



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 07:23 PM UTC

PDB ID : 7XID / pdb_00007xid
EMDB ID : EMD-33203
Title : S-ECD (Omicron) in complex with PD of ACE2
Authors : Li, Y.N.; Shen, Y.P.; Zhang, Y.Y.; Yan, R.H.
Deposited on : 2022-04-12
Resolution : 3.30 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:

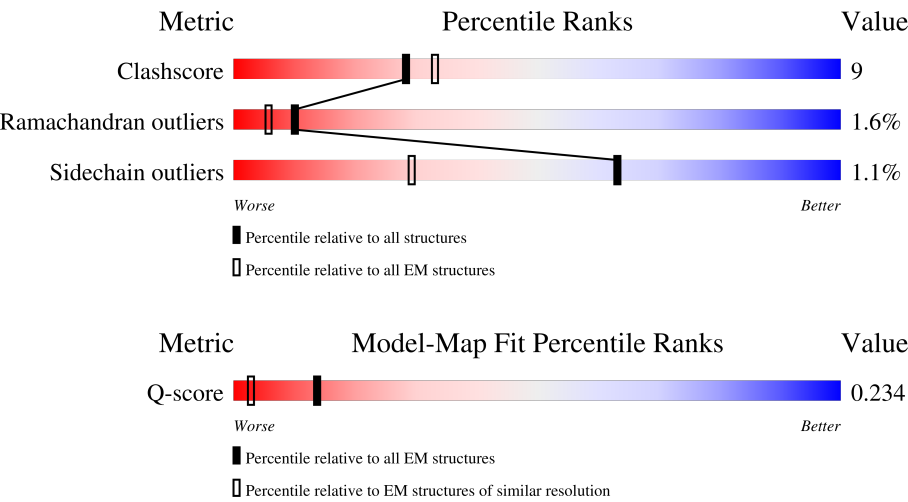
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1267	9% 67% 7% 24%
1	B	1267	11% 66% 11% 21%
1	C	1267	7% 69% 9% 21%
2	D	817	63% 58% 14% 27%

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Mol	Chain	Length	Quality of chain
2	E	817	
3	F	2	
3	G	2	
3	H	2	
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	W	2	
3	X	2	
3	Y	2	
3	Z	2	
3	a	2	
3	b	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	D	902	-	-	X	-
4	NAG	E	902	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34256 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	963	Total	C	N	O	S	0	0
			7558	4842	1255	1427	34		
1	B	998	Total	C	N	O	S	0	0
			7842	5025	1304	1477	36		
1	C	998	Total	C	N	O	S	0	0
			7842	5025	1304	1477	36		

There are 330 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	145	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	211	ILE	LEU	variant	UNP P0DTC2
A	214	GLU	-	insertion	UNP P0DTC2
A	214A	PRO	-	insertion	UNP P0DTC2
A	214B	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	GLU	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	SER	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLU	-	expression tag	UNP P0DTC2
A	1244	VAL	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	ALA	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	SER	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	SER	-	expression tag	UNP P0DTC2
A	1261	VAL	-	expression tag	UNP P0DTC2
A	1262	GLU	-	expression tag	UNP P0DTC2
A	1263	ASP	-	expression tag	UNP P0DTC2
A	1264	TYR	-	expression tag	UNP P0DTC2
A	1265	LYS	-	expression tag	UNP P0DTC2
A	1266	ASP	-	expression tag	UNP P0DTC2
A	1267	ASP	-	expression tag	UNP P0DTC2
A	1268	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1269	ASP	-	expression tag	UNP P0DTC2
A	1270	LYS	-	expression tag	UNP P0DTC2
B	69	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	145	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	211	ILE	LEU	variant	UNP P0DTC2
B	214	GLU	-	insertion	UNP P0DTC2
B	214A	PRO	-	insertion	UNP P0DTC2
B	214B	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	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	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	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	SER	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1243	GLU	-	expression tag	UNP P0DTC2
B	1244	VAL	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	ALA	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	SER	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	SER	-	expression tag	UNP P0DTC2
B	1261	VAL	-	expression tag	UNP P0DTC2
B	1262	GLU	-	expression tag	UNP P0DTC2
B	1263	ASP	-	expression tag	UNP P0DTC2
B	1264	TYR	-	expression tag	UNP P0DTC2
B	1265	LYS	-	expression tag	UNP P0DTC2
B	1266	ASP	-	expression tag	UNP P0DTC2
B	1267	ASP	-	expression tag	UNP P0DTC2
B	1268	ASP	-	expression tag	UNP P0DTC2
B	1269	ASP	-	expression tag	UNP P0DTC2
B	1270	LYS	-	expression tag	UNP P0DTC2
C	69	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	145	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	211	ILE	LEU	variant	UNP P0DTC2
C	214	GLU	-	insertion	UNP P0DTC2
C	214A	PRO	-	insertion	UNP P0DTC2
C	214B	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	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	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	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	SER	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	GLU	-	expression tag	UNP P0DTC2
C	1244	VAL	-	expression tag	UNP P0DTC2
C	1245	ASP	-	expression tag	UNP P0DTC2
C	1246	ALA	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	SER	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	SER	-	expression tag	UNP P0DTC2
C	1261	VAL	-	expression tag	UNP P0DTC2
C	1262	GLU	-	expression tag	UNP P0DTC2
C	1263	ASP	-	expression tag	UNP P0DTC2
C	1264	TYR	-	expression tag	UNP P0DTC2
C	1265	LYS	-	expression tag	UNP P0DTC2
C	1266	ASP	-	expression tag	UNP P0DTC2
C	1267	ASP	-	expression tag	UNP P0DTC2
C	1268	ASP	-	expression tag	UNP P0DTC2
C	1269	ASP	-	expression tag	UNP P0DTC2
C	1270	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		
2	E	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	MET	-	expression tag	UNP Q9BYF1
D	-10	ALA	-	expression tag	UNP Q9BYF1
D	-9	SER	-	expression tag	UNP Q9BYF1
D	-8	GLY	-	expression tag	UNP Q9BYF1
D	-7	ARG	-	expression tag	UNP Q9BYF1
D	10	TRP	-	insertion	UNP Q9BYF1
D	11	SER	-	insertion	UNP Q9BYF1
D	12	HIS	-	insertion	UNP Q9BYF1
D	13	PRO	-	insertion	UNP Q9BYF1
D	14	GLN	-	insertion	UNP Q9BYF1
D	15	PHE	-	insertion	UNP Q9BYF1
D	16	GLU	-	insertion	UNP Q9BYF1
D	17	LYS	-	insertion	UNP Q9BYF1
E	-11	MET	-	expression tag	UNP Q9BYF1
E	-10	ALA	-	expression tag	UNP Q9BYF1
E	-9	SER	-	expression tag	UNP Q9BYF1
E	-8	GLY	-	expression tag	UNP Q9BYF1
E	-7	ARG	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	TRP	-	insertion	UNP Q9BYF1
E	11	SER	-	insertion	UNP Q9BYF1
E	12	HIS	-	insertion	UNP Q9BYF1
E	13	PRO	-	insertion	UNP Q9BYF1
E	14	GLN	-	insertion	UNP Q9BYF1
E	15	PHE	-	insertion	UNP Q9BYF1
E	16	GLU	-	insertion	UNP Q9BYF1
E	17	LYS	-	insertion	UNP Q9BYF1

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



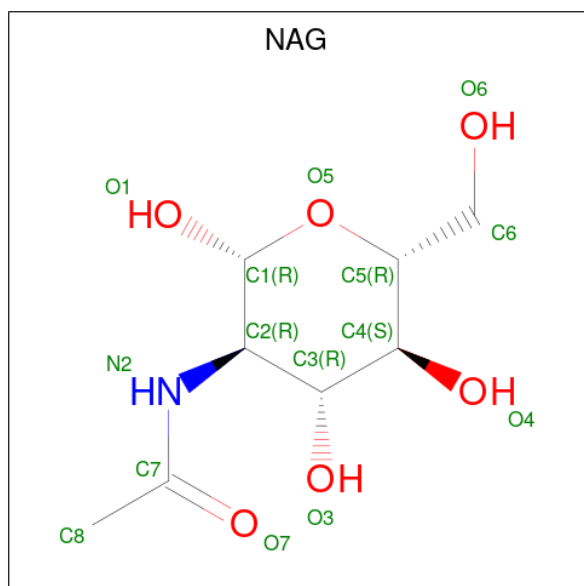
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		
3	b	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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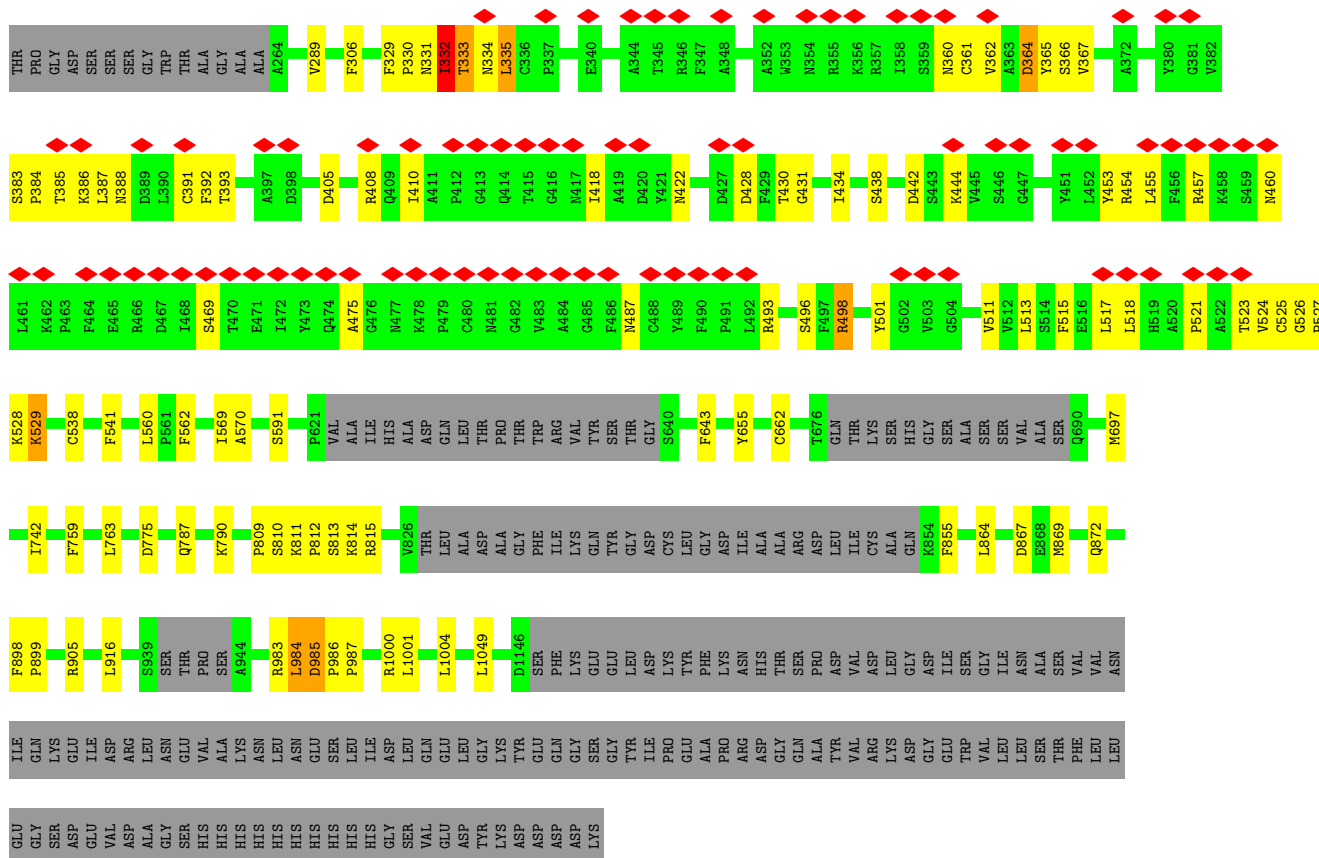
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	D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

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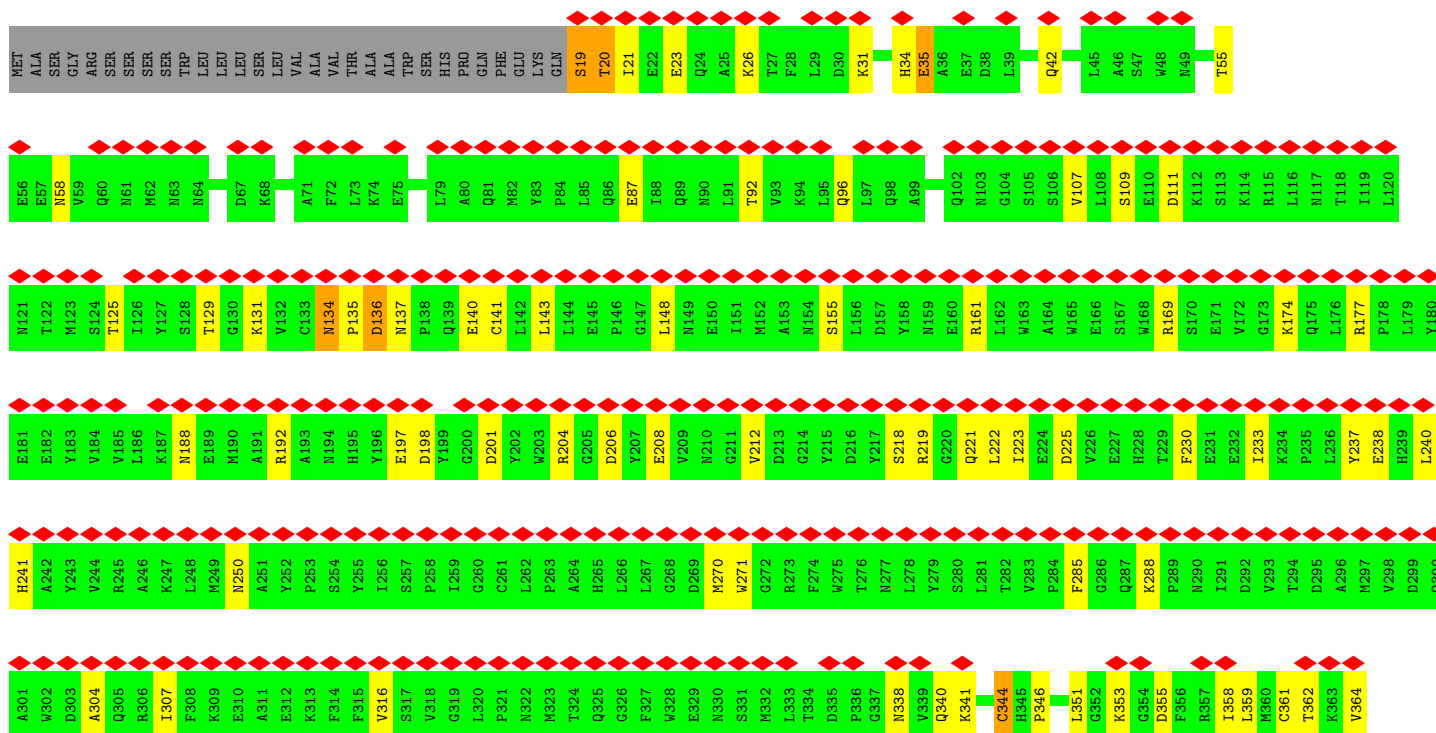
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Mol	Chain	Residues	Atoms				AltConf
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	

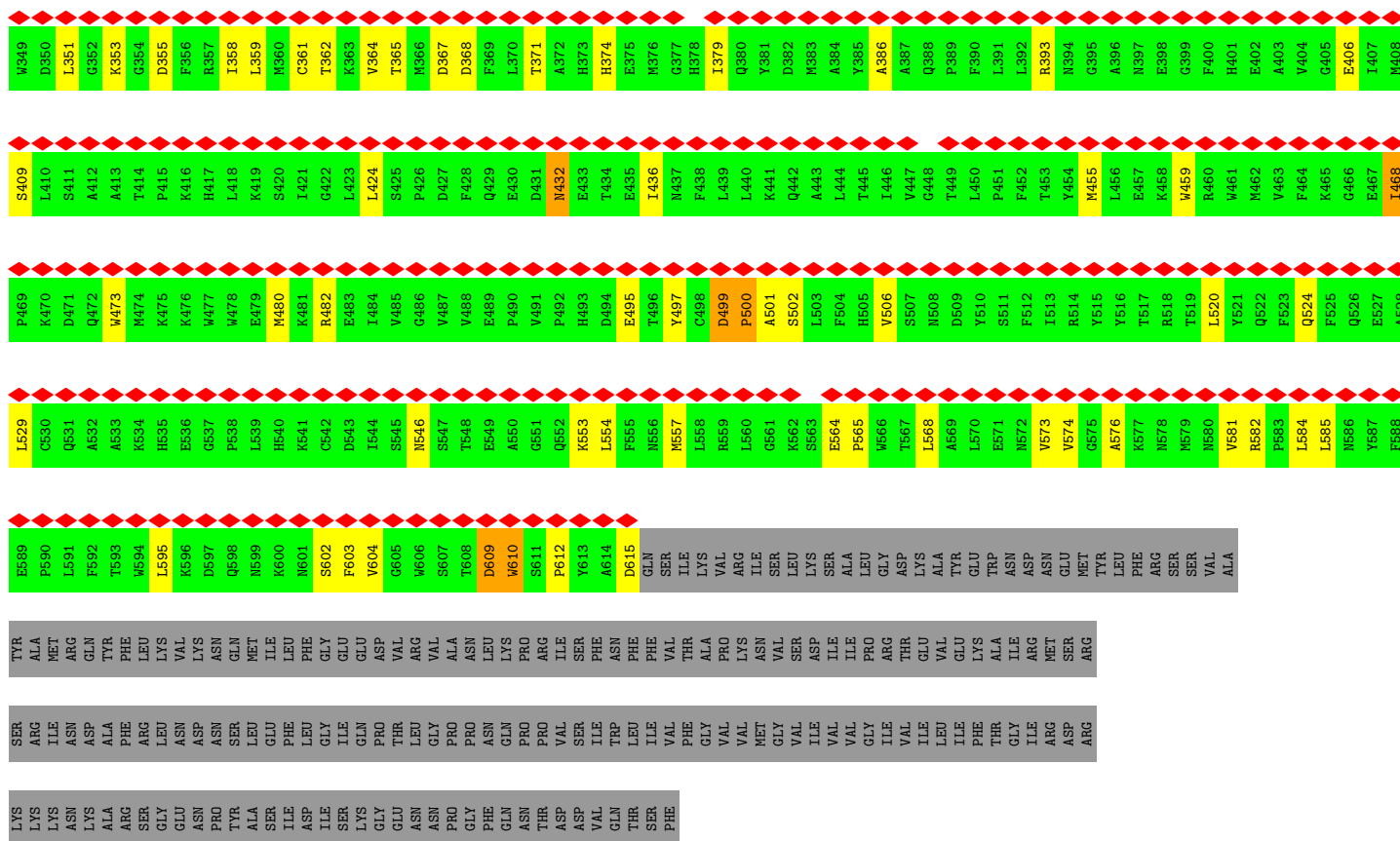




- Molecule 2: Angiotensin-converting enzyme 2



T365	M366	D367	D368	T371	A372	H373	H374	E375	M376	G377	I379	Q380	Y381	D382	M383	A384	Y385	A386	A387	Q388	P389	F390	L391	L392	R393	N394	G395	A396	G399	F400	H401	E402	A403	V404	G405	E406	I407	M408	S409	L410	S411	A412	T413	P415	K416	H417	L418	K419	S420	I421	G422	L423	L424	S425	P426																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
D427	F428	Q429	E430	M431	E433	T434	E435	I436	M437	F438	L439	L440	K441	Q442	A443	L444	T445	I446	V447	G448	T449	L450	P451	F452	T453	Y454	M455	L456	E457	K458	W459	R460	W461	M462	V463	F464	K465	G466	E467	I468	P469	K470	D471	Q472	W473	M474	K475	K476	W477	W478	E479	M480	R482	E483	I484	V485	G486																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
V487	V488	E489	P490	V491	H493	D494	E495	T496	Y497	G498	D499	P500	A501	S502	L503	F504	H505	V506	S507	N508	D509	Y510	S511	F512	I513	R514	S515	Y516	T517	R518	T519	L520	Y521	Q522	F523	Q524	F525	Q526	E527	A528	L529	C530	Q531	A532	A533	K534	H535	E536	G537	P538	L539	H540	K541	C542	D543	I544	S545	N546																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
S547	T548	E549	A550	G551	Q552	K553	L554	F555	N556	M557	K562	S563	E564	P565	M566	T567	L568	A569	L570	E571	N572	V573	V574	G575	A576	K577	N578	M579	N580	V581	R582	P583	L584	L585	N586	T587	F588	E589	P590	L591	F592	T593	M594	L595	K596	D597	Q598	N599	K600	M601	S602	F603	V604	G605	W606	S607	T608	D609																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
W610	S611	P612	Y613	A614	D615	G616	S617	E618	T619	N620	P621	L622	A623	M624	S625	T626	L627	A628	G629	P630	N631	D632	V633	G634	A635	K636	L637	N638	M639	V640	T641	R642	L643	A644	P645	S646	E647	L648	F649	T650	M651	L652	P653	N654	D655	T656	K657	S658	P659	L660	A661	M662	S663	T664	N665	D666	V667	G668	A669	K670	L671	N672	M673	V674	T675	R676	L677	A678	P679	S680	E681	L682	F683	T684	M685	L686	P687	N688	D689	V690	G691	A692	M693	S694	E695	L696	F697	T698	M699	V700	G701	A702	M703	S704	E705	L706	F707	T708	M709	V710	G711	A712	M713	S714	E715	L716	F717	T718	M719	V720	G721	A722	M723	S724	E725	L726	F727	T728	M729	V730	G731	A732	M733	S734	E735	L736	F737	T738	M739	V740	G741	A742	M743	S744	E745	L746	F747	T748	M749	V750	G751	A752	M753	S754	E755	L756	F757	T758	M759	V760	G761	A762	M763	S764	E765	L766	F767	T768	M769	V770	G771	A772	M773	S774	E775	L776	F777	T778	M779	V780	G781	A782	M783	S784	E785	L786	F787	T788	M789	V790	G791	A792	M793	S794	E795	L796	F797	T798	M799	V800	G801	A802	M803	S804	E805	L806	F807	T808	M809	V810	G811	A812	M813	S814	E815	L816	F817	T818	M819	V820	G821	A822	M823	S824	E825	L826	F827	T828	M829	V830	G831	A832	M833	S834	E835	L836	F837	T838	M839	V840	G841	A842	M843	S844	E845	L846	F847	T848	M849	V850	G851	A852	M853	S854	E855	L856	F857	T858	M859	V860	G861	A862	M863	S864	E865	L866	F867	T868	M869	V870	G871	A872	M873	S874	E875	L876	F877	T878	M879	V880	G881	A882	M883	S884	E885	L886	F887	T888	M889	V890	G891	A892	M893	S894	E895	L896	F897	T898	M899	V900	G901	A902	M903	S904	E905	L906	F907	T908	M909	V910	G911	A912	M913	S914	E915	L916	F917	T918	M919	V920	G921	A922	M923	S924	E925	L926	F927	T928	M929	V930	G931	A932	M933	S934	E935	L936	F937	T938	M939	V940	G941	A942	M943	S944	E945	L946	F947	T948	M949	V950	G951	A952	M953	S954	E955	L956	F957	T958	M959	V960	G961	A962	M963	S964	E965	L966	F967	T968	M969	V970	G971	A972	M973	S974	E975	L976	F977	T978	M979	V980	G981	A982	M983	S984	E985	L986	F987	T988	M989	V990	G991	A992	M993	S994	E995	L996	F997	T998	M999	V1000	G1001	A1002	M1003	S1004	E1005	L1006	F1007	T1008	M1009	V1010	G1011	A1012	M1013	S1014	E1015	L1016	F1017	T1018	M1019	V1020	G1021	A1022	M1023	S1024	E1025	L1026	F1027	T1028	M1029	V1030	G1031	A1032	M1033	S1034	E1035	L1036	F1037	T1038	M1039	V1040	G1041	A1042	M1043	S1044	E1045	L1046	F1047	T1048	M1049	V1050	G1051	A1052	M1053	S1054	E1055	L1056	F1057	T1058	M1059	V1060	G1061	A1062	M1063	S1064	E1065	L1066	F1067	T1068	M1069	V1070	G1071	A1072	M1073	S1074	E1075	L1076	F1077	T1078	M1079	V1080	G1081	A1082	M1083	S1084	E1085	L1086	F1087	T1088	M1089	V1090	G1091	A1092	M1093	S1094	E1095	L1096	F1097	T1098	M1099	V1100	G1101	A1102	M1103	S1104	E1105	L1106	F1107	T1108	M1109	V1110	G1111	A1112	M1113	S1114	E1115	L1116	F1117	T1118	M1119	V1120	G1121	A1122	M1123	S1124	E1125	L1126	F1127	T1128	M1129	V1130	G1131	A1132	M1133	S1134	E1135	L1136	F1137	T1138	M1139	V1140	G1141	A1142	M1143	S1144	E1145	L1146	F1147	T1148	M1149	V1150	G1151	A1152	M1153	S1154	E1155	L1156	F1157	T1158	M1159	V1160	G1161	A1162	M1163	S1164	E1165	L1166	F1167	T1168	M1169	V1170	G1171	A1172	M1173	S1174	E1175	L1176	F1177	T1178	M1179	V1180	G1181	A1182	M1183	S1184	E1185	L1186	F1187	T1188	M1189	V1190	G1191	A1192	M1193	S1194	E1195	L1196	F1197	T1198	M1199	V1200	G1201	A1202	M1203	S1204	E1205	L1206	F1207	T1208	M1209	V1210	G1211	A1212	M1213	S1214	E1215	L1216	F1217	T1218	M1219	V1220	G1221	A1222	M1223	S1224	E1225	L1226	F1227	T1228	M1229	V1230	G1231	A1232	M1233	S1234	E1235	L1236	F1237	T1238	M1239	V1240	G1241	A1242	M1243	S1244	E1245	L1246	F1247	T1248	M1249	V1250	G1251	A1252	M1253	S1254	E1255	L1256	F1257	T1258	M1259	V1260	G1261	A1262	M1263	S1264	E1265	L1266	F1267	T1268	M1269	V1270	G1271	A1272	M1273	S1274	E1275	L1276	F1277	T1278	M1279	V1280	G1281	A1282	M1283	S1284	E1285	L1286	F1287	T1288	M1289	V1290	G1291	A1292	M1293	S1294	E1295	L1296	F1297	T1298	M1299	V1300	G1301	A1302	M1303	S1304	E1305	L1306	F1307	T1308	M1309	V1310	G1311	A1312	M1313	S1314	E1315	L1316	F1317	T1318	M1319	V1320	G1321	A1322	M1323	S1324	E1325	L1326	F1327	T1328	M1329	V1330	G1331	A1332	M1333	S1334	E1335	L1336	F1337	T1338	M1339	V1340	G1341	A1342	M1343	S1344	E1345	L1346	F1347	T1348	M1349	V1350	G1351	A1352	M1353	S1354	E1355	L1356	F1357	T1358	M1359	V1360	G1361	A1362	M1363	S1364	E1365	L1366	F1367	T1368	M1369	V1370	G1371	A1372	M1373	S1374	E1375	L1376	F1377	T1378	M1379	V1380	G1381	A1382	M1383	S1384	E1385	L1386	F1387	T1388	M1389	V1390	G1391	A1392	M1393	S1394	E1395	L1396	F1397	T1398	M1399	V1400	G1401	A1402	M1403	S1404	E1405	L1406	F1407	T1408	M1409	V1410	G1411	A1412	M1413	S1414	E1415	L1416	F1417	T1418	M1419	V1420	G1421	A1422	M1423	S1424	E1425	L1426	F1427	T1428	M1429	V1430	G1431	A1432	M1433	S1434	E1435	L1436	F1437	T1438	M1439	V1440	G1441	A1442	M1443	S1444	E1445	L1446	F1447	T1448	M1449	V1450	G1451	A1452	M1453	S1454	E1455	L1456	F1457	T1458	M1459	V1460	G1461	A1462	M1463	S1464	E1465	L1466	F1467	T1468	M1469	V1470	G1471	A1472	M1473	S1474	E1475	L1476	F1477	T1478	M1479	V1480	G1481	A1482	M1483	S1484	E1485	L1486	F1487	T1488	M1489	V1490	G1491	A1492	M1493	S1494	E1495	L1496	F1497	T1498	M1499	V1500	G1501	A1502	M1503	S1504	E1505	L1506	F1507	T1508	M1509	V1510	G1511	A1512	M1513	S1514	E1515	L1516	F1517	T1518	M1519	V1520	G1521	A1522	M1523	S1524	E1525	L1526	F1527	T1528	M1529	V1530	G1531	A1532	M1533	S1534	E1535	L1536	F1537	T1538	M1539	V1540	G1541	A1542	M1543	S1544	E1545	L1546	F1547	T1548	M1549	V1550	G1551	A1552	M1553	S1554	E1555	L1556	F1557	T1558	M1559	V1560	G1561	A1562	M1563	S1564	E1565	L1566	F1567	T1568	M1569	V1570	G1571	A1572	M1573	S1574	E1575	L1576	F1577	T1578	M1579	V1580	G1581	A1582	M1583	S1584	E1585	L1586	F1587	T1588	M1589	V1590	G1591	A1592	M1593	S1594	E1595	L1596	F1597	T1598	M1599	V1600	G1601	A1602	M1603	S1604	E1605	L1606	F1607	T1608	M1609	V1610	G1611	A1612	M1613	S1614	E1615	L1616	F1617	T1618	M1619	V1620	G1621	A1622	M1623	S1624	E1625	L1626	F1627	T1628	M1629	V1630	G1631	A1632	M1633	S1634	E1635	L1636	F1637	T1638	M1639	V1640	G1641	A1642	M1643	S1644	E1645	L1646	F1647	T1648	M1649	V1650	G1651	A1652	M1653	S1654	E1655	L1656	F1657	T1658	M1659	V1660	G1661	A1662	M1663	S1664	E1665	L1666	F1667	T1668	M1669	V1670	G1671	A1672	M1673	S1674	E1675	L1676	F1677	T1678	M1679	V1680	G1681	A1682	M1683	S1684	E1685	L1686	F1687	T1688	M1689	V1690	G1691	A1692	M1693	S1694	E1695	L1696	F1697	T1698	M1699	V1700	G1701	A1702	M1703	S1704	E1705	L1706	F1707	T1708	M1709	V1710	G1711	A1712	M1713	S1714	E1715	L1716	F1717	T1718	M1719	V1720	G1721	A1722	M1723	S1724	E1725	L1726	F1727	T1728	M1729	V1730	G1731	A1732	M1733	S1734	E1735	L1736	F1737	T1738	M1739	V1740	G1741	A1742	M1743	S1744	E1745	L1746	F1747	T1748	M1749	V1750	G1751	A1752	M1753	S1754	E1755	L1756	F1757	T1758	M1759	V1760	G1761	A1762	M1763	S1764	E1765	L1766	F1767	T1768	M1769	V1770	G1771	A1772	M1773	S1774	E1775	L1776	F1777	T1778	M1779	V1780	G1781	A1782	M1783	S1784	E1785	L1786	F1787	T1788	M1789	V1790	G1791	A1792	M1793	S1794	E1795	L1796	F1797	T1798	M1799	V1800	G1801	A1802



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



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



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



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

Chain I:  100%



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

Chain J:  50% 50%



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

Chain K:  50% 50%



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

Chain L:  100%



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

Chain M:  50% 100%



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

Chain N:  50% 100%



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

Chain O:  50% 50%



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

Chain P:  50% 50%

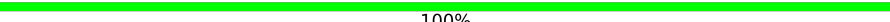


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

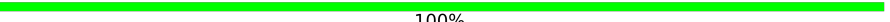


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



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

Chain S:  100%



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

Chain T:  100% 100%



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

Chain U:  50% 50% 50%



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

Chain V:  50% 50%



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

Chain W:  100%

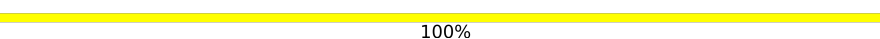


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  50% 50%

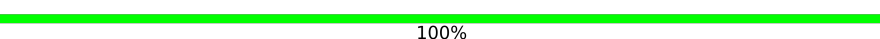


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%



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

Chain Z:  100%

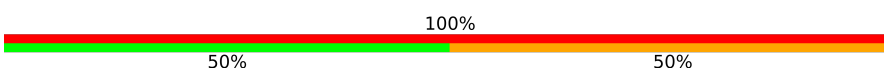


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100% 50% 50%



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

Chain b: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97021	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.014	Depositor
Minimum map value	-1.616	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.53	1/7732 (0.0%)	0.66	11/10514 (0.1%)
1	B	0.50	0/8025	0.65	7/10911 (0.1%)
1	C	0.50	0/8025	0.65	8/10911 (0.1%)
2	D	0.32	0/5007	0.68	4/6803 (0.1%)
2	E	0.32	0/5007	0.68	4/6803 (0.1%)
All	All	0.46	1/33796 (0.0%)	0.66	34/45942 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	698	SER	CA-C	-6.63	1.44	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	432	ASN	N-CA-C	7.40	120.40	111.82
2	E	432	ASN	N-CA-C	7.39	120.39	111.82
1	A	794	ILE	N-CA-C	-6.29	103.19	110.05
1	C	208	THR	CA-C-N	-6.06	114.37	120.31
1	C	208	THR	C-N-CA	-6.06	114.37	120.31
1	A	31	SER	CA-C-N	-6.00	115.30	122.44
1	A	31	SER	C-N-CA	-6.00	115.30	122.44
1	B	31	SER	CA-C-N	-6.00	115.30	122.44
1	B	31	SER	C-N-CA	-6.00	115.30	122.44
1	A	538	CYS	N-CA-C	-5.93	100.88	109.59
1	C	538	CYS	N-CA-C	-5.93	100.88	109.59
1	A	86	PHE	CA-C-N	5.91	132.83	121.54
1	A	86	PHE	C-N-CA	5.91	132.83	121.54
1	B	86	PHE	CA-C-N	5.91	132.83	121.54
1	B	86	PHE	C-N-CA	5.91	132.83	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	546	ASN	N-CA-C	-5.89	103.33	111.28
2	E	546	ASN	N-CA-C	-5.89	103.33	111.28
1	C	86	PHE	CA-C-N	5.86	132.74	121.54
1	C	86	PHE	C-N-CA	5.86	132.74	121.54
1	A	82	PRO	N-CA-C	5.79	120.59	111.38
1	C	82	PRO	N-CA-C	5.74	120.02	111.41
1	C	985	ASP	CA-C-N	-5.65	114.56	120.38
1	C	985	ASP	C-N-CA	-5.65	114.56	120.38
1	A	591	SER	N-CA-C	5.55	122.62	110.80
1	B	208	THR	CA-C-N	-5.42	114.39	120.14
1	B	208	THR	C-N-CA	-5.42	114.39	120.14
1	A	208	THR	CA-C-N	-5.41	114.41	120.14
1	A	208	THR	C-N-CA	-5.41	114.41	120.14
2	D	609	ASP	CA-C-N	5.28	131.63	121.54
2	D	609	ASP	C-N-CA	5.28	131.63	121.54
2	E	609	ASP	CA-C-N	5.26	131.59	121.54
2	E	609	ASP	C-N-CA	5.26	131.59	121.54
1	B	82	PRO	N-CA-C	5.22	119.69	111.38
1	A	697	MET	N-CA-C	5.14	117.16	110.43

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7558	0	7394	129	0
1	B	7842	0	7665	205	0
1	C	7842	0	7665	137	0
2	D	4870	0	4633	116	0
2	E	4870	0	4633	116	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	24	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	1	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	24	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	2	0
3	b	28	0	25	2	0
4	A	154	0	142	0	0
4	B	154	0	142	6	0
4	C	126	0	117	0	0
4	D	98	0	89	12	0
4	E	98	0	89	12	0
All	All	34256	0	33142	637	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 9.

All (637) 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)
4:B:1410:NAG:O4	4:B:1411:NAG:C1	1.63	1.43
4:D:905:NAG:O4	4:D:906:NAG:C1	1.65	1.43
4:E:905:NAG:O4	4:E:906:NAG:C1	1.65	1.42
1:A:230:PRO:HB3	1:C:521:PRO:CG	1.57	1.33
1:A:230:PRO:CB	1:C:521:PRO:HG2	1.59	1.32
1:A:528:LYS:O	1:A:529:LYS:CG	1.82	1.26
1:B:364:ASP:HB3	1:B:527:PRO:CB	1.66	1.25
1:A:230:PRO:CB	1:C:521:PRO:CG	2.16	1.21
1:A:386:LYS:HG2	1:B:981:PHE:O	1.36	1.21
1:C:364:ASP:HB3	1:C:527:PRO:CB	1.75	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:VAL:HG23	1:B:983:ARG:C	1.73	1.14
1:B:335:LEU:HG	1:B:363:ALA:CB	1.78	1.13
1:A:230:PRO:HB3	1:C:521:PRO:HG3	1.14	1.12
1:B:392:PHE:O	1:B:524:VAL:HG12	1.48	1.12
1:C:364:ASP:HB3	1:C:527:PRO:HB3	1.19	1.12
1:A:390:LEU:HD21	1:B:983:ARG:HD3	1.26	1.10
1:C:455:LEU:HD23	1:C:493:ARG:HG3	1.35	1.09
1:A:528:LYS:O	1:A:529:LYS:HG2	0.93	1.08
1:B:364:ASP:HB3	1:B:527:PRO:HB3	1.10	1.08
1:A:396:TYR:HE2	1:A:516:GLU:OE1	1.35	1.06
1:A:519:HIS:CE1	1:B:40:ASP:CG	2.33	1.06
1:A:230:PRO:HB2	1:C:521:PRO:HG2	1.35	1.06
1:C:332:ILE:HG23	1:C:333:THR:H	1.21	1.05
1:B:455:LEU:HD23	1:B:493:ARG:HG3	1.35	1.04
2:E:134:ASN:HB3	2:E:137:ASN:OD1	1.57	1.03
2:D:134:ASN:HB3	2:D:137:ASN:OD1	1.57	1.03
1:C:364:ASP:OD1	1:C:367:VAL:HG13	1.58	1.03
1:B:364:ASP:CB	1:B:527:PRO:HB3	1.88	1.02
2:D:31:LYS:O	2:D:35:GLU:HG2	1.59	1.02
2:E:31:LYS:O	2:E:35:GLU:HG2	1.59	1.01
1:A:390:LEU:HD21	1:B:983:ARG:CD	1.89	1.01
1:B:455:LEU:CD2	1:B:493:ARG:HG3	1.91	1.00
4:B:1410:NAG:C4	4:B:1411:NAG:C1	2.38	1.00
1:A:382:VAL:HG23	1:B:983:ARG:CA	1.90	1.00
1:C:455:LEU:CD2	1:C:493:ARG:HG3	1.91	1.00
1:A:330:PRO:O	1:A:331:ASN:CG	2.04	0.99
1:A:390:LEU:CD2	1:B:983:ARG:CG	2.42	0.97
1:B:39:PRO:O	1:B:40:ASP:CG	2.09	0.95
1:B:364:ASP:HB3	1:B:527:PRO:CG	1.98	0.93
2:E:107:VAL:HG23	4:E:902:NAG:C6	1.99	0.93
1:B:332:ILE:HD12	1:B:333:THR:H	1.32	0.92
2:E:107:VAL:CG2	4:E:902:NAG:H61	1.98	0.92
2:E:107:VAL:HG23	4:E:902:NAG:H61	1.51	0.92
1:C:493:ARG:HD3	2:D:34:HIS:CD2	2.05	0.92
2:D:107:VAL:HG23	4:D:902:NAG:C6	1.99	0.92
1:B:493:ARG:HD3	2:E:34:HIS:CD2	2.05	0.91
2:D:107:VAL:CG2	4:D:902:NAG:H61	1.98	0.91
1:A:382:VAL:CG2	1:B:983:ARG:HA	2.01	0.90
1:A:516:GLU:OE2	1:B:200:TYR:CE2	2.24	0.90
2:D:107:VAL:HG23	4:D:902:NAG:H61	1.51	0.89
1:C:364:ASP:CB	1:C:527:PRO:HB3	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:ASN:CB	2:D:137:ASN:OD1	2.21	0.89
2:D:340:GLN:HG2	3:a:1:NAG:H82	1.54	0.89
1:A:396:TYR:CE2	1:A:516:GLU:OE1	2.26	0.88
2:D:135:PRO:O	2:D:136:ASP:HB2	1.74	0.88
2:E:340:GLN:HG2	3:b:1:NAG:H82	1.55	0.87
2:E:134:ASN:CB	2:E:137:ASN:OD1	2.21	0.87
1:B:392:PHE:O	1:B:524:VAL:CG1	2.23	0.86
1:A:390:LEU:CD2	1:B:983:ARG:HG2	2.04	0.86
1:C:364:ASP:HB3	1:C:527:PRO:CG	2.06	0.85
1:A:382:VAL:CG2	1:B:983:ARG:CA	2.53	0.85
2:E:135:PRO:O	2:E:136:ASP:HB2	1.74	0.85
1:A:386:LYS:CG	1:B:981:PHE:O	2.23	0.85
2:D:316:VAL:HG21	4:D:903:NAG:H5	1.59	0.84
1:A:390:LEU:CD2	1:B:983:ARG:HD3	2.07	0.84
1:A:519:HIS:CE1	1:B:40:ASP:OD2	2.31	0.84
2:E:316:VAL:HG21	4:E:903:NAG:H5	1.59	0.84
1:C:332:ILE:HD13	1:C:333:THR:N	1.95	0.82
1:B:335:LEU:HG	1:B:363:ALA:HB1	1.60	0.81
1:B:496:SER:HB2	1:B:498:ARG:NH1	1.95	0.81
1:A:382:VAL:HB	1:B:983:ARG:HB3	1.61	0.81
1:A:528:LYS:C	1:A:529:LYS:HG2	2.03	0.81
1:A:382:VAL:HG23	1:B:983:ARG:HA	1.56	0.81
2:E:20:THR:HG23	2:E:23:GLU:HG2	1.63	0.80
2:D:20:THR:HG23	2:D:23:GLU:HG2	1.63	0.80
1:B:332:ILE:CD1	1:B:333:THR:H	1.94	0.80
1:C:496:SER:HB2	1:C:498:ARG:NH1	1.95	0.80
2:D:134:ASN:HB3	2:D:135:PRO:CD	2.13	0.79
1:A:390:LEU:HD21	1:B:983:ARG:CG	2.07	0.79
2:E:134:ASN:HB3	2:E:135:PRO:CD	2.13	0.78
1:A:390:LEU:HD22	1:B:983:ARG:CG	2.12	0.78
1:C:329:PHE:CE1	1:C:529:LYS:O	2.36	0.78
2:D:169:ARG:HD3	2:D:499:ASP:OD1	1.83	0.78
2:E:169:ARG:HD3	2:E:499:ASP:OD1	1.83	0.77
2:D:20:THR:HG22	2:D:23:GLU:CD	2.10	0.77
1:A:334:ASN:O	1:A:362:VAL:HG22	1.85	0.77
2:E:432:ASN:OD1	4:E:904:NAG:C7	2.33	0.77
2:D:432:ASN:OD1	4:D:904:NAG:C7	2.33	0.77
1:B:493:ARG:HD3	2:E:34:HIS:NE2	2.00	0.77
1:C:493:ARG:HD3	2:D:34:HIS:NE2	2.00	0.76
1:B:335:LEU:HG	1:B:363:ALA:HB2	1.65	0.76
2:E:20:THR:HG22	2:E:23:GLU:CD	2.10	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:PHE:CG	1:C:528:LYS:HB2	2.20	0.75
1:A:200:TYR:CE1	1:C:521:PRO:HG3	2.22	0.75
1:B:332:ILE:HD12	1:B:333:THR:N	2.00	0.75
1:B:392:PHE:C	1:B:524:VAL:HG12	2.11	0.74
1:B:455:LEU:HD23	1:B:493:ARG:CG	2.17	0.74
1:A:390:LEU:HD22	1:B:983:ARG:HG2	1.67	0.73
1:C:498:ARG:HD3	1:C:501:TYR:CE1	2.23	0.73
1:B:335:LEU:O	1:B:336:CYS:O	2.06	0.73
1:A:382:VAL:HA	1:B:983:ARG:O	1.89	0.72
1:A:854:LYS:O	1:A:855:PHE:HB2	1.88	0.72
1:A:332:ILE:O	1:A:333:THR:HG23	1.89	0.72
1:B:498:ARG:HD3	1:B:501:TYR:CE1	2.23	0.72
1:B:388:ASN:OD1	1:B:527:PRO:CD	2.38	0.72
1:C:455:LEU:HD23	1:C:493:ARG:CG	2.17	0.72
2:E:432:ASN:O	2:E:436:ILE:HG12	1.90	0.72
1:B:392:PHE:C	1:B:524:VAL:CG1	2.63	0.71
1:A:516:GLU:OE2	1:B:200:TYR:HE2	1.69	0.71
1:B:498:ARG:HD3	1:B:501:TYR:CZ	2.26	0.71
2:D:432:ASN:O	2:D:436:ILE:HG12	1.90	0.70
1:B:366:SER:OG	1:B:388:ASN:ND2	2.25	0.70
4:B:1410:NAG:H4	4:B:1411:NAG:C1	2.21	0.69
1:C:388:ASN:OD1	1:C:527:PRO:CG	2.39	0.69
1:C:498:ARG:HD3	1:C:501:TYR:CZ	2.26	0.69
1:A:854:LYS:O	1:A:855:PHE:CB	2.39	0.69
1:A:519:HIS:NE2	1:B:40:ASP:OD1	2.25	0.69
1:A:519:HIS:CE1	1:B:40:ASP:OD1	2.46	0.68
1:A:855:PHE:CG	1:A:856:LYS:N	2.61	0.68
1:B:498:ARG:CD	1:B:501:TYR:OH	2.42	0.68
1:A:368:LEU:O	1:A:370:ASN:N	2.25	0.68
1:A:519:HIS:CD2	1:B:40:ASP:OD1	2.47	0.68
1:B:799:GLY:O	1:B:800:PHE:C	2.37	0.68
1:C:498:ARG:CD	1:C:501:TYR:OH	2.42	0.68
1:B:498:ARG:NH2	2:E:42:GLN:OE1	2.27	0.68
1:C:329:PHE:HE1	1:C:529:LYS:O	1.75	0.68
1:C:498:ARG:NH2	2:D:42:GLN:OE1	2.27	0.68
1:C:528:LYS:O	1:C:529:LYS:O	2.12	0.67
1:A:383:SER:OG	1:A:384:PRO:CD	2.42	0.67
1:A:393:THR:HG23	1:A:516:GLU:O	1.94	0.67
1:A:382:VAL:HG21	1:B:983:ARG:HA	1.76	0.66
2:E:107:VAL:CG2	4:E:902:NAG:C6	2.67	0.66
1:B:496:SER:O	1:B:498:ARG:HD2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:ASN:OD1	1:C:527:PRO:CD	2.44	0.66
1:A:230:PRO:HB2	1:C:521:PRO:CG	2.00	0.66
1:C:332:ILE:HG23	1:C:333:THR:N	2.02	0.66
1:C:496:SER:O	1:C:498:ARG:HD2	1.94	0.66
1:A:330:PRO:C	1:A:331:ASN:CG	2.64	0.65
1:A:382:VAL:CG2	1:B:983:ARG:C	2.62	0.65
1:B:388:ASN:OD1	1:B:527:PRO:CG	2.45	0.65
1:C:332:ILE:HG12	1:C:362:VAL:O	1.96	0.65
2:D:500:PRO:O	2:D:506:VAL:HG21	1.96	0.65
1:A:516:GLU:OE2	1:B:200:TYR:CZ	2.50	0.65
2:D:582:ARG:O	2:D:585:LEU:HB2	1.96	0.65
1:A:383:SER:OG	1:A:384:PRO:HD3	1.97	0.64
1:A:382:VAL:HG22	1:A:383:SER:N	2.12	0.64
1:C:332:ILE:HD11	1:C:335:LEU:HD12	1.78	0.64
1:B:529:LYS:O	1:B:530:SER:HB2	1.95	0.64
2:E:500:PRO:O	2:E:506:VAL:HG21	1.96	0.64
2:E:582:ARG:O	2:E:585:LEU:HB2	1.97	0.64
1:B:332:ILE:CG1	1:B:333:THR:H	2.10	0.64
1:C:364:ASP:OD1	1:C:367:VAL:CG1	2.43	0.64
2:D:107:VAL:CG2	4:D:902:NAG:C6	2.68	0.64
1:A:331:ASN:O	1:A:332:ILE:HD12	1.98	0.63
1:B:455:LEU:HD22	1:B:493:ARG:HG3	1.80	0.63
1:A:528:LYS:O	1:A:529:LYS:CB	2.46	0.63
1:B:364:ASP:OD1	1:B:364:ASP:N	2.29	0.63
1:A:330:PRO:O	1:A:331:ASN:OD1	2.16	0.63
2:E:31:LYS:O	2:E:35:GLU:CG	2.42	0.63
1:B:498:ARG:HD2	1:B:501:TYR:OH	1.99	0.62
1:B:528:LYS:C	1:B:529:LYS:HG2	2.24	0.62
1:A:330:PRO:O	1:A:331:ASN:ND2	2.32	0.62
2:D:169:ARG:CD	2:D:499:ASP:OD1	2.48	0.62
1:B:528:LYS:O	1:B:529:LYS:CB	2.48	0.61
2:D:177:ARG:NH2	2:D:497:TYR:O	2.32	0.61
1:C:498:ARG:HD2	1:C:501:TYR:OH	1.99	0.61
2:E:285:PHE:HB3	2:E:288:LYS:HD3	1.83	0.61
2:D:31:LYS:O	2:D:35:GLU:CG	2.42	0.61
2:D:602:SER:OG	2:D:603:PHE:N	2.33	0.61
2:E:602:SER:OG	2:E:603:PHE:N	2.33	0.61
1:A:333:THR:O	1:A:334:ASN:HB2	1.98	0.61
2:E:169:ARG:CD	2:E:499:ASP:OD1	2.48	0.61
2:E:177:ARG:NH2	2:E:497:TYR:O	2.32	0.61
1:A:386:LYS:HB3	1:B:982:SER:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:VAL:O	1:B:524:VAL:HG13	2.00	0.61
1:C:455:LEU:HD22	1:C:493:ARG:HG3	1.80	0.61
1:B:364:ASP:CG	1:B:527:PRO:HB3	2.26	0.61
1:C:759:PHE:CD2	1:C:1001:LEU:HD21	2.36	0.60
1:B:329:PHE:HE1	1:B:529:LYS:O	1.84	0.60
1:A:230:PRO:CG	1:C:521:PRO:HG2	2.29	0.60
1:B:706:ALA:CB	4:B:1410:NAG:H5	2.32	0.60
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.83	0.60
2:D:285:PHE:HB3	2:D:288:LYS:HD3	1.83	0.60
1:B:364:ASP:HB3	1:B:527:PRO:HG3	1.83	0.60
1:B:329:PHE:CE1	1:B:529:LYS:O	2.55	0.59
1:B:699:LEU:CD1	1:C:872:GLN:OE1	2.49	0.59
1:A:200:TYR:HE1	1:C:521:PRO:HG3	1.65	0.59
2:D:109:SER:OG	2:D:111:ASP:OD1	2.21	0.59
2:E:134:ASN:HB2	2:E:137:ASN:ND2	2.18	0.59
1:C:95:ILE:O	1:C:96:GLU:HB2	2.02	0.58
1:B:364:ASP:HA	1:B:526:GLY:C	2.28	0.58
1:A:516:GLU:OE2	1:B:200:TYR:OH	2.21	0.58
1:C:332:ILE:CG2	1:C:333:THR:H	2.05	0.58
1:A:394:ASN:HB2	1:B:200:TYR:OH	2.02	0.58
1:C:332:ILE:CD1	1:C:335:LEU:HD12	2.34	0.58
2:D:529:LEU:HD11	2:D:554:LEU:HD13	1.85	0.58
1:B:496:SER:CB	1:B:498:ARG:NH1	2.66	0.58
2:D:134:ASN:HB2	2:D:137:ASN:ND2	2.18	0.58
1:B:335:LEU:O	1:B:336:CYS:C	2.46	0.57
1:A:519:HIS:ND1	1:B:40:ASP:CG	2.62	0.57
1:B:388:ASN:OD1	1:B:527:PRO:HD3	2.04	0.57
1:B:498:ARG:CD	1:B:501:TYR:CZ	2.88	0.57
1:B:39:PRO:O	1:B:40:ASP:OD1	2.22	0.57
1:B:392:PHE:HB2	1:B:524:VAL:HG13	1.86	0.57
1:C:496:SER:CB	1:C:498:ARG:NH1	2.65	0.57
2:D:344:CYS:HB2	2:D:361:CYS:HB3	1.86	0.57
1:A:368:LEU:C	1:A:370:ASN:H	2.12	0.57
2:E:499:ASP:C	2:E:501:ALA:H	2.13	0.57
2:E:529:LEU:HD11	2:E:554:LEU:HD13	1.86	0.57
2:E:344:CYS:HB2	2:E:361:CYS:HB3	1.86	0.56
1:A:362:VAL:HG23	1:A:362:VAL:O	2.05	0.56
1:B:122:ASN:OD1	1:B:122:ASN:N	2.38	0.56
1:C:498:ARG:CD	1:C:501:TYR:CZ	2.88	0.56
2:D:459:TRP:CH2	2:D:500:PRO:HG3	2.40	0.56
2:D:581:VAL:O	2:D:584:LEU:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:21:ILE:HD13	2:E:87:GLU:HG2	1.87	0.56
2:E:109:SER:OG	2:E:111:ASP:OD1	2.21	0.56
2:E:19:SER:N	2:E:23:GLU:OE2	2.39	0.56
1:C:815:ARG:NH2	1:C:867:ASP:OD2	2.38	0.56
2:E:107:VAL:HG23	4:E:902:NAG:O6	2.06	0.56
2:E:107:VAL:CG2	4:E:902:NAG:O5	2.54	0.56
1:B:496:SER:OG	2:E:353:LYS:NZ	2.39	0.56
1:C:405:ASP:O	1:C:408:ARG:NH1	2.39	0.56
2:E:134:ASN:CB	2:E:135:PRO:CD	2.84	0.56
2:E:459:TRP:CH2	2:E:500:PRO:HG3	2.40	0.56
2:D:553:LYS:NZ	2:D:573:VAL:O	2.39	0.56
1:B:405:ASP:O	1:B:408:ARG:NH1	2.39	0.55
1:C:496:SER:OG	2:D:353:LYS:NZ	2.39	0.55
2:D:107:VAL:CG2	4:D:902:NAG:O5	2.54	0.55
1:A:390:LEU:CD2	1:B:983:ARG:HG3	2.32	0.55
2:E:609:ASP:OD1	2:E:609:ASP:N	2.39	0.55
1:B:95:ILE:O	1:B:96:GLU:HB2	2.06	0.55
1:C:364:ASP:CB	1:C:527:PRO:CG	2.84	0.55
1:C:364:ASP:HA	1:C:526:GLY:C	2.31	0.55
2:D:338:ASN:OD1	2:D:341:LYS:NZ	2.40	0.55
2:D:499:ASP:C	2:D:501:ALA:H	2.13	0.55
1:C:332:ILE:HD13	1:C:334:ASN:H	1.70	0.55
2:D:21:ILE:HD13	2:D:87:GLU:HG2	1.87	0.55
2:E:553:LYS:NZ	2:E:573:VAL:O	2.39	0.55
2:E:581:VAL:O	2:E:584:LEU:HB3	2.06	0.55
1:A:390:LEU:HD22	1:B:983:ARG:HG3	1.88	0.55
1:B:365:TYR:OH	1:B:524:VAL:O	2.25	0.55
1:B:528:LYS:O	1:B:529:LYS:CG	2.55	0.55
2:D:19:SER:N	2:D:23:GLU:OE2	2.39	0.55
2:E:137:ASN:ND2	2:E:140:GLU:O	2.39	0.55
1:A:354:ASN:O	1:A:398:ASP:HA	2.06	0.55
1:C:393:THR:HG23	1:C:517:LEU:HD12	1.89	0.55
2:D:107:VAL:HG23	4:D:902:NAG:O6	2.06	0.55
1:B:659:SER:HA	1:B:696:THR:O	2.07	0.54
1:A:363:ALA:O	1:A:526:GLY:HA2	2.07	0.54
1:B:434:ILE:HB	1:B:511:VAL:HG23	1.89	0.54
2:D:137:ASN:ND2	2:D:140:GLU:O	2.39	0.54
1:A:122:ASN:OD1	1:A:122:ASN:N	2.39	0.54
1:A:898:PHE:N	1:A:899:PRO:CD	2.70	0.54
1:B:703:ASN:HB3	1:C:787:GLN:OE1	2.07	0.54
1:C:431:GLY:HA3	1:C:513:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:THR:CG2	2:D:23:GLU:HG2	2.35	0.54
2:E:20:THR:CG2	2:E:23:GLU:HG2	2.35	0.54
2:E:482:ARG:NH1	2:E:609:ASP:O	2.41	0.54
1:A:331:ASN:C	1:A:332:ILE:HG13	2.31	0.54
1:B:431:GLY:HA3	1:B:513:LEU:O	2.07	0.54
1:A:502:GLY:O	1:A:506:GLN:HG3	2.07	0.54
1:C:122:ASN:N	1:C:122:ASN:OD1	2.40	0.54
1:C:334:ASN:HB3	1:C:362:VAL:HB	1.90	0.54
1:C:434:ILE:HB	1:C:511:VAL:HG23	1.89	0.54
1:A:382:VAL:CB	1:B:983:ARG:O	2.55	0.54
1:B:393:THR:HG23	1:B:517:LEU:HD12	1.89	0.54
2:E:338:ASN:OD1	2:E:341:LYS:NZ	2.40	0.54
1:A:796:TYR:O	1:A:798:GLY:N	2.39	0.54
2:D:134:ASN:HB2	2:D:137:ASN:HD21	1.73	0.54
1:C:392:PHE:O	1:C:524:VAL:HG12	2.07	0.54
2:D:134:ASN:HB2	2:D:137:ASN:OD1	2.07	0.54
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.44	0.53
2:D:482:ARG:NH1	2:D:609:ASP:O	2.41	0.53
1:A:382:VAL:CB	1:B:983:ARG:HB3	2.35	0.53
2:E:134:ASN:HB2	2:E:137:ASN:HD21	1.73	0.53
2:D:134:ASN:HB2	2:D:137:ASN:CG	2.34	0.53
1:A:394:ASN:ND2	1:B:200:TYR:OH	2.35	0.53
2:E:55:THR:OG1	2:E:58:ASN:OD1	2.26	0.53
2:E:499:ASP:C	2:E:501:ALA:N	2.67	0.53
1:B:335:LEU:HD13	1:B:335:LEU:H	1.72	0.53
1:B:528:LYS:O	1:B:529:LYS:HB2	2.09	0.53
2:D:134:ASN:CB	2:D:135:PRO:CD	2.84	0.53
2:D:499:ASP:C	2:D:501:ALA:N	2.67	0.53
2:D:192:ARG:HG2	2:D:197:GLU:HG3	1.91	0.53
1:B:48:LEU:CD2	1:B:305:SER:HA	2.39	0.53
1:C:388:ASN:CG	1:C:527:PRO:CD	2.82	0.53
2:E:192:ARG:HG2	2:E:197:GLU:HG3	1.91	0.52
1:A:371:LEU:C	1:A:373:PRO:HD2	2.34	0.52
1:B:392:PHE:HB2	1:B:524:VAL:CG1	2.39	0.52
1:C:524:VAL:O	1:C:524:VAL:HG13	2.09	0.52
2:D:55:THR:OG1	2:D:58:ASN:OD1	2.26	0.52
2:E:134:ASN:HB2	2:E:137:ASN:OD1	2.07	0.52
1:A:916:LEU:HD13	1:A:916:LEU:C	2.34	0.52
1:B:660:TYR:HB2	1:B:695:TYR:CE2	2.45	0.52
1:A:390:LEU:CD2	1:B:983:ARG:CD	2.64	0.52
2:D:169:ARG:HG2	2:D:499:ASP:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:N	1:B:335:LEU:CD1	2.73	0.52
4:D:905:NAG:O4	4:D:906:NAG:O5	2.26	0.52
1:B:898:PHE:N	1:B:899:PRO:CD	2.73	0.52
1:C:457:ARG:NH1	1:C:460:ASN:O	2.43	0.52
2:E:169:ARG:HG2	2:E:499:ASP:OD1	2.10	0.52
2:D:499:ASP:O	2:D:501:ALA:N	2.44	0.52
2:E:134:ASN:HB2	2:E:137:ASN:CG	2.34	0.52
1:B:457:ARG:NH1	1:B:460:ASN:O	2.42	0.51
1:C:388:ASN:OD1	1:C:527:PRO:HG2	2.10	0.51
1:A:95:ILE:O	1:A:96:GLU:HB2	2.09	0.51
2:D:125:THR:O	2:D:129:THR:OG1	2.28	0.51
2:D:222:LEU:O	2:D:225:ASP:HB2	2.11	0.51
2:D:520:LEU:HD22	2:D:581:VAL:HG12	1.92	0.51
1:B:41:LYS:O	1:B:42:VAL:HB	2.09	0.51
1:A:295:PRO:O	1:A:296:LEU:C	2.54	0.51
1:B:528:LYS:O	1:B:529:LYS:HG2	2.10	0.51
2:D:459:TRP:HB2	2:D:480:MET:HE1	1.93	0.51
2:E:222:LEU:O	2:E:225:ASP:HB2	2.11	0.51
1:C:430:THR:OG1	1:C:515:PHE:O	2.27	0.51
1:B:312:ILE:HD11	1:B:665:PRO:O	2.11	0.51
2:E:499:ASP:O	2:E:501:ALA:N	2.43	0.51
1:C:41:LYS:O	1:C:42:VAL:HB	2.11	0.51
1:A:382:VAL:CA	1:B:983:ARG:O	2.56	0.51
1:B:47:VAL:O	1:B:49:HIS:N	2.44	0.51
2:D:137:ASN:OD1	2:D:137:ASN:N	2.44	0.51
1:C:329:PHE:CD1	1:C:528:LYS:HB2	2.45	0.51
1:A:377:PHE:O	1:A:378:LYS:HG3	2.11	0.50
2:D:134:ASN:CB	2:D:137:ASN:CG	2.84	0.50
4:E:905:NAG:O4	4:E:906:NAG:O5	2.26	0.50
1:A:342:PHE:CZ	1:A:368:LEU:HD21	2.47	0.50
1:C:43:PHE:CG	1:C:44:ARG:N	2.79	0.50
1:C:454:ARG:NH2	1:C:469:SER:O	2.41	0.50
1:A:371:LEU:HG	1:A:375:PHE:CE1	2.47	0.50
1:B:702:GLU:OE2	1:C:790:LYS:NZ	2.44	0.50
1:C:898:PHE:N	1:C:899:PRO:CD	2.75	0.50
2:E:137:ASN:OD1	2:E:137:ASN:N	2.44	0.50
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.75	0.50
1:C:388:ASN:ND2	1:C:527:PRO:HD3	2.26	0.50
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.75	0.50
2:E:125:THR:O	2:E:129:THR:OG1	2.28	0.50
2:E:134:ASN:CB	2:E:137:ASN:CG	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:O	1:A:42:VAL:HB	2.10	0.50
1:A:391:CYS:HG	1:A:525:CYS:CB	2.16	0.50
2:E:459:TRP:HB2	2:E:480:MET:HE1	1.93	0.50
1:A:230:PRO:HB2	1:C:521:PRO:CD	2.40	0.50
2:E:520:LEU:HD22	2:E:581:VAL:HG12	1.92	0.50
2:D:155:SER:O	2:D:161:ARG:NH1	2.45	0.50
1:B:43:PHE:CG	1:B:44:ARG:N	2.80	0.50
2:D:20:THR:CG2	2:D:23:GLU:CD	2.85	0.50
2:E:155:SER:O	2:E:161:ARG:NH1	2.45	0.50
2:E:198:ASP:OD2	2:E:204:ARG:NH2	2.45	0.50
1:A:357:ARG:HH11	1:B:230:PRO:HG2	1.77	0.49
1:C:364:ASP:HA	1:C:526:GLY:HA2	1.94	0.49
2:D:198:ASP:OD2	2:D:204:ARG:NH2	2.45	0.49
2:E:212:VAL:HG21	2:E:565:PRO:HG3	1.93	0.49
2:E:368:ASP:HA	2:E:371:THR:HG22	1.93	0.49
1:B:388:ASN:O	1:B:527:PRO:HD3	2.12	0.49
1:C:331:ASN:O	1:C:332:ILE:HB	2.12	0.49
1:C:388:ASN:HD21	1:C:527:PRO:HG3	1.75	0.49
2:E:406:GLU:O	2:E:409:SER:OG	2.29	0.49
1:C:493:ARG:CD	2:D:34:HIS:CD2	2.90	0.49
1:A:331:ASN:C	1:A:332:ILE:CG1	2.86	0.49
1:B:335:LEU:H	1:B:335:LEU:CD1	2.26	0.49
1:B:430:THR:OG1	1:B:515:PHE:O	2.27	0.49
1:C:45:SER:O	1:C:47:VAL:N	2.46	0.49
2:D:212:VAL:HG21	2:D:565:PRO:HG3	1.93	0.49
1:B:643:PHE:CE1	1:B:655:TYR:CD2	3.01	0.49
2:D:368:ASP:HA	2:D:371:THR:HG22	1.94	0.49
1:A:391:CYS:SG	1:A:525:CYS:CB	3.01	0.49
1:B:744:GLY:O	1:B:745:ASP:HB2	2.13	0.49
2:E:364:VAL:HG13	2:E:364:VAL:O	2.12	0.49
2:D:92:THR:O	2:D:96:GLN:NE2	2.41	0.49
2:D:364:VAL:HG13	2:D:364:VAL:O	2.12	0.49
1:A:45:SER:O	1:A:47:VAL:N	2.46	0.48
1:B:383:SER:HG	1:B:385:THR:HG1	1.60	0.48
1:C:388:ASN:O	1:C:527:PRO:CD	2.61	0.48
2:E:201:ASP:OD2	2:E:219:ARG:NH2	2.46	0.48
1:B:364:ASP:CB	1:B:527:PRO:CG	2.84	0.48
1:B:103:GLY:HA3	1:B:119:ILE:O	2.13	0.48
1:A:382:VAL:CG2	1:A:383:SER:N	2.77	0.48
1:A:382:VAL:HG22	1:A:383:SER:H	1.78	0.48
1:B:672:ALA:HA	1:B:693:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:SER:OG	1:A:498:ARG:NH2	2.47	0.48
1:B:916:LEU:C	1:B:916:LEU:HD23	2.39	0.48
1:C:365:TYR:HB2	1:C:388:ASN:HA	1.95	0.48
1:C:385:THR:HG1	1:C:386:LYS:N	2.11	0.48
2:E:20:THR:CG2	2:E:23:GLU:CD	2.85	0.48
2:E:340:GLN:HG2	3:b:1:NAG:C8	2.36	0.48
2:E:92:THR:O	2:E:96:GLN:NE2	2.41	0.48
1:C:388:ASN:O	1:C:527:PRO:HD2	2.13	0.48
2:D:201:ASP:OD2	2:D:219:ARG:NH2	2.46	0.48
2:D:406:GLU:O	2:D:409:SER:OG	2.29	0.48
1:A:43:PHE:CG	1:A:44:ARG:N	2.82	0.48
1:B:329:PHE:HE1	1:B:529:LYS:C	2.22	0.48
2:E:230:PHE:HD1	2:E:233:ILE:HD12	1.79	0.48
1:C:47:VAL:O	1:C:49:HIS:N	2.46	0.47
2:D:201:ASP:OD1	2:D:219:ARG:NE	2.47	0.47
2:D:230:PHE:HD1	2:D:233:ILE:HD12	1.79	0.47
1:B:332:ILE:CG1	1:B:333:THR:N	2.77	0.47
1:B:365:TYR:HB2	1:B:388:ASN:HA	1.95	0.47
1:B:1082:CYS:SG	1:B:1132:ILE:HD13	2.54	0.47
1:C:763:LEU:HD13	1:C:1004:LEU:CD2	2.44	0.47
1:B:45:SER:O	1:B:47:VAL:N	2.48	0.47
1:B:310:LYS:HE3	1:B:664:ILE:HG12	1.96	0.47
2:E:111:ASP:OD1	2:E:111:ASP:N	2.47	0.47
1:C:332:ILE:HD13	1:C:334:ASN:N	2.29	0.47
1:C:384:PRO:HA	1:C:387:LEU:HG	1.96	0.47
2:D:609:ASP:OD1	2:D:609:ASP:N	2.40	0.47
2:E:131:LYS:HE3	2:E:141:CYS:HB2	1.97	0.47
1:A:47:VAL:O	1:A:49:HIS:N	2.47	0.47
1:B:384:PRO:HA	1:B:387:LEU:HG	1.96	0.47
1:C:332:ILE:CD1	1:C:333:THR:N	2.73	0.47
1:C:364:ASP:HA	1:C:526:GLY:CA	2.45	0.47
2:D:177:ARG:NH1	2:D:495:GLU:OE1	2.48	0.47
2:D:346:PRO:HA	2:D:359:LEU:O	2.14	0.47
2:E:107:VAL:HG21	4:E:902:NAG:H61	1.90	0.47
2:E:238:GLU:HB3	2:E:604:VAL:HG22	1.96	0.47
2:E:304:ALA:HA	2:E:307:ILE:HD12	1.96	0.47
2:E:346:PRO:HA	2:E:359:LEU:O	2.14	0.47
1:B:493:ARG:CD	2:E:34:HIS:CD2	2.90	0.47
1:C:360:ASN:HD22	1:C:523:THR:HB	1.80	0.47
1:C:366:SER:H	1:C:388:ASN:HD22	1.63	0.47
2:D:134:ASN:HB3	2:D:135:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:20:THR:CG2	2:E:23:GLU:CG	2.93	0.47
1:A:295:PRO:O	1:A:298:GLU:N	2.48	0.47
1:A:330:PRO:C	1:A:331:ASN:ND2	2.73	0.47
1:A:382:VAL:CG2	1:B:983:ARG:CB	2.93	0.47
2:D:131:LYS:HE3	2:D:141:CYS:HB2	1.97	0.47
2:E:177:ARG:NH1	2:E:495:GLU:OE1	2.48	0.47
2:E:201:ASP:OD1	2:E:219:ARG:NE	2.47	0.47
1:B:706:ALA:HB1	4:B:1410:NAG:H5	1.97	0.46
1:C:388:ASN:CG	1:C:527:PRO:HD3	2.40	0.46
2:E:134:ASN:HB3	2:E:135:PRO:HD2	1.95	0.46
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.50	0.46
1:B:364:ASP:CB	1:B:527:PRO:HG3	2.45	0.46
1:C:383:SER:HG	1:C:385:THR:HG1	1.63	0.46
2:E:386:ALA:HA	2:E:393:ARG:HE	1.80	0.46
1:C:916:LEU:C	1:C:916:LEU:HD23	2.41	0.46
2:D:20:THR:CG2	2:D:23:GLU:CG	2.93	0.46
2:D:524:GLN:HB3	2:D:574:VAL:HG11	1.98	0.46
2:E:365:THR:HG22	2:E:367:ASP:H	1.80	0.46
1:A:560:LEU:O	1:A:562:PHE:N	2.49	0.46
1:C:364:ASP:HA	1:C:527:PRO:N	2.31	0.46
2:D:107:VAL:HG21	4:D:902:NAG:H61	1.90	0.46
2:D:471:ASP:OD1	2:D:471:ASP:N	2.37	0.46
1:A:388:ASN:O	1:A:388:ASN:ND2	2.35	0.46
1:B:364:ASP:HA	1:B:527:PRO:N	2.30	0.46
2:D:238:GLU:HB3	2:D:604:VAL:HG22	1.96	0.46
2:D:351:LEU:HB2	2:D:355:ASP:HB3	1.98	0.46
2:D:386:ALA:HA	2:D:393:ARG:HE	1.80	0.46
1:A:888:PHE:CZ	1:A:1034:LEU:CD2	2.98	0.46
1:C:428:ASP:OD1	1:C:428:ASP:N	2.47	0.46
2:D:304:ALA:HA	2:D:307:ILE:HD12	1.96	0.46
1:A:382:VAL:HG23	1:B:983:ARG:O	2.07	0.46
1:B:385:THR:HG1	1:B:386:LYS:N	2.13	0.46
1:C:475:ALA:HB3	1:C:487:ASN:HD22	1.81	0.46
1:B:388:ASN:O	1:B:526:GLY:HA3	2.16	0.46
2:D:365:THR:HG22	2:D:367:ASP:H	1.80	0.46
2:E:237:TYR:O	2:E:240:LEU:HB3	2.16	0.46
2:E:362:THR:HG23	2:E:368:ASP:HB3	1.97	0.46
1:A:330:PRO:HG2	1:A:331:ASN:H	1.81	0.45
1:B:38:TYR:CE1	1:B:285:ILE:HG13	2.51	0.45
2:D:111:ASP:OD1	2:D:111:ASP:N	2.47	0.45
2:D:362:THR:HG23	2:D:368:ASP:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:VAL:HG23	1:B:306:PHE:CE2	2.52	0.45
1:C:983:ARG:O	1:C:984:LEU:HB2	2.15	0.45
2:E:524:GLN:HB3	2:E:574:VAL:HG11	1.98	0.45
1:B:335:LEU:CG	1:B:363:ALA:HB2	2.40	0.45
1:C:388:ASN:OD1	1:C:527:PRO:HD2	2.17	0.45
1:C:643:PHE:CZ	1:C:655:TYR:CD1	3.05	0.45
2:D:107:VAL:HG21	4:D:902:NAG:O5	2.16	0.45
1:B:329:PHE:HB2	1:B:330:PRO:HD2	1.98	0.45
1:B:600:PRO:HB3	1:B:674:TYR:HE2	1.81	0.45
1:C:332:ILE:C	1:C:334:ASN:N	2.73	0.45
1:B:294:ASP:HB2	1:B:295:PRO:CD	2.47	0.45
1:B:569:ILE:O	1:B:570:ALA:HB3	2.16	0.45
1:C:444:LYS:HB3	1:C:444:LYS:HE2	1.82	0.45
1:B:699:LEU:HD11	1:C:872:GLN:OE1	2.15	0.45
2:D:237:TYR:O	2:D:240:LEU:HB3	2.16	0.45
2:D:169:ARG:CG	2:D:499:ASP:OD1	2.64	0.45
2:E:169:ARG:CG	2:E:499:ASP:OD1	2.64	0.45
1:C:569:ILE:O	1:C:570:ALA:HB3	2.17	0.45
2:D:455:MET:HE3	2:D:455:MET:HB3	1.73	0.45
2:E:107:VAL:HG21	4:E:902:NAG:O5	2.16	0.45
1:B:428:ASP:N	1:B:428:ASP:OD1	2.47	0.45
1:C:811:LYS:HB3	1:C:812:PRO:HD2	1.99	0.45
2:D:218:SER:HB3	2:D:221:GLN:HB2	1.99	0.45
2:D:340:GLN:HG2	3:a:1:NAG:C8	2.35	0.45
1:B:335:LEU:C	1:B:336:CYS:O	2.60	0.44
1:B:475:ALA:HB3	1:B:487:ASN:HD22	1.81	0.44
1:B:542:ASN:HA	1:B:546:LEU:O	2.17	0.44
1:B:560:LEU:O	1:B:562:PHE:N	2.50	0.44
1:C:112:SER:O	1:C:113:LYS:HB2	2.17	0.44
1:C:332:ILE:O	1:C:334:ASN:N	2.50	0.44
1:C:364:ASP:CB	1:C:527:PRO:HG3	2.47	0.44
1:C:811:LYS:HB3	1:C:812:PRO:CD	2.48	0.44
1:B:718:PHE:CD1	1:B:718:PHE:C	2.96	0.44
2:E:351:LEU:HB2	2:E:355:ASP:HB3	1.98	0.44
1:C:541:PHE:CD1	1:C:541:PHE:C	2.96	0.44
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.49	0.44
1:A:326:ILE:HA	1:A:531:THR:CG2	2.47	0.44
1:B:358:ILE:HD13	1:B:358:ILE:HA	1.90	0.44
1:C:438:SER:OG	1:C:442:ASP:OD2	2.35	0.44
2:D:20:THR:OG1	2:D:21:ILE:N	2.50	0.44
2:D:177:ARG:NH2	2:D:495:GLU:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:218:SER:HB3	2:E:221:GLN:HB2	1.99	0.44
1:B:674:TYR:CE1	1:B:691:SER:O	2.71	0.44
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.99	0.44
1:C:63:THR:HG22	1:C:64:TRP:N	2.32	0.44
1:C:364:ASP:HB3	1:C:527:PRO:HG3	1.96	0.44
2:E:143:LEU:O	2:E:148:LEU:N	2.48	0.44
1:B:33:THR:HG22	1:B:58:PHE:CD2	2.52	0.44
1:B:360:ASN:HA	1:B:523:THR:HB	1.99	0.44
1:B:1126:CYS:SG	1:B:1132:ILE:HD13	2.58	0.44
1:C:388:ASN:O	1:C:526:GLY:HA3	2.18	0.44
1:C:364:ASP:HB3	1:C:527:PRO:CD	2.48	0.43
2:E:188:ASN:HB3	2:E:192:ARG:HH11	1.83	0.43
1:A:569:ILE:O	1:A:570:ALA:HB3	2.19	0.43
2:D:574:VAL:HG23	2:D:576:ALA:H	1.84	0.43
1:B:318:PHE:CE1	1:B:620:VAL:O	2.72	0.43
1:B:985:ASP:C	1:B:985:ASP:OD1	2.60	0.43
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.51	0.43
1:A:733:LYS:NZ	1:A:862:PRO:O	2.45	0.43
1:B:712:ILE:O	1:B:1074:ASN:HA	2.18	0.43
1:C:391:CYS:O	1:C:392:PHE:CD1	2.71	0.43
2:D:143:LEU:O	2:D:148:LEU:N	2.48	0.43
2:E:20:THR:OG1	2:E:21:ILE:N	2.50	0.43
1:A:372:ALA:N	1:A:373:PRO:HD2	2.34	0.43
1:A:382:VAL:CG1	1:A:387:LEU:HD23	2.49	0.43
1:A:541:PHE:CD1	1:A:541:PHE:C	2.97	0.43
1:B:335:LEU:CG	1:B:363:ALA:CB	2.72	0.43
1:B:655:TYR:HA	1:B:694:ALA:O	2.19	0.43
1:A:357:ARG:NH1	1:B:230:PRO:HG2	2.34	0.43
2:D:371:THR:HA	2:D:374:HIS:HB3	2.01	0.43
1:A:898:PHE:HB3	1:A:899:PRO:HD3	1.99	0.43
1:B:391:CYS:O	1:B:392:PHE:CD1	2.71	0.43
1:B:453:TYR:HE2	1:B:455:LEU:HD13	1.83	0.43
1:B:498:ARG:HD3	1:B:501:TYR:OH	2.14	0.43
1:C:332:ILE:HD13	1:C:333:THR:CA	2.48	0.43
2:D:474:MET:SD	2:D:499:ASP:N	2.85	0.43
2:E:208:GLU:HB2	2:E:219:ARG:HG2	2.00	0.43
2:E:574:VAL:HG23	2:E:576:ALA:H	1.84	0.43
1:B:363:ALA:O	1:B:525:CYS:O	2.37	0.43
2:D:35:GLU:HG2	2:D:35:GLU:H	1.57	0.43
2:E:177:ARG:NH2	2:E:495:GLU:O	2.51	0.43
1:A:112:SER:O	1:A:113:LYS:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:PHE:O	1:B:42:VAL:HA	2.19	0.42
1:C:366:SER:H	1:C:388:ASN:ND2	2.17	0.42
1:C:453:TYR:HE2	1:C:455:LEU:HD13	1.83	0.42
1:C:986:PRO:HB2	1:C:987:PRO:HD3	2.01	0.42
2:E:137:ASN:HD22	2:E:140:GLU:HB3	1.84	0.42
1:A:230:PRO:CB	1:C:521:PRO:CD	2.92	0.42
1:A:368:LEU:C	1:A:370:ASN:N	2.73	0.42
1:B:699:LEU:HD21	1:C:869:MET:HE3	2.00	0.42
1:B:980:ILE:O	1:B:984:LEU:HB3	2.19	0.42
2:E:371:THR:HA	2:E:374:HIS:HB3	2.01	0.42
1:B:85:PRO:O	1:B:238:PHE:CE1	2.72	0.42
1:B:792:PRO:HA	1:B:793:PRO:HD3	1.91	0.42
2:D:358:ILE:HD11	2:D:379:ILE:HG13	2.01	0.42
2:E:424:LEU:HD12	2:E:424:LEU:HA	1.89	0.42
2:E:455:MET:HB3	2:E:455:MET:HE3	1.73	0.42
2:D:188:ASN:HB3	2:D:192:ARG:HH11	1.83	0.42
3:Q:1:NAG:H4	3:Q:2:NAG:C7	2.49	0.42
1:B:39:PRO:C	1:B:40:ASP:CG	2.82	0.42
1:B:112:SER:O	1:B:113:LYS:HB2	2.18	0.42
2:E:42:GLN:HE21	2:E:42:GLN:HB3	1.68	0.42
1:B:444:LYS:HE2	1:B:444:LYS:HB3	1.82	0.42
4:B:1410:NAG:O4	4:B:1411:NAG:O5	2.28	0.42
2:D:208:GLU:HB2	2:D:219:ARG:HG2	2.00	0.42
2:D:612:PRO:HA	2:D:615:ASP:HB2	2.02	0.42
2:E:358:ILE:HD11	2:E:379:ILE:HG13	2.01	0.42
1:A:437:ASN:HB2	1:A:508:TYR:CZ	2.54	0.42
1:B:541:PHE:CD1	1:B:541:PHE:C	2.97	0.42
1:B:674:TYR:CD1	1:B:691:SER:O	2.72	0.42
1:C:438:SER:OG	1:C:438:SER:O	2.36	0.42
1:B:366:SER:H	1:B:388:ASN:ND2	2.16	0.42
1:C:289:VAL:HG23	1:C:306:PHE:CE2	2.55	0.42
2:E:134:ASN:CB	2:E:137:ASN:HD21	2.32	0.42
1:B:63:THR:HG22	1:B:64:TRP:N	2.35	0.42
1:B:393:THR:OG1	1:B:518:LEU:N	2.53	0.42
2:D:137:ASN:HD22	2:D:140:GLU:HB3	1.85	0.42
1:B:898:PHE:HB3	1:B:899:PRO:HD3	2.01	0.41
1:B:388:ASN:OD1	1:B:527:PRO:HG3	2.17	0.41
1:B:454:ARG:NH2	1:B:469:SER:O	2.41	0.41
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.36	0.41
2:D:134:ASN:CB	2:D:137:ASN:HD21	2.32	0.41
2:E:206:ASP:OD1	2:E:206:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:564:GLU:HB3	2:E:568:LEU:HD23	2.02	0.41
2:E:612:PRO:HA	2:E:615:ASP:HB2	2.02	0.41
1:A:970:PHE:O	1:A:995:ARG:NH2	2.53	0.41
1:A:986:PRO:N	1:A:987:PRO:HD2	2.35	0.41
1:B:335:LEU:HD23	1:B:367:VAL:HG11	2.02	0.41
1:B:392:PHE:CA	1:B:524:VAL:HG13	2.50	0.41
2:D:174:LYS:HG2	2:D:497:TYR:HA	2.02	0.41
1:A:200:TYR:CZ	1:C:521:PRO:HD3	2.56	0.41
1:A:394:ASN:ND2	1:B:200:TYR:CE1	2.88	0.41
1:C:204:TYR:CE2	1:C:225:PRO:HG3	2.55	0.41
2:D:468:ILE:HD11	2:D:473:TRP:HA	2.03	0.41
1:B:438:SER:O	1:B:438:SER:OG	2.36	0.41
2:D:206:ASP:OD1	2:D:206:ASP:N	2.53	0.41
1:A:379:CYS:HB3	1:A:382:VAL:O	2.20	0.41
2:D:442:GLN:O	2:D:445:THR:OG1	2.32	0.41
2:E:168:TRP:HE1	2:E:502:SER:HB2	1.86	0.41
2:E:238:GLU:HA	2:E:241:HIS:HB3	2.03	0.41
1:B:360:ASN:HD22	1:B:523:THR:HB	1.86	0.41
1:B:361:CYS:C	1:B:362:VAL:HG23	2.46	0.41
1:C:662:CYS:HB2	1:C:697:MET:SD	2.61	0.41
1:A:516:GLU:CD	1:B:200:TYR:HH	2.28	0.41
1:A:393:THR:HA	1:A:522:ALA:HA	2.01	0.41
1:A:736:VAL:HG22	1:A:858:LEU:CD2	2.51	0.41
1:B:590:CYS:O	1:B:591:SER:C	2.63	0.41
1:B:702:GLU:OE2	1:C:790:LYS:CE	2.69	0.41
1:B:986:PRO:N	1:B:987:PRO:CD	2.83	0.41
1:C:361:CYS:C	1:C:362:VAL:HG23	2.46	0.41
1:C:393:THR:OG1	1:C:518:LEU:N	2.53	0.41
1:C:560:LEU:C	1:C:562:PHE:H	2.29	0.41
2:D:26:LYS:HB2	2:D:26:LYS:HE3	1.78	0.41
2:E:134:ASN:CB	2:E:135:PRO:HD3	2.51	0.41
2:E:595:LEU:HD23	2:E:595:LEU:HA	1.91	0.41
2:D:238:GLU:HA	2:D:241:HIS:HB3	2.03	0.41
2:D:250:ASN:OD1	2:D:250:ASN:N	2.54	0.41
2:E:169:ARG:HD3	2:E:499:ASP:CG	2.46	0.41
1:A:382:VAL:CG2	1:B:983:ARG:HB3	2.50	0.40
2:D:169:ARG:HD3	2:D:499:ASP:CG	2.46	0.40
2:D:564:GLU:HB3	2:D:568:LEU:HD23	2.02	0.40
1:C:985:ASP:O	1:C:986:PRO:C	2.64	0.40
2:D:198:ASP:O	2:D:201:ASP:N	2.49	0.40
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:237:TYR:O	2:D:241:HIS:N	2.53	0.40
2:E:174:LYS:HG2	2:E:497:TYR:HA	2.03	0.40
1:A:382:VAL:HG21	1:B:983:ARG:CA	2.41	0.40
1:B:392:PHE:CB	1:B:524:VAL:HG13	2.51	0.40
1:C:385:THR:HG1	1:C:386:LYS:H	1.69	0.40
1:C:775:ASP:OD1	1:C:864:LEU:HB3	2.22	0.40
2:E:122:THR:HA	2:E:125:THR:HG22	2.04	0.40
2:E:468:ILE:HD11	2:E:473:TRP:HA	2.03	0.40
2:E:557:MET:HE3	2:E:557:MET:HB3	2.00	0.40
1:B:103:GLY:CA	1:B:119:ILE:O	2.68	0.40
1:C:560:LEU:O	1:C:562:PHE:N	2.50	0.40
2:E:223:ILE:H	2:E:223:ILE:HG12	1.66	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	941/1267 (74%)	868 (92%)	52 (6%)	21 (2%)	5	26
1	B	978/1267 (77%)	904 (92%)	61 (6%)	13 (1%)	9	35
1	C	978/1267 (77%)	899 (92%)	62 (6%)	17 (2%)	7	30
2	D	595/817 (73%)	553 (93%)	35 (6%)	7 (1%)	10	37
2	E	595/817 (73%)	553 (93%)	35 (6%)	7 (1%)	10	37
All	All	4087/5435 (75%)	3777 (92%)	245 (6%)	65 (2%)	10	31

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	46	SER

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Mol	Chain	Res	Type
1	A	332	ILE
1	A	591	SER
1	A	855	PHE
1	B	41	LYS
1	B	46	SER
1	B	336	CYS
1	B	524	VAL
1	B	530	SER
1	C	46	SER
1	C	332	ILE
1	C	529	LYS
1	C	984	LEU
2	D	134	ASN
2	D	136	ASP
2	E	134	ASN
2	E	136	ASP
1	A	48	LEU
1	A	370	ASN
1	A	701	ALA
1	B	48	LEU
1	B	96	GLU
1	B	529	LYS
1	B	591	SER
1	C	41	LYS
1	C	96	GLU
1	C	591	SER
1	C	814	LYS
1	C	855	PHE
2	D	20	THR
2	E	20	THR
1	A	96	GLU
1	A	330	PRO
1	A	331	ASN
1	A	529	LYS
1	A	797	PHE
1	B	217	PRO
1	B	333	THR
1	C	48	LEU
1	C	333	THR
1	C	810	SER
1	A	217	PRO
1	A	334	ASN

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Mol	Chain	Res	Type
1	A	798	GLY
1	C	217	PRO
1	C	330	PRO
1	C	813	SER
2	D	270	MET
2	D	610	TRP
2	E	270	MET
2	E	610	TRP
1	A	42	VAL
1	A	368	LEU
1	B	42	VAL
1	C	42	VAL
2	D	271	TRP
2	E	271	TRP
1	A	382	VAL
1	A	527	PRO
1	C	809	PRO
1	A	295	PRO
1	B	742	ILE
2	D	500	PRO
2	E	500	PRO

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	848/1108 (76%)	836 (99%)	12 (1%)	59	73
1	B	878/1108 (79%)	870 (99%)	8 (1%)	70	78
1	C	878/1108 (79%)	871 (99%)	7 (1%)	73	79
2	D	527/721 (73%)	520 (99%)	7 (1%)	61	74
2	E	527/721 (73%)	520 (99%)	7 (1%)	61	74
All	All	3658/4766 (77%)	3617 (99%)	41 (1%)	63	76

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	332	ILE
1	A	333	THR
1	A	356	LYS
1	A	366	SER
1	A	371	LEU
1	A	374	PHE
1	A	386	LYS
1	A	388	ASN
1	A	393	THR
1	A	434	ILE
1	A	1074	ASN
1	B	122	ASN
1	B	332	ILE
1	B	335	LEU
1	B	364	ASP
1	B	410	ILE
1	B	498	ARG
1	B	528	LYS
1	B	1074	ASN
1	C	122	ASN
1	C	332	ILE
1	C	335	LEU
1	C	364	ASP
1	C	410	ILE
1	C	498	ARG
1	C	525	CYS
2	D	19	SER
2	D	35	GLU
2	D	223	ILE
2	D	344	CYS
2	D	468	ILE
2	D	499	ASP
2	D	610	TRP
2	E	19	SER
2	E	35	GLU
2	E	223	ILE
2	E	344	CYS
2	E	468	ILE
2	E	499	ASP
2	E	610	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	188	ASN
1	A	519	HIS
1	A	607	GLN
1	A	787	GLN
1	A	804	GLN
1	A	949	GLN
1	A	1058	HIS
1	A	1083	HIS
1	A	1088	HIS
1	B	218	GLN
1	B	354	ASN
1	B	360	ASN
1	B	422	ASN
1	B	448	ASN
1	B	487	ASN
1	B	536	ASN
1	B	949	GLN
1	B	1002	GLN
1	B	1083	HIS
1	C	354	ASN
1	C	360	ASN
1	C	422	ASN
1	C	448	ASN
1	C	487	ASN
1	C	536	ASN
1	C	606	ASN
1	C	949	GLN
1	C	992	GLN
2	D	49	ASN
2	D	51	ASN
2	D	61	ASN
2	D	96	GLN
2	D	149	ASN
2	D	194	ASN
2	D	241	HIS
2	D	508	ASN
2	D	524	GLN
2	D	552	GLN
2	D	572	ASN
2	D	578	ASN
2	D	586	ASN
2	E	49	ASN

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Mol	Chain	Res	Type
2	E	51	ASN
2	E	61	ASN
2	E	96	GLN
2	E	149	ASN
2	E	194	ASN
2	E	241	HIS
2	E	508	ASN
2	E	524	GLN
2	E	552	GLN
2	E	572	ASN
2	E	578	ASN
2	E	586	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

46 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	F	1	3,1	14,14,15	0.52	0	17,19,21	0.51	0
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	G	1	3,1	14,14,15	0.30	0	17,19,21	0.63	0
3	NAG	G	2	3	14,14,15	0.54	0	17,19,21	0.49	0
3	NAG	H	1	3,1	14,14,15	0.36	0	17,19,21	0.74	0
3	NAG	H	2	3	14,14,15	0.30	0	17,19,21	1.39	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	I	1	3,1	14,14,15	0.67	1 (7%)	17,19,21	0.71	0
3	NAG	I	2	3	14,14,15	0.40	0	17,19,21	1.49	3 (17%)
3	NAG	J	1	3,1	14,14,15	0.67	1 (7%)	17,19,21	0.68	0
3	NAG	J	2	3	14,14,15	0.27	0	17,19,21	0.68	0
3	NAG	K	1	3,1	14,14,15	0.24	0	17,19,21	0.70	1 (5%)
3	NAG	K	2	3	14,14,15	0.17	0	17,19,21	0.49	0
3	NAG	L	1	3,1	14,14,15	0.51	0	17,19,21	0.52	0
3	NAG	L	2	3	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	M	1	3,1	14,14,15	0.57	0	17,19,21	0.59	0
3	NAG	M	2	3	14,14,15	0.29	0	17,19,21	0.46	0
3	NAG	N	1	3,1	14,14,15	0.29	0	17,19,21	0.41	0
3	NAG	N	2	3	14,14,15	0.38	0	17,19,21	0.38	0
3	NAG	O	1	3,1	14,14,15	0.35	0	17,19,21	1.17	1 (5%)
3	NAG	O	2	3	14,14,15	0.26	0	17,19,21	0.47	0
3	NAG	P	1	3,1	14,14,15	0.31	0	17,19,21	0.71	1 (5%)
3	NAG	P	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	Q	1	3,1	14,14,15	0.71	1 (7%)	17,19,21	0.92	1 (5%)
3	NAG	Q	2	3	14,14,15	0.37	0	17,19,21	0.74	1 (5%)
3	NAG	R	1	3,1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	R	2	3	14,14,15	0.29	0	17,19,21	0.39	0
3	NAG	S	1	3,1	14,14,15	0.50	0	17,19,21	0.52	0
3	NAG	S	2	3	14,14,15	0.24	0	17,19,21	0.60	0
3	NAG	T	1	3,1	14,14,15	0.57	0	17,19,21	0.58	0
3	NAG	T	2	3	14,14,15	0.29	0	17,19,21	0.47	0
3	NAG	U	1	3,1	14,14,15	0.23	0	17,19,21	1.45	2 (11%)
3	NAG	U	2	3	14,14,15	0.16	0	17,19,21	0.51	0
3	NAG	V	1	3,1	14,14,15	0.51	0	17,19,21	0.72	1 (5%)
3	NAG	V	2	3	14,14,15	0.40	0	17,19,21	0.49	0
3	NAG	W	1	3,1	14,14,15	0.41	0	17,19,21	0.41	0
3	NAG	W	2	3	14,14,15	0.21	0	17,19,21	0.77	0
3	NAG	X	1	3,1	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	X	2	3	14,14,15	0.61	1 (7%)	17,19,21	1.38	2 (11%)
3	NAG	Y	1	3,1	14,14,15	0.62	1 (7%)	17,19,21	0.43	0
3	NAG	Y	2	3	14,14,15	0.34	0	17,19,21	1.43	2 (11%)
3	NAG	Z	1	3,1	14,14,15	0.38	0	17,19,21	0.47	0
3	NAG	Z	2	3	14,14,15	0.24	0	17,19,21	0.52	0
3	NAG	a	1	2,3	14,14,15	0.57	0	17,19,21	0.74	0
3	NAG	a	2	3	14,14,15	0.55	0	17,19,21	0.39	0
3	NAG	b	1	2,3	14,14,15	0.59	1 (7%)	17,19,21	0.74	0
3	NAG	b	2	3	14,14,15	0.54	0	17,19,21	0.39	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	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	3/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	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	NAG	S	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	3/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	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	NAG	W	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	NAG	X	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Y	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Z	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
3	NAG	a	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	1	NAG	O5-C1	-2.58	1.39	1.43
3	J	1	NAG	O5-C1	-2.44	1.39	1.43
3	I	1	NAG	O5-C1	-2.18	1.40	1.43
3	X	2	NAG	C1-C2	2.07	1.55	1.52
3	b	1	NAG	O5-C1	-2.07	1.40	1.43
3	Y	1	NAG	O5-C1	-2.05	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	1	NAG	C2-N2-C7	5.01	129.62	122.90
3	I	2	NAG	C2-N2-C7	4.73	129.24	122.90
3	Y	2	NAG	C2-N2-C7	4.59	129.06	122.90
3	X	2	NAG	C2-N2-C7	4.58	129.04	122.90
3	H	2	NAG	C2-N2-C7	4.52	128.96	122.90
3	O	1	NAG	C1-O5-C5	3.35	116.68	112.19
3	I	2	NAG	C1-C2-N2	2.63	114.58	110.43
3	H	2	NAG	C1-C2-N2	2.61	114.54	110.43
3	Y	2	NAG	C1-C2-N2	2.45	114.29	110.43
3	Q	1	NAG	O4-C4-C3	-2.36	104.80	110.38
3	V	1	NAG	C1-O5-C5	2.27	115.23	112.19
3	P	1	NAG	C1-O5-C5	2.26	115.22	112.19
3	U	1	NAG	C1-C2-N2	2.12	113.78	110.43
3	K	1	NAG	C1-O5-C5	2.12	115.02	112.19
3	Q	2	NAG	C1-O5-C5	2.10	115.00	112.19
3	I	2	NAG	C1-O5-C5	2.08	114.97	112.19
3	X	2	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (14) torsion outliers are listed below:

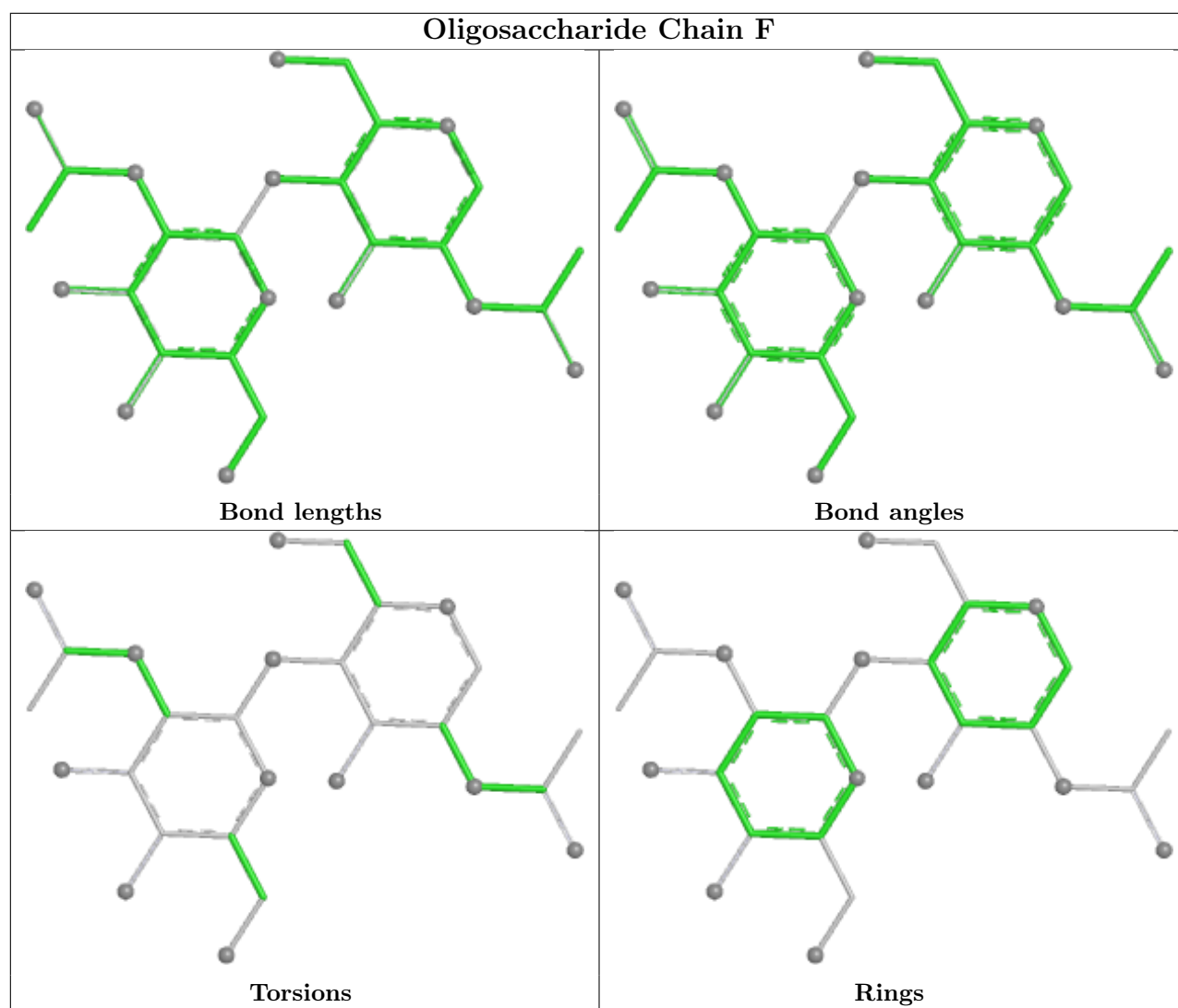
Mol	Chain	Res	Type	Atoms
3	a	1	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C3-C2-N2-C7
3	T	2	NAG	C3-C2-N2-C7
3	M	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6

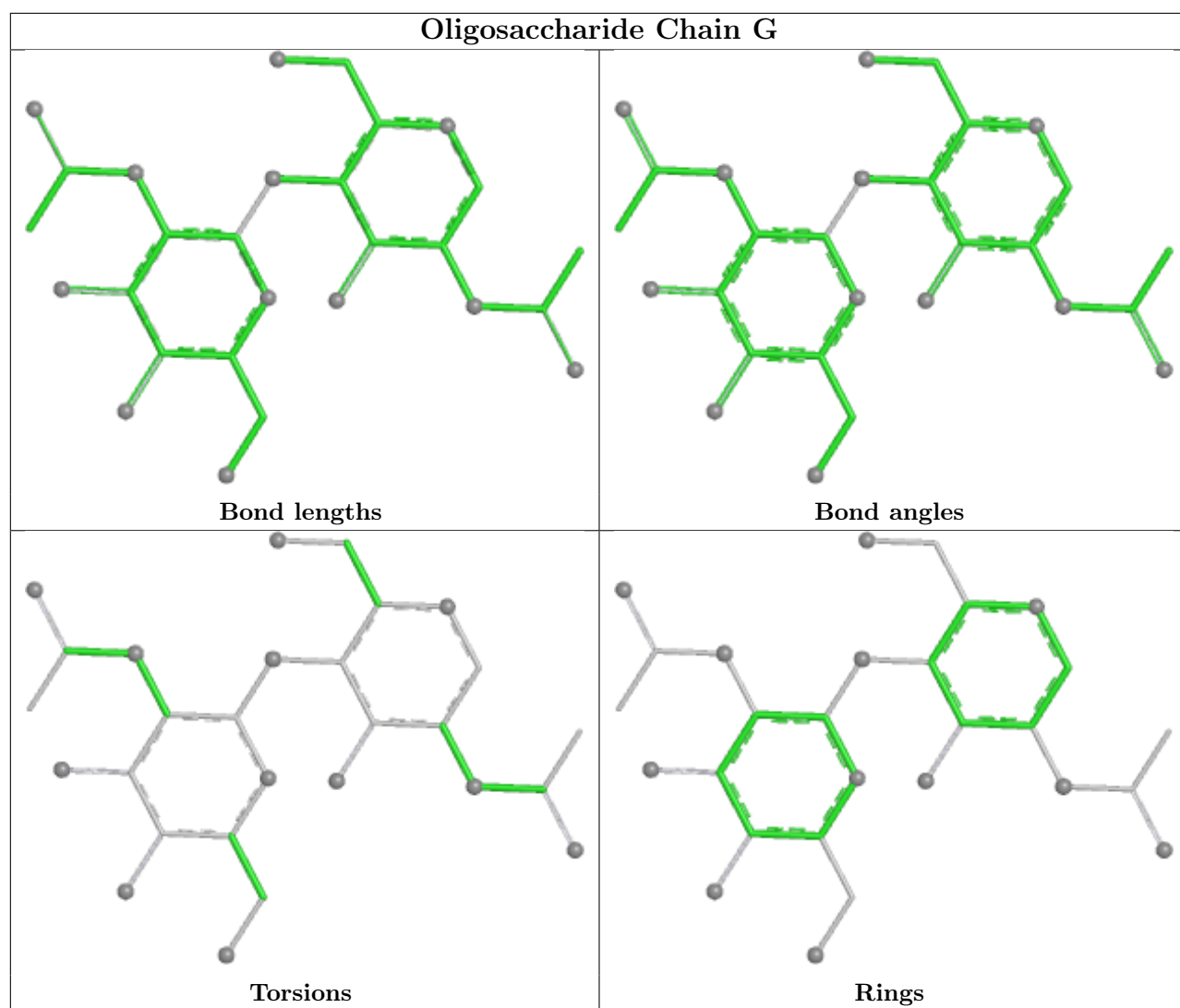
There are no ring outliers.

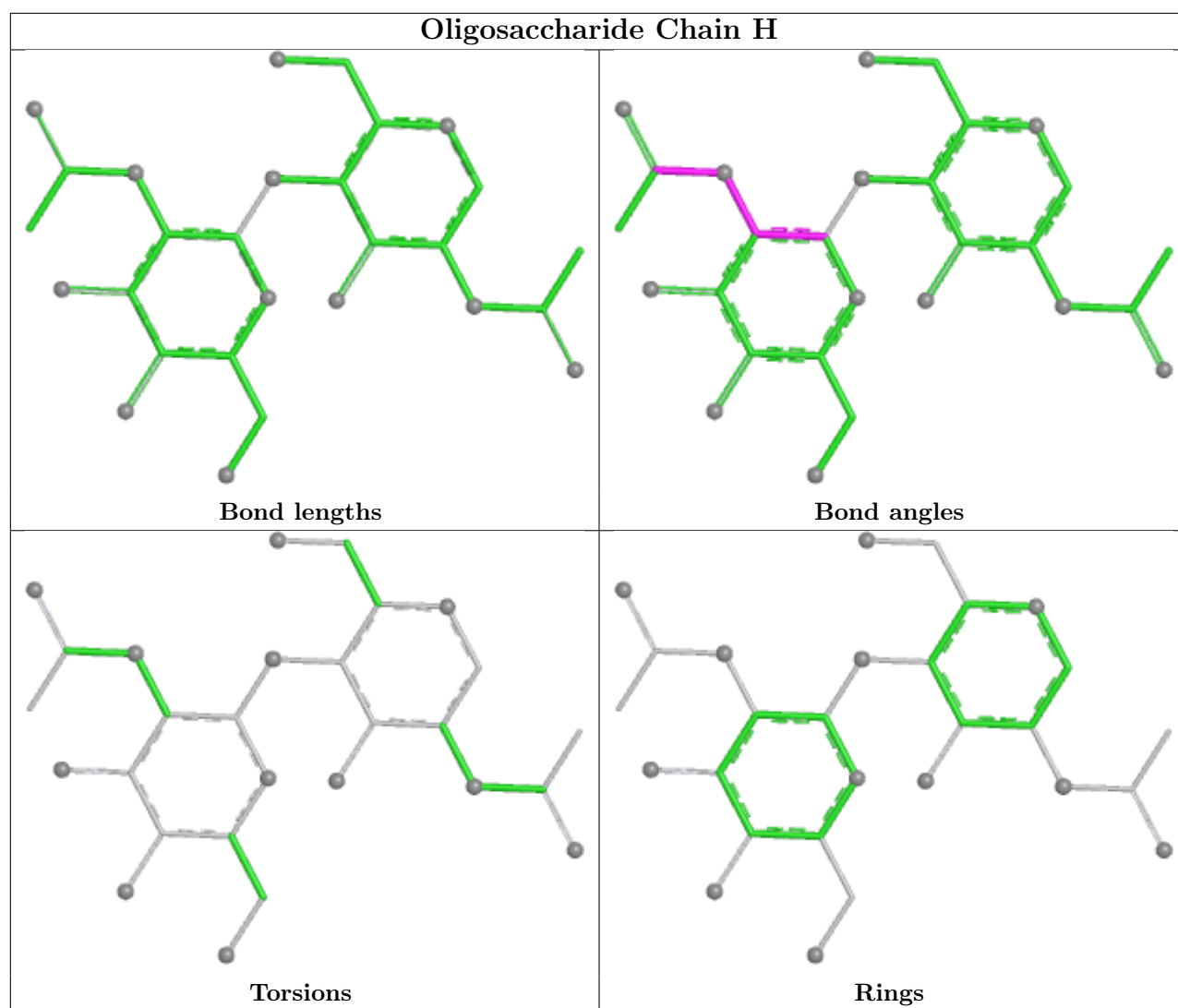
4 monomers are involved in 5 short contacts:

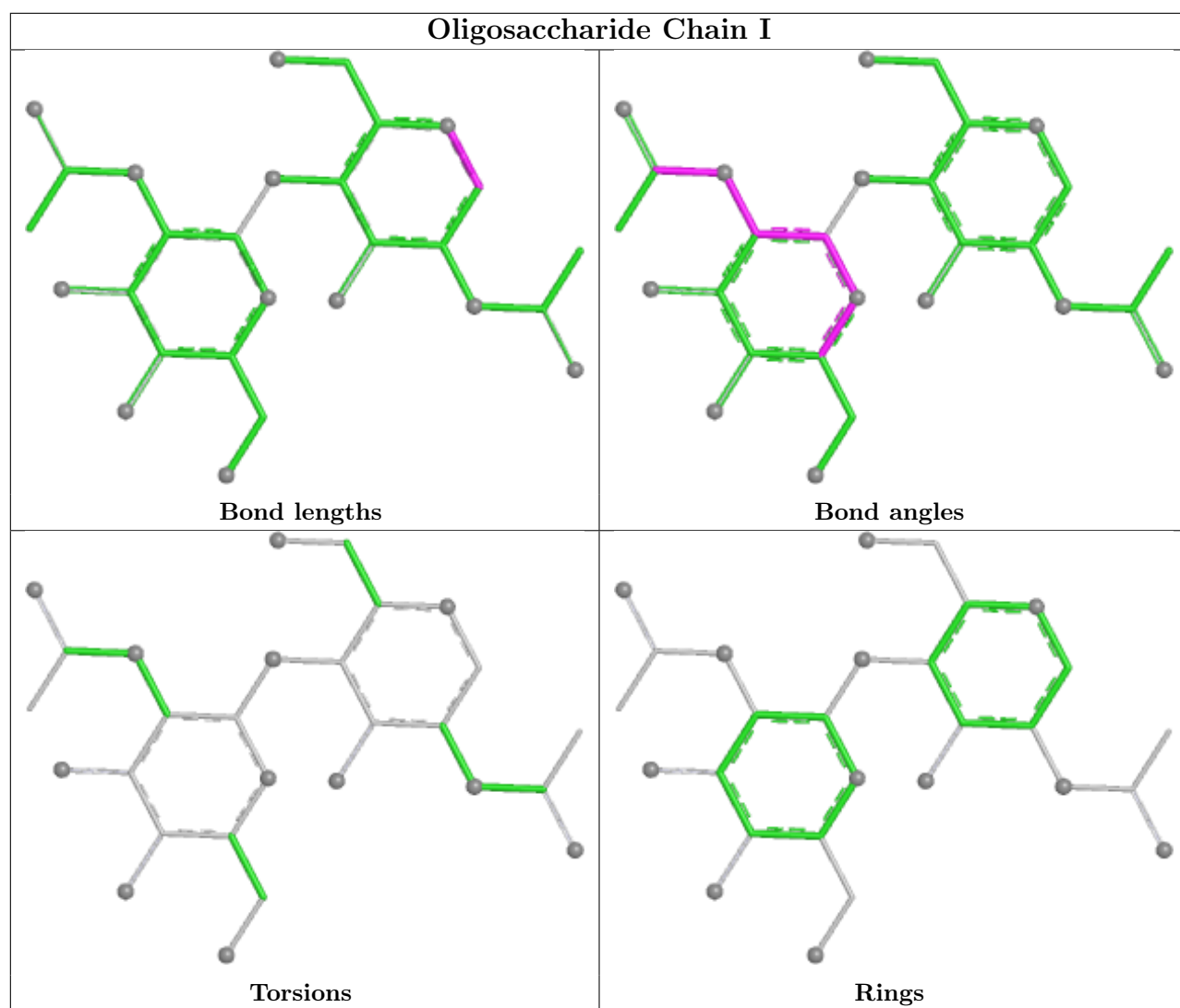
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	a	1	NAG	2	0
3	b	1	NAG	2	0
3	Q	1	NAG	1	0
3	Q	2	NAG	1	0

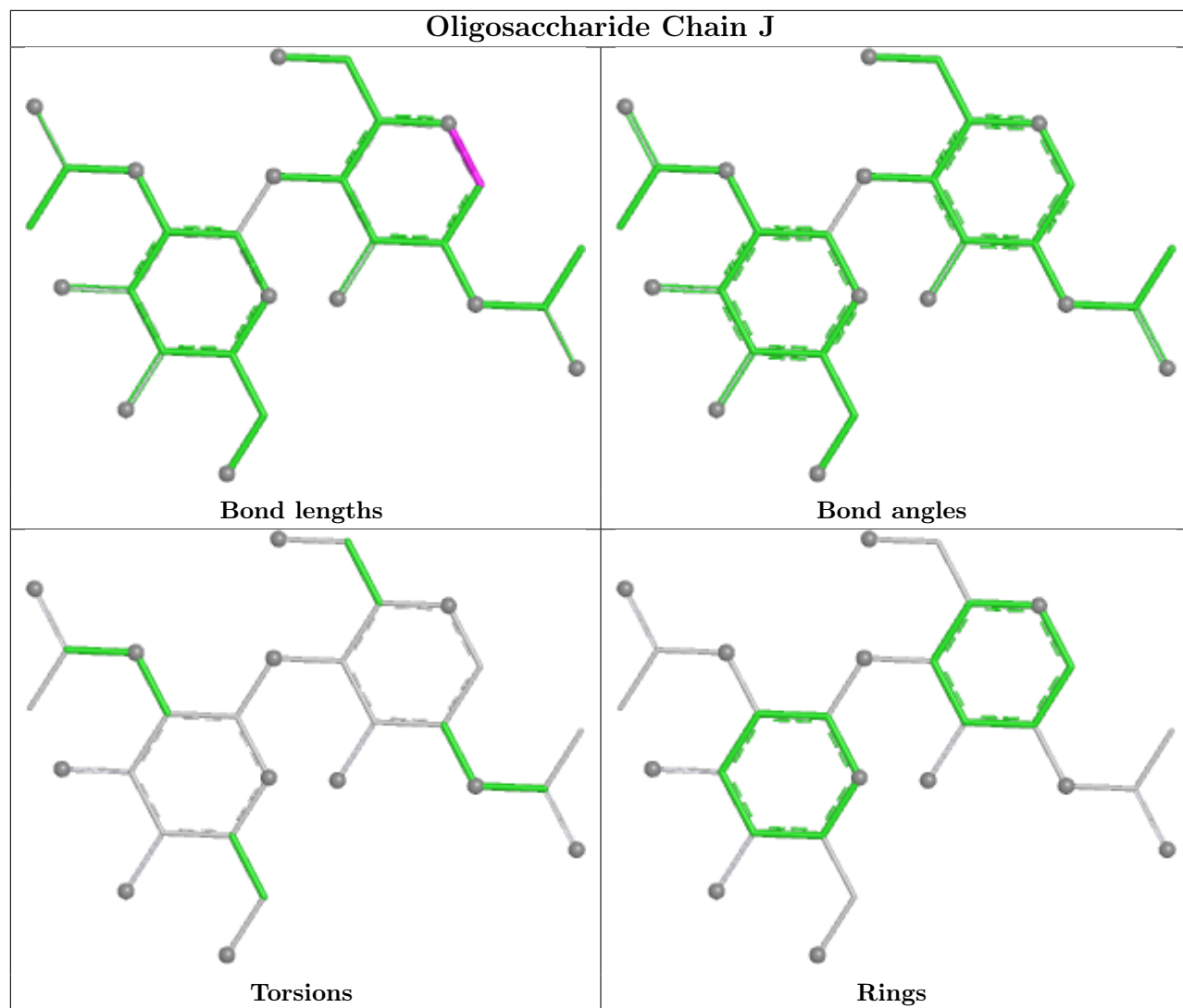
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

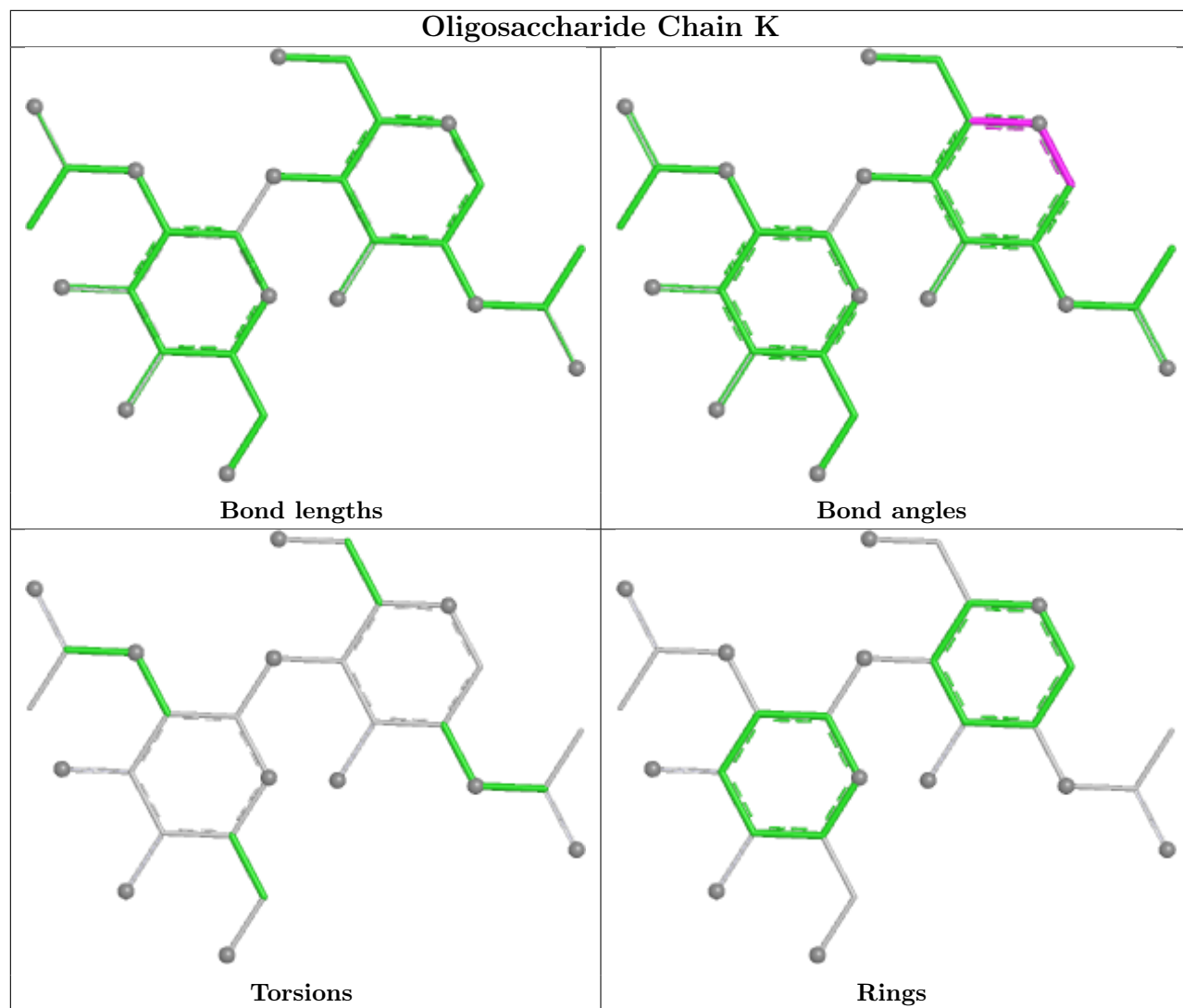


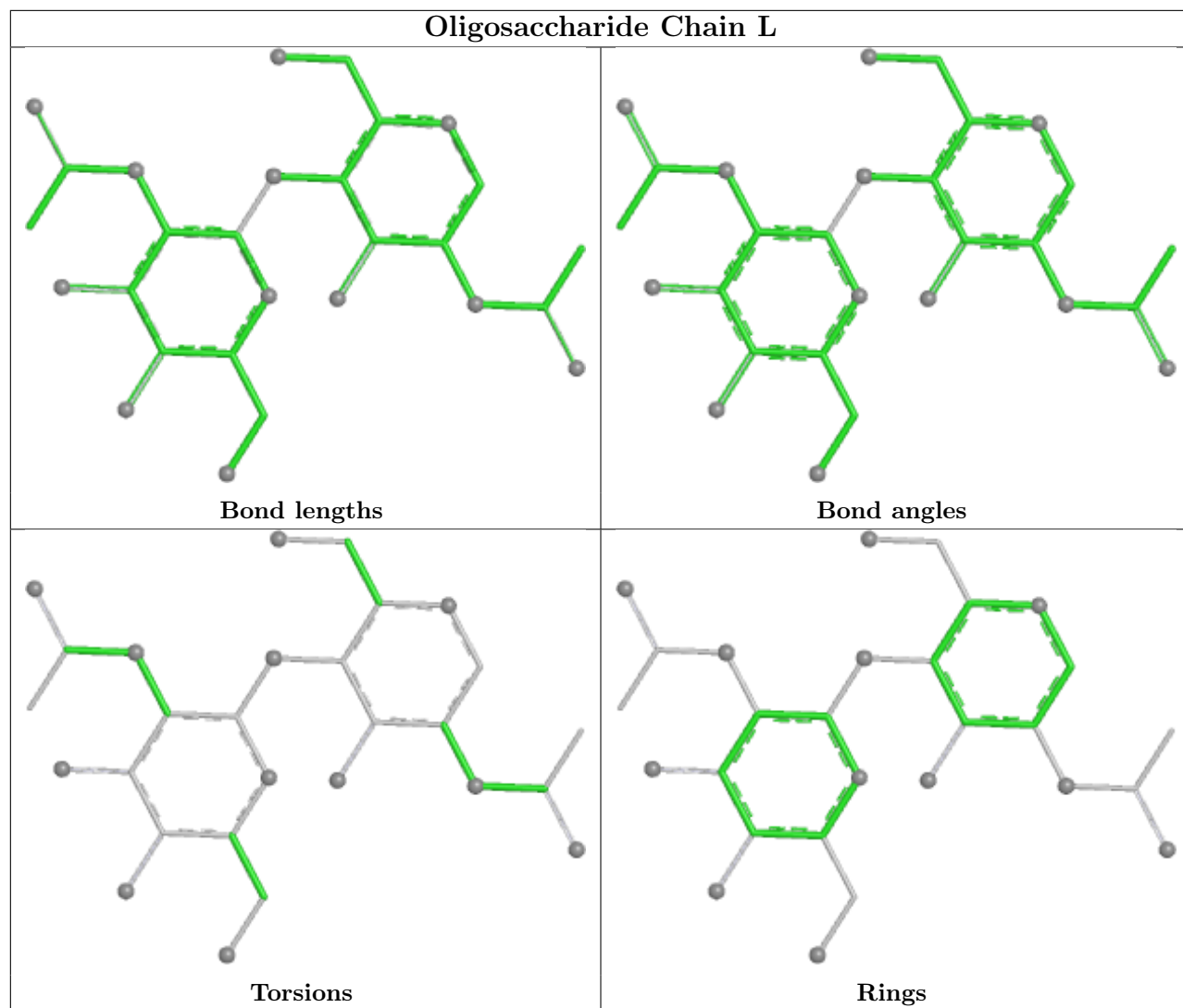


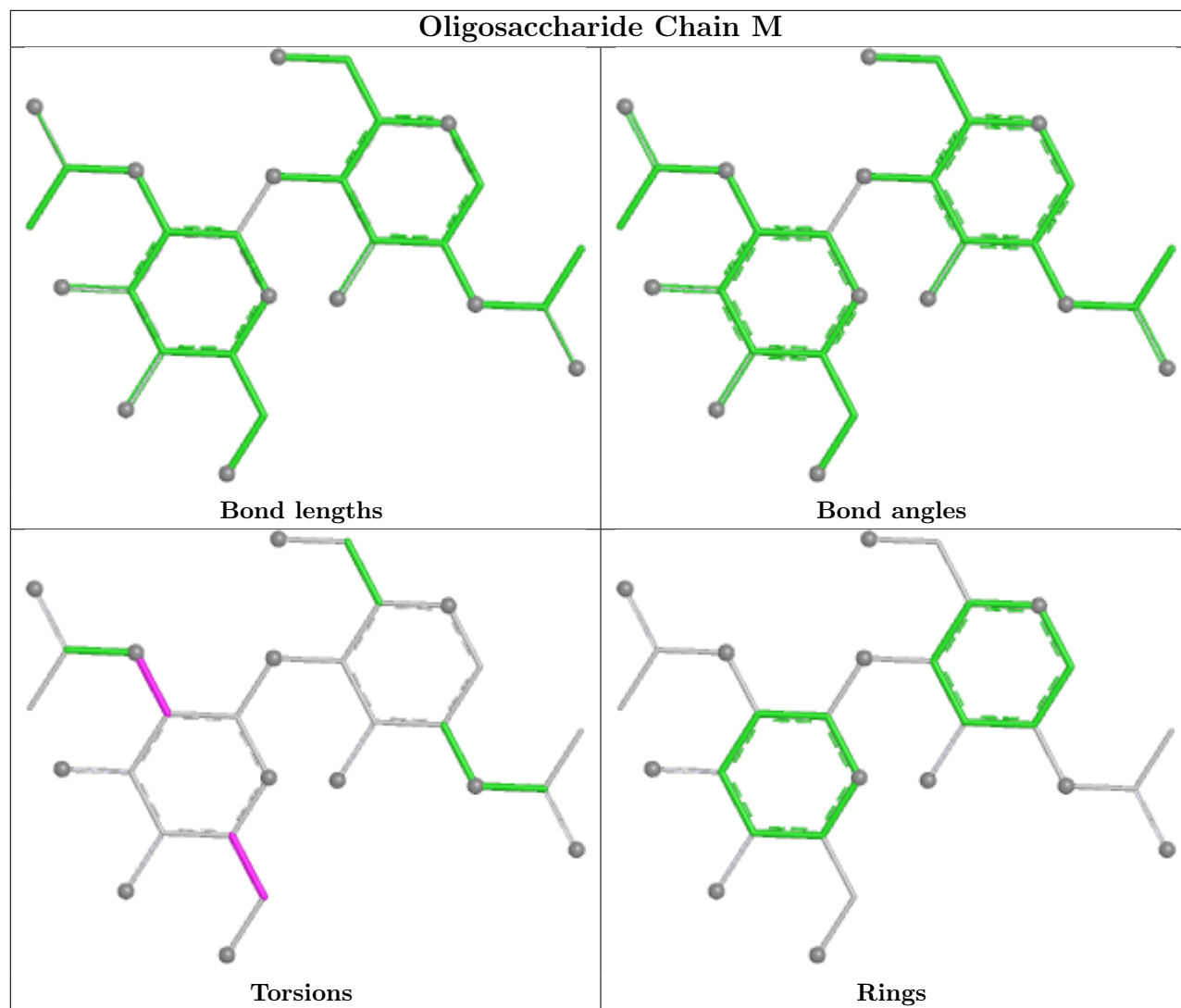


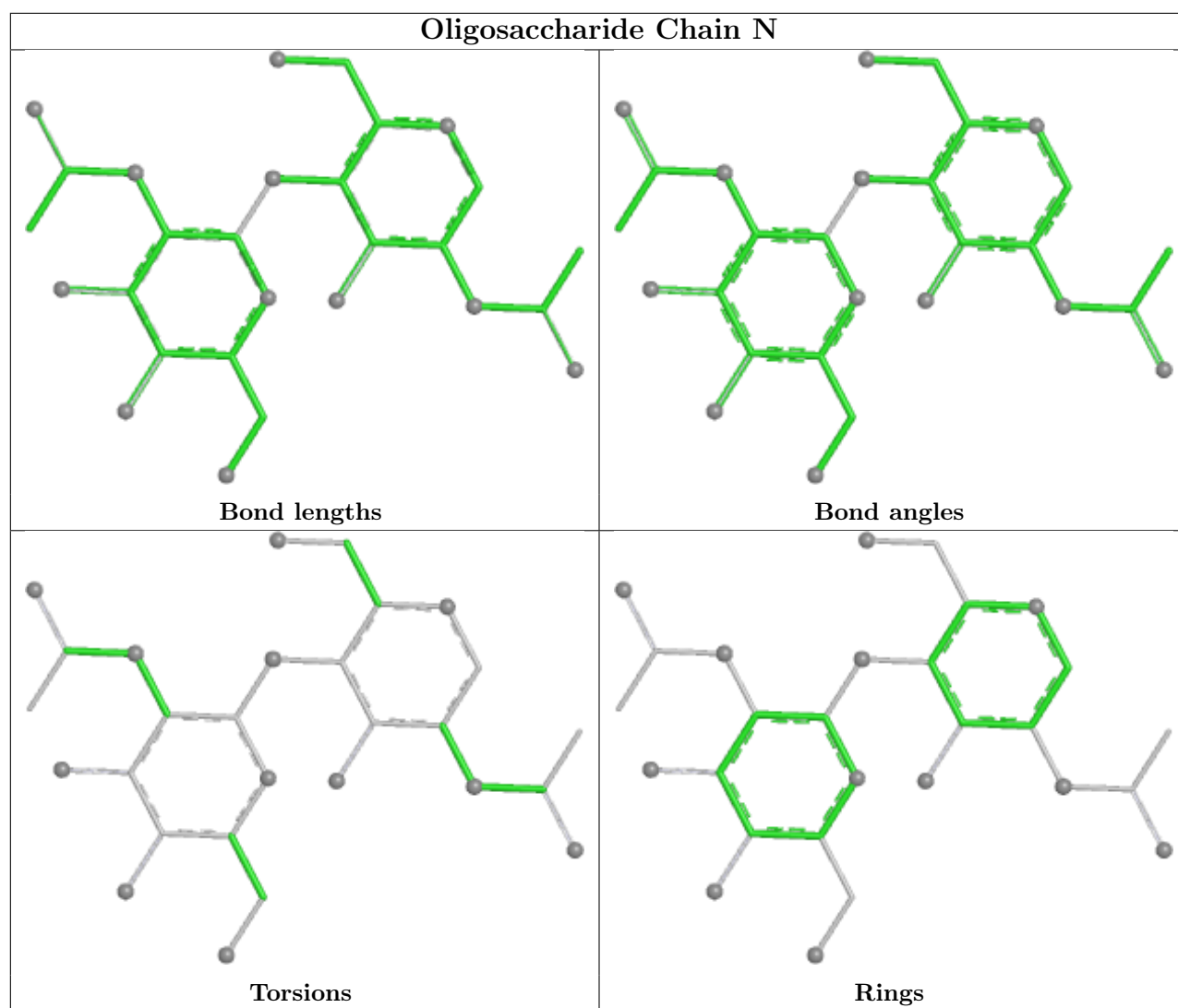


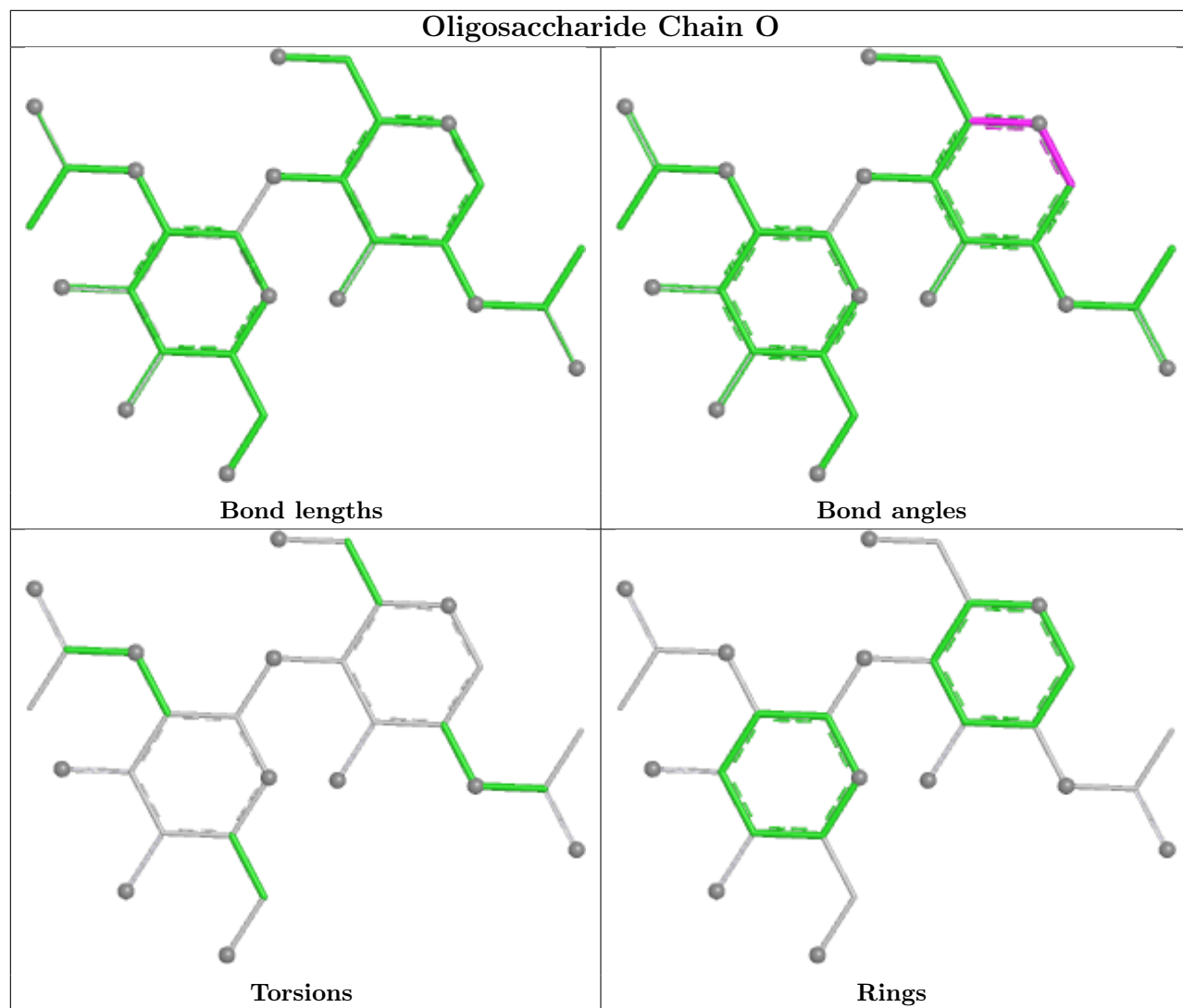


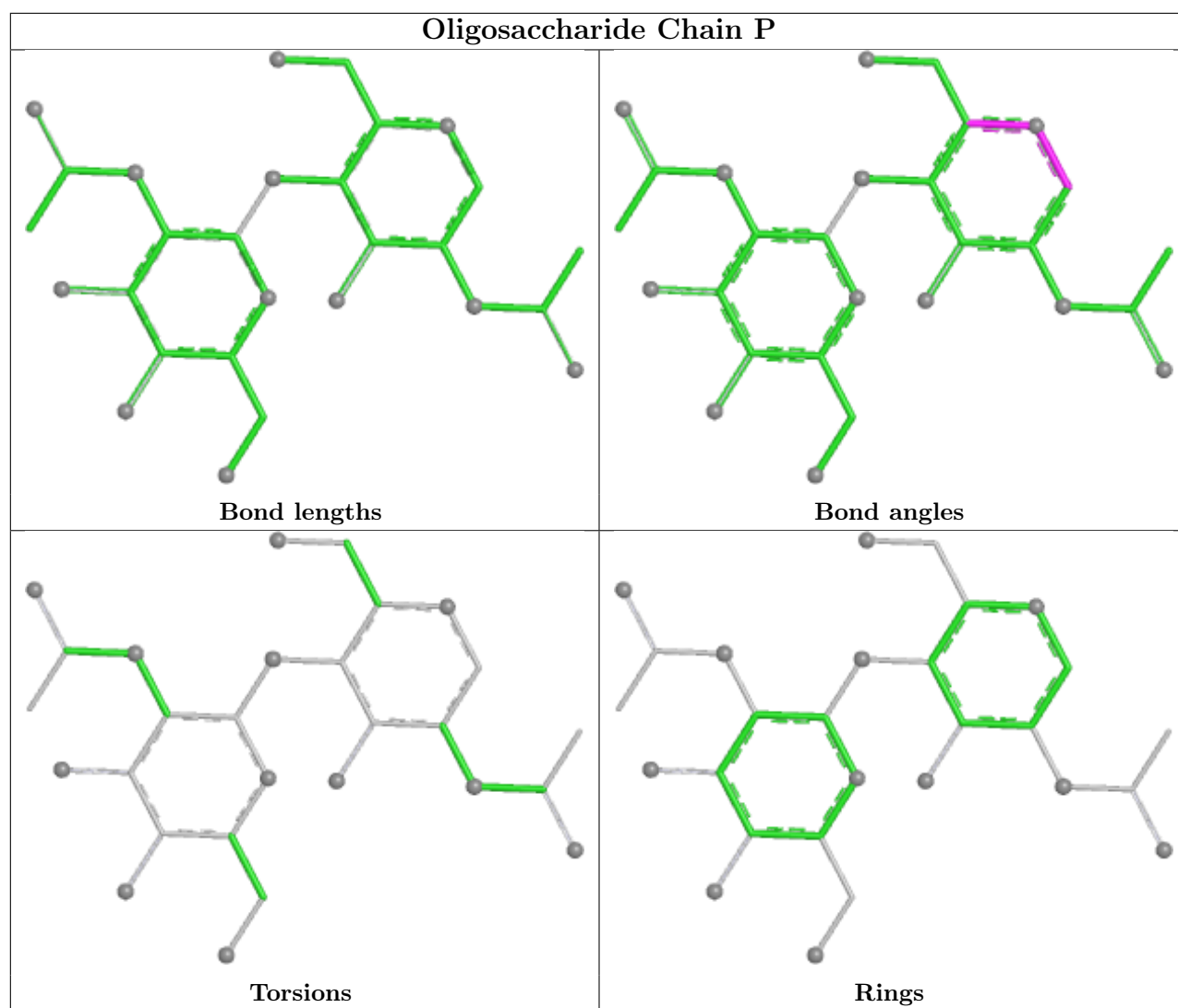


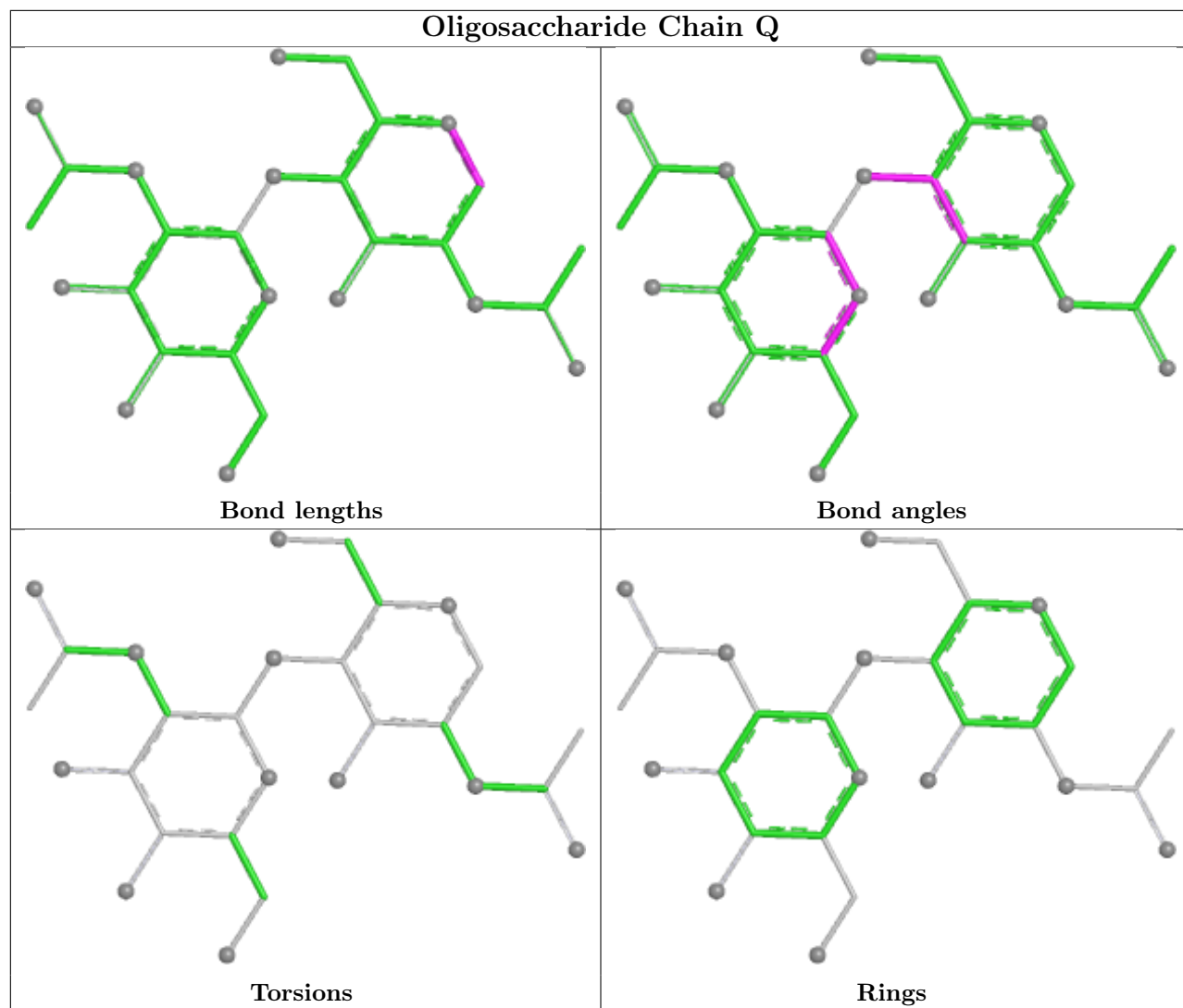


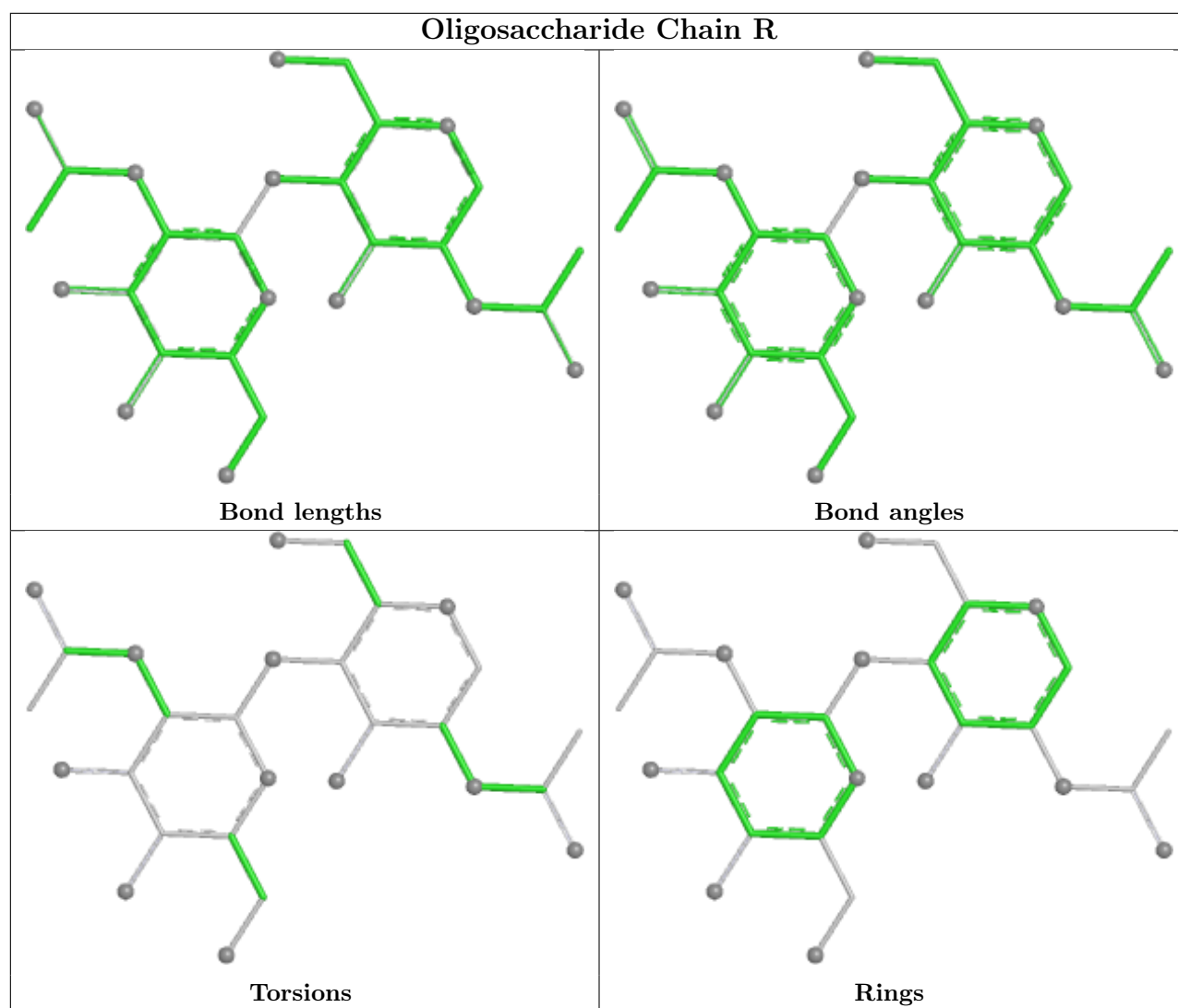


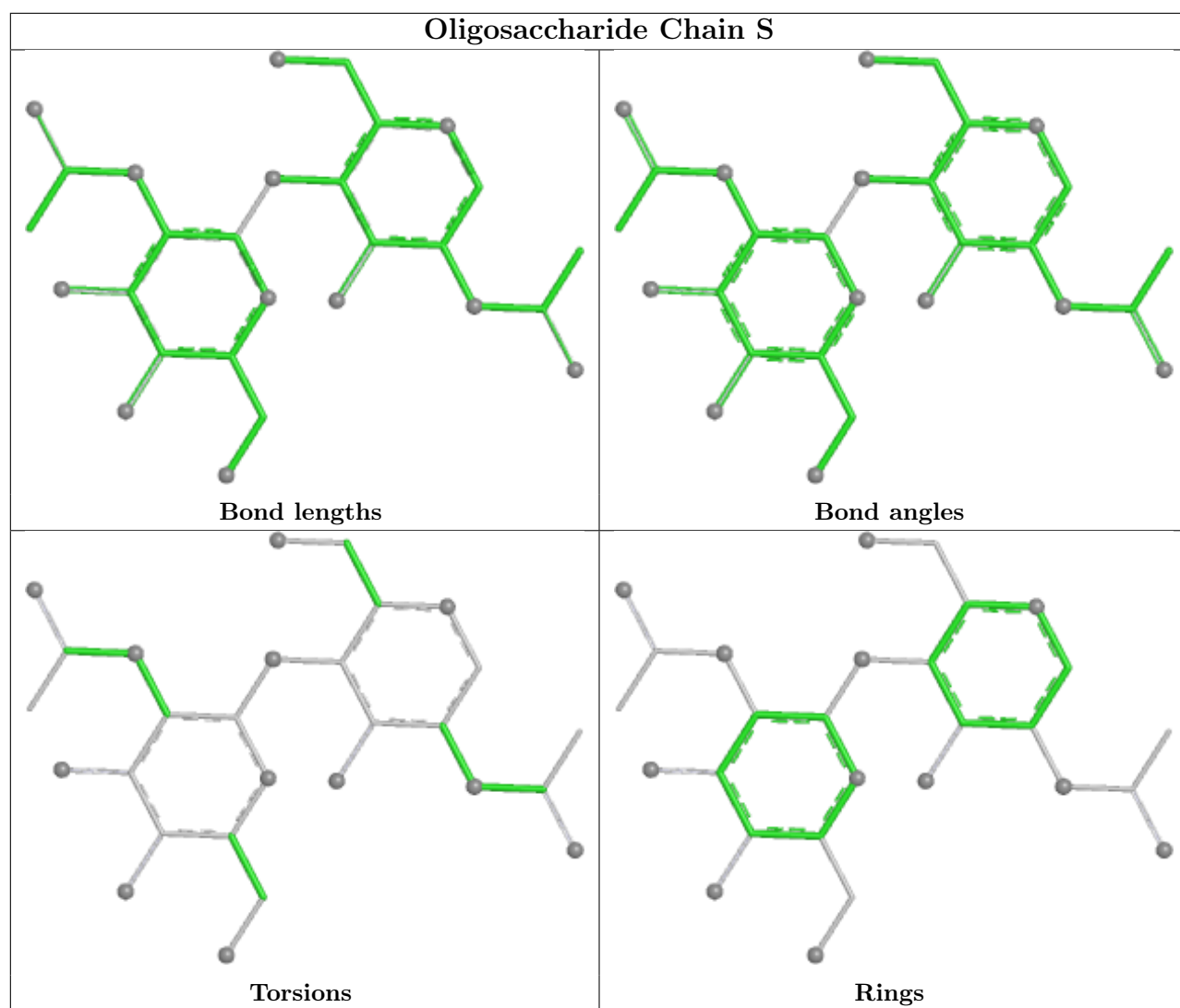


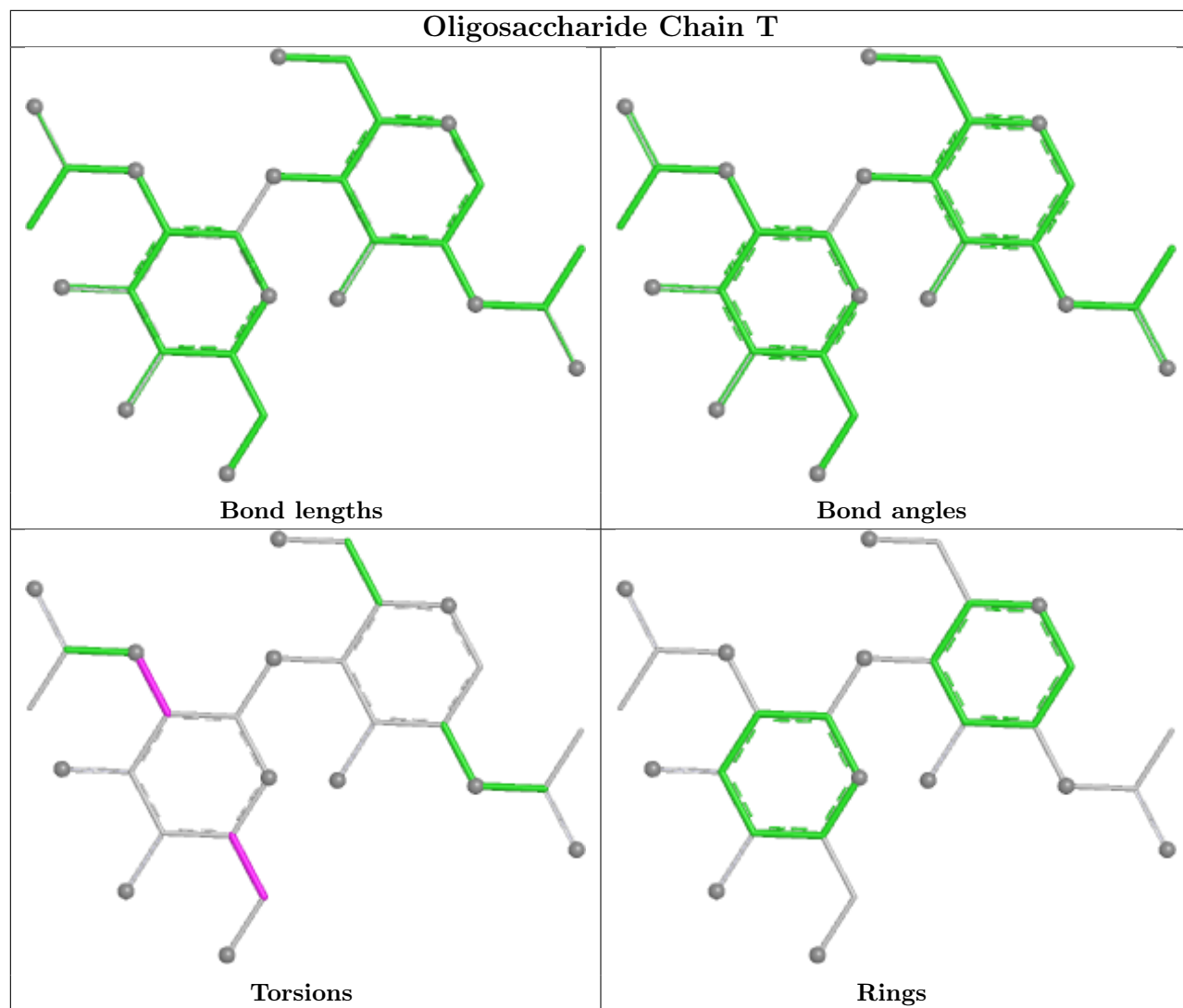


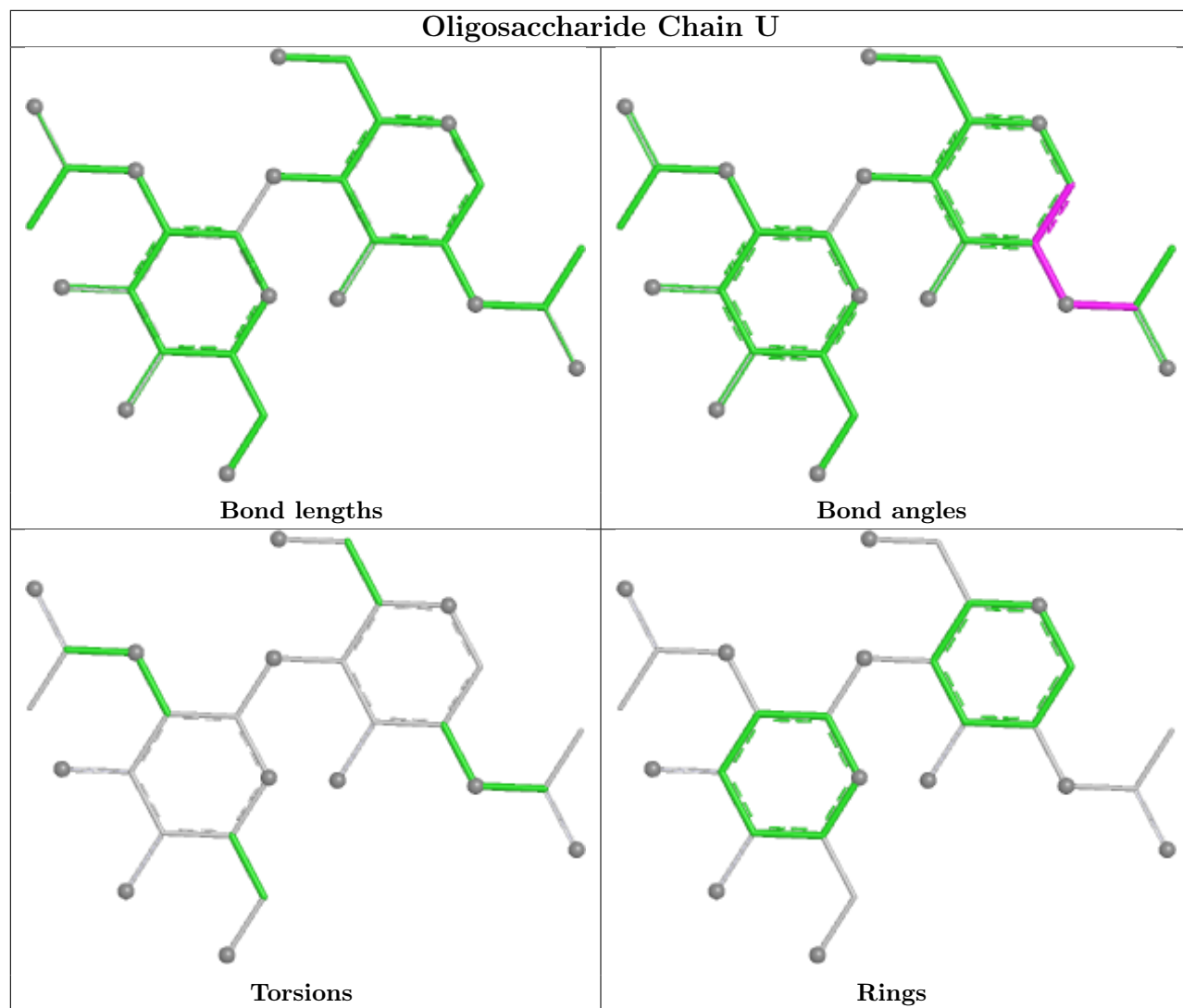


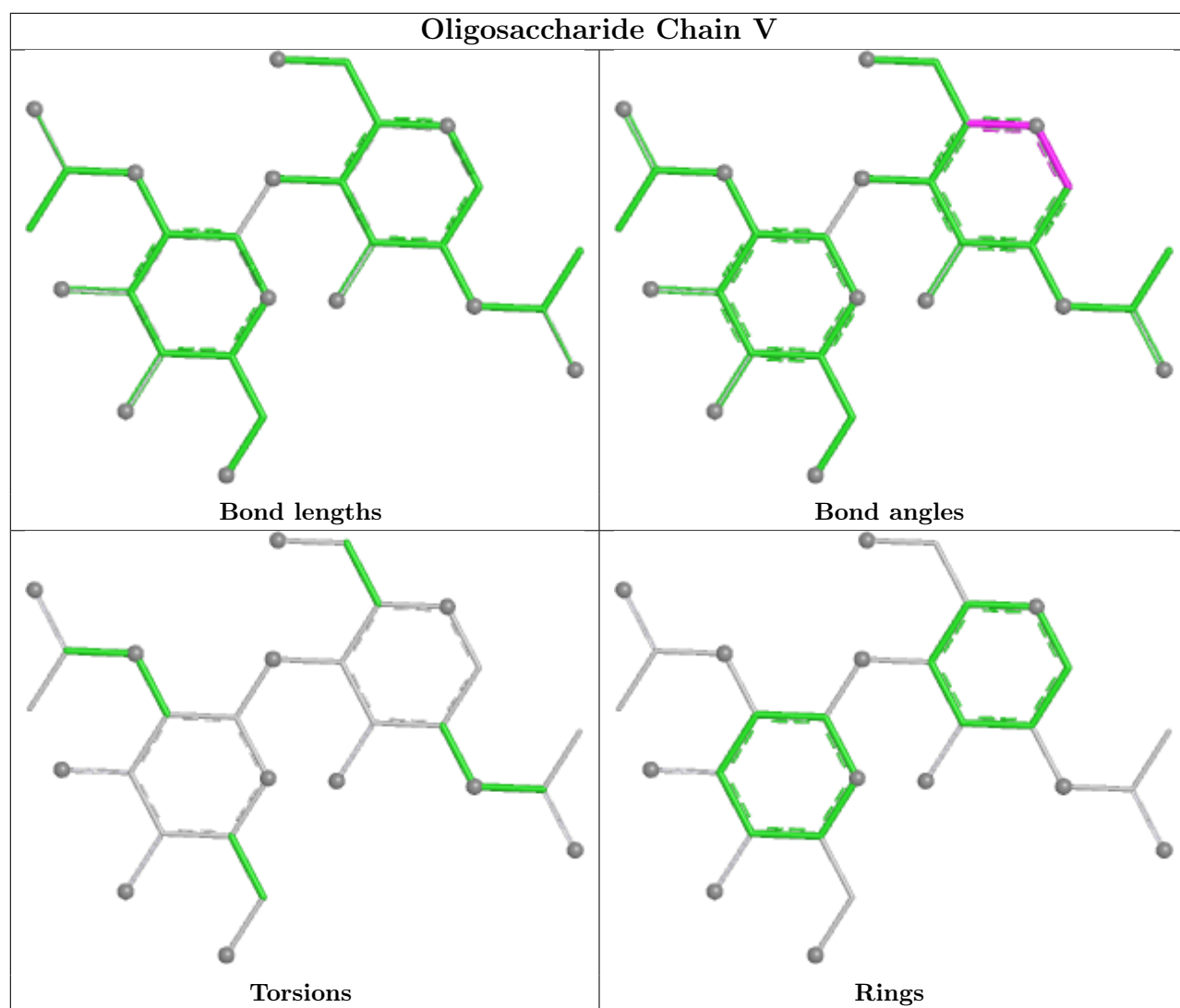


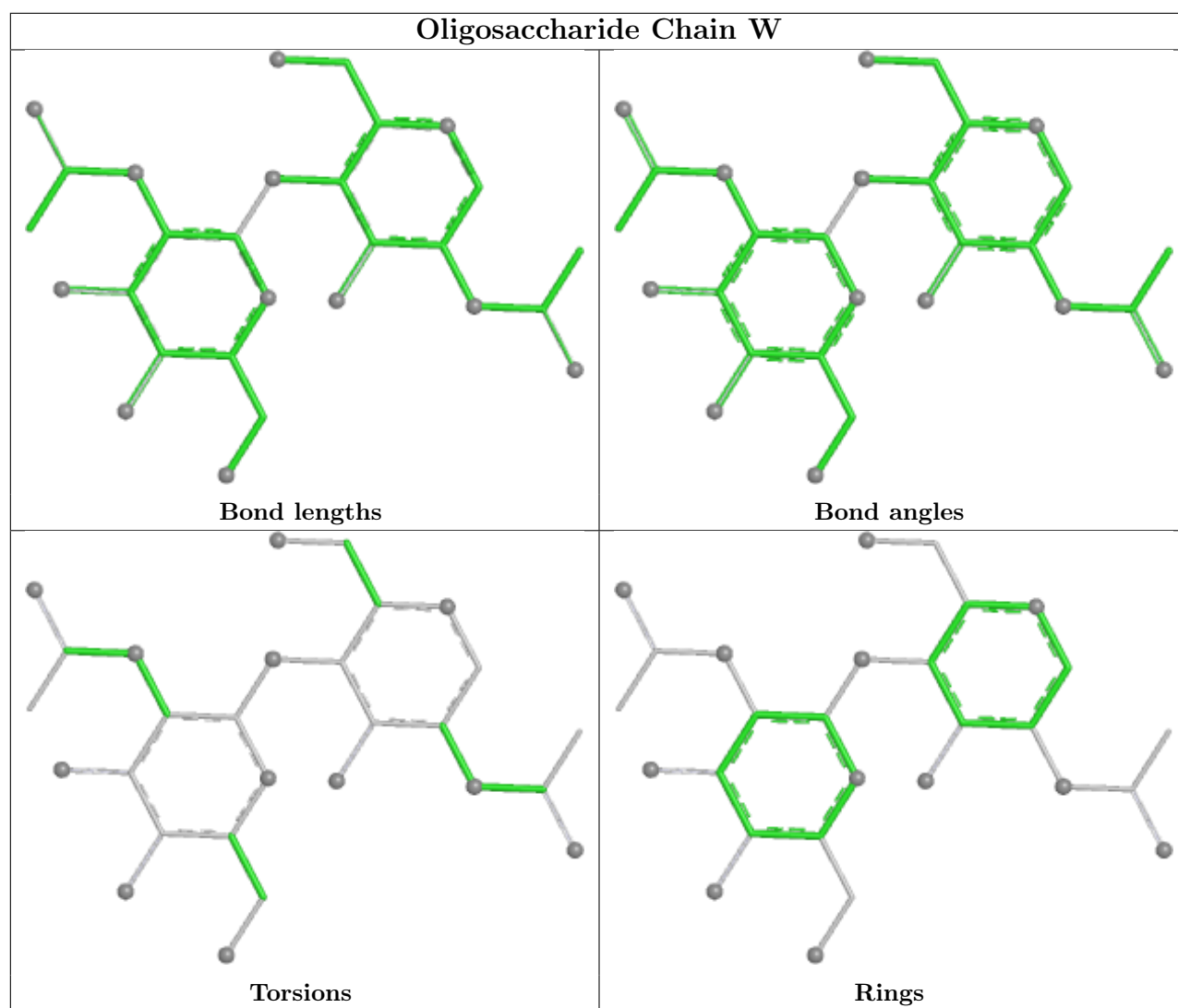


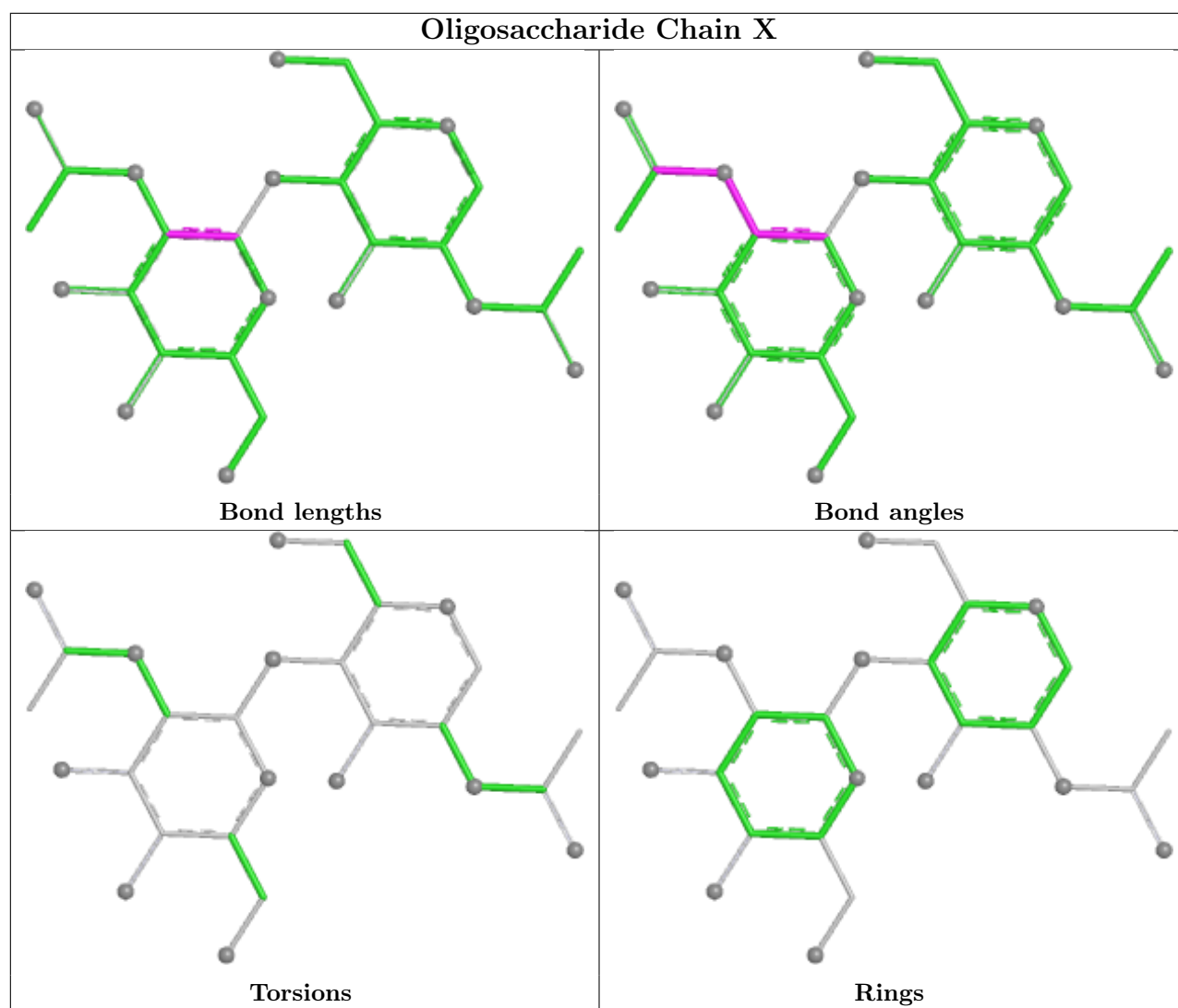


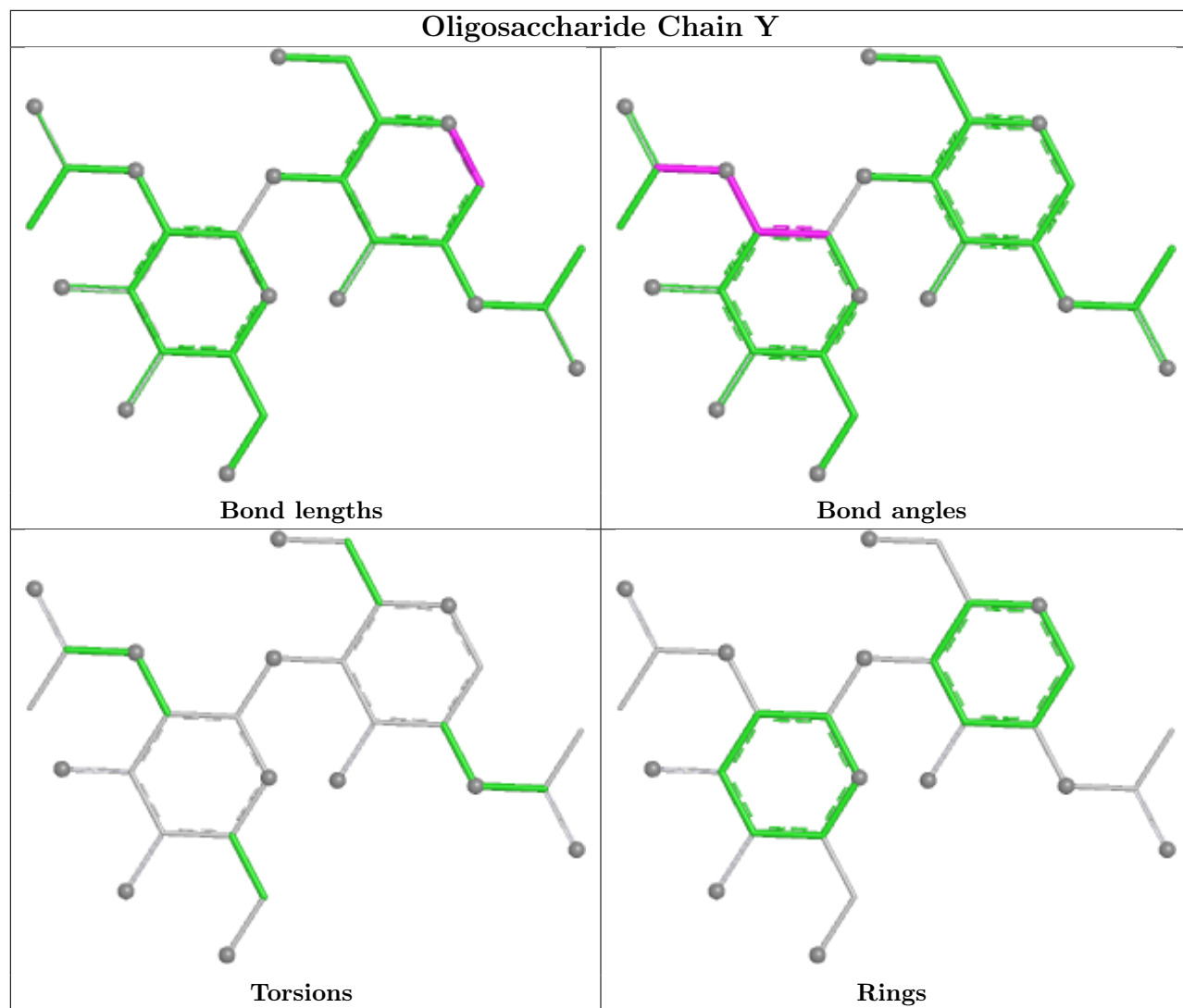


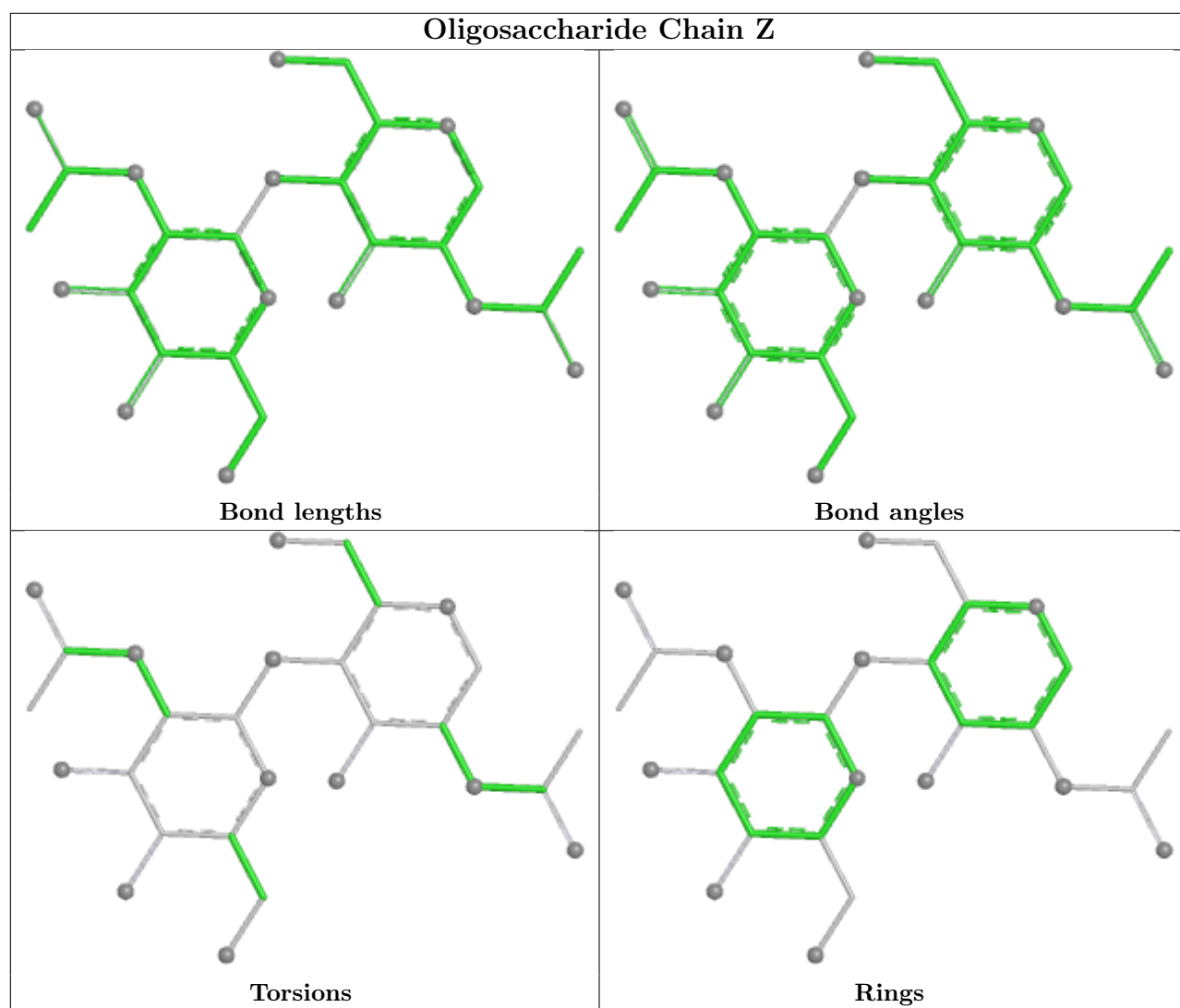


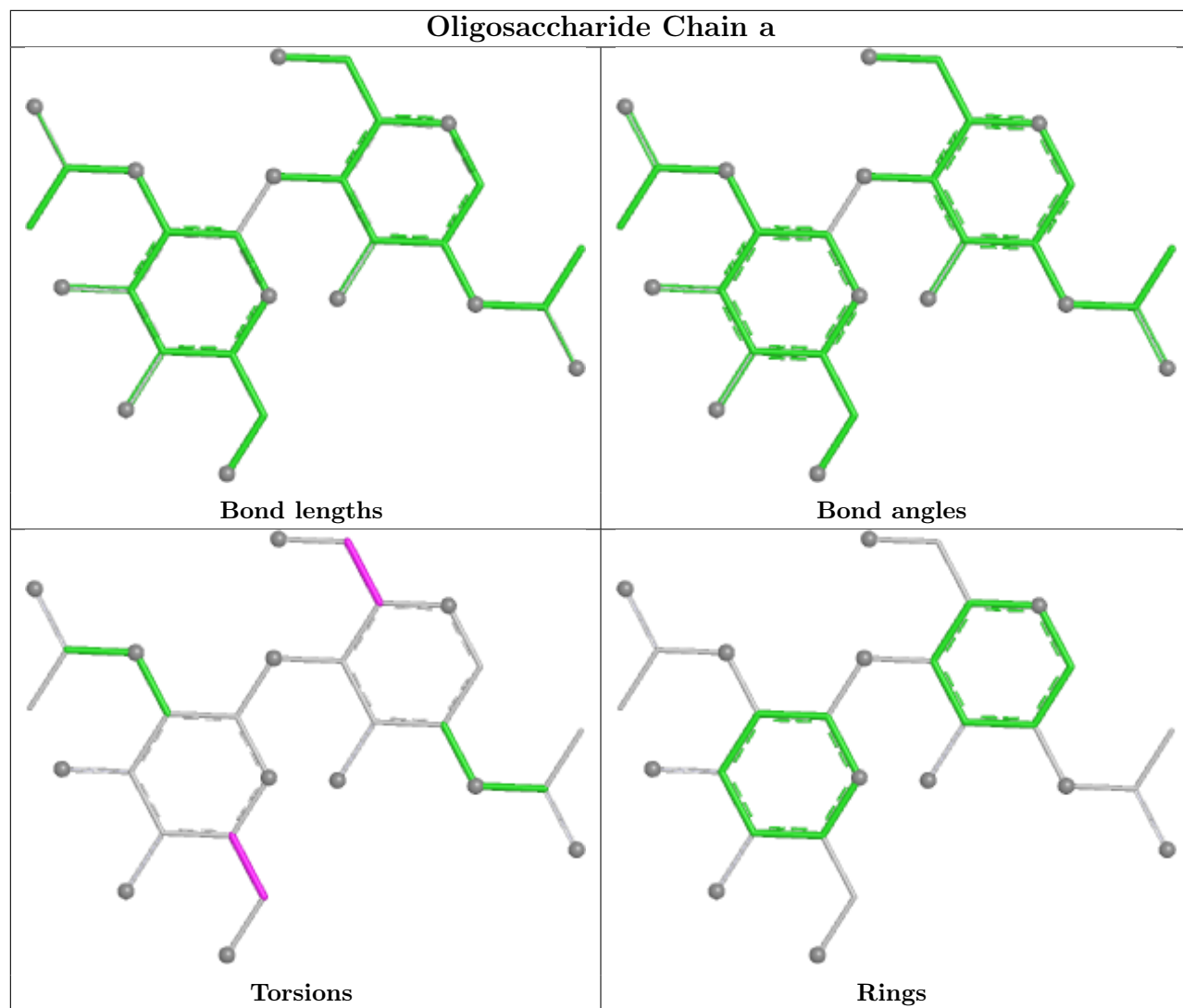


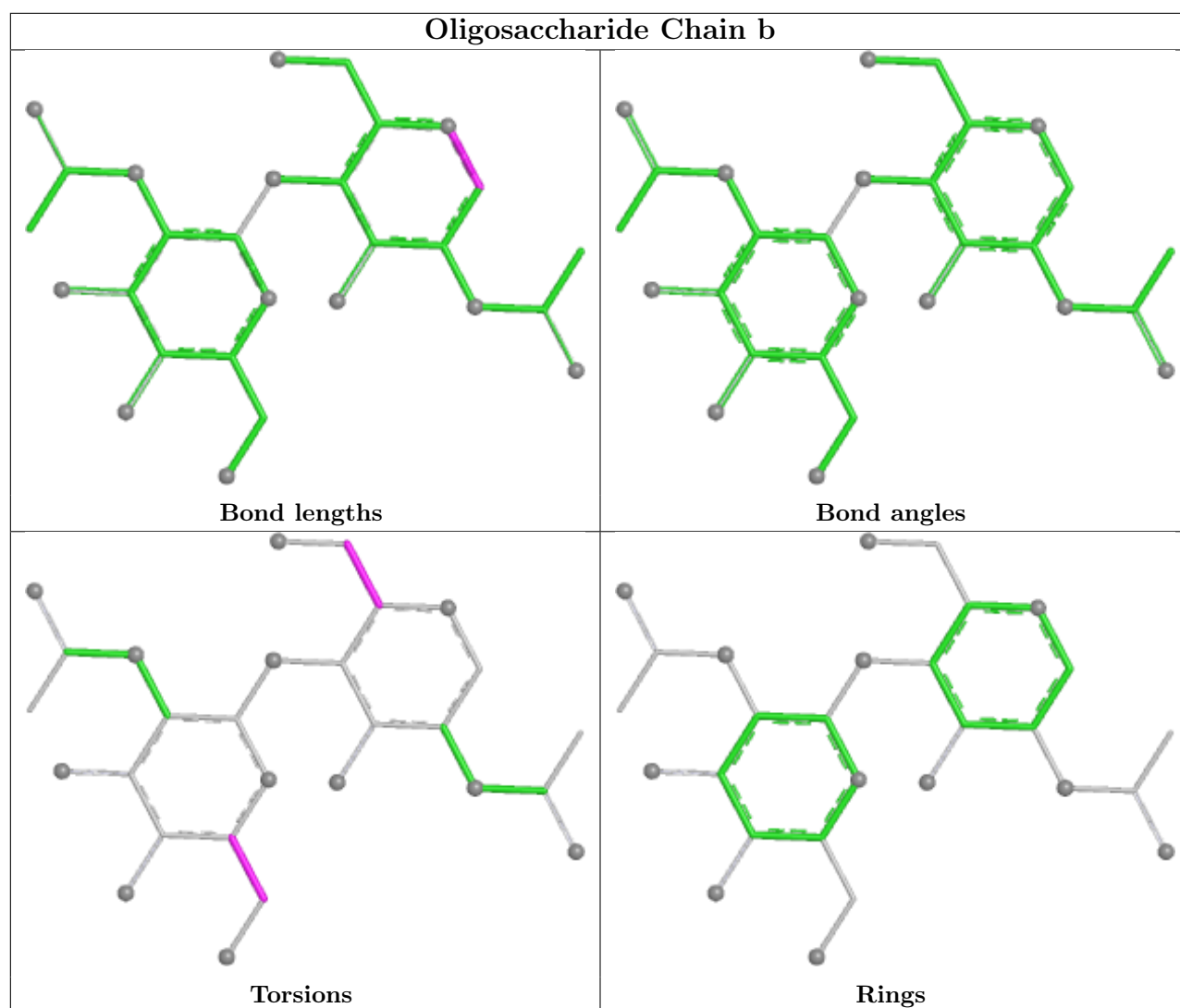












5.6 Ligand geometry [i](#)

45 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	E	905	-	14,14,15	0.34	0	17,19,21	0.50	0
4	NAG	A	1405	1	14,14,15	0.61	0	17,19,21	1.34	2 (11%)
4	NAG	B	1401	1	14,14,15	0.33	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1408	1	14,14,15	0.23	0	17,19,21	0.51	0
4	NAG	B	1407	1	14,14,15	0.27	0	17,19,21	0.40	0
4	NAG	E	902	-	14,14,15	0.27	0	17,19,21	0.58	0
4	NAG	A	1411	1	14,14,15	0.49	0	17,19,21	0.37	0
4	NAG	A	1409	1	14,14,15	0.24	0	17,19,21	0.51	0
4	NAG	E	903	2	14,14,15	0.43	0	17,19,21	1.16	2 (11%)
4	NAG	C	1401	1	14,14,15	0.29	0	17,19,21	0.35	0
4	NAG	D	901	2	14,14,15	0.40	0	17,19,21	0.67	0
4	NAG	A	1404	1	14,14,15	0.50	0	17,19,21	0.55	0
4	NAG	E	906	-	14,14,15	0.23	0	17,19,21	0.64	0
4	NAG	B	1411	-	14,14,15	0.37	0	17,19,21	0.43	0
4	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.66	0
4	NAG	D	905	-	14,14,15	0.35	0	17,19,21	0.49	0
4	NAG	B	1404	1	14,14,15	0.49	0	17,19,21	0.55	0
4	NAG	B	1405	1	14,14,15	0.62	0	17,19,21	1.35	2 (11%)
4	NAG	C	1405	1	14,14,15	0.64	0	17,19,21	1.35	2 (11%)
4	NAG	E	904	2	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	C	1409	1	14,14,15	0.32	0	17,19,21	0.41	0
4	NAG	B	1409	1	14,14,15	0.32	0	17,19,21	0.41	0
4	NAG	A	1401	1	14,14,15	0.31	0	17,19,21	0.35	0
4	NAG	A	1403	1	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	D	902	-	14,14,15	0.28	0	17,19,21	0.58	0
4	NAG	B	1410	1	14,14,15	0.42	0	17,19,21	1.13	2 (11%)
4	NAG	D	907	-	14,14,15	0.34	0	17,19,21	0.62	1 (5%)
4	NAG	C	1406	-	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
4	NAG	B	1406	-	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
4	NAG	D	906	-	14,14,15	0.23	0	17,19,21	0.63	0
4	NAG	A	1408	1	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	B	1403	1	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.65	0
4	NAG	A	1407	-	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	C	1403	1	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	A	1410	1	14,14,15	0.33	0	17,19,21	0.40	0
4	NAG	D	904	2	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	C	1407	1	14,14,15	0.26	0	17,19,21	0.40	0
4	NAG	E	907	-	14,14,15	0.34	0	17,19,21	0.61	1 (5%)
4	NAG	A	1406	1	14,14,15	0.56	0	17,19,21	0.58	0
4	NAG	B	1402	1	14,14,15	0.21	0	17,19,21	0.66	0
4	NAG	E	901	2	14,14,15	0.39	0	17,19,21	0.67	0
4	NAG	C	1404	1	14,14,15	0.51	0	17,19,21	0.54	0
4	NAG	D	903	2	14,14,15	0.42	0	17,19,21	1.15	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1408	1	14,14,15	0.23	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	905	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	E	902	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1411	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	E	903	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	D	901	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	E	906	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1411	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	1/6/23/26	0/1/1/1
4	NAG	D	905	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	E	904	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	D	902	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1410	1	-	0/6/23/26	0/1/1/1
4	NAG	D	907	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1406	-	-	0/6/23/26	0/1/1/1
4	NAG	D	906	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1407	-	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1410	1	-	0/6/23/26	0/1/1/1
4	NAG	D	904	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	E	907	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	E	901	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	D	903	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1405	NAG	C2-N2-C7	4.67	129.16	122.90
4	C	1405	NAG	C2-N2-C7	4.65	129.14	122.90
4	A	1405	NAG	C2-N2-C7	4.62	129.09	122.90
4	C	1406	NAG	C8-C7-N2	2.40	120.09	116.12
4	B	1406	NAG	C8-C7-N2	2.39	120.08	116.12
4	E	903	NAG	C8-C7-N2	2.36	120.03	116.12
4	D	903	NAG	C8-C7-N2	2.34	120.00	116.12
4	B	1410	NAG	C8-C7-N2	2.25	119.85	116.12
4	B	1410	NAG	C2-N2-C7	-2.21	119.94	122.90
4	E	903	NAG	C2-N2-C7	-2.16	120.00	122.90
4	C	1405	NAG	C1-C2-N2	2.15	113.82	110.43
4	D	903	NAG	C2-N2-C7	-2.14	120.03	122.90
4	B	1405	NAG	C1-C2-N2	2.14	113.80	110.43
4	A	1405	NAG	C1-C2-N2	2.13	113.79	110.43
4	D	907	NAG	C1-O5-C5	2.13	115.04	112.19
4	E	907	NAG	C1-O5-C5	2.10	115.00	112.19
4	C	1406	NAG	C2-N2-C7	-2.09	120.10	122.90
4	B	1406	NAG	C2-N2-C7	-2.07	120.12	122.90

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	902	NAG	O7-C7-N2-C2
4	E	902	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	D	902	NAG	C8-C7-N2-C2
4	E	902	NAG	C8-C7-N2-C2
4	D	907	NAG	O5-C5-C6-O6
4	E	907	NAG	O5-C5-C6-O6
4	D	901	NAG	O5-C5-C6-O6
4	E	901	NAG	O5-C5-C6-O6
4	D	907	NAG	C4-C5-C6-O6
4	E	907	NAG	C4-C5-C6-O6
4	D	901	NAG	C4-C5-C6-O6
4	E	901	NAG	C4-C5-C6-O6
4	A	1402	NAG	O5-C5-C6-O6
4	A	1407	NAG	C3-C2-N2-C7
4	A	1407	NAG	C4-C5-C6-O6
4	A	1407	NAG	O5-C5-C6-O6

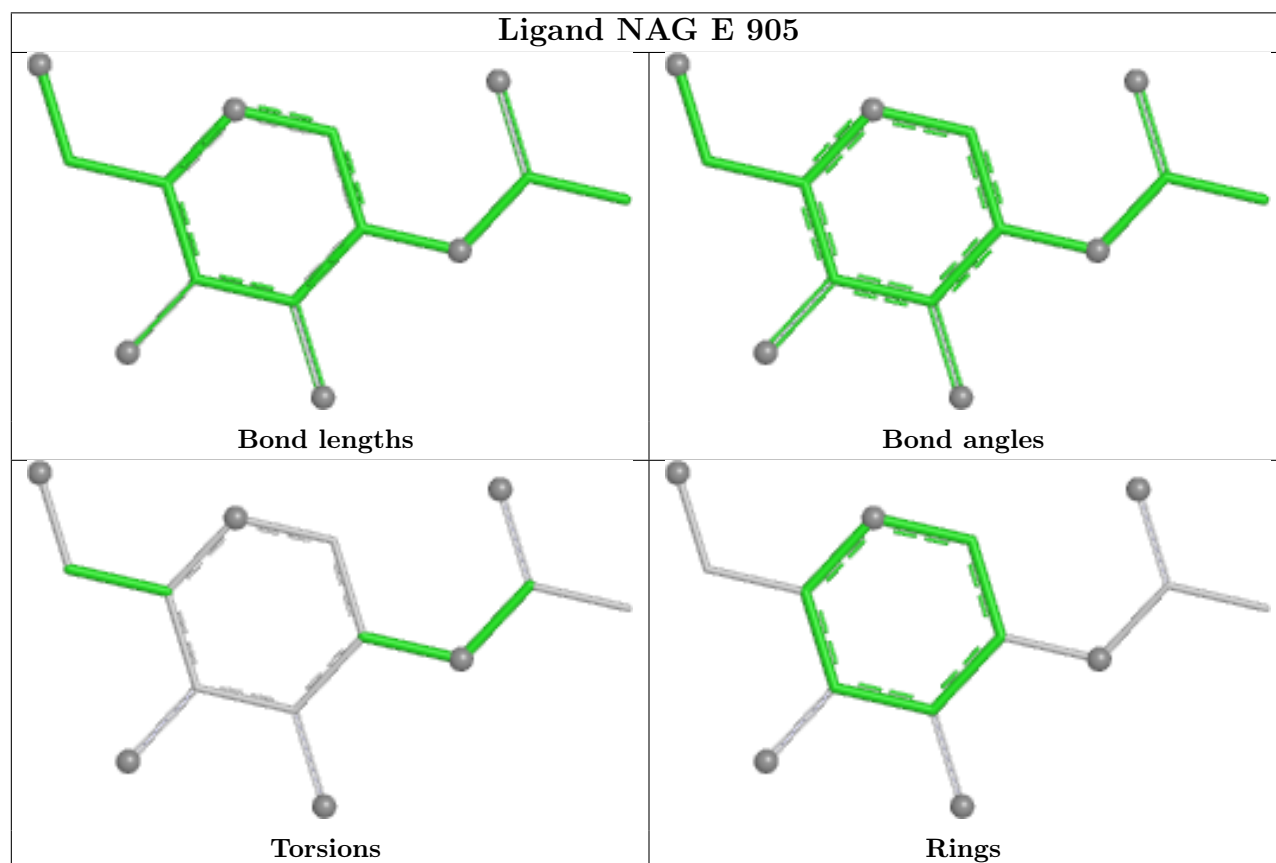
There are no ring outliers.

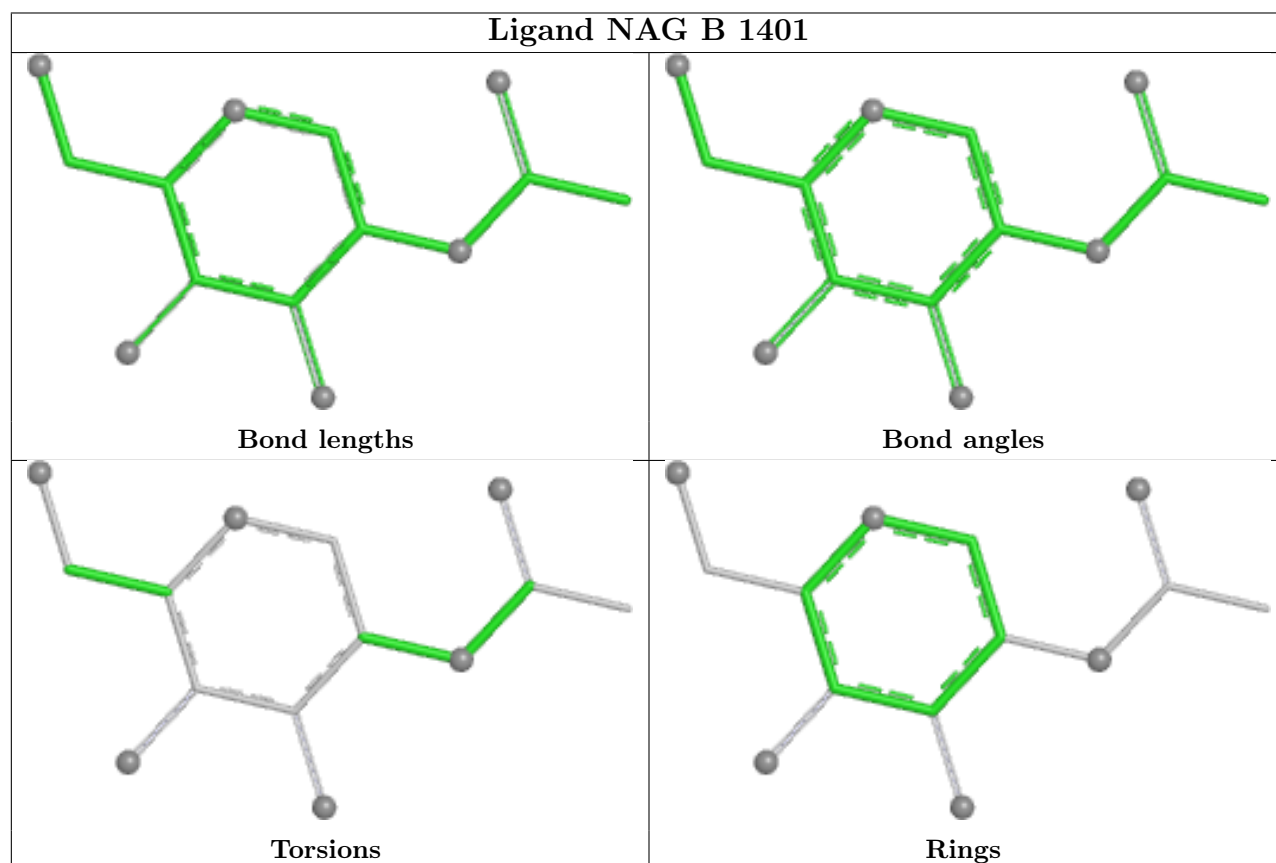
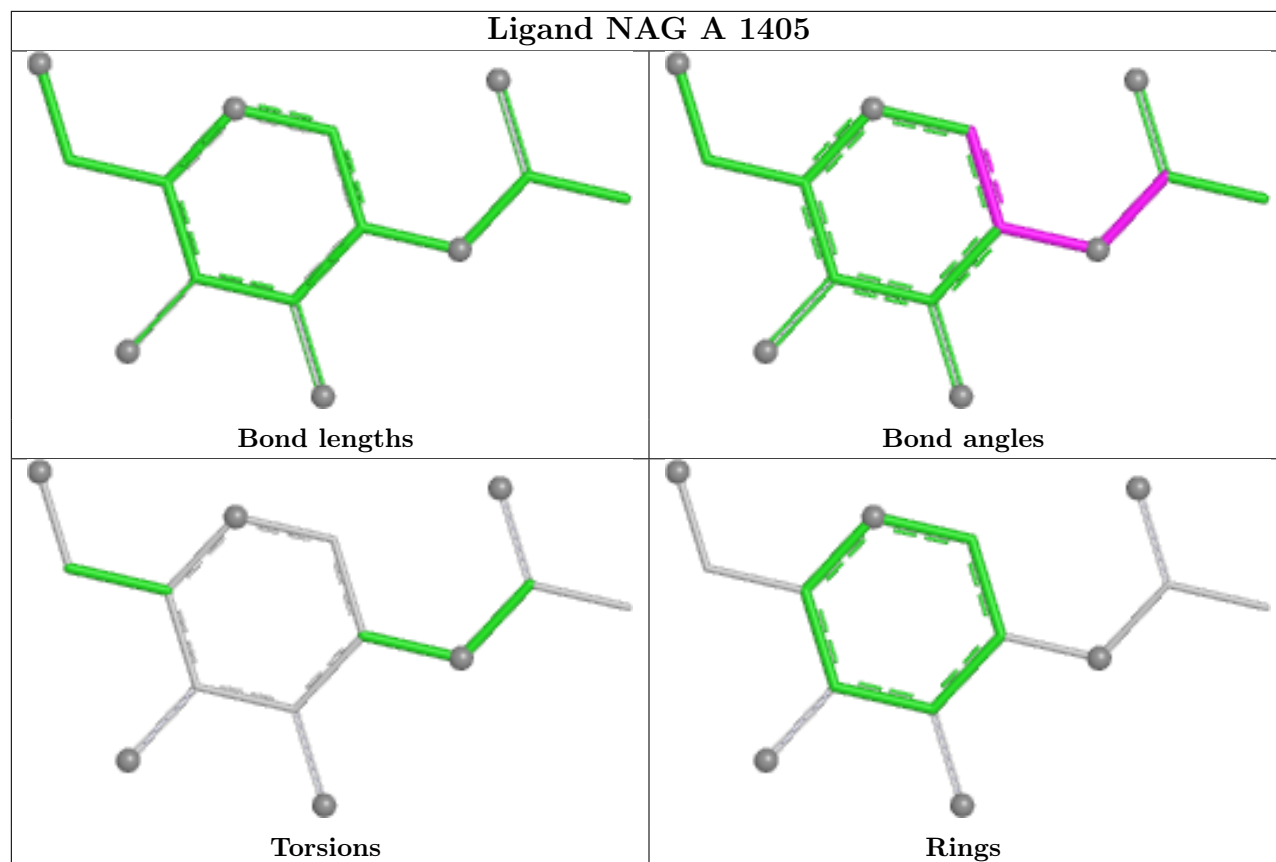
12 monomers are involved in 30 short contacts:

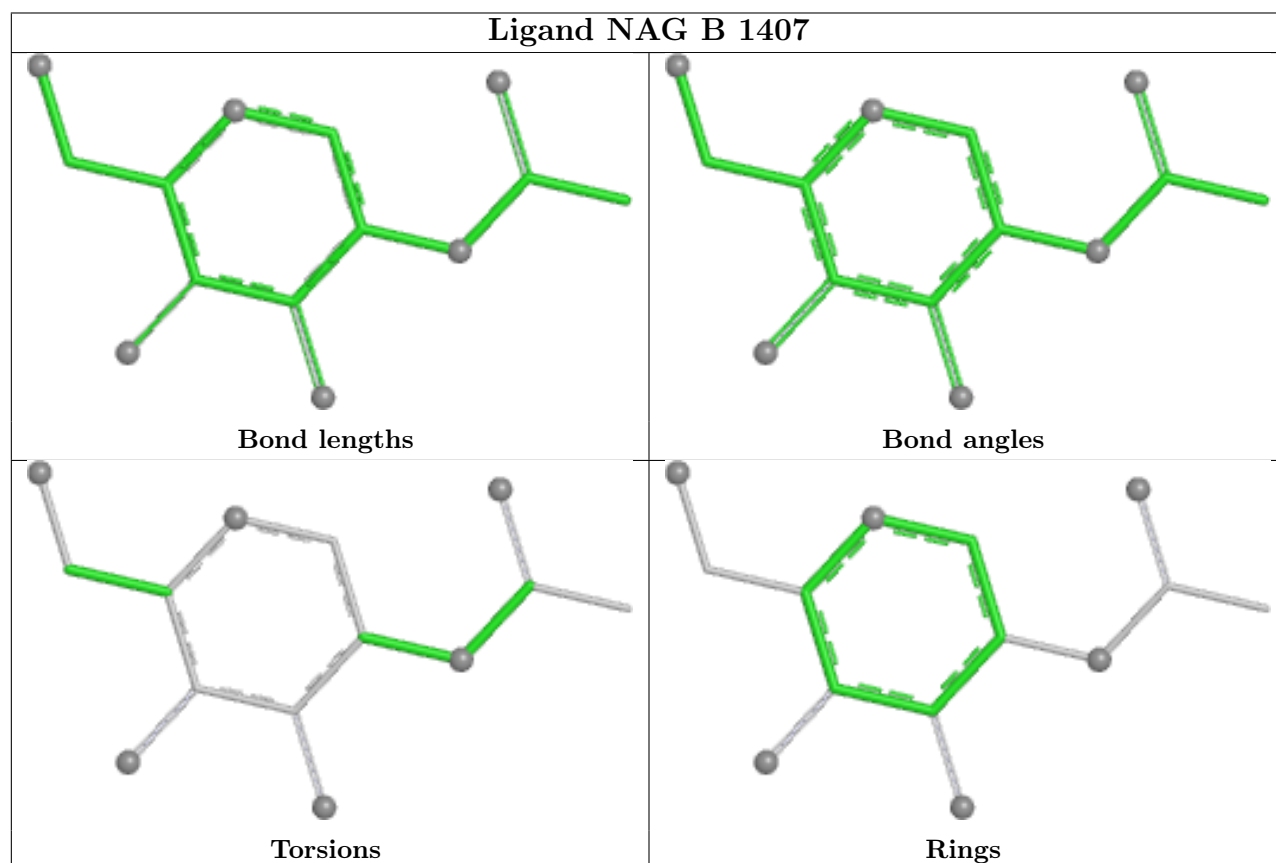
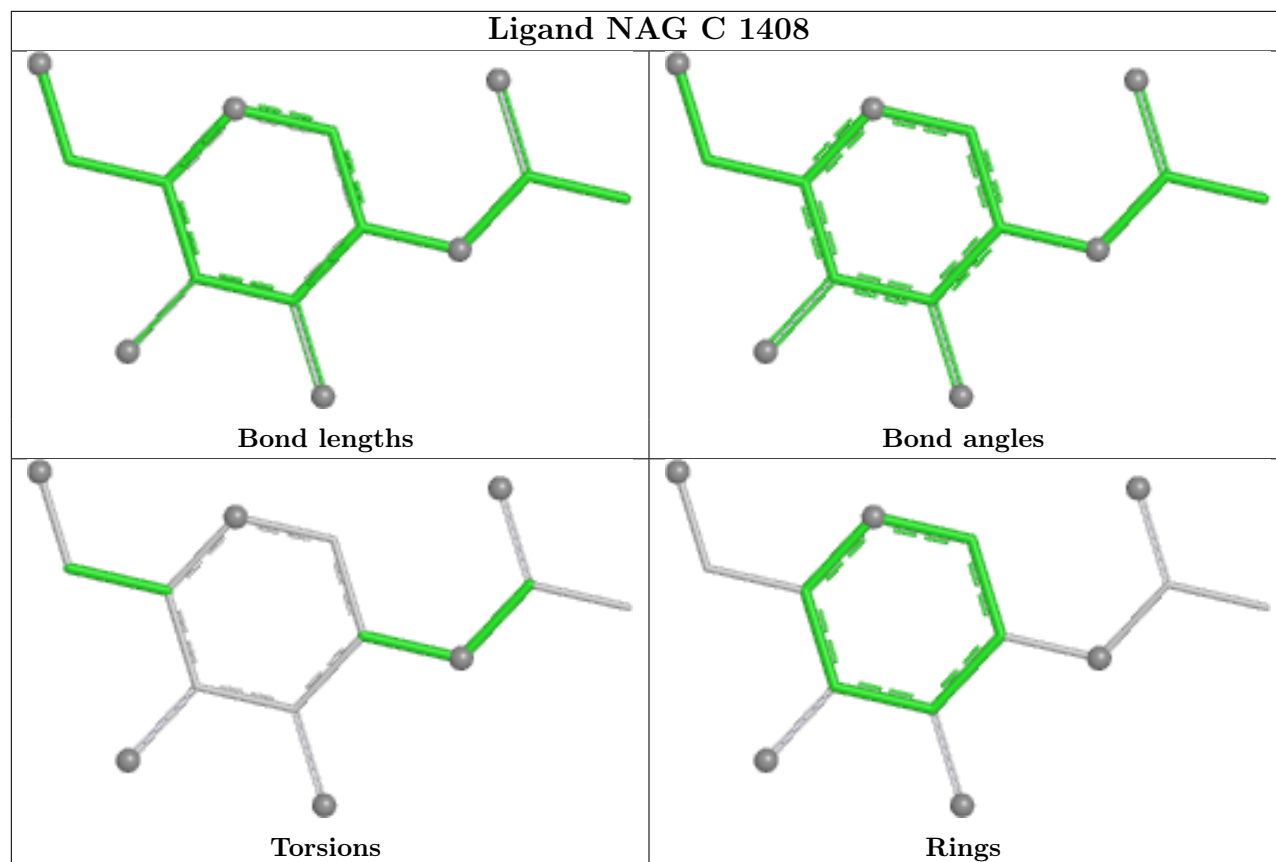
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	905	NAG	2	0
4	E	902	NAG	8	0
4	E	903	NAG	1	0
4	E	906	NAG	2	0
4	B	1411	NAG	4	0
4	D	905	NAG	2	0
4	E	904	NAG	1	0
4	D	902	NAG	8	0
4	B	1410	NAG	6	0
4	D	906	NAG	2	0
4	D	904	NAG	1	0
4	D	903	NAG	1	0

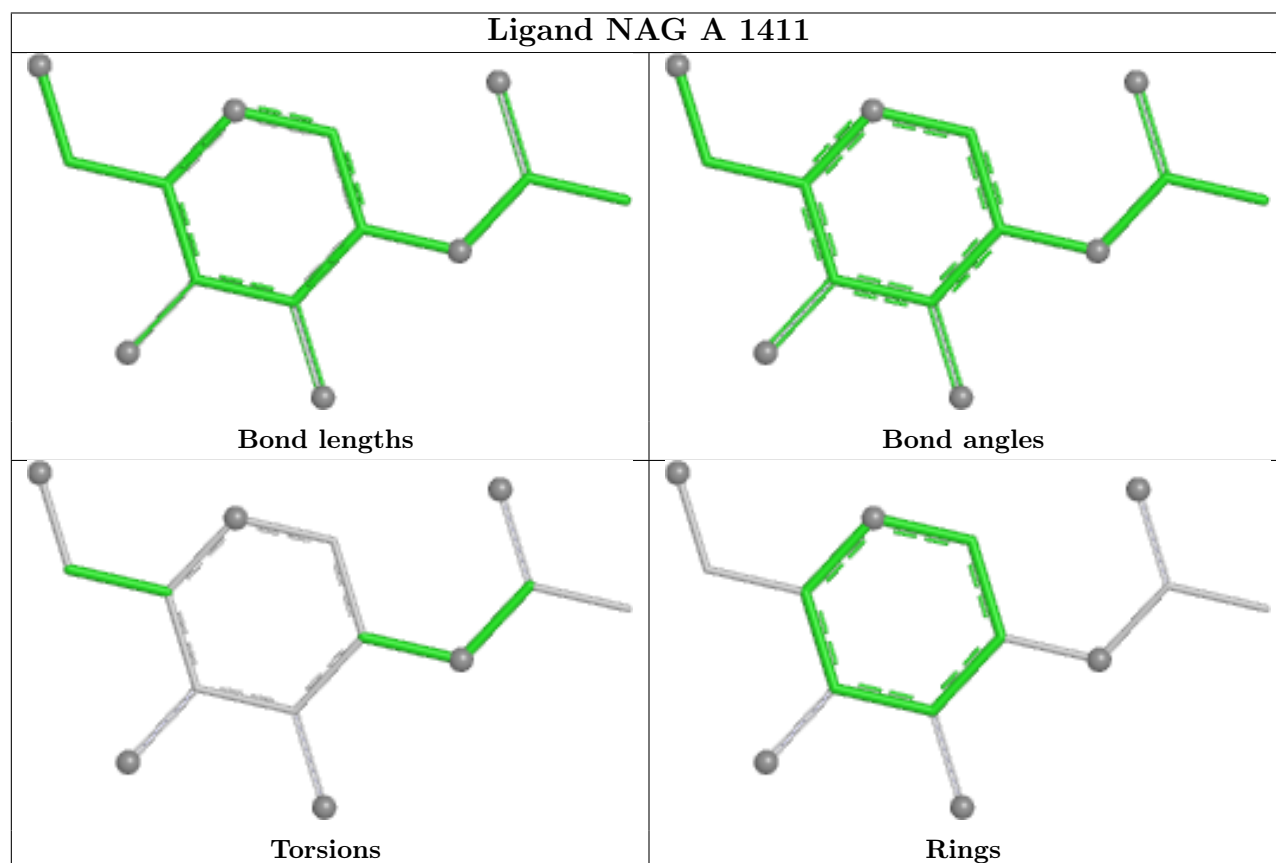
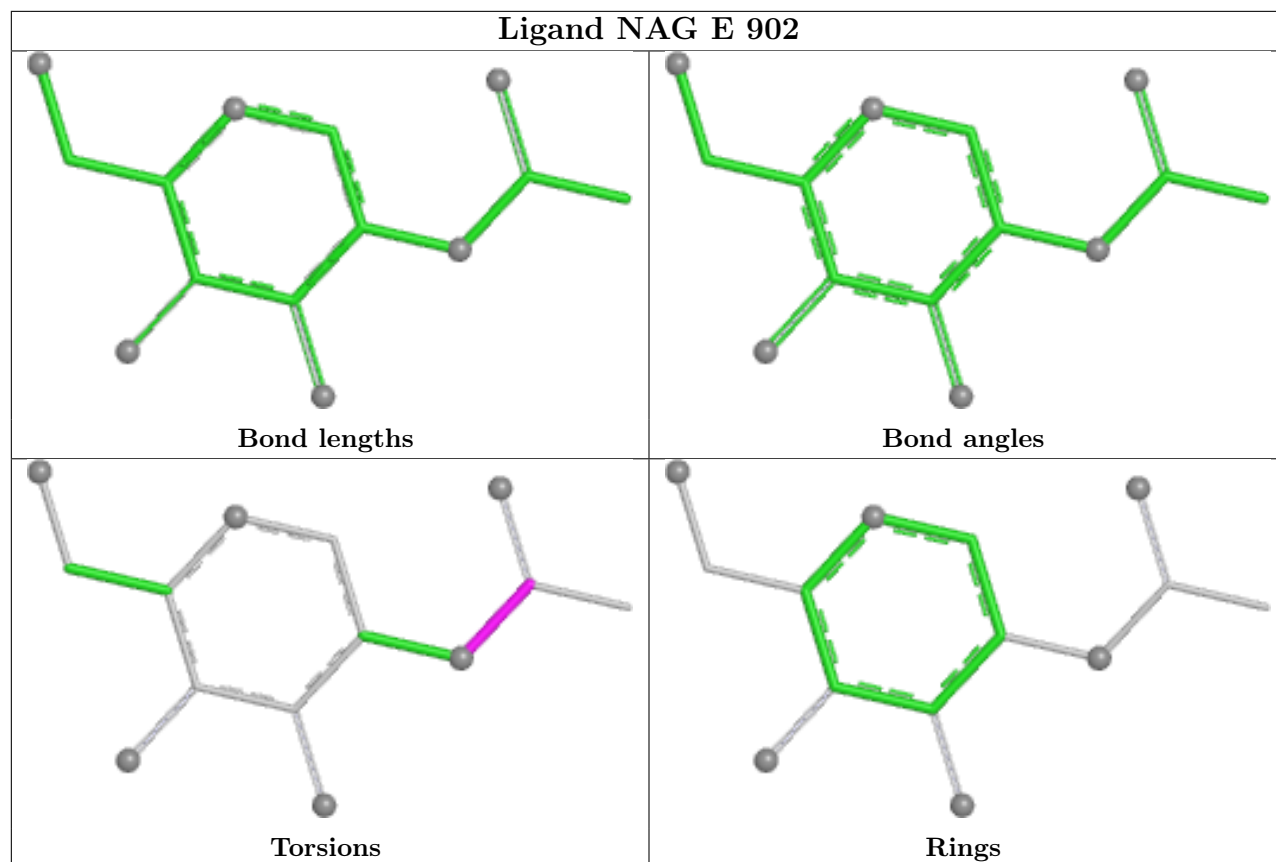
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

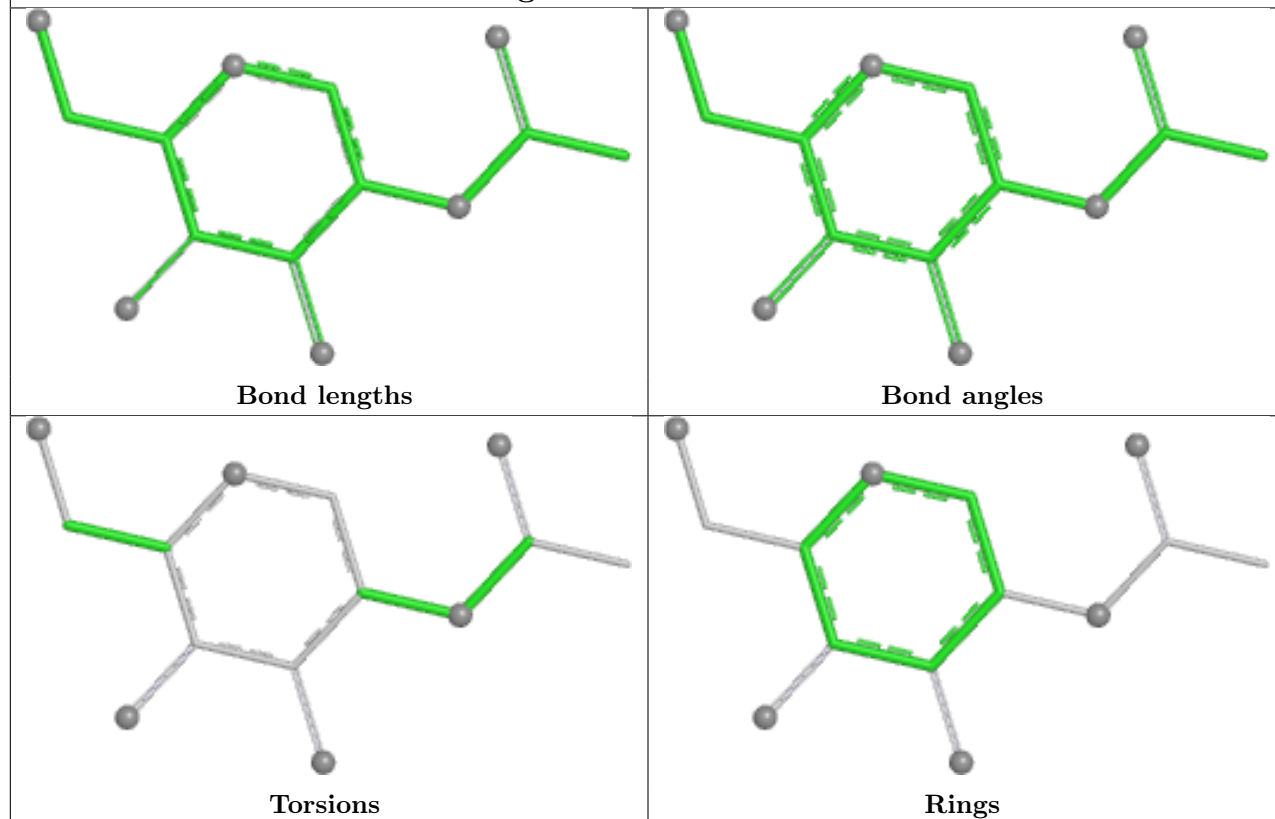




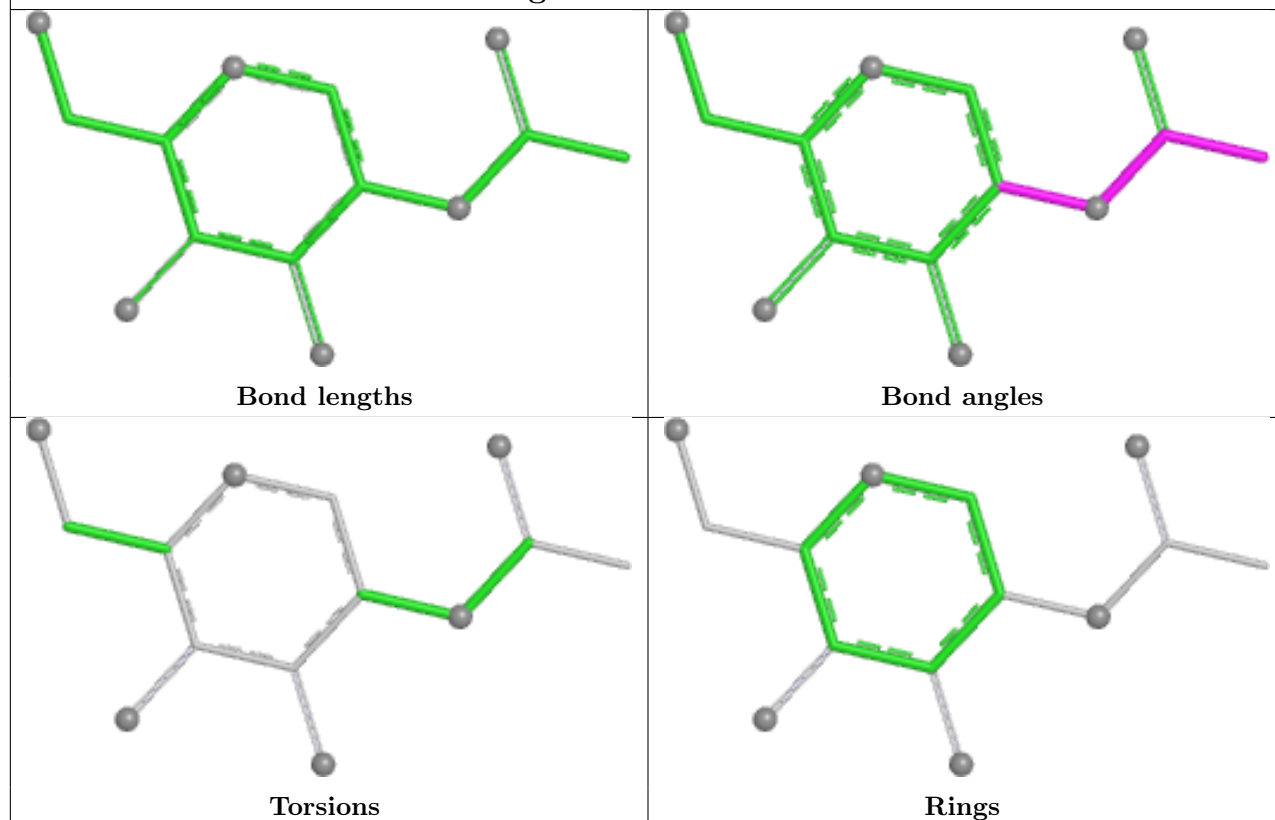




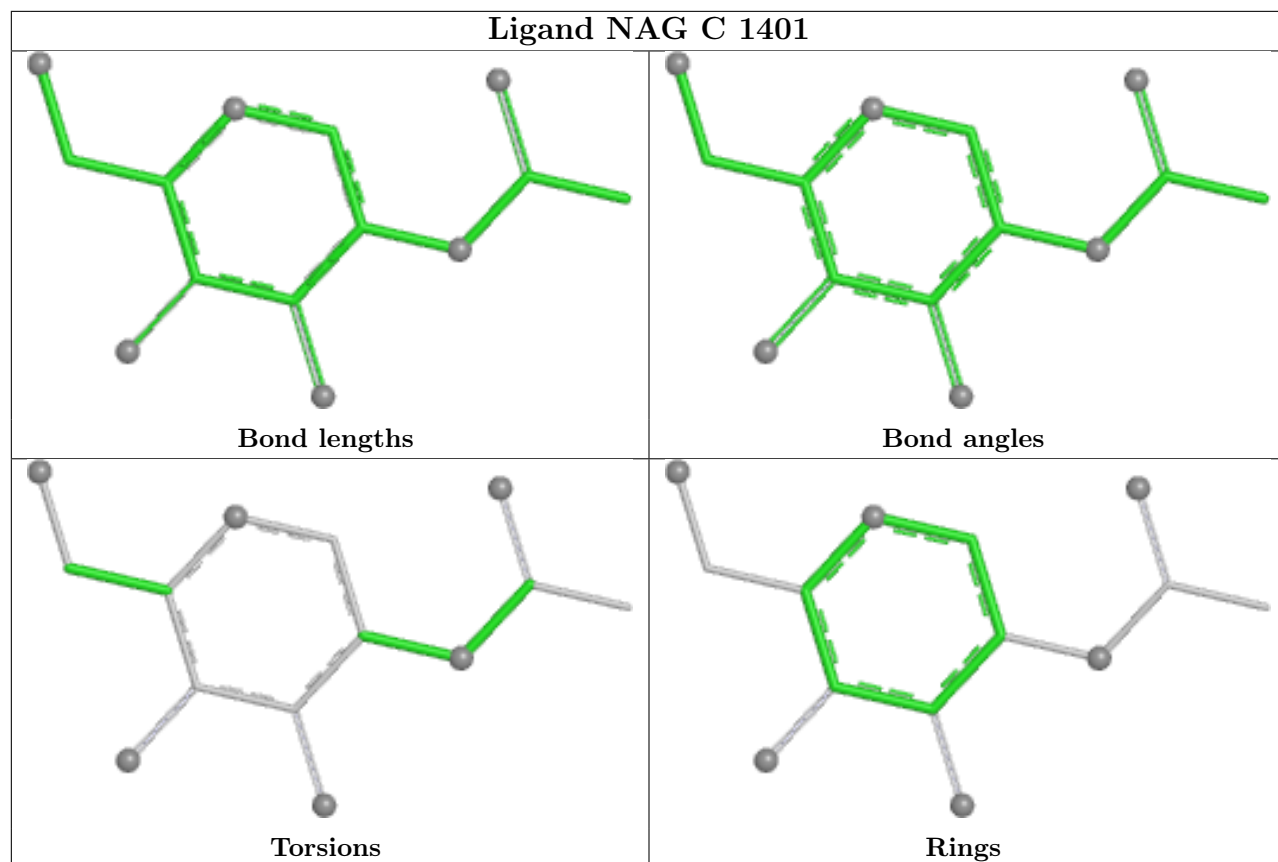
Ligand NAG A 1409



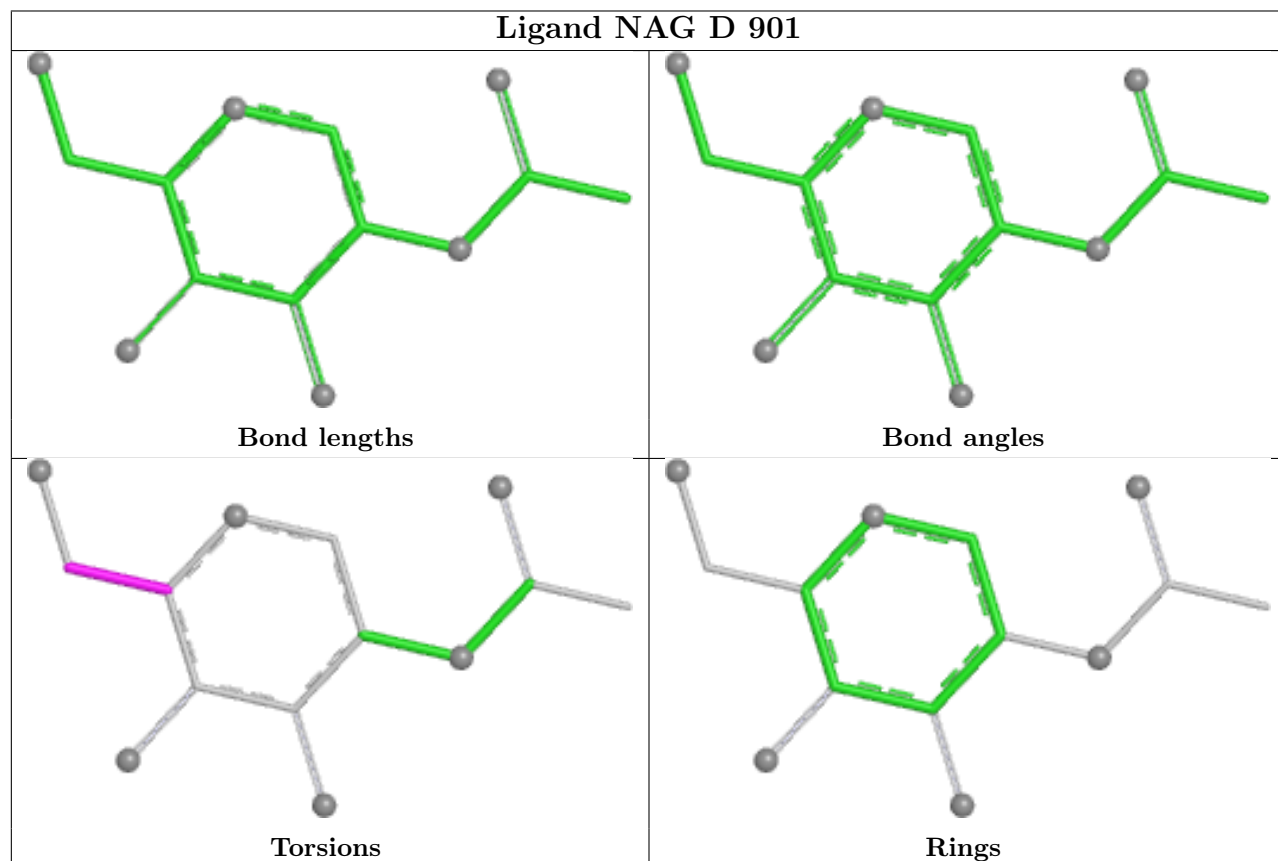
Ligand NAG E 903



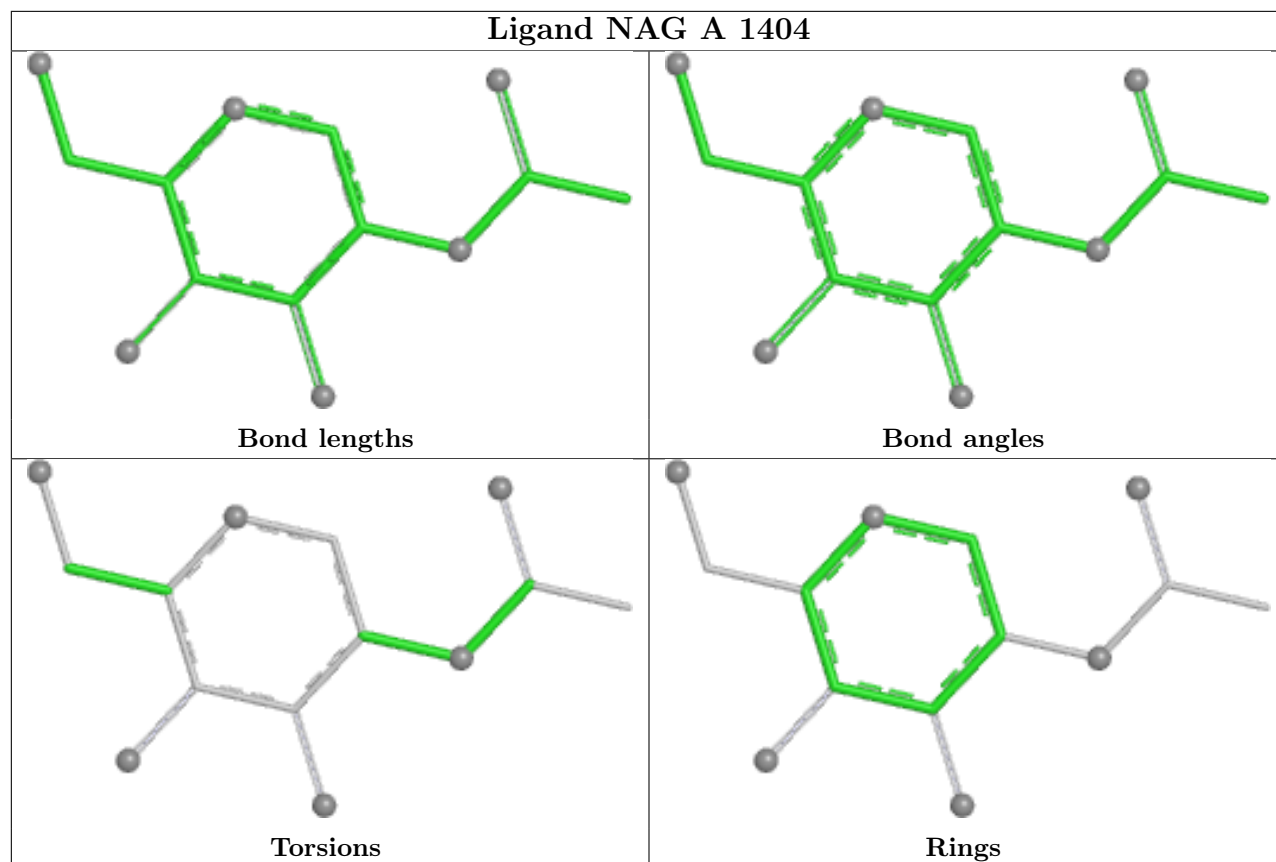
Ligand NAG C 1401



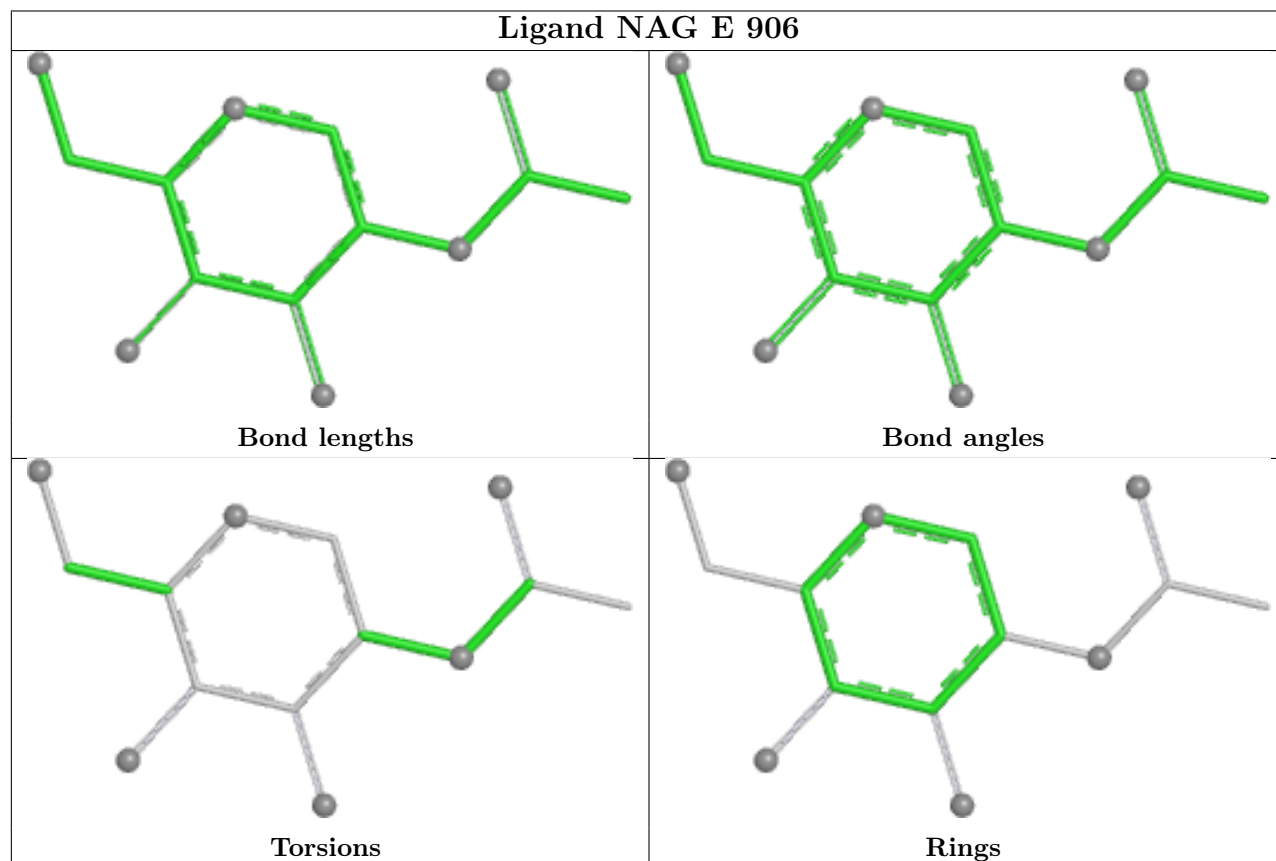
Ligand NAG D 901



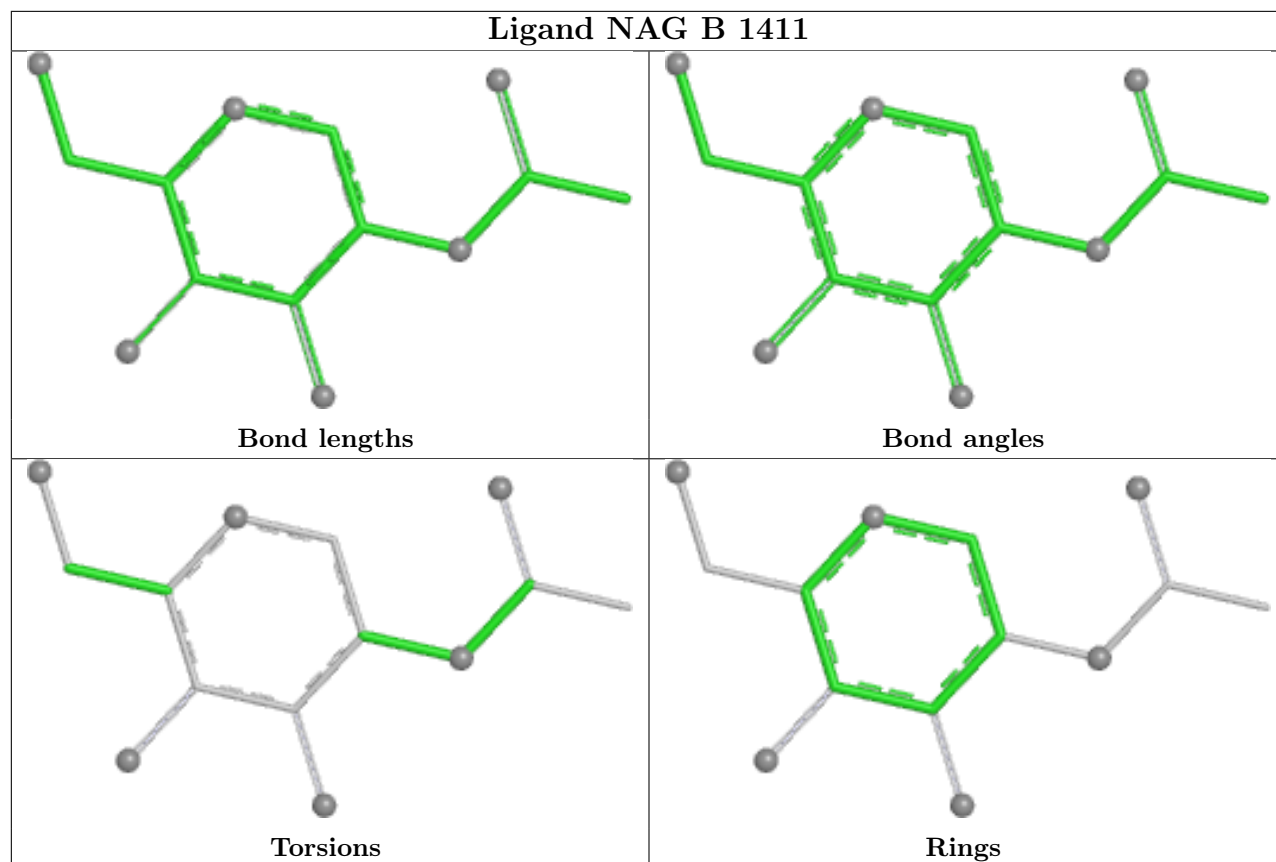
Ligand NAG A 1404



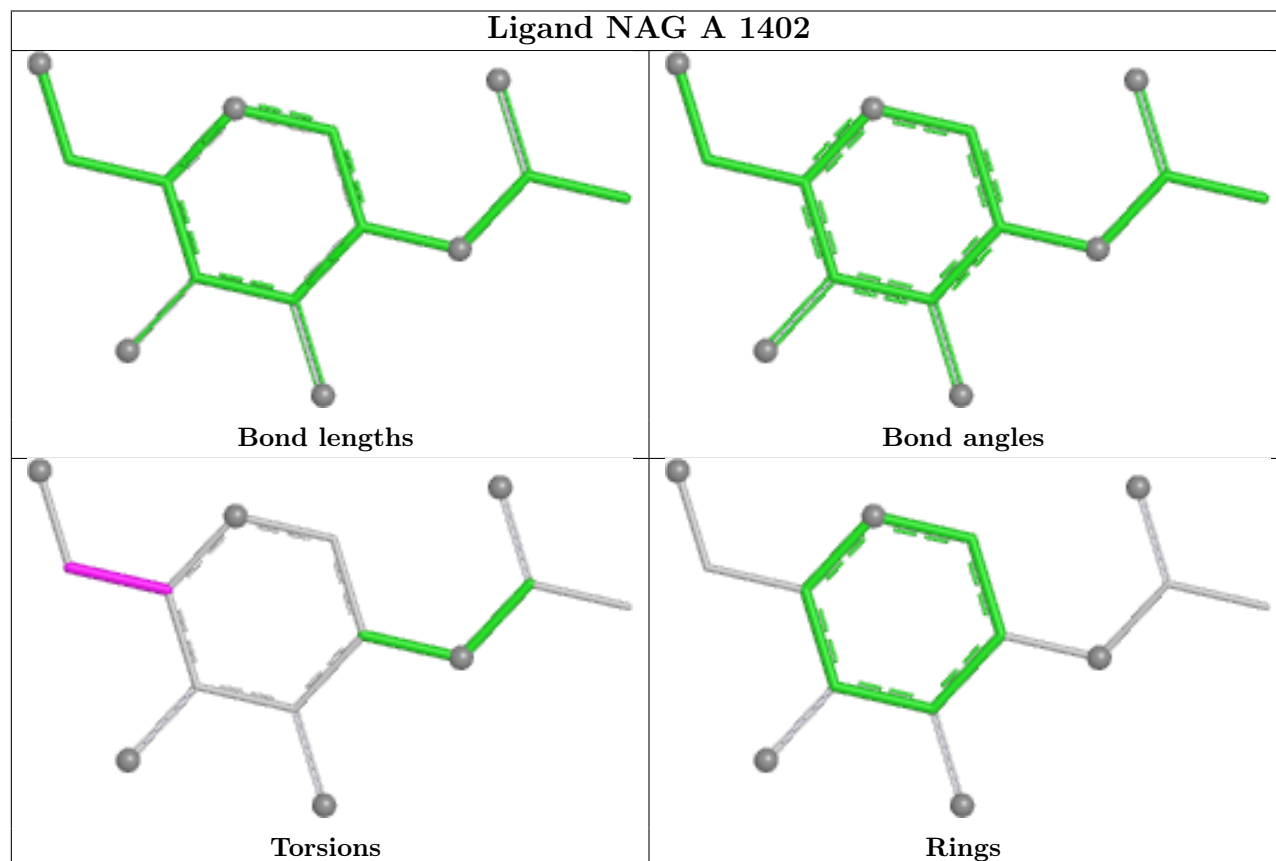
Ligand NAG E 906

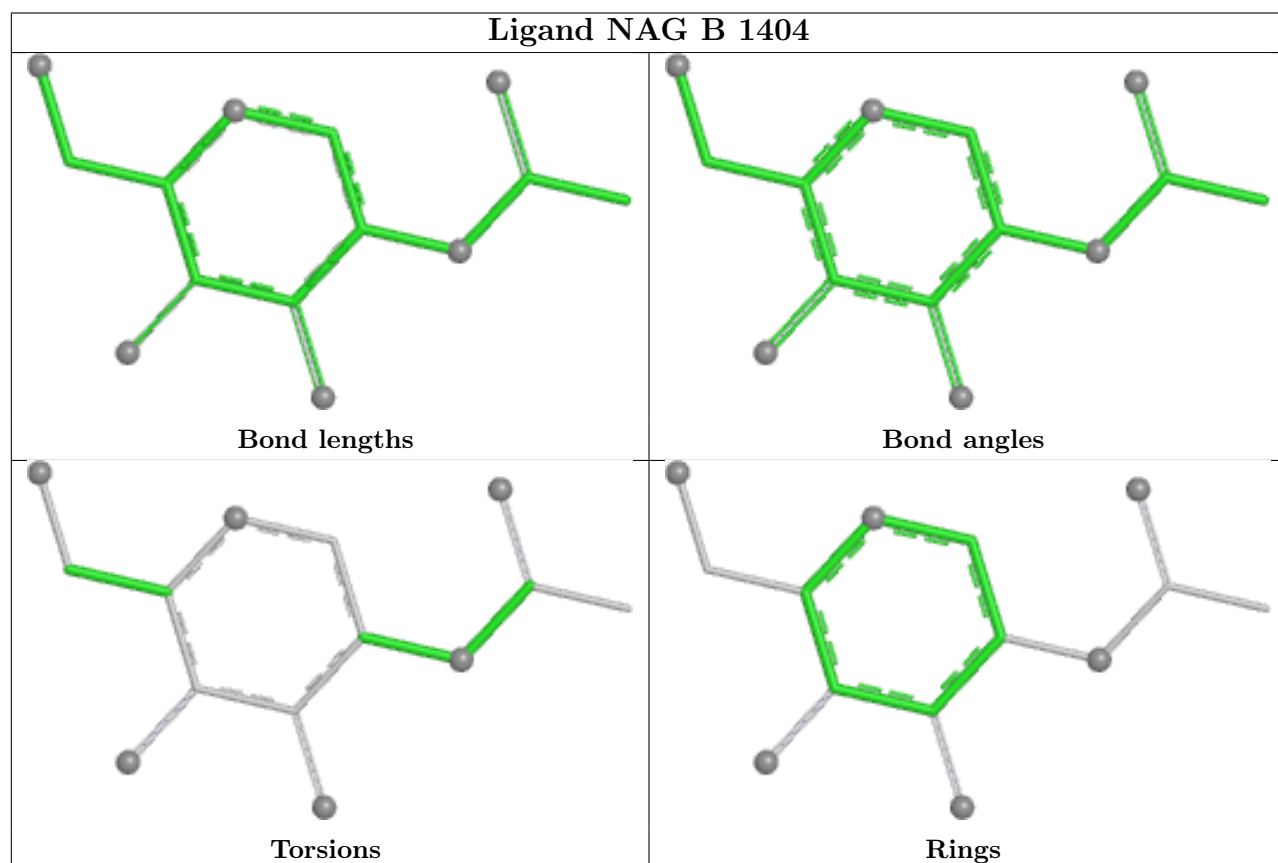
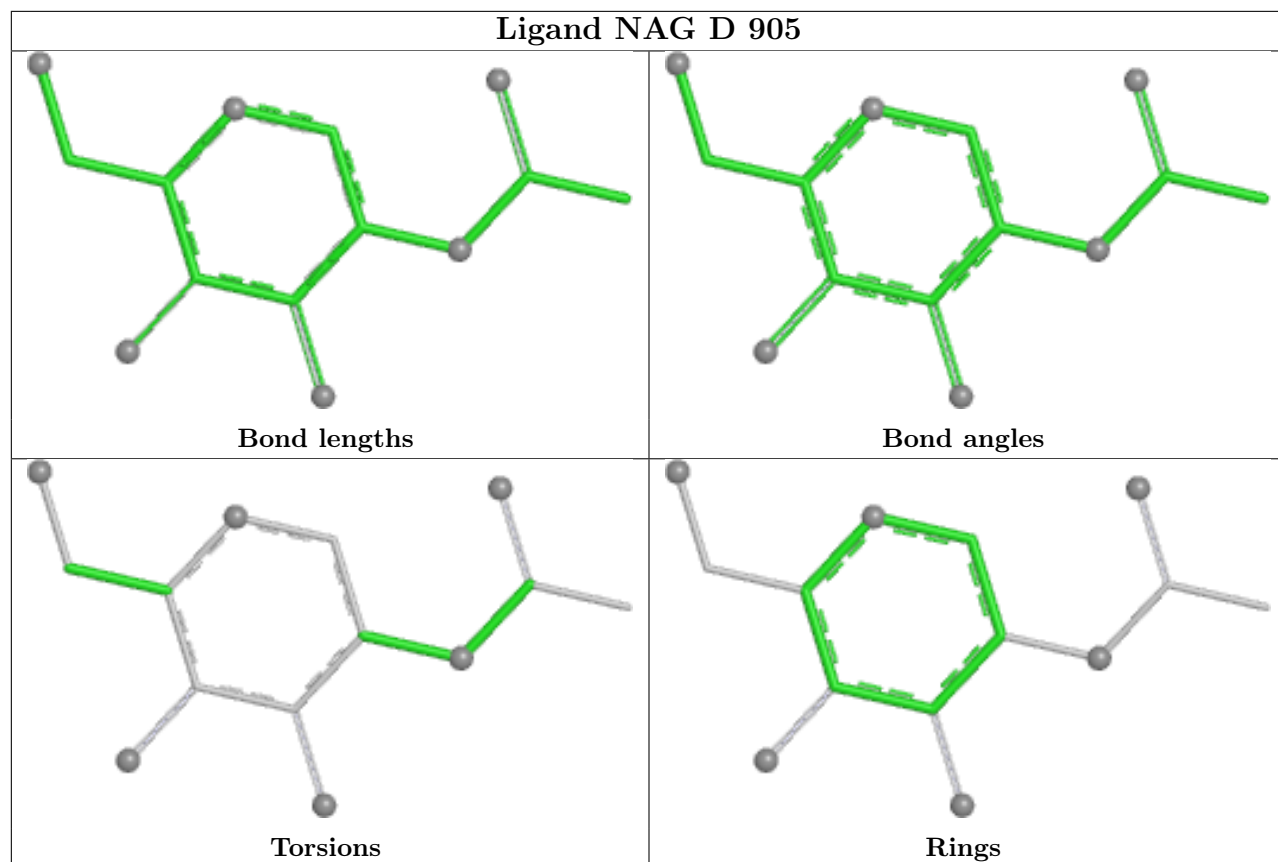


Ligand NAG B 1411

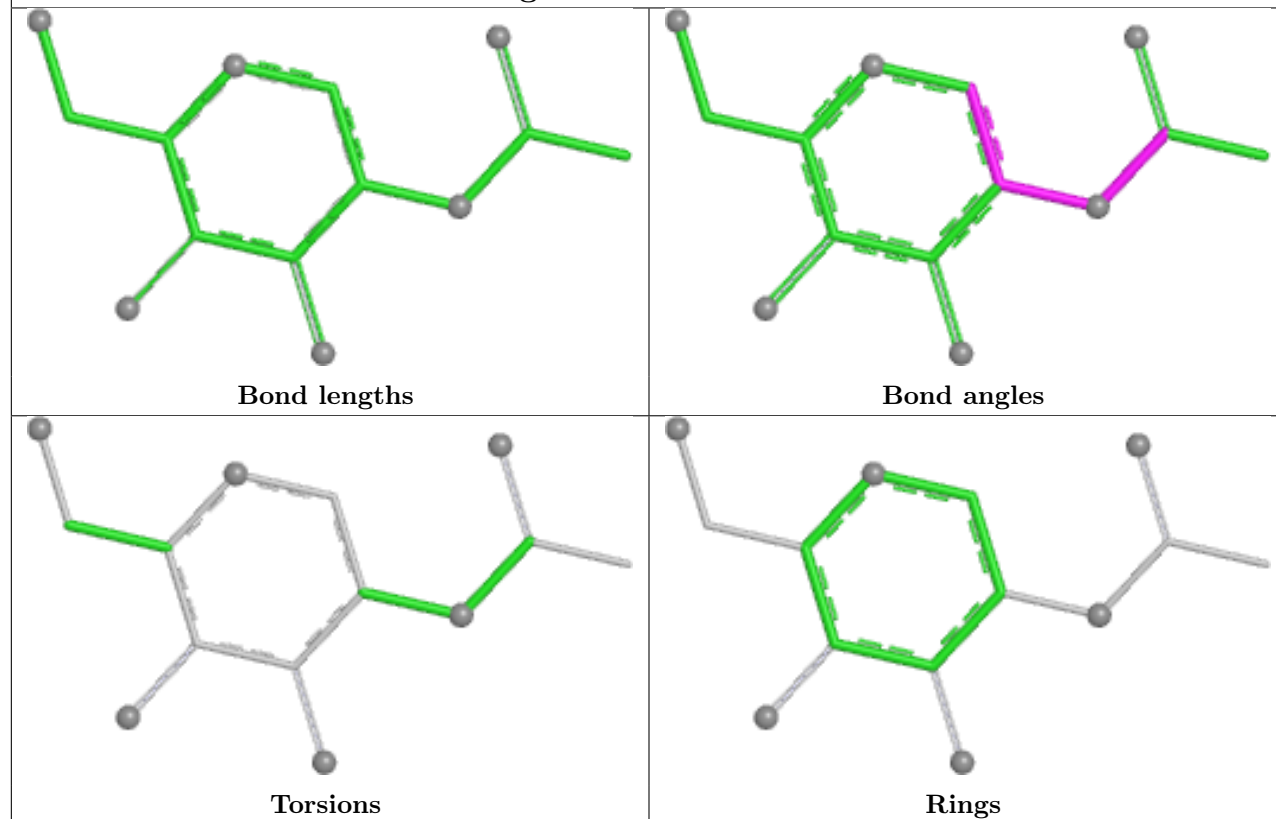


Ligand NAG A 1402

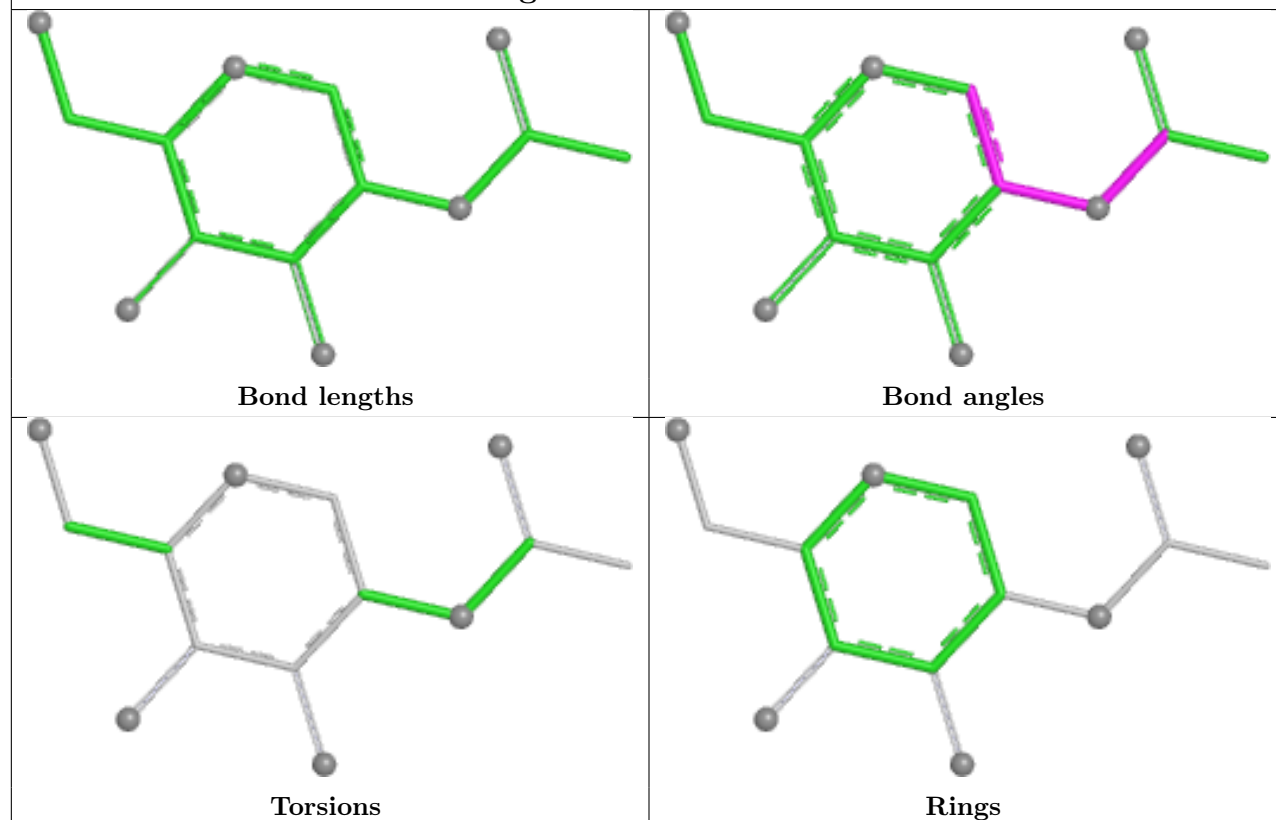


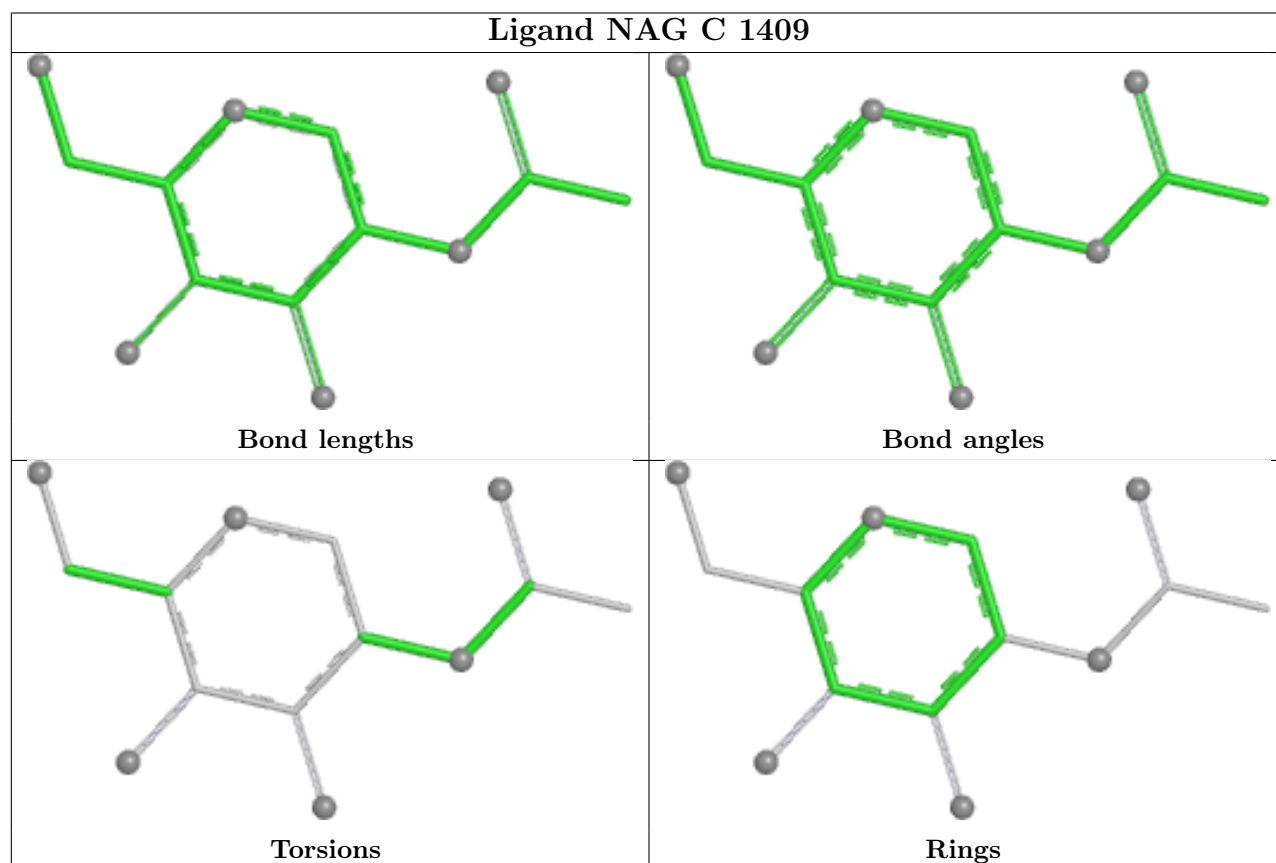
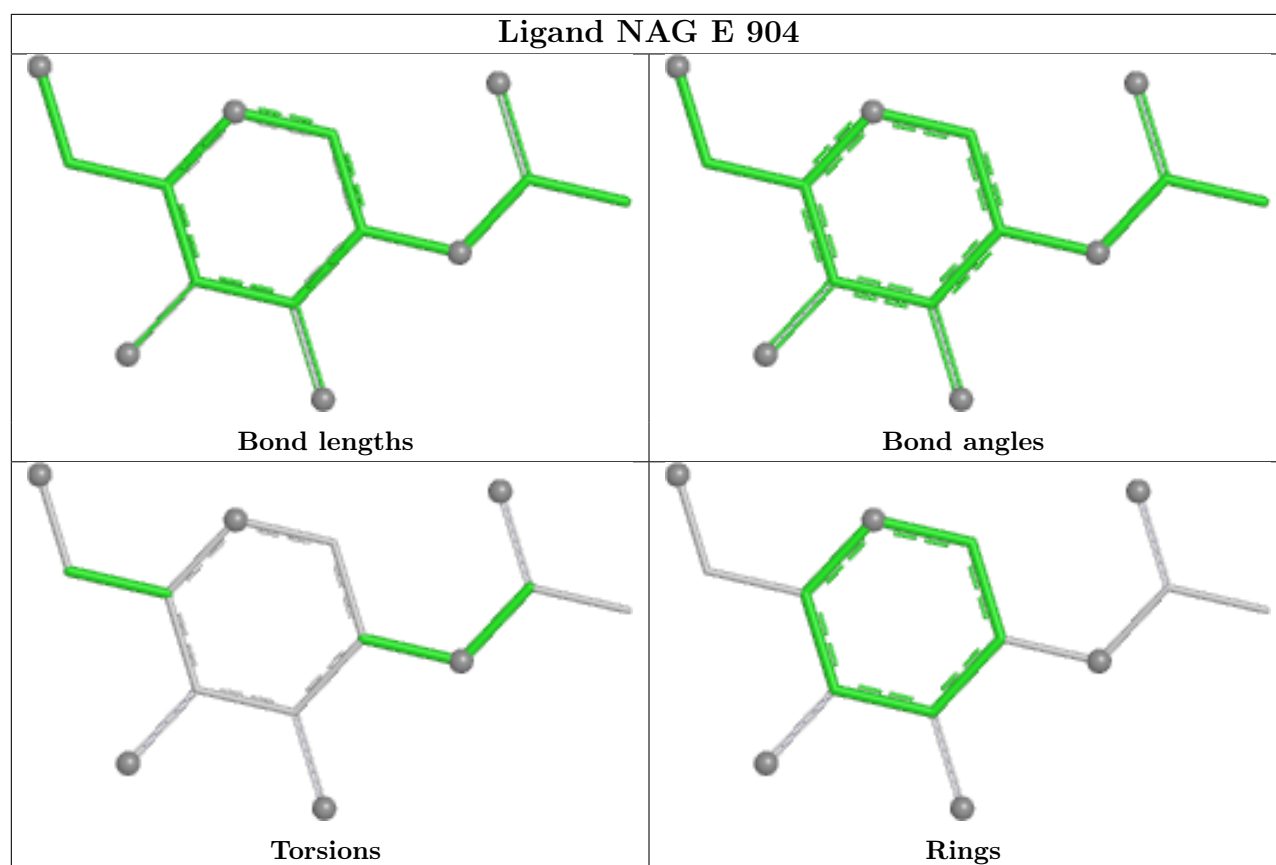


Ligand NAG B 1405

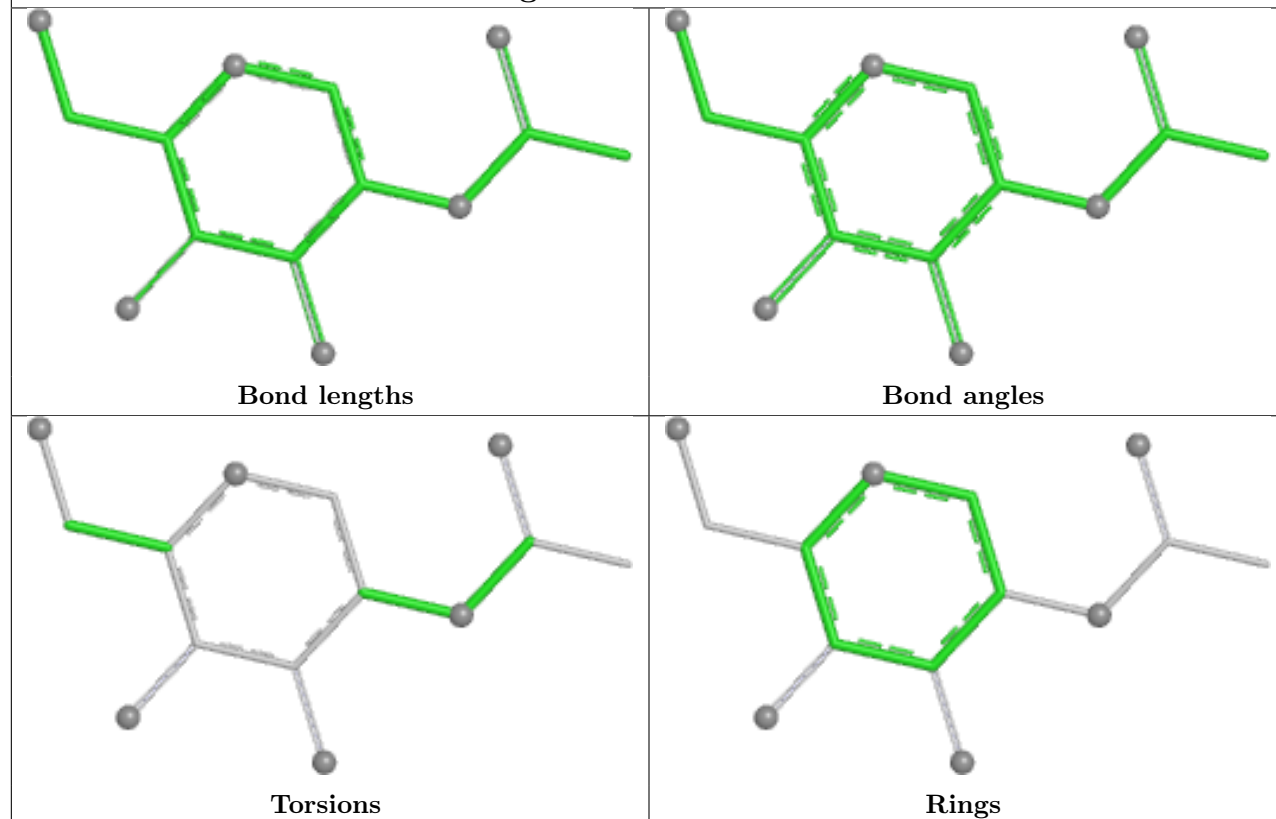


Ligand NAG C 1405

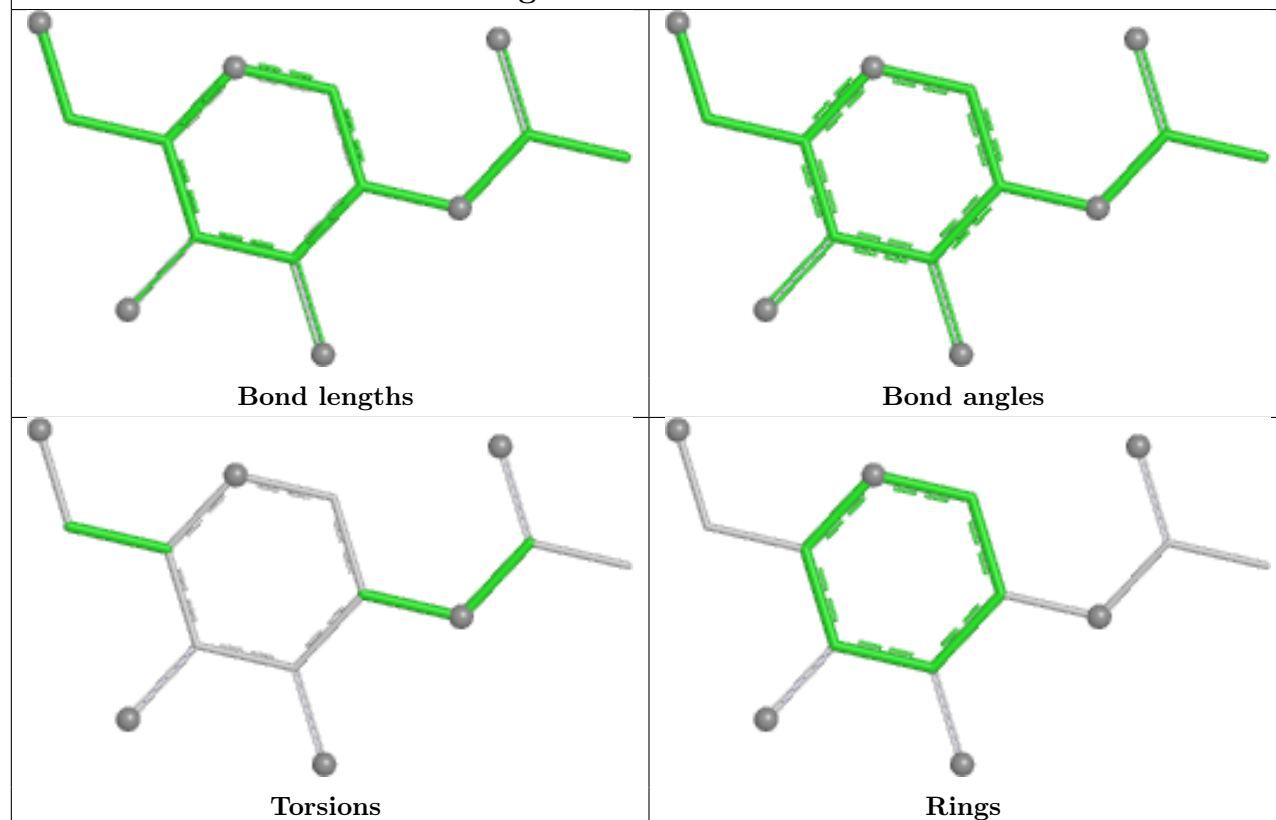




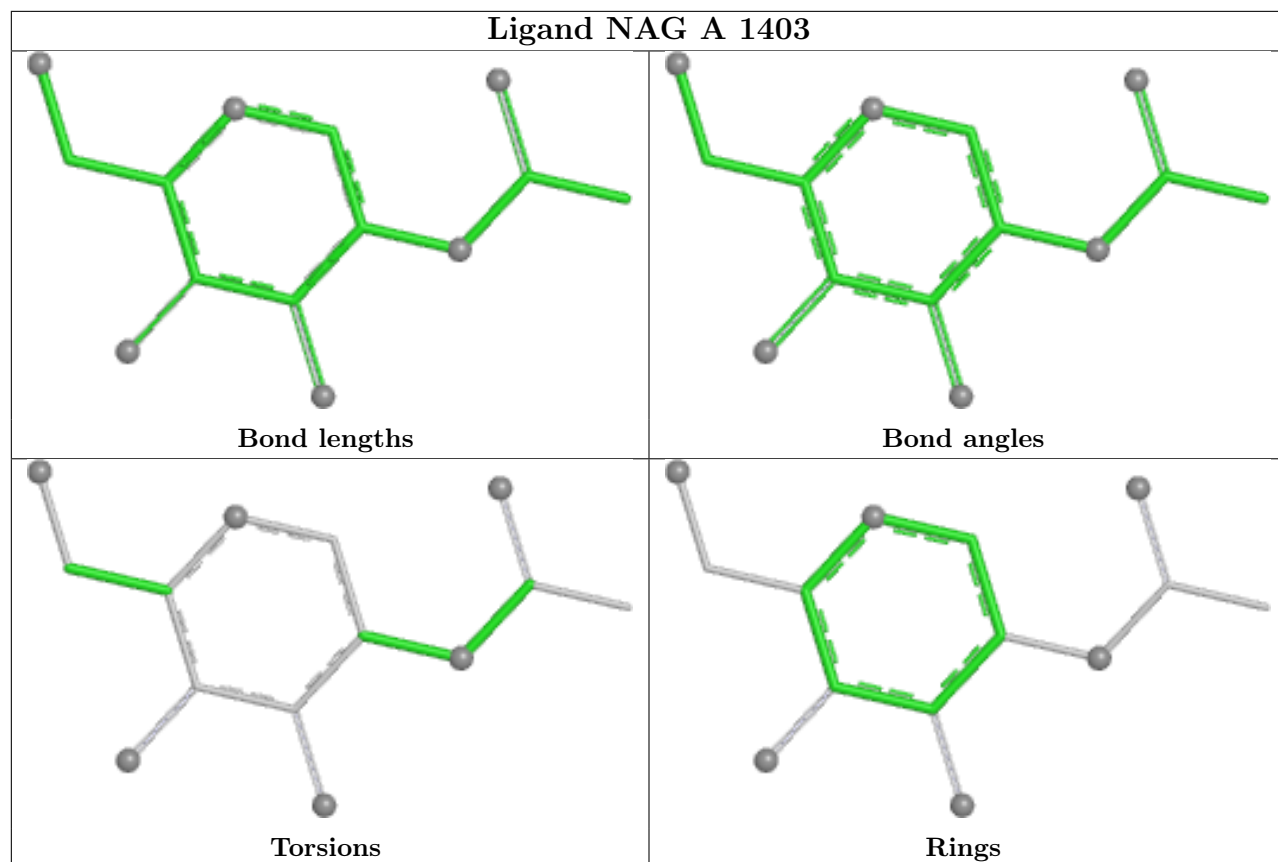
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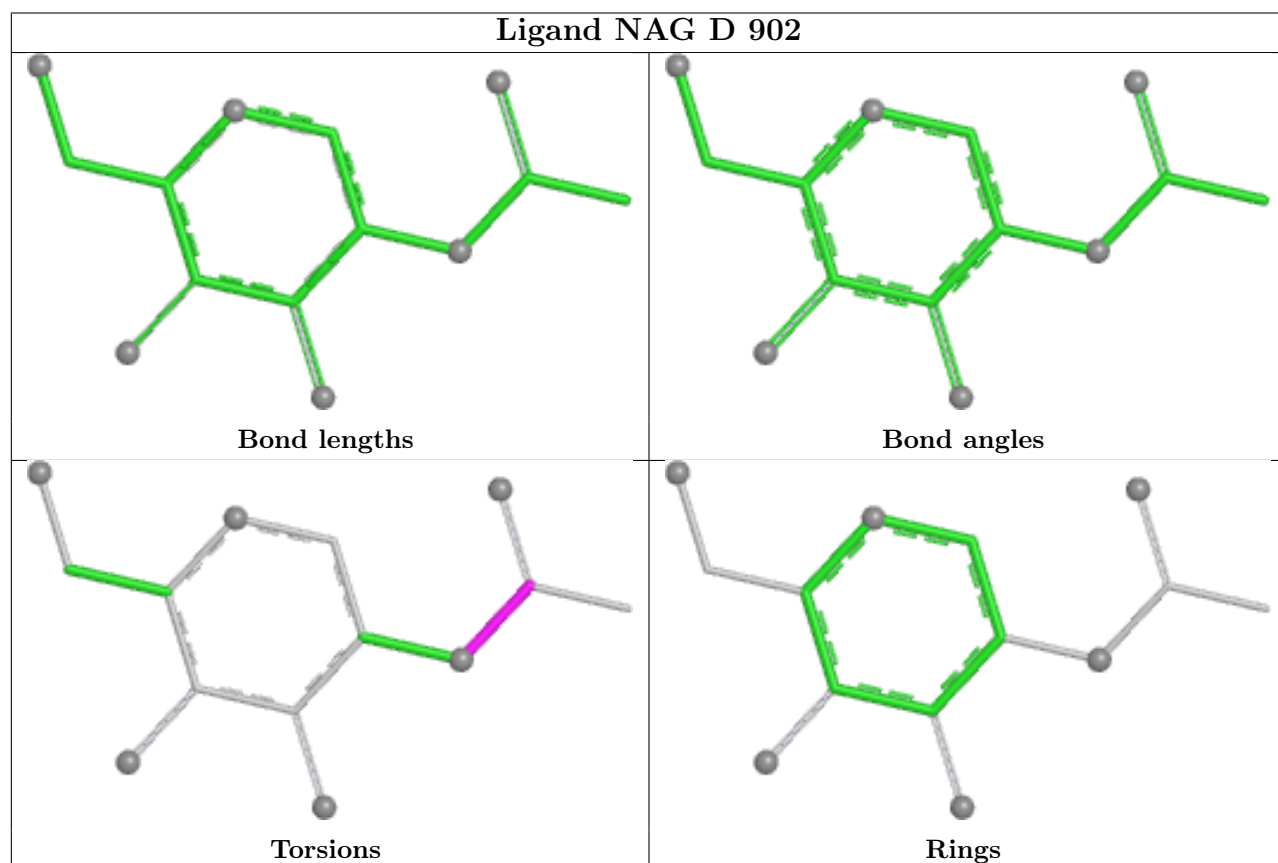
Ligand NAG A 1401



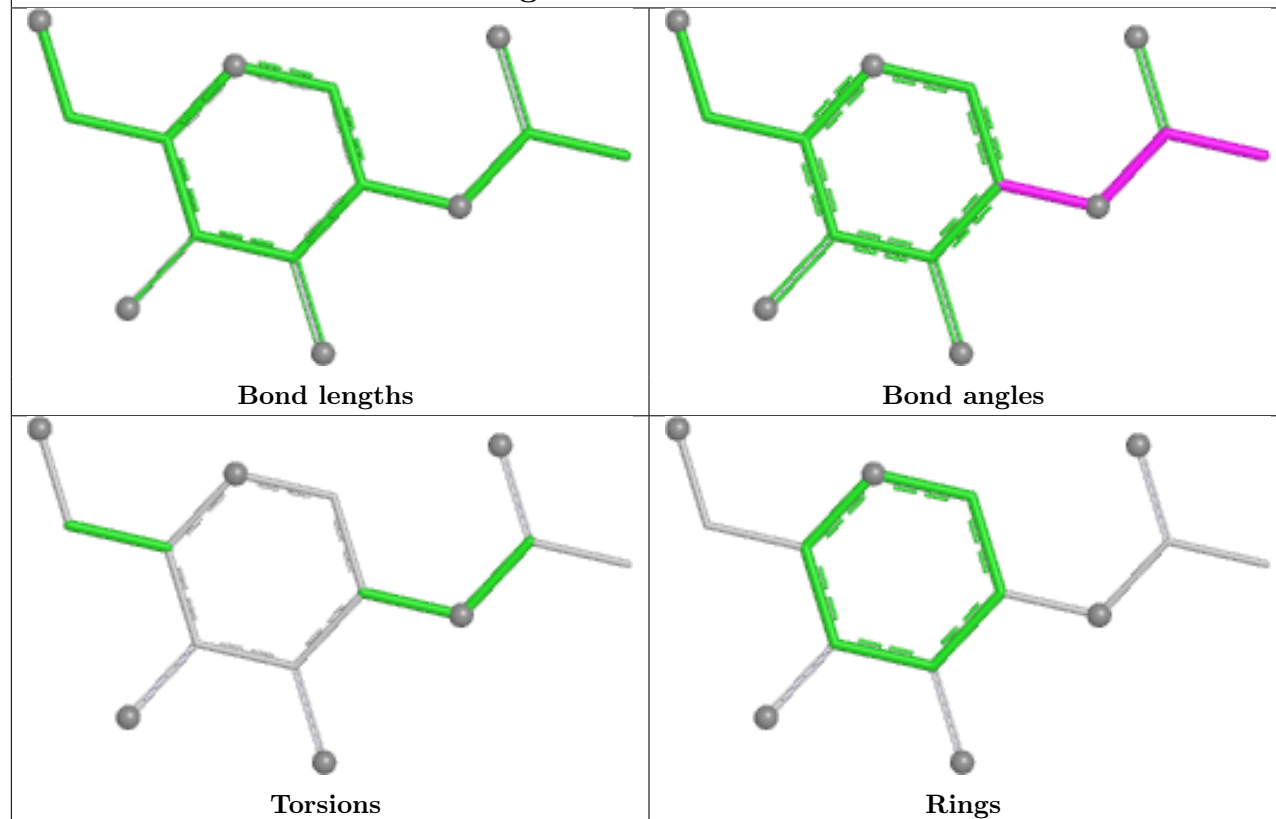
Ligand NAG A 1403



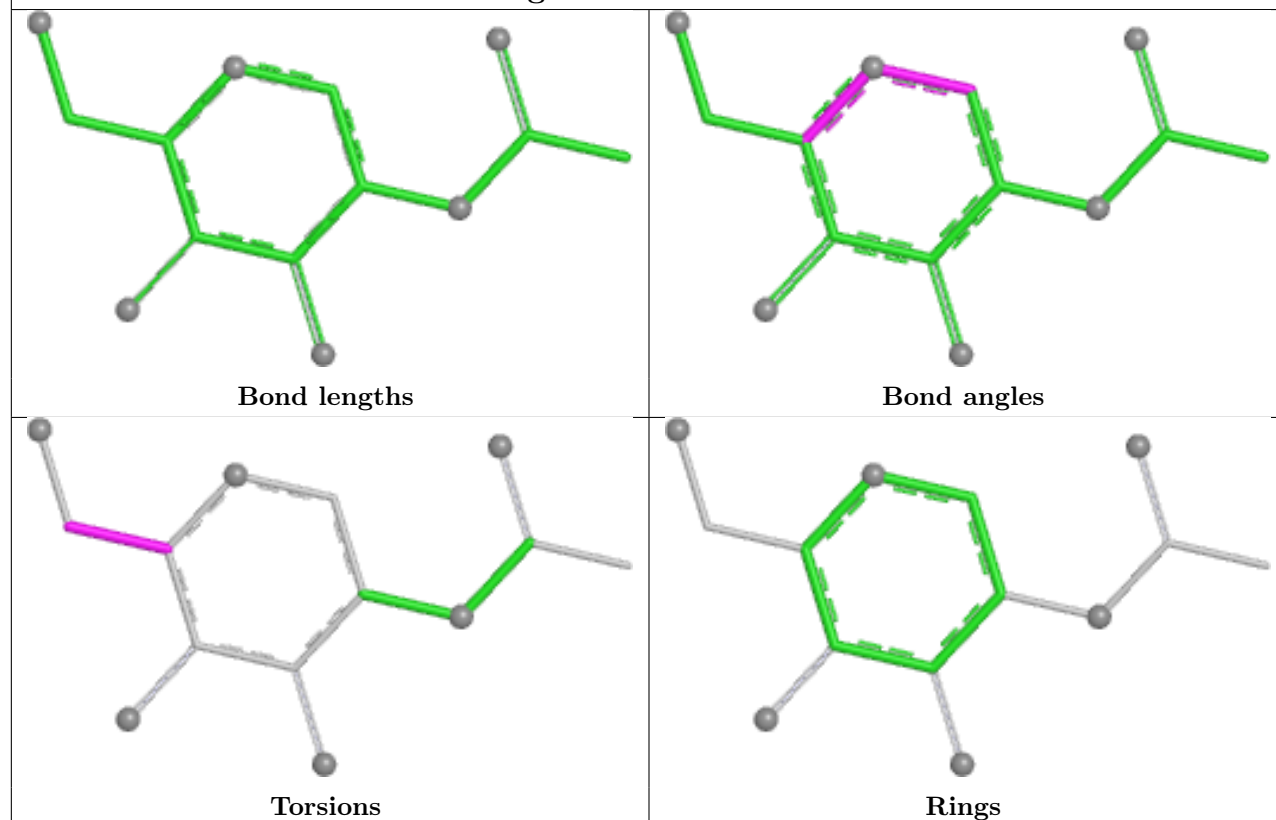
Ligand NAG D 902



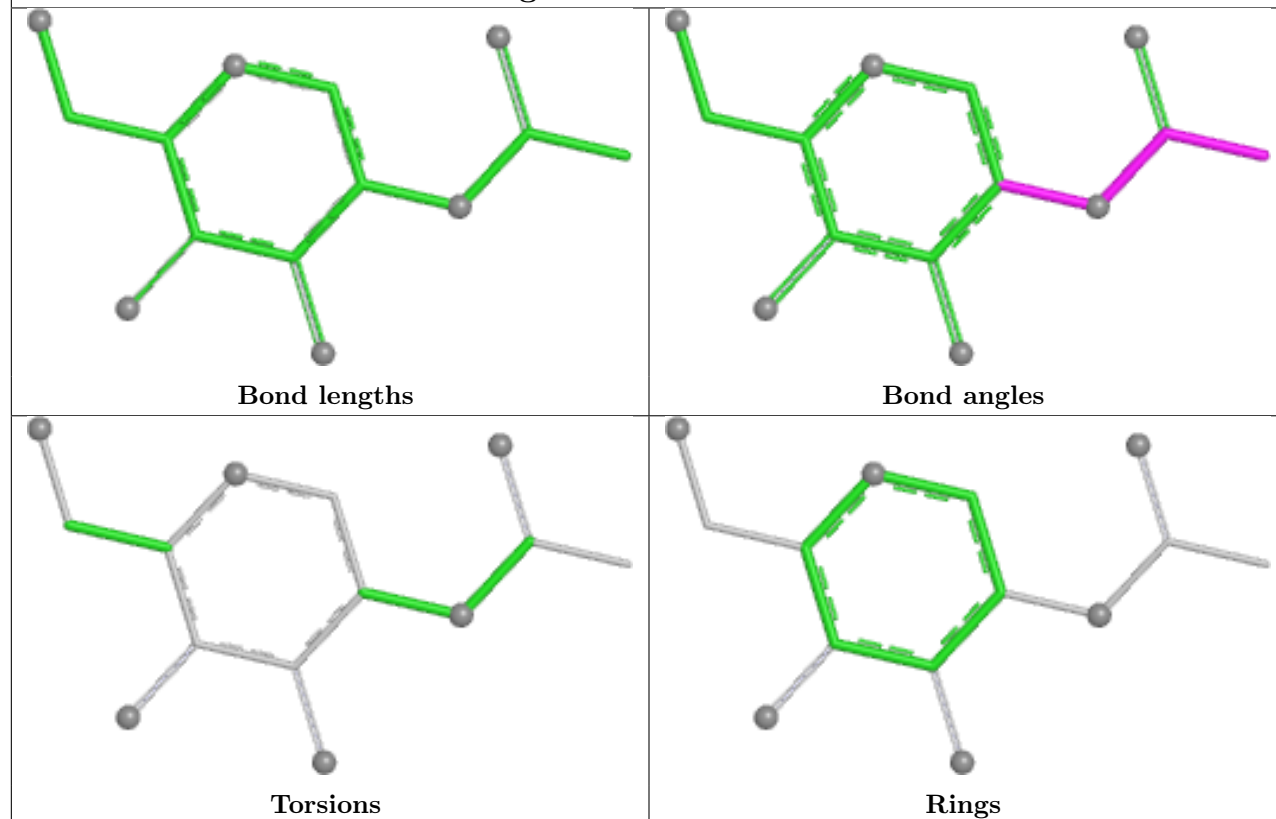
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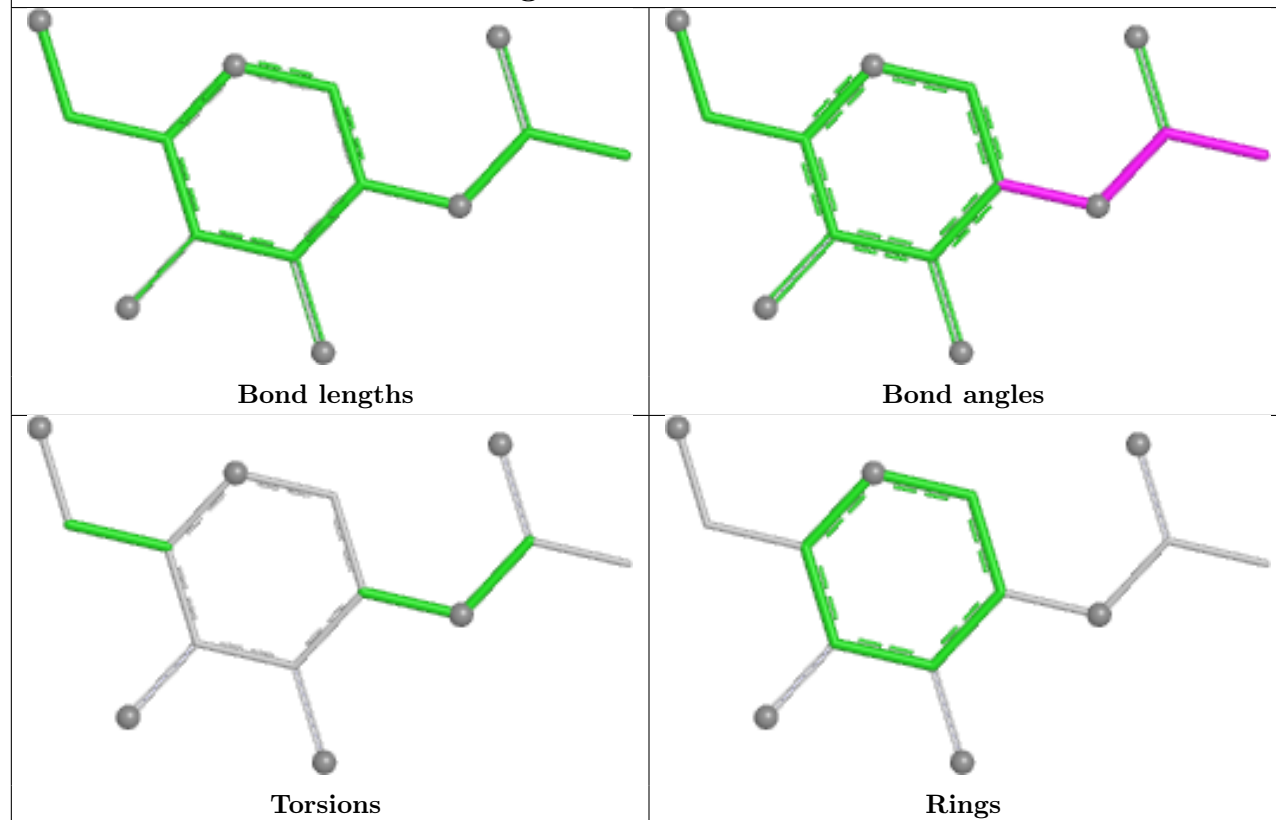
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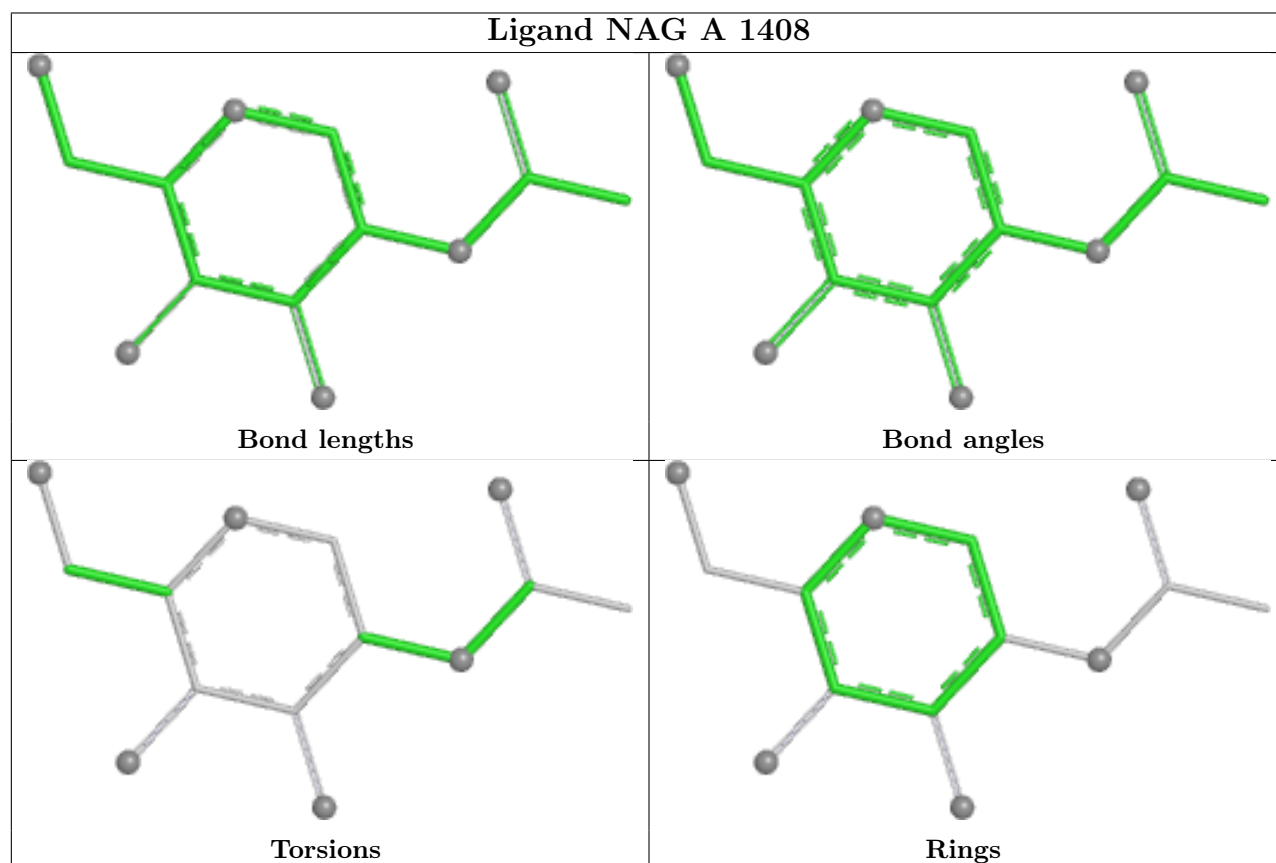
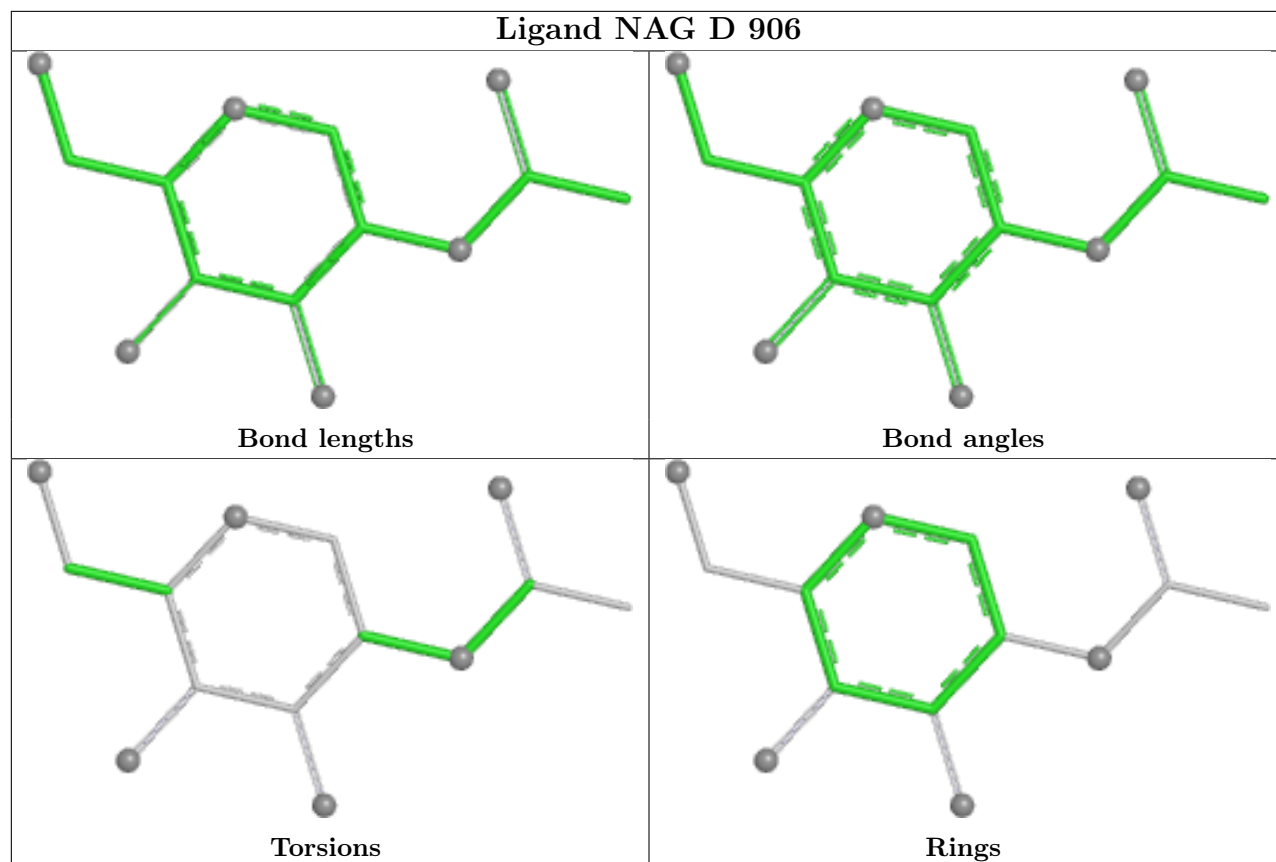


Ligand NAG C 1406

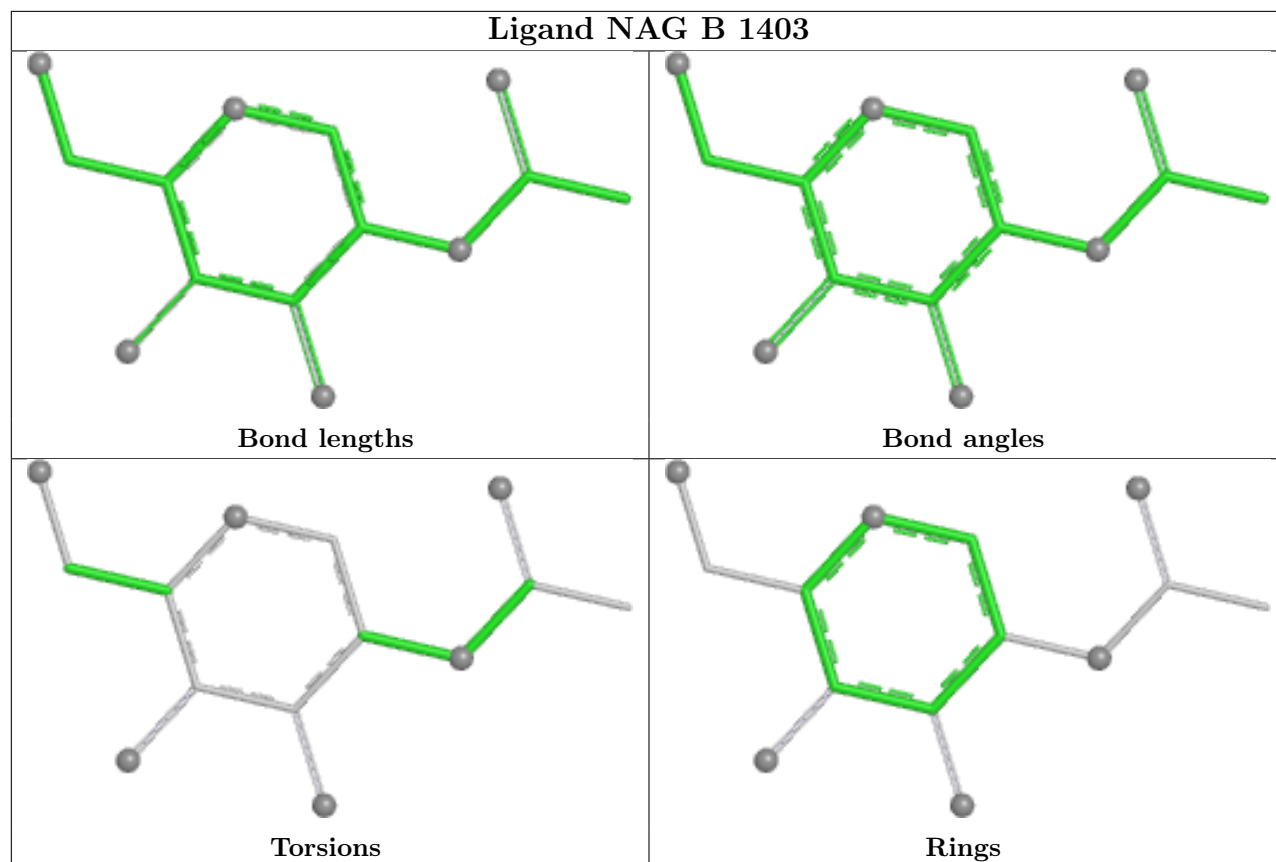


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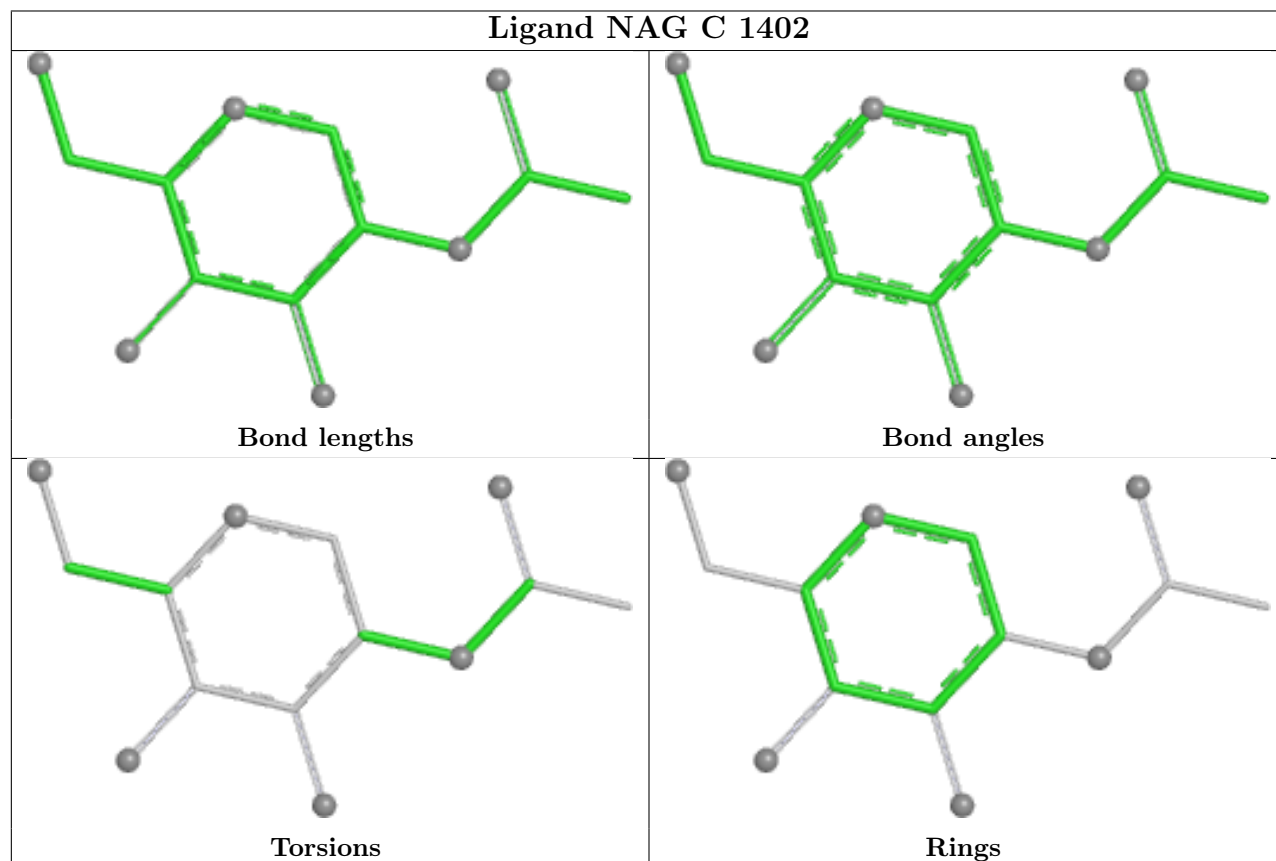




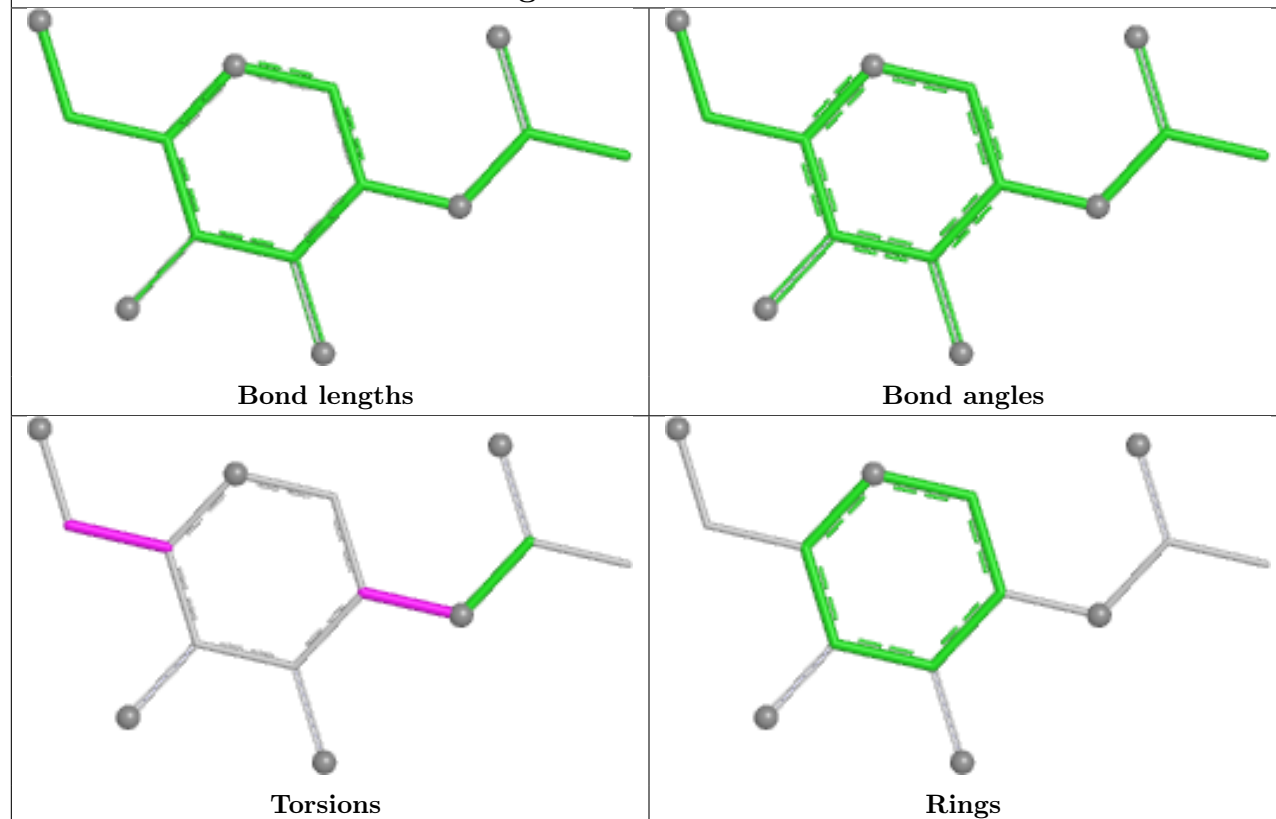
Ligand NAG B 1403



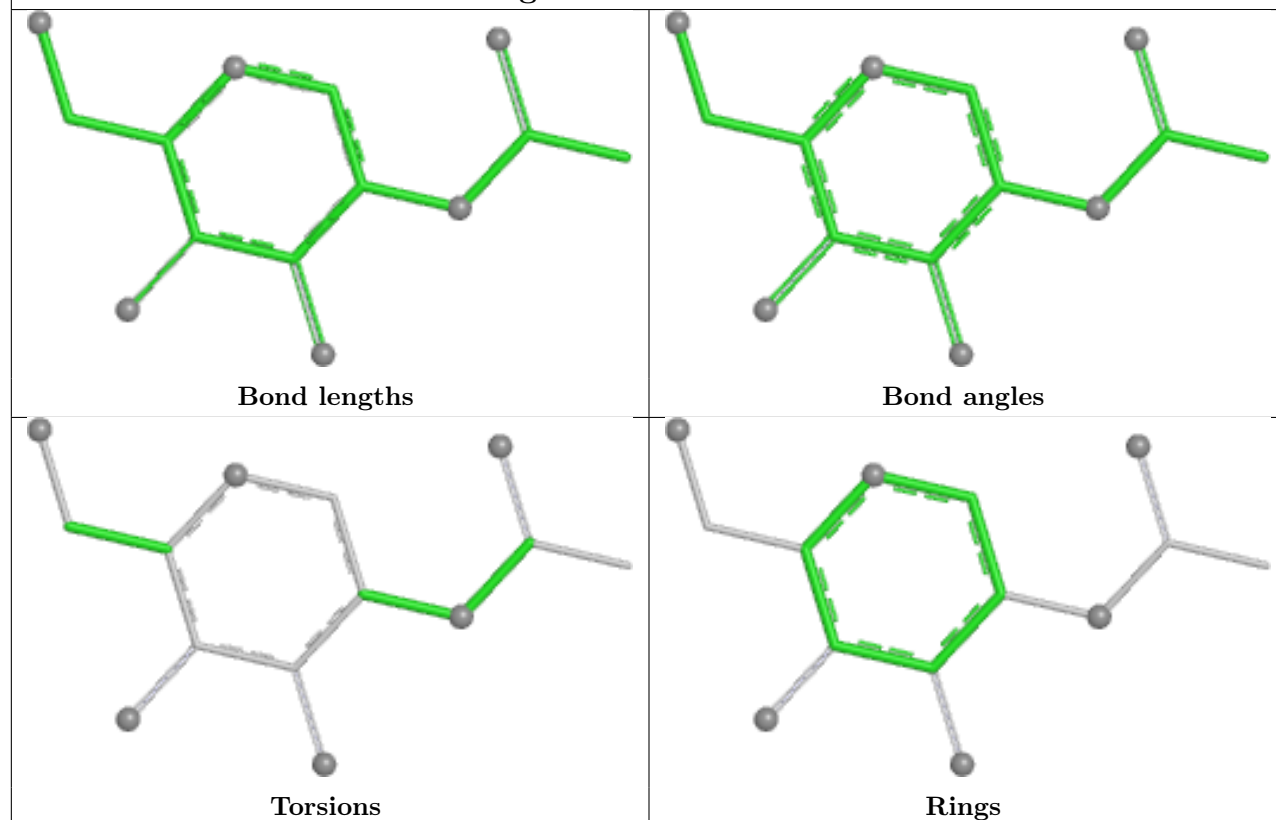
Ligand NAG C 1402



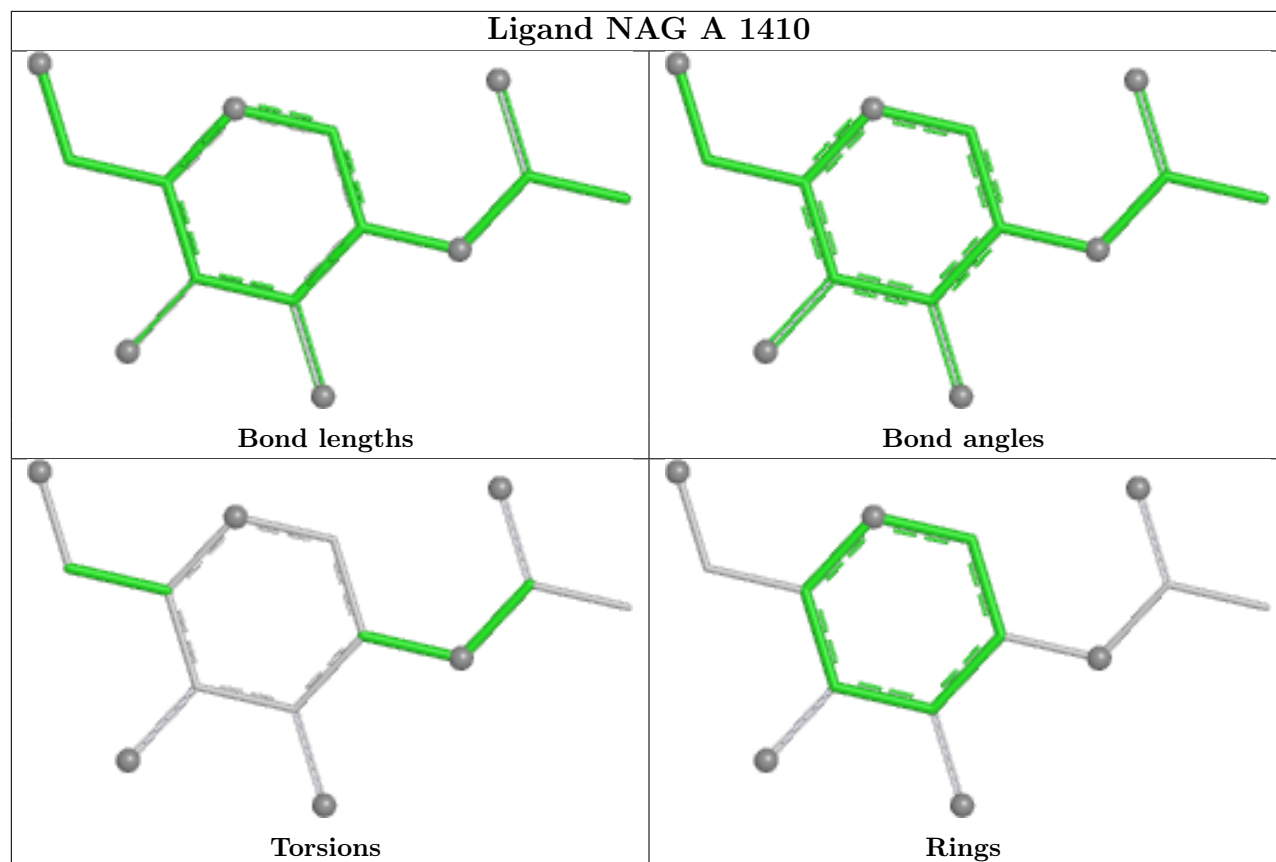
Ligand NAG A 1407



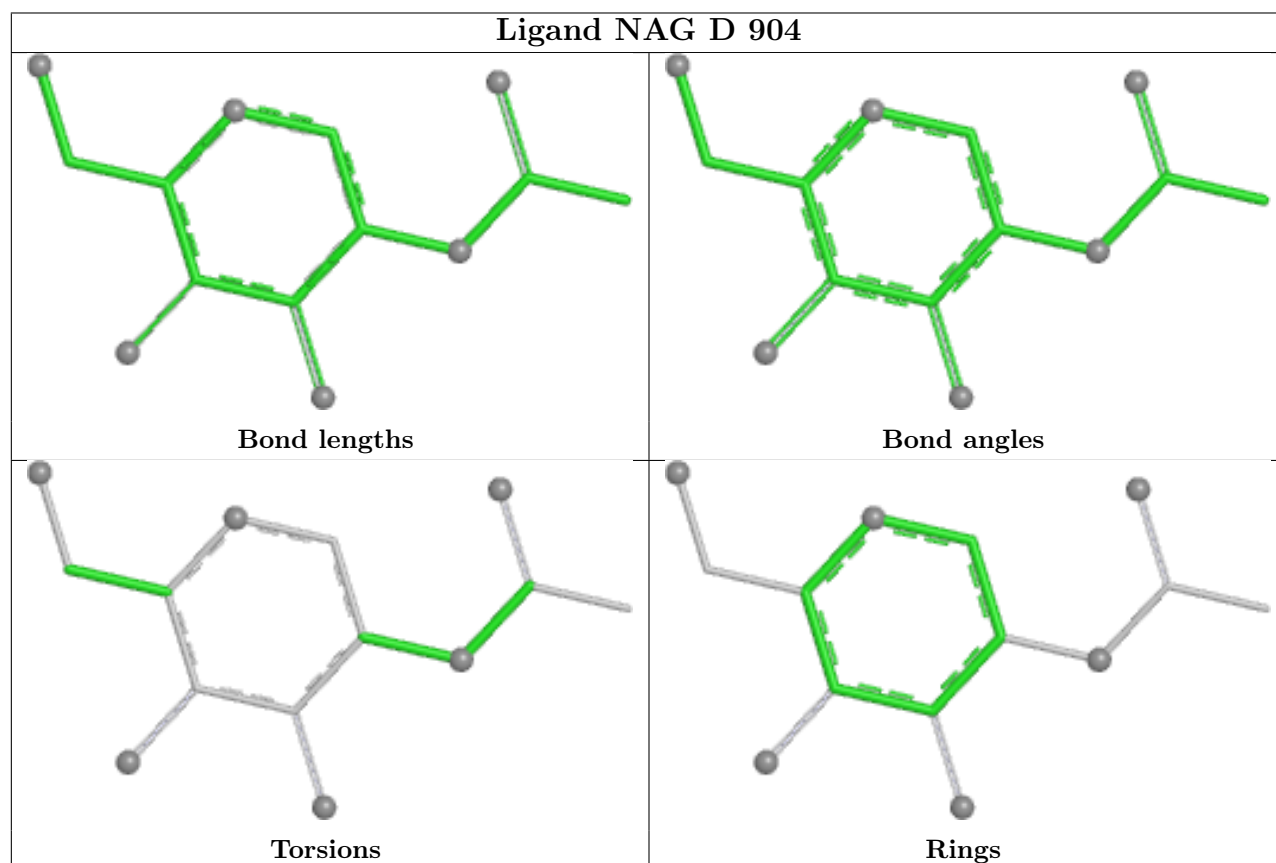
Ligand NAG C 1403

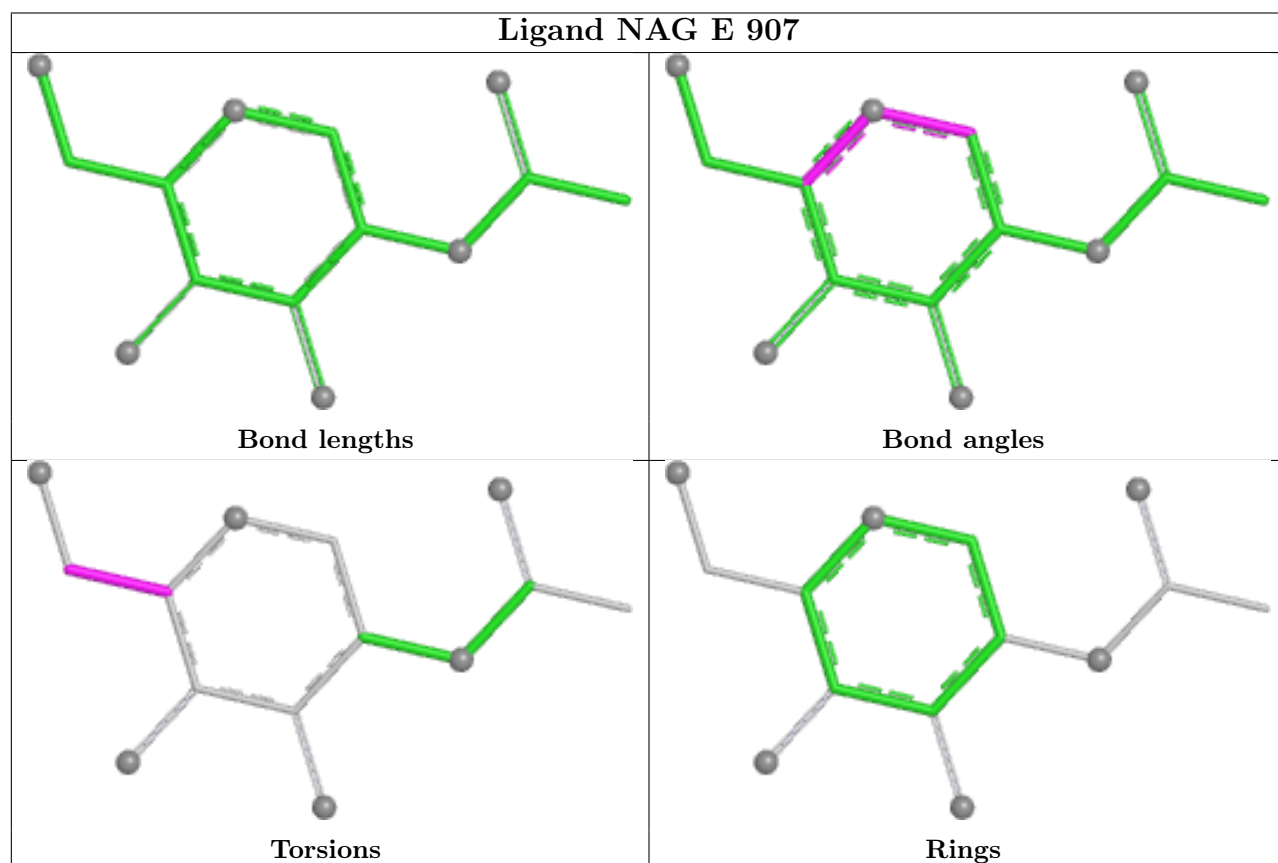
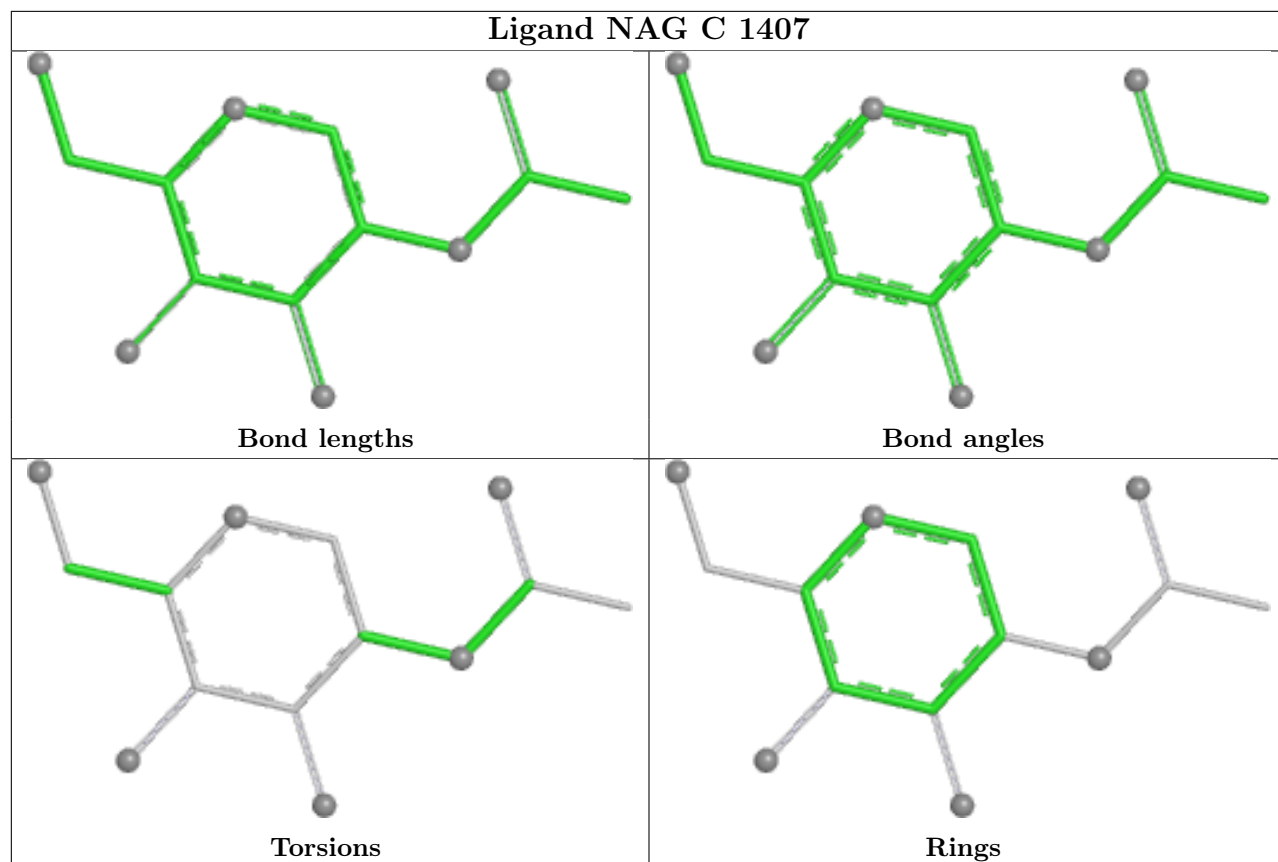


Ligand NAG A 1410

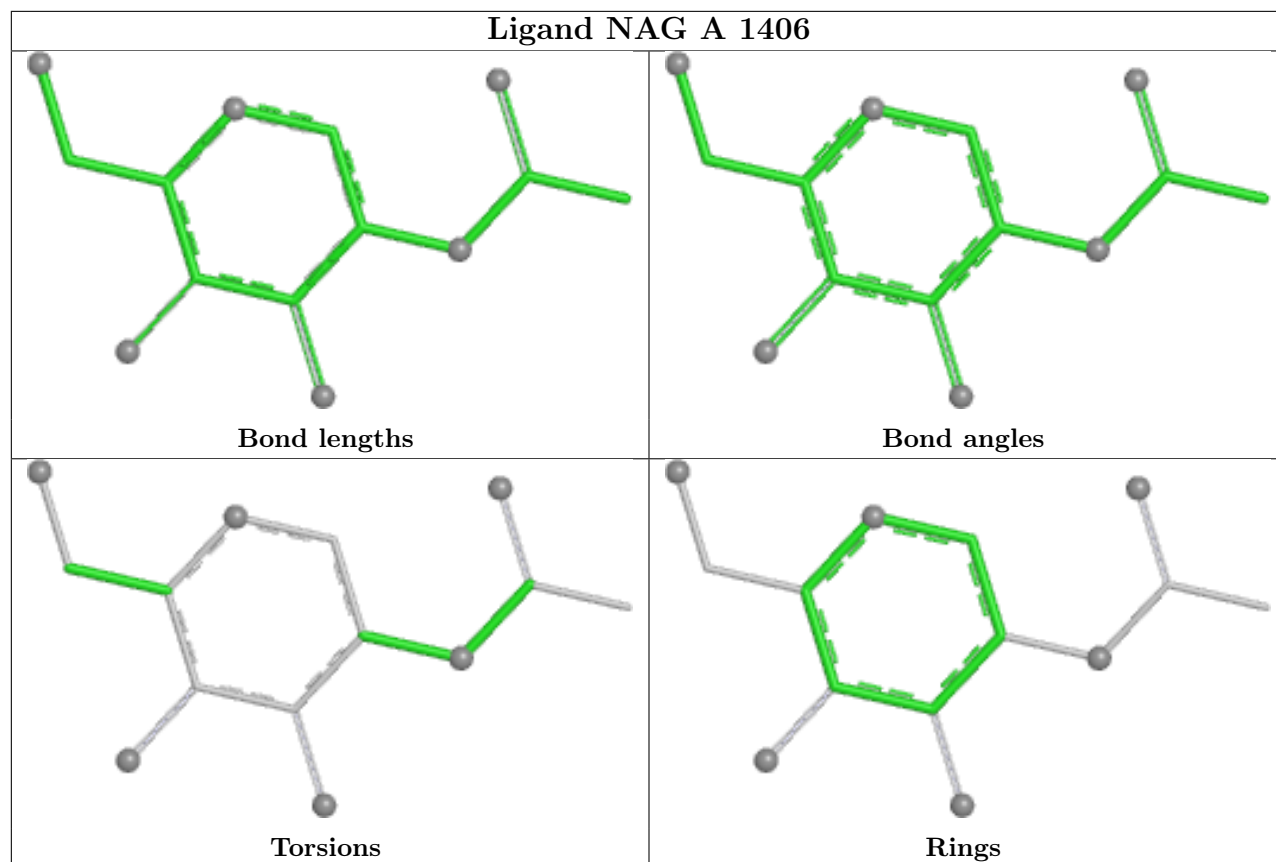


Ligand NAG D 904

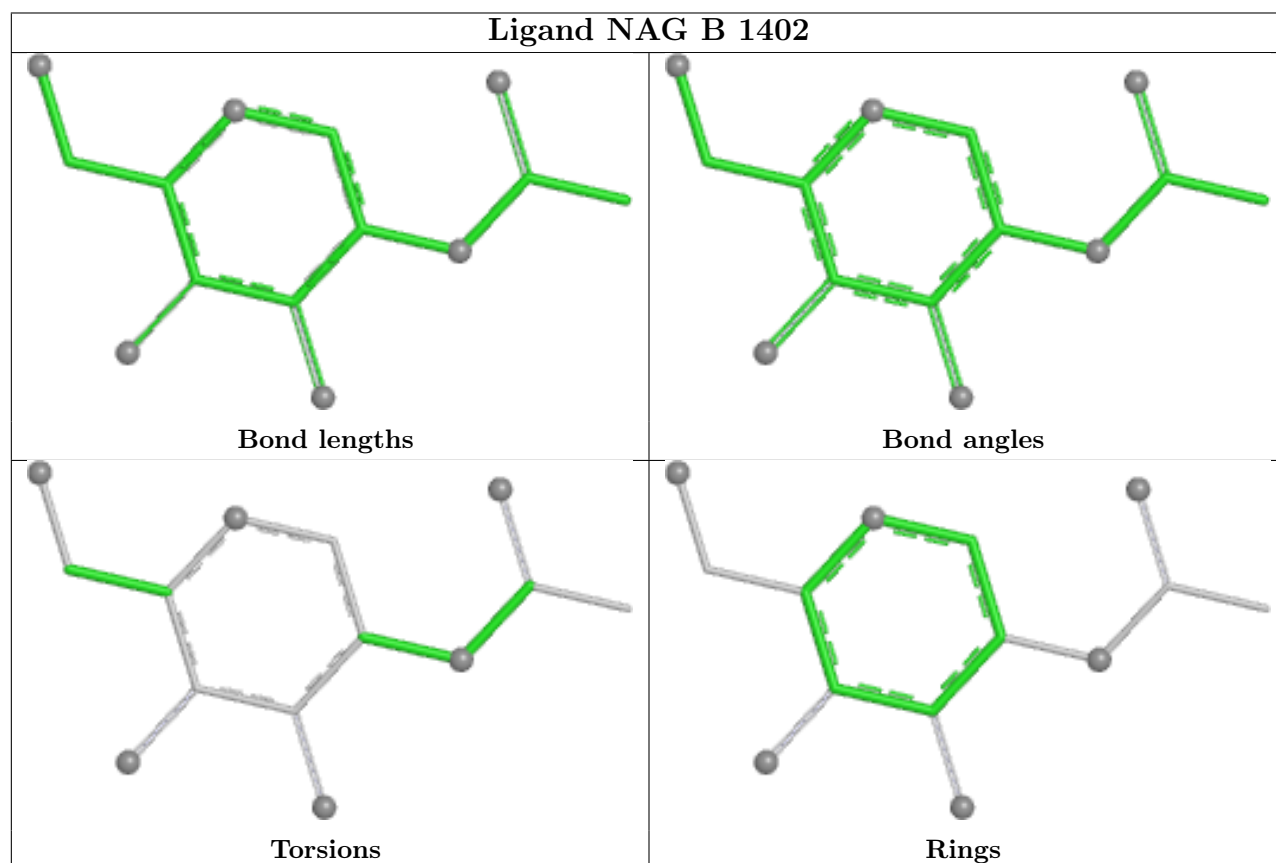


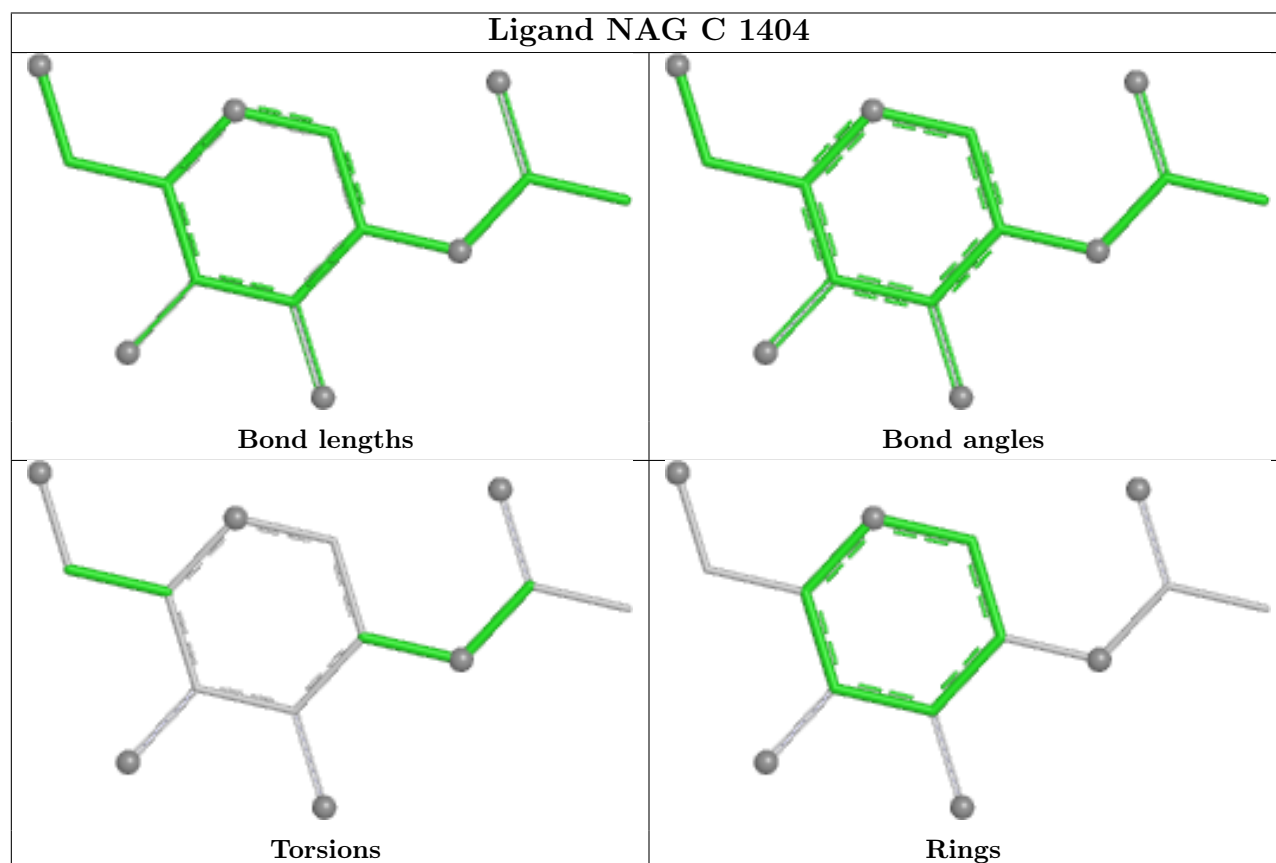
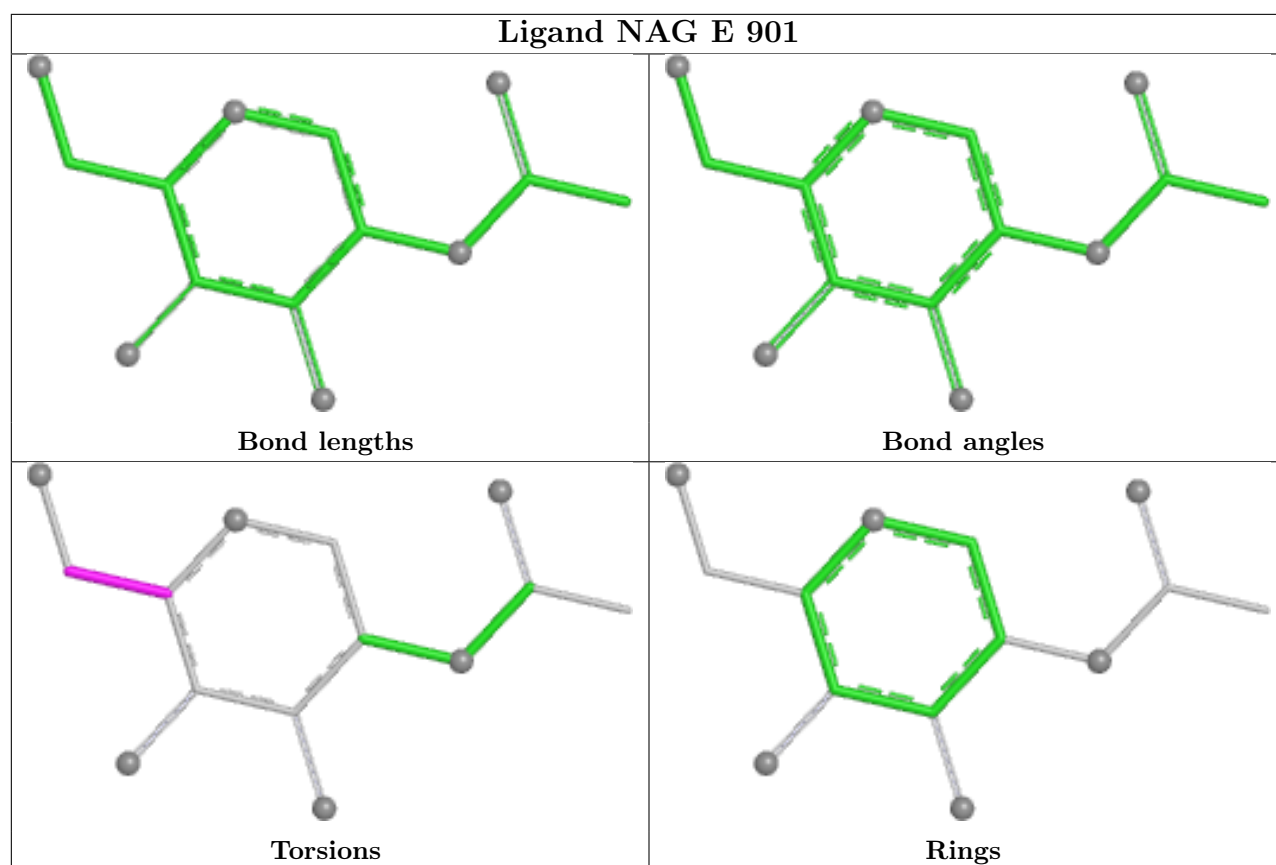


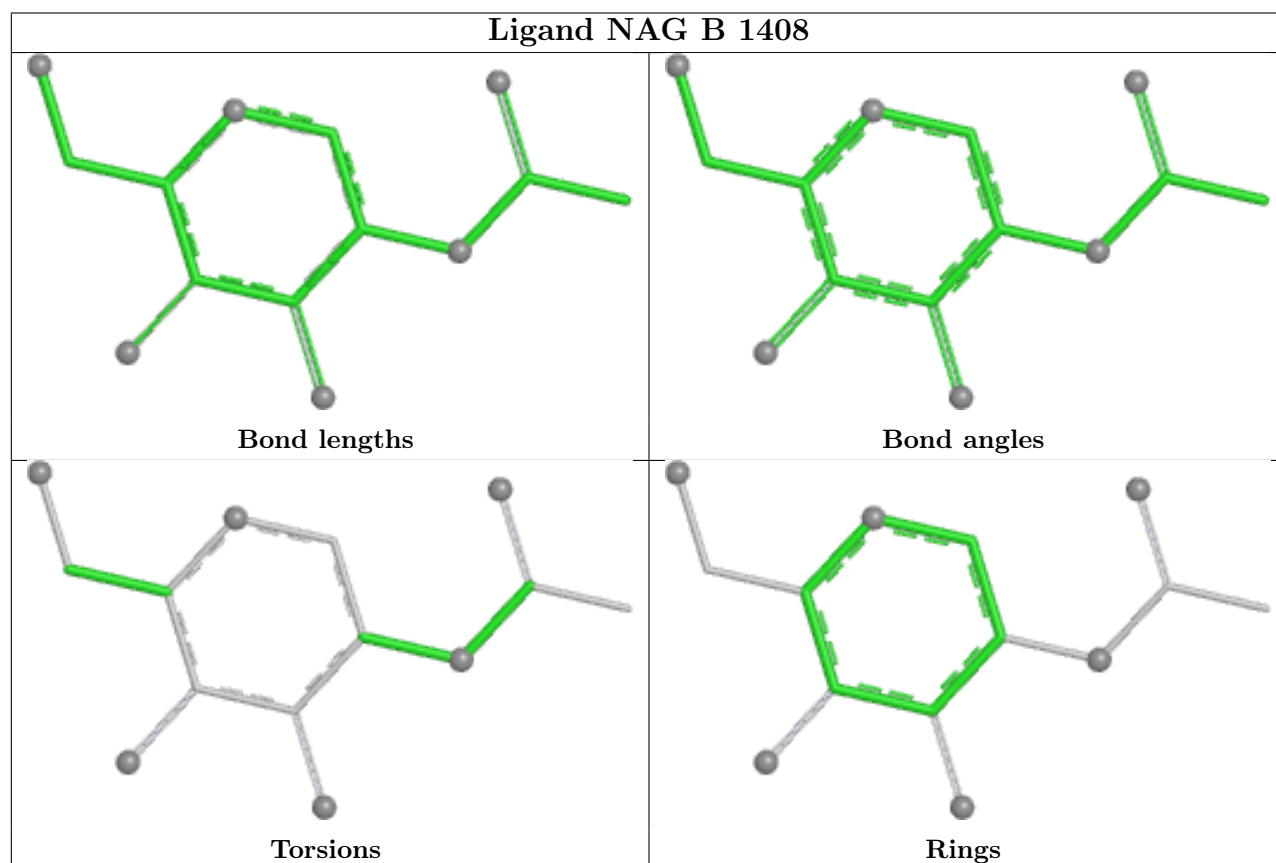
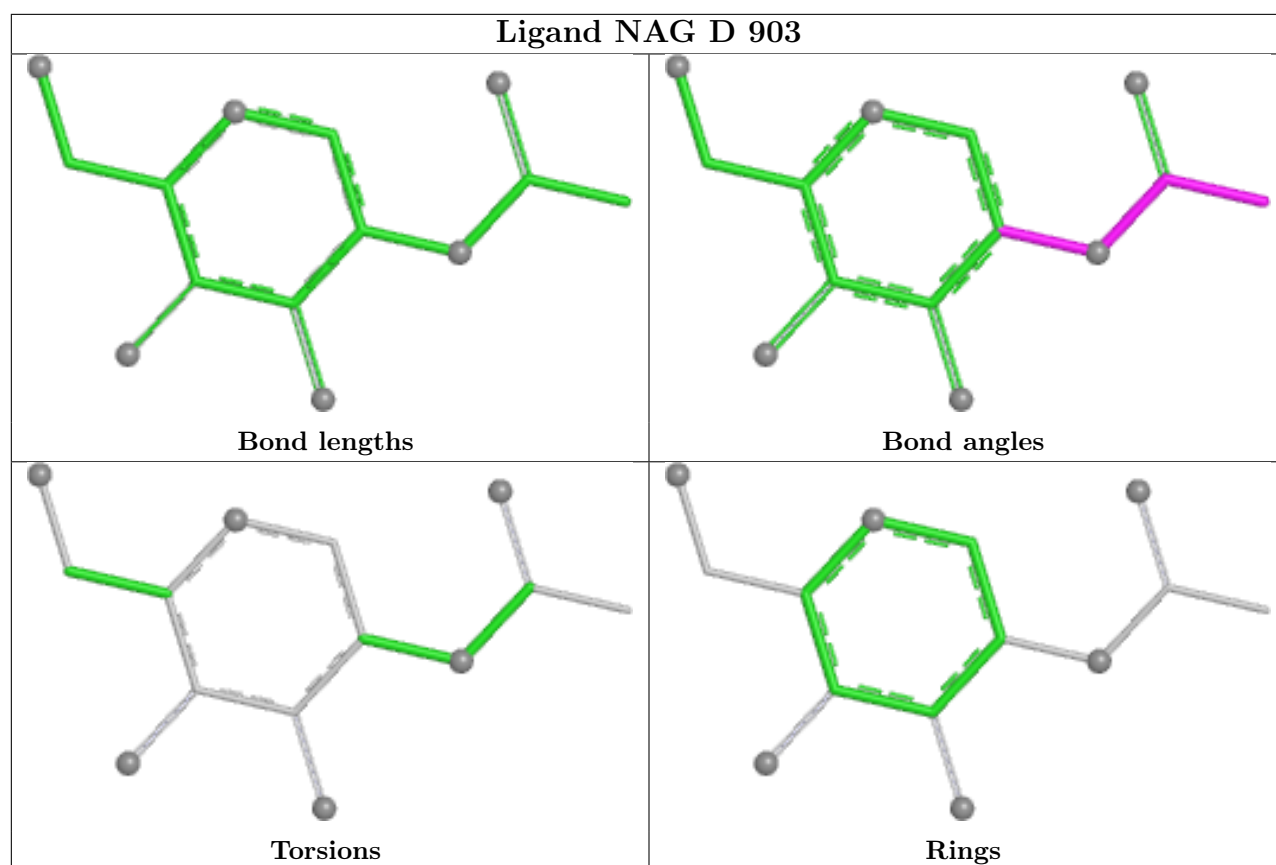
Ligand NAG A 1406



Ligand NAG B 1402







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.

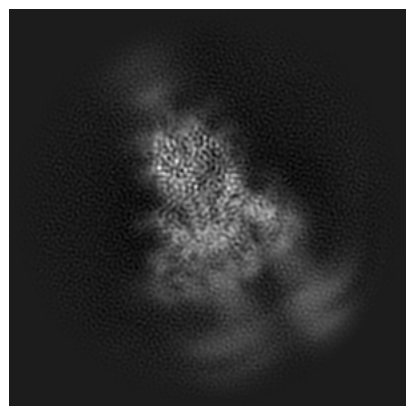
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33203. These allow visual inspection of the internal detail of the map and identification of artifacts.

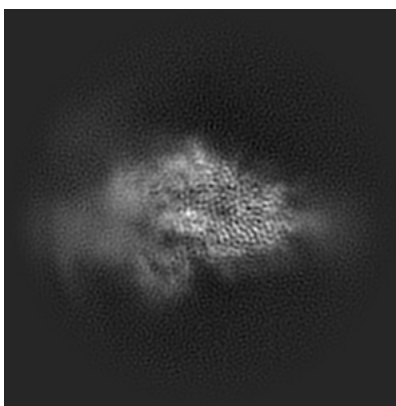
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

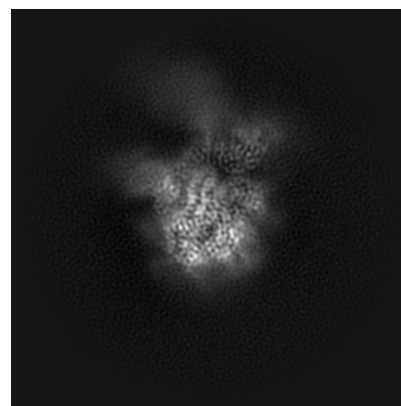
6.1.1 Primary map



X

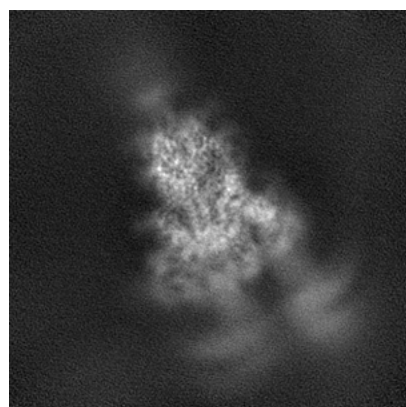


Y

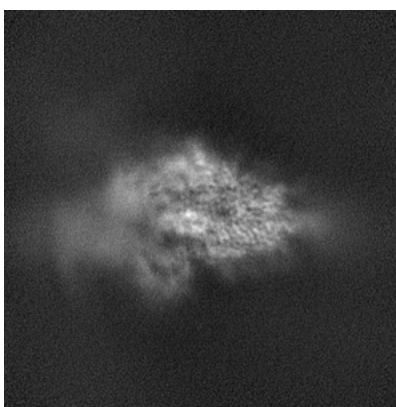


Z

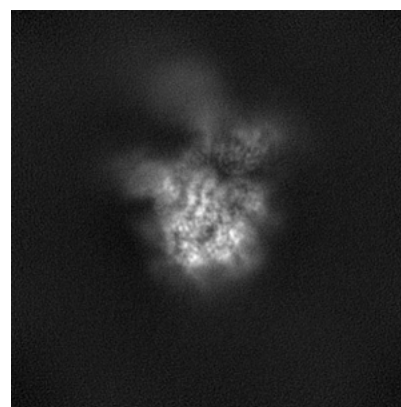
6.1.2 Raw map



X



Y

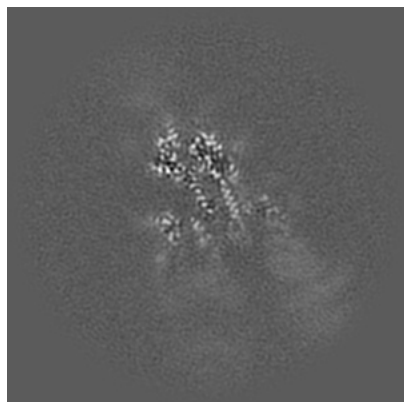


Z

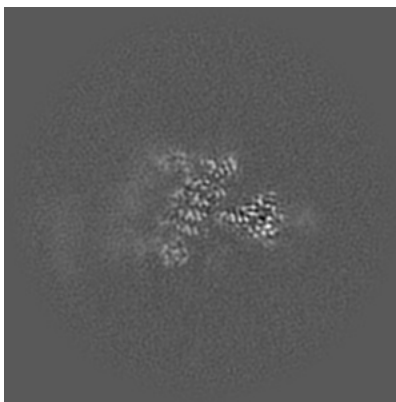
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

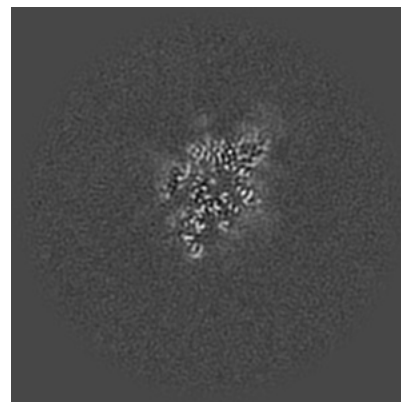
6.2.1 Primary map



X Index: 144

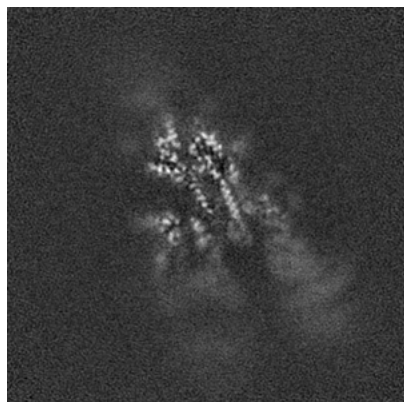


Y Index: 144

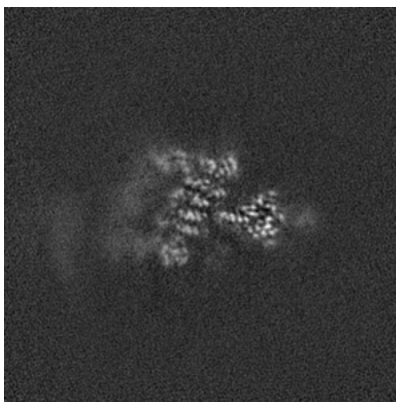


Z Index: 144

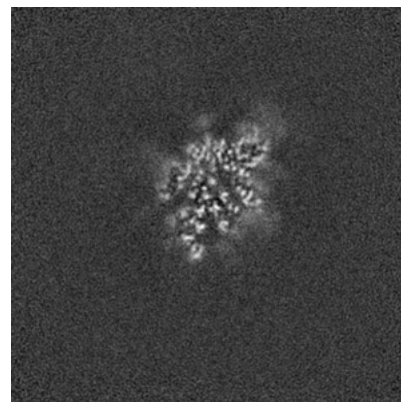
6.2.2 Raw map



X Index: 144



Y Index: 144

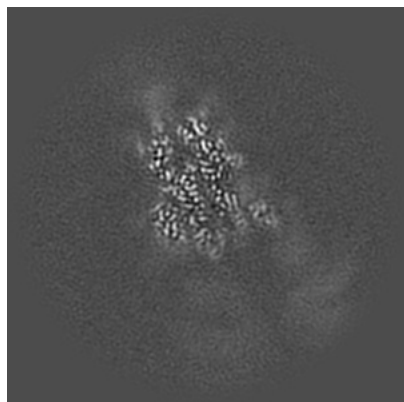


Z Index: 144

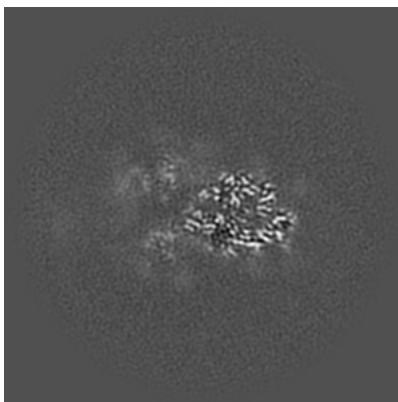
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

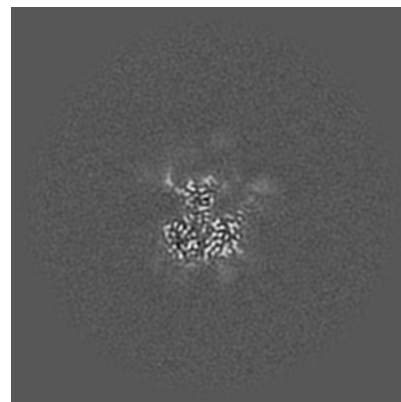
6.3.1 Primary map



X Index: 133

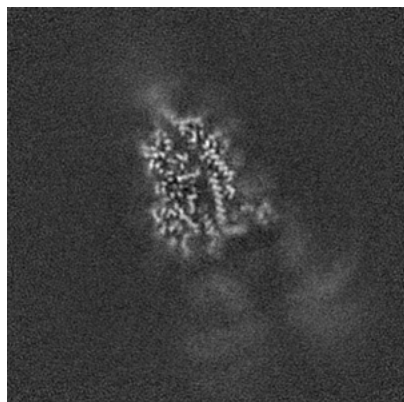


Y Index: 132

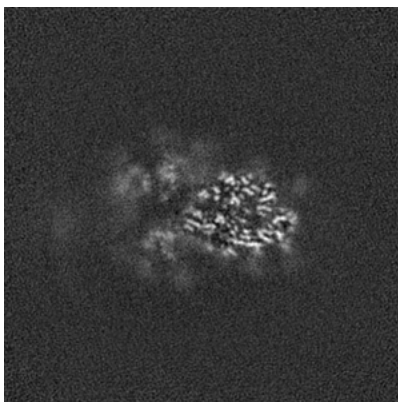


Z Index: 168

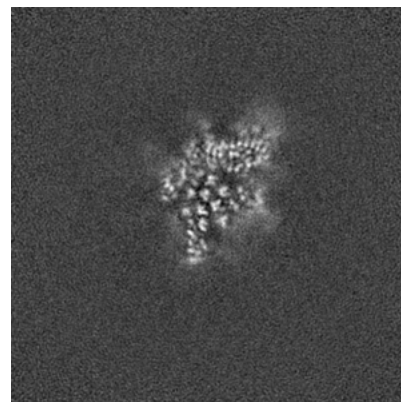
6.3.2 Raw map



X Index: 129



Y Index: 132

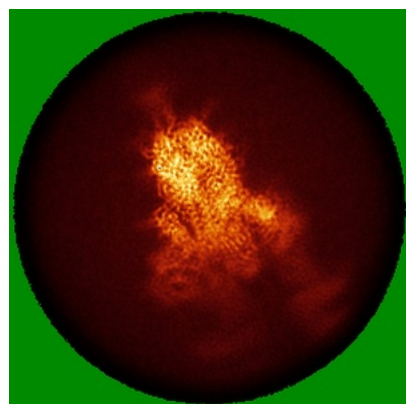


Z Index: 141

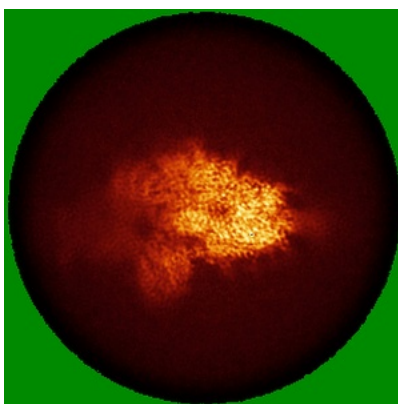
The images above show the largest variance slices of the map in three orthogonal directions.

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

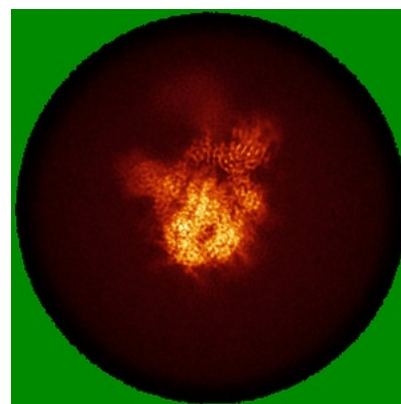
6.4.1 Primary map



X

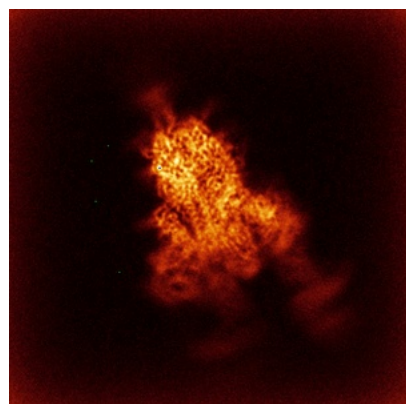


Y



Z

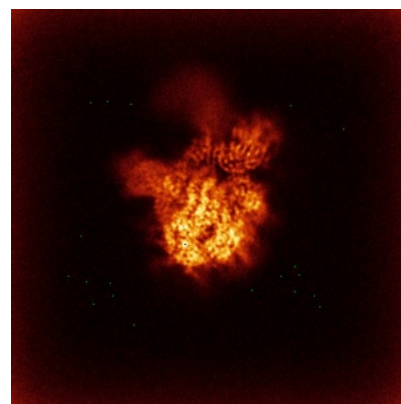
6.4.2 Raw map



X



Y

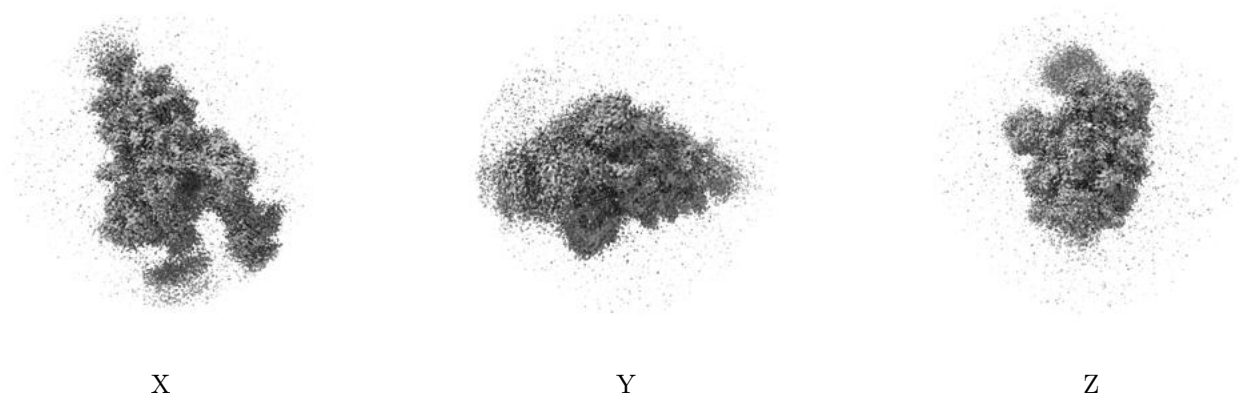


Z

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.

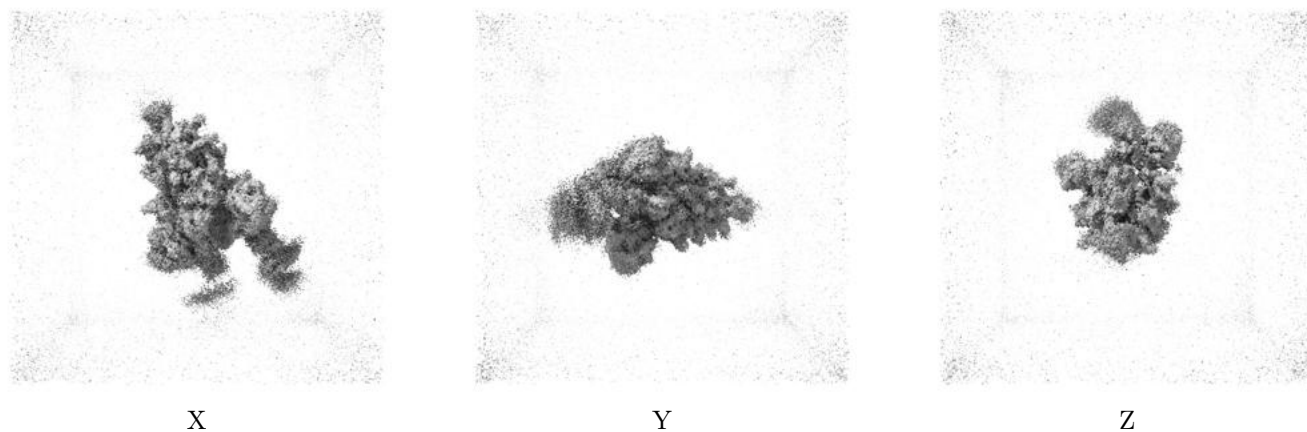
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

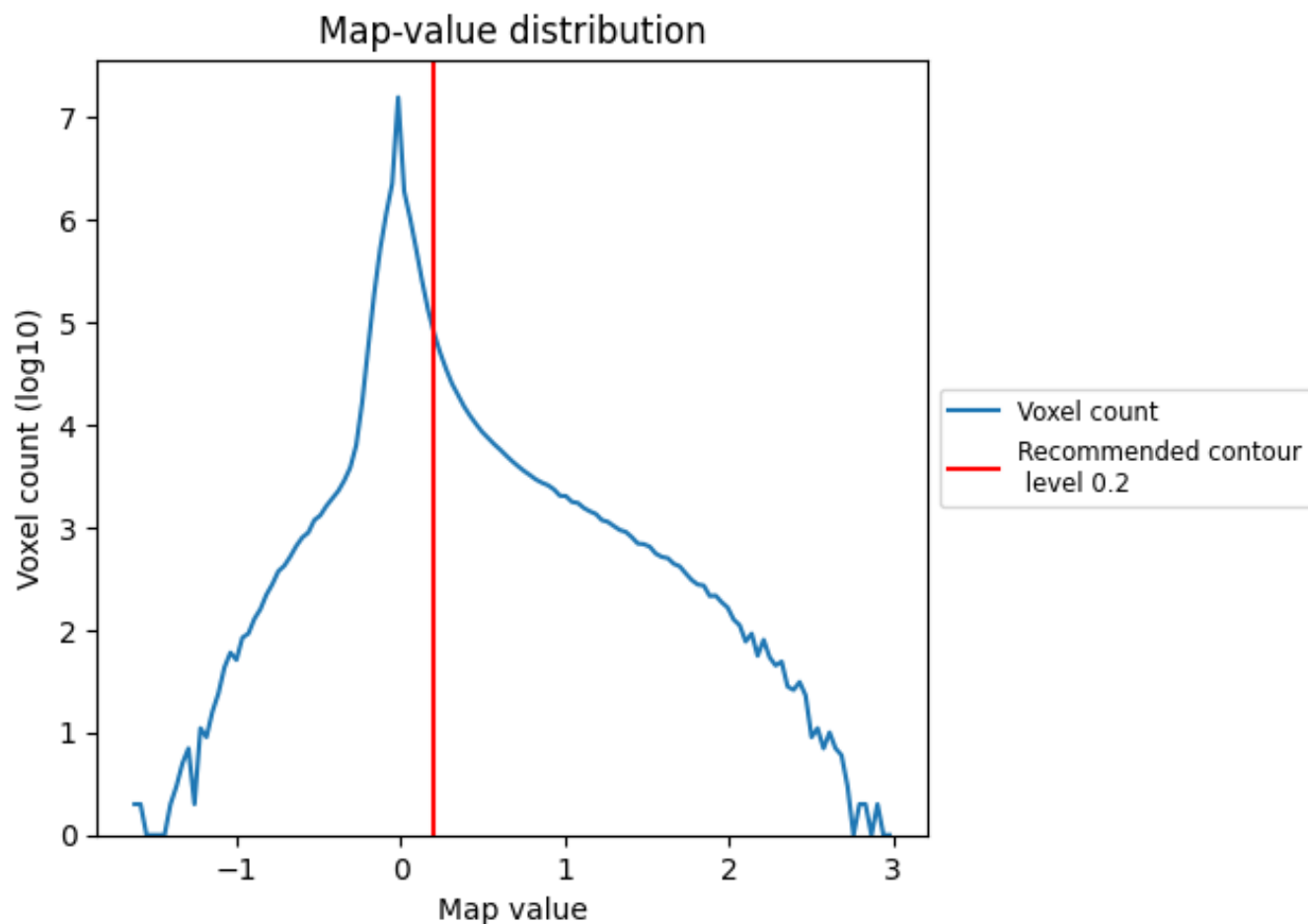
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

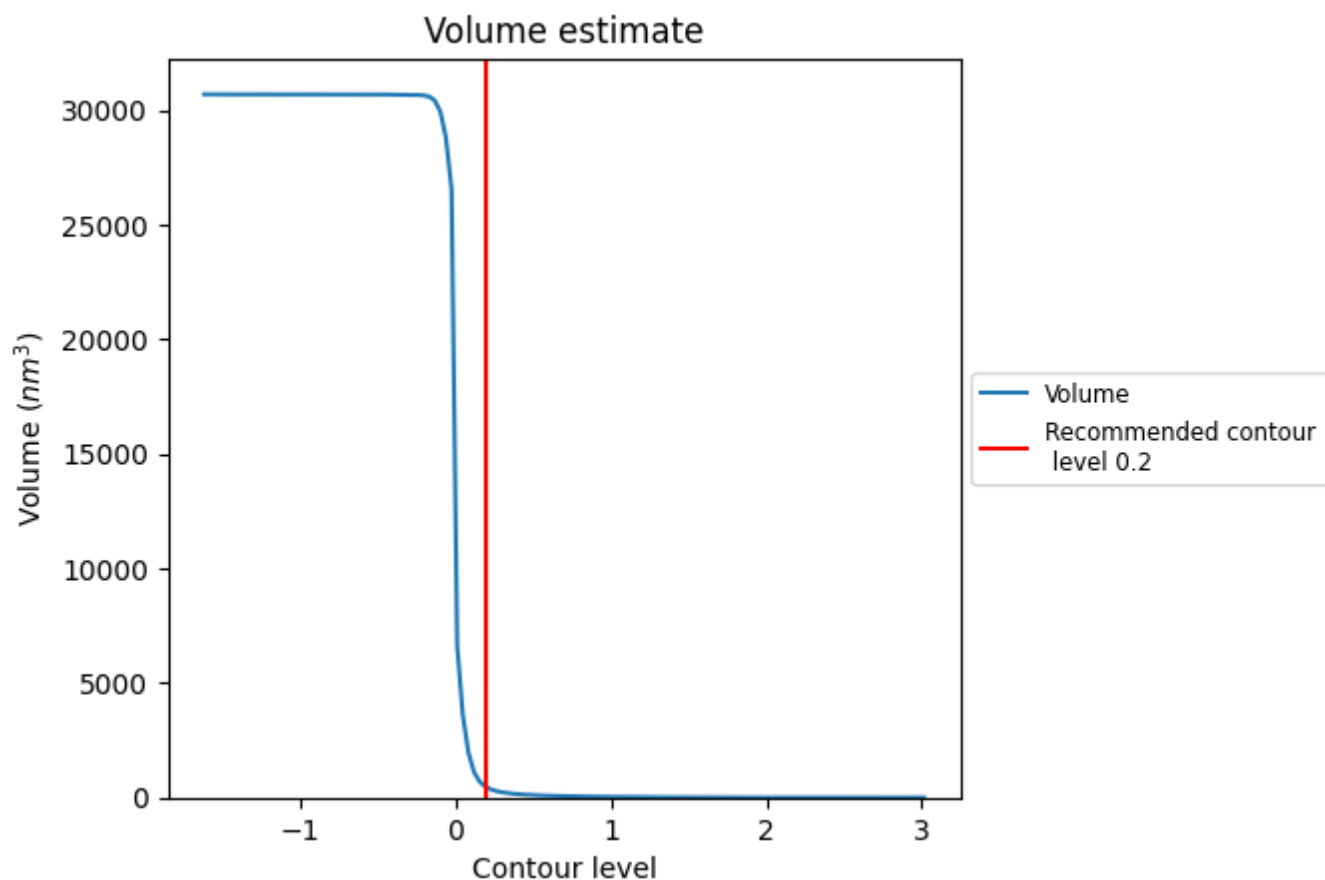
This section contains the results of statistical analysis of the map.

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.

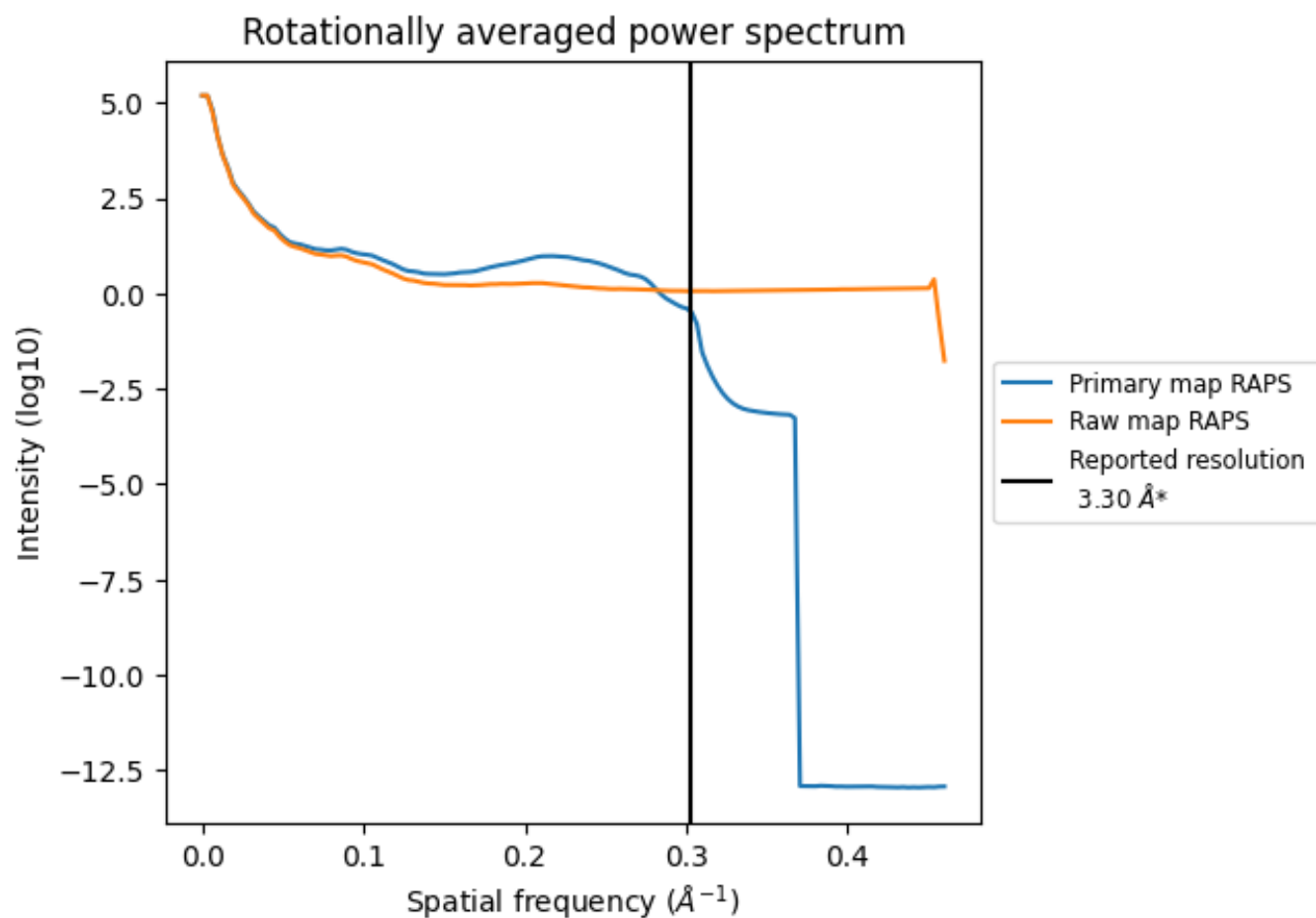
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 452 nm³; this corresponds to an approximate mass of 408 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 ⓘ

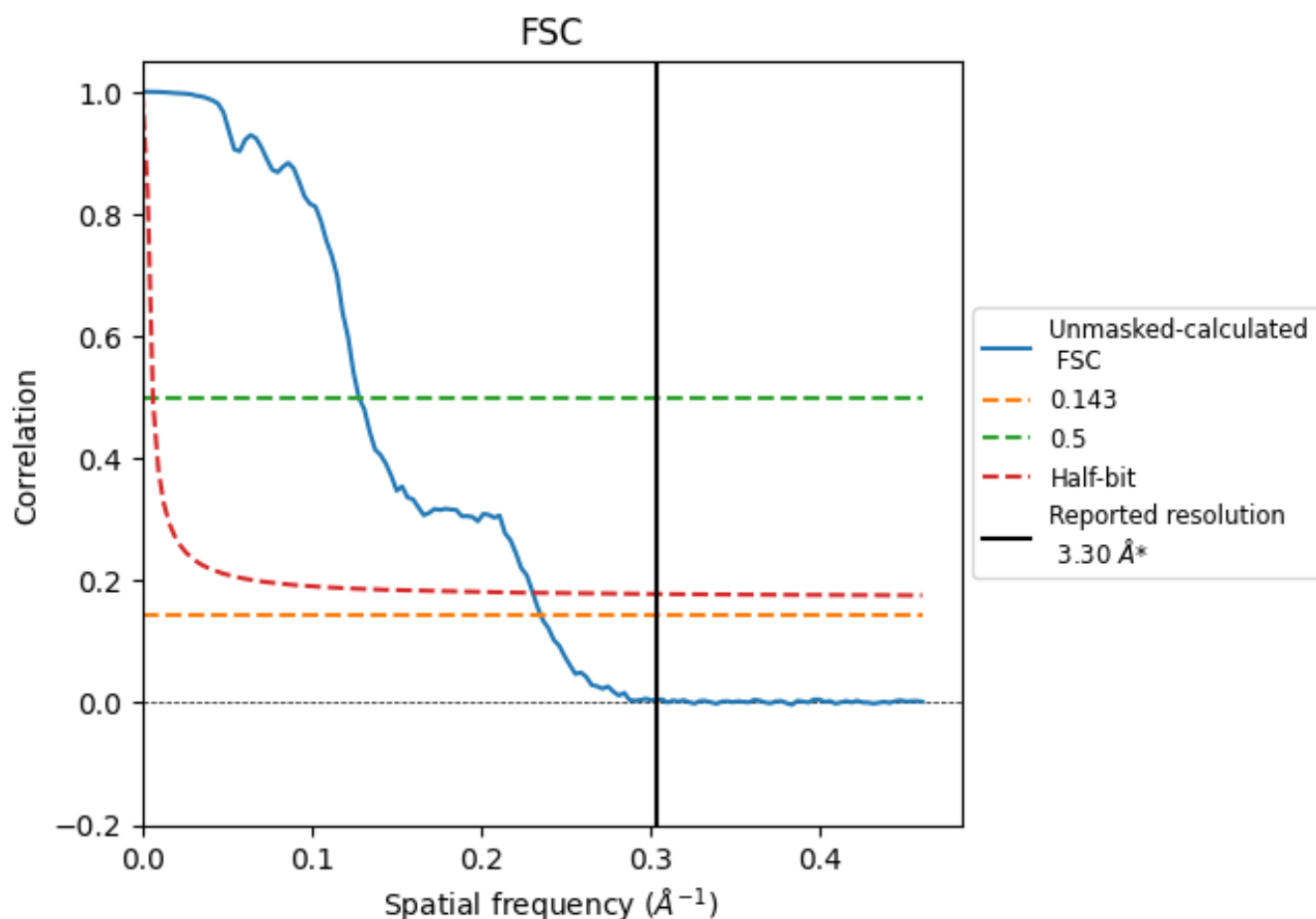


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

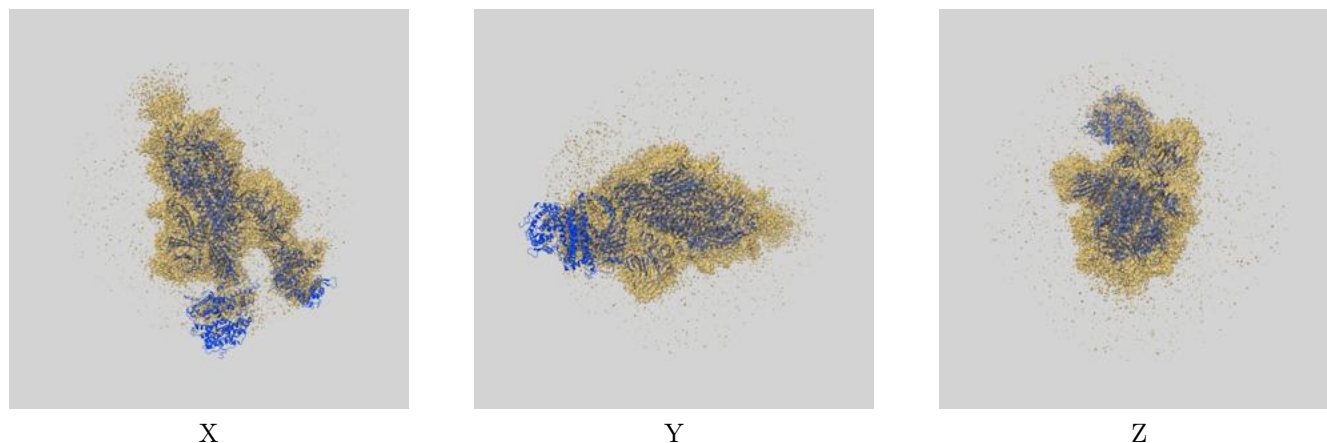
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.25	7.83	4.34

*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 4.25 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

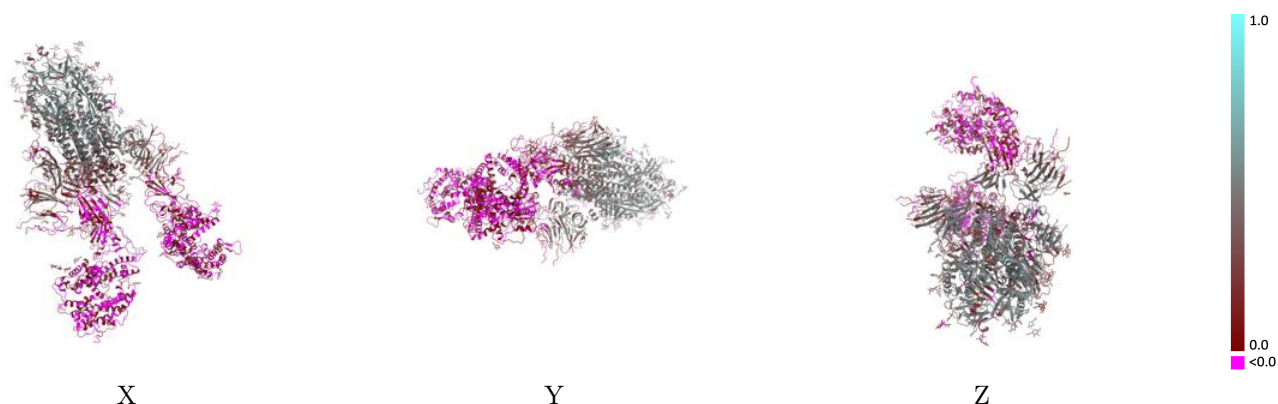
This section contains information regarding the fit between EMDB map EMD-33203 and PDB model 7XID. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



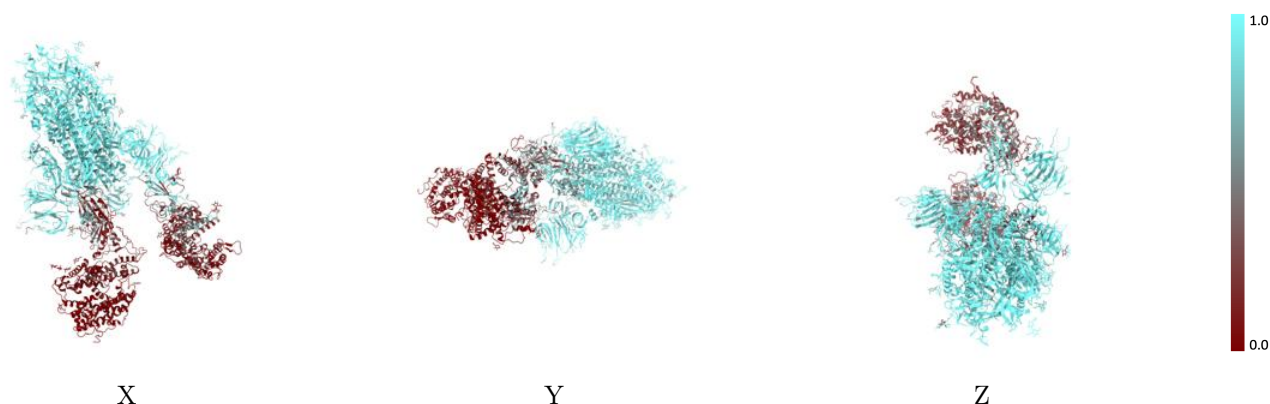
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



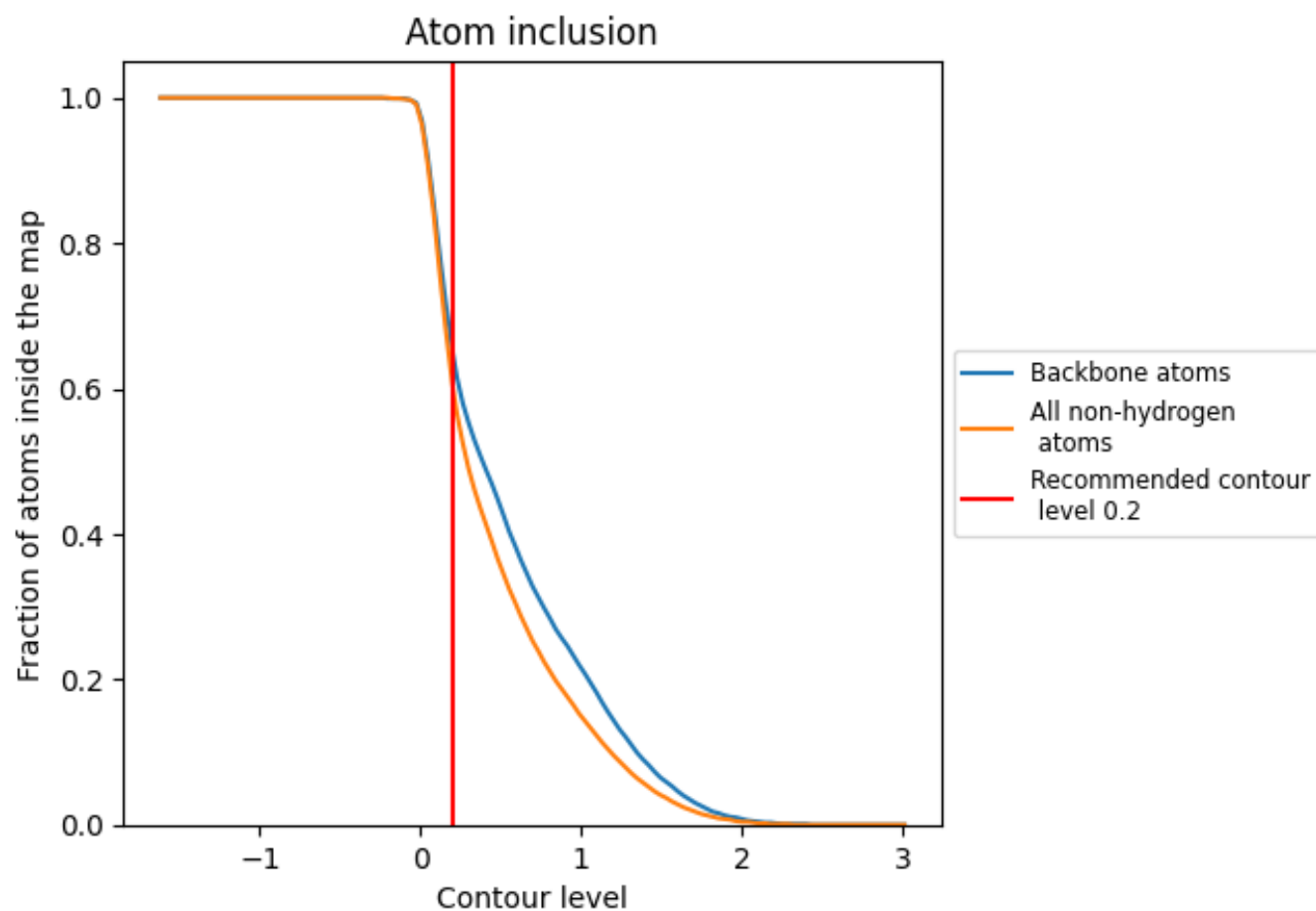
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 60% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6050	 0.2340
A	 0.8250	 0.3430
B	 0.7820	 0.2950
C	 0.8350	 0.3350
D	 0.1560	 0.0170
E	 0.0400	 0.0150
F	 0.5000	 0.0540
G	 0.9640	 0.4330
H	 0.9290	 0.3310
I	 0.8570	 0.3310
J	 1.0000	 0.4650
K	 0.9640	 0.4130
L	 0.8570	 0.2420
M	 0.3930	 0.1630
N	 0.4290	 0.0570
O	 0.9290	 0.3700
P	 0.9290	 0.3030
Q	 0.9640	 0.3670
R	 0.8570	 0.3030
S	 0.8930	 0.3210
T	 0.3210	 -0.0170
U	 0.5360	 0.1110
V	 1.0000	 0.4560
W	 0.8210	 0.3020
X	 0.9290	 0.3490
Y	 0.8930	 0.3180
Z	 0.8930	 0.2670
a	 0.1070	 -0.0600
b	 0.0710	 0.0160

