



# wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 07:03 PM JST

PDB ID : 7WUH  
EMDB ID : EMD-32832  
Title : SARS-CoV-2 Spike in complex with Fab of m31A7  
Authors : Chen, X.; Wu, Y.-M.  
Deposited on : 2022-02-08  
Resolution : 4.70 Å (reported)  
Based on initial model : 7CN9

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

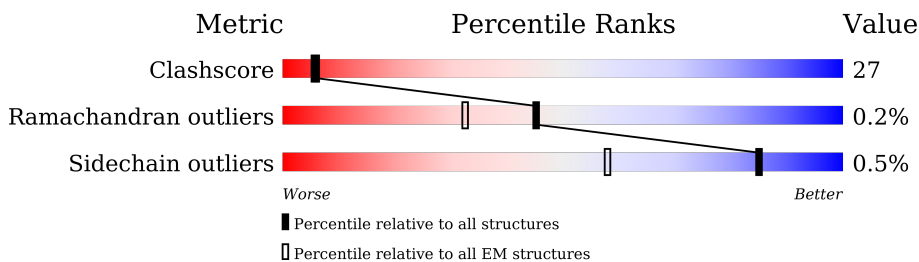
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001) 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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1242	
1	C	1242	
1	E	1242	
2	D	239	
2	H	239	
2	K	239	
3	F	240	
3	I	240	

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Mol	Chain	Length	Quality of chain
3	L	240	
4	B	3	
4	b	3	
5	G	2	
5	N	2	
5	O	2	
5	P	2	
5	R	2	
5	T	2	
5	V	2	
5	X	2	
6	J	4	
6	Y	4	
7	M	3	
7	Q	3	
7	Z	3	
7	e	3	
8	S	5	
8	W	5	
9	U	5	
10	a	4	
10	g	4	
11	c	2	
12	d	6	
13	f	6	

## 2 Entry composition i

There are 14 unique types of molecules in this entry. The entry contains 35569 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1038	8062	5137	1354	1535	36	0	0
1	C	1038	8072	5145	1353	1538	36	0	0
1	E	1044	8123	5177	1361	1549	36	0	0

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	GLY	ARG	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	ASP	-	expression tag	UNP P0DTC2
A	1210	ILE	-	expression tag	UNP P0DTC2
A	1211	ARG	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	LEU	-	expression tag	UNP P0DTC2
A	1214	VAL	-	expression tag	UNP P0DTC2
A	1215	PRO	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	GLY	-	expression tag	UNP P0DTC2
A	1218	SER	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	SER	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	ILE	-	expression tag	UNP P0DTC2
A	1225	PRO	-	expression tag	UNP P0DTC2
A	1226	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ALA	-	expression tag	UNP P0DTC2
A	1228	PRO	-	expression tag	UNP P0DTC2
A	1229	ARG	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLN	-	expression tag	UNP P0DTC2
A	1233	ALA	-	expression tag	UNP P0DTC2
A	1234	TYR	-	expression tag	UNP P0DTC2
A	1235	VAL	-	expression tag	UNP P0DTC2
A	1236	ARG	-	expression tag	UNP P0DTC2
A	1237	LYS	-	expression tag	UNP P0DTC2
A	1238	ASP	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	GLU	-	expression tag	UNP P0DTC2
A	1241	TRP	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	SER	-	expression tag	UNP P0DTC2
A	1246	THR	-	expression tag	UNP P0DTC2
A	1247	PHE	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	GLY	ARG	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	ASP	-	expression tag	UNP P0DTC2
C	1210	ILE	-	expression tag	UNP P0DTC2
C	1211	ARG	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	LEU	-	expression tag	UNP P0DTC2
C	1214	VAL	-	expression tag	UNP P0DTC2
C	1215	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	GLY	-	expression tag	UNP P0DTC2
C	1218	SER	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	SER	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	ILE	-	expression tag	UNP P0DTC2
C	1225	PRO	-	expression tag	UNP P0DTC2
C	1226	GLU	-	expression tag	UNP P0DTC2
C	1227	ALA	-	expression tag	UNP P0DTC2
C	1228	PRO	-	expression tag	UNP P0DTC2
C	1229	ARG	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2
C	1232	GLN	-	expression tag	UNP P0DTC2
C	1233	ALA	-	expression tag	UNP P0DTC2
C	1234	TYR	-	expression tag	UNP P0DTC2
C	1235	VAL	-	expression tag	UNP P0DTC2
C	1236	ARG	-	expression tag	UNP P0DTC2
C	1237	LYS	-	expression tag	UNP P0DTC2
C	1238	ASP	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	GLU	-	expression tag	UNP P0DTC2
C	1241	TRP	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	SER	-	expression tag	UNP P0DTC2
C	1246	THR	-	expression tag	UNP P0DTC2
C	1247	PHE	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
E	614	GLY	ASP	engineered mutation	UNP P0DTC2
E	682	GLY	ARG	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	683	SER	ARG	variant	UNP P0DTC2
E	685	GLY	ARG	variant	UNP P0DTC2
E	986	PRO	LYS	variant	UNP P0DTC2
E	987	PRO	VAL	variant	UNP P0DTC2
E	1209	ASP	-	expression tag	UNP P0DTC2
E	1210	ILE	-	expression tag	UNP P0DTC2
E	1211	ARG	-	expression tag	UNP P0DTC2
E	1212	SER	-	expression tag	UNP P0DTC2
E	1213	LEU	-	expression tag	UNP P0DTC2
E	1214	VAL	-	expression tag	UNP P0DTC2
E	1215	PRO	-	expression tag	UNP P0DTC2
E	1216	ARG	-	expression tag	UNP P0DTC2
E	1217	GLY	-	expression tag	UNP P0DTC2
E	1218	SER	-	expression tag	UNP P0DTC2
E	1219	PRO	-	expression tag	UNP P0DTC2
E	1220	GLY	-	expression tag	UNP P0DTC2
E	1221	SER	-	expression tag	UNP P0DTC2
E	1222	GLY	-	expression tag	UNP P0DTC2
E	1223	TYR	-	expression tag	UNP P0DTC2
E	1224	ILE	-	expression tag	UNP P0DTC2
E	1225	PRO	-	expression tag	UNP P0DTC2
E	1226	GLU	-	expression tag	UNP P0DTC2
E	1227	ALA	-	expression tag	UNP P0DTC2
E	1228	PRO	-	expression tag	UNP P0DTC2
E	1229	ARG	-	expression tag	UNP P0DTC2
E	1230	ASP	-	expression tag	UNP P0DTC2
E	1231	GLY	-	expression tag	UNP P0DTC2
E	1232	GLN	-	expression tag	UNP P0DTC2
E	1233	ALA	-	expression tag	UNP P0DTC2
E	1234	TYR	-	expression tag	UNP P0DTC2
E	1235	VAL	-	expression tag	UNP P0DTC2
E	1236	ARG	-	expression tag	UNP P0DTC2
E	1237	LYS	-	expression tag	UNP P0DTC2
E	1238	ASP	-	expression tag	UNP P0DTC2
E	1239	GLY	-	expression tag	UNP P0DTC2
E	1240	GLU	-	expression tag	UNP P0DTC2
E	1241	TRP	-	expression tag	UNP P0DTC2
E	1242	VAL	-	expression tag	UNP P0DTC2
E	1243	LEU	-	expression tag	UNP P0DTC2
E	1244	LEU	-	expression tag	UNP P0DTC2
E	1245	SER	-	expression tag	UNP P0DTC2
E	1246	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1247	PHE	-	expression tag	UNP P0DTC2
E	1248	LEU	-	expression tag	UNP P0DTC2
E	1249	GLY	-	expression tag	UNP P0DTC2
E	1250	HIS	-	expression tag	UNP P0DTC2
E	1251	HIS	-	expression tag	UNP P0DTC2
E	1252	HIS	-	expression tag	UNP P0DTC2
E	1253	HIS	-	expression tag	UNP P0DTC2
E	1254	HIS	-	expression tag	UNP P0DTC2
E	1255	HIS	-	expression tag	UNP P0DTC2

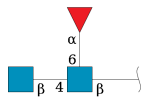
- Molecule 2 is a protein called m31A7 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	218	Total	C	N	O	S	0	0
			1641	1039	265	331	6		
2	H	218	Total	C	N	O	S	0	0
			1641	1039	265	331	6		
2	K	218	Total	C	N	O	S	0	0
			1641	1039	265	331	6		

- Molecule 3 is a protein called m31A7 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	219	Total	C	N	O	S	0	0
			1705	1073	283	343	6		
3	I	219	Total	C	N	O	S	0	0
			1705	1073	283	343	6		
3	L	219	Total	C	N	O	S	0	0
			1705	1073	283	343	6		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	B	3	Total	C	N	O	0	0
			38	22	2	14		
4	b	3	Total	C	N	O	0	0
			38	22	2	14		

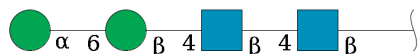


- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	2	28	16	2	10	0	0
5	N	2	28	16	2	10	0	0
5	O	2	28	16	2	10	0	0
5	P	2	28	16	2	10	0	0
5	R	2	28	16	2	10	0	0
5	T	2	28	16	2	10	0	0
5	V	2	28	16	2	10	0	0
5	X	2	28	16	2	10	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



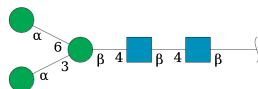
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	J	4	50	28	2	20	0	0
6	Y	4	50	28	2	20	0	0

- Molecule 7 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.



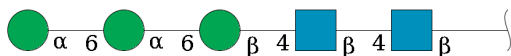
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	M	3	39	22	2	15	0	0
7	Q	3	39	22	2	15	0	0
7	Z	3	39	22	2	15	0	0
7	e	3	39	22	2	15	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



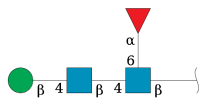
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	S	5	61	34	2	25	0	0
8	W	5	61	34	2	25	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-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
			Total	C	N	O		
9	U	5	61	34	2	25	0	0

- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



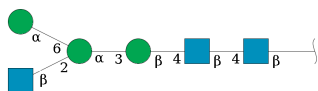
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	a	4	49	28	2	19	0	0
10	g	4	49	28	2	19	0	0

- Molecule 11 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



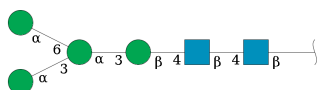
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	c	2	24	14	1	9	0	0

- Molecule 12 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-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
			Total	C	N	O		
12	d	6	75	42	3	30	0	0

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-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
			Total	C	N	O		
13	f	6	72	40	2	30	0	0

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

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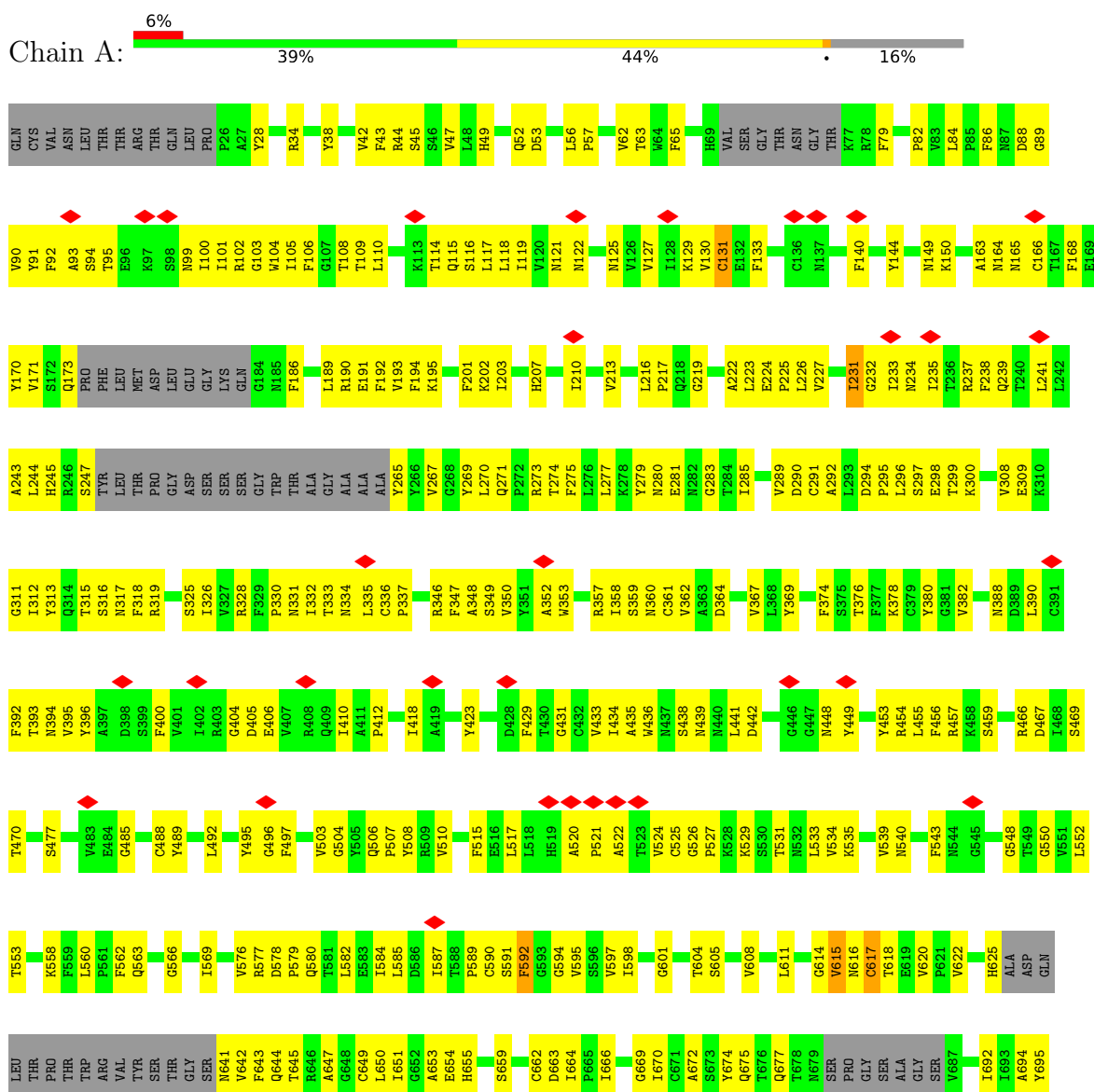
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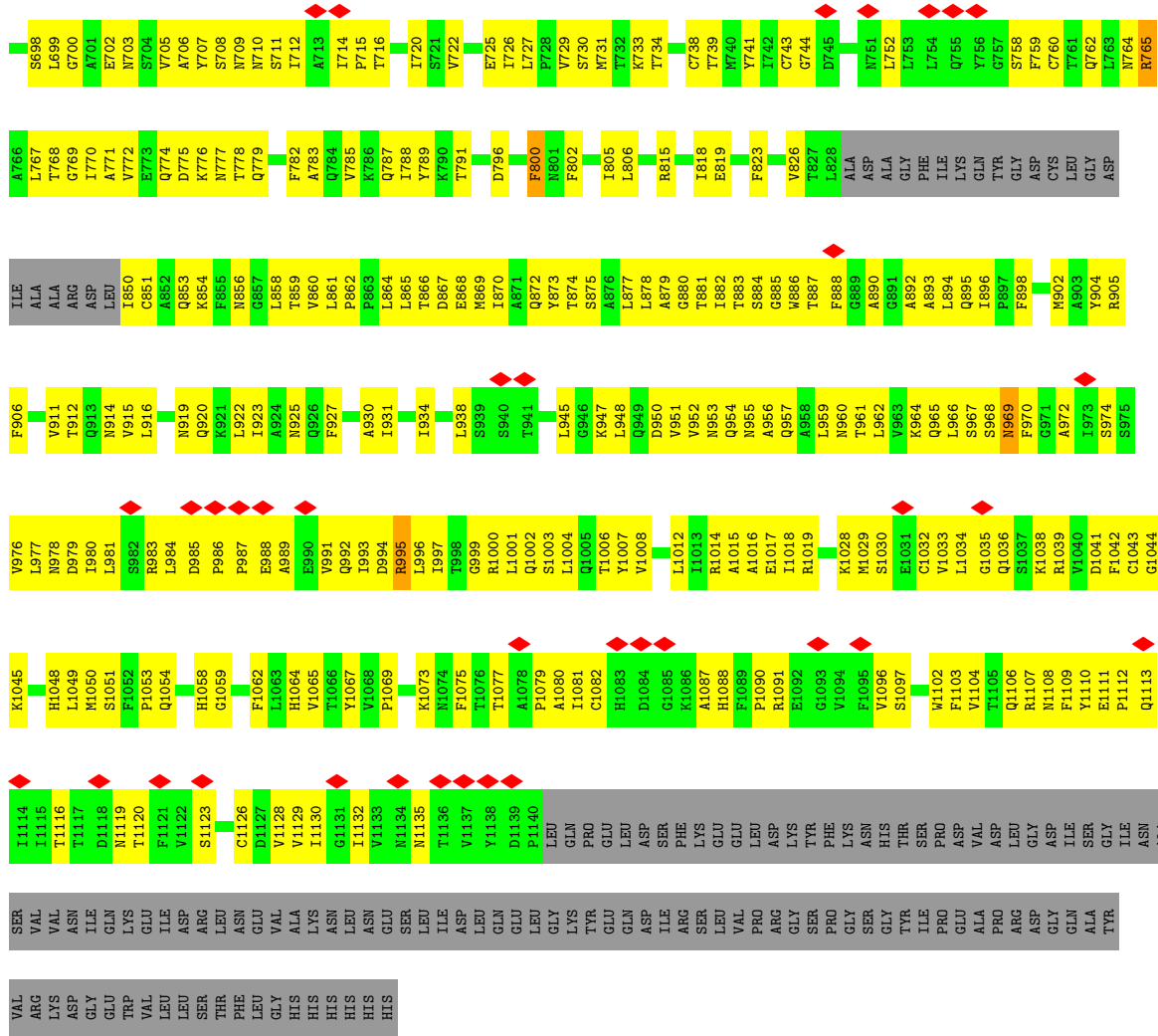
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>AltConf</b>
14	C	1	Total 14	C 8	N 1	O 5	0
14	C	1	Total 14	C 8	N 1	O 5	0
14	C	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
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14	K	1	Total 14	C 8	N 1	O 5	0

### 3 Residue-property plots [i](#)

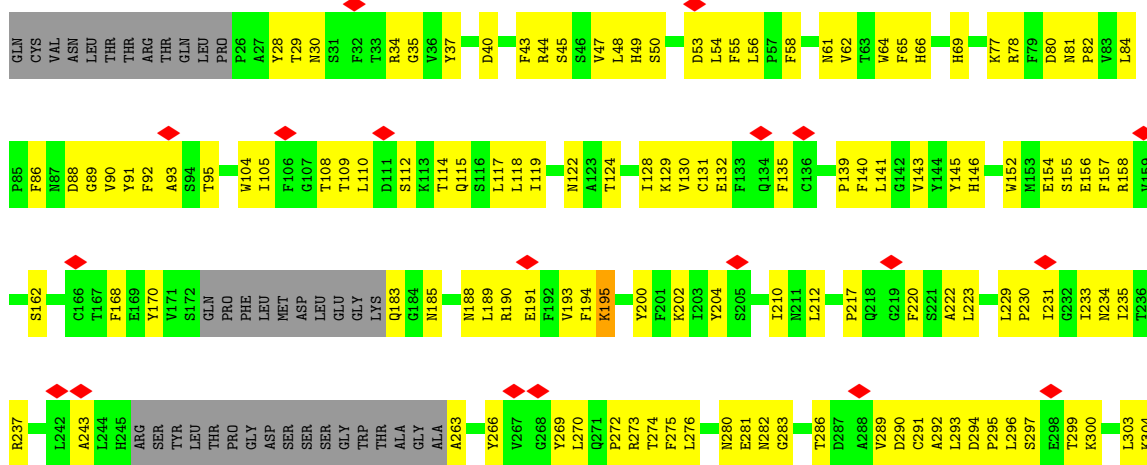
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Spike glycoprotein



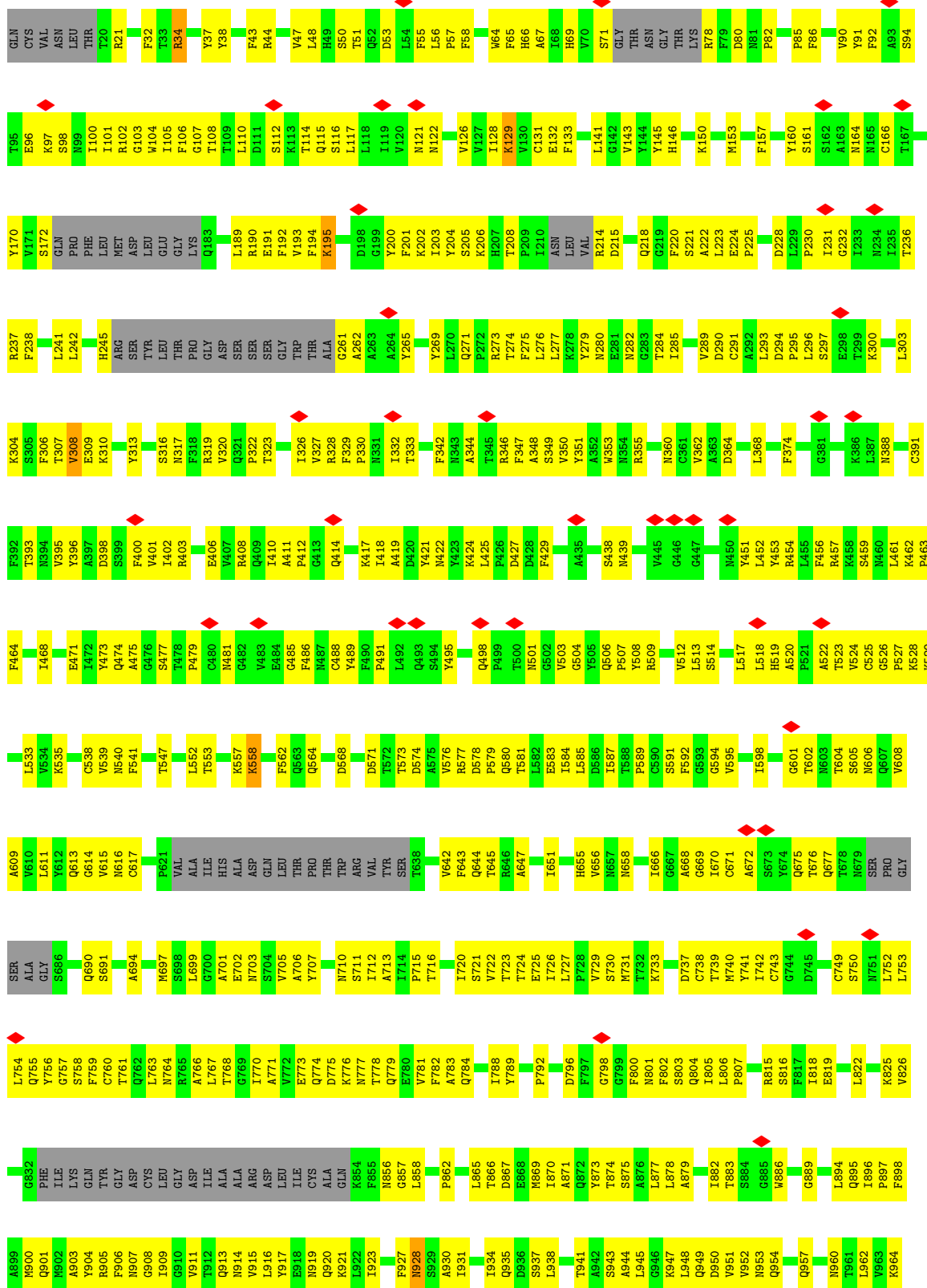


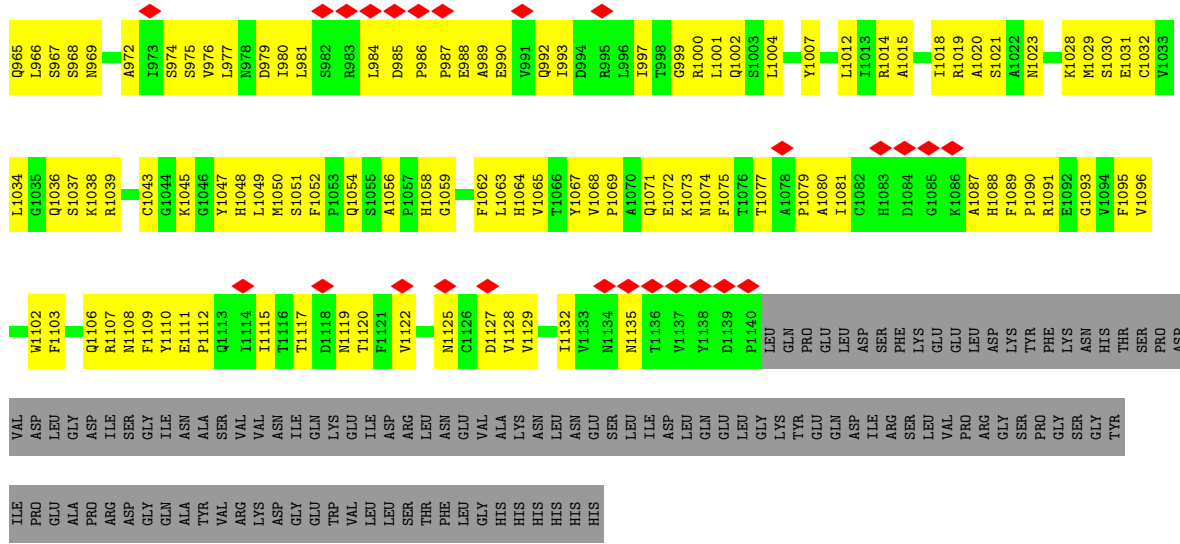
• Molecule 1: Spike glycoprotein



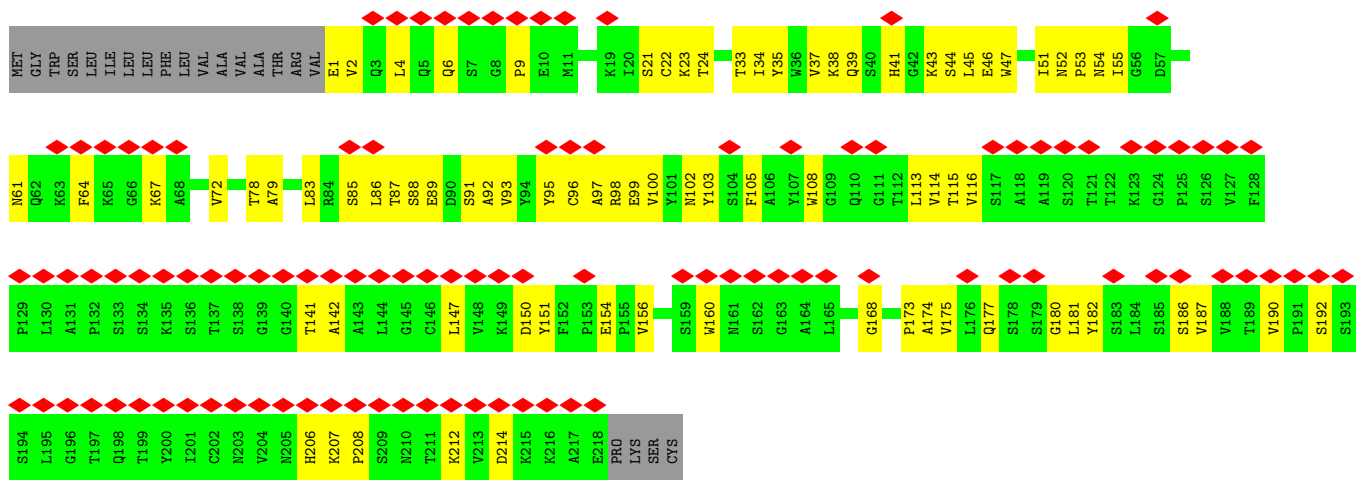
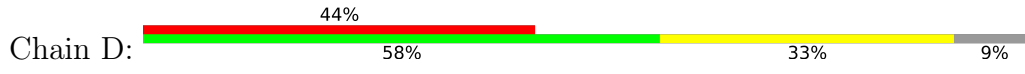
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ASP	G311	L390	D467	N642	V621	VAL	Q755	A829	P897	L962	L1034	V1104	ASP
GLY	I312	C391	I468	F543	P622	ALA	Y756	ASP	F898	V963	G1035	T1106	GLY
ALA	S316	F392	S469	T549	G690	GLY	G757	ALA	A699	K964	Q1036	Q1107	ALA
VAL	N317	T393	T470	T550	Q691	PHE	S758	PHE	Q901	Q965	S1037	R1107	VAL
VAL	N318	N994	C480	G485	S691	ILE	F759	ILE	N902	S968	F1042	Y1110	VAL
LYS	F318	V996	M481	M482	I692	LYS	T760	LYS	A903	N969	C1043	E1111	LYS
ASN	R319	Y396	G482	N555	I693	GLN	T761	GLN	Y904	F970	Y1047	P1112	ASN
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TRP	T323	D398	V483	K558	E484	GLY	L763	GLY	F906	A972	M1049	F1092	TRP
VAL	F400	S399	F484	K558	ASP	ASP	N764	ASP	N907	I973	M1050	N1118	VAL
LEU	F401	F400	G485	F562	CYS	LEU	A766	CYS	G908	S974	S1051	T1120	LEU
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LEU	R404	R404	C488	G567	ALA	ALA	E773	ALA	G912	D979	S1055	S1123	LEU
LEU	D405	D405	P491	R567	ARG	ARG	O774	ARG	N913	I980	A1056	G1124	LEU
LEU	E406	E406	L492	R567	ASP	ASP	O775	ASP	N914	L981	P1057	N1125	LEU
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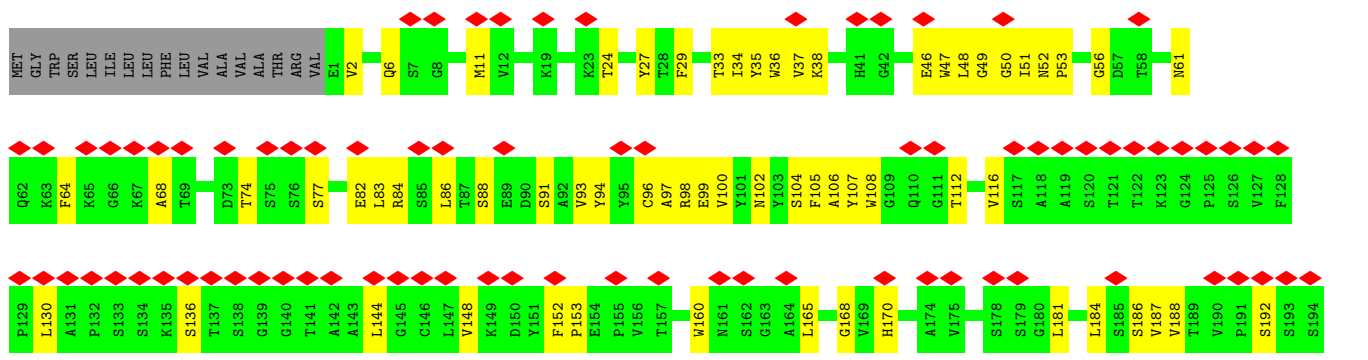
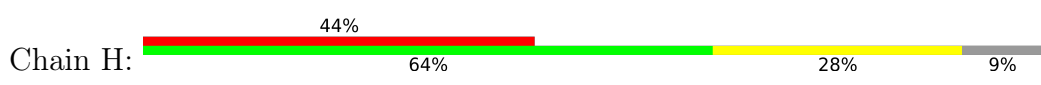


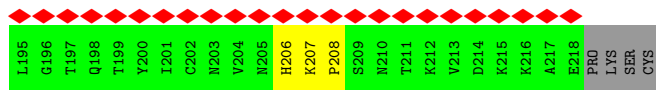


• Molecule 2: m31A7 Fab heavy chain

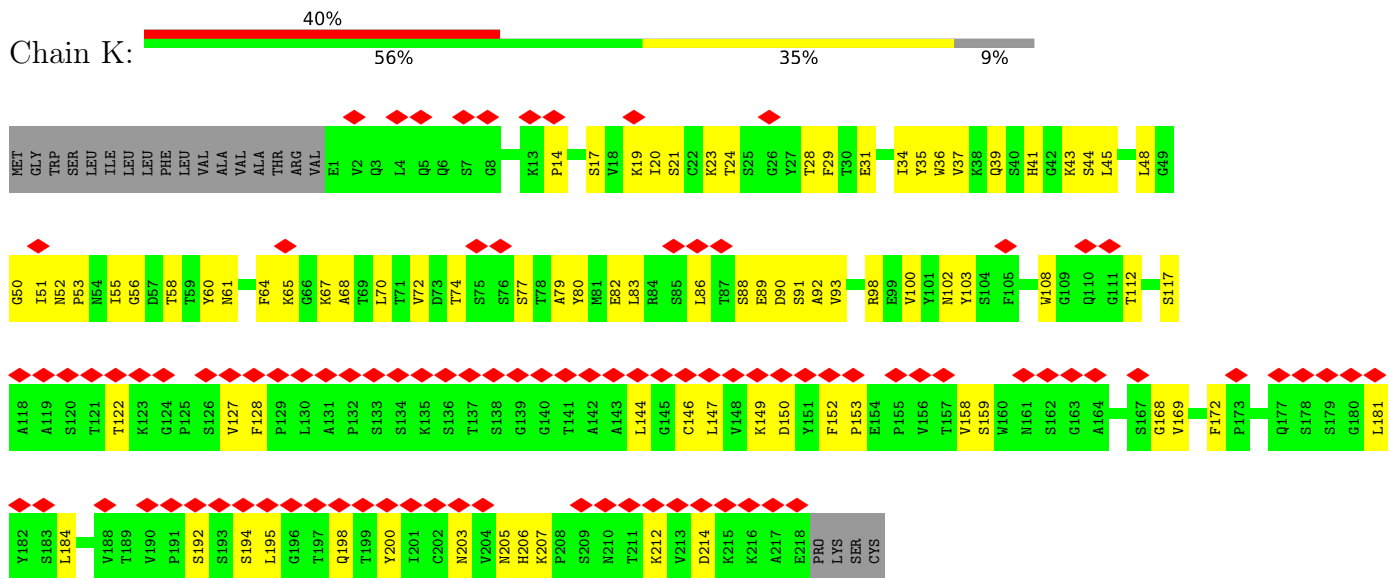


• Molecule 2: m31A7 Fab heavy chain

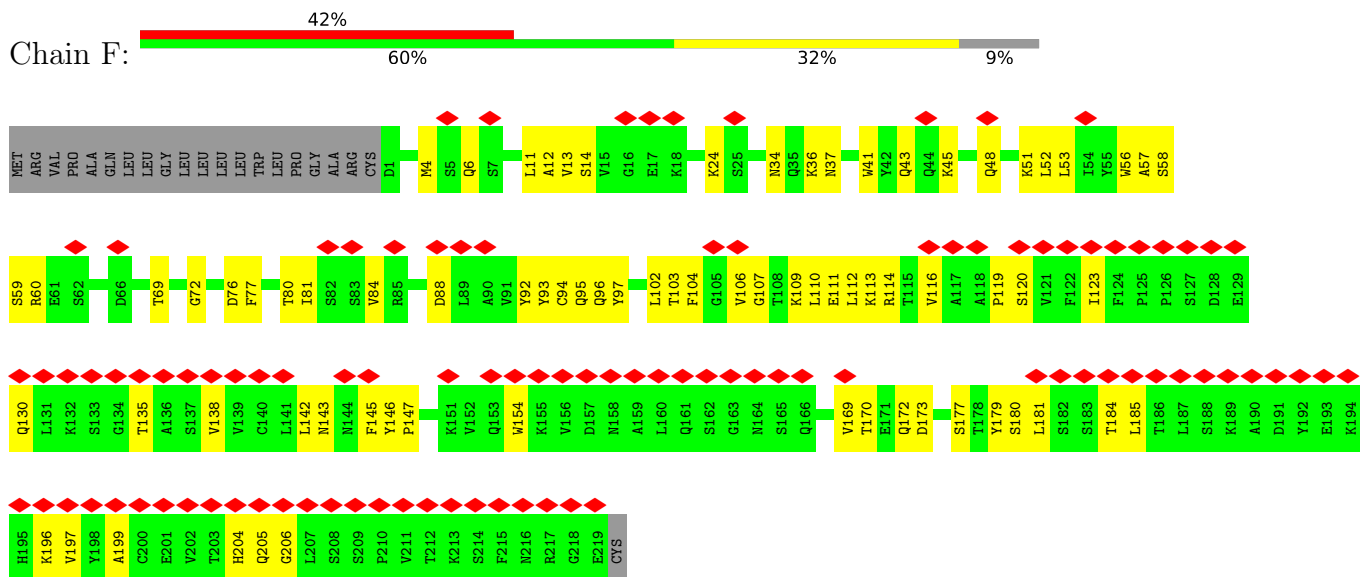




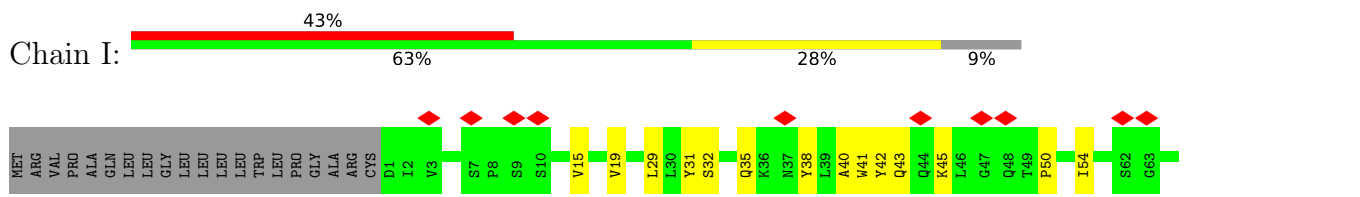
• Molecule 2: m31A7 Fab heavy chain

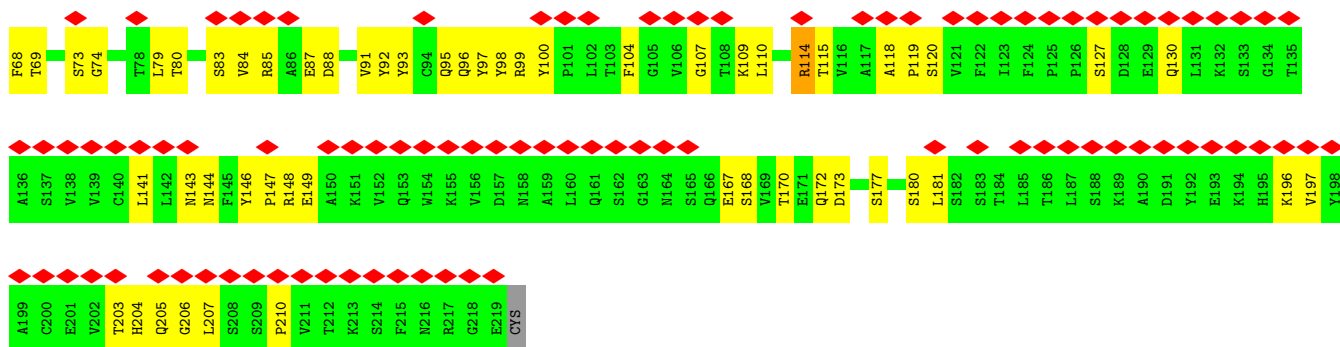


• Molecule 3: m31A7 Fab light chain

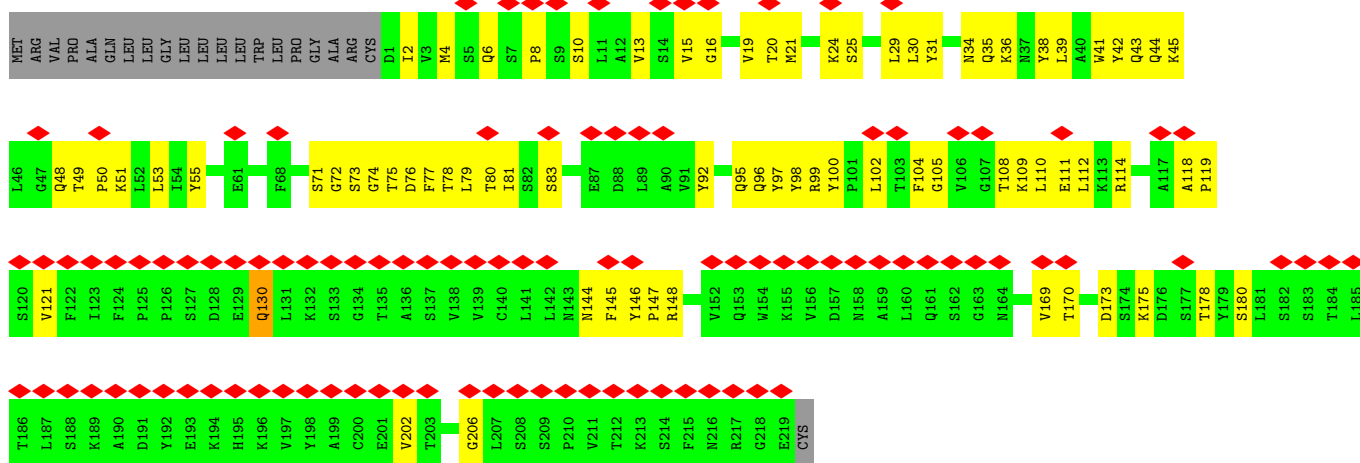
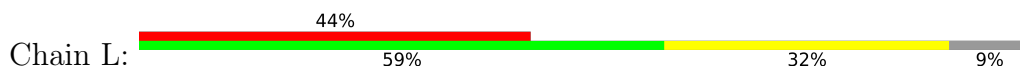


• Molecule 3: m31A7 Fab light chain





- Molecule 3: m31A7 Fab light chain



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

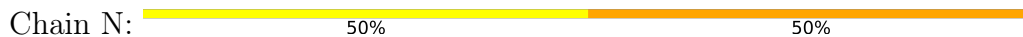


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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



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



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



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



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



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

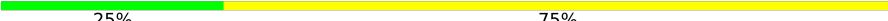


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

MAG1  
MAG2

- Molecule 6: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  25% 75%

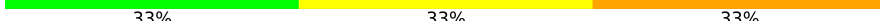
MAG1  
MAG2  
BMA3  
MAN4

- Molecule 6: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  50% 50%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 33% 33%

MAG1  
MAG2  
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  67% 33%

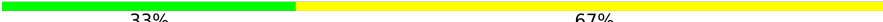
MAG1  
MAG2  
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

MAG1  
MAG2  
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  33% 67%




- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  60% 40%

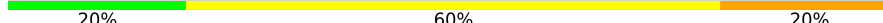


- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  20% 40% 40%



- Molecule 9: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  20% 60% 20%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50% 50%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  75% 25%

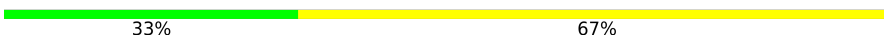


- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%

MAG1  
FUC2

- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  33% 67%

MAG1  
MAG2  
BMA3  
MAN4  
MAG5  
MAN6

- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  17% 83%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108565	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.1	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	11.642	Depositor
Minimum map value	-3.915	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.385	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	315.4, 315.4, 315.4	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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, MAN, FUC, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/8245	0.56	0/11227
1	C	0.31	0/8256	0.57	1/11234 (0.0%)
1	E	0.30	0/8308	0.55	1/11306 (0.0%)
2	D	0.26	0/1681	0.51	0/2292
2	H	0.27	0/1681	0.51	0/2292
2	K	0.26	0/1681	0.50	0/2292
3	F	0.26	0/1741	0.52	0/2361
3	I	0.26	0/1741	0.55	0/2361
3	L	0.27	0/1741	0.51	0/2361
All	All	0.29	0/35075	0.55	2/47726 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	995	ARG	CA-CB-CG	5.79	126.15	113.40
1	E	571	ASP	CB-CG-OD1	5.12	122.90	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	CYS	Peptide
1	A	800	PHE	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8062	0	7808	563	0
1	C	8072	0	7852	528	0
1	E	8123	0	7890	537	0
2	D	1641	0	1604	69	0
2	H	1641	0	1603	56	0
2	K	1641	0	1603	59	0
3	F	1705	0	1669	71	0
3	I	1705	0	1669	56	0
3	L	1705	0	1669	67	0
4	B	38	0	32	3	0
4	b	38	0	34	0	0
5	G	28	0	25	0	0
5	N	28	0	25	2	0
5	O	28	0	25	1	0
5	P	28	0	25	5	0
5	R	28	0	25	0	0
5	T	28	0	25	1	0
5	V	28	0	25	2	0
5	X	28	0	25	2	0
6	J	50	0	43	1	0
6	Y	50	0	43	6	0
7	M	39	0	34	2	0
7	Q	39	0	34	1	0
7	Z	39	0	34	0	0
7	e	39	0	34	0	0
8	S	61	0	52	3	0
8	W	61	0	52	2	0
9	U	61	0	52	2	0
10	a	49	0	43	0	0
10	g	49	0	43	0	0
11	c	24	0	22	0	0
12	d	75	0	63	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	f	72	0	61	0	0
14	A	70	0	65	1	0
14	C	112	0	104	5	0
14	E	70	0	65	4	0
14	K	14	0	13	0	0
All	All	35569	0	34490	1880	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 27.

The worst 5 of 1880 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:SER:O	1:A:615:VAL:HG13	1.48	1.12
1:A:591:SER:C	1:A:615:VAL:HG13	1.77	1.04
1:C:866:THR:H	1:C:869:MET:HE2	1.31	0.96
1:A:591:SER:CA	1:A:615:VAL:HG13	1.96	0.95
1:C:1028:LYS:O	1:C:1032:CYS:HB3	1.68	0.93

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1024/1242 (82%)	873 (85%)	148 (14%)	3 (0%)	37	72
1	C	1026/1242 (83%)	870 (85%)	156 (15%)	0	100	100
1	E	1028/1242 (83%)	884 (86%)	140 (14%)	4 (0%)	30	68
2	D	216/239 (90%)	202 (94%)	14 (6%)	0	100	100
2	H	216/239 (90%)	198 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	216/239 (90%)	206 (95%)	10 (5%)	0	100	100
3	F	217/240 (90%)	203 (94%)	14 (6%)	0	100	100
3	I	217/240 (90%)	202 (93%)	15 (7%)	0	100	100
3	L	217/240 (90%)	201 (93%)	16 (7%)	0	100	100
All	All	4377/5163 (85%)	3839 (88%)	531 (12%)	7 (0%)	45	78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	592	PHE
1	A	617	CYS
1	A	231	ILE
1	E	153	MET
1	E	1127	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	894/1077 (83%)	889 (99%)	5 (1%)	84	88
1	C	898/1077 (83%)	891 (99%)	7 (1%)	79	85
1	E	903/1077 (84%)	897 (99%)	6 (1%)	81	87
2	D	186/204 (91%)	186 (100%)	0	100	100
2	H	186/204 (91%)	186 (100%)	0	100	100
2	K	186/204 (91%)	186 (100%)	0	100	100
3	F	195/212 (92%)	195 (100%)	0	100	100
3	I	195/212 (92%)	193 (99%)	2 (1%)	73	82
3	L	195/212 (92%)	194 (100%)	1 (0%)	86	90
All	All	3838/4479 (86%)	3817 (100%)	21 (0%)	85	90

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	129	LYS
1	E	928	ASN
3	L	130	GLN
3	I	114	ARG
1	E	558	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1036	GLN
1	E	439	ASN
2	H	6	GLN
1	E	121	ASN
1	E	644	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

79 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	B	1	1,4	14,14,15	0.19	0	17,19,21	0.53	0
4	NAG	B	2	4	14,14,15	0.24	0	17,19,21	0.59	0
4	FUC	B	3	4	10,10,11	0.63	0	14,14,16	0.88	0
5	NAG	G	1	5,1	14,14,15	0.29	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	G	2	5	14,14,15	0.30	0	17,19,21	0.39	0
6	NAG	J	1	1,6	14,14,15	0.23	0	17,19,21	0.36	0
6	NAG	J	2	6	14,14,15	0.19	0	17,19,21	0.46	0
6	BMA	J	3	6	11,11,12	0.47	0	15,15,17	0.82	0
6	MAN	J	4	6	11,11,12	0.77	1 (9%)	15,15,17	1.25	2 (13%)
7	NAG	M	1	7,1	14,14,15	0.92	1 (7%)	17,19,21	1.29	1 (5%)
7	NAG	M	2	7	14,14,15	0.90	1 (7%)	17,19,21	1.25	1 (5%)
7	BMA	M	3	7	11,11,12	0.53	0	15,15,17	0.86	0
5	NAG	N	1	5,1	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	N	2	5	14,14,15	0.32	0	17,19,21	1.32	2 (11%)
5	NAG	O	1	5,1	14,14,15	0.77	1 (7%)	17,19,21	0.66	0
5	NAG	O	2	5	14,14,15	0.40	0	17,19,21	1.30	2 (11%)
5	NAG	P	1	5,1	14,14,15	0.44	0	17,19,21	0.45	0
5	NAG	P	2	5	14,14,15	0.23	0	17,19,21	0.52	0
7	NAG	Q	1	7,1	14,14,15	0.37	0	17,19,21	0.61	0
7	NAG	Q	2	7	14,14,15	0.52	0	17,19,21	1.24	1 (5%)
7	BMA	Q	3	7	11,11,12	0.59	0	15,15,17	0.74	0
5	NAG	R	1	5,1	14,14,15	0.47	0	17,19,21	0.94	1 (5%)
5	NAG	R	2	5	14,14,15	0.26	0	17,19,21	0.43	0
8	NAG	S	1	8,1	14,14,15	0.28	0	17,19,21	0.49	0
8	NAG	S	2	8	14,14,15	0.39	0	17,19,21	0.92	1 (5%)
8	BMA	S	3	8	11,11,12	0.65	0	15,15,17	0.80	1 (6%)
8	MAN	S	4	8	11,11,12	0.57	0	15,15,17	1.07	2 (13%)
8	MAN	S	5	8	11,11,12	0.61	0	15,15,17	1.10	2 (13%)
5	NAG	T	1	5,1	14,14,15	0.36	0	17,19,21	0.39	0
5	NAG	T	2	5	14,14,15	0.41	0	17,19,21	1.24	1 (5%)
9	NAG	U	1	1,9	14,14,15	0.30	0	17,19,21	0.64	0
9	NAG	U	2	9	14,14,15	0.26	0	17,19,21	0.59	0
9	BMA	U	3	9	11,11,12	0.61	0	15,15,17	0.98	1 (6%)
9	MAN	U	4	9	11,11,12	0.61	0	15,15,17	1.19	2 (13%)
9	MAN	U	5	9	11,11,12	0.62	0	15,15,17	1.61	5 (33%)
5	NAG	V	1	5,1	14,14,15	0.56	0	17,19,21	0.53	0
5	NAG	V	2	5	14,14,15	0.24	0	17,19,21	0.41	0
8	NAG	W	1	8,1	14,14,15	0.16	0	17,19,21	0.69	0
8	NAG	W	2	8	14,14,15	0.26	0	17,19,21	0.39	0
8	BMA	W	3	8	11,11,12	0.74	1 (9%)	15,15,17	1.19	1 (6%)
8	MAN	W	4	8	11,11,12	0.94	1 (9%)	15,15,17	1.09	3 (20%)
8	MAN	W	5	8	11,11,12	0.64	0	15,15,17	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	X	1	5,1	14,14,15	0.66	1 (7%)	17,19,21	0.60	0
5	NAG	X	2	5	14,14,15	0.42	0	17,19,21	1.24	1 (5%)
6	NAG	Y	1	1,6	14,14,15	0.69	0	17,19,21	1.22	3 (17%)
6	NAG	Y	2	6	14,14,15	0.90	0	17,19,21	2.81	8 (47%)
6	BMA	Y	3	6	11,11,12	0.62	0	15,15,17	2.15	7 (46%)
6	MAN	Y	4	6	11,11,12	0.56	0	15,15,17	1.21	2 (13%)
7	NAG	Z	1	7,1	14,14,15	0.54	0	17,19,21	0.60	0
7	NAG	Z	2	7	14,14,15	0.23	0	17,19,21	0.62	0
7	BMA	Z	3	7	11,11,12	0.61	0	15,15,17	0.74	0
10	NAG	a	1	1,10	14,14,15	0.30	0	17,19,21	0.64	1 (5%)
10	NAG	a	2	10	14,14,15	0.55	0	17,19,21	1.31	1 (5%)
10	BMA	a	3	10	11,11,12	0.49	0	15,15,17	0.83	0
10	FUC	a	4	10	10,10,11	0.64	0	14,14,16	0.79	0
4	NAG	b	1	1,4	14,14,15	0.87	1 (7%)	17,19,21	0.80	0
4	NAG	b	2	4	14,14,15	0.19	0	17,19,21	0.47	0
4	FUC	b	3	4	10,10,11	0.75	0	14,14,16	1.00	0
11	NAG	c	1	1,11	14,14,15	0.20	0	17,19,21	0.48	0
11	FUC	c	2	11	10,10,11	0.65	0	14,14,16	0.82	0
12	NAG	d	1	1,12	14,14,15	0.49	0	17,19,21	0.87	1 (5%)
12	NAG	d	2	12	14,14,15	0.28	0	17,19,21	0.50	0
12	BMA	d	3	12	11,11,12	0.95	0	15,15,17	1.19	2 (13%)
12	MAN	d	4	12	11,11,12	1.06	2 (18%)	15,15,17	1.63	2 (13%)
12	NAG	d	5	12	14,14,15	0.25	0	17,19,21	0.36	0
12	MAN	d	6	12	11,11,12	0.60	0	15,15,17	1.17	2 (13%)
7	NAG	e	1	7,1	14,14,15	0.64	0	17,19,21	1.01	1 (5%)
7	NAG	e	2	7	14,14,15	0.29	0	17,19,21	0.41	0
7	BMA	e	3	7	11,11,12	0.50	0	15,15,17	0.96	1 (6%)
13	NAG	f	1	13,1	14,14,15	0.43	0	17,19,21	0.95	2 (11%)
13	NAG	f	2	13	14,14,15	0.27	0	17,19,21	0.52	0
13	BMA	f	3	13	11,11,12	1.22	2 (18%)	15,15,17	1.61	3 (20%)
13	MAN	f	4	13	11,11,12	0.83	0	15,15,17	1.07	1 (6%)
13	MAN	f	5	13	11,11,12	0.53	0	15,15,17	1.03	2 (13%)
13	MAN	f	6	13	11,11,12	0.88	0	15,15,17	0.98	1 (6%)
10	NAG	g	1	10,2	14,14,15	0.20	0	17,19,21	0.54	0
10	NAG	g	2	10	14,14,15	0.21	0	17,19,21	0.41	0
10	BMA	g	3	10	11,11,12	0.77	1 (9%)	15,15,17	0.91	1 (6%)
10	FUC	g	4	10	10,10,11	0.71	0	14,14,16	0.94	0



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	B	2	4	-	3/6/23/26	0/1/1/1
4	FUC	B	3	4	-	-	0/1/1/1
5	NAG	G	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	4/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
7	NAG	M	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	M	2	7	-	0/6/23/26	0/1/1/1
7	BMA	M	3	7	-	0/2/19/22	0/1/1/1
5	NAG	N	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	5/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	5/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
7	NAG	Q	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	5/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	2/2/19/22	0/1/1/1
5	NAG	R	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	4/6/23/26	0/1/1/1
8	NAG	S	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	S	2	8	-	2/6/23/26	0/1/1/1
8	BMA	S	3	8	-	2/2/19/22	0/1/1/1
8	MAN	S	4	8	-	0/2/19/22	0/1/1/1
8	MAN	S	5	8	-	1/2/19/22	0/1/1/1
5	NAG	T	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	3/6/23/26	0/1/1/1
9	NAG	U	1	1,9	-	3/6/23/26	0/1/1/1
9	NAG	U	2	9	-	2/6/23/26	0/1/1/1
9	BMA	U	3	9	-	2/2/19/22	0/1/1/1
9	MAN	U	4	9	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	U	5	9	-	2/2/19/22	0/1/1/1
5	NAG	V	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	V	2	5	-	2/6/23/26	0/1/1/1
8	NAG	W	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	W	2	8	-	1/6/23/26	0/1/1/1
8	BMA	W	3	8	-	1/2/19/22	0/1/1/1
8	MAN	W	4	8	-	1/2/19/22	0/1/1/1
8	MAN	W	5	8	-	0/2/19/22	0/1/1/1
5	NAG	X	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	4/6/23/26	0/1/1/1
6	NAG	Y	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	5/6/23/26	0/1/1/1
6	BMA	Y	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Y	4	6	-	0/2/19/22	0/1/1/1
7	NAG	Z	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1
7	BMA	Z	3	7	-	0/2/19/22	0/1/1/1
10	NAG	a	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	a	2	10	-	5/6/23/26	0/1/1/1
10	BMA	a	3	10	-	1/2/19/22	0/1/1/1
10	FUC	a	4	10	-	-	0/1/1/1
4	NAG	b	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	FUC	b	3	4	-	-	0/1/1/1
11	NAG	c	1	1,11	-	4/6/23/26	0/1/1/1
11	FUC	c	2	11	-	-	0/1/1/1
12	NAG	d	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	d	2	12	-	3/6/23/26	0/1/1/1
12	BMA	d	3	12	-	2/2/19/22	0/1/1/1
12	MAN	d	4	12	-	1/2/19/22	1/1/1/1
12	NAG	d	5	12	-	1/6/23/26	0/1/1/1
12	MAN	d	6	12	-	0/2/19/22	0/1/1/1
7	NAG	e	1	7,1	-	3/6/23/26	0/1/1/1
7	NAG	e	2	7	-	2/6/23/26	0/1/1/1
7	BMA	e	3	7	-	2/2/19/22	0/1/1/1
13	NAG	f	1	13,1	-	2/6/23/26	0/1/1/1
13	NAG	f	2	13	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BMA	f	3	13	-	0/2/19/22	0/1/1/1
13	MAN	f	4	13	-	2/2/19/22	0/1/1/1
13	MAN	f	5	13	-	1/2/19/22	0/1/1/1
13	MAN	f	6	13	-	2/2/19/22	0/1/1/1
10	NAG	g	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	g	2	10	-	2/6/23/26	0/1/1/1
10	BMA	g	3	10	-	2/2/19/22	0/1/1/1
10	FUC	g	4	10	-	-	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1	NAG	O5-C1	3.32	1.49	1.43
7	M	2	NAG	O5-C1	3.20	1.48	1.43
4	b	1	NAG	O5-C1	-3.00	1.38	1.43
13	f	3	BMA	C1-C2	2.77	1.58	1.52
12	d	4	MAN	C1-C2	2.65	1.58	1.52

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	2	NAG	C1-C2-N2	-6.05	100.15	110.49
6	Y	2	NAG	O3-C3-C2	-5.46	98.16	109.47
7	M	1	NAG	C1-O5-C5	5.09	119.09	112.19
7	M	2	NAG	C1-O5-C5	4.87	118.79	112.19
12	d	4	MAN	C1-O5-C5	4.54	118.35	112.19

There are no chirality outliers.

5 of 145 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Y	1	NAG	C8-C7-N2-C2
6	Y	1	NAG	O7-C7-N2-C2
6	Y	2	NAG	C8-C7-N2-C2
6	Y	2	NAG	O7-C7-N2-C2
7	Z	1	NAG	C4-C5-C6-O6

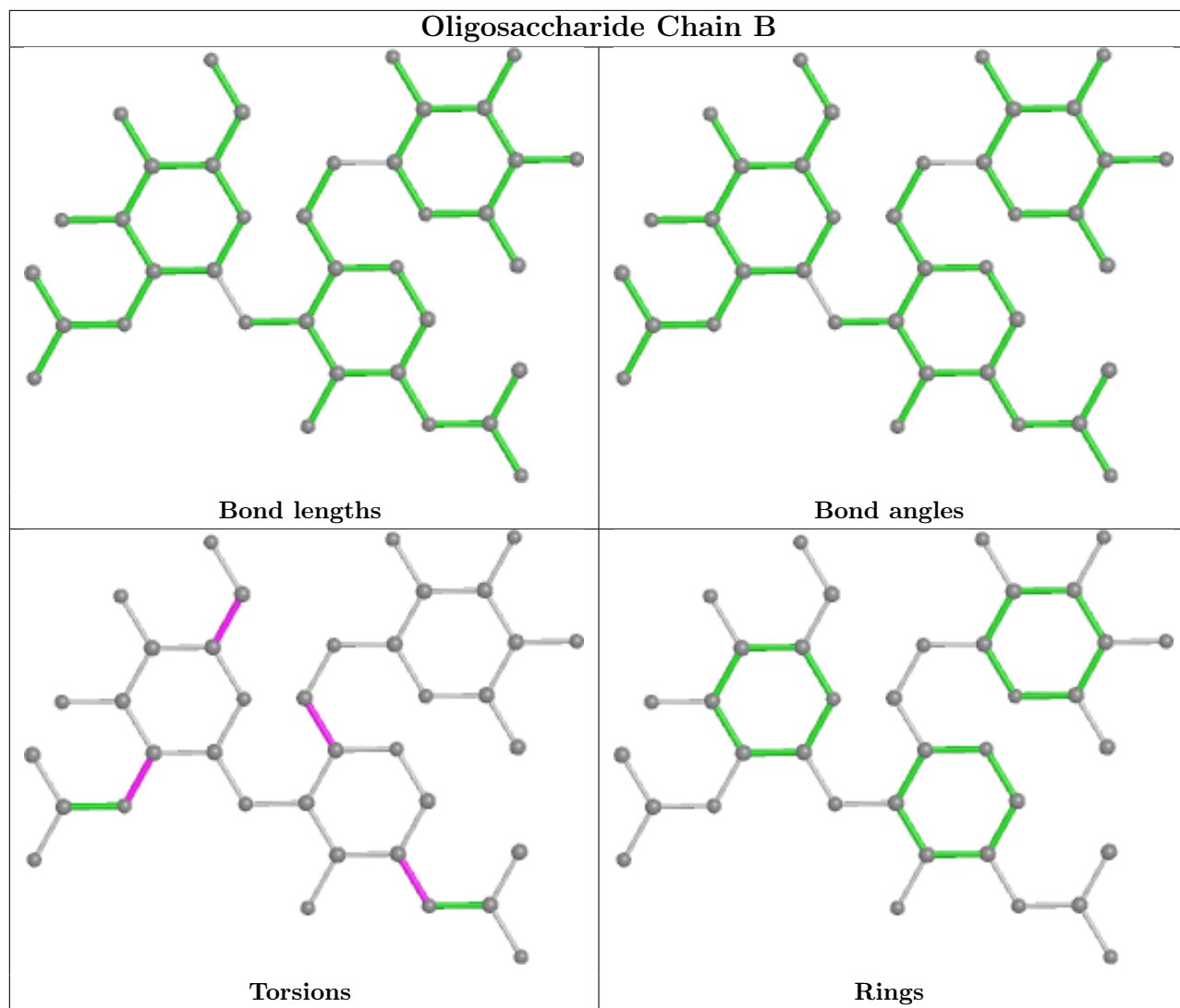
All (1) ring outliers are listed below:

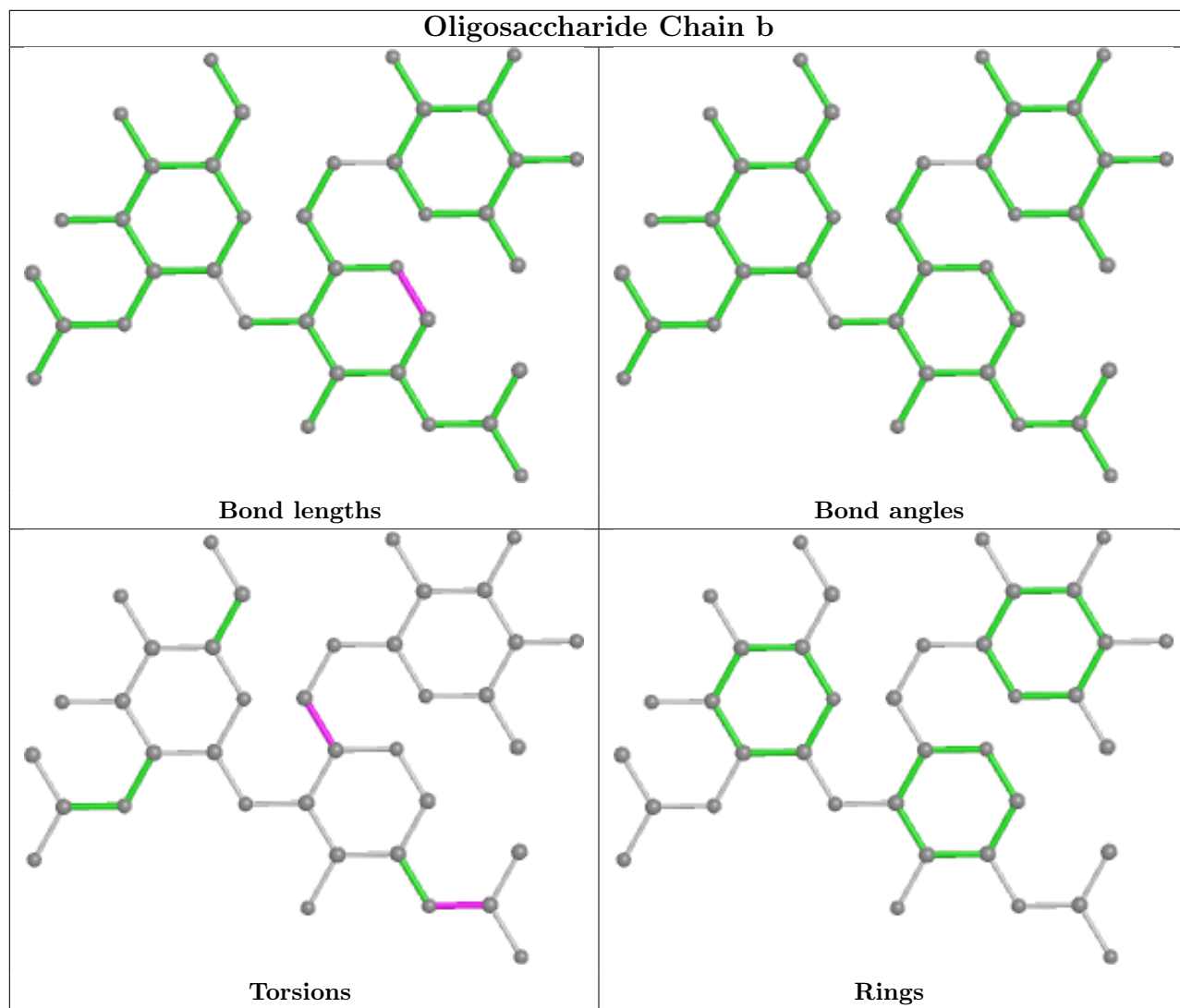
Mol	Chain	Res	Type	Atoms
12	d	4	MAN	C1-C2-C3-C4-C5-O5

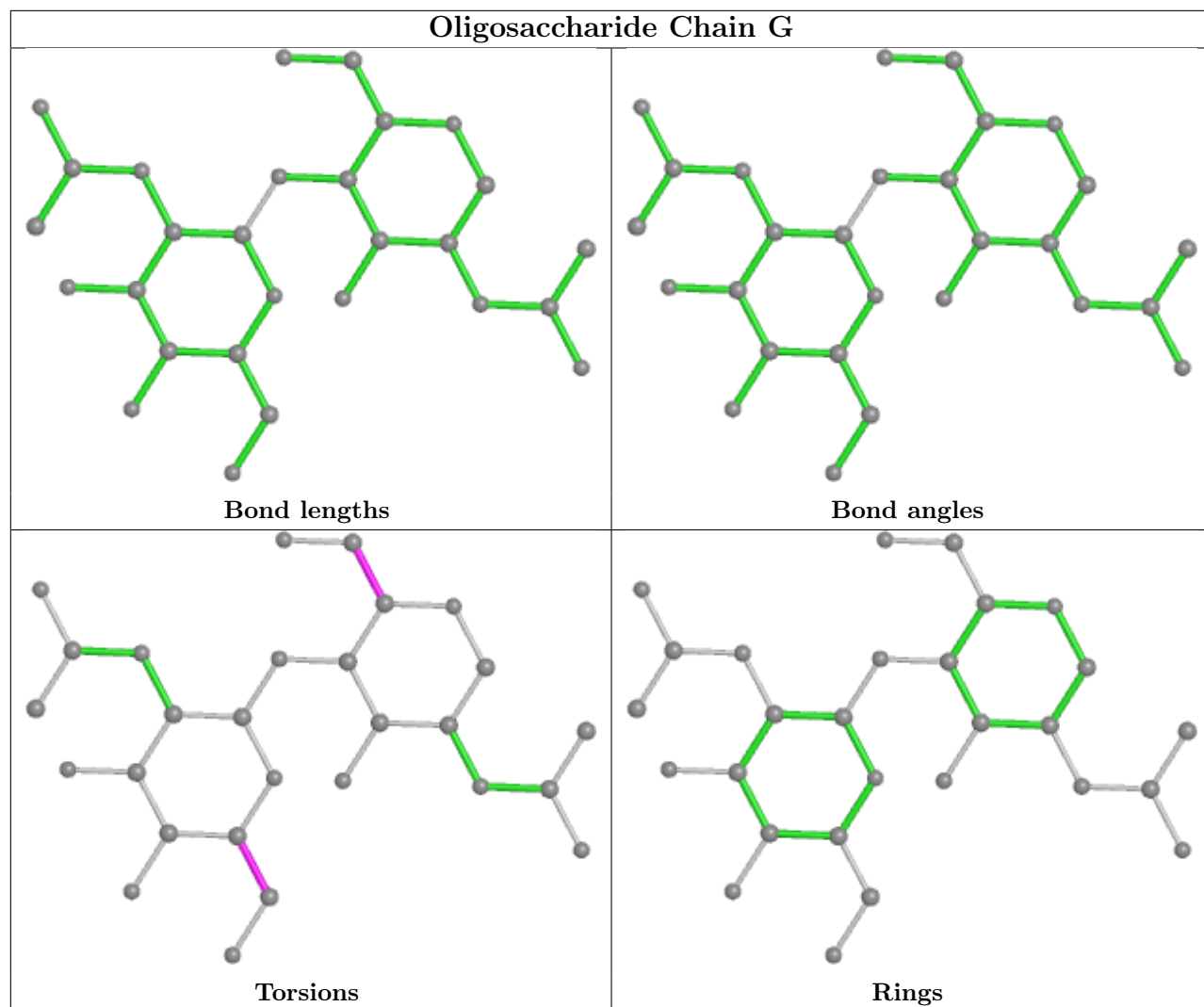
26 monomers are involved in 33 short contacts:

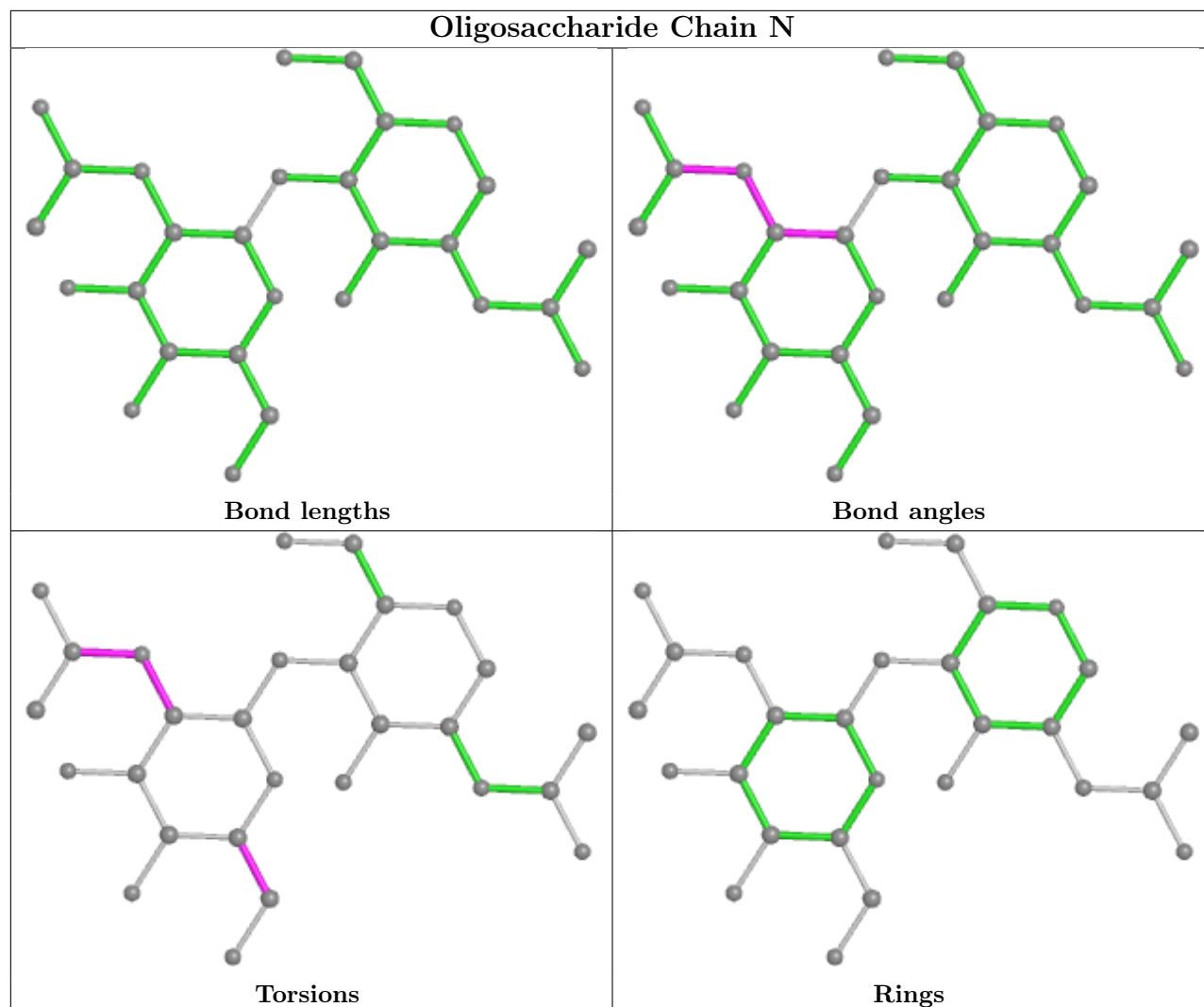
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	1	NAG	5	0
8	S	3	BMA	2	0
5	X	2	NAG	1	0
6	Y	2	NAG	5	0
6	J	2	NAG	1	0
5	N	2	NAG	2	0
5	V	1	NAG	2	0
6	J	3	BMA	1	0
4	B	1	NAG	1	0
4	B	3	FUC	2	0
5	P	2	NAG	1	0
8	W	3	BMA	2	0
6	Y	1	NAG	1	0
9	U	1	NAG	1	0
8	W	2	NAG	1	0
8	S	1	NAG	1	0
5	V	2	NAG	1	0
7	M	1	NAG	2	0
5	T	2	NAG	1	0
5	N	1	NAG	1	0
8	S	2	NAG	3	0
8	W	4	MAN	1	0
7	Q	2	NAG	1	0
5	O	2	NAG	1	0
5	X	1	NAG	1	0
9	U	5	MAN	1	0

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

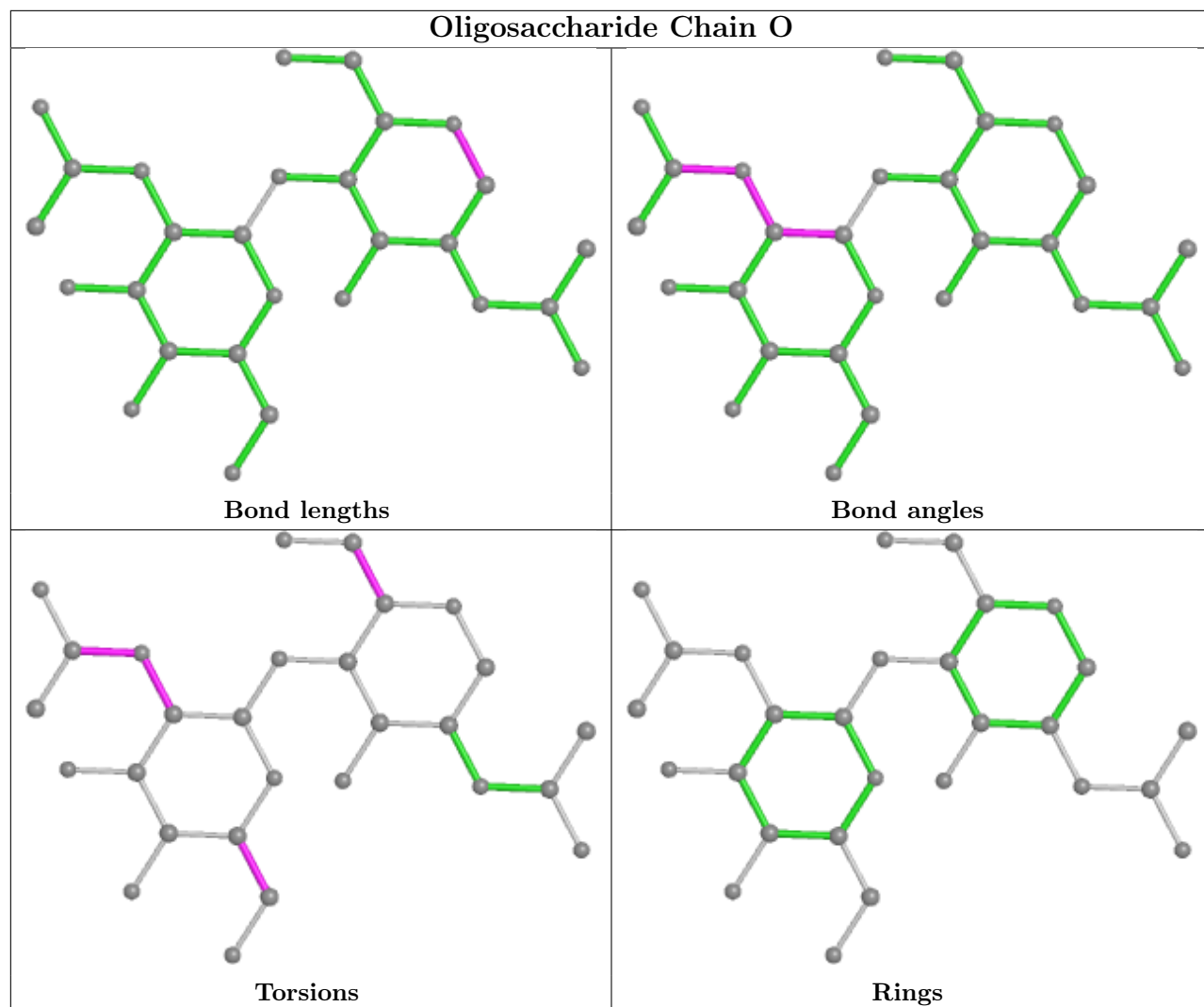


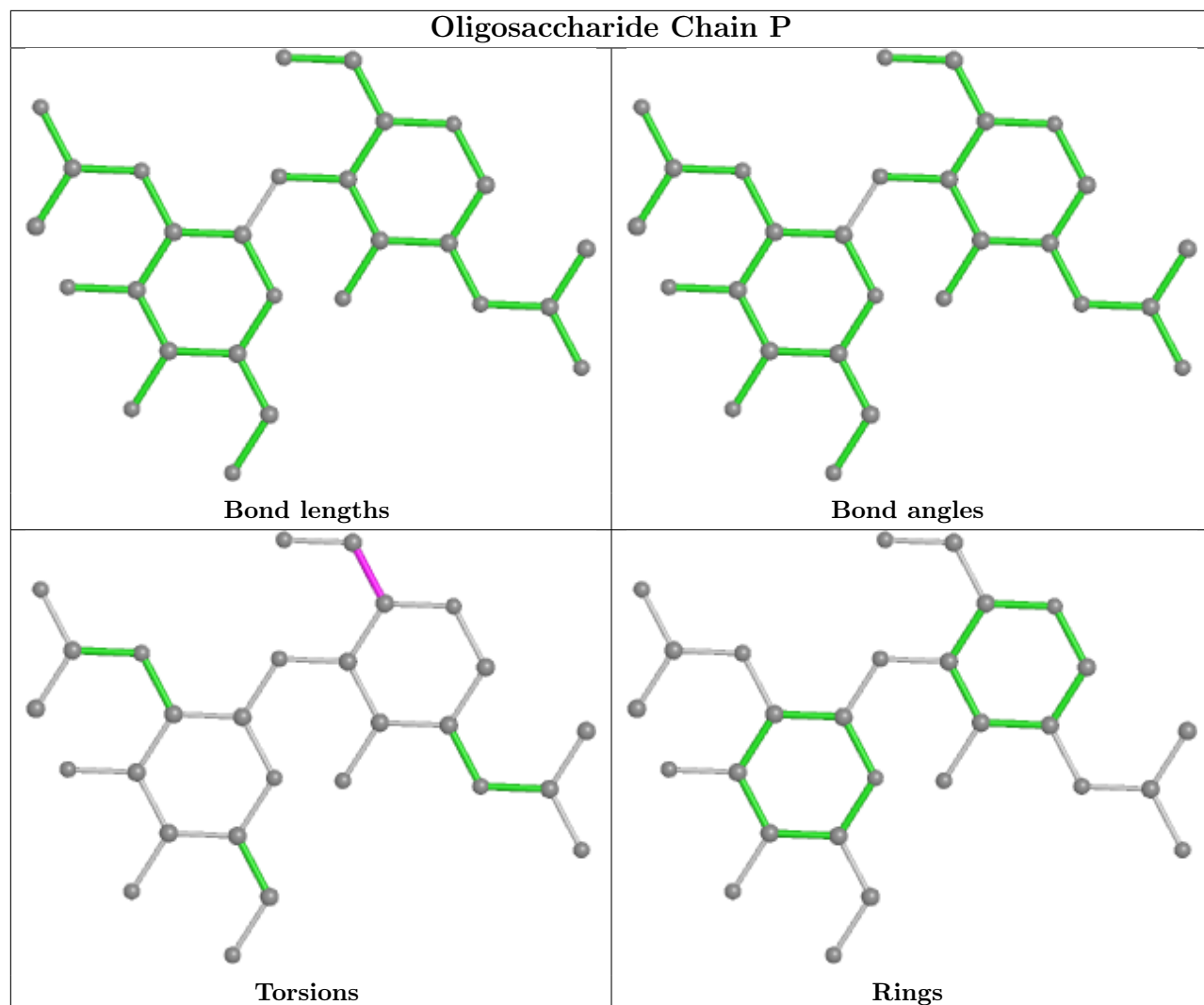


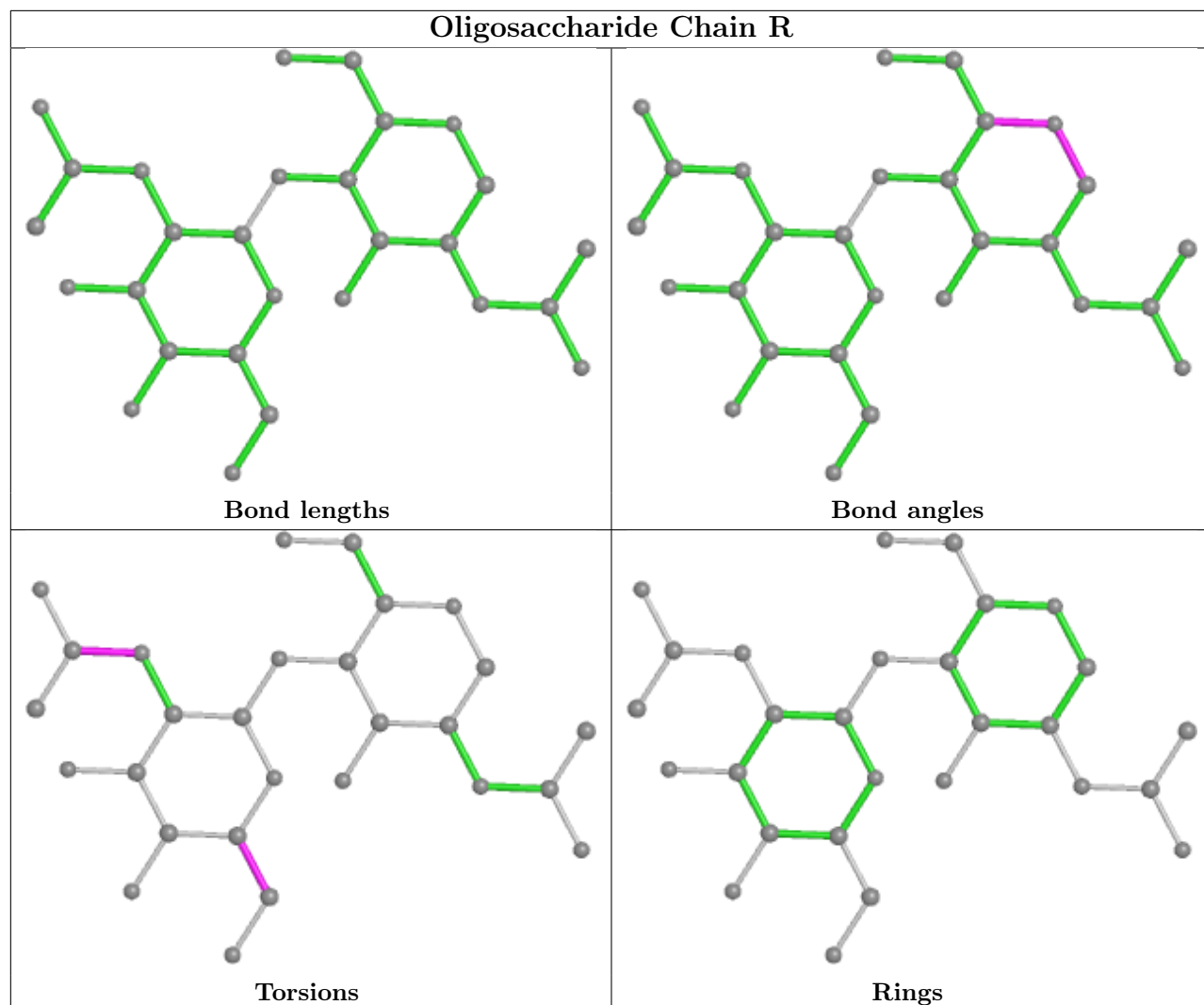


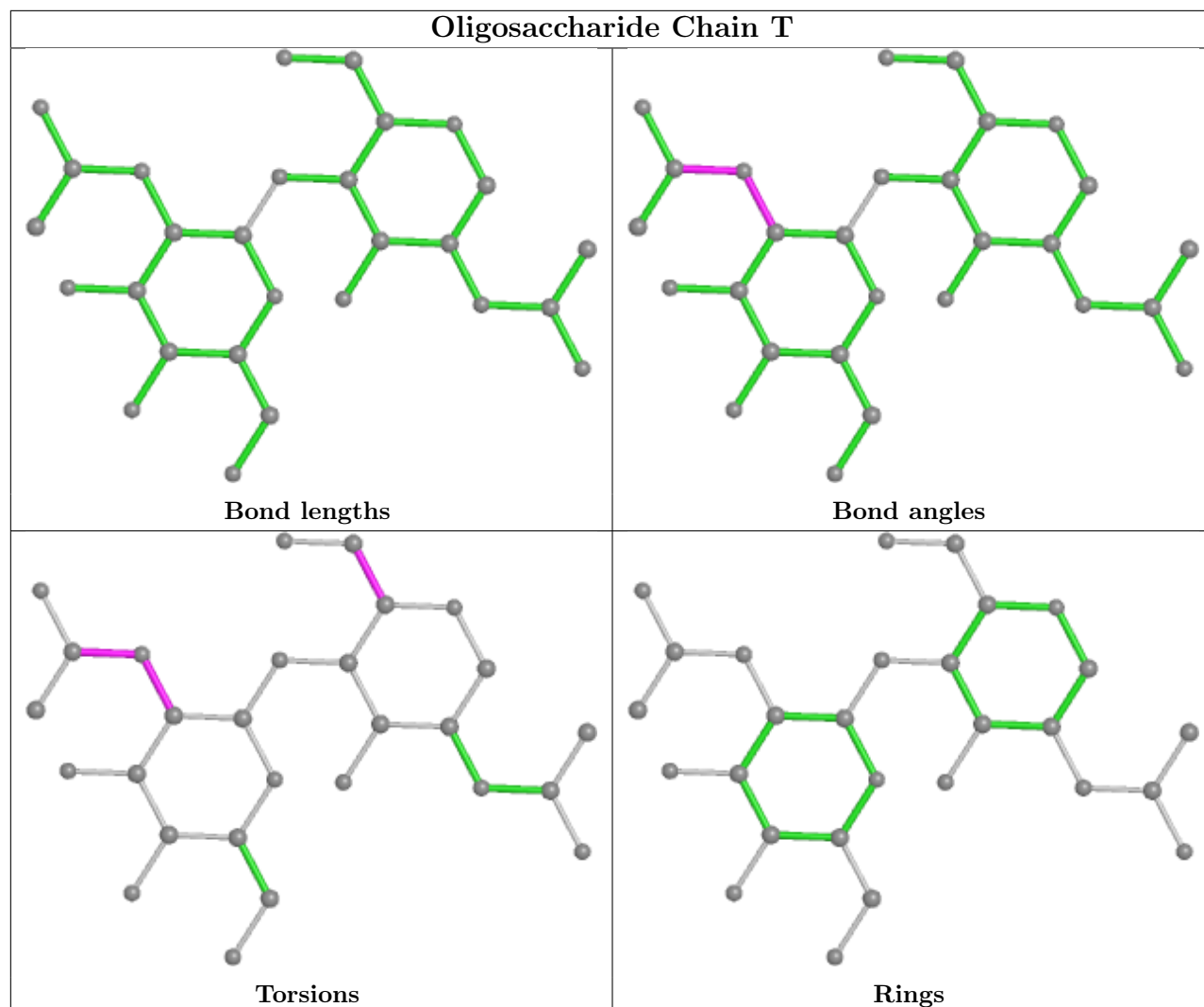


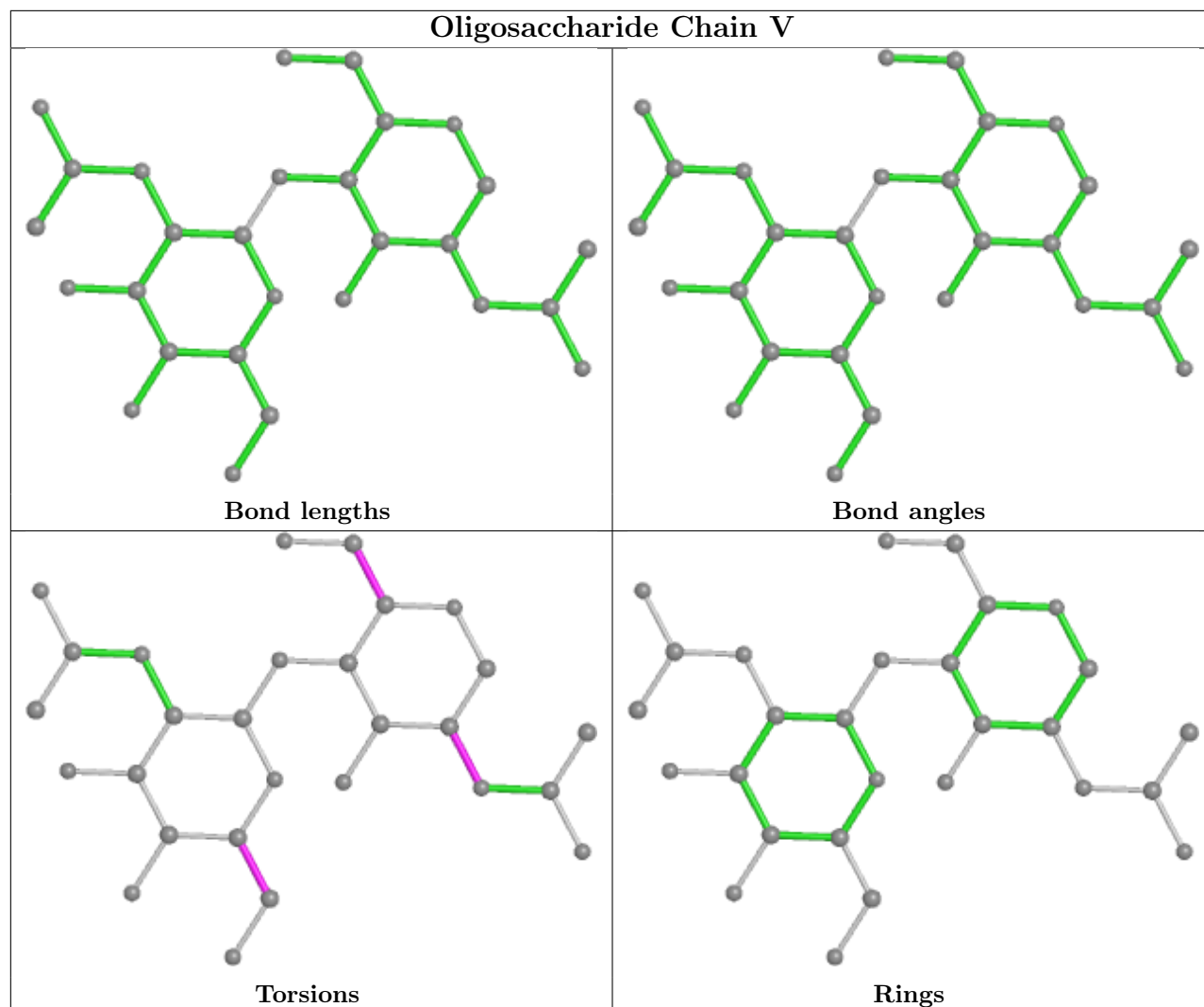


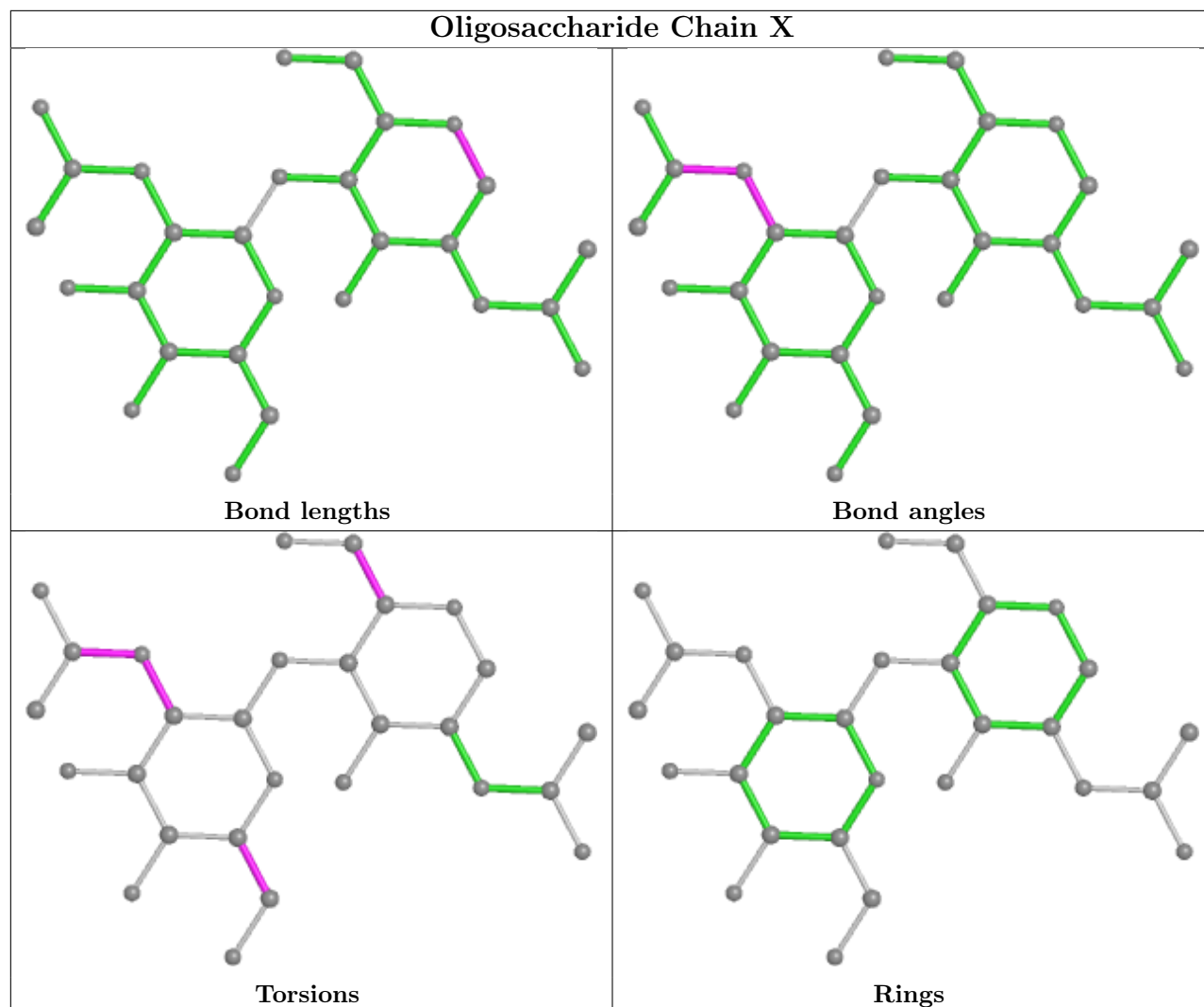


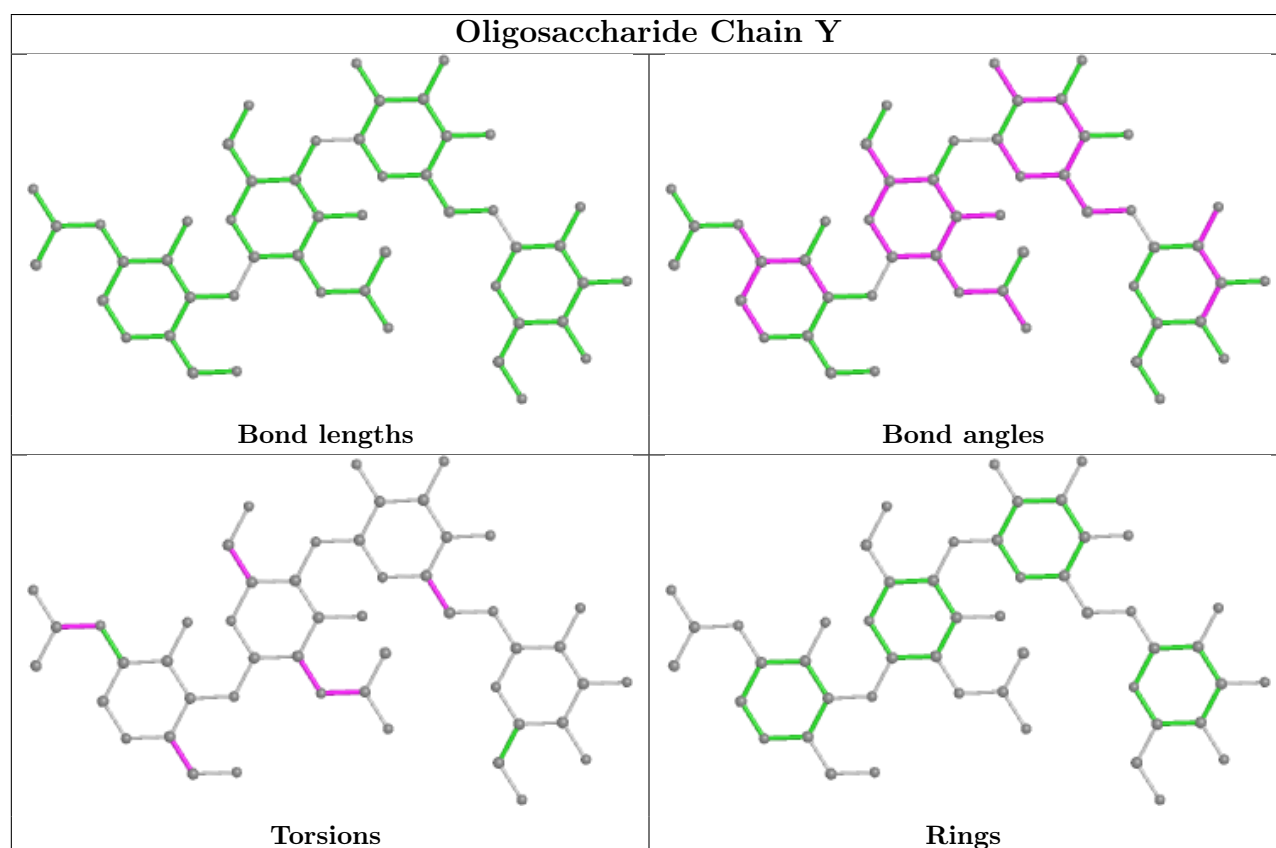
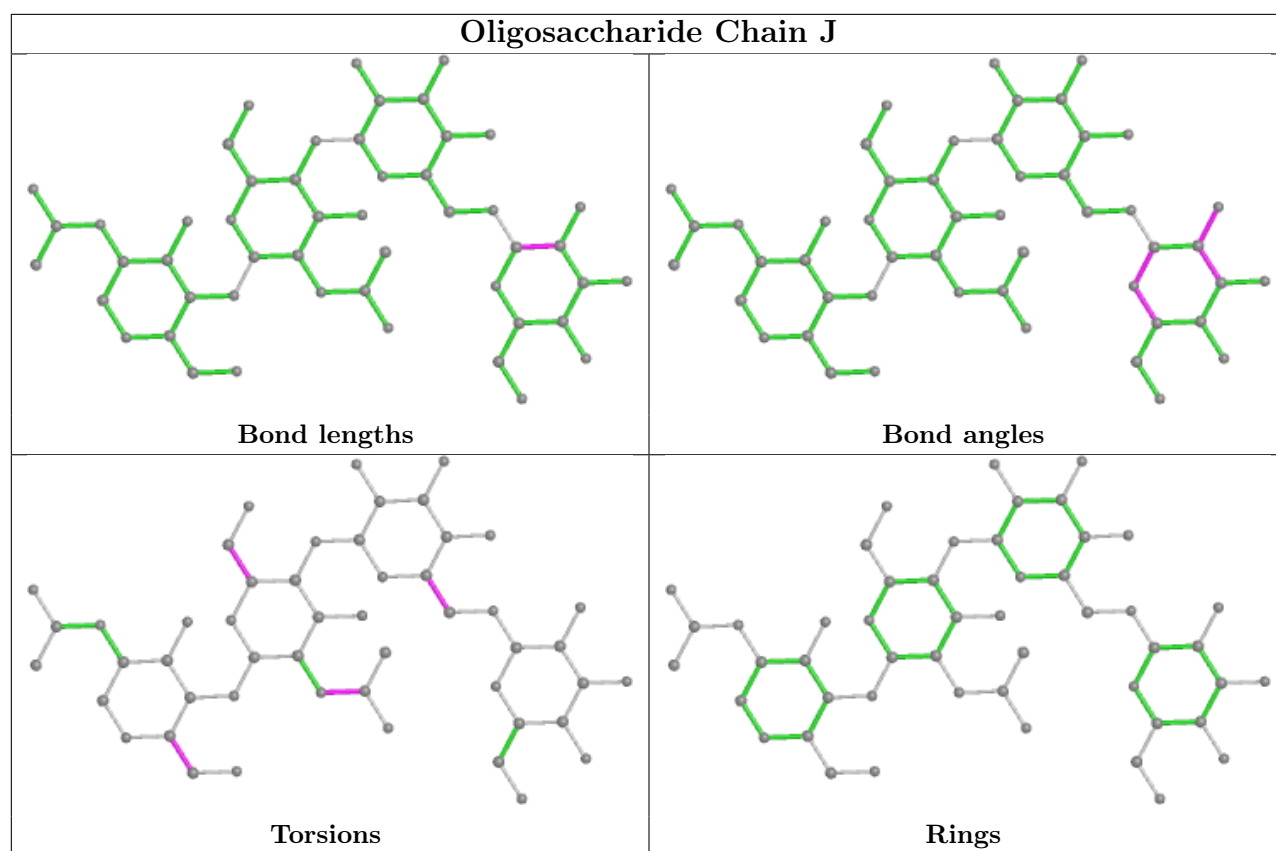


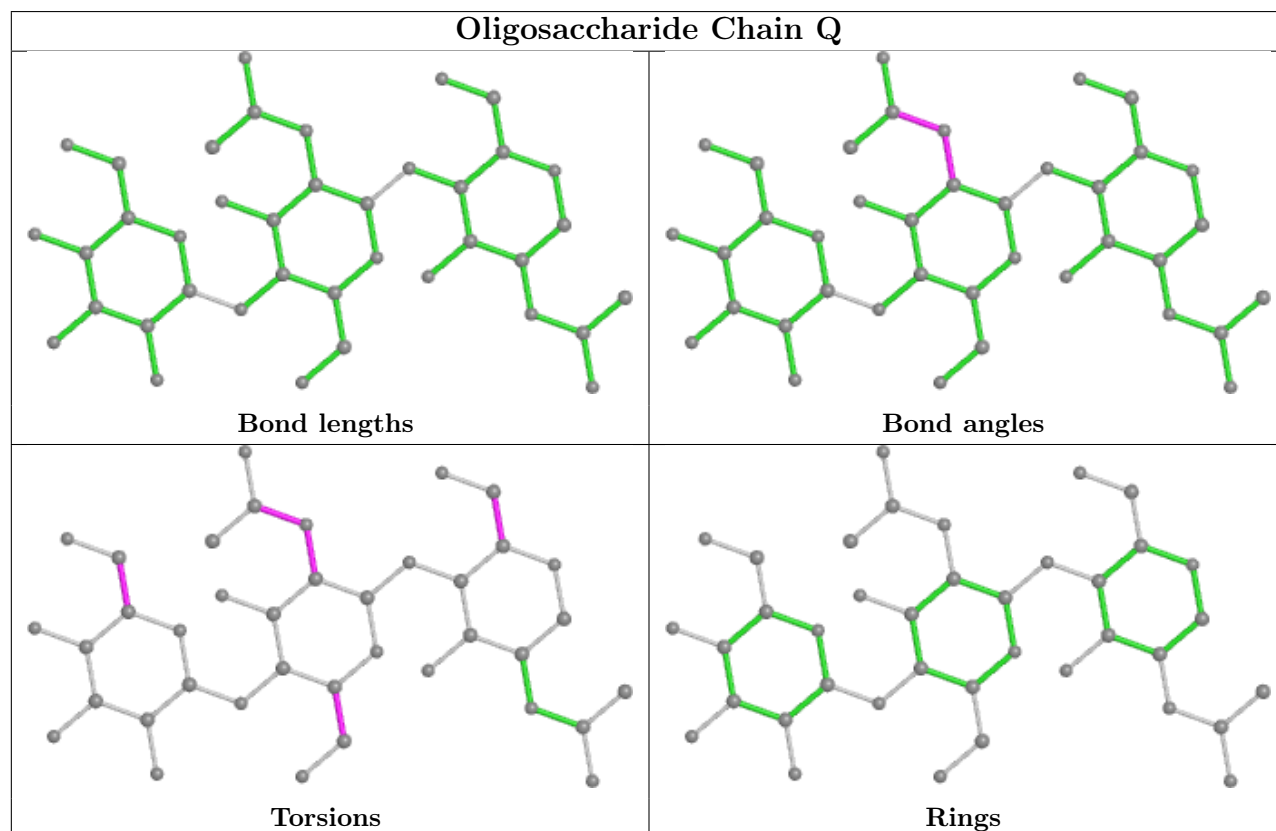
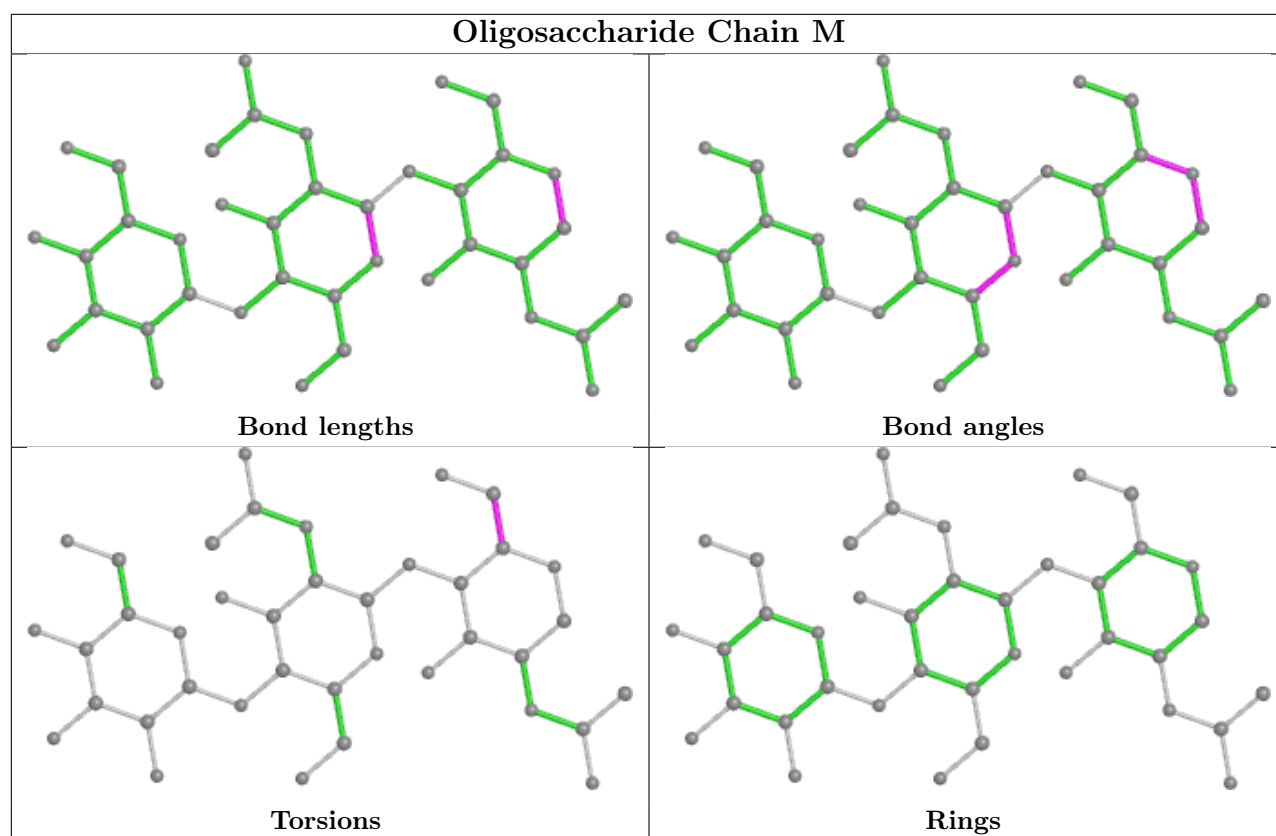




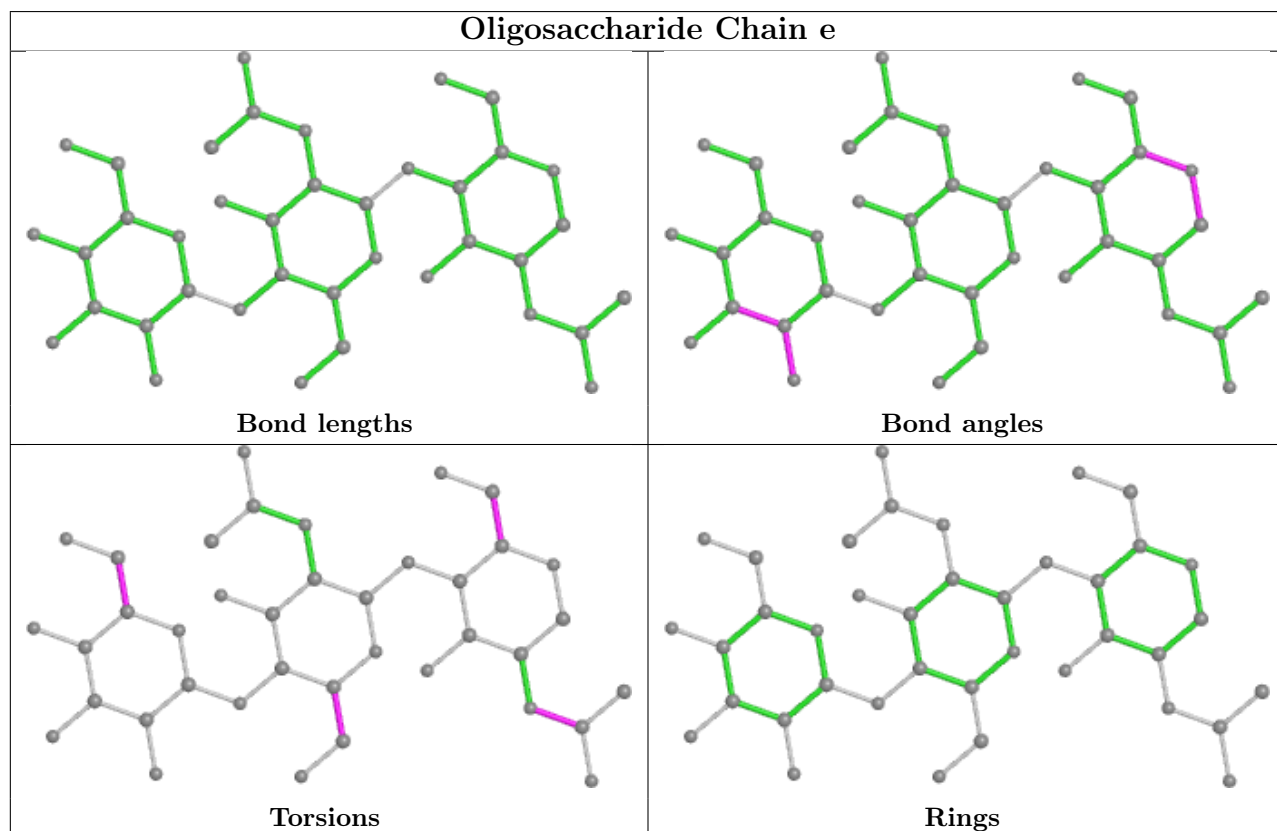
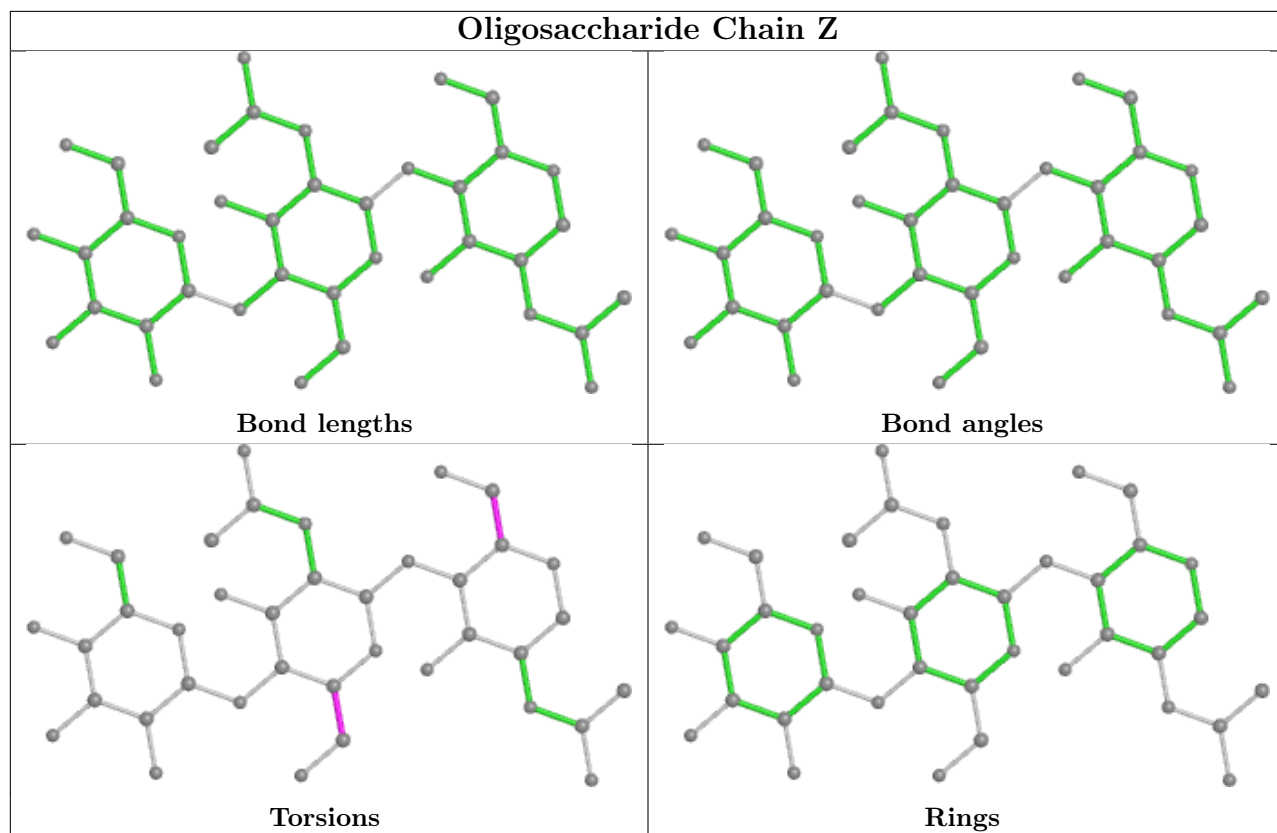


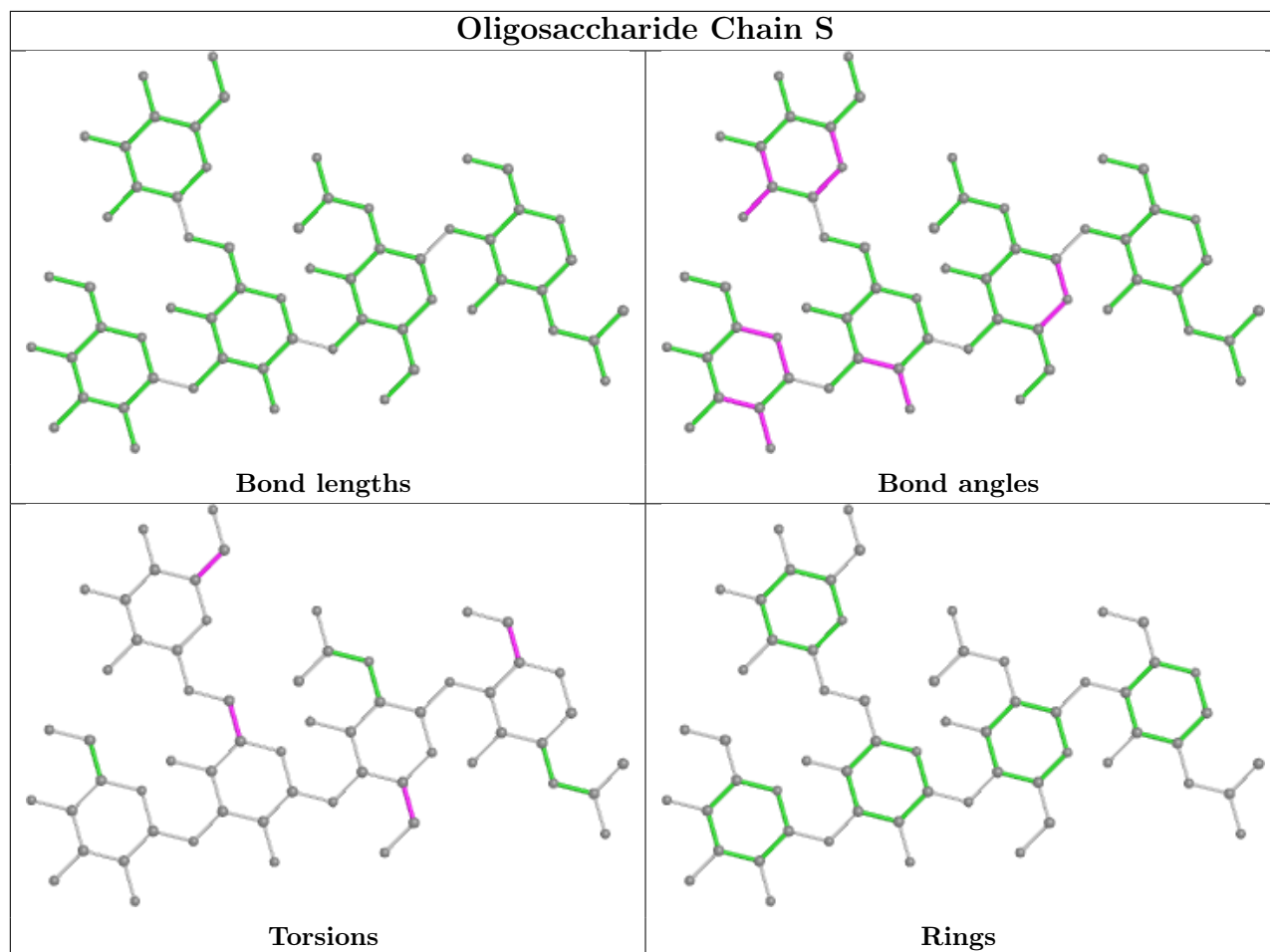


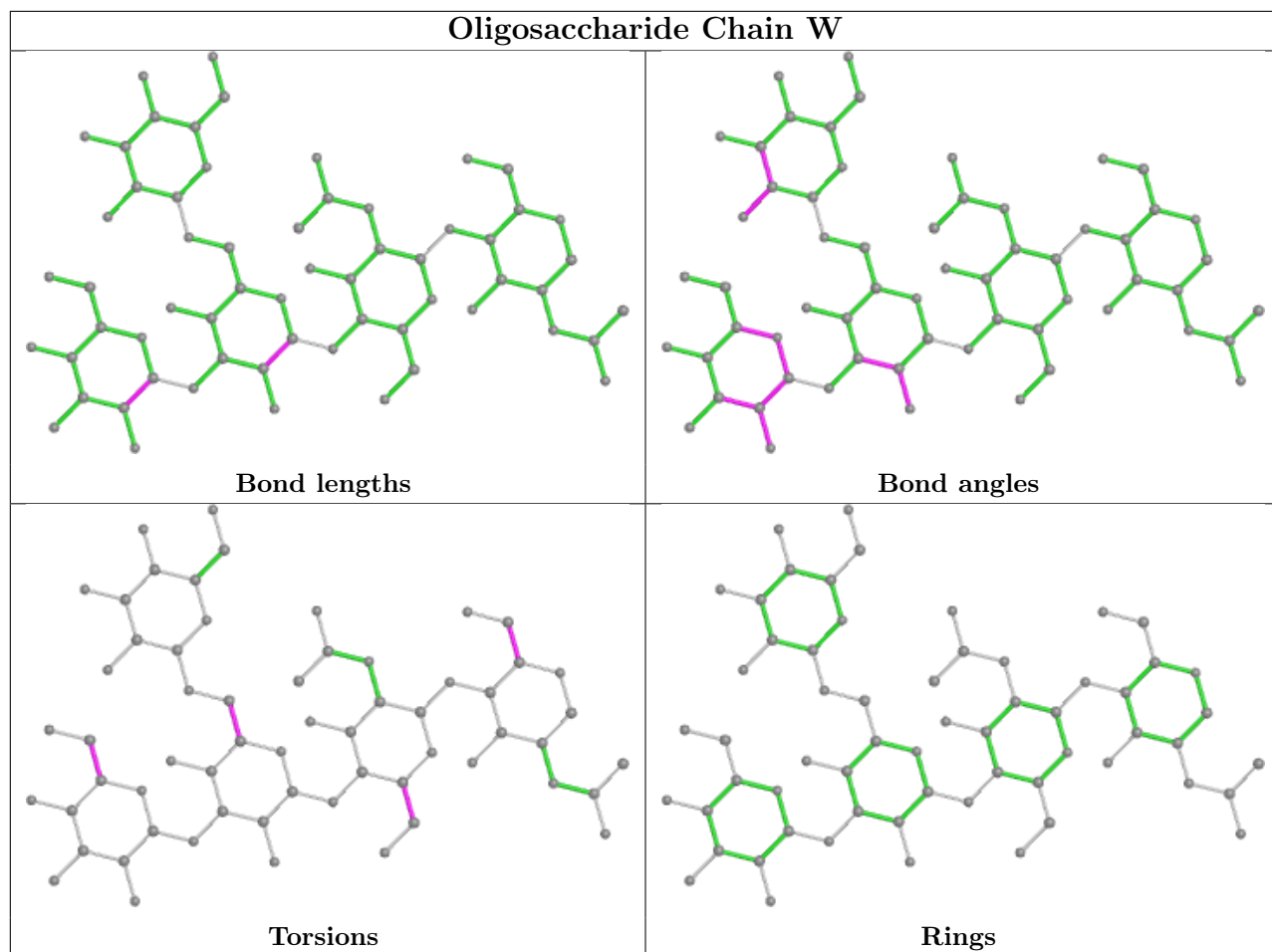


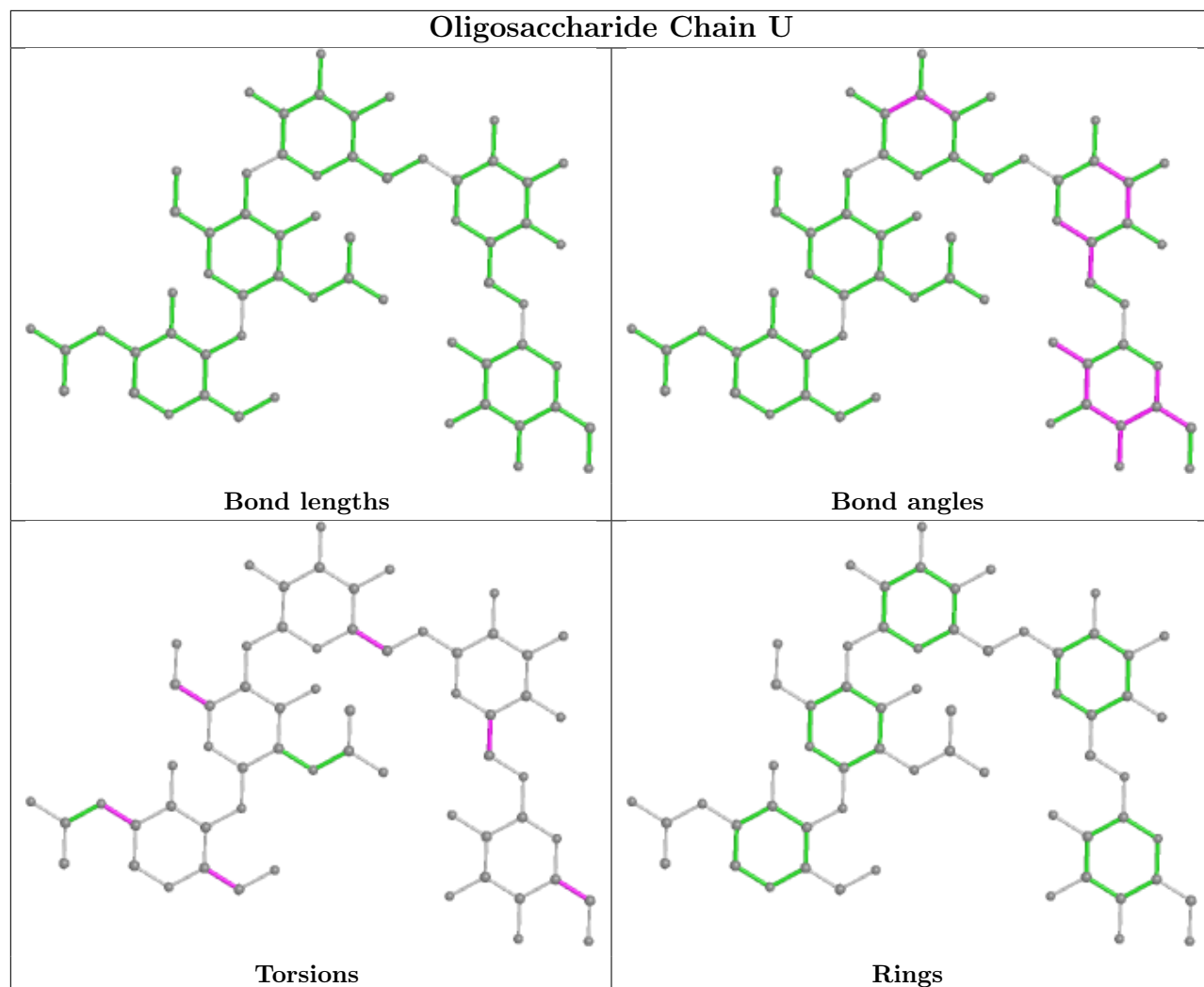


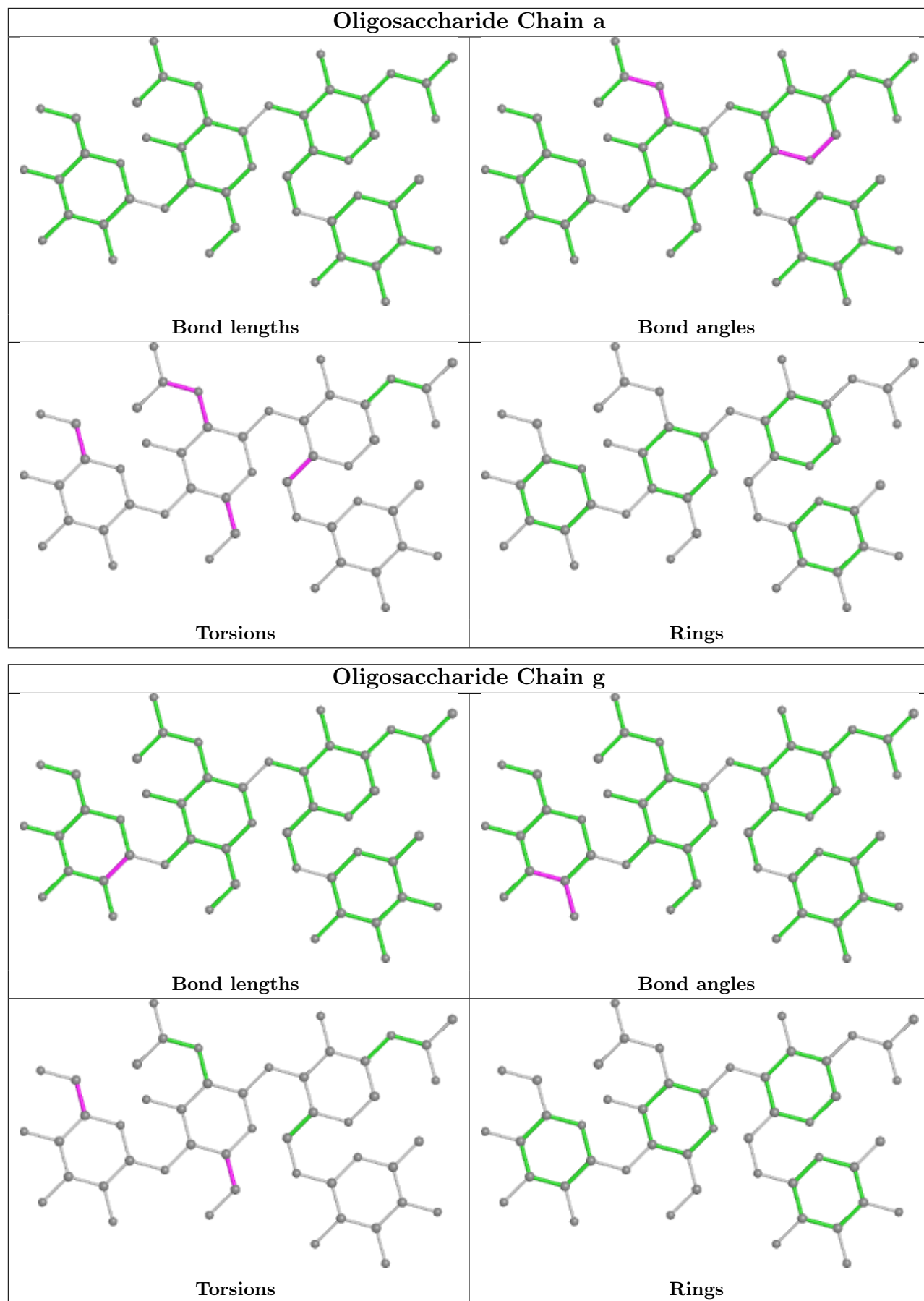


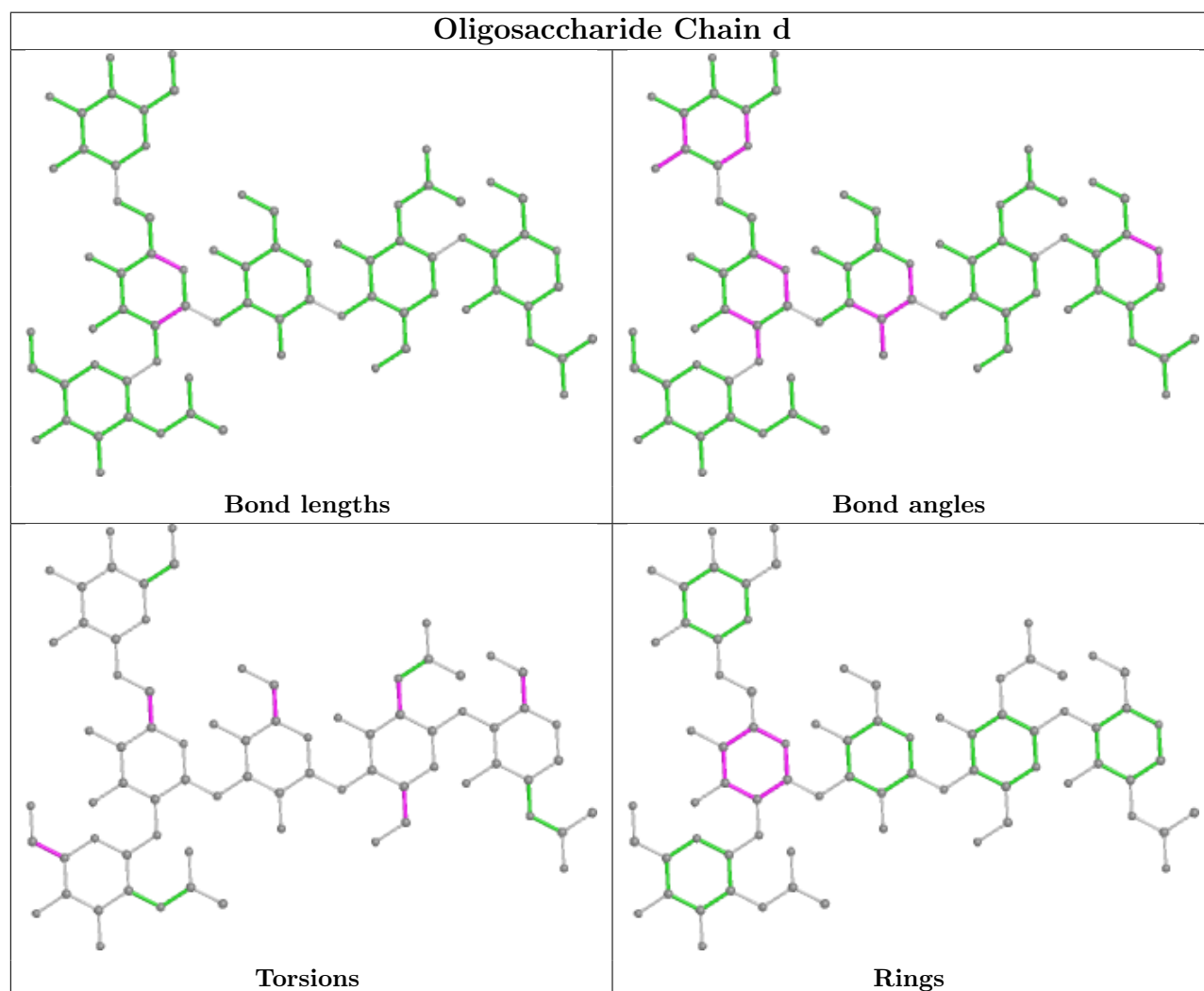
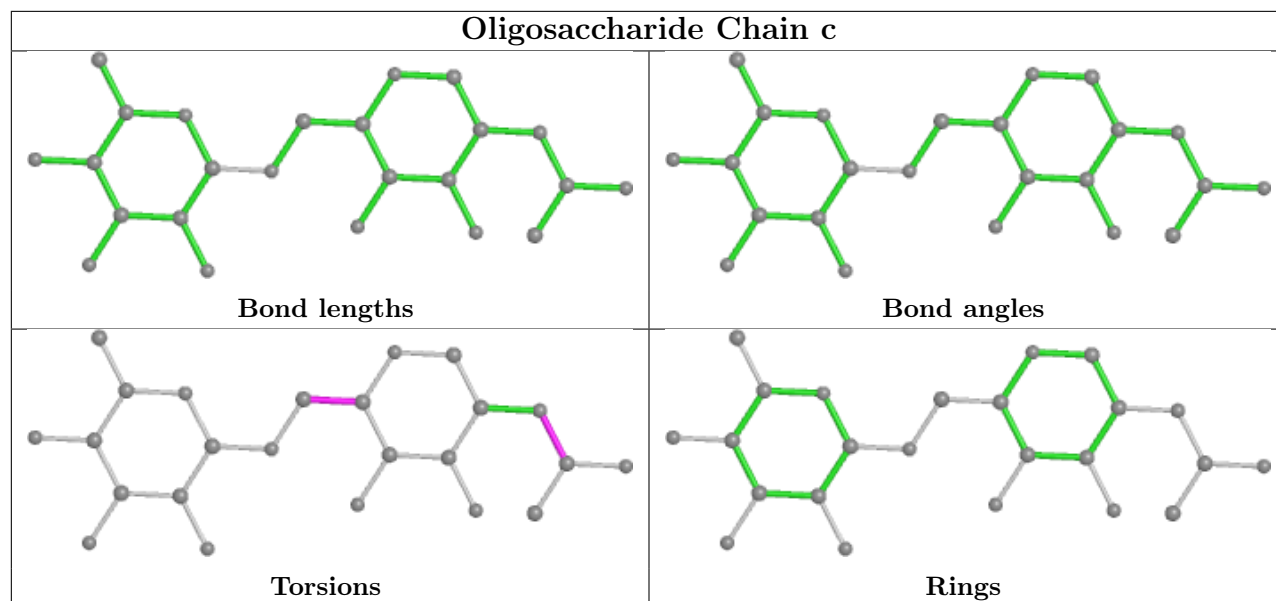


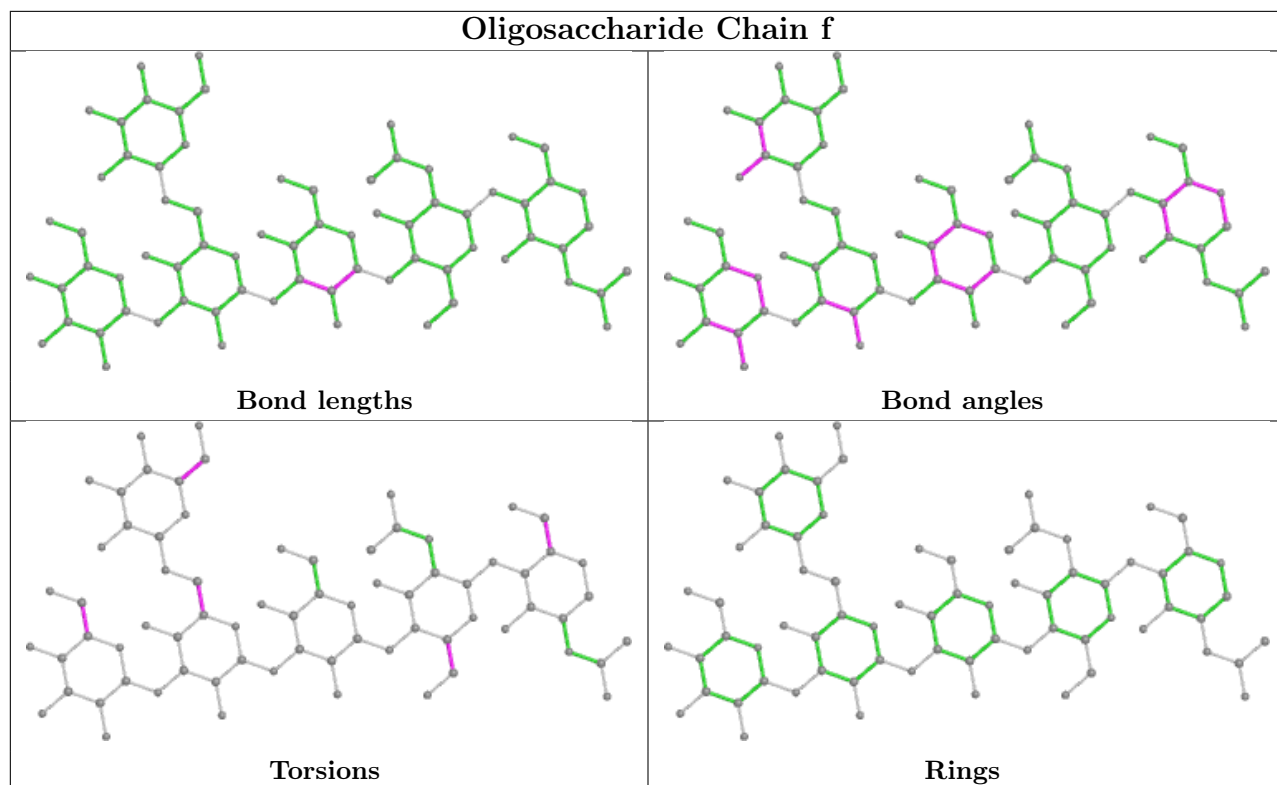












## 5.6 Ligand geometry [i](#)

19 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	$\# Z  > 2$
14	NAG	C	1304	1	14,14,15	0.22	0	17,19,21	0.32	0
14	NAG	C	1306	1	14,14,15	0.32	0	17,19,21	0.37	0
14	NAG	E	1301	1	14,14,15	0.35	0	17,19,21	0.41	0
14	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.35	0
14	NAG	E	1305	1	14,14,15	0.25	0	17,19,21	0.43	0
14	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.40	0
14	NAG	C	1302	1	14,14,15	0.44	0	17,19,21	0.68	1 (5%)
14	NAG	C	1305	1	14,14,15	0.29	0	17,19,21	0.50	0
14	NAG	A	1303	1	14,14,15	0.47	0	17,19,21	0.44	0
14	NAG	A	1304	1	14,14,15	0.48	0	17,19,21	1.16	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	NAG	A	1305	1	14,14,15	0.26	0	17,19,21	0.71	0
14	NAG	C	1307	1	14,14,15	0.24	0	17,19,21	0.51	0
14	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.51	0
14	NAG	C	1301	1	14,14,15	0.25	0	17,19,21	0.57	0
14	NAG	K	301	2	14,14,15	0.19	0	17,19,21	0.39	0
14	NAG	E	1302	1	14,14,15	0.25	0	17,19,21	0.36	0
14	NAG	E	1303	1	14,14,15	0.51	0	17,19,21	0.65	1 (5%)
14	NAG	C	1308	1	14,14,15	0.85	1 (7%)	17,19,21	0.96	1 (5%)
14	NAG	E	1304	1	14,14,15	0.17	0	17,19,21	0.58	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
14	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
14	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
14	NAG	E	1301	1	-	2/6/23/26	0/1/1/1
14	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
14	NAG	E	1305	1	-	2/6/23/26	0/1/1/1
14	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
14	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
14	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
14	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
14	NAG	A	1304	1	-	4/6/23/26	0/1/1/1
14	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
14	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
14	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
14	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
14	NAG	K	301	2	-	2/6/23/26	0/1/1/1
14	NAG	E	1302	1	-	2/6/23/26	0/1/1/1
14	NAG	E	1303	1	-	4/6/23/26	0/1/1/1
14	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
14	NAG	E	1304	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	1308	NAG	O5-C1	2.61	1.47	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	1308	NAG	C1-O5-C5	3.55	117.00	112.19
14	A	1304	NAG	O5-C5-C6	2.26	110.75	107.20
14	A	1304	NAG	C6-C5-C4	-2.19	107.87	113.00
14	E	1303	NAG	C1-O5-C5	2.16	115.12	112.19
14	A	1304	NAG	C2-N2-C7	2.09	125.88	122.90

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	1304	NAG	C8-C7-N2-C2
14	A	1304	NAG	O7-C7-N2-C2
14	A	1305	NAG	C8-C7-N2-C2
14	A	1305	NAG	O7-C7-N2-C2
14	E	1303	NAG	C4-C5-C6-O6

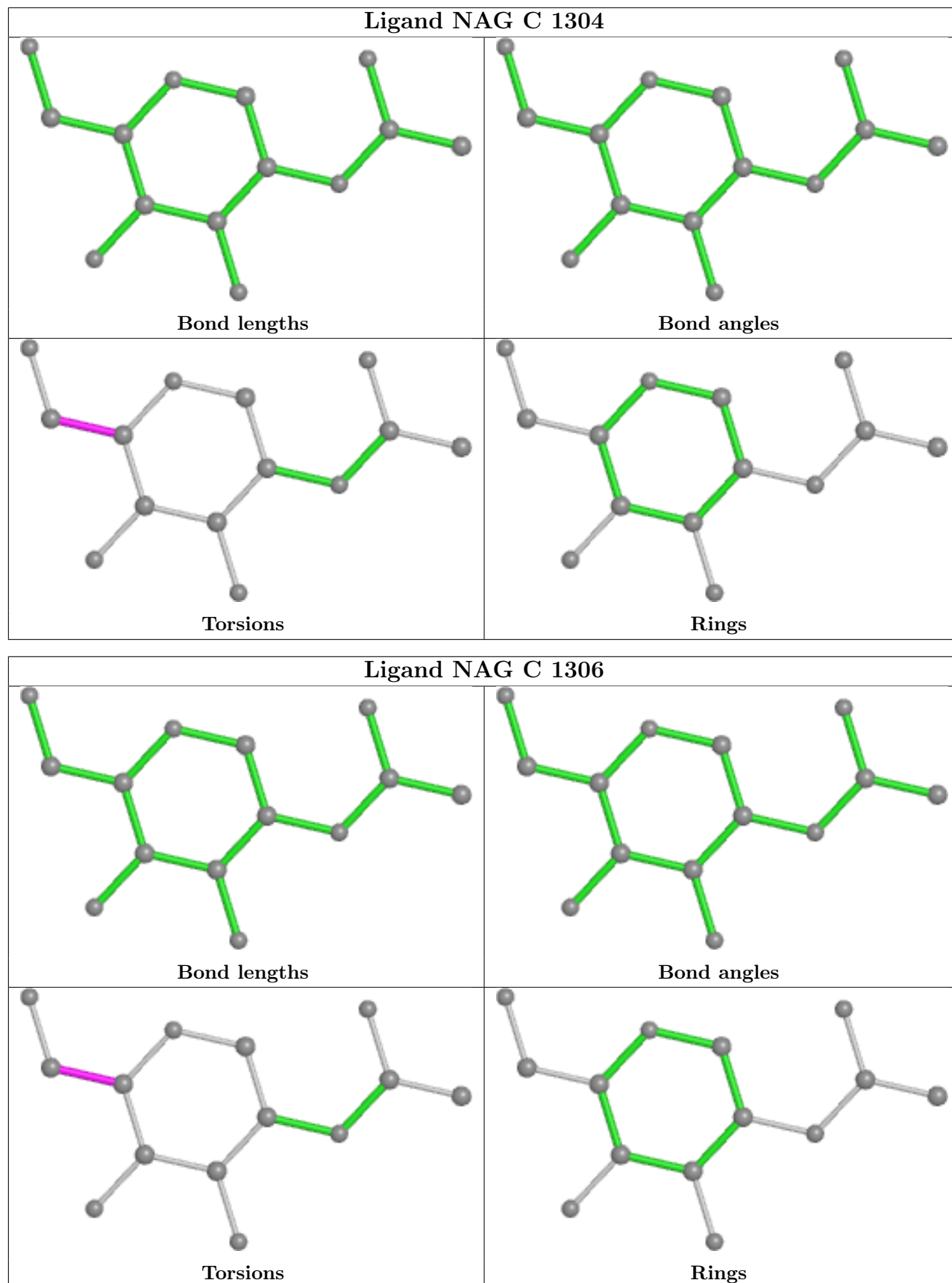
There are no ring outliers.

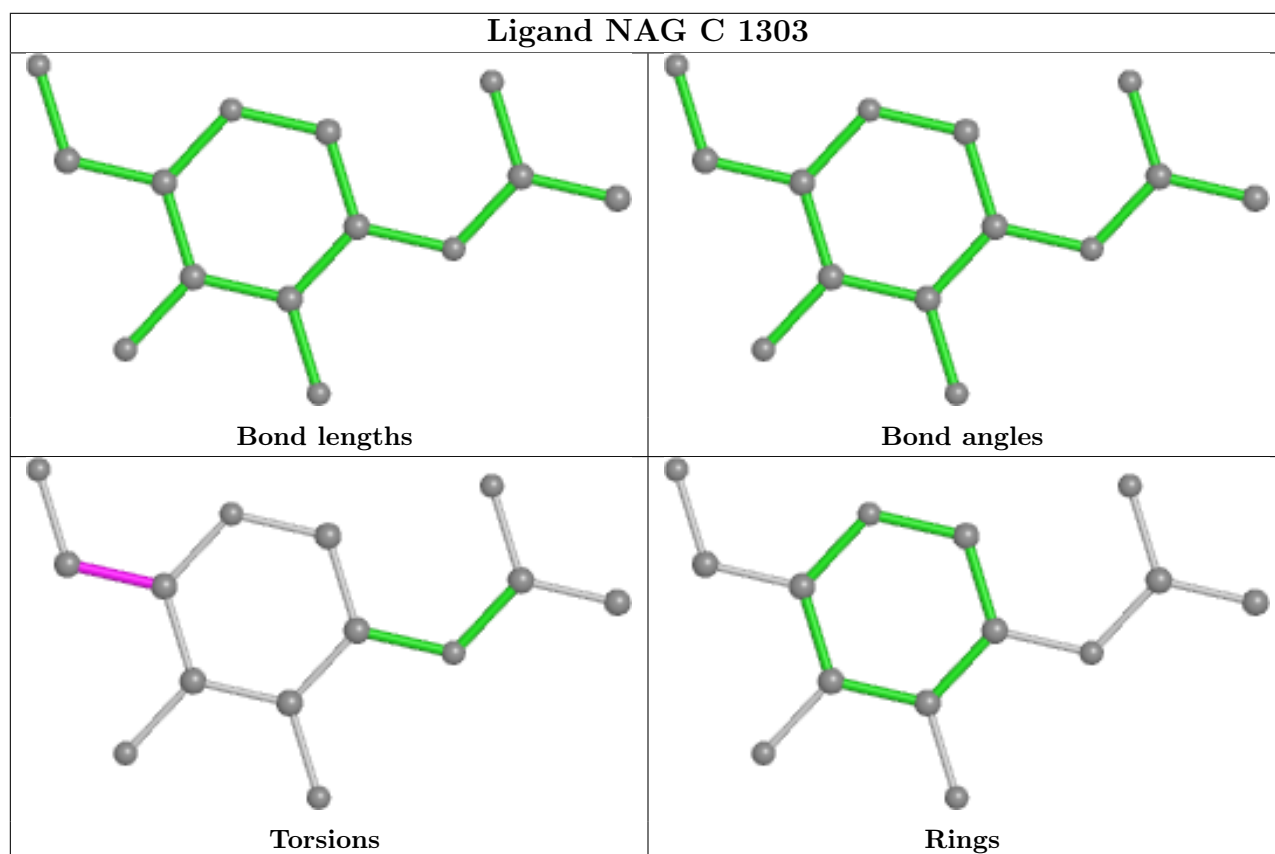
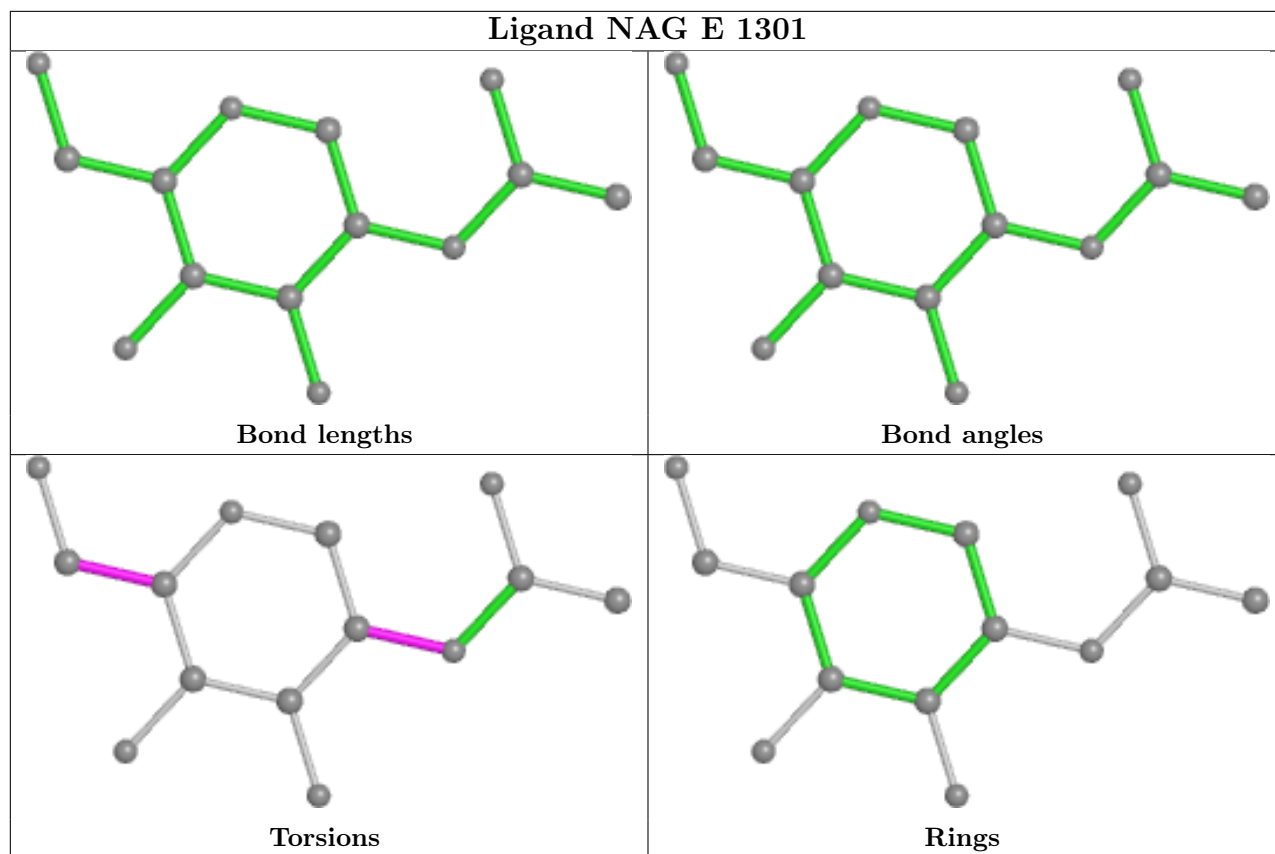
6 monomers are involved in 10 short contacts:

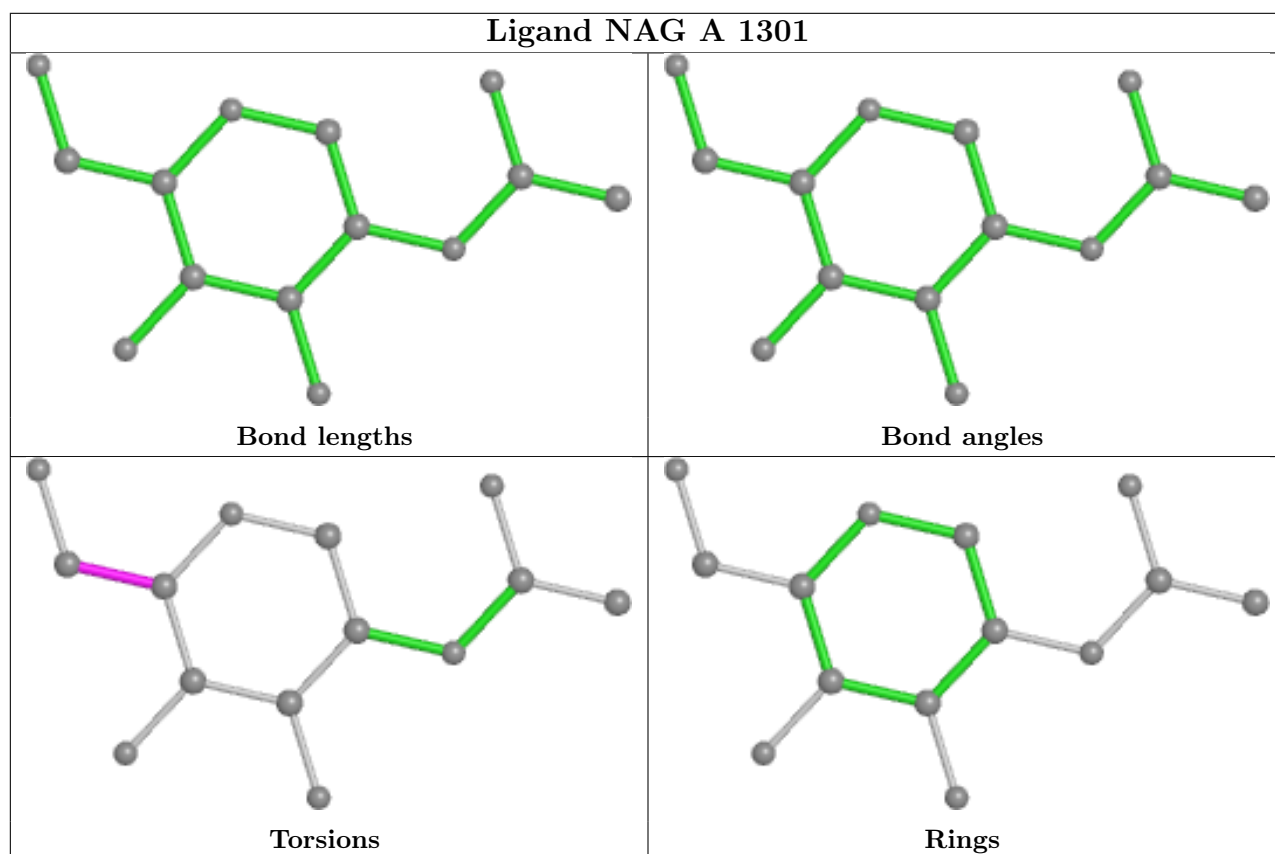
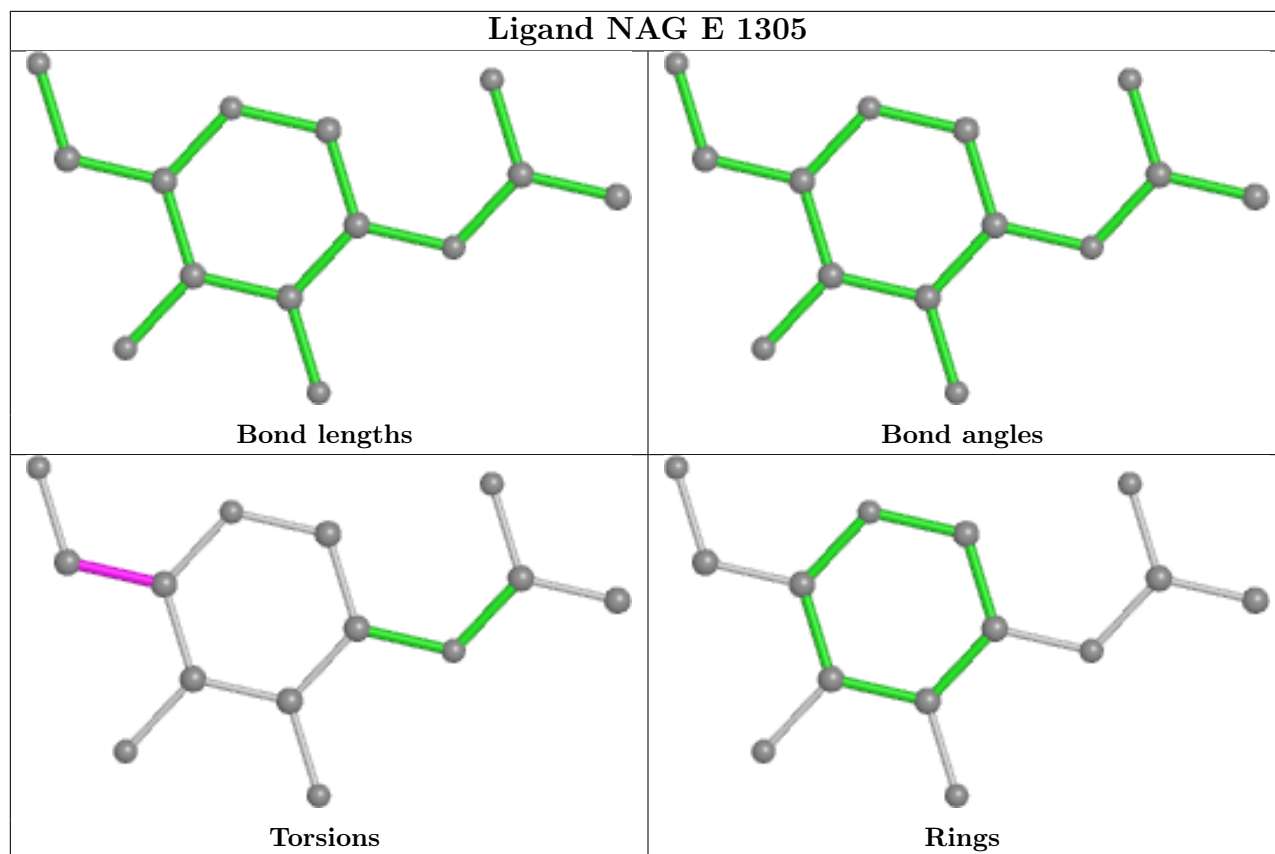
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	1304	NAG	1	0
14	C	1307	NAG	1	0
14	C	1301	NAG	3	0
14	E	1303	NAG	1	0
14	C	1308	NAG	1	0
14	E	1304	NAG	3	0

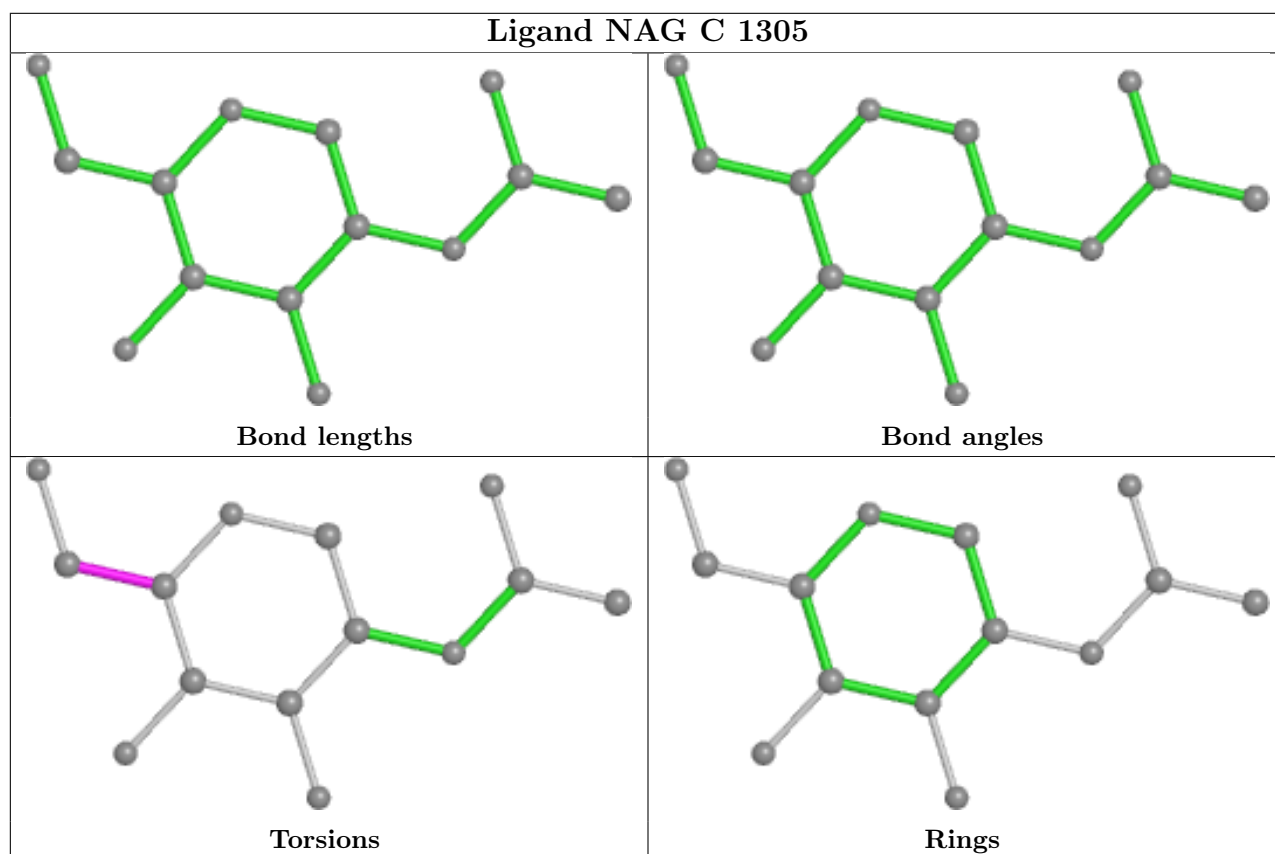
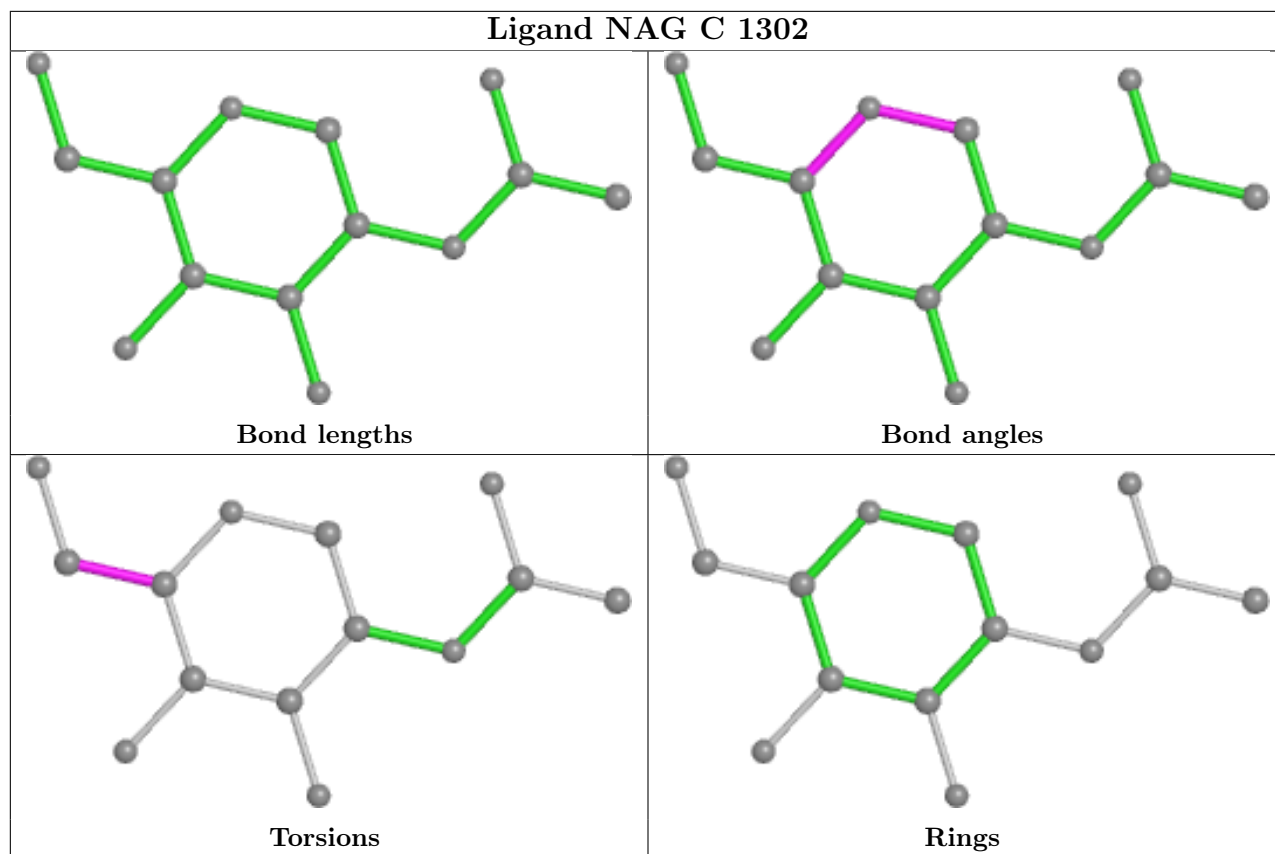
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

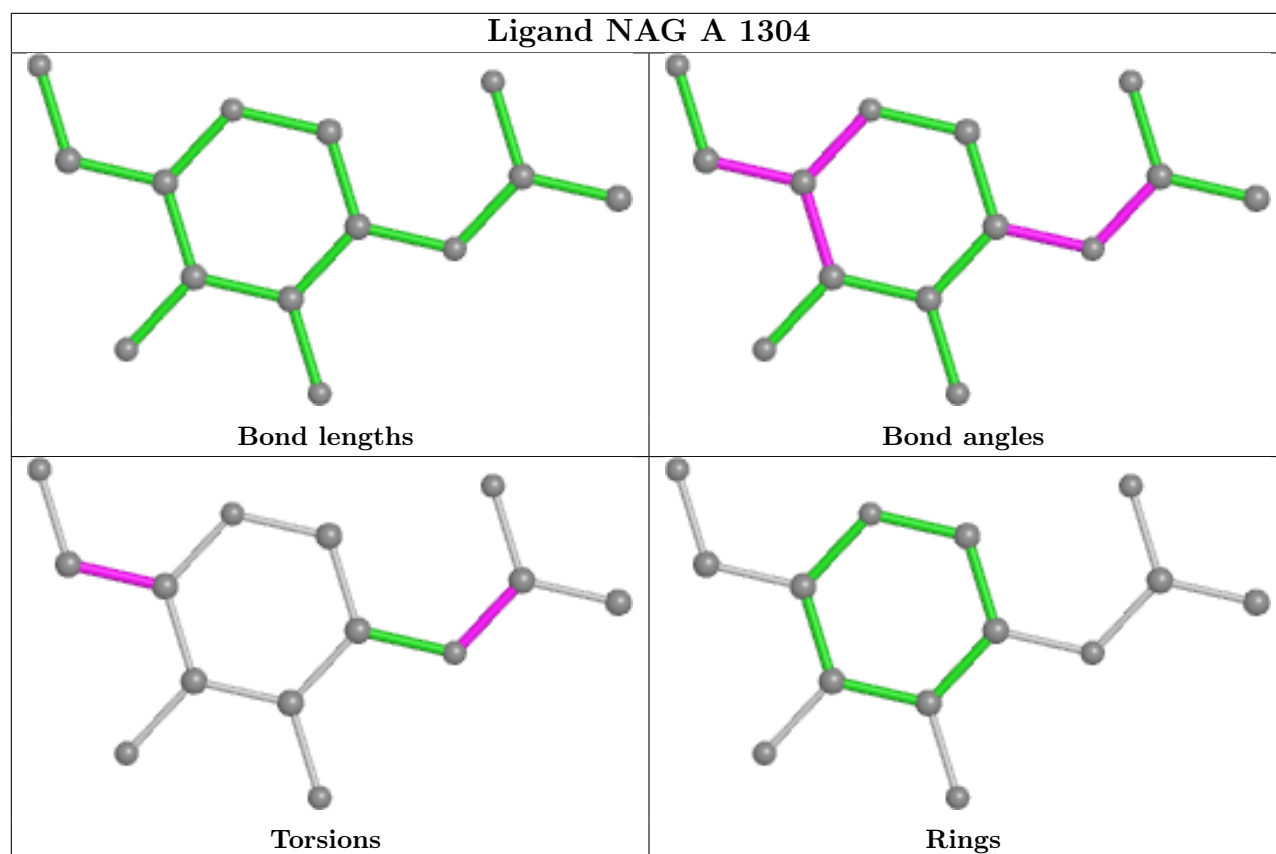
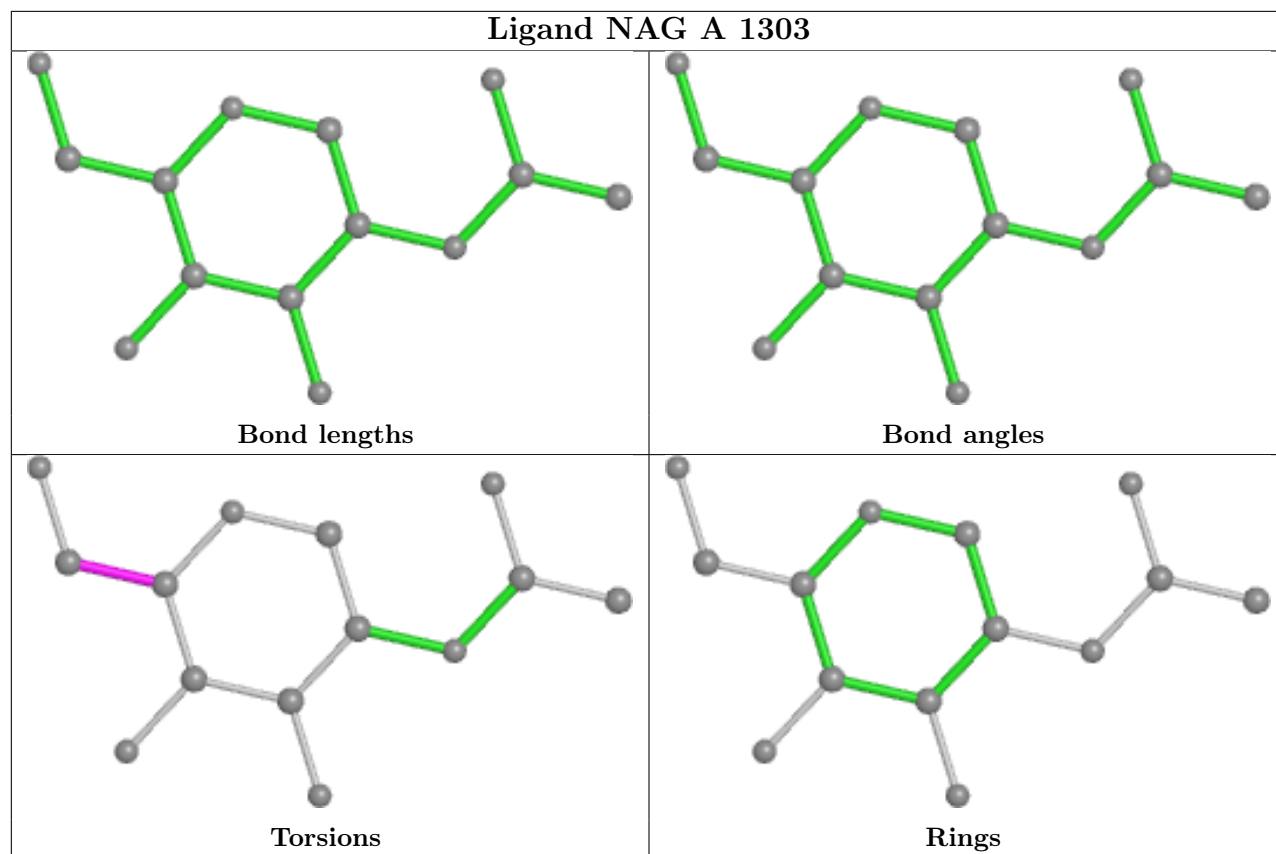
equivalents in the CSD to analyse the geometry.

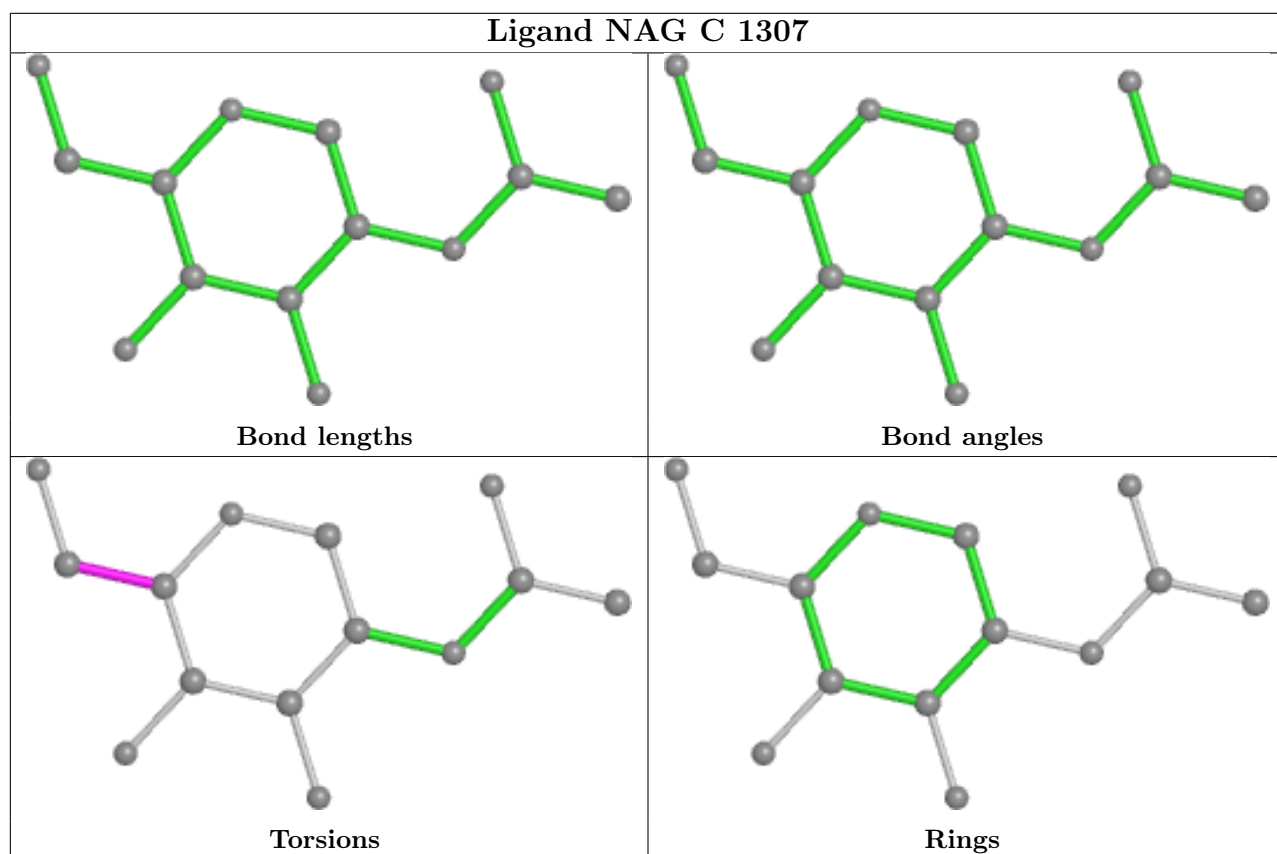
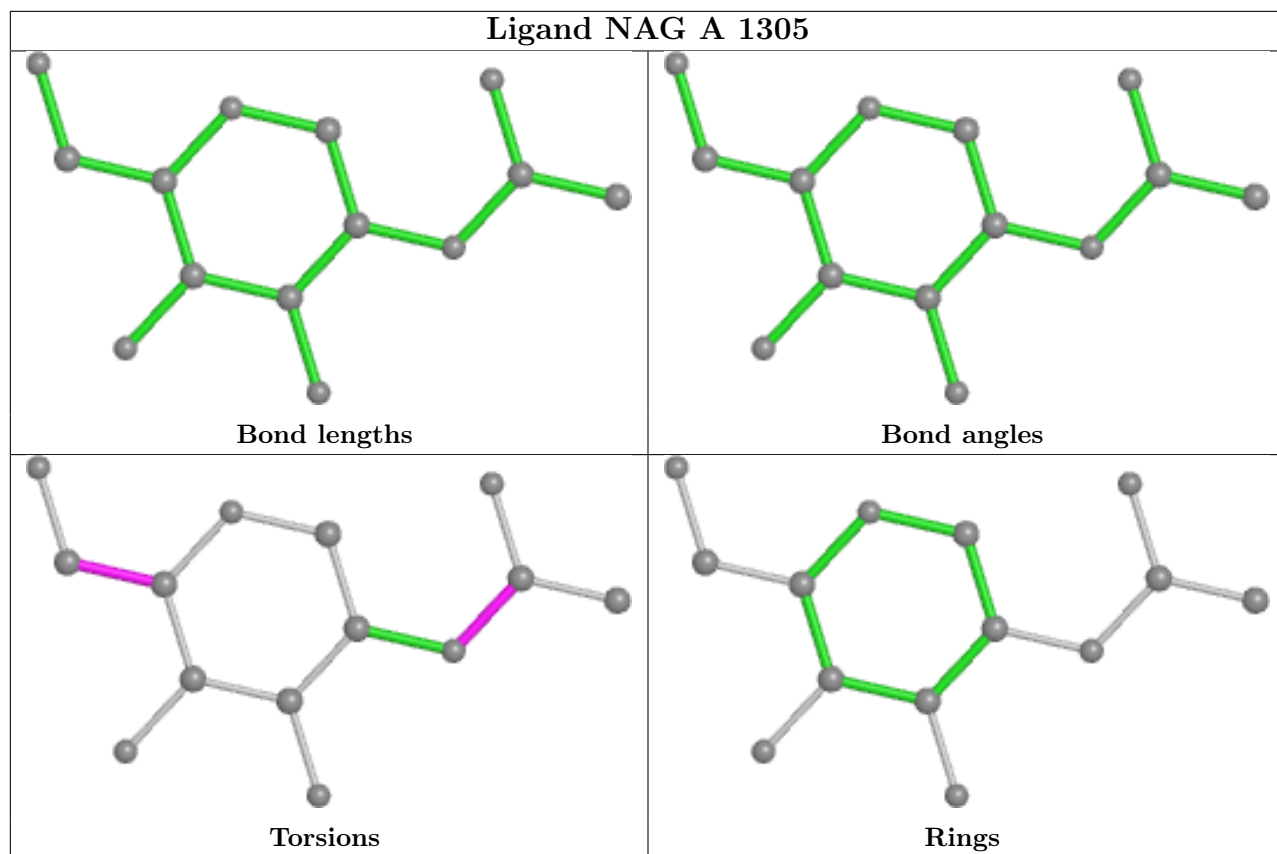


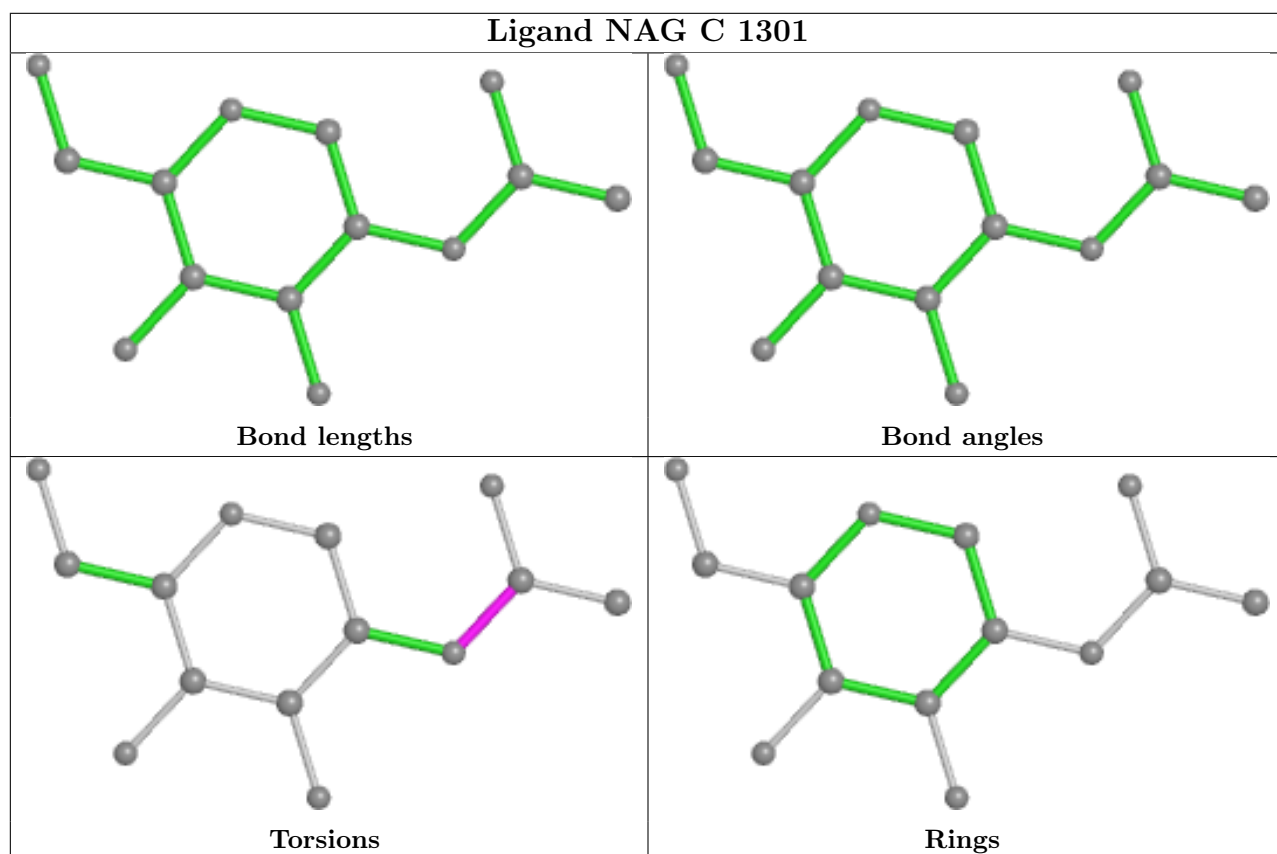
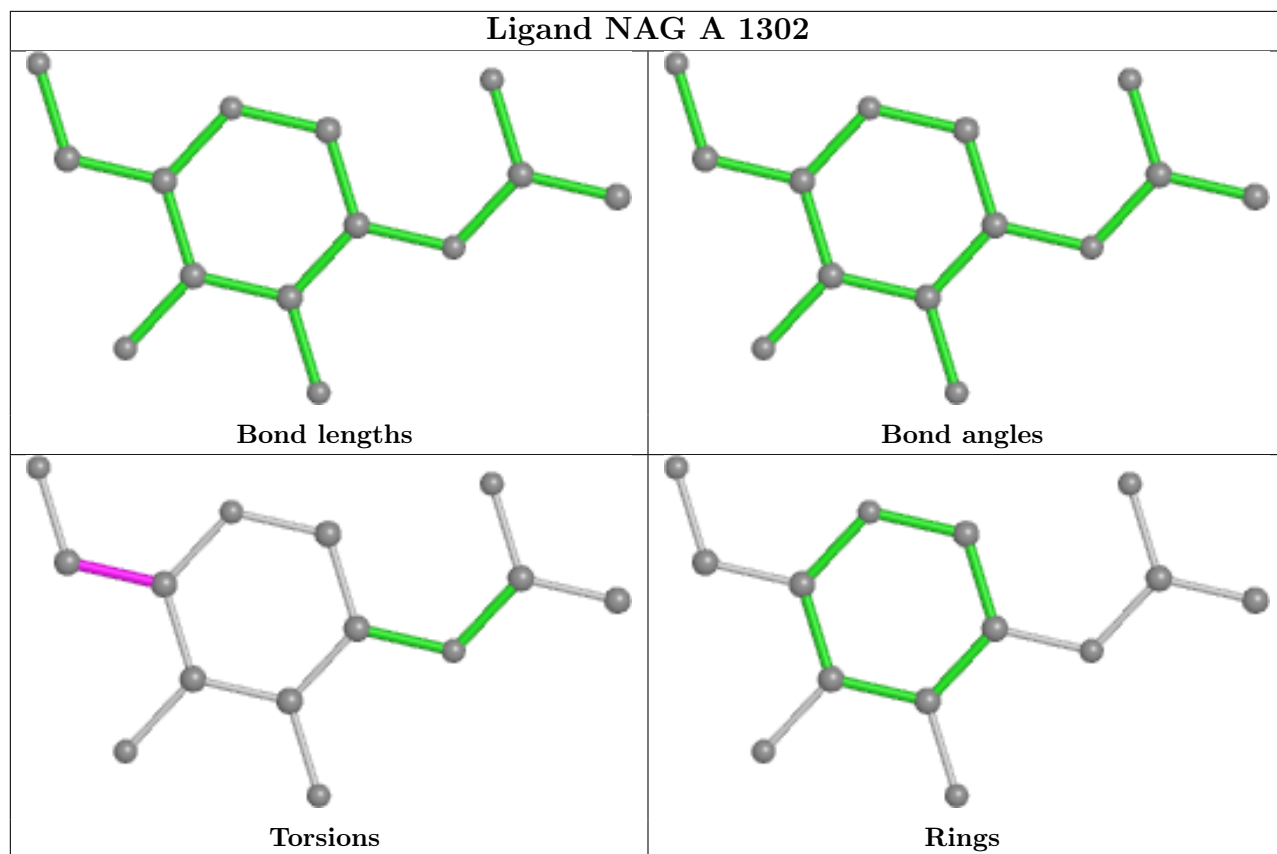




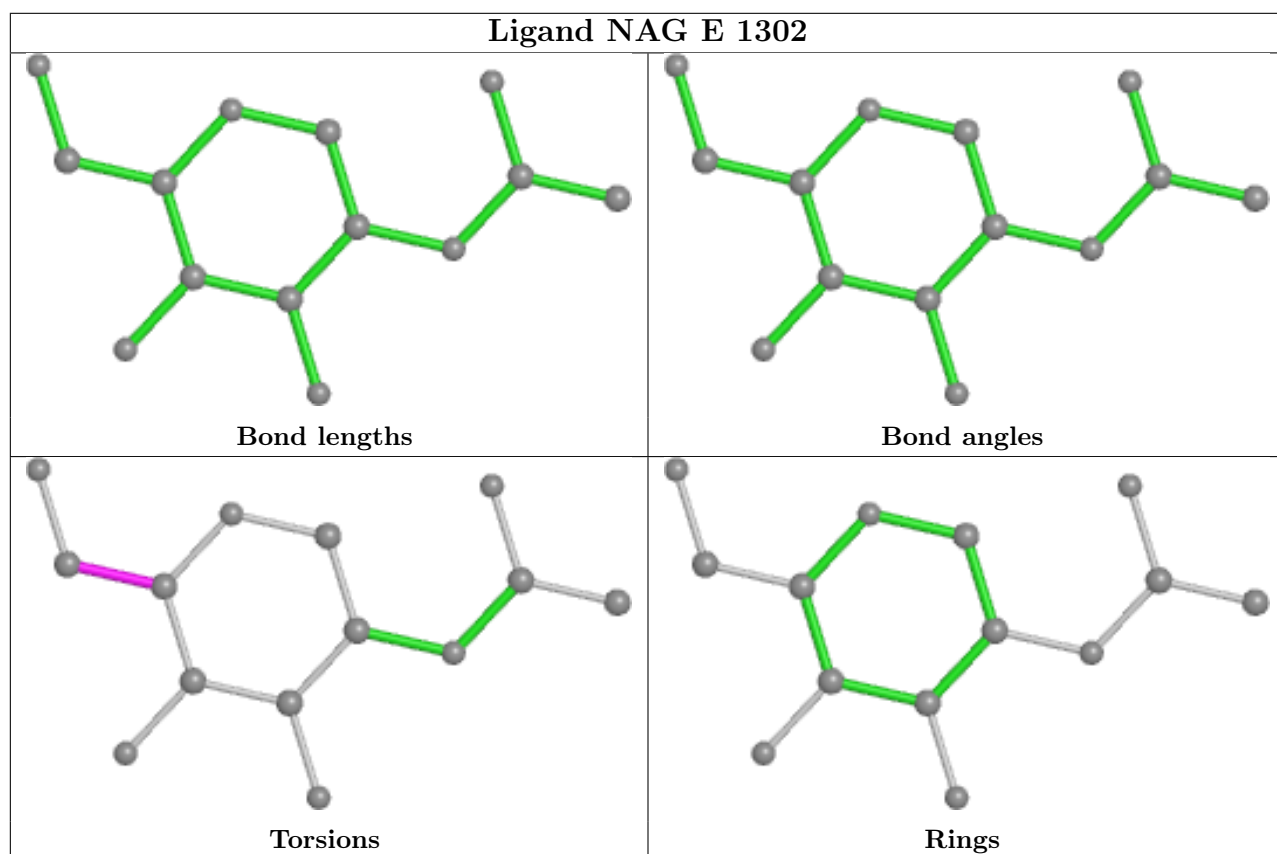
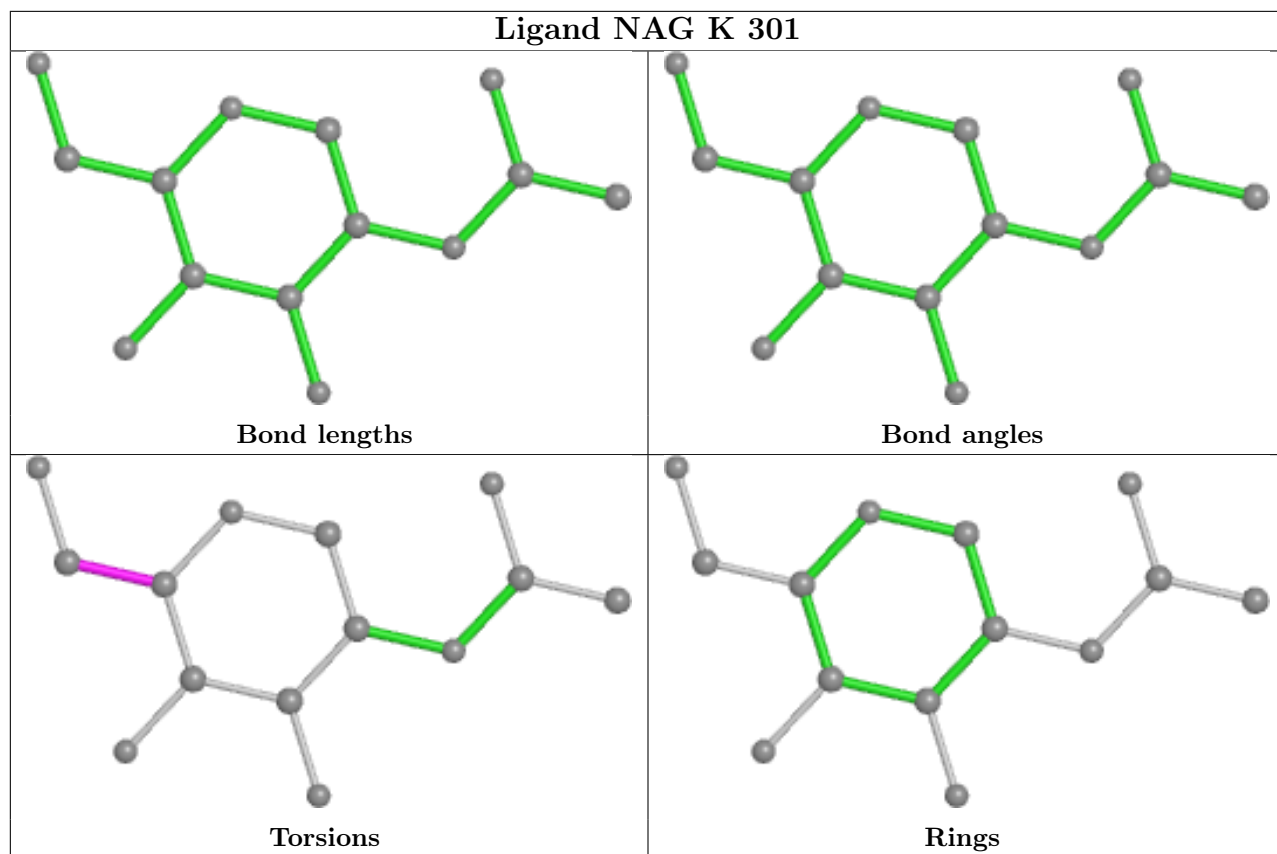


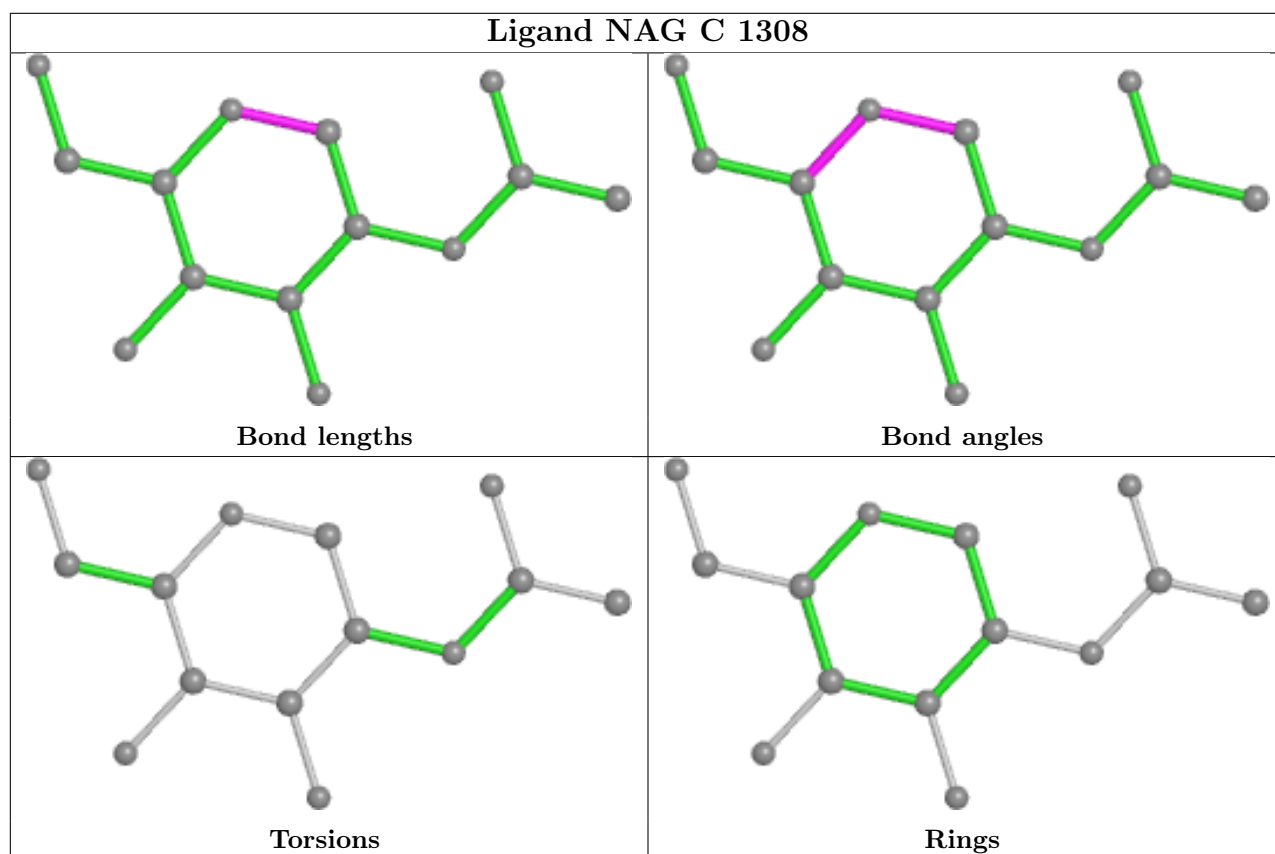
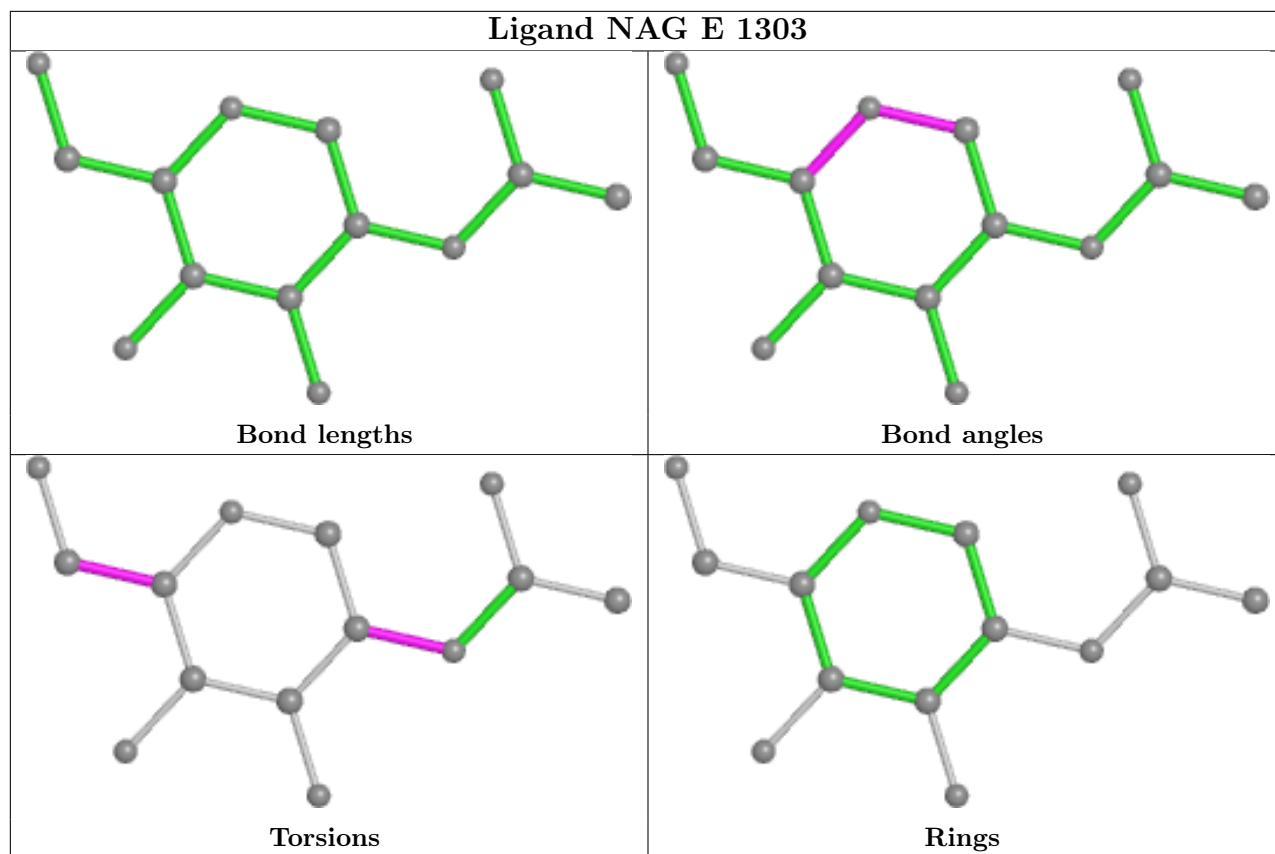


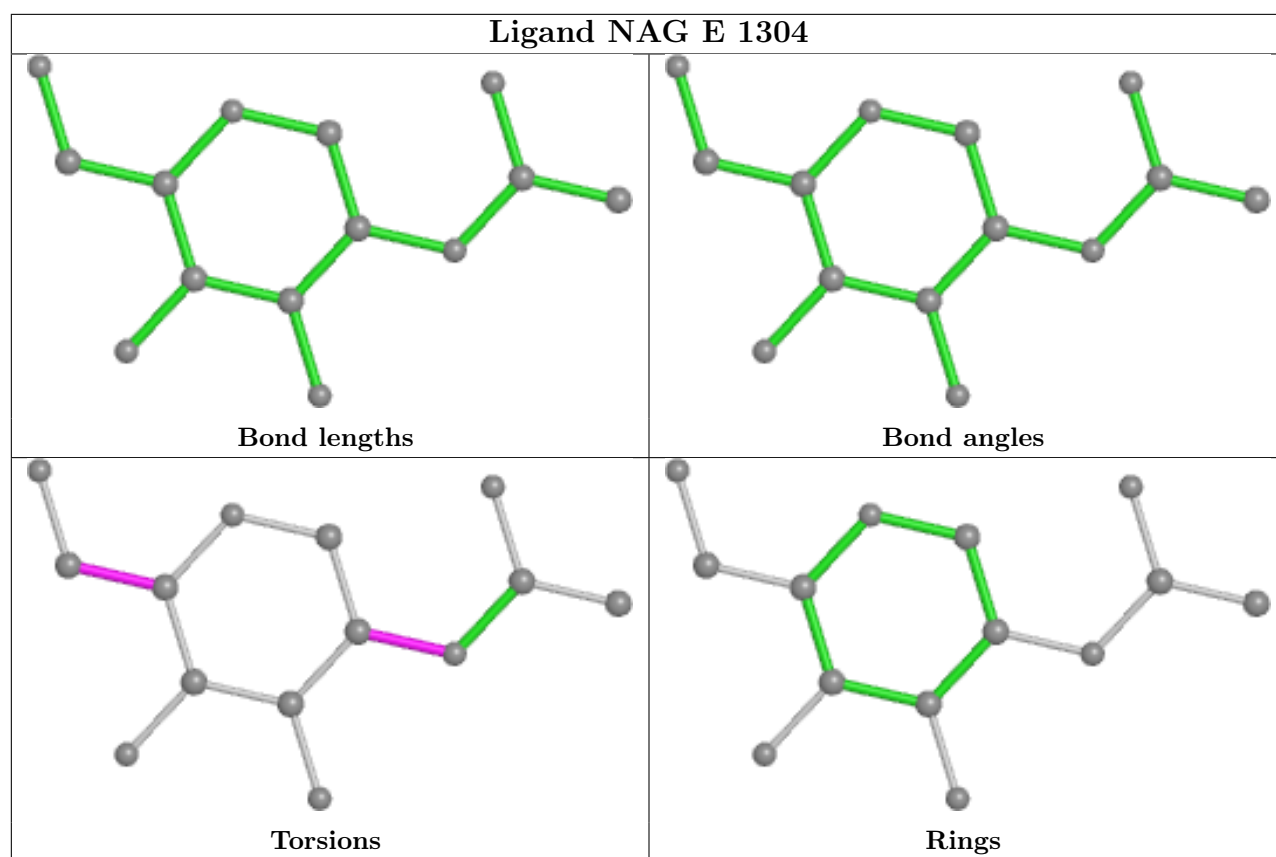












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

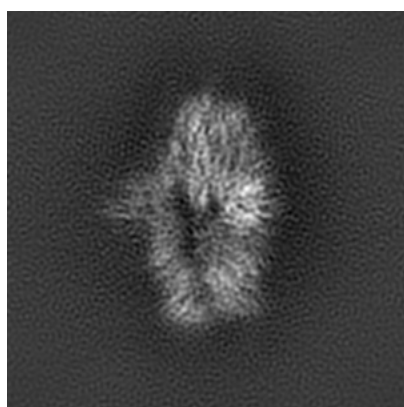
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32832. These allow visual inspection of the internal detail of the map and identification of artifacts.

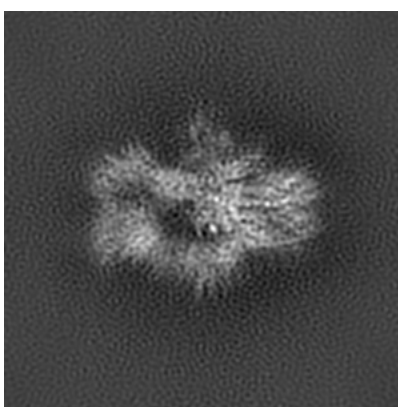
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

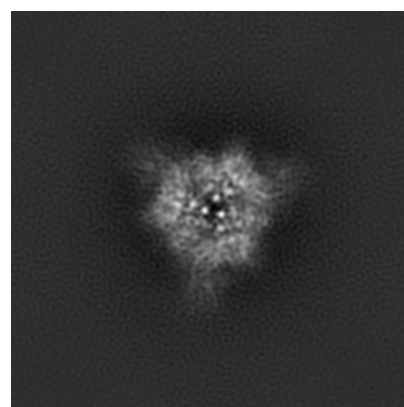
#### 6.1.1 Primary map



X



Y

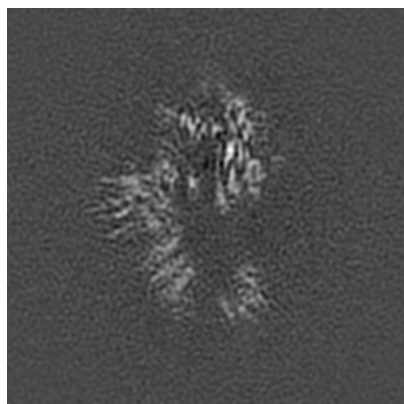


Z

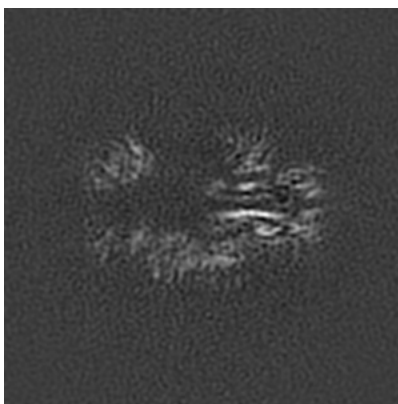
The images above show the map projected in three orthogonal directions.

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

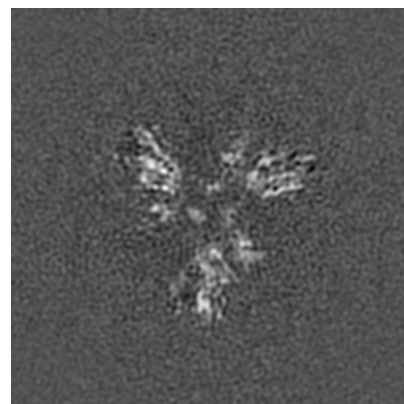
#### 6.2.1 Primary map



X Index: 190



Y Index: 190

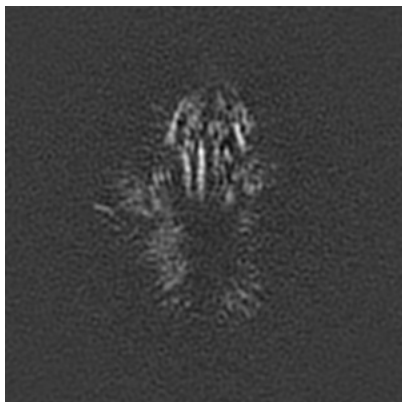


Z Index: 190

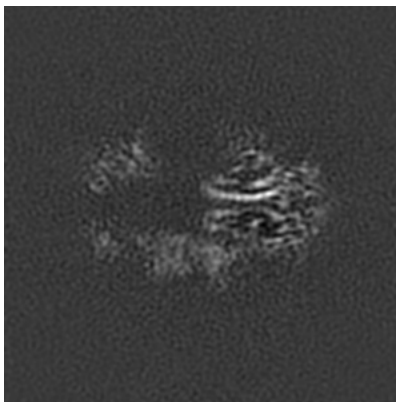
The images above show central slices of the map in three orthogonal directions.

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

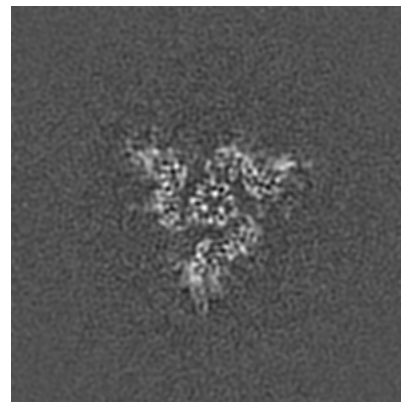
### 6.3.1 Primary map



X Index: 198



Y Index: 186

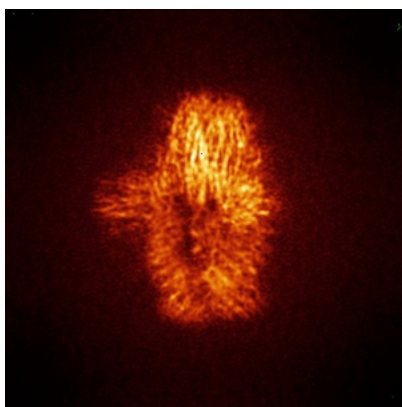


Z Index: 211

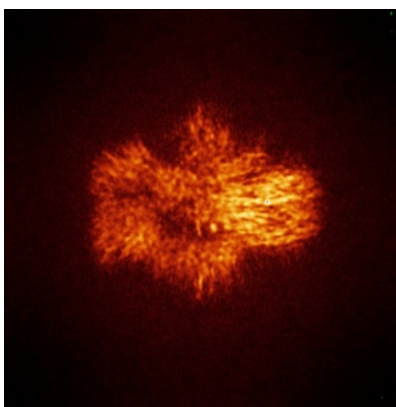
The images above show the largest variance slices of the map in three orthogonal directions.

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

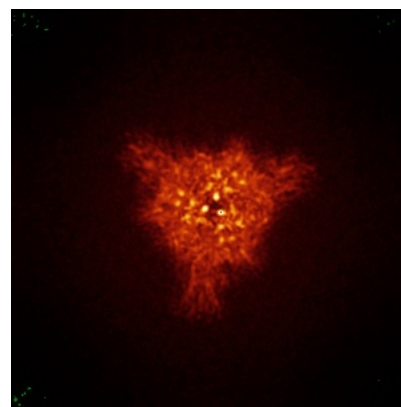
### 6.4.1 Primary map



X



Y

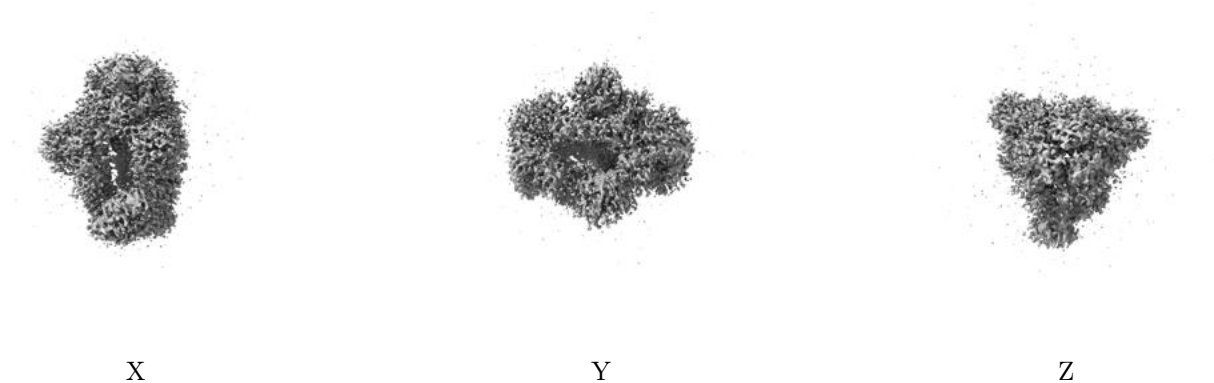


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

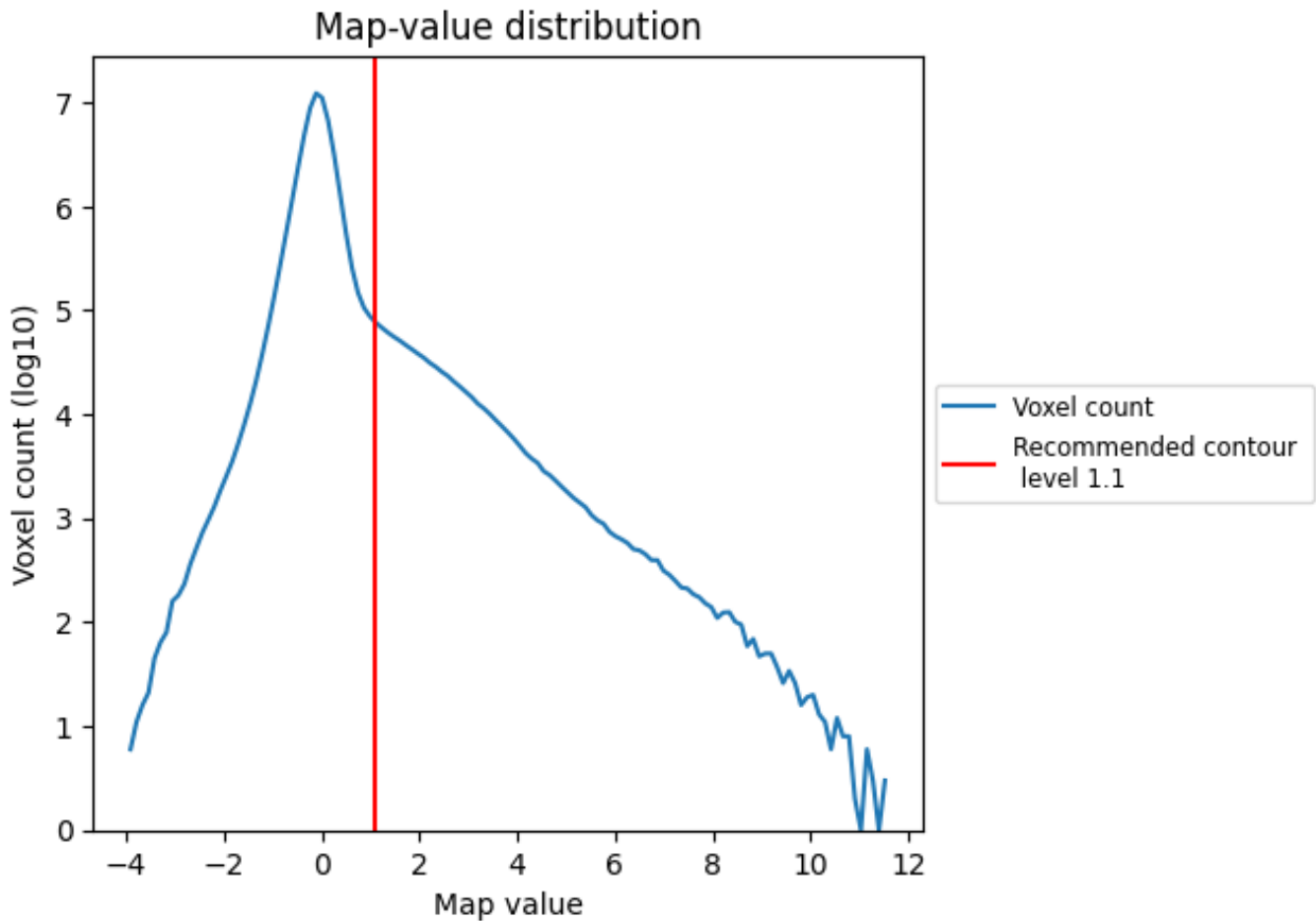
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

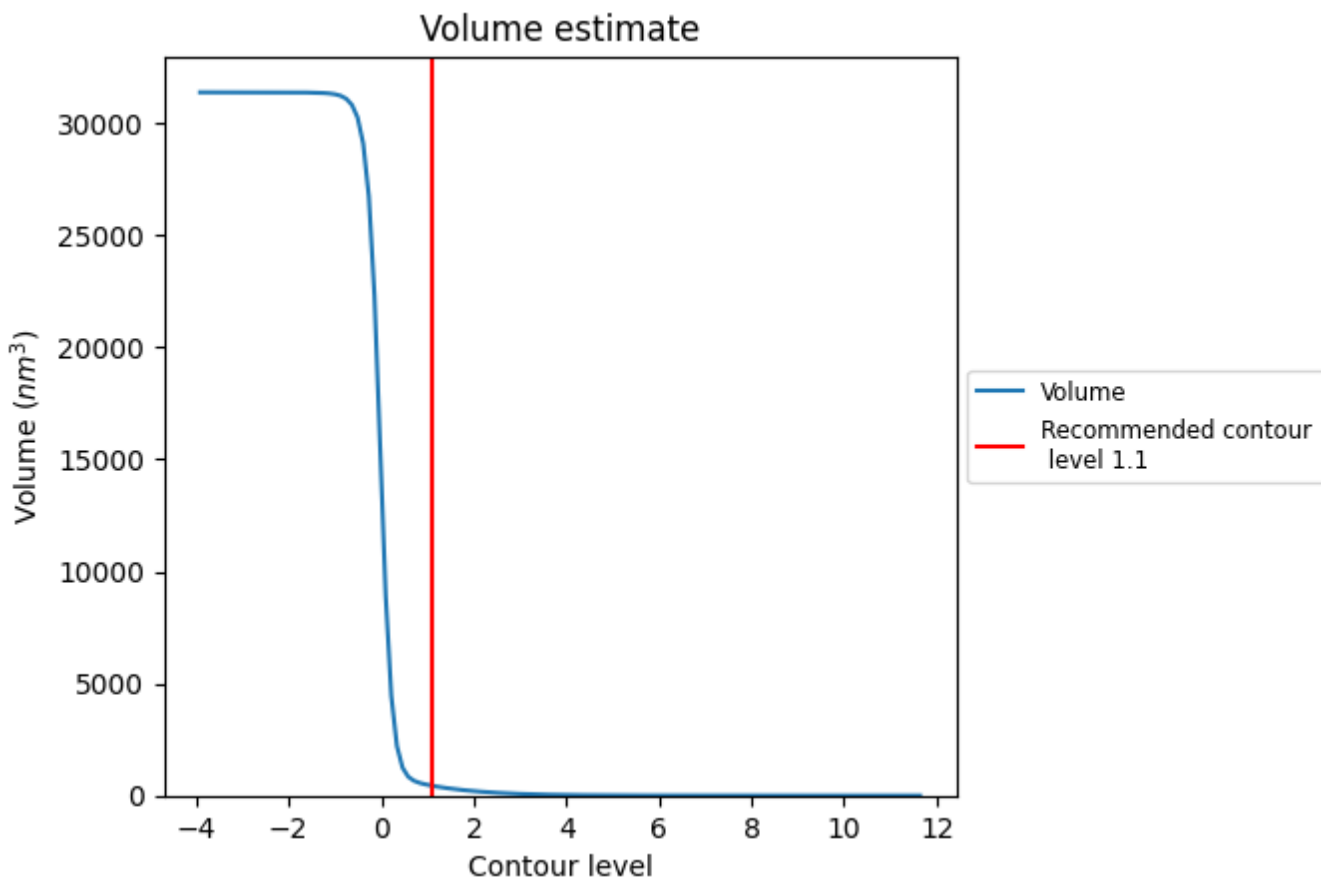
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

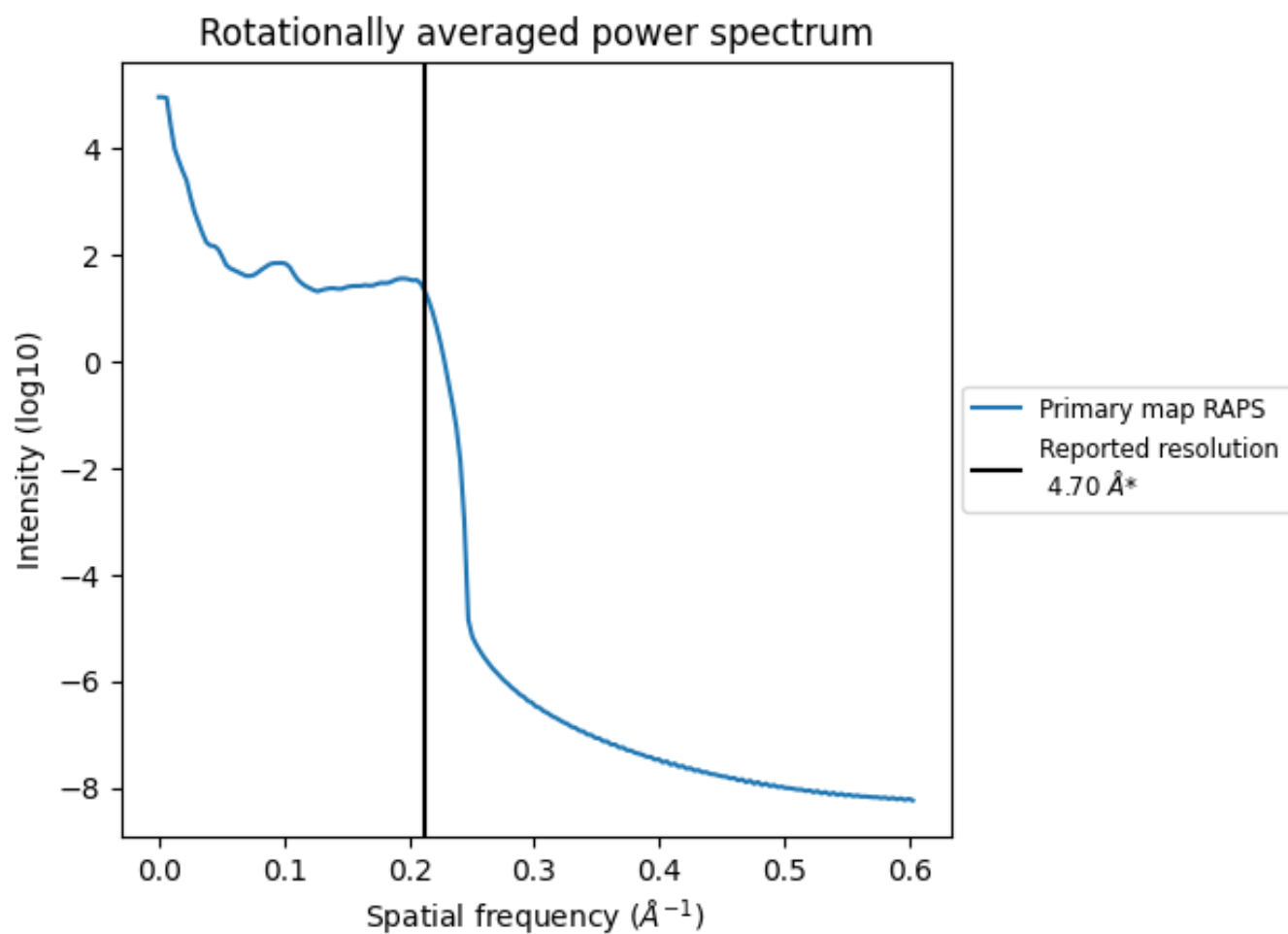


The volume at the recommended contour level is 438 nm<sup>3</sup>; this corresponds to an approximate mass of 395 kDa.

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 0.213 Å<sup>-1</sup>

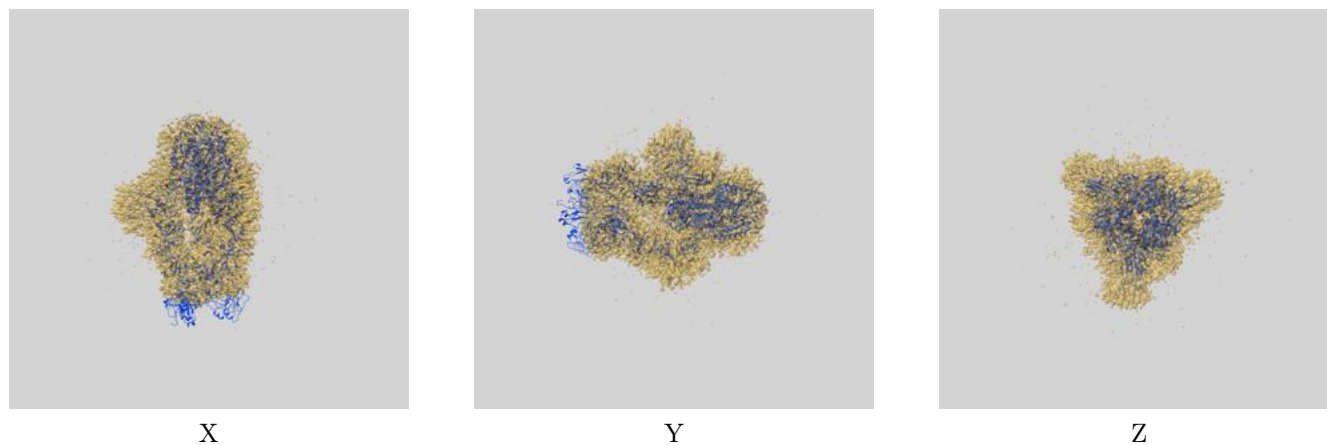
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

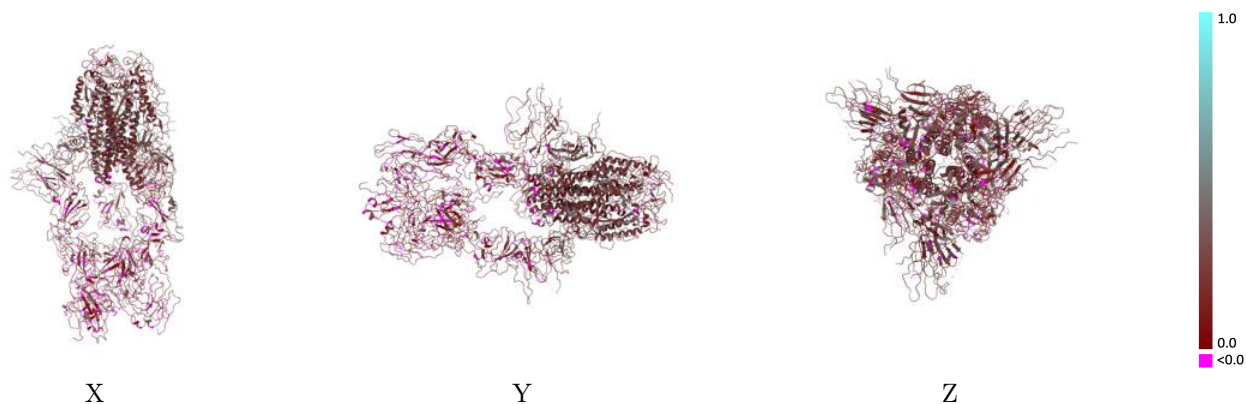
This section contains information regarding the fit between EMDB map EMD-32832 and PDB model 7WUH. Per-residue inclusion information can be found in section 3 on page 14.

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



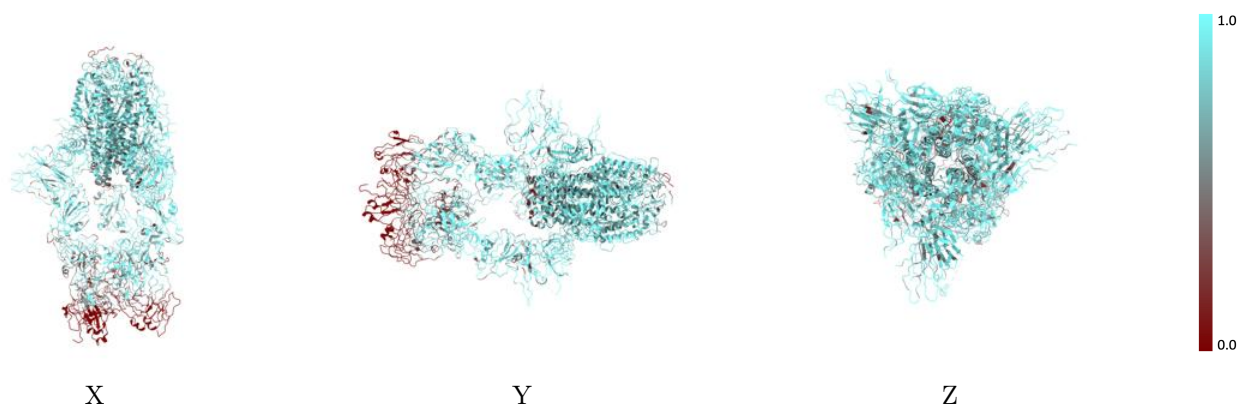
The images above show the 3D surface view of the map at the recommended contour level 1.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



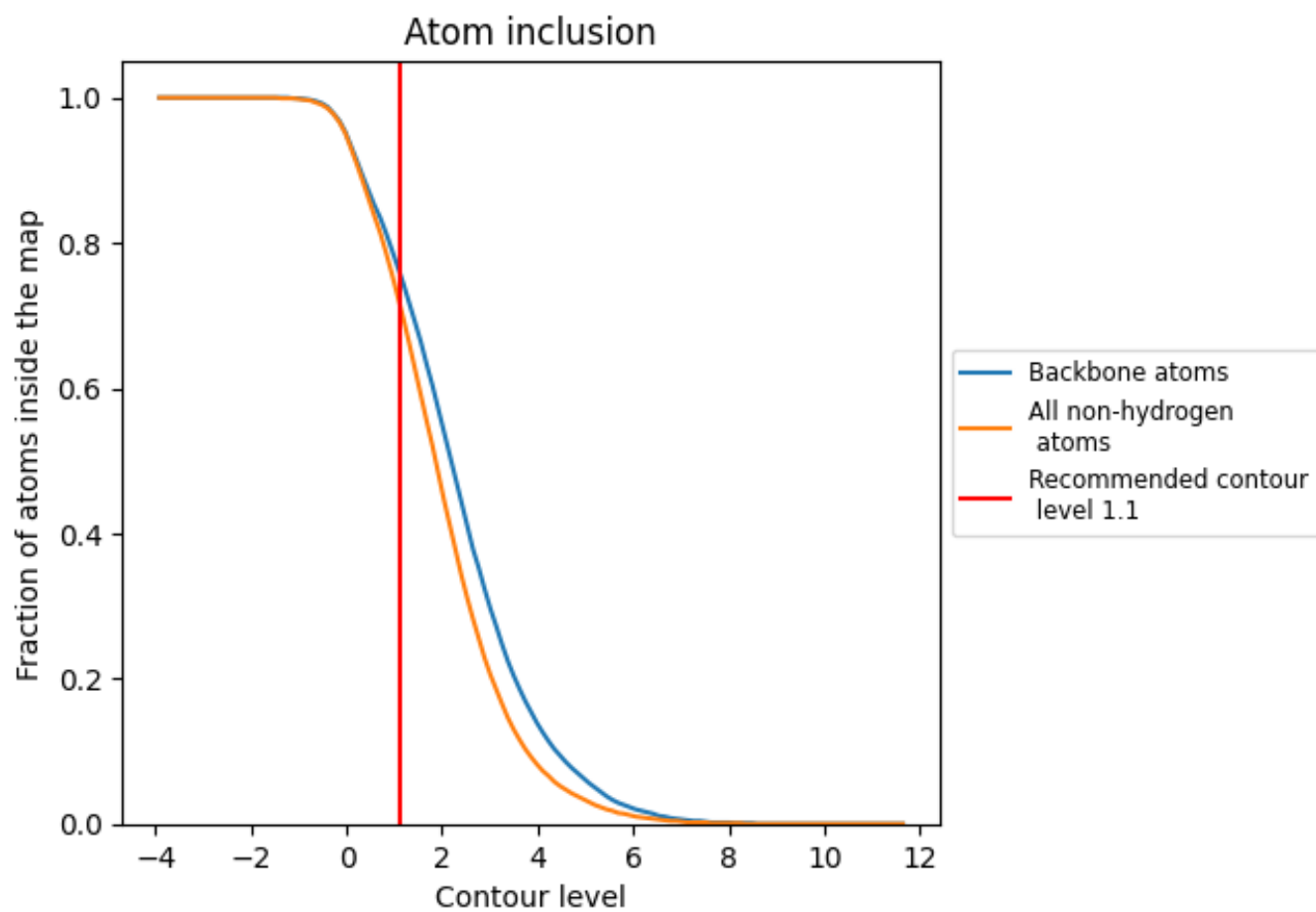
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.1).





































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.2450
A	 0.8210	 0.2660
B	 0.7890	 0.3650
C	 0.8190	 0.2670
D	 0.4650	 0.1830
E	 0.8100	 0.2630
F	 0.4720	 0.1970
G	 0.5360	 0.3730
H	 0.4750	 0.1840
I	 0.4690	 0.1820
J	 0.8400	 0.3700
K	 0.5010	 0.1850
L	 0.4440	 0.1560
M	 0.9490	 0.3480
N	 0.9290	 0.4250
O	 0.8930	 0.3810
P	 0.9640	 0.4010
Q	 0.7950	 0.2830
R	 0.7500	 0.4520
S	 0.9020	 0.4280
T	 1.0000	 0.4440
U	 0.8850	 0.4100
V	 0.7140	 0.3780
W	 0.7380	 0.4040
X	 0.7500	 0.3580
Y	 0.8600	 0.3810
Z	 0.7950	 0.4160
a	 0.8370	 0.4420
b	 0.7370	 0.3940
c	 0.7500	 0.3630
d	 0.9470	 0.4620
e	 0.9490	 0.4430
f	 0.7500	 0.4300
g	 0.8370	 0.3510

