
1:C:352:TRP:N	1:C:465:ARG:HH12	2.08	0.51
1:C:577:PRO:HG2	1:C:578:GLN:HE21	1.75	0.51
1:A:402:LYS:HB2	1:A:405:GLU:HG2	1.92	0.51
1:B:969:GLY:HA3	1:B:993:ARG:HH21	1.75	0.51
1:C:420:TYR:HA	1:C:460:LEU:HD23	1.91	0.51
1:A:731:LYS:NZ	1:A:773:ASP:OD2	2.43	0.51
1:A:326:VAL:HG22	1:A:540:ASN:HB3	1.91	0.51
1:B:368:TYR:H	1:B:372:PRO:HG3	1.76	0.51
1:C:188:ASN:N	1:C:210:ILE:HG22	2.25	0.51
1:C:355:THR:N	1:C:396:ALA:O	2.35	0.51
1:A:977:ASP:OD2	1:A:981:ARG:NH2	2.44	0.51
1:B:738:MET:SD	1:C:318:ARG:NH1	2.72	0.51
1:C:659:GLU:O	1:C:693:TYR:OH	2.28	0.51
1:B:903:ARG:NH1	1:B:1047:LEU:O	2.44	0.51
1:A:166:CYS:HB3	1:A:169:GLU:CD	2.36	0.50
1:A:133:PHE:CG	1:A:160:TYR:HB2	2.46	0.50
1:C:455:PHE:HB2	1:C:489:PRO:HA	1.92	0.50
1:A:286:ASP:HB3	1:A:305:PHE:HE2	1.77	0.50
1:A:328:PHE:O	1:A:578:GLN:NE2	2.45	0.50
1:B:115:GLN:HB3	1:B:130:VAL:HG22	1.94	0.50
1:B:28:TYR:HD1	1:B:61:ASN:HB2	1.77	0.50
1:B:981:ARG:HG3	1:C:381:VAL:HG12	1.94	0.50
1:C:142:ASP:N	1:C:142:ASP:OD1	2.44	0.50
1:C:453:ARG:HH12	1:C:468:SER:N	2.10	0.50
1:A:375:ALA:HB3	1:A:434:ALA:H	1.77	0.49
1:A:438:ASN:HB3	1:A:504:GLN:HB3	1.94	0.49
1:A:61:ASN:HB3	3:A:1301:NAG:C7	2.43	0.49
1:A:341:PHE:HZ	1:A:367:LEU:HD23	1.76	0.49
1:B:306:THR:HA	1:B:600:THR:HG21	1.94	0.49
1:B:339:GLU:HG2	1:B:340:VAL:HG13	1.94	0.49
1:B:823:LYS:HD2	1:B:943:LEU:HD12	1.94	0.49
1:A:355:THR:OG1	1:A:396:ALA:O	2.31	0.49
1:A:452:TYR:O	1:A:491:GLN:N	2.46	0.49
1:B:352:TRP:CD1	1:B:399:PHE:HB3	2.47	0.49
1:C:103:GLY:HA3	1:C:240:LEU:HD12	1.93	0.49
1:C:95:THR:HB	1:C:189:LEU:HD12	1.94	0.49
1:A:395:TYR:HB2	1:A:512:SER:HB2	1.93	0.49
1:B:109:THR:OG1	1:B:110:LEU:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ARG:HH21	1:A:469:THR:HG22	1.78	0.49
1:A:359:ASN:HB3	1:A:521:THR:HB	1.94	0.49
1:A:126:VAL:HG12	1:A:173:GLN:HE21	1.78	0.48
1:B:408:GLN:O	1:B:413:GLN:NE2	2.45	0.48
1:C:631:TRP:HD1	1:C:649:ILE:HG22	1.78	0.48
1:A:392:THR:O	1:A:521:THR:OG1	2.28	0.48
1:B:397:ASP:N	1:B:397:ASP:OD1	2.45	0.48
1:C:413:GLN:O	1:C:423:LYS:NZ	2.46	0.48
1:A:173:GLN:OE1	1:A:173:GLN:N	2.43	0.48
1:B:420:TYR:HB3	1:B:456:ARG:HD3	1.96	0.48
1:C:105:ILE:HD12	1:C:238:GLN:HB2	1.95	0.48
1:A:275:LEU:HD23	1:A:305:PHE:HE1	1.79	0.48
1:B:293:ASP:OD1	1:B:293:ASP:N	2.46	0.48
1:B:117:LEU:HD13	1:B:130:VAL:HB	1.96	0.48
1:B:424:LEU:HD12	1:B:425:PRO:HD2	1.96	0.47
1:C:496:ARG:HB2	1:C:499:TYR:HD2	1.79	0.47
1:A:36:VAL:HG11	1:A:219:PHE:CZ	2.49	0.47
1:A:200:TYR:CZ	1:A:229:PRO:HB3	2.49	0.47
1:B:107:GLY:H	1:B:234:ILE:HG23	1.80	0.47
1:A:983:ASP:OD1	1:A:983:ASP:N	2.48	0.47
1:B:363:ASP:N	1:B:363:ASP:OD1	2.47	0.47
1:C:906:GLY:O	1:C:1036:LYS:NZ	2.45	0.47
1:C:976:ASN:HA	1:C:979:LEU:HB2	1.96	0.47
1:C:344:THR:CG2	1:C:345:ARG:H	2.18	0.47
1:C:674:THR:HG1	1:C:688:GLN:HE22	1.60	0.47
1:C:65:PHE:HE2	1:C:84:LEU:HD11	1.80	0.46
1:C:359:ASN:HA	1:C:521:THR:HG21	1.98	0.46
1:A:572:ASP:OD1	1:A:572:ASP:N	2.48	0.46
1:C:320:GLN:H	1:C:625:ASP:HB3	1.80	0.46
1:A:981:ARG:HG3	1:B:381:VAL:HG23	1.98	0.46
1:B:130:VAL:O	1:B:130:VAL:HG13	2.16	0.46
1:C:402:LYS:HZ1	1:C:505:PRO:HG3	1.80	0.46
1:A:351:ALA:HA	1:A:467:ILE:HG12	1.96	0.46
1:C:83:VAL:HG23	1:C:84:LEU:HG	1.98	0.46
1:A:189:LEU:HG	1:A:210:ILE:HD13	1.97	0.46
1:C:141:LEU:HD12	1:C:242:ALA:HB2	1.98	0.46
1:B:388:ASP:N	1:B:388:ASP:OD1	2.49	0.46
1:B:433:ILE:HD12	1:B:511:LEU:HD13	1.98	0.46
1:A:352:TRP:HE1	1:A:465:ARG:HA	1.81	0.45
1:A:416:ASN:HD21	1:A:452:TYR:HE2	1.63	0.45
1:B:101:ILE:HD12	1:B:241:LEU:HD11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:502:GLY:N	1:C:504:GLN:OE1	2.49	0.45
1:A:436:ASN:HB2	1:A:506:TYR:CZ	2.51	0.45
1:B:430:GLY:HA2	1:B:513:PHE:CE1	2.52	0.45
1:B:335:CYS:HB2	1:B:360:CYS:HB2	1.75	0.45
1:B:522:VAL:HG13	1:B:522:VAL:O	2.16	0.45
1:A:531:LEU:HD23	1:A:531:LEU:HA	1.82	0.45
1:A:164:ASN:HB2	3:A:1303:NAG:H83	1.97	0.45
1:A:230:ILE:HG22	1:A:232:ILE:HG23	1.99	0.45
1:B:206:LYS:HB3	1:B:222:LEU:HD22	1.98	0.45
1:A:984:PRO:N	1:A:985:PRO:HD2	2.31	0.45
1:B:375:ALA:HB3	1:B:434:ALA:HB2	1.98	0.45
1:B:738:MET:HE1	1:C:318:ARG:HH22	1.82	0.45
1:B:904:PHE:CD2	1:B:914:LEU:HB2	2.52	0.45
1:C:618:VAL:O	1:C:622:ILE:HG12	2.16	0.45
1:B:426:ASP:N	1:B:426:ASP:OD1	2.50	0.44
1:A:618:VAL:O	1:A:622:ILE:HG13	2.16	0.44
1:C:1120:VAL:HG13	1:C:1121:SER:N	2.31	0.44
1:B:403:GLY:HA3	1:B:504:GLN:HB3	2.00	0.44
1:C:423:LYS:HD2	1:C:423:LYS:HA	1.78	0.44
1:A:170:TYR:CD2	1:A:228:LEU:HD21	2.53	0.44
1:A:460:LEU:HD23	1:A:460:LEU:HA	1.88	0.44
1:B:713:PRO:HA	1:B:1070:GLU:HA	2.00	0.44
1:A:100:ILE:HG13	1:A:101:ILE:H	1.83	0.44
1:A:108:THR:HA	1:A:235:THR:H	1.82	0.44
1:A:202:LYS:HB3	1:A:204:TYR:CZ	2.52	0.44
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.53	0.44
1:B:195:LYS:HG2	1:B:197:ILE:HG12	1.99	0.44
1:A:356:ARG:HE	1:A:393:ASN:HB3	1.83	0.44
1:B:210:ILE:HD12	1:B:216:PRO:HG2	2.00	0.44
1:B:343:ALA:H	1:B:435:TRP:HH2	1.65	0.44
1:A:128:ILE:HD13	1:A:228:LEU:HD11	1.99	0.43
1:A:380:GLY:HA3	1:A:429:THR:HA	2.00	0.43
1:C:352:TRP:HA	1:C:398:SER:O	2.17	0.43
1:C:449:ASP:OD1	1:C:449:ASP:N	2.50	0.43
1:A:455:PHE:CE1	1:A:489:PRO:HA	2.53	0.43
1:B:99:ASN:C	1:B:101:ILE:H	2.26	0.43
1:C:28:TYR:CE1	1:C:63:THR:HG22	2.53	0.43
1:C:174:PRO:HB2	1:C:176:LEU:HD23	1.99	0.43
1:C:204:TYR:HB3	1:C:222:LEU:HB3	1.99	0.43
1:A:633:VAL:HG12	1:A:634:TYR:CD1	2.53	0.43
1:A:825:THR:OG1	1:A:826:LEU:N	2.40	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:PHE:HB3	1:B:435:TRP:HZ3	1.82	0.43
1:A:768:ILE:HD11	1:A:1010:LEU:HD23	2.01	0.43
1:B:95:THR:HG23	1:B:96:GLU:N	2.33	0.43
1:B:819:LEU:HD21	1:B:937:PHE:CE2	2.54	0.43
1:C:95:THR:HG23	1:C:96:GLU:N	2.34	0.43
1:C:350:TYR:HB2	1:C:466:ASP:HB3	1.99	0.43
1:A:112:SER:O	1:A:113:LYS:HG3	2.18	0.43
1:C:404:ASN:OD1	1:C:503:HIS:ND1	2.52	0.43
1:C:139:PRO:HG2	1:C:240:LEU:HD22	1.99	0.43
1:A:172:SER:O	1:A:174:PRO:HD3	2.19	0.43
1:C:626:GLN:HG3	1:C:627:LEU:H	1.84	0.43
1:C:190:ARG:NH1	1:C:206:LYS:O	2.51	0.43
1:C:447:ASN:HD21	1:C:450:TYR:HD2	1.66	0.43
1:C:1026:LYS:NZ	1:C:1040:PHE:O	2.52	0.43
1:A:364:TYR:HD2	1:A:386:LEU:HG	1.84	0.42
1:C:96:GLU:HB3	1:C:97:LYS:H	1.70	0.42
1:A:224:PRO:HD2	1:B:560:PHE:CZ	2.53	0.42
1:A:448:TYR:CD1	1:A:494:GLY:HA2	2.53	0.42
1:B:30:ASN:HD21	1:B:59:PHE:HD1	1.68	0.42
1:A:903:ARG:NH1	1:A:1047:LEU:O	2.49	0.42
1:C:168:PHE:CE2	1:C:170:TYR:HB2	2.55	0.42
1:C:430:GLY:HA2	1:C:513:PHE:HD2	1.83	0.42
1:A:904:PHE:CD2	1:A:914:LEU:HB2	2.55	0.42
1:C:1095:SER:HB2	1:C:1100:TRP:CD2	2.54	0.42
1:A:202:LYS:HB3	1:A:204:TYR:CE2	2.55	0.42
1:B:190:ARG:NE	1:B:207:HIS:HB2	2.35	0.42
1:C:553:SER:OG	1:C:554:ASN:N	2.53	0.42
1:A:90:VAL:HG12	1:A:92:PHE:H	1.85	0.42
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.87	0.42
1:B:983:ASP:OD1	1:B:986:GLU:HB2	2.19	0.42
1:A:430:GLY:HA3	1:A:511:LEU:O	2.20	0.42
1:A:652:GLU:HG3	1:A:691:ILE:HG22	2.02	0.42
1:A:409:ILE:O	1:A:409:ILE:HG13	2.20	0.42
1:A:336:PRO:HD2	1:A:357:ILE:HG23	2.02	0.41
1:A:809:LYS:HD2	1:A:810:PRO:HD2	2.01	0.41
1:B:199:GLY:HA2	1:B:231:GLY:HA2	2.01	0.41
1:B:446:GLY:HA2	1:B:495:PHE:N	2.35	0.41
1:C:31:SER:HG	1:C:60:SER:H	1.67	0.41
1:A:204:TYR:HD1	1:A:224:PRO:HA	1.85	0.41
1:A:633:VAL:HG12	1:A:634:TYR:HD1	1.84	0.41
1:A:92:PHE:CE1	1:A:94:SER:HB3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:PHE:CE1	1:A:505:PRO:HG3	2.54	0.41
1:C:230:ILE:HG22	1:C:232:ILE:HG23	2.02	0.41
1:A:824:VAL:HG11	1:A:1055:PRO:HG2	2.02	0.41
1:B:371:ALA:HB3	1:B:435:TRP:CD1	2.55	0.41
1:B:652:GLU:HG3	1:B:691:ILE:HG22	2.01	0.41
1:B:952:HIS:HD2	1:B:1012:ARG:HH21	1.69	0.41
1:B:208:THR:HA	1:B:209:PRO:HD3	1.90	0.41
1:B:457:LYS:HB3	1:B:457:LYS:HE3	1.88	0.41
1:C:280:GLU:HG2	1:C:281:ASN:OD1	2.21	0.41
1:C:784:LYS:H	1:C:784:LYS:HG2	1.57	0.41
1:A:453:ARG:HG3	1:A:490:LEU:HD23	2.02	0.41
1:B:102:ARG:HG3	1:B:121:ASN:HB3	2.03	0.41
1:B:128:ILE:HD13	1:B:170:TYR:HD2	1.84	0.41
1:A:983:ASP:OD1	1:A:986:GLU:HB3	2.21	0.41
1:B:106:PHE:HB2	1:B:117:LEU:HB2	2.03	0.41
1:B:113:LYS:NZ	1:B:233:ASN:HB2	2.36	0.41
1:B:159:VAL:O	1:B:162:SER:OG	2.37	0.41
1:B:447:ASN:HB2	1:B:493:TYR:CD2	2.56	0.41
1:C:402:LYS:HZ1	1:C:495:PHE:HB2	1.85	0.41
1:C:452:TYR:CE1	1:C:491:GLN:HB3	2.56	0.41
1:A:121:ASN:HB3	1:A:126:VAL:HG22	2.02	0.41
1:A:598:PRO:HD3	1:A:690:ILE:HD11	2.03	0.41
1:A:697:LEU:HD21	1:C:867:MET:HG2	2.03	0.41
1:B:127:PHE:HB3	1:B:171:VAL:HG22	2.02	0.41
1:C:987:ALA:O	1:C:991:ILE:HG12	2.21	0.41
1:A:289:ASP:O	1:A:296:SER:HB3	2.21	0.41
1:A:346:PHE:CE2	1:A:507:ARG:HD3	2.56	0.41
1:B:164:ASN:ND2	1:B:165:ASN:OD1	2.50	0.41
1:B:352:TRP:HZ2	1:B:422:TYR:HB2	1.86	0.41
1:B:957:LEU:HD23	1:B:957:LEU:HA	1.87	0.41
1:C:34:ARG:HH21	1:C:216:PRO:HG2	1.86	0.41
1:C:350:TYR:HE1	1:C:451:TRP:HB2	1.84	0.41
1:B:350:TYR:CD2	1:B:453:ARG:HB2	2.56	0.40
1:B:392:THR:OG1	1:B:517:HIS:HB2	2.21	0.40
1:B:402:LYS:HA	1:B:495:PHE:CZ	2.55	0.40
1:A:92:PHE:HE1	1:A:94:SER:HB3	1.86	0.40
1:A:807:PRO:O	1:A:812:LYS:NZ	2.38	0.40
1:B:230:ILE:HG22	1:B:232:ILE:HG23	2.03	0.40
1:B:404:ASN:OD1	1:B:404:ASN:N	2.53	0.40
1:A:119:ILE:HD12	1:A:119:ILE:H	1.85	0.40
1:A:101:ILE:HD11	1:A:262:ALA:HB1	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ASN:O	1:B:125:ASN:N	2.54	0.40
1:B:848:ILE:HD12	1:B:848:ILE:HA	1.96	0.40
1:A:133:PHE:HD1	1:A:163:ALA:HA	1.87	0.40
1:A:195:LYS:HG2	1:A:197:ILE:HG22	2.03	0.40
1:A:375:ALA:HB3	1:A:434:ALA:N	2.37	0.40
1:A:450:TYR:O	1:A:493:TYR:N	2.50	0.40
1:B:141:LEU:HD12	1:B:242:ALA:HB2	2.03	0.40
1:B:540:ASN:O	1:B:542:ASN:N	2.54	0.40
1:B:817:GLU:OE1	1:B:1053:SER:OG	2.29	0.40
1:C:206:LYS:HD2	1:C:206:LYS:HA	1.85	0.40
1:C:984:PRO:HB2	1:C:985:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1020/1235 (83%)	942 (92%)	78 (8%)	0	100	100
1	B	1000/1235 (81%)	897 (90%)	103 (10%)	0	100	100
1	C	998/1235 (81%)	925 (93%)	73 (7%)	0	100	100
All	All	3018/3705 (82%)	2764 (92%)	254 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	906/1077 (84%)	906 (100%)	0	100	100
1	B	892/1077 (83%)	892 (100%)	0	100	100
1	C	890/1077 (83%)	890 (100%)	0	100	100
All	All	2688/3231 (83%)	2688 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	ASN
1	A	540	ASN
1	A	642	GLN
1	A	753	GLN
1	A	772	GLN
1	A	802	GLN
1	A	822	ASN
1	A	911	GLN
1	A	933	GLN
1	A	1008	GLN
1	B	49	HIS
1	B	115	GLN
1	B	320	GLN
1	B	333	ASN
1	B	413	GLN
1	B	639	ASN
1	B	933	GLN
1	B	1104	GLN
1	C	447	ASN
1	C	578	GLN
1	C	688	GLN
1	C	854	ASN
1	C	951	ASN
1	C	1009	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 ⓘ

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	E	2	2	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	F	1	2,1	14,14,15	0.23	0	17,19,21	0.48	0
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	G	1	2,1	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	G	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	H	1	2,1	14,14,15	0.29	0	17,19,21	0.43	0
2	NAG	H	2	2	14,14,15	0.24	0	17,19,21	0.41	0
2	NAG	I	1	2,1	14,14,15	0.32	0	17,19,21	0.55	0
2	NAG	I	2	2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	J	1	2,1	14,14,15	0.20	0	17,19,21	0.44	0
2	NAG	J	2	2	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	K	1	2,1	14,14,15	0.23	0	17,19,21	0.49	0
2	NAG	K	2	2	14,14,15	0.20	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

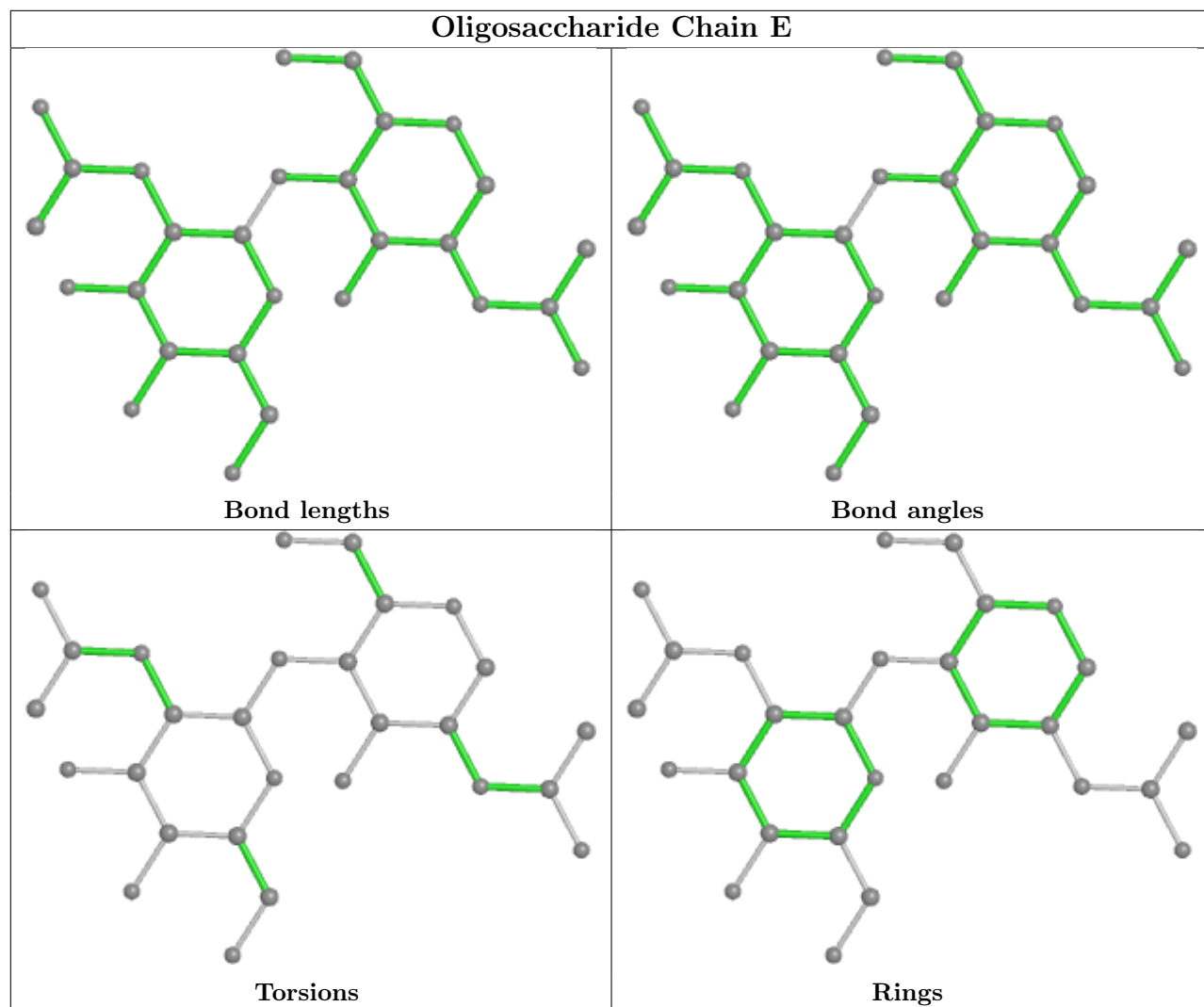
All (11) torsion outliers are listed below:

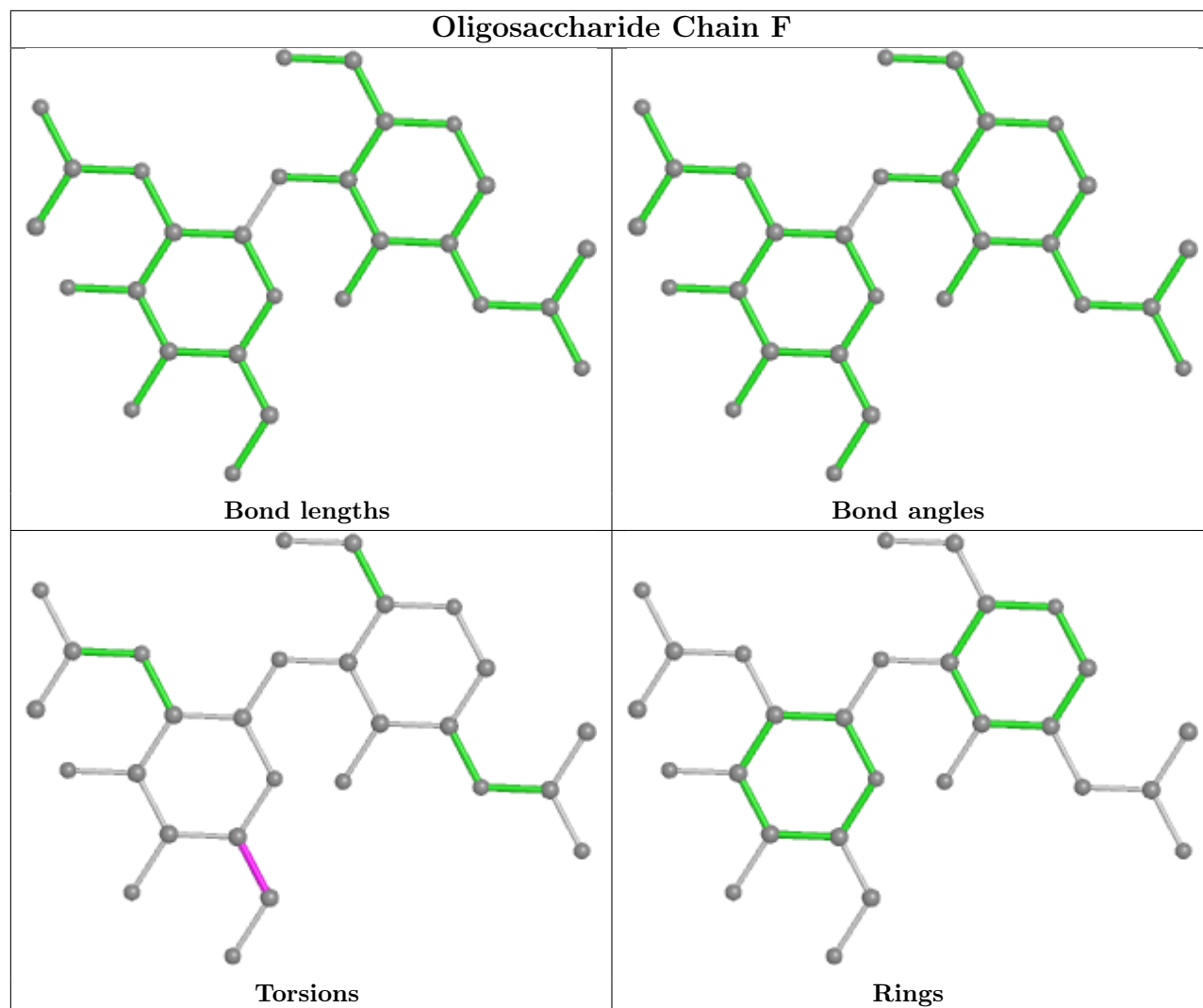
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C3-C2-N2-C7

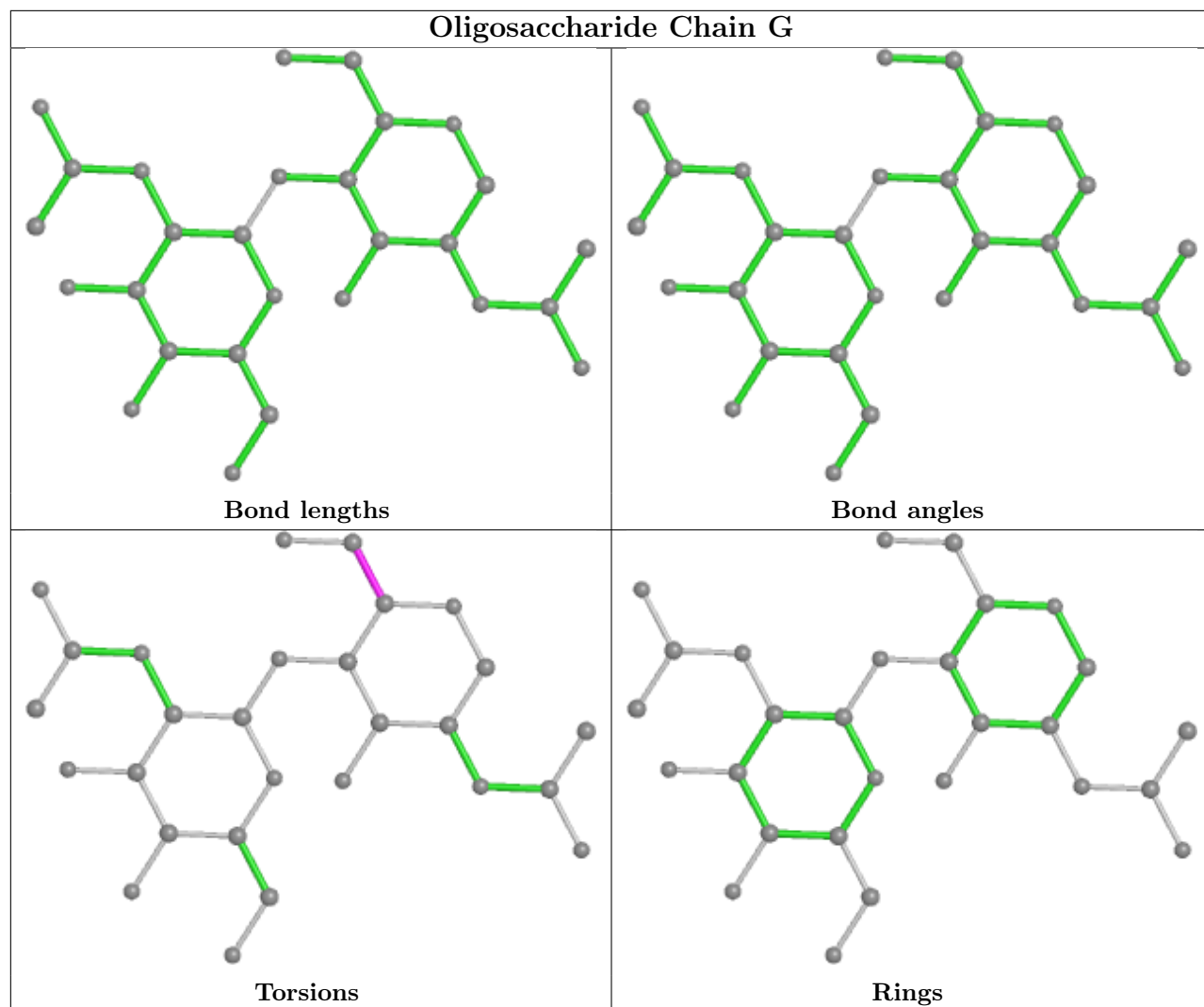
There are no ring outliers.

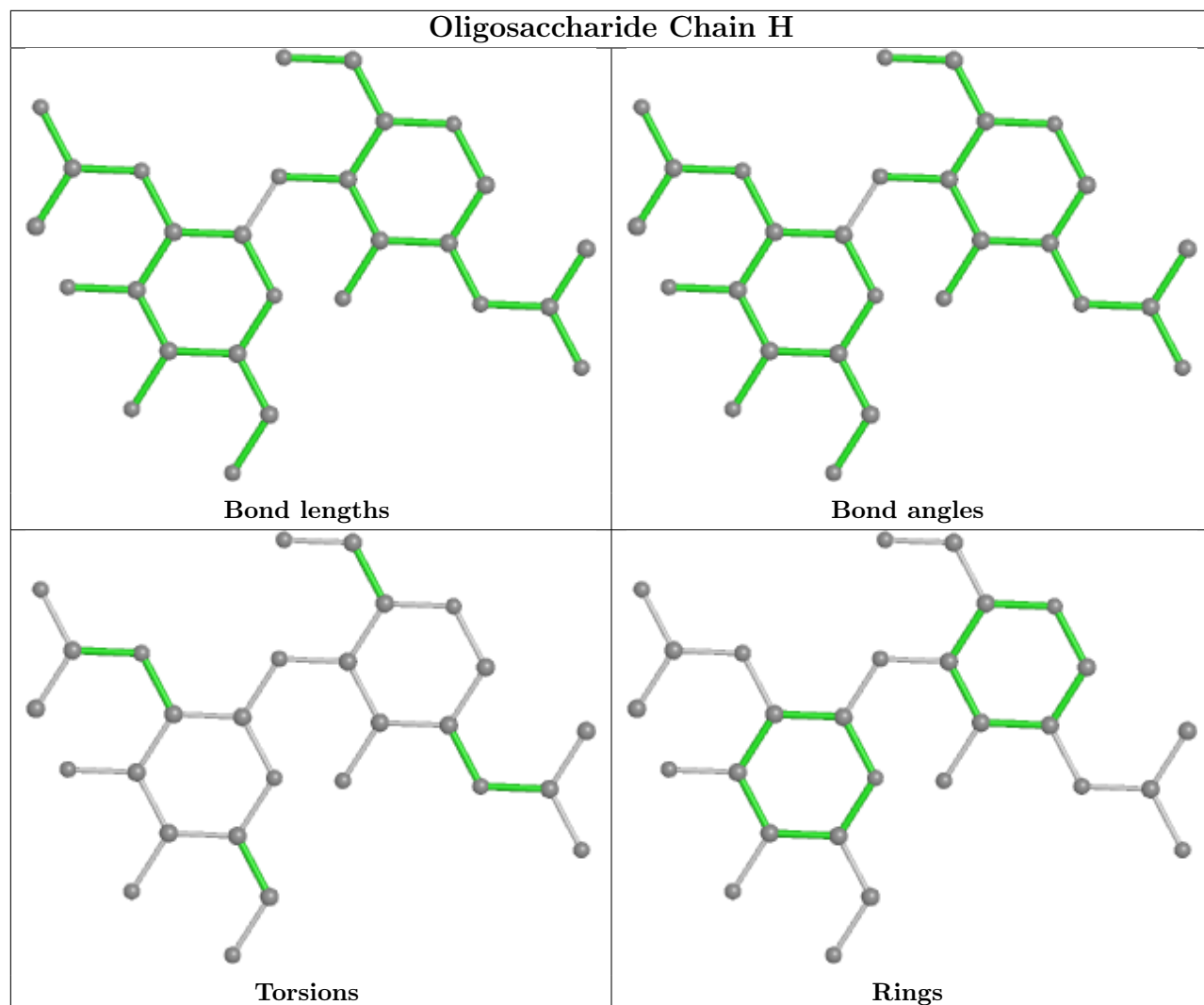
No monomer is involved in short contacts.

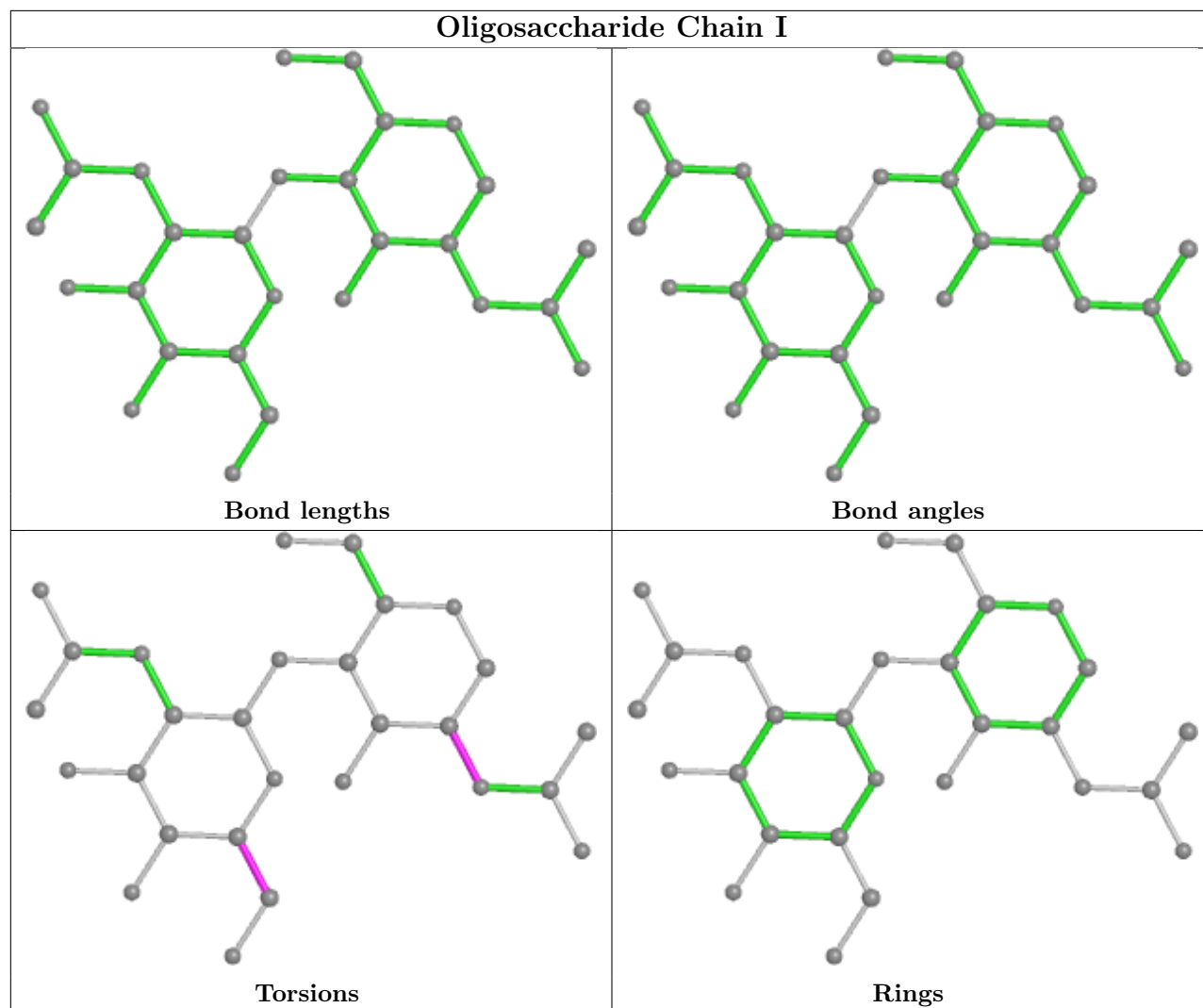
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

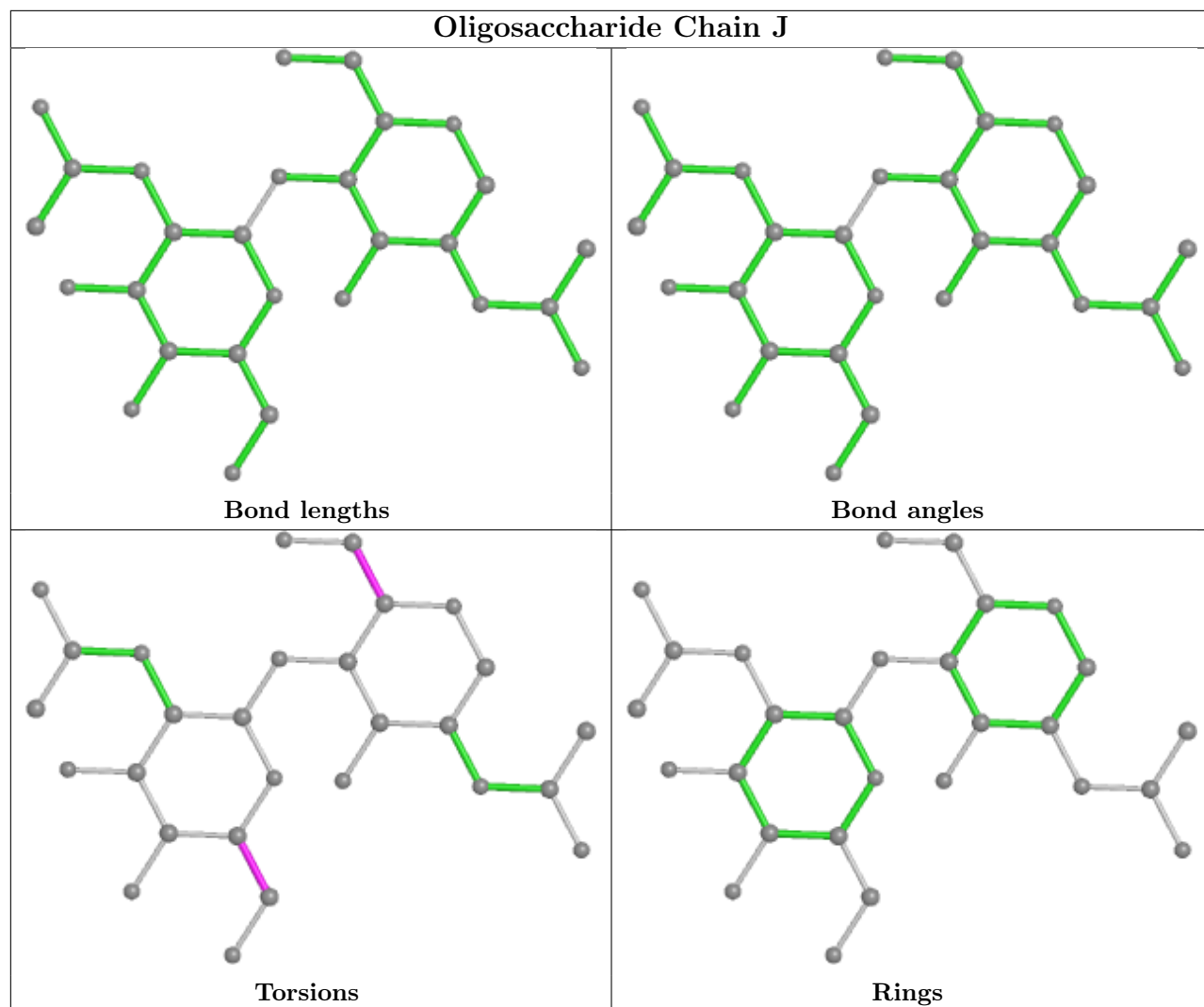


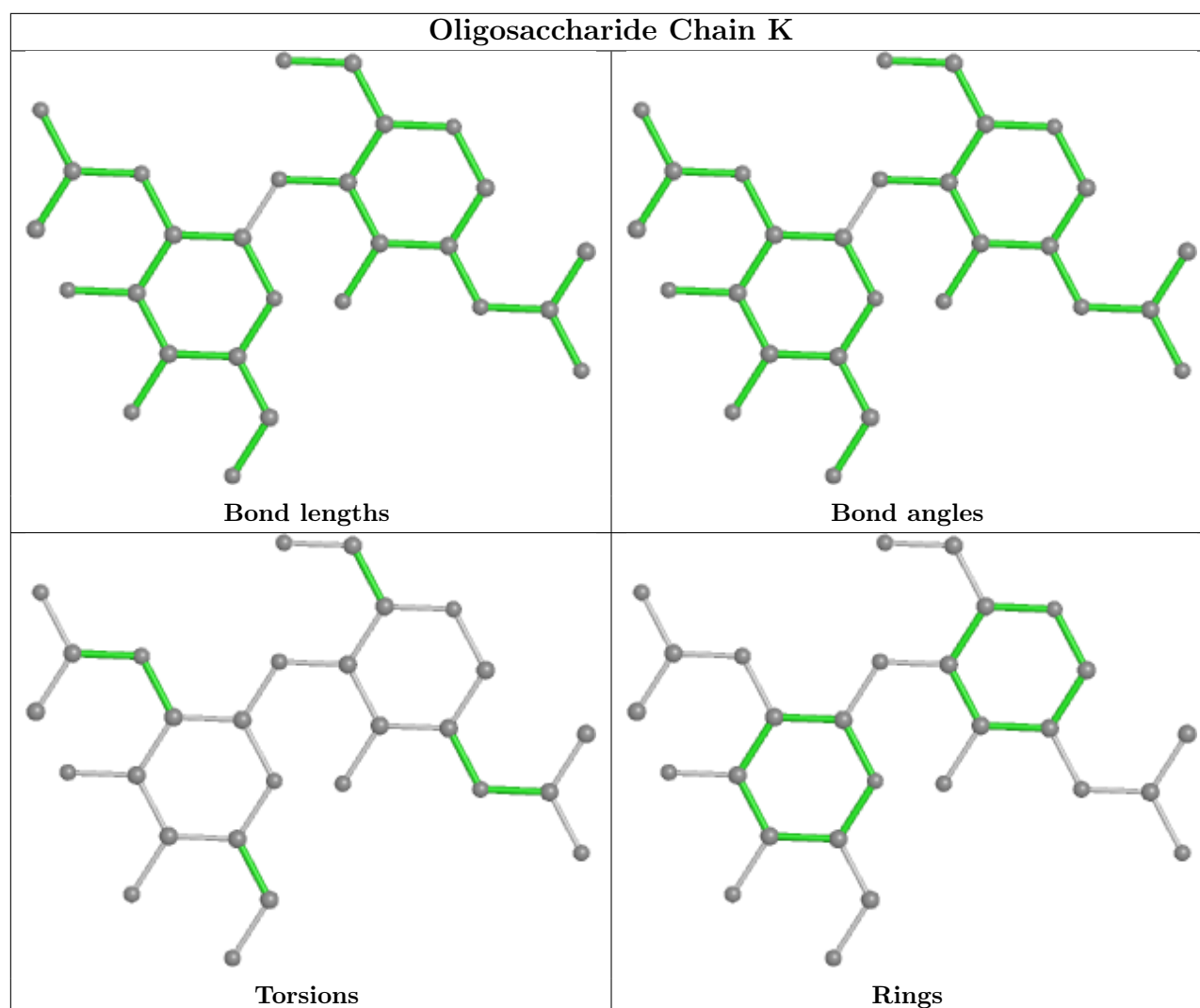












5.6 Ligand geometry [i](#)

35 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	1301	1	14,14,15	0.18	0	17,19,21	0.37	0
3	NAG	B	1303	1	14,14,15	0.27	0	17,19,21	0.60	0
3	NAG	B	1310	1	14,14,15	0.29	0	17,19,21	0.35	0
3	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1310	1	14,14,15	0.28	0	17,19,21	0.44	0
3	NAG	C	1304	1	14,14,15	0.22	0	17,19,21	0.31	0
3	NAG	C	1310	1	14,14,15	0.18	0	17,19,21	0.44	0
3	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	A	1313	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	B	1311	1	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	A	1306	1	14,14,15	0.18	0	17,19,21	0.46	0
3	NAG	A	1302	1	14,14,15	0.28	0	17,19,21	0.42	0
3	NAG	A	1314	1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	A	1309	1	14,14,15	0.29	0	17,19,21	0.57	0
3	NAG	A	1312	1	14,14,15	0.45	0	17,19,21	0.47	0
3	NAG	C	1306	1	14,14,15	0.24	0	17,19,21	0.35	0
3	NAG	A	1301	1	14,14,15	0.29	0	17,19,21	0.62	0
3	NAG	A	1311	1	14,14,15	0.26	0	17,19,21	0.51	0
3	NAG	A	1305	1	14,14,15	0.26	0	17,19,21	0.53	0
3	NAG	B	1302	1	14,14,15	0.28	0	17,19,21	0.57	0
3	NAG	C	1307	1	14,14,15	0.33	0	17,19,21	0.53	0
3	NAG	C	1302	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	C	1308	1	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	C	1305	1	14,14,15	0.18	0	17,19,21	0.38	0
3	NAG	A	1304	1	14,14,15	0.19	0	17,19,21	0.53	0
3	NAG	A	1308	1	14,14,15	0.25	0	17,19,21	0.38	0
3	NAG	B	1309	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	C	1301	1	14,14,15	0.96	1 (7%)	17,19,21	1.06	1 (5%)
3	NAG	C	1309	1	14,14,15	0.27	0	17,19,21	0.43	0
3	NAG	B	1306	1	14,14,15	0.94	1 (7%)	17,19,21	1.20	1 (5%)
3	NAG	A	1303	1	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	A	1307	1	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	B	1308	1	14,14,15	0.22	0	17,19,21	0.49	0
3	NAG	B	1307	1	14,14,15	0.24	0	17,19,21	0.37	0
3	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1313	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1314	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1312	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1306	NAG	O5-C1	3.28	1.49	1.43
3	C	1301	NAG	O5-C1	3.07	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1306	NAG	C1-O5-C5	4.72	118.59	112.19
3	C	1301	NAG	C1-O5-C5	4.02	117.64	112.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1309	NAG	O5-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	A	1311	NAG	C4-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	A	1311	NAG	O5-C5-C6-O6
3	B	1309	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1304	NAG	C4-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	A	1305	NAG	C8-C7-N2-C2
3	A	1305	NAG	O7-C7-N2-C2
3	A	1307	NAG	C8-C7-N2-C2
3	A	1307	NAG	O7-C7-N2-C2
3	A	1313	NAG	C8-C7-N2-C2
3	A	1313	NAG	O7-C7-N2-C2
3	B	1304	NAG	C8-C7-N2-C2
3	B	1304	NAG	O7-C7-N2-C2
3	B	1306	NAG	C8-C7-N2-C2
3	B	1306	NAG	O7-C7-N2-C2
3	C	1303	NAG	C8-C7-N2-C2
3	C	1303	NAG	O7-C7-N2-C2
3	C	1305	NAG	C8-C7-N2-C2
3	C	1305	NAG	O7-C7-N2-C2
3	B	1304	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1308	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	B	1309	NAG	C4-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	A	1312	NAG	O5-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	B	1311	NAG	O5-C5-C6-O6
3	A	1313	NAG	O5-C5-C6-O6
3	A	1309	NAG	C4-C5-C6-O6
3	A	1301	NAG	C3-C2-N2-C7
3	A	1303	NAG	C3-C2-N2-C7
3	B	1302	NAG	C3-C2-N2-C7
3	B	1303	NAG	C3-C2-N2-C7
3	C	1301	NAG	C3-C2-N2-C7
3	C	1303	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	A	1304	NAG	C3-C2-N2-C7

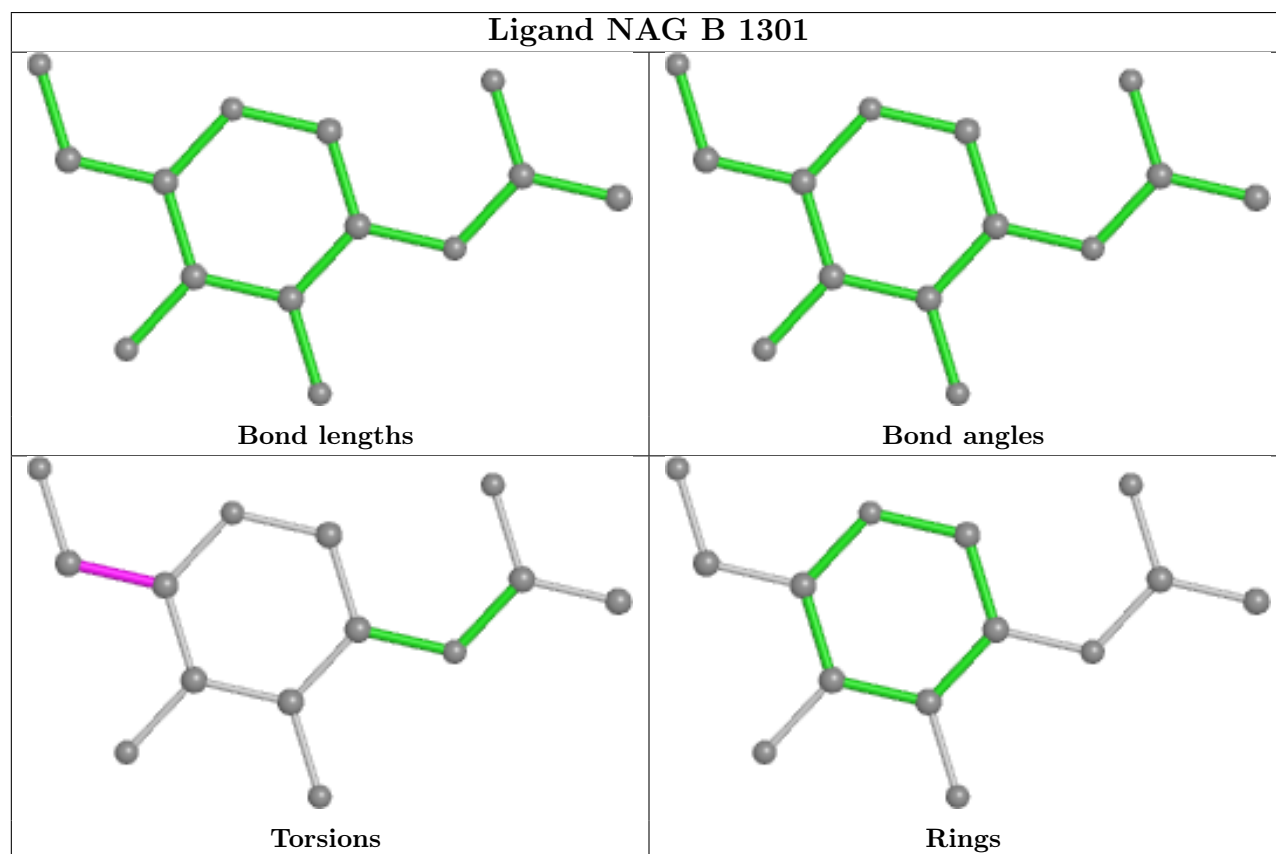
There are no ring outliers.

5 monomers are involved in 5 short contacts:

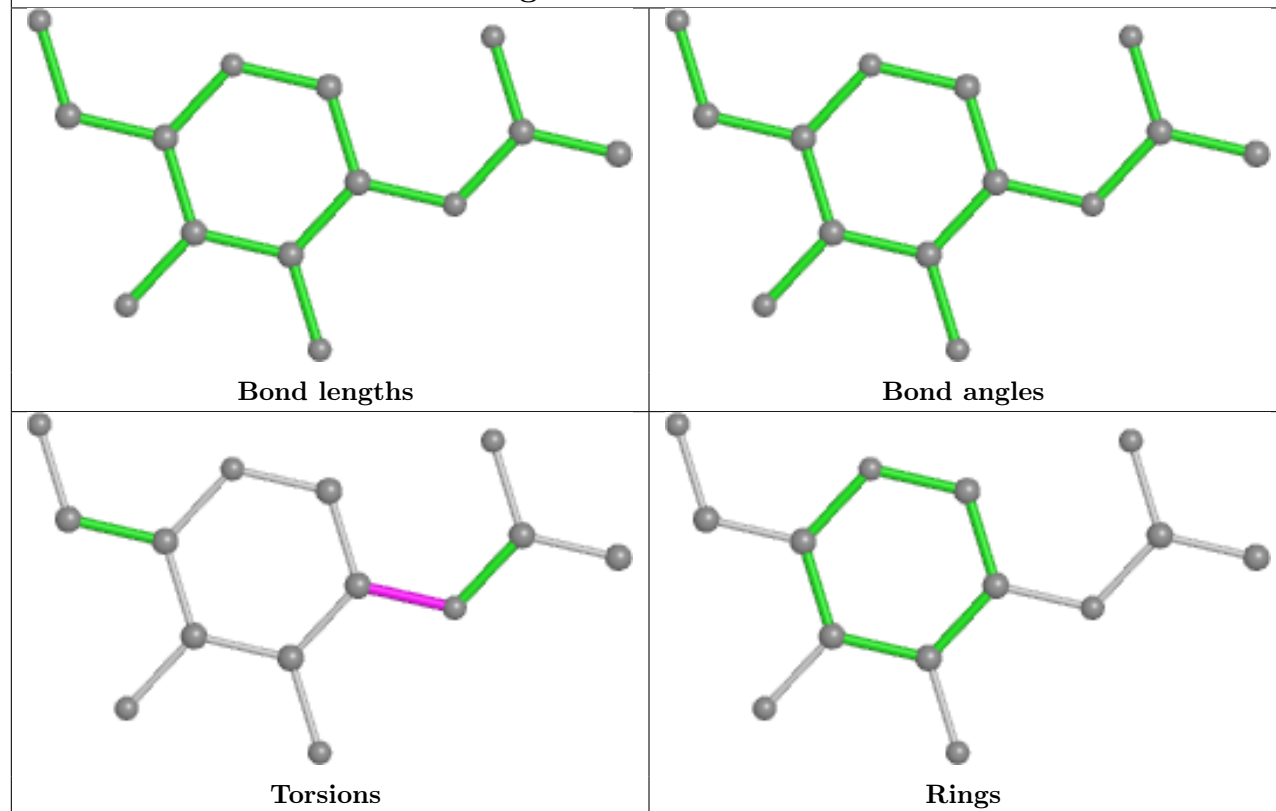
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1303	NAG	1	0
3	A	1312	NAG	1	0
3	A	1301	NAG	1	0
3	A	1303	NAG	1	0
3	B	1307	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

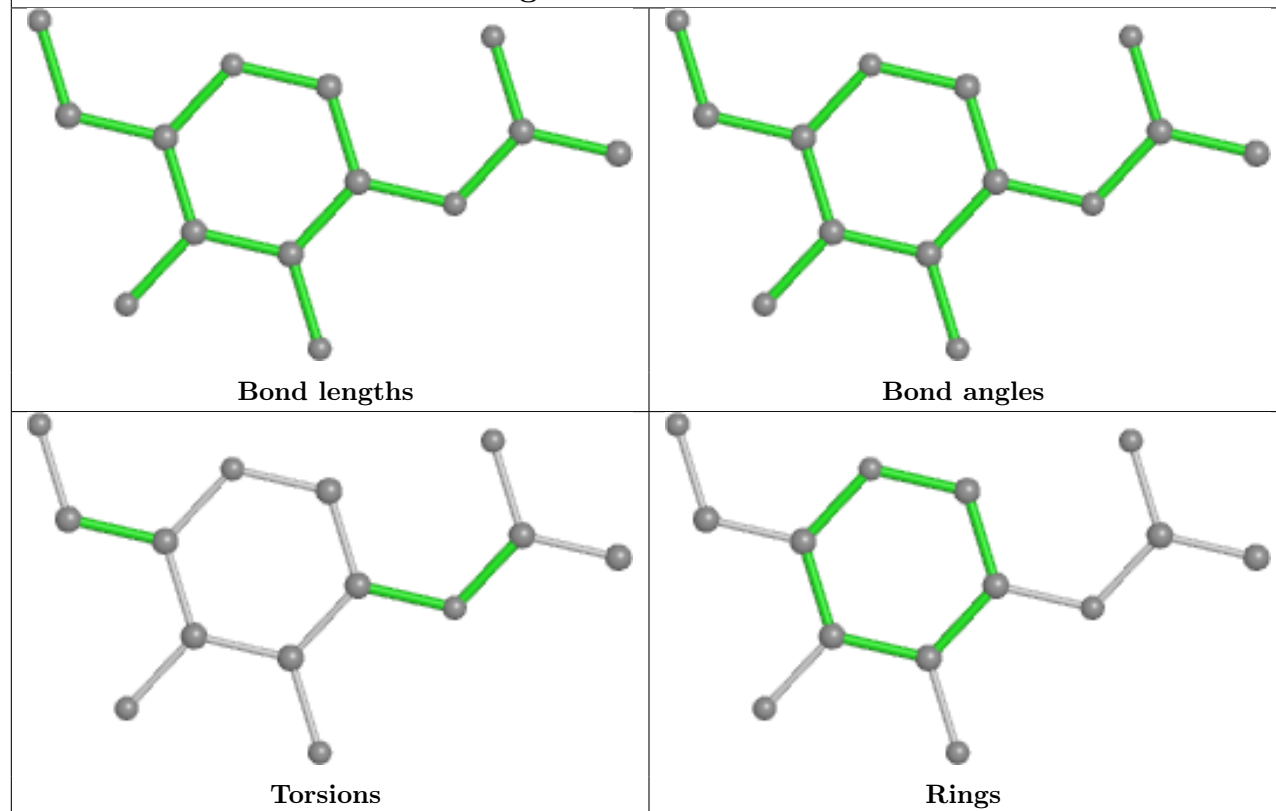
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

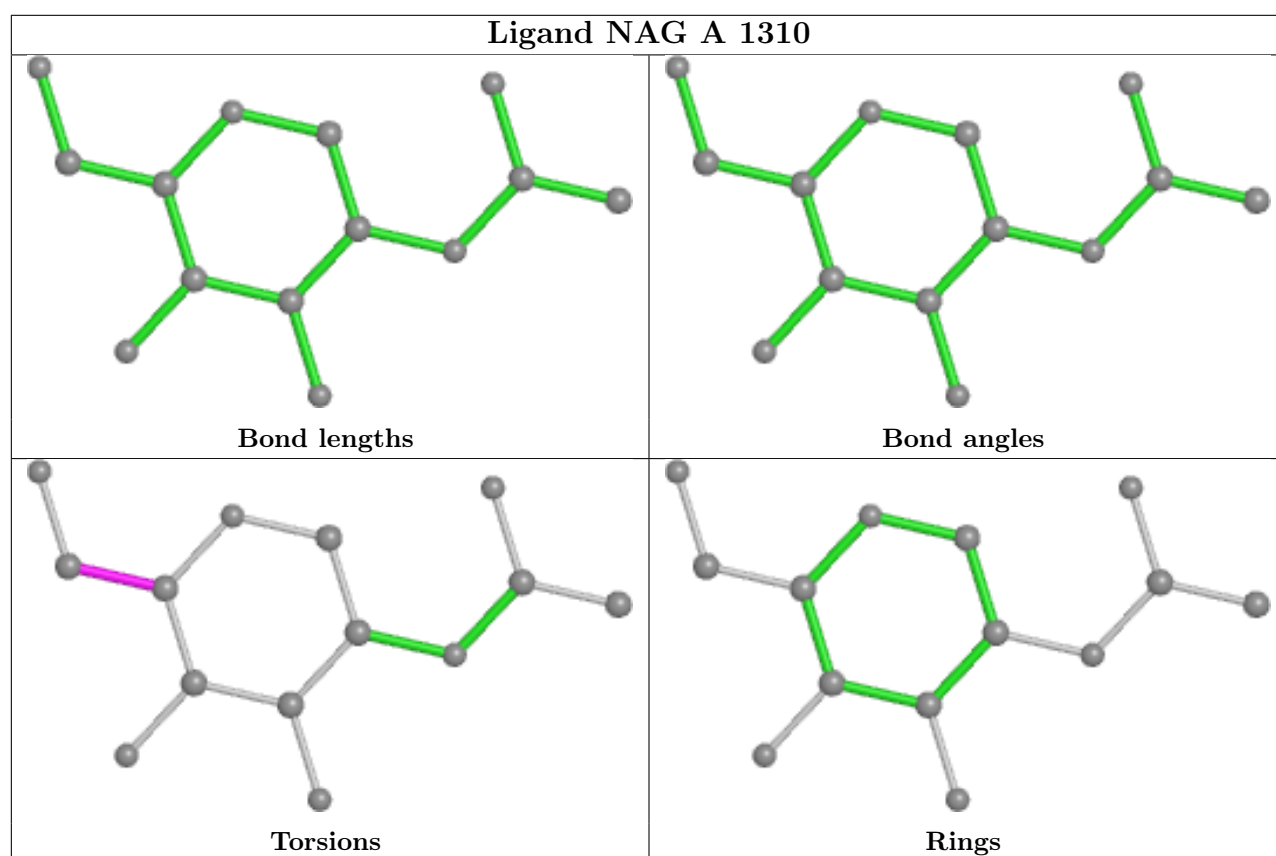
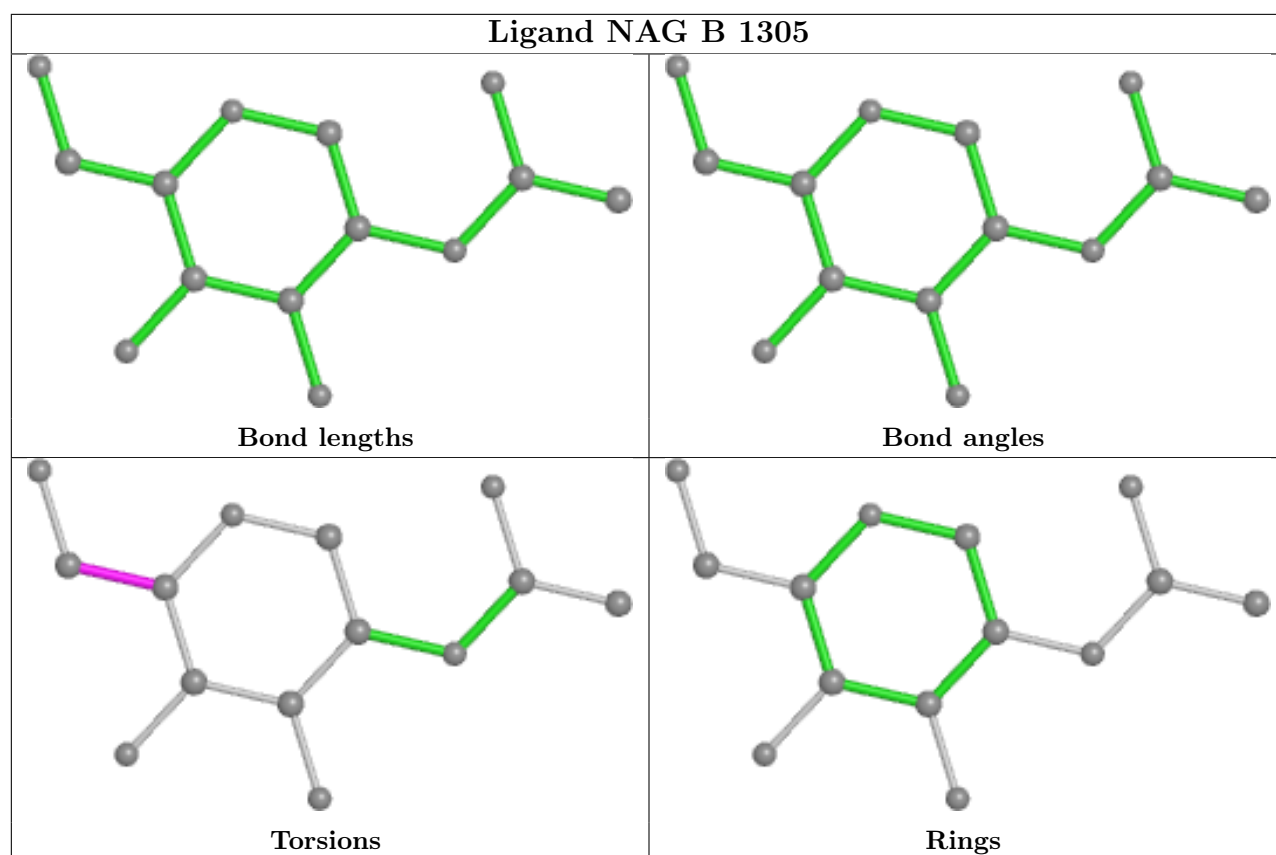


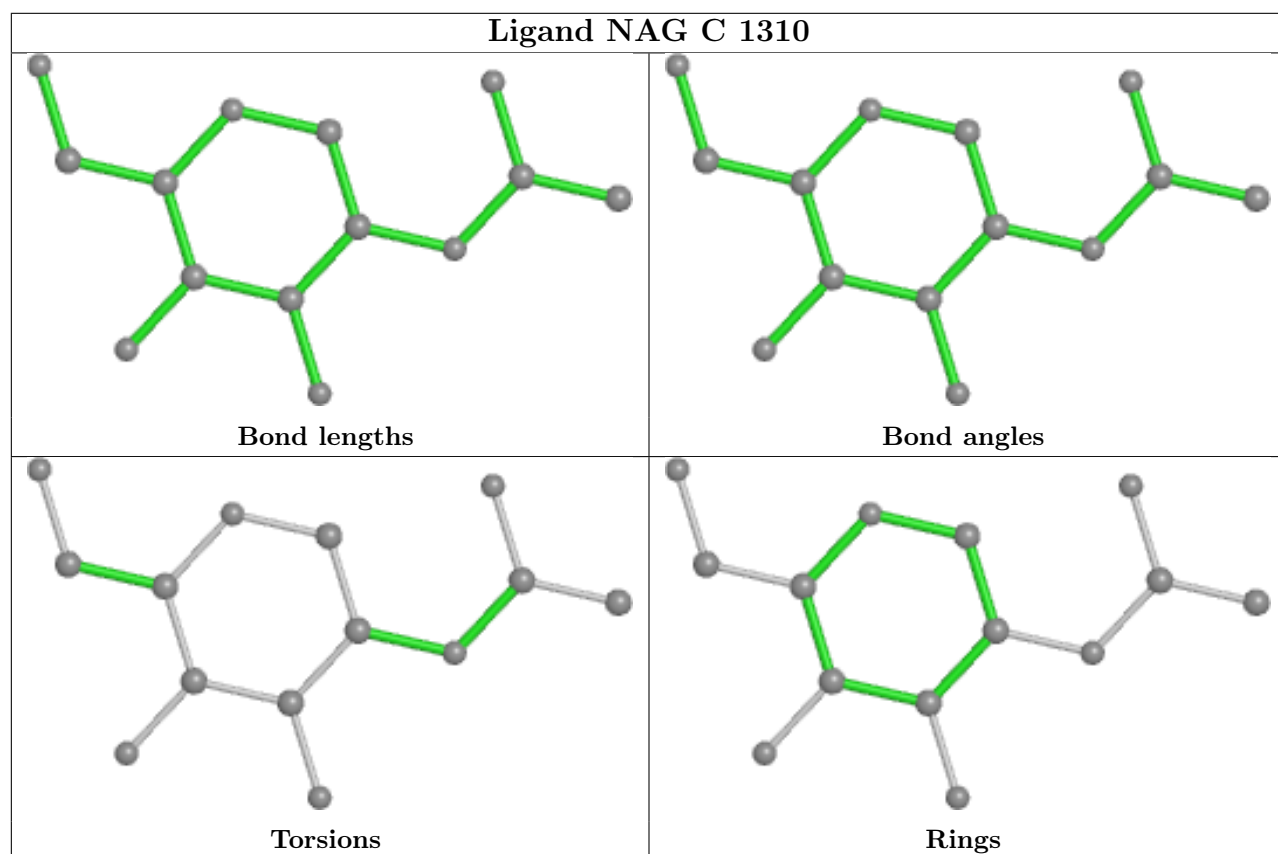
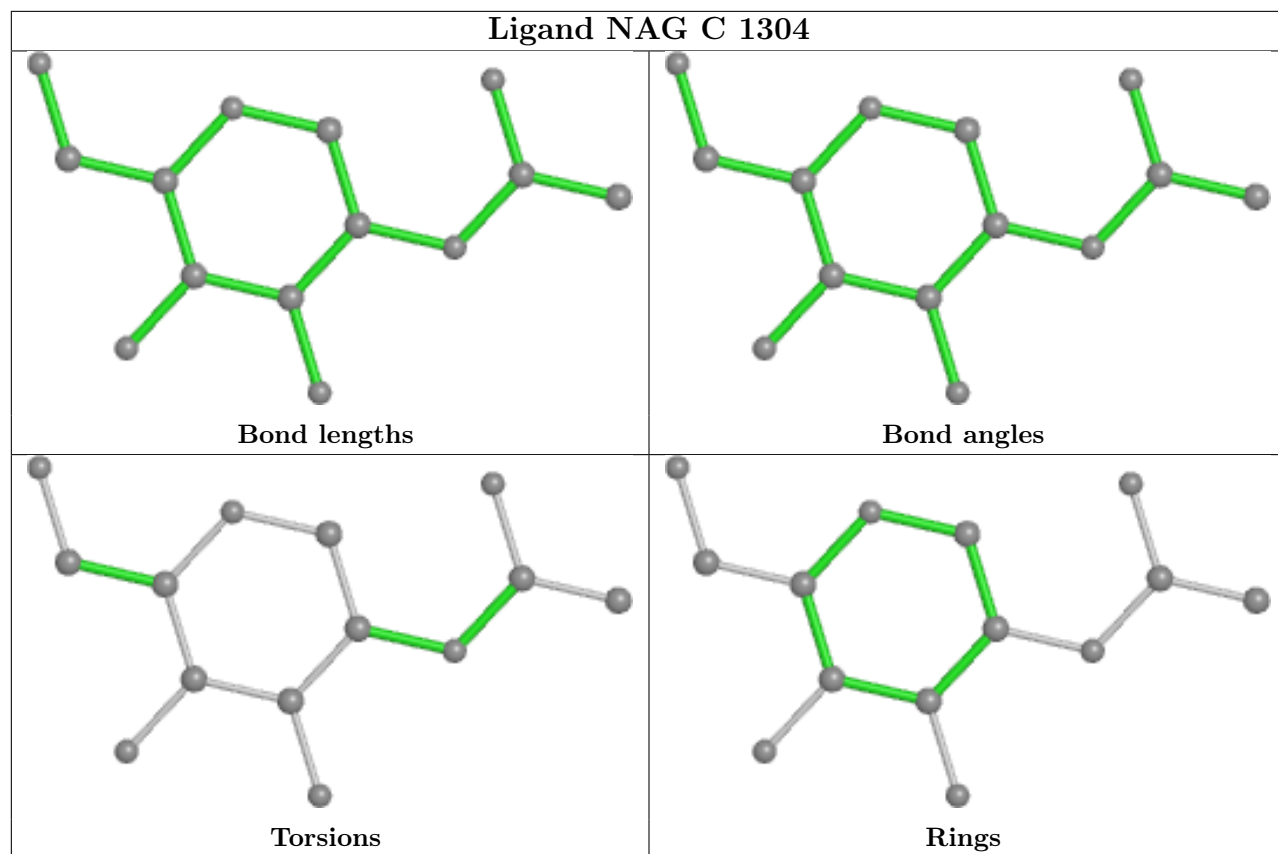
Ligand NAG B 1303



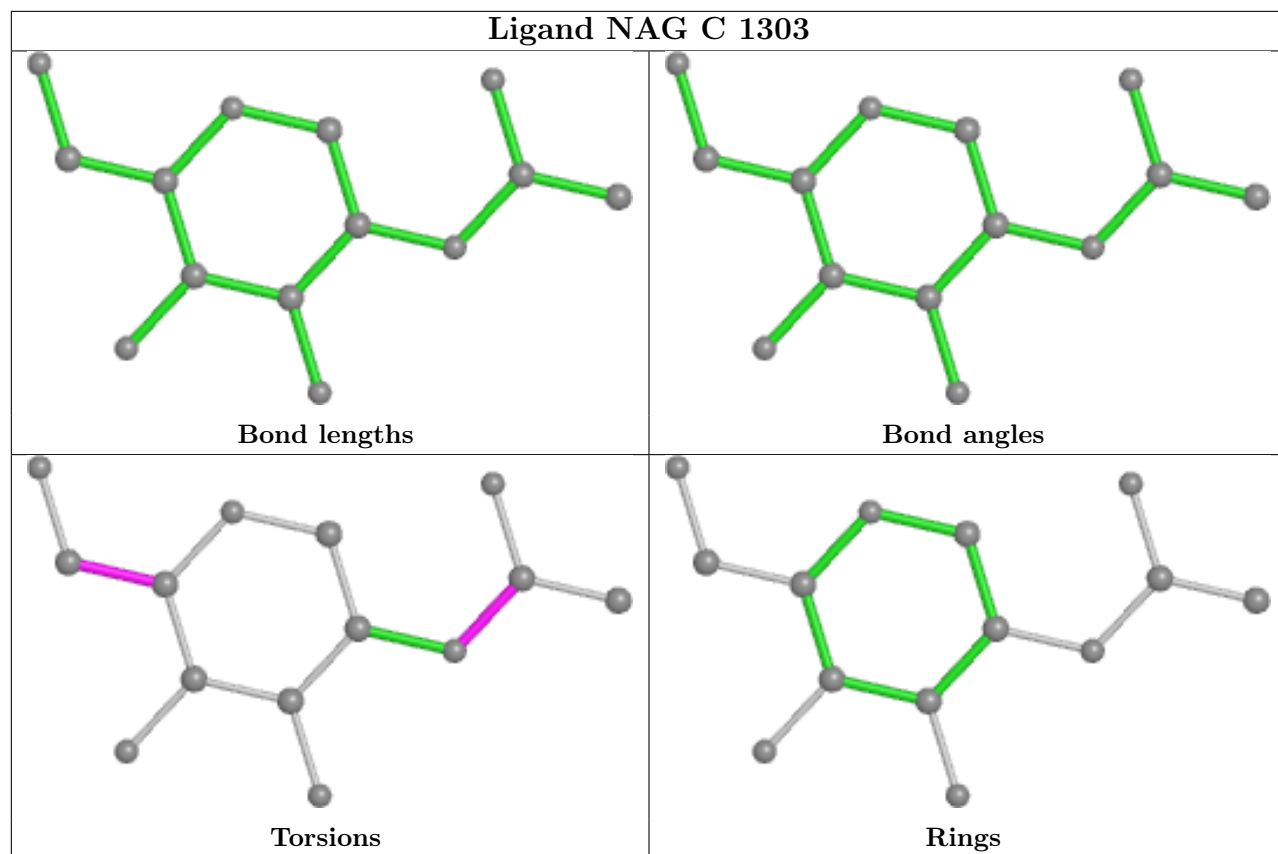
Ligand NAG B 1310



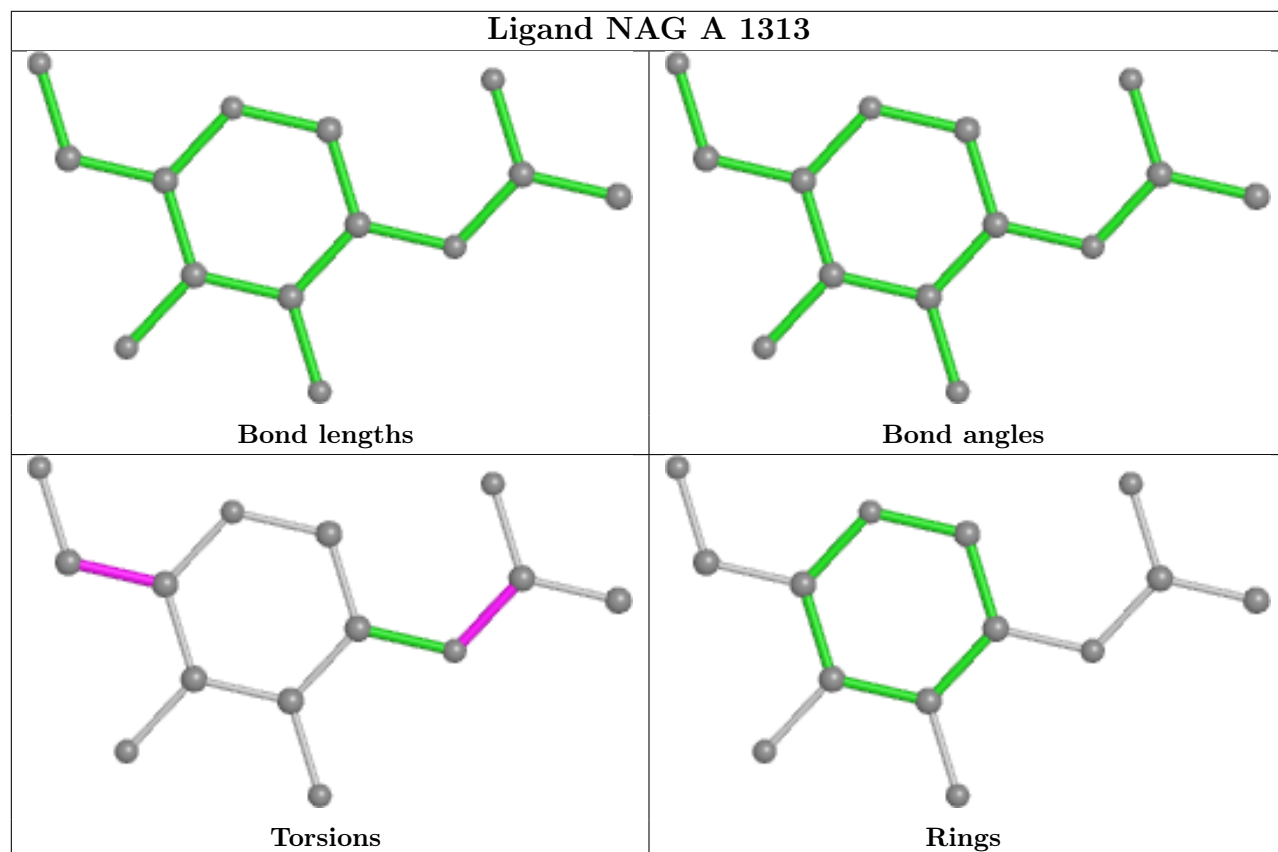


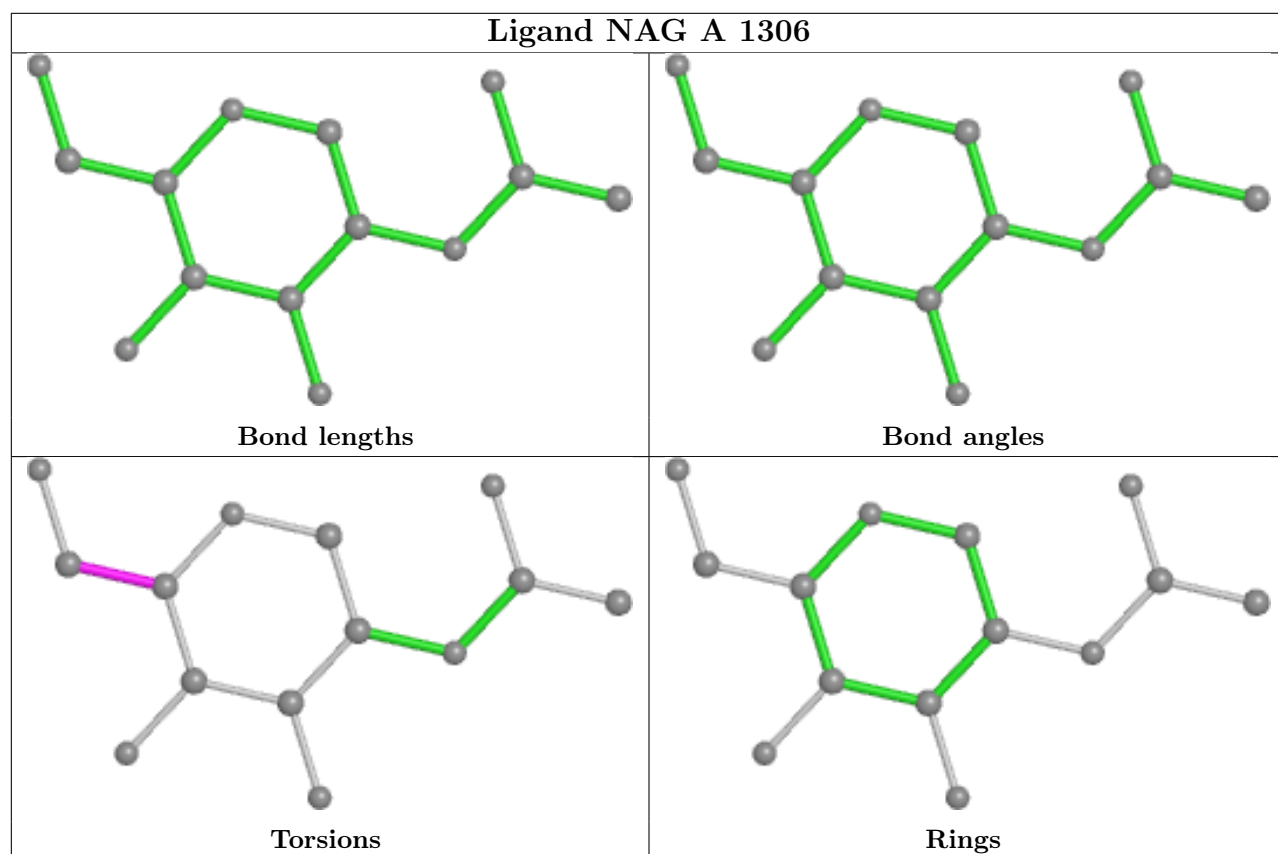
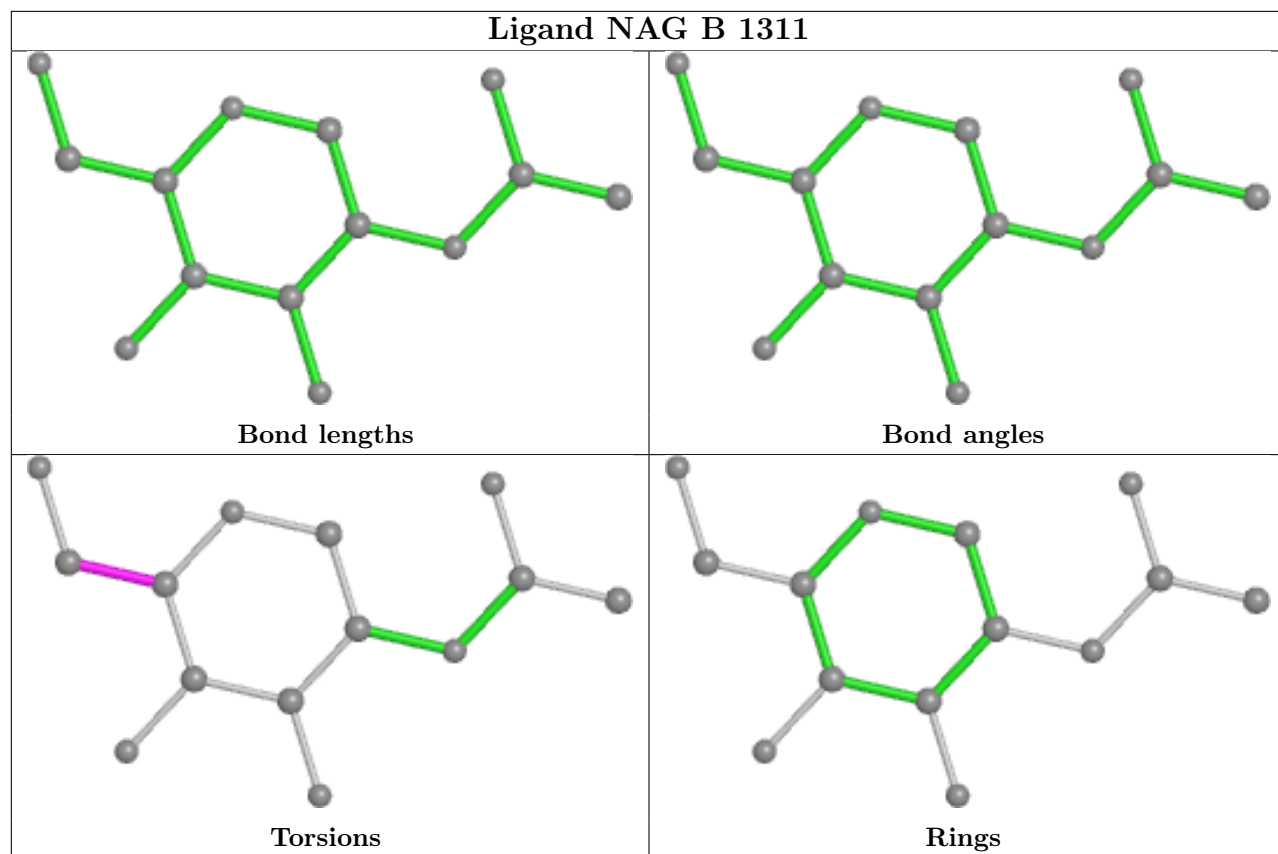


Ligand NAG C 1303

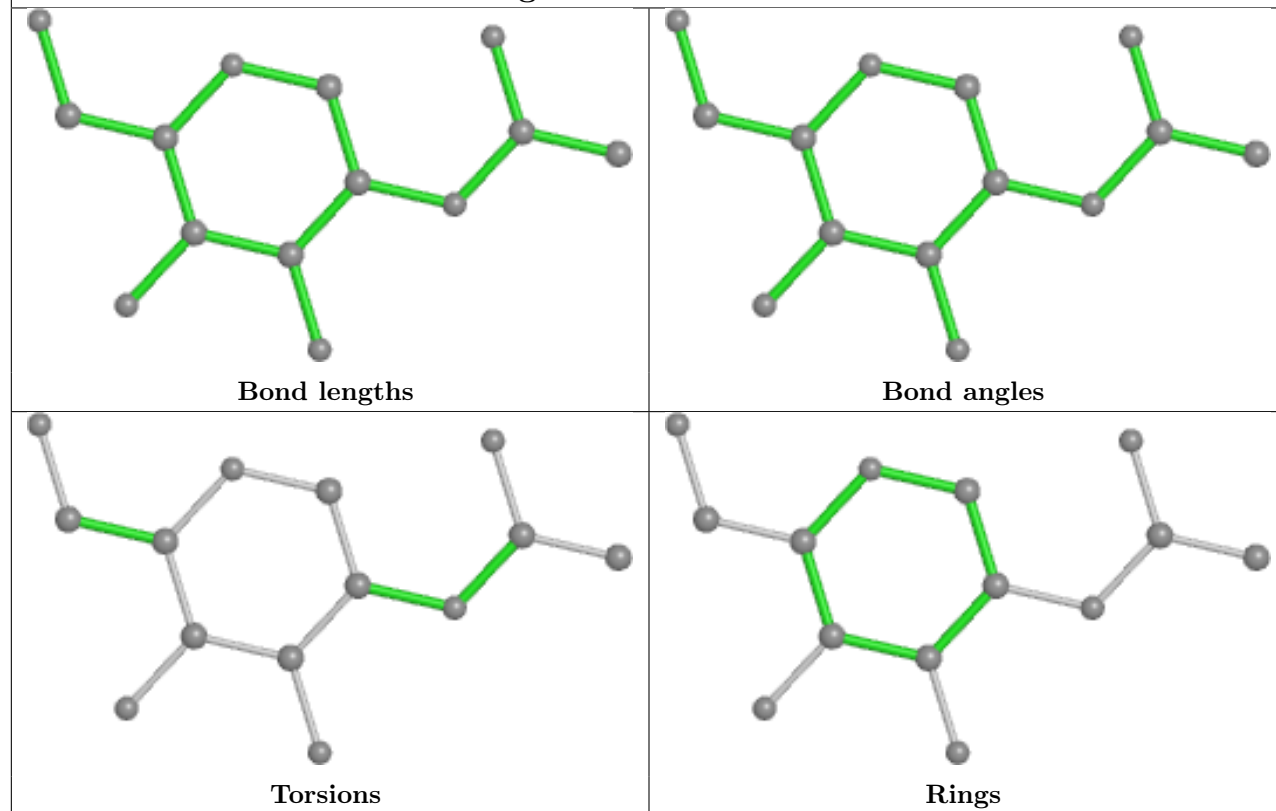


Ligand NAG A 1313

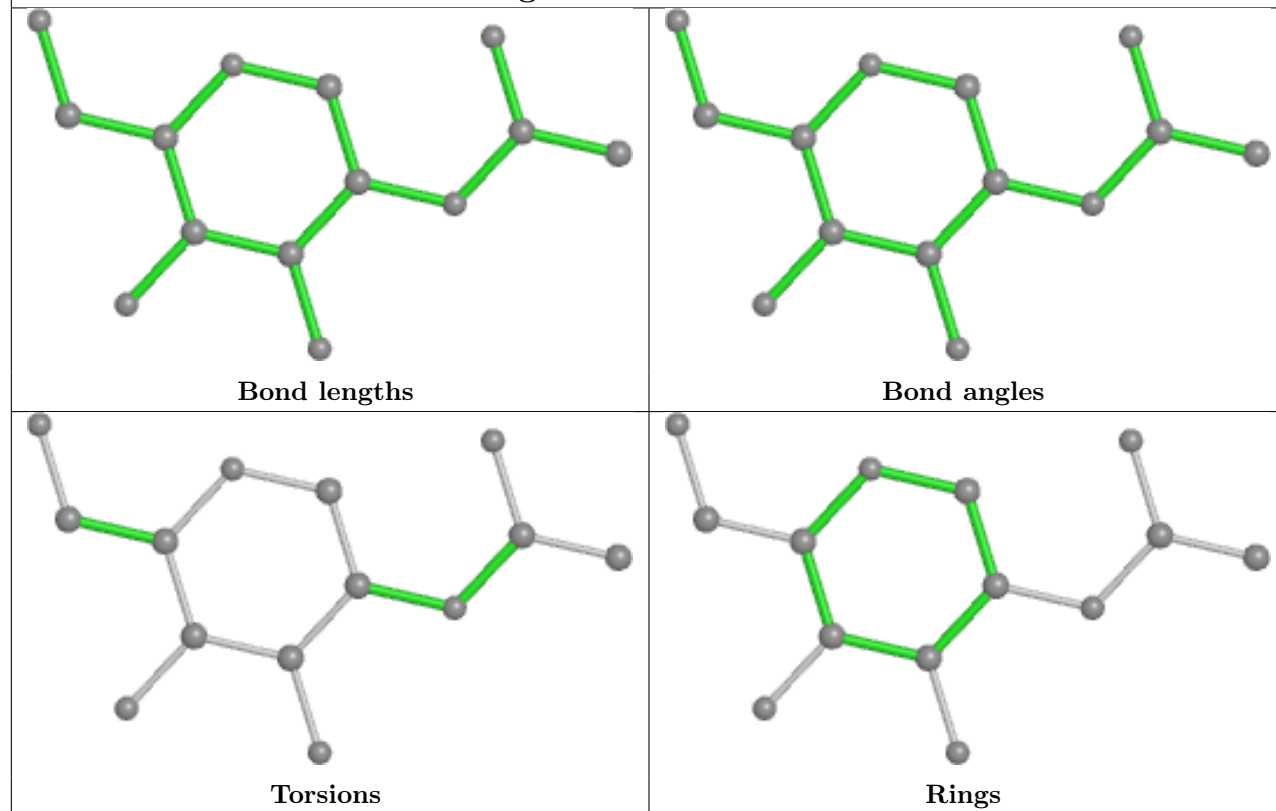


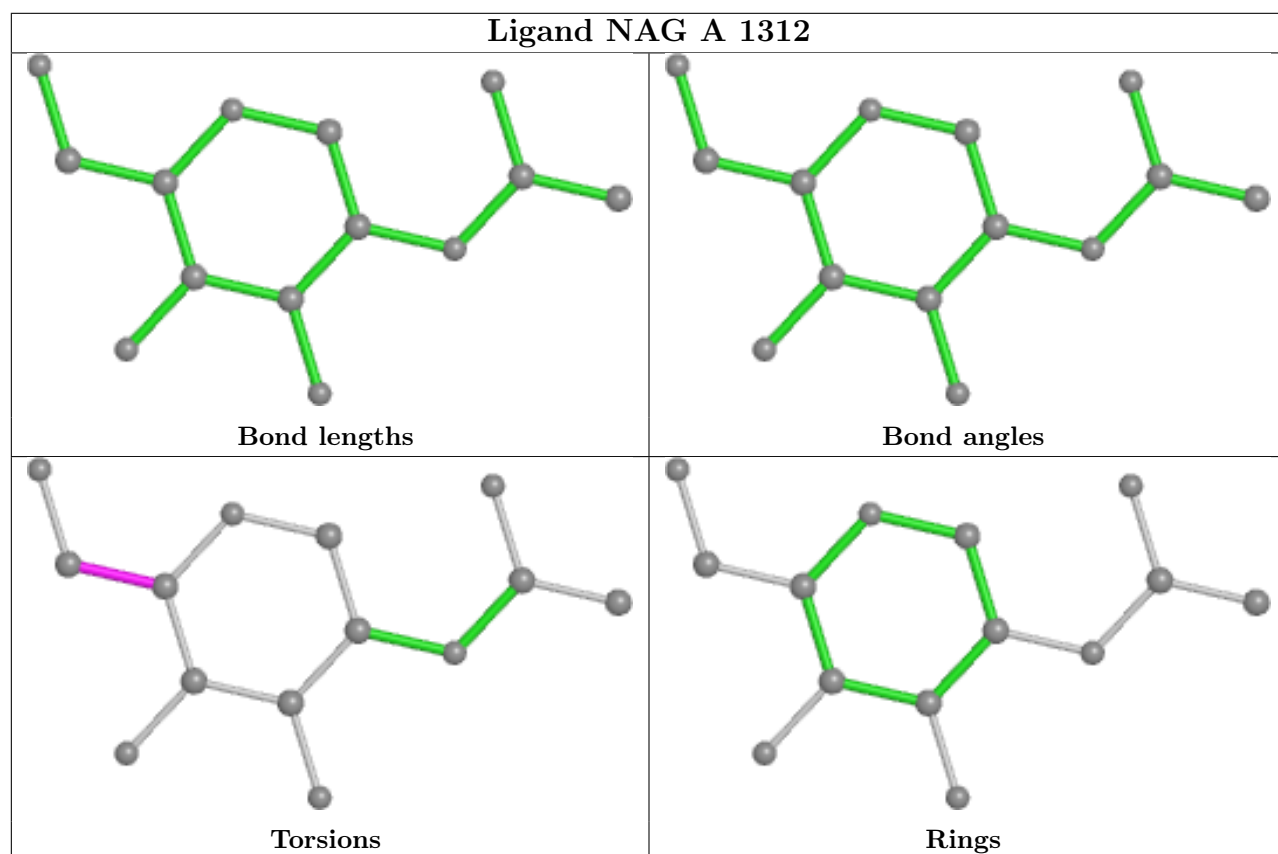
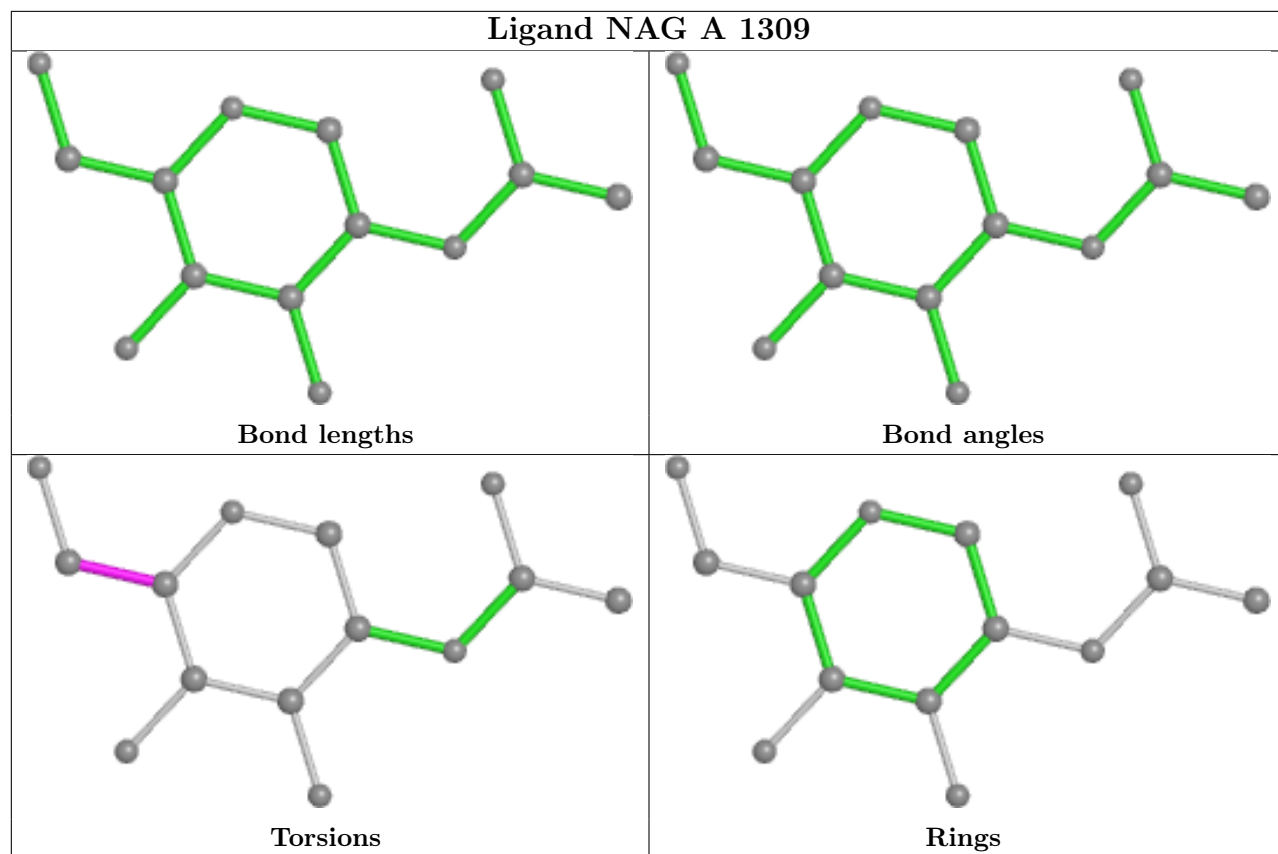


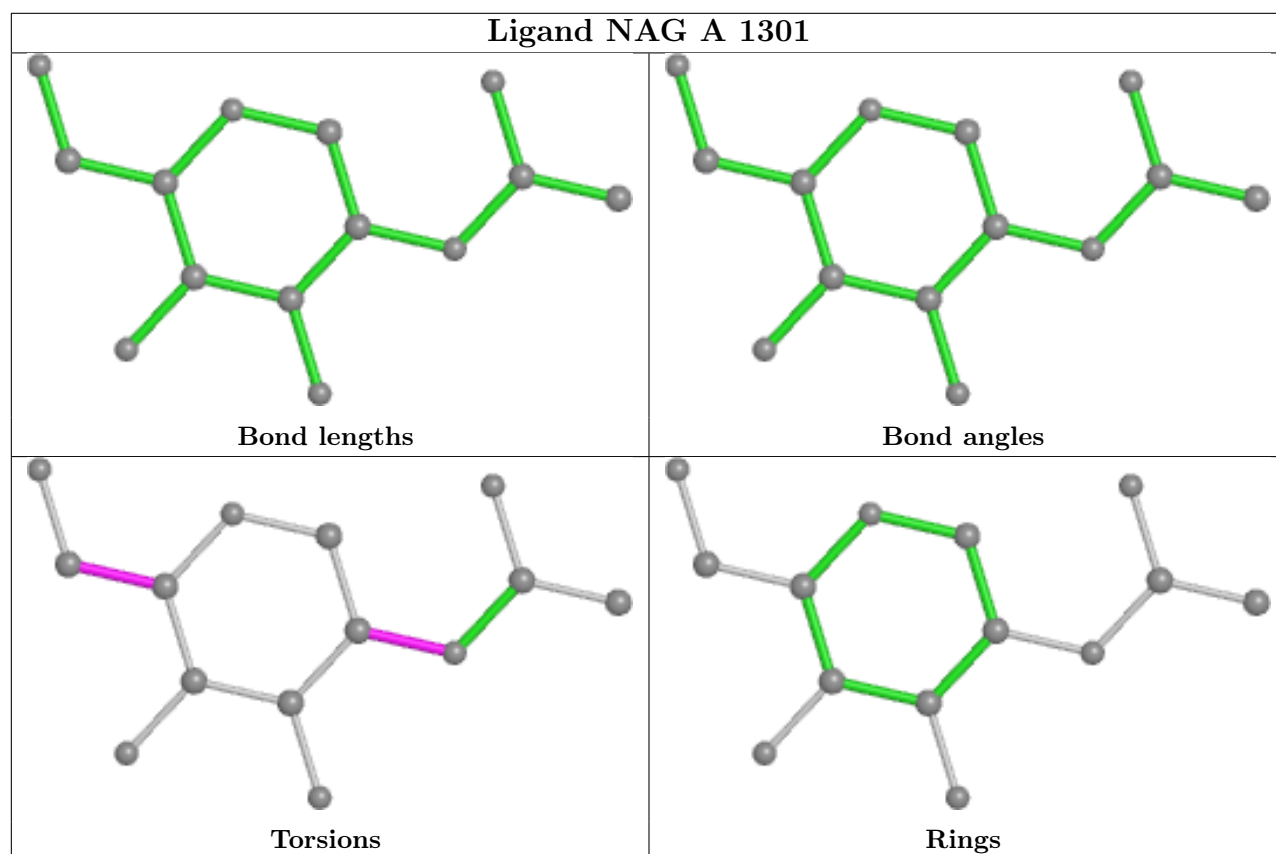
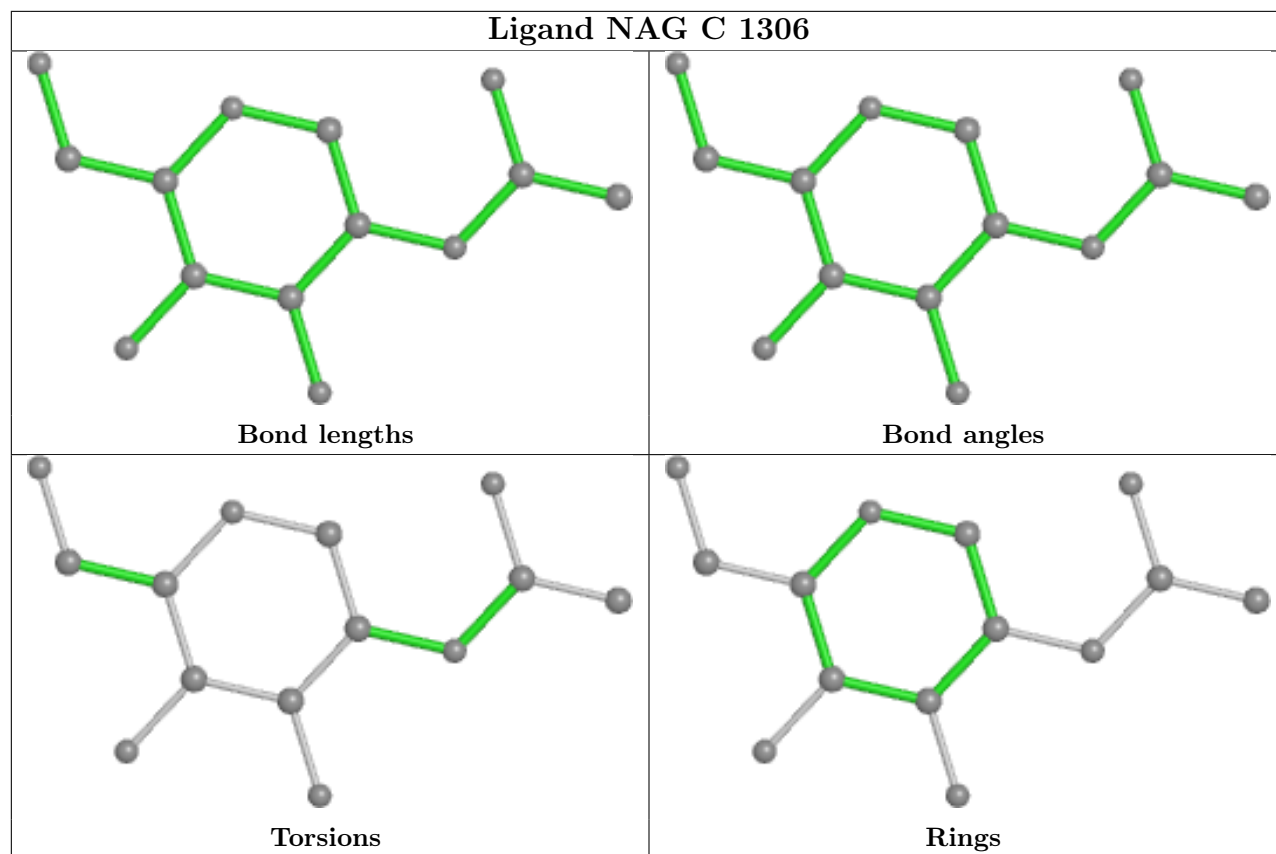
Ligand NAG A 1302

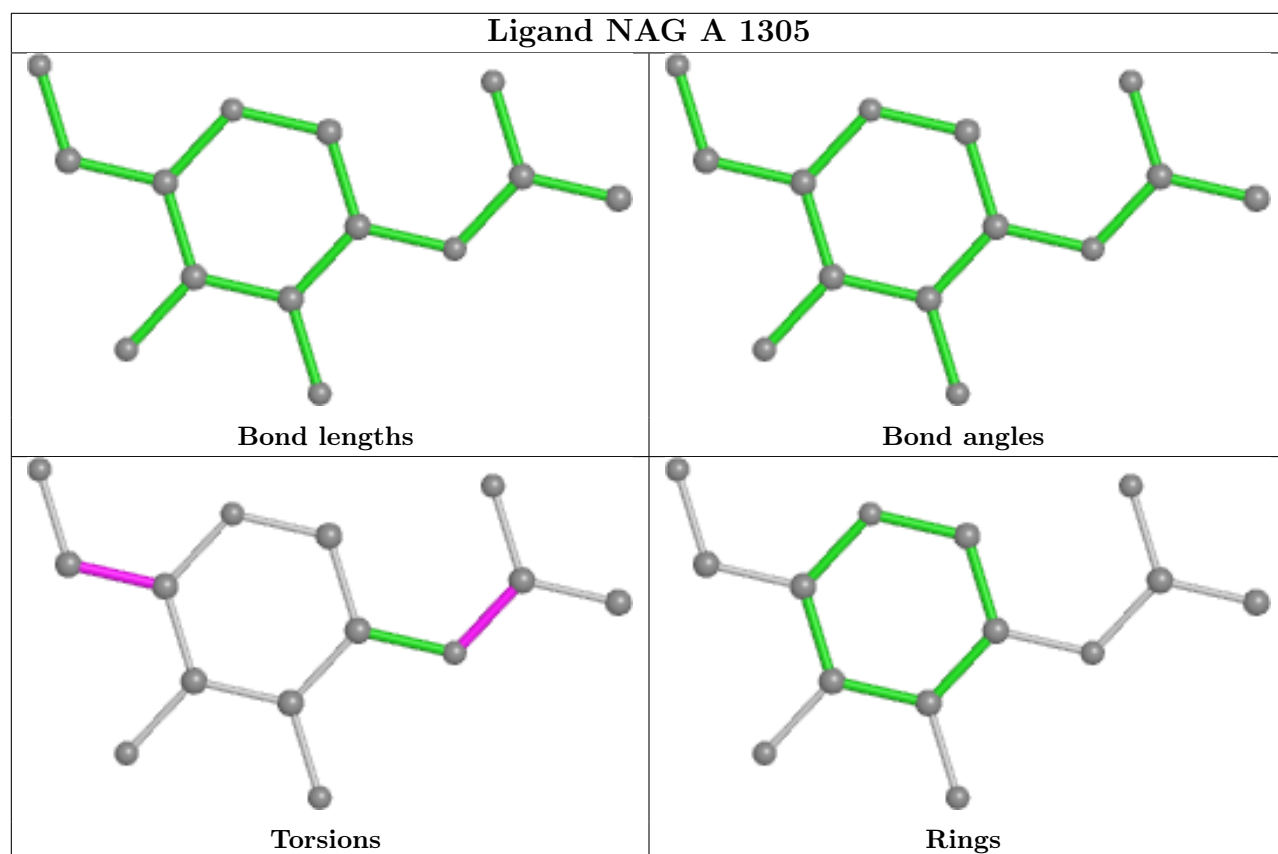
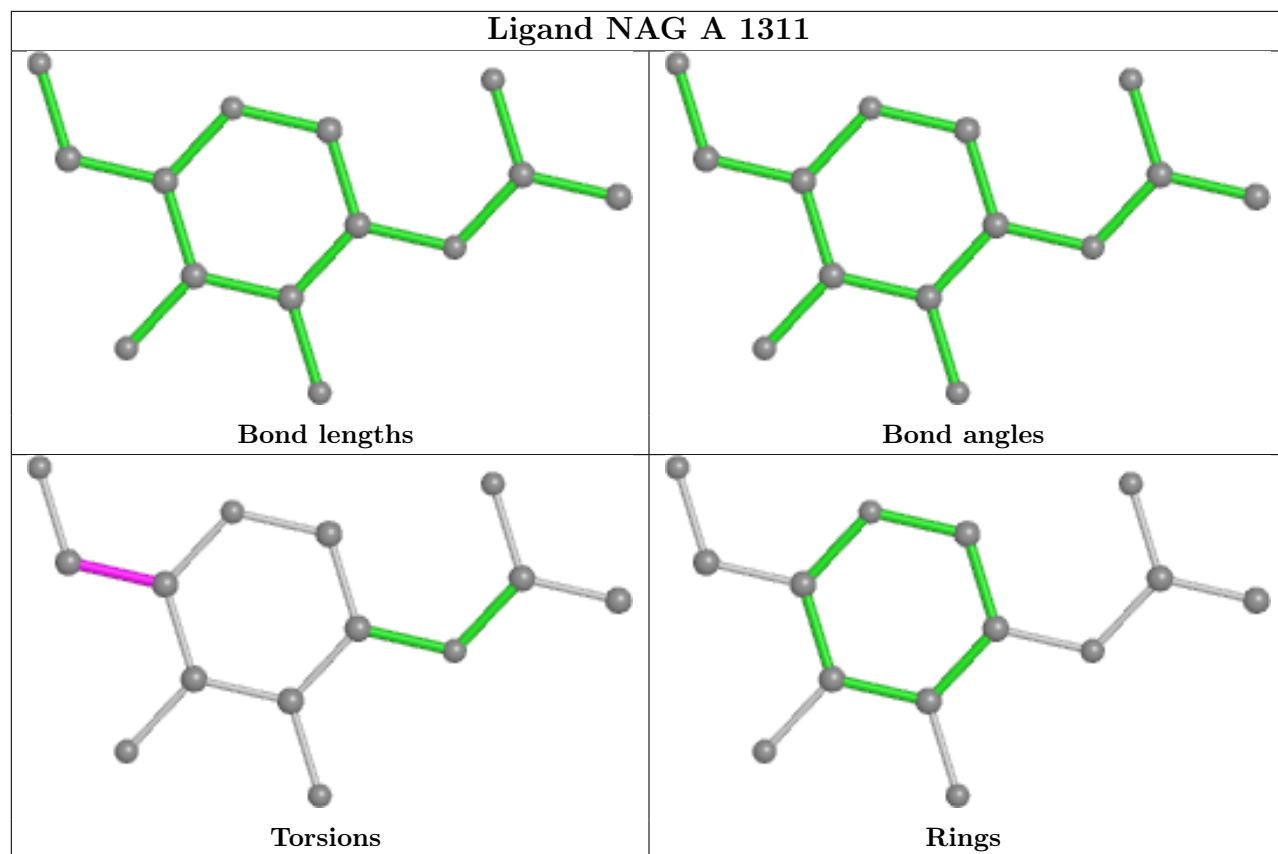


Ligand NAG A 1314

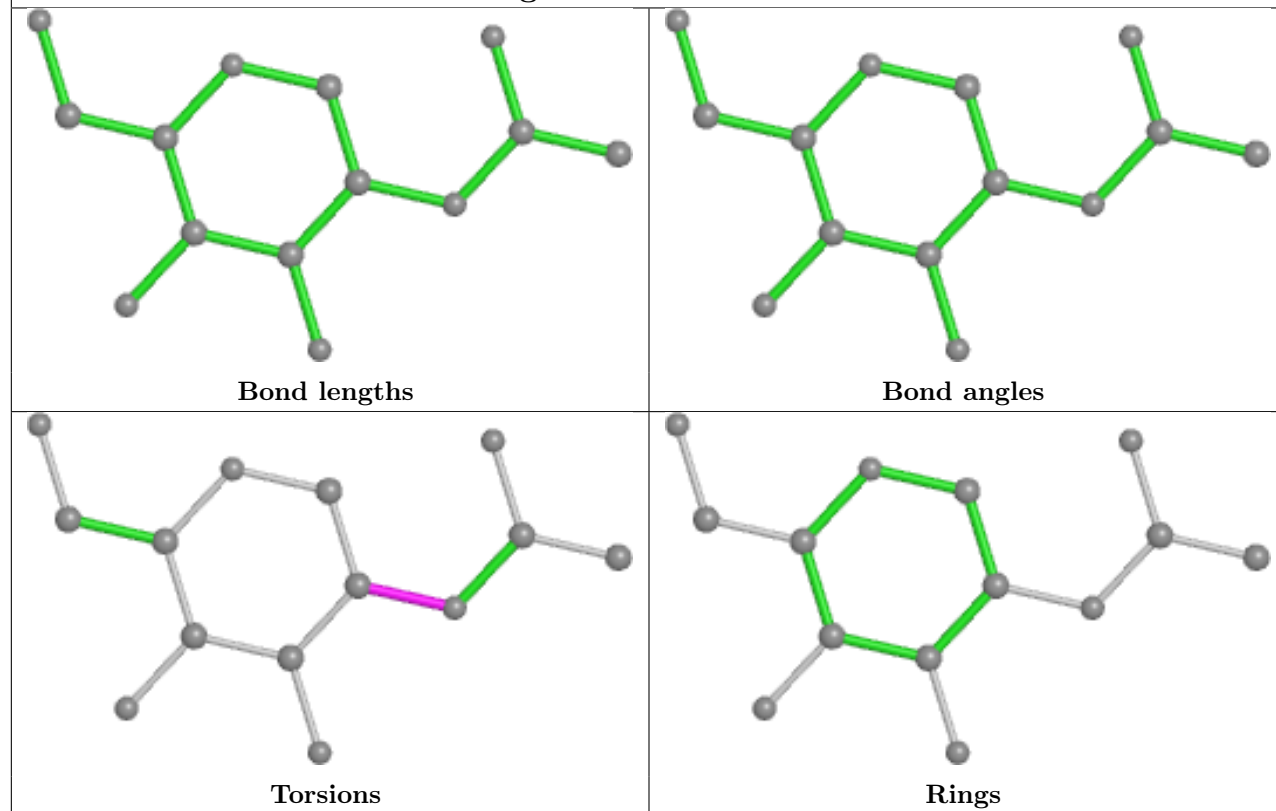




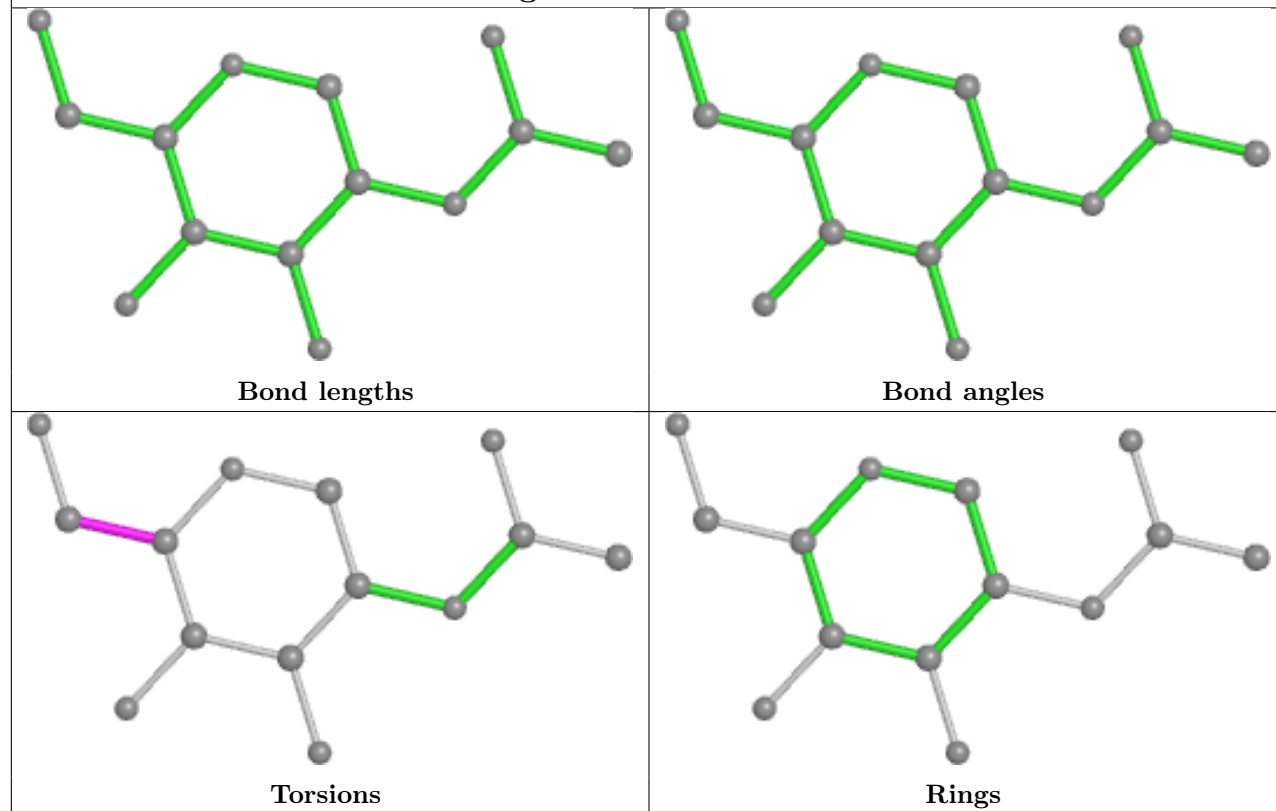


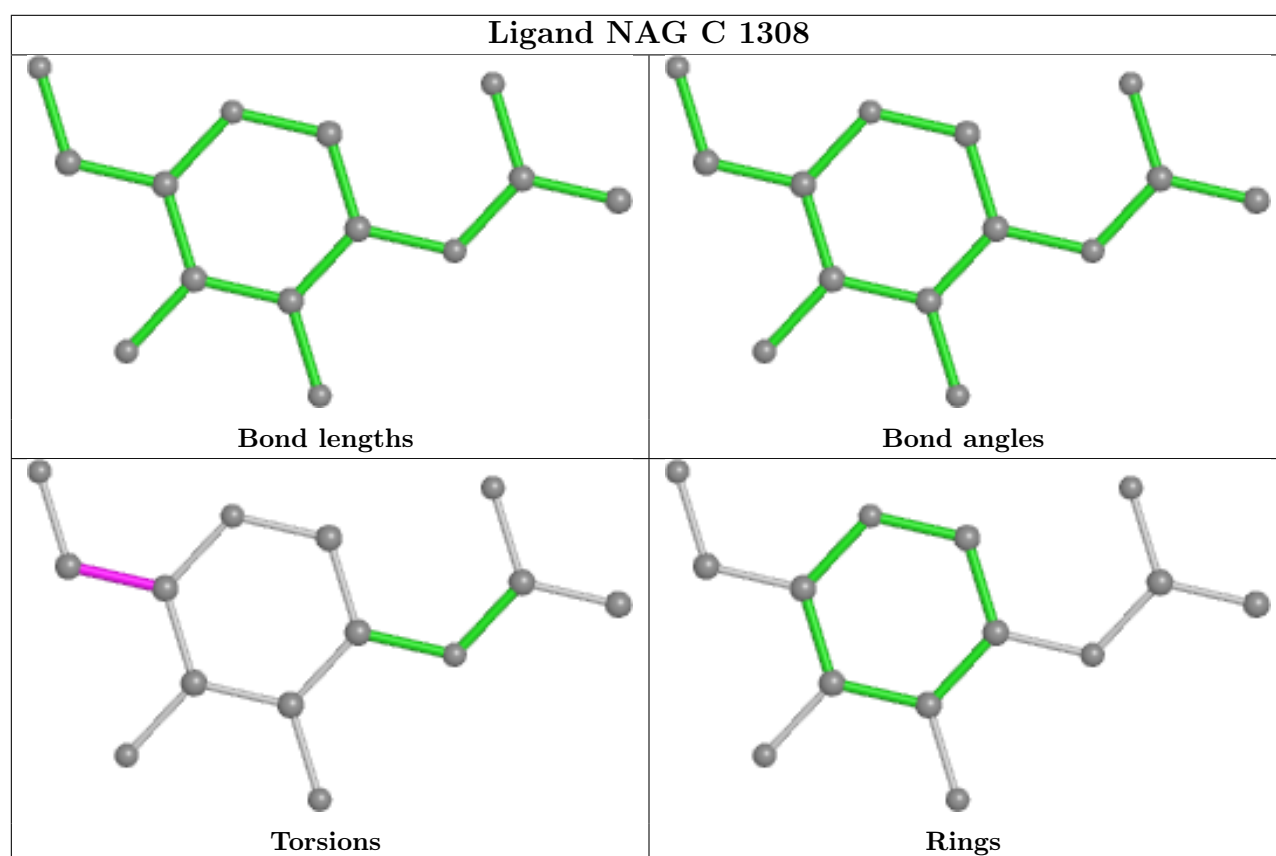
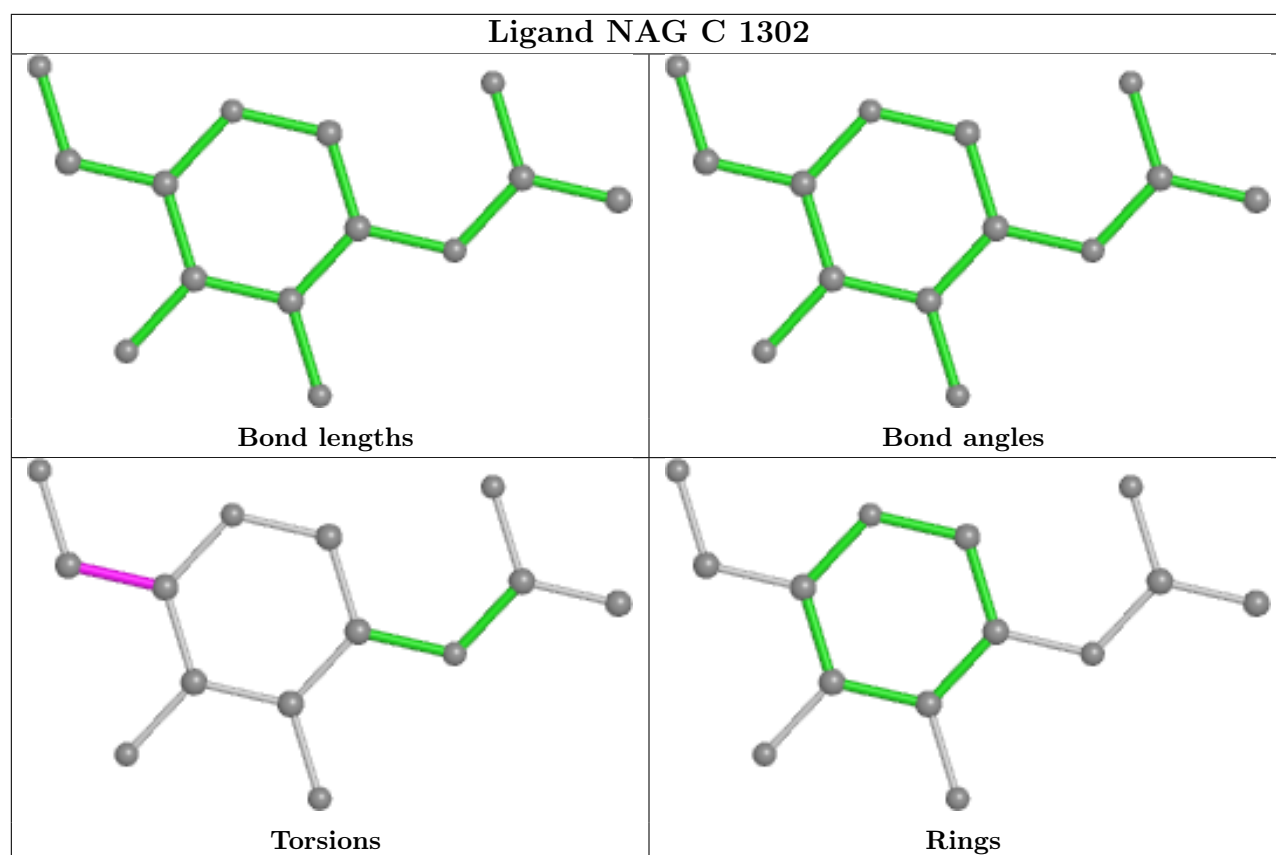


Ligand NAG B 1302

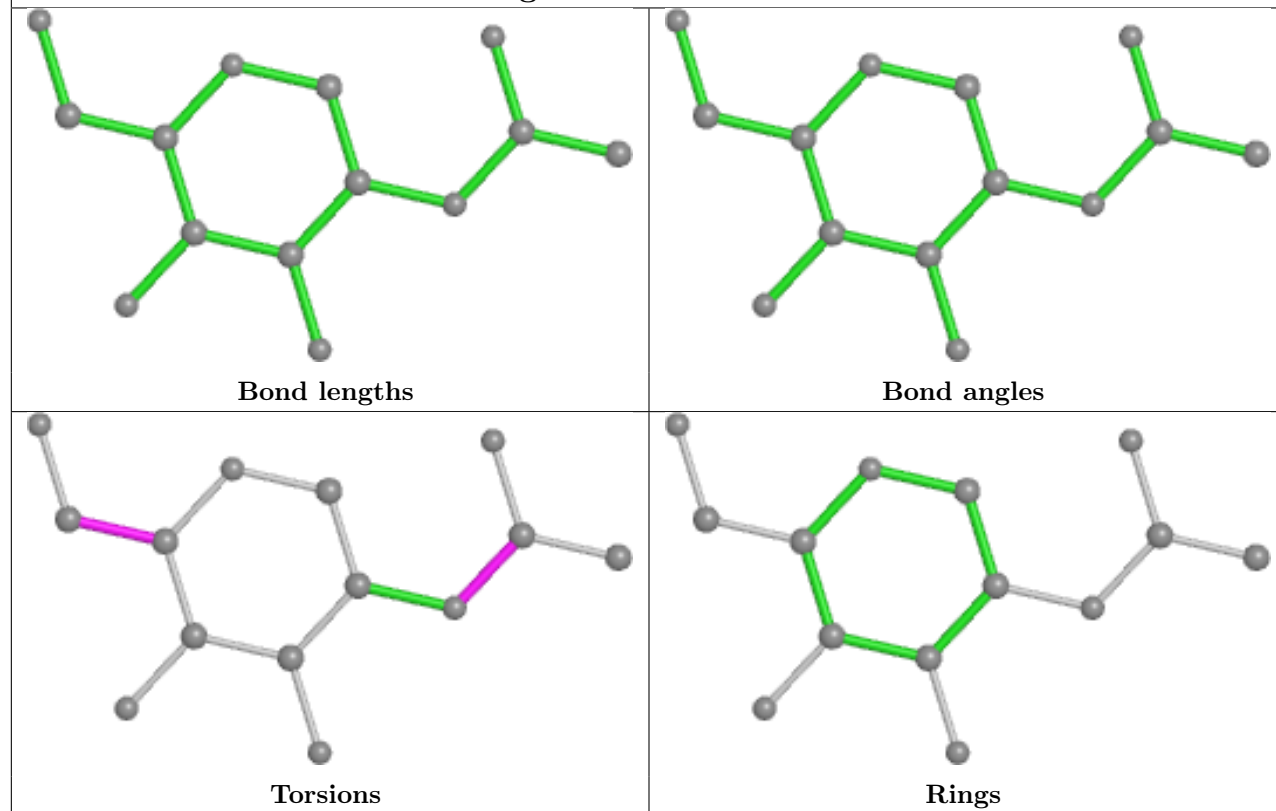


Ligand NAG C 1307

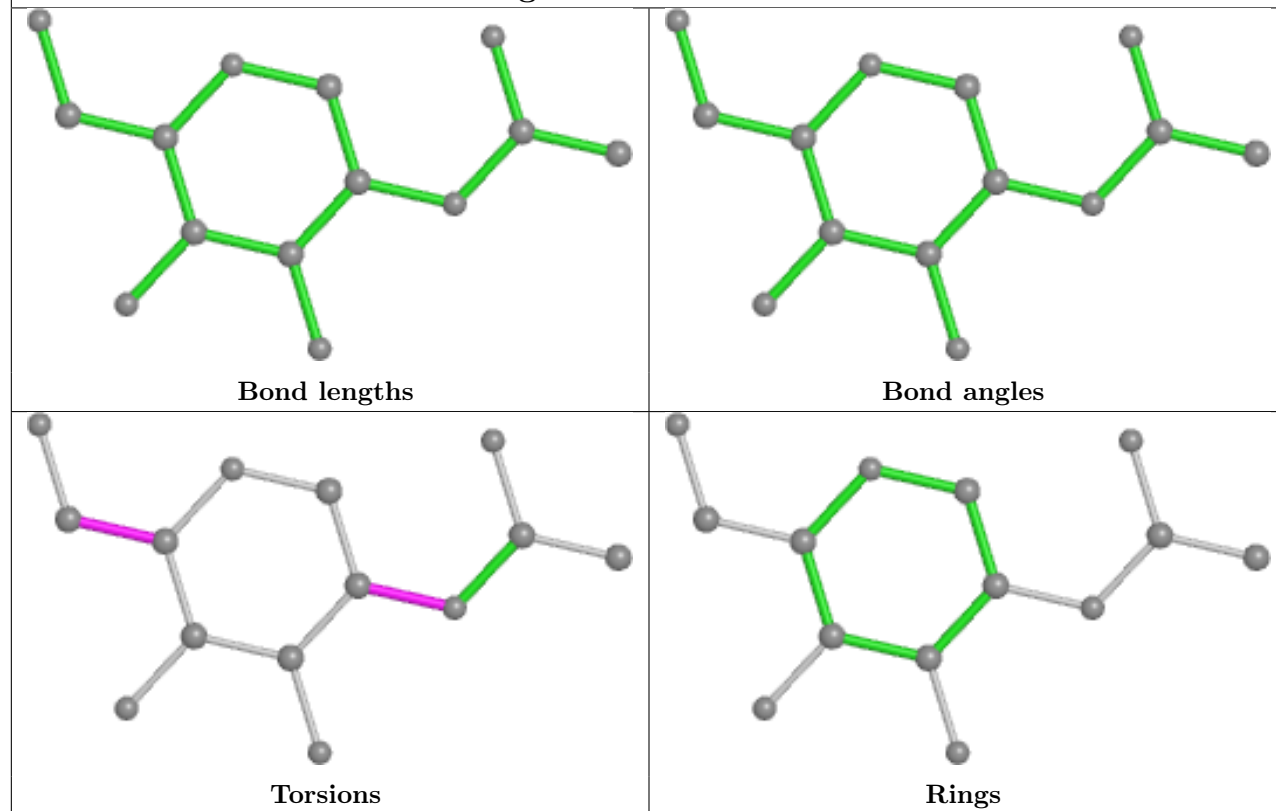




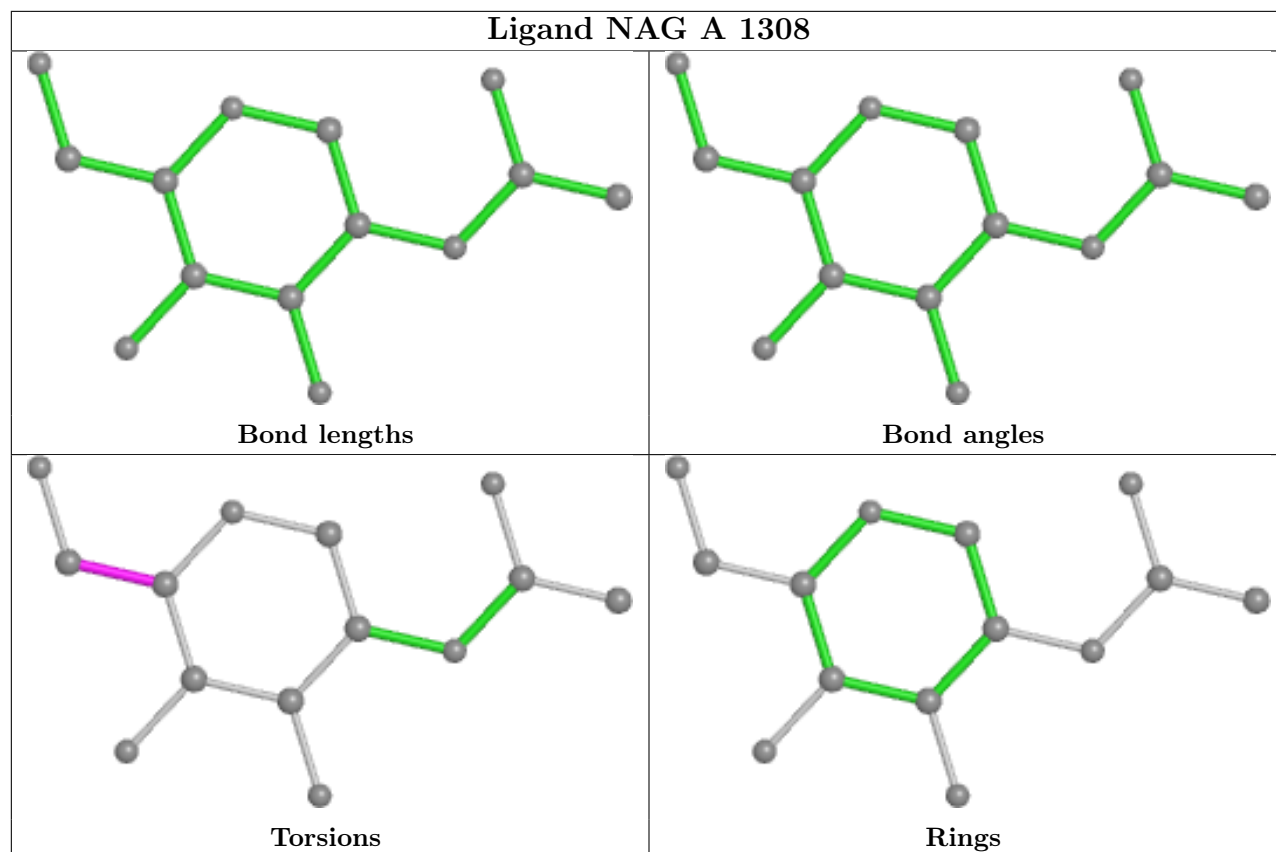
Ligand NAG C 1305



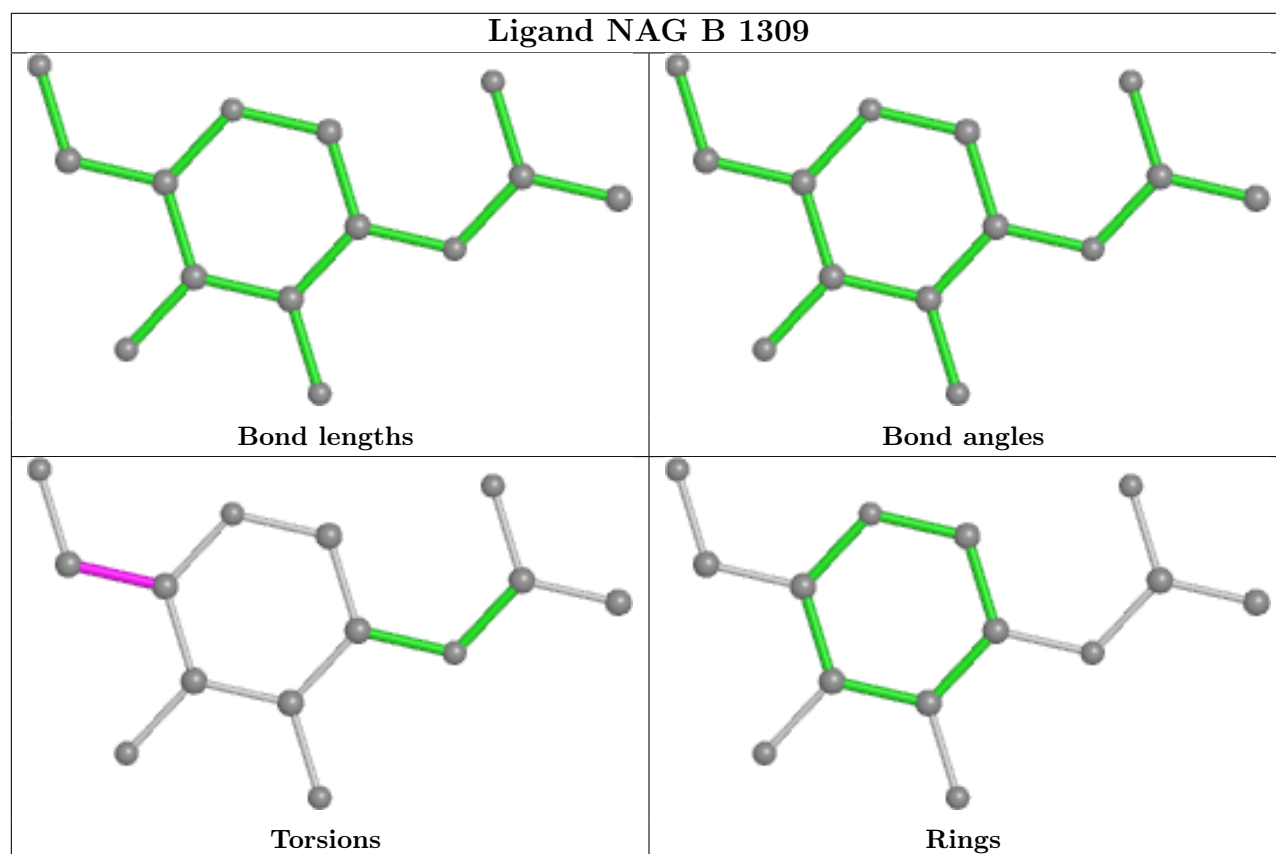
Ligand NAG A 1304



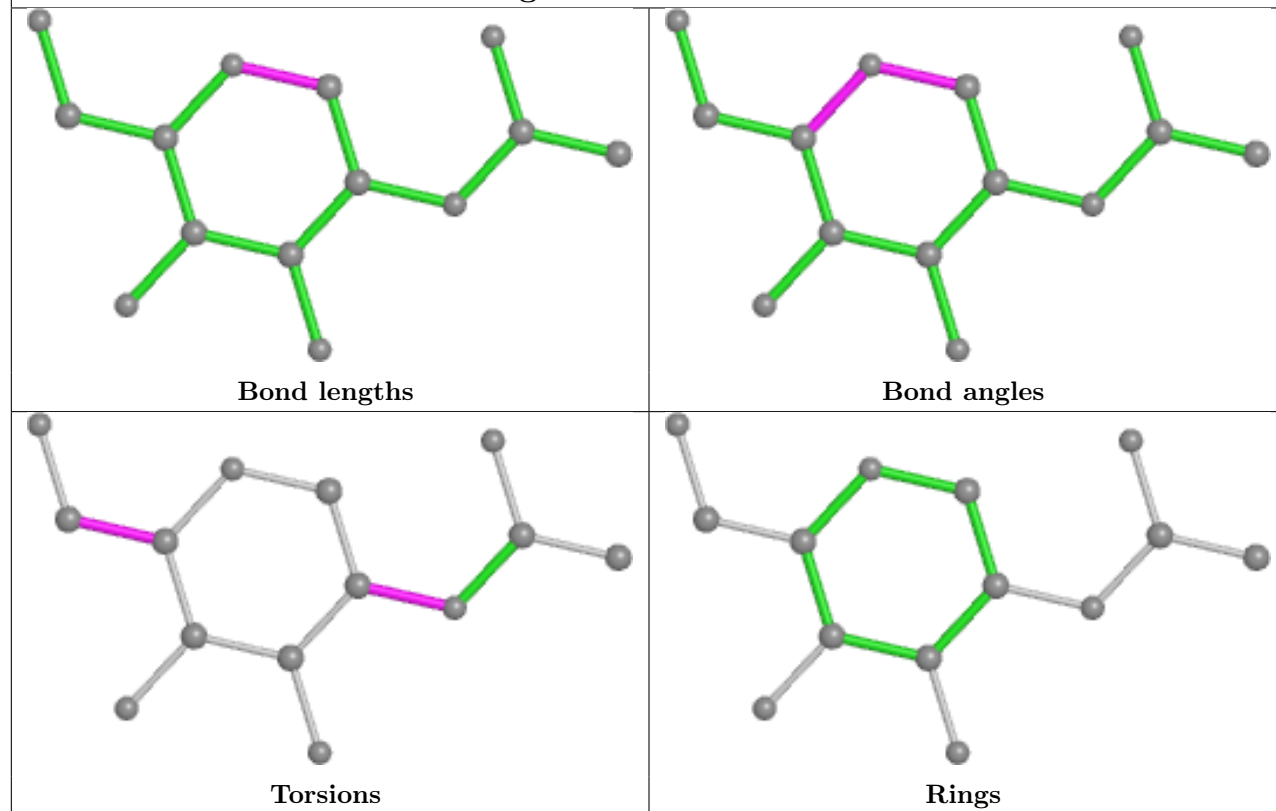
Ligand NAG A 1308



Ligand NAG B 1309



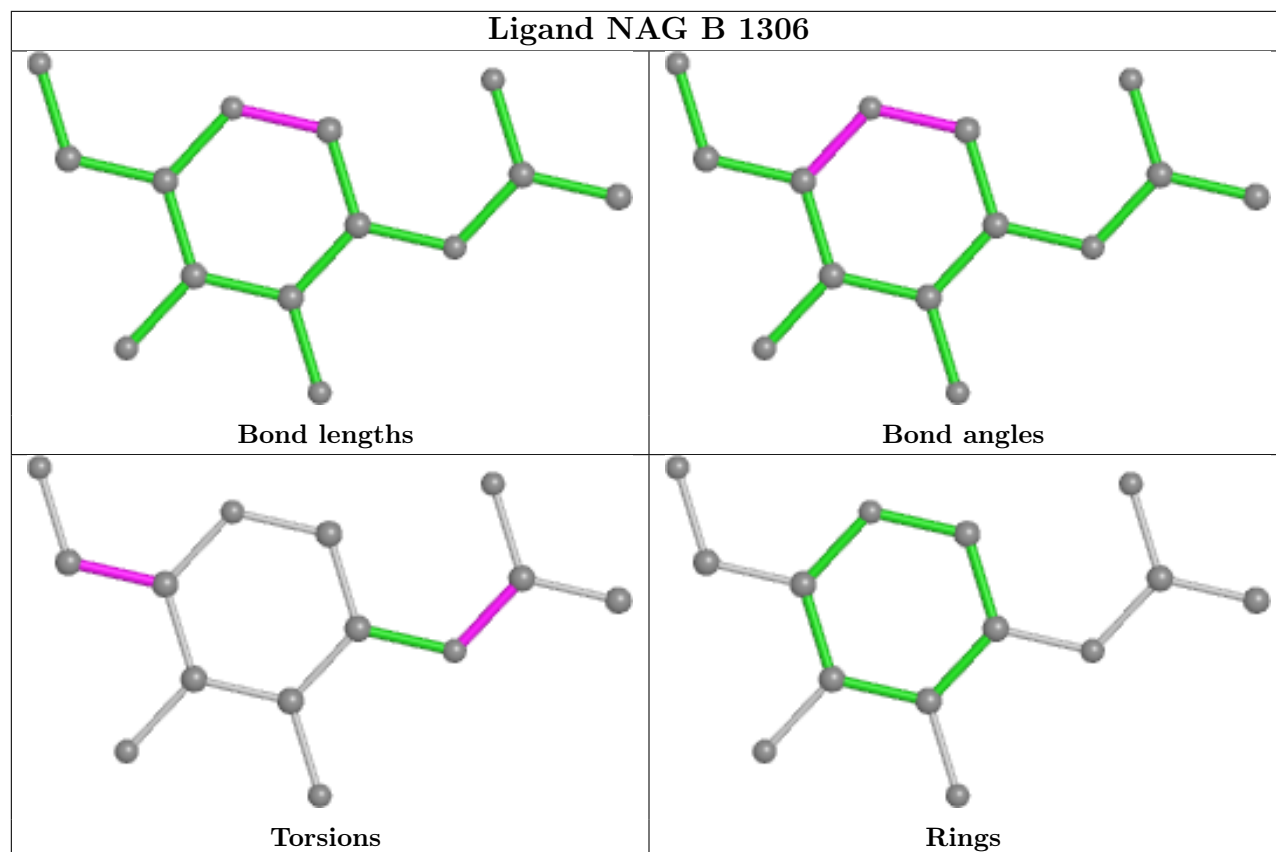
Ligand NAG C 1301



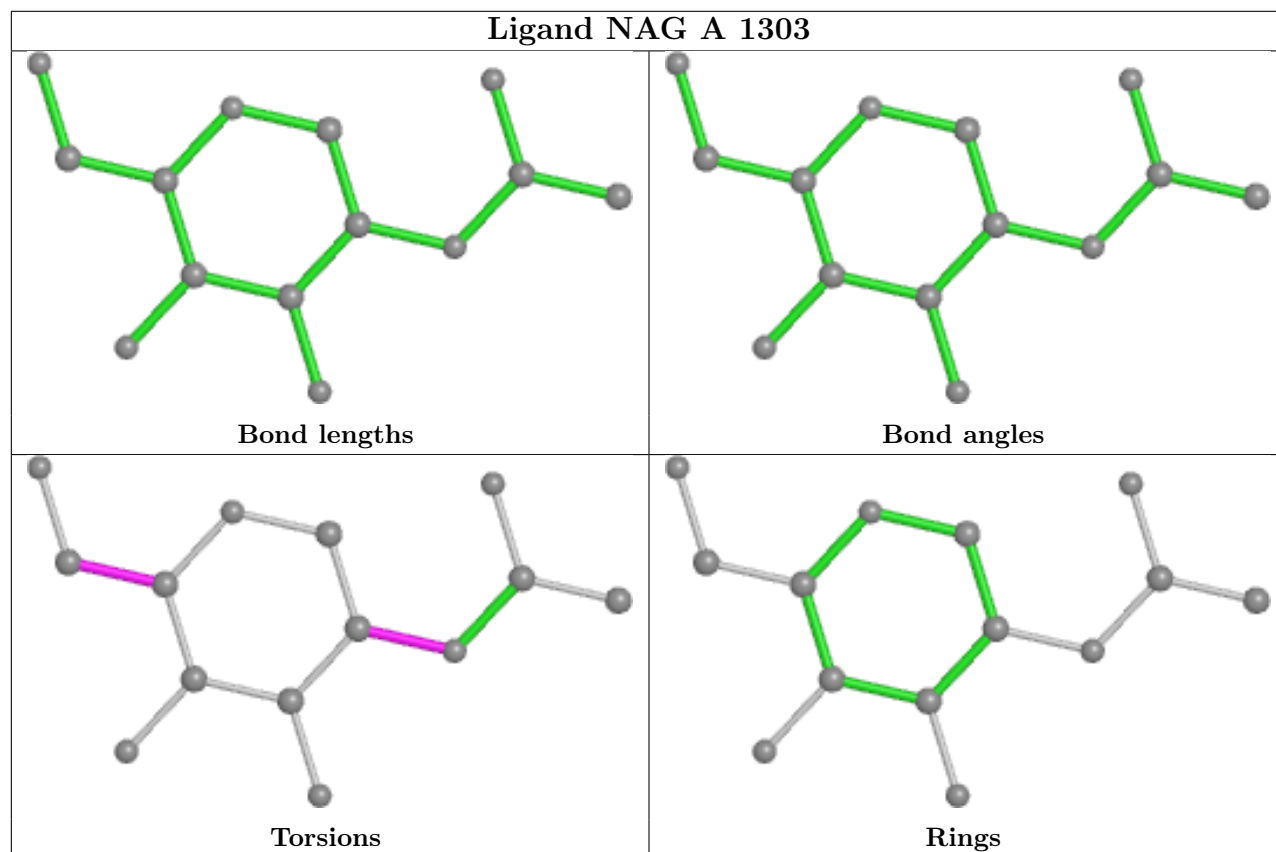
Ligand NAG C 1309



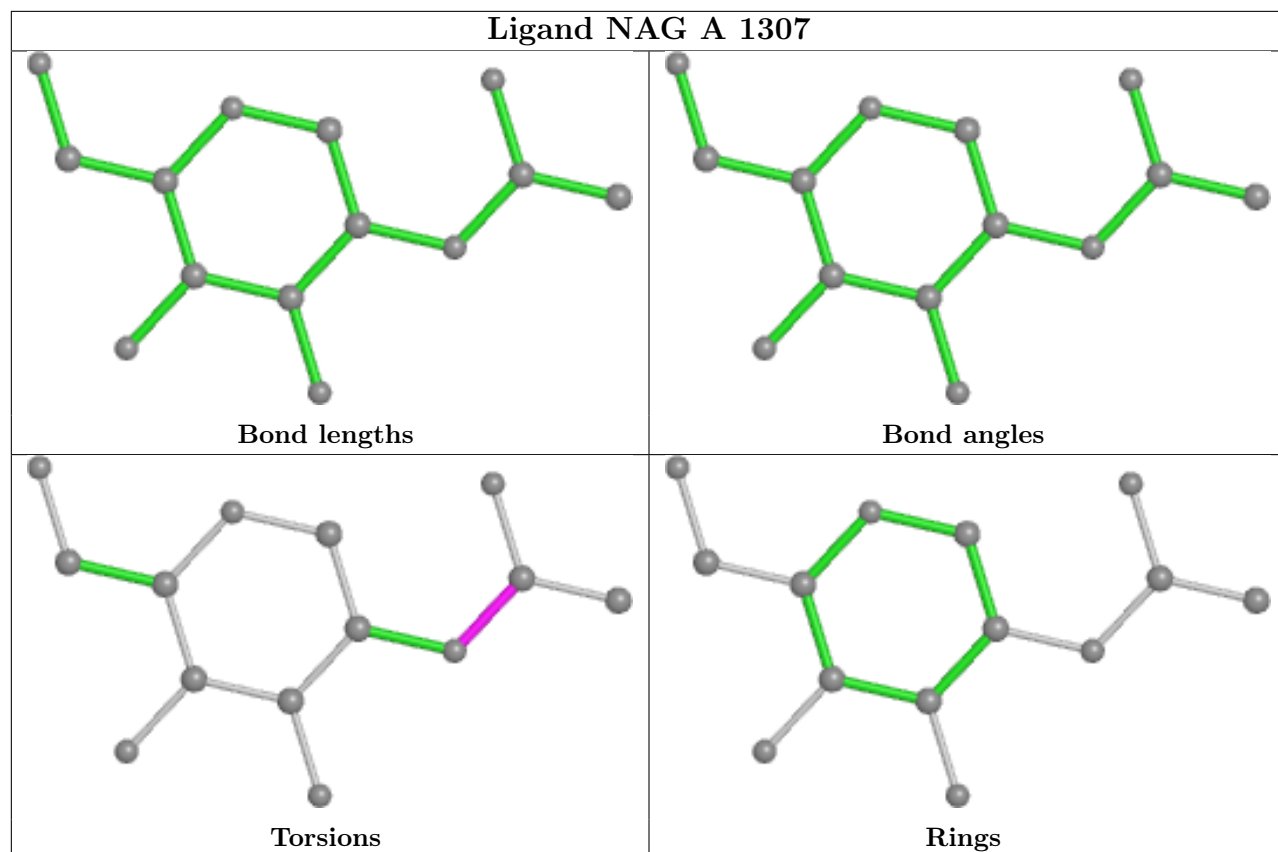
Ligand NAG B 1306



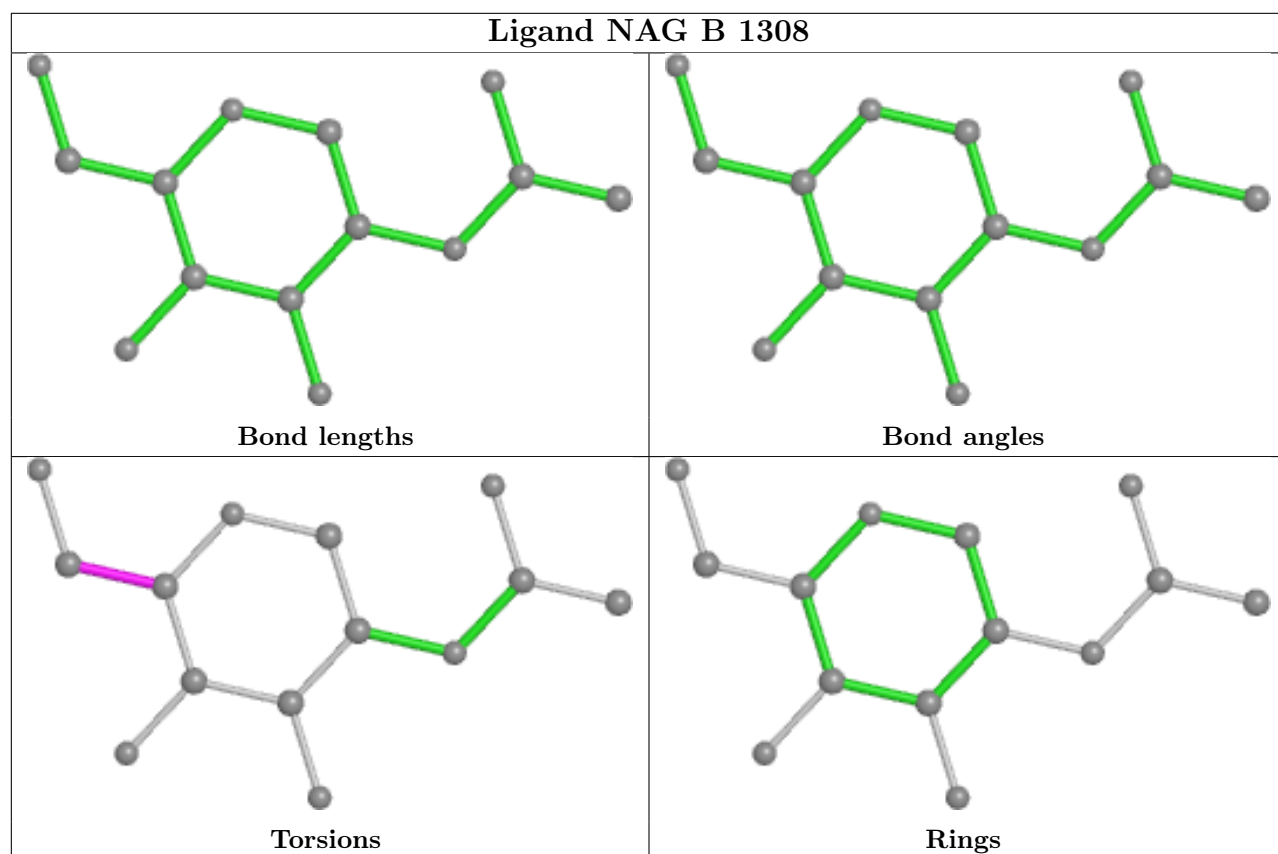
Ligand NAG A 1303

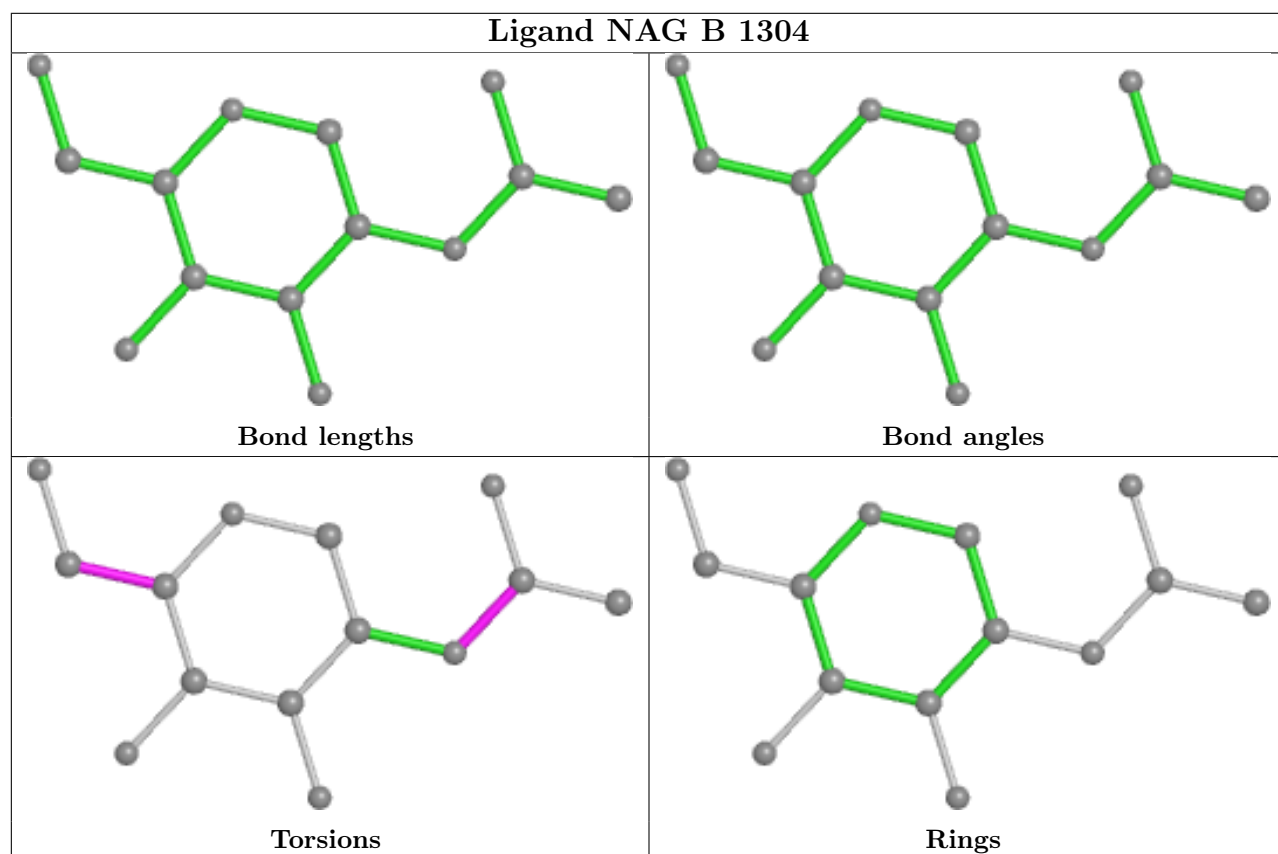
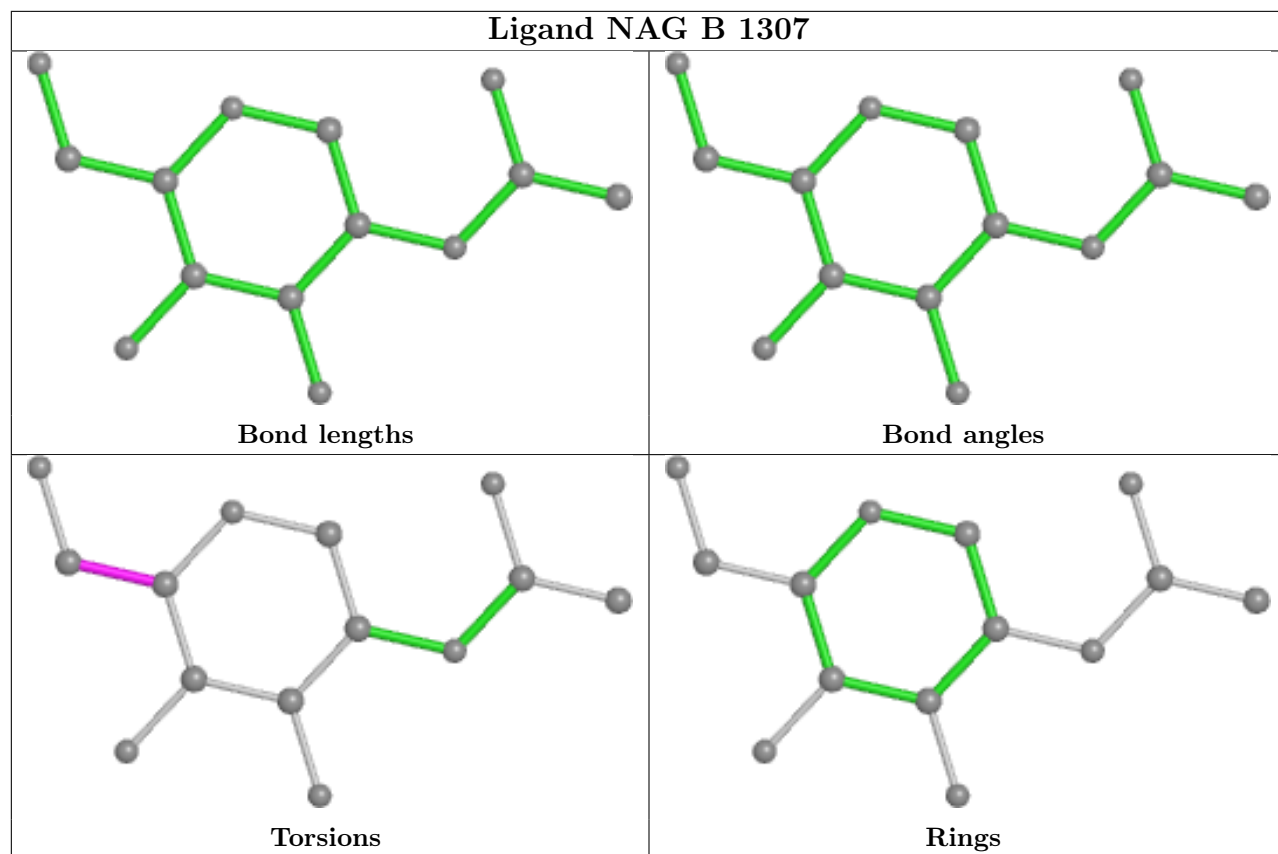


Ligand NAG A 1307



Ligand NAG B 1308





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

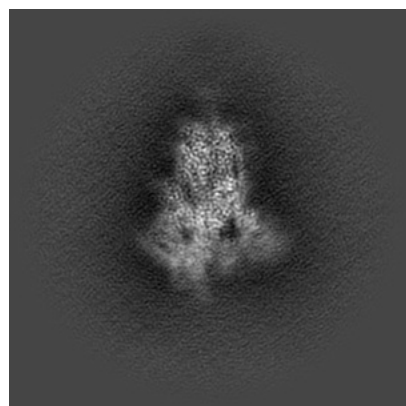
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38459. These allow visual inspection of the internal detail of the map and identification of artifacts.

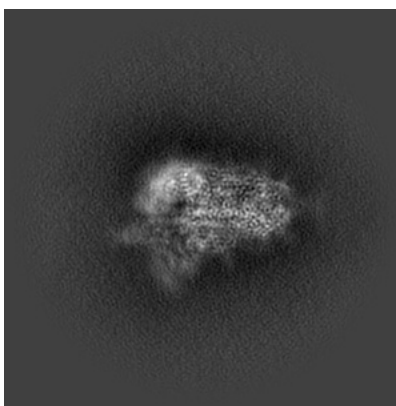
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

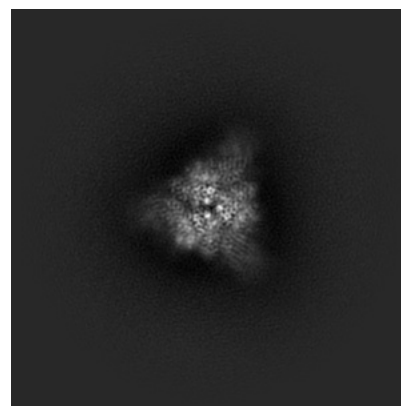
6.1.1 Primary map



X

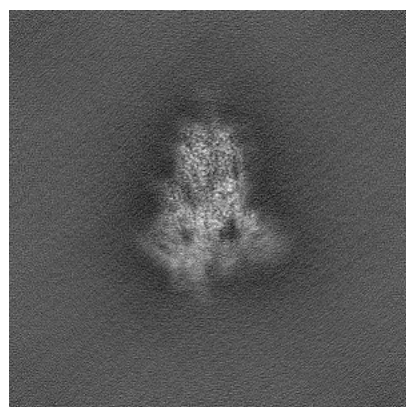


Y

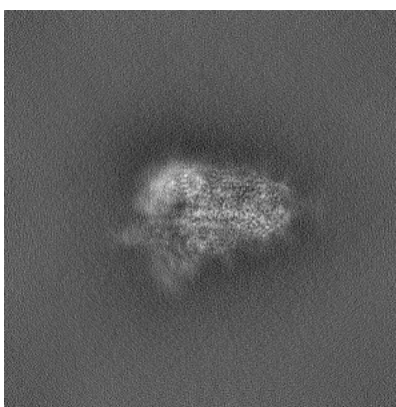


Z

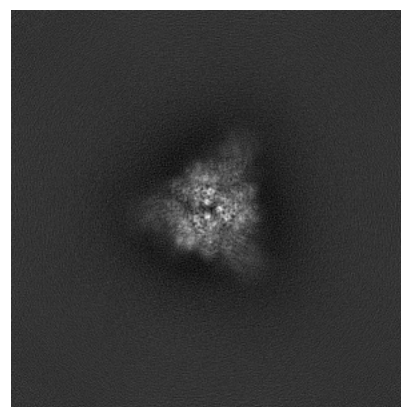
6.1.2 Raw map



X



Y

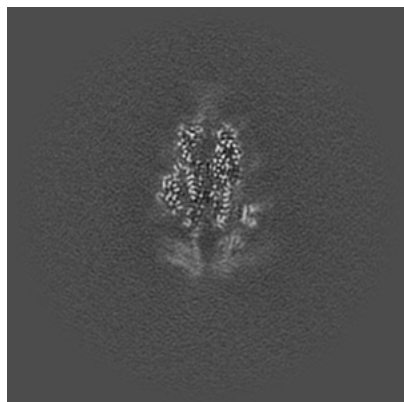


Z

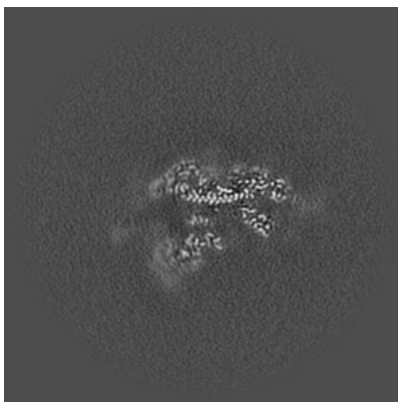
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

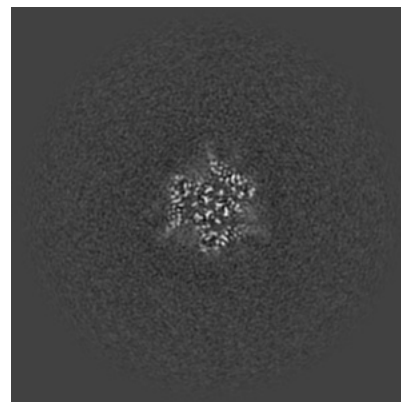
6.2.1 Primary map



X Index: 192

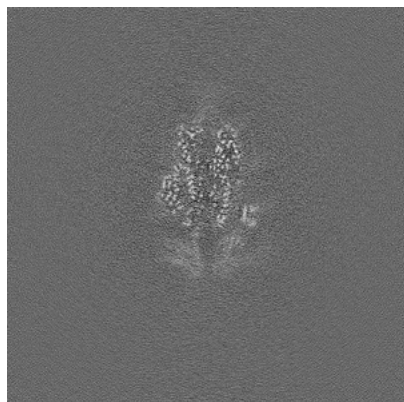


Y Index: 192

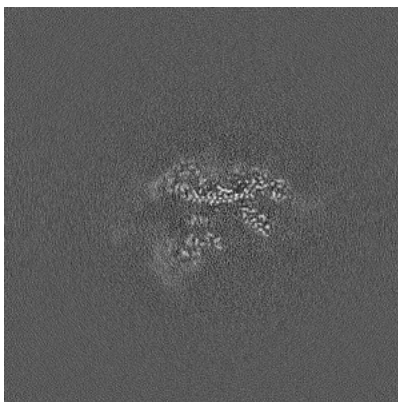


Z Index: 192

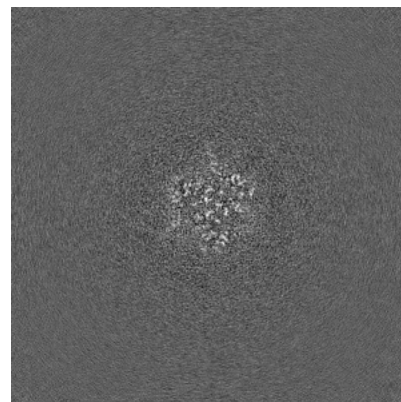
6.2.2 Raw map



X Index: 192



Y Index: 192

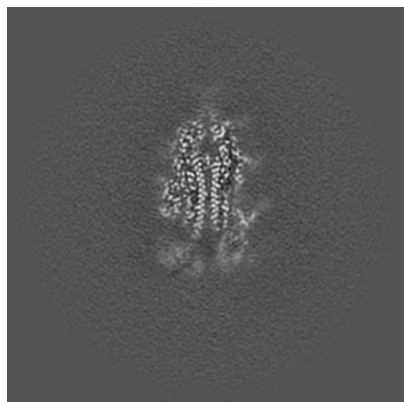


Z Index: 192

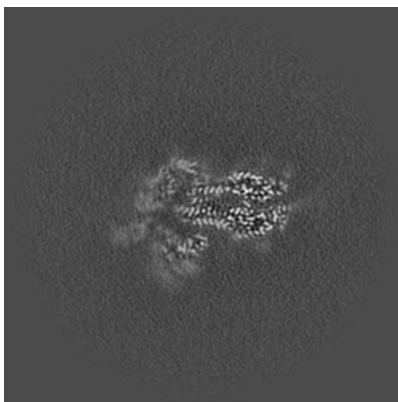
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

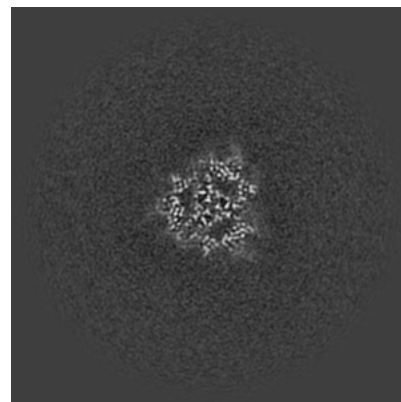
6.3.1 Primary map



X Index: 188

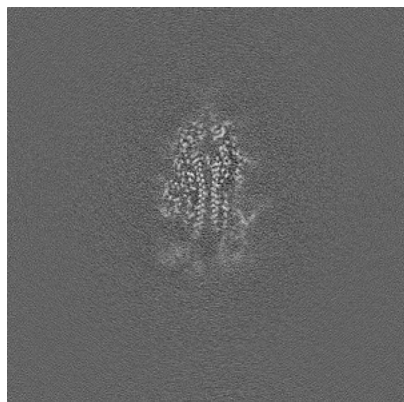


Y Index: 183

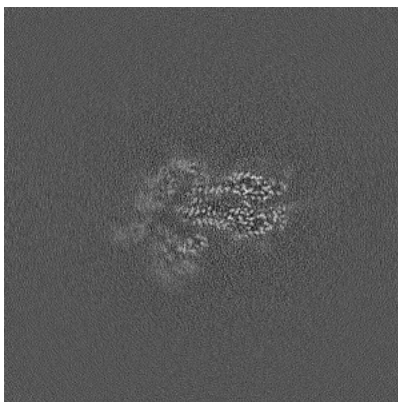


Z Index: 188

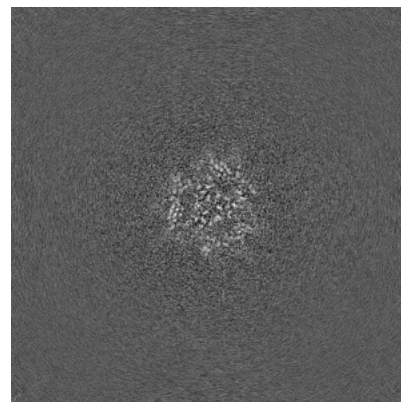
6.3.2 Raw map



X Index: 188



Y Index: 183

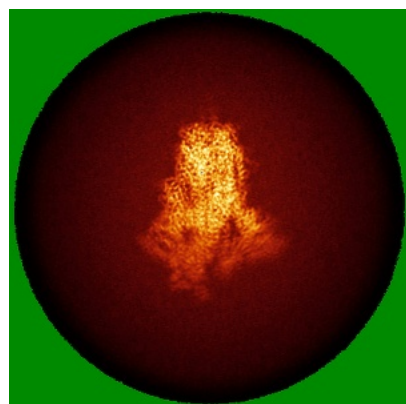


Z Index: 189

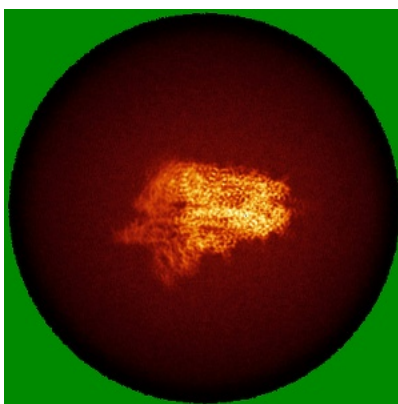
The images above show the largest variance slices of the map in three orthogonal directions.

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

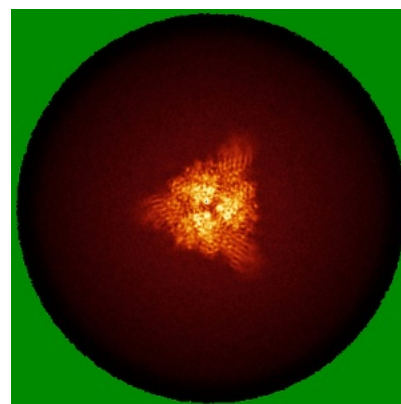
6.4.1 Primary map



X

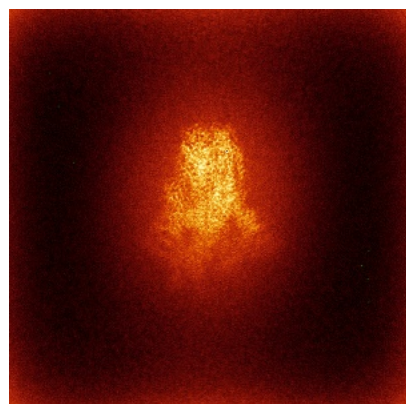


Y

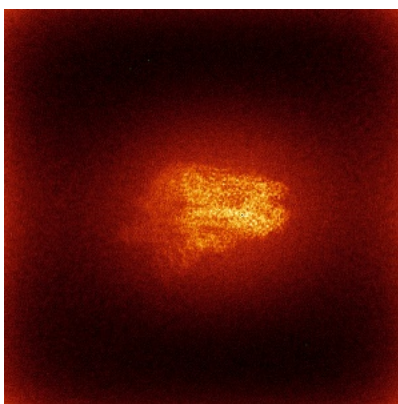


Z

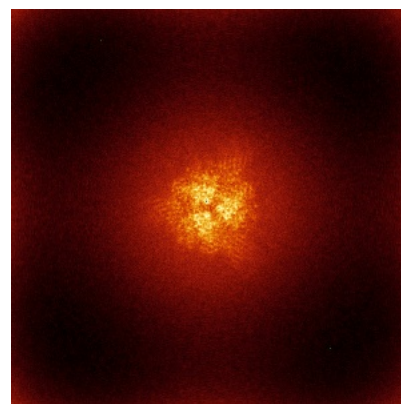
6.4.2 Raw map



X



Y

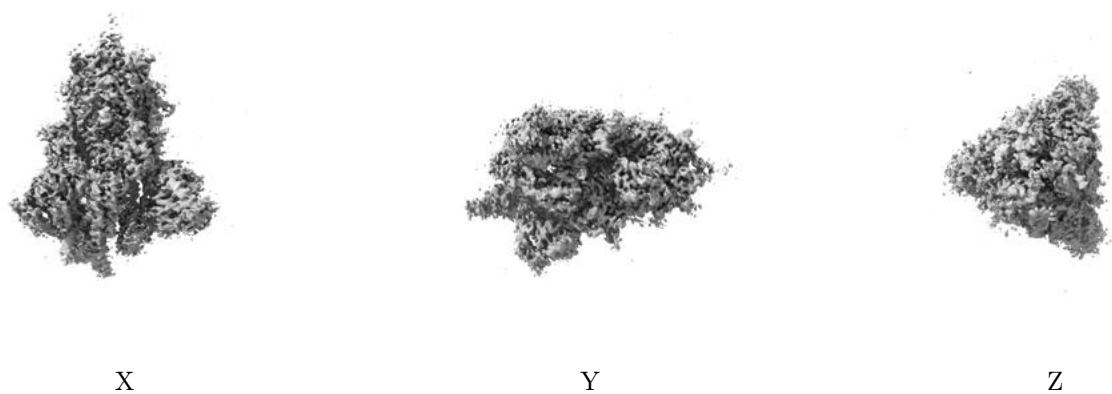


Z

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.

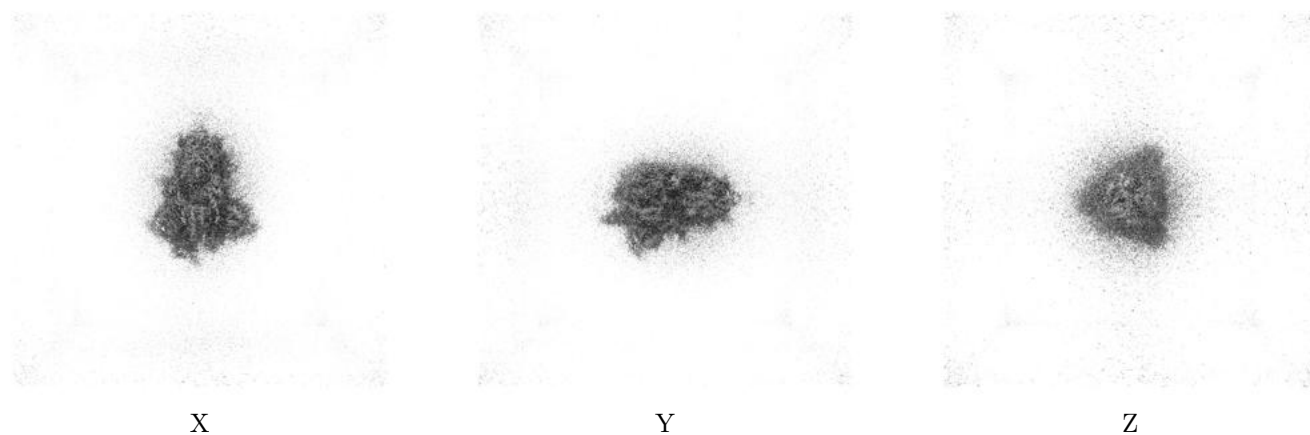
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0802. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

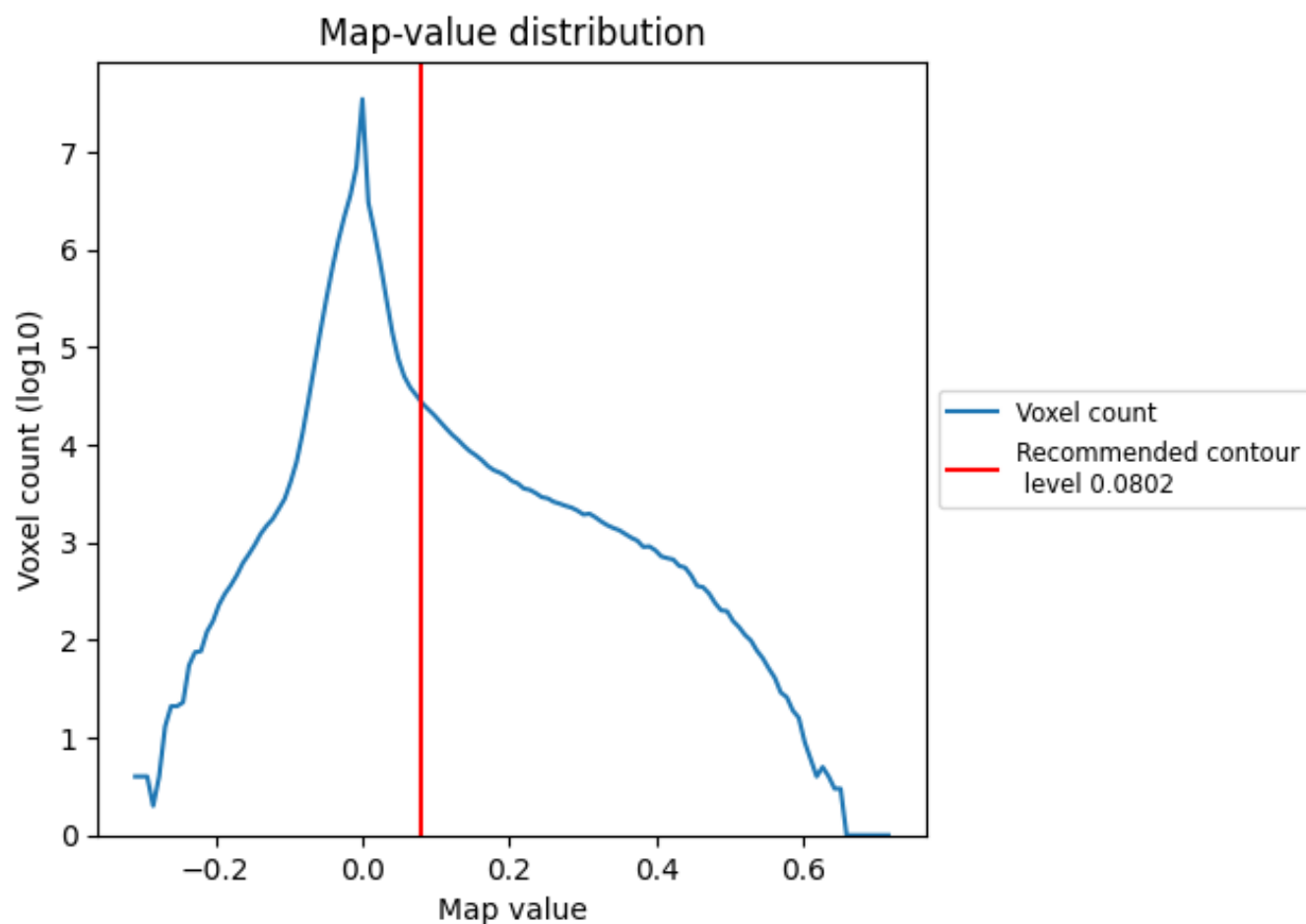
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

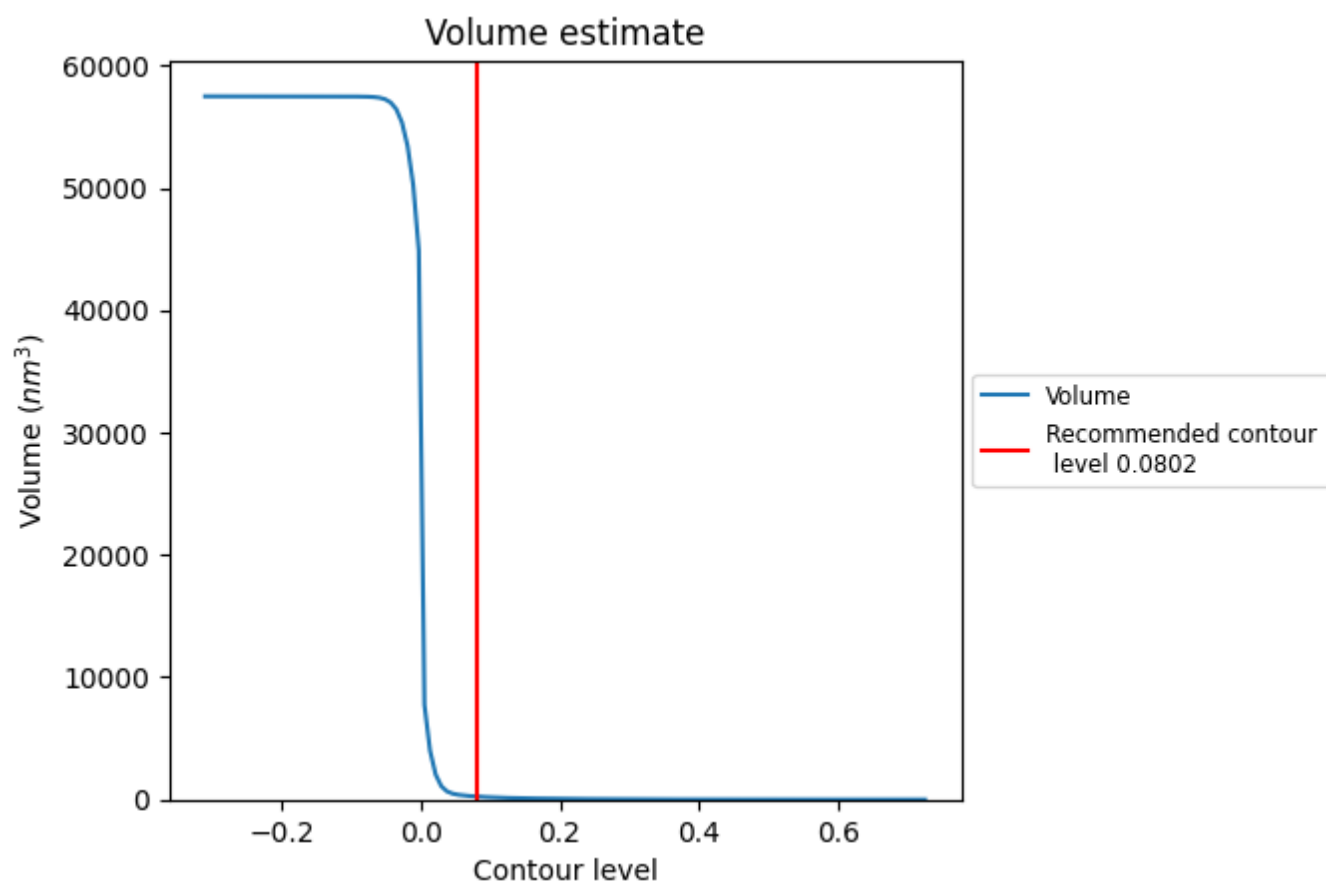
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

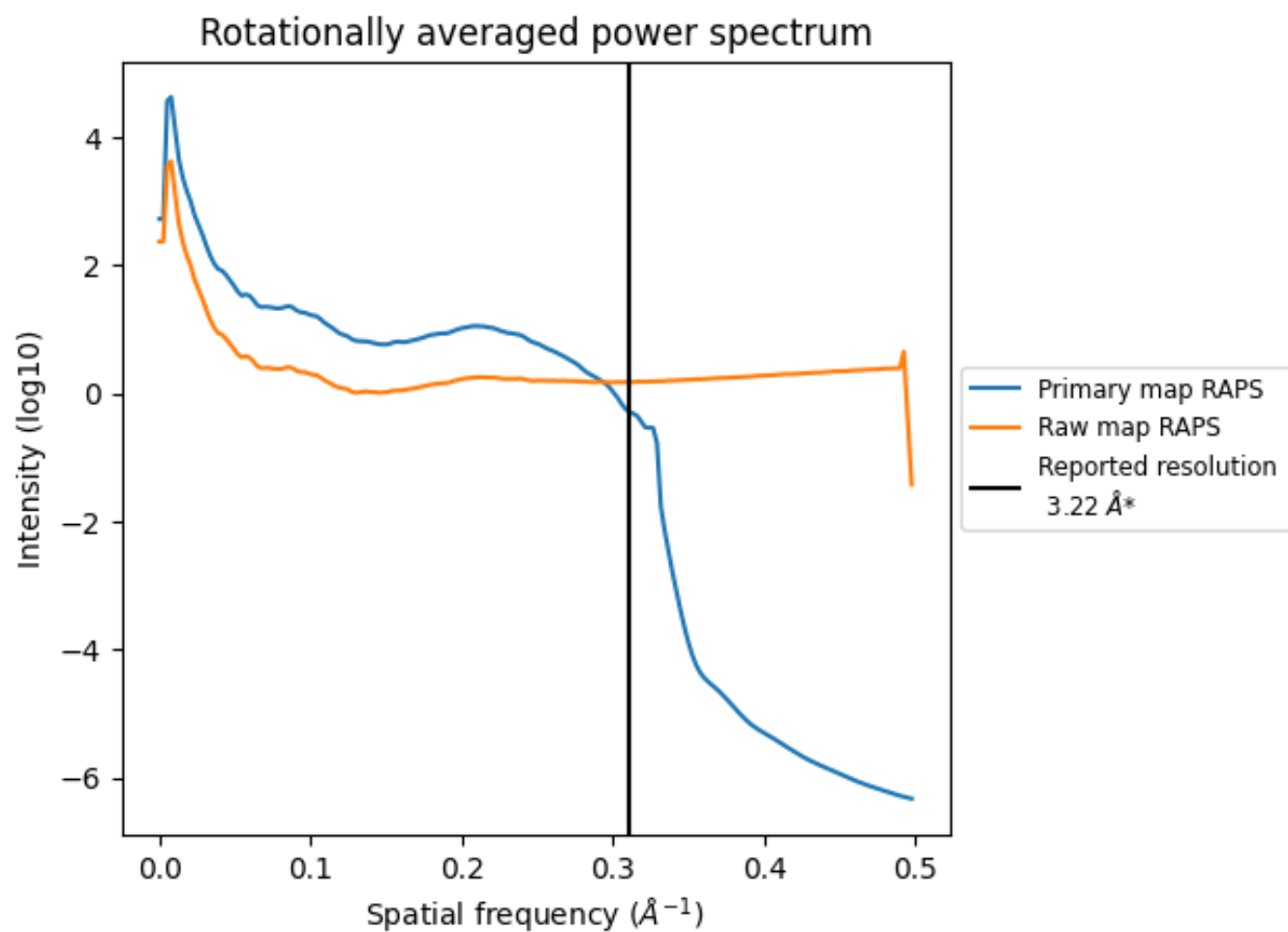
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 250 nm³; this corresponds to an approximate mass of 225 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

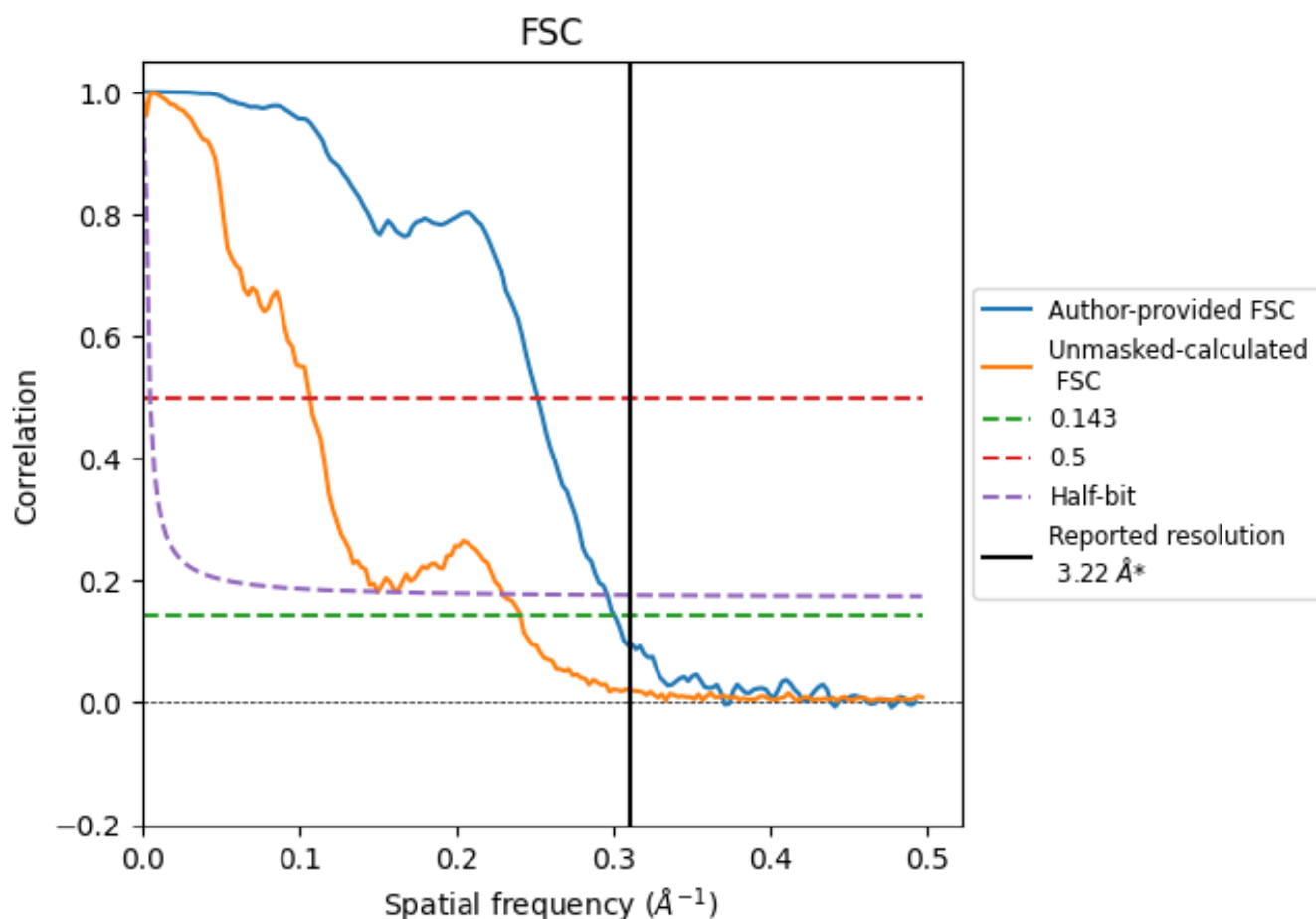


*Reported resolution corresponds to spatial frequency of 0.311 \AA^{-1}

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 0.311 \AA^{-1}

8.2 Resolution estimates [i](#)

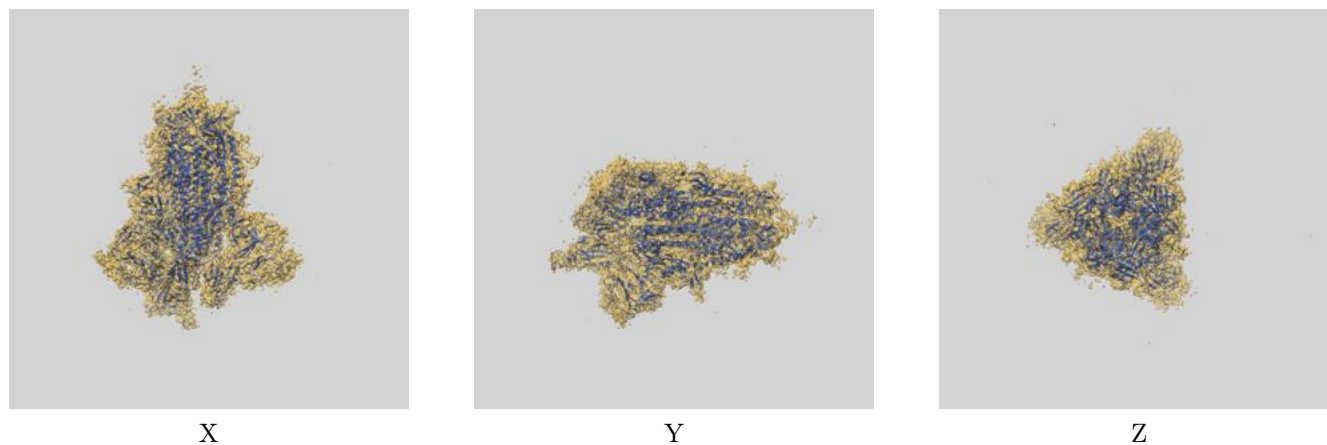
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	3.32	3.97	3.37
Unmasked-calculated*	4.14	9.35	6.66

*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 4.14 differs from the reported value 3.22 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38459 and PDB model 8XUX. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



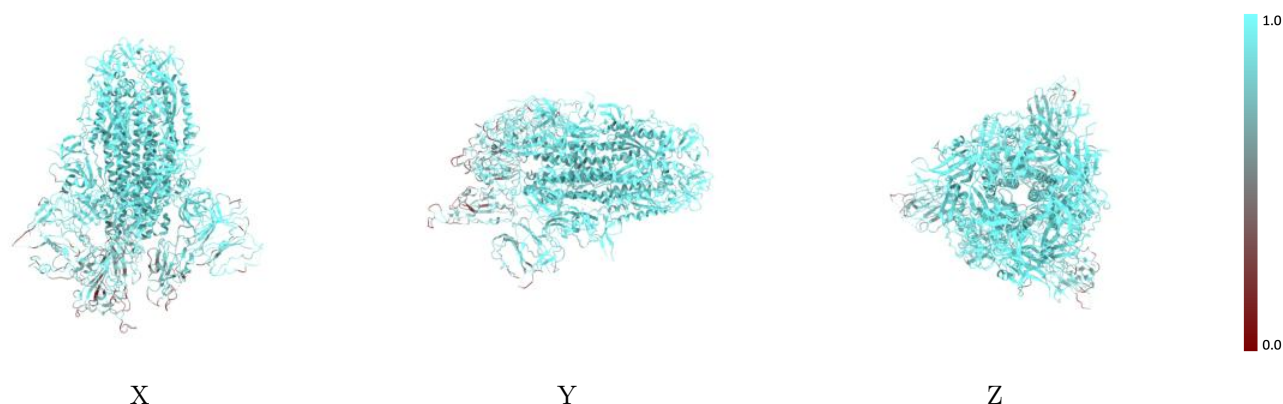
The images above show the 3D surface view of the map at the recommended contour level 0.0802 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



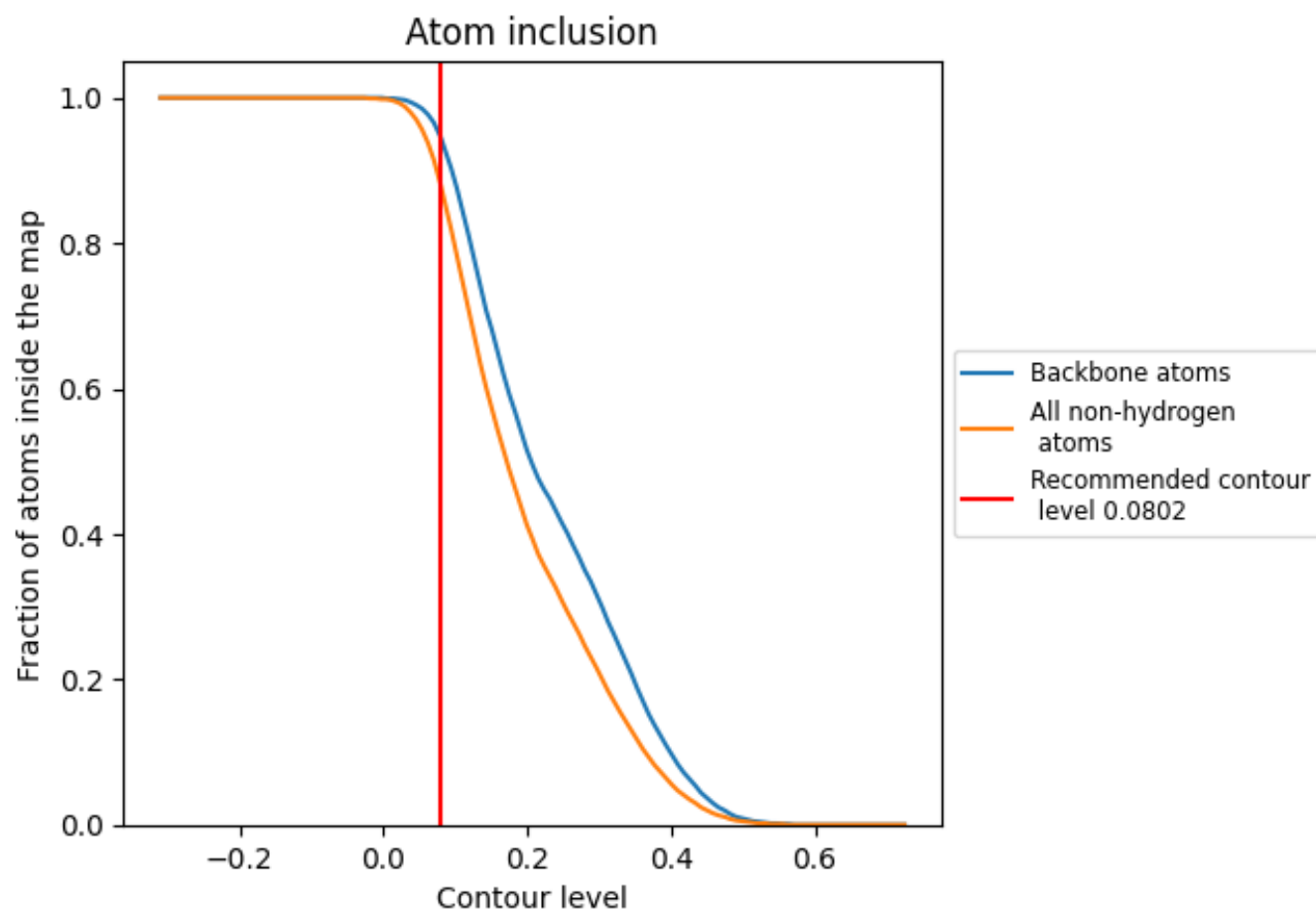
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0802).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.0802) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8790	<div></div> 0.4600
A	<div></div> 0.8620	<div></div> 0.4450
B	<div></div> 0.8940	<div></div> 0.4650
C	<div></div> 0.8810	<div></div> 0.4700
E	<div></div> 1.0000	<div></div> 0.5040
F	<div></div> 0.9290	<div></div> 0.4840
G	<div></div> 0.9640	<div></div> 0.4870
H	<div></div> 0.8570	<div></div> 0.4500
I	<div></div> 0.4290	<div></div> 0.2260
J	<div></div> 0.9640	<div></div> 0.5200
K	<div></div> 0.9640	<div></div> 0.4940

