



## Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 06:25 PM JST

PDB ID : 7WRH  
EMDB ID : EMD-32726  
Title : Cryo-EM structure of SARS-CoV-2 Omicron BA.1 spike protein in complex with mouse ACE2  
Authors : Han, P.; Xie, Y.; Qi, J.  
Deposited on : 2022-01-26  
Resolution : 2.66 Å(reported)  
Based on initial model : 7XD7

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

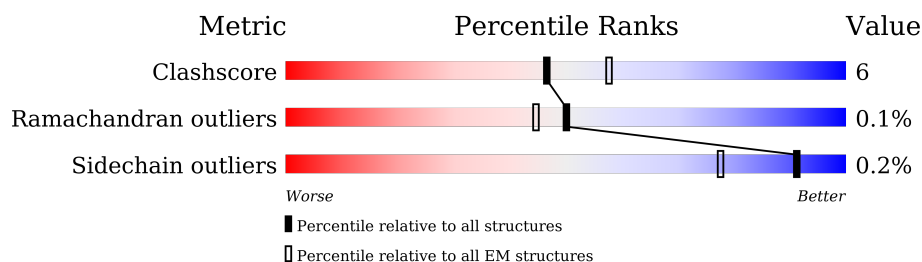
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.66 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1243	<div> <div>14%</div> <div>73%</div> <div>12%</div> <div>15%</div> </div>
1	B	1243	<div> <div>12%</div> <div>73%</div> <div>12%</div> <div>15%</div> </div>
1	C	1243	<div> <div>8%</div> <div>74%</div> <div>12%</div> <div>15%</div> </div>
2	D	598	<div> <div>99%</div> <div>77%</div> <div>22%</div> <div>..</div> </div>
3	E	2	<div> <div>100%</div> <div>50%</div> <div>50%</div> </div>
3	F	2	<div> <div>50%</div> <div>50%</div> </div>
3	G	2	<div> <div>50%</div> <div>100%</div> </div>
3	H	2	<div> <div>100%</div> </div>

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

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30771 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	1061	Total	C	N	O	S	0	0
			8327	5334	1387	1568	38		
1	B	1061	Total	C	N	O	S	0	0
			8327	5334	1387	1568	38		
1	C	1061	Total	C	N	O	S	0	0
			8327	5334	1387	1568	38		

There are 300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP P0DTC2
A	-3	PRO	-	expression tag	UNP P0DTC2
A	-2	ARG	-	expression tag	UNP P0DTC2
A	-1	GLY	-	expression tag	UNP P0DTC2
A	0	PRO	-	expression tag	UNP P0DTC2
A	1	VAL	-	expression tag	UNP P0DTC2
A	2	ALA	-	expression tag	UNP P0DTC2
A	3	ALA	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	LEU	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	ILE	-	expression tag	UNP P0DTC2
A	9	LEU	-	expression tag	UNP P0DTC2
A	10	HIS	-	expression tag	UNP P0DTC2
A	11	GLY	-	expression tag	UNP P0DTC2
A	12	ALA	-	expression tag	UNP P0DTC2
A	13	TRP	-	expression tag	UNP P0DTC2
A	14	SER	-	expression tag	UNP P0DTC2
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	142	ASP	TYR	variant	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	210A	ILE	LEU	variant	UNP P0DTC2
A	210D	GLU	-	insertion	UNP P0DTC2
A	210E	PRO	-	insertion	UNP P0DTC2
A	210F	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
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	engineered mutation	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	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	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	LEU	-	expression tag	UNP P0DTC2
A	1210	VAL	-	expression tag	UNP P0DTC2
A	1211	PRO	-	expression tag	UNP P0DTC2
A	1212	ARG	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	TYR	-	expression tag	UNP P0DTC2
A	1217	ILE	-	expression tag	UNP P0DTC2
A	1218	PRO	-	expression tag	UNP P0DTC2
A	1219	GLU	-	expression tag	UNP P0DTC2
A	1220	ALA	-	expression tag	UNP P0DTC2
A	1221	PRO	-	expression tag	UNP P0DTC2
A	1222	ARG	-	expression tag	UNP P0DTC2
A	1223	ASP	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLN	-	expression tag	UNP P0DTC2
A	1226	ALA	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	VAL	-	expression tag	UNP P0DTC2
A	1229	ARG	-	expression tag	UNP P0DTC2
A	1230	LYS	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLU	-	expression tag	UNP P0DTC2
A	1234	TRP	-	expression tag	UNP P0DTC2
A	1235	VAL	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	THR	-	expression tag	UNP P0DTC2
A	1240	PHE	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
B	-4	MET	-	initiating methionine	UNP P0DTC2
B	-3	PRO	-	expression tag	UNP P0DTC2
B	-2	ARG	-	expression tag	UNP P0DTC2
B	-1	GLY	-	expression tag	UNP P0DTC2
B	0	PRO	-	expression tag	UNP P0DTC2
B	1	VAL	-	expression tag	UNP P0DTC2
B	2	ALA	-	expression tag	UNP P0DTC2
B	3	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	LEU	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	ILE	-	expression tag	UNP P0DTC2
B	9	LEU	-	expression tag	UNP P0DTC2
B	10	HIS	-	expression tag	UNP P0DTC2
B	11	GLY	-	expression tag	UNP P0DTC2
B	12	ALA	-	expression tag	UNP P0DTC2
B	13	TRP	-	expression tag	UNP P0DTC2
B	14	SER	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	142	ASP	TYR	variant	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	210A	ILE	LEU	variant	UNP P0DTC2
B	210D	GLU	-	insertion	UNP P0DTC2
B	210E	PRO	-	insertion	UNP P0DTC2
B	210F	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	engineered mutation	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	LEU	-	expression tag	UNP P0DTC2
B	1210	VAL	-	expression tag	UNP P0DTC2
B	1211	PRO	-	expression tag	UNP P0DTC2
B	1212	ARG	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	TYR	-	expression tag	UNP P0DTC2
B	1217	ILE	-	expression tag	UNP P0DTC2
B	1218	PRO	-	expression tag	UNP P0DTC2
B	1219	GLU	-	expression tag	UNP P0DTC2
B	1220	ALA	-	expression tag	UNP P0DTC2
B	1221	PRO	-	expression tag	UNP P0DTC2
B	1222	ARG	-	expression tag	UNP P0DTC2
B	1223	ASP	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLN	-	expression tag	UNP P0DTC2
B	1226	ALA	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	VAL	-	expression tag	UNP P0DTC2
B	1229	ARG	-	expression tag	UNP P0DTC2
B	1230	LYS	-	expression tag	UNP P0DTC2
B	1231	ASP	-	expression tag	UNP P0DTC2
B	1232	GLY	-	expression tag	UNP P0DTC2
B	1233	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1234	TRP	-	expression tag	UNP P0DTC2
B	1235	VAL	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	THR	-	expression tag	UNP P0DTC2
B	1240	PHE	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
C	-4	MET	-	initiating methionine	UNP P0DTC2
C	-3	PRO	-	expression tag	UNP P0DTC2
C	-2	ARG	-	expression tag	UNP P0DTC2
C	-1	GLY	-	expression tag	UNP P0DTC2
C	0	PRO	-	expression tag	UNP P0DTC2
C	1	VAL	-	expression tag	UNP P0DTC2
C	2	ALA	-	expression tag	UNP P0DTC2
C	3	ALA	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	LEU	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	ILE	-	expression tag	UNP P0DTC2
C	9	LEU	-	expression tag	UNP P0DTC2
C	10	HIS	-	expression tag	UNP P0DTC2
C	11	GLY	-	expression tag	UNP P0DTC2
C	12	ALA	-	expression tag	UNP P0DTC2
C	13	TRP	-	expression tag	UNP P0DTC2
C	14	SER	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	142	ASP	TYR	variant	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	210A	ILE	LEU	variant	UNP P0DTC2
C	210D	GLU	-	insertion	UNP P0DTC2
C	210E	PRO	-	insertion	UNP P0DTC2
C	210F	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	engineered mutation	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	LEU	-	expression tag	UNP P0DTC2
C	1210	VAL	-	expression tag	UNP P0DTC2
C	1211	PRO	-	expression tag	UNP P0DTC2
C	1212	ARG	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	TYR	-	expression tag	UNP P0DTC2
C	1217	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1218	PRO	-	expression tag	UNP P0DTC2
C	1219	GLU	-	expression tag	UNP P0DTC2
C	1220	ALA	-	expression tag	UNP P0DTC2
C	1221	PRO	-	expression tag	UNP P0DTC2
C	1222	ARG	-	expression tag	UNP P0DTC2
C	1223	ASP	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLN	-	expression tag	UNP P0DTC2
C	1226	ALA	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	VAL	-	expression tag	UNP P0DTC2
C	1229	ARG	-	expression tag	UNP P0DTC2
C	1230	LYS	-	expression tag	UNP P0DTC2
C	1231	ASP	-	expression tag	UNP P0DTC2
C	1232	GLY	-	expression tag	UNP P0DTC2
C	1233	GLU	-	expression tag	UNP P0DTC2
C	1234	TRP	-	expression tag	UNP P0DTC2
C	1235	VAL	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	THR	-	expression tag	UNP P0DTC2
C	1240	PHE	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	595	Total	C	N	O	S	0	0
			4851	3091	815	916	29		

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



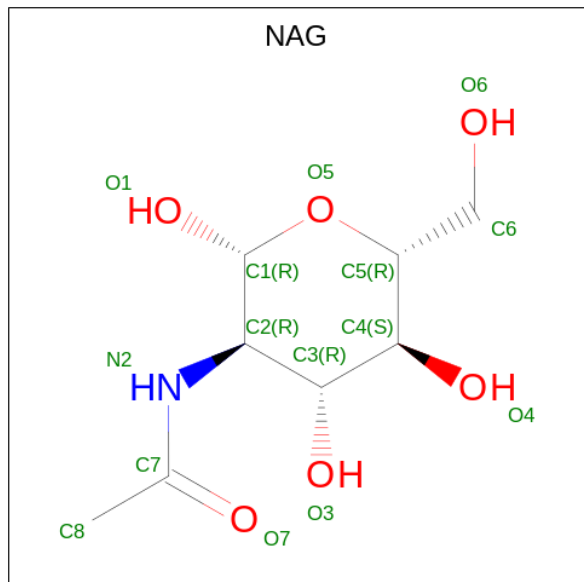
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		

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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		
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		

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



Mol	Chain	Residues	Atoms				AltConf
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	

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


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

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Zn	0
			1	1	




ASP	ILE	GLY	ILE	ASN	ALA	SER	VAL	VAL	ASN	ASN	ILE	GLN	LYS	GLU	ILE	ASP	ARG	LEU	ASN	ASN	GLU	ASN	GLY	GLY	LYS	TYR	GLN	GLY	VAL	PRO	ARG	GLY	SER	GLY	TYR	ILE	PRO	GLU	ALA	ALA	GLY	ALA	TYR			
VAL	ARG	LYS	ASP	GLY	GLU	TRP	VAL	LEU	LEU	LEU	SER	THR	PHE	LEU																																

• Molecule 1: Spike glycoprotein

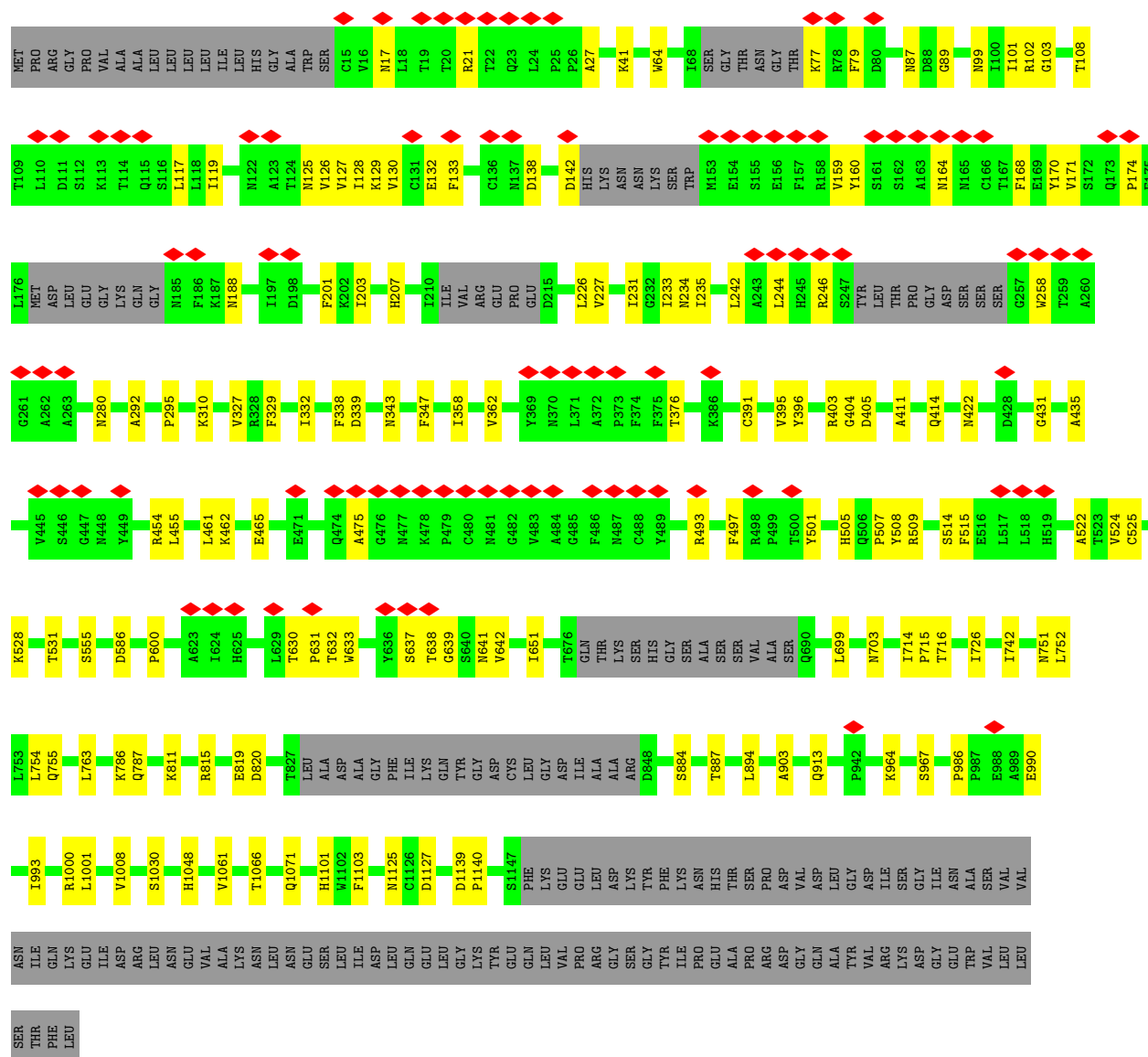
Chain B: 

ASN	LEU	LEU	ASN	GLU	SER	LEU	ILE	ASP	LEU	GLY	LEU	GLY	LYS	TYR	GLN	LEU	VAL	PRO	ARG	GLY	ASP	GLY	ILE	PRO	ASN	HIS	ALA	THR	SER	PRO	ARG	ASP	VAL	GLN	ALA	LEU	VAL	TYR	VAL	LEU	LEU	SER	THR	PHE	LEU												
K1038	D1041	H1048	H1064	V1065	T1066	W1102	N1135	S1147	PHE	LYS	GLU	GLU	VAL	PRO	ASN	HIS	ALA	THR	SER	PRO	ARG	ASP	VAL	GLY	ASN	GLY	ILE	TYR	PHE	LYS	ASN	GLY	ILE	ASN	VAL	ASP	GLY	ILE	ASN	VAL	LEU	LEU	SER	THR	PHE	LEU											
ILE	LYS	GLN	TYR	GLY	ASP	ILE	ALA	ALA	ARG	D848	G885	L894	Q901	M902	A903	Y904	R905	Q913	L916	Q935	L938	P942	L959	G971	V976	L977	N978	D979	R983	L984	D985	P986	P987	E988	A989	E990	D994	R995	R1000	V1008																	
S637	T638	G639	S640	H641	V642	I651	G652	Q675	T676	GLN	THR	LYS	HIS	SER	GLY	ALA	SER	SER	VAL	ALA	SER	Q690	I693	A713	V722	I742	C743	T747	E748	C749	Y756	L763	K786	Q787	Y796	Q804	L821	T827	ASN	ALA	ASP	ALA	GLY	PHE													
R493	S494	Y495	S496	R498	P499	T500	Y501	G502	V503	G504	H505	V512	F515	E516	L517	L518	H519	A520	P521	A522	T523	V524	C525	K537	V551	F562	A570	D571	D578	T581	Y612	V620	P621	V622	A623	I624	H625	A626	D627	Q628	L629	T630	P631	T632	V633	R634	V635	Y636									
G431	C432	I433	I434	A435	N437	S438	N439	K440	L441	D442	S443	K444	V445	S446	G447	N448	Y449	N450	Y451	L452	F456	R457	K458	S459	N460	L461	K462	P463	F464	E465	R466	D467	I468	S469	T470	E471	I472	Y473	Q474	A475	G476	N477	K478	P479	C480	N481	G482	V483	A484	G485	F486	N487	C488	Y489	F490	P491	L492
Y351	A352	W353	N354	R355	K356	K357	I358	S366	V367	L368	T369	N370	L371	A372	P373	F374	F375	T376	F377	K378	K386	C391	N394	V395	D398	I402	R403	G404	D405	E406	V407	Q409	I410	A411	P412	G413	Q414	T415	G416	N417	I418	A419	D420	Y421	N422	Y423	P426	D427	D428	F429	T430						
L226	V227	T231	I233	R237	F238	Q239	L244	H245	R246	S247	TYR	THR	PRO	GLY	ASP	SER	SER	SER	G257	W258	T259	A260	G261	A262	R273	G283	D290	C291	A292	L293	D294	P295	F318	R319	V320	Q321	T333	N334	L335	C336	D339	E340	A419	D420	R346	S349	V350										
I128	K129	V130	C131	E132	N137	D138	F139	L141	D142	HIS	LYS	ASN	ASN	LYS	SER	TRP	M153	E154	S155	E156	F157	R158	M164	F168	E169	Y170	S172	Q173	L176	MET	ASP	LEU	GLY	LYS	GLN	GLY	N185	F186	K187	N188	K206	T210	ILE	VAL	ARG	GLU	PRO	GLU	D215								
MET	PRO	ARG	GLY	PRO	VAL	ALA	ALA	LEU	LEU	LEU	ILE	LEU	HIS	ASN	GLY	ALA	TRP	SER	C15	V16	N17	L18	T19	T20	R21	T22	Q23	L24	P25	T29	R44	V62	I68	SER	GLY	THR	ASN	ASN	GLY	THR	K77	R78	F79	D80	N81	E96	N99	T108	T114	N121							

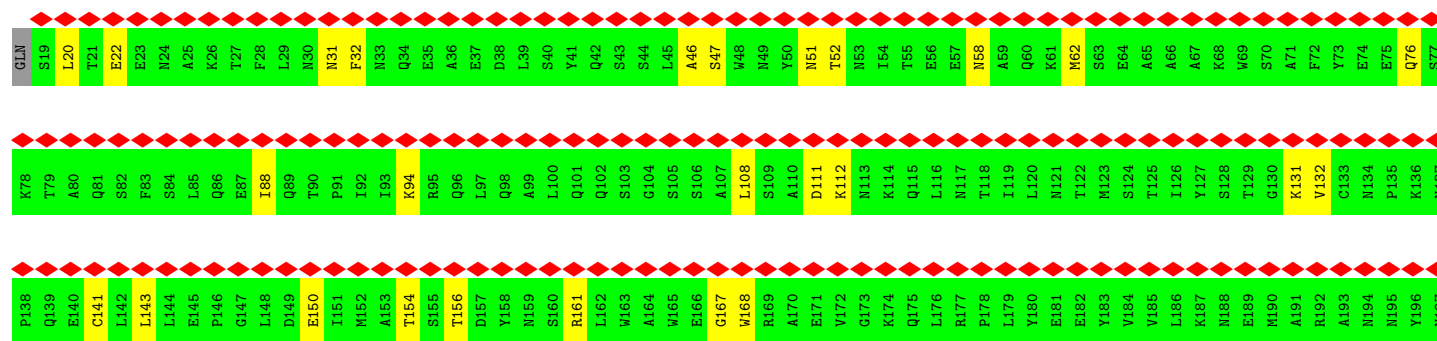
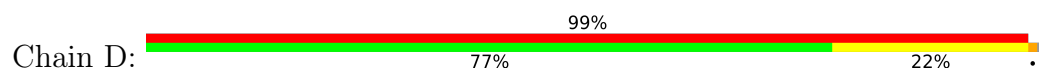
• Molecule 1: Spike glycoprotein

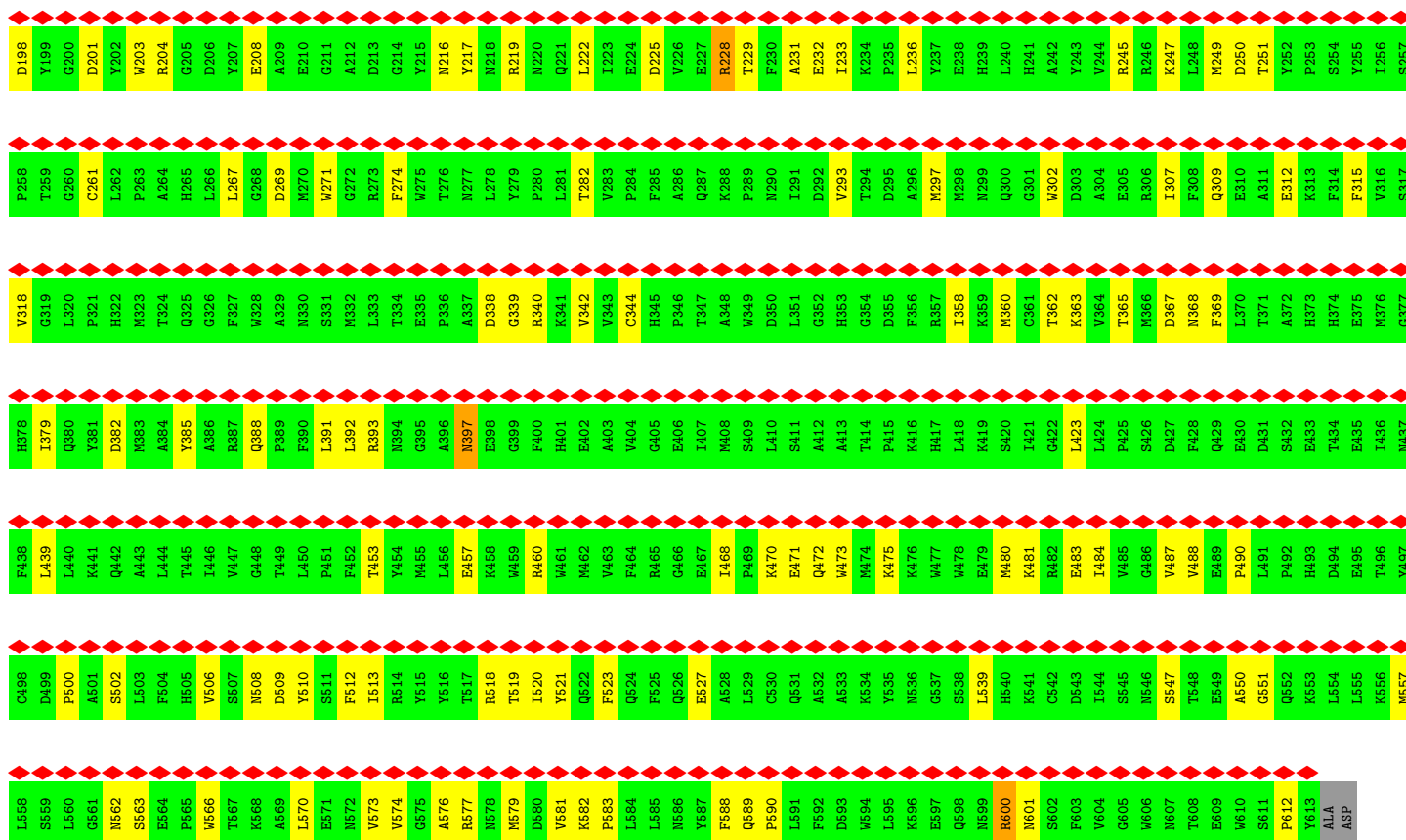
Chain C: 





● Molecule 2: Processed angiotensin-converting enzyme 2





- 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 H:  100%



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

Chain I:  50% 50%



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

Chain J:  100%



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

Chain K:  100%



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

Chain L:  50% 50%



- 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



- 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



- 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



- 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 Z:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	503967	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.444	Depositor
Minimum map value	-3.692	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.489	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.28	0/8526	0.51	1/11605 (0.0%)
1	B	0.28	0/8526	0.50	0/11605
1	C	0.30	0/8526	0.52	1/11605 (0.0%)
2	D	0.25	0/4986	0.45	0/6769
All	All	0.28	0/30564	0.50	2/41584 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	CYS	CA-CB-SG	7.55	127.59	114.00
1	C	964	LYS	O-C-N	-5.17	114.44	122.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8327	0	8149	99	0
1	B	8327	0	8145	90	0
1	C	8327	0	8145	92	0
2	D	4851	0	4631	84	0
3	E	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	28	0	25	1	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	1	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	1	0
3	M	28	0	25	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	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	3	0
3	U	28	0	25	1	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	2	0
3	Z	28	0	25	0	0
4	A	84	0	78	1	0
4	B	126	0	117	0	0
4	C	112	0	104	1	0
5	D	1	0	0	0	0
All	All	30771	0	29919	359	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 6.

All (359) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:CYS:HA	1:A:432:CYS:HB3	1.51	0.92
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.53	0.88
1:A:96:GLU:O	1:A:188:ASN:HB2	1.74	0.87
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.56	0.86
1:A:327:VAL:HG12	1:A:531:THR:HG23	1.62	0.79
1:A:379:CYS:HA	1:A:432:CYS:CB	2.14	0.77
1:C:226:LEU:HG	1:C:227:VAL:HG23	1.67	0.77
1:C:786:LYS:HG3	1:C:787:GLN:HG2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:HB3	1:A:190:ARG:HH12	1.49	0.76
1:C:126:VAL:HG23	1:C:174:PRO:HA	1.67	0.75
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.70	0.73
1:A:226:LEU:HG	1:A:227:VAL:HG23	1.70	0.73
1:A:902:MET:HB3	1:A:916:LEU:HD11	1.70	0.73
1:B:786:LYS:HG3	1:B:787:GLN:HG2	1.72	0.71
1:C:188:ASN:OD1	1:C:207:HIS:NE2	2.23	0.70
2:D:457:GLU:HG2	2:D:513:ILE:HD13	1.73	0.70
1:A:318:PHE:O	1:A:592:PHE:HA	1.92	0.70
2:D:228:ARG:NH1	2:D:229:THR:OG1	2.25	0.70
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.73	0.69
1:B:901:GLN:HE21	1:B:905:ARG:HH21	1.39	0.69
2:D:392:LEU:HD13	2:D:563:SER:HB3	1.76	0.68
2:D:573:VAL:HG13	2:D:574:VAL:HG13	1.76	0.68
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.76	0.68
1:C:1125:ASN:ND2	1:C:1127:ASP:OD2	2.28	0.67
2:D:20:LEU:HD12	2:D:22:GLU:H	1.59	0.67
1:B:640:SER:HB3	1:B:652:GLY:HA2	1.77	0.67
1:A:622:VAL:O	1:A:634:ARG:NH1	2.28	0.67
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.29	0.66
2:D:32:PHE:HE2	2:D:391:LEU:HD11	1.62	0.65
1:C:752:LEU:HD13	1:C:993:ILE:HD11	1.79	0.65
1:C:903:ALA:HB1	1:C:913:GLN:HG2	1.79	0.65
1:B:804:GLN:HE21	1:B:935:GLN:HE21	1.46	0.64
1:C:716:THR:HB	1:C:1071:GLN:O	1.98	0.64
1:B:226:LEU:HG	1:B:227:VAL:HG23	1.79	0.64
2:D:557:MET:HG3	2:D:573:VAL:HB	1.79	0.64
1:C:637:SER:O	1:C:639:GLY:N	2.31	0.64
1:A:433:VAL:HG12	1:A:512:VAL:HG22	1.80	0.64
1:A:490:PHE:O	1:A:493:ARG:NH1	2.31	0.63
1:A:203:ILE:HB	1:A:227:VAL:HB	1.79	0.63
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.81	0.63
1:B:139:PRO:HA	1:B:158:ARG:O	1.99	0.62
1:B:490:PHE:O	1:B:493:ARG:NH1	2.33	0.62
2:D:271:TRP:HZ2	2:D:502:SER:HB3	1.64	0.62
1:A:371:LEU:HG	1:A:372:ALA:H	1.65	0.61
2:D:168:TRP:NE1	2:D:502:SER:OG	2.32	0.61
1:A:318:PHE:CE1	1:A:621:PRO:HG3	2.35	0.61
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.34	0.61
1:A:328:ARG:HH21	1:A:580:GLN:HB2	1.64	0.61
1:B:81:ASN:HB3	1:B:239:GLN:HE21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:ARG:HH22	2:D:579:MET:HB2	1.66	0.60
1:A:131:CYS:HB3	1:A:166:CYS:HA	1.82	0.60
1:C:751:ASN:HA	1:C:754:LEU:HD13	1.84	0.60
1:C:130:VAL:HG21	1:C:231:ILE:HG23	1.83	0.60
2:D:216:ASN:O	2:D:577:ARG:NH2	2.34	0.59
1:B:885:GLY:HA2	1:B:901:GLN:NE2	2.17	0.59
1:C:99:ASN:O	1:C:102:ARG:NH2	2.34	0.59
1:C:884:SER:OG	1:C:887:THR:OG1	2.21	0.59
1:B:971:GLY:HA3	1:B:995:ARG:HH21	1.68	0.59
2:D:297:MET:HB3	2:D:302:TRP:HB2	1.84	0.59
2:D:481:LYS:HG2	2:D:487:VAL:HB	1.83	0.59
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.67	0.59
1:C:103:GLY:HA3	1:C:119:ILE:O	2.02	0.58
2:D:397:ASN:C	2:D:397:ASN:HD22	2.06	0.58
1:B:295:PRO:HG3	1:B:633:TRP:CE3	2.39	0.58
2:D:88:ILE:HB	2:D:94:LYS:HE3	1.85	0.58
1:C:497:PHE:CD1	1:C:507:PRO:HD3	2.39	0.58
1:C:391:CYS:HA	1:C:525:CYS:CB	2.31	0.58
1:A:96:GLU:OE2	1:A:100:ILE:N	2.37	0.58
1:B:351:TYR:HE1	1:B:452:LEU:HB2	1.69	0.58
1:A:31:SER:O	1:A:59:PHE:HA	2.04	0.57
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.86	0.57
1:A:176:LEU:HD21	1:A:190:ARG:HE	1.68	0.57
1:A:378:LYS:O	1:A:432:CYS:HB2	2.05	0.57
2:D:338:ASP:OD1	2:D:339:GLY:N	2.37	0.57
1:A:319:ARG:HG3	1:A:629:LEU:HD12	1.87	0.57
1:B:675:GLN:HG3	1:B:693:ILE:HD11	1.87	0.56
1:C:108:THR:OG1	1:C:234:ASN:O	2.23	0.56
1:C:358:ILE:HB	1:C:395:VAL:HB	1.87	0.56
2:D:582:LYS:N	2:D:583:PRO:HD3	2.21	0.56
1:C:501:TYR:HB3	1:C:505:HIS:HB2	1.85	0.56
1:B:903:ALA:HB1	1:B:913:GLN:HG2	1.88	0.56
2:D:271:TRP:HH2	2:D:500:PRO:HA	1.71	0.56
1:B:29:THR:HG23	1:B:62:VAL:HG23	1.86	0.55
3:E:1:NAG:H3	3:E:1:NAG:H83	1.88	0.55
1:B:21:ARG:HE	1:B:79:PHE:HD2	1.55	0.55
2:D:229:THR:O	2:D:232:GLU:HG3	2.06	0.55
2:D:547:SER:HB3	2:D:550:ALA:HB3	1.88	0.55
2:D:52:THR:HB	2:D:340:ARG:HH22	1.70	0.55
2:D:518:ARG:NH2	2:D:519:THR:OG1	2.40	0.54
1:A:105:ILE:HD12	1:A:110:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:HG23	1:B:395:VAL:HB	1.88	0.54
1:C:332:ILE:HG22	1:C:362:VAL:HG23	1.89	0.54
2:D:250:ASP:OD1	2:D:251:THR:N	2.41	0.54
1:A:231:ILE:HD12	1:A:233:ILE:HD12	1.89	0.54
2:D:228:ARG:O	2:D:231:ALA:HB3	2.07	0.54
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.30	0.54
1:A:122:ASN:HB2	1:A:125:ASN:H	1.73	0.53
1:A:142:ASP:HB2	1:A:156:GLU:HB2	1.89	0.53
1:A:351:TYR:HE1	1:A:452:LEU:HB2	1.72	0.53
1:A:493:ARG:NH2	2:D:31:ASN:OD1	2.41	0.53
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.27	0.53
2:D:490:PRO:HA	2:D:612:PRO:HG2	1.90	0.53
2:D:460:ARG:NH2	2:D:506:VAL:HG22	2.24	0.53
1:B:231:ILE:HD12	1:B:233:ILE:HG12	1.89	0.53
1:B:355:ARG:NE	1:B:398:ASP:OD1	2.41	0.53
1:B:984:LEU:HD13	1:B:988:GLU:HB3	1.90	0.53
1:A:393:THR:HG21	1:A:518:LEU:HB2	1.90	0.53
1:C:455:LEU:HD22	1:C:493:ARG:HE	1.73	0.53
1:C:339:ASP:OD1	1:C:343:ASN:ND2	2.42	0.53
1:C:396:TYR:HB2	1:C:514:SER:HB3	1.91	0.53
2:D:161:ARG:NH2	2:D:267:LEU:O	2.41	0.53
2:D:508:ASN:OD1	2:D:509:ASP:N	2.38	0.53
1:B:376:THR:HB	1:B:435:ALA:HB3	1.91	0.52
1:C:203:ILE:HB	1:C:227:VAL:HB	1.89	0.52
1:A:986:PRO:HG2	1:A:987:PRO:HD3	1.91	0.52
1:B:130:VAL:HG12	1:B:168:PHE:HB3	1.91	0.52
1:A:945:LEU:HD12	1:A:948:LEU:HD12	1.92	0.52
1:A:805:ILE:HD12	1:A:878:LEU:HD11	1.92	0.52
1:C:77:LYS:HB2	1:C:79:PHE:CE2	2.45	0.52
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.91	0.52
1:C:726:ILE:HG13	1:C:1061:VAL:HG22	1.92	0.52
2:D:527:GLU:HA	2:D:539:LEU:HD11	1.92	0.52
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.92	0.52
1:C:630:THR:O	1:C:632:THR:N	2.35	0.52
1:A:752:LEU:HD12	1:A:993:ILE:HG21	1.92	0.51
1:C:125:ASN:HA	1:C:174:PRO:HD3	1.91	0.51
1:C:132:GLU:HB2	1:C:164:ASN:HB2	1.90	0.51
2:D:508:ASN:HB3	2:D:510:TYR:CE2	2.46	0.51
1:B:621:PRO:O	1:B:623:ALA:N	2.43	0.51
1:B:638:THR:OG1	1:B:639:GLY:N	2.43	0.51
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:TYR:HB3	1:A:505:HIS:HB2	1.93	0.51
1:C:159:VAL:HG13	1:C:160:TYR:HD1	1.76	0.51
1:A:386:LYS:NZ	1:C:475:ALA:O	2.42	0.51
1:C:376:THR:HB	1:C:435:ALA:HB3	1.91	0.51
2:D:382:ASP:OD1	2:D:385:TYR:OH	2.28	0.51
1:A:544:ASN:HD21	1:A:579:PRO:HB3	1.76	0.51
1:A:821:LEU:HD23	1:A:938:LEU:HD23	1.92	0.51
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.46	0.51
2:D:108:LEU:HD22	2:D:112:LYS:HD3	1.93	0.50
1:B:394:ASN:H	1:B:516:GLU:HB3	1.77	0.50
1:A:344:ALA:HB3	1:A:347:PHE:CE1	2.46	0.50
1:C:246:ARG:HA	1:C:258:TRP:HB3	1.92	0.50
2:D:589:GLN:HB3	2:D:590:PRO:HD3	1.93	0.50
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.11	0.50
1:C:338:PHE:HE1	1:C:358:ILE:HD13	1.77	0.50
2:D:523:PHE:HB3	2:D:583:PRO:HB2	1.94	0.50
2:D:198:ASP:OD1	2:D:201:ASP:N	2.39	0.50
2:D:245:ARG:O	2:D:249:MET:HG2	2.12	0.50
2:D:247:LYS:HG3	2:D:282:THR:HG23	1.93	0.49
1:C:422:ASN:HD21	1:C:454:ARG:H	1.59	0.49
2:D:480:MET:HA	2:D:483:GLU:HG2	1.94	0.49
1:B:628:GLN:NE2	1:B:630:THR:OG1	2.46	0.49
2:D:233:ILE:HG22	2:D:236:LEU:HD21	1.94	0.49
1:C:117:LEU:HD11	1:C:231:ILE:HG21	1.94	0.49
1:C:391:CYS:HB3	1:C:522:ALA:HB1	1.95	0.49
2:D:342:VAL:HG12	2:D:344:CYS:H	1.76	0.49
1:C:329:PHE:HE2	1:C:528:LYS:HD3	1.78	0.49
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.95	0.48
1:B:756:TYR:OH	1:B:994:ASP:OD1	2.29	0.48
1:B:108:THR:O	1:B:237:ARG:NH1	2.46	0.48
1:C:129:LYS:HD3	1:C:133:PHE:HZ	1.77	0.48
2:D:382:ASP:HA	2:D:385:TYR:CZ	2.48	0.48
1:B:15:CYS:HA	1:B:158:ARG:HD2	1.95	0.48
1:C:233:ILE:HG23	1:C:235:ILE:HG13	1.95	0.48
1:C:119:ILE:HG13	1:C:128:ILE:HG23	1.94	0.48
1:C:403:ARG:NH1	1:C:405:ASP:OD1	2.46	0.48
1:A:1031:GLU:OE1	1:A:1039:ARG:NH1	2.47	0.48
1:B:578:ASP:HB3	1:B:581:THR:O	2.14	0.48
2:D:363:LYS:HE2	2:D:368:ASN:HD21	1.77	0.48
1:B:398:ASP:OD2	1:B:423:TYR:OH	2.20	0.48
1:C:347:PHE:HE2	1:C:509:ARG:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:358:ILE:HD11	2:D:379:ILE:HG13	1.96	0.48
2:D:521:TYR:HE1	2:D:570:LEU:HD11	1.78	0.47
2:D:388:GLN:HB2	2:D:393:ARG:HG2	1.96	0.47
1:B:612:TYR:HE1	1:B:651:ILE:HD12	1.79	0.47
2:D:203:TRP:HZ3	2:D:460:ARG:HH11	1.61	0.47
1:A:360:ASN:H	1:A:523:THR:HG23	1.78	0.47
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.95	0.47
2:D:360:MET:SD	2:D:362:THR:OG1	2.67	0.47
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.95	0.47
1:B:433:VAL:HG22	1:B:512:VAL:HG22	1.96	0.47
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.96	0.47
1:B:985:ASP:HB2	1:B:987:PRO:HD2	1.97	0.47
1:B:562:PHE:HD2	1:C:41:LYS:HG2	1.80	0.47
1:A:748:GLU:O	1:A:752:LEU:HG	2.15	0.46
1:C:986:PRO:O	1:C:990:GLU:HG2	2.15	0.46
1:A:1072:GLU:HG2	1:B:894:LEU:CD2	2.46	0.46
1:B:336:CYS:HB3	1:B:358:ILE:HD11	1.97	0.46
1:A:980:ILE:HD13	1:A:992:GLN:HB3	1.97	0.46
1:C:130:VAL:O	1:C:130:VAL:HG13	2.16	0.46
2:D:204:ARG:HG2	2:D:222:LEU:HD23	1.97	0.46
1:C:462:LYS:HB2	1:C:465:GLU:CD	2.36	0.46
2:D:132:VAL:HG23	2:D:167:GLY:HA3	1.96	0.46
2:D:520:ILE:HG12	2:D:581:VAL:HG21	1.97	0.46
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.48	0.46
1:B:295:PRO:HG3	1:B:633:TRP:CZ3	2.51	0.46
2:D:261:CYS:HB2	2:D:488:VAL:HB	1.97	0.46
2:D:468:ILE:HG22	2:D:473:TRP:HD1	1.80	0.46
1:A:201:PHE:HD2	1:A:203:ILE:HD11	1.80	0.46
1:A:323:THR:O	1:A:324:GLU:HG2	2.16	0.46
1:B:96:GLU:O	1:B:188:ASN:HB2	2.16	0.46
1:B:394:ASN:ND2	1:B:516:GLU:OE1	2.41	0.46
1:B:411:ALA:HB3	1:B:414:GLN:HG3	1.98	0.46
1:B:571:ASP:OD2	1:C:967:SER:HB2	2.15	0.46
1:A:287:ASP:OD1	1:A:288:ALA:N	2.49	0.46
1:B:68:ILE:HG22	1:B:78:ARG:HB2	1.97	0.46
1:A:159:VAL:HG23	1:A:160:TYR:CD2	2.51	0.46
2:D:453:THR:HA	2:D:512:PHE:HE2	1.81	0.46
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.97	0.45
1:A:630:THR:O	1:A:632:THR:N	2.38	0.45
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.74	0.45
1:C:395:VAL:HG23	1:C:524:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:VAL:HG22	1:C:651:ILE:HG12	1.98	0.45
3:T:1:NAG:H4	3:T:2:NAG:H83	1.97	0.45
1:B:132:GLU:HB2	1:B:164:ASN:HB3	1.98	0.45
1:B:334:ASN:OD1	1:B:335:LEU:N	2.43	0.45
1:C:292:ALA:HB1	1:C:631:PRO:HB2	1.97	0.45
2:D:46:ALA:O	2:D:62:MET:HE1	2.17	0.45
1:A:322:PRO:HB3	1:A:538:CYS:SG	2.57	0.45
1:A:46:SER:HA	1:A:279:TYR:O	2.17	0.45
1:A:108:THR:OG1	3:F:1:NAG:O5	2.35	0.45
1:A:578:ASP:HB3	1:A:581:THR:O	2.16	0.45
2:D:217:TYR:OH	2:D:225:ASP:OD2	2.28	0.45
2:D:309:GLN:O	2:D:312:GLU:HG3	2.17	0.45
1:A:203:ILE:O	1:A:226:LEU:HD23	2.17	0.45
1:B:128:ILE:HD13	1:B:170:TYR:HD2	1.82	0.45
1:A:231:ILE:HG13	1:A:232:GLY:N	2.32	0.45
2:D:47:SER:O	2:D:51:ASN:ND2	2.34	0.45
1:A:327:VAL:HG13	1:A:530:SER:HA	1.99	0.45
1:B:376:THR:OG1	1:B:408:ARG:NH2	2.48	0.45
2:D:397:ASN:C	2:D:397:ASN:ND2	2.71	0.44
2:D:470:LYS:HE3	2:D:470:LYS:HB3	1.85	0.44
1:A:24:LEU:HD12	1:A:25:PRO:HD2	1.99	0.44
1:B:321:GLN:HB2	1:B:627:ASP:HA	1.99	0.44
1:B:821:LEU:HD22	1:B:938:LEU:HB3	1.98	0.44
1:B:80:ASP:N	1:B:80:ASP:OD1	2.50	0.44
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.49	0.44
1:B:986:PRO:HA	1:B:989:ALA:HB3	1.99	0.44
2:D:581:VAL:HG13	2:D:581:VAL:O	2.17	0.44
1:A:68:ILE:HG22	1:A:78:ARG:HB2	1.98	0.44
1:A:137:ASN:HB2	4:A:1301:NAG:H62	1.99	0.44
1:B:121:ASN:HD21	1:B:176:LEU:HB2	1.83	0.44
1:C:1103:PHE:HZ	3:Y:1:NAG:H62	1.82	0.44
2:D:483:GLU:HG3	2:D:484:ILE:HG12	1.98	0.44
1:A:787:GLN:HG2	1:C:703:ASN:HD22	1.83	0.44
1:B:292:ALA:HB1	1:B:631:PRO:HB2	1.99	0.44
1:C:201:PHE:HD2	1:C:203:ILE:HD11	1.82	0.44
1:C:1101:HIS:ND1	3:Y:1:NAG:H5	2.33	0.44
2:D:471:GLU:HG2	2:D:472:GLN:HG2	2.00	0.44
1:A:394:ASN:OD1	1:A:516:GLU:HB3	2.17	0.44
2:D:570:LEU:HA	2:D:573:VAL:HG12	1.99	0.44
3:T:1:NAG:H4	3:T:2:NAG:H2	1.79	0.44
1:A:328:ARG:NH1	1:A:533:LEU:HD23	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ARG:HH21	1:C:138:ASP:HB3	1.83	0.44
1:A:233:ILE:HG22	1:A:234:ASN:N	2.33	0.43
1:B:1041:ASP:HB2	1:C:1030:SER:OG	2.17	0.43
1:C:17:ASN:OD1	4:C:1301:NAG:N2	2.51	0.43
1:A:821:LEU:O	1:A:825:LYS:HG2	2.18	0.43
1:C:203:ILE:O	1:C:226:LEU:HD23	2.18	0.43
2:D:131:LYS:HG2	2:D:141:CYS:HB3	2.01	0.43
1:B:81:ASN:HB3	1:B:239:GLN:NE2	2.33	0.43
1:B:977:LEU:HD23	1:B:977:LEU:H	1.81	0.43
1:C:815:ARG:HD2	1:C:819:GLU:HB3	1.99	0.43
1:A:170:TYR:CZ	1:A:172:SER:HB2	2.54	0.43
1:C:329:PHE:CE2	1:C:528:LYS:HB2	2.54	0.43
1:A:411:ALA:HB3	1:A:414:GLN:HG3	2.01	0.43
1:A:760:CYS:HA	1:A:763:LEU:HD12	2.00	0.43
2:D:473:TRP:C	2:D:475:LYS:H	2.21	0.43
1:A:122:ASN:N	1:A:125:ASN:O	2.48	0.43
1:B:319:ARG:HB2	1:B:629:LEU:HB2	2.01	0.43
1:C:329:PHE:CE2	1:C:528:LYS:HD3	2.54	0.43
1:B:431:GLY:HA2	1:B:515:PHE:CD2	2.54	0.43
1:C:27:ALA:HB3	1:C:64:TRP:HB3	2.01	0.42
1:C:497:PHE:CG	1:C:507:PRO:HD3	2.54	0.42
2:D:271:TRP:CH2	2:D:500:PRO:HA	2.51	0.42
1:A:620:VAL:HG22	1:A:621:PRO:HD2	2.01	0.42
1:A:722:VAL:HA	1:A:1064:HIS:O	2.19	0.42
1:A:1101:HIS:ND1	3:L:1:NAG:H5	2.34	0.42
1:B:902:MET:CG	1:B:916:LEU:HD11	2.49	0.42
1:C:405:ASP:OD1	1:C:405:ASP:N	2.51	0.42
1:A:703:ASN:OD1	1:A:704:SER:N	2.52	0.42
1:A:985:ASP:CG	1:A:986:PRO:HD2	2.40	0.42
1:B:294:ASP:N	1:B:294:ASP:OD1	2.52	0.42
1:A:124:THR:C	1:A:174:PRO:HG3	2.39	0.42
1:C:280:ASN:HD22	3:T:1:NAG:H83	1.84	0.42
1:A:715:PRO:HA	1:A:1072:GLU:HA	2.01	0.42
1:B:318:PHE:CZ	1:B:621:PRO:HD3	2.54	0.42
1:B:722:VAL:HA	1:B:1064:HIS:O	2.20	0.42
1:B:902:MET:HG3	1:B:916:LEU:HD11	2.02	0.42
1:C:714:ILE:HA	1:C:715:PRO:HD3	1.95	0.42
2:D:143:LEU:H	2:D:143:LEU:HD23	1.85	0.42
1:A:31:SER:O	1:A:59:PHE:CA	2.68	0.42
1:A:105:ILE:HG23	1:A:241:LEU:HD11	2.02	0.42
1:B:367:VAL:O	1:B:368:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1038:LYS:HA	1:B:1038:LYS:HD3	1.83	0.42
1:B:172:SER:OG	1:B:173:GLN:N	2.52	0.42
2:D:315:PHE:O	2:D:318:VAL:HG12	2.20	0.42
2:D:574:VAL:HG23	2:D:576:ALA:H	1.84	0.42
1:A:986:PRO:O	1:A:990:GLU:HG2	2.20	0.42
1:B:462:LYS:HB3	1:B:462:LYS:HE2	1.77	0.42
1:C:87:ASN:O	1:C:89:GLY:N	2.52	0.42
2:D:439:LEU:HD22	2:D:588:PHE:CD1	2.55	0.42
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	2.01	0.42
1:C:327:VAL:H	1:C:531:THR:HB	1.85	0.42
1:C:1001:LEU:HD23	1:C:1001:LEU:HA	1.93	0.42
1:B:44:ARG:O	1:B:283:GLY:HA2	2.20	0.41
2:D:269:ASP:HB2	2:D:274:PHE:O	2.20	0.41
1:B:796:TYR:HB3	3:I:1:NAG:O6	2.20	0.41
1:B:959:LEU:HD23	1:B:959:LEU:HA	1.91	0.41
2:D:208:GLU:OE1	2:D:219:ARG:N	2.53	0.41
1:A:277:LEU:HD13	1:A:285:ILE:HD13	2.02	0.41
1:A:201:PHE:CD2	1:A:203:ILE:HD11	2.56	0.41
1:A:379:CYS:HA	1:A:432:CYS:HB2	2.00	0.41
1:B:206:LYS:HA	1:B:206:LYS:HD3	1.92	0.41
1:B:713:ALA:HB3	1:C:894:LEU:HB3	2.02	0.41
1:C:1048:HIS:HA	1:C:1066:THR:HG22	2.02	0.41
2:D:365:THR:HG22	2:D:367:ASP:H	1.85	0.41
1:A:364:ASP:O	1:A:366:SER:N	2.47	0.41
1:B:537:LYS:C	1:B:551:VAL:HG12	2.40	0.41
1:C:101:ILE:HD13	1:C:242:LEU:HD23	2.03	0.41
1:C:127:VAL:HG12	1:C:171:VAL:HG22	2.02	0.41
1:C:142:ASP:OD1	1:C:244:LEU:HB2	2.20	0.41
1:C:168:PHE:HZ	1:C:170:TYR:HD2	1.68	0.41
2:D:293:VAL:HG21	2:D:423:LEU:HD13	2.03	0.41
2:D:392:LEU:HA	2:D:562:ASN:HD21	1.85	0.41
3:U:1:NAG:H4	3:U:2:NAG:H2	1.72	0.41
1:A:130:VAL:CG1	1:A:168:PHE:HB3	2.50	0.41
1:A:130:VAL:HG21	1:A:233:ILE:HD11	2.01	0.41
1:A:873:TYR:CE1	1:C:699:LEU:HD13	2.56	0.41
1:B:403:ARG:HE	1:B:406:GLU:HG3	1.85	0.41
1:C:201:PHE:CD2	1:C:203:ILE:HD11	2.55	0.41
1:A:40:ASP:OD2	1:A:44:ARG:NH1	2.44	0.41
1:B:976:VAL:HG23	1:B:979:ASP:HB2	2.01	0.41
2:D:111:ASP:OD1	2:D:111:ASP:N	2.53	0.41
2:D:566:TRP:HE3	2:D:570:LEU:HD12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:ASN:OD1	1:A:1125:ASN:N	2.50	0.41
1:B:620:VAL:HG11	1:B:636:TYR:CE1	2.56	0.41
1:B:642:VAL:HG22	1:B:651:ILE:HG12	2.03	0.41
1:C:461:LEU:HD11	1:C:465:GLU:HB2	2.03	0.41
2:D:150:GLU:OE2	2:D:154:THR:OG1	2.39	0.41
2:D:307:ILE:HG23	2:D:369:PHE:HD1	1.85	0.41
1:B:350:VAL:HG22	1:B:422:ASN:HB3	2.03	0.41
2:D:58:ASN:O	2:D:62:MET:HG2	2.20	0.41
2:D:600:ARG:HG2	2:D:601:ASN:N	2.36	0.41
1:A:206:LYS:HB3	1:A:223:LEU:HD23	2.03	0.40
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.56	0.40
1:A:139:PRO:HD2	1:A:239:GLN:HE22	1.86	0.40
1:B:971:GLY:HA2	1:C:755:GLN:HE22	1.86	0.40
1:C:79:PHE:CE2	1:C:258:TRP:HZ3	2.39	0.40
1:B:141:LEU:O	1:B:244:LEU:N	2.50	0.40
1:B:403:ARG:HD3	1:B:495:TYR:CE1	2.57	0.40
1:B:675:GLN:HG3	1:B:693:ILE:CD1	2.52	0.40
1:C:1139:ASP:HA	1:C:1140:PRO:HD3	1.95	0.40
2:D:32:PHE:CD1	2:D:76:GLN:HG3	2.56	0.40
2:D:318:VAL:HG22	2:D:551:GLY:HA3	2.03	0.40
1:A:736:VAL:HG11	1:A:1004:LEU:HD11	2.03	0.40
1:A:855:PHE:O	1:A:856:LYS:HD3	2.21	0.40
1:C:295:PRO:HG3	1:C:633:TRP:CE3	2.57	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	1045/1243 (84%)	978 (94%)	66 (6%)	1 (0%)	48 67
1	B	1045/1243 (84%)	998 (96%)	45 (4%)	2 (0%)	44 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1045/1243 (84%)	980 (94%)	63 (6%)	2 (0%)	44	61
2	D	593/598 (99%)	554 (93%)	39 (7%)	0	100	100
All	All	3728/4327 (86%)	3510 (94%)	213 (6%)	5 (0%)	50	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	638	THR
1	A	235	ILE
1	B	638	THR
1	C	641	ASN
1	B	622	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	932/1083 (86%)	932 (100%)	0	100	100
1	B	932/1083 (86%)	930 (100%)	2 (0%)	92	97
1	C	932/1083 (86%)	932 (100%)	0	100	100
2	D	520/522 (100%)	516 (99%)	4 (1%)	79	89
All	All	3316/3771 (88%)	3310 (100%)	6 (0%)	91	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	188	ASN
1	B	690	GLN
2	D	156	THR
2	D	228	ARG
2	D	397	ASN
2	D	600	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	239	GLN
1	B	690	GLN
1	B	901	GLN
1	B	935	GLN
1	C	675	GLN
1	C	690	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

44 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	E	1	1,3	14,14,15	0.30	0	17,19,21	1.29	2 (11%)
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	F	1	1,3	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	F	2	3	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	G	1	1,3	14,14,15	0.26	0	17,19,21	0.45	0
3	NAG	G	2	3	14,14,15	0.21	0	17,19,21	0.38	0
3	NAG	H	1	1,3	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	H	2	3	14,14,15	0.23	0	17,19,21	0.38	0
3	NAG	I	1	1,3	14,14,15	1.12	1 (7%)	17,19,21	1.65	1 (5%)
3	NAG	I	2	3	14,14,15	0.34	0	17,19,21	0.45	0
3	NAG	J	1	1,3	14,14,15	0.24	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	J	2	3	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	K	1	1,3	14,14,15	0.26	0	17,19,21	0.52	0
3	NAG	K	2	3	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	L	1	1,3	14,14,15	0.28	0	17,19,21	0.47	0
3	NAG	L	2	3	14,14,15	0.23	0	17,19,21	0.39	0
3	NAG	M	1	1,3	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	M	2	3	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	N	1	1,3	14,14,15	0.60	1 (7%)	17,19,21	0.53	0
3	NAG	N	2	3	14,14,15	0.33	0	17,19,21	0.42	0
3	NAG	O	1	1,3	14,14,15	0.22	0	17,19,21	0.50	0
3	NAG	O	2	3	14,14,15	0.28	0	17,19,21	0.36	0
3	NAG	P	1	1,3	14,14,15	0.25	0	17,19,21	0.72	1 (5%)
3	NAG	P	2	3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	Q	1	1,3	14,14,15	0.18	0	17,19,21	0.47	0
3	NAG	Q	2	3	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	R	1	1,3	14,14,15	0.64	0	17,19,21	0.97	2 (11%)
3	NAG	R	2	3	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	S	1	1,3	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	S	2	3	14,14,15	0.24	0	17,19,21	0.39	0
3	NAG	T	1	1,3	14,14,15	0.27	0	17,19,21	0.62	0
3	NAG	T	2	3	14,14,15	0.58	0	17,19,21	0.49	0
3	NAG	U	1	1,3	14,14,15	0.53	0	17,19,21	0.50	0
3	NAG	U	2	3	14,14,15	0.55	0	17,19,21	0.56	0
3	NAG	V	1	1,3	14,14,15	0.22	0	17,19,21	0.51	0
3	NAG	V	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	W	1	1,3	14,14,15	0.27	0	17,19,21	0.68	0
3	NAG	W	2	3	14,14,15	0.24	0	17,19,21	0.39	0
3	NAG	X	1	1,3	14,14,15	0.23	0	17,19,21	0.50	0
3	NAG	X	2	3	14,14,15	0.32	0	17,19,21	0.37	0
3	NAG	Y	1	1,3	14,14,15	0.31	0	17,19,21	0.43	0
3	NAG	Y	2	3	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	Z	1	1,3	14,14,15	0.20	0	17,19,21	0.56	0
3	NAG	Z	2	3	14,14,15	0.25	0	17,19,21	0.54	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	E	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	T	2	3	-	4/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	U	2	3	-	3/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	1/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	O5-C1	4.08	1.50	1.43
3	N	1	NAG	O5-C1	-2.15	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	NAG	C1-O5-C5	6.47	120.96	112.19
3	E	1	NAG	C2-N2-C7	4.40	129.16	122.90
3	R	1	NAG	O5-C1-C2	2.32	114.95	111.29
3	R	1	NAG	O5-C5-C4	-2.27	105.30	110.83
3	E	1	NAG	C1-C2-N2	2.16	114.18	110.49
3	P	1	NAG	C1-O5-C5	2.12	115.06	112.19

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	O	2	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	S	2	NAG	C4-C5-C6-O6
3	Z	1	NAG	O5-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	Z	1	NAG	C4-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C1-C2-N2-C7

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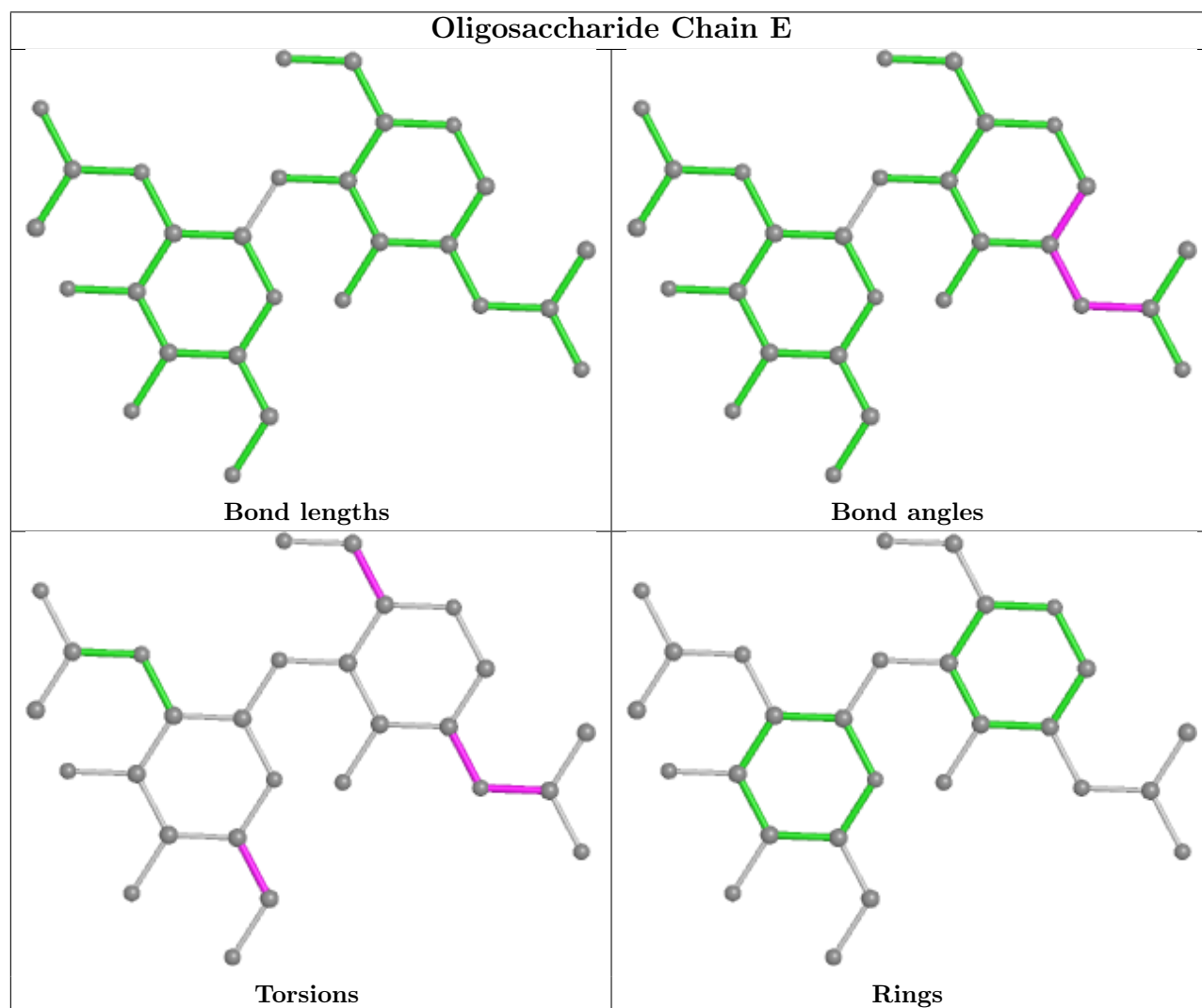
Mol	Chain	Res	Type	Atoms
3	H	1	NAG	O5-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	Z	2	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C1-C2-N2-C7
3	P	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C1-C2-N2-C7
3	G	1	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C3-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7
3	T	1	NAG	C3-C2-N2-C7
3	U	1	NAG	C3-C2-N2-C7
3	U	2	NAG	C3-C2-N2-C7
3	W	1	NAG	C3-C2-N2-C7
3	Z	1	NAG	C3-C2-N2-C7
3	Z	2	NAG	C3-C2-N2-C7
3	G	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	V	2	NAG	C4-C5-C6-O6

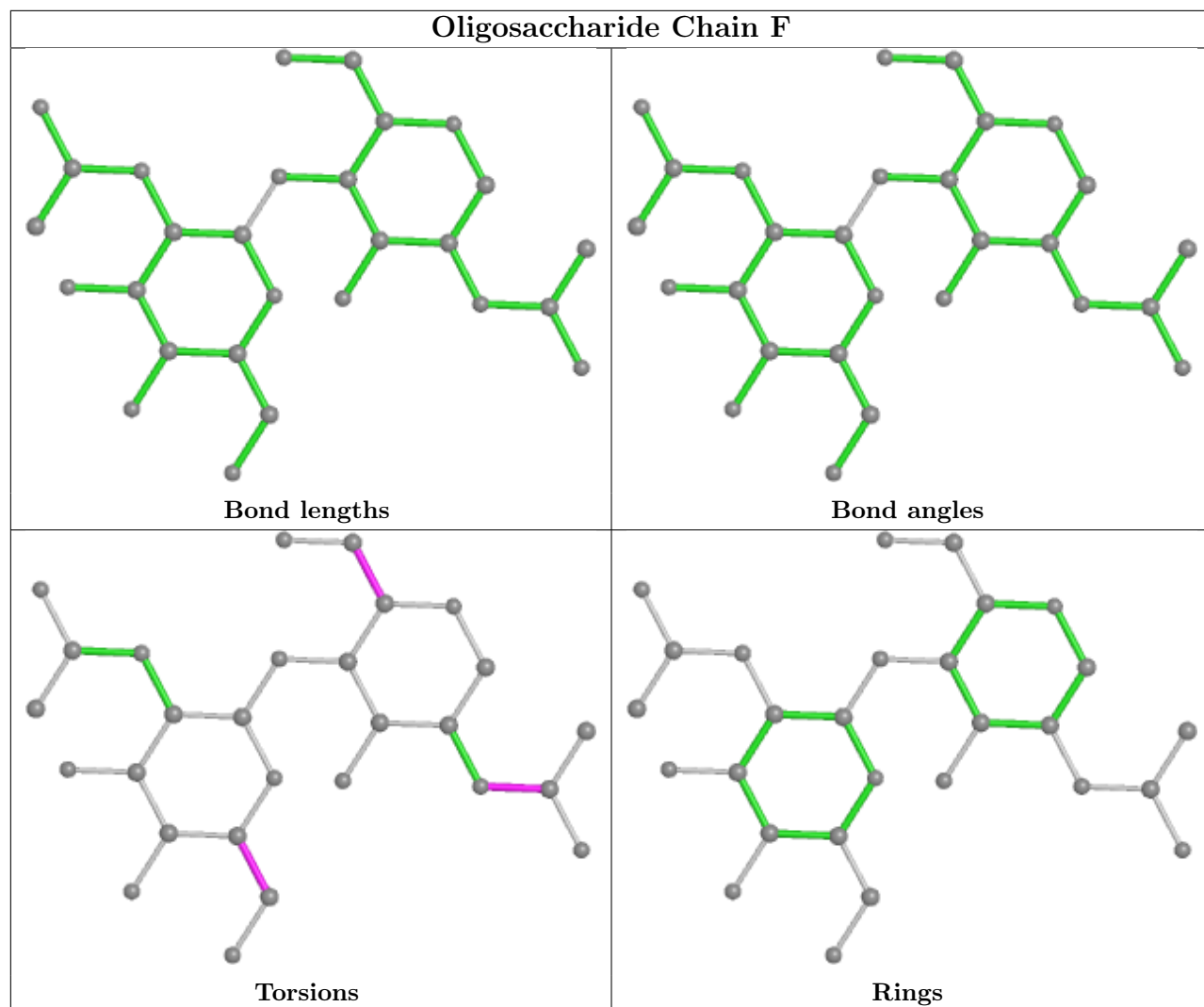
There are no ring outliers.

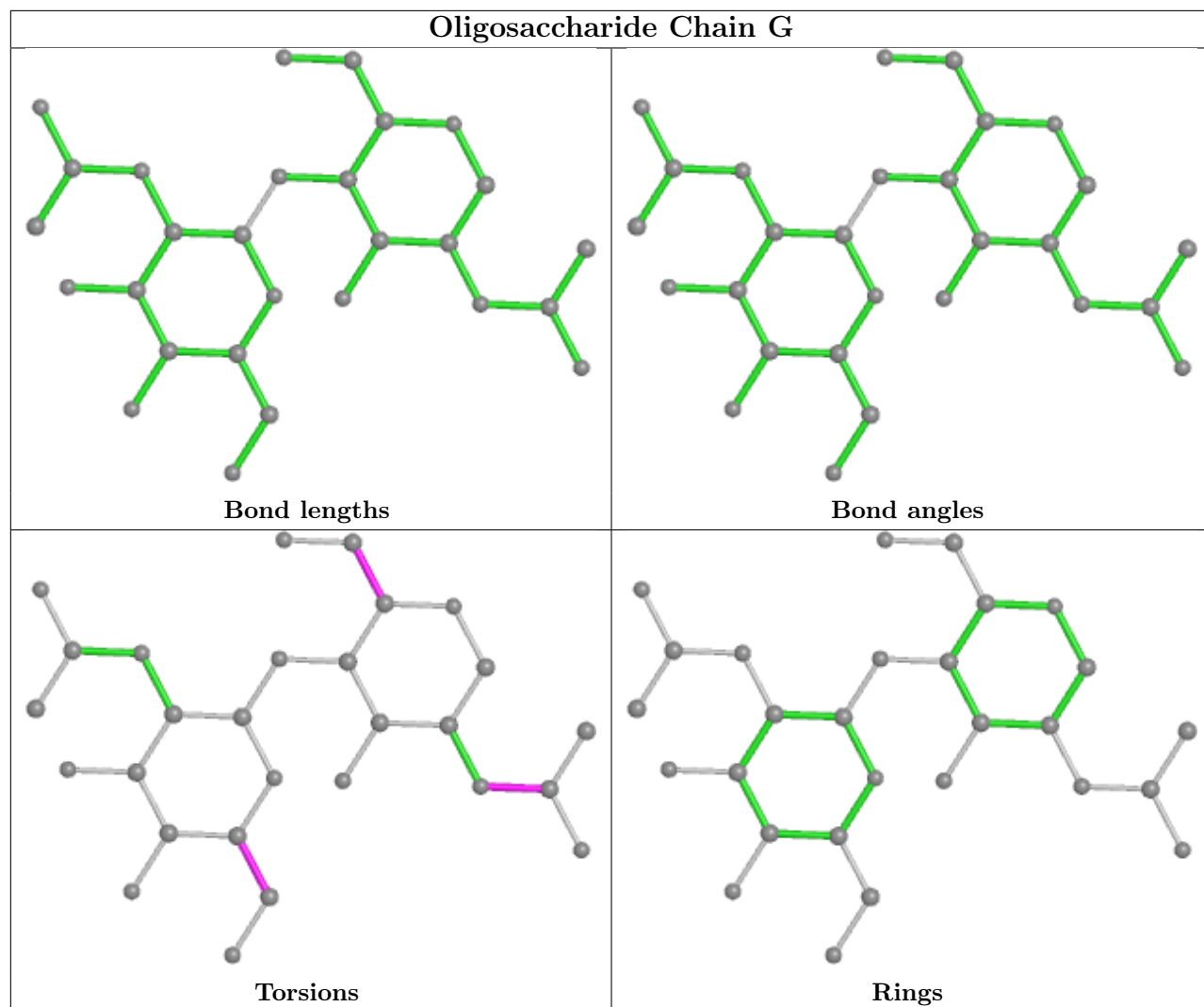
9 monomers are involved in 10 short contacts:

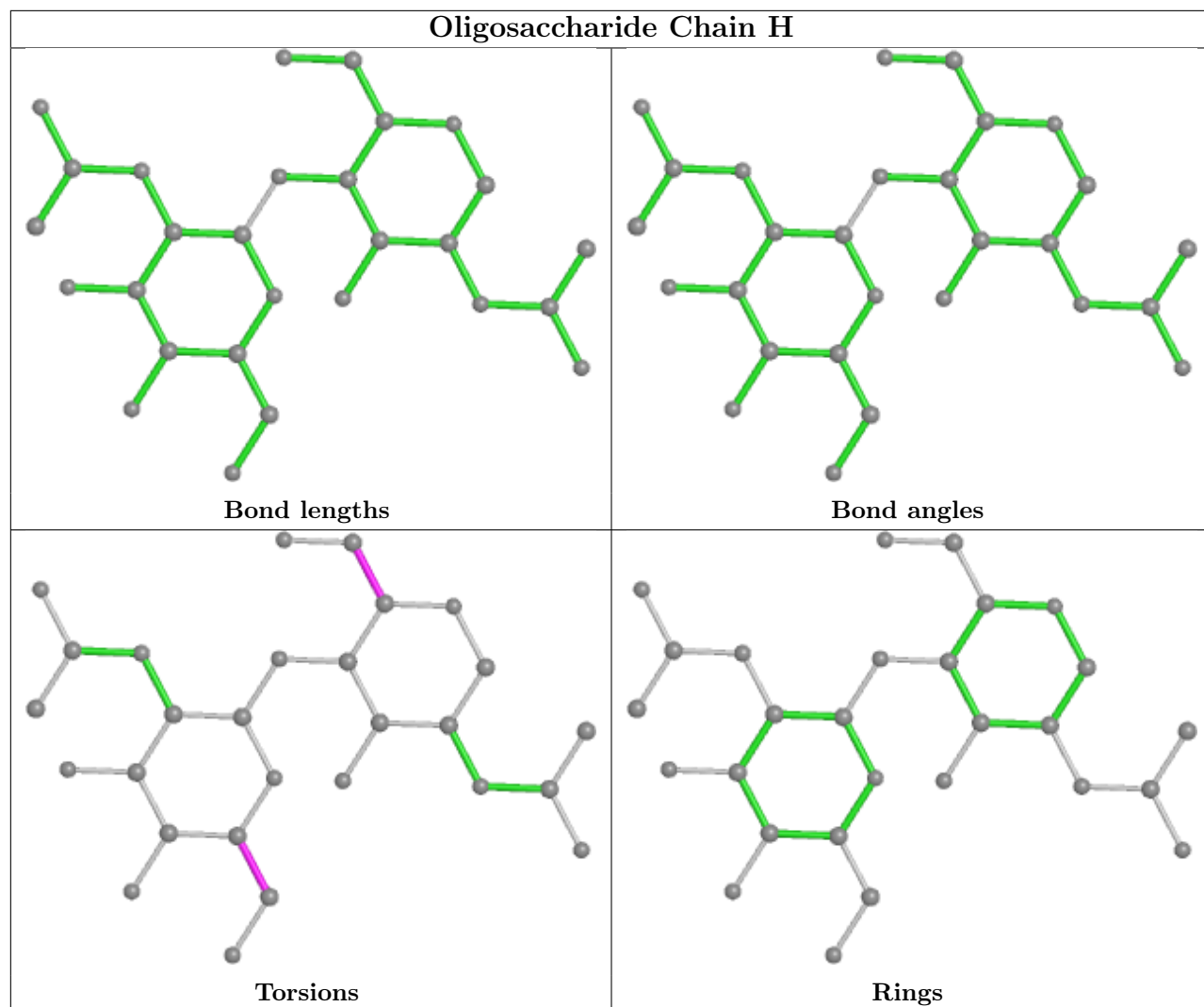
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1	NAG	1	0
3	T	2	NAG	2	0
3	E	1	NAG	1	0
3	Y	1	NAG	2	0
3	U	1	NAG	1	0
3	I	1	NAG	1	0
3	T	1	NAG	3	0
3	U	2	NAG	1	0
3	F	1	NAG	1	0

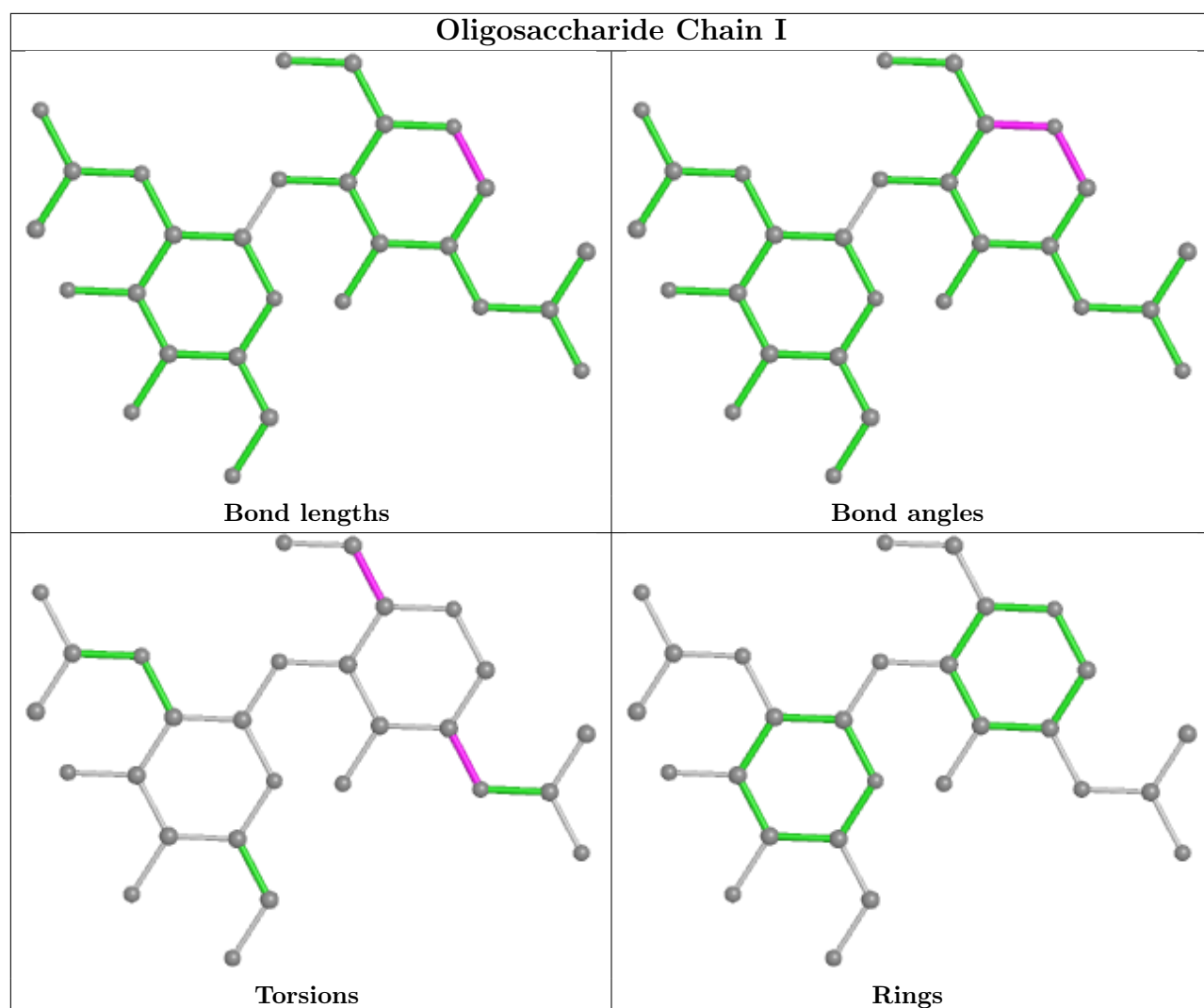
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

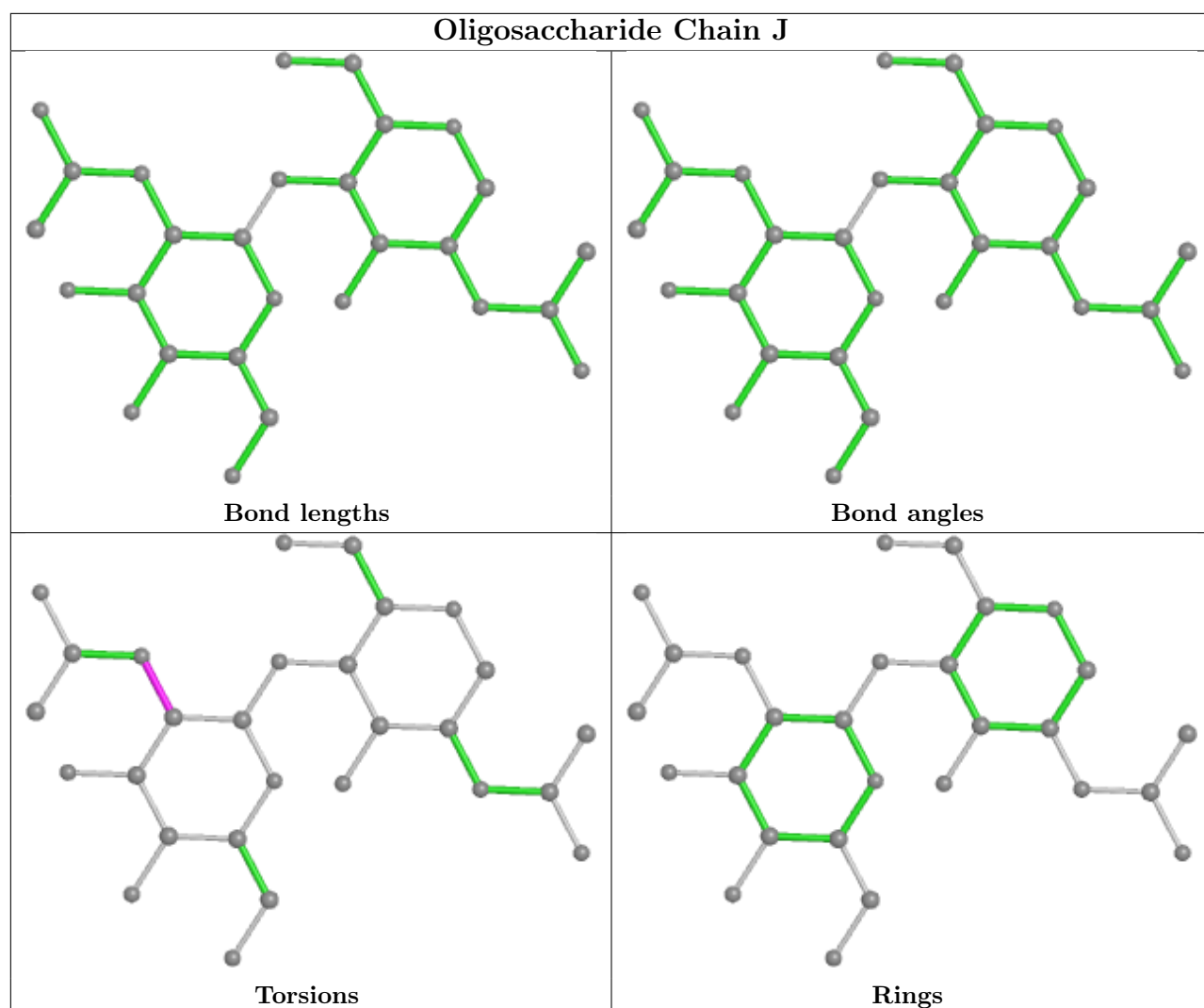


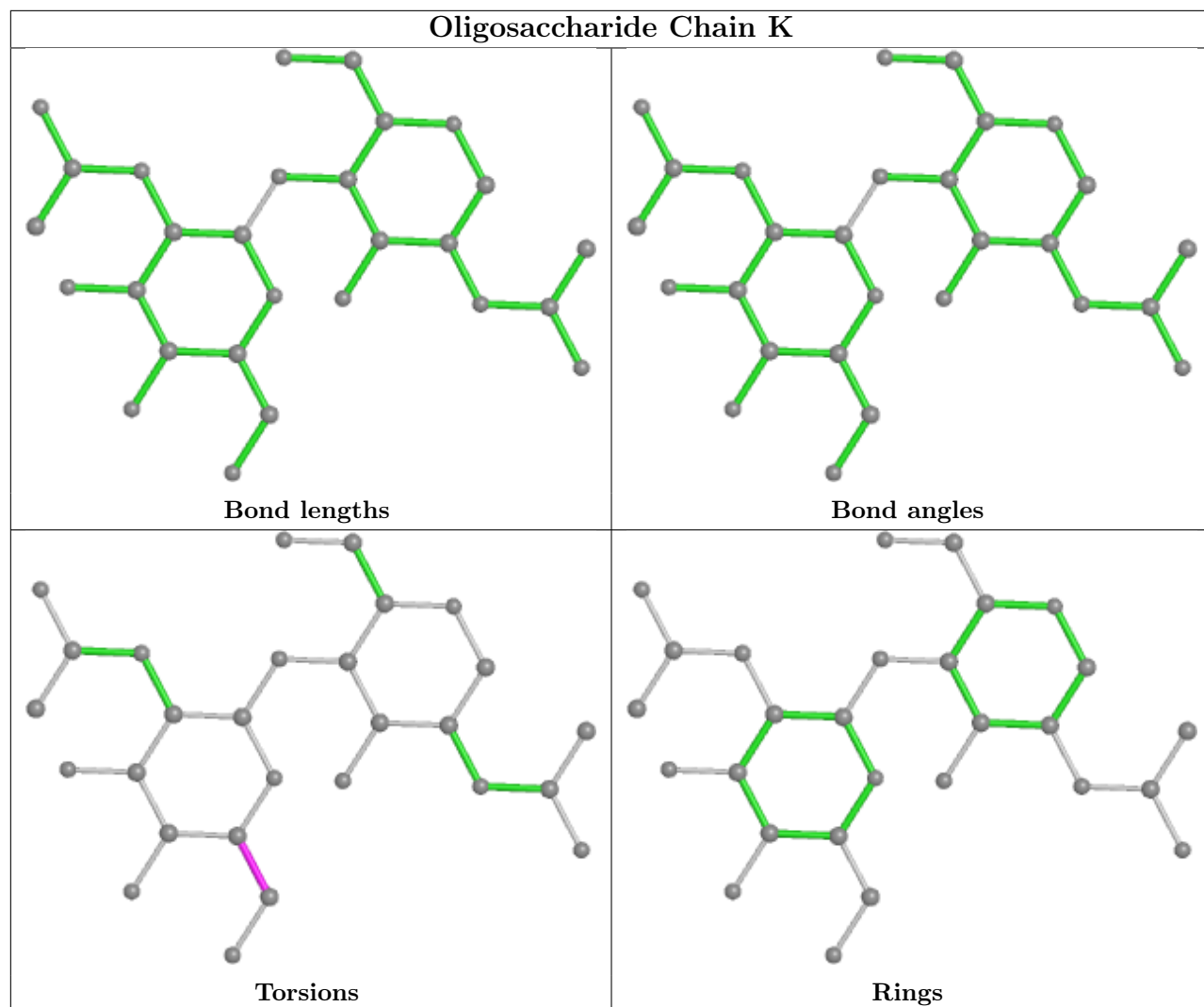




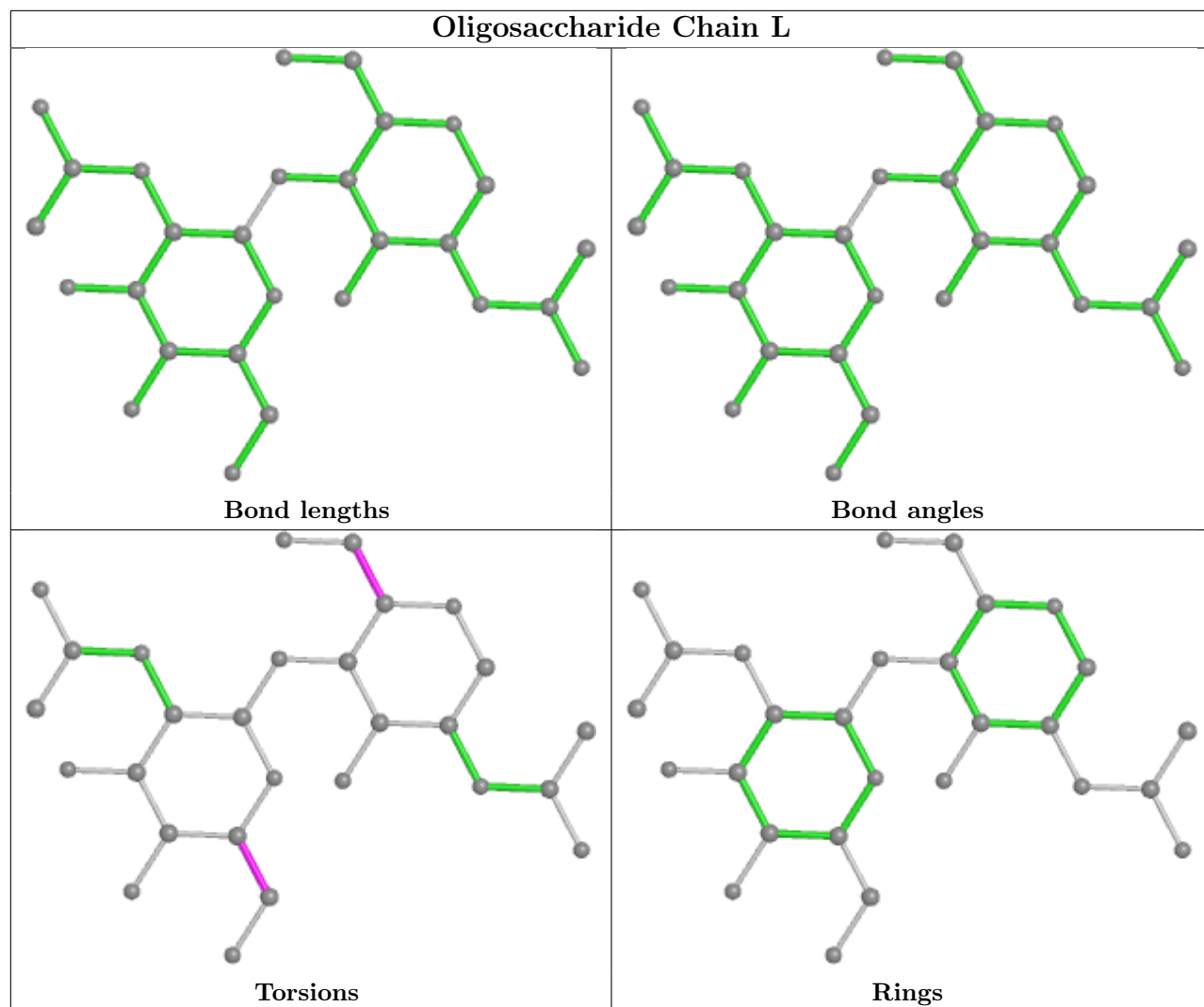


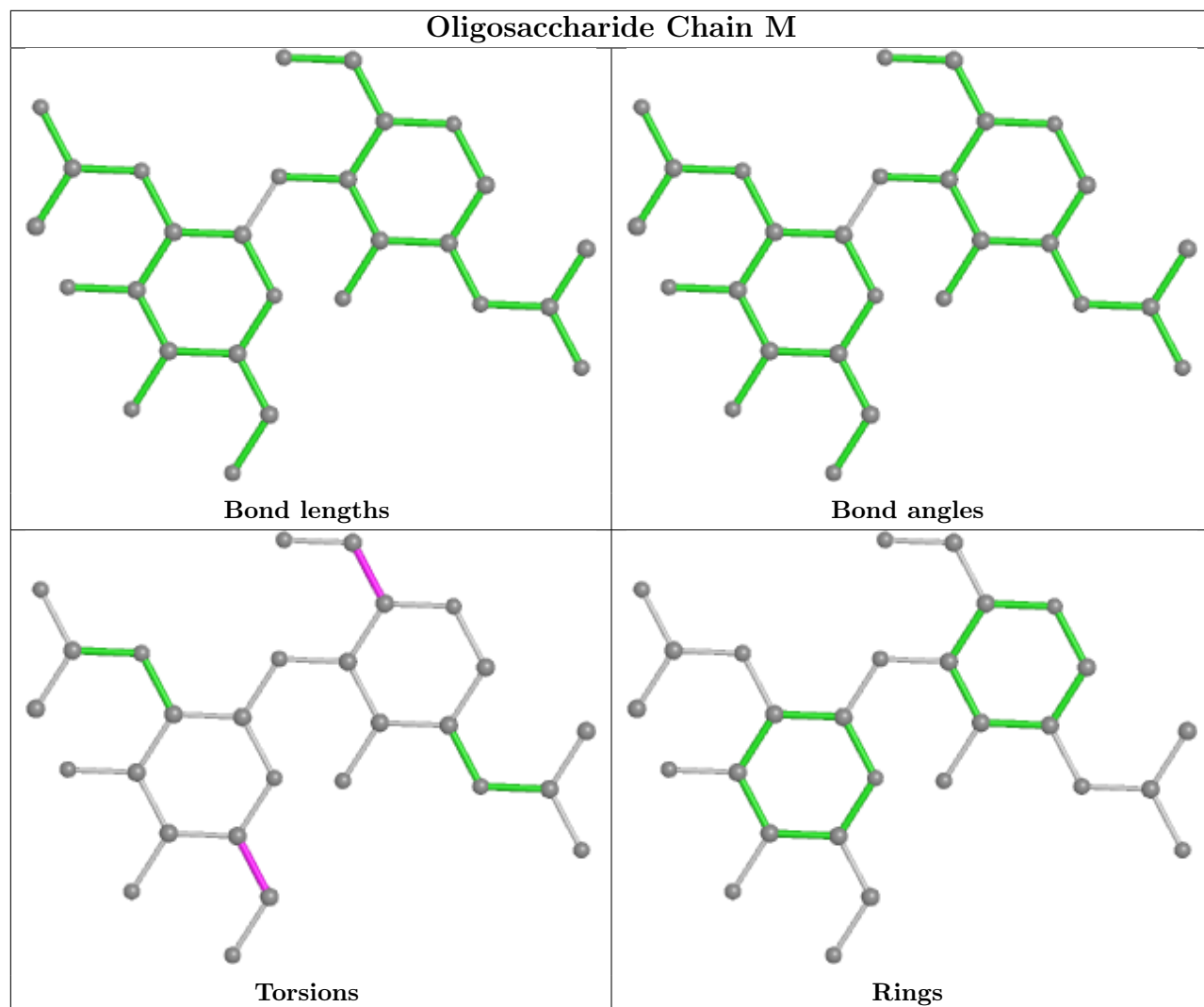


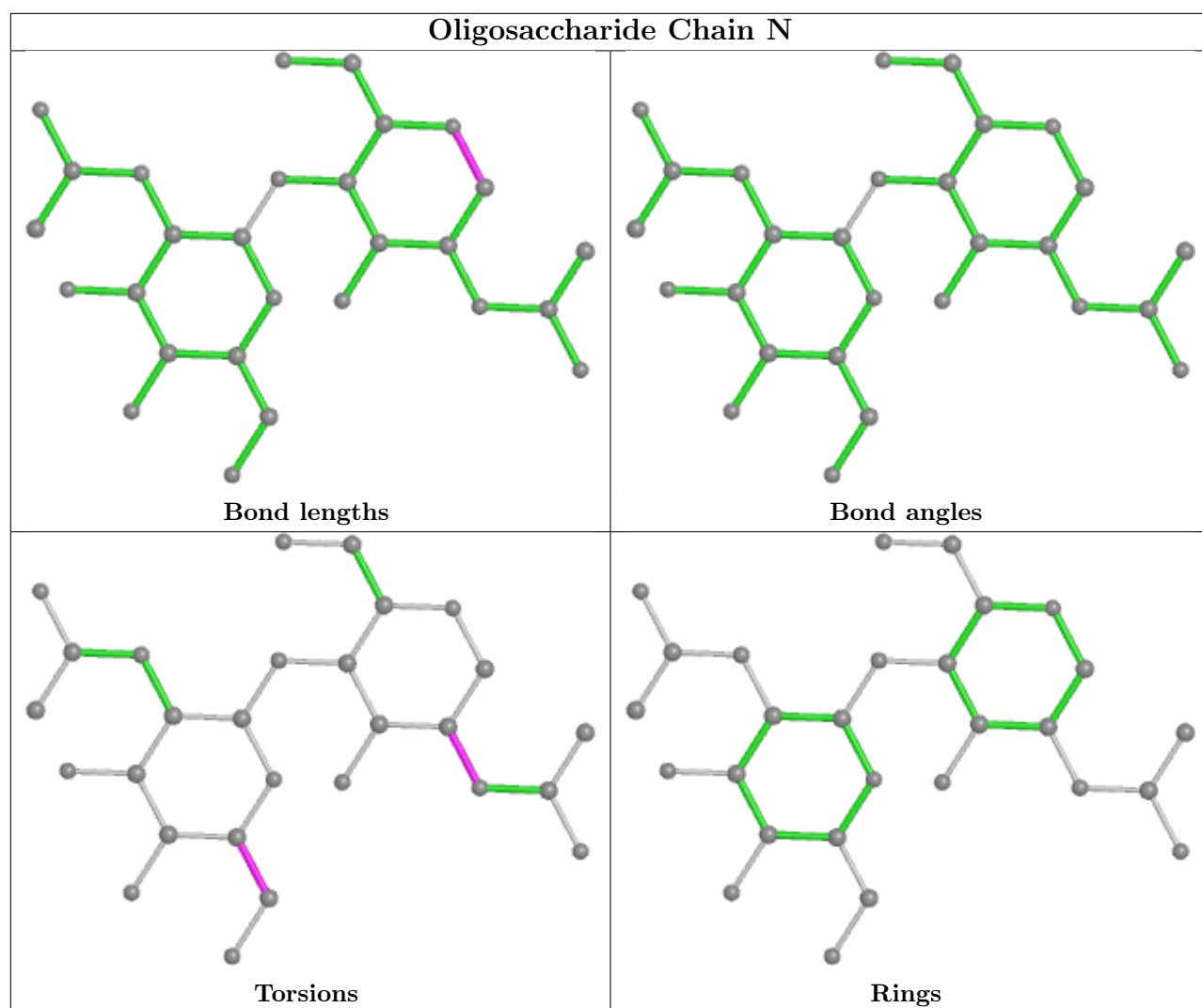


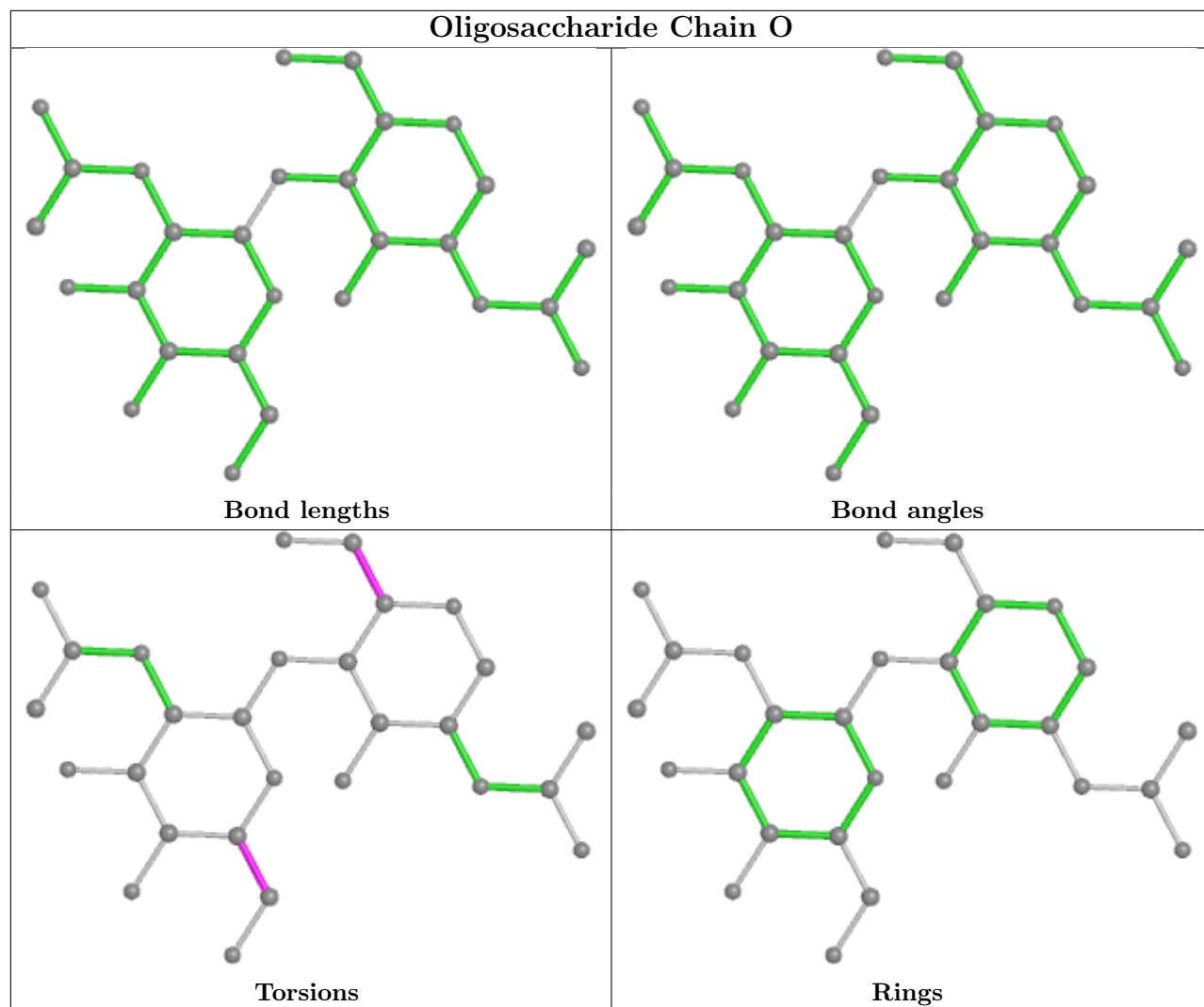


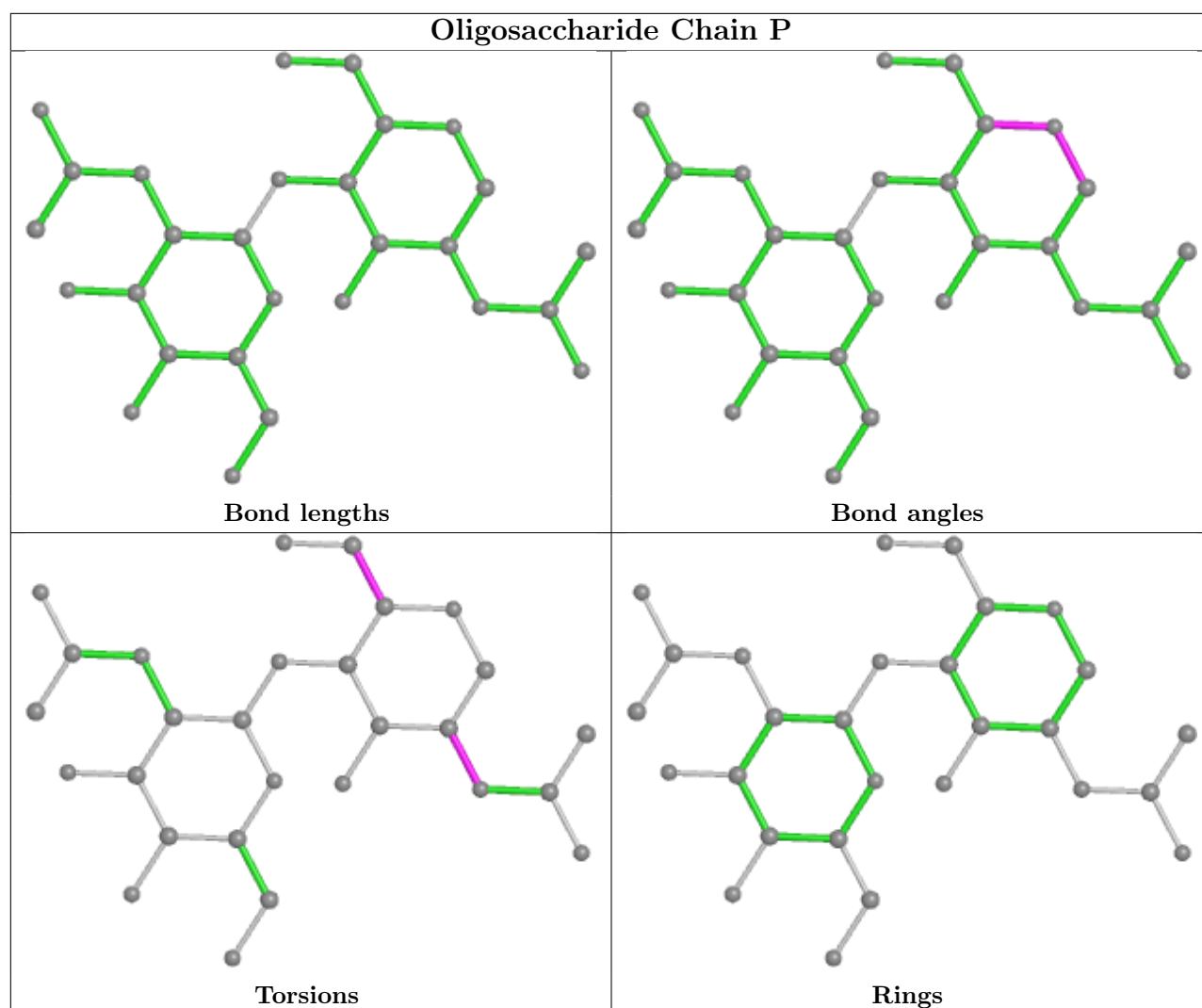


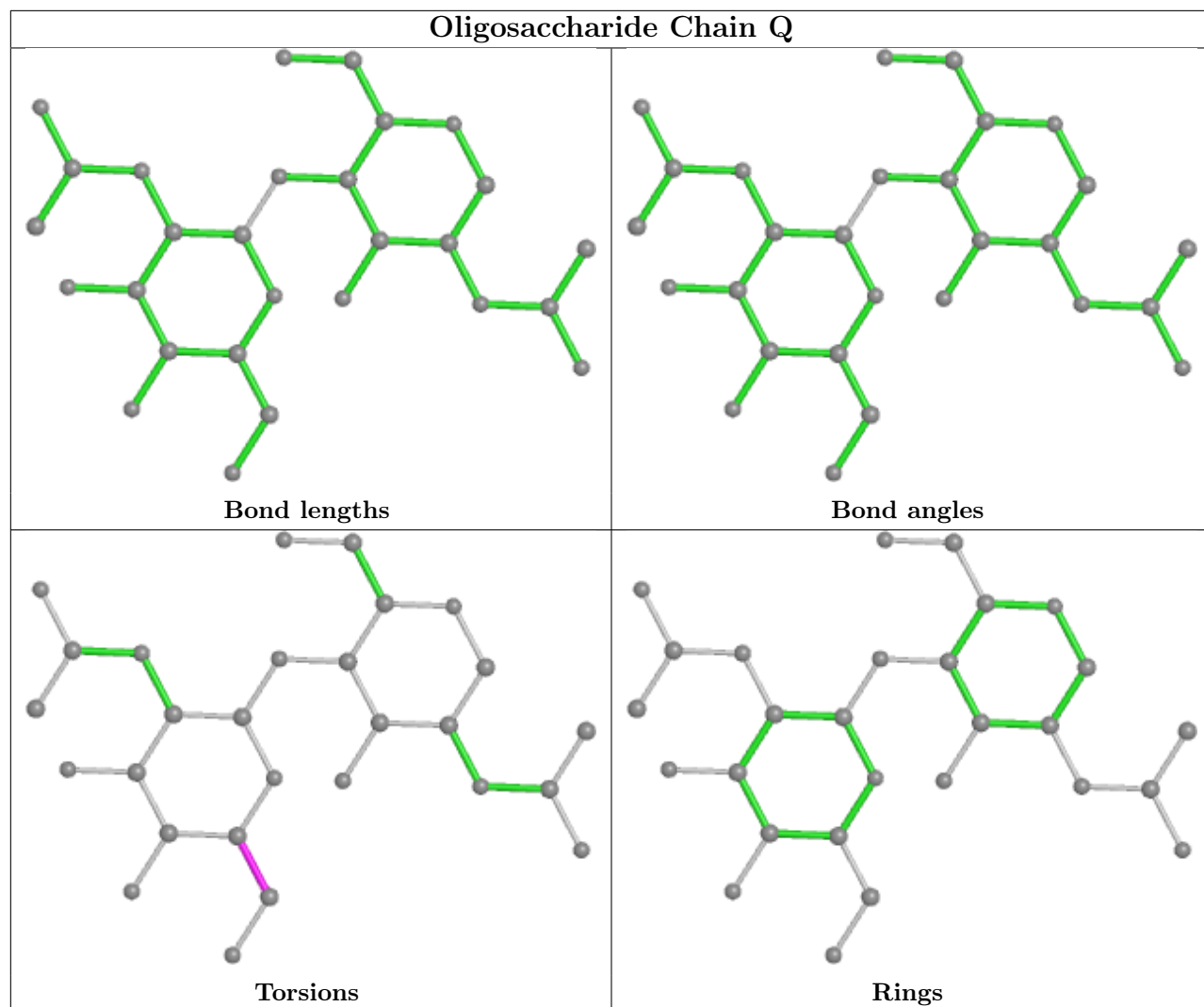


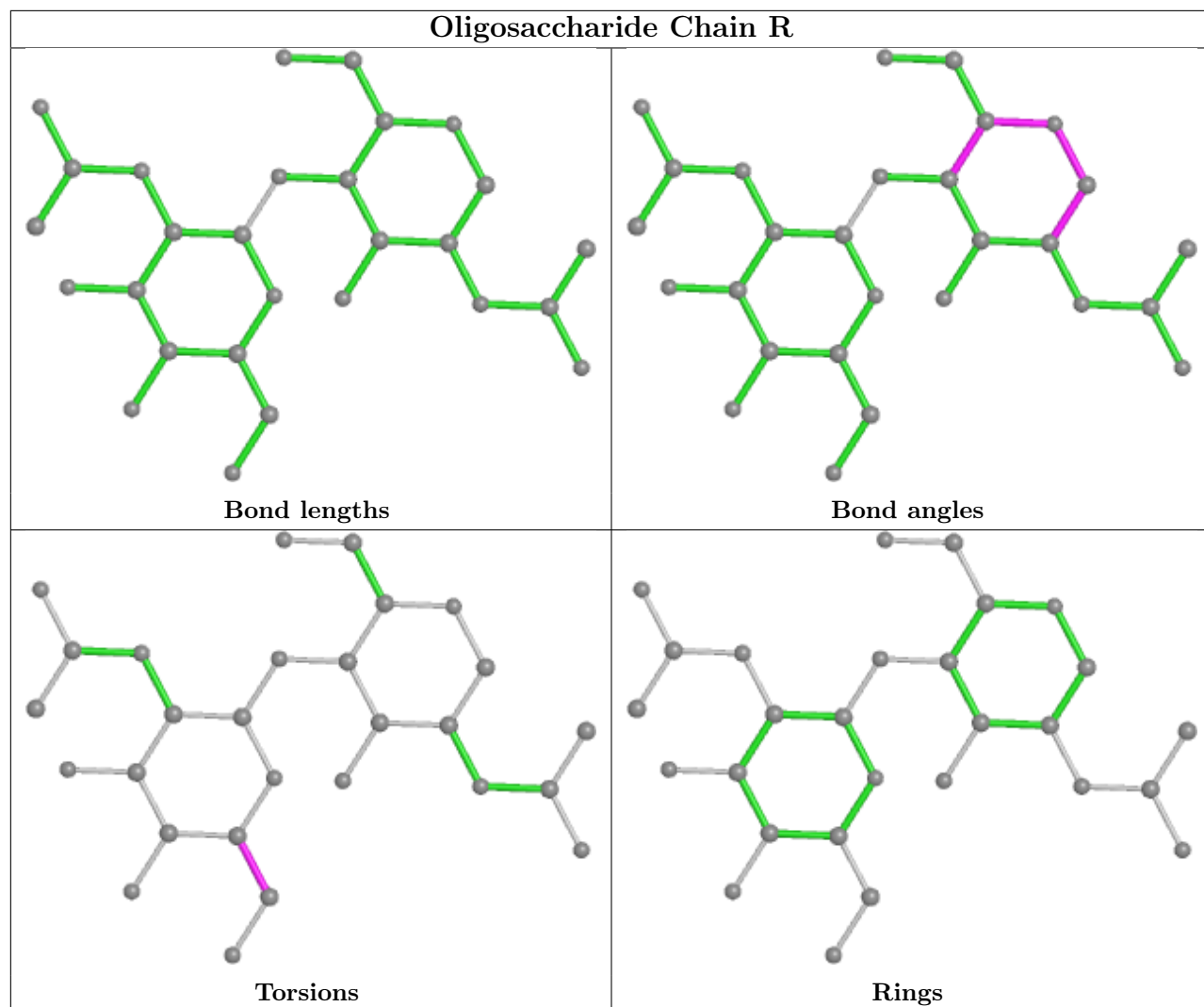


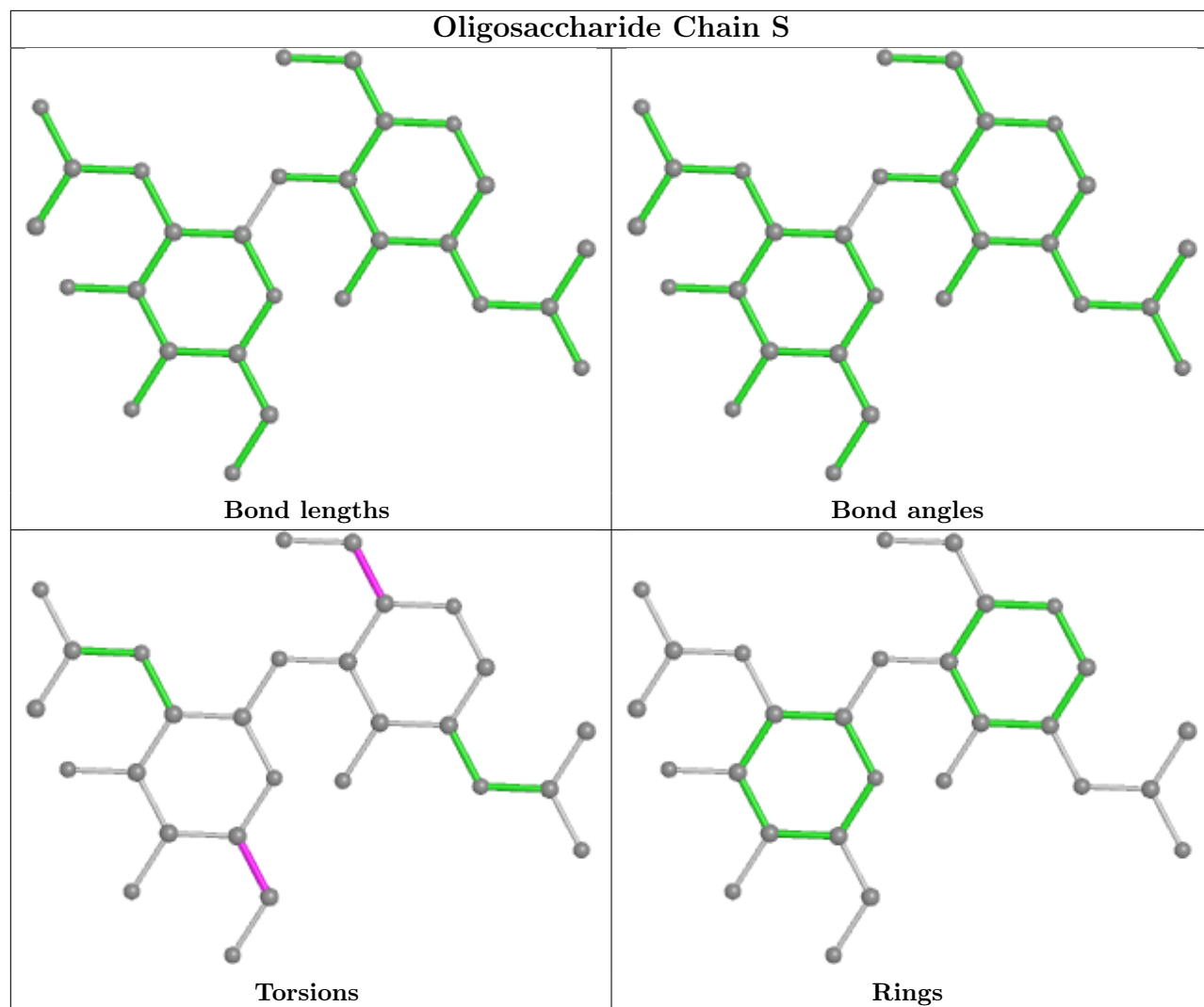




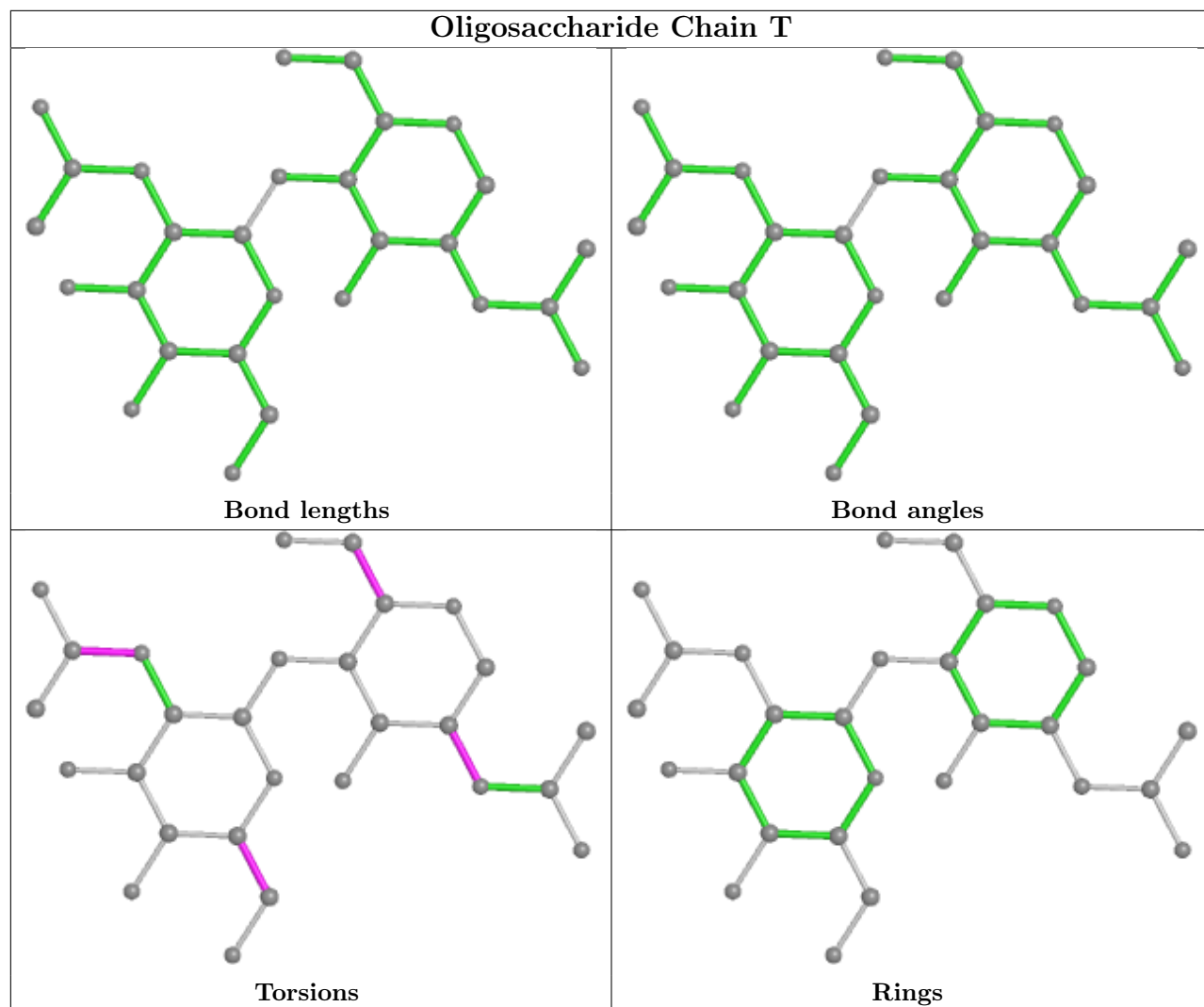


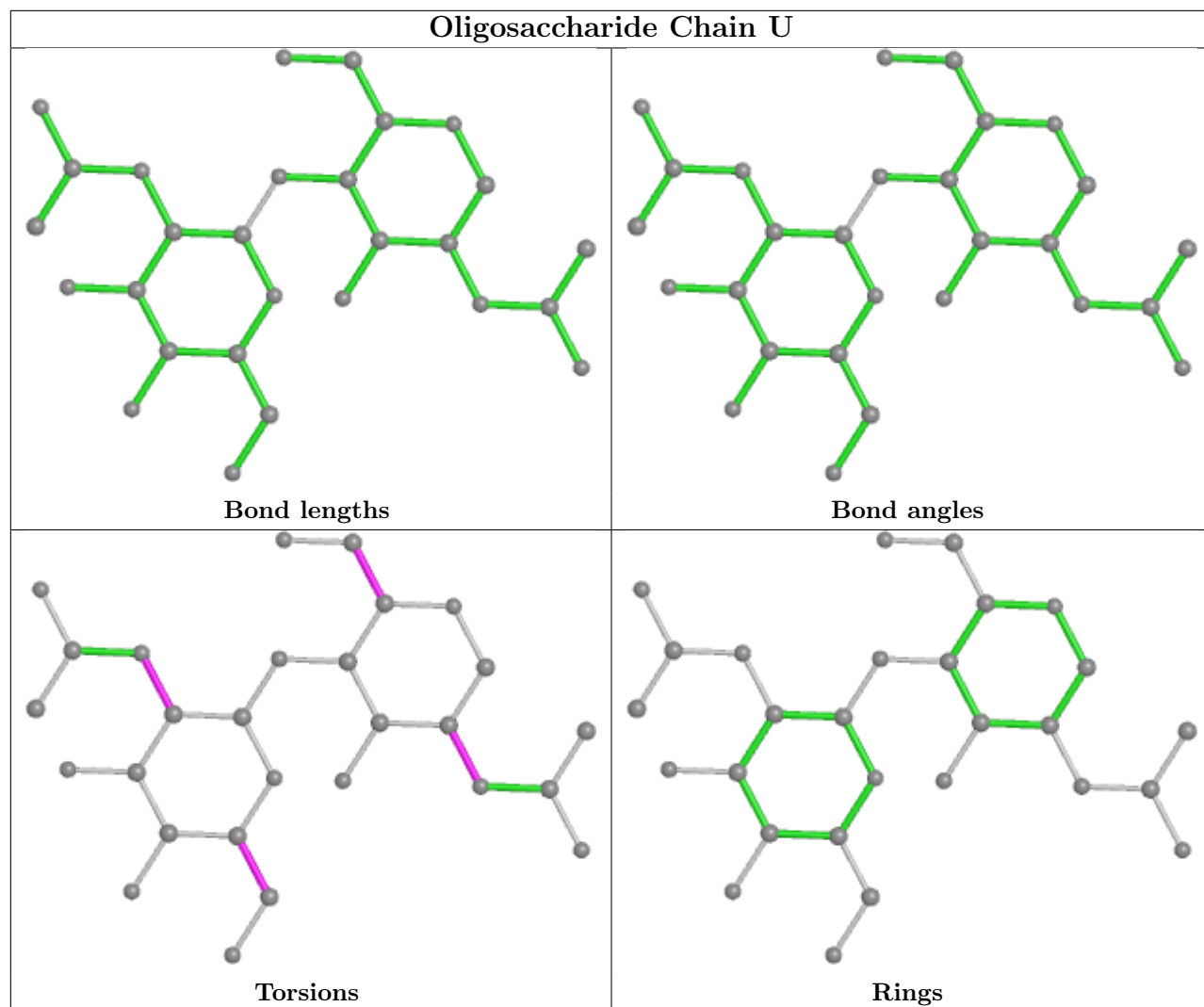


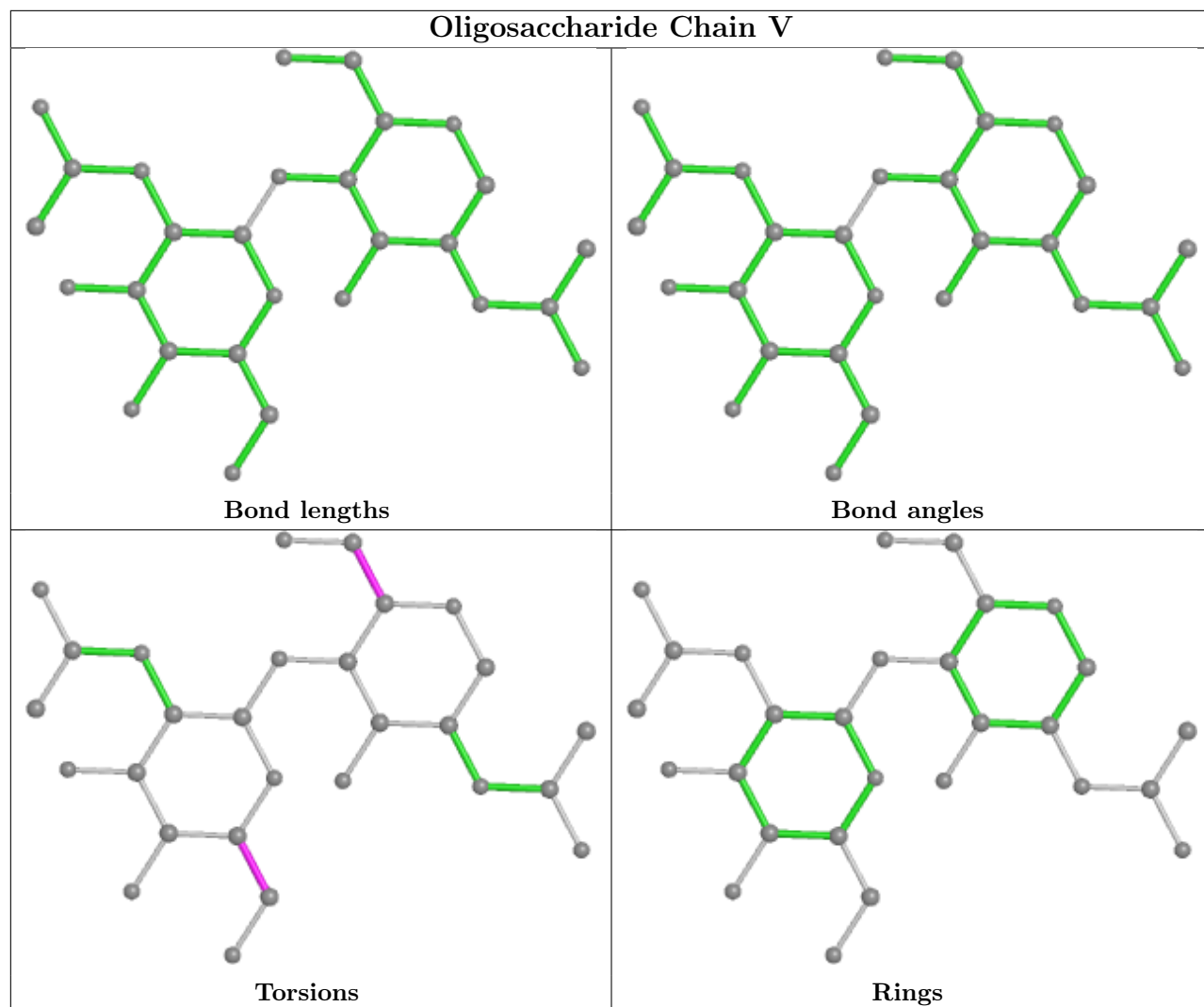


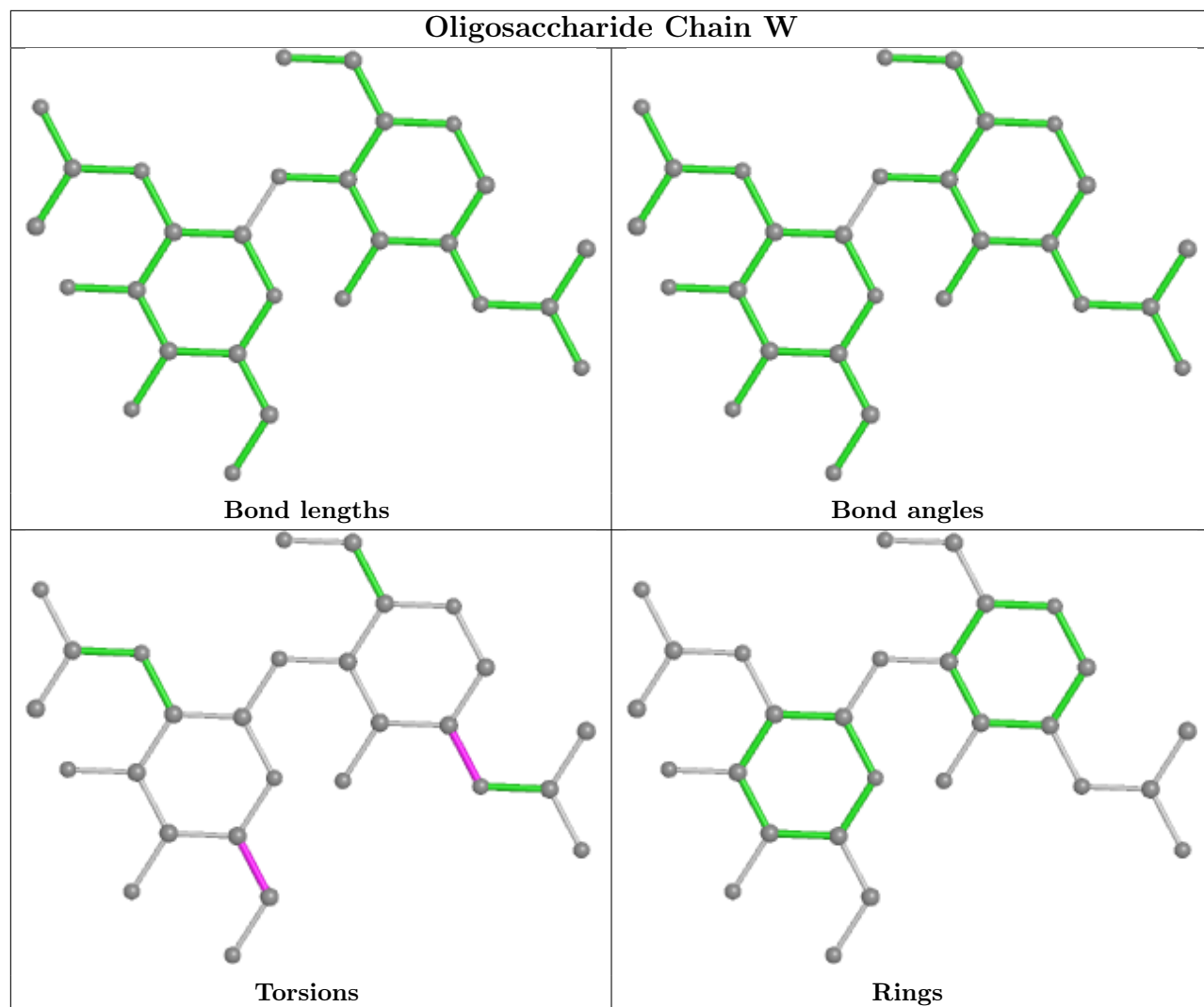


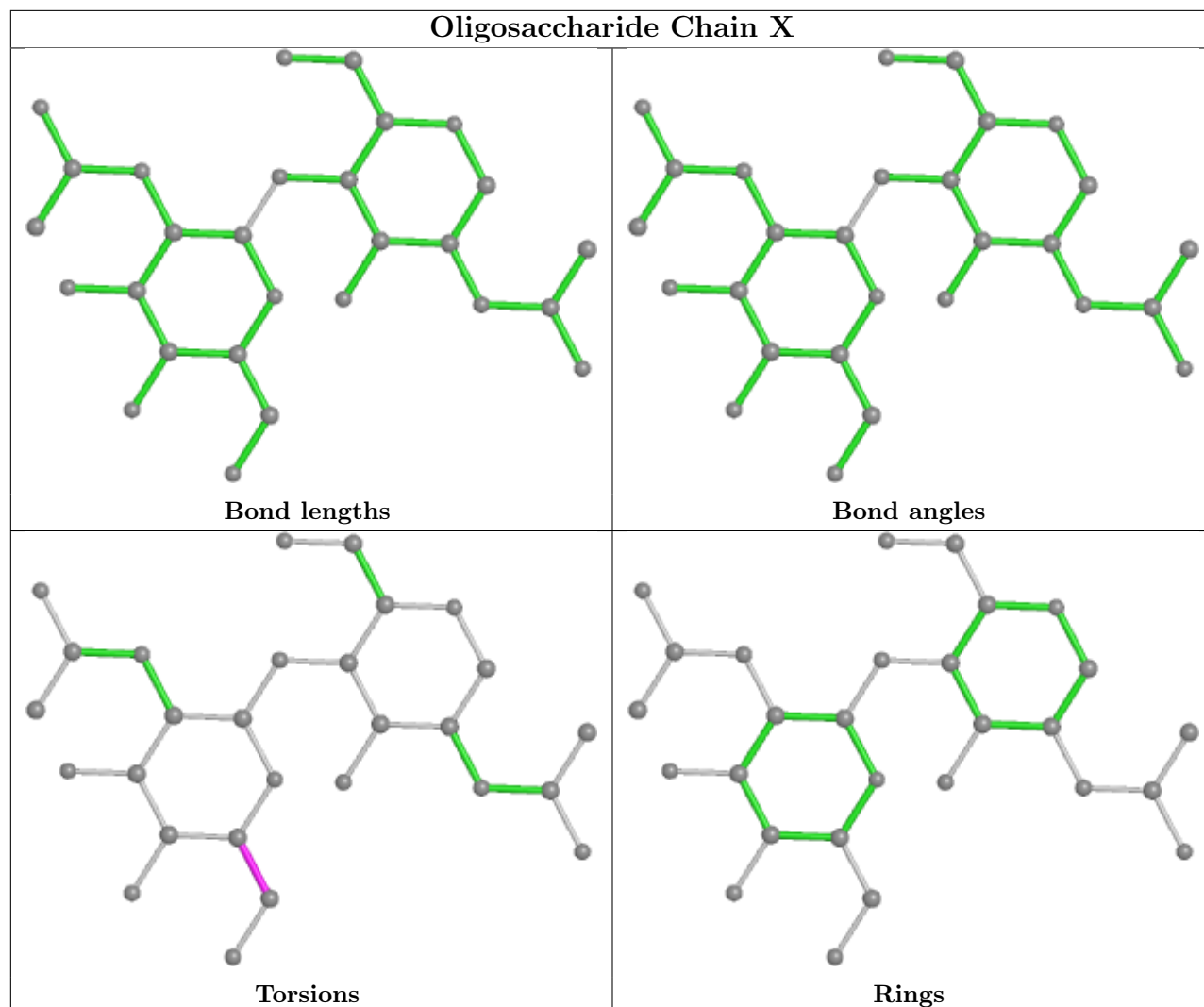


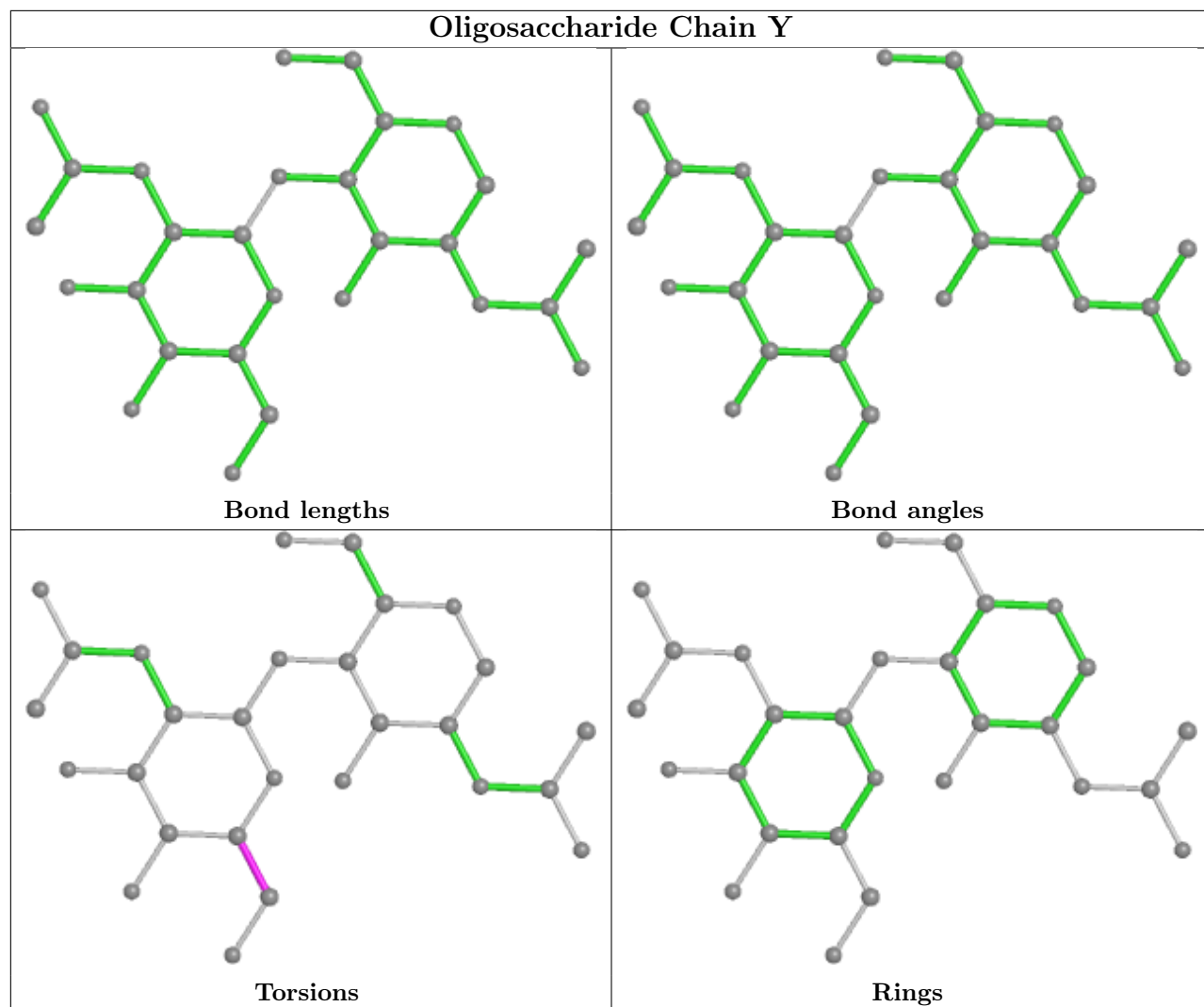


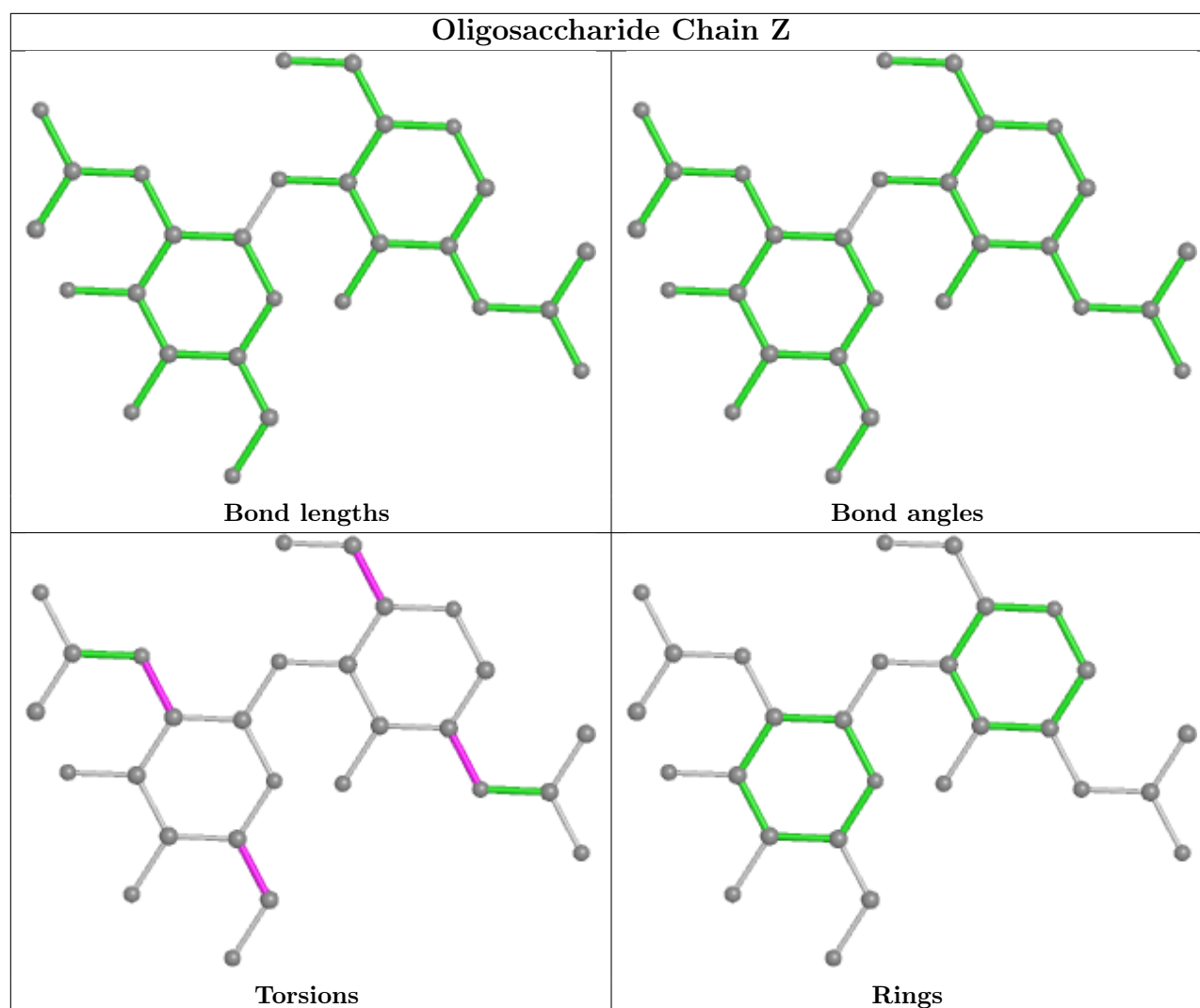












## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	B	1306	1	14,14,15	0.25	0	17,19,21	0.55	0
4	NAG	B	1302	1	14,14,15	0.25	0	17,19,21	0.54	0
4	NAG	A	1303	1	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	A	1305	1	14,14,15	0.29	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	1307	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	B	1305	1	14,14,15	0.30	0	17,19,21	0.46	0
4	NAG	C	1305	1	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	B	1308	1	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	C	1306	1	14,14,15	0.48	0	17,19,21	0.35	0
4	NAG	C	1304	1	14,14,15	0.30	0	17,19,21	0.43	0
4	NAG	B	1309	1	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	C	1301	1	14,14,15	0.49	0	17,19,21	0.68	1 (5%)
4	NAG	B	1303	1	14,14,15	0.25	0	17,19,21	0.39	0
4	NAG	C	1303	1	14,14,15	0.28	0	17,19,21	0.36	0
4	NAG	A	1306	1	14,14,15	0.26	0	17,19,21	0.55	0
4	NAG	A	1304	1	14,14,15	0.29	0	17,19,21	0.46	0
4	NAG	C	1307	1	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	A	1302	1	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	B	1304	1	14,14,15	0.19	0	17,19,21	0.45	0
4	NAG	A	1301	1	14,14,15	0.25	0	17,19,21	0.39	0
4	NAG	C	1308	1	14,14,15	0.18	0	17,19,21	0.49	0
4	NAG	B	1301	1	14,14,15	0.24	0	17,19,21	0.57	0
4	NAG	C	1302	1	14,14,15	0.29	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	B	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1301	NAG	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1309	NAG	O5-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	B	1309	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	B	1308	NAG	C8-C7-N2-C2
4	B	1308	NAG	O7-C7-N2-C2
4	B	1309	NAG	C8-C7-N2-C2
4	B	1309	NAG	O7-C7-N2-C2
4	A	1303	NAG	C4-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1302	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	A	1306	NAG	C3-C2-N2-C7
4	B	1301	NAG	C3-C2-N2-C7
4	B	1302	NAG	C3-C2-N2-C7
4	B	1306	NAG	C3-C2-N2-C7
4	C	1301	NAG	C3-C2-N2-C7
4	B	1305	NAG	C1-C2-N2-C7

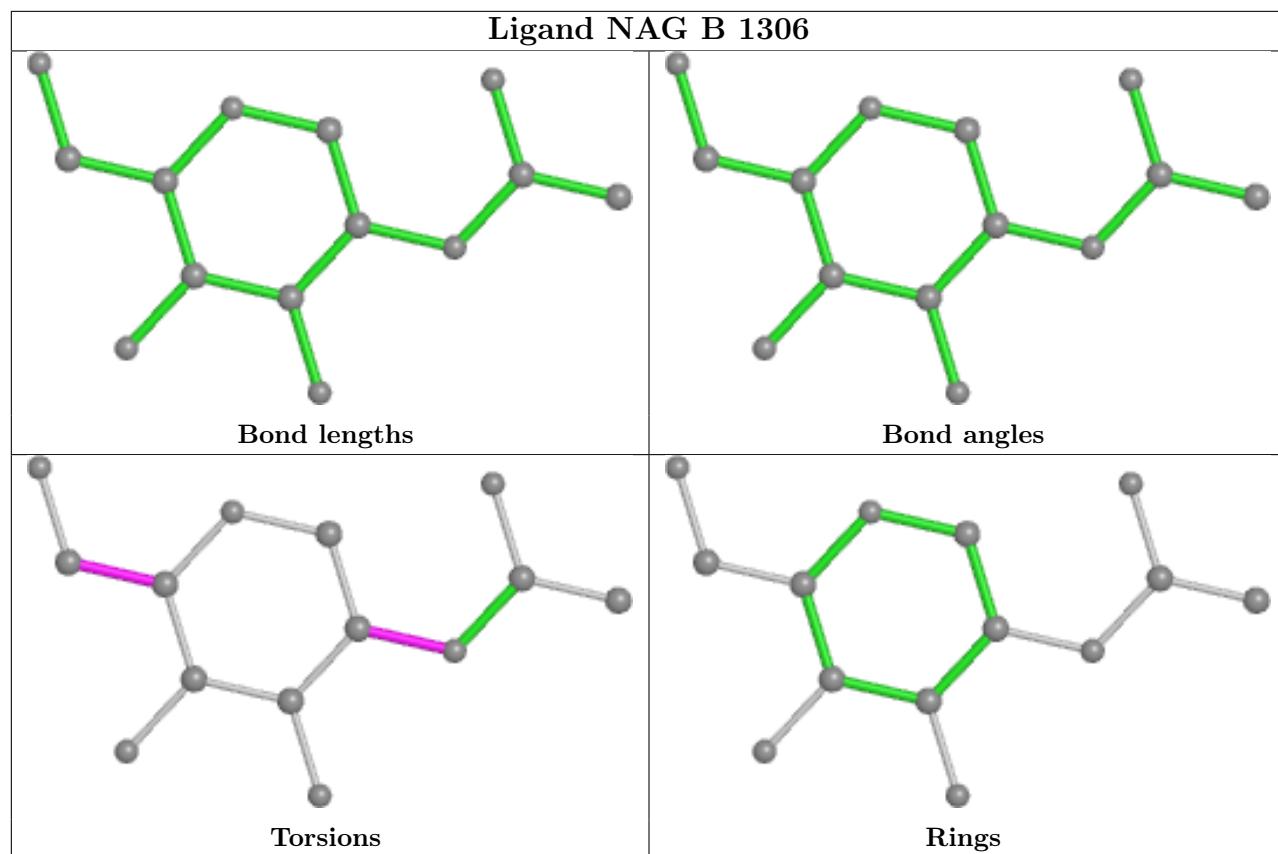
There are no ring outliers.

2 monomers are involved in 2 short contacts:

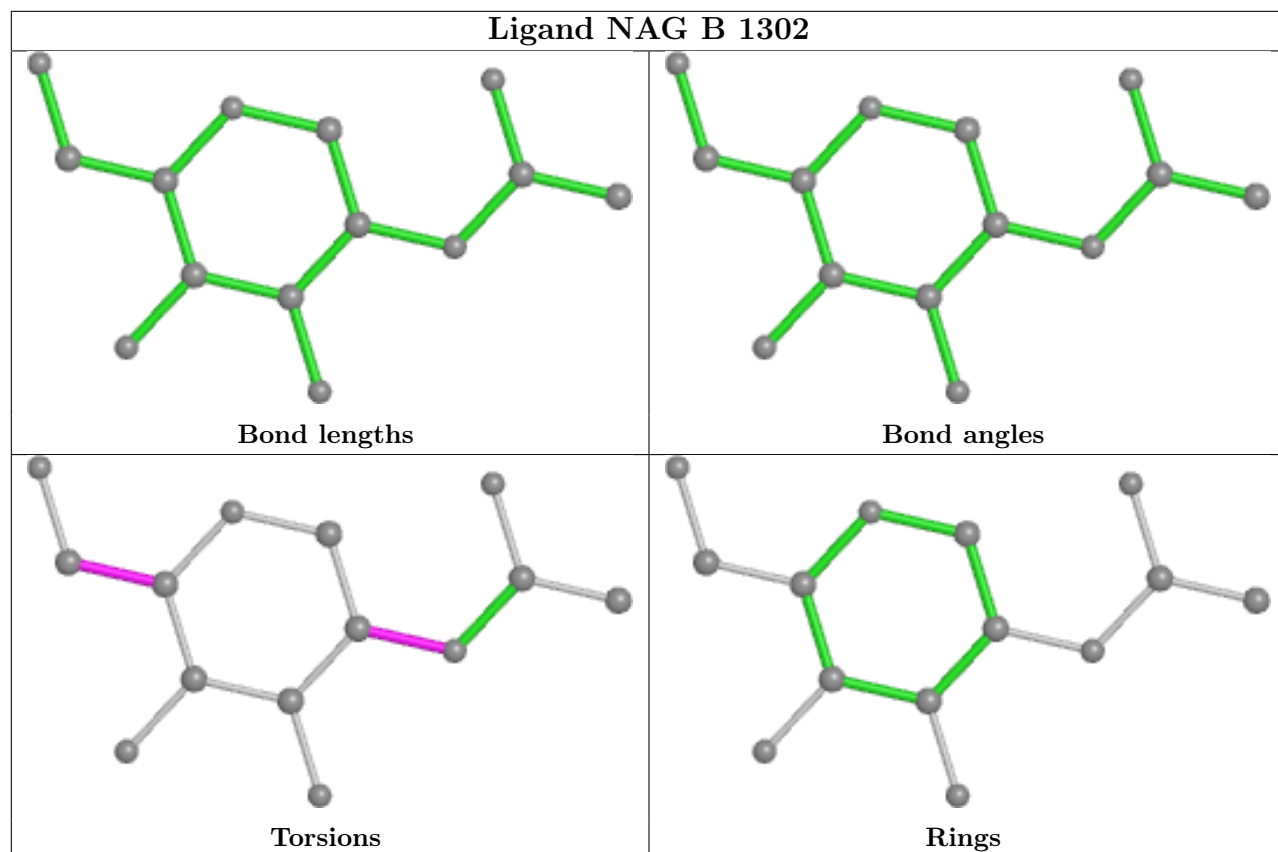
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1301	NAG	1	0
4	A	1301	NAG	1	0

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

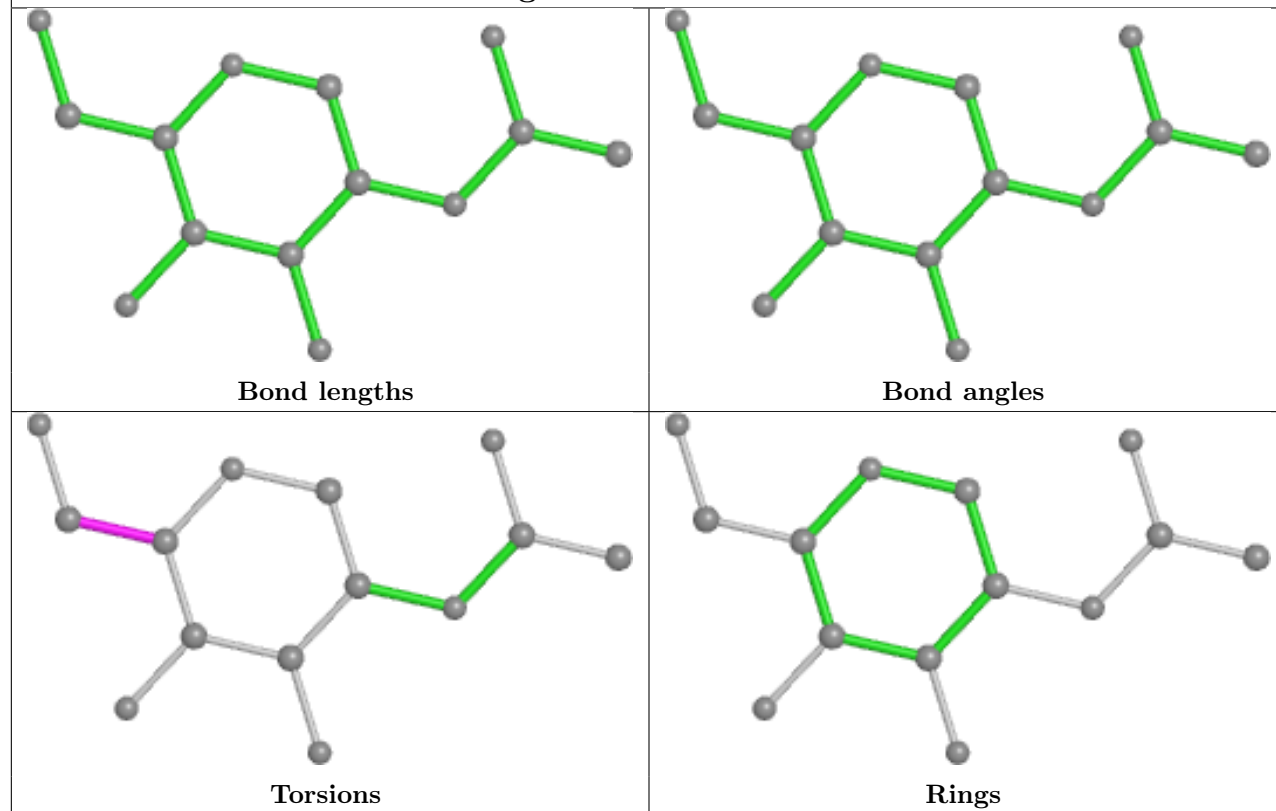
## Ligand NAG B 1306



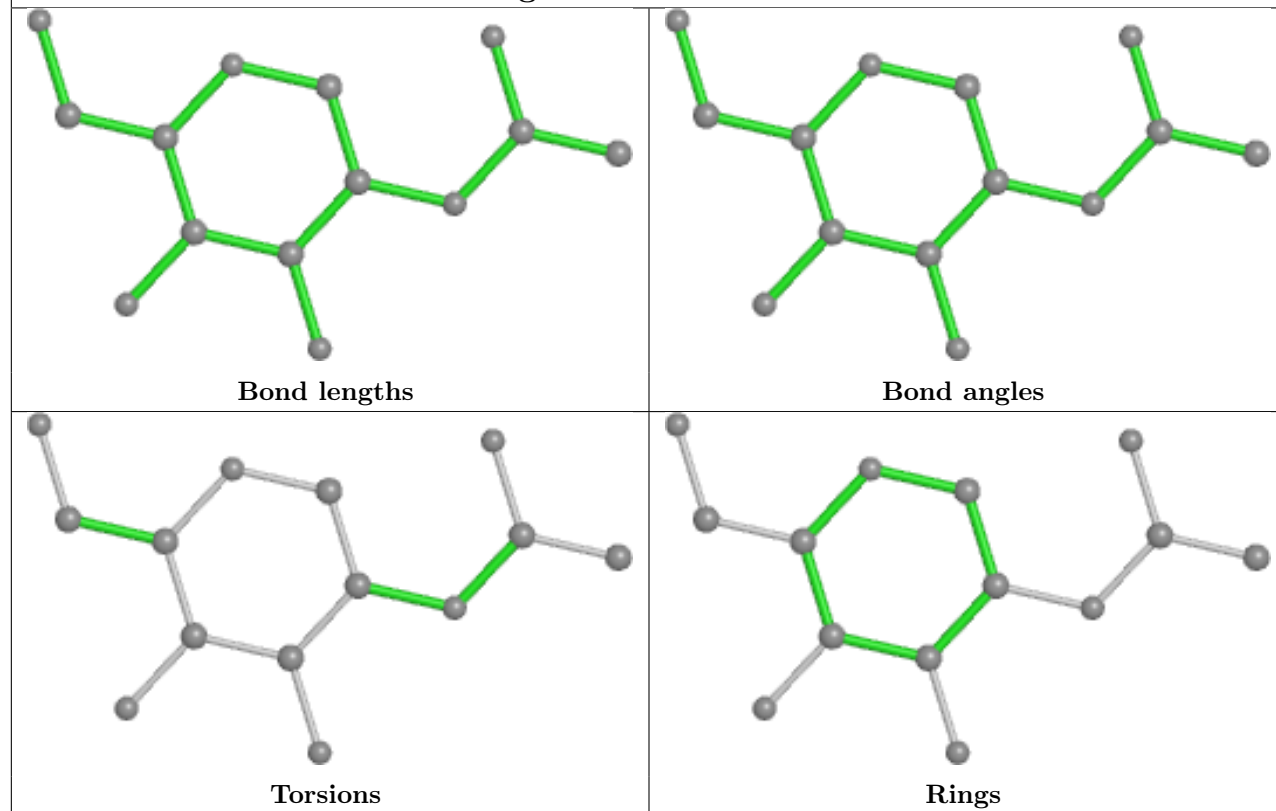
## Ligand NAG B 1302



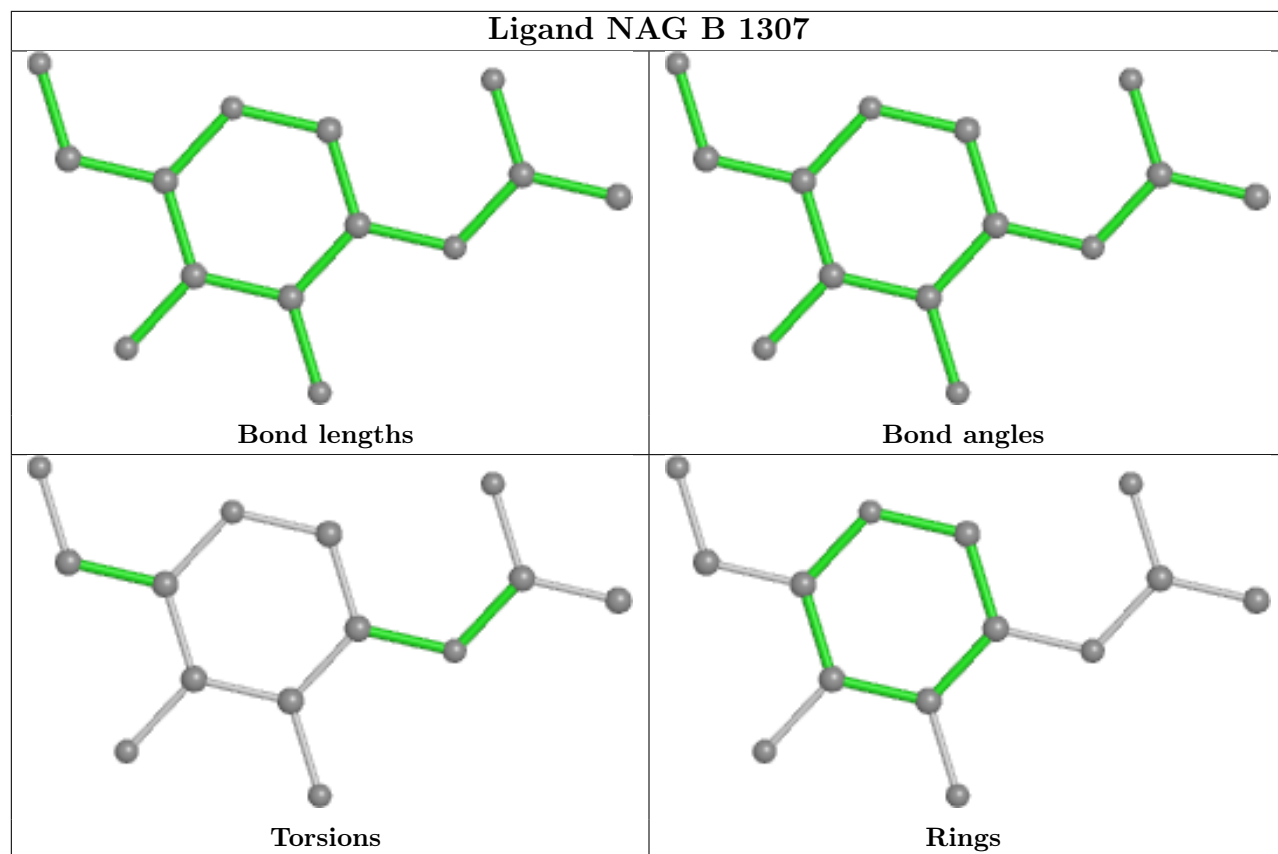
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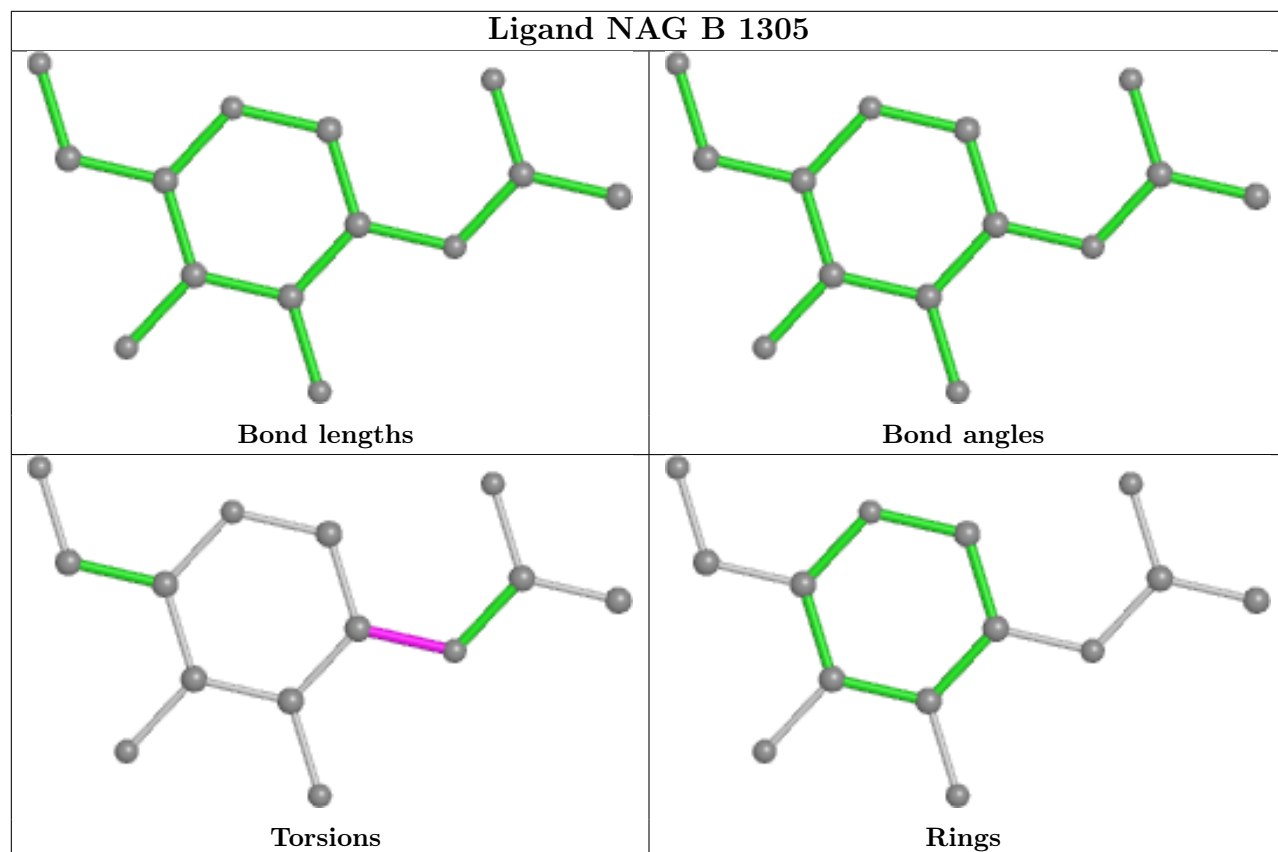
## Ligand NAG A 1305



## Ligand NAG B 1307



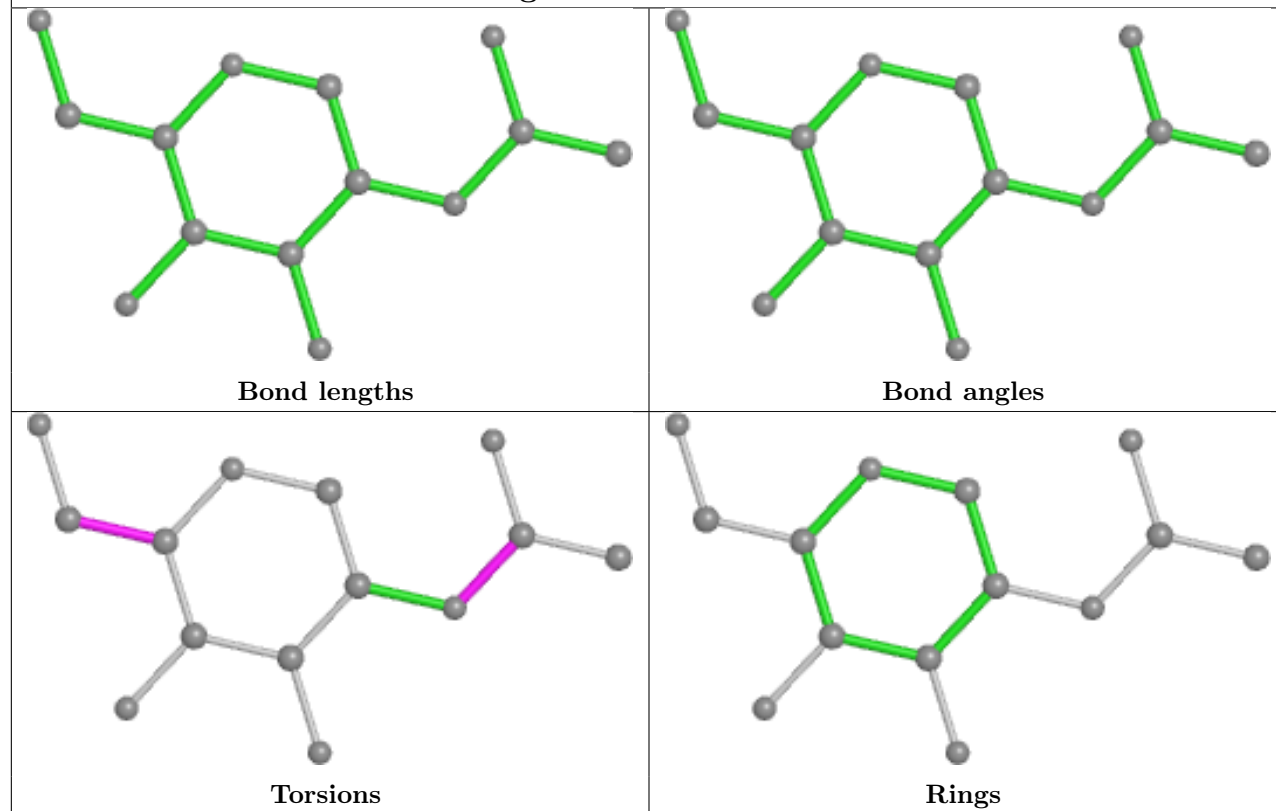
## Ligand NAG B 1305



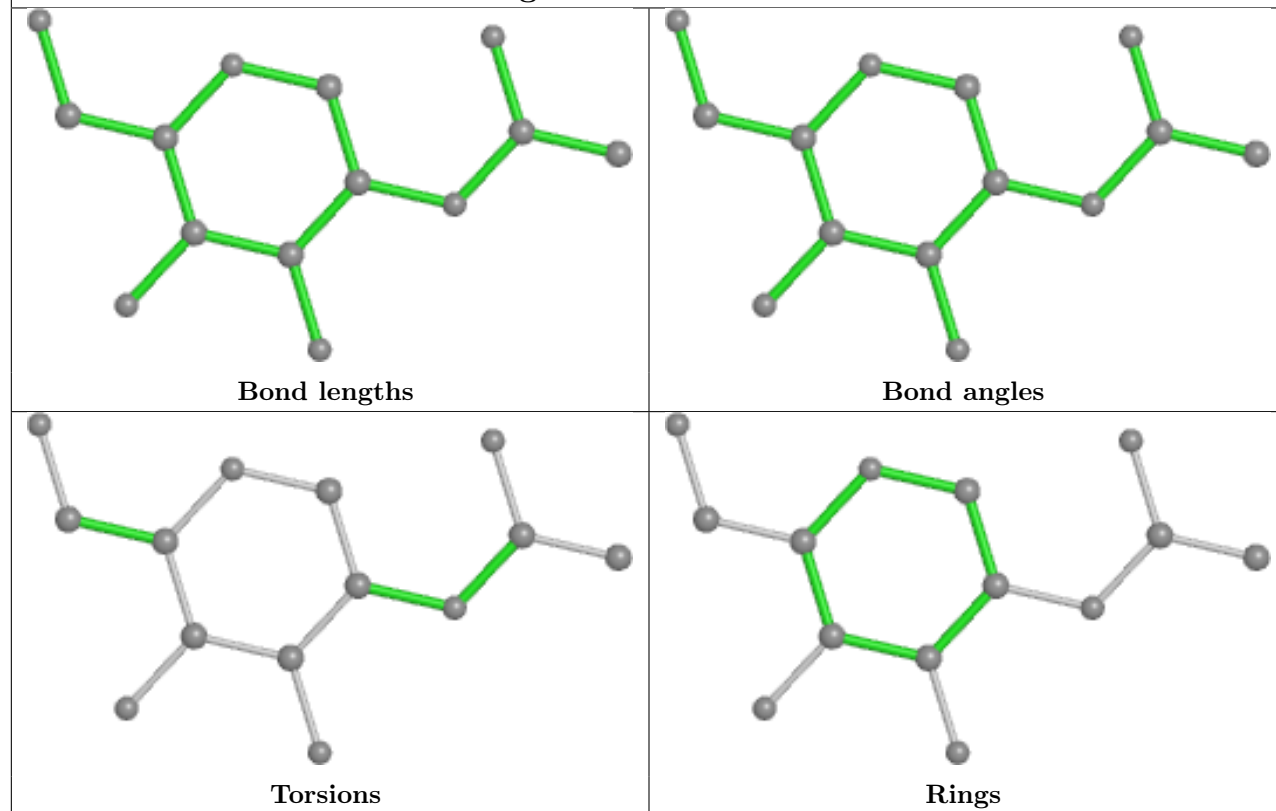
## Ligand NAG C 1305



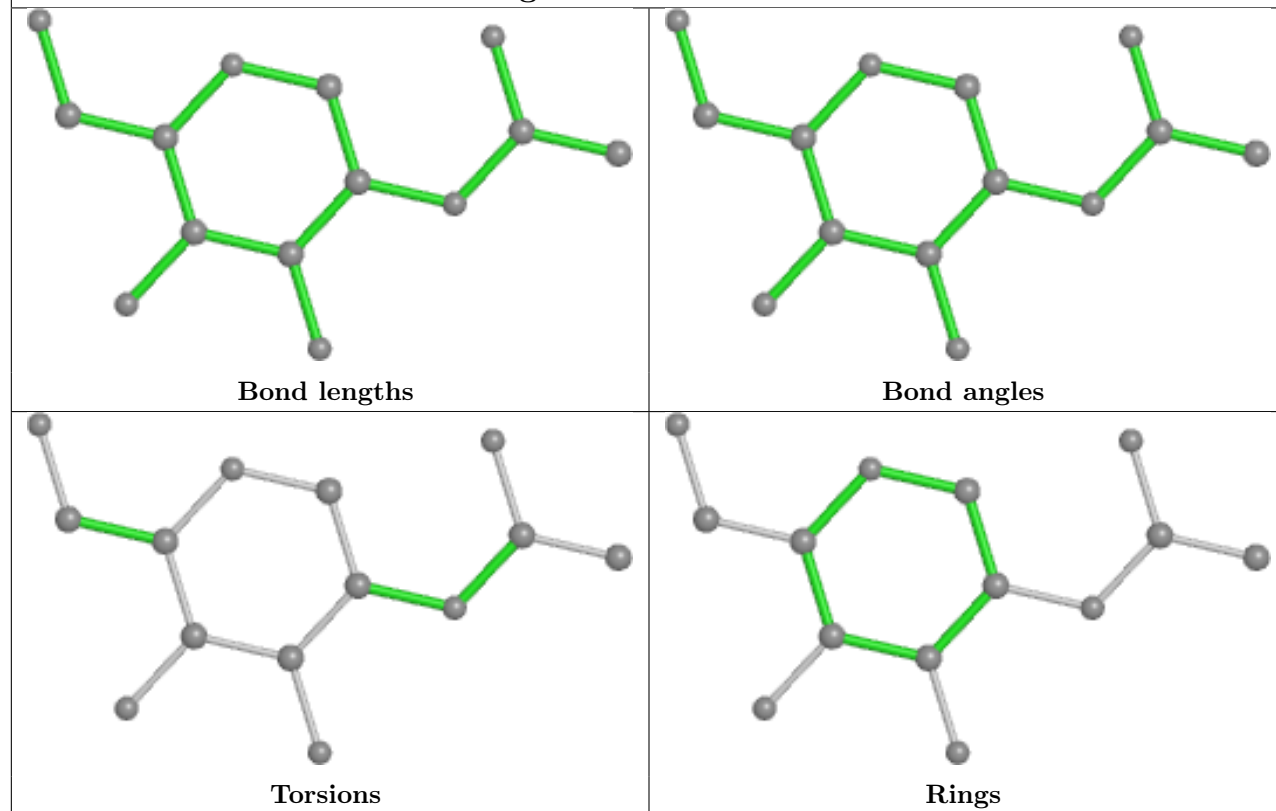
## Ligand NAG B 1308



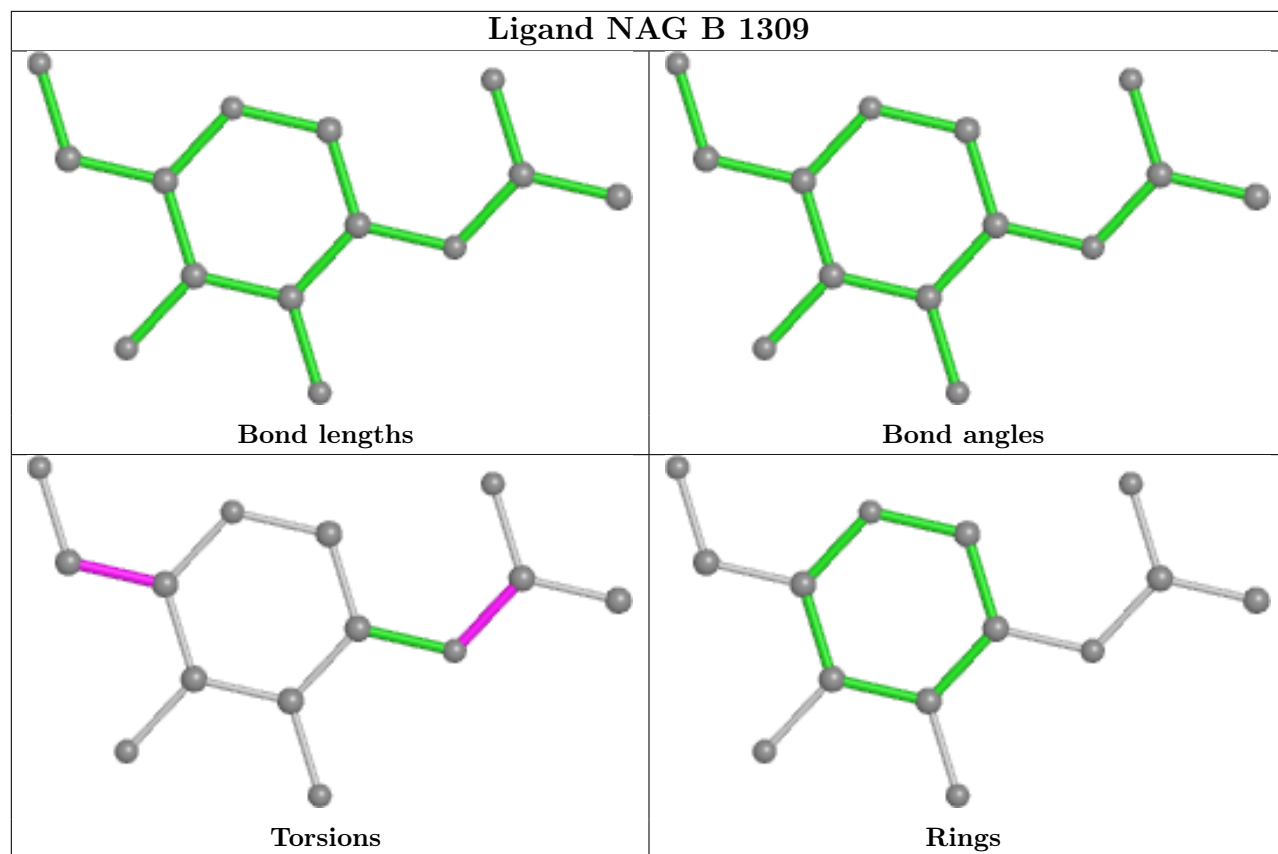
## Ligand NAG C 1306



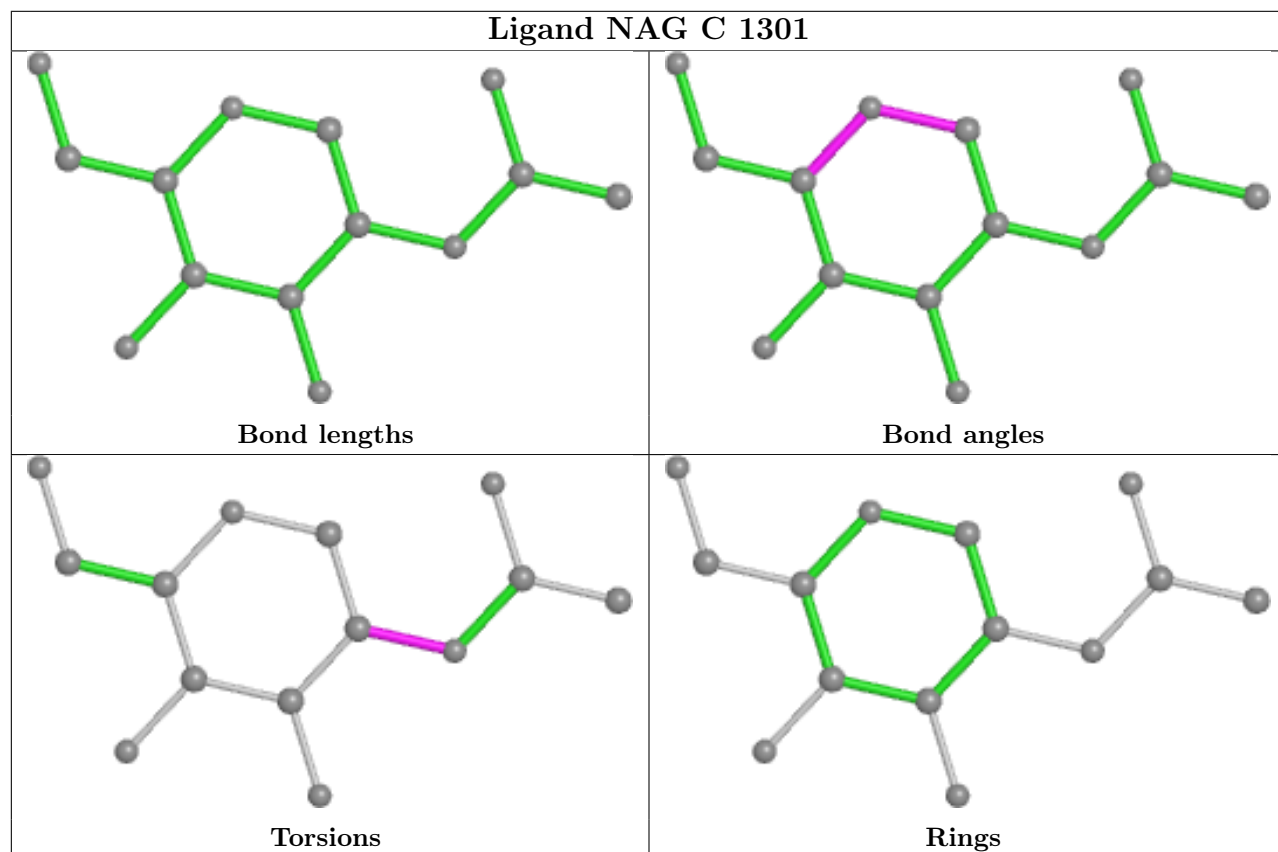
## Ligand NAG C 1304



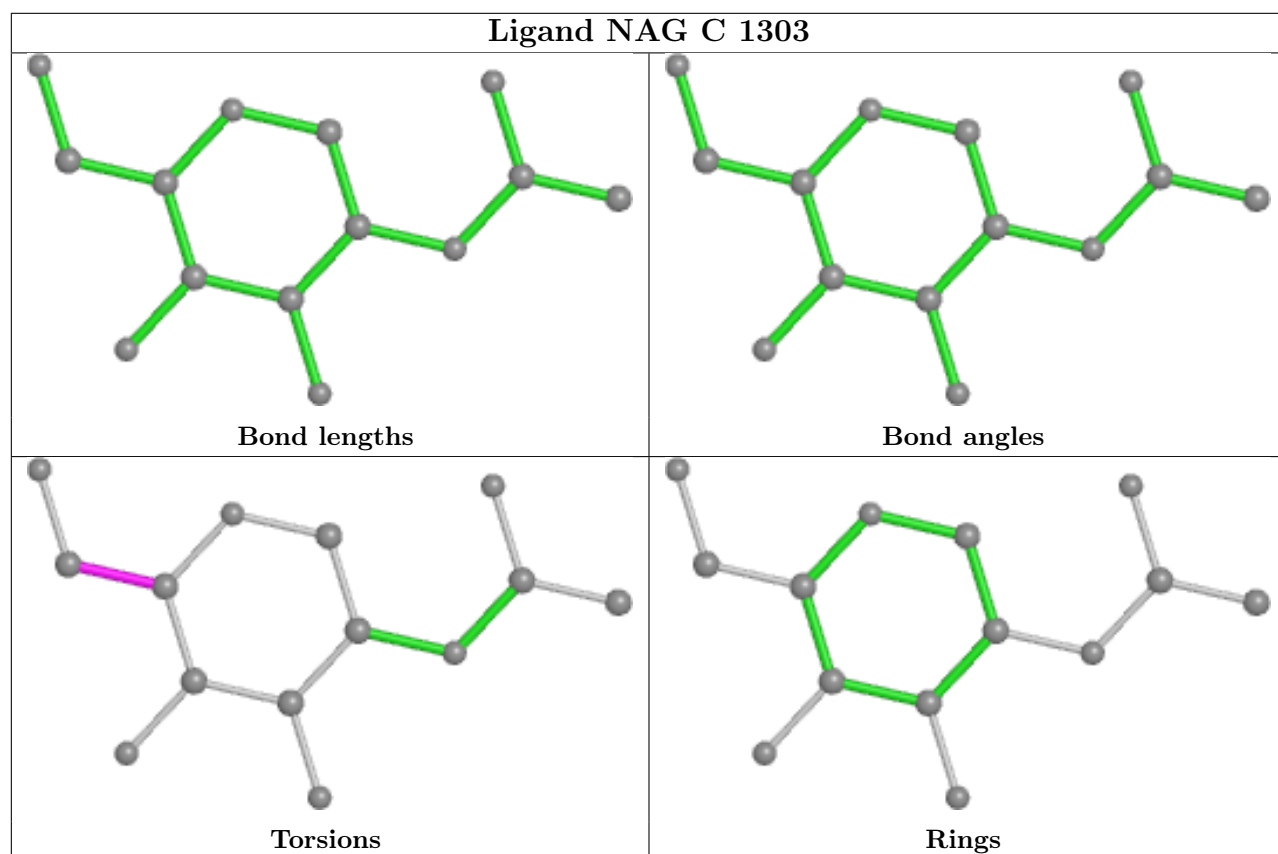
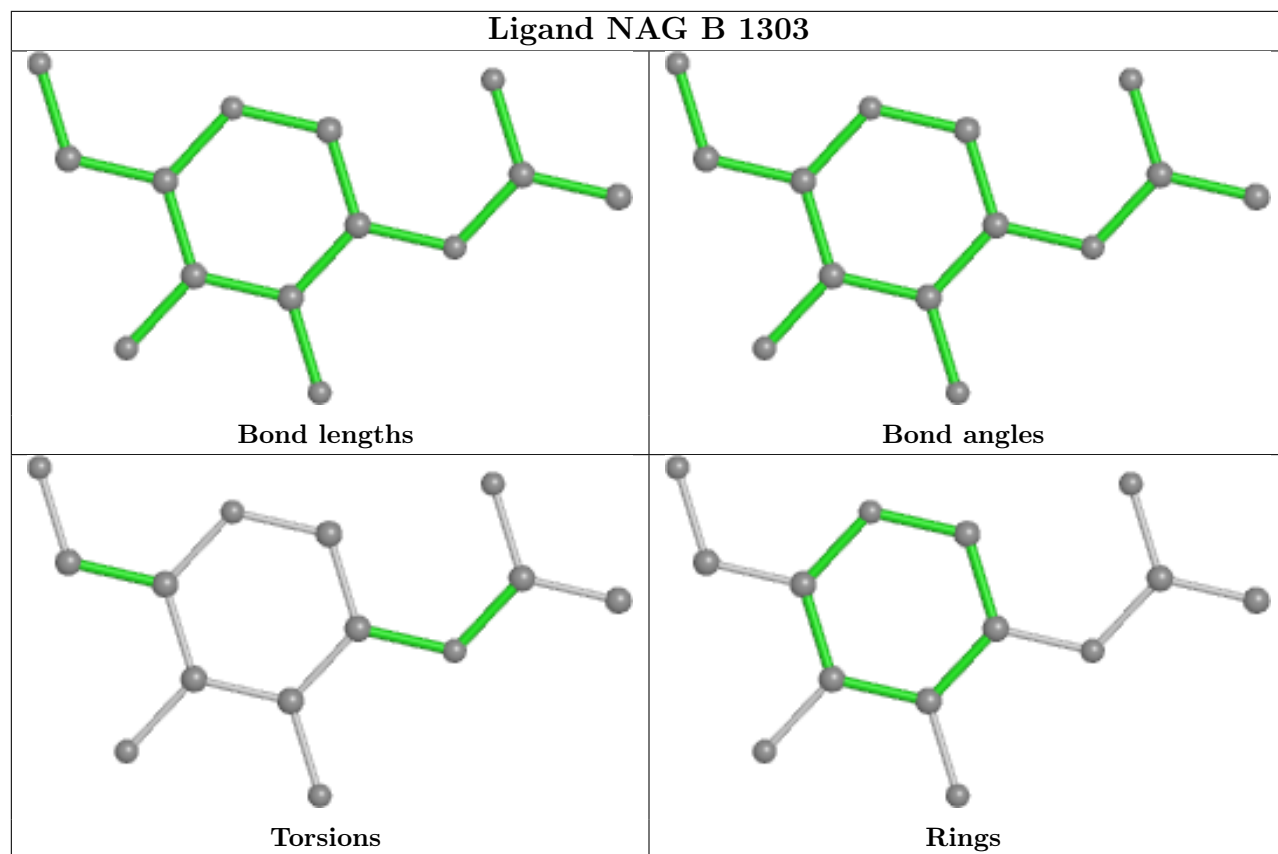
## Ligand NAG B 1309



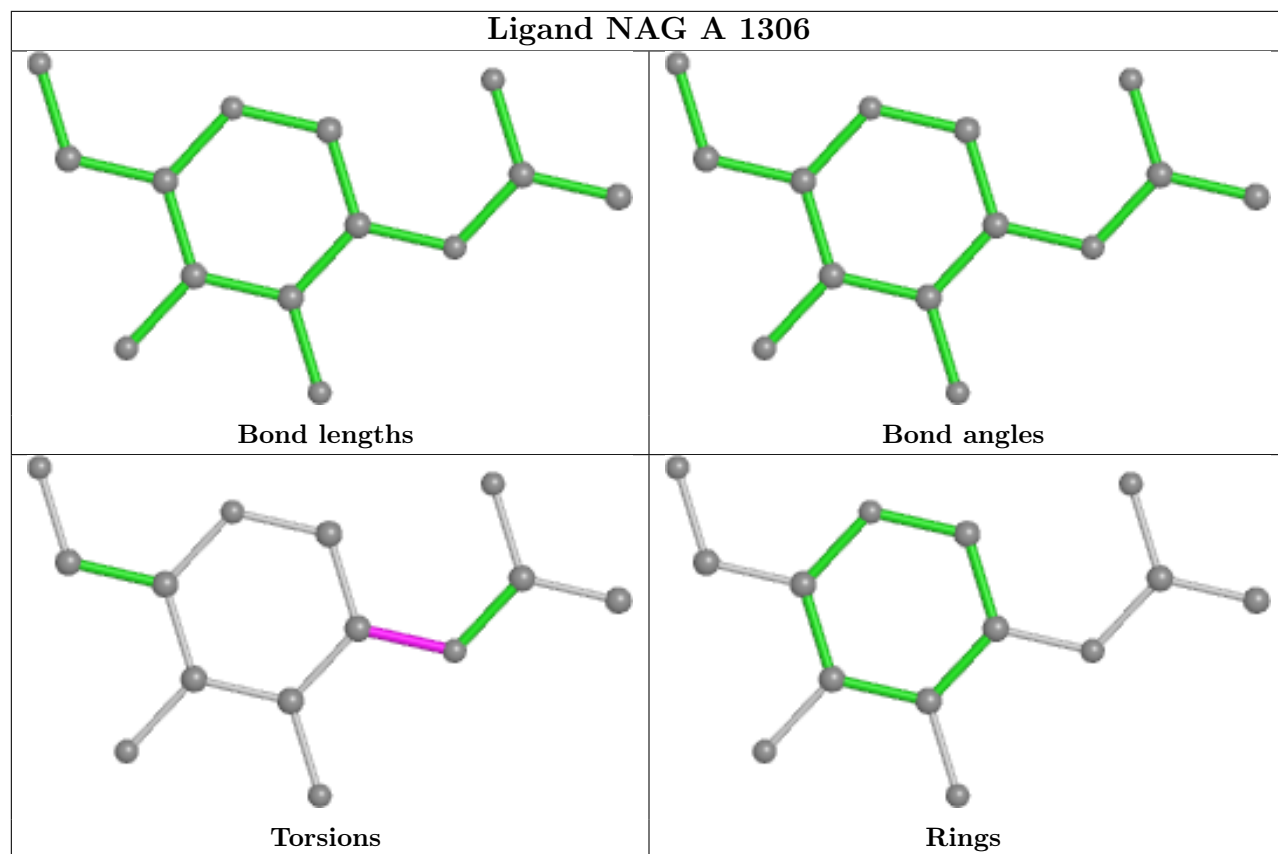
## Ligand NAG C 1301



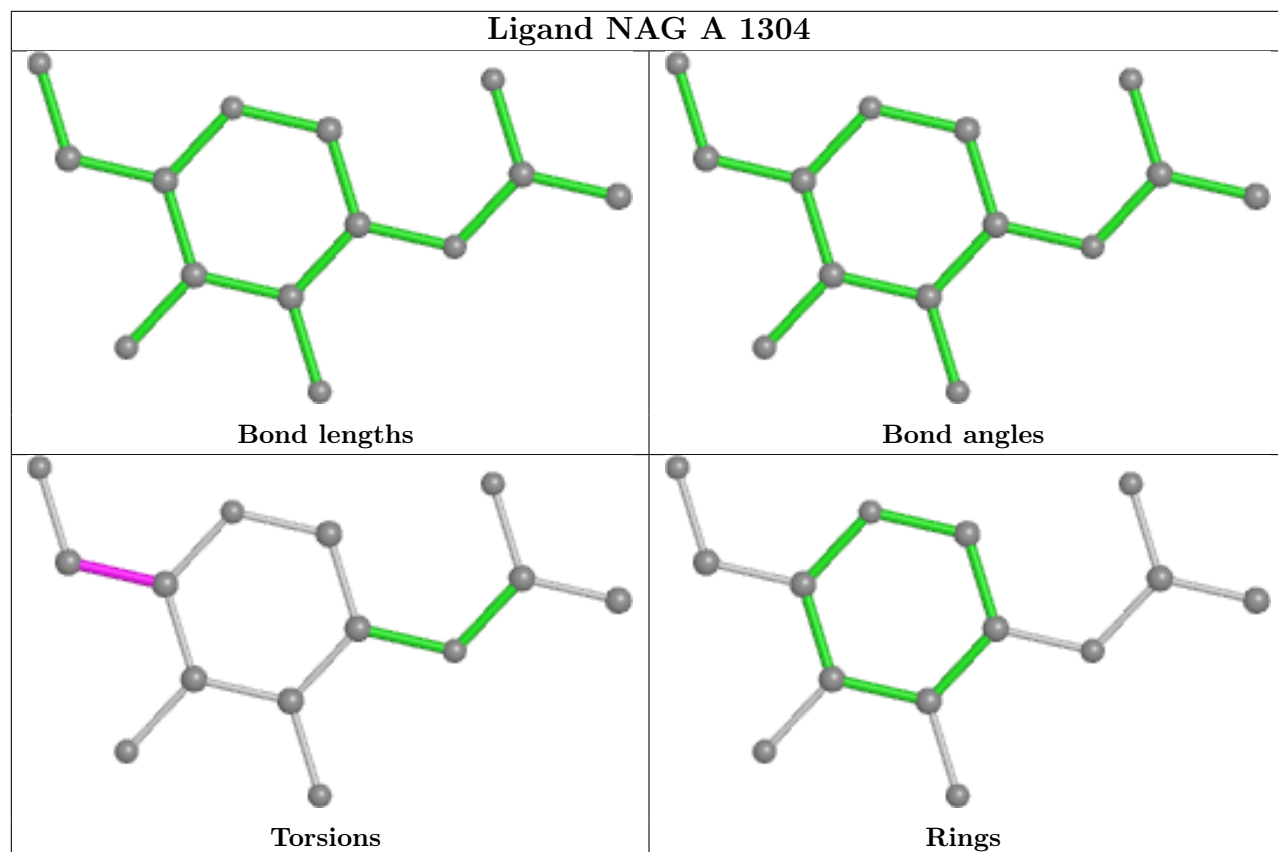


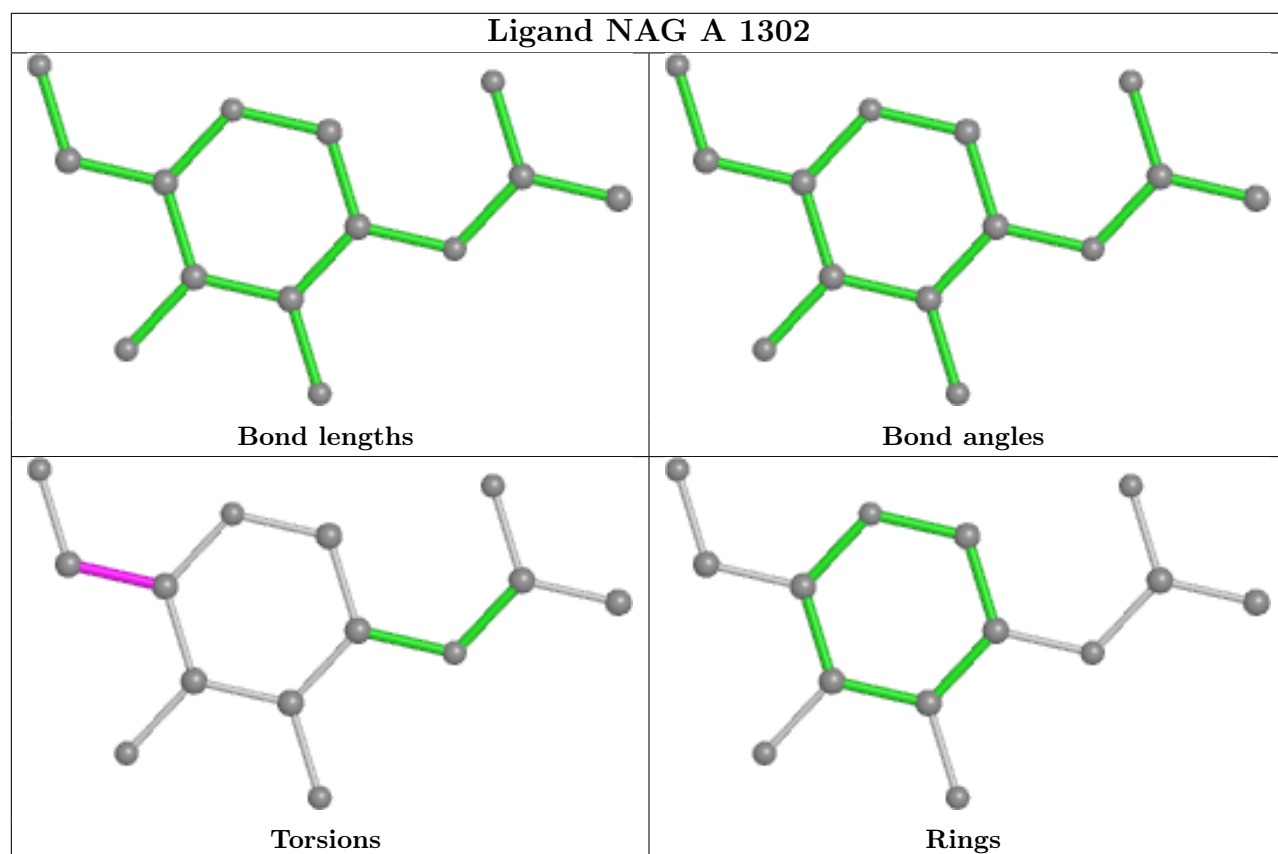
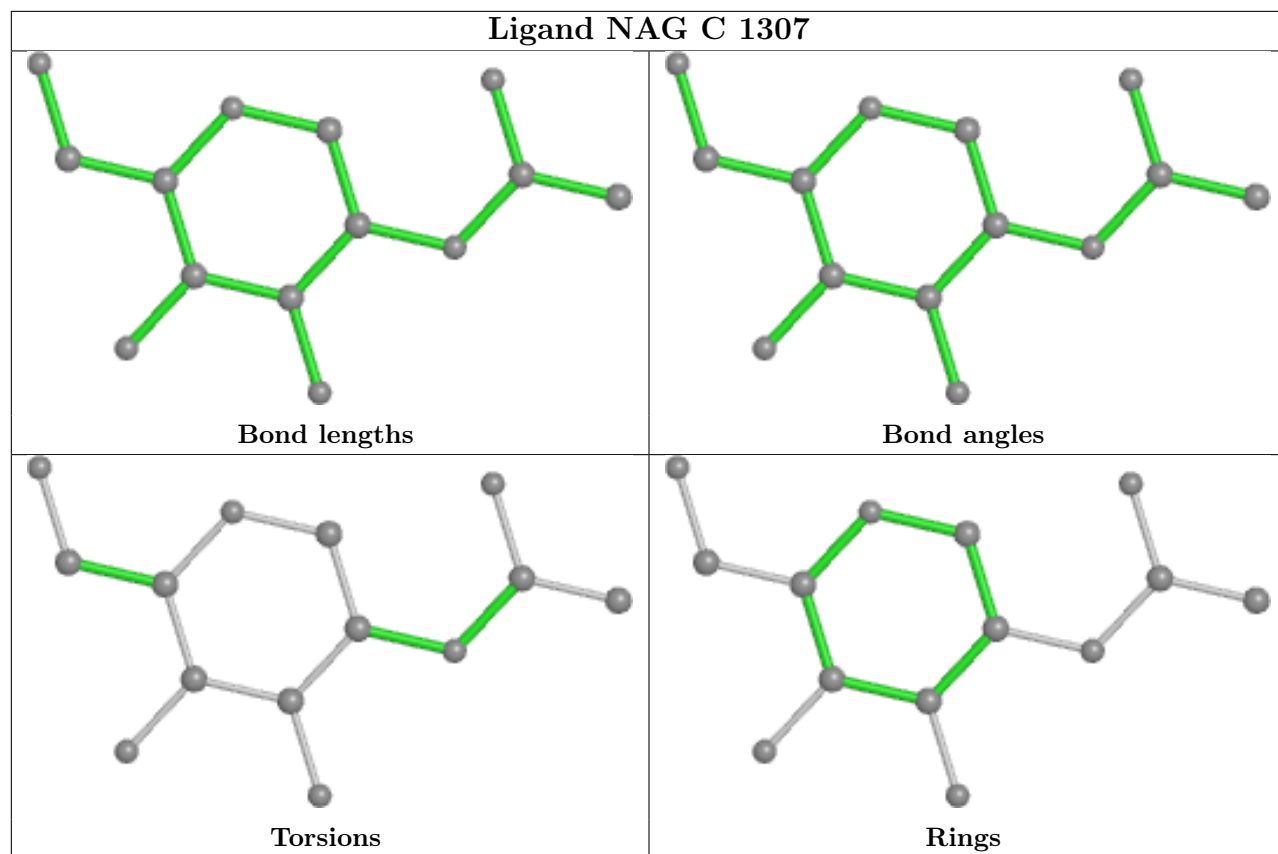


## Ligand NAG A 1306

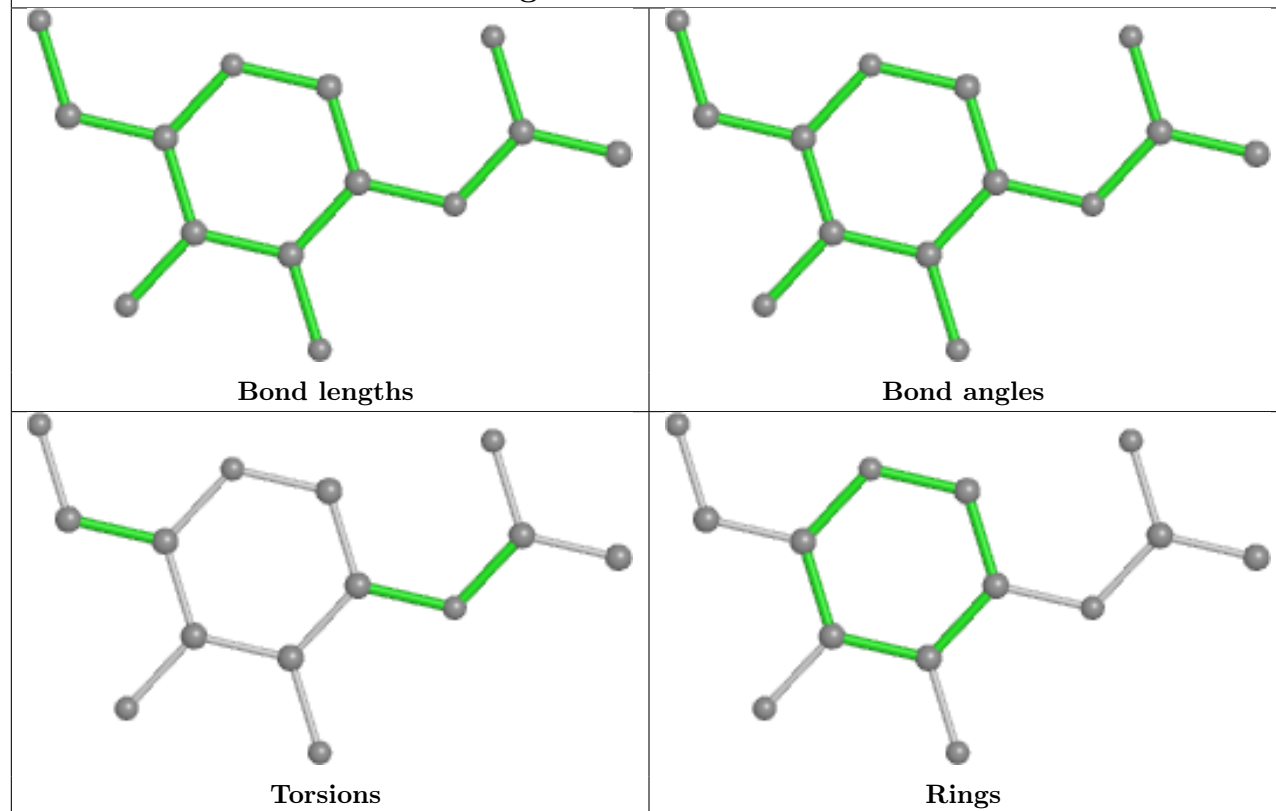


## Ligand NAG A 1304

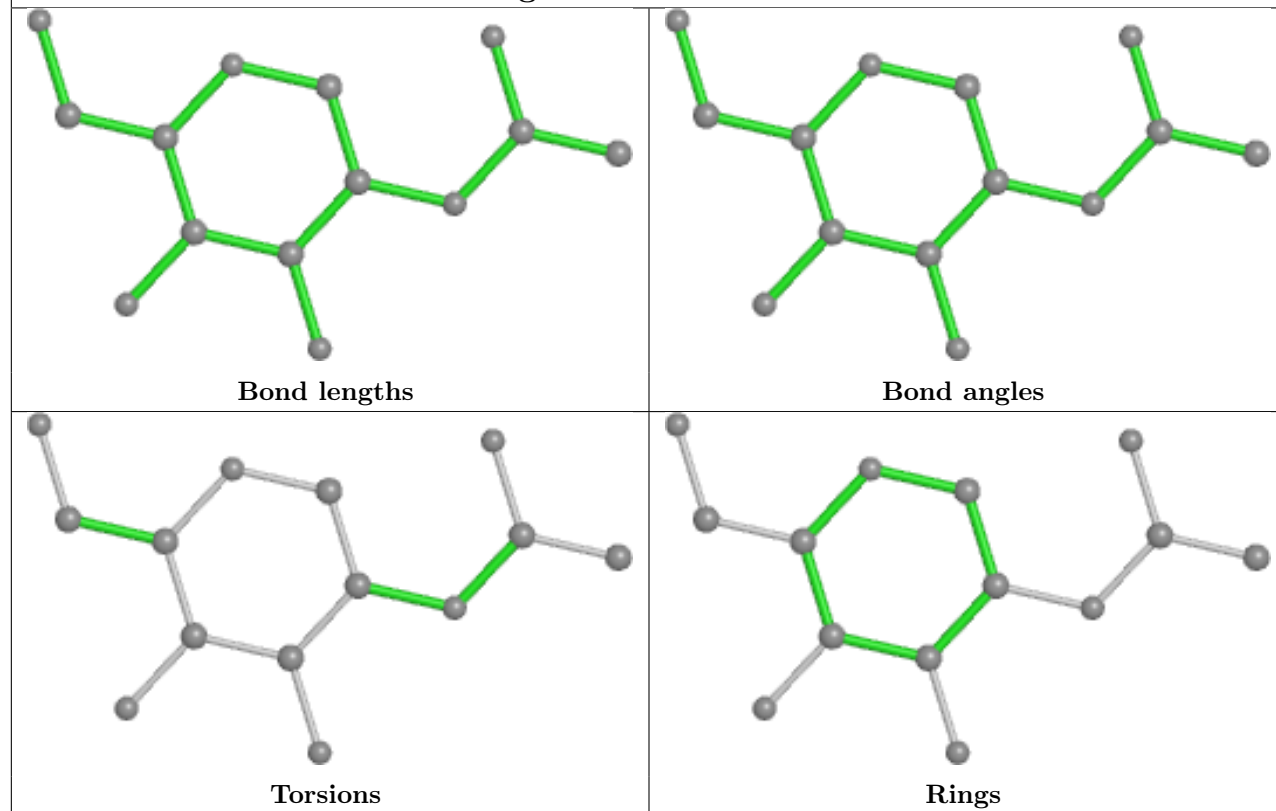




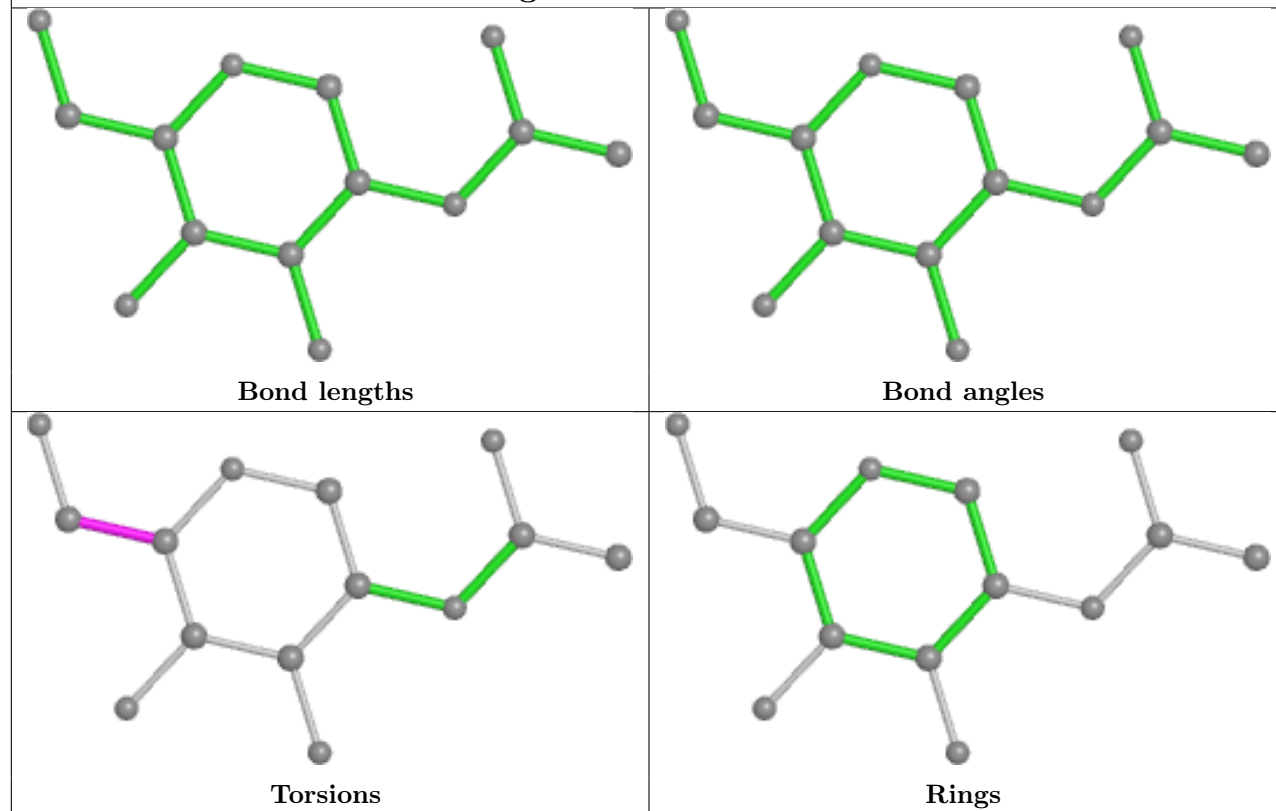
## Ligand NAG B 1304



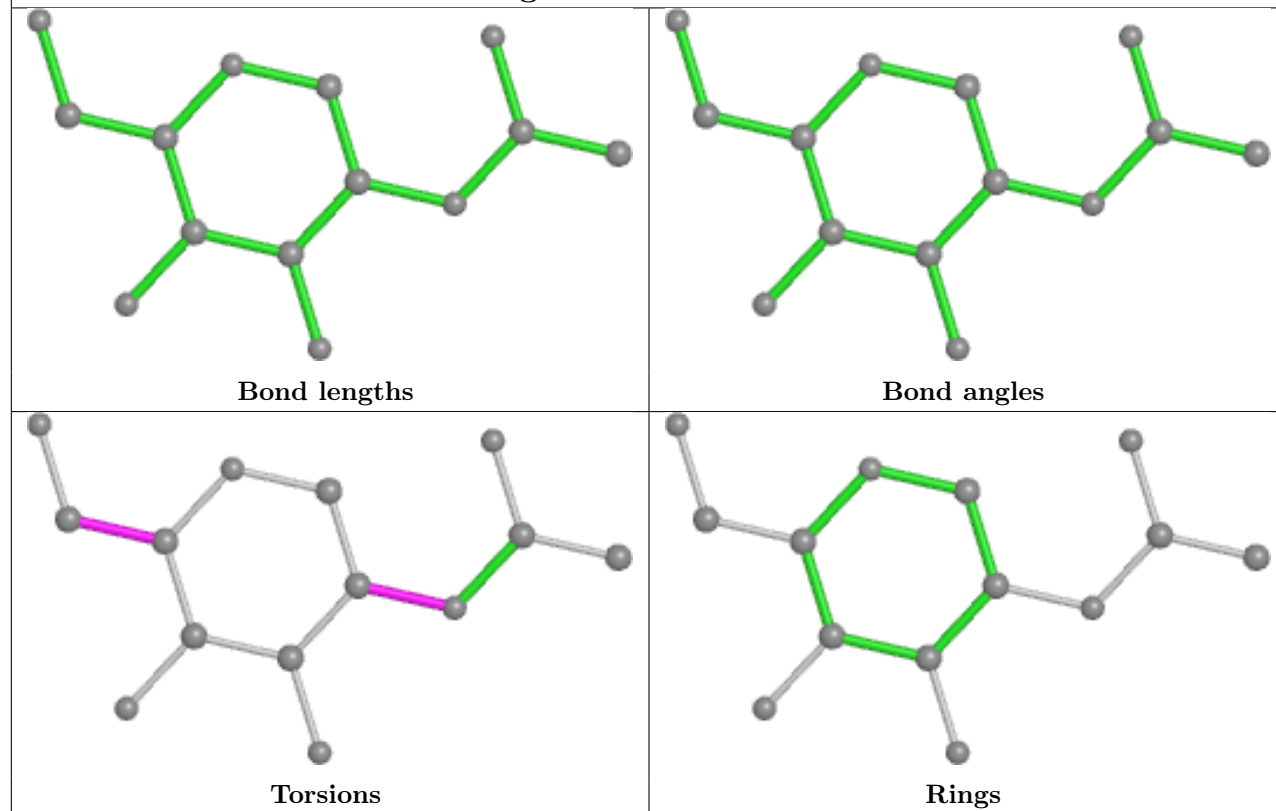
## Ligand NAG A 1301

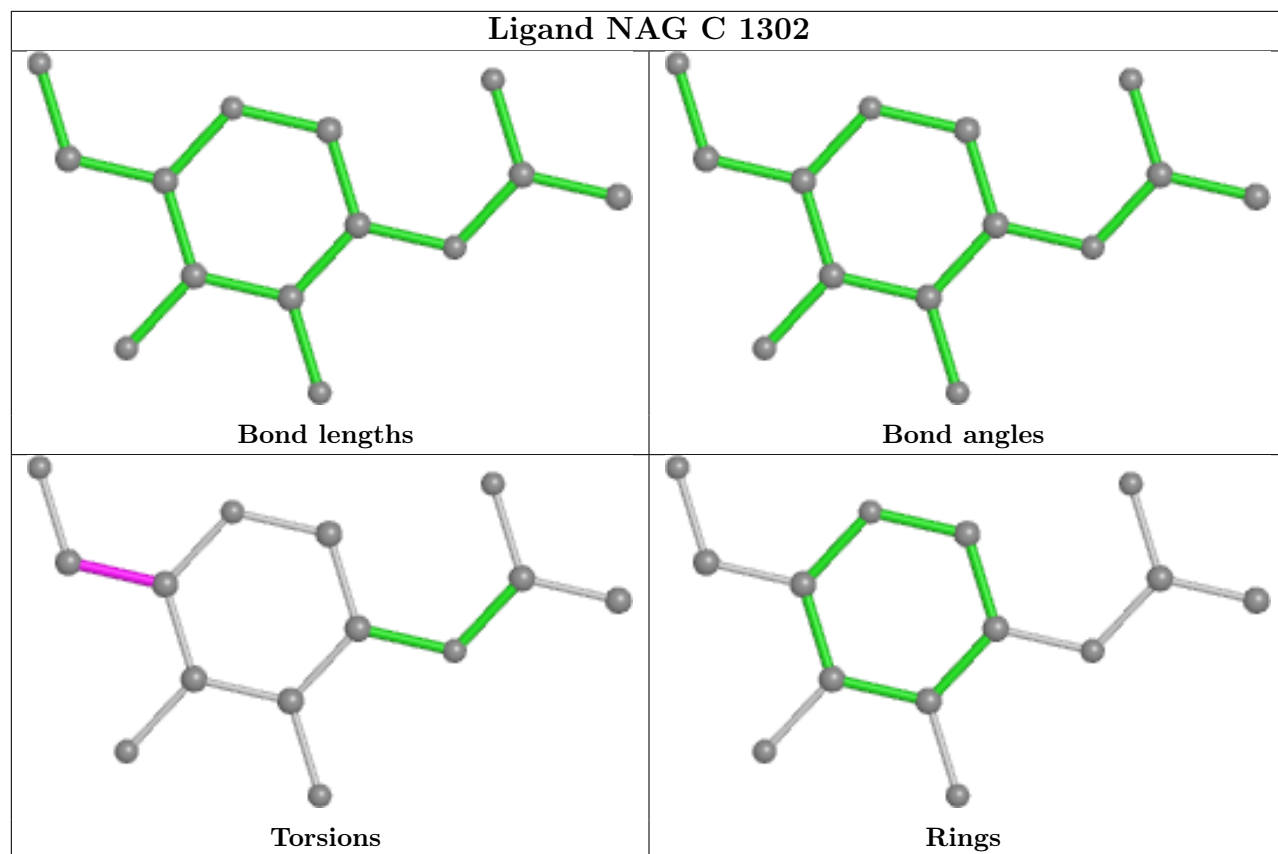


## Ligand NAG C 1308



## Ligand NAG B 1301





## 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.

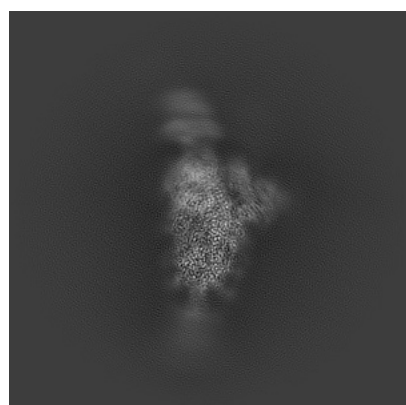
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32726. These allow visual inspection of the internal detail of the map and identification of artifacts.

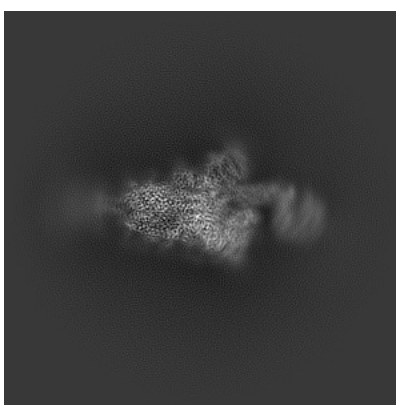
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

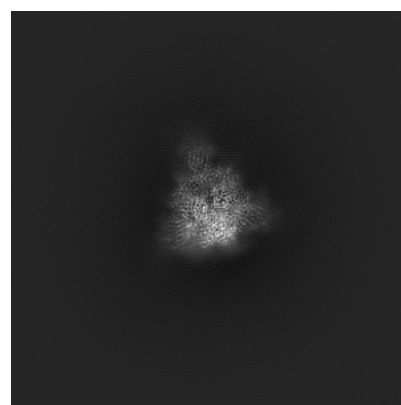
#### 6.1.1 Primary map



X



Y

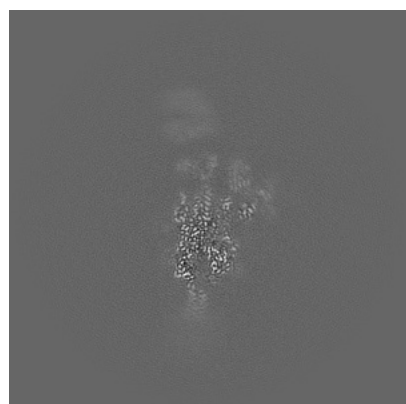


Z

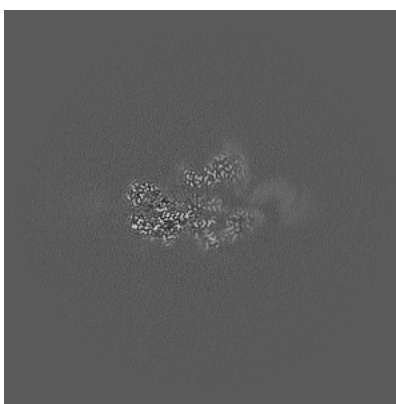
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

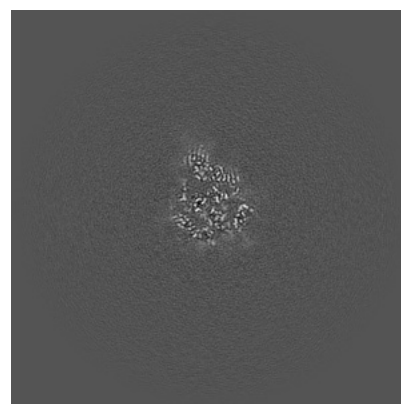
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

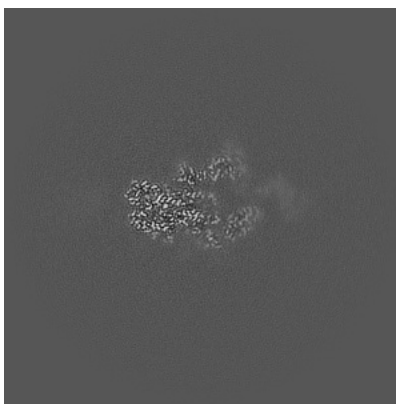
The images above show central slices of the map in three orthogonal directions.

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

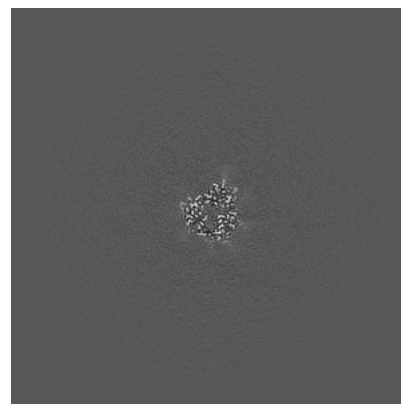
### 6.3.1 Primary map



X Index: 203



Y Index: 203

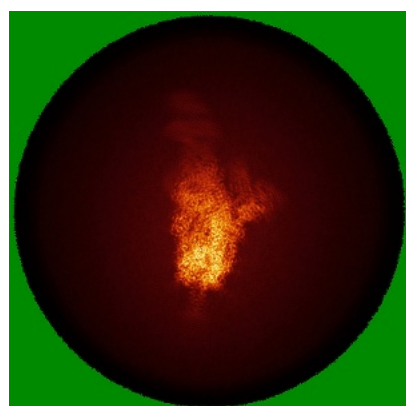


Z Index: 149

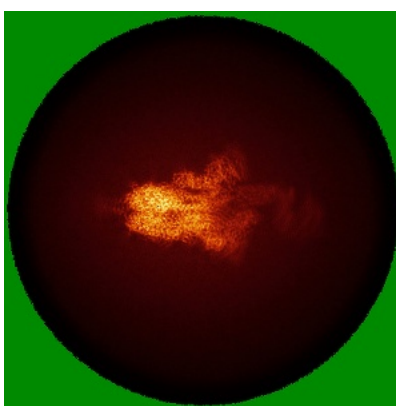
The images above show the largest variance slices of the map in three orthogonal directions.

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

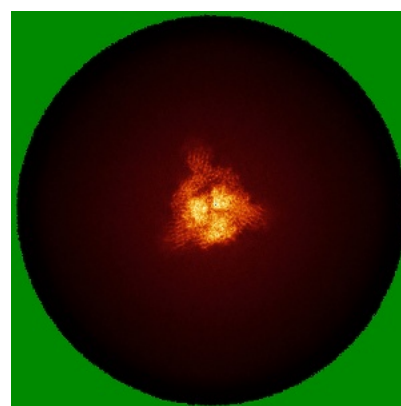
### 6.4.1 Primary map



X



Y



Z

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 0.489. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

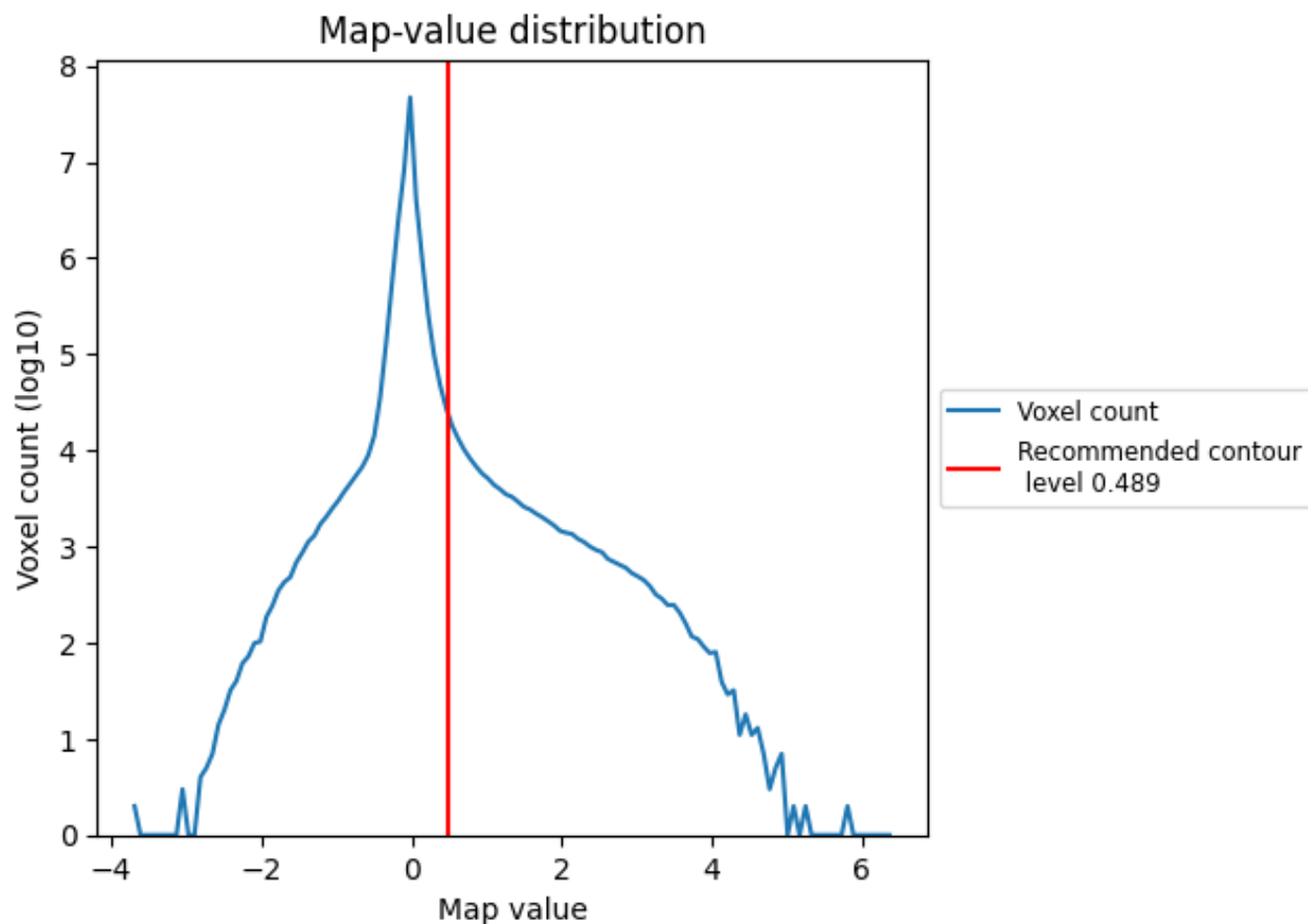
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

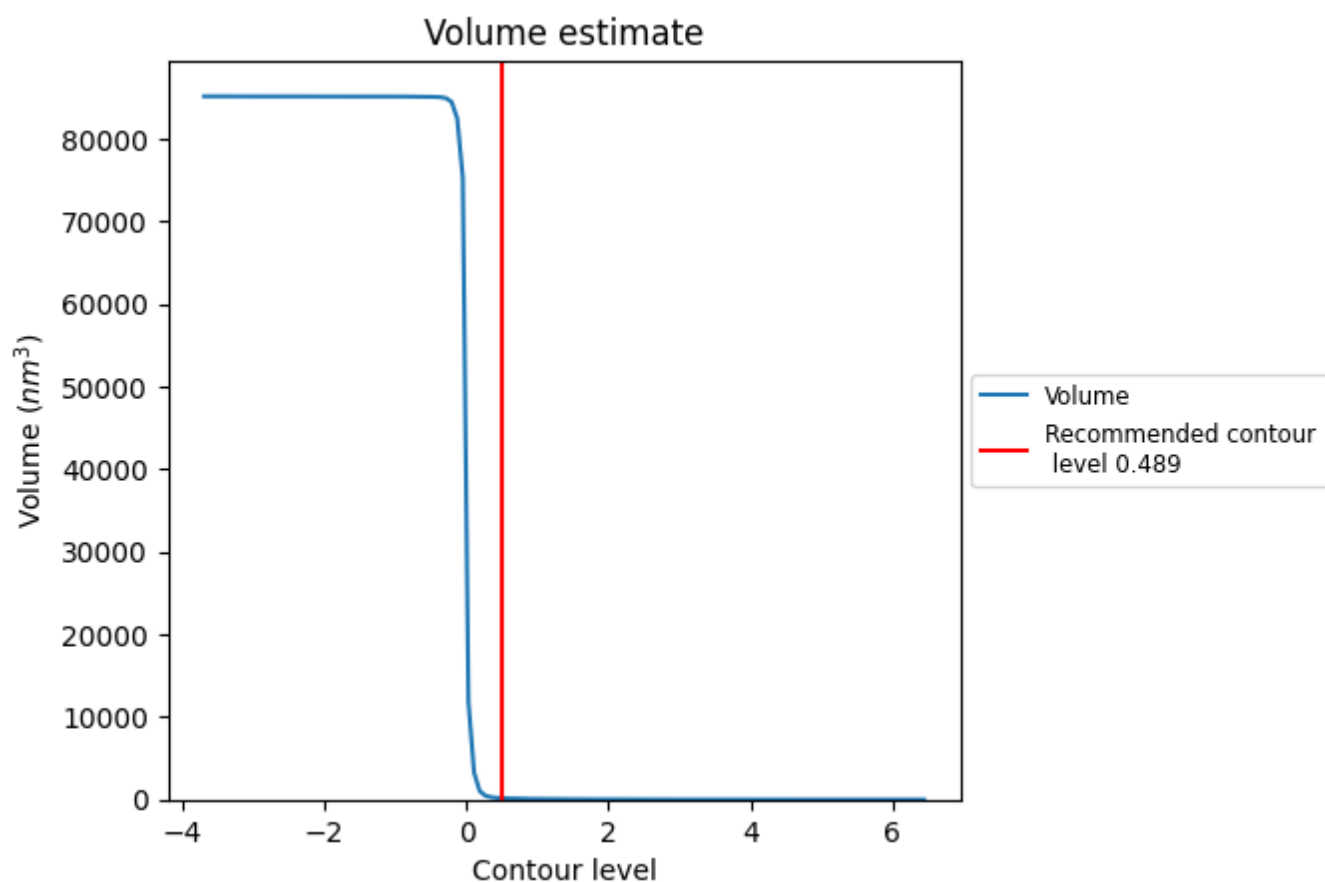
This section contains the results of statistical analysis of the map.

### 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.

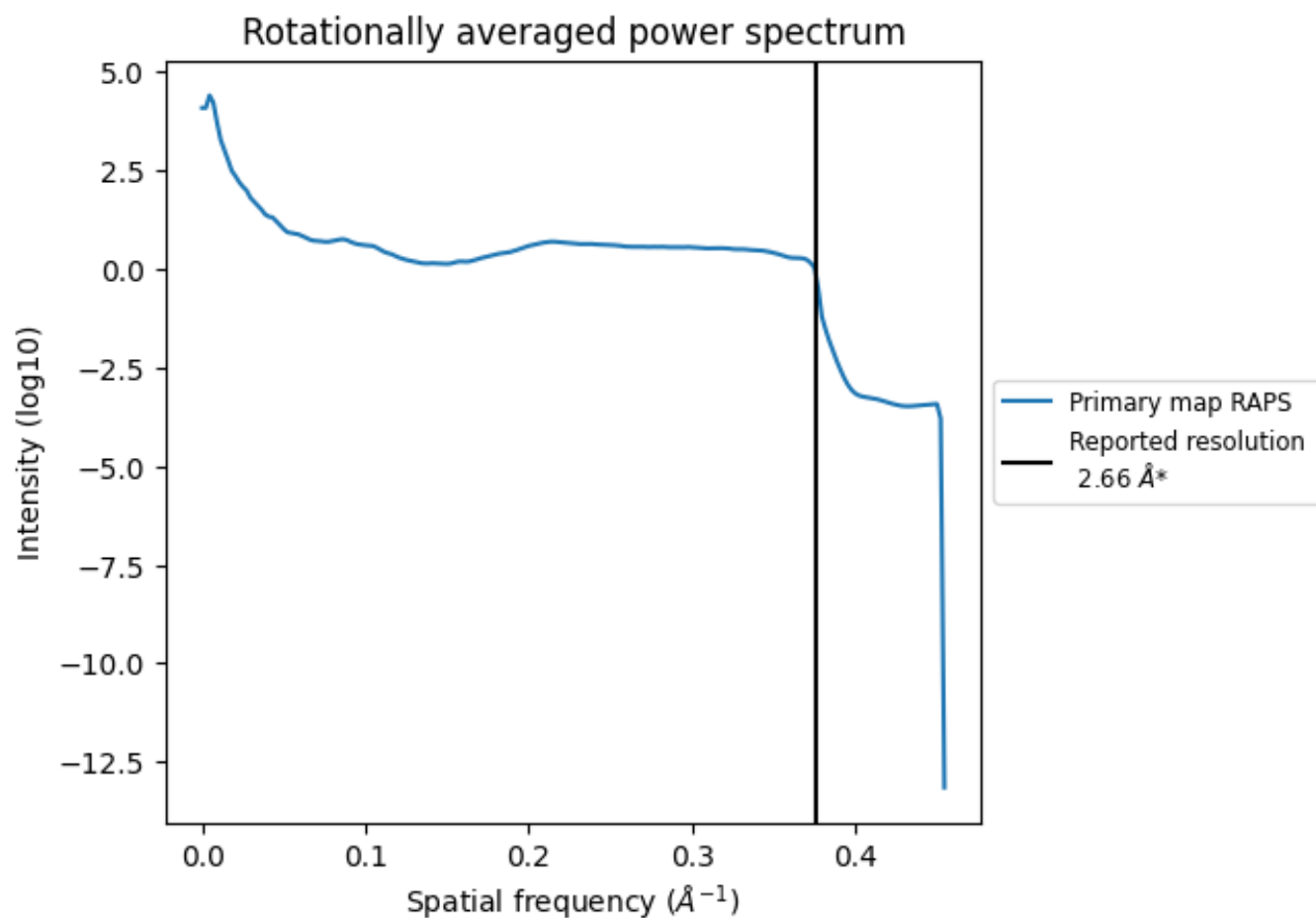
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm<sup>3</sup>; this corresponds to an approximate mass of 158 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 ⓘ

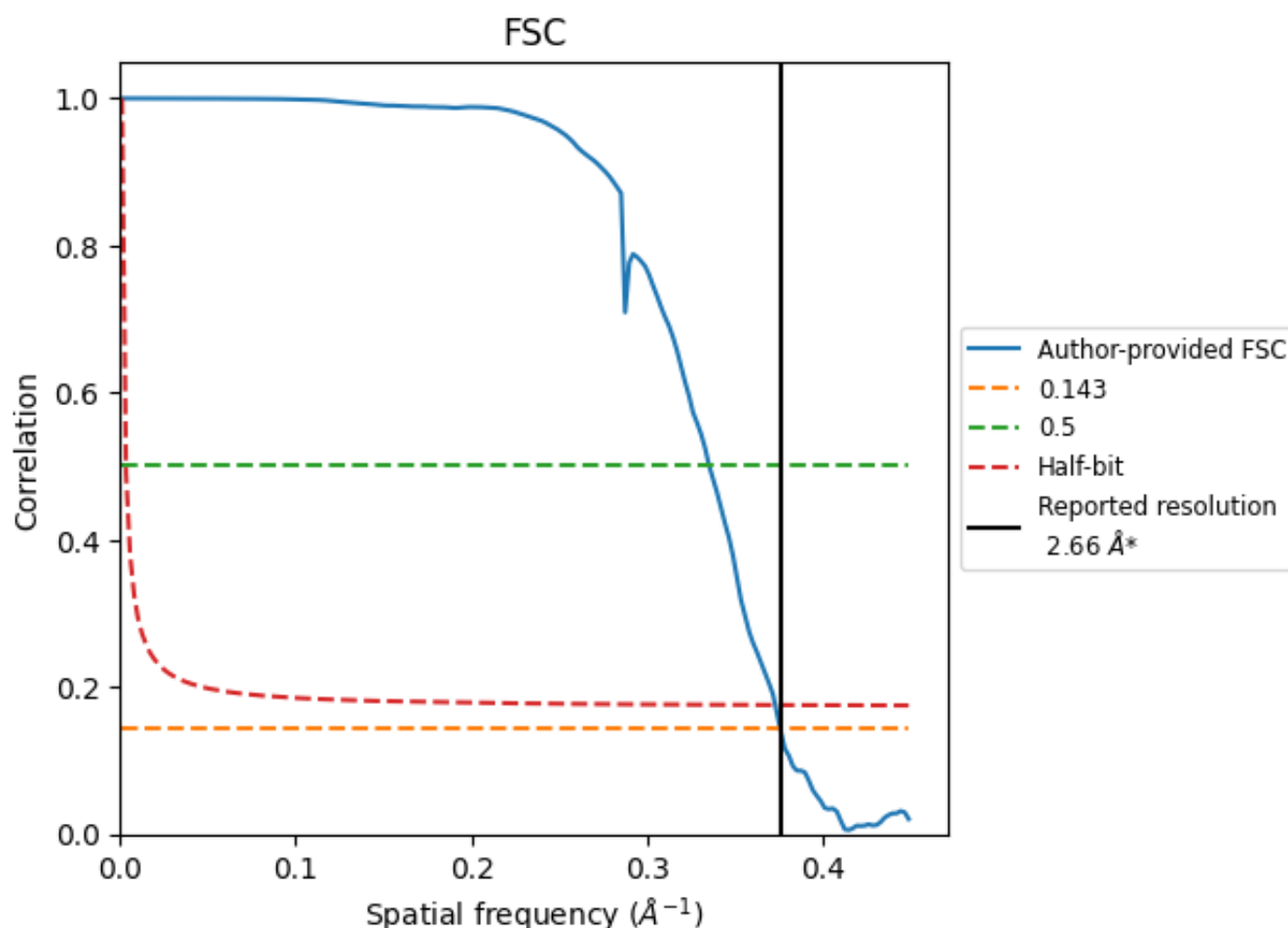


\*Reported resolution corresponds to spatial frequency of 0.376 Å<sup>-1</sup>

## 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 0.376 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

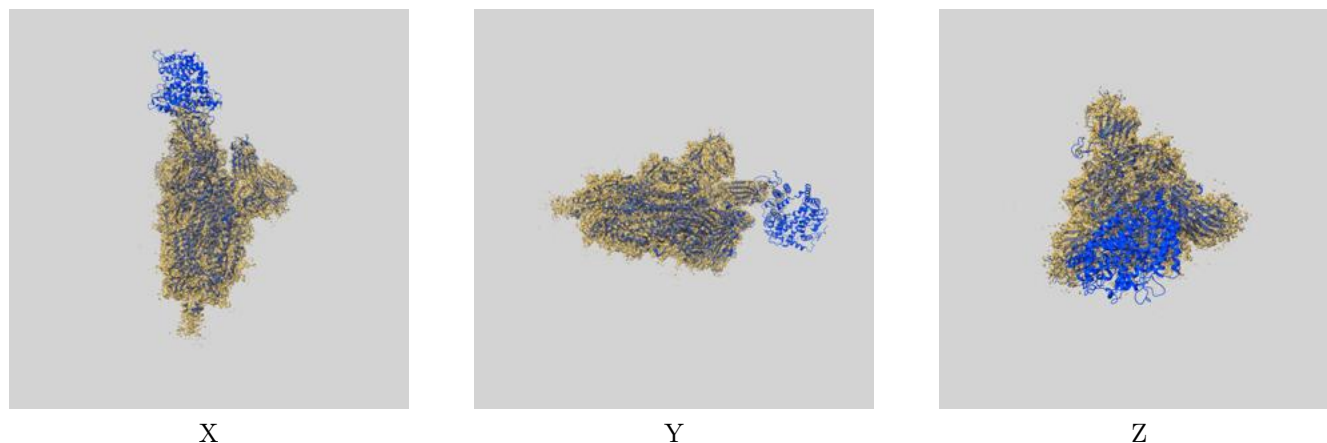
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.66	2.98	2.68
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

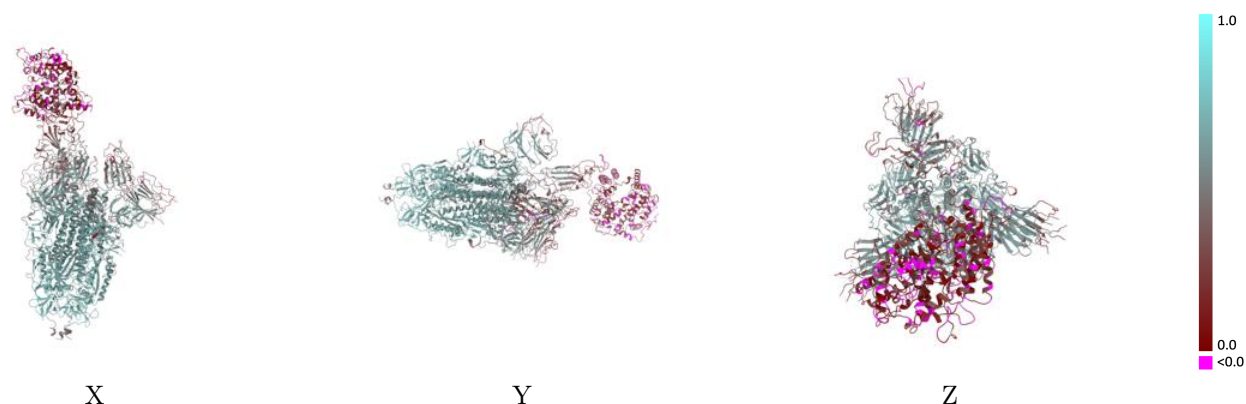
This section contains information regarding the fit between EMDB map EMD-32726 and PDB model 7WRH. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

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



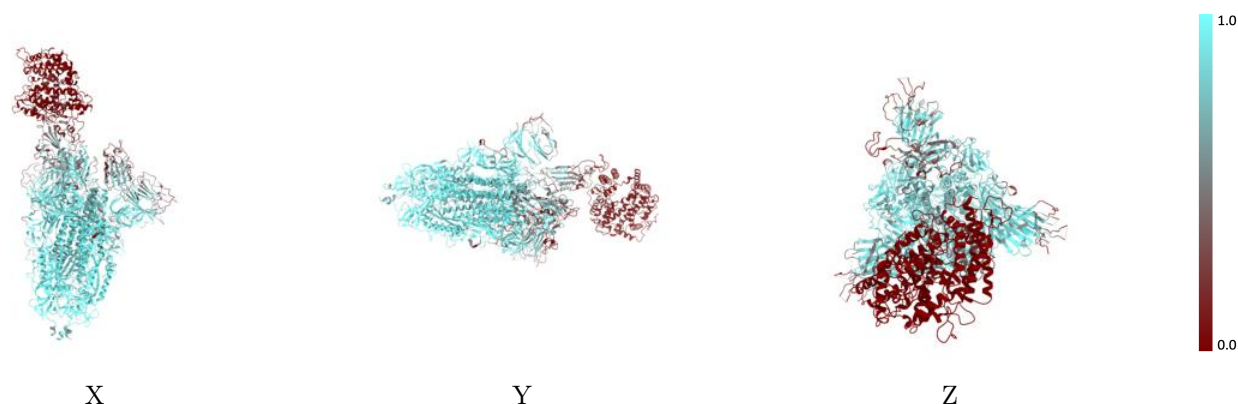
The images above show the 3D surface view of the map at the recommended contour level 0.489 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

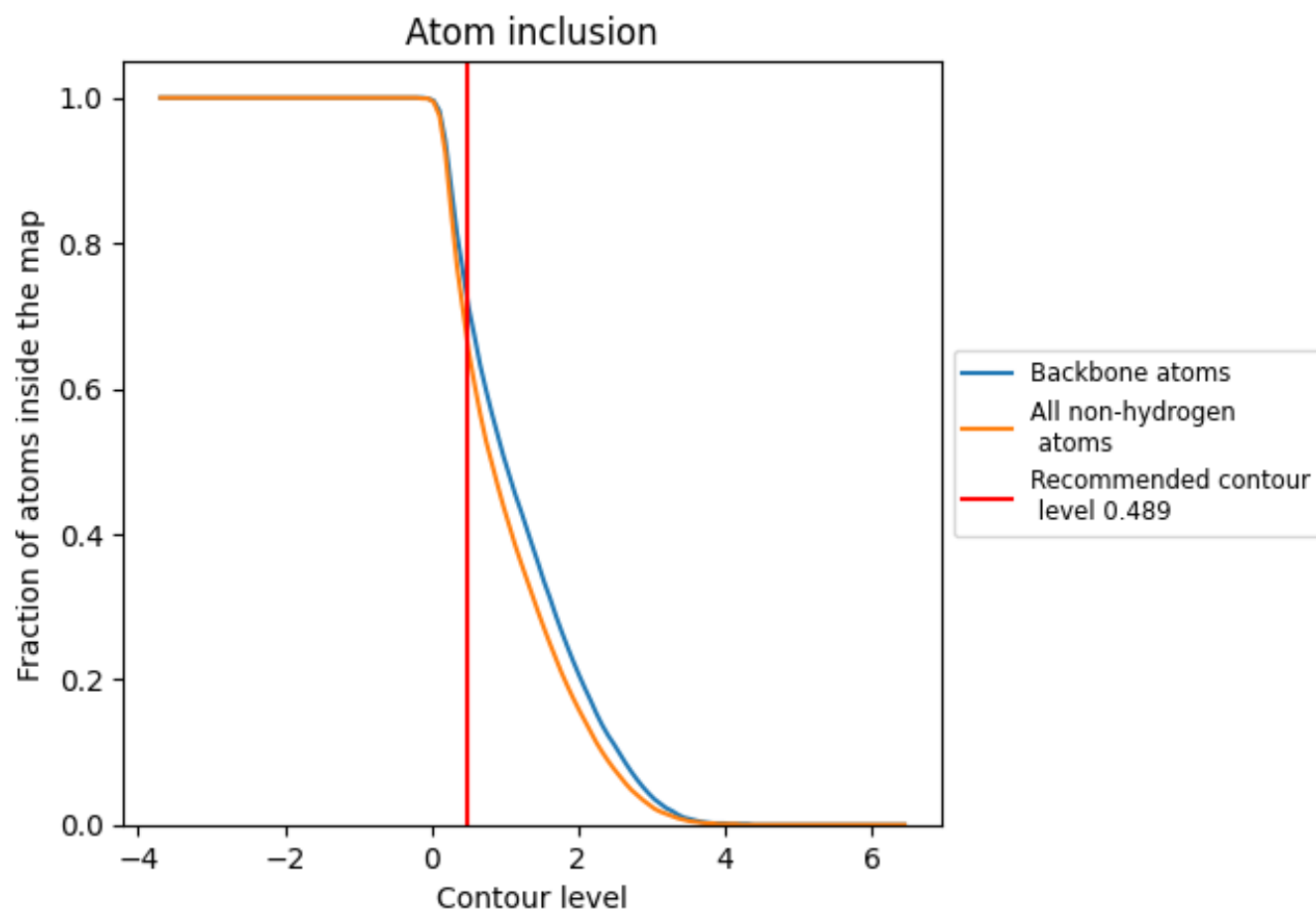
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.489).

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 66% 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 (0.489) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6630	 0.4680
A	 0.7680	 0.5220
B	 0.7780	 0.5350
C	 0.8220	 0.5450
D	 0.0050	 0.1270
E	 0.2140	 0.2650
F	 0.2500	 0.3400
G	 0.3210	 0.3740
H	 0.7860	 0.5030
I	 0.3570	 0.3100
J	 0.8930	 0.5960
K	 0.7500	 0.4780
L	 0.8210	 0.5390
M	 0.5710	 0.3860
N	 0.4640	 0.3240
O	 0.8570	 0.5550
P	 0.8570	 0.5120
Q	 0.6430	 0.5440
R	 0.7500	 0.5060
S	 0.6070	 0.4240
T	 0.2860	 0.3690
U	 0.4290	 0.2790
V	 0.8570	 0.5750
W	 0.7860	 0.4920
X	 0.5360	 0.4930
Y	 0.7500	 0.5130
Z	 0.6790	 0.5230

