



Full wwPDB EM Validation Report ⓘ

Dec 2, 2025 – 04:52 AM JST

PDB ID : 9KZZ / pdb_00009kzz
EMDB ID : EMD-62680
Title : Structure of SARS-CoV-2 EG.5.1 Variant Spike protein complexed with anti-body XGi-171
Authors : Qiu, Y.N.; Sun, L.
Deposited on : 2024-12-11
Resolution : 3.18 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

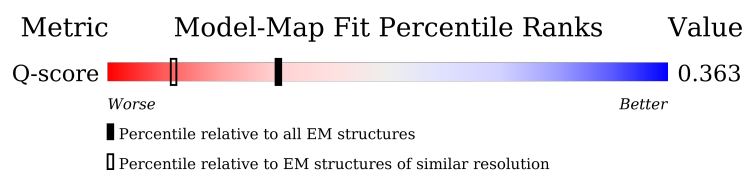
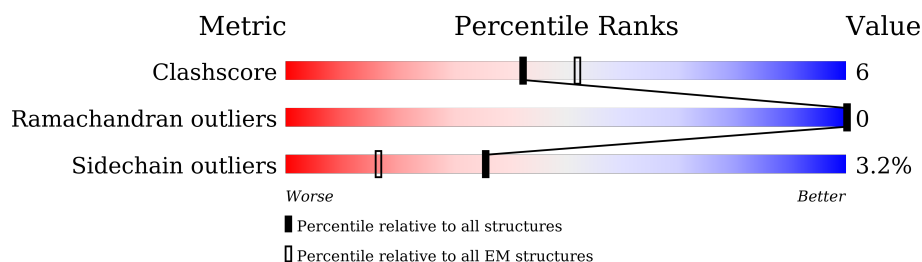
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 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.








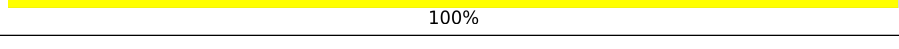
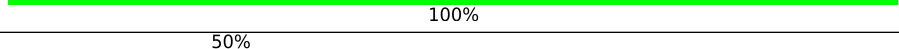

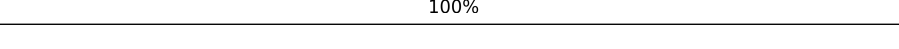
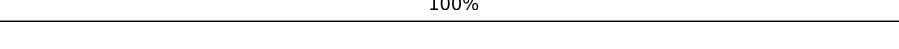
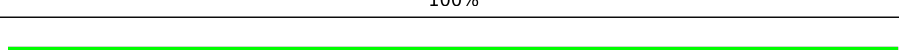
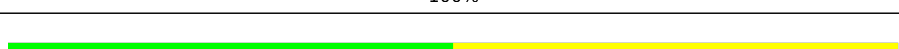
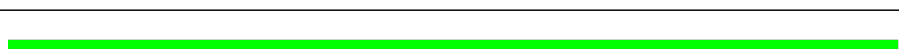
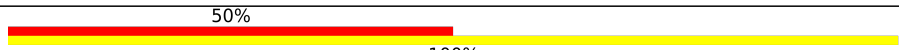
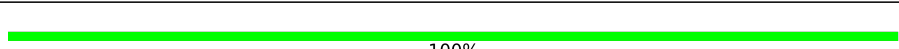

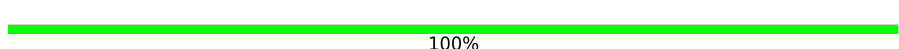
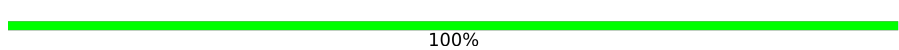
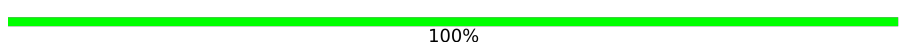

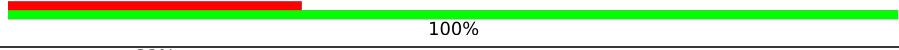
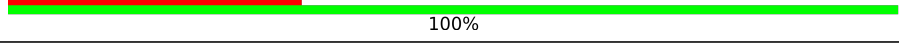
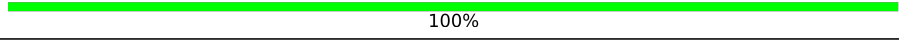
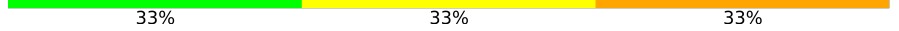

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14470 (2.68 - 3.68)

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	H	449	
1	I	449	
1	J	449	
2	L	215	





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Mol	Chain	Length	Quality of chain
2	M	215	
2	N	215	
3	A	1295	
3	B	1295	
3	C	1295	
4	D	2	
4	F	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	U	2	
4	V	2	
4	W	2	
4	a	2	
4	c	2	
4	e	2	
4	g	2	
4	h	2	
4	i	2	
5	E	3	
5	G	3	
5	K	3	
5	T	3	

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Mol	Chain	Length	Quality of chain
5	X	3	 100%
5	Y	3	 33%100%
5	Z	3	 33%100%
5	b	3	 33%100%
5	d	3	 100%
5	f	3	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 34280 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 XGi-171 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	202	Total	C	N	O	S	0	0
			1517	960	258	294	5		
1	I	202	Total	C	N	O	S	0	0
			1517	960	258	294	5		
1	J	202	Total	C	N	O	S	0	0
			1517	960	258	294	5		

- Molecule 2 is a protein called XGi-171 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	209	Total	C	N	O	S	0	0
			1608	1008	272	322	6		
2	M	209	Total	C	N	O	S	0	0
			1608	1008	272	322	6		
2	N	209	Total	C	N	O	S	0	0
			1608	1008	272	322	6		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1020	Total	C	N	O	S	0	0
			7980	5103	1330	1511	36		
3	B	1016	Total	C	N	O	S	0	0
			7950	5085	1322	1507	36		
3	A	1016	Total	C	N	O	S	0	0
			7955	5092	1323	1503	37		

There are 471 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	initiating methionine	UNP P0DTC2
C	-9	PRO	-	expression tag	UNP P0DTC2
C	-8	MET	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLY	-	expression tag	UNP P0DTC2
C	-6	SER	-	expression tag	UNP P0DTC2
C	-5	LEU	-	expression tag	UNP P0DTC2
C	-4	GLN	-	expression tag	UNP P0DTC2
C	-3	PRO	-	expression tag	UNP P0DTC2
C	-2	LEU	-	expression tag	UNP P0DTC2
C	-1	ALA	-	expression tag	UNP P0DTC2
C	0	THR	-	expression tag	UNP P0DTC2
C	1	LEU	-	expression tag	UNP P0DTC2
C	2	TYR	-	expression tag	UNP P0DTC2
C	3	LEU	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	GLY	-	expression tag	UNP P0DTC2
C	6	MET	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	VAL	-	expression tag	UNP P0DTC2
C	9	ALA	-	expression tag	UNP P0DTC2
C	10	SER	-	expression tag	UNP P0DTC2
C	11	VAL	-	expression tag	UNP P0DTC2
C	12	LEU	-	expression tag	UNP P0DTC2
C	13	ALA	-	expression tag	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	52	HIS	GLN	variant	UNP P0DTC2
C	83	ALA	VAL	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	146	GLN	HIS	variant	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	456	LEU	PHE	variant	UNP P0DTC2
C	460	LYS	ASN	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	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	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	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	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
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	PHE	-	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	SER	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLN	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	PRO	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	TRP	-	expression tag	UNP P0DTC2
C	1251	SER	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	GLN	-	expression tag	UNP P0DTC2
C	1255	PHE	-	expression tag	UNP P0DTC2
C	1256	GLU	-	expression tag	UNP P0DTC2
C	1257	LYS	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	HIS	-	expression tag	UNP P0DTC2
B	-10	MET	-	initiating methionine	UNP P0DTC2
B	-9	PRO	-	expression tag	UNP P0DTC2
B	-8	MET	-	expression tag	UNP P0DTC2
B	-7	GLY	-	expression tag	UNP P0DTC2
B	-6	SER	-	expression tag	UNP P0DTC2
B	-5	LEU	-	expression tag	UNP P0DTC2
B	-4	GLN	-	expression tag	UNP P0DTC2
B	-3	PRO	-	expression tag	UNP P0DTC2
B	-2	LEU	-	expression tag	UNP P0DTC2
B	-1	ALA	-	expression tag	UNP P0DTC2
B	0	THR	-	expression tag	UNP P0DTC2
B	1	LEU	-	expression tag	UNP P0DTC2
B	2	TYR	-	expression tag	UNP P0DTC2
B	3	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	GLY	-	expression tag	UNP P0DTC2
B	6	MET	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	VAL	-	expression tag	UNP P0DTC2
B	9	ALA	-	expression tag	UNP P0DTC2
B	10	SER	-	expression tag	UNP P0DTC2
B	11	VAL	-	expression tag	UNP P0DTC2
B	12	LEU	-	expression tag	UNP P0DTC2
B	13	ALA	-	expression tag	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	52	HIS	GLN	variant	UNP P0DTC2
B	83	ALA	VAL	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	variant	UNP P0DTC2
B	183	GLU	GLN	variant	UNP P0DTC2
B	213	GLU	VAL	variant	UNP P0DTC2
B	252	VAL	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	368	ILE	LEU	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	PRO	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	456	LEU	PHE	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	490	SER	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	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	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	PHE	-	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	SER	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	PRO	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	TRP	-	expression tag	UNP P0DTC2
B	1251	SER	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	GLN	-	expression tag	UNP P0DTC2
B	1255	PHE	-	expression tag	UNP P0DTC2
B	1256	GLU	-	expression tag	UNP P0DTC2
B	1257	LYS	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
A	-10	MET	-	initiating methionine	UNP P0DTC2
A	-9	PRO	-	expression tag	UNP P0DTC2
A	-8	MET	-	expression tag	UNP P0DTC2
A	-7	GLY	-	expression tag	UNP P0DTC2
A	-6	SER	-	expression tag	UNP P0DTC2
A	-5	LEU	-	expression tag	UNP P0DTC2
A	-4	GLN	-	expression tag	UNP P0DTC2
A	-3	PRO	-	expression tag	UNP P0DTC2
A	-2	LEU	-	expression tag	UNP P0DTC2
A	-1	ALA	-	expression tag	UNP P0DTC2
A	0	THR	-	expression tag	UNP P0DTC2
A	1	LEU	-	expression tag	UNP P0DTC2
A	2	TYR	-	expression tag	UNP P0DTC2
A	3	LEU	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	GLY	-	expression tag	UNP P0DTC2
A	6	MET	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	VAL	-	expression tag	UNP P0DTC2
A	9	ALA	-	expression tag	UNP P0DTC2
A	10	SER	-	expression tag	UNP P0DTC2
A	11	VAL	-	expression tag	UNP P0DTC2
A	12	LEU	-	expression tag	UNP P0DTC2
A	13	ALA	-	expression tag	UNP P0DTC2
A	19	ILE	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	52	HIS	GLN	variant	UNP P0DTC2
A	83	ALA	VAL	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	PRO	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	456	LEU	PHE	variant	UNP P0DTC2
A	460	LYS	ASN	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	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	PHE	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	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	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	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
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	PHE	-	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	SER	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2

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



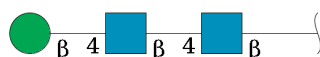
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		

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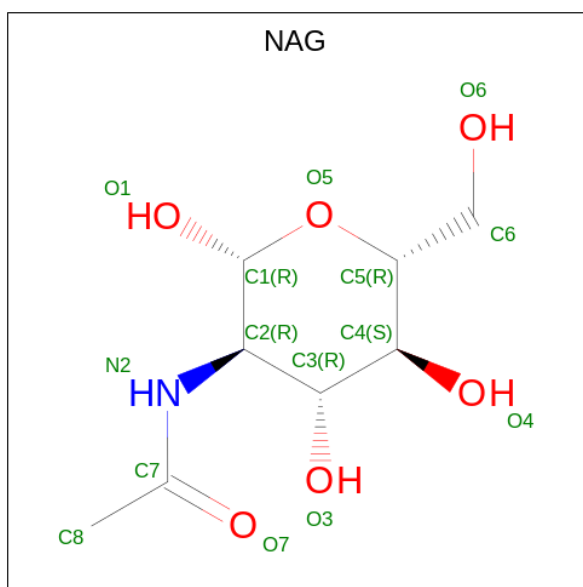
Mol	Chain	Residues	Atoms				AltConf	Trace
4	h	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	3	Total	C	N	O	0	0
			39	22	2	15		
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	K	3	Total	C	N	O	0	0
			39	22	2	15		
5	T	3	Total	C	N	O	0	0
			39	22	2	15		
5	X	3	Total	C	N	O	0	0
			39	22	2	15		
5	Y	3	Total	C	N	O	0	0
			39	22	2	15		
5	Z	3	Total	C	N	O	0	0
			39	22	2	15		
5	b	3	Total	C	N	O	0	0
			39	22	2	15		
5	d	3	Total	C	N	O	0	0
			39	22	2	15		
5	f	3	Total	C	N	O	0	0
			39	22	2	15		


- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

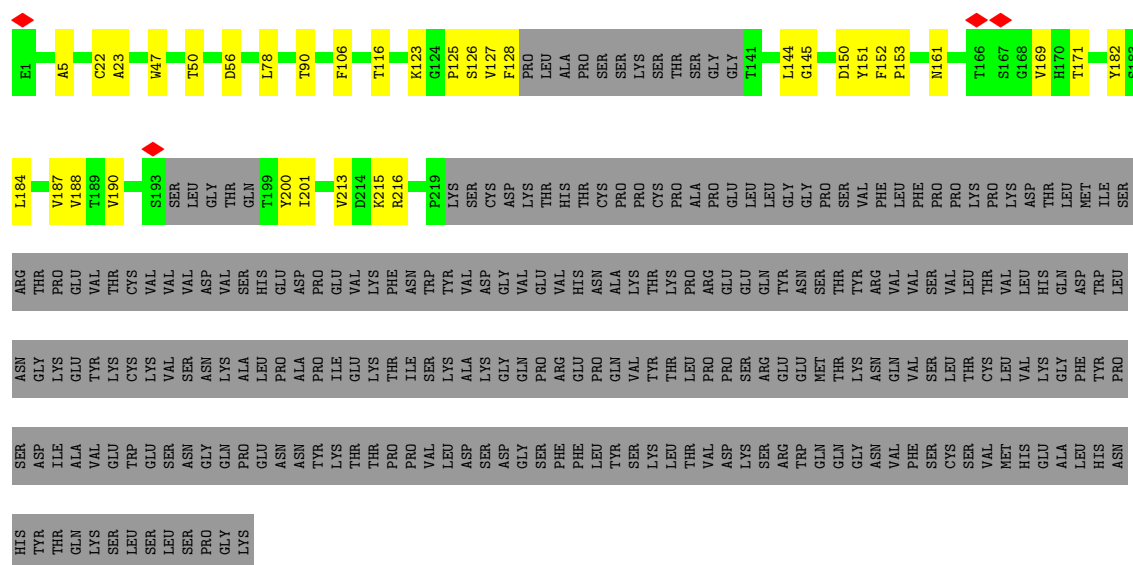


Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6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

ALA
LEU
HIS
ASN
HIS
TYR
THR
GLN
LYS
SER
LEU
SER
SER
LEU
SER
PRO
GLY
LYS

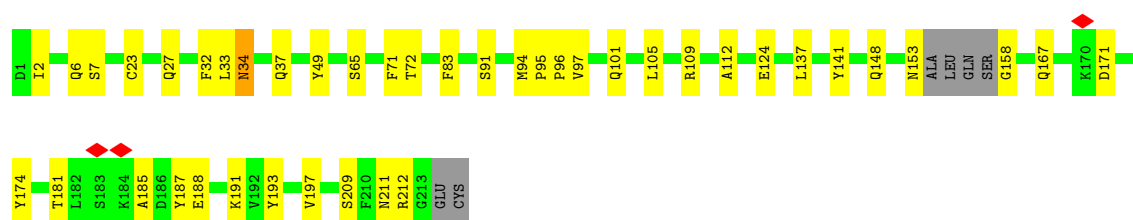
• Molecule 1: XGi-171 heavy chain

Chain J:  37% 8% 55%




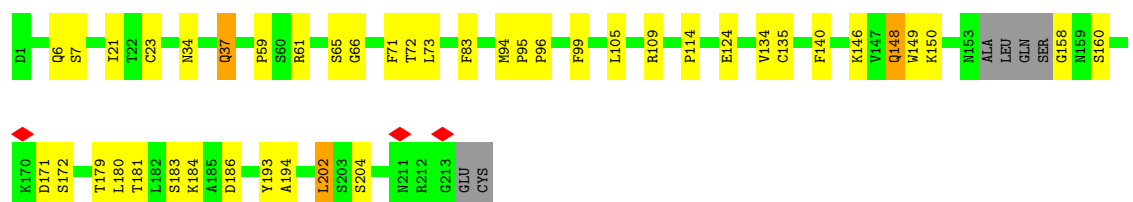
• Molecule 2: XGi-171 light chain

Chain L:  78% 19%




• Molecule 2: XGi-171 light chain

Chain M:  77% 19%



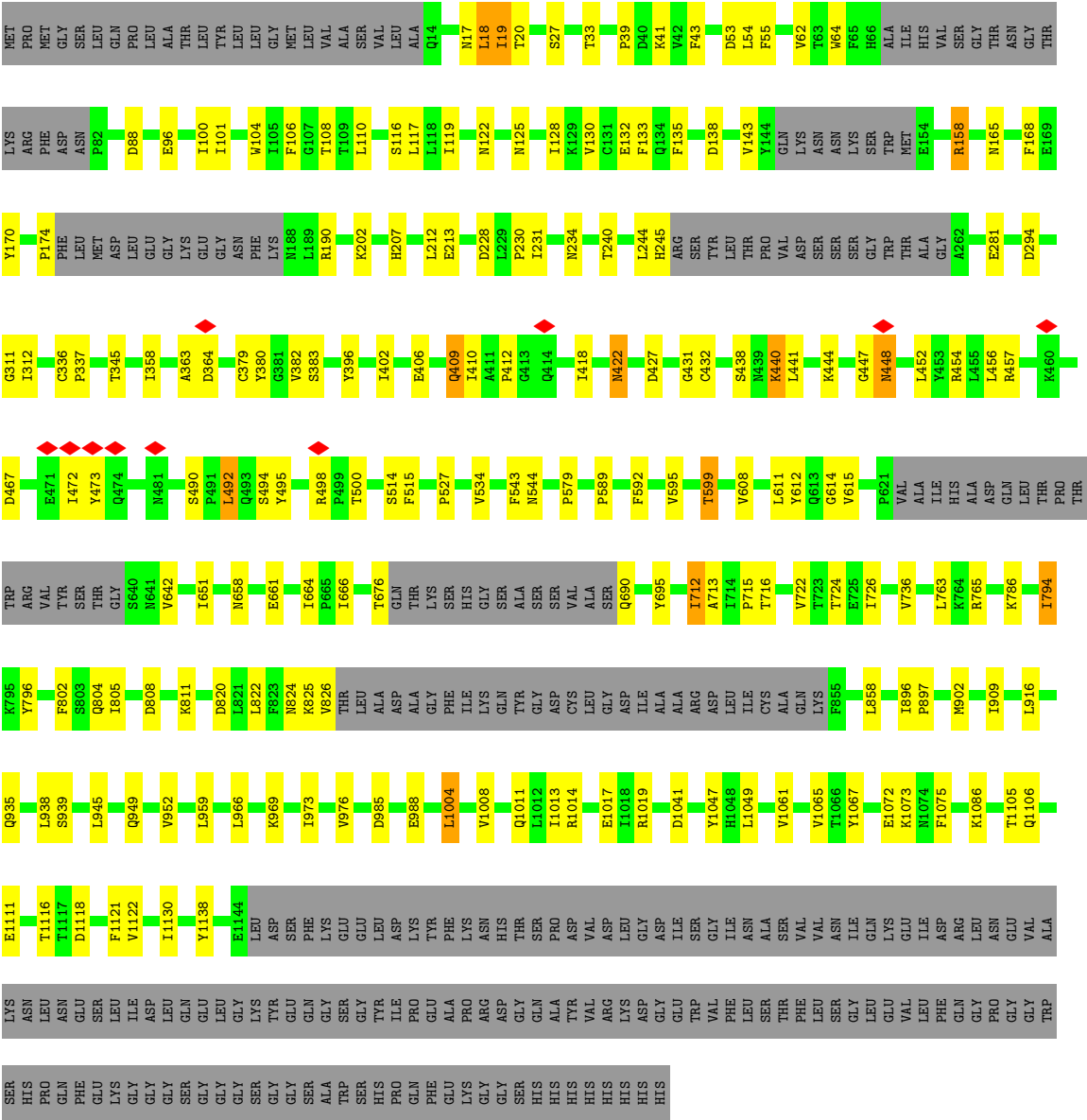
• Molecule 2: XGi-171 light chain

Chain N:  76% 20%

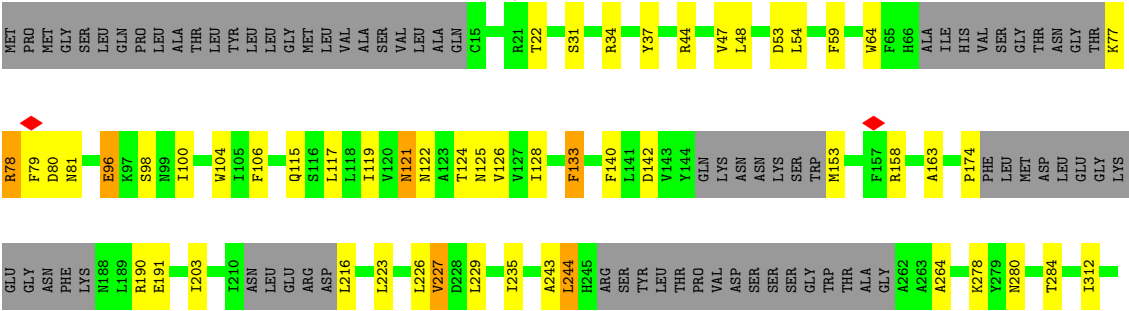
- Molecule 3: Spike glycoprotein

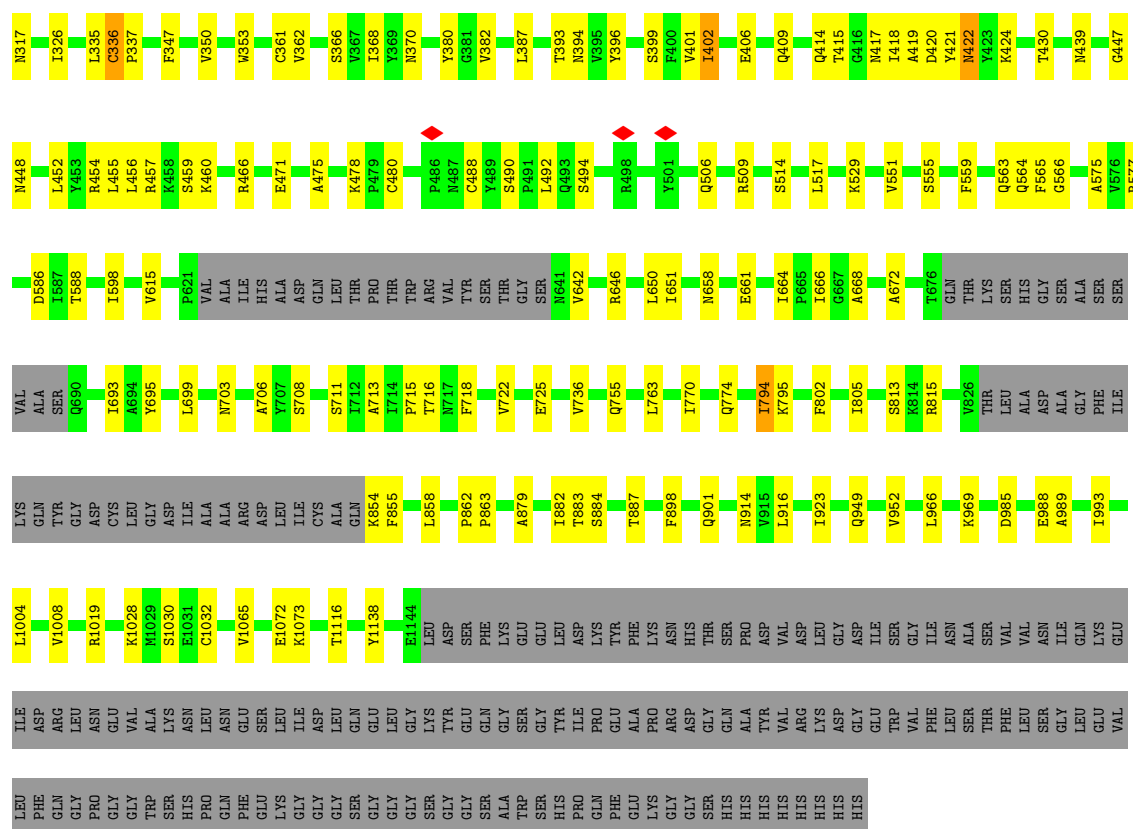
- Molecule 3: Spike glycoprotein





• Molecule 3: Spike glycoprotein





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

Chain D: 100%

MAG1
MAG2

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

Chain F: 100%

MAG1
MAG2

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

Chain O: 50%

MAG1
MAG2

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

Chain P:  100%



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

Chain Q:  100%



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

Chain R:  100%



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

Chain S:  100%



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

Chain U:  50% 50%



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

Chain V:  100%



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

Chain W:  50% 100%



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

Chain a:  100%



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

Chain c:  50% 50%



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

Chain e:  100%



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

Chain g:  100%



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

Chain h:  100%



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

Chain i:  50% 100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33% 100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  33% 33% 33%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  33% 100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  33% 100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  33% 100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	30115	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.039	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	633.76, 633.76, 633.76	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93200004, 0.93200004, 0.93200004	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: BMA, 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	H	0.10	0/1553	0.29	0/2113
1	I	0.10	0/1553	0.30	0/2113
1	J	0.11	0/1553	0.31	0/2113
2	L	0.12	0/1642	0.36	0/2226
2	M	0.13	0/1642	0.37	0/2226
2	N	0.14	0/1642	0.36	0/2226
3	A	0.12	0/8144	0.36	0/11085
3	B	0.13	0/8139	0.35	0/11082
3	C	0.13	0/8168	0.37	0/11118
All	All	0.12	0/34036	0.35	0/46302

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1517	0	1464	10	0
1	I	1517	0	1464	18	0
1	J	1517	0	1464	17	0
2	L	1608	0	1574	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1608	0	1574	27	0
2	N	1608	0	1574	34	0
3	A	7955	0	7773	107	0
3	B	7950	0	7761	108	0
3	C	7980	0	7799	117	0
4	D	28	0	25	1	0
4	F	28	0	25	0	0
4	O	28	0	25	1	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	U	28	0	25	1	0
4	V	28	0	25	0	0
4	W	28	0	25	1	0
4	a	28	0	25	0	0
4	c	28	0	25	1	0
4	e	28	0	25	0	0
4	g	28	0	25	0	0
4	h	28	0	25	0	0
4	i	28	0	25	0	0
5	E	39	0	34	0	0
5	G	39	0	34	0	0
5	K	39	0	34	0	0
5	T	39	0	34	1	0
5	X	39	0	34	0	0
5	Y	39	0	34	0	0
5	Z	39	0	34	0	0
5	b	39	0	34	0	0
5	d	39	0	34	0	0
5	f	39	0	34	0	0
6	A	70	0	65	0	0
6	B	70	0	65	2	0
6	C	42	0	39	1	0
All	All	34280	0	33356	437	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 (437) 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)
3:C:965:GLN:HA	3:C:968:SER:HB3	1.60	0.80
2:L:6:GLN:HG3	2:L:23:CYS:HB2	1.76	0.67
3:C:1017:GLU:HG2	3:B:1019:ARG:HH12	1.59	0.67
2:N:137:LEU:HD21	2:N:197:VAL:HG11	1.78	0.66
3:B:110:LEU:HB3	3:B:135:PHE:HB2	1.78	0.66
3:B:447:GLY:O	3:B:448:ASN:ND2	2.29	0.66
3:A:366:SER:O	3:A:370:ASN:ND2	2.29	0.66
3:A:312:ILE:HG22	3:A:598:ILE:HG12	1.79	0.65
3:B:125:ASN:HA	3:B:174:PRO:HD3	1.79	0.64
3:A:447:GLY:O	3:A:448:ASN:ND2	2.31	0.64
3:C:128:ILE:HB	3:C:170:TYR:HB3	1.79	0.64
3:A:226:LEU:HG	3:A:227:VAL:HG22	1.80	0.63
3:A:642:VAL:HG12	3:A:651:ILE:HG12	1.80	0.63
3:C:575:ALA:HB1	3:C:584:ILE:HD11	1.80	0.62
3:C:378:LYS:HA	2:N:95:PRO:HG2	1.81	0.62
3:B:457:ARG:NH2	3:B:467:ASP:OD2	2.33	0.62
3:C:820:ASP:O	3:C:824:ASN:ND2	2.30	0.62
3:A:452:LEU:HA	3:A:494:SER:HA	1.80	0.62
3:B:418:ILE:HG23	3:B:422:ASN:HB3	1.82	0.62
3:C:895:GLN:HE22	3:A:706:ALA:HB3	1.65	0.61
2:N:6:GLN:HG3	2:N:23:CYS:HB2	1.81	0.61
3:C:121:ASN:ND2	3:C:122:ASN:O	2.32	0.61
3:A:121:ASN:ND2	3:A:122:ASN:O	2.33	0.61
3:A:140:PHE:HB2	3:A:244:LEU:HB2	1.83	0.61
3:A:393:THR:HG23	3:A:517:LEU:HD12	1.82	0.61
2:N:112:ALA:H	2:N:141:TYR:HB3	1.65	0.61
3:B:1017:GLU:OE1	3:A:1019:ARG:NH1	2.33	0.61
3:A:353:TRP:O	3:A:466:ARG:NH1	2.32	0.60
3:C:804:GLN:OE1	3:C:935:GLN:NE2	2.34	0.60
3:A:898:PHE:HA	3:A:901:GLN:HG2	1.83	0.60
2:N:39:LYS:HB3	2:N:42:LYS:HE2	1.84	0.60
3:A:96:GLU:OE2	3:A:190:ARG:NH1	2.35	0.59
3:A:191:GLU:HG2	3:A:223:LEU:HD21	1.83	0.59
2:M:6:GLN:HG3	2:M:23:CYS:HB2	1.82	0.59
3:B:804:GLN:OE1	3:B:935:GLN:NE2	2.35	0.59
3:C:642:VAL:HG12	3:C:651:ILE:HG12	1.83	0.59
3:A:716:THR:HG21	3:A:1073:LYS:HE2	1.85	0.59
3:C:492:LEU:HD13	3:C:492:LEU:H	1.67	0.59
3:A:122:ASN:HB2	3:A:125:ASN:H	1.68	0.59
3:A:153:MET:SD	3:A:153:MET:N	2.76	0.59
3:C:106:PHE:HB2	3:C:118:LEU:HD23	1.83	0.59
3:C:560:LEU:O	3:C:562:PHE:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:108:THR:OG1	3:B:234:ASN:O	2.20	0.59
3:A:126:VAL:HG13	3:A:174:PRO:HG3	1.85	0.59
3:A:1116:THR:HG22	3:A:1138:TYR:HB3	1.84	0.58
2:N:182:LEU:HD22	2:N:187:TYR:HA	1.86	0.58
3:B:614:GLY:O	3:A:854:LYS:NZ	2.36	0.58
3:A:555:SER:HB2	3:A:586:ASP:HB2	1.85	0.58
2:N:94:MET:HB2	2:N:95:PRO:HD3	1.86	0.58
3:C:167:THR:HG23	3:A:394:ASN:HD21	1.68	0.58
3:C:1116:THR:HG22	3:C:1138:TYR:HB3	1.84	0.58
3:B:969:LYS:NZ	3:B:973:ILE:O	2.37	0.58
3:B:589:PRO:HG2	3:A:855:PHE:HA	1.86	0.57
3:C:951:VAL:O	3:C:955:ASN:ND2	2.37	0.57
3:A:456:LEU:HD11	3:A:490:SER:HB3	1.85	0.57
3:B:825:LYS:HD2	3:B:945:LEU:HD12	1.86	0.57
3:B:1086:LYS:HD3	3:B:1122:VAL:HG21	1.84	0.57
2:L:112:ALA:H	2:L:141:TYR:HB3	1.70	0.57
3:A:396:TYR:HB2	3:A:514:SER:HB3	1.86	0.56
3:B:820:ASP:OD1	3:B:824:ASN:ND2	2.38	0.56
3:C:118:LEU:HD12	3:C:119:ILE:HG13	1.86	0.56
2:M:66:GLY:HA3	2:M:71:PHE:HA	1.87	0.56
2:N:196:GLU:HA	2:N:206:VAL:HG12	1.88	0.56
3:C:1086:LYS:HD3	3:C:1122:VAL:HG21	1.86	0.56
2:L:2:ILE:HG12	2:L:27:GLN:HE22	1.71	0.56
3:A:454:ARG:HH11	3:A:457:ARG:HB3	1.71	0.56
3:A:478:LYS:HG2	3:A:480:CYS:H	1.71	0.56
2:M:109:ARG:NH2	2:M:171:ASP:O	2.38	0.55
3:C:518:LEU:HD12	4:U:2:NAG:H83	1.88	0.55
3:B:17:ASN:ND2	3:B:138:ASP:OD2	2.37	0.55
1:H:5:ALA:HB3	1:H:23:ALA:HB3	1.87	0.55
3:B:1106:GLN:NE2	3:B:1111:GLU:OE1	2.40	0.55
3:B:642:VAL:HG12	3:B:651:ILE:HG12	1.88	0.55
3:B:820:ASP:O	3:B:824:ASN:ND2	2.32	0.55
3:B:396:TYR:HB2	3:B:514:SER:HB3	1.87	0.55
3:B:716:THR:HG21	3:B:1073:LYS:HE2	1.88	0.55
1:I:5:ALA:HB3	1:I:23:ALA:HB3	1.89	0.55
1:J:123:LYS:HD3	1:J:150:ASP:HB3	1.87	0.55
2:N:133:VAL:O	2:N:180:LEU:N	2.39	0.55
1:J:127:VAL:HG11	1:J:215:LYS:HB3	1.89	0.55
3:A:106:PHE:HB2	3:A:117:LEU:HB3	1.88	0.55
3:B:128:ILE:HB	3:B:170:TYR:HB3	1.89	0.54
3:C:453:TYR:HB2	3:C:495:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:559:PHE:HB3	3:A:563:GLN:HB2	1.89	0.54
3:A:882:ILE:HG13	3:A:883:THR:HG23	1.88	0.54
3:C:117:LEU:HD13	3:C:118:LEU:H	1.72	0.54
3:C:737:ASP:OD1	3:A:317:ASN:ND2	2.40	0.54
3:A:661:GLU:O	3:A:695:TYR:OH	2.24	0.54
2:L:109:ARG:NH2	2:L:171:ASP:O	2.38	0.54
3:C:884:SER:OG	3:C:887:THR:OG1	2.24	0.54
3:C:1075:PHE:HA	6:C:1302:NAG:H82	1.89	0.53
2:N:150:LYS:HB2	2:N:194:ALA:HB3	1.89	0.53
3:A:78:ARG:O	3:A:78:ARG:NH2	2.30	0.53
2:M:146:LYS:NZ	2:M:148:GLN:OE1	2.33	0.53
2:N:133:VAL:HB	2:N:180:LEU:HB3	1.90	0.53
3:C:39:PRO:HG3	3:C:55:PHE:HZ	1.73	0.53
3:C:108:THR:OG1	3:C:234:ASN:O	2.27	0.53
3:B:985:ASP:HB2	3:B:988:GLU:HG2	1.91	0.53
3:A:646:ARG:HE	3:A:668:ALA:HB1	1.74	0.53
3:A:725:GLU:OE2	3:A:1028:LYS:NZ	2.38	0.53
3:C:448:ASN:ND2	3:C:448:ASN:O	2.42	0.53
3:B:202:LYS:NZ	3:B:228:ASP:OD2	2.42	0.53
2:M:160:SER:HB2	2:M:181:THR:HG23	1.91	0.53
3:C:825:LYS:NZ	3:C:938:LEU:O	2.33	0.53
3:B:88:ASP:OD1	3:B:88:ASP:N	2.39	0.53
3:A:401:VAL:HG22	3:A:509:ARG:HG2	1.91	0.53
3:B:726:ILE:HG12	3:B:1061:VAL:HG22	1.90	0.52
3:A:884:SER:OG	3:A:887:THR:OG1	2.26	0.52
3:C:442:ASP:OD2	3:C:451:TYR:OH	2.26	0.52
3:B:119:ILE:HG12	3:B:128:ILE:HD12	1.91	0.52
1:J:145:GLY:HA3	1:J:187:VAL:HA	1.91	0.52
3:C:43:PHE:N	3:A:565:PHE:O	2.35	0.52
3:C:581:THR:OG1	3:C:583:GLU:OE1	2.20	0.52
3:C:968:SER:OG	3:C:969:LYS:N	2.42	0.52
2:N:125:GLN:HG2	2:N:131:ALA:HA	1.91	0.52
3:C:499:PRO:HB2	3:C:503:VAL:HB	1.90	0.52
3:C:726:ILE:HG12	3:C:1061:VAL:HG22	1.91	0.52
3:A:100:ILE:HD12	3:A:243:ALA:HB3	1.91	0.52
1:J:5:ALA:HB3	1:J:23:ALA:HB3	1.92	0.52
3:C:287:ASP:N	3:C:287:ASP:OD1	2.41	0.52
3:C:645:THR:HG23	3:C:647:ALA:H	1.74	0.52
3:B:383:SER:HA	2:M:94:MET:HG3	1.92	0.52
3:B:736:VAL:HA	3:B:858:LEU:HA	1.92	0.52
3:A:566:GLY:HA3	3:A:575:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:21:ILE:HB	2:N:73:LEU:HB3	1.90	0.52
1:J:22:CYS:HB3	1:J:78:LEU:HB3	1.92	0.52
3:C:661:GLU:O	3:C:695:TYR:OH	2.25	0.52
3:A:421:TYR:CE1	3:A:459:SER:HB3	2.44	0.51
1:I:215:LYS:HE2	2:M:124:GLU:HB2	1.93	0.51
3:C:455:LEU:HB2	3:C:493:GLN:HG3	1.92	0.51
2:M:94:MET:HB2	2:M:95:PRO:HD3	1.91	0.51
3:C:725:GLU:OE2	3:C:1028:LYS:NZ	2.36	0.51
3:C:858:LEU:HD21	3:C:962:LEU:HD23	1.93	0.51
3:C:646:ARG:HE	3:C:668:ALA:HB1	1.76	0.51
3:B:96:GLU:OE2	3:B:190:ARG:NH2	2.43	0.51
2:M:6:GLN:HG2	2:M:7:SER:H	1.75	0.51
2:M:149:TRP:CD2	2:M:180:LEU:HB2	2.45	0.51
3:B:380:TYR:OH	3:B:410:ILE:O	2.27	0.51
2:M:202:LEU:HD13	2:M:204:SER:H	1.76	0.51
3:B:336:CYS:HB2	3:B:364:ASP:HB2	1.92	0.50
3:B:1116:THR:HG22	3:B:1138:TYR:HB3	1.93	0.50
3:A:104:TRP:H	3:A:119:ILE:HB	1.75	0.50
2:L:191:LYS:NZ	2:L:211:ASN:OD1	2.40	0.50
3:B:452:LEU:HA	3:B:494:SER:HA	1.94	0.50
3:B:27:SER:N	3:B:64:TRP:O	2.42	0.50
1:H:47:TRP:HZ2	1:H:50:THR:HG22	1.76	0.50
3:C:131:CYS:HB2	3:C:133:PHE:HE1	1.77	0.50
3:B:969:LYS:HD3	3:A:755:GLN:HG3	1.93	0.50
3:C:882:ILE:HG13	3:C:883:THR:HG23	1.94	0.50
3:C:64:TRP:HE1	3:C:264:ALA:HB1	1.77	0.50
3:B:796:TYR:HB2	4:O:2:NAG:H62	1.93	0.50
3:A:420:ASP:O	3:A:460:LYS:N	2.44	0.50
1:I:68:THR:HB	1:I:81:GLN:HB2	1.93	0.50
2:L:153:ASN:ND2	2:L:209:SER:OG	2.45	0.50
3:C:646:ARG:NH1	3:C:668:ALA:O	2.43	0.49
3:C:1139:ASP:HB3	3:C:1142:GLN:HB2	1.93	0.49
2:L:158:GLY:N	2:L:181:THR:O	2.45	0.49
2:L:191:LYS:NZ	2:L:212:ARG:O	2.37	0.49
3:C:895:GLN:HG2	3:A:713:ALA:HB2	1.94	0.49
3:B:143:VAL:HB	3:B:245:HIS:HA	1.94	0.49
2:L:6:GLN:HG2	2:L:7:SER:H	1.77	0.49
3:B:726:ILE:HD13	3:B:945:LEU:HD23	1.93	0.49
3:C:203:ILE:HB	3:C:227:VAL:HB	1.95	0.49
3:C:787:GLN:OE1	3:A:703:ASN:ND2	2.38	0.49
2:M:186:ASP:O	2:M:193:TYR:OH	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:558:LYS:HE2	6:B:1303:NAG:H62	1.93	0.49
3:B:473:TYR:HB3	3:B:490:SER:HB2	1.95	0.49
3:B:909:ILE:HD13	3:B:1049:LEU:HD21	1.95	0.49
3:A:106:PHE:HB3	3:A:235:ILE:HD13	1.94	0.49
2:L:65:SER:OG	2:L:72:THR:OG1	2.28	0.49
3:C:563:GLN:HA	3:B:41:LYS:HB3	1.95	0.49
3:A:598:ILE:HG23	3:A:664:ILE:HG21	1.95	0.49
3:A:722:VAL:HG22	3:A:1065:VAL:HG22	1.95	0.49
3:C:909:ILE:HD13	3:C:1049:LEU:HD21	1.94	0.48
2:N:34:ASN:OD1	2:N:89:GLN:NE2	2.44	0.48
3:C:454:ARG:HD3	3:C:492:LEU:HB3	1.95	0.48
3:B:822:LEU:HD22	3:B:945:LEU:HD21	1.95	0.48
3:C:131:CYS:HB2	3:C:133:PHE:CE1	2.48	0.48
3:C:343:ASN:HB3	3:C:371:PHE:HE1	1.77	0.48
3:C:107:GLY:O	3:C:237:ARG:N	2.45	0.48
3:A:1028:LYS:HG3	3:A:1032:CYS:SG	2.53	0.48
3:B:18:LEU:HD12	3:B:19:ILE:HD13	1.96	0.48
3:B:722:VAL:HG22	3:B:1065:VAL:HG22	1.96	0.48
2:L:112:ALA:HB3	2:L:141:TYR:H	1.79	0.48
3:C:189:LEU:HD13	3:C:217:PRO:HD3	1.94	0.48
3:C:598:ILE:HG23	3:C:664:ILE:HG21	1.96	0.48
3:B:1116:THR:OG1	3:B:1118:ASP:OD1	2.22	0.48
3:A:142:ASP:OD2	3:A:158:ARG:NH2	2.45	0.48
3:A:382:VAL:HG13	3:A:430:THR:HB	1.96	0.48
3:A:715:PRO:HA	3:A:1072:GLU:HA	1.95	0.48
3:C:116:SER:HB3	3:C:233:ILE:HG21	1.95	0.47
2:L:94:MET:HB2	2:L:95:PRO:HD3	1.96	0.47
3:C:53:ASP:OD1	3:C:54:LEU:N	2.43	0.47
3:A:457:ARG:NH1	3:A:471:GLU:O	2.45	0.47
3:A:564:GLN:HA	3:A:577:ARG:HB2	1.96	0.47
3:B:444:LYS:HD2	3:B:447:GLY:HA2	1.96	0.47
3:B:858:LEU:HD22	3:B:959:LEU:HD22	1.96	0.47
3:A:335:LEU:H	3:A:335:LEU:HD22	1.78	0.47
3:B:736:VAL:HG11	3:B:1004:LEU:HD21	1.96	0.47
1:I:151:TYR:HB3	1:I:182:TYR:HB2	1.96	0.47
1:H:171:THR:HG23	1:H:184:LEU:HD21	1.97	0.47
1:I:47:TRP:HZ2	1:I:50:THR:HG22	1.78	0.47
2:L:6:GLN:HA	2:L:23:CYS:HA	1.97	0.47
3:C:497:PHE:CD1	3:C:499:PRO:HD2	2.49	0.47
3:C:898:PHE:HA	3:C:901:GLN:HG2	1.97	0.47
3:B:104:TRP:HD1	3:B:240:THR:HG22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:412:PRO:HB3	3:B:427:ASP:HA	1.96	0.47
3:A:133:PHE:HB3	3:A:163:ALA:HA	1.95	0.47
2:N:112:ALA:HB3	2:N:141:TYR:H	1.79	0.47
1:J:47:TRP:HZ2	1:J:50:THR:HG22	1.79	0.47
3:C:87:ASN:OD1	3:C:87:ASN:N	2.48	0.47
3:B:1121:PHE:HE2	3:A:914:ASN:HD21	1.63	0.47
1:I:22:CYS:HB3	1:I:78:LEU:HB3	1.96	0.47
2:M:158:GLY:O	2:M:181:THR:OG1	2.28	0.47
5:T:1:NAG:H61	5:T:2:NAG:C7	2.45	0.47
3:C:379:CYS:HA	3:C:432:CYS:HA	1.96	0.47
3:C:949:GLN:HA	3:C:952:VAL:HG22	1.97	0.47
1:J:169:VAL:HG22	1:J:188:VAL:HG23	1.97	0.47
3:C:298:GLU:HB3	3:C:315:THR:HG21	1.97	0.46
3:B:1041:ASP:HB2	3:A:1030:SER:HB2	1.95	0.46
1:J:126:SER:HA	1:J:213:VAL:HG21	1.97	0.46
2:N:145:ALA:HB2	2:N:199:HIS:HD2	1.80	0.46
3:A:48:LEU:HD21	3:A:278:LYS:HD3	1.97	0.46
3:B:379:CYS:HA	3:B:432:CYS:HA	1.97	0.46
1:J:201:ILE:HG12	1:J:216:ARG:HB3	1.97	0.46
3:C:755:GLN:HB2	3:A:969:LYS:HE3	1.97	0.46
3:B:168:PHE:CZ	3:B:230:PRO:HD2	2.50	0.46
3:C:383:SER:HA	2:N:94:MET:HG3	1.98	0.46
3:B:454:ARG:HA	3:B:492:LEU:HB3	1.97	0.46
2:L:34:ASN:HB3	2:L:49:TYR:HA	1.98	0.46
3:B:431:GLY:HA2	3:B:515:PHE:HD2	1.79	0.46
3:B:409:GLN:O	3:B:409:GLN:NE2	2.49	0.46
1:J:128:PHE:CG	2:N:125:GLN:HB2	2.51	0.46
3:C:396:TYR:HB2	3:C:514:SER:HB3	1.98	0.46
3:C:722:VAL:HG22	3:C:1065:VAL:HG22	1.97	0.46
3:C:989:ALA:O	3:C:993:ILE:HG12	2.15	0.46
3:A:125:ASN:HA	3:A:174:PRO:HD3	1.97	0.46
2:M:21:ILE:HB	2:M:73:LEU:HB3	1.97	0.46
3:C:196:ASN:HD22	3:C:201:PHE:HD1	1.63	0.45
3:C:336:CYS:HB2	3:C:364:ASP:OD2	2.17	0.45
3:C:1028:LYS:HG3	3:C:1032:CYS:SG	2.56	0.45
3:B:825:LYS:HE3	3:B:939:SER:HA	1.97	0.45
3:B:106:PHE:O	3:B:116:SER:HB2	2.15	0.45
2:M:135:CYS:HB2	2:M:149:TRP:CZ2	2.51	0.45
1:J:171:THR:HG23	1:J:184:LEU:HD21	1.98	0.45
3:C:763:LEU:HD22	3:C:1008:VAL:HG21	1.99	0.45
3:A:64:TRP:HE1	3:A:264:ALA:HB1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:551:VAL:HB	3:A:588:THR:HG23	1.98	0.45
3:B:39:PRO:HG3	3:B:55:PHE:HZ	1.82	0.45
3:B:661:GLU:O	3:B:695:TYR:OH	2.26	0.45
3:B:763:LEU:HD22	3:B:1008:VAL:HG21	1.97	0.45
3:B:794:ILE:HD13	3:B:794:ILE:H	1.81	0.45
2:N:147:VAL:HG13	2:N:197:VAL:HG22	1.99	0.45
3:B:826:VAL:HG23	3:B:945:LEU:HD13	1.99	0.45
2:N:147:VAL:HG22	2:N:197:VAL:HG13	1.99	0.45
1:H:154:GLU:OE1	1:H:154:GLU:N	2.50	0.45
2:L:167:GLN:HB2	2:L:174:TYR:CZ	2.51	0.45
3:C:916:LEU:HD12	3:C:923:ILE:HD12	1.99	0.45
3:B:611:LEU:HD22	3:B:666:ILE:HG23	1.98	0.45
3:A:409:GLN:HG3	3:A:419:ALA:HB2	1.99	0.45
2:N:114:PRO:HD2	2:N:202:LEU:HB2	1.98	0.45
3:B:543:PHE:HD1	3:B:579:PRO:HD3	1.81	0.45
3:B:1047:TYR:HB2	3:B:1067:TYR:HB3	1.97	0.45
3:C:735:SER:OG	3:C:859:THR:OG1	2.34	0.44
3:B:336:CYS:HB2	3:B:364:ASP:CB	2.46	0.44
3:A:763:LEU:HD22	3:A:1008:VAL:HG21	1.98	0.44
1:I:161:ASN:O	1:I:161:ASN:ND2	2.47	0.44
2:L:95:PRO:HB2	2:L:96:PRO:HD3	1.98	0.44
3:C:113:LYS:HG3	3:C:114:THR:H	1.82	0.44
3:B:132:GLU:HG2	3:B:165:ASN:HB2	2.00	0.44
3:B:383:SER:OG	1:I:102:GLN:O	2.29	0.44
3:A:37:TYR:OH	3:A:54:LEU:O	2.30	0.44
3:C:327:VAL:H	3:C:531:THR:HG22	1.83	0.44
3:B:808:ASP:OD2	3:B:811:LYS:NZ	2.50	0.44
3:A:128:ILE:HD13	3:A:229:LEU:HD11	1.99	0.44
3:C:802:PHE:HD1	3:C:805:ILE:HD11	1.82	0.44
3:C:227:VAL:CG1	3:C:229:LEU:HG	2.48	0.44
3:A:80:ASP:OD1	3:A:81:ASN:N	2.51	0.44
3:B:802:PHE:HD1	3:B:805:ILE:HD11	1.83	0.44
2:M:109:ARG:HD2	2:M:172:SER:HB2	1.98	0.44
2:M:150:LYS:HB2	2:M:194:ALA:HB3	2.00	0.44
3:A:280:ASN:ND2	3:A:284:THR:OG1	2.44	0.44
3:A:414:GLN:OE1	3:A:424:LYS:HA	2.18	0.44
2:M:6:GLN:HA	2:M:23:CYS:HA	1.98	0.44
2:N:146:LYS:NZ	2:N:148:GLN:OE1	2.33	0.44
3:C:336:CYS:O	3:C:338:PHE:N	2.50	0.44
3:B:380:TYR:O	3:B:382:VAL:N	2.51	0.44
3:A:336:CYS:SG	3:A:337:PRO:HD2	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:989:ALA:O	3:A:993:ILE:HG12	2.18	0.44
2:N:6:GLN:HG2	2:N:7:SER:H	1.83	0.44
3:C:353:TRP:CZ2	3:C:466:ARG:HG2	2.53	0.44
3:B:456:LEU:HG	3:B:457:ARG:HG3	2.00	0.44
3:B:676:THR:HB	3:B:690:GLN:HG2	2.00	0.44
3:B:1011:GLN:OE1	3:B:1014:ARG:NH1	2.51	0.44
4:D:1:NAG:H4	4:D:2:NAG:H2	1.70	0.44
1:I:90:THR:HG23	1:I:116:THR:HA	2.00	0.43
4:W:1:NAG:O3	4:W:2:NAG:N2	2.51	0.43
3:C:214:ARG:O	3:C:266:TYR:OH	2.32	0.43
2:M:37:GLN:HE21	2:M:37:GLN:HB3	1.62	0.43
2:M:59:PRO:HB2	2:M:61:ARG:HG2	1.99	0.43
2:N:59:PRO:HB2	2:N:61:ARG:HG2	2.00	0.43
3:C:414:GLN:HG2	3:C:415:THR:H	1.83	0.43
3:C:563:GLN:HE22	3:B:43:PHE:HD2	1.65	0.43
3:B:19:ILE:HD11	3:B:138:ASP:HB3	1.99	0.43
3:B:311:GLY:HA2	3:B:664:ILE:HG23	2.00	0.43
3:A:666:ILE:HD11	3:A:672:ALA:HB2	1.99	0.43
2:L:6:GLN:H	2:L:101:GLN:HE22	1.65	0.43
3:C:398:ASP:OD2	3:C:423:TYR:OH	2.29	0.43
3:A:53:ASP:OD1	3:A:54:LEU:N	2.44	0.43
3:A:115:GLN:NE2	4:c:1:NAG:O5	2.52	0.43
1:I:158:VAL:HG13	1:I:204:VAL:HG22	1.99	0.43
2:M:114:PRO:HB3	2:M:140:PHE:HB3	2.00	0.43
1:H:90:THR:HG23	1:H:116:THR:HA	1.99	0.43
3:A:457:ARG:HH22	3:A:471:GLU:H	1.66	0.43
3:A:949:GLN:HA	3:A:952:VAL:HG22	2.00	0.43
1:I:145:GLY:HA3	1:I:187:VAL:HG12	2.00	0.43
3:B:902:MET:HE3	3:B:1049:LEU:HD13	2.01	0.43
3:B:715:PRO:HA	3:B:1072:GLU:HA	2.00	0.43
3:A:96:GLU:OE1	3:A:98:SER:N	2.50	0.43
2:M:134:VAL:HA	2:M:179:THR:HA	2.01	0.43
1:H:22:CYS:HB3	1:H:78:LEU:HB3	2.01	0.43
3:C:498:ARG:N	3:C:499:PRO:HD3	2.33	0.43
3:C:1047:TYR:HB2	3:C:1067:TYR:HB3	2.01	0.43
3:A:34:ARG:HB2	3:A:216:LEU:HD21	2.01	0.43
3:A:879:ALA:O	3:A:883:THR:OG1	2.30	0.43
1:I:56:ASP:N	1:I:56:ASP:OD1	2.52	0.43
3:C:54:LEU:HD13	3:C:88:ASP:HB3	2.01	0.43
3:C:658:ASN:HD22	3:C:660:TYR:HE2	1.66	0.43
3:C:1028:LYS:HE3	3:C:1028:LYS:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:LEU:HD22	3:C:117:LEU:HA	1.88	0.42
3:B:440:LYS:H	3:B:440:LYS:HG3	1.69	0.42
3:A:736:VAL:HG22	3:A:858:LEU:HD22	2.01	0.42
2:M:95:PRO:HB2	2:M:96:PRO:HD3	2.01	0.42
3:A:44:ARG:HB3	3:A:47:VAL:HG22	2.02	0.42
3:B:363:ALA:HB2	3:B:527:PRO:HD3	2.00	0.42
3:B:1075:PHE:HA	6:B:1305:NAG:H82	2.01	0.42
2:L:193:TYR:HE2	2:L:212:ARG:HB2	1.84	0.42
2:N:21:ILE:HD12	2:N:73:LEU:HD23	2.01	0.42
2:N:37:GLN:HE21	2:N:37:GLN:HB3	1.62	0.42
3:B:117:LEU:HD22	3:B:231:ILE:HD13	2.00	0.42
3:B:190:ARG:HG2	3:B:207:HIS:CD2	2.54	0.42
3:A:203:ILE:HB	3:A:227:VAL:HG23	2.02	0.42
3:C:195:LYS:HB2	3:C:202:LYS:HB2	2.00	0.42
3:C:826:VAL:HG23	3:C:945:LEU:HD23	2.00	0.42
3:C:895:GLN:OE1	3:A:711:SER:OG	2.35	0.42
3:B:498:ARG:O	3:B:500:THR:N	2.52	0.42
3:A:794:ILE:HD13	3:A:795:LYS:H	1.85	0.42
1:I:106:PHE:HE2	2:M:99:PHE:HZ	1.68	0.42
2:N:33:LEU:HD13	2:N:71:PHE:CD1	2.55	0.42
1:H:51:ILE:HD13	1:H:71:ARG:HB3	2.02	0.42
2:L:33:LEU:HD13	2:L:71:PHE:CD1	2.55	0.42
2:L:137:LEU:HD21	2:L:197:VAL:HG13	2.01	0.42
3:A:80:ASP:OD1	3:A:81:ASN:ND2	2.52	0.42
3:A:813:SER:OG	3:A:815:ARG:NE	2.53	0.42
2:L:32:PHE:O	2:L:91:SER:N	2.45	0.42
3:C:108:THR:HG22	3:C:109:THR:HG23	2.02	0.42
3:C:408:SER:O	3:C:409:GLN:NE2	2.41	0.42
3:B:1013:ILE:O	3:B:1017:GLU:HG2	2.19	0.42
3:A:770:ILE:O	3:A:774:GLN:HG2	2.20	0.42
1:I:92:VAL:HG22	1:I:114:LEU:HD13	2.00	0.42
3:B:96:GLU:HB2	3:B:100:ILE:HG22	2.01	0.42
3:B:612:TYR:HE2	3:B:651:ILE:HD12	1.84	0.42
2:N:140:PHE:HZ	2:N:176:LEU:HB2	1.85	0.42
3:C:912:THR:OG1	3:C:1106:GLN:NE2	2.53	0.42
3:A:439:ASN:HB2	3:A:506:GLN:HB3	2.02	0.42
1:H:128:PHE:HD1	2:L:124:GLU:HB3	1.85	0.41
3:C:560:LEU:HB3	3:C:562:PHE:CE1	2.55	0.41
3:A:31:SER:O	3:A:59:PHE:HA	2.20	0.41
1:I:215:LYS:HG3	1:I:216:ARG:H	1.85	0.41
2:M:183:SER:OG	2:M:184:LYS:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:LEU:HB3	3:C:276:LEU:HD11	2.02	0.41
3:C:92:PHE:O	3:C:192:PHE:N	2.49	0.41
3:B:337:PRO:HD2	3:B:358:ILE:HG23	2.01	0.41
3:B:19:ILE:HG12	3:B:20:THR:H	1.86	0.41
3:B:1105:THR:OG1	3:B:1106:GLN:N	2.52	0.41
3:B:53:ASP:OD1	3:B:54:LEU:N	2.44	0.41
3:C:600:PRO:HB3	3:C:674:TYR:HB2	2.01	0.41
3:C:927:PHE:HE1	3:C:1065:VAL:HG21	1.85	0.41
3:C:957:GLN:OE1	3:B:765:ARG:NE	2.54	0.41
3:B:96:GLU:OE1	3:B:101:ILE:N	2.39	0.41
3:B:599:THR:HB	3:B:608:VAL:HG12	2.02	0.41
3:A:335:LEU:O	3:A:362:VAL:N	2.46	0.41
1:J:106:PHE:HE2	2:N:99:PHE:HZ	1.67	0.41
3:C:227:VAL:HG12	3:C:229:LEU:HG	2.02	0.41
3:C:611:LEU:HD22	3:C:666:ILE:HG23	2.02	0.41
3:B:724:THR:HG21	3:B:938:LEU:HD11	2.03	0.41
3:B:896:ILE:HD12	3:B:897:PRO:HD2	2.03	0.41
3:B:949:GLN:HA	3:B:952:VAL:HG22	2.02	0.41
1:J:56:ASP:OD1	1:J:56:ASP:N	2.50	0.41
3:A:402:ILE:HB	3:A:406:GLU:HB2	2.03	0.41
3:A:916:LEU:HD12	3:A:923:ILE:HD12	2.02	0.41
2:M:65:SER:OG	2:M:72:THR:OG1	2.28	0.41
3:C:108:THR:HB	3:C:114:THR:HG21	2.02	0.41
3:B:712:ILE:HD13	3:B:713:ALA:H	1.84	0.41
3:A:475:ALA:HB3	3:A:488:CYS:HA	2.02	0.41
3:A:347:PHE:CE2	3:A:399:SER:HB2	2.56	0.41
1:J:152:PHE:CG	1:J:153:PRO:HD2	2.56	0.41
1:J:190:VAL:HG12	1:J:200:TYR:HD2	1.85	0.41
2:N:21:ILE:N	2:N:73:LEU:O	2.47	0.41
1:H:56:ASP:OD1	1:H:56:ASP:N	2.54	0.41
3:C:31:SER:O	3:C:59:PHE:HA	2.21	0.41
3:A:417:ASN:HD22	3:A:418:ILE:HD12	1.86	0.41
1:J:90:THR:HG23	1:J:116:THR:HA	2.03	0.41
1:J:125:PRO:HB3	1:J:151:TYR:HD1	1.86	0.41
1:H:15:GLY:N	1:H:85:LEU:O	2.53	0.40
2:L:185:ALA:HA	2:L:188:GLU:HG2	2.03	0.40
2:L:191:LYS:HD3	2:L:212:ARG:HB3	2.03	0.40
3:C:676:THR:HG22	3:C:690:GLN:HG3	2.02	0.40
3:B:158:ARG:CZ	3:B:158:ARG:HA	2.51	0.40
3:B:294:ASP:OD1	3:B:294:ASP:N	2.52	0.40
3:A:81:ASN:H	3:A:81:ASN:HD22	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:350:VAL:O	3:A:422:ASN:ND2	2.50	0.40
3:A:862:PRO:HA	3:A:863:PRO:HD3	1.99	0.40
1:I:148:VAL:HB	1:I:184:LEU:HB2	2.03	0.40
3:C:117:LEU:HB3	3:C:129:LYS:O	2.21	0.40
3:C:561:PRO:HA	3:C:577:ARG:HH22	1.86	0.40
2:N:61:ARG:NH1	2:N:81:GLU:OE2	2.50	0.40
3:C:168:PHE:CE2	3:C:229:LEU:HD22	2.56	0.40
3:C:412:PRO:HG2	2:N:92:TYR:CE2	2.56	0.40
3:B:122:ASN:HB2	3:B:125:ASN:H	1.85	0.40
3:B:438:SER:HB2	3:B:441:LEU:HD11	2.02	0.40
3:A:380:TYR:O	3:A:382:VAL:N	2.54	0.40
1:I:100:SER:O	1:I:105:TYR:OH	2.30	0.40
2:N:109:ARG:HH11	2:N:110:THR:HG1	1.68	0.40
2:L:83:PHE:HA	2:L:105:LEU:HD23	2.03	0.40
3:C:193:VAL:HG23	3:C:223:LEU:HD22	2.02	0.40
3:C:226:LEU:HG	3:C:227:VAL:HG23	2.02	0.40
3:A:77:LYS:HB3	3:A:79:PHE:CE1	2.57	0.40
3:A:718:PHE:HE1	3:A:923:ILE:HG12	1.86	0.40
3:A:985:ASP:HB3	3:A:988:GLU:HB3	2.03	0.40
1:I:154:GLU:N	1:I:154:GLU:OE1	2.54	0.40
2:M:83:PHE:HA	2:M:105:LEU:HD23	2.03	0.40
3:C:344:ALA:C	3:C:346:THR:H	2.30	0.40
3:B:213:GLU:CD	3:B:213:GLU:H	2.29	0.40
3:B:592:PHE:CZ	3:A:854:LYS:HB2	2.56	0.40
3:A:802:PHE:HD1	3:A:805:ILE:HD11	1.87	0.40
2:N:65:SER:OG	2:N:72:THR:OG1	2.27	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	H	196/449 (44%)	194 (99%)	2 (1%)	0	100	100
1	I	196/449 (44%)	194 (99%)	2 (1%)	0	100	100
1	J	196/449 (44%)	192 (98%)	4 (2%)	0	100	100
2	L	205/215 (95%)	198 (97%)	7 (3%)	0	100	100
2	M	205/215 (95%)	196 (96%)	9 (4%)	0	100	100
2	N	205/215 (95%)	200 (98%)	5 (2%)	0	100	100
3	A	998/1295 (77%)	948 (95%)	50 (5%)	0	100	100
3	B	1000/1295 (77%)	933 (93%)	67 (7%)	0	100	100
3	C	1004/1295 (78%)	938 (93%)	66 (7%)	0	100	100
All	All	4205/5877 (72%)	3993 (95%)	212 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	H	165/391 (42%)	164 (99%)	1 (1%)	84	92
1	I	165/391 (42%)	163 (99%)	2 (1%)	67	83
1	J	165/391 (42%)	162 (98%)	3 (2%)	54	75
2	L	184/189 (97%)	179 (97%)	5 (3%)	40	67
2	M	184/189 (97%)	180 (98%)	4 (2%)	47	71
2	N	184/189 (97%)	181 (98%)	3 (2%)	58	78
3	A	892/1118 (80%)	864 (97%)	28 (3%)	35	63
3	B	892/1118 (80%)	857 (96%)	35 (4%)	27	57
3	C	894/1118 (80%)	857 (96%)	37 (4%)	26	56
All	All	3725/5094 (73%)	3607 (97%)	118 (3%)	36	63

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	144	LEU
2	L	34	ASN
2	L	37	GLN
2	L	97	VAL
2	L	148	GLN
2	L	187	TYR
3	C	21	ARG
3	C	87	ASN
3	C	117	LEU
3	C	118	LEU
3	C	121	ASN
3	C	160	TYR
3	C	197	ILE
3	C	210	ILE
3	C	213	GLU
3	C	236	THR
3	C	281	GLU
3	C	301	CYS
3	C	310	LYS
3	C	332	ILE
3	C	347	PHE
3	C	355	ARG
3	C	362	VAL
3	C	364	ASP
3	C	387	LEU
3	C	402	ILE
3	C	440	LYS
3	C	448	ASN
3	C	453	TYR
3	C	460	LYS
3	C	488	CYS
3	C	492	LEU
3	C	559	PHE
3	C	650	LEU
3	C	658	ASN
3	C	740	MET
3	C	753	LEU
3	C	786	LYS
3	C	855	PHE
3	C	878	LEU
3	C	1004	LEU
3	C	1045	LYS
3	C	1104	VAL

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Mol	Chain	Res	Type
3	B	18	LEU
3	B	19	ILE
3	B	33	THR
3	B	62	VAL
3	B	130	VAL
3	B	133	PHE
3	B	158	ARG
3	B	212	LEU
3	B	244	LEU
3	B	281	GLU
3	B	312	ILE
3	B	345	THR
3	B	402	ILE
3	B	406	GLU
3	B	409	GLN
3	B	422	ASN
3	B	440	LYS
3	B	448	ASN
3	B	472	ILE
3	B	492	LEU
3	B	495	TYR
3	B	534	VAL
3	B	544	ASN
3	B	595	VAL
3	B	599	THR
3	B	615	VAL
3	B	658	ASN
3	B	712	ILE
3	B	786	LYS
3	B	794	ILE
3	B	916	LEU
3	B	966	LEU
3	B	976	VAL
3	B	1004	LEU
3	B	1130	ILE
3	A	22	THR
3	A	78	ARG
3	A	96	GLU
3	A	121	ASN
3	A	124	THR
3	A	133	PHE
3	A	227	VAL

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Mol	Chain	Res	Type
3	A	244	LEU
3	A	326	ILE
3	A	336	CYS
3	A	361	CYS
3	A	368	ILE
3	A	387	LEU
3	A	402	ILE
3	A	415	THR
3	A	422	ASN
3	A	455	LEU
3	A	492	LEU
3	A	529	LYS
3	A	615	VAL
3	A	650	LEU
3	A	658	ASN
3	A	693	ILE
3	A	699	LEU
3	A	708	SER
3	A	794	ILE
3	A	966	LEU
3	A	1004	LEU
1	I	144	LEU
1	I	161	ASN
2	M	34	ASN
2	M	37	GLN
2	M	148	GLN
2	M	202	LEU
1	J	144	LEU
1	J	161	ASN
1	J	182	TYR
2	N	34	ASN
2	N	37	GLN
2	N	148	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	39	GLN
1	H	81	GLN
2	L	37	GLN
2	L	38	GLN

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Mol	Chain	Res	Type
2	L	89	GLN
3	C	17	ASN
3	C	99	ASN
3	C	173	GLN
3	C	188	ASN
3	C	196	ASN
3	C	239	GLN
3	C	321	GLN
3	C	394	ASN
3	C	563	GLN
3	C	580	GLN
3	C	644	GLN
3	C	895	GLN
3	C	913	GLN
3	C	935	GLN
3	C	965	GLN
3	C	1010	GLN
3	C	1106	GLN
3	C	1135	ASN
3	B	14	GLN
3	B	52	HIS
3	B	99	ASN
3	B	196	ASN
3	B	207	HIS
3	B	239	GLN
3	B	317	ASN
3	B	409	GLN
3	B	450	ASN
3	B	580	GLN
3	B	675	GLN
3	B	901	GLN
3	B	919	ASN
3	B	935	GLN
3	B	955	ASN
3	B	957	GLN
3	B	1058	HIS
3	B	1106	GLN
3	A	49	HIS
3	A	81	ASN
3	A	188	ASN
3	A	207	HIS
3	A	245	HIS

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Mol	Chain	Res	Type
3	A	280	ASN
3	A	314	GLN
3	A	317	ASN
3	A	388	ASN
3	A	394	ASN
3	A	414	GLN
3	A	422	ASN
3	A	536	ASN
3	A	542	ASN
3	A	563	GLN
3	A	762	GLN
3	A	907	ASN
3	A	919	ASN
3	A	935	GLN
3	A	1011	GLN
1	I	39	GLN
2	M	34	ASN
2	M	37	GLN
2	M	38	GLN
2	M	89	GLN
2	M	190	HIS
1	J	39	GLN
1	J	81	GLN
2	N	34	ASN
2	N	37	GLN
2	N	38	GLN
2	N	89	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 ⓘ

62 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	$\# Z > 2$
4	NAG	D	1	3,4	14,14,15	0.21	0	17,19,21	0.51	0
4	NAG	D	2	4	14,14,15	0.54	0	17,19,21	0.49	0
5	NAG	E	1	3,5	14,14,15	0.48	0	17,19,21	0.65	0
5	NAG	E	2	5	14,14,15	0.22	0	17,19,21	0.52	0
5	BMA	E	3	5	11,11,12	0.59	0	15,15,17	0.73	0
4	NAG	F	1	3,4	14,14,15	0.19	0	17,19,21	0.53	0
4	NAG	F	2	4	14,14,15	0.54	0	17,19,21	0.49	0
5	NAG	G	1	3,5	14,14,15	0.21	0	17,19,21	0.46	0
5	NAG	G	2	5	14,14,15	0.21	0	17,19,21	0.42	0
5	BMA	G	3	5	11,11,12	0.60	0	15,15,17	0.76	0
5	NAG	K	1	3,5	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	K	2	5	14,14,15	0.26	0	17,19,21	0.52	0
5	BMA	K	3	5	11,11,12	0.58	0	15,15,17	0.78	0
4	NAG	O	1	3,4	14,14,15	0.33	0	17,19,21	0.37	0
4	NAG	O	2	4	14,14,15	0.42	0	17,19,21	0.35	0
4	NAG	P	1	3,4	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	P	2	4	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	Q	1	3,4	14,14,15	0.27	0	17,19,21	0.57	0
4	NAG	Q	2	4	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	R	1	3,4	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	R	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	S	1	3,4	14,14,15	0.19	0	17,19,21	0.42	0
4	NAG	S	2	4	14,14,15	0.27	0	17,19,21	0.55	0
5	NAG	T	1	3,5	14,14,15	0.82	1 (7%)	17,19,21	0.84	0
5	NAG	T	2	5	14,14,15	0.23	0	17,19,21	0.60	0
5	BMA	T	3	5	11,11,12	0.58	0	15,15,17	0.77	0
4	NAG	U	1	3,4	14,14,15	0.19	0	17,19,21	0.40	0
4	NAG	U	2	4	14,14,15	0.27	0	17,19,21	0.54	0
4	NAG	V	1	3,4	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	V	2	4	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	W	1	3,4	14,14,15	0.26	0	17,19,21	0.41	0
4	NAG	W	2	4	14,14,15	0.46	0	17,19,21	0.53	0
5	NAG	X	1	3,5	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	X	2	5	14,14,15	0.21	0	17,19,21	0.39	0
5	BMA	X	3	5	11,11,12	0.59	0	15,15,17	0.76	0
5	NAG	Y	1	3,5	14,14,15	0.24	0	17,19,21	0.49	0
5	NAG	Y	2	5	14,14,15	0.25	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	Y	3	5	11,11,12	0.58	0	15,15,17	0.80	0
5	NAG	Z	1	3,5	14,14,15	0.26	0	17,19,21	0.47	0
5	NAG	Z	2	5	14,14,15	0.46	0	17,19,21	0.43	0
5	BMA	Z	3	5	11,11,12	0.59	0	15,15,17	0.75	0
4	NAG	a	1	3,4	14,14,15	0.26	0	17,19,21	0.36	0
4	NAG	a	2	4	14,14,15	0.27	0	17,19,21	0.40	0
5	NAG	b	1	3,5	14,14,15	0.28	0	17,19,21	0.42	0
5	NAG	b	2	5	14,14,15	0.29	0	17,19,21	0.56	0
5	BMA	b	3	5	11,11,12	0.60	0	15,15,17	0.78	0
4	NAG	c	1	3,4	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	c	2	4	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	d	1	3,5	14,14,15	0.24	0	17,19,21	0.52	0
5	NAG	d	2	5	14,14,15	0.21	0	17,19,21	0.44	0
5	BMA	d	3	5	11,11,12	0.59	0	15,15,17	0.74	0
4	NAG	e	1	3,4	14,14,15	0.20	0	17,19,21	0.39	0
4	NAG	e	2	4	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	f	1	3,5	14,14,15	0.24	0	17,19,21	0.49	0
5	NAG	f	2	5	14,14,15	0.22	0	17,19,21	0.39	0
5	BMA	f	3	5	11,11,12	0.60	0	15,15,17	0.77	0
4	NAG	g	1	3,4	14,14,15	0.32	0	17,19,21	0.63	0
4	NAG	g	2	4	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	h	1	3,4	14,14,15	0.25	0	17,19,21	0.36	0
4	NAG	h	2	4	14,14,15	0.27	0	17,19,21	0.38	0
4	NAG	i	1	3,4	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	i	2	4	14,14,15	0.23	0	17,19,21	0.42	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	D	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
5	NAG	E	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	1/2/19/22	0/1/1/1
4	NAG	F	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
5	NAG	G	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	K	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
4	NAG	O	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
4	NAG	R	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	1/6/23/26	0/1/1/1
5	NAG	T	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	T	2	5	-	1/6/23/26	0/1/1/1
5	BMA	T	3	5	-	0/2/19/22	0/1/1/1
4	NAG	U	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	1/6/23/26	0/1/1/1
4	NAG	V	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	NAG	W	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	3/6/23/26	0/1/1/1
5	NAG	X	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	X	2	5	-	0/6/23/26	0/1/1/1
5	BMA	X	3	5	-	0/2/19/22	0/1/1/1
5	NAG	Y	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	1/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	0/2/19/22	0/1/1/1
5	NAG	Z	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	0/2/19/22	0/1/1/1
4	NAG	a	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	a	2	4	-	1/6/23/26	0/1/1/1
5	NAG	b	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1
5	BMA	b	3	5	-	0/2/19/22	0/1/1/1
4	NAG	c	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	0/6/23/26	0/1/1/1
5	NAG	d	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	d	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	d	3	5	-	0/2/19/22	0/1/1/1
4	NAG	e	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
5	NAG	f	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	f	2	5	-	0/6/23/26	0/1/1/1
5	BMA	f	3	5	-	0/2/19/22	0/1/1/1
4	NAG	g	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	g	2	4	-	0/6/23/26	0/1/1/1
4	NAG	h	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	h	2	4	-	2/6/23/26	0/1/1/1
4	NAG	i	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	i	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	1	NAG	O5-C1	-2.91	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	2	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	g	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	g	1	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	h	2	NAG	C4-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	i	1	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	i	1	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	h	2	NAG	O5-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6

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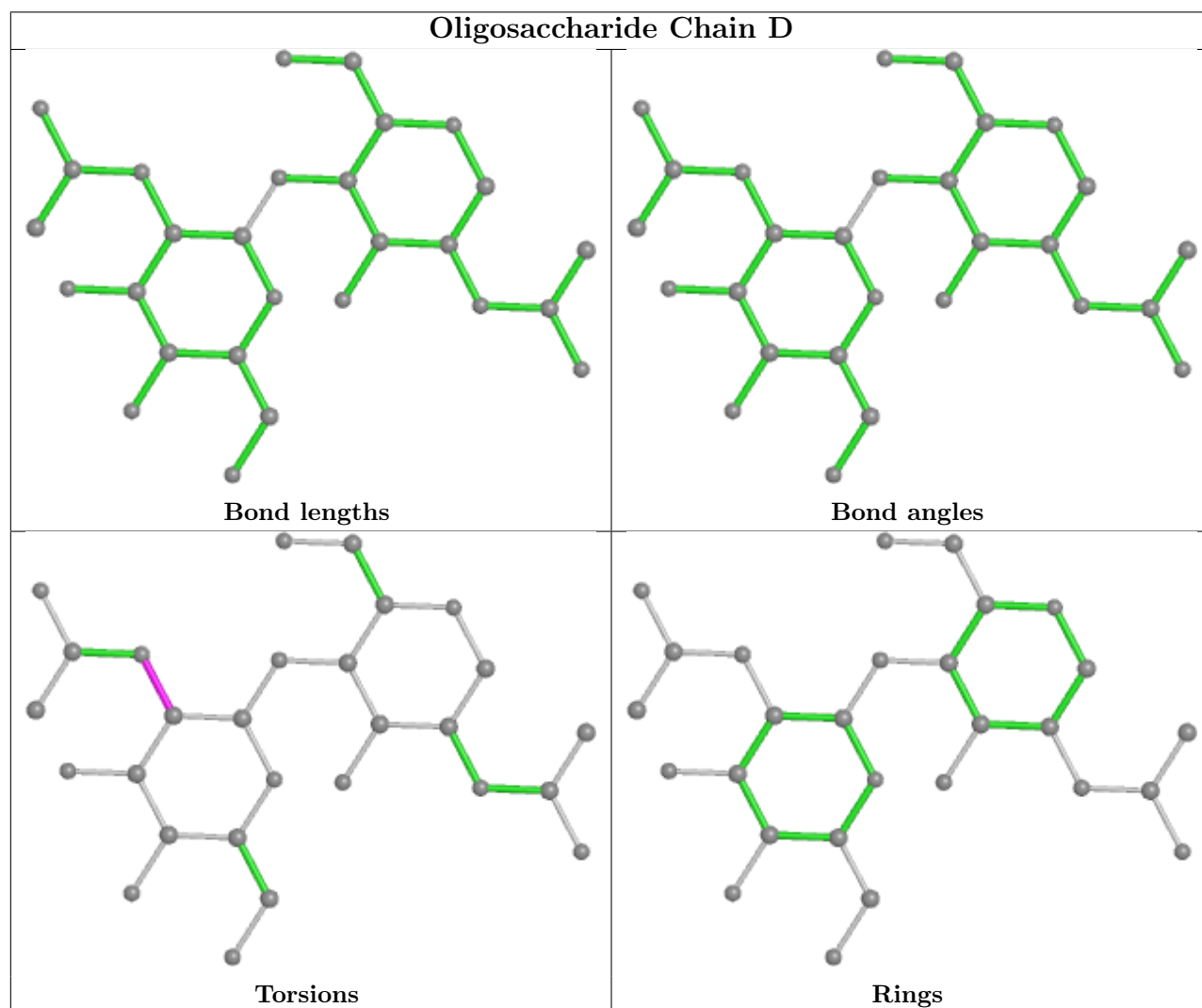
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C4-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
5	d	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C3-C2-N2-C7
4	S	2	NAG	C3-C2-N2-C7
4	U	2	NAG	C3-C2-N2-C7
4	W	2	NAG	C3-C2-N2-C7
4	g	1	NAG	C3-C2-N2-C7
5	E	1	NAG	C3-C2-N2-C7
5	K	2	NAG	C3-C2-N2-C7
5	T	1	NAG	C3-C2-N2-C7
5	T	2	NAG	C3-C2-N2-C7
5	Y	2	NAG	C3-C2-N2-C7
5	d	1	NAG	C3-C2-N2-C7
5	d	1	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C1-C2-N2-C7
4	Q	2	NAG	C4-C5-C6-O6

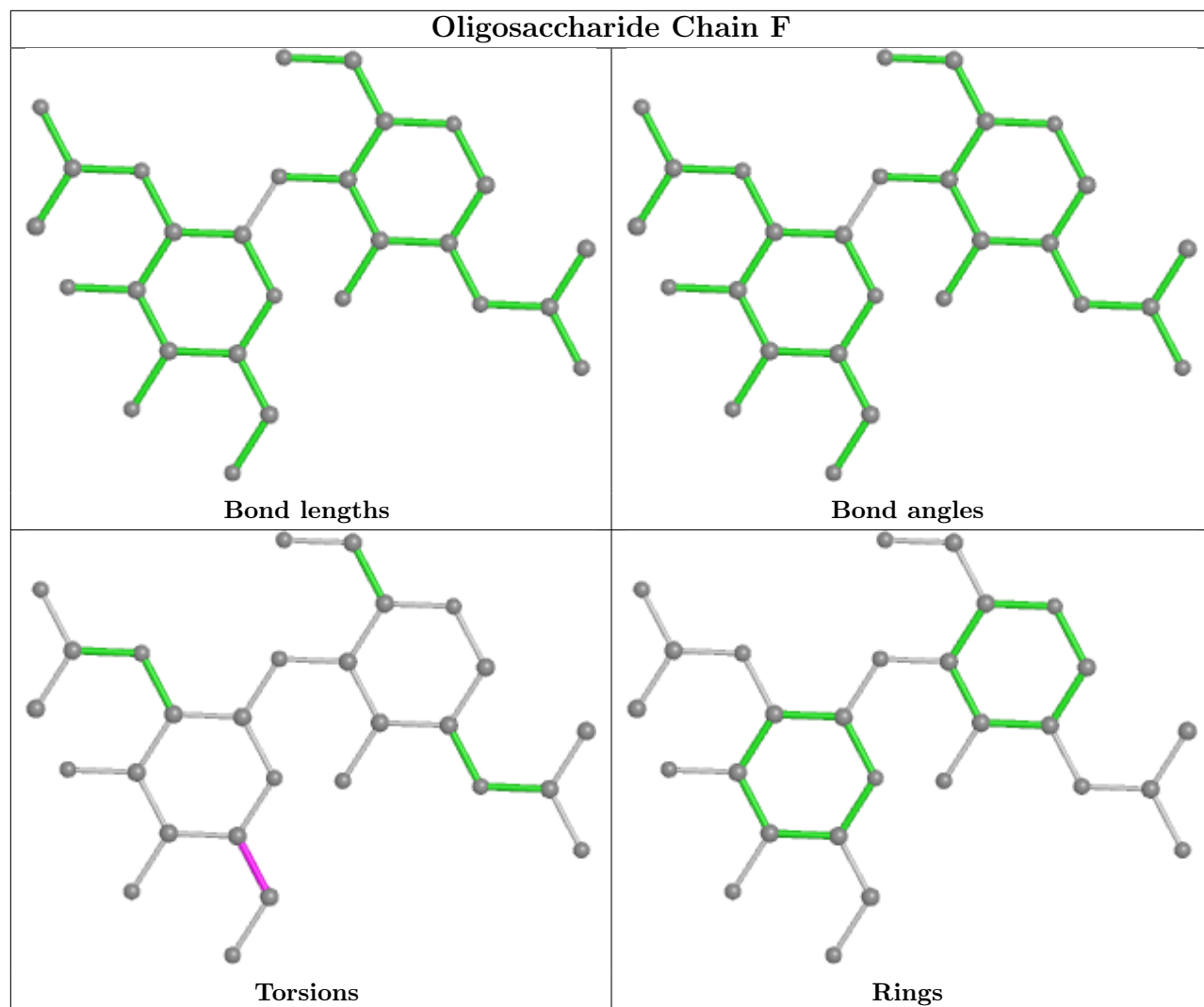
There are no ring outliers.

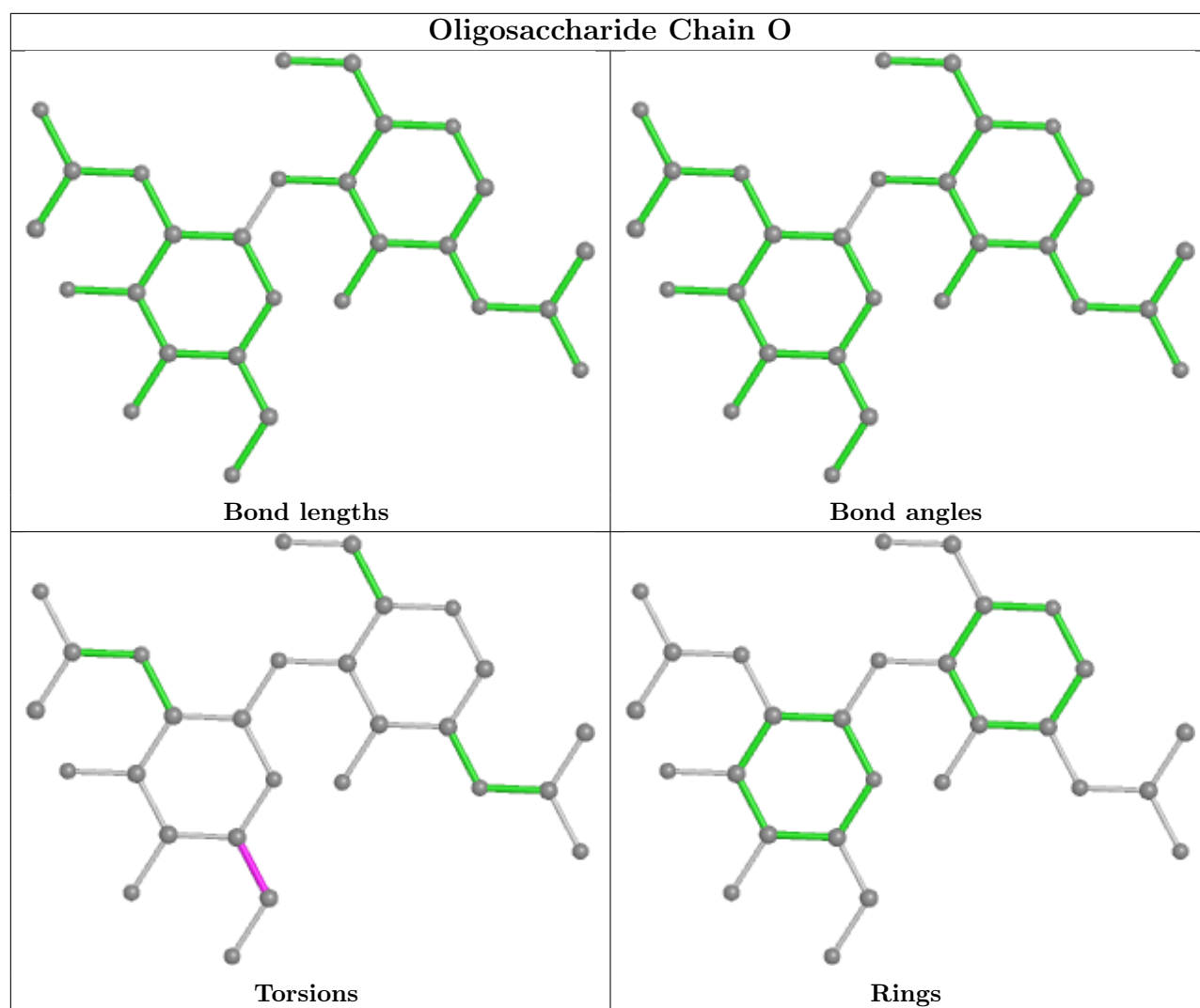
9 monomers are involved in 6 short contacts:

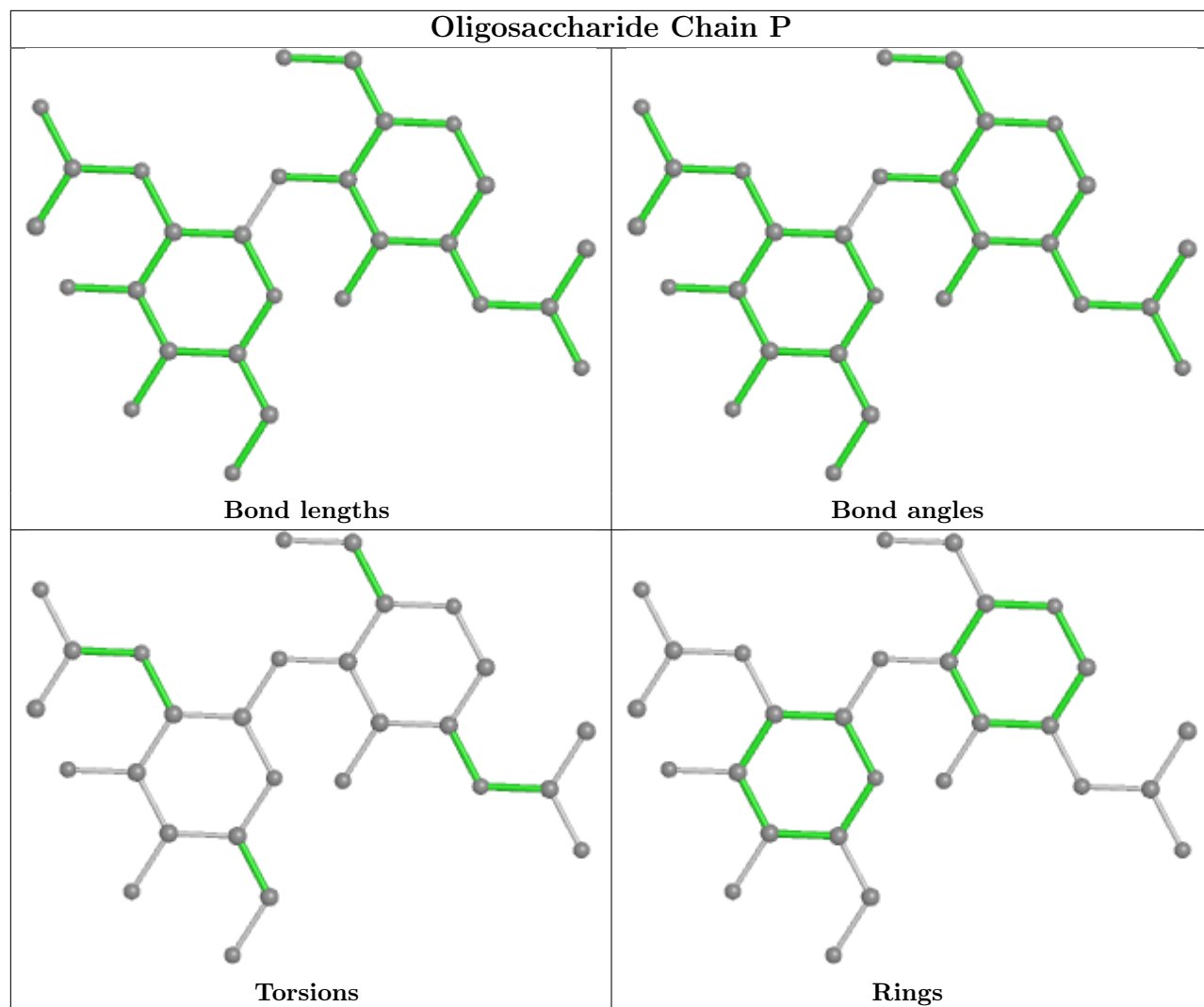
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	1	NAG	1	0
4	c	1	NAG	1	0
4	W	1	NAG	1	0
4	O	2	NAG	1	0
5	T	2	NAG	1	0
4	D	2	NAG	1	0
4	D	1	NAG	1	0
4	W	2	NAG	1	0
4	U	2	NAG	1	0

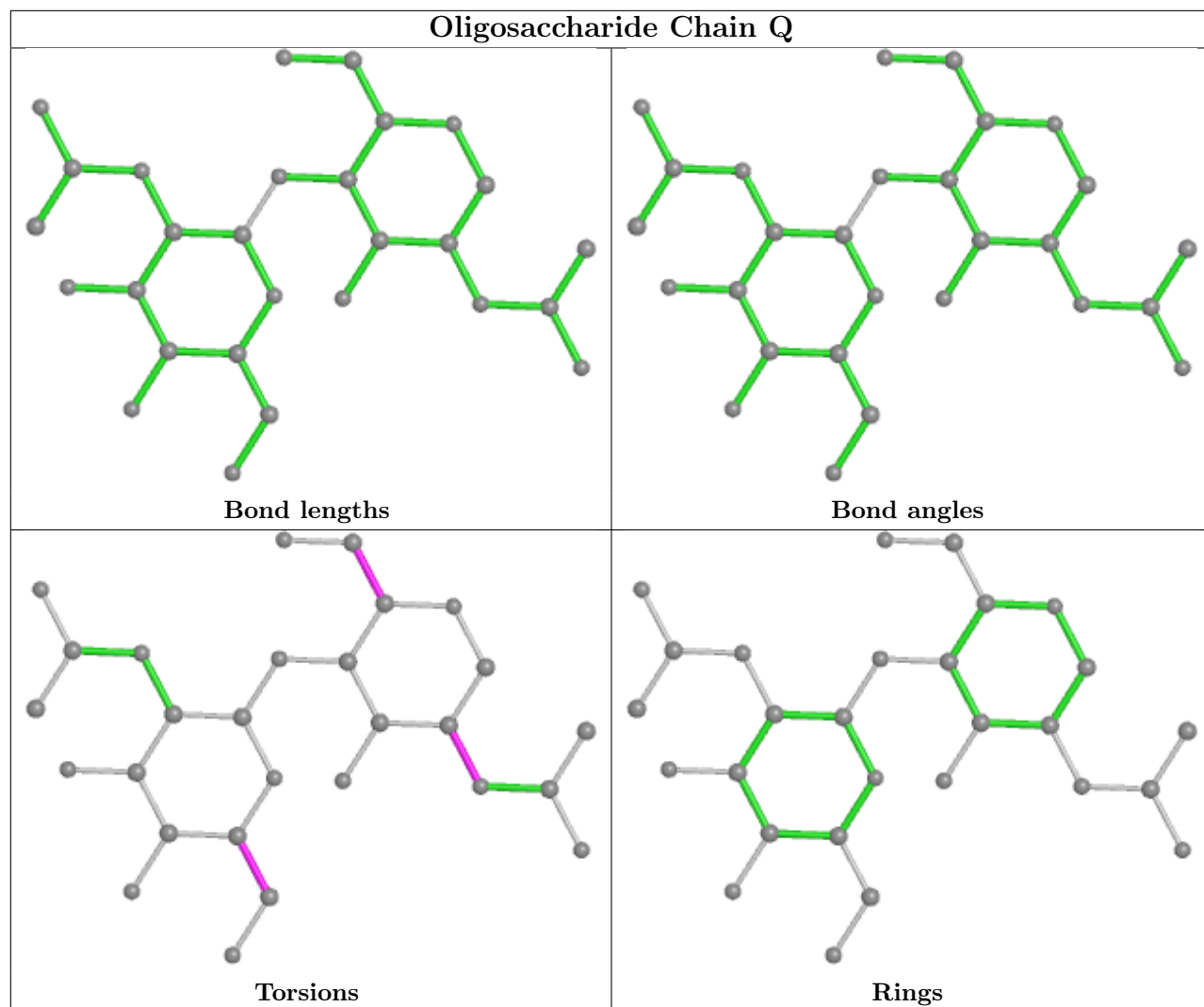
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

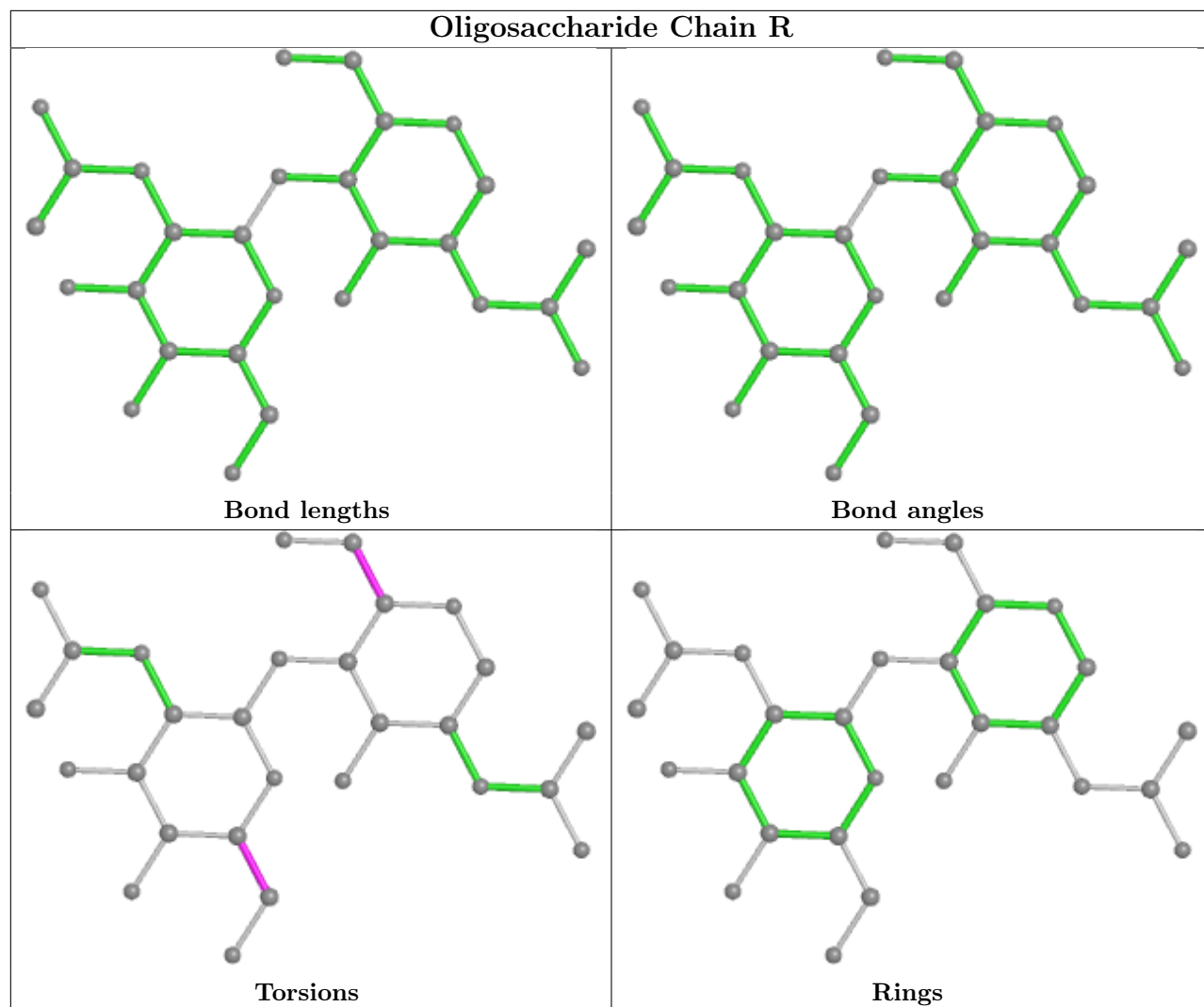


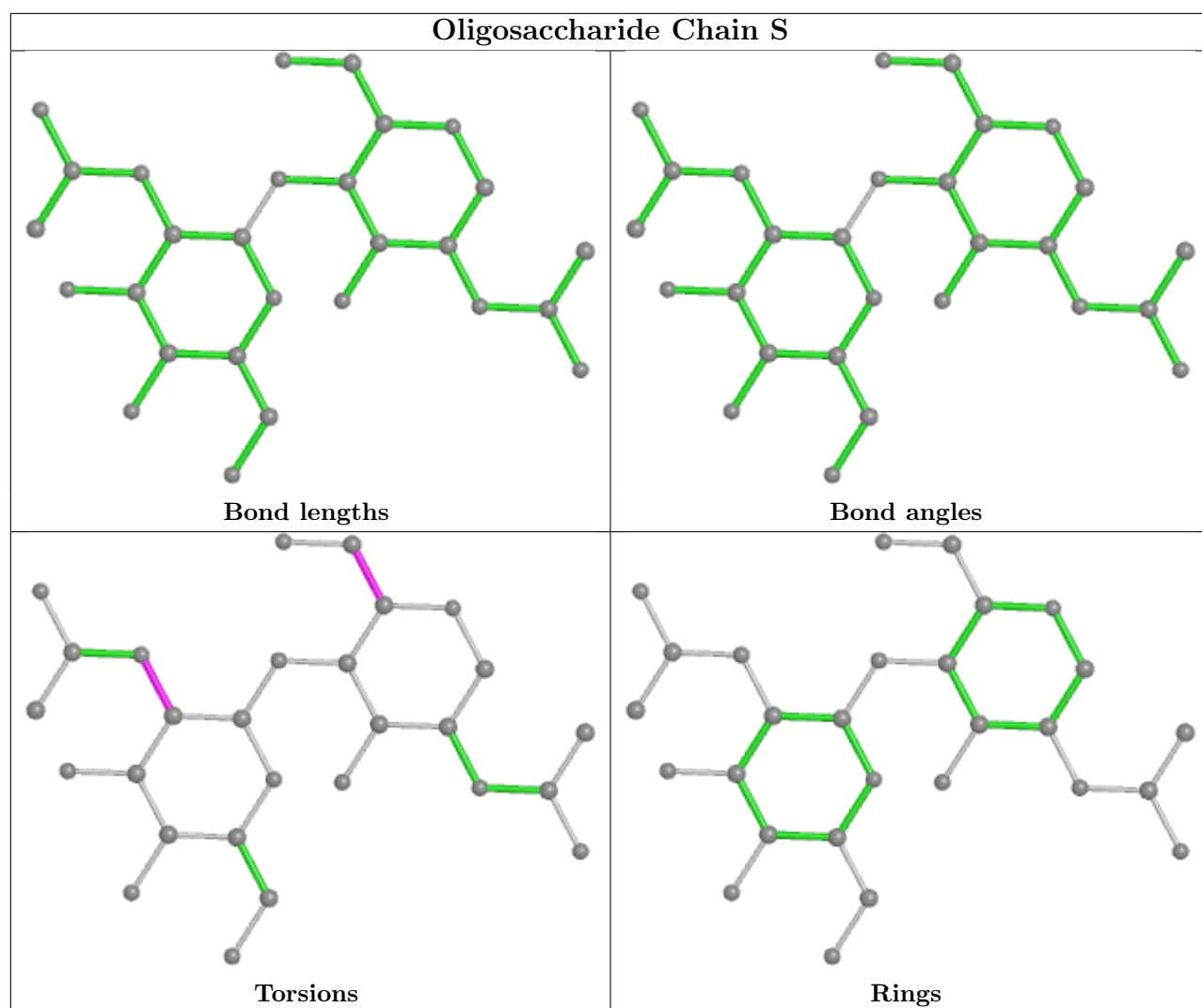


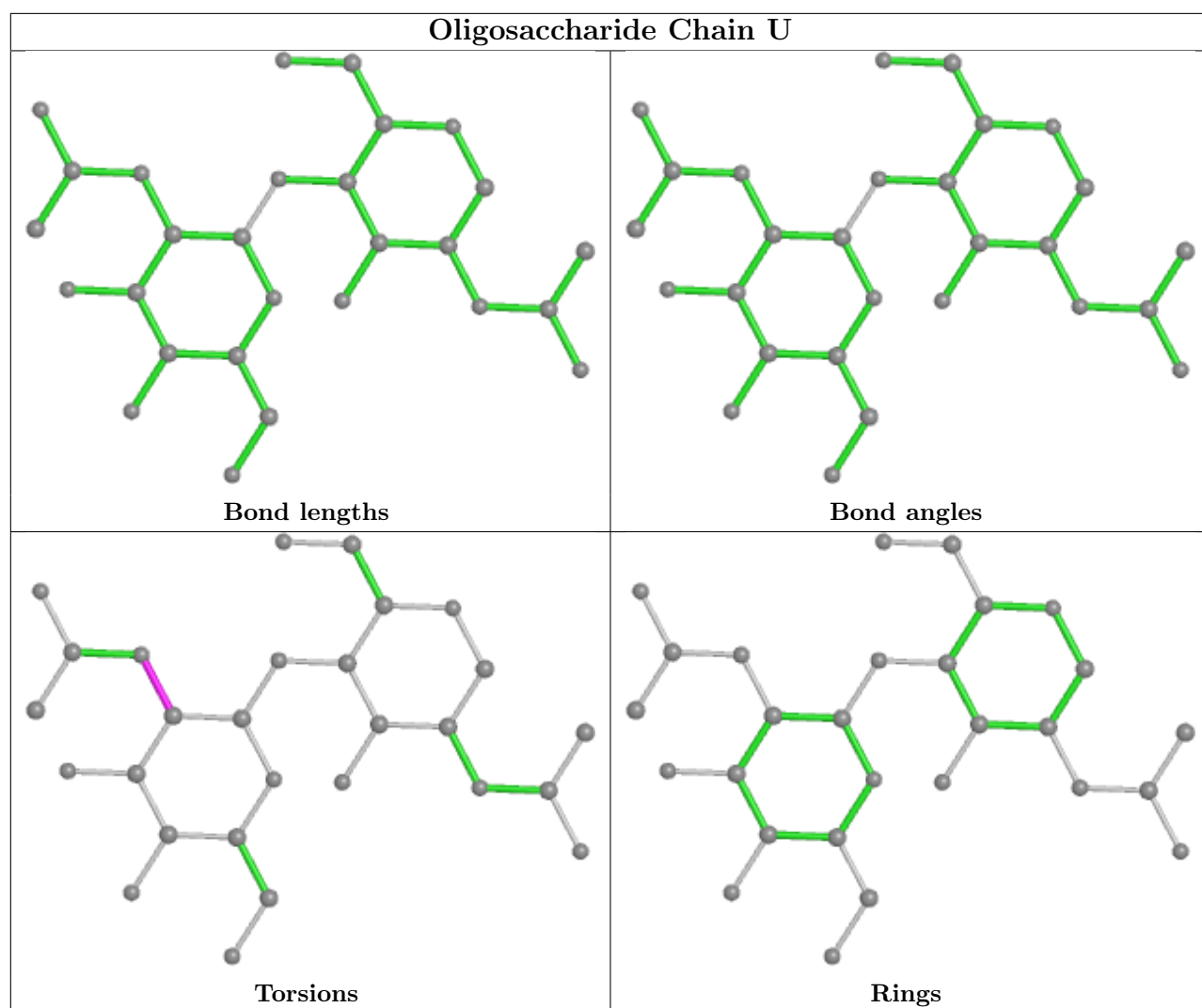


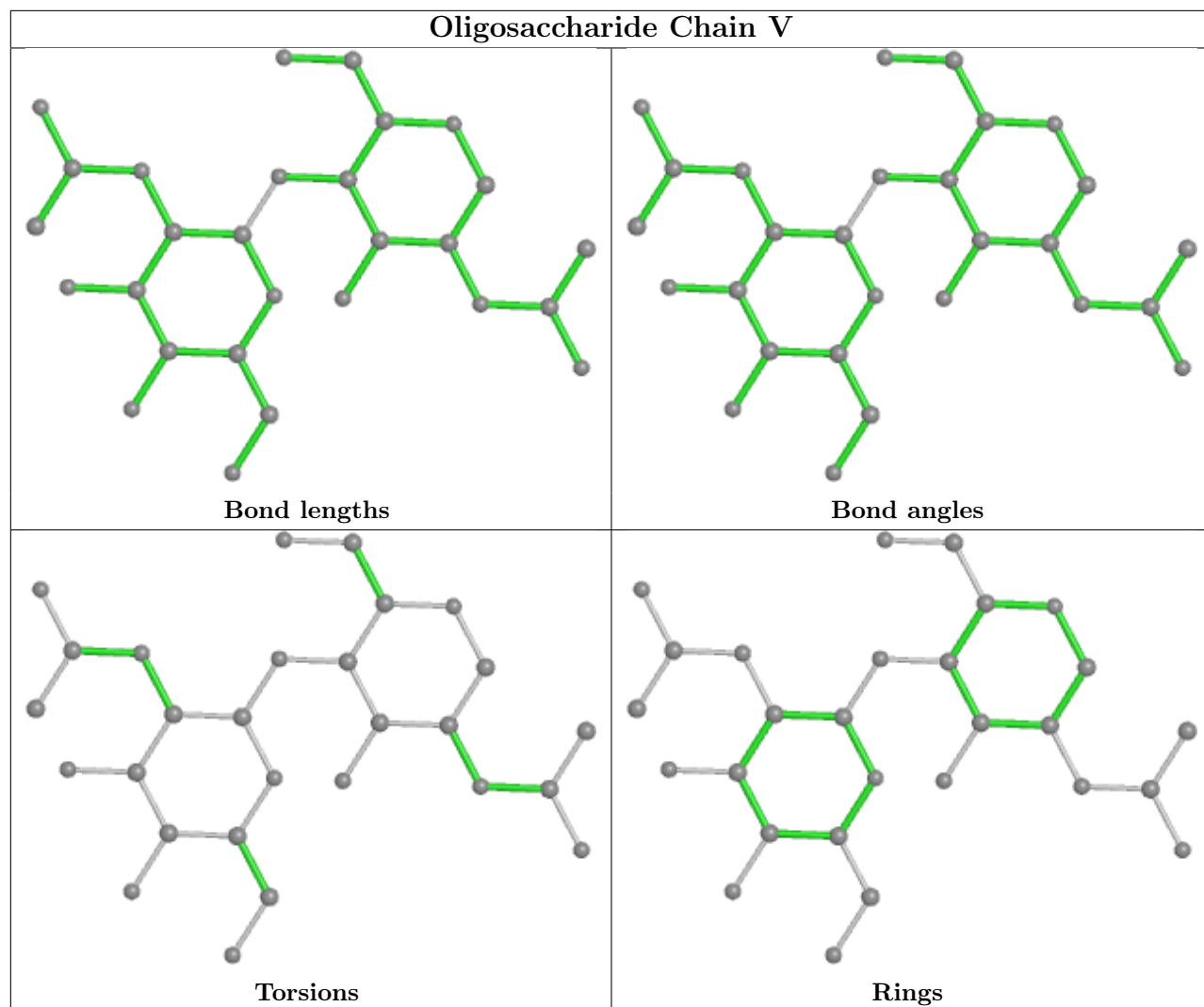


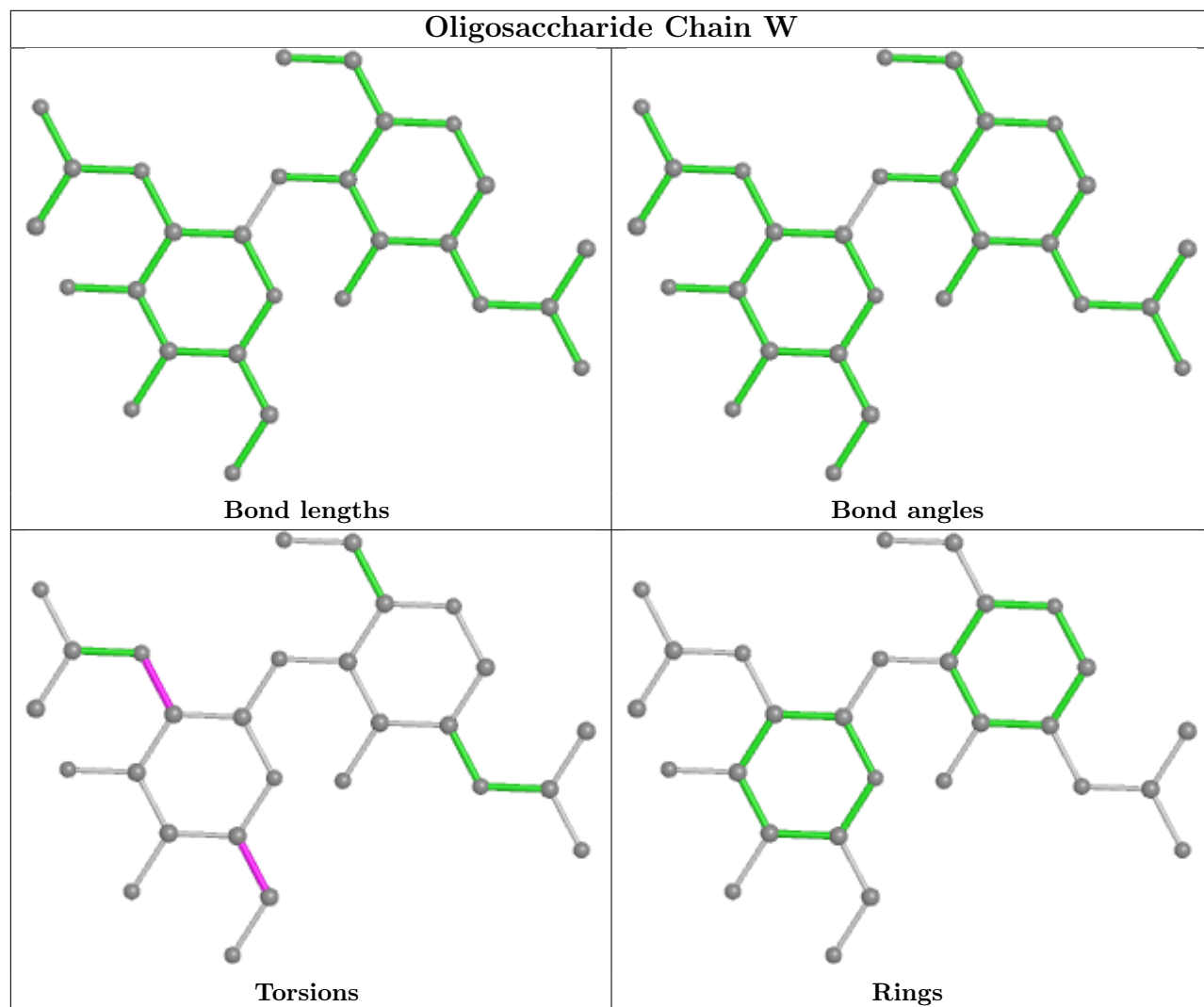


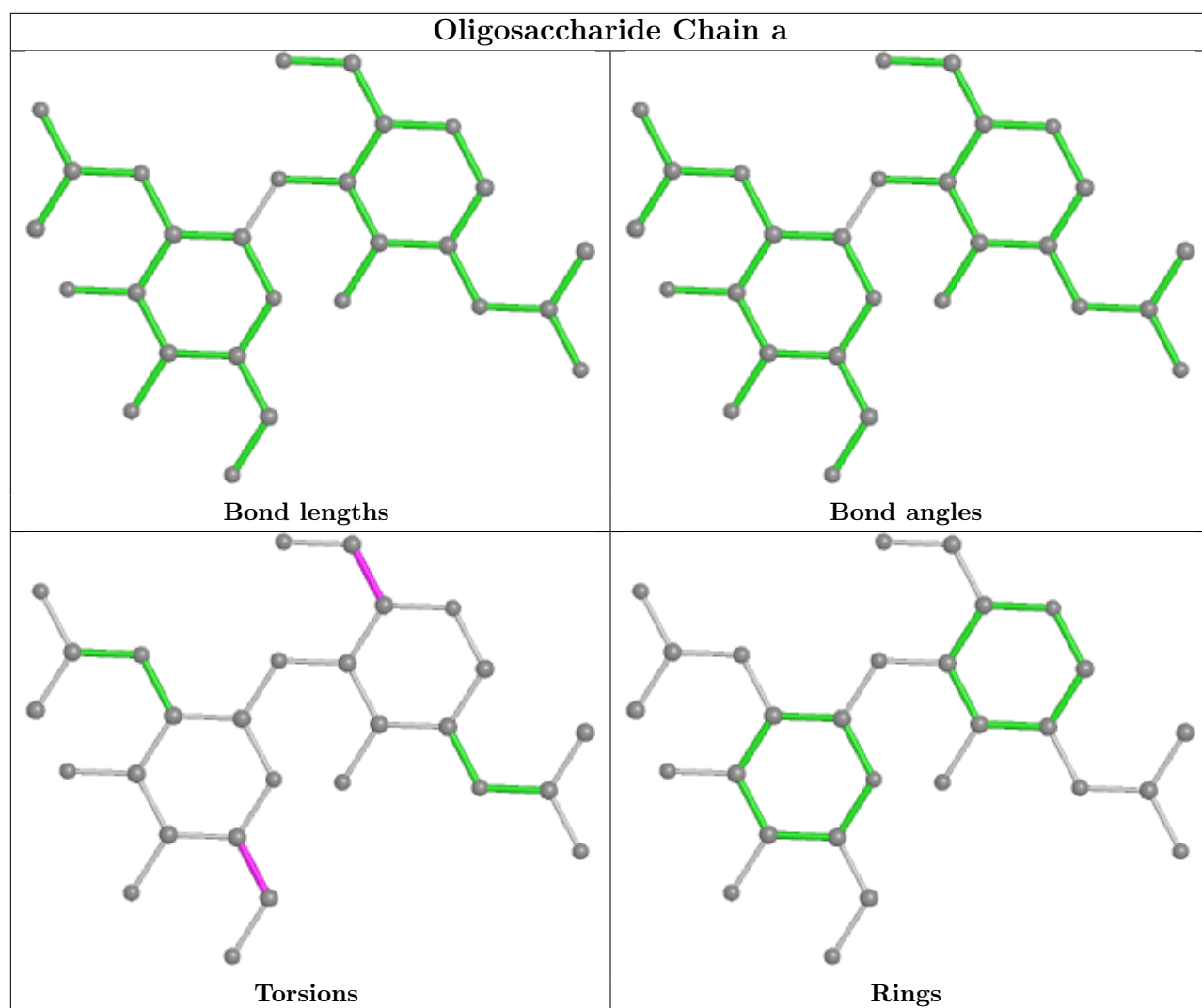


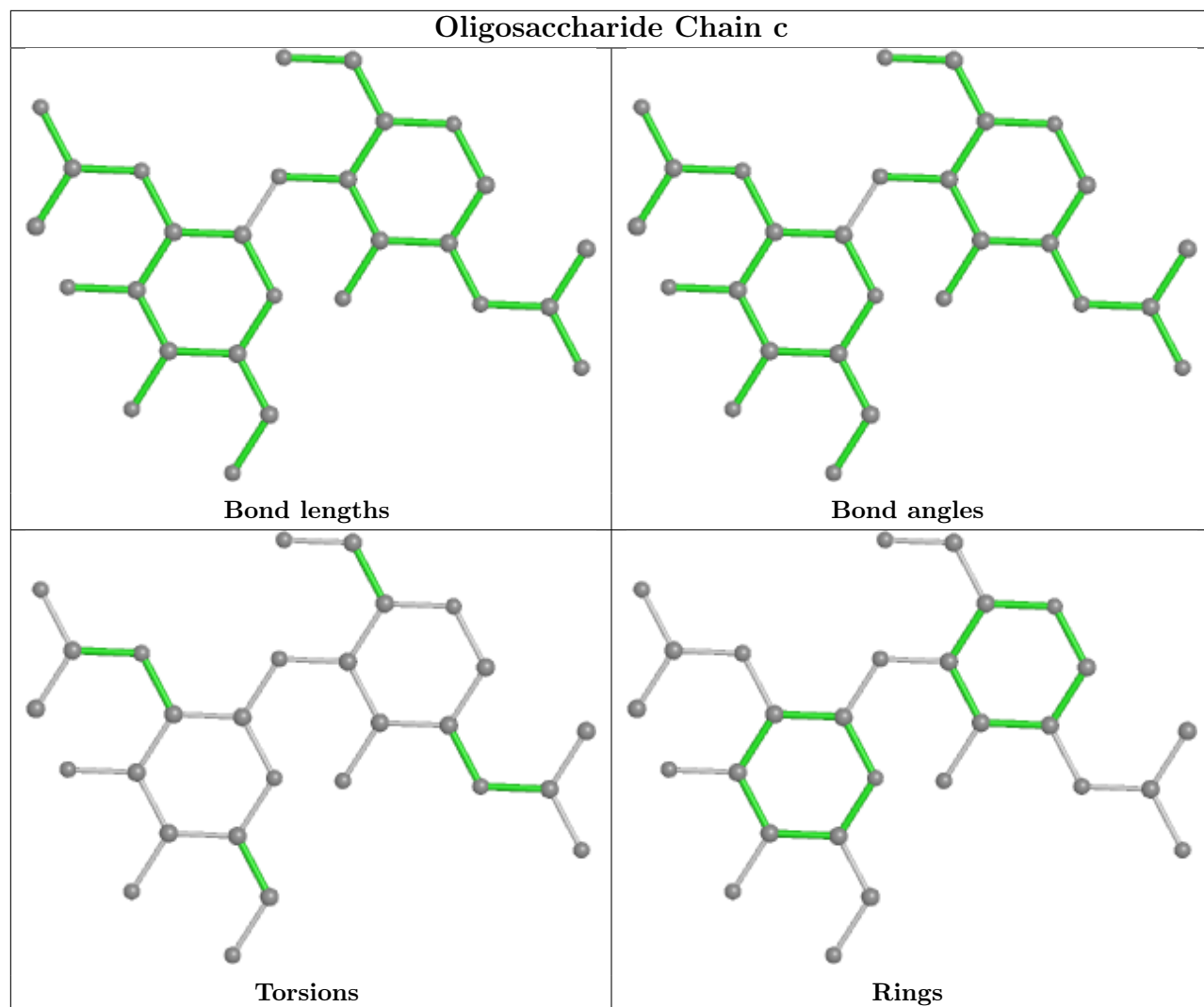


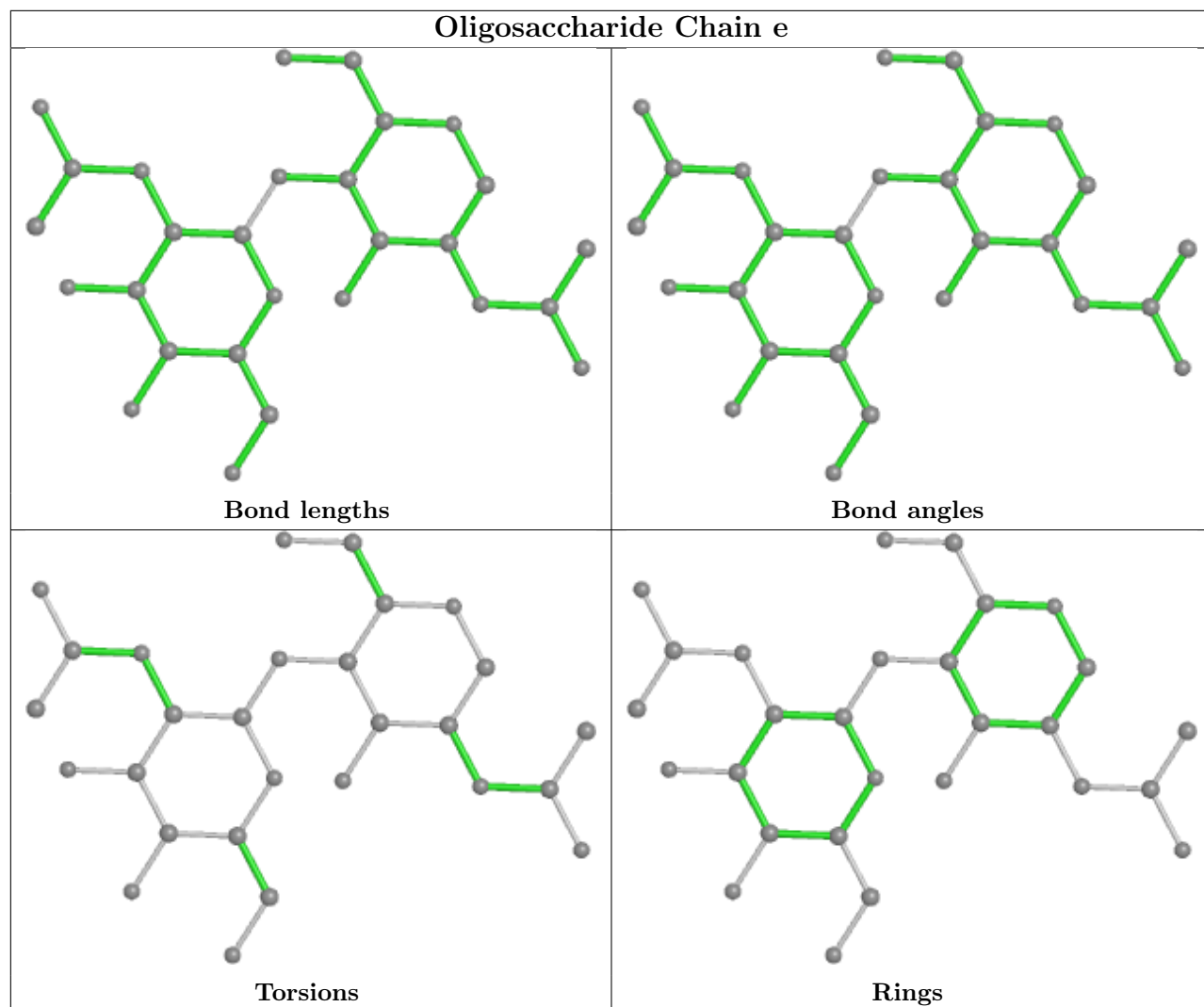


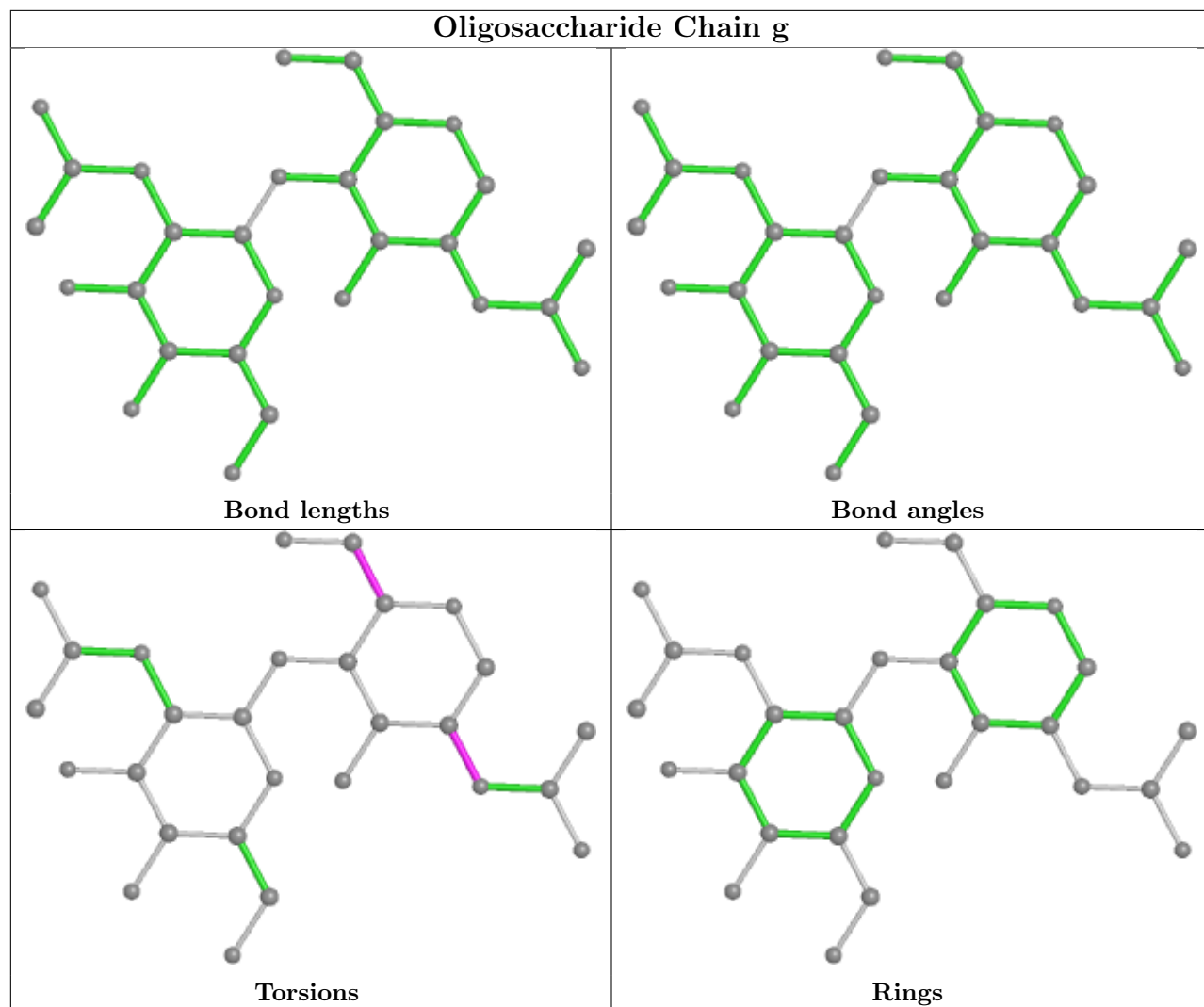


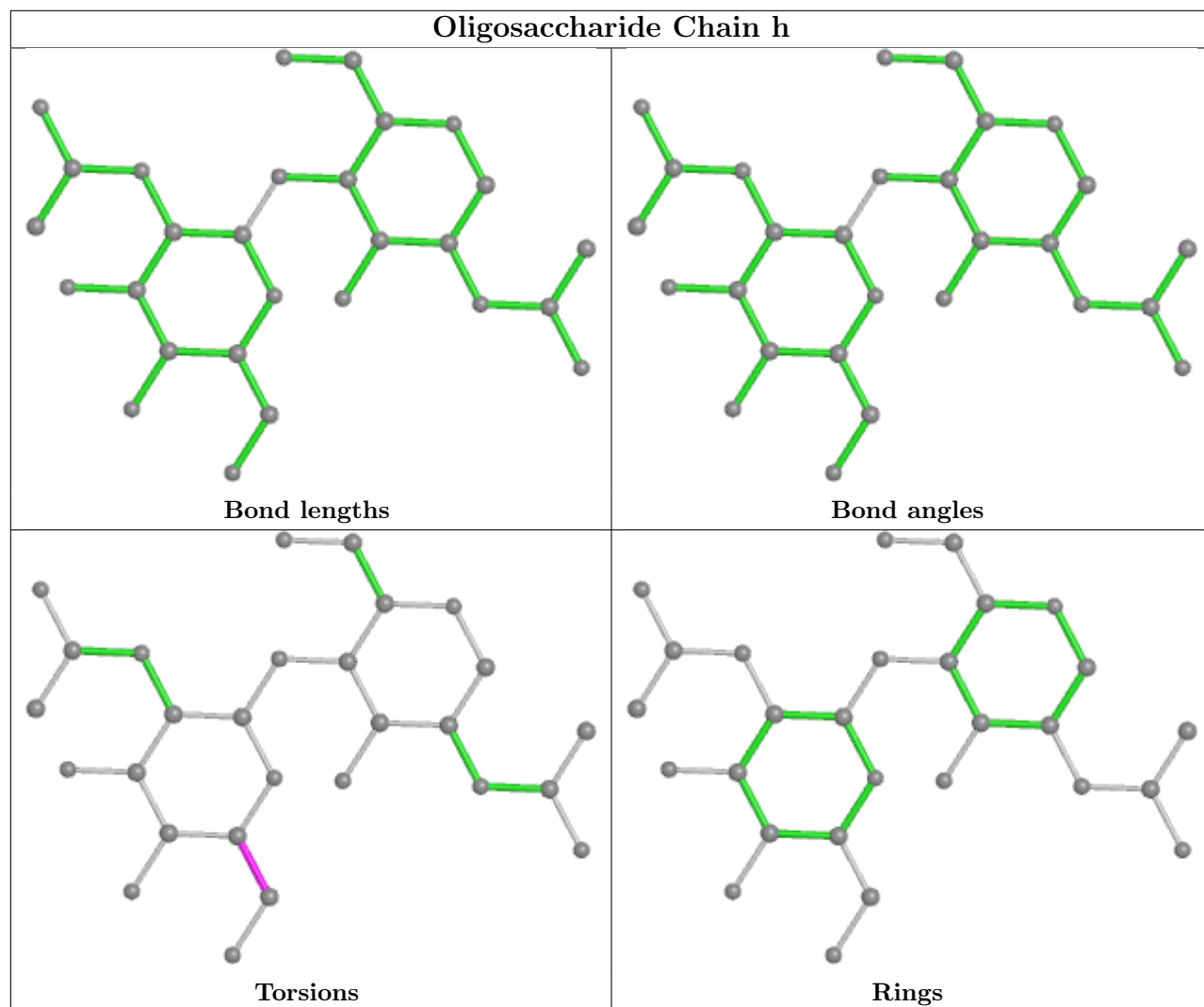


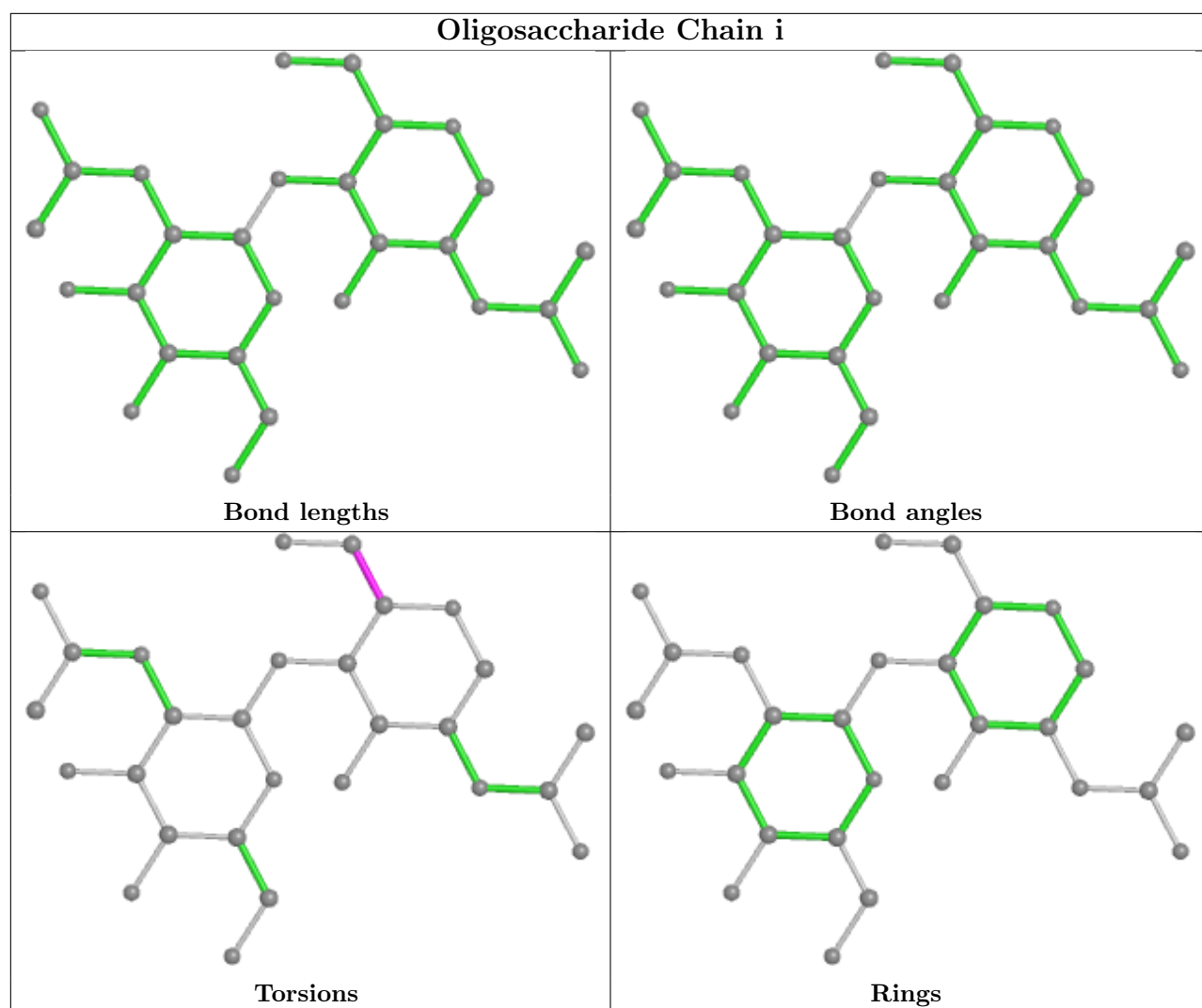


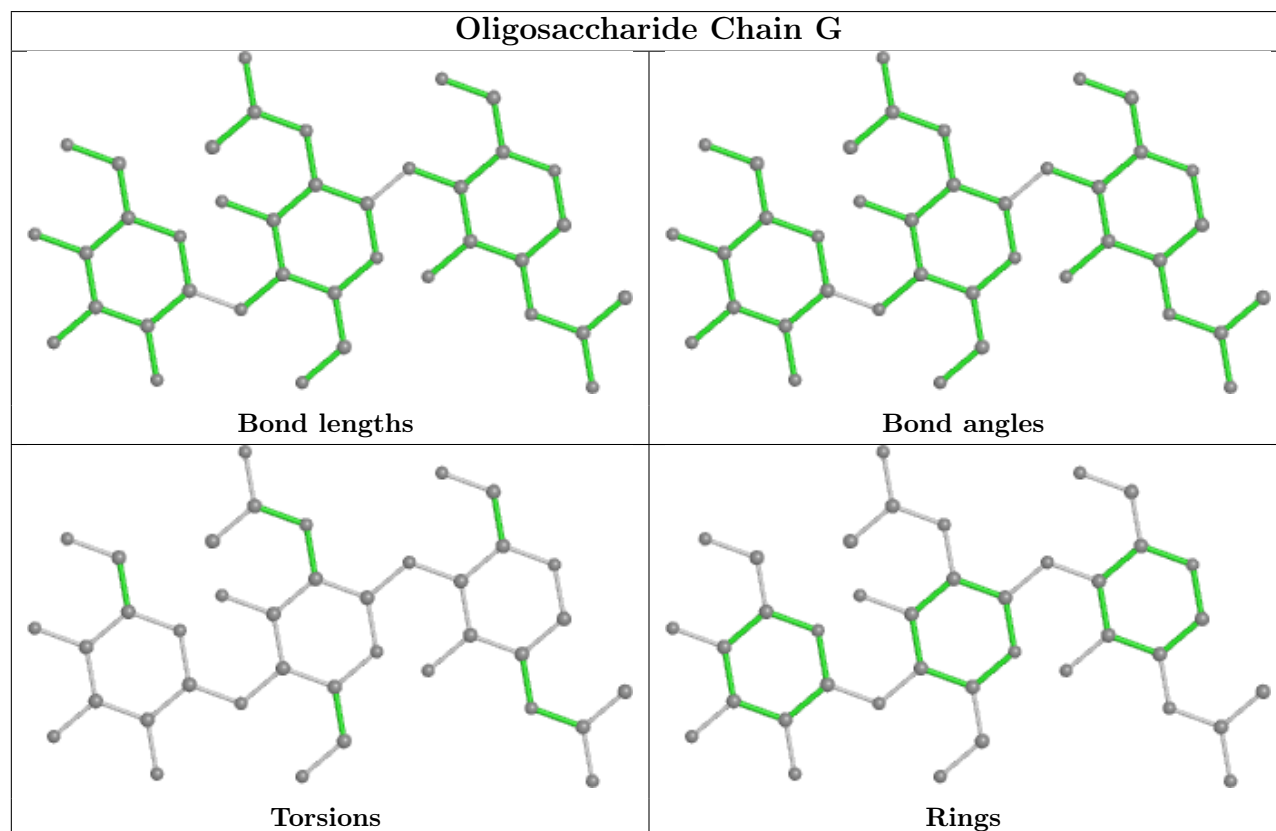
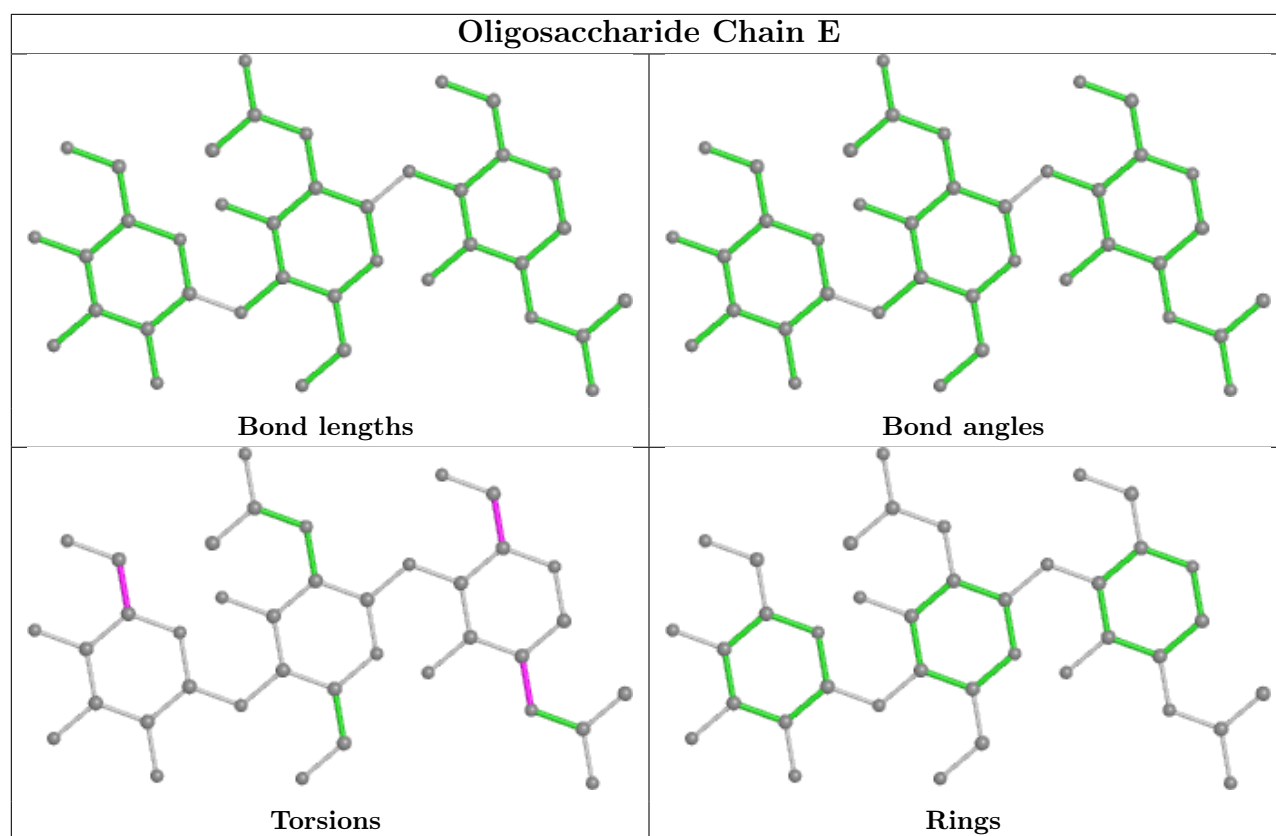


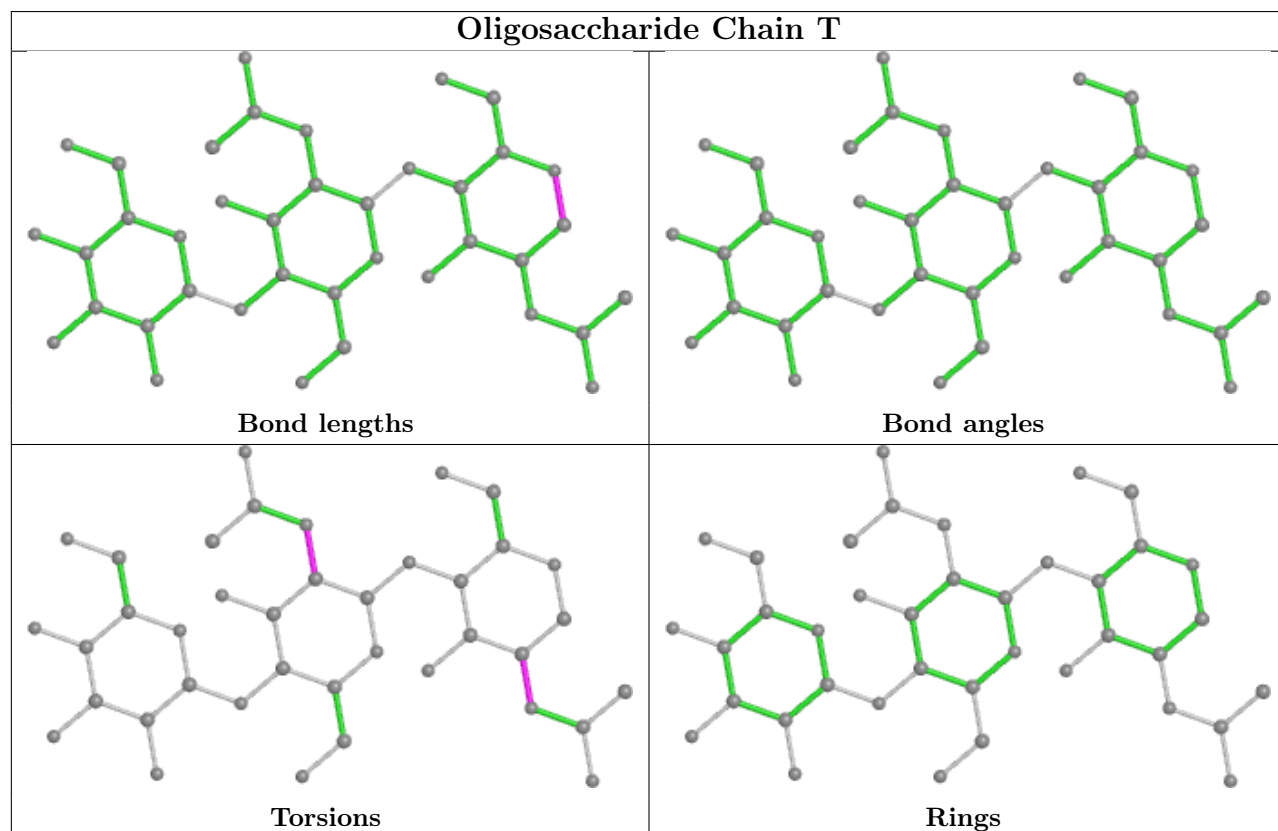
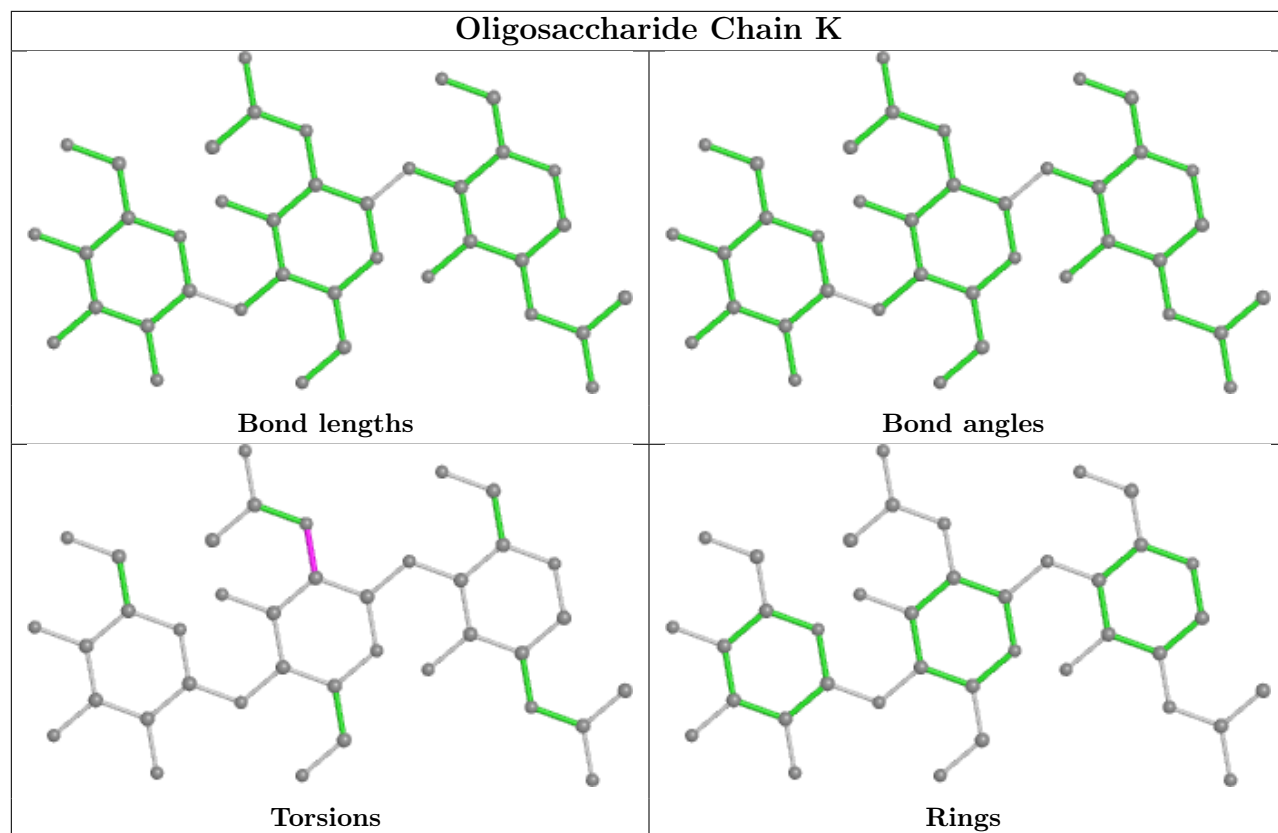


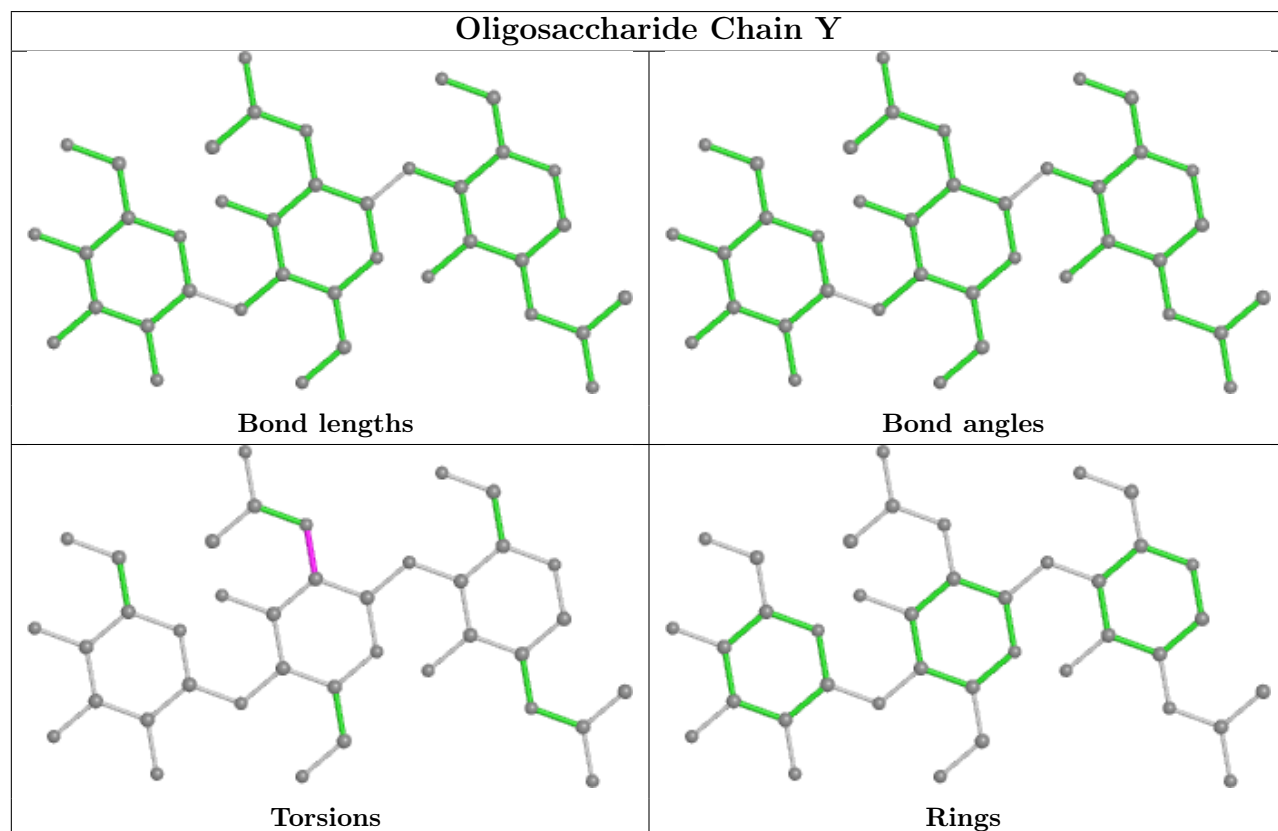
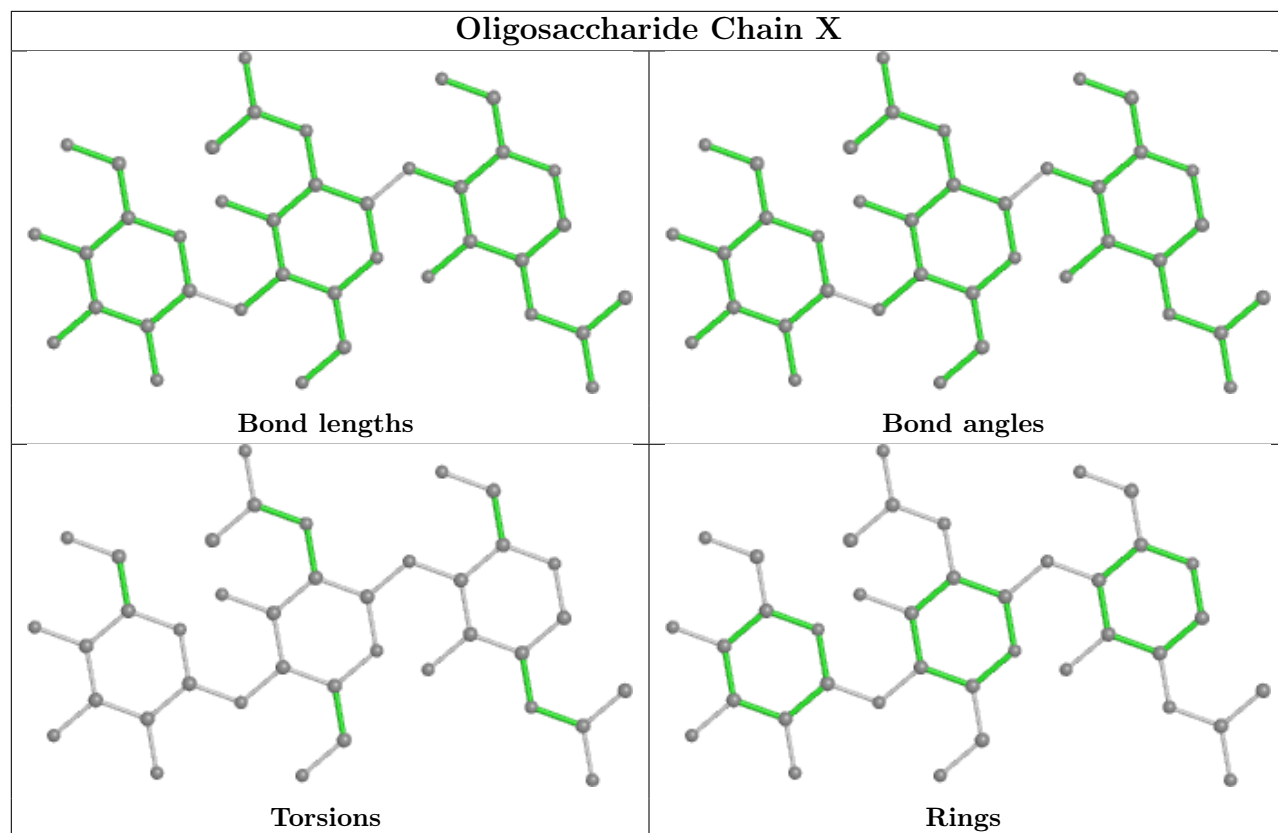


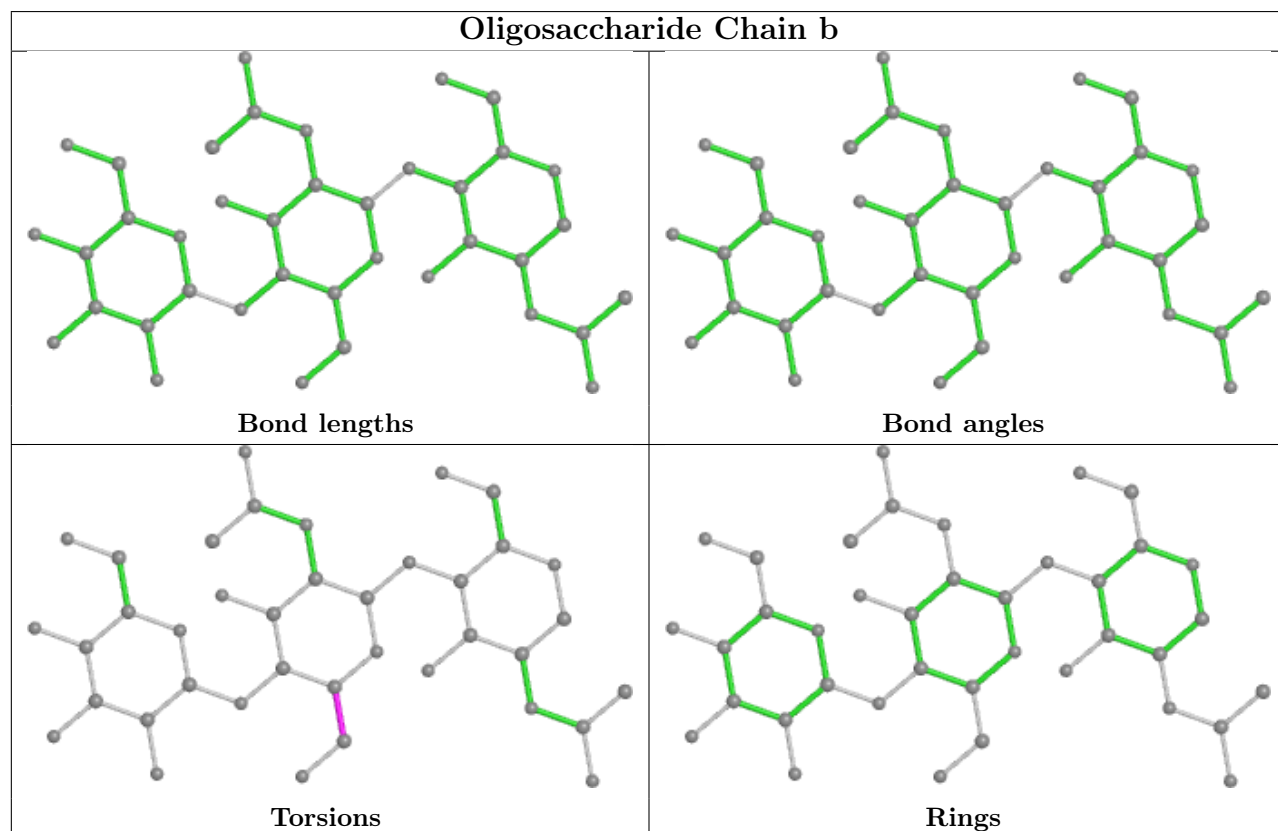
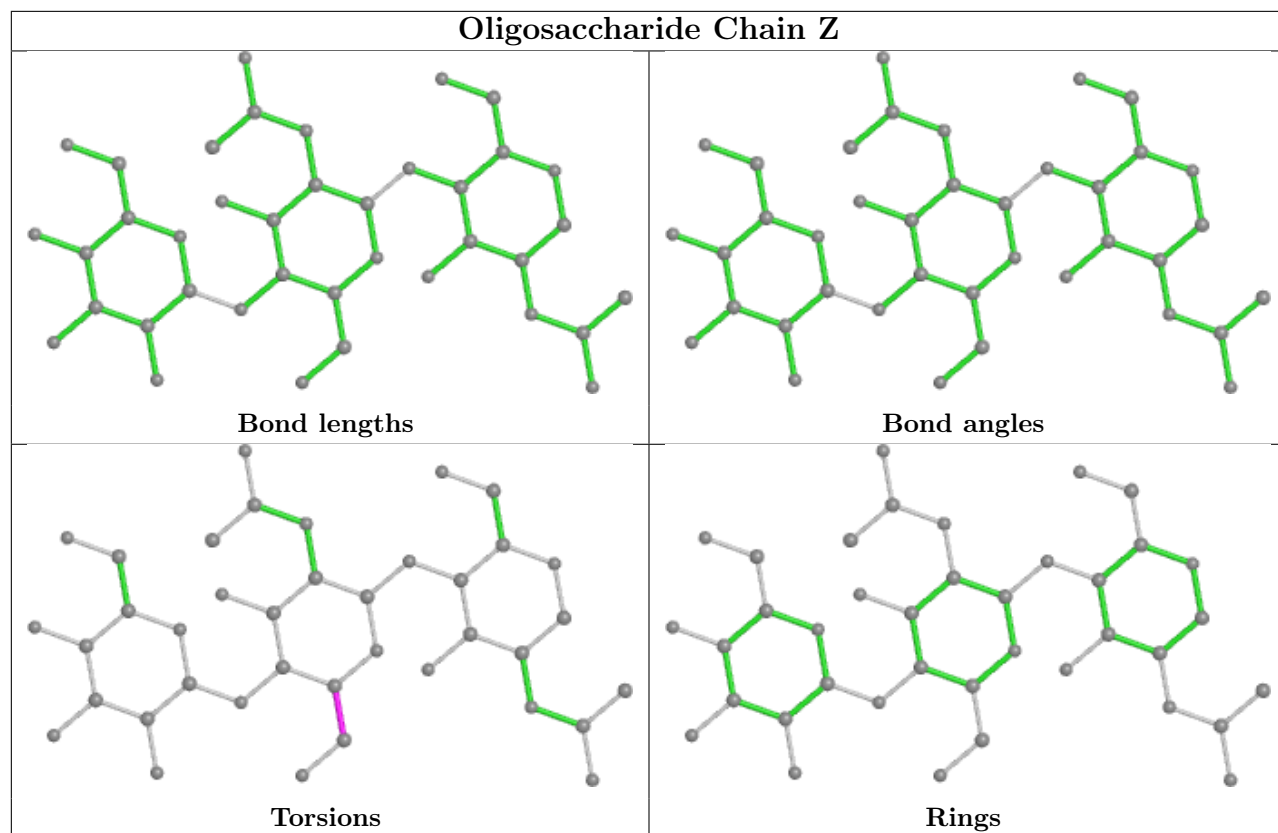


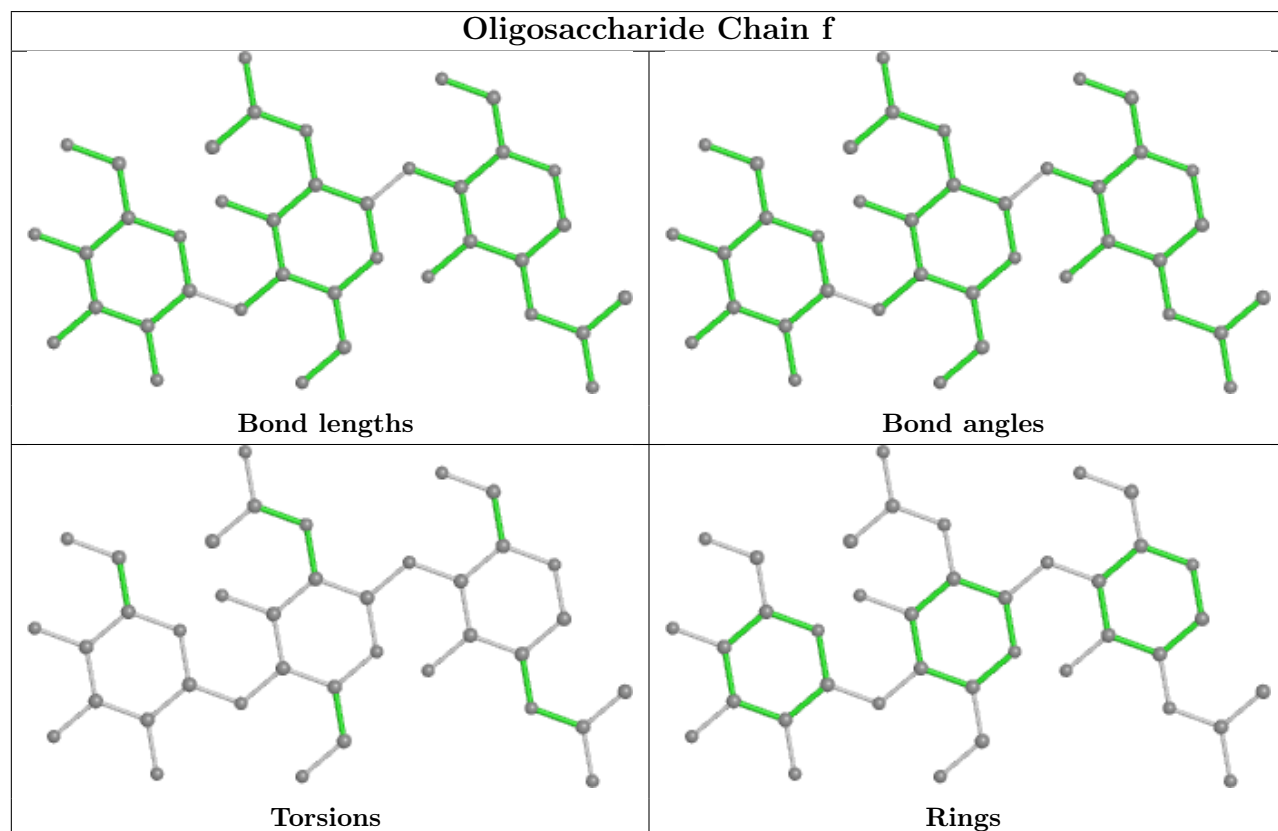
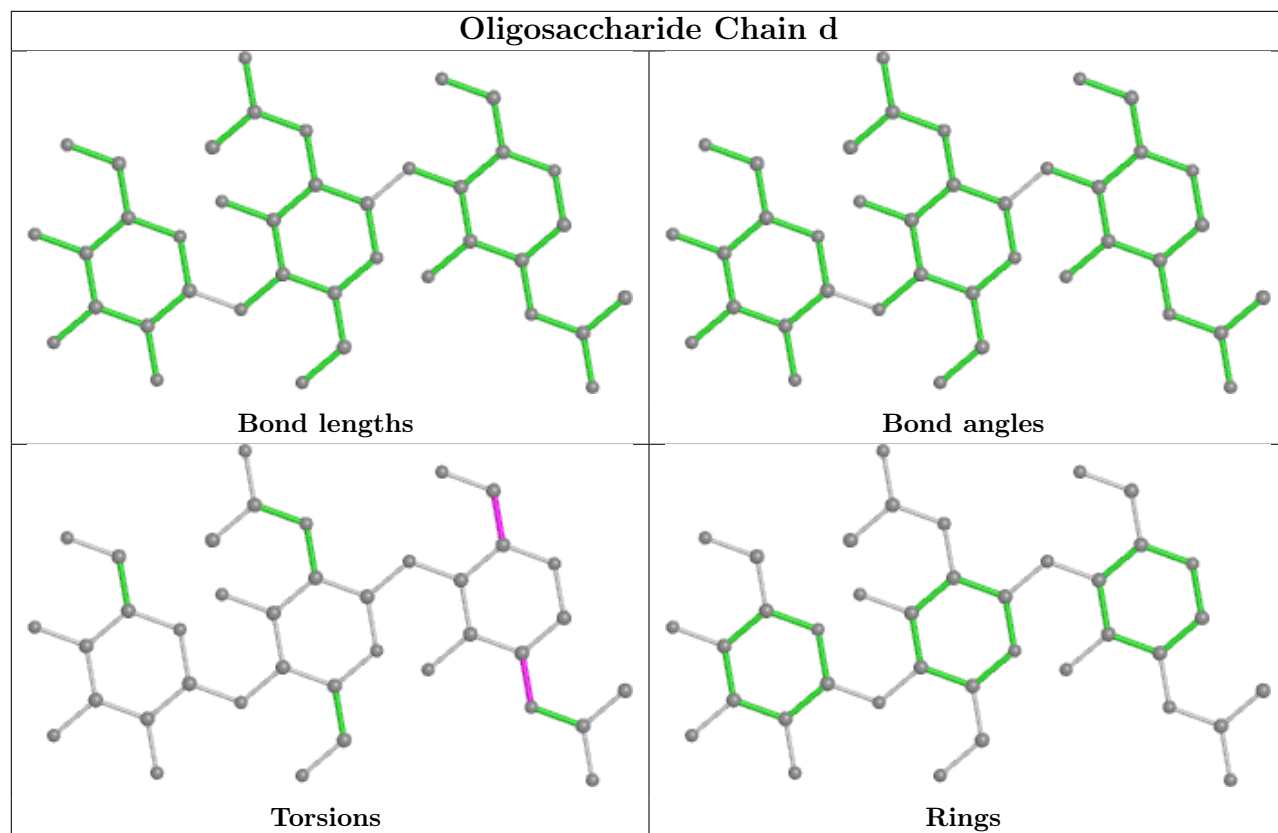












5.6 Ligand geometry

13 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
6	NAG	A	1304	3	14,14,15	0.21	0	17,19,21	0.40	0
6	NAG	A	1302	3	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	C	1303	3	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	B	1304	3	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	A	1303	3	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	A	1301	3	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	B	1302	3	14,14,15	0.27	0	17,19,21	0.51	0
6	NAG	C	1302	3	14,14,15	0.25	0	17,19,21	0.44	0
6	NAG	C	1301	3	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	B	1301	3	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	B	1303	3	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	B	1305	3	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	A	1305	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
6	NAG	A	1304	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1302	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1303	3	-	0/6/23/26	0/1/1/1
6	NAG	B	1304	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1303	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1301	3	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	3	-	3/6/23/26	0/1/1/1
6	NAG	C	1302	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1301	3	-	0/6/23/26	0/1/1/1
6	NAG	B	1301	3	-	0/6/23/26	0/1/1/1
6	NAG	B	1303	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1305	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1305	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1304	NAG	O5-C5-C6-O6
6	B	1304	NAG	C4-C5-C6-O6
6	A	1305	NAG	O5-C5-C6-O6
6	B	1302	NAG	C4-C5-C6-O6
6	A	1305	NAG	C4-C5-C6-O6
6	B	1302	NAG	O5-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6
6	B	1302	NAG	C3-C2-N2-C7
6	A	1305	NAG	C3-C2-N2-C7

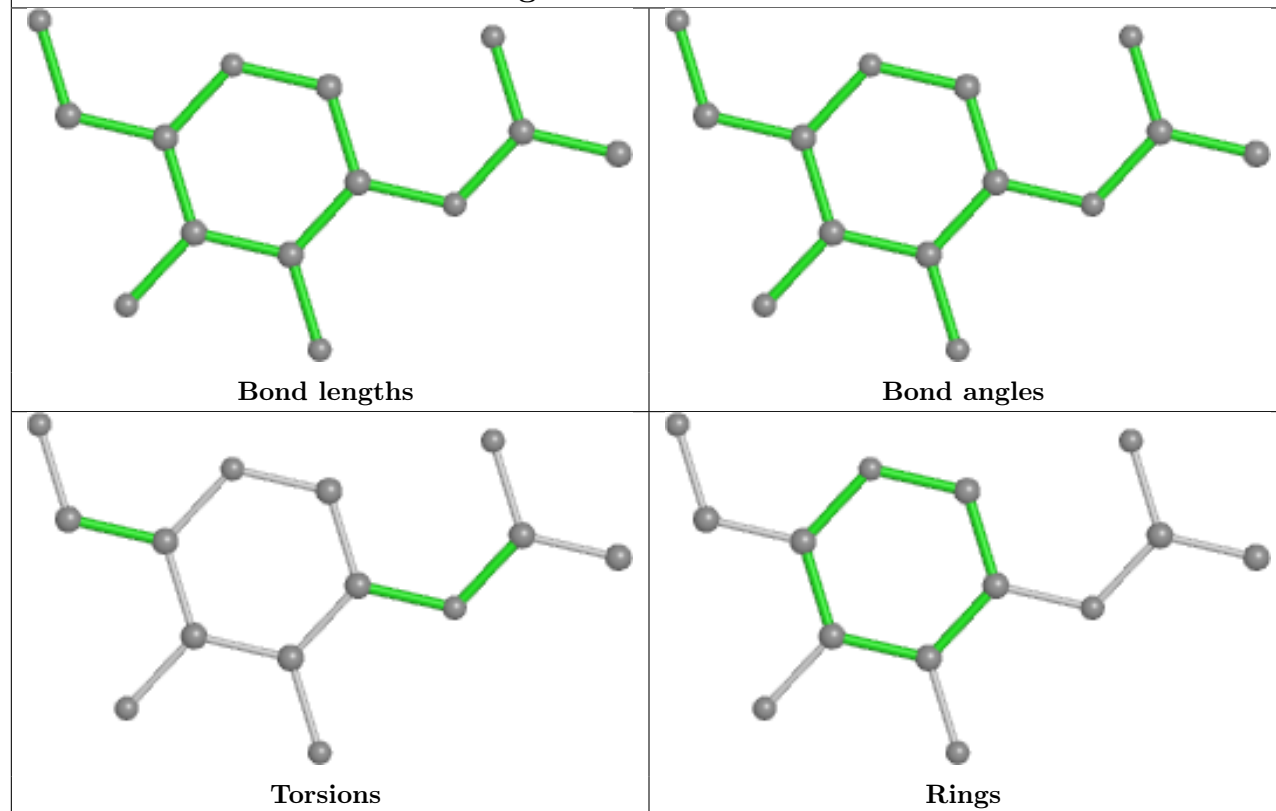
There are no ring outliers.

3 monomers are involved in 3 short contacts:

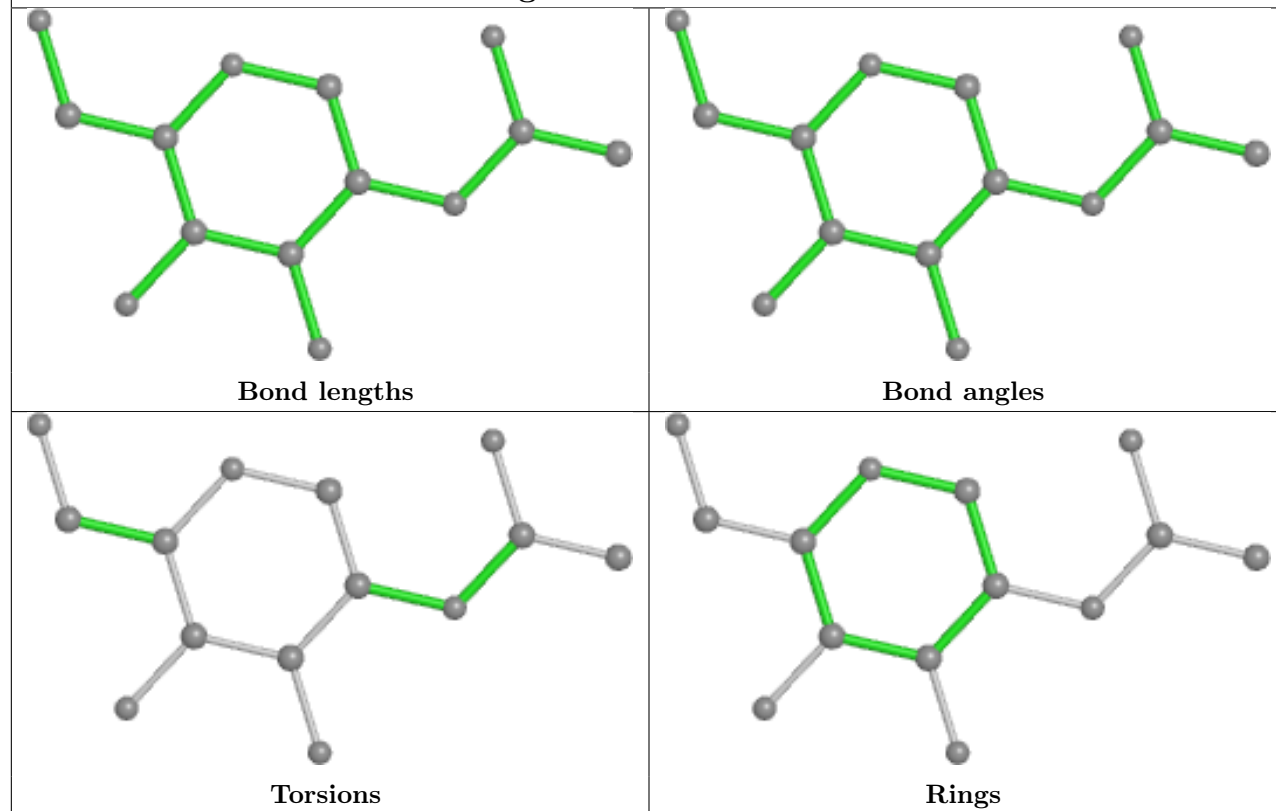
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1302	NAG	1	0
6	B	1303	NAG	1	0
6	B	1305	NAG	1	0

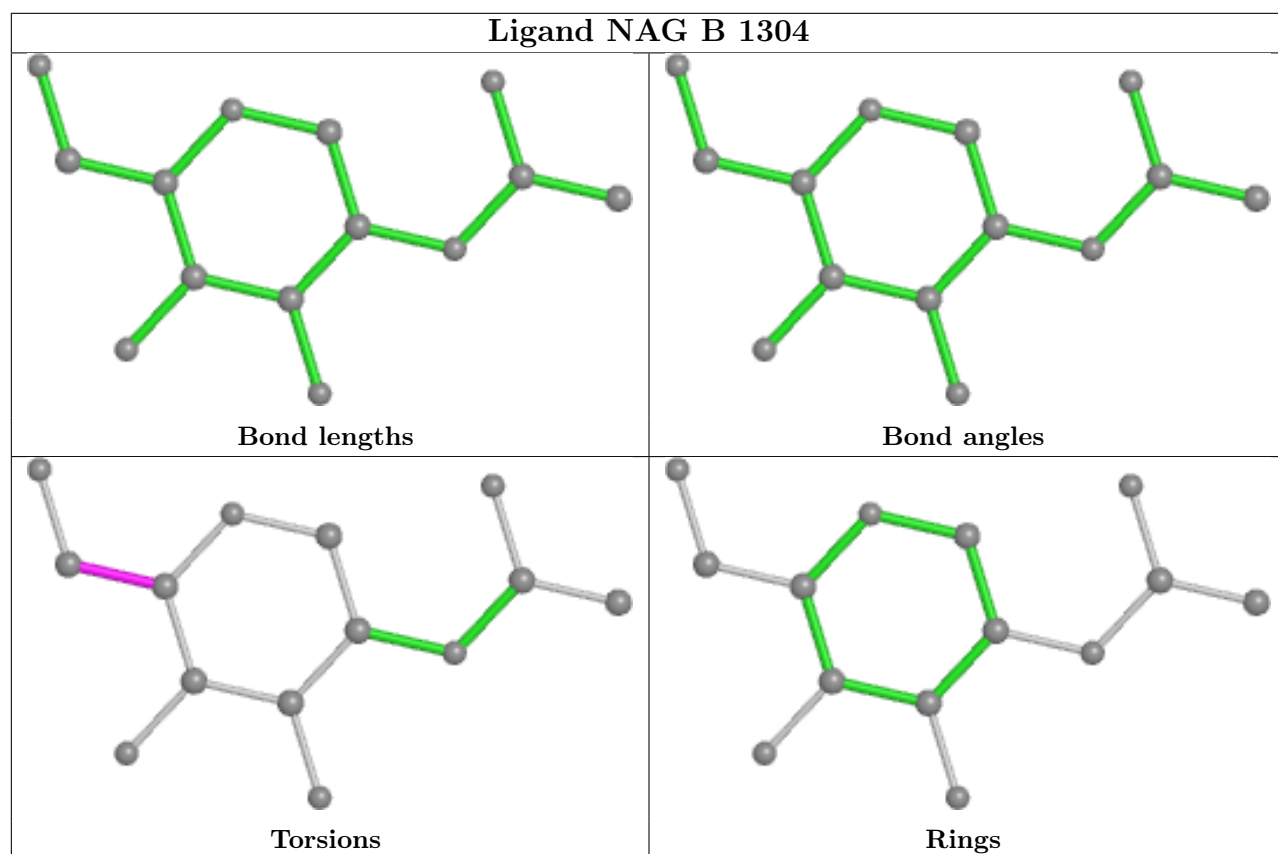
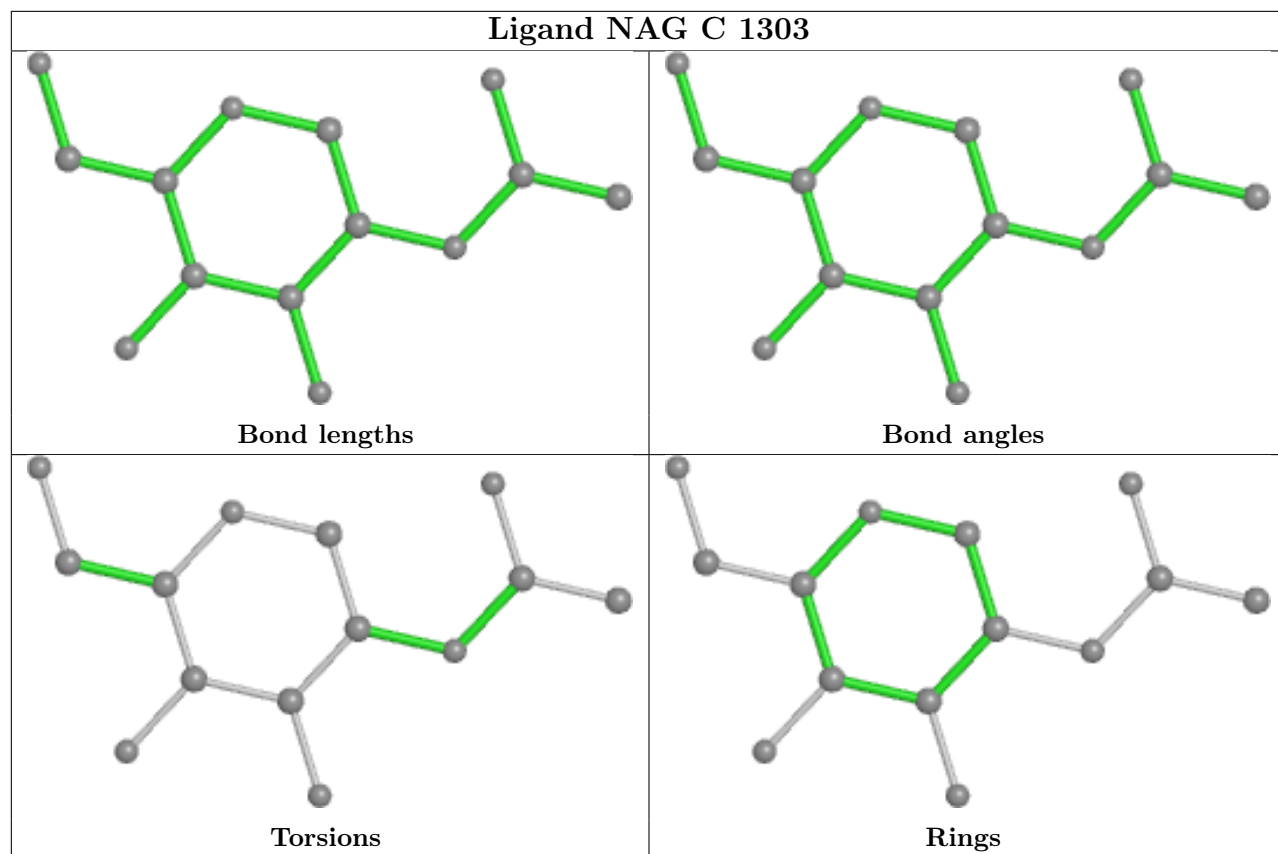
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

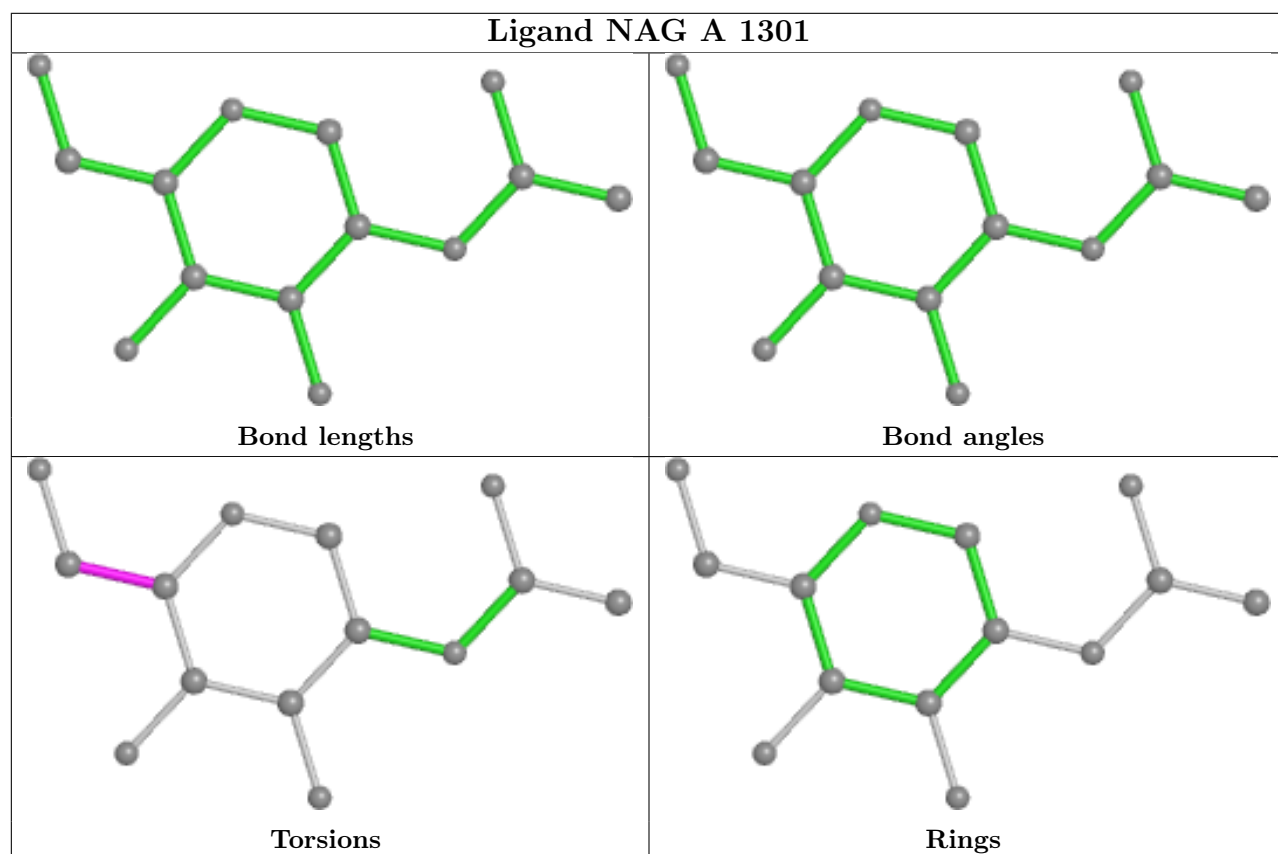
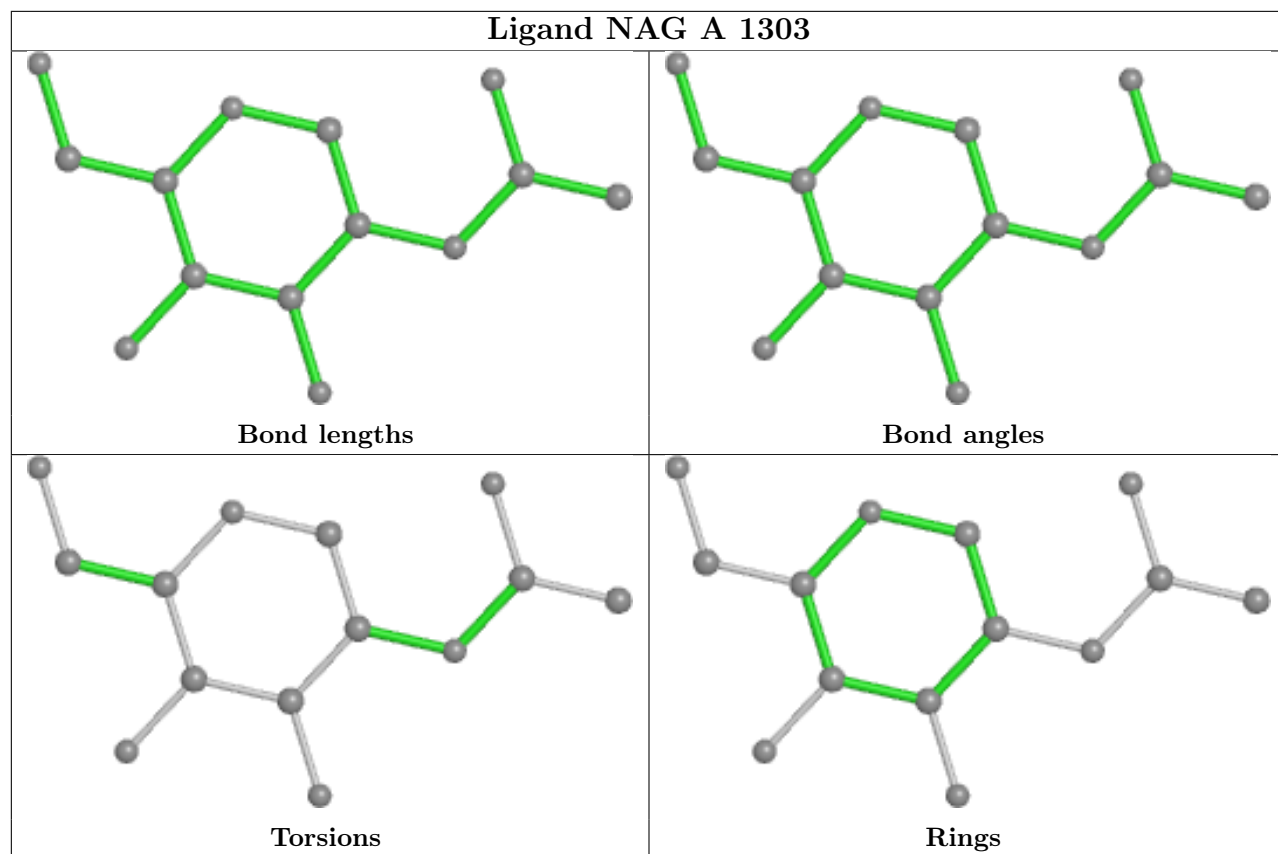
Ligand NAG A 1304



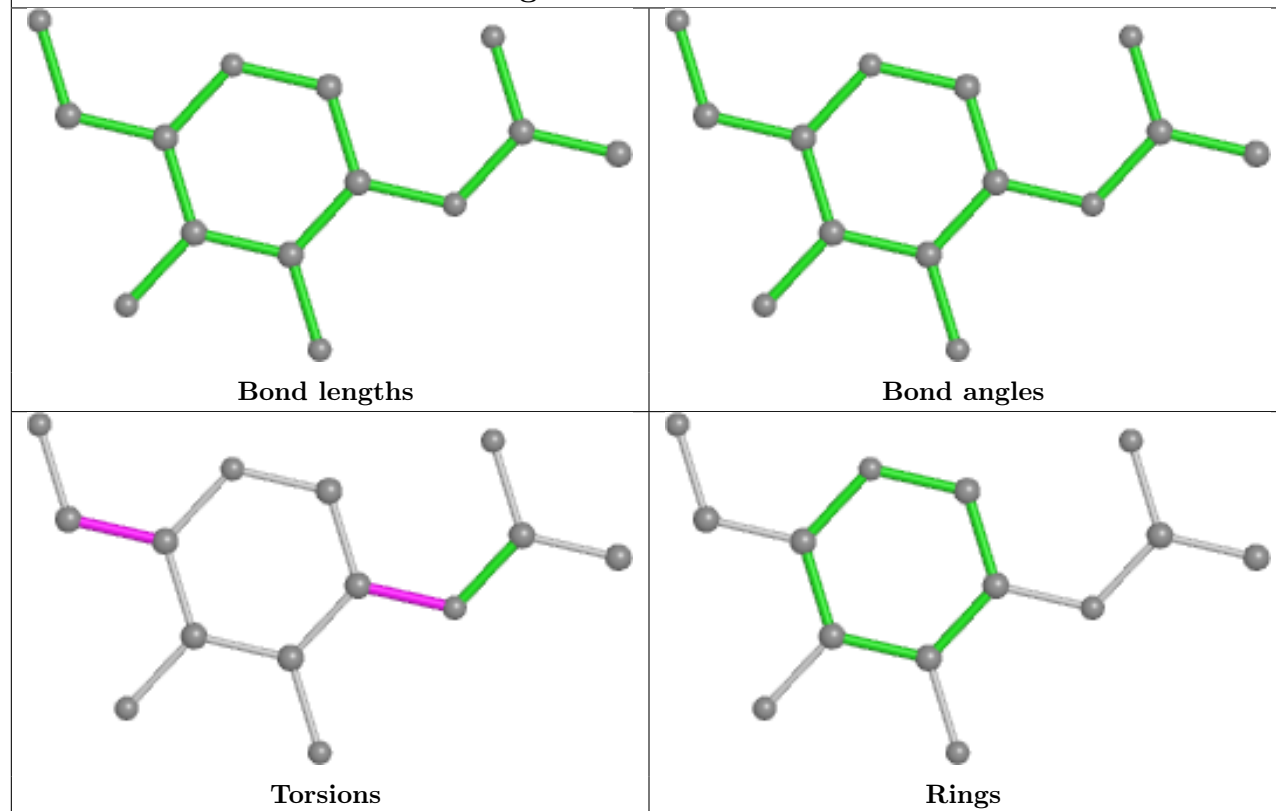
Ligand NAG A 1302



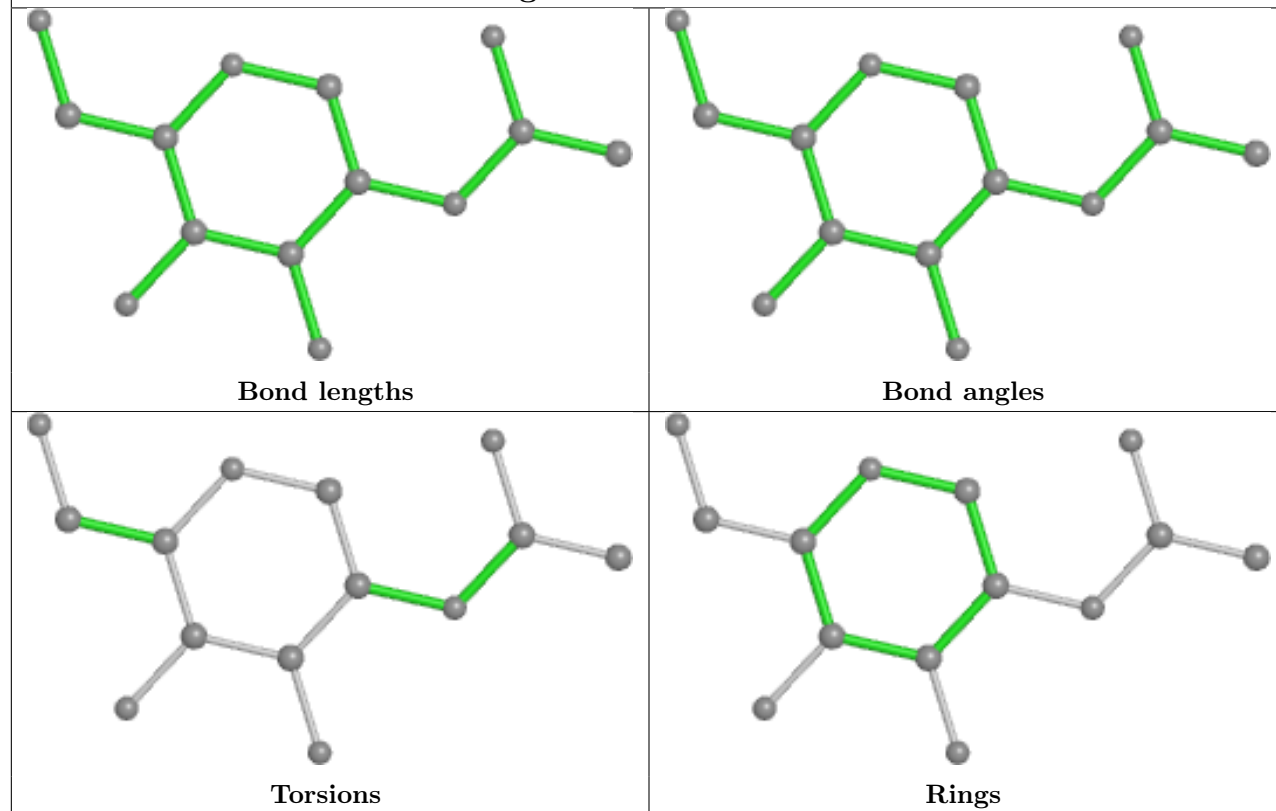




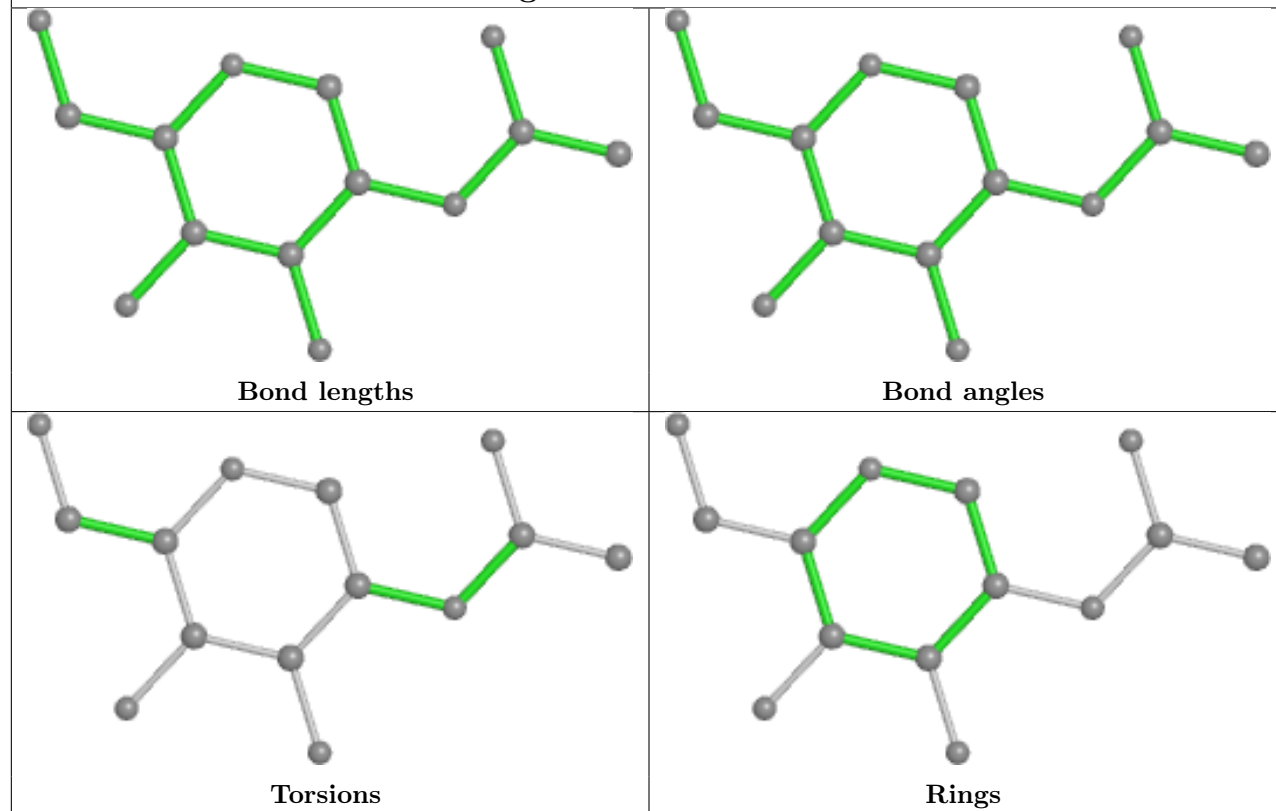
Ligand NAG B 1302



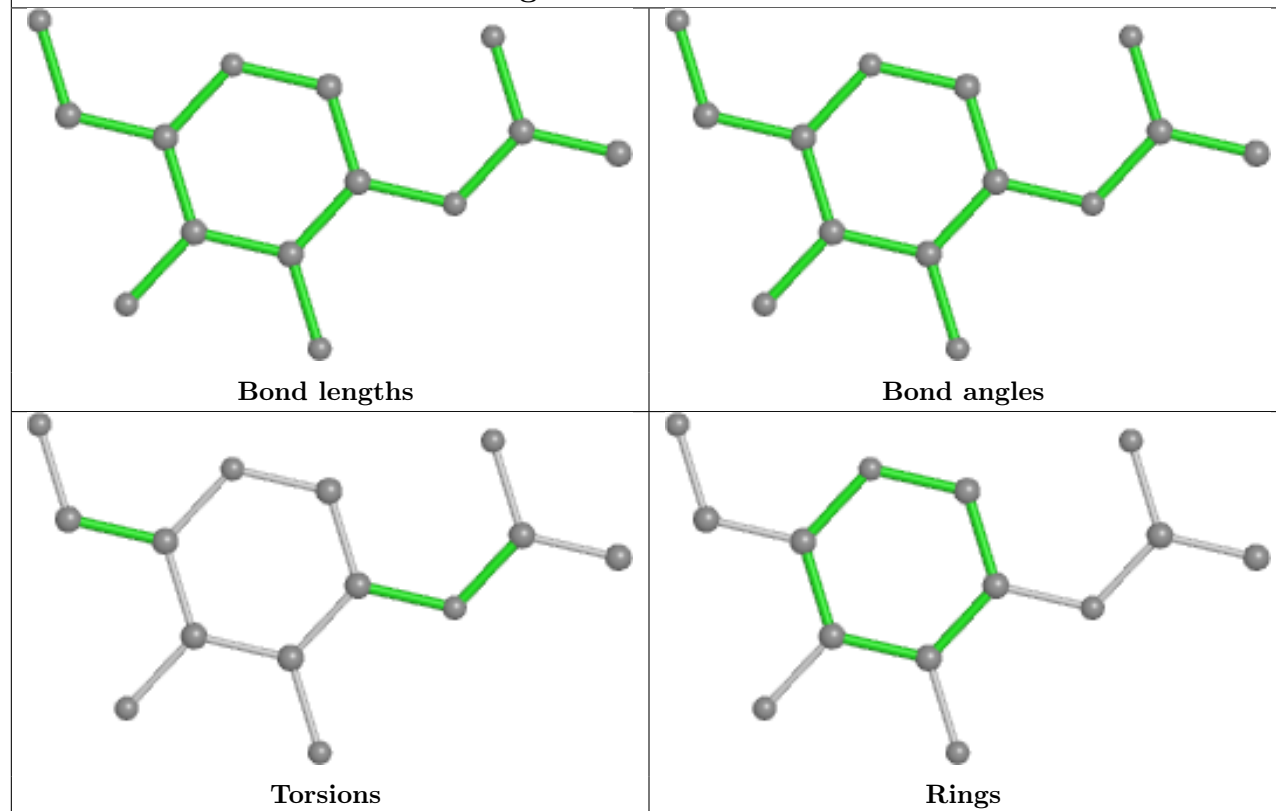
Ligand NAG C 1302

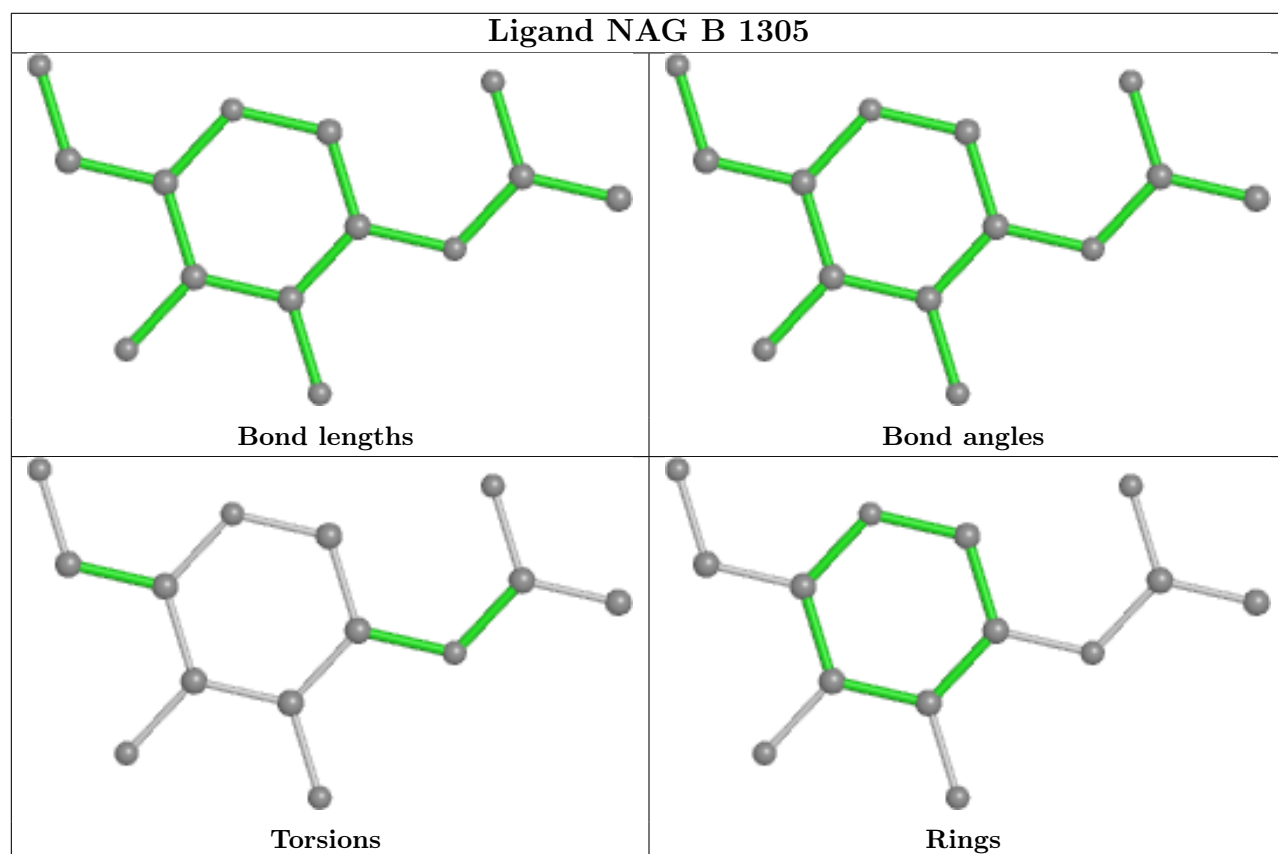
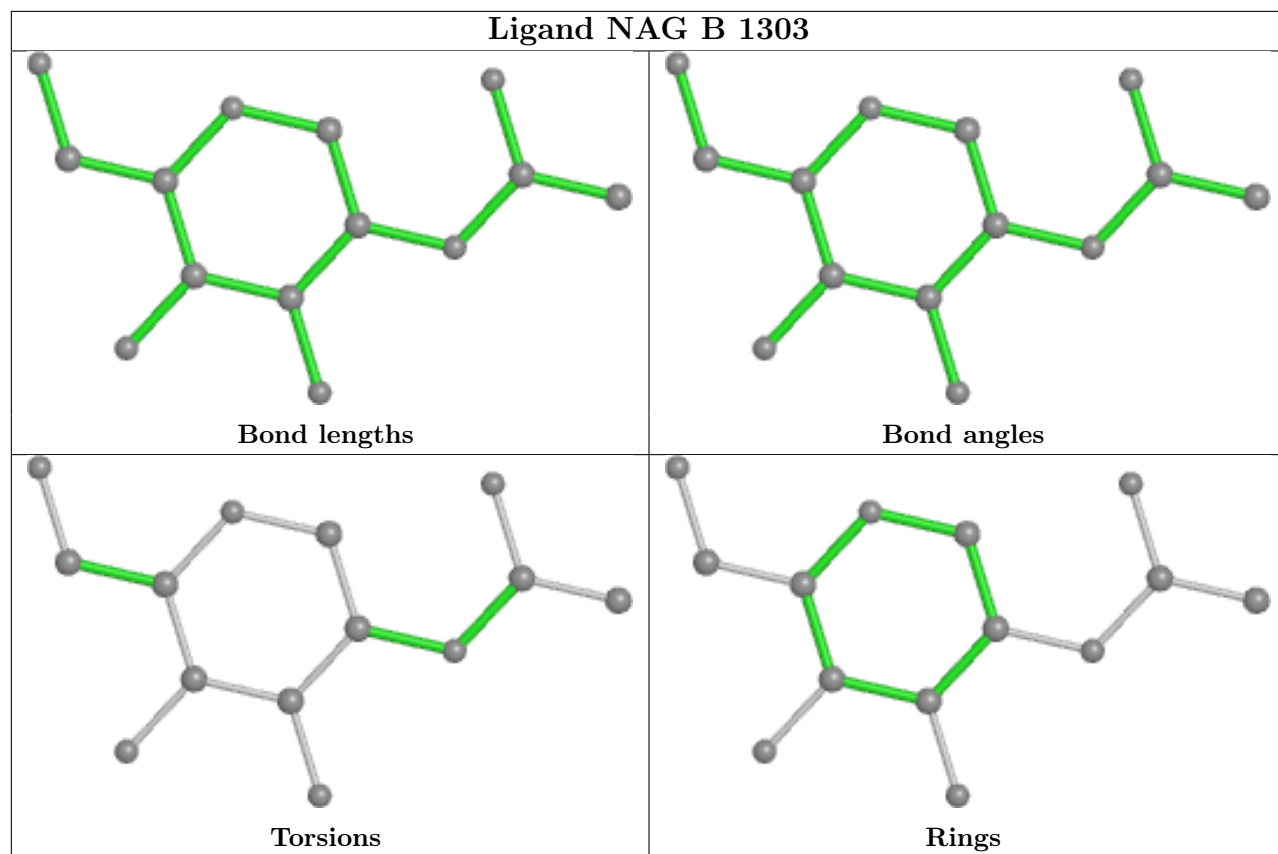


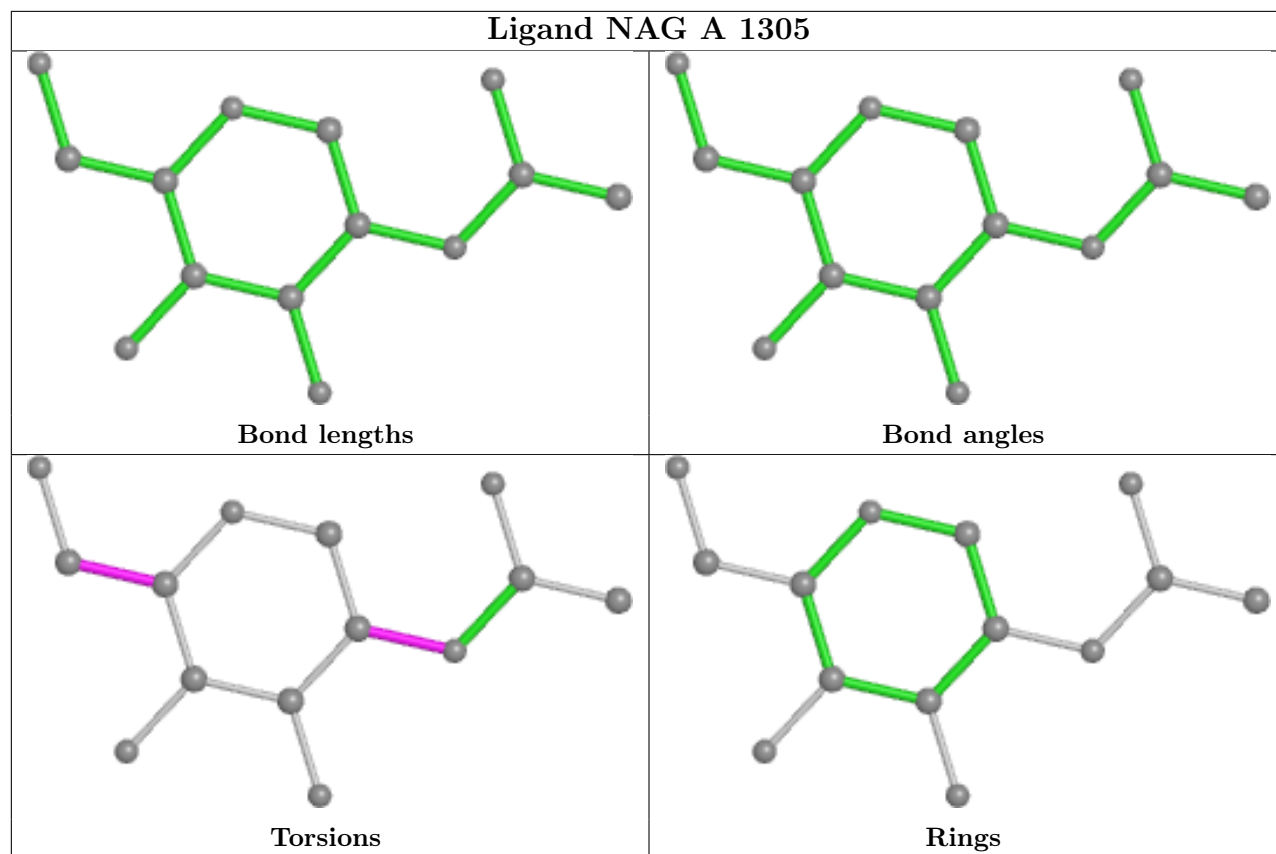
Ligand NAG C 1301



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.

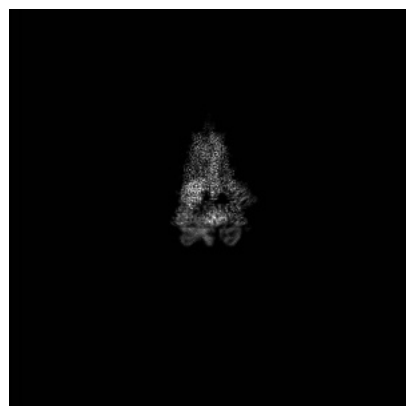
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62680. These allow visual inspection of the internal detail of the map and identification of artifacts.

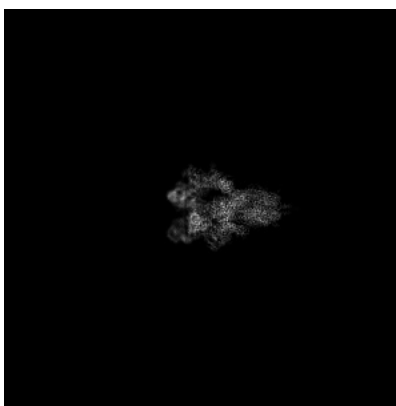
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

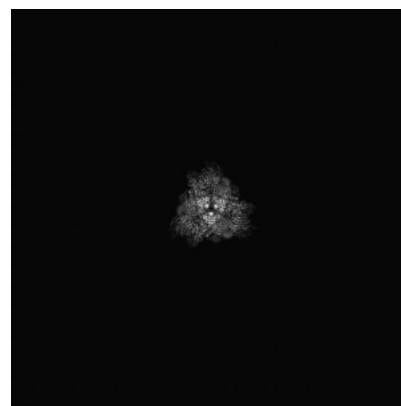
6.1.1 Primary map



X

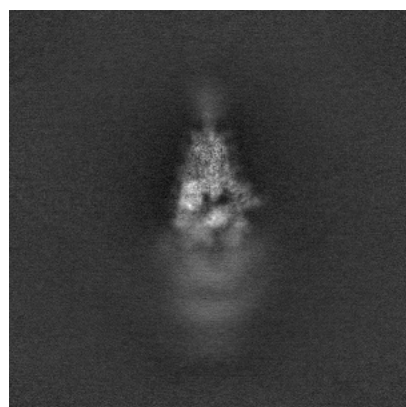


Y

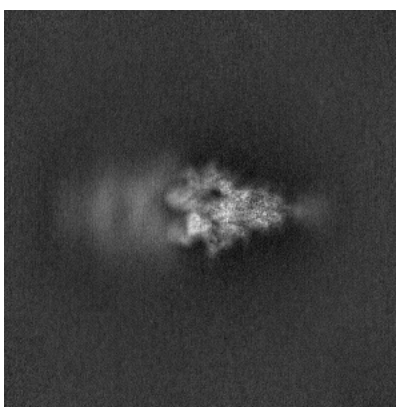


Z

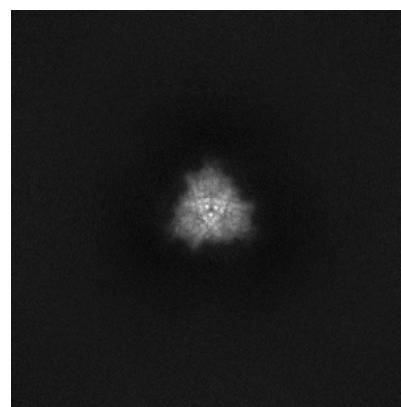
6.1.2 Raw map



X



Y

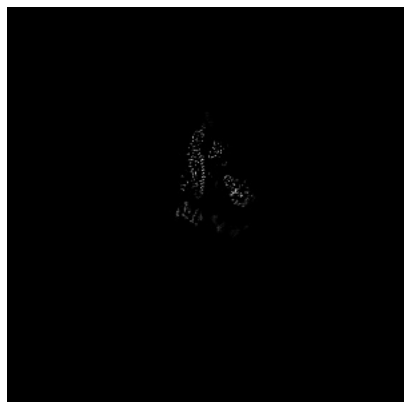


Z

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

6.2 Central slices [i](#)

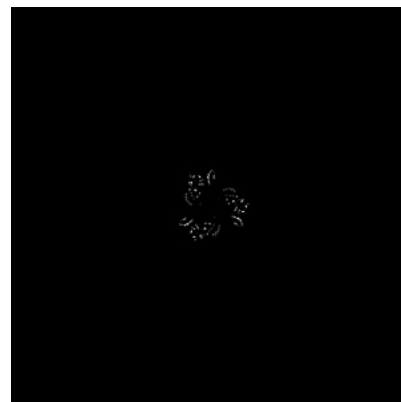
6.2.1 Primary map



X Index: 340



Y Index: 340



Z Index: 340

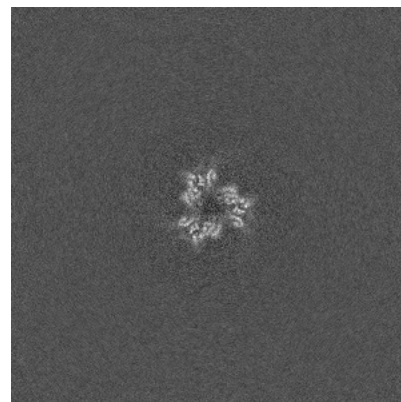
6.2.2 Raw map



X Index: 340



Y Index: 340



Z Index: 340

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

6.3 Largest variance slices [i](#)

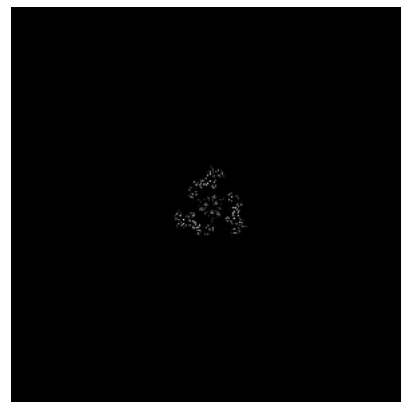
6.3.1 Primary map



X Index: 331



Y Index: 344



Z Index: 373

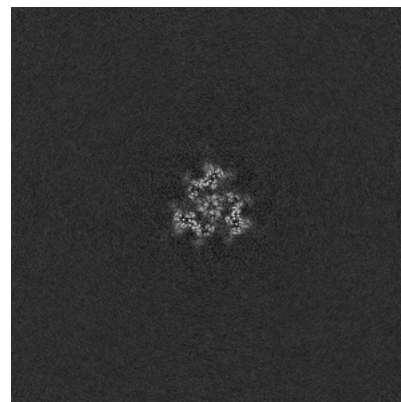
6.3.2 Raw map



X Index: 332



Y Index: 345

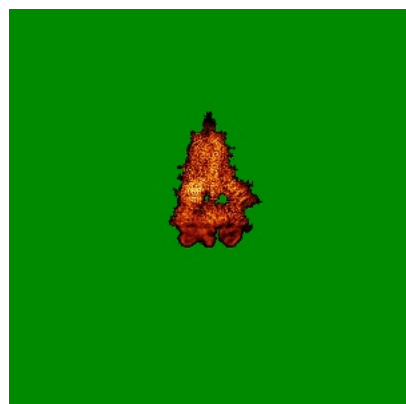


Z Index: 373

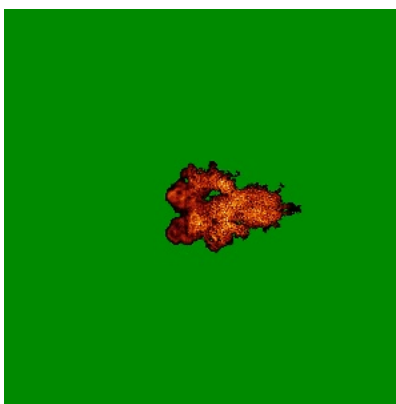
The images above show the largest variance slices of the map in three orthogonal directions.

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

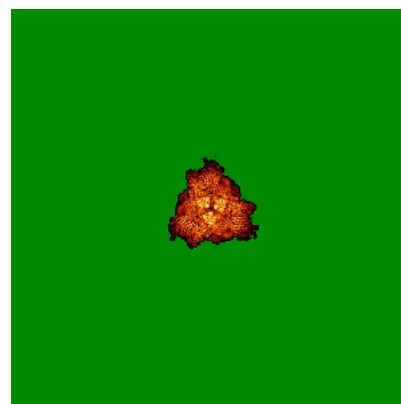
6.4.1 Primary map



X

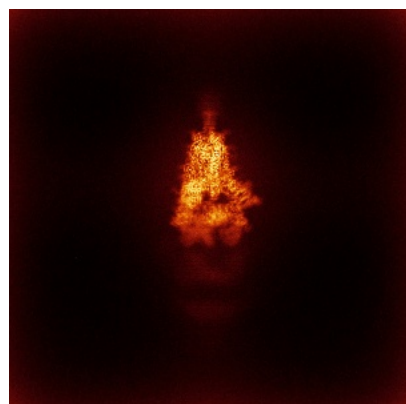


Y

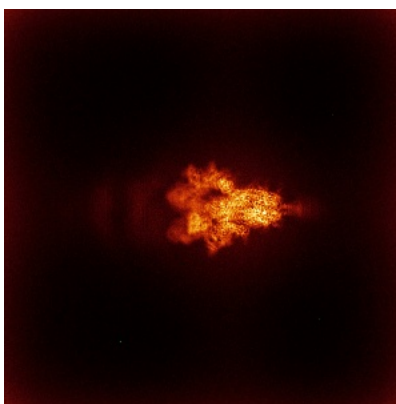


Z

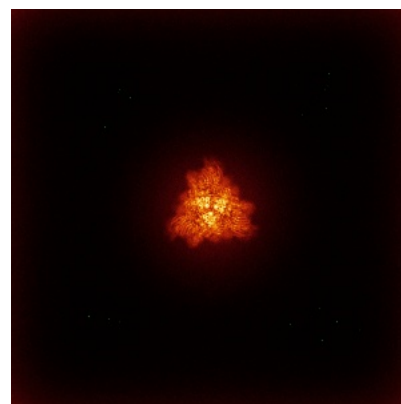
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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



X



Y



Z

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.

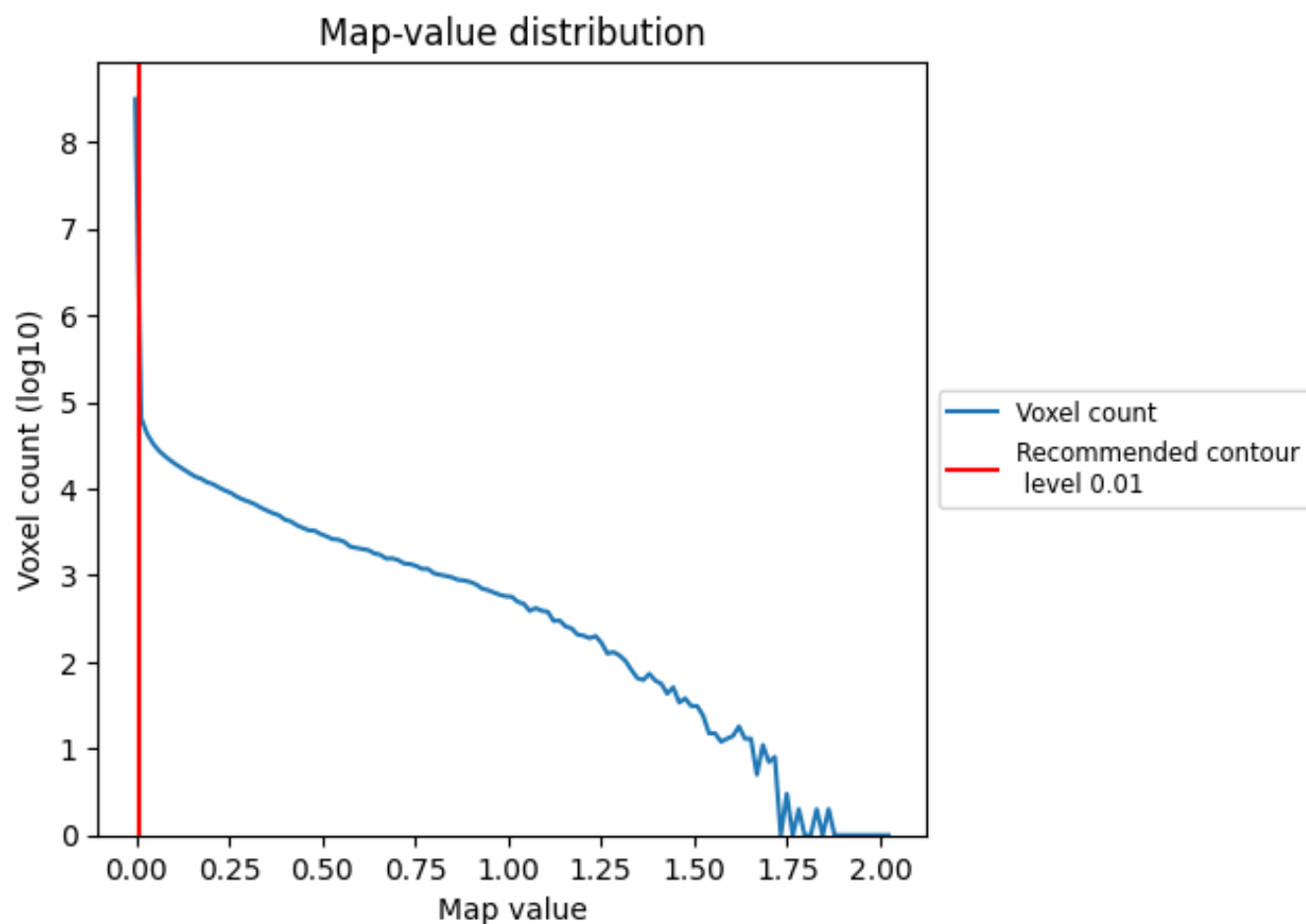
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

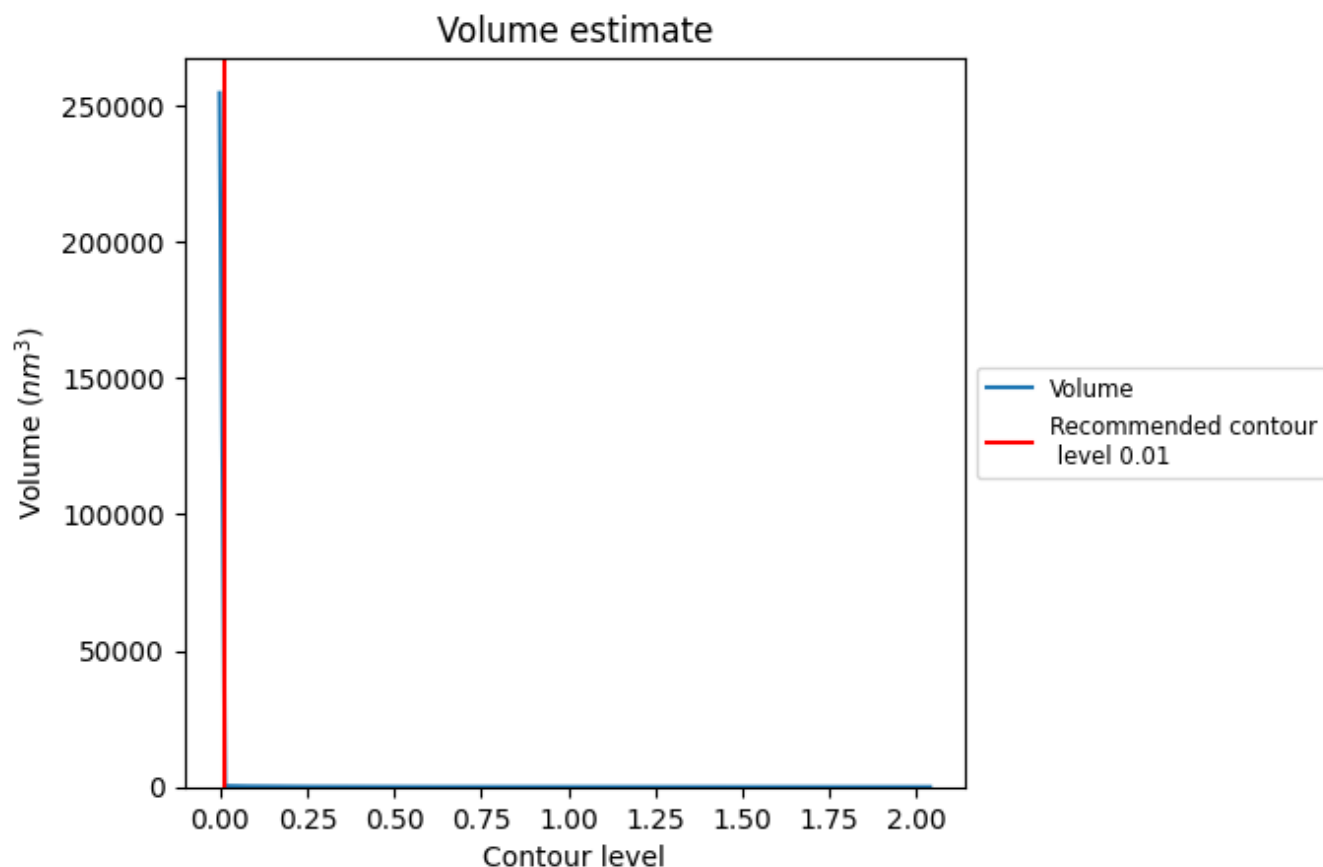
This section contains the results of statistical analysis of the map.

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.

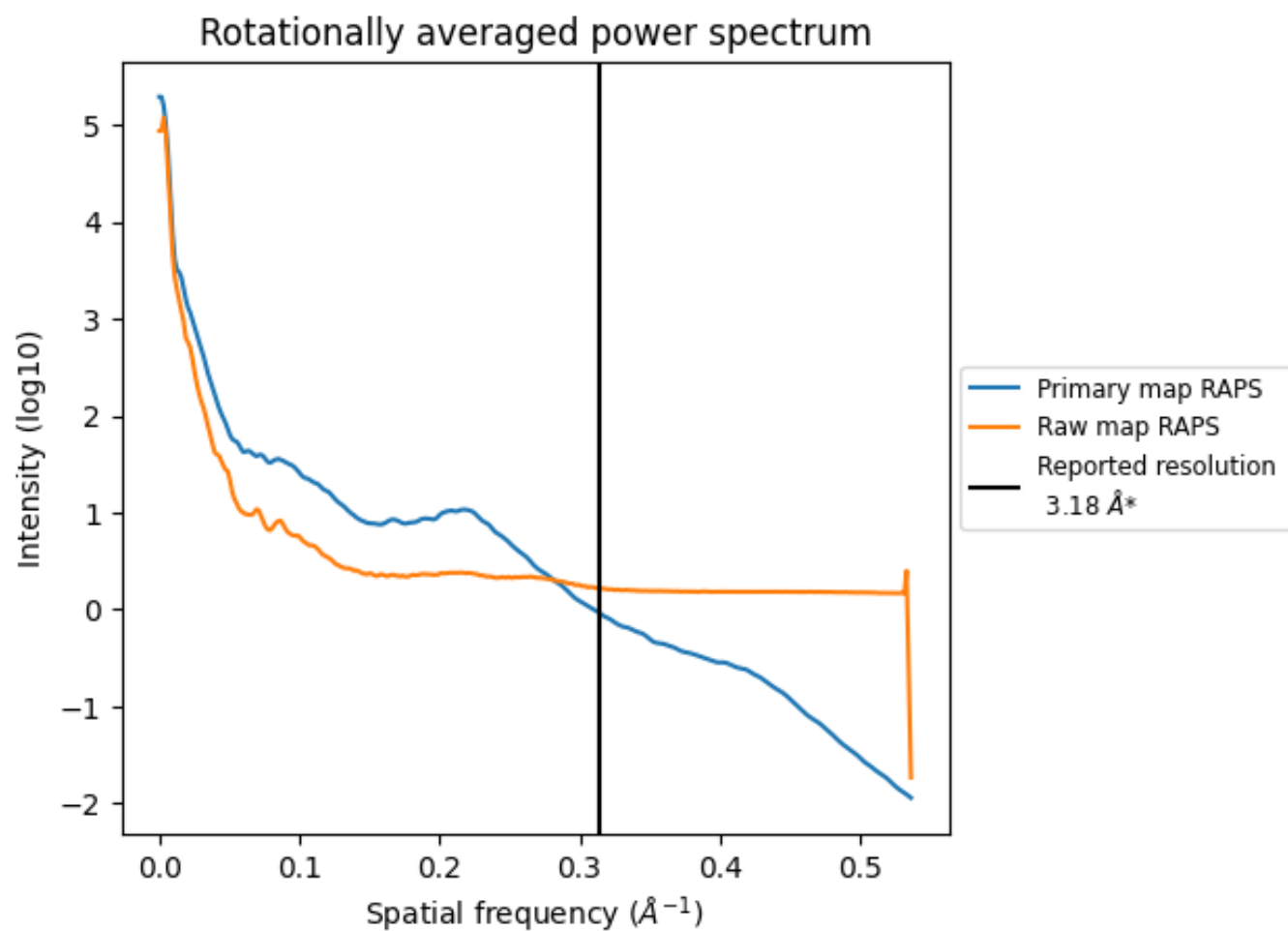
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66982 nm^3 ; this corresponds to an approximate mass of 60507 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

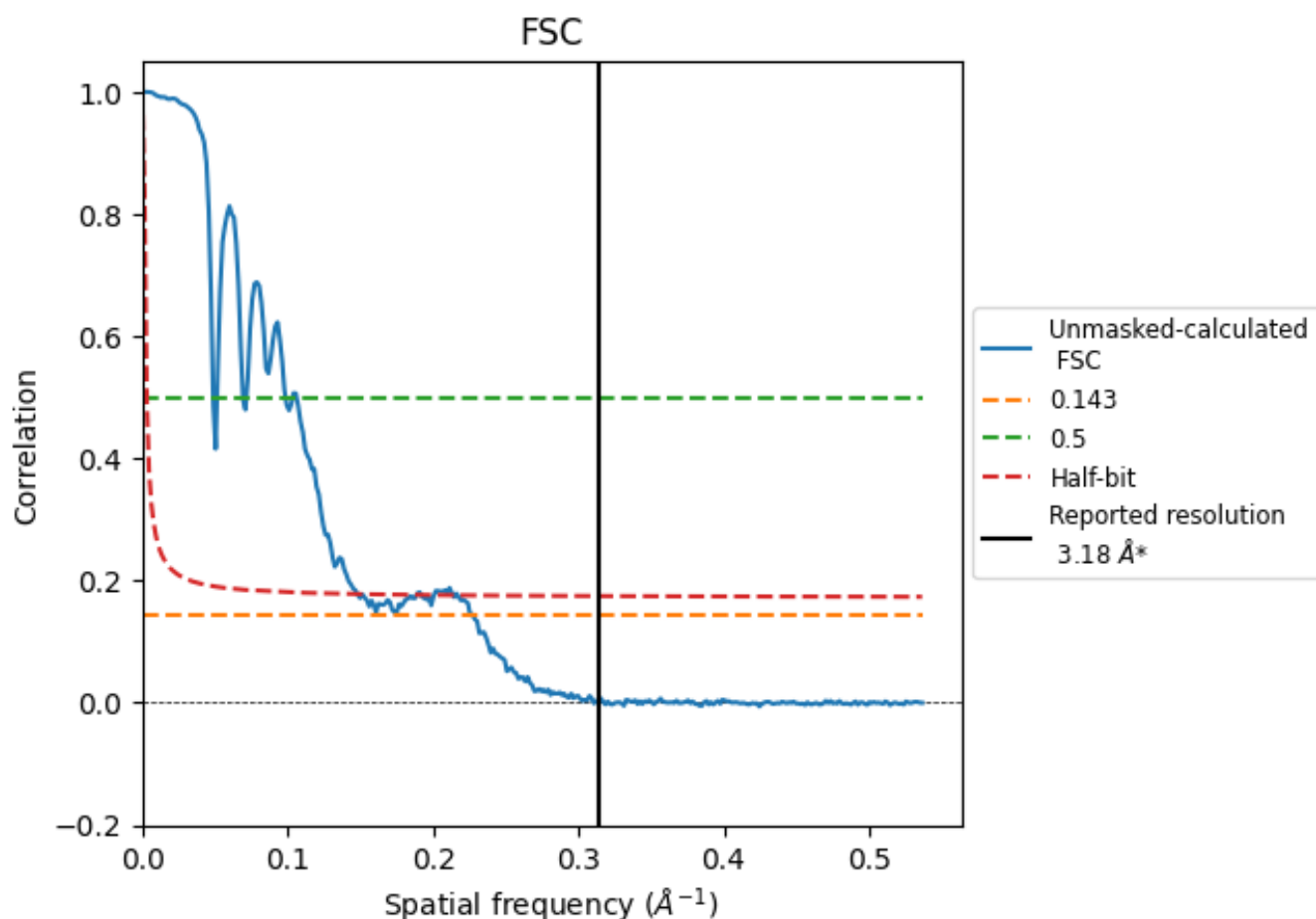


*Reported resolution corresponds to spatial frequency of 0.314 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.314 \AA^{-1}

8.2 Resolution estimates [i](#)

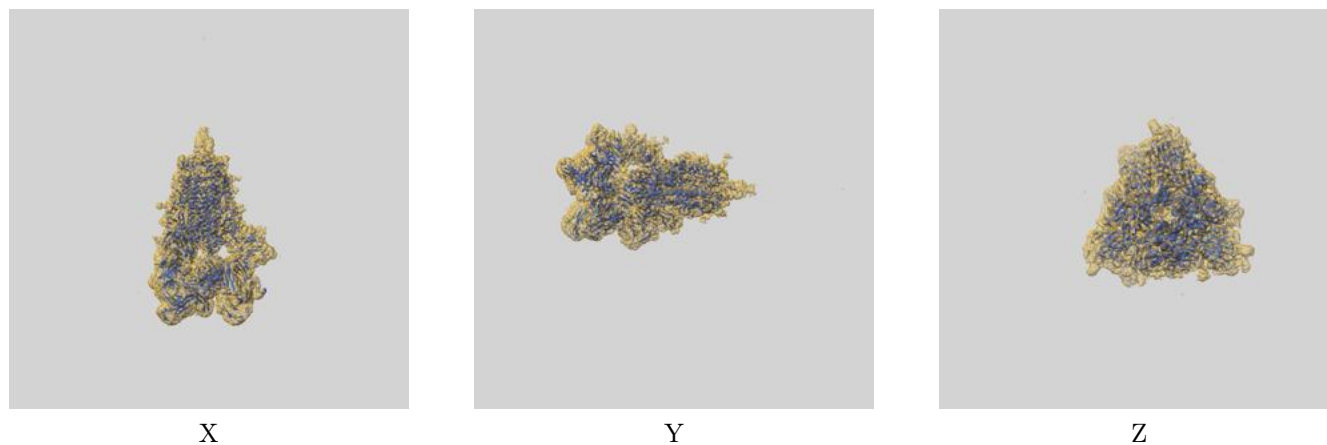
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.40	20.49	6.76

*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 4.40 differs from the reported value 3.18 by more than 10 %

9 Map-model fit [i](#)

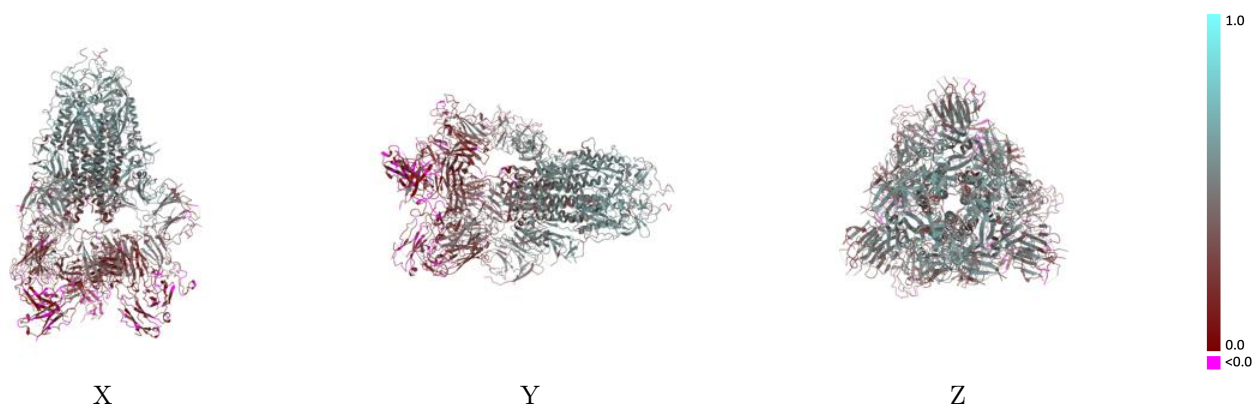
This section contains information regarding the fit between EMDB map EMD-62680 and PDB model 9KZZ. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



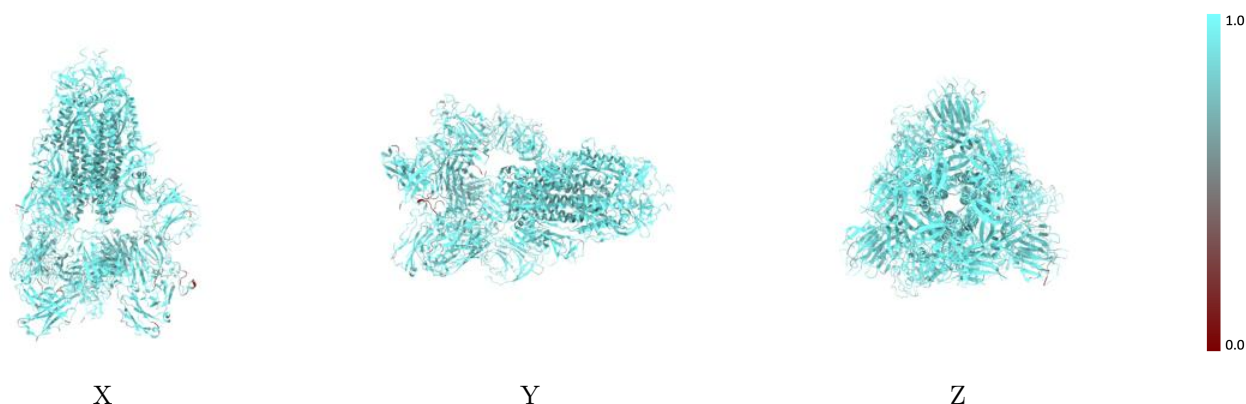
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



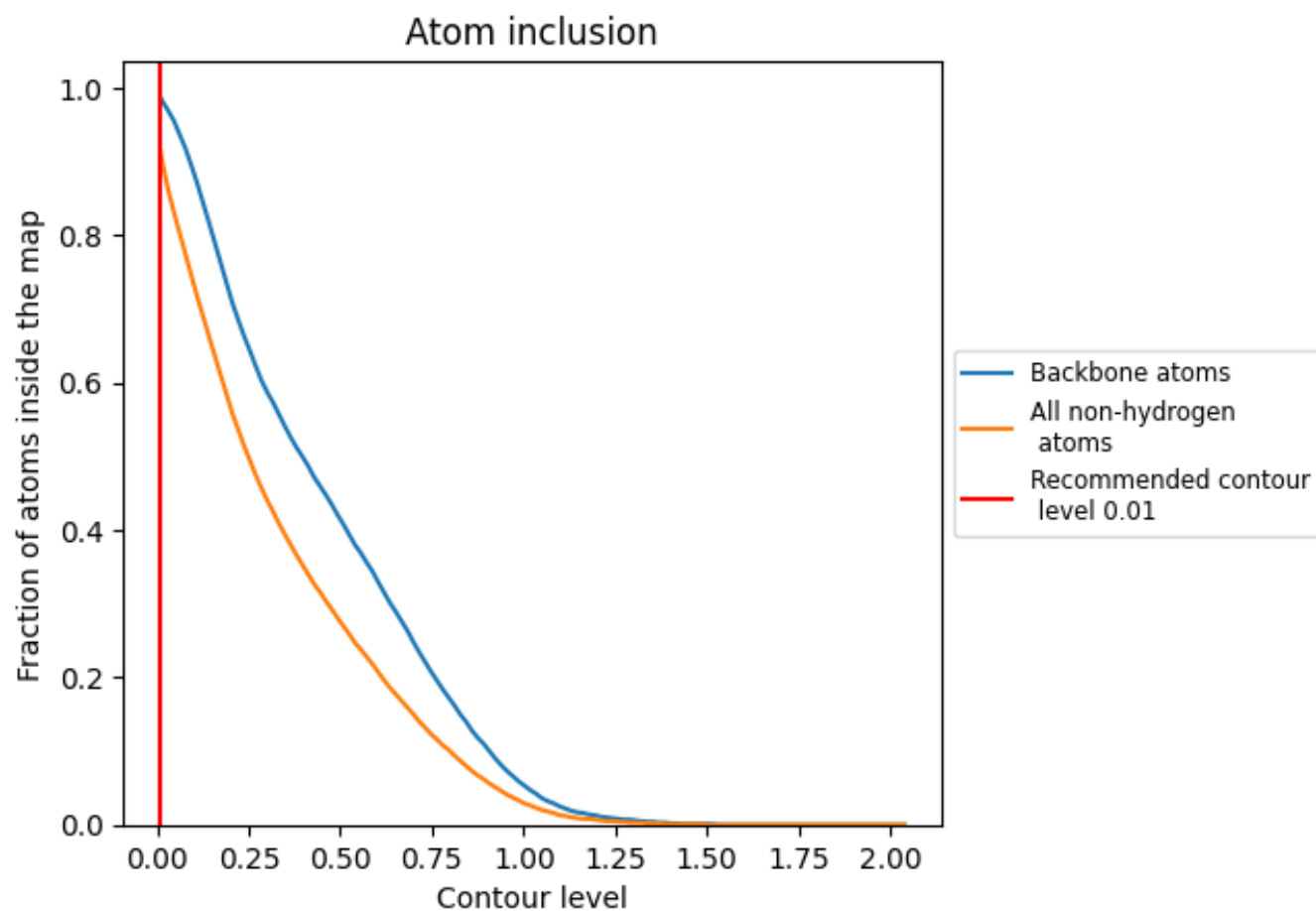
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 91% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9140	 0.3630
A	 0.9310	 0.4350
B	 0.9280	 0.4350
C	 0.9230	 0.4280
D	 0.7500	 0.2030
E	 0.5130	 0.0710
F	 0.7140	 0.1570
G	 0.8210	 0.3910
H	 0.8820	 0.1960
I	 0.8930	 0.2000
J	 0.9040	 0.2060
K	 0.7180	 0.2560
L	 0.8900	 0.1870
M	 0.8950	 0.1780
N	 0.9080	 0.1950
O	 0.5000	 0.1500
P	 0.8210	 0.3790
Q	 0.8570	 0.3740
R	 0.8570	 0.3580
S	 0.8210	 0.3220
T	 0.8460	 0.1740
U	 0.6790	 0.1830
V	 0.9640	 0.4180
W	 0.4640	 0.1970
X	 0.9490	 0.4320
Y	 0.7180	 0.2420
Z	 0.6150	 0.1990
a	 0.6430	 0.2560
b	 0.7440	 0.1710
c	 0.7140	 0.1640
d	 0.8210	 0.3690
e	 0.6430	 0.2810
f	 0.8460	 0.3870
g	 0.8930	 0.3840
h	 0.7140	 0.2270
i	 0.6070	 0.2130

