



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 03:07 PM UTC

PDB ID : 9UBX / pdb_00009ubx
EMDB ID : EMD-64028
Title : The atomic coordinates of the mouse CatSper trimer
Authors : Xu, Q.; Lin, S.; Zhao, Q.; Yan, Z.; Wu, J.
Deposited on : 2025-04-03
Resolution : 6.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

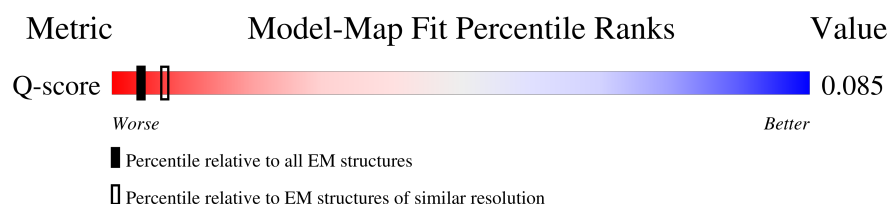
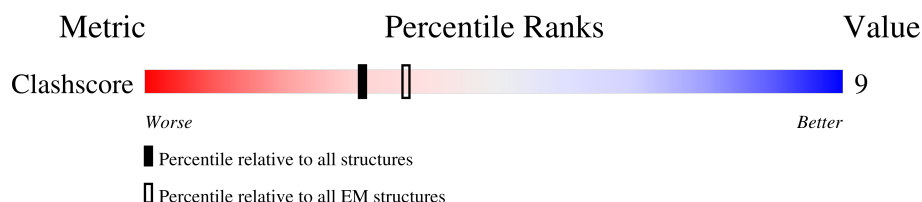
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

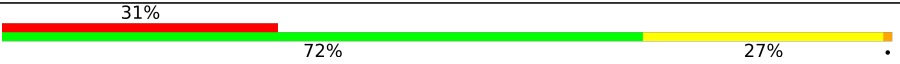
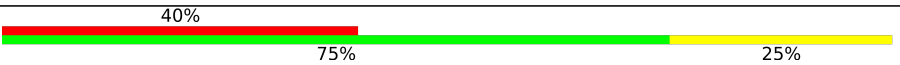
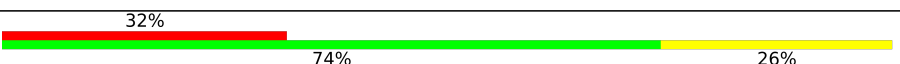
The reported resolution of this entry is 6.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	503 (6.30 - 7.30)

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

Mol	Chain	Length	Quality of chain
1	A	251	
1	a	251	
1	n	251	
2	B	281	
2	b	281	
2	o	281	

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Mol	Chain	Length	Quality of chain
3	C	278	41% 79%21%
3	c	278	59% 79%20%
3	p	278	35% 76%24%
4	D	250	42% 76%23%
4	d	250	61% 77%22%
4	q	250	29% 77%22%
5	E	1065	81% 18%
5	e	1065	17% 78%21%
5	r	1065	77% 22%
6	F	1042	82% 17%
6	f	1042	8% 70%30%
6	s	1042	13% 69%31%
7	G	733	10% 79%18%
7	g	733	26% 80%18%
7	t	733	9% 75%22%
8	H	921	9% 76%23%
8	h	921	23% 77%22%
8	u	921	8% 75%24%
9	I	174	97% 100%
9	Q	174	97% 100%
9	i	174	97% 100%
10	J	168	44% 70%30%
10	j	168	96% 74%26%
10	w	168	45% 66%34%
11	K	149	100% 99%

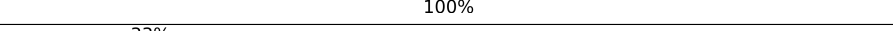
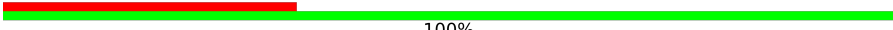
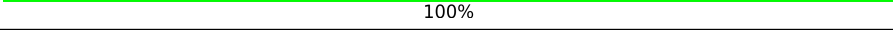
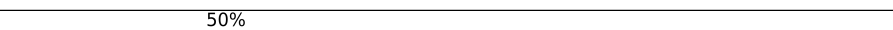
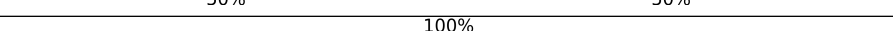
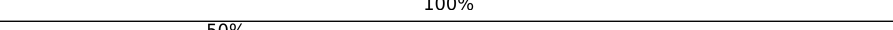
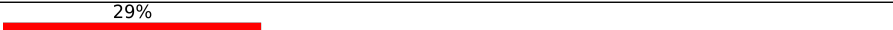
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Mol	Chain	Length	Quality of chain
11	k	149	100%
11	x	149	99%
12	L	610	98%
12	l	610	99%
12	y	610	93%
13	M	115	84%
13	m	115	14%
13	z	115	97%
13	M	115	85%
13	m	115	93%
13	z	115	83%
13	M	115	12%
13	m	115	64%
13	z	115	80%
13	M	115	77%
13	m	115	5%
13	z	115	68%
14	N	28	32%
14	O	28	18%
14	P	28	100%
14	N	28	79%
14	O	28	100%
14	P	28	7%
14	N	28	100%
15	0	7	86%
15	AA	7	29%
15	AA	7	100%
15	R	7	57%
15	R	7	29%
15	R	7	14%
16	1	3	33%
16	1	3	67%
16	2	3	67%
16	2	3	100%
16	4	3	33%
16	4	3	100%
16	5	3	100%
16	5	3	100%
16	6	3	100%
16	6	3	100%
16	BA	3	33%
16	BA	3	67%
16	CA	3	100%
16	CA	3	67%
16	CA	3	33%
16	EA	3	100%
16	EA	3	100%
16	FA	3	100%
16	FA	3	100%
16	GA	3	100%
16	GA	3	100%
16	S	3	33%
16	S	3	67%

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Mol	Chain	Length	Quality of chain
16	T	3	 67% 33%
16	V	3	 67% 100%
16	W	3	 33% 100%
16	X	3	 100%
17	3	2	 50% 50%
17	8	2	 50% 50%
17	DA	2	 50% 50%
17	IA	2	 100% 100%
17	U	2	 50% 100%
17	Z	2	 50% 50%
18	7	7	 29% 71% 29%
18	HA	7	 57% 86% 14%
18	Y	7	 29% 71% 14% 14%
19	9	5	 40% 20% 80%
19	JA	5	 40% 20% 80%
19	v	5	 20% 60% 40%

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 144816 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 Cation channel sperm-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	251	Total	C	N	O	S	0	0
			2053	1383	313	346	11		
1	n	251	Total	C	N	O	S	0	0
			2053	1383	313	346	11		
1	a	251	Total	C	N	O	S	0	0
			2053	1383	313	346	11		

- Molecule 2 is a protein called Cation channel sperm-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	281	Total	C	N	O	S	0	0
			2343	1585	363	384	11		
2	o	281	Total	C	N	O	S	0	0
			2343	1585	363	384	11		
2	b	281	Total	C	N	O	S	0	0
			2343	1585	363	384	11		

- Molecule 3 is a protein called Cation channel sperm-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	278	Total	C	N	O	S	0	0
			2277	1506	359	400	12		
3	p	278	Total	C	N	O	S	0	0
			2277	1506	359	400	12		
3	c	278	Total	C	N	O	S	0	0
			2277	1506	359	400	12		

- Molecule 4 is a protein called Cation channel sperm-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	250	Total	C	N	O	S	0	0
			2035	1370	311	338	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	q	250	Total	C	N	O	S	0	0
			2035	1370	311	338	16		
4	d	250	Total	C	N	O	S	0	0
			2035	1370	311	338	16		

- Molecule 5 is a protein called Cation channel sperm-associated auxiliary subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	1058	Total	C	N	O	S	0	0
			8510	5524	1395	1547	44		
5	r	1058	Total	C	N	O	S	0	0
			8510	5524	1395	1547	44		
5	e	1058	Total	C	N	O	S	0	0
			8510	5524	1395	1547	44		

- Molecule 6 is a protein called Cation channel sperm-associated auxiliary subunit gamma 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	1042	Total	C	N	O	S	0	0
			8454	5515	1354	1538	47		
6	f	1042	Total	C	N	O	S	0	0
			8454	5515	1354	1538	47		
6	s	1042	Total	C	N	O	S	0	0
			8454	5515	1354	1538	47		

- Molecule 7 is a protein called Cation channel sperm-associated auxiliary subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	714	Total	C	N	O	S	0	0
			5680	3669	923	1056	32		
7	t	714	Total	C	N	O	S	0	0
			5680	3669	923	1056	32		
7	g	714	Total	C	N	O	S	0	0
			5680	3669	923	1056	32		

- Molecule 8 is a protein called Cation channel sperm-associated auxiliary subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	916	Total	C	N	O	S	0	0
			7502	4865	1208	1389	40		
8	u	916	Total	C	N	O	S	0	0
			7502	4865	1208	1389	40		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	916	Total	C	N	O	S	0	0
			7502	4865	1208	1389	40		

- Molecule 9 is a protein called EF-hand calcium-binding domain-containing protein 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	174	Total	C	N	O	0	0
			863	515	174	174		
9	i	174	Total	C	N	O	0	0
			863	515	174	174		
9	Q	174	Total	C	N	O	0	0
			863	515	174	174		

- Molecule 10 is a protein called Cation channel sperm-associated auxiliary subunit TMEM249.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	168	Total	C	N	O	S	0	0
			1398	921	238	225	14		
10	w	168	Total	C	N	O	S	0	0
			1398	921	238	225	14		
10	j	168	Total	C	N	O	S	0	0
			1398	921	238	225	14		

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	initiating methionine	UNP A0A2R8VHF7
J	2	CYS	-	expression tag	UNP A0A2R8VHF7
J	3	TRP	-	expression tag	UNP A0A2R8VHF7
J	4	VAL	-	expression tag	UNP A0A2R8VHF7
J	5	MET	-	expression tag	UNP A0A2R8VHF7
J	6	PRO	-	expression tag	UNP A0A2R8VHF7
J	7	PRO	-	expression tag	UNP A0A2R8VHF7
J	8	SER	-	expression tag	UNP A0A2R8VHF7
J	9	VAL	-	expression tag	UNP A0A2R8VHF7
J	10	PHE	-	expression tag	UNP A0A2R8VHF7
J	11	VAL	-	expression tag	UNP A0A2R8VHF7
J	12	LEU	-	expression tag	UNP A0A2R8VHF7
J	13	GLU	-	expression tag	UNP A0A2R8VHF7
J	14	TYR	-	expression tag	UNP A0A2R8VHF7
J	15	TYR	-	expression tag	UNP A0A2R8VHF7
J	16	LEU	-	expression tag	UNP A0A2R8VHF7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	17	ASP	-	expression tag	UNP A0A2R8VHF7
J	18	THR	-	expression tag	UNP A0A2R8VHF7
J	19	LEU	-	expression tag	UNP A0A2R8VHF7
J	20	TRP	-	expression tag	UNP A0A2R8VHF7
J	21	LYS	-	expression tag	UNP A0A2R8VHF7
J	22	GLY	-	expression tag	UNP A0A2R8VHF7
J	23	THR	-	expression tag	UNP A0A2R8VHF7
w	1	MET	-	initiating methionine	UNP A0A2R8VHF7
w	2	CYS	-	expression tag	UNP A0A2R8VHF7
w	3	TRP	-	expression tag	UNP A0A2R8VHF7
w	4	VAL	-	expression tag	UNP A0A2R8VHF7
w	5	MET	-	expression tag	UNP A0A2R8VHF7
w	6	PRO	-	expression tag	UNP A0A2R8VHF7
w	7	PRO	-	expression tag	UNP A0A2R8VHF7
w	8	SER	-	expression tag	UNP A0A2R8VHF7
w	9	VAL	-	expression tag	UNP A0A2R8VHF7
w	10	PHE	-	expression tag	UNP A0A2R8VHF7
w	11	VAL	-	expression tag	UNP A0A2R8VHF7
w	12	LEU	-	expression tag	UNP A0A2R8VHF7
w	13	GLU	-	expression tag	UNP A0A2R8VHF7
w	14	TYR	-	expression tag	UNP A0A2R8VHF7
w	15	TYR	-	expression tag	UNP A0A2R8VHF7
w	16	LEU	-	expression tag	UNP A0A2R8VHF7
w	17	ASP	-	expression tag	UNP A0A2R8VHF7
w	18	THR	-	expression tag	UNP A0A2R8VHF7
w	19	LEU	-	expression tag	UNP A0A2R8VHF7
w	20	TRP	-	expression tag	UNP A0A2R8VHF7
w	21	LYS	-	expression tag	UNP A0A2R8VHF7
w	22	GLY	-	expression tag	UNP A0A2R8VHF7
w	23	THR	-	expression tag	UNP A0A2R8VHF7
j	1	MET	-	initiating methionine	UNP A0A2R8VHF7
j	2	CYS	-	expression tag	UNP A0A2R8VHF7
j	3	TRP	-	expression tag	UNP A0A2R8VHF7
j	4	VAL	-	expression tag	UNP A0A2R8VHF7
j	5	MET	-	expression tag	UNP A0A2R8VHF7
j	6	PRO	-	expression tag	UNP A0A2R8VHF7
j	7	PRO	-	expression tag	UNP A0A2R8VHF7
j	8	SER	-	expression tag	UNP A0A2R8VHF7
j	9	VAL	-	expression tag	UNP A0A2R8VHF7
j	10	PHE	-	expression tag	UNP A0A2R8VHF7
j	11	VAL	-	expression tag	UNP A0A2R8VHF7
j	12	LEU	-	expression tag	UNP A0A2R8VHF7

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Chain	Residue	Modelled	Actual	Comment	Reference
j	13	GLU	-	expression tag	UNP A0A2R8VHF7
j	14	TYR	-	expression tag	UNP A0A2R8VHF7
j	15	TYR	-	expression tag	UNP A0A2R8VHF7
j	16	LEU	-	expression tag	UNP A0A2R8VHF7
j	17	ASP	-	expression tag	UNP A0A2R8VHF7
j	18	THR	-	expression tag	UNP A0A2R8VHF7
j	19	LEU	-	expression tag	UNP A0A2R8VHF7
j	20	TRP	-	expression tag	UNP A0A2R8VHF7
j	21	LYS	-	expression tag	UNP A0A2R8VHF7
j	22	GLY	-	expression tag	UNP A0A2R8VHF7
j	23	THR	-	expression tag	UNP A0A2R8VHF7

- Molecule 11 is a protein called Cation channel sperm-associated auxiliary subunit zeta.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	149	Total	C	N	O	0	0
			755	453	152	150		
11	x	149	Total	C	N	O	0	0
			755	453	152	150		
11	k	149	Total	C	N	O	0	0
			755	453	152	150		

- Molecule 12 is a protein called Solute carrier organic anion transporter family member 6C1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	597	Total	C	N	O	S	0	0
			4694	3079	747	829	39		
12	y	597	Total	C	N	O	S	0	0
			4694	3079	747	829	39		
12	l	597	Total	C	N	O	S	0	0
			4694	3079	747	829	39		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	224	GLY	ALA	engineered mutation	UNP Q8C0X7
y	224	GLY	ALA	engineered mutation	UNP Q8C0X7
l	224	GLY	ALA	engineered mutation	UNP Q8C0X7

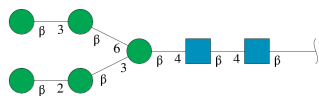
- Molecule 13 is a protein called Cation channel sperm-associated auxiliary subunit TMEM262.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	115	Total	C	N	O	S	0	0
			936	619	156	150	11		
13	z	115	Total	C	N	O	S	0	0
			936	619	156	150	11		
13	m	115	Total	C	N	O	S	0	0
			936	619	156	150	11		

- Molecule 14 is a protein called Unknown protein.

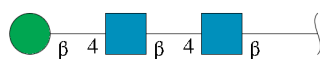
Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	28	Total	C	N	O	0	0
			140	84	28	28		
14	P	28	Total	C	N	O	0	0
			140	84	28	28		
14	O	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 15 is an oligosaccharide called beta-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-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.



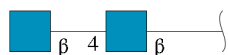
Mol	Chain	Residues	Atoms				AltConf	Trace
15	R	7	Total	C	N	O	0	0
			83	46	2	35		
15	0	7	Total	C	N	O	0	0
			83	46	2	35		
15	AA	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 16 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
16	S	3	Total	C	N	O	0	0
			39	22	2	15		
16	T	3	Total	C	N	O	0	0
			39	22	2	15		
16	V	3	Total	C	N	O	0	0
			39	22	2	15		
16	W	3	Total	C	N	O	0	0
			39	22	2	15		
16	X	3	Total	C	N	O	0	0
			39	22	2	15		
16	1	3	Total	C	N	O	0	0
			39	22	2	15		
16	2	3	Total	C	N	O	0	0
			39	22	2	15		
16	4	3	Total	C	N	O	0	0
			39	22	2	15		
16	5	3	Total	C	N	O	0	0
			39	22	2	15		
16	6	3	Total	C	N	O	0	0
			39	22	2	15		
16	BA	3	Total	C	N	O	0	0
			39	22	2	15		
16	CA	3	Total	C	N	O	0	0
			39	22	2	15		
16	EA	3	Total	C	N	O	0	0
			39	22	2	15		
16	FA	3	Total	C	N	O	0	0
			39	22	2	15		
16	GA	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 17 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



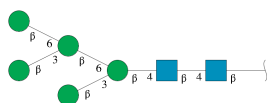
Mol	Chain	Residues	Atoms				AltConf	Trace
17	U	2	Total	C	N	O	0	0
			28	16	2	10		
17	Z	2	Total	C	N	O	0	0
			28	16	2	10		

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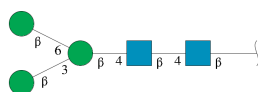
Mol	Chain	Residues	Atoms				AltConf	Trace
17	3	2	Total	C	N	O	0	0
			28	16	2	10		
17	8	2	Total	C	N	O	0	0
			28	16	2	10		
17	DA	2	Total	C	N	O	0	0
			28	16	2	10		
17	IA	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 18 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-[beta-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.



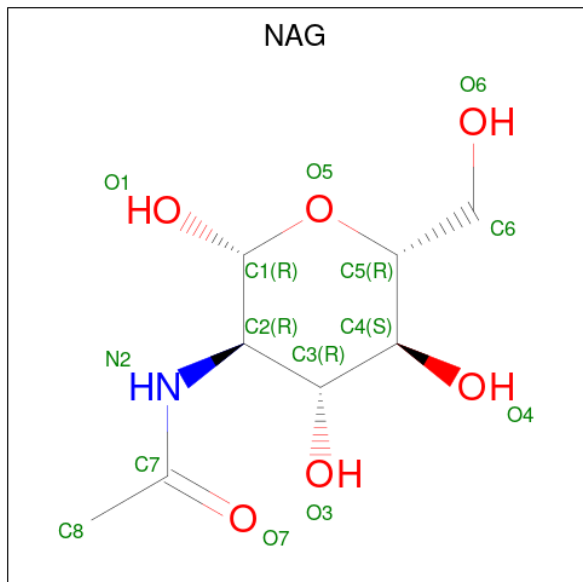
Mol	Chain	Residues	Atoms				AltConf	Trace
18	Y	7	Total	C	N	O	0	0
			83	46	2	35		
18	7	7	Total	C	N	O	0	0
			83	46	2	35		
18	HA	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 19 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-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
19	v	5	Total	C	N	O	0	0
			61	34	2	25		
19	9	5	Total	C	N	O	0	0
			61	34	2	25		
19	JA	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 20 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



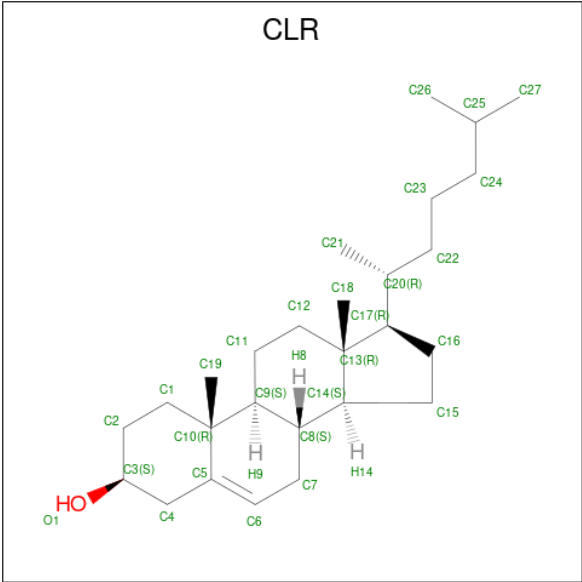
Mol	Chain	Residues	Atoms				AltConf
20	E	1	Total	C	N	O	0
			14	8	1	5	
20	E	1	Total	C	N	O	0
			14	8	1	5	
20	E	1	Total	C	N	O	0
			14	8	1	5	
20	E	1	Total	C	N	O	0
			14	8	1	5	
20	E	1	Total	C	N	O	0
			14	8	1	5	
20	E	1	Total	C	N	O	0
			14	8	1	5	
20	F	1	Total	C	N	O	0
			14	8	1	5	
20	G	1	Total	C	N	O	0
			14	8	1	5	
20	G	1	Total	C	N	O	0
			14	8	1	5	
20	r	1	Total	C	N	O	0
			14	8	1	5	
20	r	1	Total	C	N	O	0
			14	8	1	5	
20	r	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
20	r	1	Total	C	N	O	0
			14	8	1	5	
20	r	1	Total	C	N	O	0
			14	8	1	5	
20	r	1	Total	C	N	O	0
			14	8	1	5	
20	f	1	Total	C	N	O	0
			14	8	1	5	
20	t	1	Total	C	N	O	0
			14	8	1	5	
20	t	1	Total	C	N	O	0
			14	8	1	5	
20	e	1	Total	C	N	O	0
			14	8	1	5	
20	e	1	Total	C	N	O	0
			14	8	1	5	
20	e	1	Total	C	N	O	0
			14	8	1	5	
20	e	1	Total	C	N	O	0
			14	8	1	5	
20	e	1	Total	C	N	O	0
			14	8	1	5	
20	e	1	Total	C	N	O	0
			14	8	1	5	
20	s	1	Total	C	N	O	0
			14	8	1	5	
20	g	1	Total	C	N	O	0
			14	8	1	5	
20	g	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 21 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).

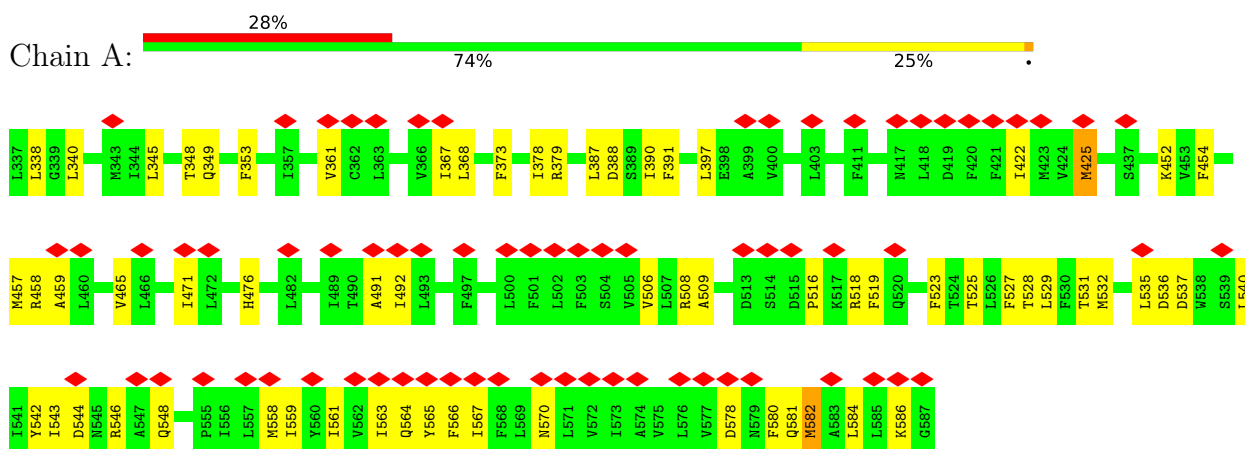


Mol	Chain	Residues	Atoms			AltConf
21	M	1	Total	C	O	0
			28	27	1	
21	z	1	Total	C	O	0
			28	27	1	
21	m	1	Total	C	O	0
			28	27	1	

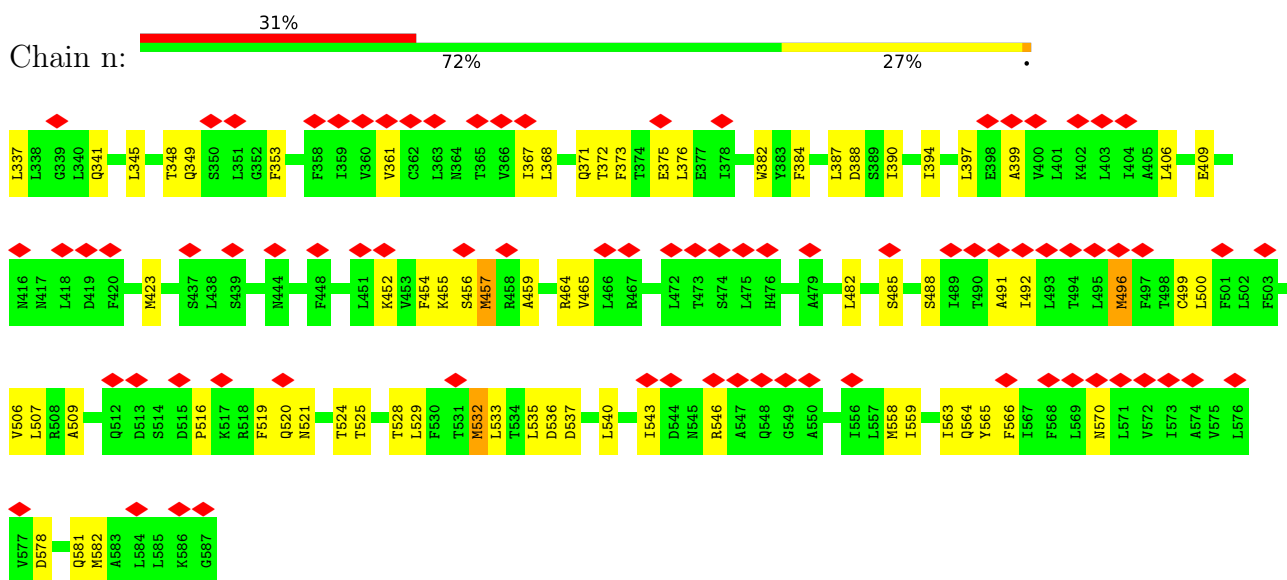
3 Residue-property plots

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

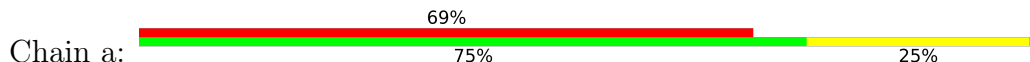
- Molecule 1: Cation channel sperm-associated protein 1

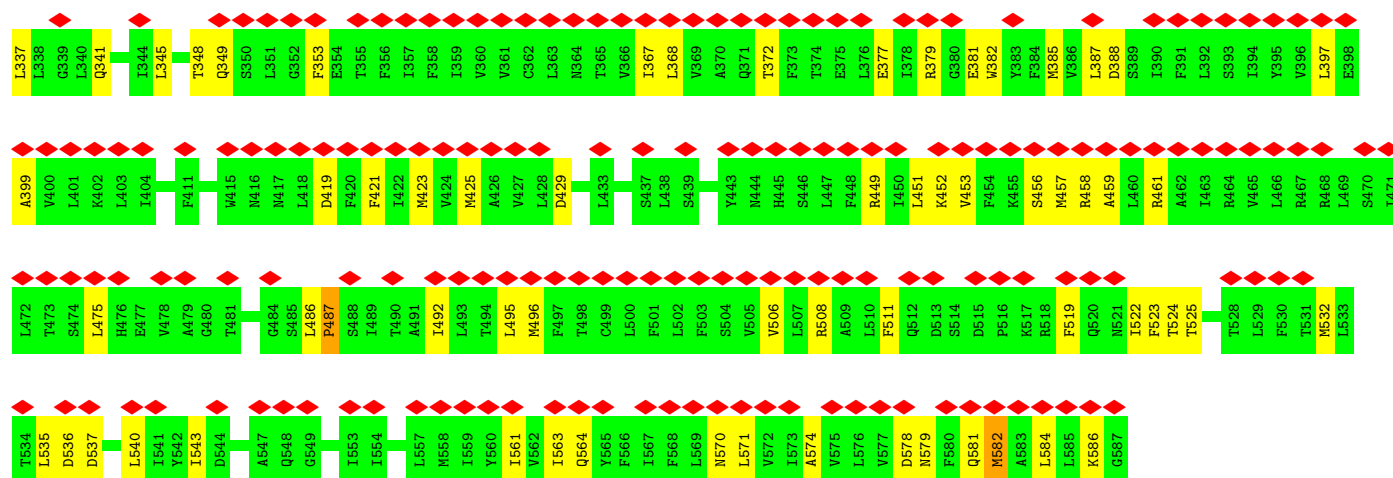


- Molecule 1: Cation channel sperm-associated protein 1

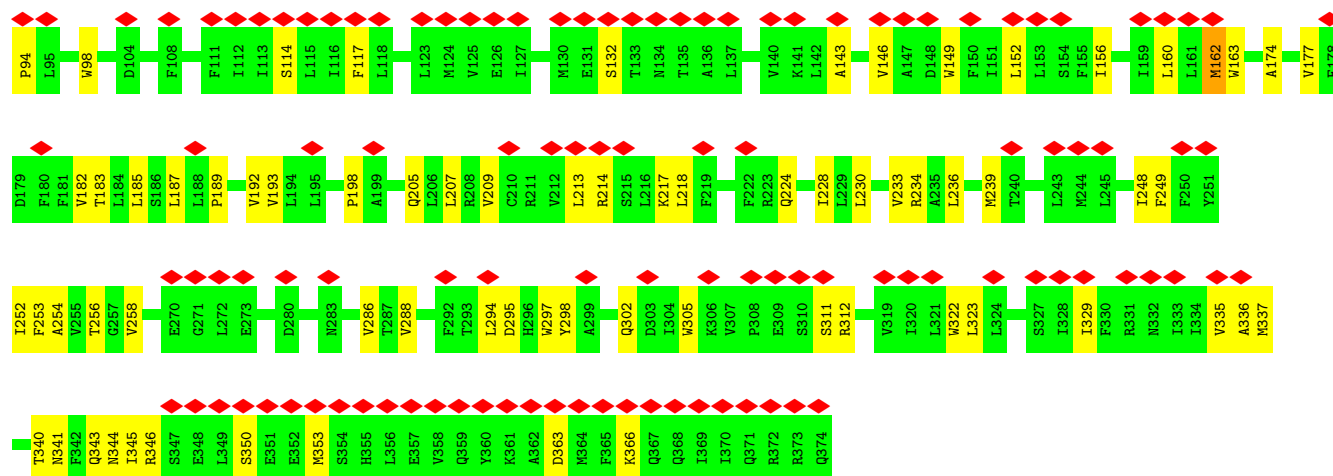
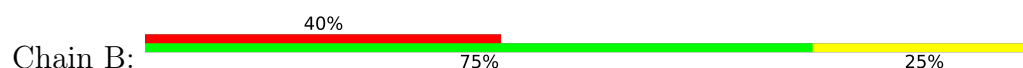


- Molecule 1: Cation channel sperm-associated protein 1

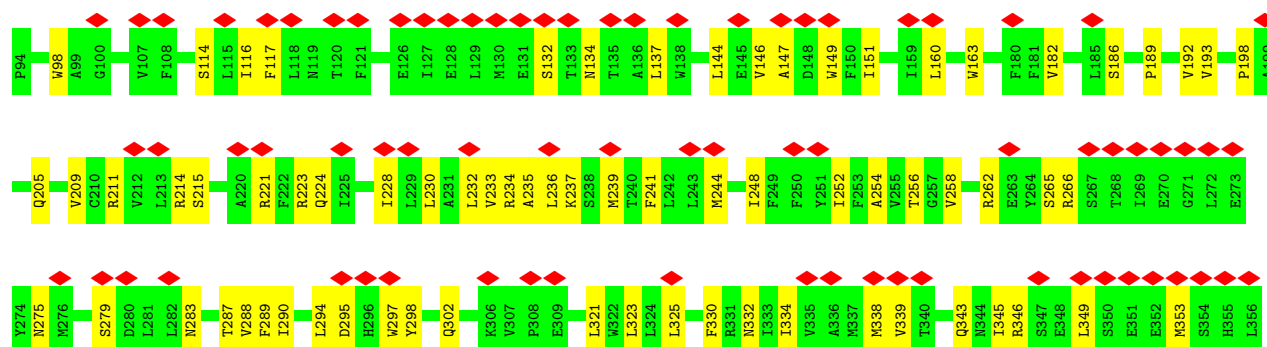
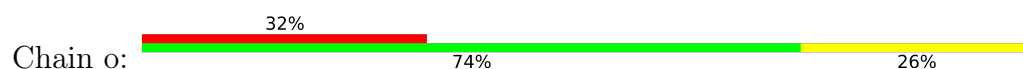


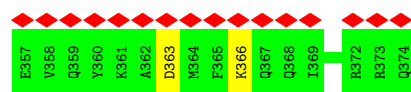


• Molecule 2: Cation channel sperm-associated protein 2

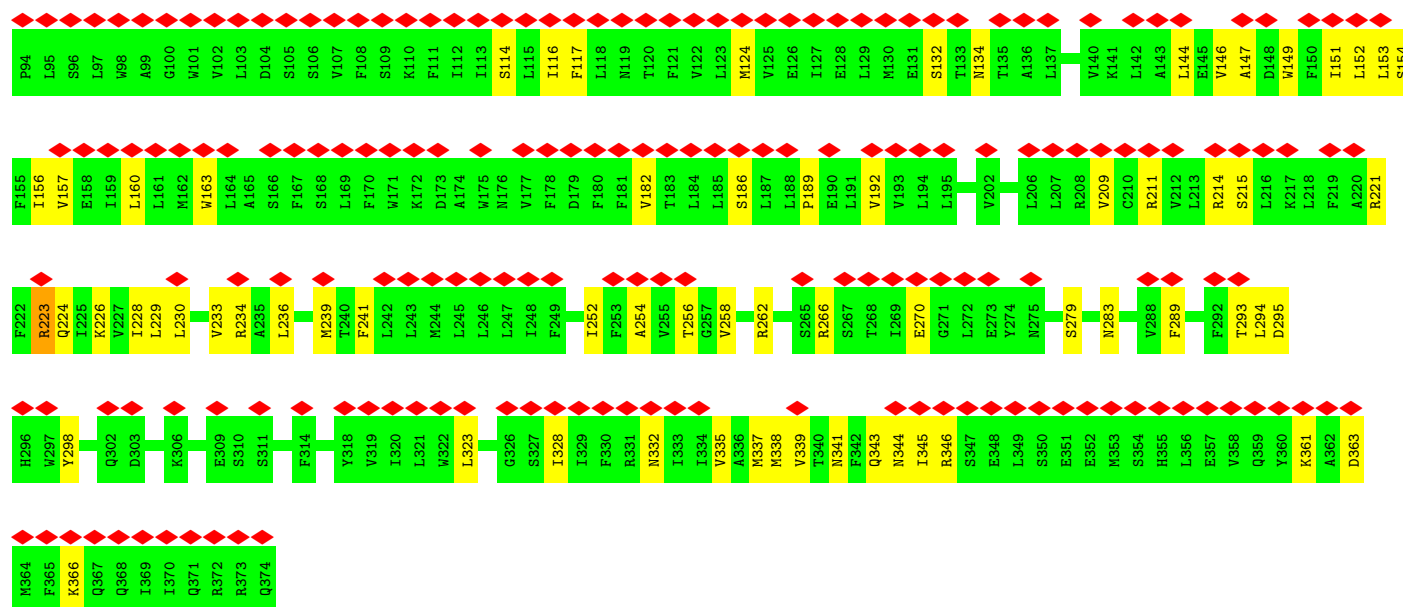
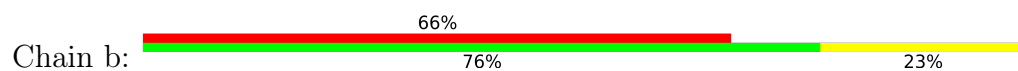


• Molecule 2: Cation channel sperm-associated protein 2

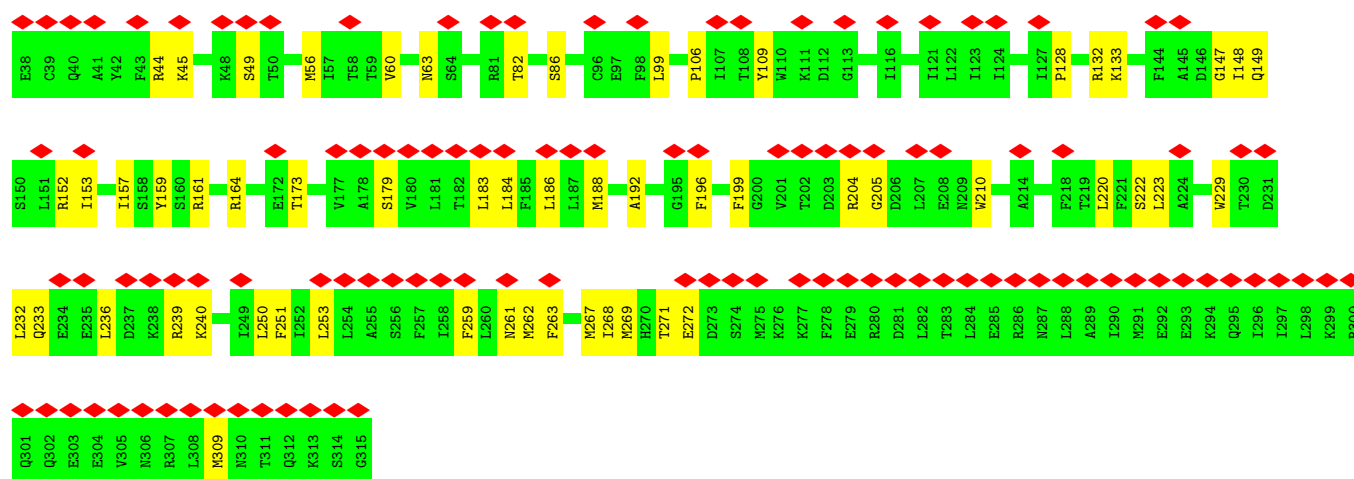
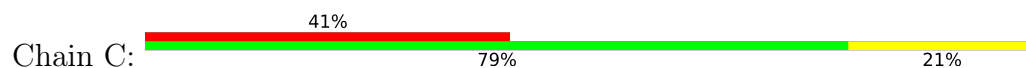




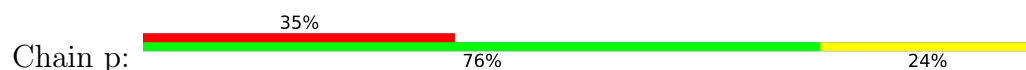
• Molecule 2: Cation channel sperm-associated protein 2

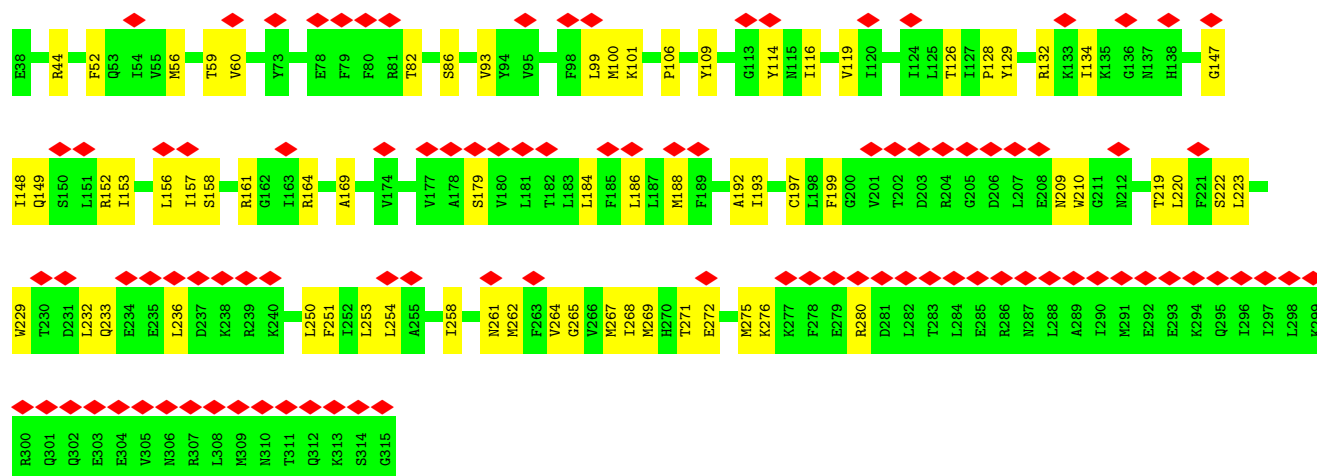


• Molecule 3: Cation channel sperm-associated protein 3

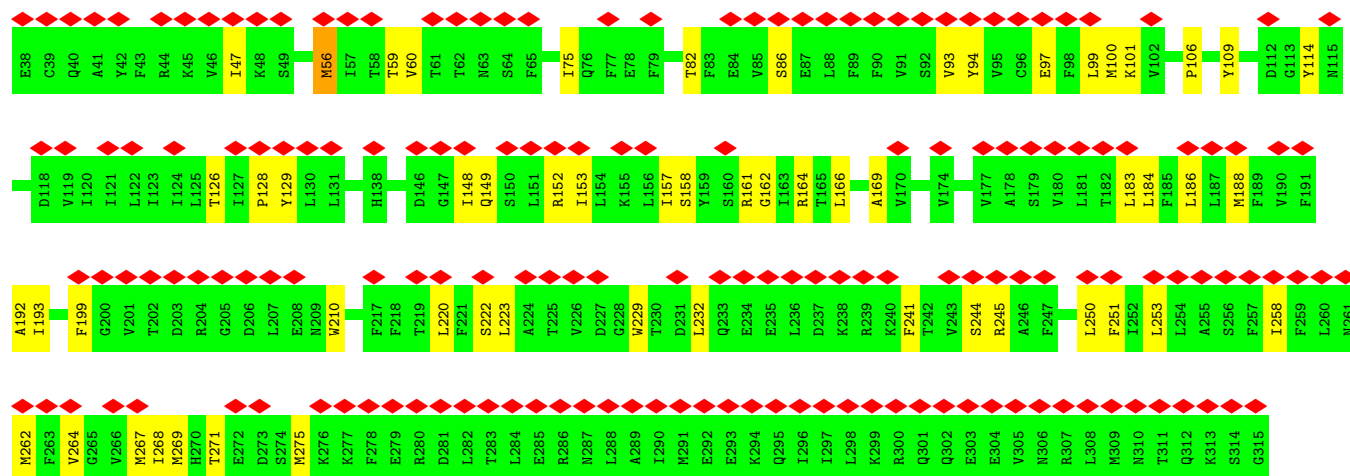
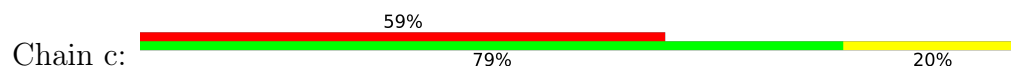


• Molecule 3: Cation channel sperm-associated protein 3

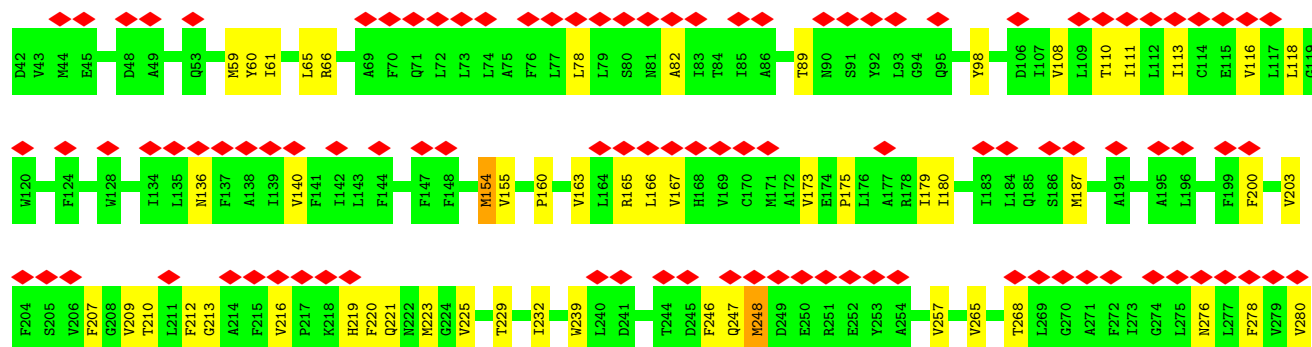
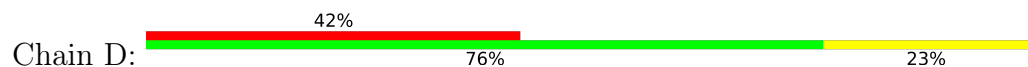


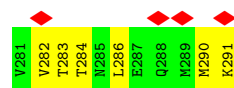


• Molecule 3: Cation channel sperm-associated protein 3

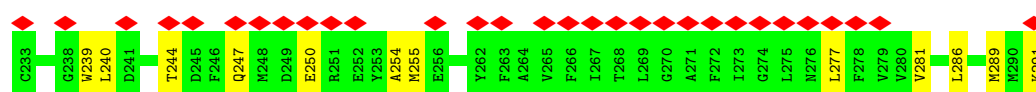
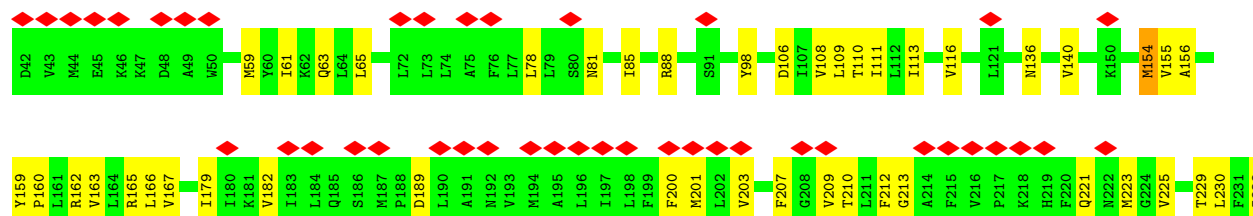
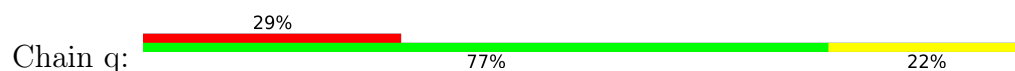


• Molecule 4: Cation channel sperm-associated protein 4

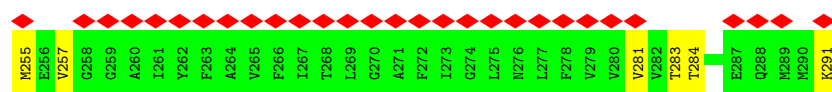
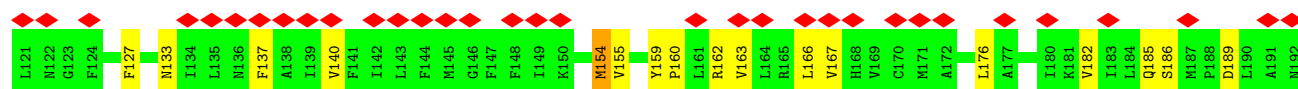
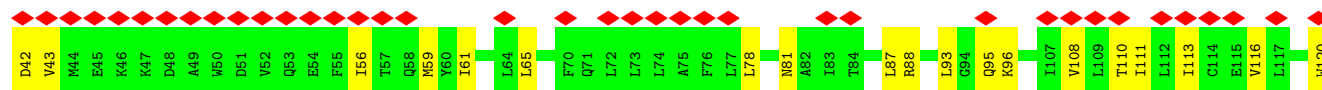
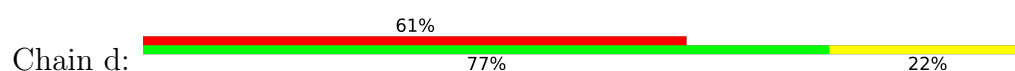




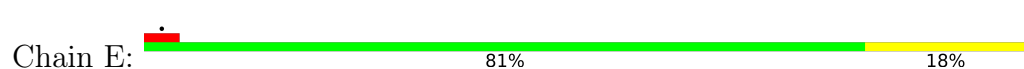
• Molecule 4: Cation channel sperm-associated protein 4

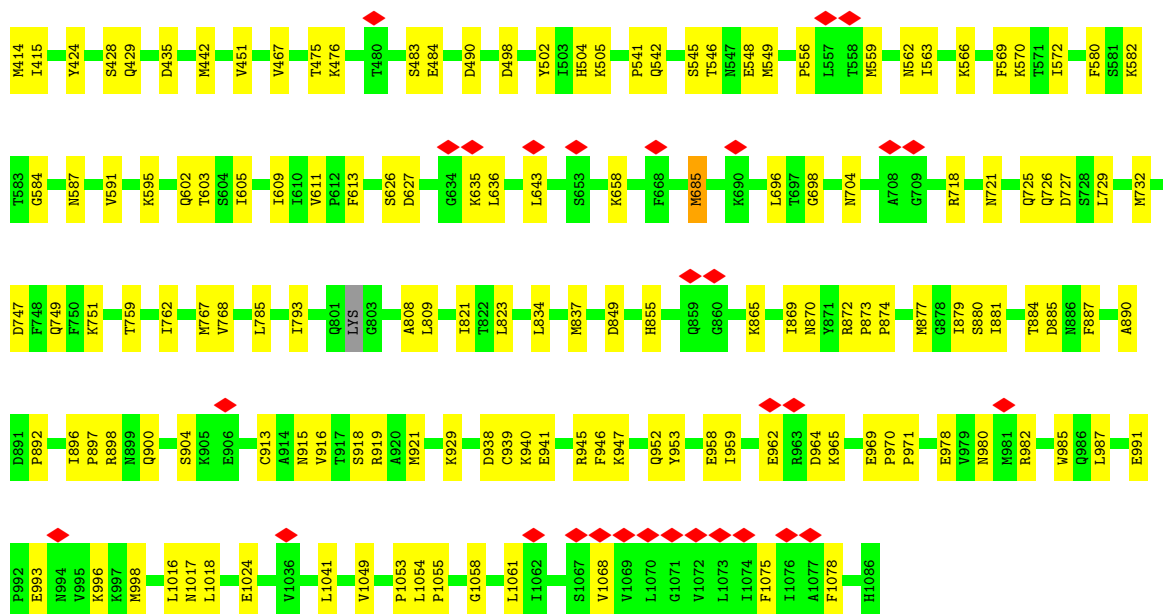


• Molecule 4: Cation channel sperm-associated protein 4



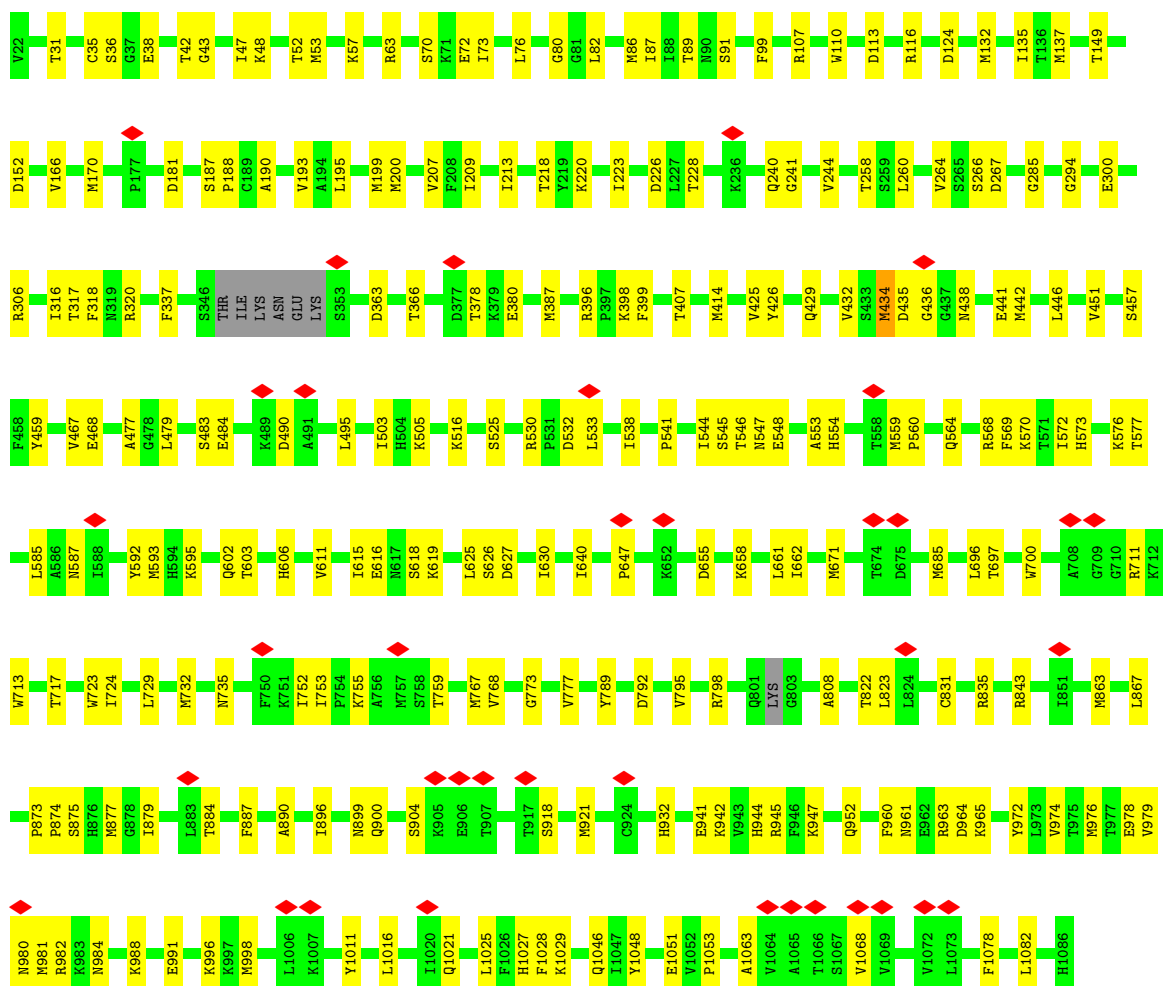
• Molecule 5: Cation channel sperm-associated auxiliary subunit beta



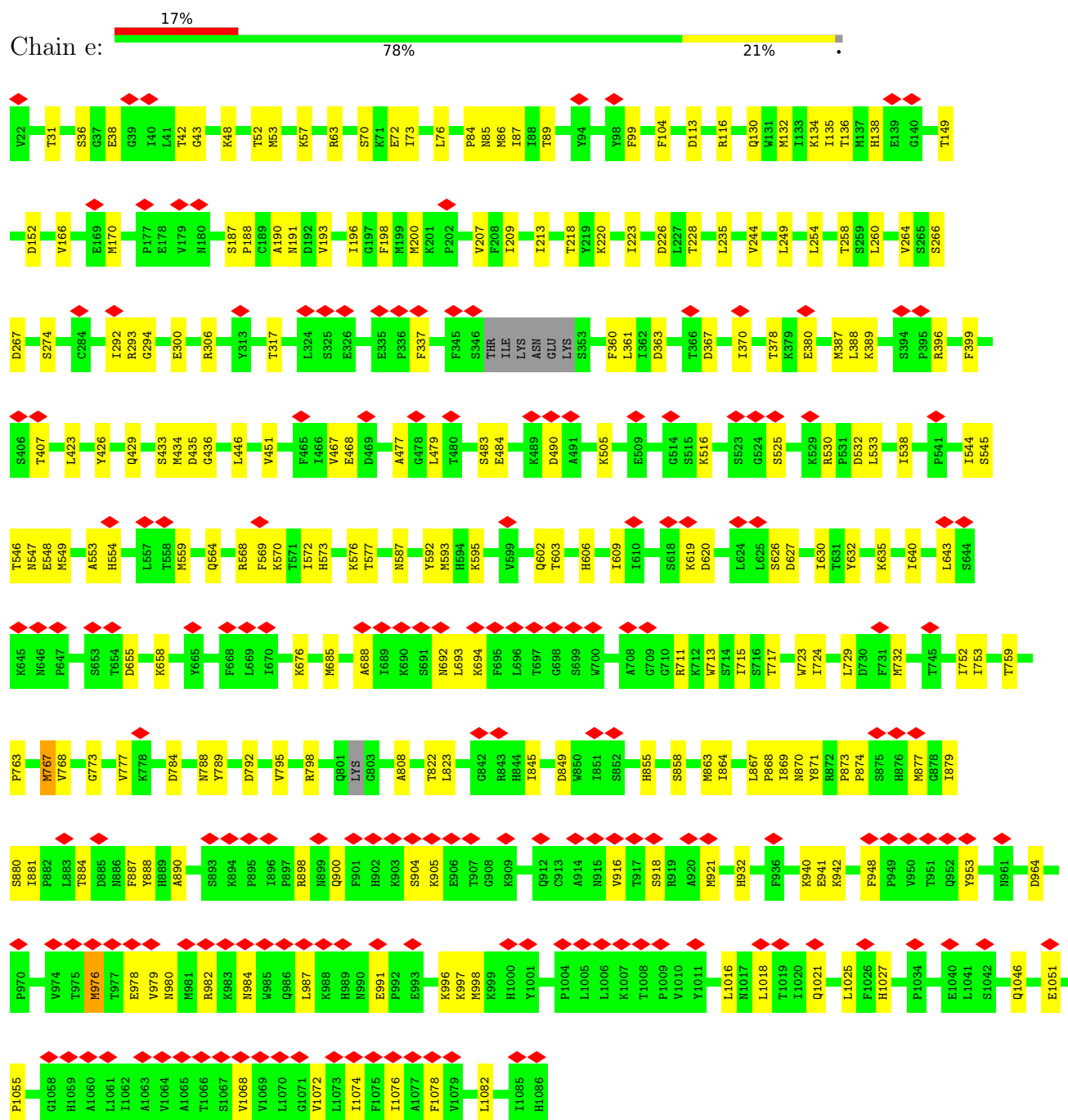


• Molecule 5: Cation channel sperm-associated auxiliary subunit beta

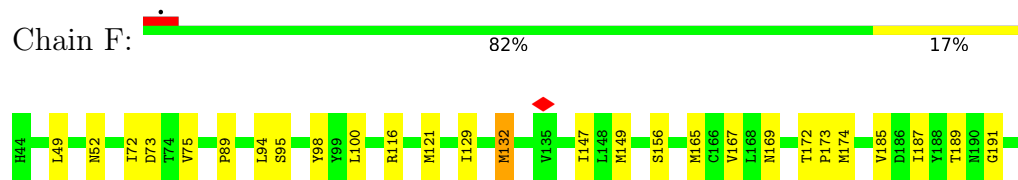
Chain r: 77% 22%

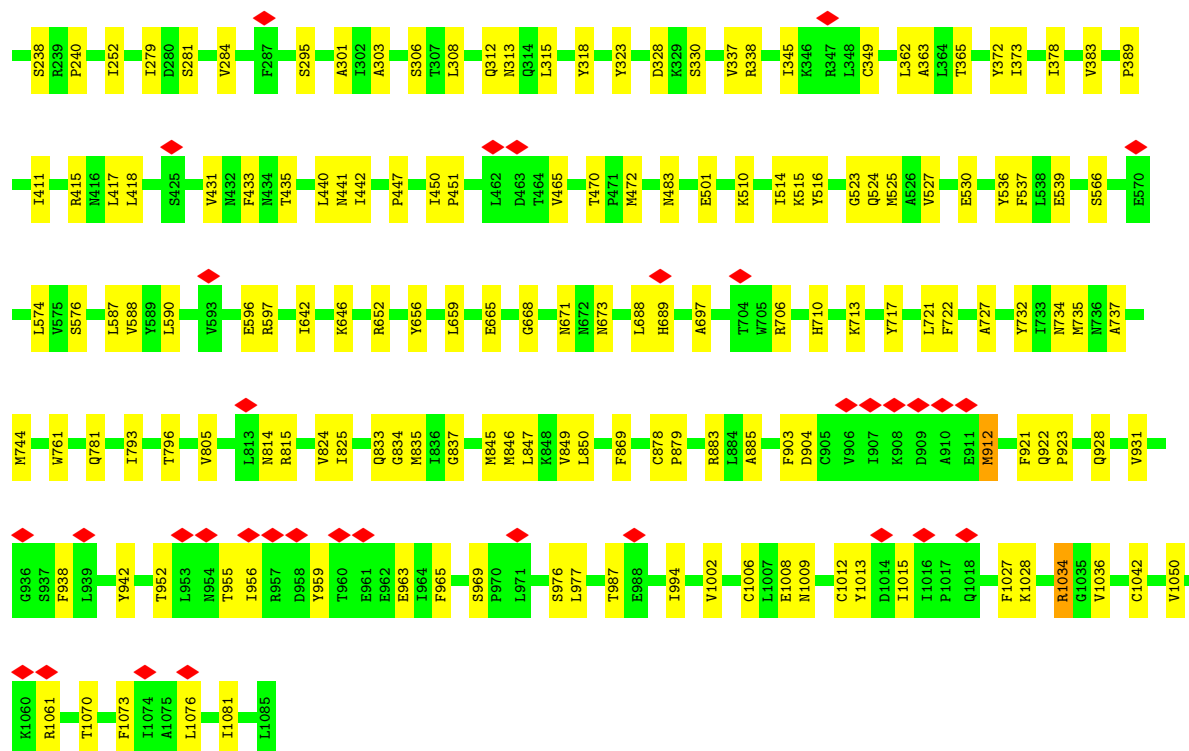


• Molecule 5: Cation channel sperm-associated auxiliary subunit beta

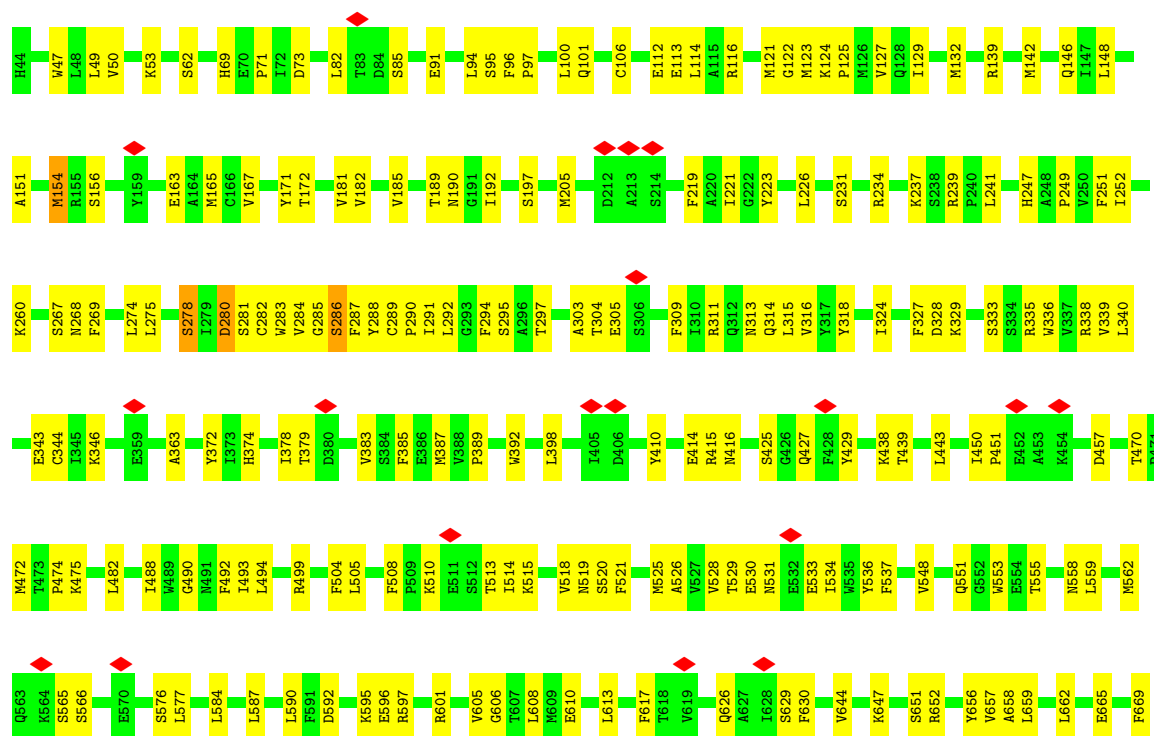


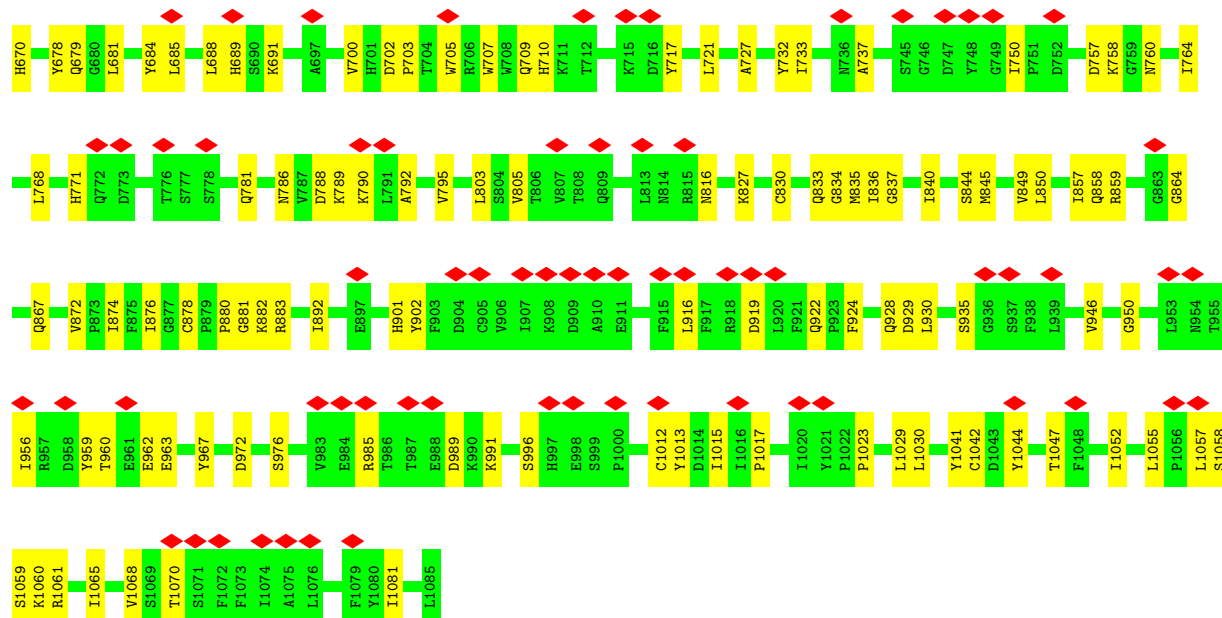
• Molecule 6: Cation channel sperm-associated auxiliary subunit gamma 2



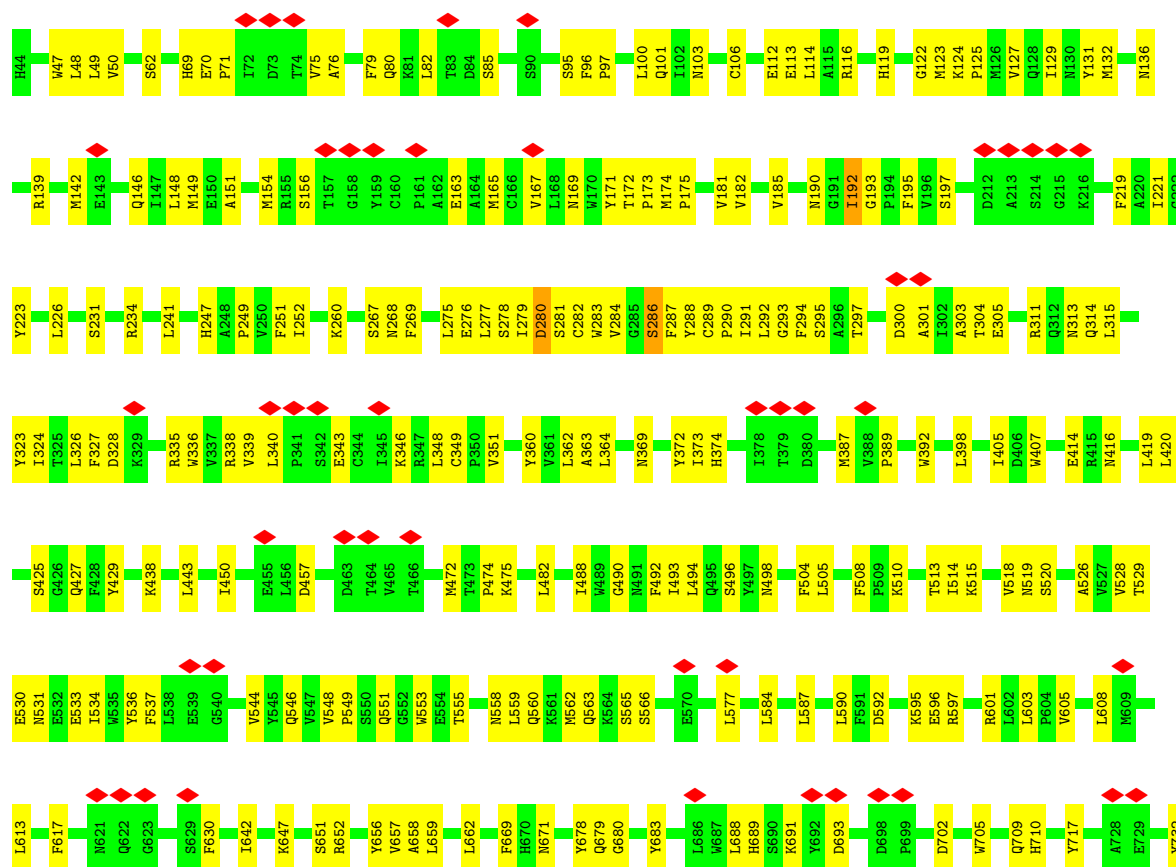


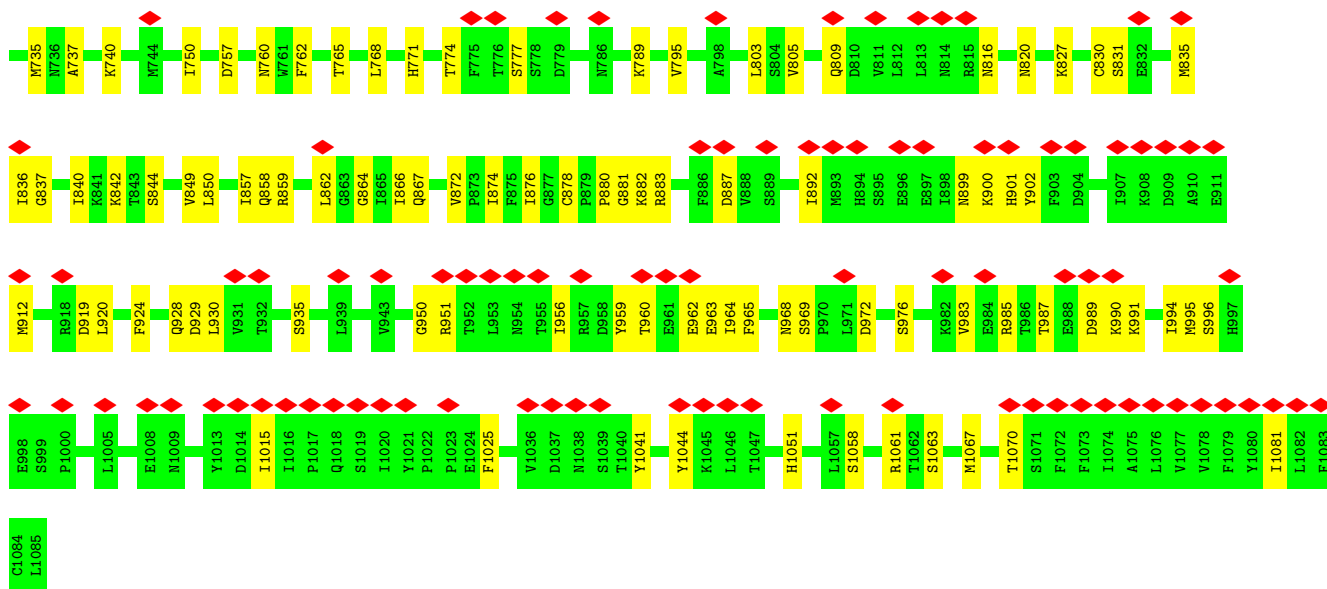
• Molecule 6: Cation channel sperm-associated auxiliary subunit gamma 2



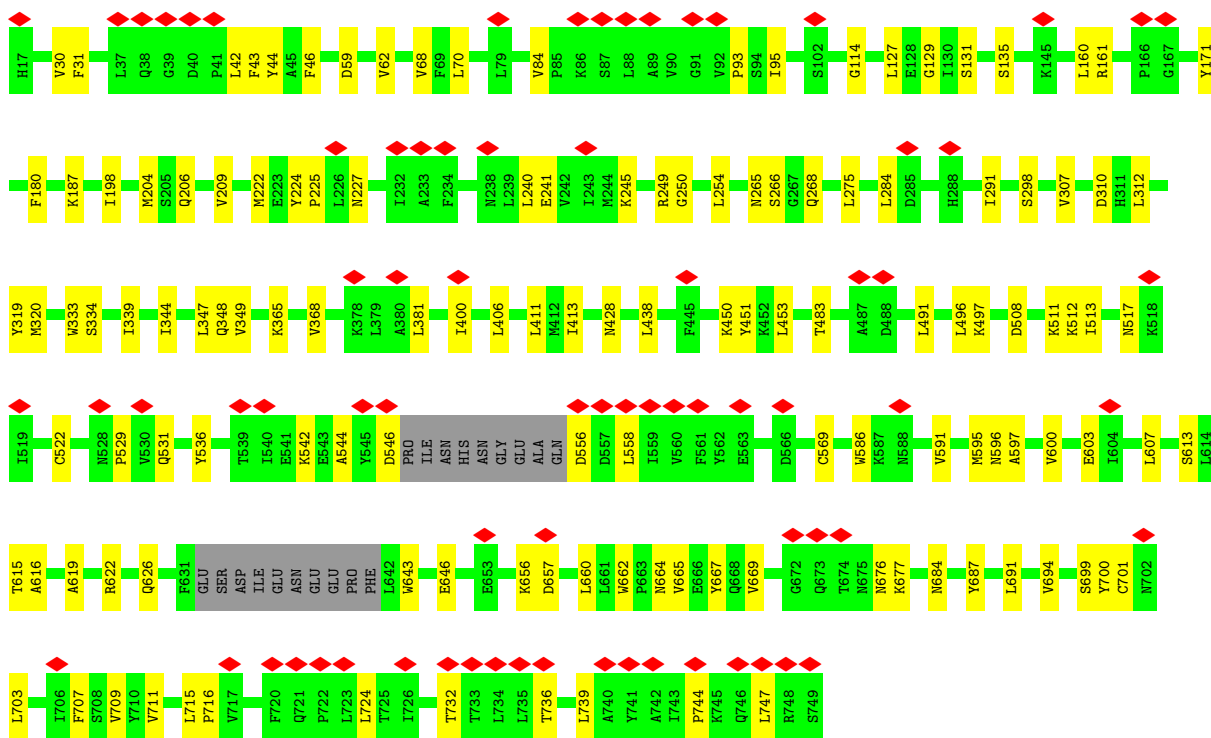
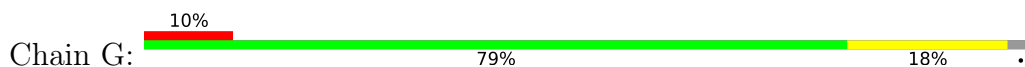


• Molecule 6: Cation channel sperm-associated auxiliary subunit gamma 2

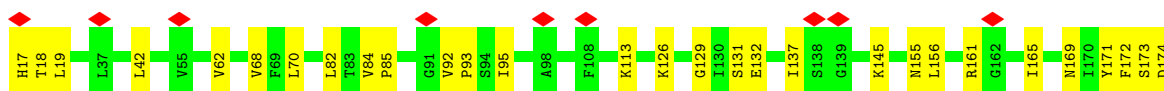


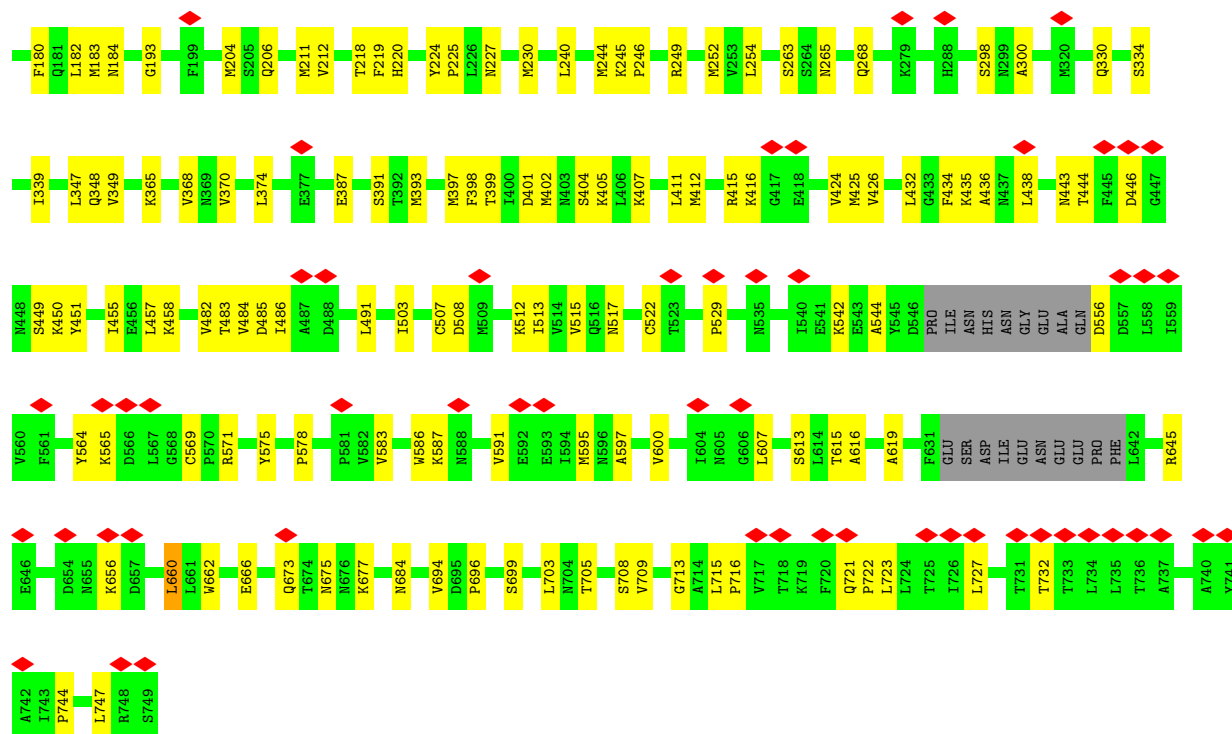


• Molecule 7: Cation channel sperm-associated auxiliary subunit delta

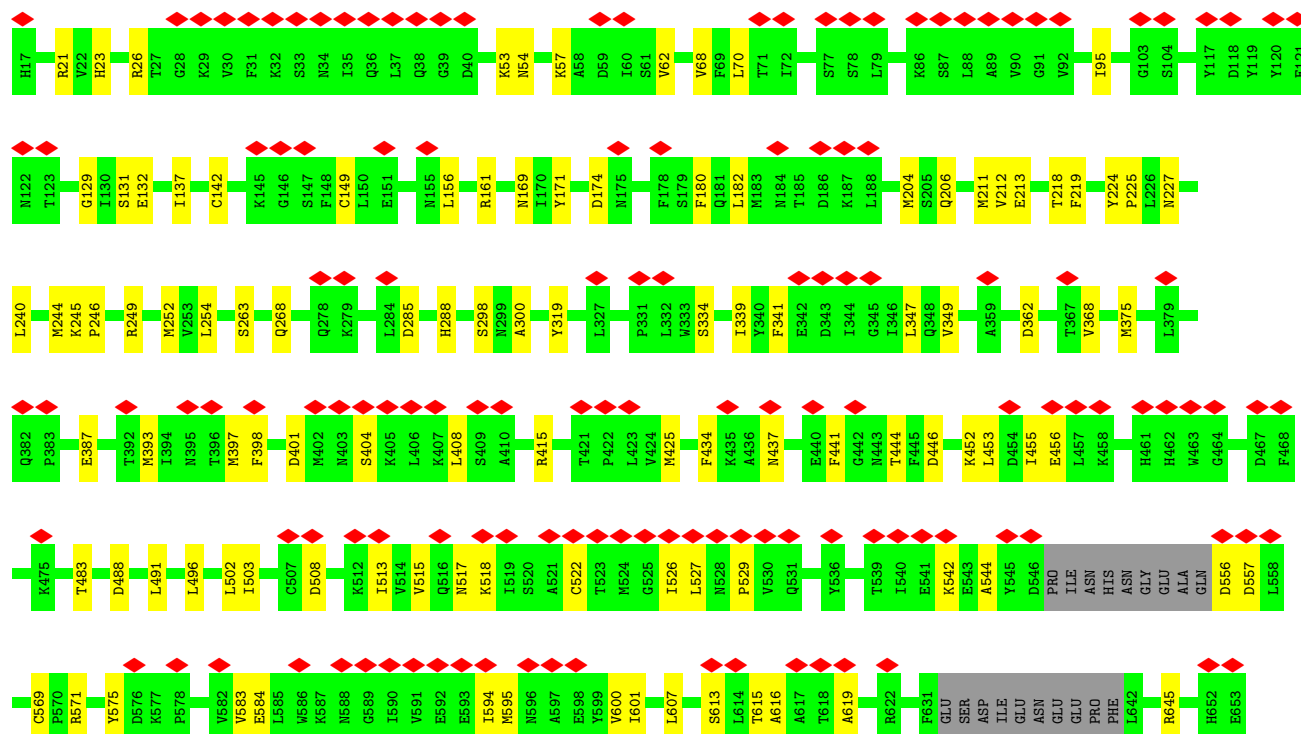
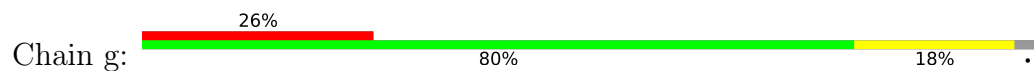


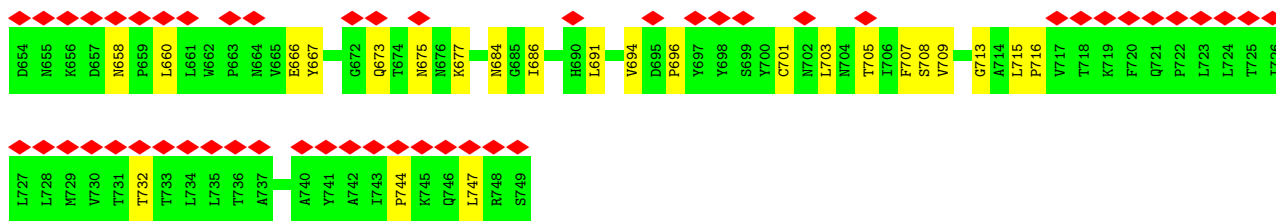
• Molecule 7: Cation channel sperm-associated auxiliary subunit delta



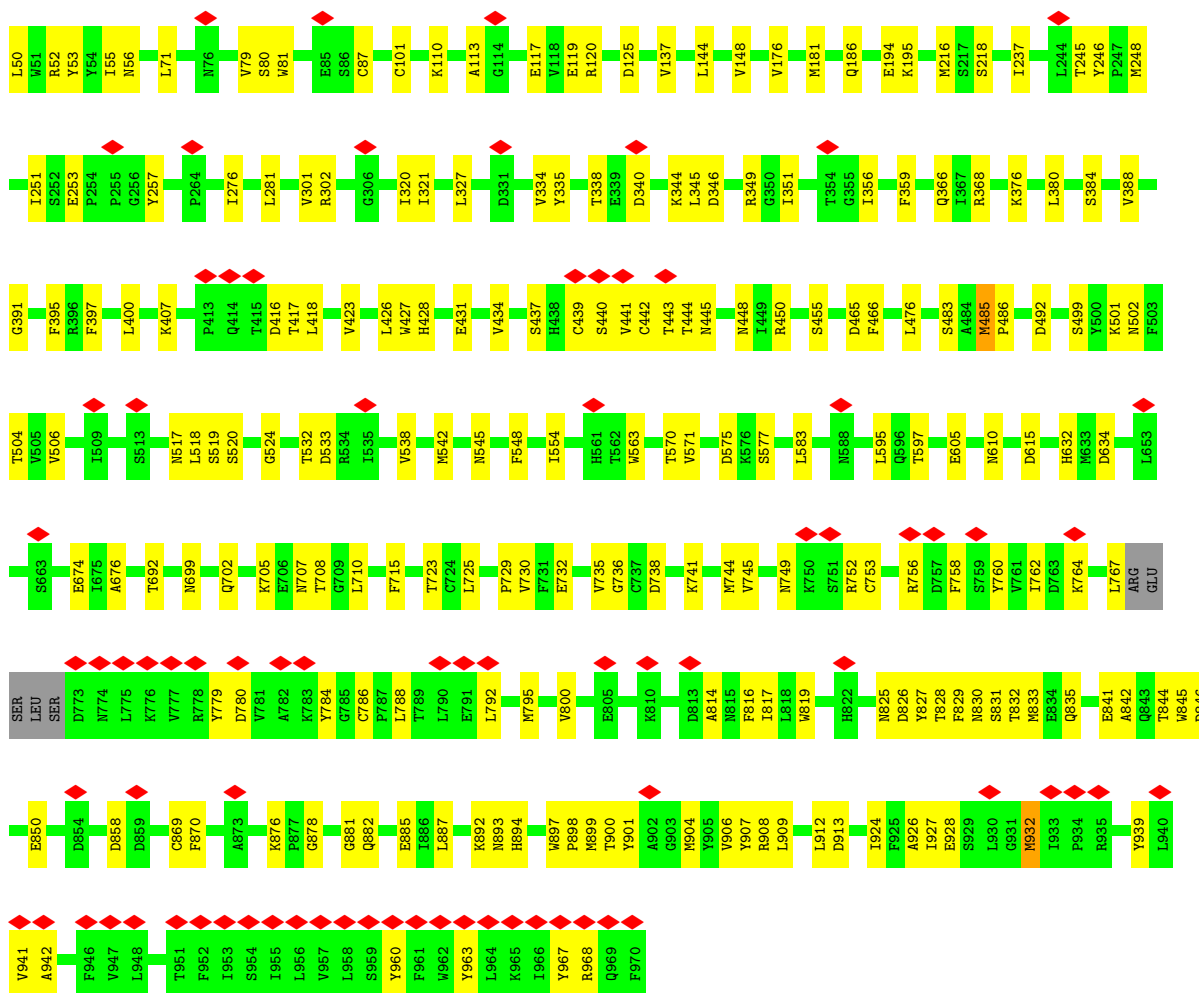
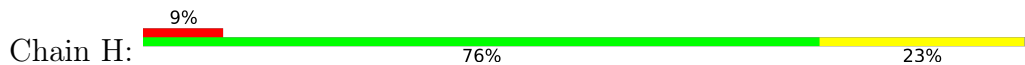


• Molecule 7: Cation channel sperm-associated auxiliary subunit delta

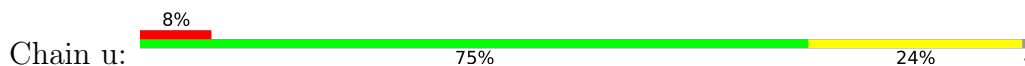


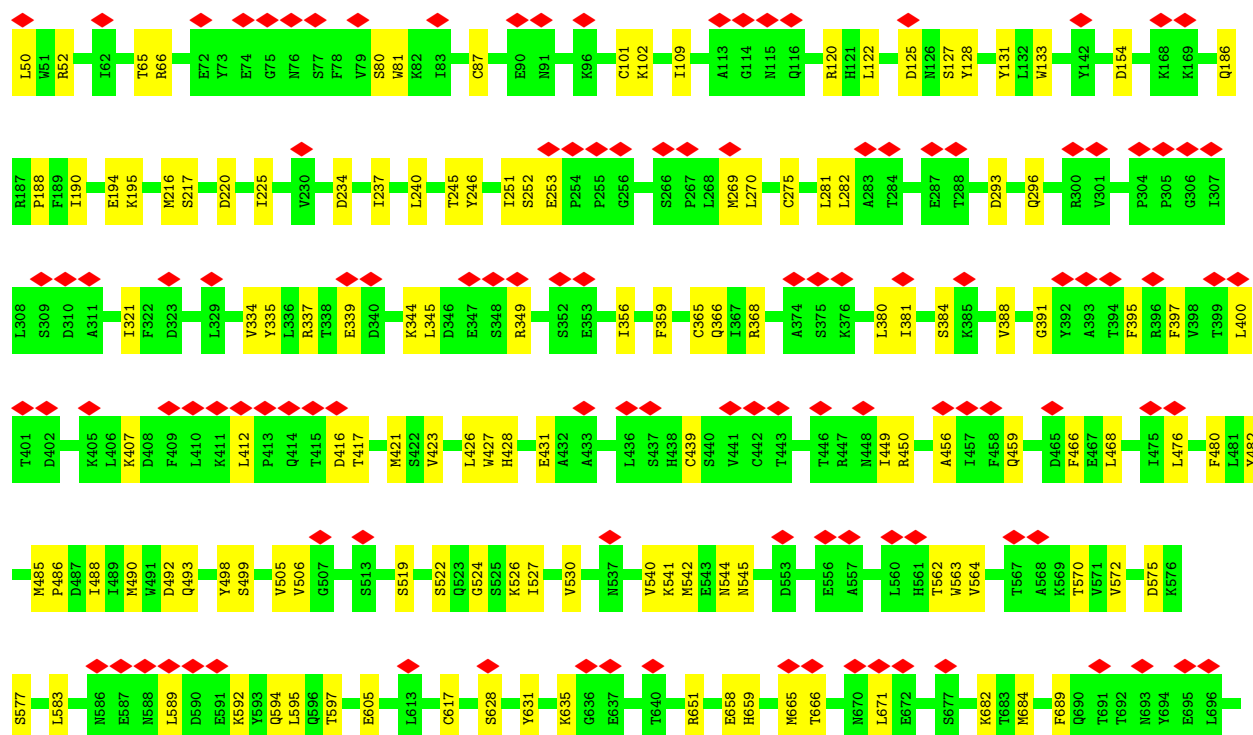


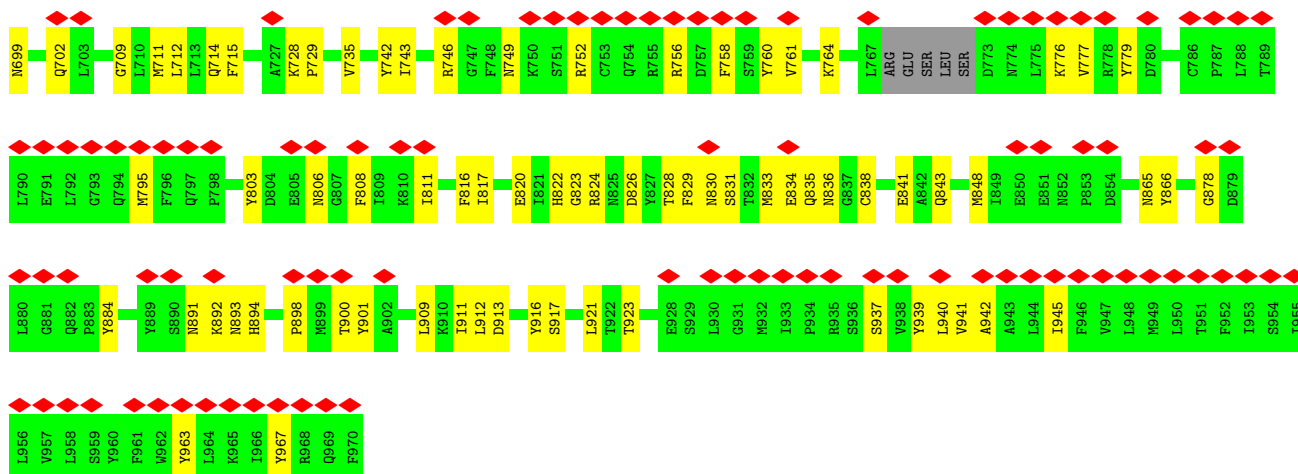
• Molecule 8: Cation channel sperm-associated auxiliary subunit epsilon



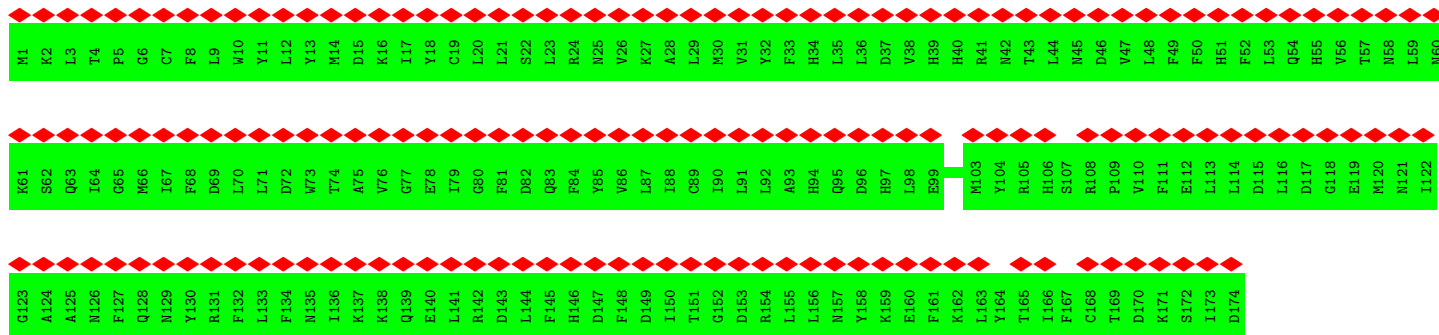
• Molecule 8: Cation channel sperm-associated auxiliary subunit epsilon



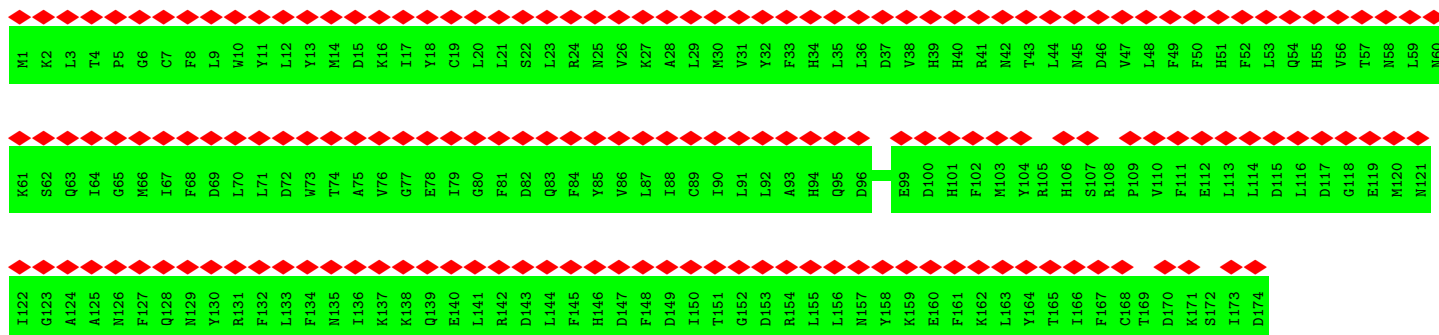




• Molecule 9: EF-hand calcium-binding domain-containing protein 9

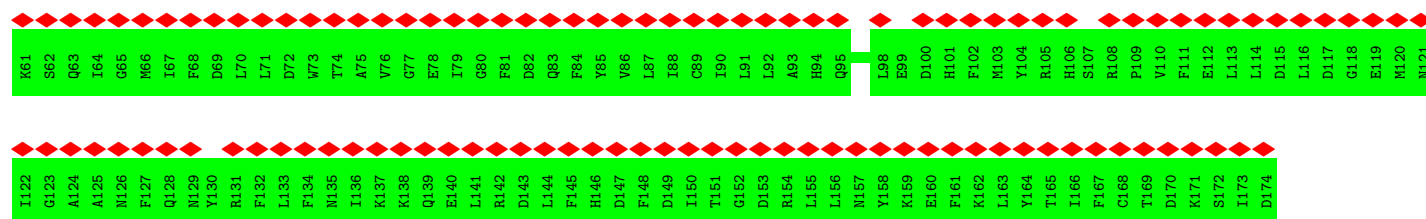


• Molecule 9: EF-hand calcium-binding domain-containing protein 9

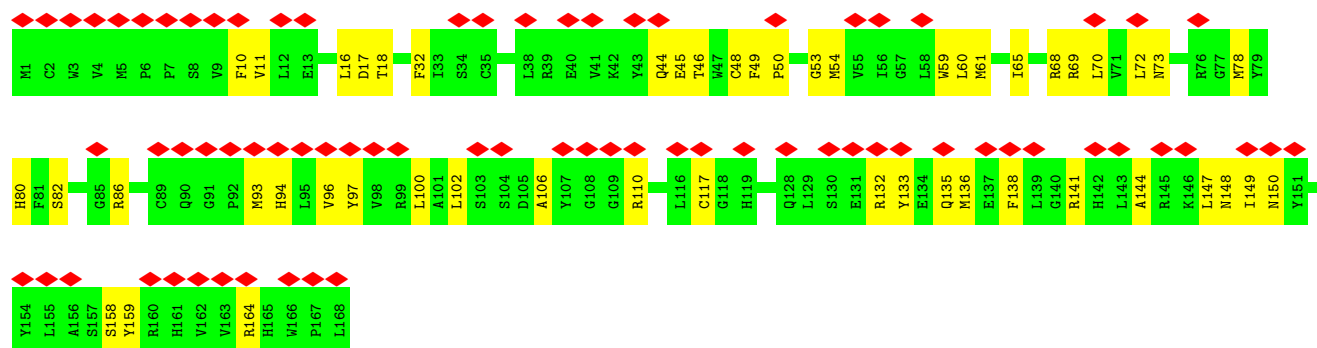
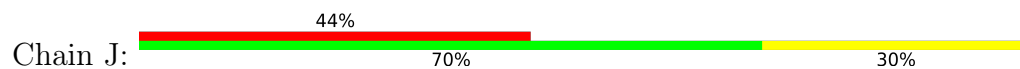


• Molecule 9: EF-hand calcium-binding domain-containing protein 9

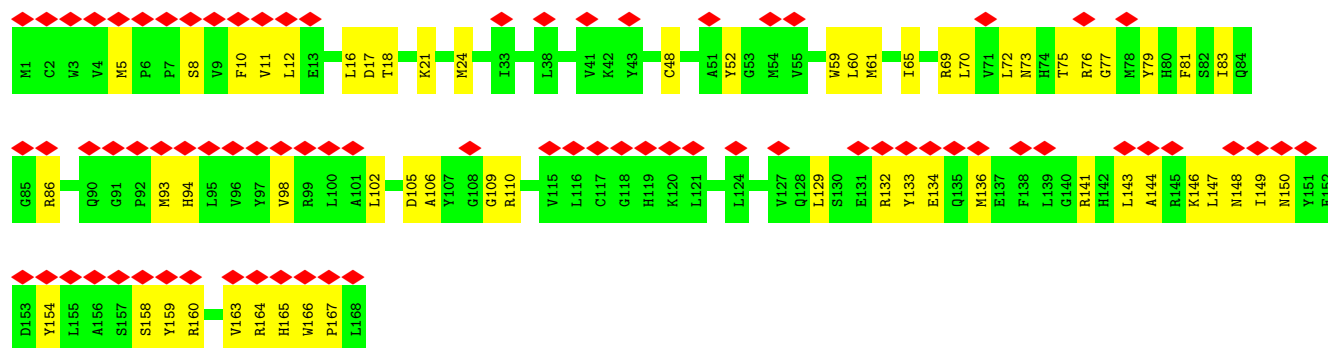




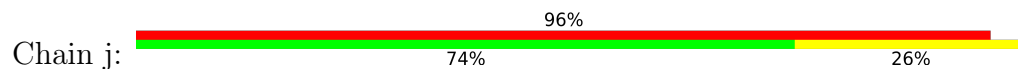
• Molecule 10: Cation channel sperm-associated auxiliary subunit TMEM249

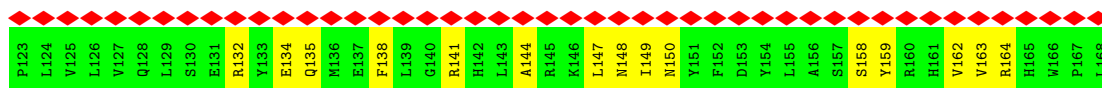


• Molecule 10: Cation channel sperm-associated auxiliary subunit TMEM249

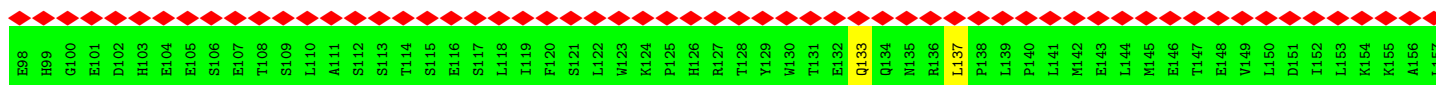
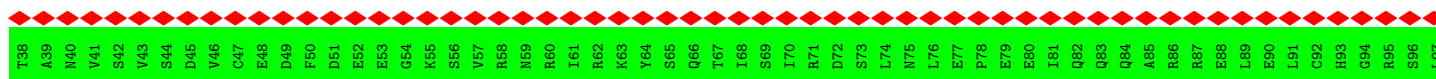


• Molecule 10: Cation channel sperm-associated auxiliary subunit TMEM249

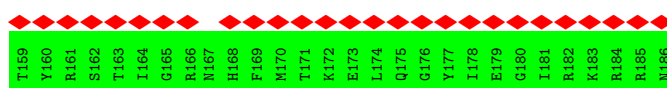
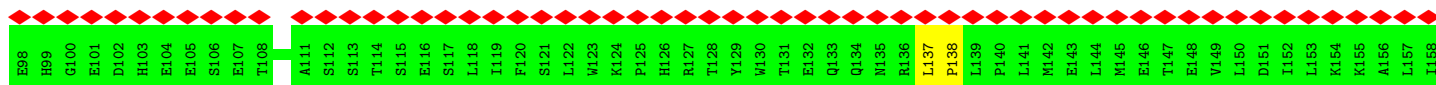
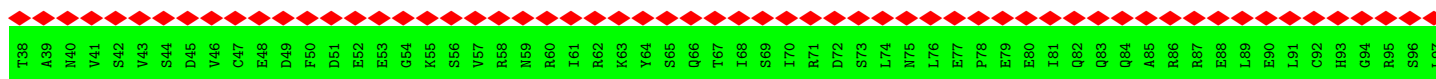




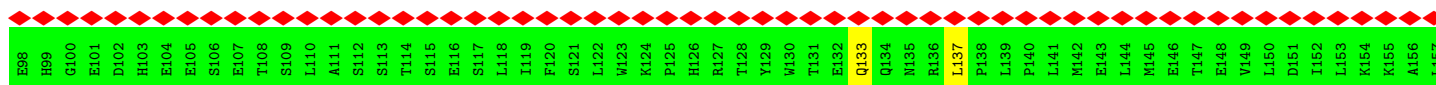
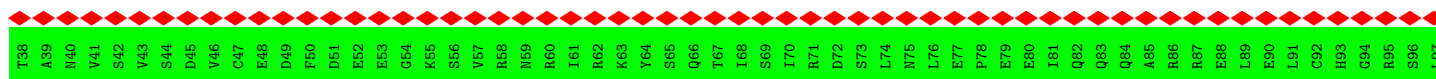
- Molecule 11: Cation channel sperm-associated auxiliary subunit zeta



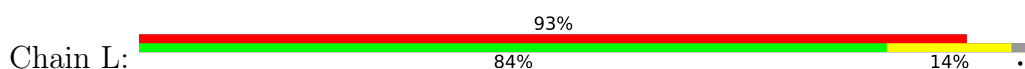
- Molecule 11: Cation channel sperm-associated auxiliary subunit zeta

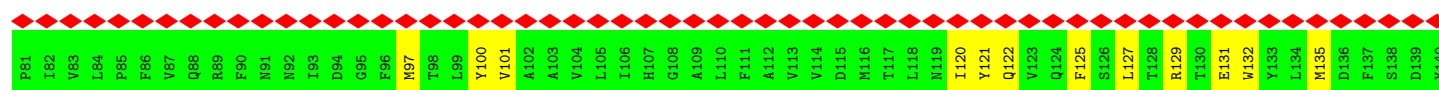


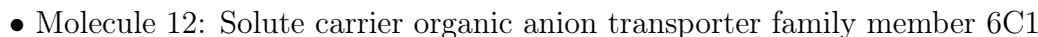
- Molecule 11: Cation channel sperm-associated auxiliary subunit zeta



- Molecule 12: Solute carrier organic anion transporter family member 6C1

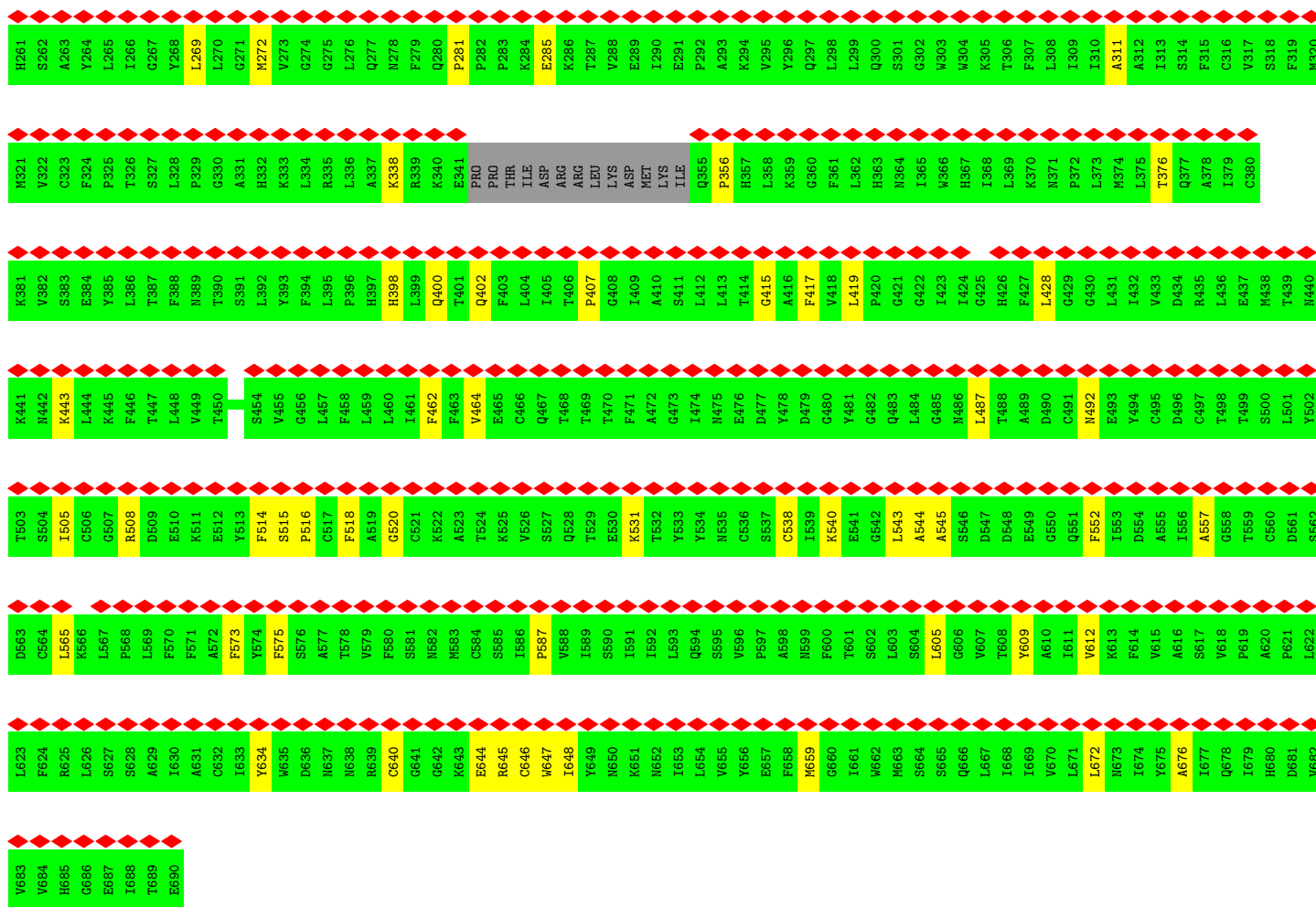




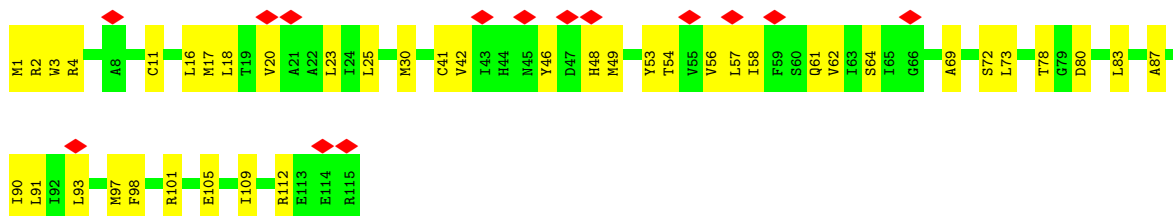


Response	Percentage
Agree	97%
Disagree	85%
Don't know	12%

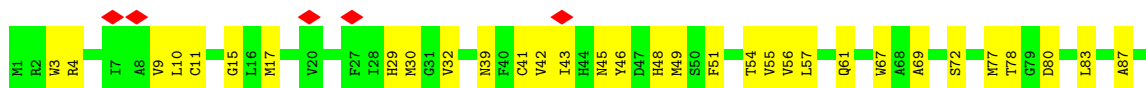




• Molecule 13: Cation channel sperm-associated auxiliary subunit TMEM262

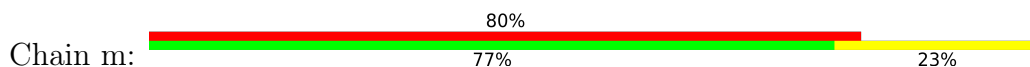


• Molecule 13: Cation channel sperm-associated auxiliary subunit TMEM262

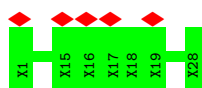




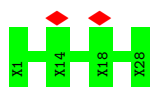
- Molecule 13: Cation channel sperm-associated auxiliary subunit TMEM262



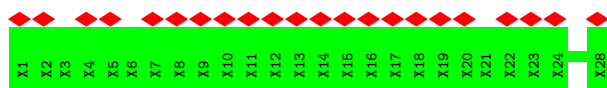
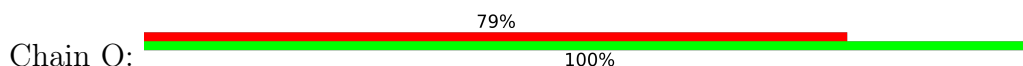
- Molecule 14: Unknown protein



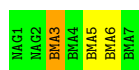
- Molecule 14: Unknown protein



- Molecule 14: Unknown protein

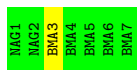


- Molecule 15: beta-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

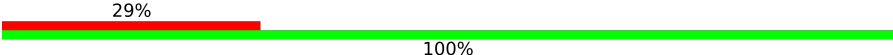


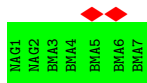
- Molecule 15: beta-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:  86% 14%



- Molecule 15: beta-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-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 AA:  29% 100%



- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  33% 67%



- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  67% 33%



- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  67% 100%



- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  33% 100%



- Molecule 16: 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 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:  33% 67% 33%



- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:  67% 100%



- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:  33% 100%



- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:  100%

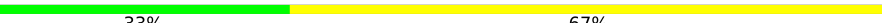


- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:  100%



- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA:  33% 67%



- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 16: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 17: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



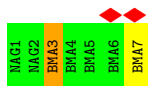
- Molecule 17: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

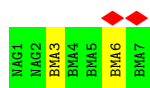


- Molecule 18: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

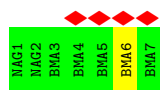
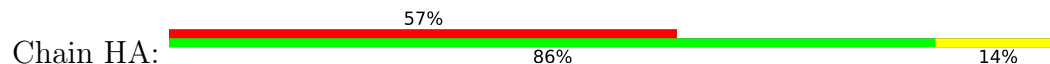


- Molecule 18: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

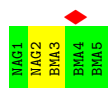
lucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



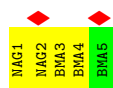
● Molecule 18: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



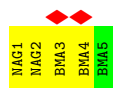
● Molecule 19: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 19: beta-D-mannopyranose-(1-3)-[beta-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



● Molecule 19: beta-D-mannopyranose-(1-3)-[beta-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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69708	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.000	Depositor
Minimum map value	-0.376	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.245	Depositor
Map size (Å)	652.2, 652.2, 652.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: CLR, NAG, BMA

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	0.24	0/2100	0.63	3/2855 (0.1%)
1	a	0.30	0/2100	0.63	2/2855 (0.1%)
1	n	0.26	0/2100	0.64	6/2855 (0.2%)
2	B	0.19	0/2406	0.50	1/3270 (0.0%)
2	b	0.19	0/2406	0.49	1/3270 (0.0%)
2	o	0.20	0/2406	0.49	0/3270
3	C	0.19	0/2324	0.45	0/3141
3	c	0.21	0/2324	0.47	1/3141 (0.0%)
3	p	0.19	0/2324	0.45	0/3141
4	D	0.23	0/2087	0.61	3/2835 (0.1%)
4	d	0.21	0/2087	0.57	1/2835 (0.0%)
4	q	0.24	0/2087	0.59	2/2835 (0.1%)
5	E	0.23	0/8746	0.51	3/11874 (0.0%)
5	e	0.22	1/8746 (0.0%)	0.53	3/11874 (0.0%)
5	r	0.20	0/8746	0.51	6/11874 (0.1%)
6	F	0.21	0/8695	0.47	4/11809 (0.0%)
6	f	0.28	1/8695 (0.0%)	0.55	6/11809 (0.1%)
6	s	0.28	1/8695 (0.0%)	0.55	6/11809 (0.1%)
7	G	0.18	0/5823	0.48	0/7921
7	g	0.17	0/5823	0.46	0/7921
7	t	0.18	0/5823	0.48	0/7921
8	H	0.20	0/7706	0.51	4/10491 (0.0%)
8	h	0.17	0/7706	0.48	1/10491 (0.0%)
8	u	0.18	0/7706	0.49	0/10491
9	I	0.11	0/862	0.34	0/1201
9	Q	0.11	0/862	0.34	0/1201
9	i	0.11	0/862	0.34	0/1201
10	J	0.23	0/1441	0.60	0/1955
10	j	0.20	0/1441	0.59	0/1955
10	w	0.25	0/1441	0.65	1/1955 (0.1%)
11	K	0.12	0/755	0.32	0/1051
11	k	0.11	0/755	0.31	0/1051

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	x	0.14	0/755	0.38	0/1051
12	L	0.18	0/4817	0.43	0/6543
12	l	0.18	0/4817	0.43	0/6543
12	y	0.18	0/4817	0.43	0/6543
13	M	0.19	0/961	0.53	0/1299
13	m	0.19	0/961	0.54	0/1299
13	z	0.27	0/961	0.62	0/1299
All	All	0.21	3/146169 (0.0%)	0.51	54/198735 (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	1
1	n	0	1
5	E	0	1
5	e	0	2
5	r	0	1
6	f	0	3
7	G	0	1
7	g	0	1
7	t	0	1
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	280	ASP	CA-C	-7.04	1.43	1.53
6	s	280	ASP	CA-C	-6.28	1.44	1.52
5	e	388	LEU	CG-CD2	-5.41	1.34	1.52

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	MET	CG-SD-CE	-11.14	76.38	100.90
5	r	647	PRO	CA-N-CD	-10.56	97.21	112.00
1	a	487	PRO	CA-N-CD	-9.88	98.17	112.00
8	H	485	MET	CG-SD-CE	-7.99	83.32	100.90
8	H	485	MET	CB-CA-C	7.90	119.66	108.68

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	916	VAL	Peptide
7	G	660	LEU	Peptide
6	f	278	SER	Mainchain
1	n	372	THR	Peptide
5	r	468	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2053	0	2142	55	0
1	a	2053	0	2142	53	0
1	n	2053	0	2142	54	0
2	B	2343	0	2435	56	0
2	b	2343	0	2435	52	0
2	o	2343	0	2435	57	0
3	C	2277	0	2339	48	0
3	c	2277	0	2339	41	0
3	p	2277	0	2339	51	0
4	D	2035	0	2088	47	0
4	d	2035	0	2088	46	0
4	q	2035	0	2088	49	0
5	E	8510	0	8442	128	0
5	e	8510	0	8442	148	0
5	r	8510	0	8442	157	0
6	F	8454	0	8307	116	0
6	f	8454	0	8308	241	0
6	s	8454	0	8309	258	0
7	G	5680	0	5597	83	0
7	g	5680	0	5597	85	0
7	t	5680	0	5597	108	0
8	H	7502	0	7358	144	0
8	h	7502	0	7358	134	0
8	u	7502	0	7358	143	0
9	I	863	0	370	0	0
9	Q	863	0	370	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	i	863	0	370	0	0
10	J	1398	0	1410	39	0
10	j	1398	0	1410	29	0
10	w	1398	0	1410	41	0
11	K	755	0	351	1	0
11	k	755	0	351	1	0
11	x	755	0	351	1	0
12	L	4694	0	4700	52	0
12	l	4694	0	4700	49	0
12	y	4694	0	4700	62	0
13	M	936	0	943	38	0
13	m	936	0	943	21	0
13	z	936	0	943	31	0
14	N	140	0	31	0	0
14	O	140	0	31	0	0
14	P	140	0	31	0	0
15	0	83	0	70	0	0
15	AA	83	0	70	0	0
15	R	83	0	70	1	0
16	1	39	0	34	1	0
16	2	39	0	34	0	0
16	4	39	0	34	0	0
16	5	39	0	34	0	0
16	6	39	0	34	0	0
16	BA	39	0	34	1	0
16	CA	39	0	34	0	0
16	EA	39	0	34	0	0
16	FA	39	0	34	0	0
16	GA	39	0	34	0	0
16	S	39	0	34	1	0
16	T	39	0	34	0	0
16	V	39	0	34	0	0
16	W	39	0	34	0	0
16	X	39	0	34	0	0
17	3	28	0	25	0	0
17	8	28	0	25	1	0
17	DA	28	0	25	0	0
17	IA	28	0	25	2	0
17	U	28	0	25	2	0
17	Z	28	0	25	1	0
18	7	83	0	70	0	0
18	HA	83	0	70	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Y	83	0	70	1	0
19	9	61	0	52	1	0
19	JA	61	0	52	1	0
19	v	61	0	52	1	0
20	E	84	0	78	0	0
20	F	14	0	13	0	0
20	G	28	0	26	0	0
20	e	84	0	78	0	0
20	f	14	0	13	0	0
20	g	28	0	26	0	0
20	r	84	0	78	0	0
20	s	14	0	13	0	0
20	t	28	0	26	0	0
21	M	28	0	46	0	0
21	m	28	0	46	1	0
21	z	28	0	46	1	0
All	All	144816	0	141267	2517	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 2517 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)
6:s:291:ILE:CD1	6:s:314:GLN:HG2	1.40	1.47
6:s:291:ILE:CD1	6:s:314:GLN:CG	2.21	1.18
8:H:485:MET:HE1	8:H:502:ASN:HB2	1.31	1.12
6:s:291:ILE:HD12	6:s:314:GLN:CG	1.76	1.12
6:s:291:ILE:HG13	6:s:314:GLN:CD	1.76	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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](#)

114 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	$\# Z > 2$
15	NAG	0	1	15,5	14,14,15	0.22	0	17,19,21	0.46	0
15	NAG	0	2	15	14,14,15	0.20	0	17,19,21	0.45	0
15	BMA	0	3	15	11,11,12	0.99	1 (9%)	15,15,17	0.81	0
15	BMA	0	4	15	11,11,12	0.62	0	15,15,17	0.80	0
15	BMA	0	5	15	11,11,12	0.68	0	15,15,17	0.75	0
15	BMA	0	6	15	11,11,12	0.65	0	15,15,17	0.73	0
15	BMA	0	7	15	11,11,12	0.64	0	15,15,17	0.69	0
16	NAG	1	1	6,16	14,14,15	0.53	0	17,19,21	0.56	0
16	NAG	1	2	16	14,14,15	0.28	0	17,19,21	0.66	0
16	BMA	1	3	16	11,11,12	0.59	0	15,15,17	0.73	0
16	NAG	2	1	6,16	14,14,15	0.58	0	17,19,21	0.69	0
16	NAG	2	2	16	14,14,15	0.24	0	17,19,21	0.42	0
16	BMA	2	3	16	11,11,12	0.63	0	15,15,17	0.78	0
17	NAG	3	1	7,17	14,14,15	0.60	0	17,19,21	0.72	0
17	NAG	3	2	17	14,14,15	0.69	1 (7%)	17,19,21	0.61	0
16	NAG	4	1	7,16	14,14,15	0.20	0	17,19,21	0.43	0
16	NAG	4	2	16	14,14,15	0.22	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BMA	4	3	16	11,11,12	0.64	0	15,15,17	0.70	0
16	NAG	5	1	8,16	14,14,15	0.33	0	17,19,21	0.49	0
16	NAG	5	2	16	14,14,15	0.20	0	17,19,21	0.42	0
16	BMA	5	3	16	11,11,12	0.75	0	15,15,17	0.72	0
16	NAG	6	1	8,16	14,14,15	0.29	0	17,19,21	0.46	0
16	NAG	6	2	16	14,14,15	0.23	0	17,19,21	0.47	0
16	BMA	6	3	16	11,11,12	0.59	0	15,15,17	0.76	0
18	NAG	7	1	8,18	14,14,15	0.27	0	17,19,21	0.53	0
18	NAG	7	2	18	14,14,15	0.21	0	17,19,21	0.46	0
18	BMA	7	3	18	11,11,12	0.54	0	15,15,17	0.93	1 (6%)
18	BMA	7	4	18	11,11,12	0.57	0	15,15,17	0.73	0
18	BMA	7	5	18	11,11,12	0.61	0	15,15,17	0.78	0
18	BMA	7	6	18	11,11,12	0.86	1 (9%)	15,15,17	0.85	0
18	BMA	7	7	18	11,11,12	0.59	0	15,15,17	0.75	0
17	NAG	8	1	8,17	14,14,15	0.74	1 (7%)	17,19,21	0.99	1 (5%)
17	NAG	8	2	17	14,14,15	0.30	0	17,19,21	0.67	1 (5%)
19	NAG	9	1	8,19	14,14,15	0.23	0	17,19,21	0.50	0
19	NAG	9	2	19	14,14,15	0.37	0	17,19,21	0.72	1 (5%)
19	BMA	9	3	19	11,11,12	0.86	1 (9%)	15,15,17	1.09	1 (6%)
19	BMA	9	4	19	11,11,12	0.77	1 (9%)	15,15,17	0.77	0
19	BMA	9	5	19	11,11,12	0.65	0	15,15,17	0.70	0
15	NAG	AA	1	15,5	14,14,15	0.18	0	17,19,21	0.43	0
15	NAG	AA	2	15	14,14,15	0.17	0	17,19,21	0.46	0
15	BMA	AA	3	15	11,11,12	0.95	0	15,15,17	0.82	0
15	BMA	AA	4	15	11,11,12	0.56	0	15,15,17	0.78	0
15	BMA	AA	5	15	11,11,12	0.67	0	15,15,17	0.75	0
15	BMA	AA	6	15	11,11,12	0.67	0	15,15,17	0.72	0
15	BMA	AA	7	15	11,11,12	0.67	0	15,15,17	0.70	0
16	NAG	BA	1	6,16	14,14,15	0.58	1 (7%)	17,19,21	0.60	0
16	NAG	BA	2	16	14,14,15	0.27	0	17,19,21	0.67	0
16	BMA	BA	3	16	11,11,12	0.58	0	15,15,17	0.71	0
16	NAG	CA	1	6,16	14,14,15	0.61	1 (7%)	17,19,21	0.67	0
16	NAG	CA	2	16	14,14,15	0.22	0	17,19,21	0.41	0
16	BMA	CA	3	16	11,11,12	0.60	0	15,15,17	0.75	0
17	NAG	DA	1	7,17	14,14,15	0.58	0	17,19,21	0.70	0
17	NAG	DA	2	17	14,14,15	0.66	1 (7%)	17,19,21	0.64	1 (5%)
16	NAG	EA	1	7,16	14,14,15	0.22	0	17,19,21	0.41	0
16	NAG	EA	2	16	14,14,15	0.25	0	17,19,21	0.46	0
16	BMA	EA	3	16	11,11,12	0.67	0	15,15,17	0.69	0
16	NAG	FA	1	8,16	14,14,15	0.36	0	17,19,21	0.44	0
16	NAG	FA	2	16	14,14,15	0.21	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BMA	FA	3	16	11,11,12	0.74	0	15,15,17	0.70	0
16	NAG	GA	1	8,16	14,14,15	0.40	0	17,19,21	0.46	0
16	NAG	GA	2	16	14,14,15	0.21	0	17,19,21	0.48	0
16	BMA	GA	3	16	11,11,12	0.62	0	15,15,17	0.73	0
18	NAG	HA	1	8,18	14,14,15	0.27	0	17,19,21	0.52	0
18	NAG	HA	2	18	14,14,15	0.24	0	17,19,21	0.47	0
18	BMA	HA	3	18	11,11,12	0.53	0	15,15,17	0.94	0
18	BMA	HA	4	18	11,11,12	0.56	0	15,15,17	0.76	0
18	BMA	HA	5	18	11,11,12	0.63	0	15,15,17	0.78	0
18	BMA	HA	6	18	11,11,12	0.87	1 (9%)	15,15,17	0.88	0
18	BMA	HA	7	18	11,11,12	0.60	0	15,15,17	0.75	0
17	NAG	IA	1	8,17	14,14,15	0.54	0	17,19,21	0.75	0
17	NAG	IA	2	17	14,14,15	0.25	0	17,19,21	0.59	1 (5%)
19	NAG	JA	1	8,19	14,14,15	0.23	0	17,19,21	0.48	0
19	NAG	JA	2	19	14,14,15	0.35	0	17,19,21	0.72	1 (5%)
19	BMA	JA	3	19	11,11,12	0.86	1 (9%)	15,15,17	1.11	1 (6%)
19	BMA	JA	4	19	11,11,12	0.78	1 (9%)	15,15,17	0.77	0
19	BMA	JA	5	19	11,11,12	0.65	0	15,15,17	0.73	0
15	NAG	R	1	15,5	14,14,15	0.27	0	17,19,21	0.51	0
15	NAG	R	2	15	14,14,15	0.29	0	17,19,21	0.42	0
15	BMA	R	3	15	11,11,12	0.81	0	15,15,17	0.95	1 (6%)
15	BMA	R	4	15	11,11,12	0.47	0	15,15,17	0.80	0
15	BMA	R	5	15	11,11,12	0.73	1 (9%)	15,15,17	0.78	0
15	BMA	R	6	15	11,11,12	0.77	0	15,15,17	0.85	0
15	BMA	R	7	15	11,11,12	0.65	0	15,15,17	0.67	0
16	NAG	S	1	6,16	14,14,15	0.26	0	17,19,21	0.44	0
16	NAG	S	2	16	14,14,15	0.16	0	17,19,21	0.51	0
16	BMA	S	3	16	11,11,12	0.62	0	15,15,17	0.97	1 (6%)
16	NAG	T	1	6,16	14,14,15	0.78	1 (7%)	17,19,21	0.80	0
16	NAG	T	2	16	14,14,15	0.26	0	17,19,21	0.41	0
16	BMA	T	3	16	11,11,12	0.59	0	15,15,17	0.74	0
17	NAG	U	1	7,17	14,14,15	0.45	0	17,19,21	0.71	1 (5%)
17	NAG	U	2	17	14,14,15	0.65	1 (7%)	17,19,21	0.70	1 (5%)
16	NAG	V	1	7,16	14,14,15	0.35	0	17,19,21	0.48	0
16	NAG	V	2	16	14,14,15	0.23	0	17,19,21	0.54	0
16	BMA	V	3	16	11,11,12	0.70	0	15,15,17	0.67	0
16	NAG	W	1	8,16	14,14,15	0.28	0	17,19,21	0.47	0
16	NAG	W	2	16	14,14,15	0.21	0	17,19,21	0.45	0
16	BMA	W	3	16	11,11,12	0.74	0	15,15,17	0.70	0
16	NAG	X	1	8,16	14,14,15	0.33	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	NAG	X	2	16	14,14,15	0.26	0	17,19,21	0.46	0
16	BMA	X	3	16	11,11,12	0.58	0	15,15,17	0.68	0
18	NAG	Y	1	8,18	14,14,15	0.29	0	17,19,21	0.59	0
18	NAG	Y	2	18	14,14,15	0.27	0	17,19,21	0.46	0
18	BMA	Y	3	18	11,11,12	0.61	0	15,15,17	1.08	1 (6%)
18	BMA	Y	4	18	11,11,12	0.48	0	15,15,17	0.97	0
18	BMA	Y	5	18	11,11,12	0.61	0	15,15,17	0.83	0
18	BMA	Y	6	18	11,11,12	0.65	0	15,15,17	0.86	0
18	BMA	Y	7	18	11,11,12	0.57	0	15,15,17	0.98	1 (6%)
17	NAG	Z	1	8,17	14,14,15	0.89	1 (7%)	17,19,21	0.86	1 (5%)
17	NAG	Z	2	17	14,14,15	0.27	0	17,19,21	0.60	1 (5%)
19	NAG	v	1	8,19	14,14,15	0.25	0	17,19,21	0.48	0
19	NAG	v	2	19	14,14,15	0.25	0	17,19,21	0.55	0
19	BMA	v	3	19	11,11,12	0.91	0	15,15,17	1.25	3 (20%)
19	BMA	v	4	19	11,11,12	0.88	0	15,15,17	0.70	0
19	BMA	v	5	19	11,11,12	0.58	0	15,15,17	0.72	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
15	NAG	0	1	15,5	-	1/6/23/26	0/1/1/1
15	NAG	0	2	15	-	2/6/23/26	0/1/1/1
15	BMA	0	3	15	-	0/2/19/22	0/1/1/1
15	BMA	0	4	15	-	2/2/19/22	0/1/1/1
15	BMA	0	5	15	-	0/2/19/22	0/1/1/1
15	BMA	0	6	15	-	0/2/19/22	0/1/1/1
15	BMA	0	7	15	-	0/2/19/22	0/1/1/1
16	NAG	1	1	6,16	-	2/6/23/26	0/1/1/1
16	NAG	1	2	16	-	2/6/23/26	0/1/1/1
16	BMA	1	3	16	-	2/2/19/22	0/1/1/1
16	NAG	2	1	6,16	-	0/6/23/26	0/1/1/1
16	NAG	2	2	16	-	2/6/23/26	0/1/1/1
16	BMA	2	3	16	-	0/2/19/22	0/1/1/1
17	NAG	3	1	7,17	-	1/6/23/26	0/1/1/1
17	NAG	3	2	17	-	2/6/23/26	0/1/1/1
16	NAG	4	1	7,16	-	2/6/23/26	0/1/1/1
16	NAG	4	2	16	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BMA	4	3	16	-	1/2/19/22	0/1/1/1
16	NAG	5	1	8,16	-	1/6/23/26	0/1/1/1
16	NAG	5	2	16	-	0/6/23/26	0/1/1/1
16	BMA	5	3	16	-	1/2/19/22	0/1/1/1
16	NAG	6	1	8,16	-	2/6/23/26	0/1/1/1
16	NAG	6	2	16	-	0/6/23/26	0/1/1/1
16	BMA	6	3	16	-	0/2/19/22	0/1/1/1
18	NAG	7	1	8,18	-	0/6/23/26	0/1/1/1
18	NAG	7	2	18	-	2/6/23/26	0/1/1/1
18	BMA	7	3	18	-	2/2/19/22	0/1/1/1
18	BMA	7	4	18	-	2/2/19/22	0/1/1/1
18	BMA	7	5	18	-	2/2/19/22	0/1/1/1
18	BMA	7	6	18	-	1/2/19/22	0/1/1/1
18	BMA	7	7	18	-	2/2/19/22	0/1/1/1
17	NAG	8	1	8,17	-	2/6/23/26	0/1/1/1
17	NAG	8	2	17	-	0/6/23/26	0/1/1/1
19	NAG	9	1	8,19	-	0/6/23/26	0/1/1/1
19	NAG	9	2	19	-	0/6/23/26	0/1/1/1
19	BMA	9	3	19	-	1/2/19/22	0/1/1/1
19	BMA	9	4	19	-	1/2/19/22	0/1/1/1
19	BMA	9	5	19	-	0/2/19/22	0/1/1/1
15	NAG	AA	1	15,5	-	1/6/23/26	0/1/1/1
15	NAG	AA	2	15	-	2/6/23/26	0/1/1/1
15	BMA	AA	3	15	-	0/2/19/22	0/1/1/1
15	BMA	AA	4	15	-	2/2/19/22	0/1/1/1
15	BMA	AA	5	15	-	0/2/19/22	0/1/1/1
15	BMA	AA	6	15	-	0/2/19/22	0/1/1/1
15	BMA	AA	7	15	-	0/2/19/22	0/1/1/1
16	NAG	BA	1	6,16	-	2/6/23/26	0/1/1/1
16	NAG	BA	2	16	-	2/6/23/26	0/1/1/1
16	BMA	BA	3	16	-	2/2/19/22	0/1/1/1
16	NAG	CA	1	6,16	-	2/6/23/26	0/1/1/1
16	NAG	CA	2	16	-	2/6/23/26	0/1/1/1
16	BMA	CA	3	16	-	0/2/19/22	0/1/1/1
17	NAG	DA	1	7,17	-	2/6/23/26	0/1/1/1
17	NAG	DA	2	17	-	2/6/23/26	0/1/1/1
16	NAG	EA	1	7,16	-	3/6/23/26	0/1/1/1
16	NAG	EA	2	16	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BMA	EA	3	16	-	1/2/19/22	0/1/1/1
16	NAG	FA	1	8,16	-	1/6/23/26	0/1/1/1
16	NAG	FA	2	16	-	0/6/23/26	0/1/1/1
16	BMA	FA	3	16	-	1/2/19/22	0/1/1/1
16	NAG	GA	1	8,16	-	1/6/23/26	0/1/1/1
16	NAG	GA	2	16	-	0/6/23/26	0/1/1/1
16	BMA	GA	3	16	-	0/2/19/22	0/1/1/1
18	NAG	HA	1	8,18	-	0/6/23/26	0/1/1/1
18	NAG	HA	2	18	-	2/6/23/26	0/1/1/1
18	BMA	HA	3	18	-	2/2/19/22	0/1/1/1
18	BMA	HA	4	18	-	2/2/19/22	0/1/1/1
18	BMA	HA	5	18	-	2/2/19/22	0/1/1/1
18	BMA	HA	6	18	-	1/2/19/22	0/1/1/1
18	BMA	HA	7	18	-	2/2/19/22	0/1/1/1
17	NAG	IA	1	8,17	-	2/6/23/26	0/1/1/1
17	NAG	IA	2	17	-	2/6/23/26	0/1/1/1
19	NAG	JA	1	8,19	-	1/6/23/26	0/1/1/1
19	NAG	JA	2	19	-	0/6/23/26	0/1/1/1
19	BMA	JA	3	19	-	1/2/19/22	0/1/1/1
19	BMA	JA	4	19	-	1/2/19/22	0/1/1/1
19	BMA	JA	5	19	-	0/2/19/22	0/1/1/1
15	NAG	R	1	15,5	-	1/6/23/26	0/1/1/1
15	NAG	R	2	15	-	0/6/23/26	0/1/1/1
15	BMA	R	3	15	-	0/2/19/22	0/1/1/1
15	BMA	R	4	15	-	0/2/19/22	0/1/1/1
15	BMA	R	5	15	-	0/2/19/22	0/1/1/1
15	BMA	R	6	15	-	2/2/19/22	0/1/1/1
15	BMA	R	7	15	-	0/2/19/22	0/1/1/1
16	NAG	S	1	6,16	-	3/6/23/26	0/1/1/1
16	NAG	S	2	16	-	2/6/23/26	0/1/1/1
16	BMA	S	3	16	-	2/2/19/22	0/1/1/1
16	NAG	T	1	6,16	-	2/6/23/26	0/1/1/1
16	NAG	T	2	16	-	2/6/23/26	0/1/1/1
16	BMA	T	3	16	-	0/2/19/22	0/1/1/1
17	NAG	U	1	7,17	-	1/6/23/26	0/1/1/1
17	NAG	U	2	17	-	2/6/23/26	0/1/1/1
16	NAG	V	1	7,16	-	1/6/23/26	0/1/1/1
16	NAG	V	2	16	-	2/6/23/26	0/1/1/1
16	BMA	V	3	16	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	NAG	W	1	8,16	-	2/6/23/26	0/1/1/1
16	NAG	W	2	16	-	1/6/23/26	0/1/1/1
16	BMA	W	3	16	-	2/2/19/22	0/1/1/1
16	NAG	X	1	8,16	-	0/6/23/26	0/1/1/1
16	NAG	X	2	16	-	0/6/23/26	0/1/1/1
16	BMA	X	3	16	-	0/2/19/22	0/1/1/1
18	NAG	Y	1	8,18	-	2/6/23/26	0/1/1/1
18	NAG	Y	2	18	-	2/6/23/26	0/1/1/1
18	BMA	Y	3	18	-	2/2/19/22	0/1/1/1
18	BMA	Y	4	18	-	2/2/19/22	0/1/1/1
18	BMA	Y	5	18	-	2/2/19/22	0/1/1/1
18	BMA	Y	6	18	-	2/2/19/22	0/1/1/1
18	BMA	Y	7	18	-	2/2/19/22	0/1/1/1
17	NAG	Z	1	8,17	-	2/6/23/26	0/1/1/1
17	NAG	Z	2	17	-	1/6/23/26	0/1/1/1
19	NAG	v	1	8,19	-	2/6/23/26	0/1/1/1
19	NAG	v	2	19	-	2/6/23/26	0/1/1/1
19	BMA	v	3	19	-	2/2/19/22	0/1/1/1
19	BMA	v	4	19	-	2/2/19/22	0/1/1/1
19	BMA	v	5	19	-	1/2/19/22	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Z	1	NAG	O5-C1	-3.15	1.38	1.43
16	T	1	NAG	O5-C1	-2.77	1.39	1.43
17	8	1	NAG	O5-C1	-2.51	1.39	1.43
18	HA	6	BMA	C1-C2	2.47	1.58	1.52
18	7	6	BMA	C1-C2	2.46	1.58	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	JA	3	BMA	C1-O5-C5	3.54	116.93	112.19
19	9	3	BMA	C1-O5-C5	3.41	116.75	112.19
19	v	3	BMA	C1-C2-C3	-2.67	105.76	109.64
17	U	2	NAG	C1-O5-C5	2.43	115.44	112.19
17	8	1	NAG	O4-C4-C5	-2.42	103.37	109.32

There are no chirality outliers.

5 of 133 torsion outliers are listed below:

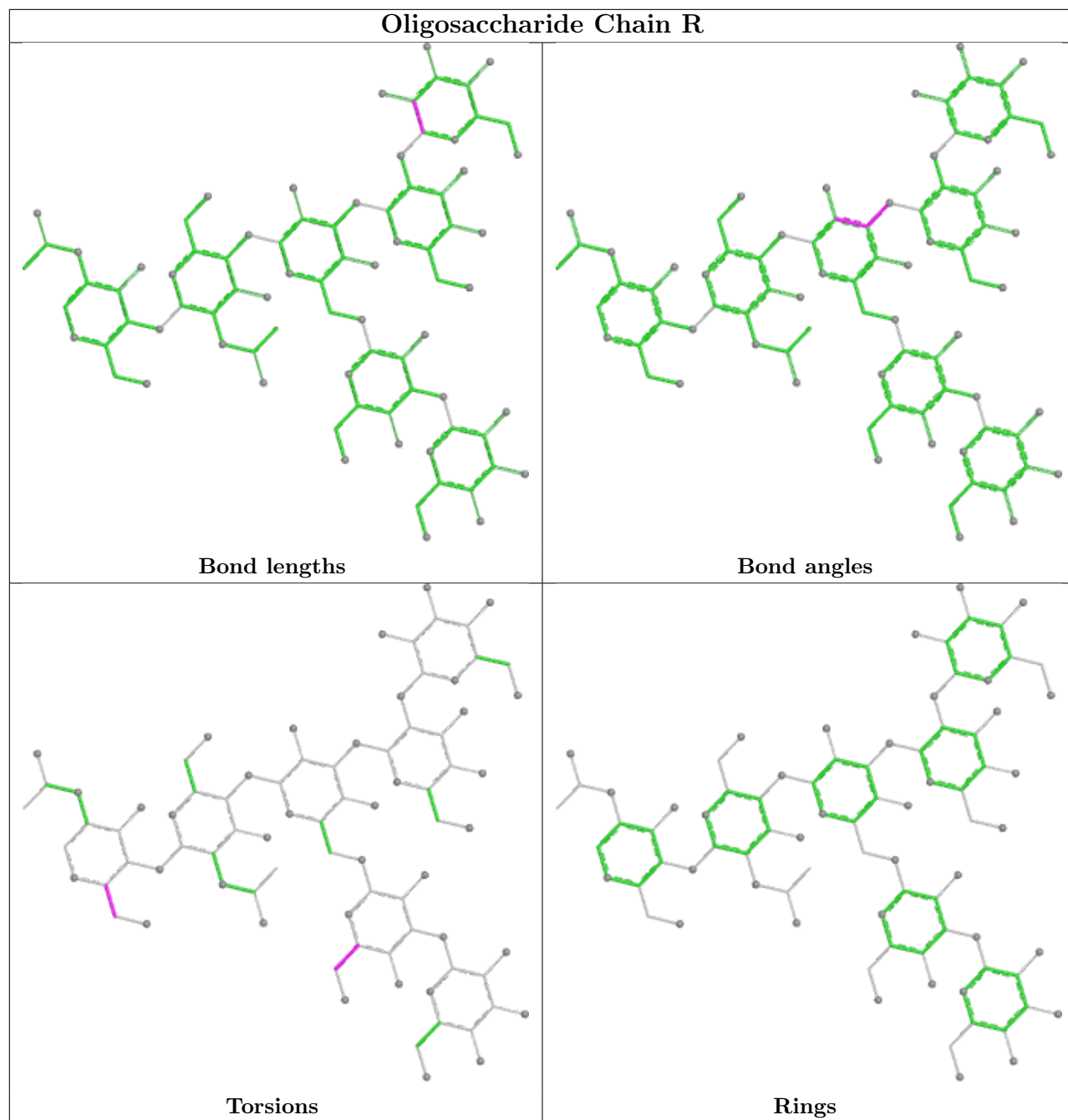
Mol	Chain	Res	Type	Atoms
16	S	1	NAG	O5-C5-C6-O6
15	0	2	NAG	O5-C5-C6-O6
16	1	2	NAG	O5-C5-C6-O6
16	4	1	NAG	O5-C5-C6-O6
17	Z	1	NAG	O5-C5-C6-O6

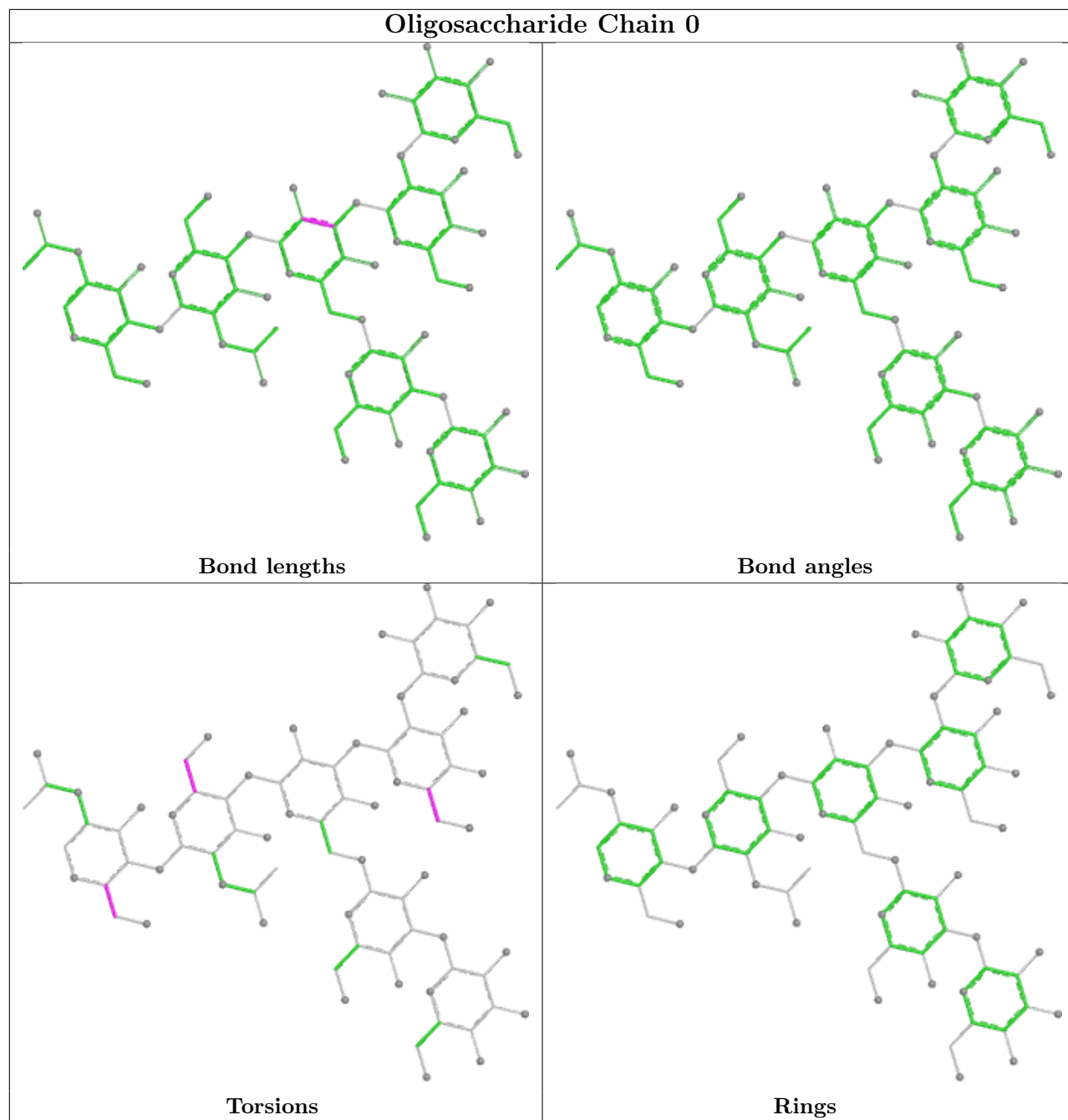
There are no ring outliers.

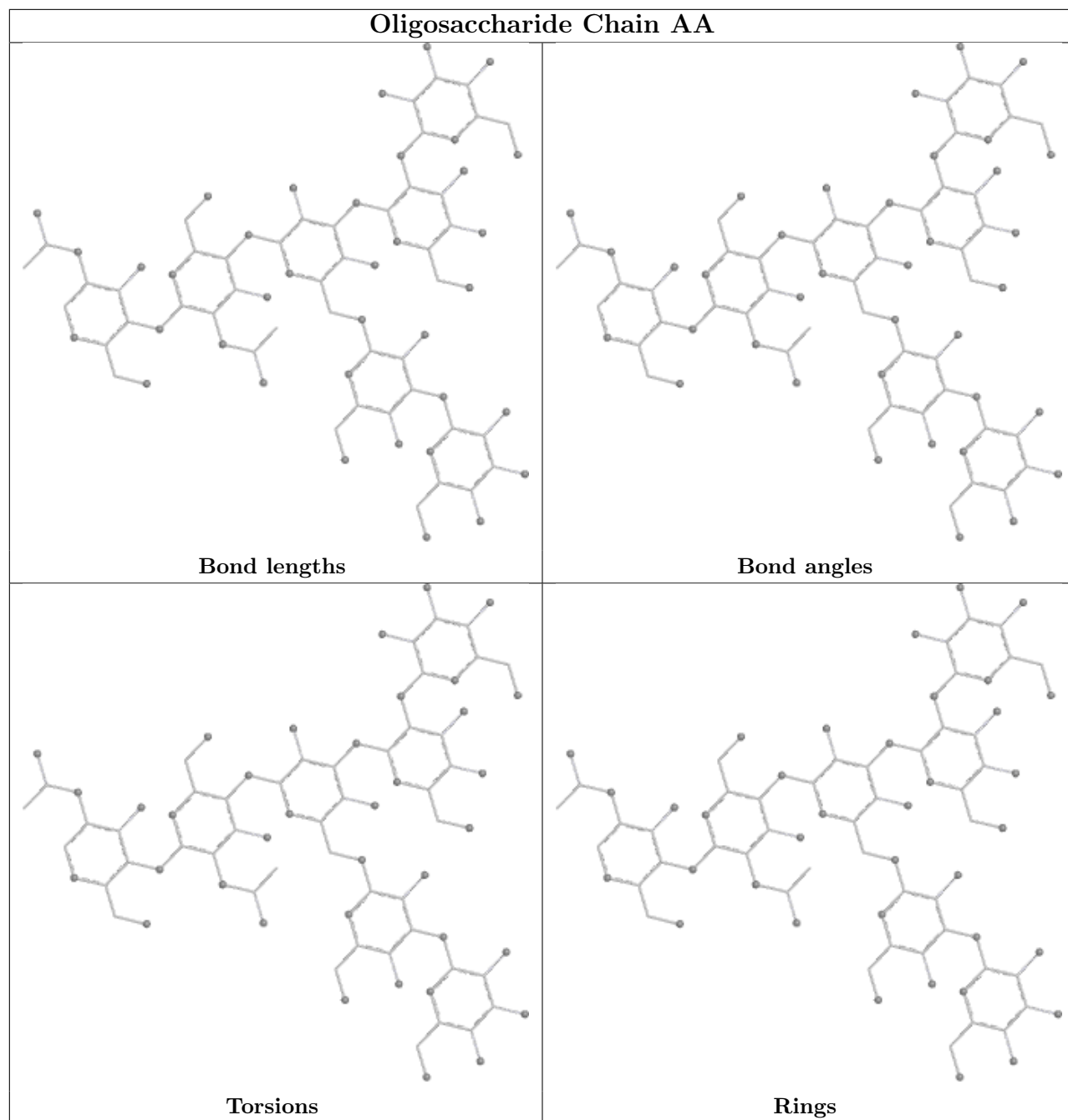
14 monomers are involved in 14 short contacts:

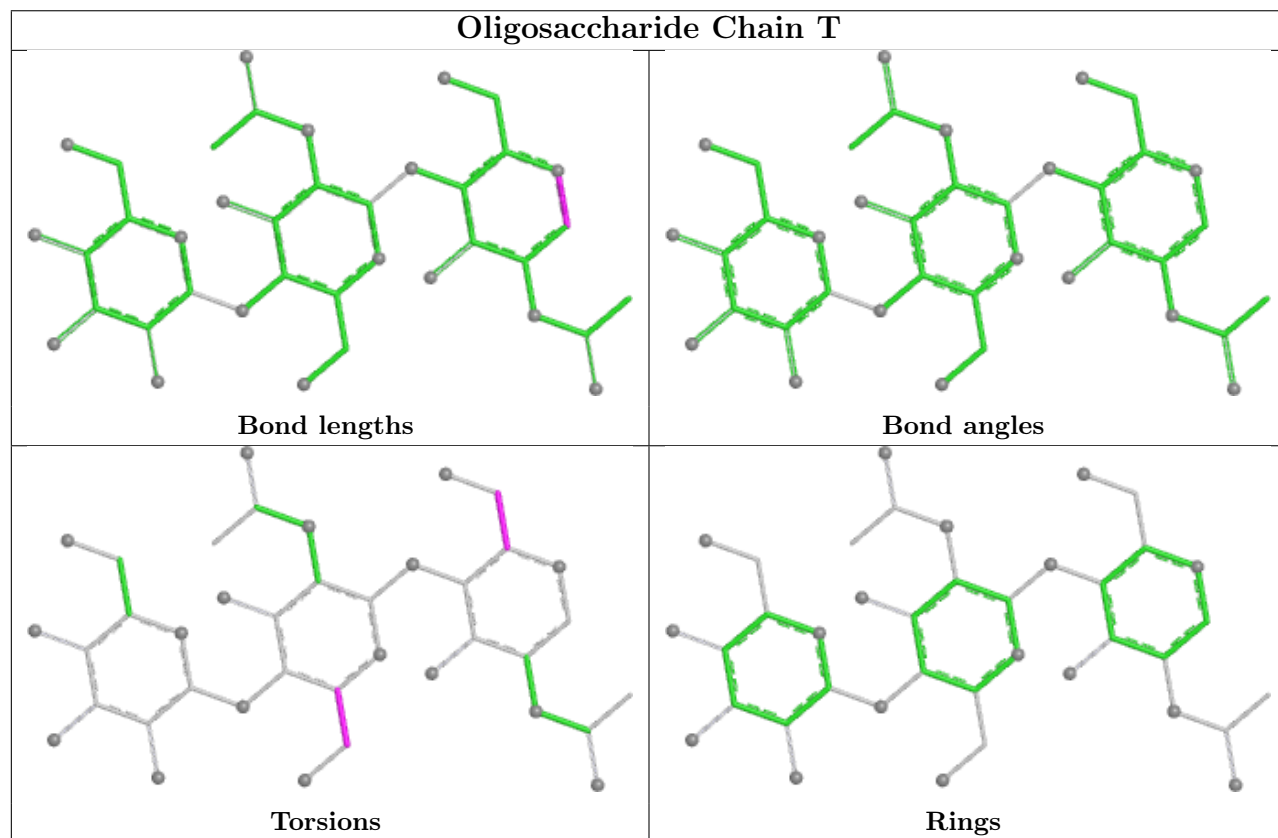
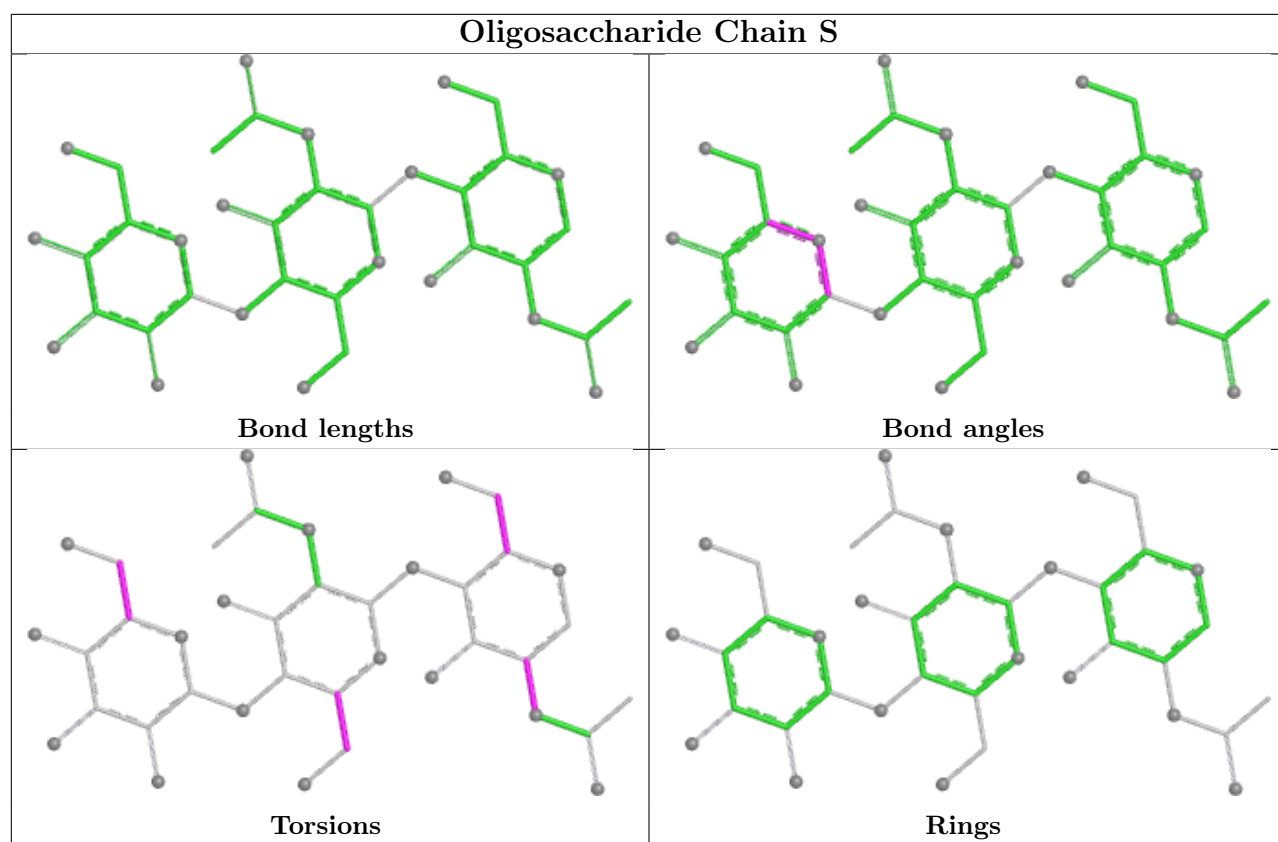
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	1	2	NAG	1	0
19	9	1	NAG	1	0
16	S	1	NAG	1	0
16	BA	2	NAG	1	0
19	JA	1	NAG	1	0
18	Y	3	BMA	1	0
15	R	3	BMA	1	0
17	8	1	NAG	1	0
17	U	2	NAG	2	0
17	IA	1	NAG	2	0
19	v	2	NAG	1	0
17	Z	1	NAG	1	0
15	R	6	BMA	1	0
17	U	1	NAG	1	0

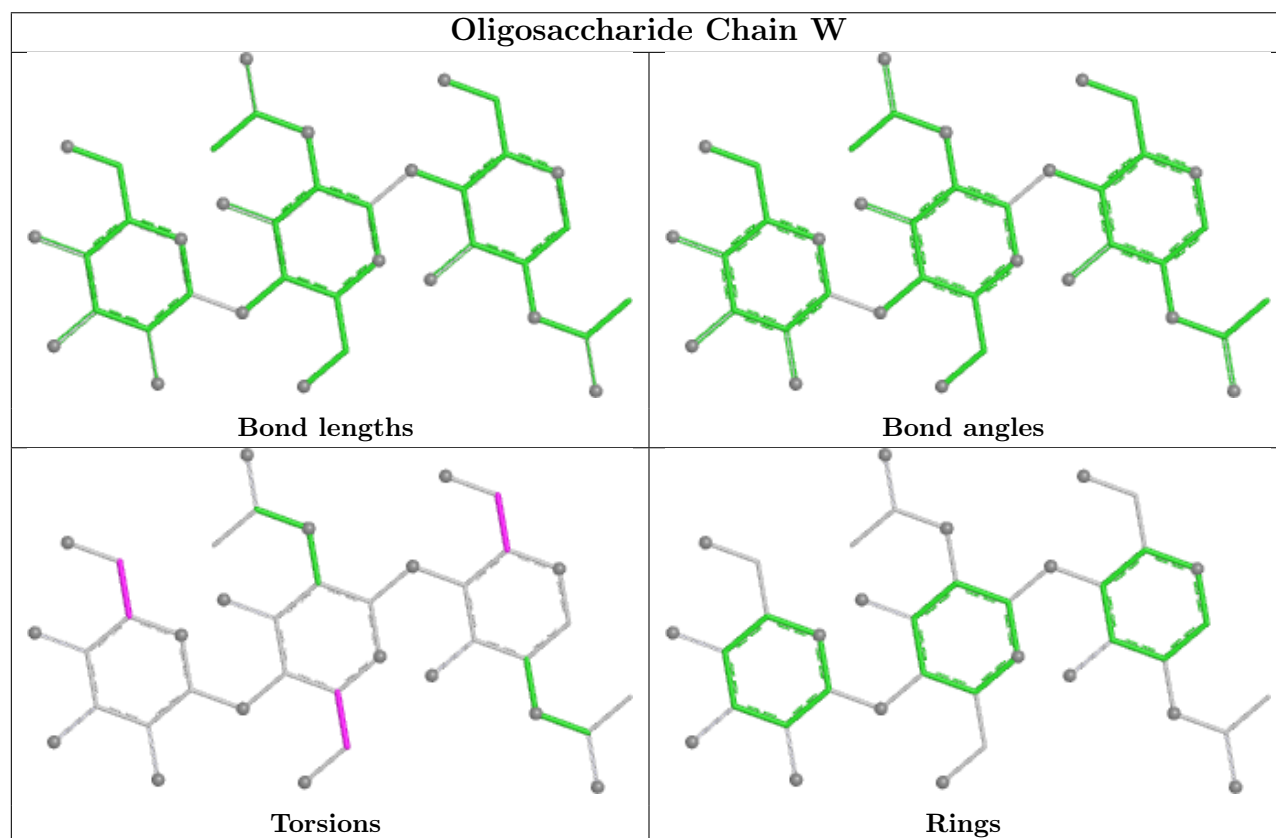
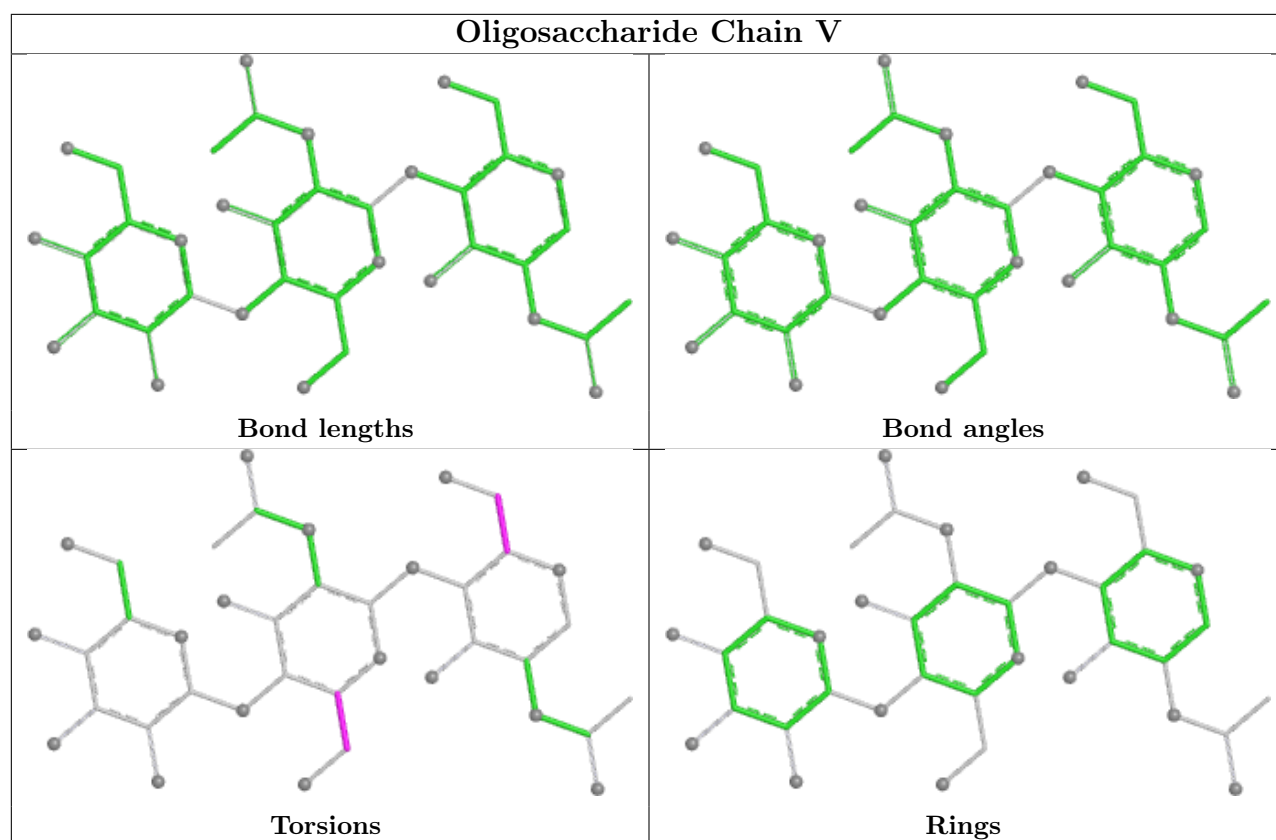
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

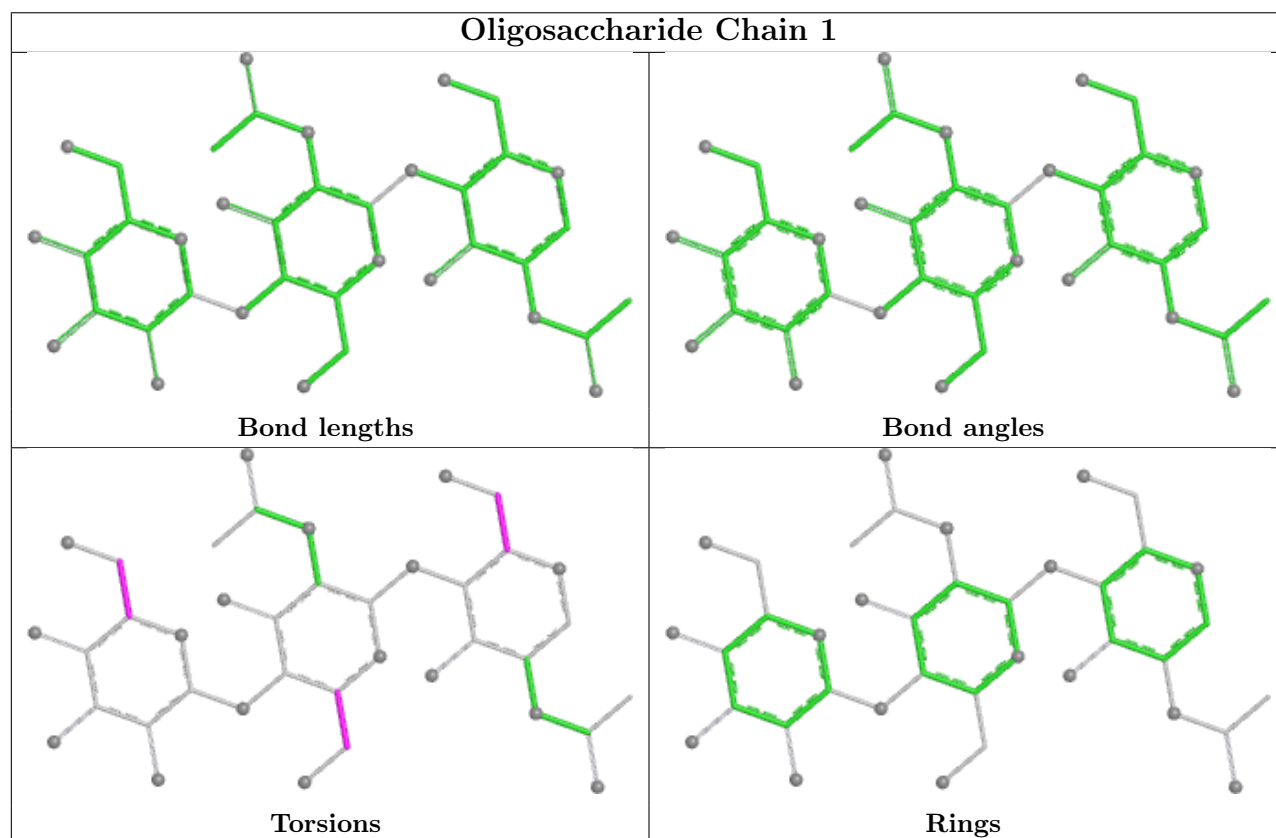
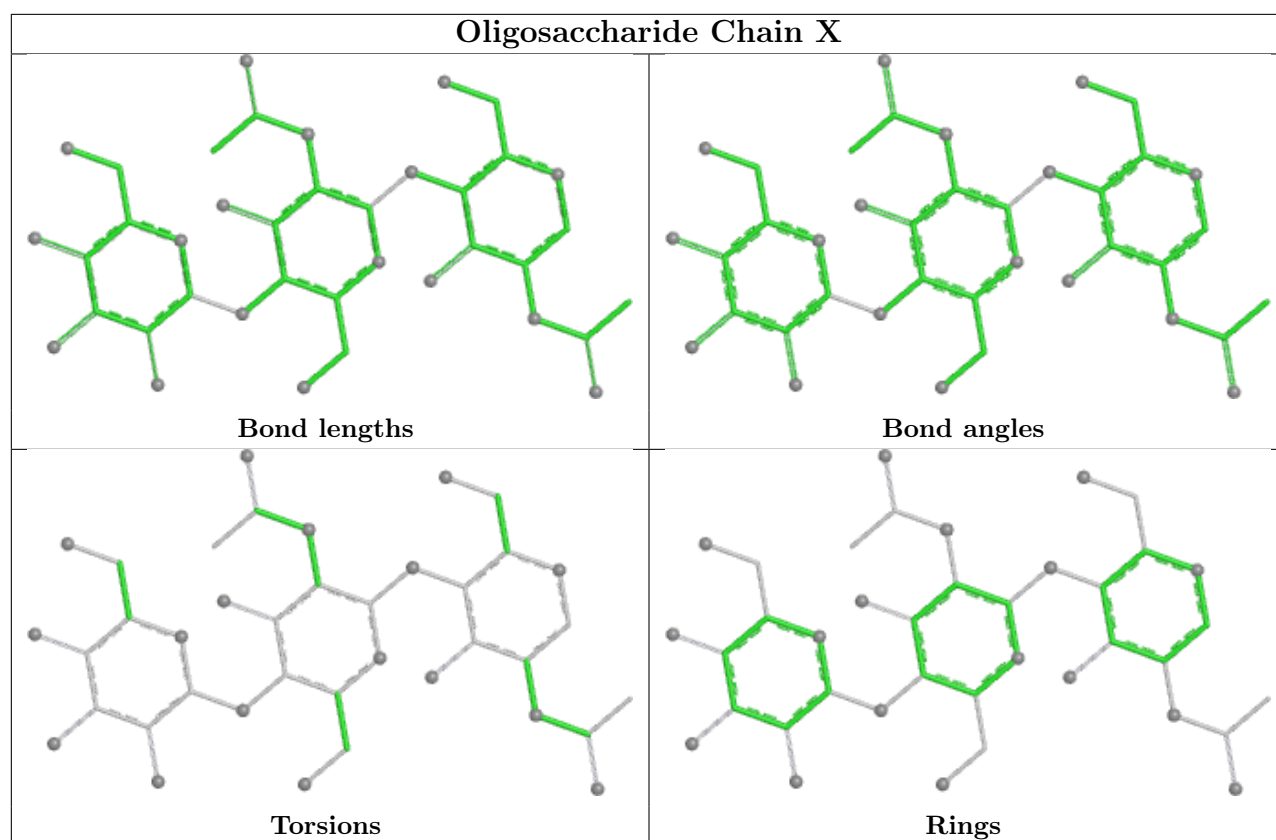


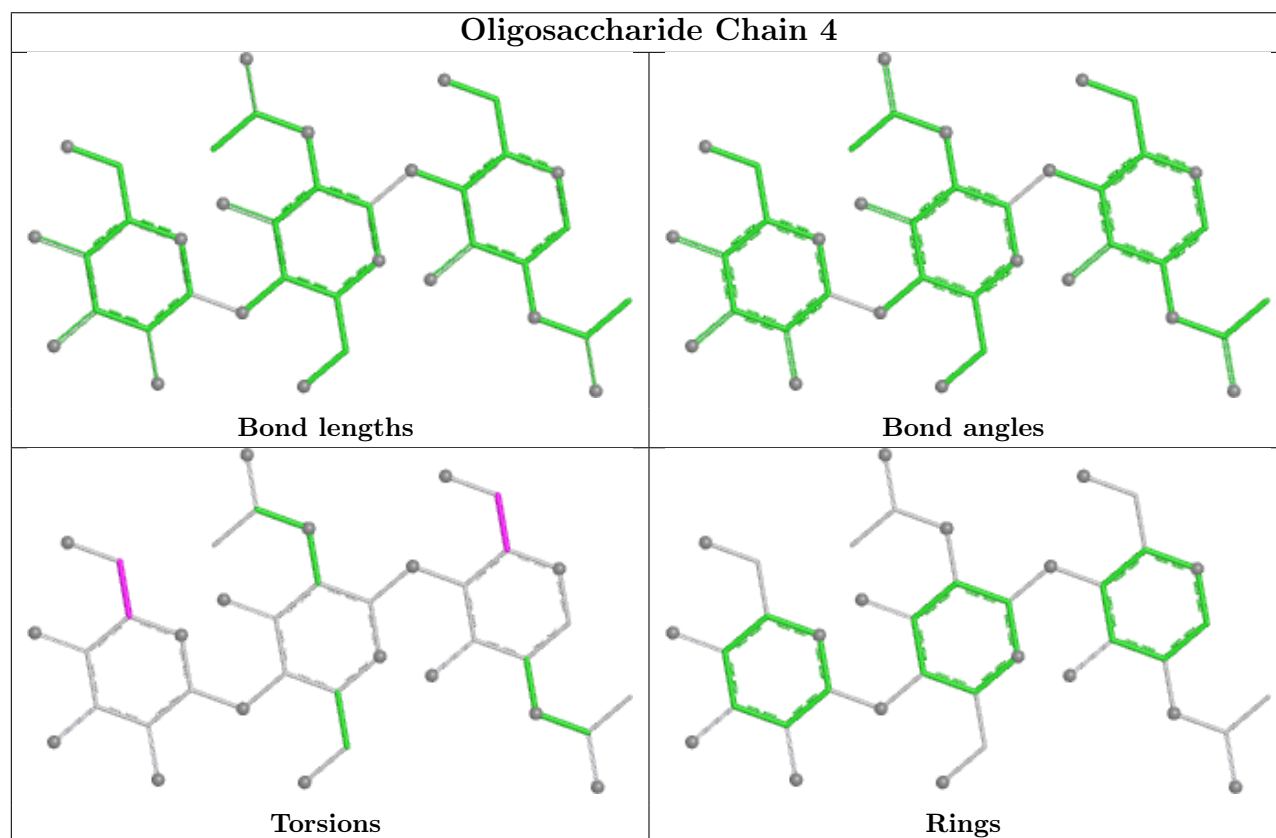
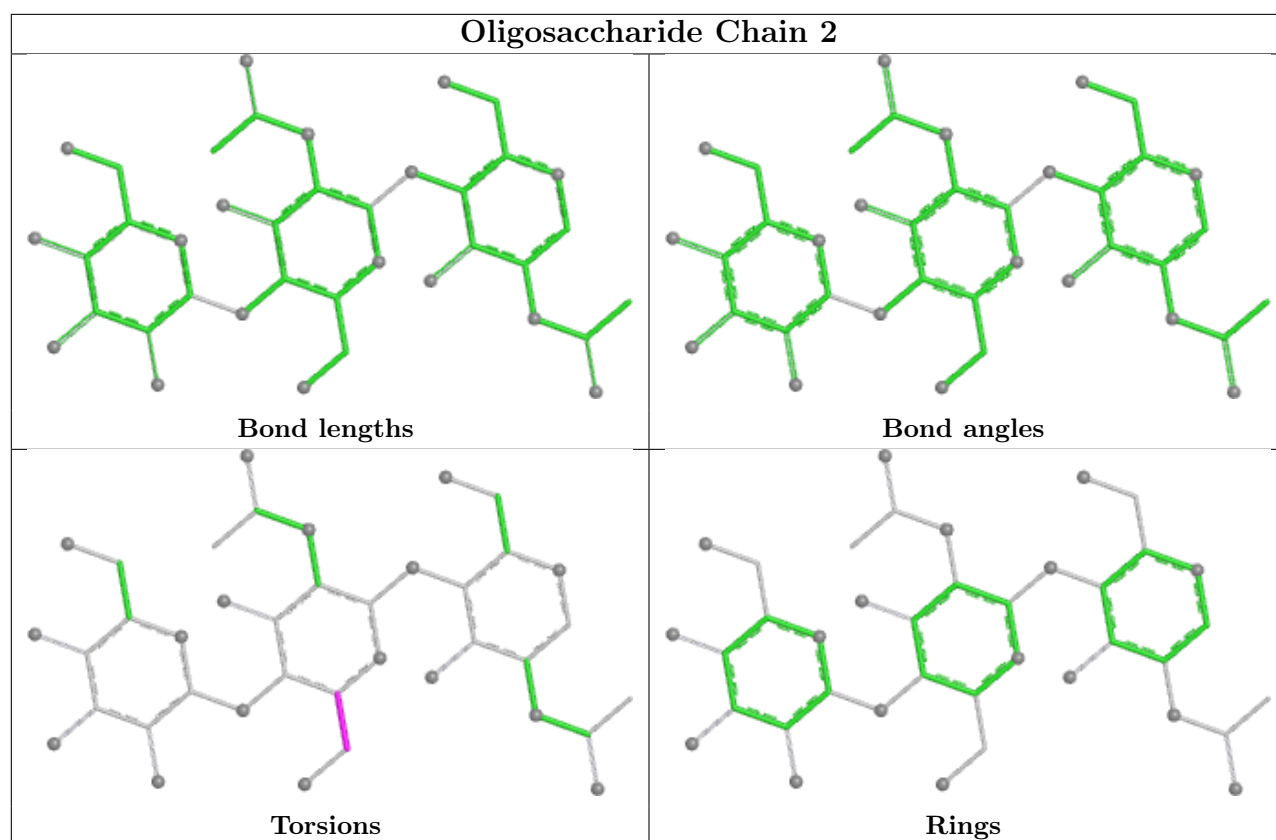


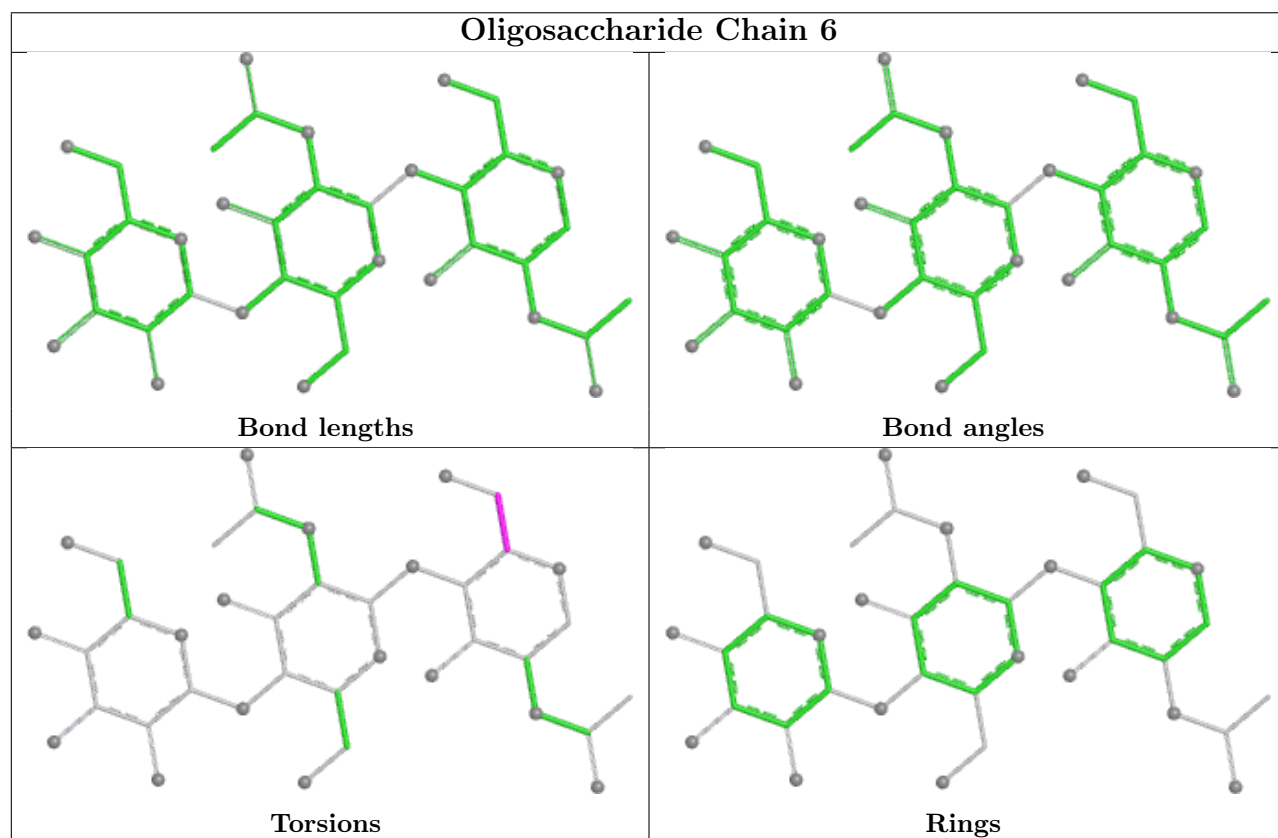
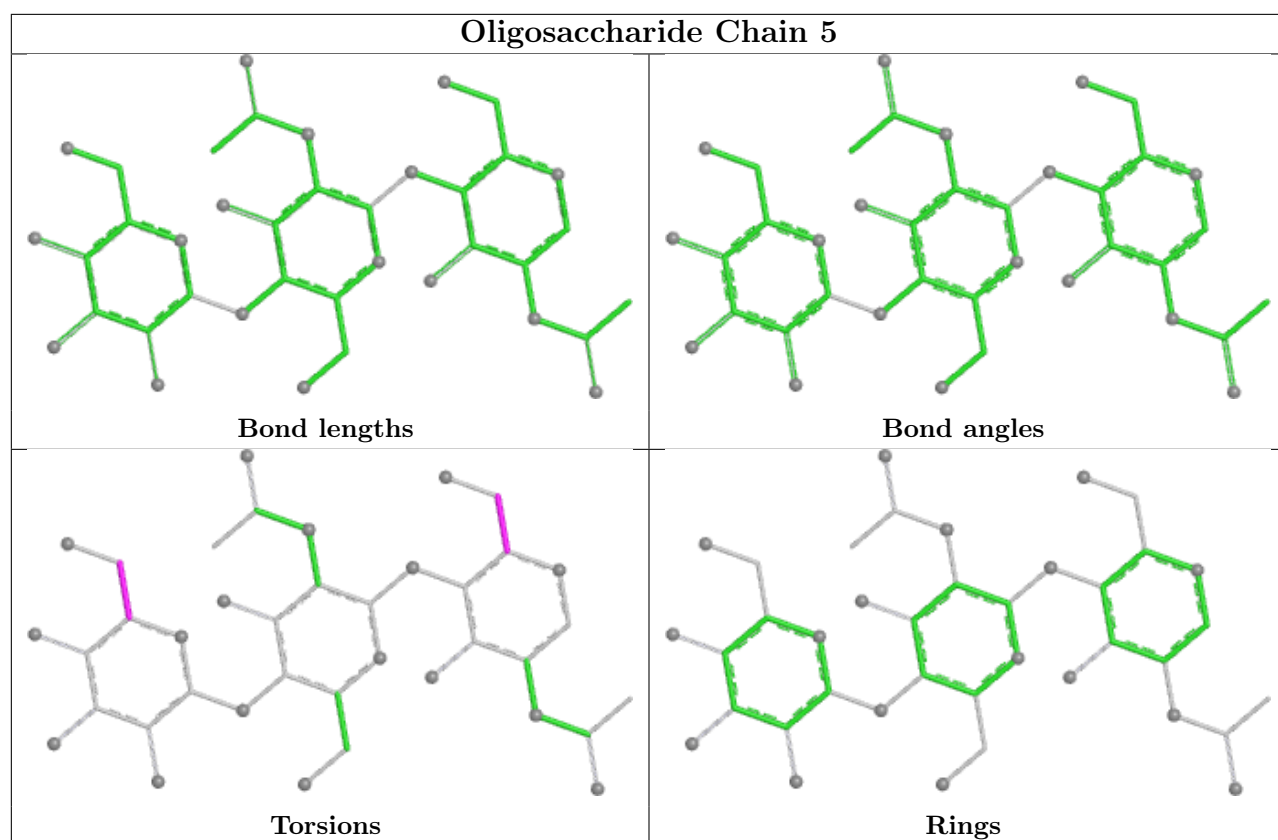


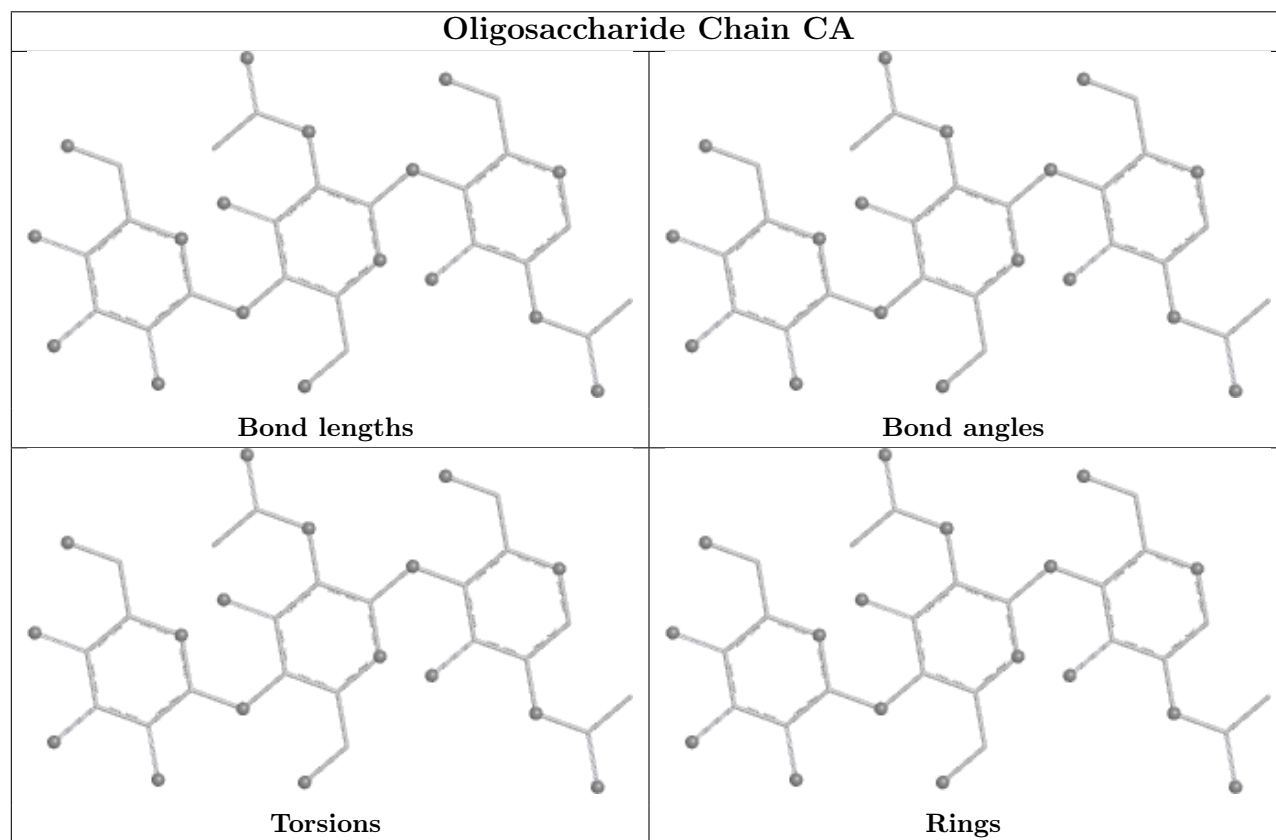
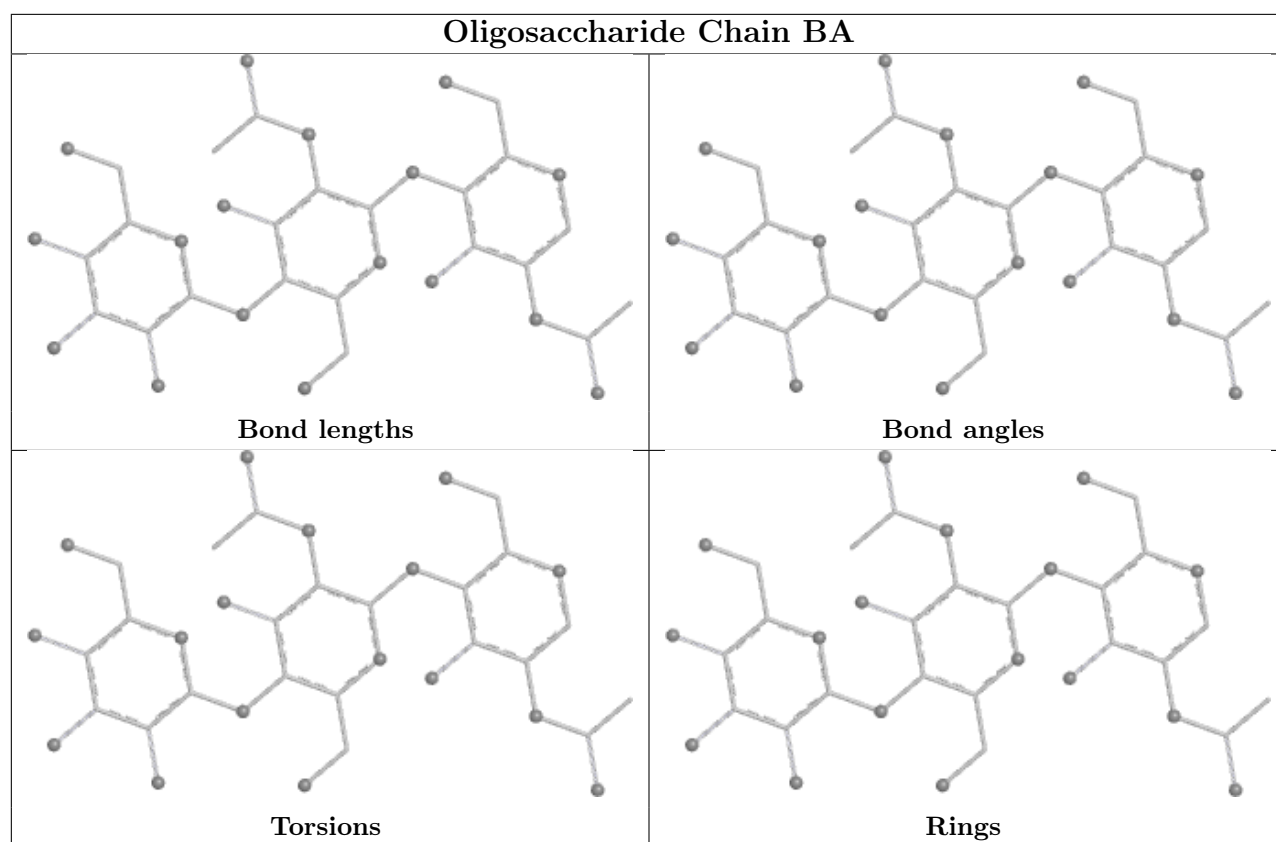


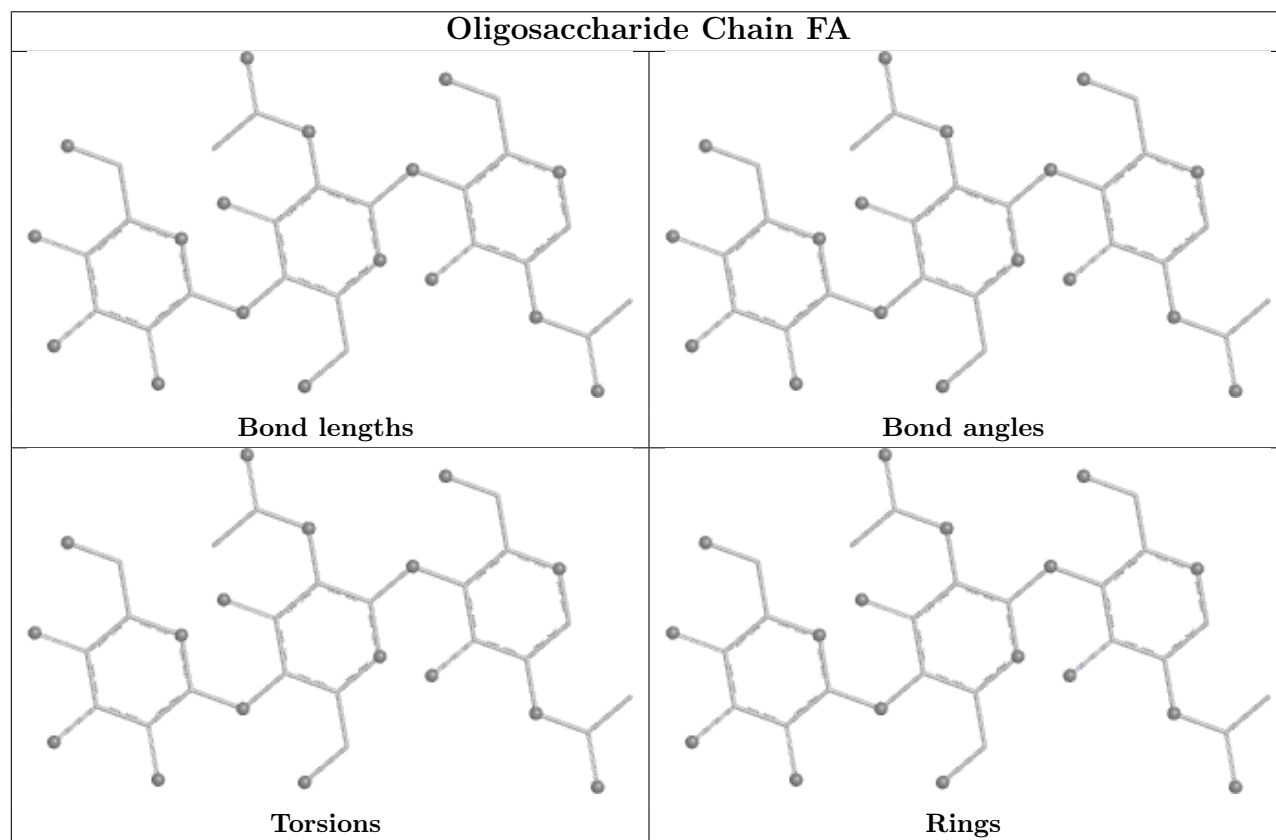
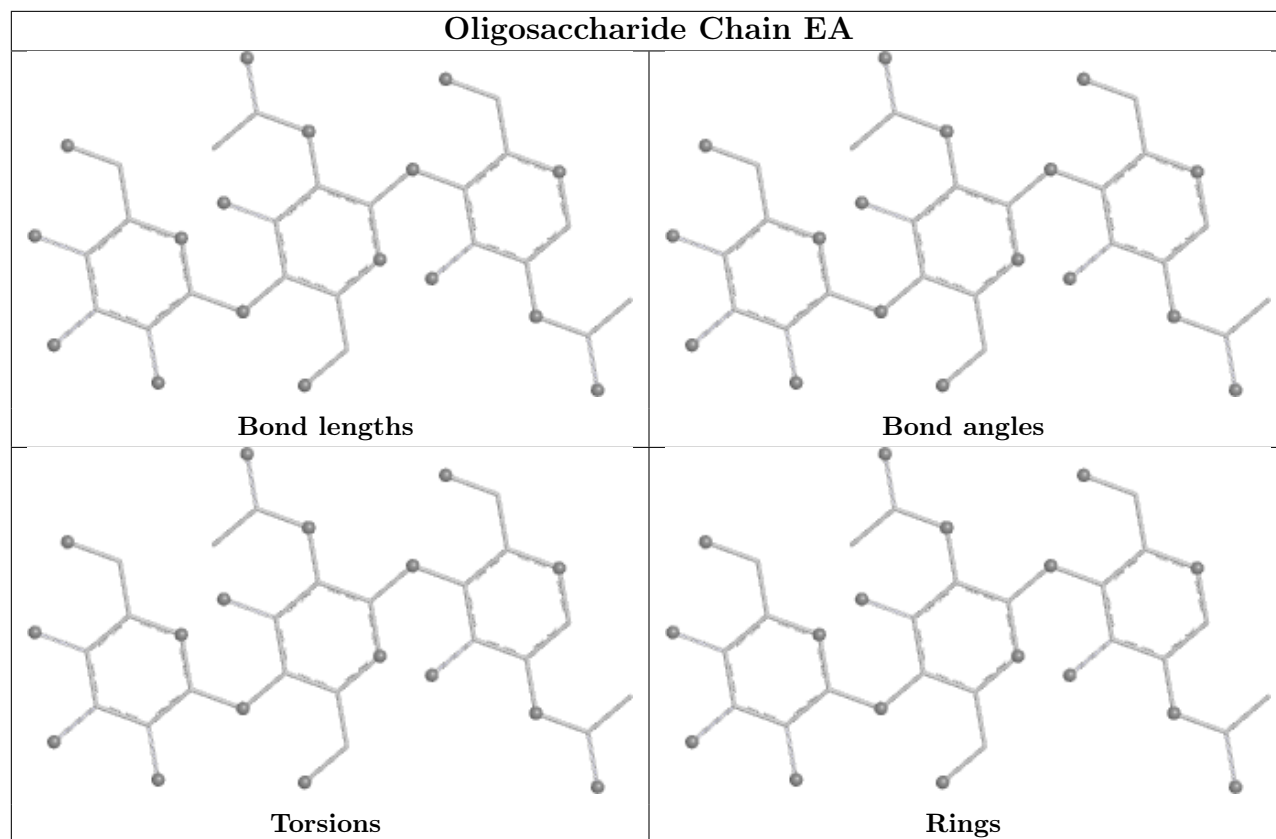


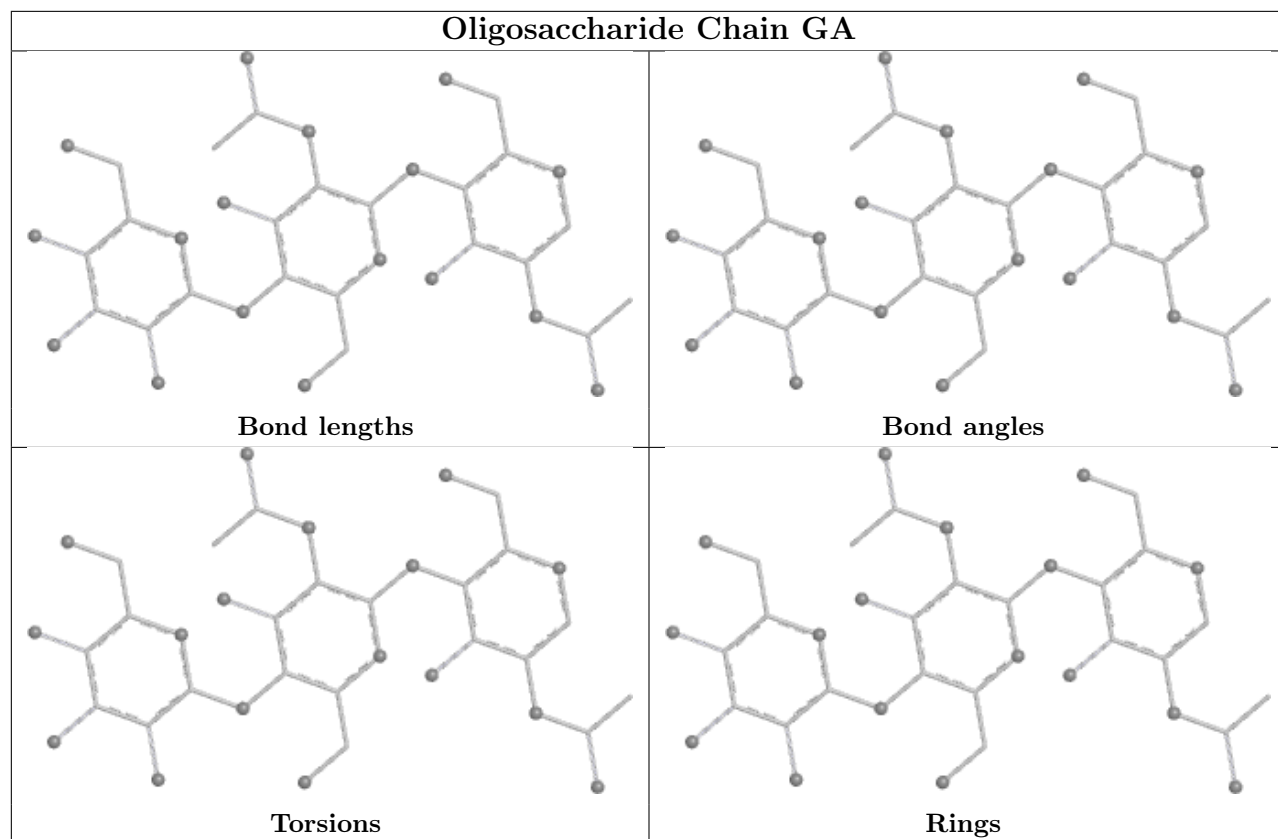


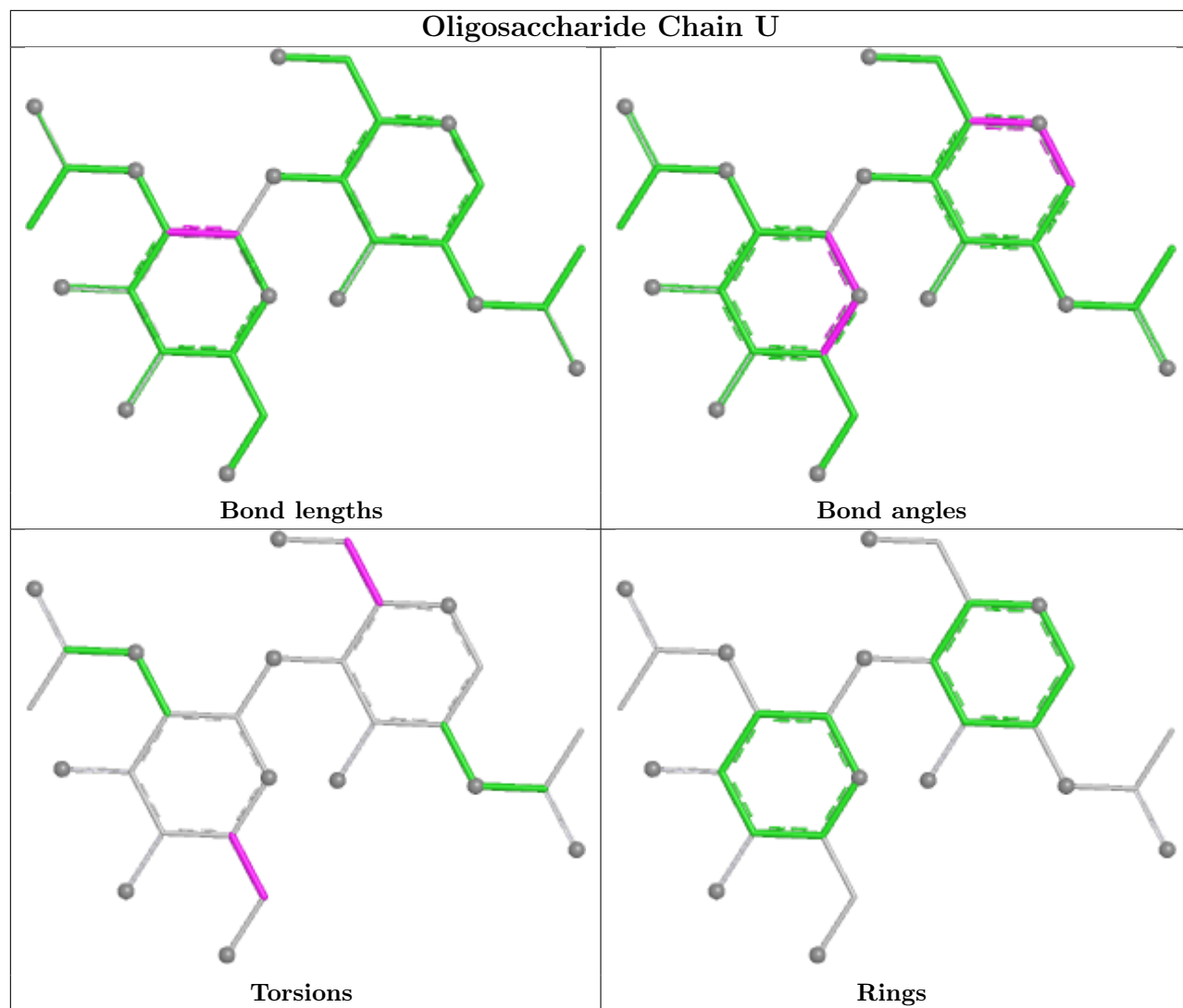


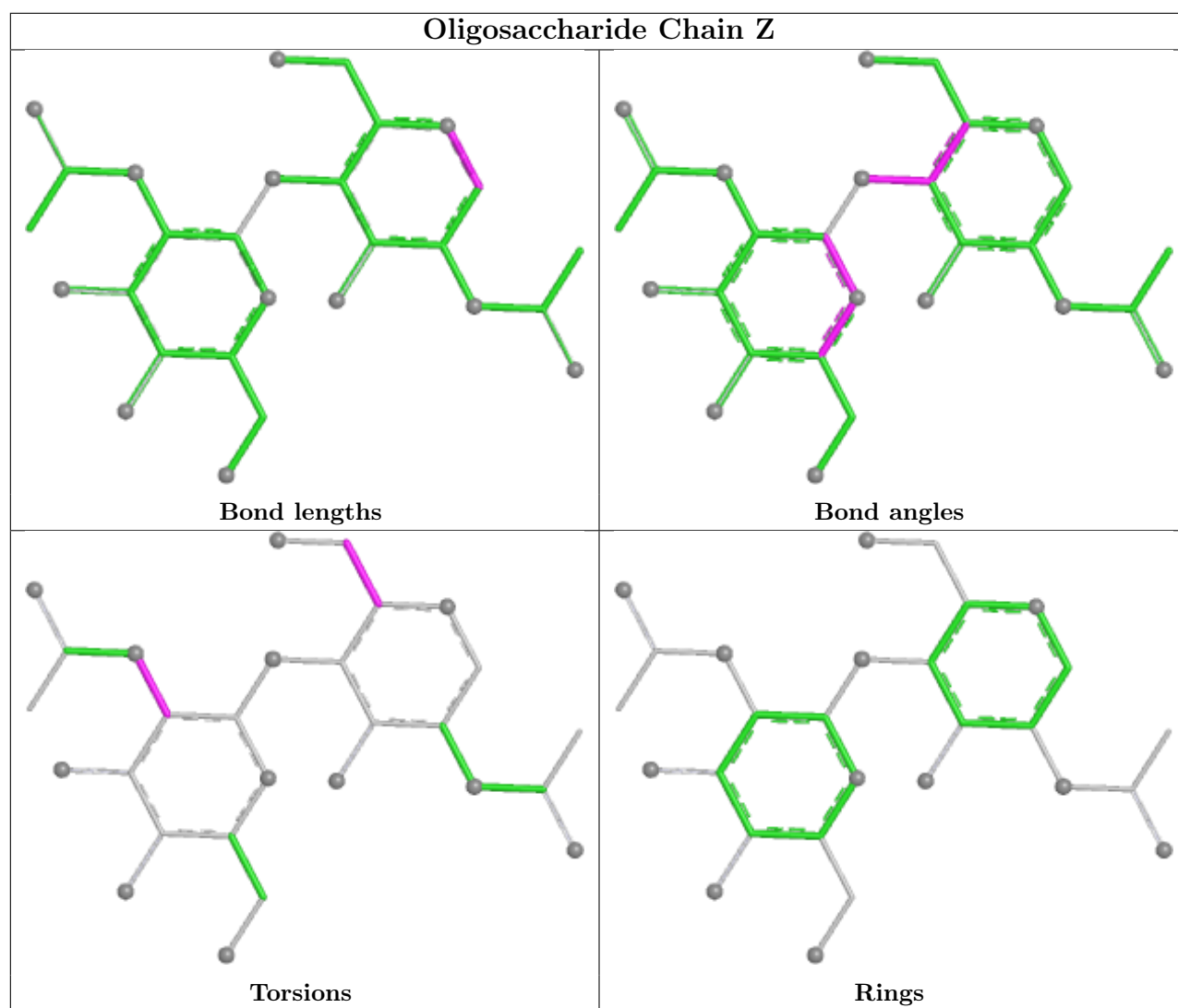


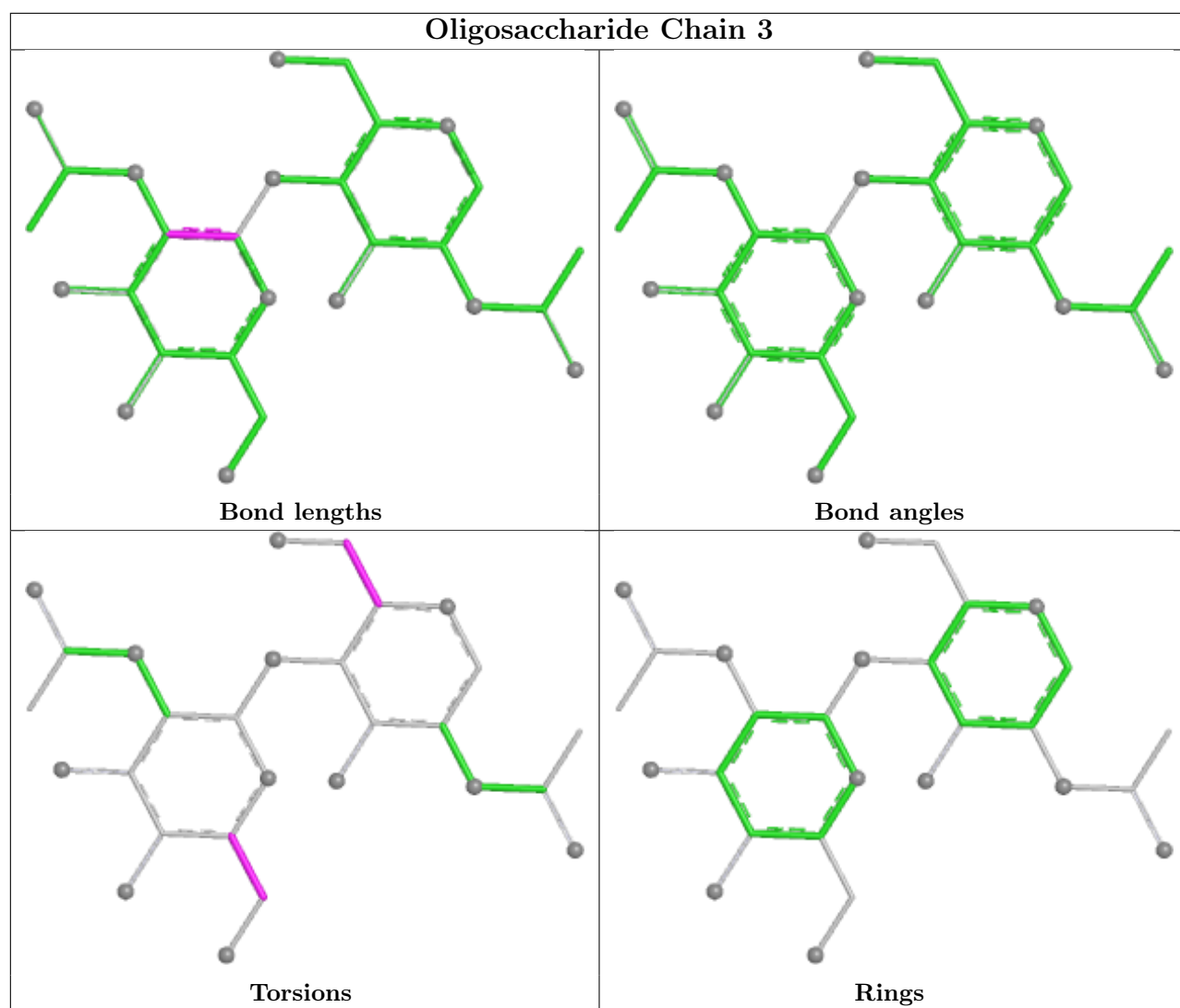


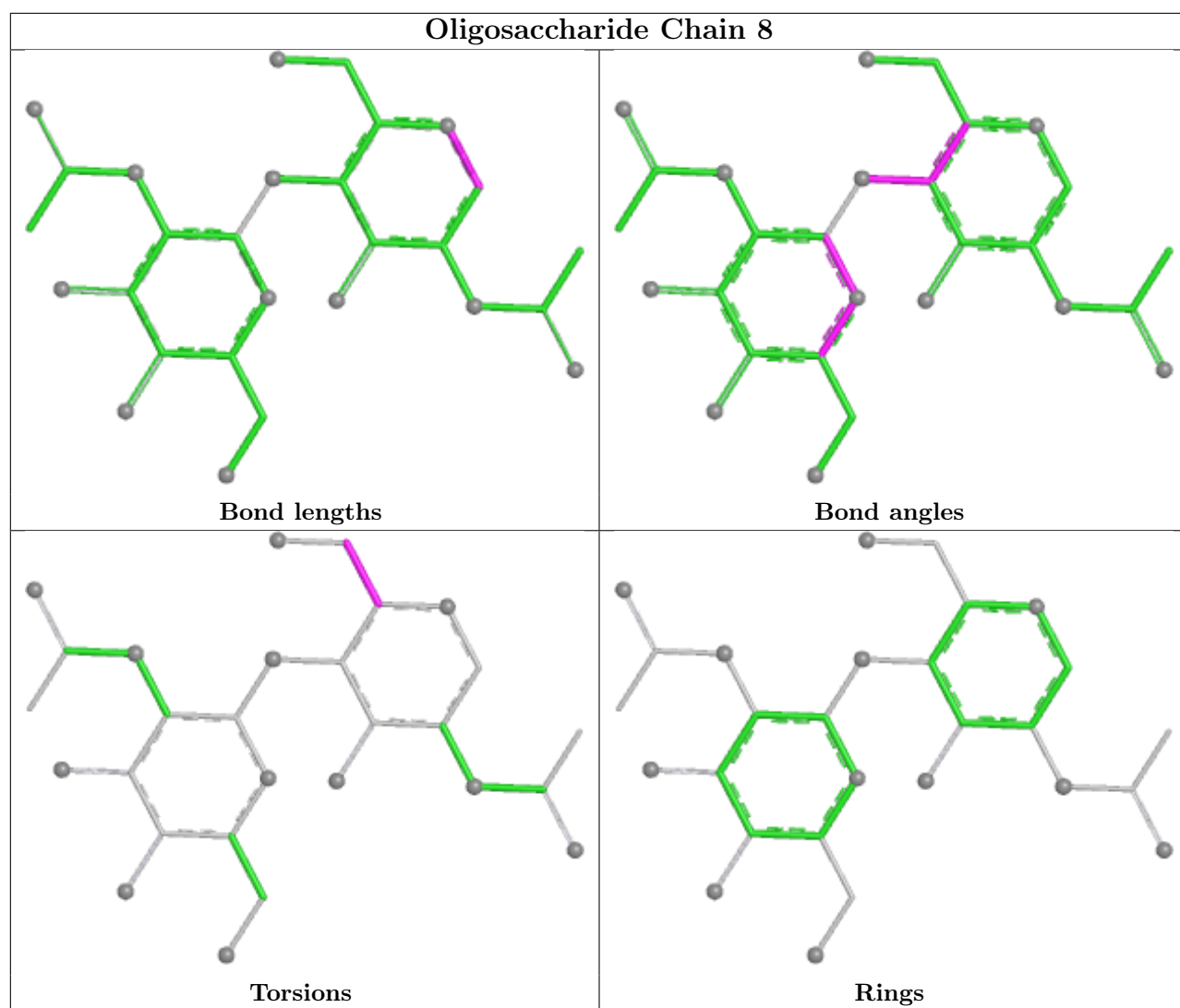


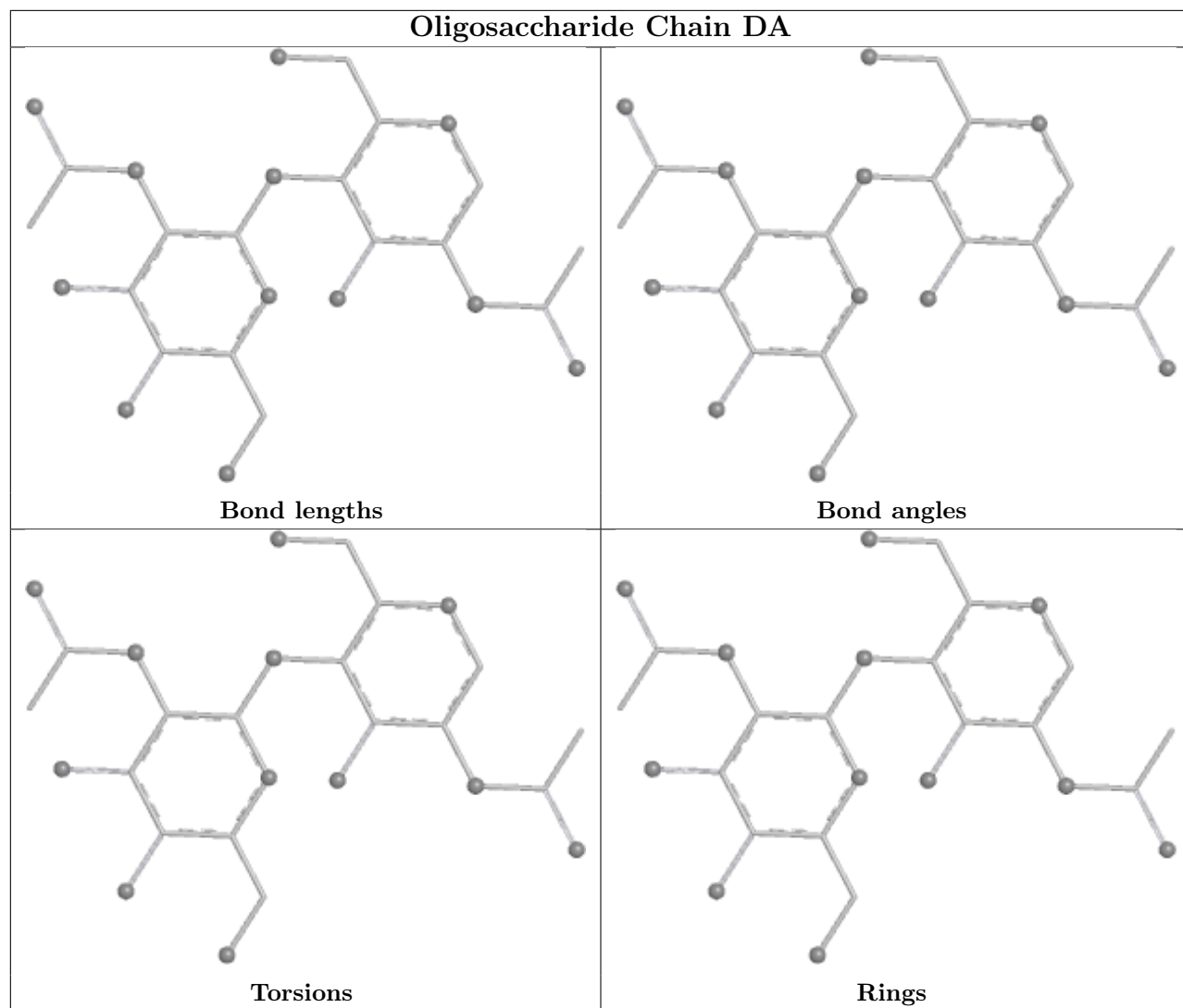


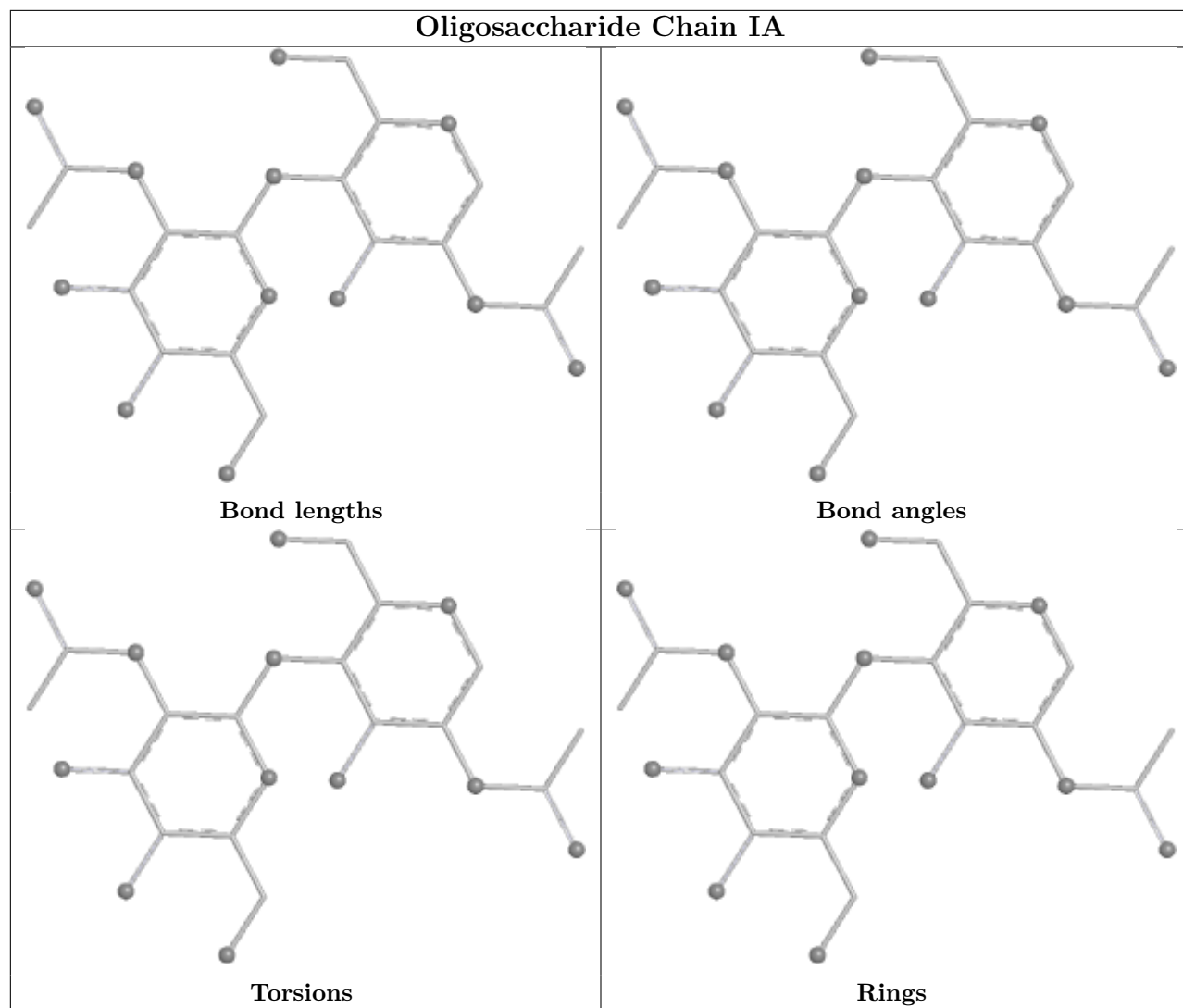


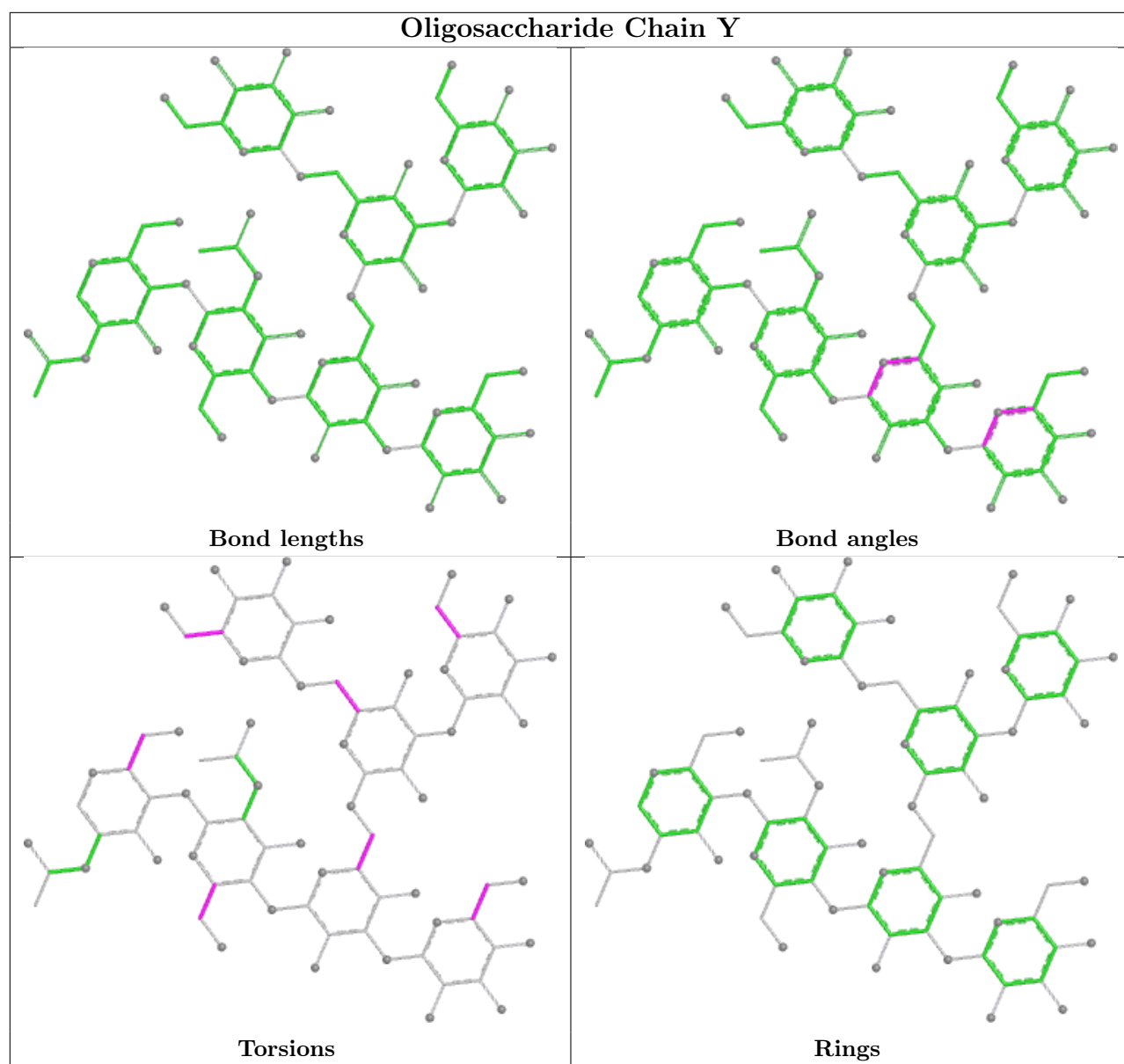


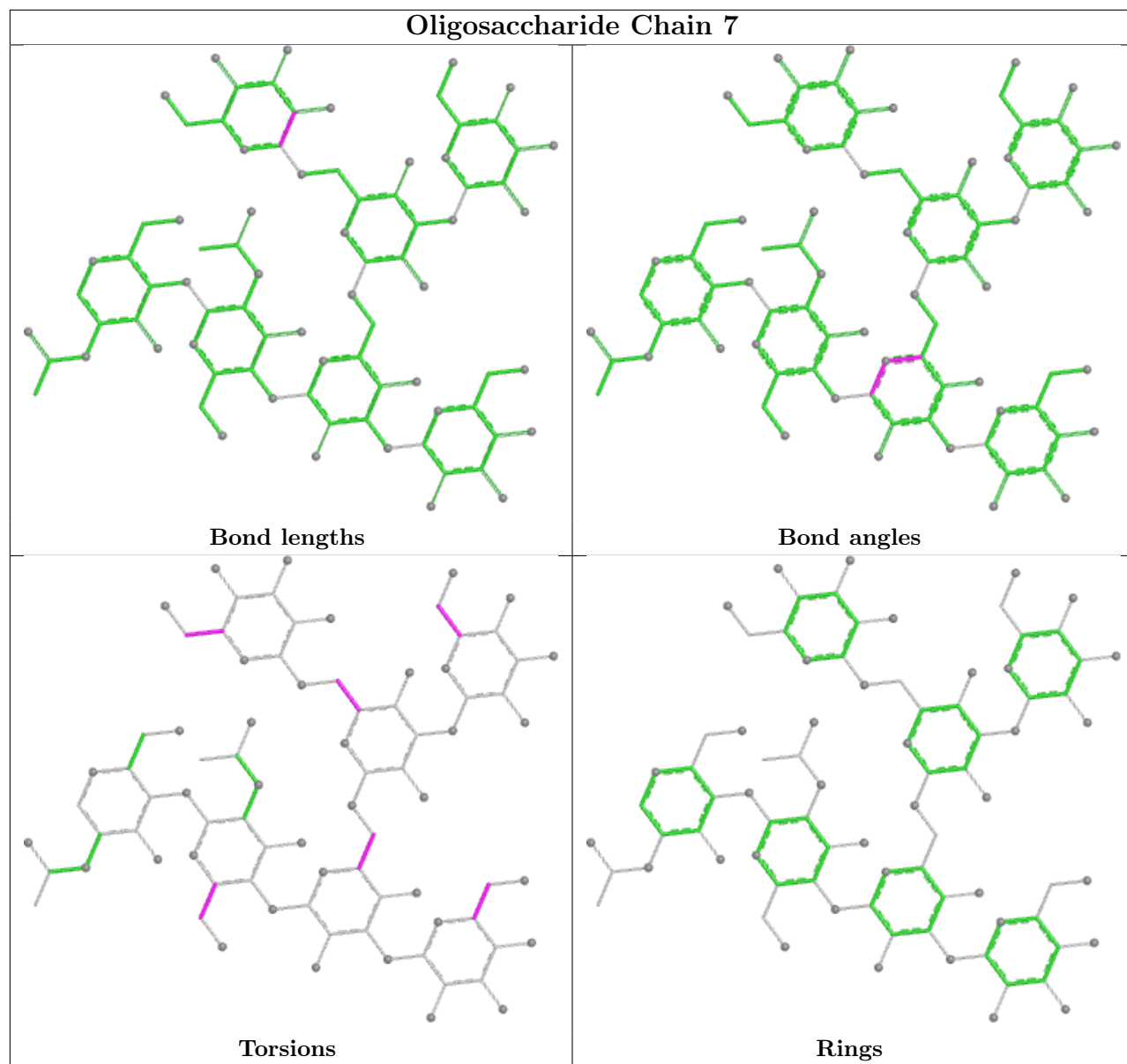


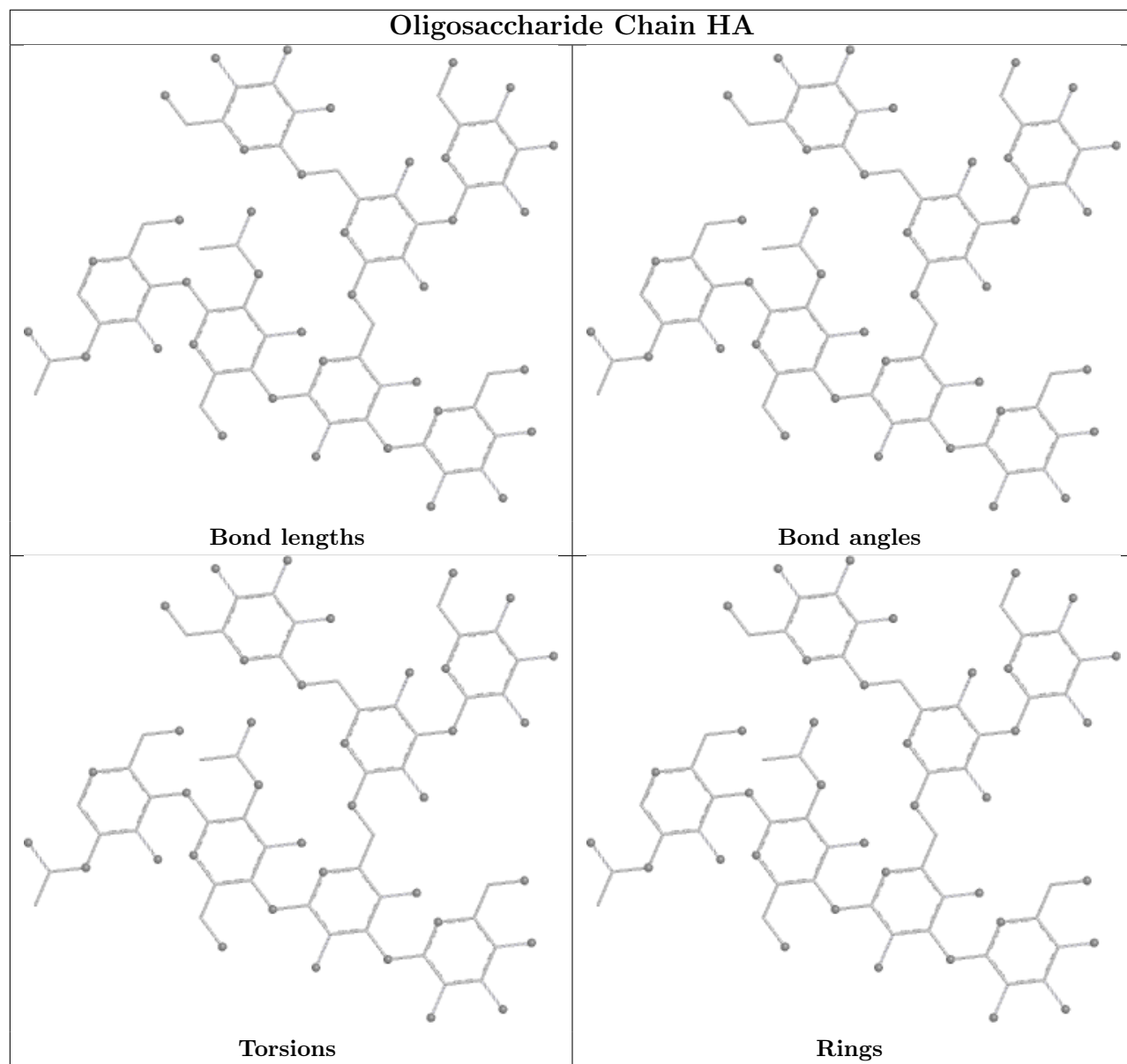


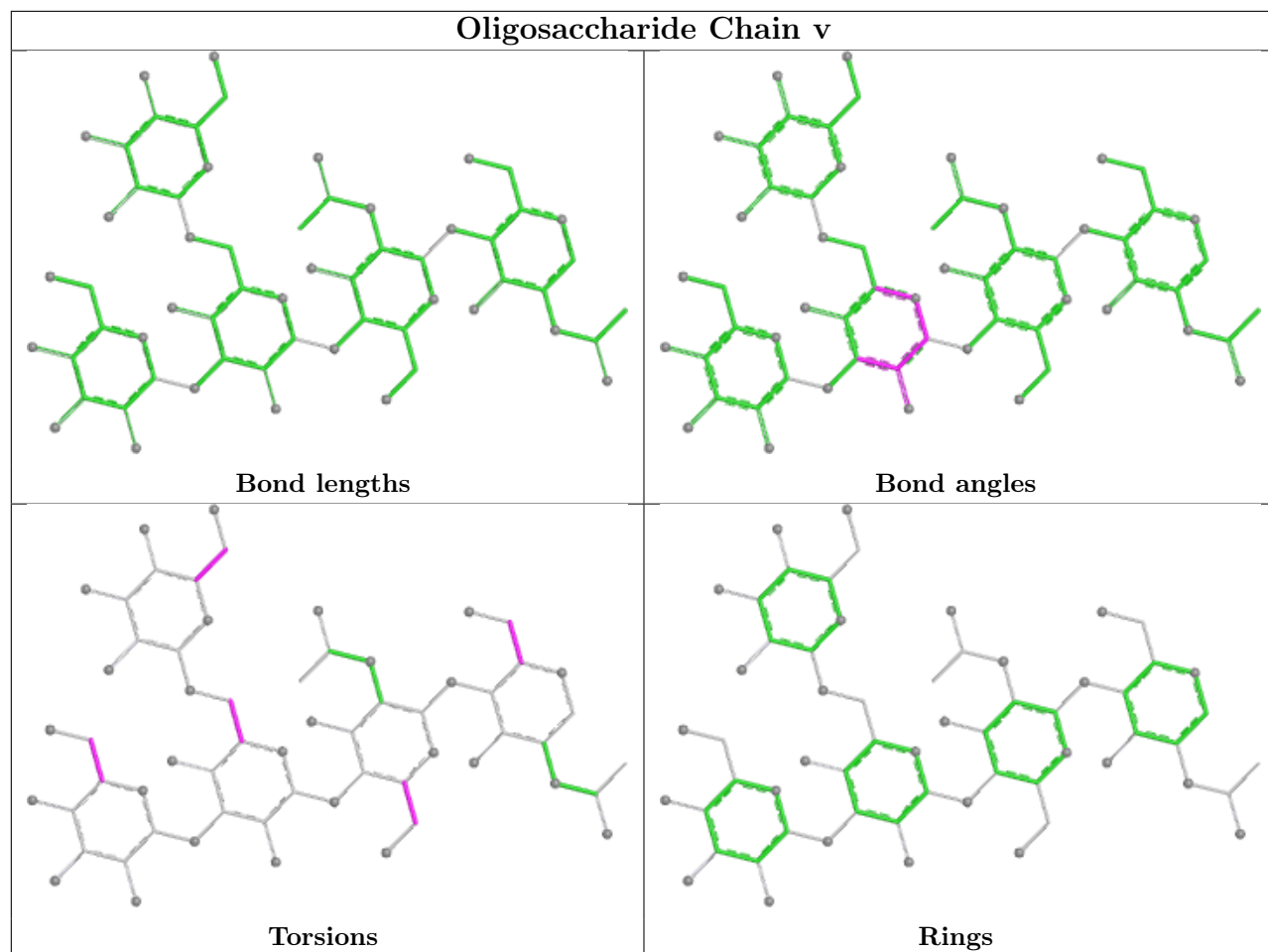


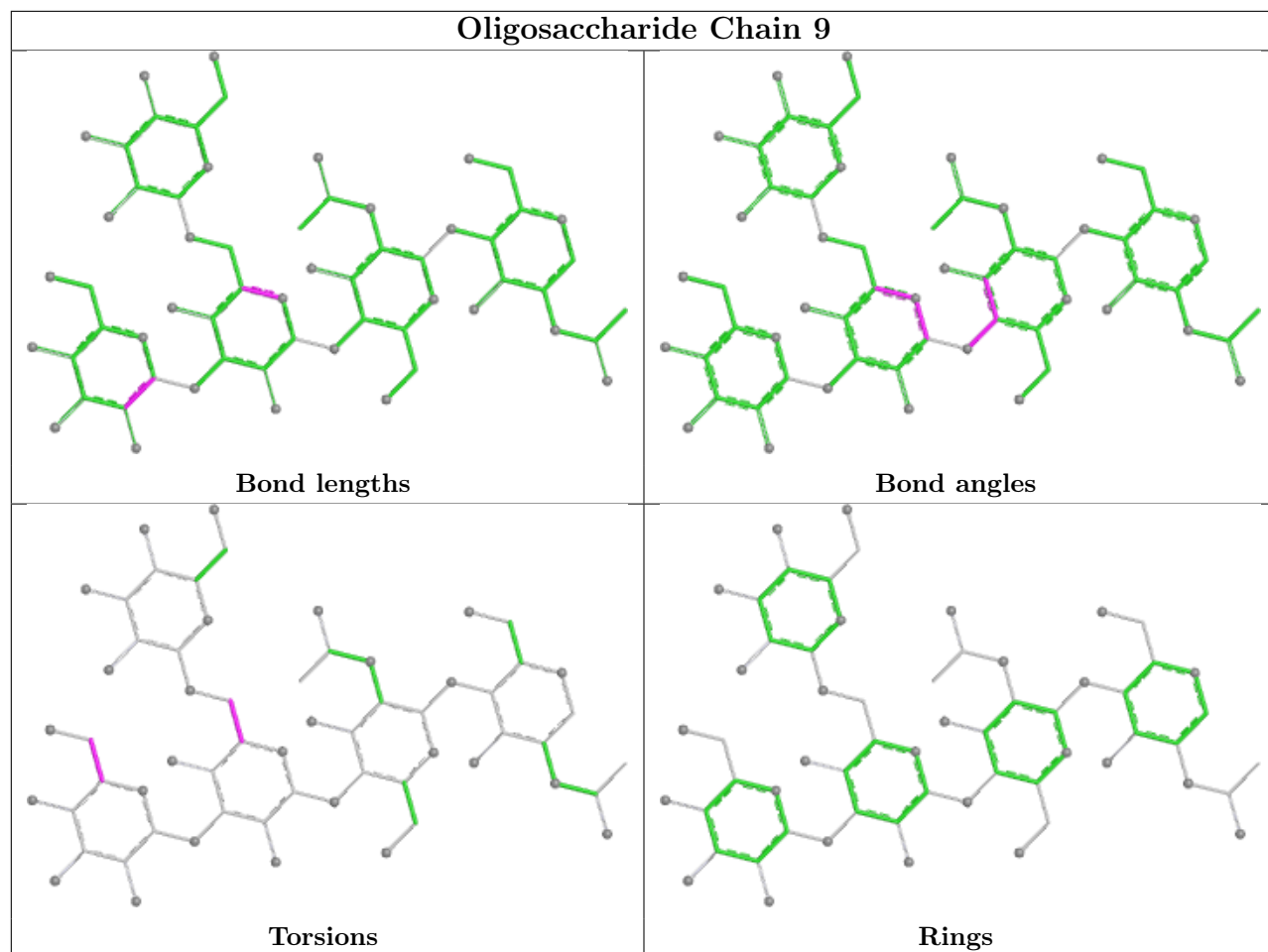


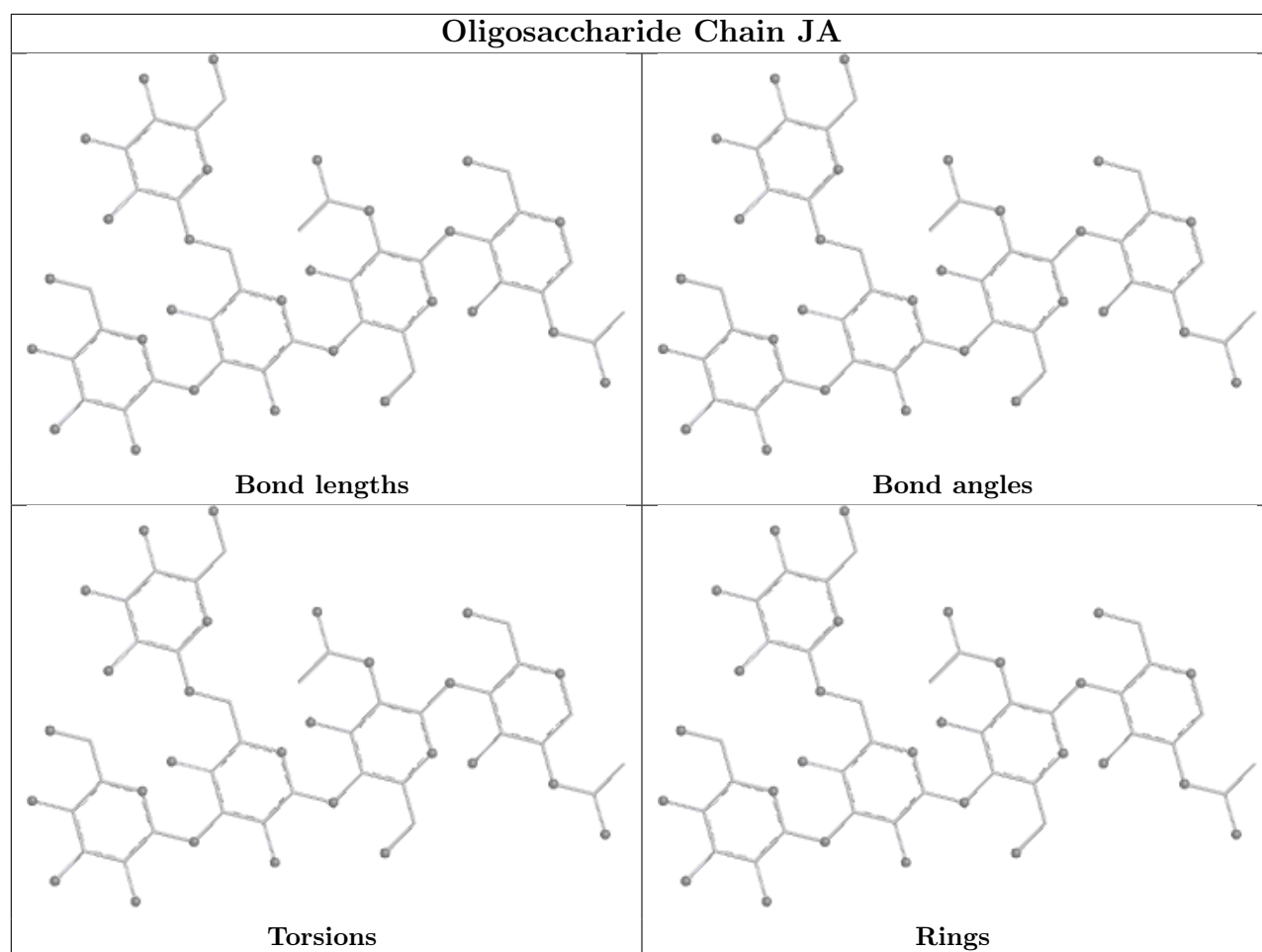












5.6 Ligand geometry [i](#)

30 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	$\# Z > 2$
20	NAG	r	1104	5	14,14,15	0.30	0	17,19,21	0.47	0
20	NAG	e	1104	5	14,14,15	0.29	0	17,19,21	0.47	0
20	NAG	f	1101	6	14,14,15	0.59	0	17,19,21	0.54	0
20	NAG	E	1106	5	14,14,15	0.39	0	17,19,21	0.54	0
21	CLR	z	201	-	31,31,31	0.41	0	48,48,48	0.73	0
20	NAG	e	1106	5	14,14,15	0.24	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	NAG	r	1103	5	14,14,15	0.27	0	17,19,21	0.44	0
20	NAG	E	1104	5	14,14,15	0.25	0	17,19,21	0.48	0
20	NAG	g	801	7	14,14,15	0.36	0	17,19,21	0.49	0
20	NAG	r	1106	5	14,14,15	0.31	0	17,19,21	0.44	0
20	NAG	G	802	7	14,14,15	0.26	0	17,19,21	0.46	0
20	NAG	F	1101	6	14,14,15	0.29	0	17,19,21	0.44	0
20	NAG	r	1101	5	14,14,15	0.23	0	17,19,21	0.47	0
20	NAG	e	1105	5	14,14,15	0.25	0	17,19,21	0.49	0
21	CLR	m	201	-	31,31,31	0.38	0	48,48,48	0.56	0
20	NAG	e	1102	5	14,14,15	1.45	2 (14%)	17,19,21	2.55	1 (5%)
20	NAG	E	1101	5	14,14,15	0.18	0	17,19,21	0.52	0
20	NAG	s	1101	6	14,14,15	0.59	0	17,19,21	0.54	0
20	NAG	r	1105	5	14,14,15	0.24	0	17,19,21	0.48	0
20	NAG	e	1103	5	14,14,15	0.31	0	17,19,21	0.45	0
20	NAG	r	1102	5	14,14,15	0.30	0	17,19,21	0.46	0
20	NAG	t	802	7	14,14,15	0.46	0	17,19,21	0.51	0
20	NAG	e	1101	5	14,14,15	0.29	0	17,19,21	0.51	0
20	NAG	E	1102	5	14,14,15	0.88	2 (14%)	17,19,21	0.89	1 (5%)
21	CLR	M	201	-	31,31,31	0.42	0	48,48,48	0.88	1 (2%)
20	NAG	E	1105	5	14,14,15	0.22	0	17,19,21	0.44	0
20	NAG	E	1103	5	14,14,15	0.35	0	17,19,21	0.53	0
20	NAG	G	801	7	14,14,15	0.35	0	17,19,21	0.52	0
20	NAG	t	801	7	14,14,15	0.36	0	17,19,21	0.48	0
20	NAG	g	802	7	14,14,15	0.48	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	NAG	r	1104	5	-	0/6/23/26	0/1/1/1
20	NAG	e	1104	5	-	0/6/23/26	0/1/1/1
20	NAG	f	1101	6	-	0/6/23/26	0/1/1/1
20	NAG	E	1106	5	-	2/6/23/26	0/1/1/1
21	CLR	z	201	-	-	4/10/68/68	0/4/4/4
20	NAG	e	1106	5	-	2/6/23/26	0/1/1/1
20	NAG	r	1103	5	-	1/6/23/26	0/1/1/1
20	NAG	E	1104	5	-	0/6/23/26	0/1/1/1
20	NAG	g	801	7	-	3/6/23/26	0/1/1/1
20	NAG	r	1106	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	NAG	G	802	7	-	2/6/23/26	0/1/1/1
20	NAG	F	1101	6	-	0/6/23/26	0/1/1/1
20	NAG	r	1101	5	-	2/6/23/26	0/1/1/1
20	NAG	e	1105	5	-	0/6/23/26	0/1/1/1
21	CLR	m	201	-	-	3/10/68/68	0/4/4/4
20	NAG	e	1102	5	-	0/6/23/26	0/1/1/1
20	NAG	E	1101	5	-	0/6/23/26	0/1/1/1
20	NAG	s	1101	6	-	0/6/23/26	0/1/1/1
20	NAG	r	1105	5	-	0/6/23/26	0/1/1/1
20	NAG	e	1103	5	-	1/6/23/26	0/1/1/1
20	NAG	r	1102	5	-	2/6/23/26	0/1/1/1
20	NAG	t	802	7	-	2/6/23/26	0/1/1/1
20	NAG	e	1101	5	-	0/6/23/26	0/1/1/1
20	NAG	E	1102	5	-	2/6/23/26	0/1/1/1
21	CLR	M	201	-	-	5/10/68/68	0/4/4/4
20	NAG	E	1105	5	-	0/6/23/26	0/1/1/1
20	NAG	E	1103	5	-	2/6/23/26	0/1/1/1
20	NAG	G	801	7	-	0/6/23/26	0/1/1/1
20	NAG	t	801	7	-	3/6/23/26	0/1/1/1
20	NAG	g	802	7	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	e	1102	NAG	O5-C1	4.89	1.51	1.43
20	E	1102	NAG	O5-C1	2.54	1.48	1.43
20	e	1102	NAG	C1-C2	2.19	1.55	1.52
20	E	1102	NAG	C1-C2	2.01	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	e	1102	NAG	C1-O5-C5	10.24	125.91	112.19
20	E	1102	NAG	C1-O5-C5	3.36	116.69	112.19
21	M	201	CLR	C16-C15-C14	-2.12	101.00	105.14

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

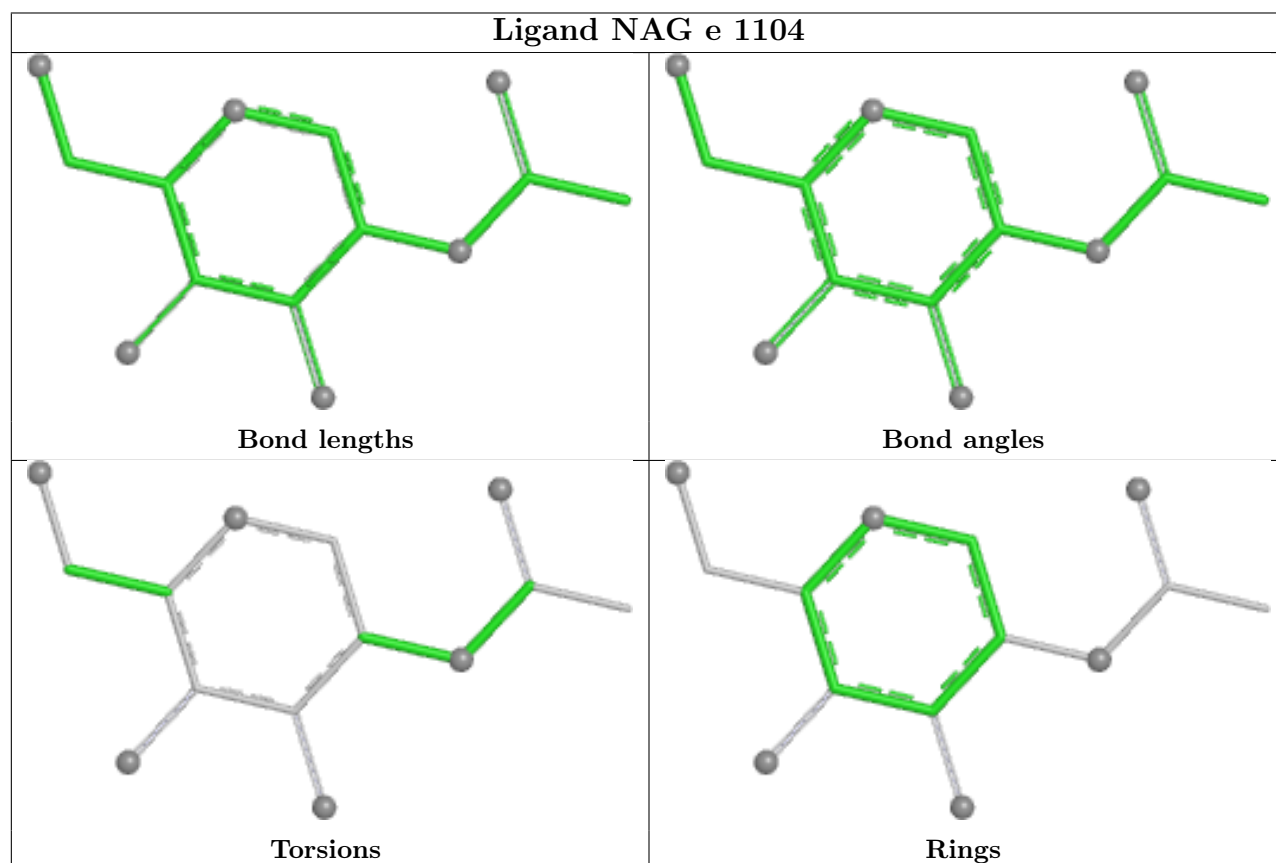
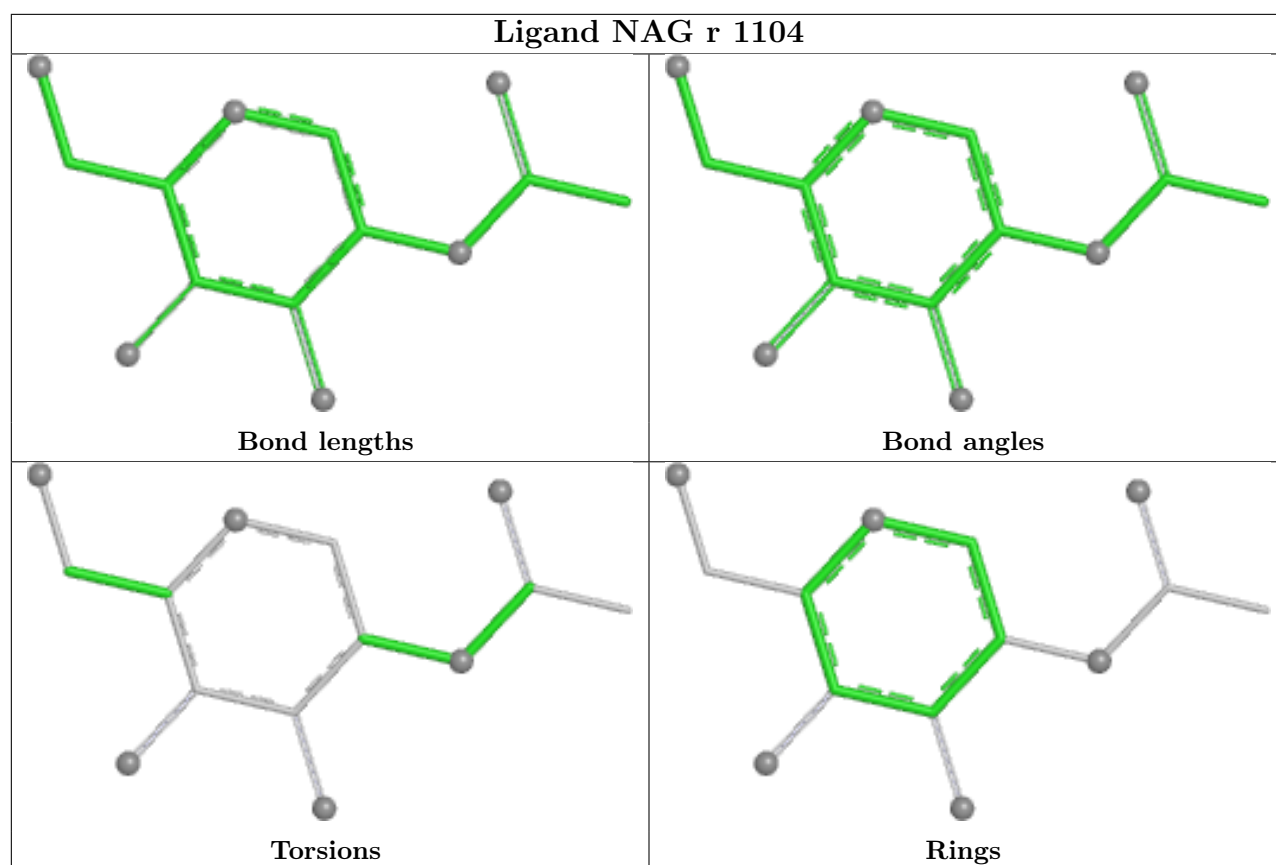
Mol	Chain	Res	Type	Atoms
20	E	1103	NAG	C4-C5-C6-O6
20	G	802	NAG	O5-C5-C6-O6
20	r	1106	NAG	O5-C5-C6-O6
21	M	201	CLR	C17-C20-C22-C23
20	E	1106	NAG	O5-C5-C6-O6

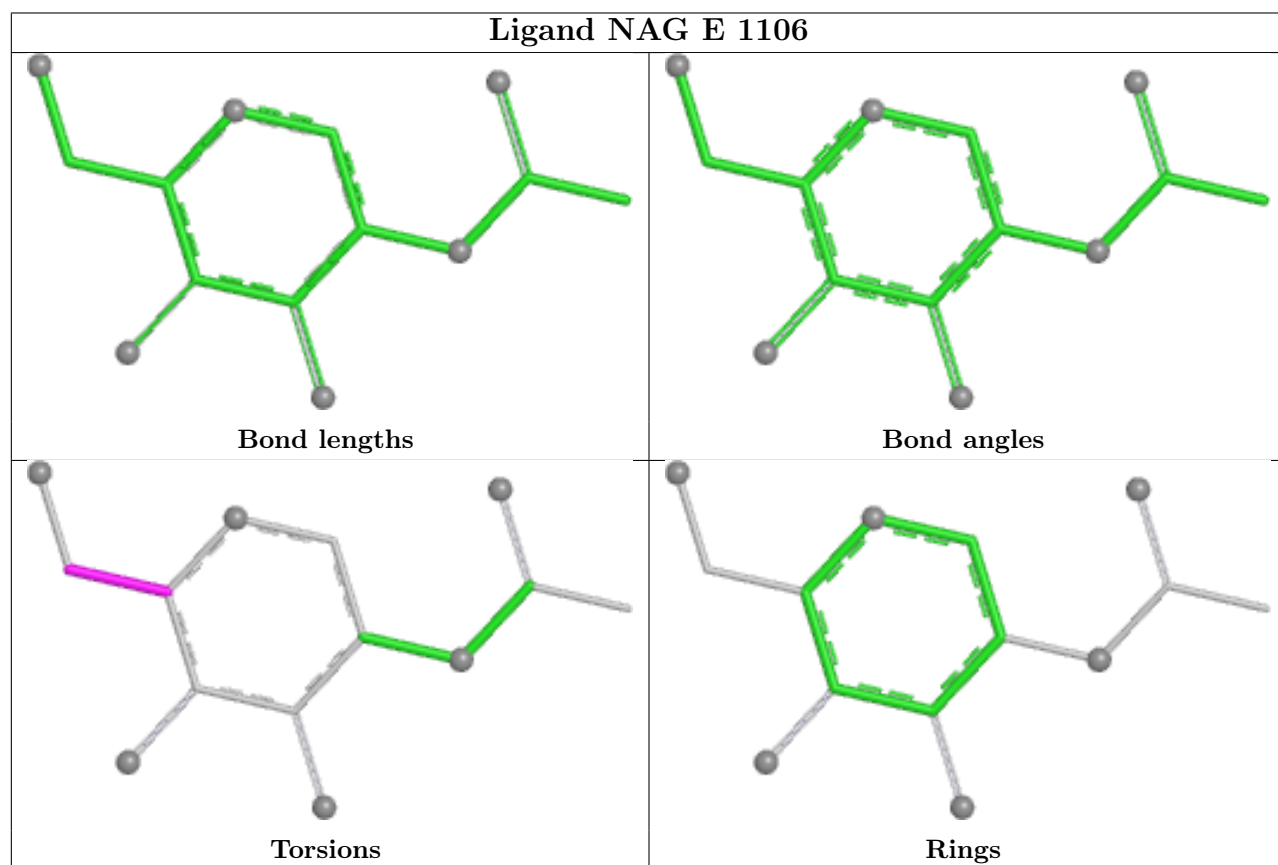
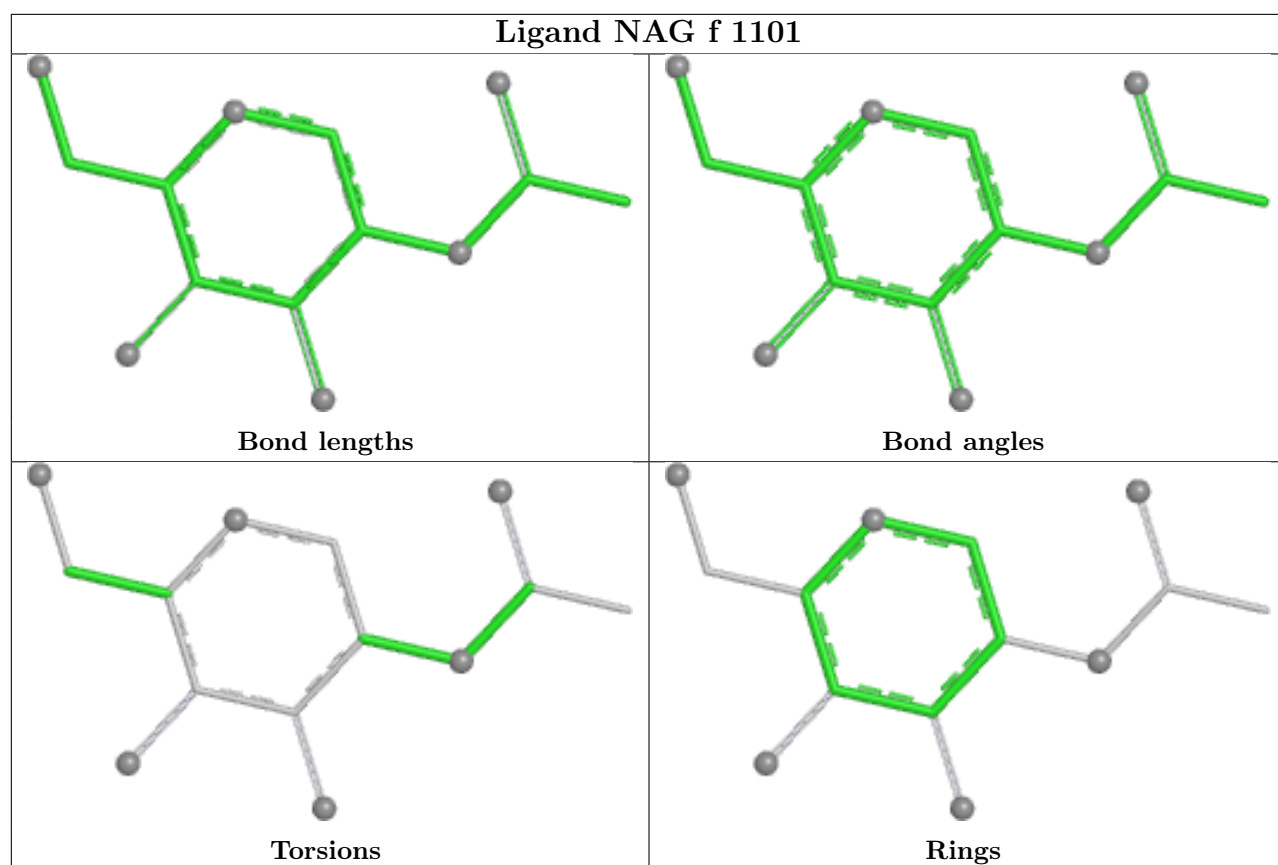
There are no ring outliers.

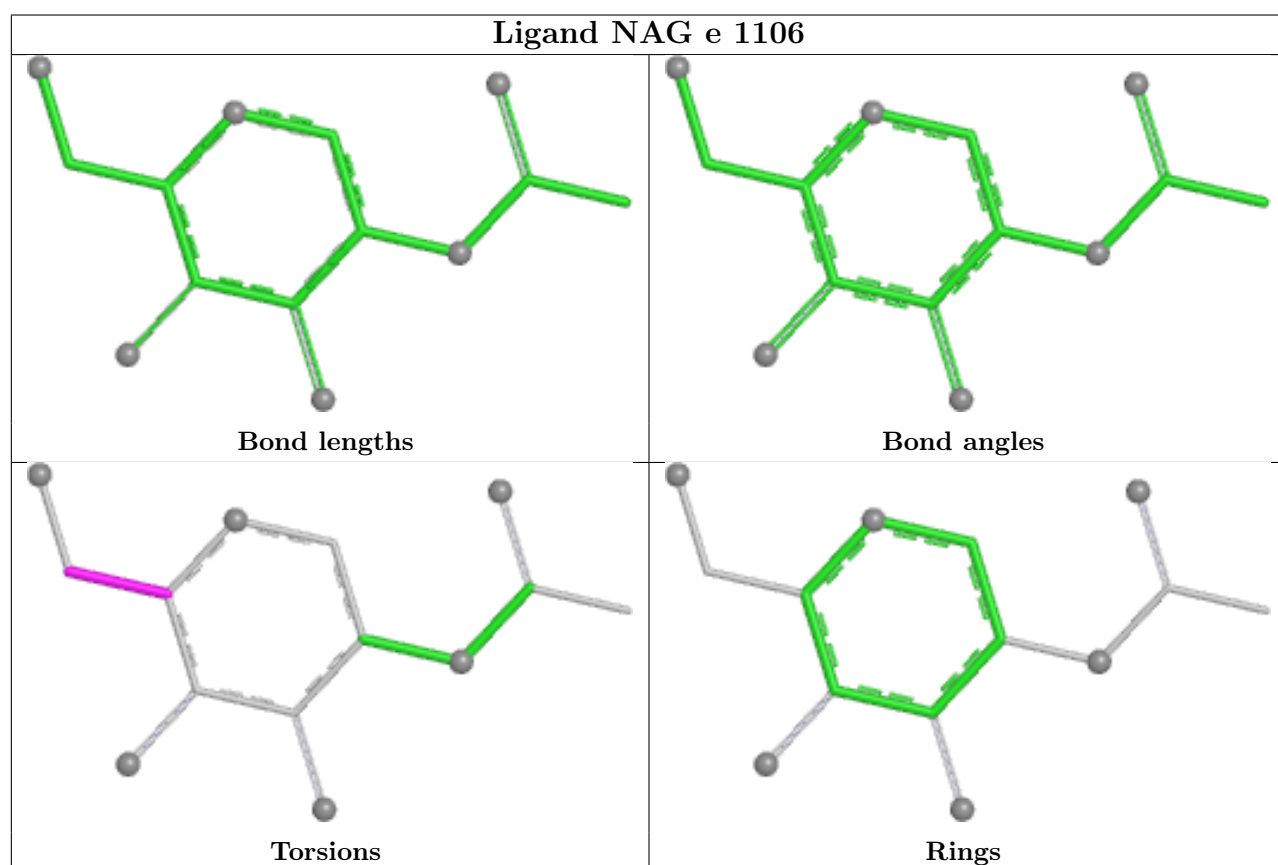
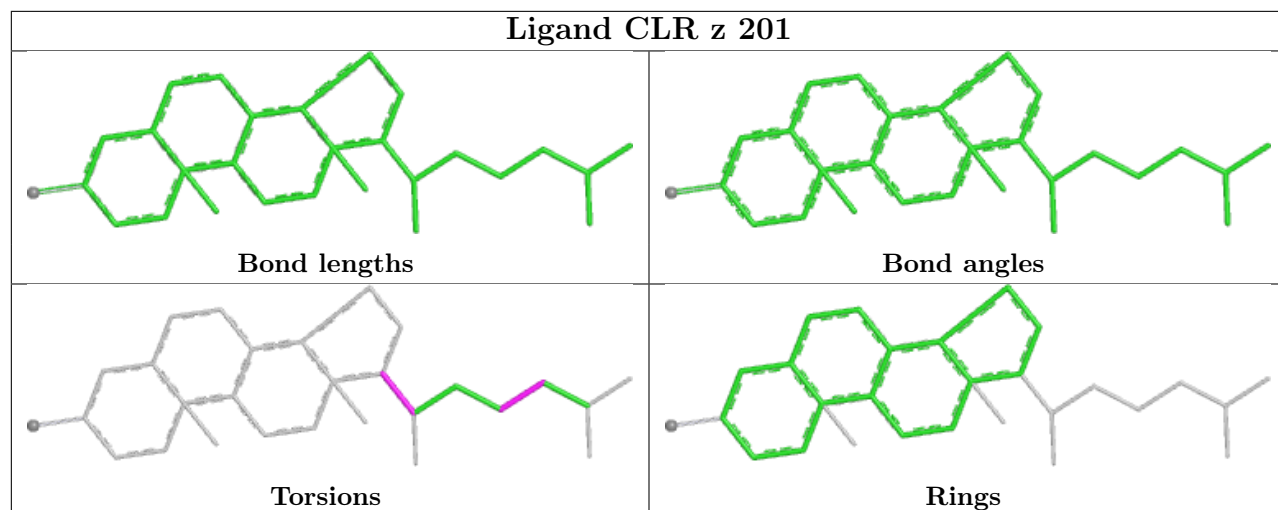
2 monomers are involved in 2 short contacts:

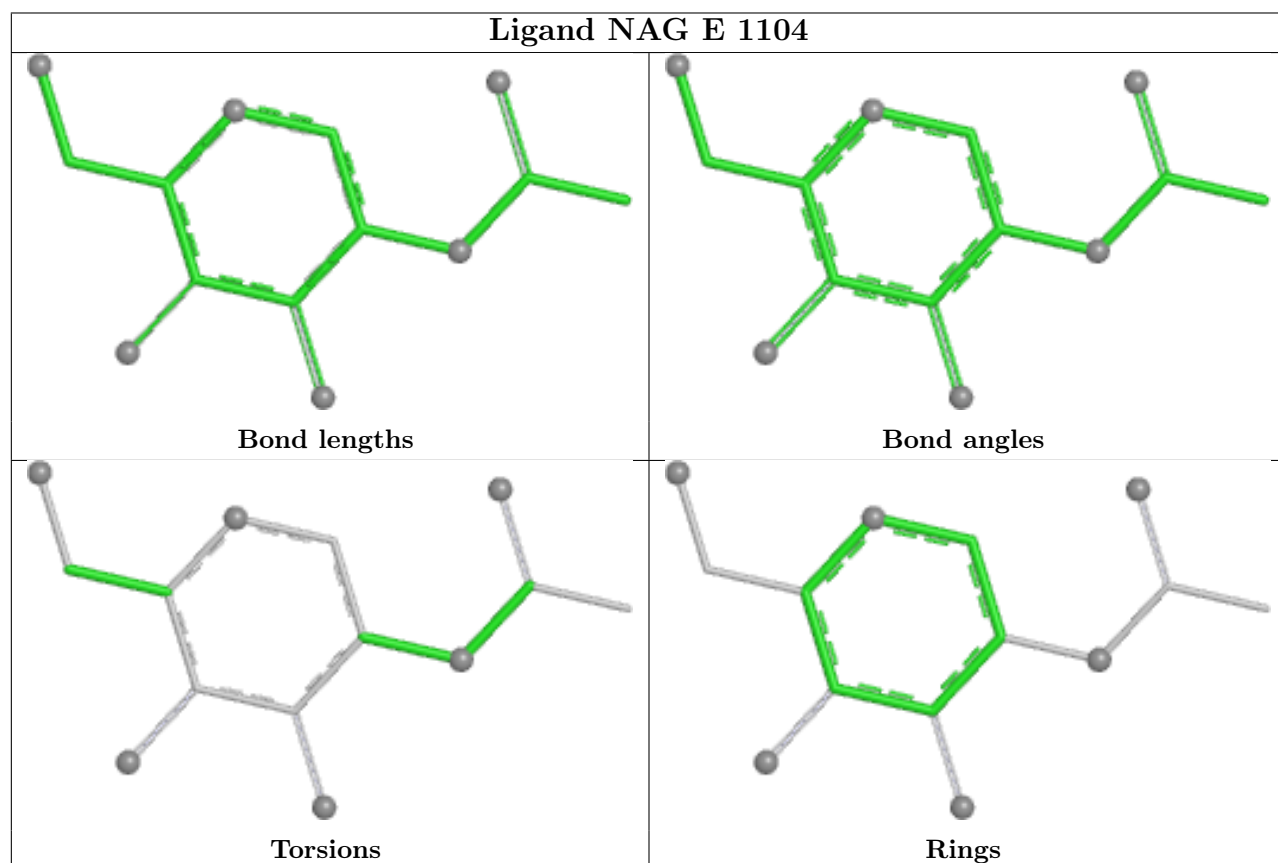
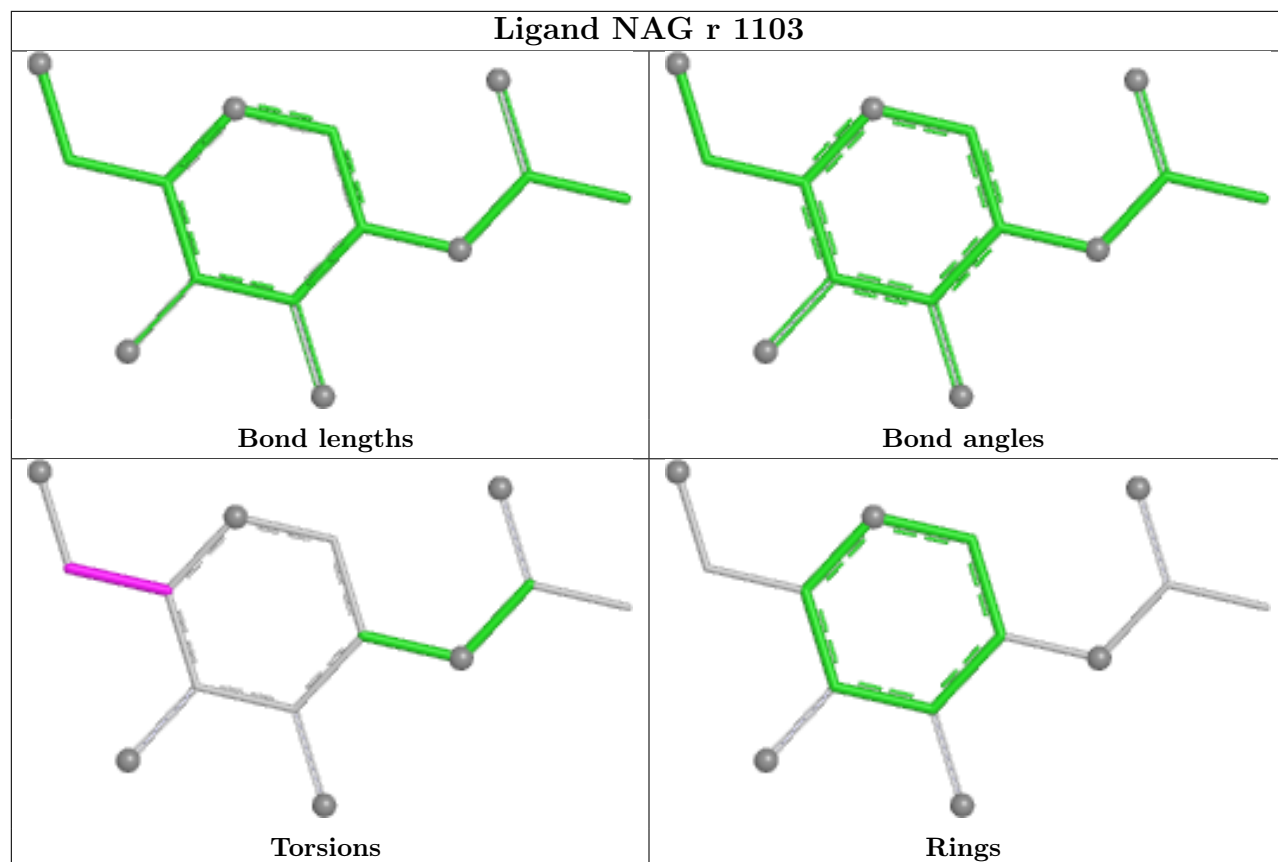
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	z	201	CLR	1	0
21	m	201	CLR	1	0

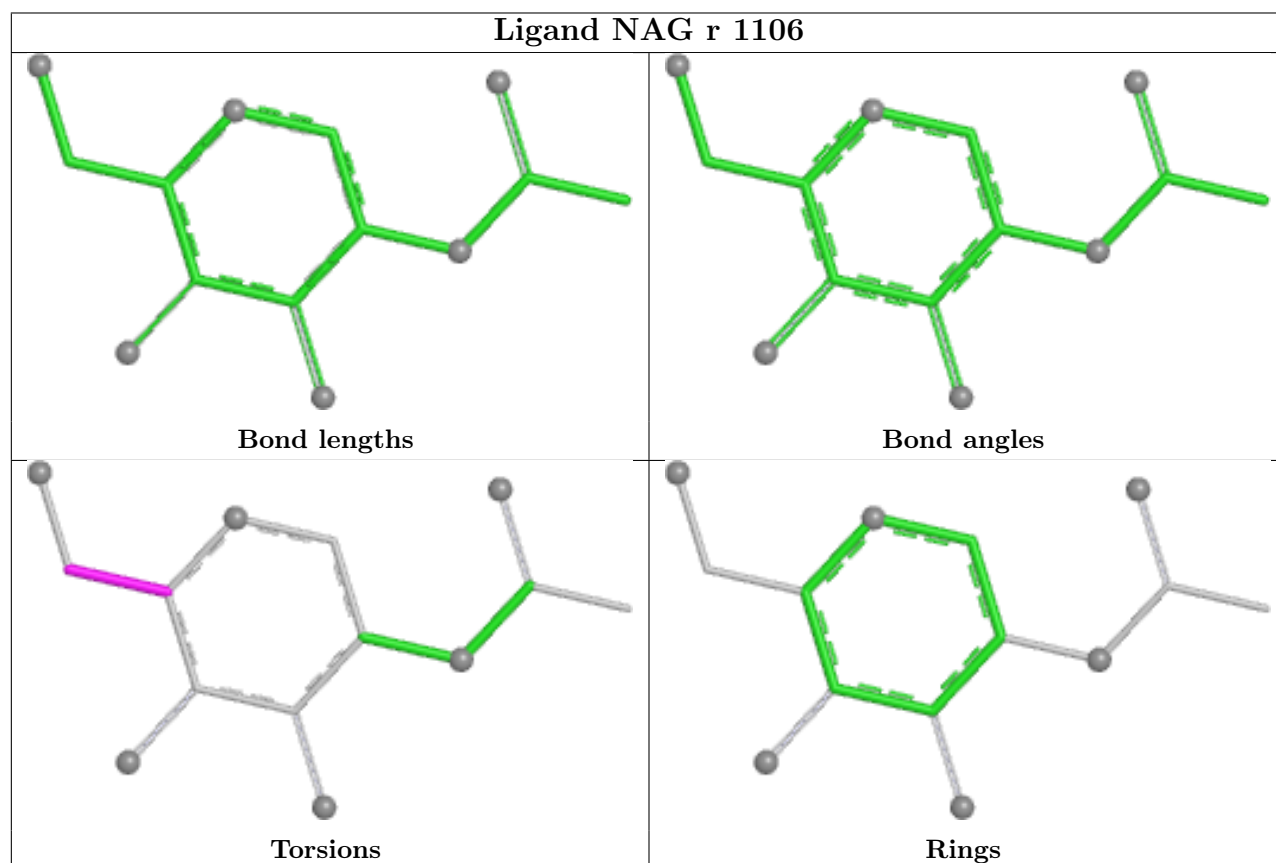
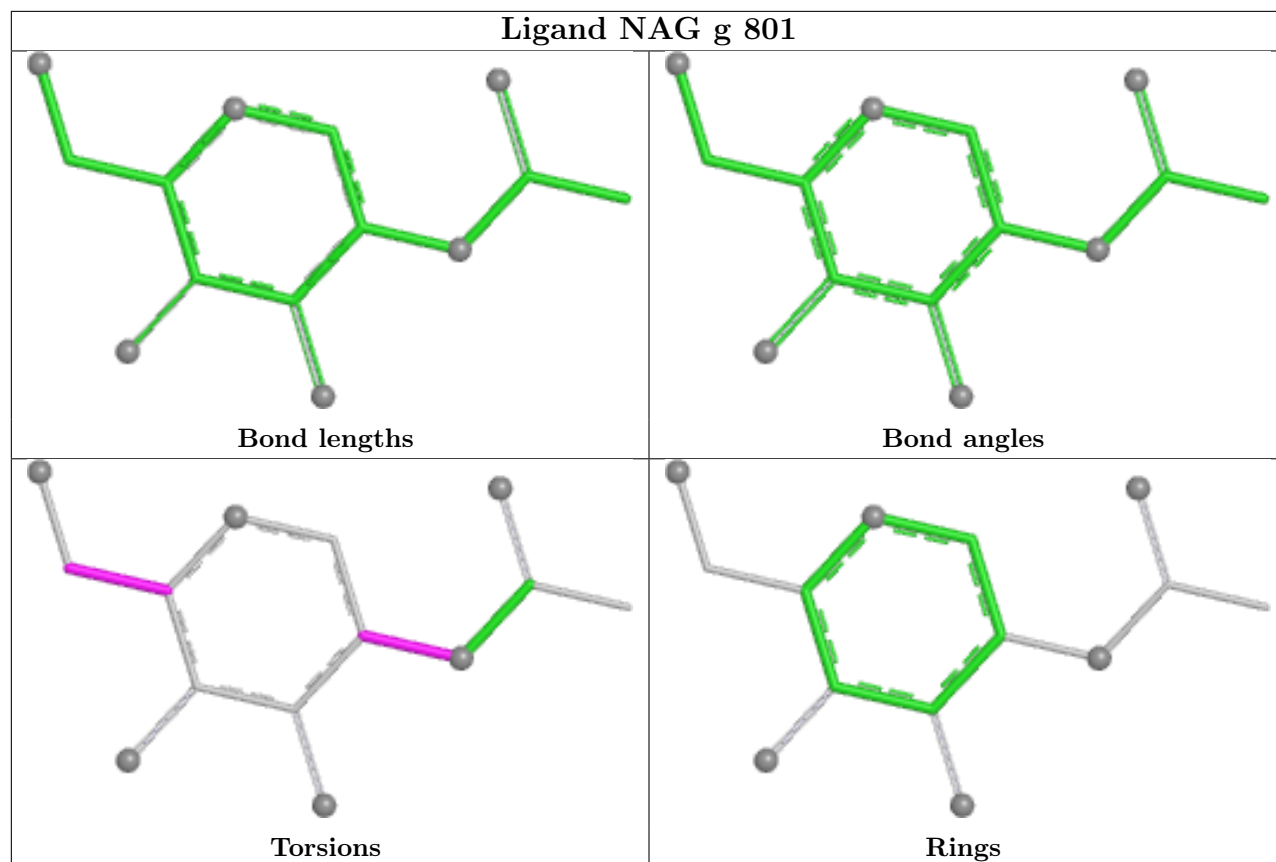
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

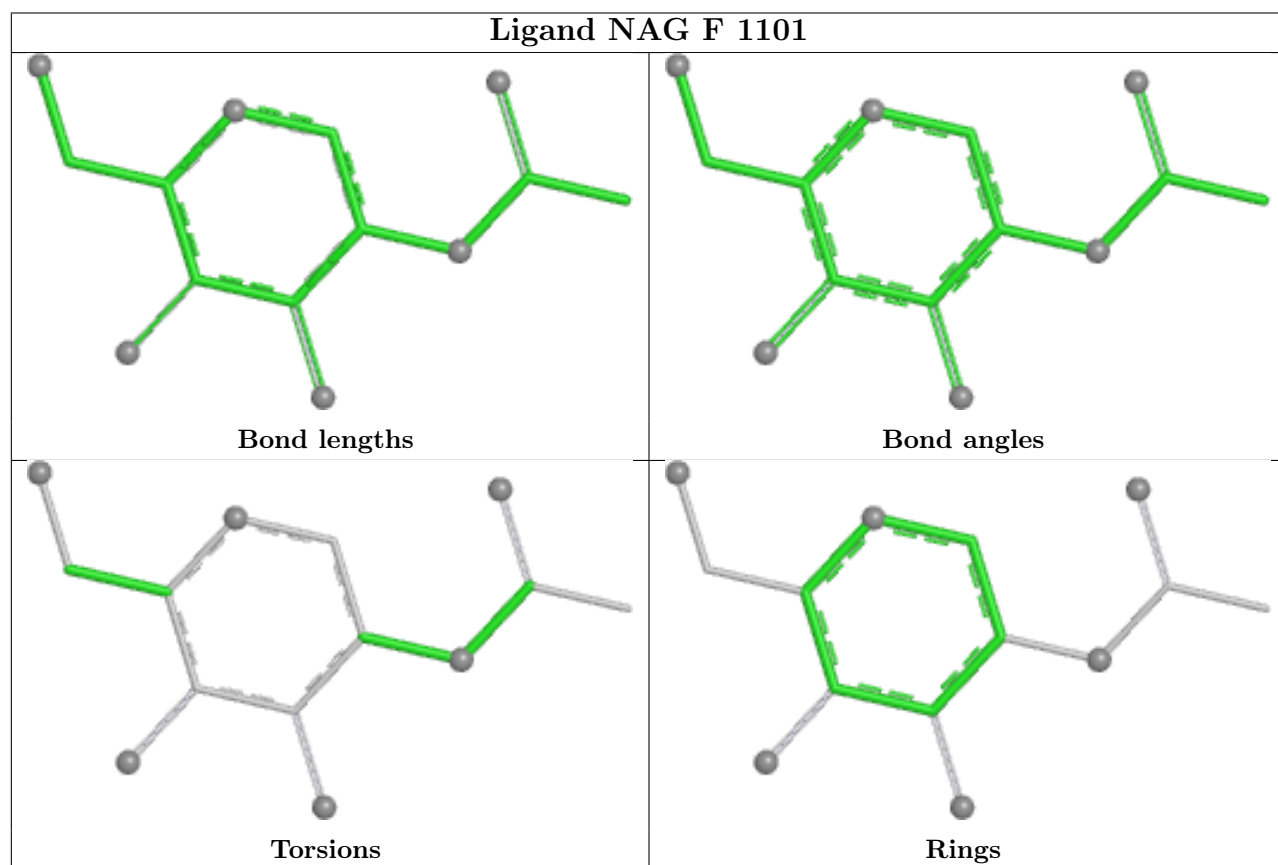
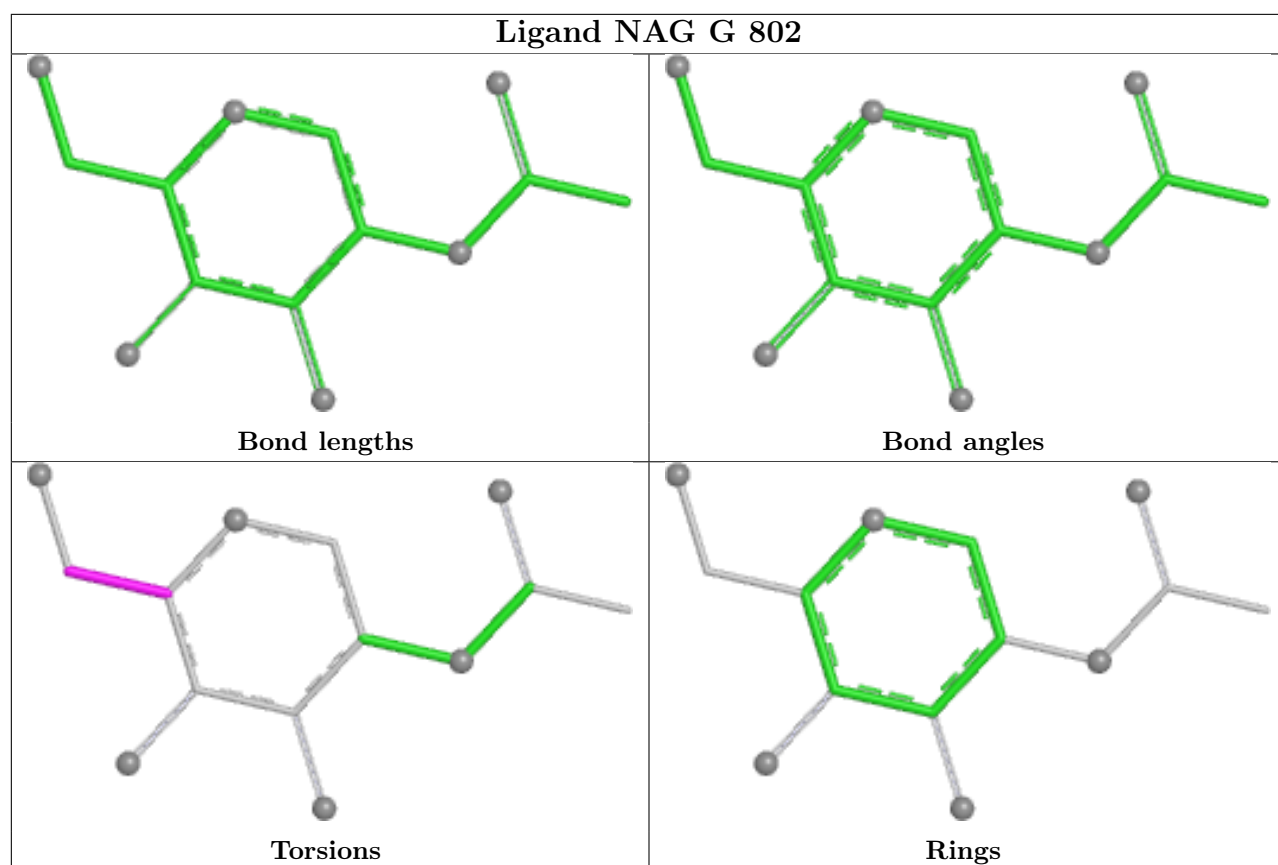


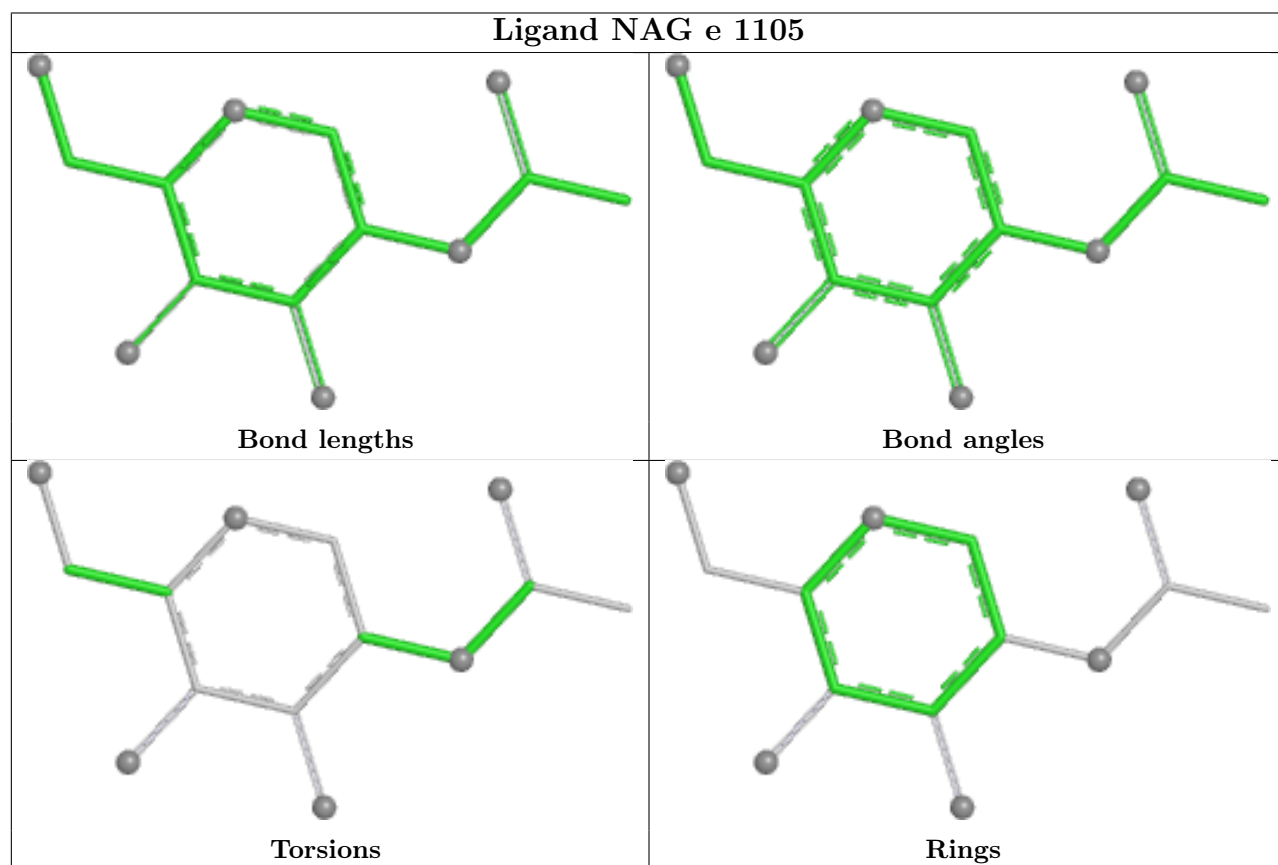
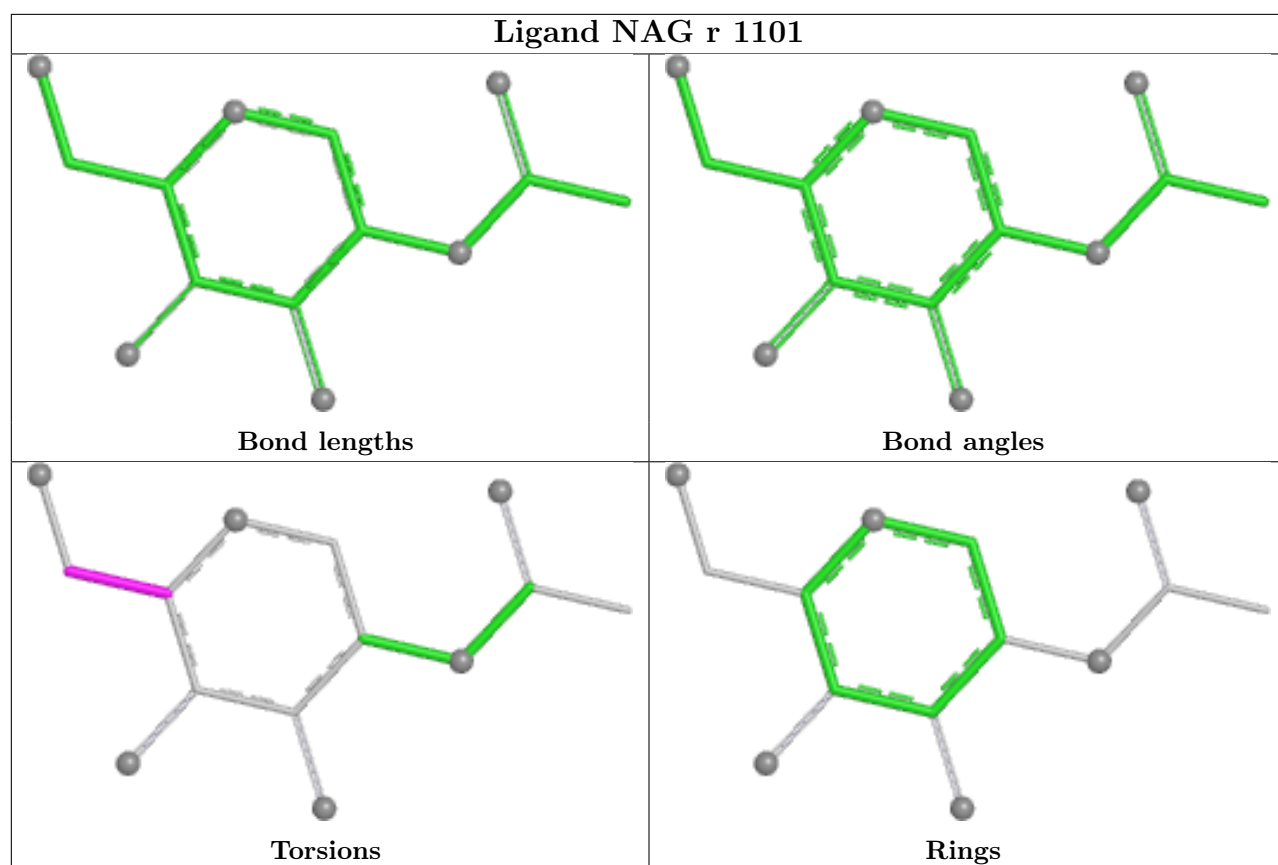


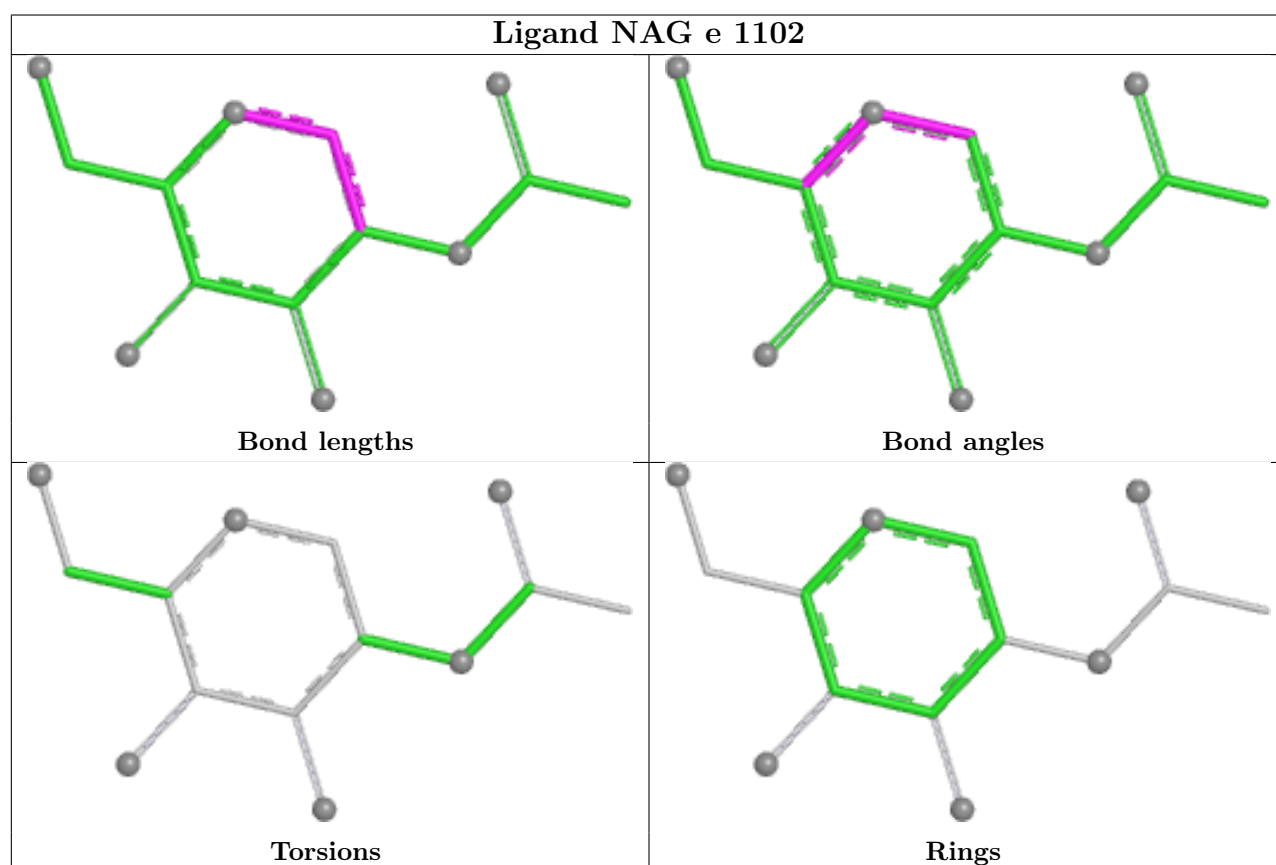
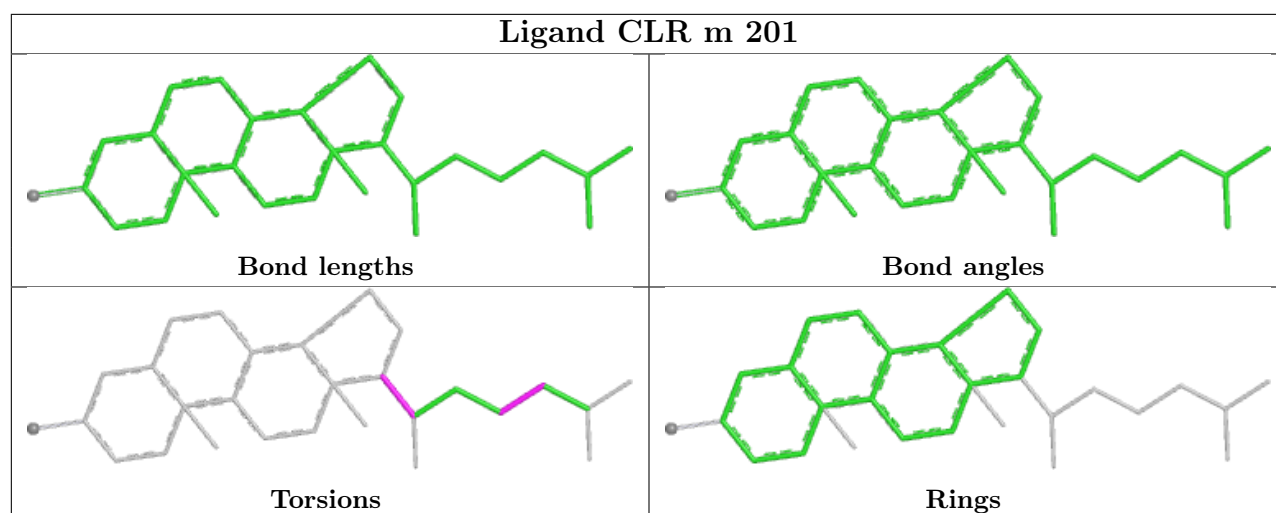


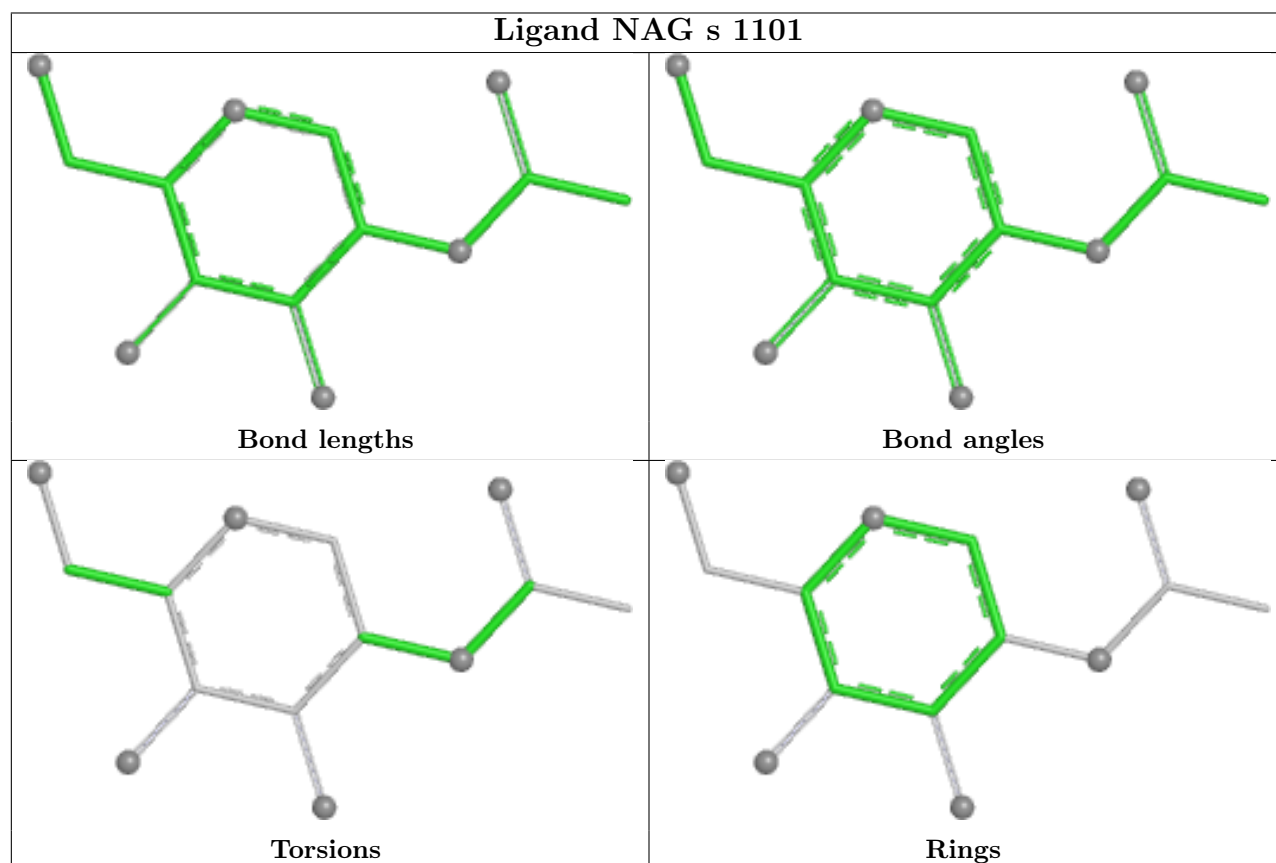
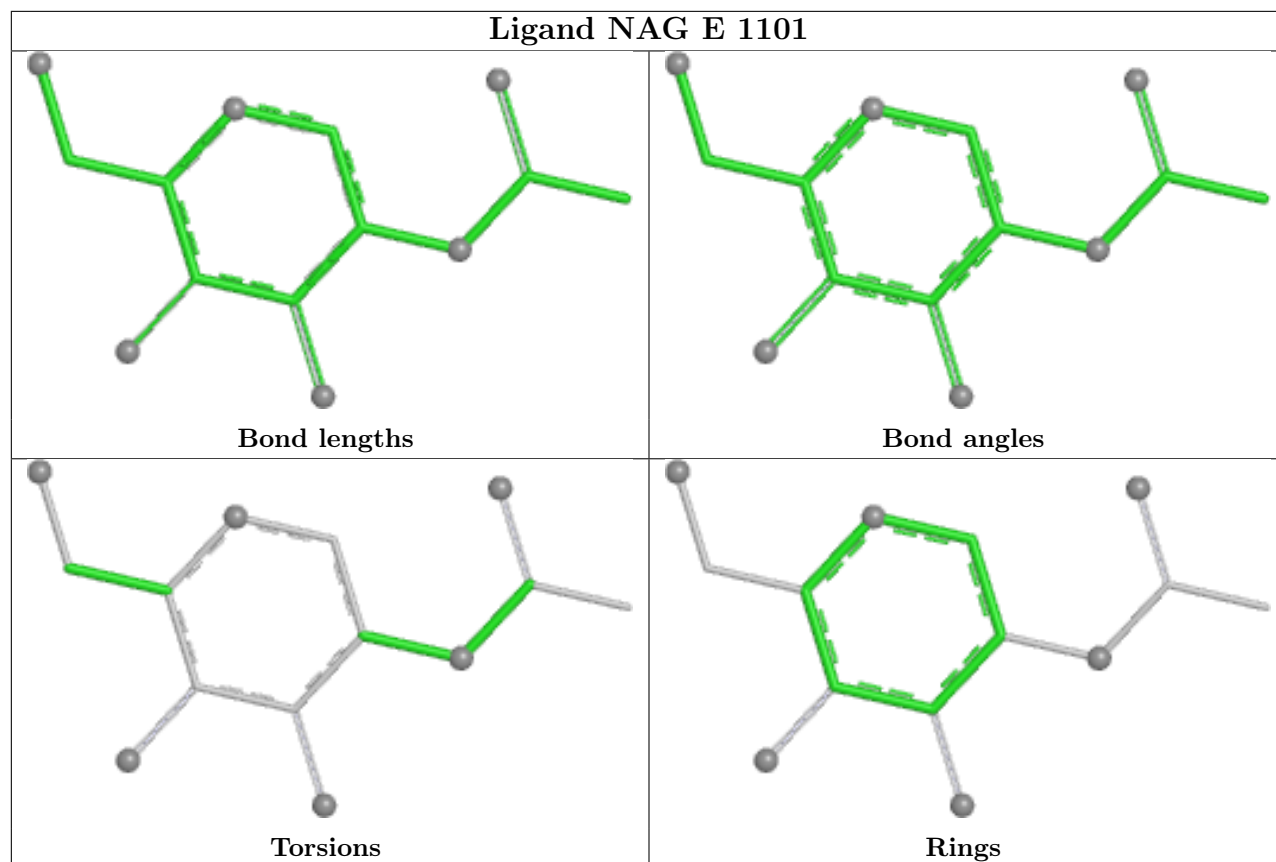


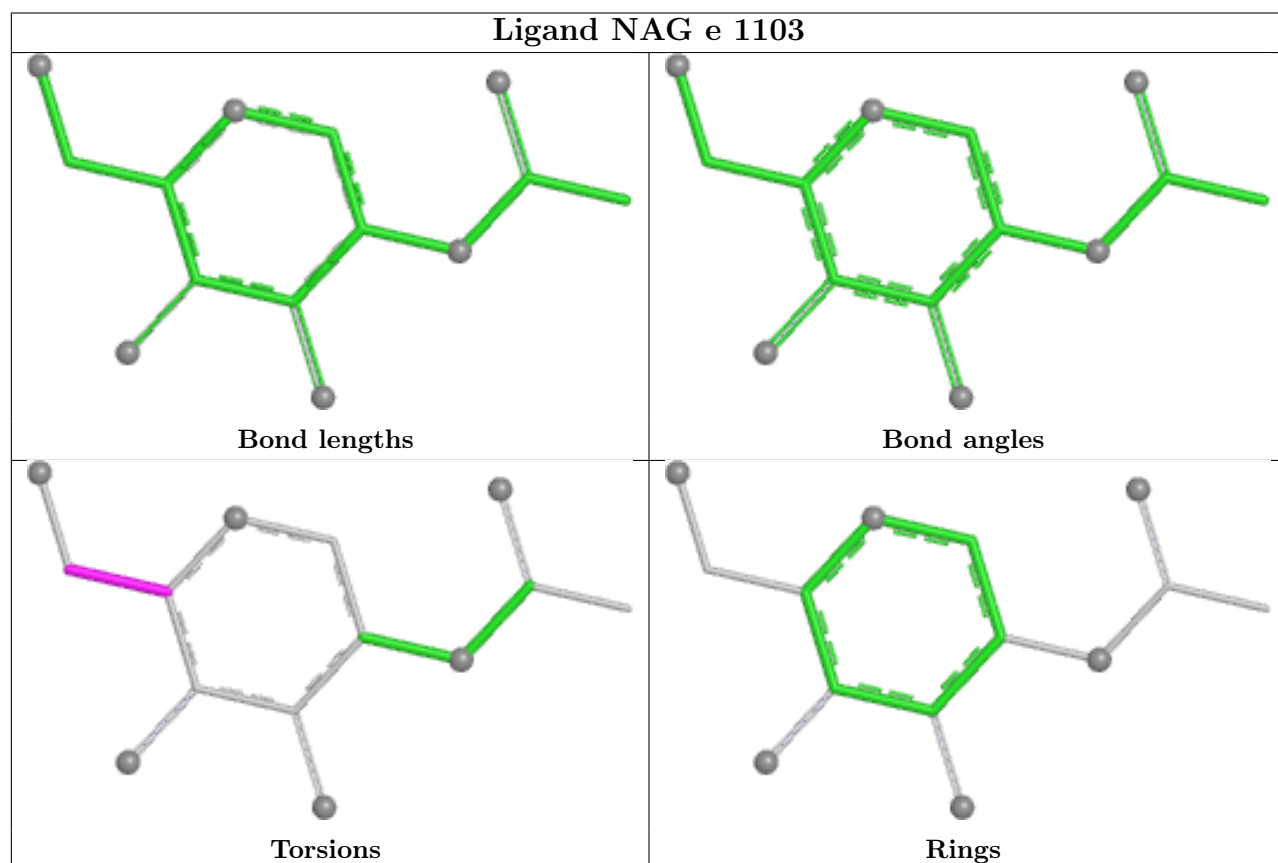
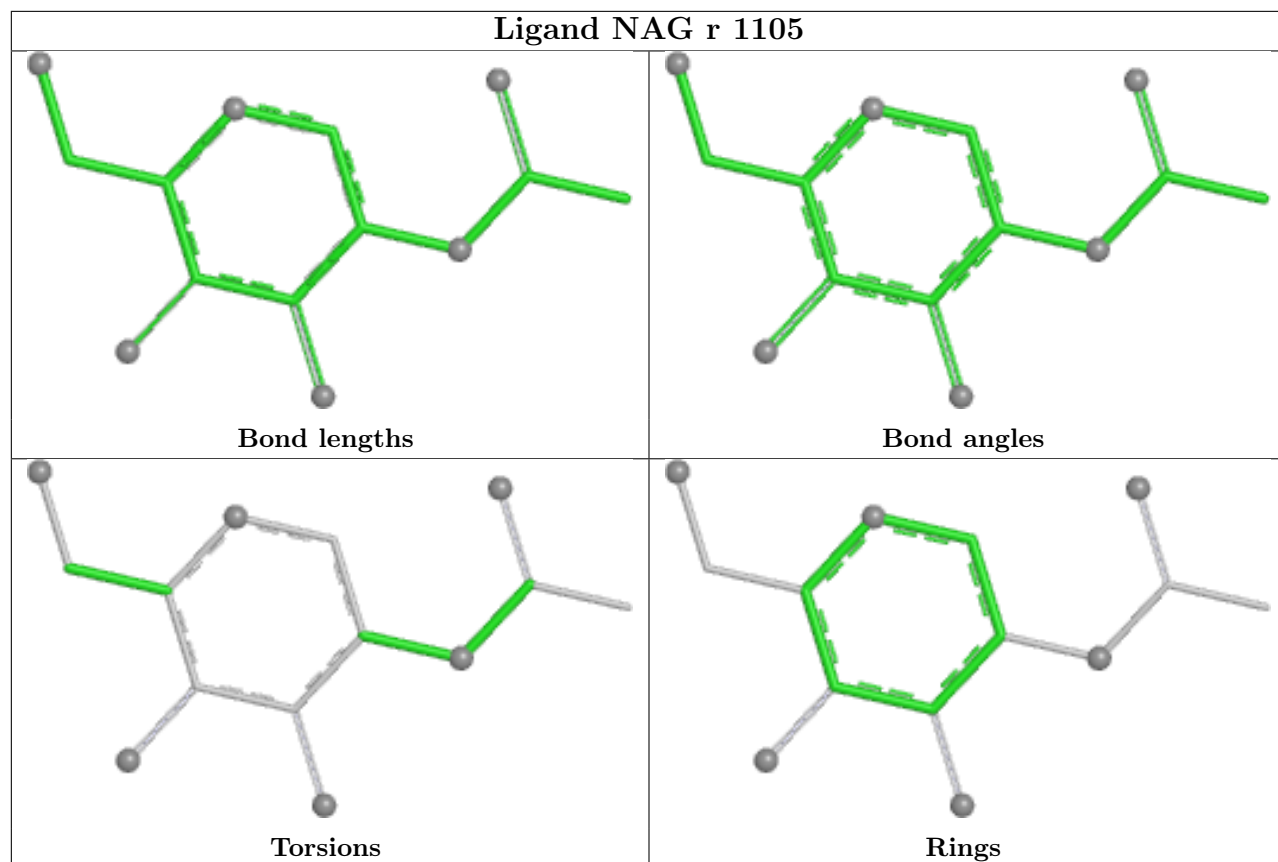


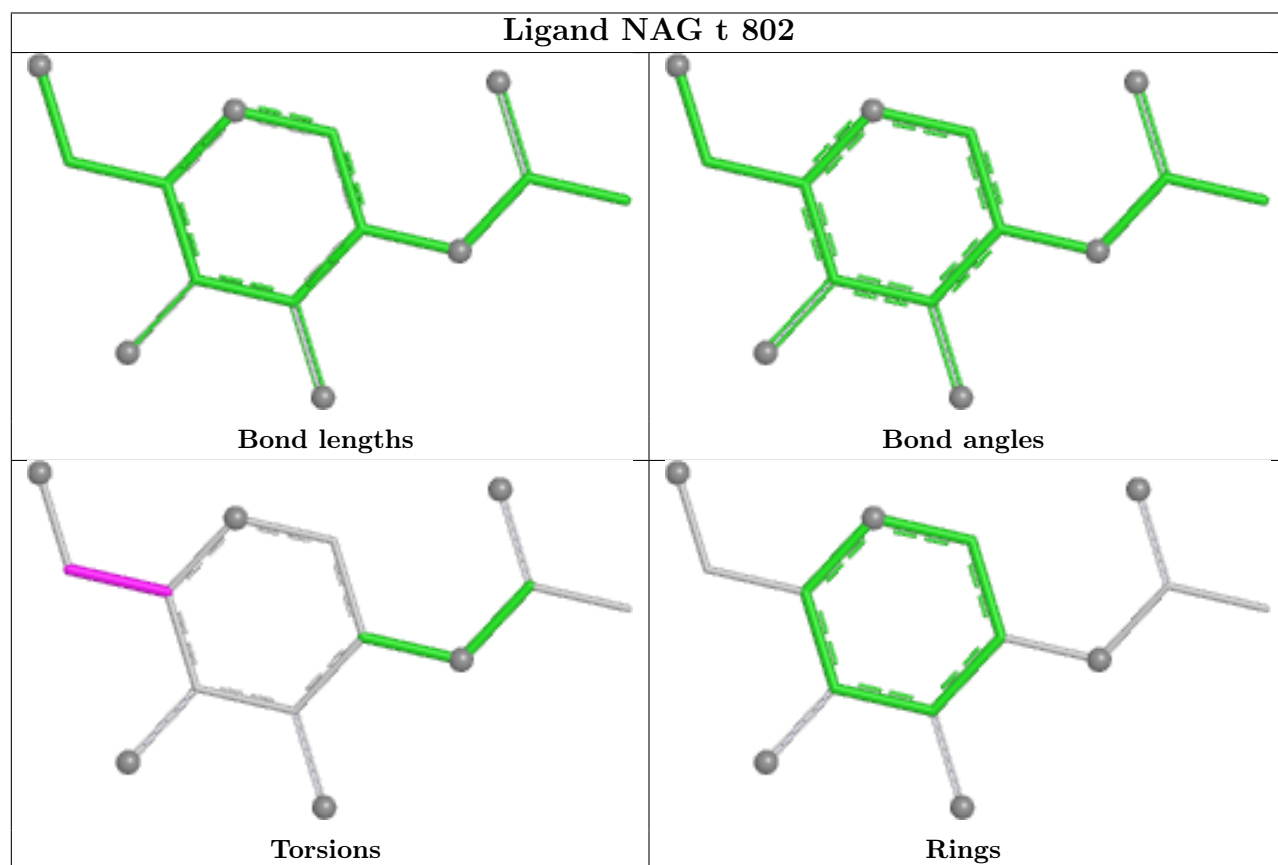
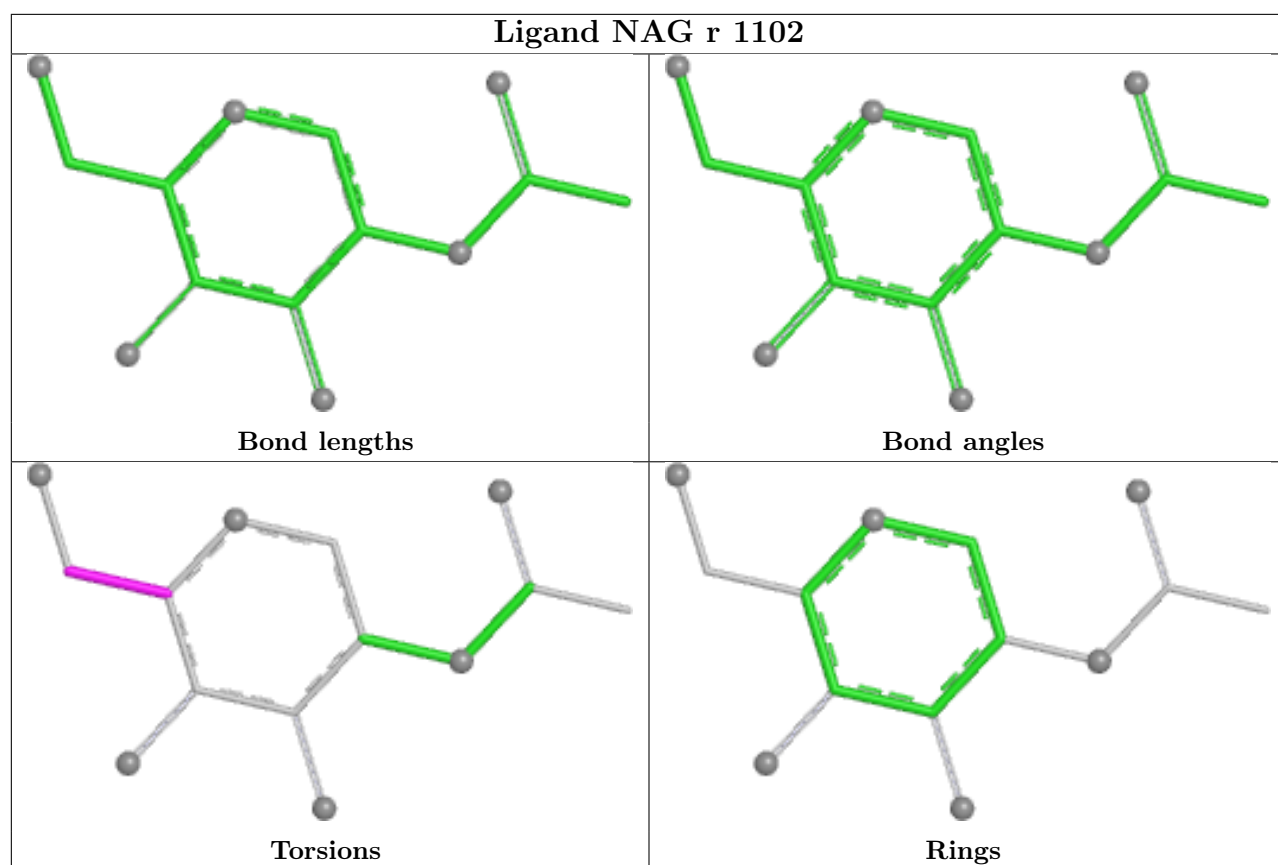


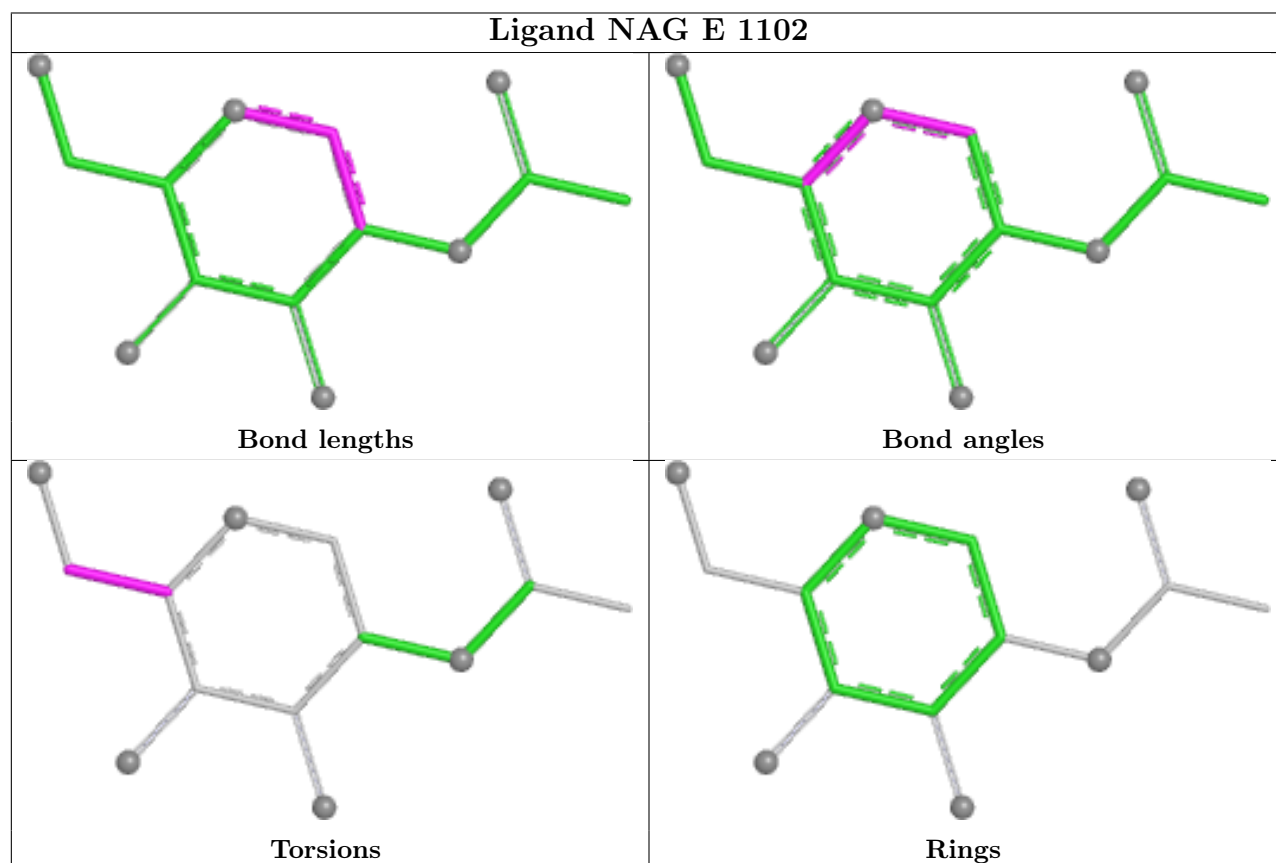
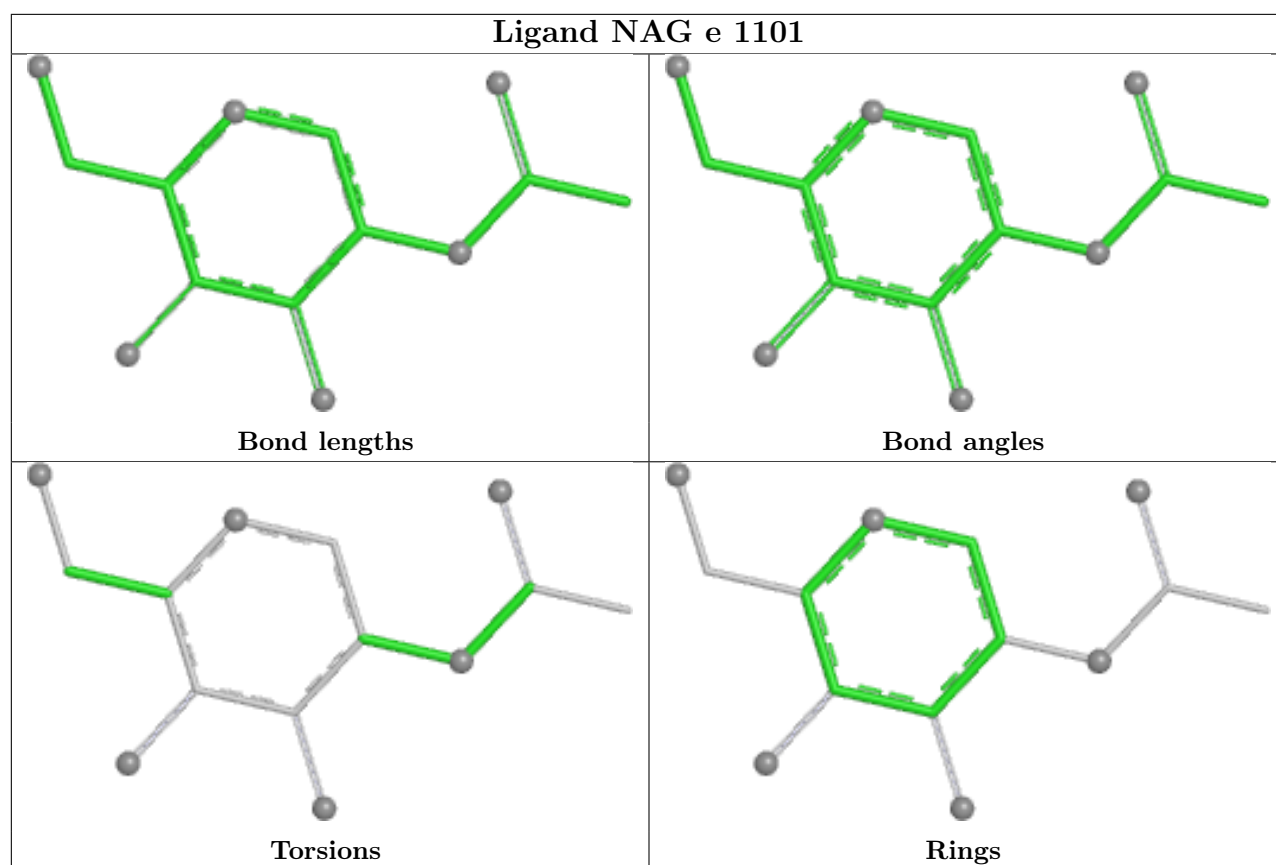


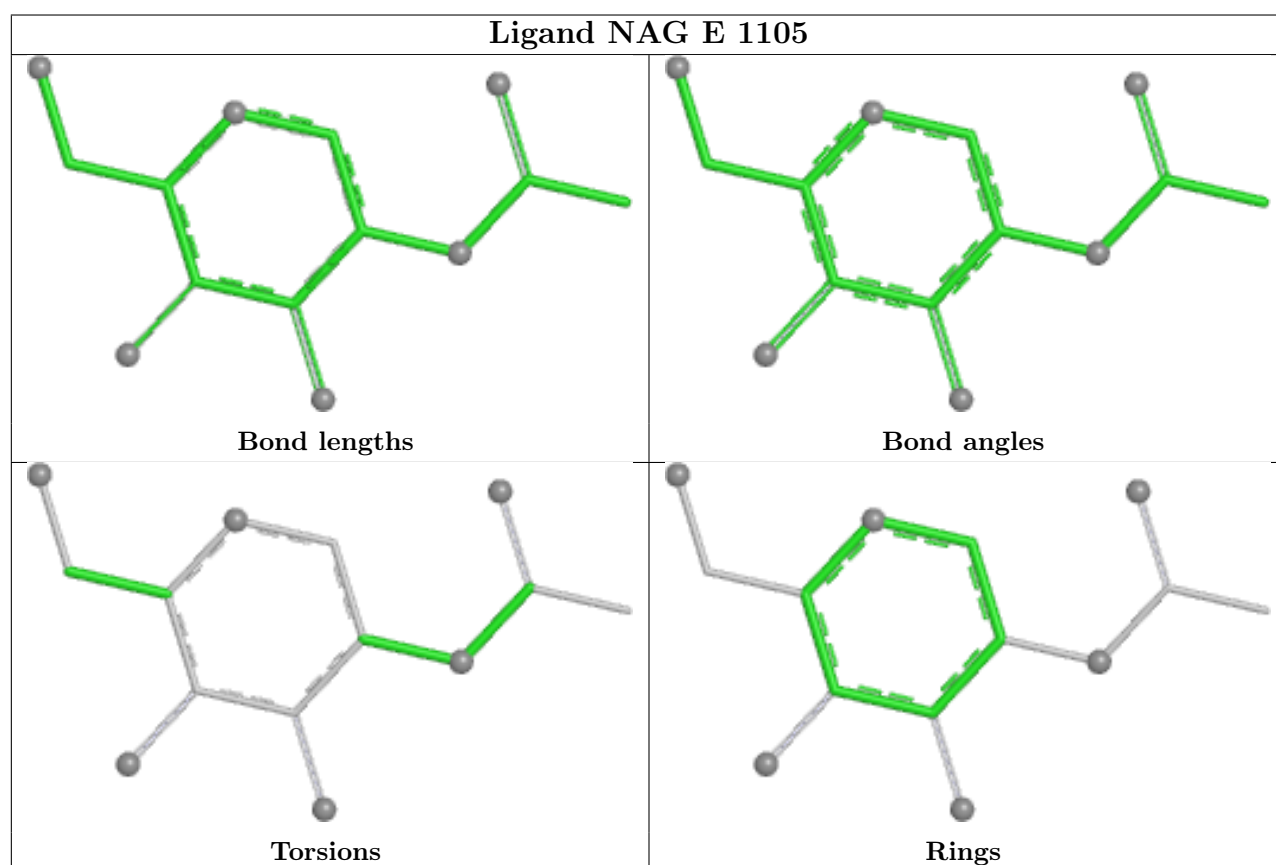
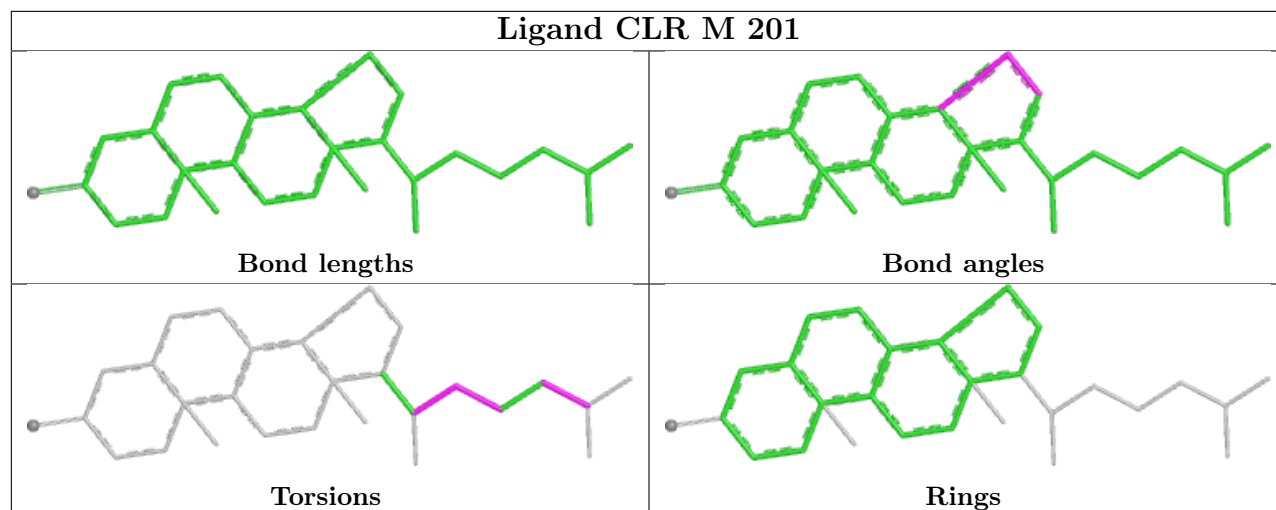


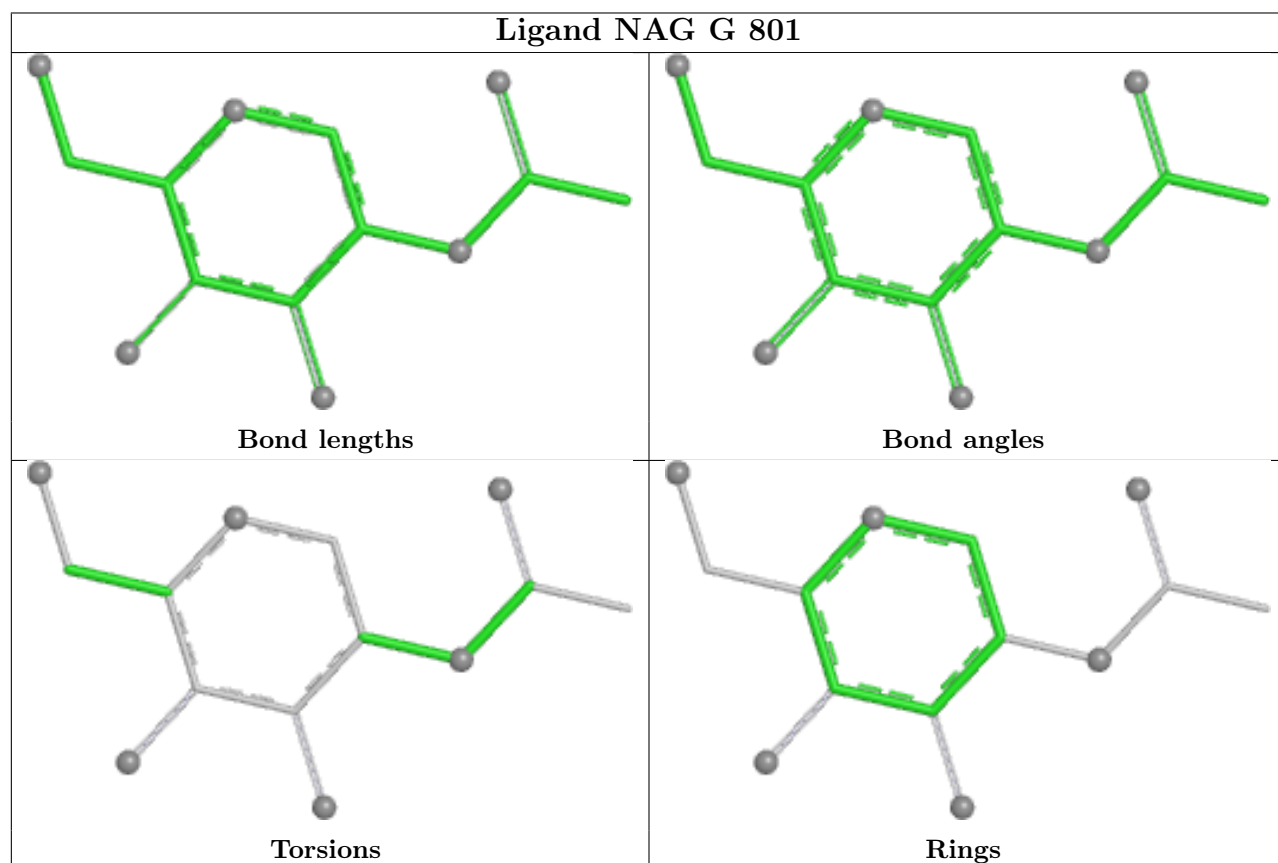
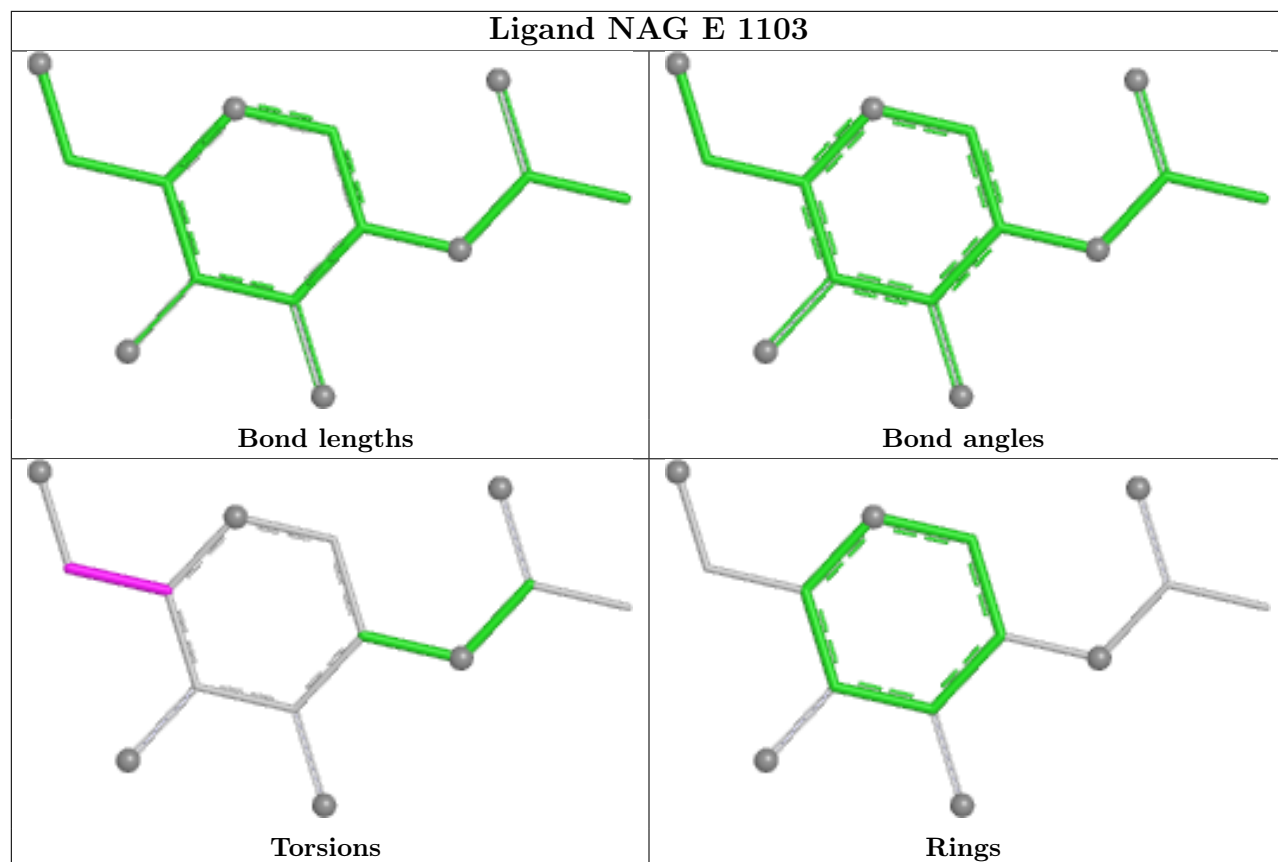


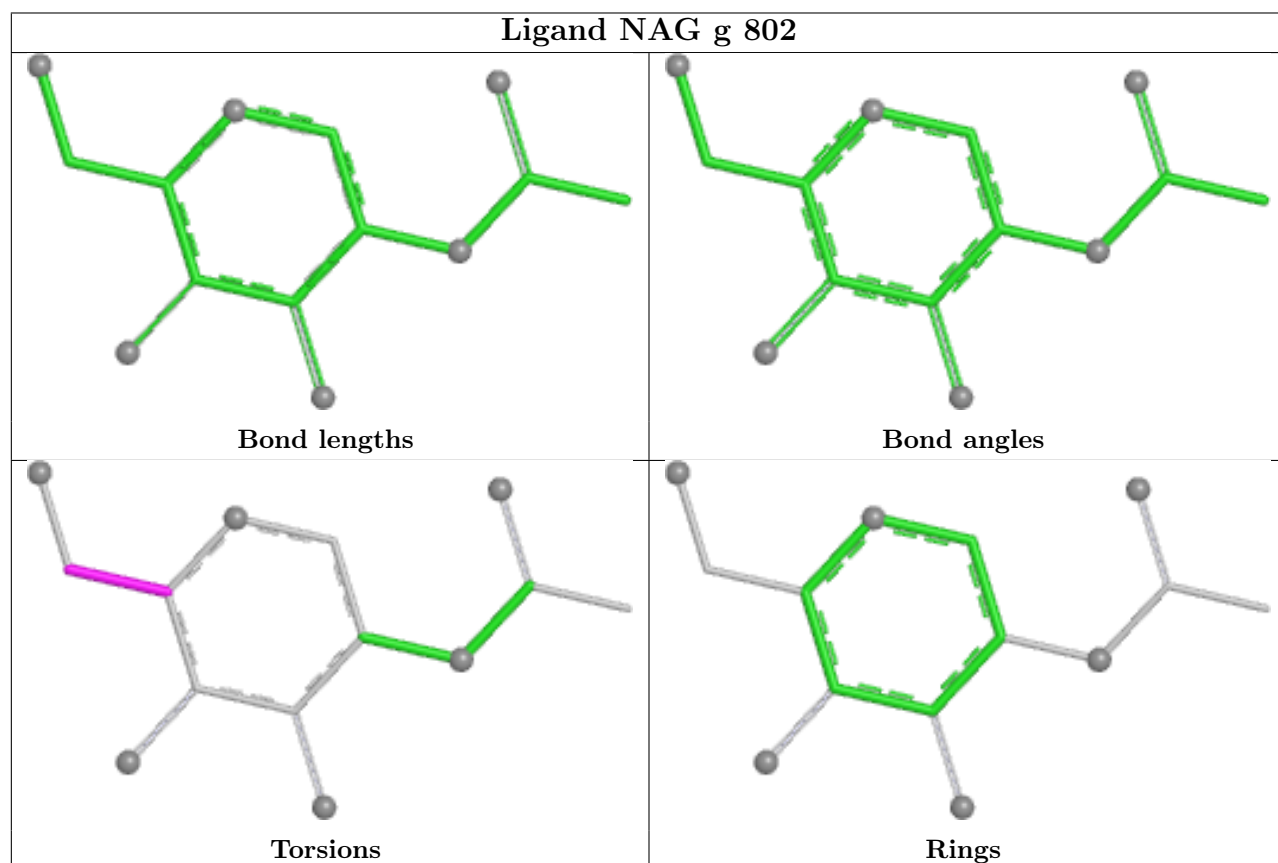
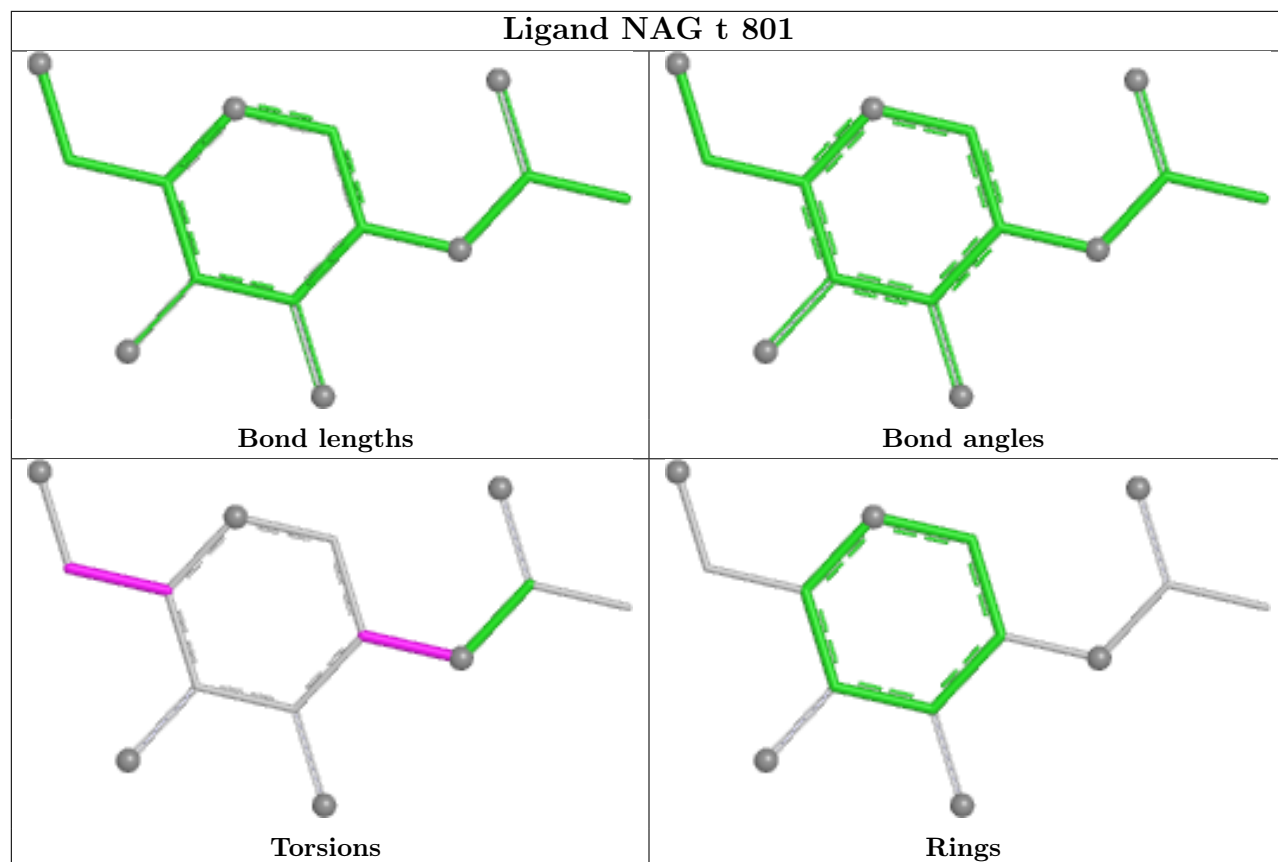












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

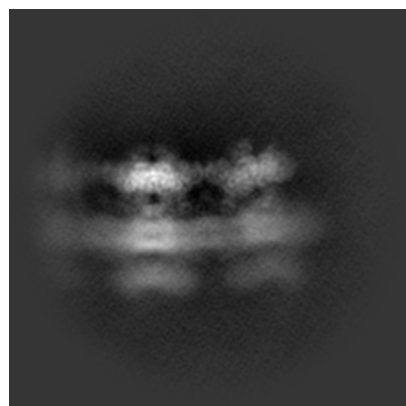
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64028. These allow visual inspection of the internal detail of the map and identification of artifacts.

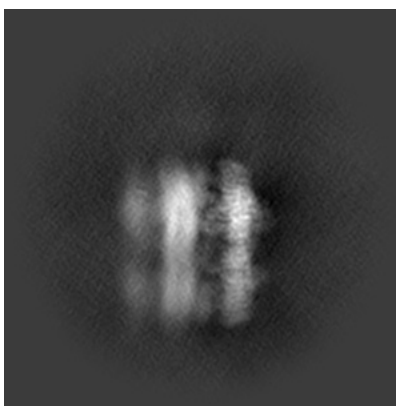
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

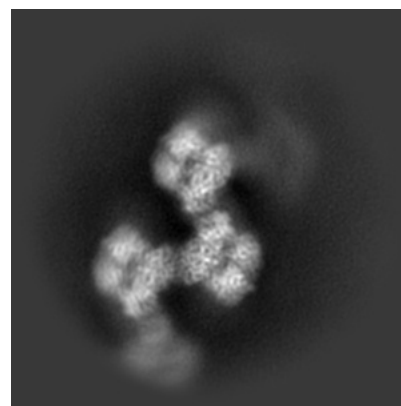
6.1.1 Primary map



X

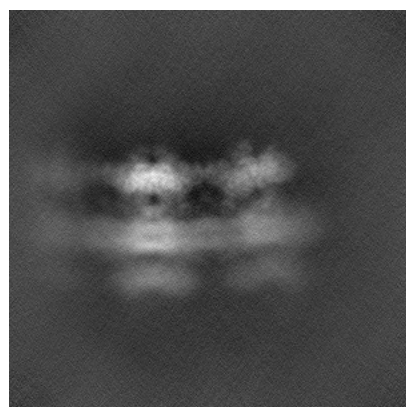


Y

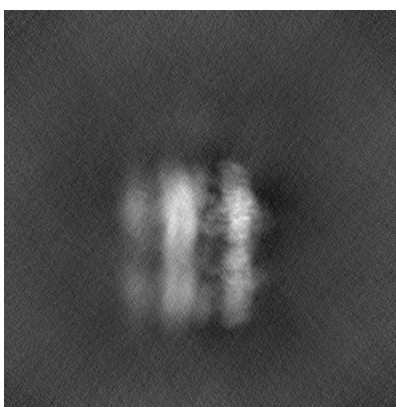


Z

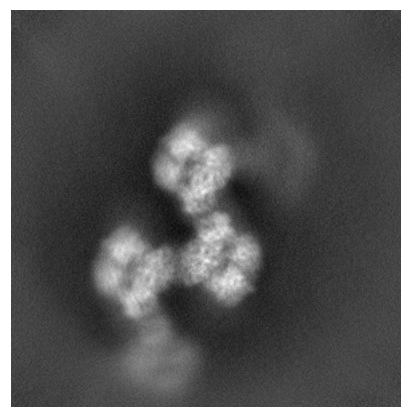
6.1.2 Raw map



X



Y

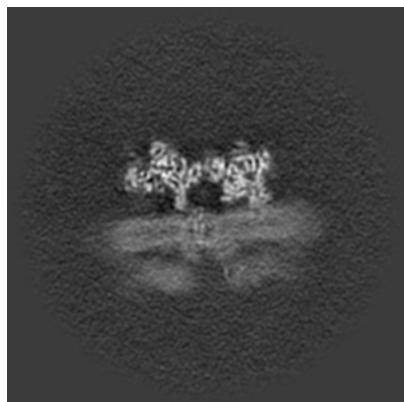


Z

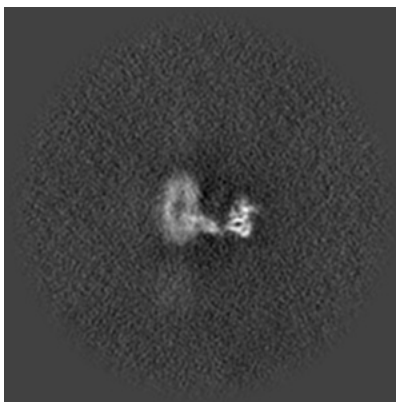
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

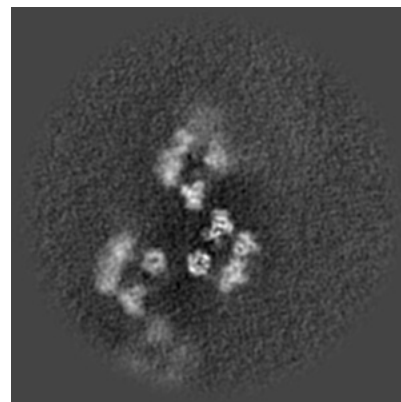
6.2.1 Primary map



X Index: 300

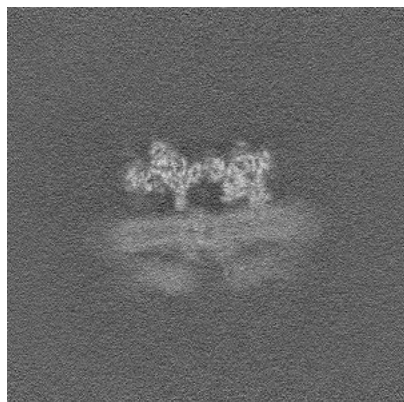


Y Index: 300

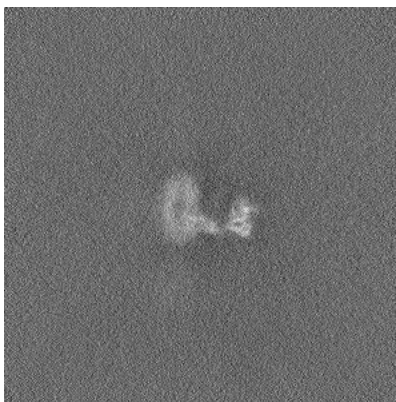


Z Index: 300

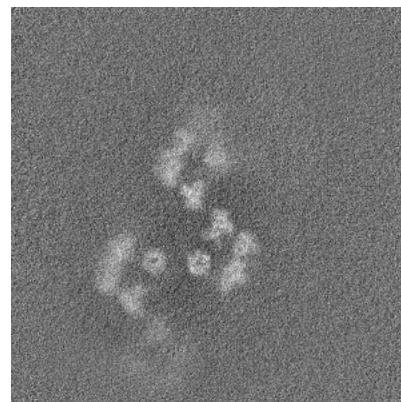
6.2.2 Raw map



X Index: 300



Y Index: 300

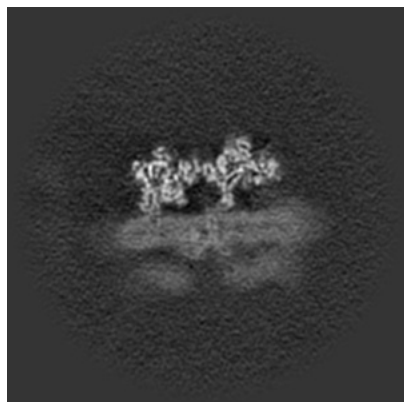


Z Index: 300

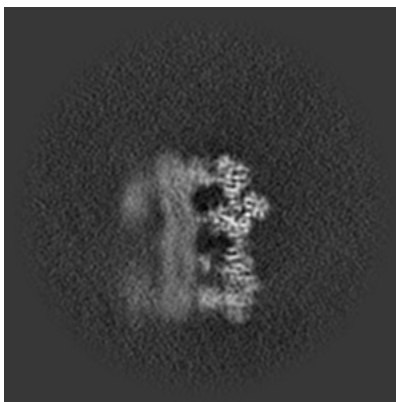
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

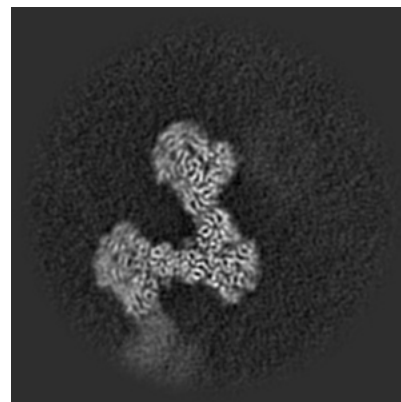
6.3.1 Primary map



X Index: 287

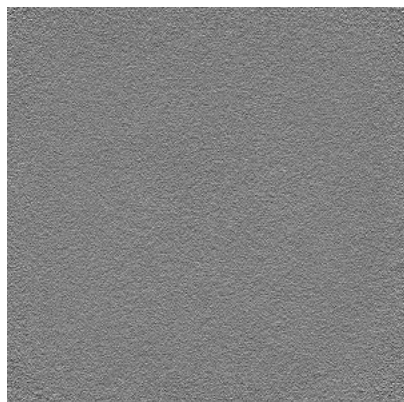


Y Index: 231

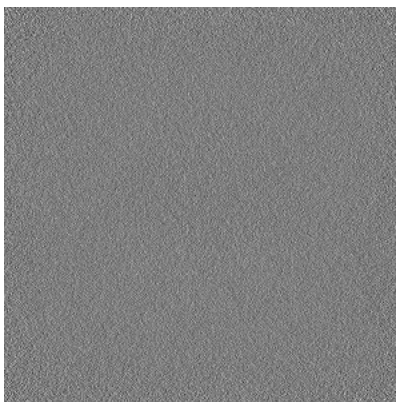


Z Index: 352

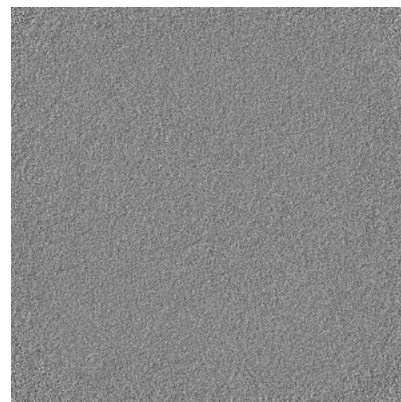
6.3.2 Raw map



X Index: 0



Y Index: 0

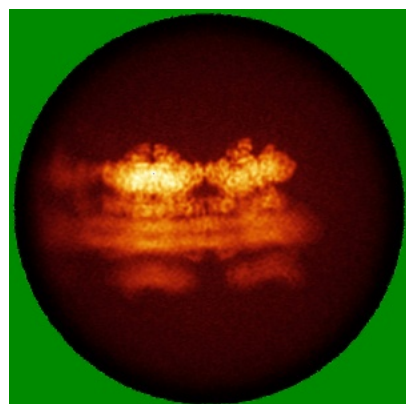


Z Index: 599

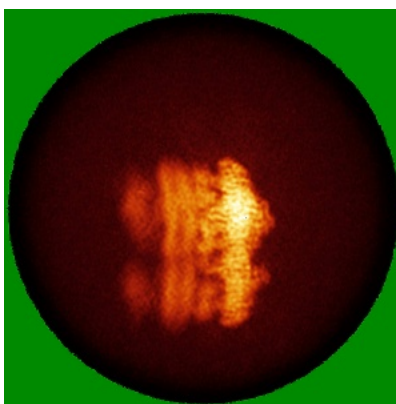
The images above show the largest variance slices of the map in three orthogonal directions.

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

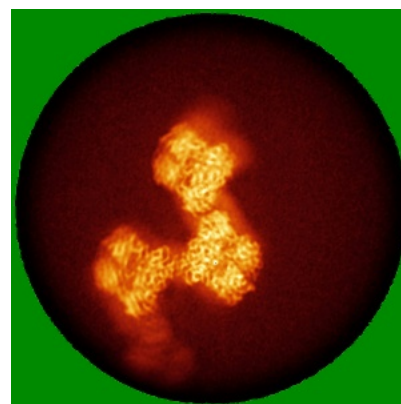
6.4.1 Primary map



X

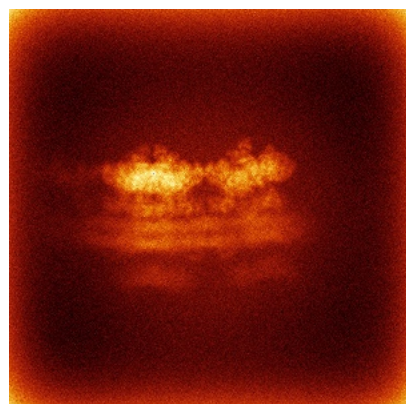


Y

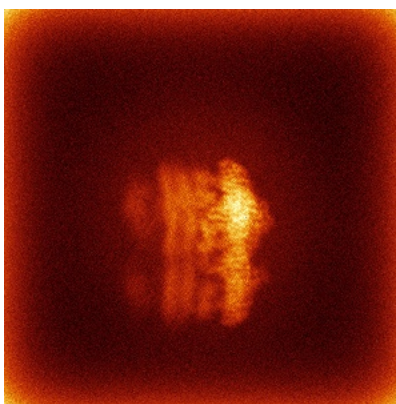


Z

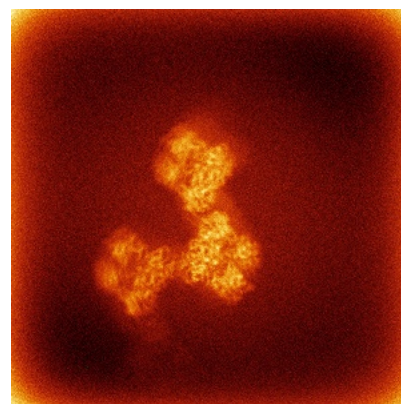
6.4.2 Raw map



X



Y

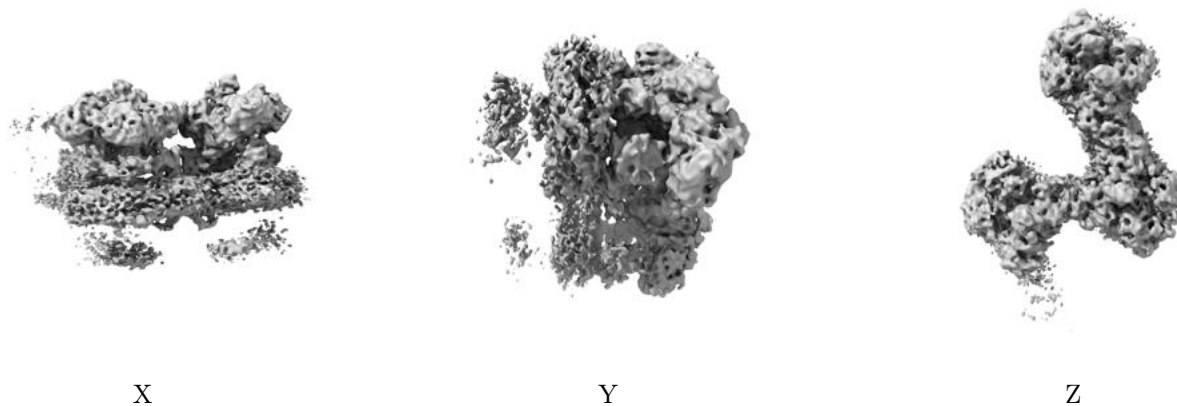


Z

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

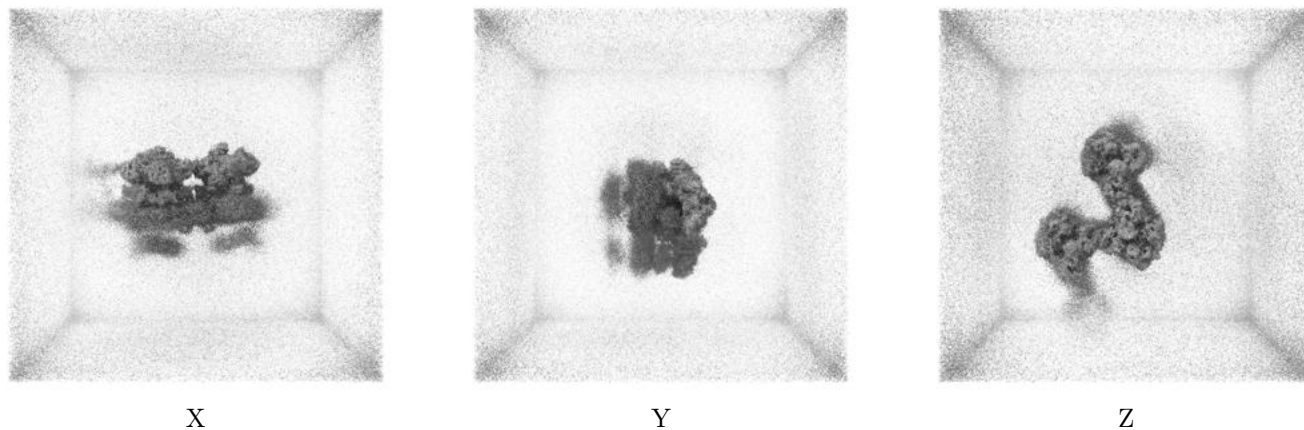
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.245. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

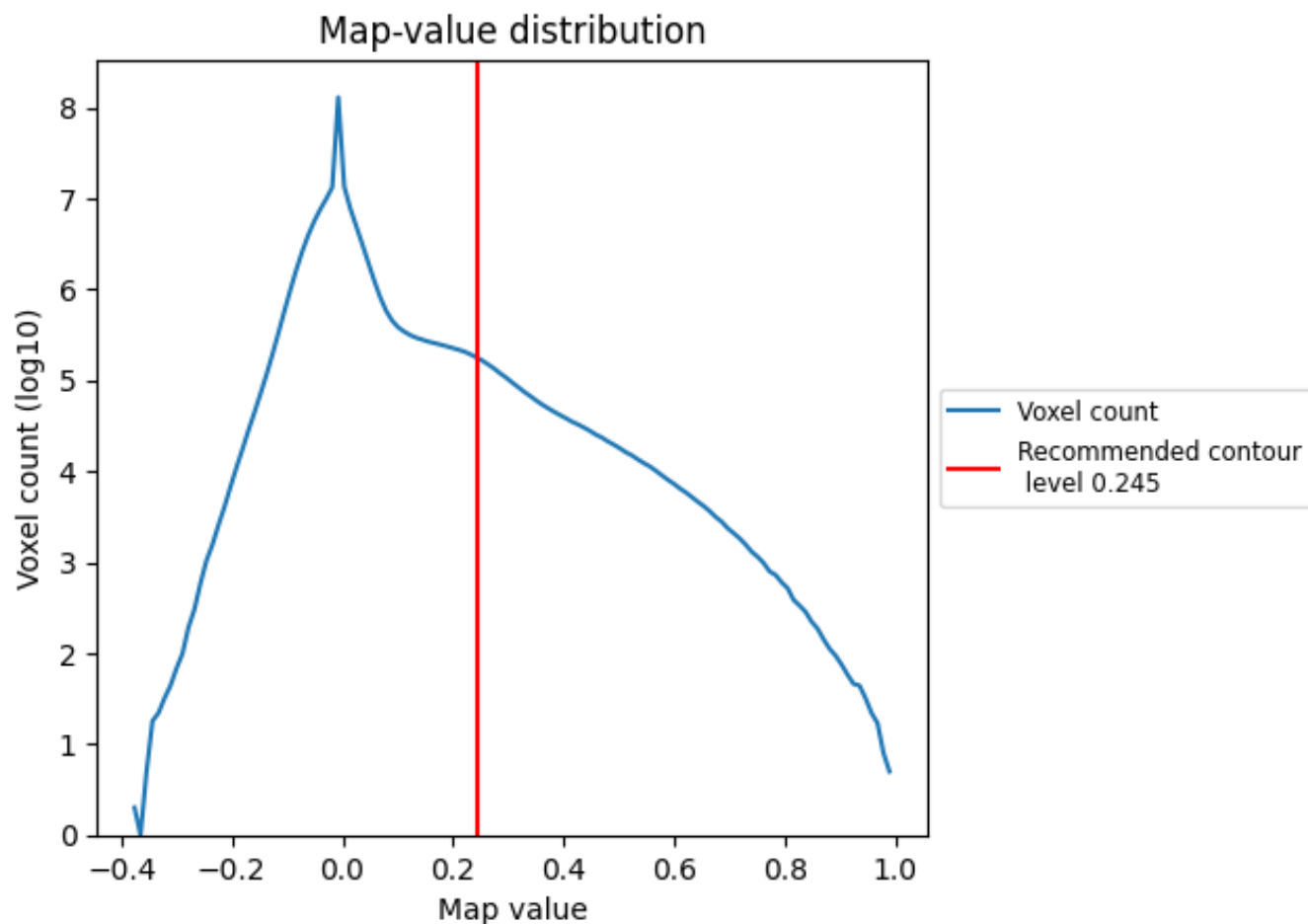
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

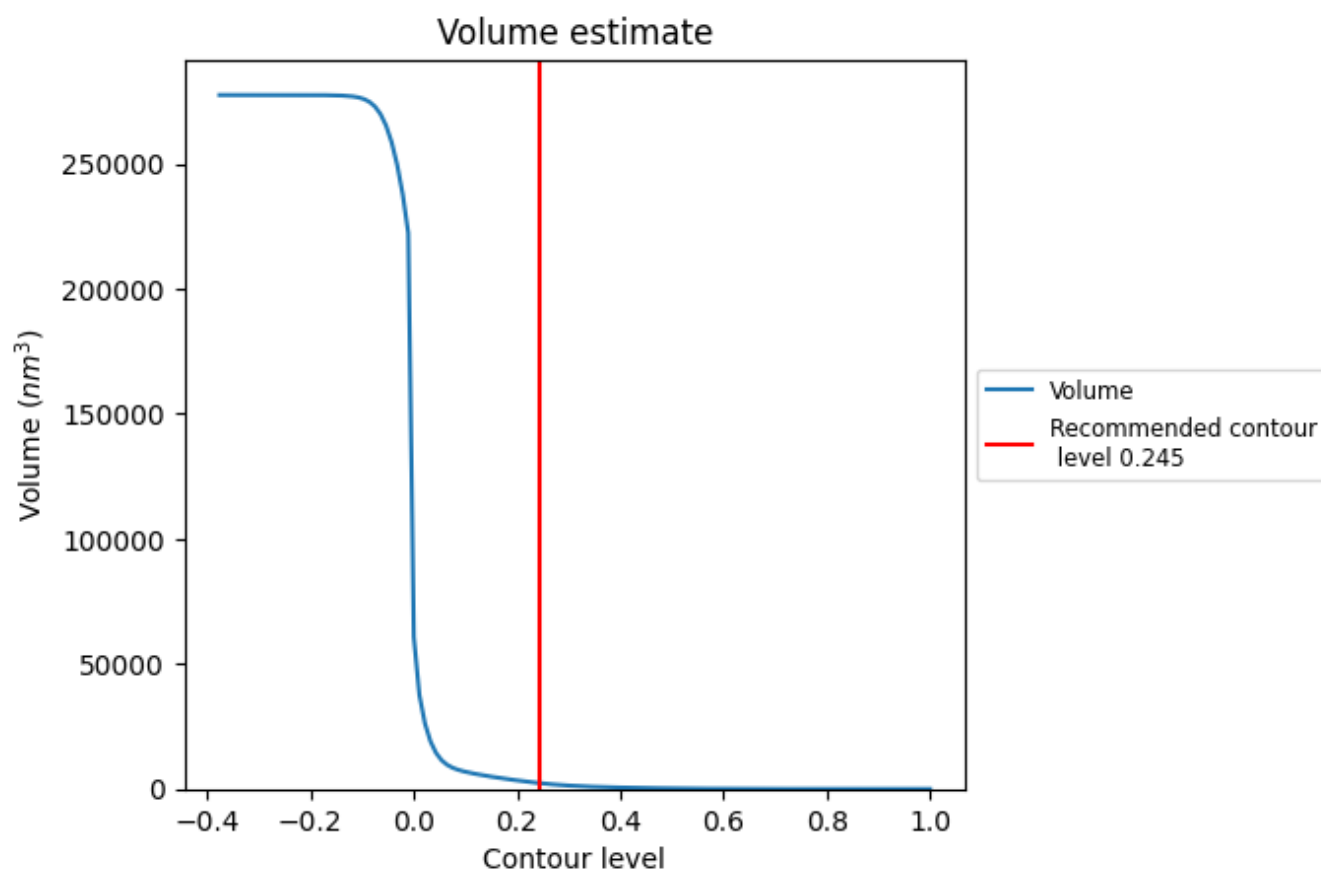
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

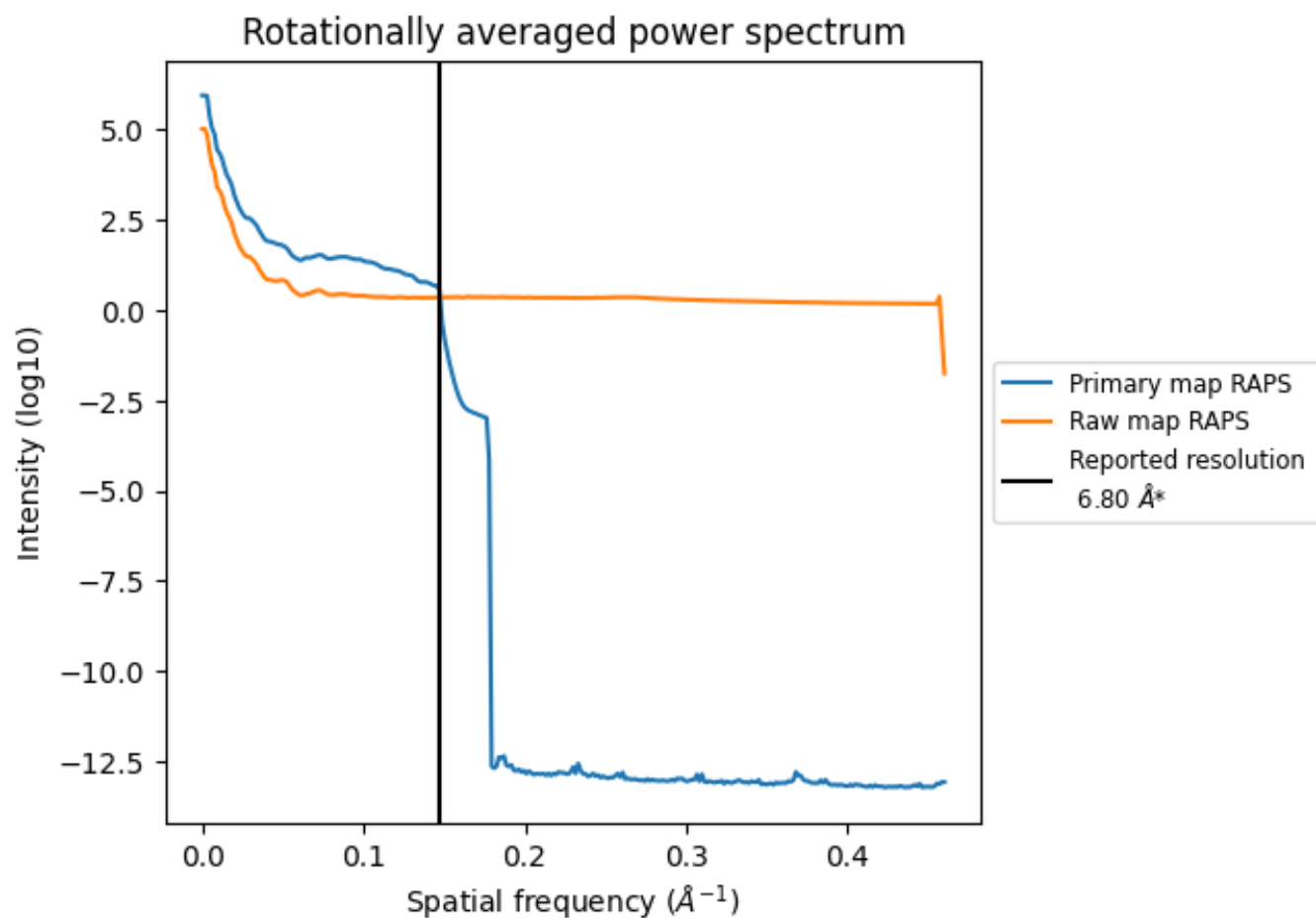
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2309 nm³; this corresponds to an approximate mass of 2086 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

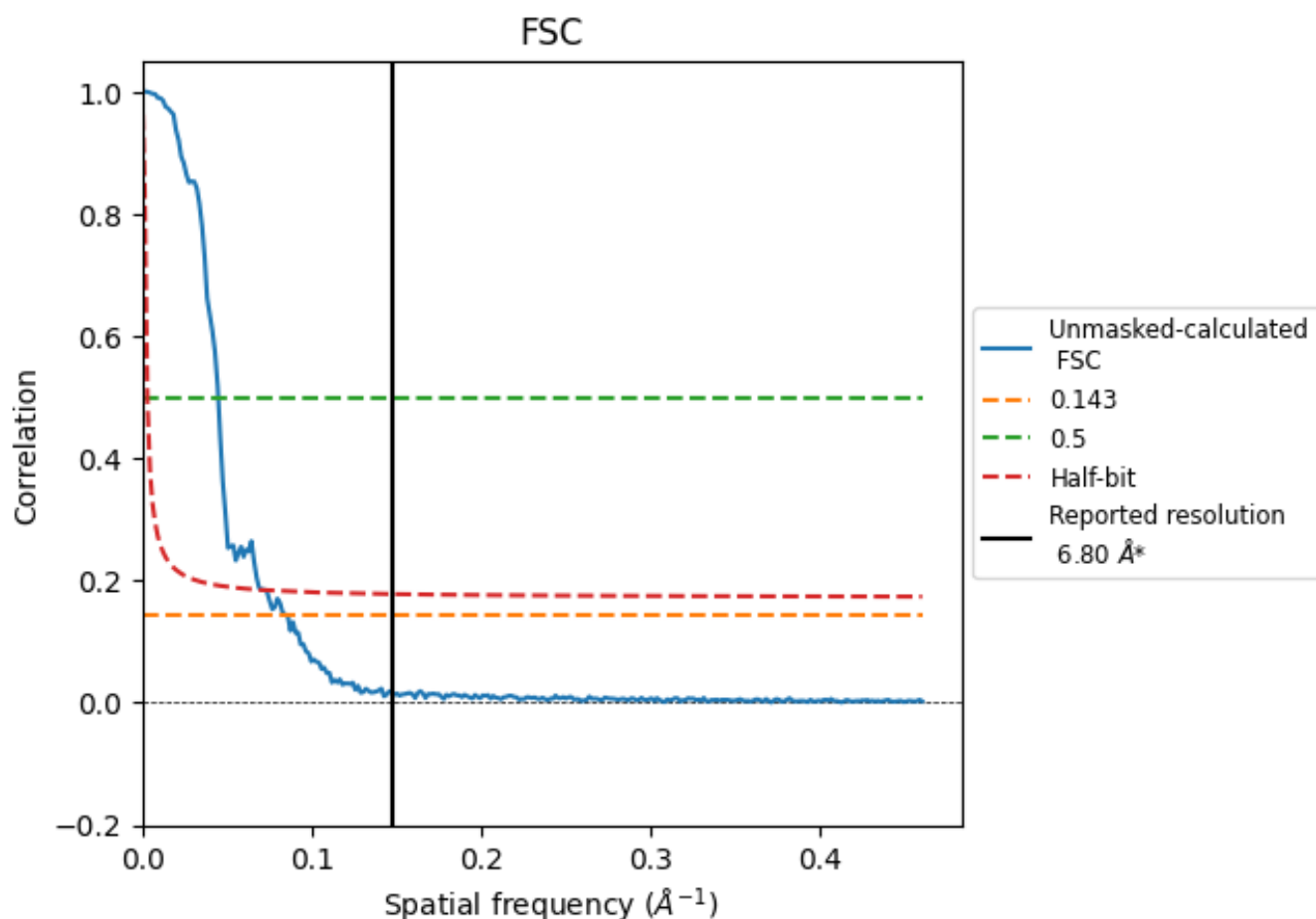


*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8.2 Resolution estimates [i](#)

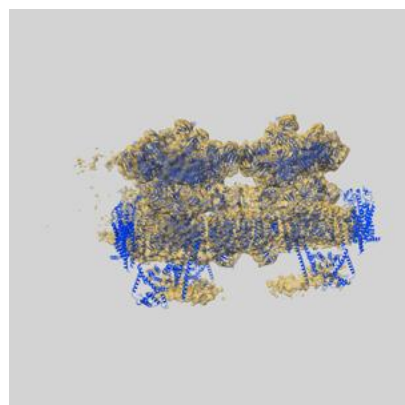
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	11.78	22.32	13.79

*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 11.78 differs from the reported value 6.8 by more than 10 %

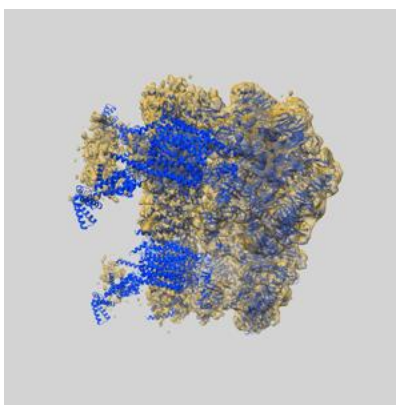
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64028 and PDB model 9UBX. Per-residue inclusion information can be found in section [3](#) on page [17](#).

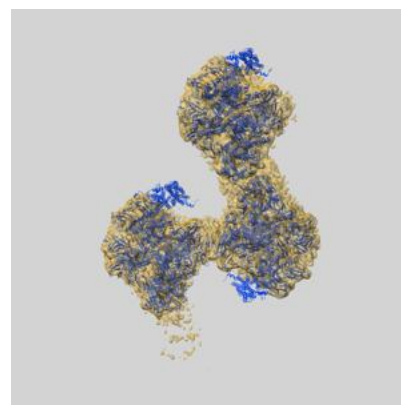
9.1 Map-model overlay [i](#)



X



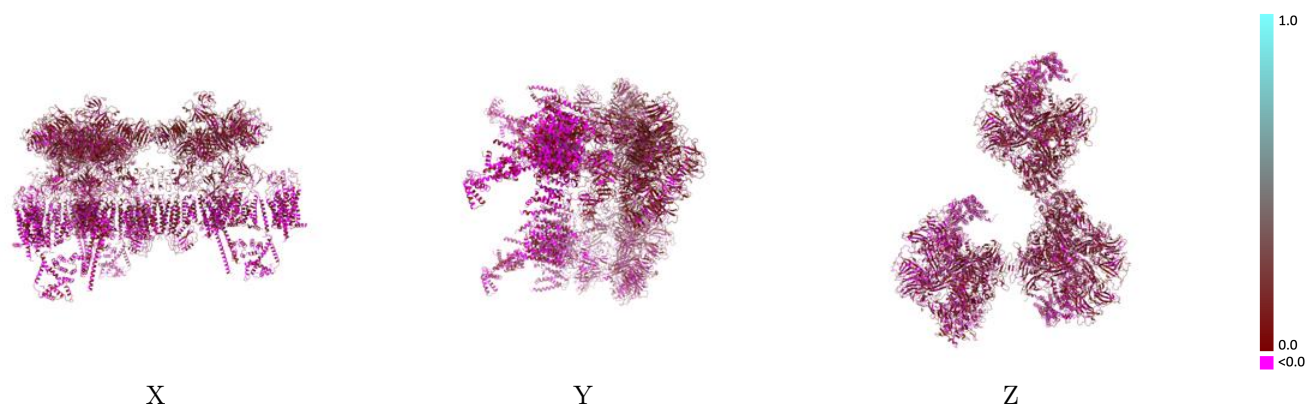
Y



Z

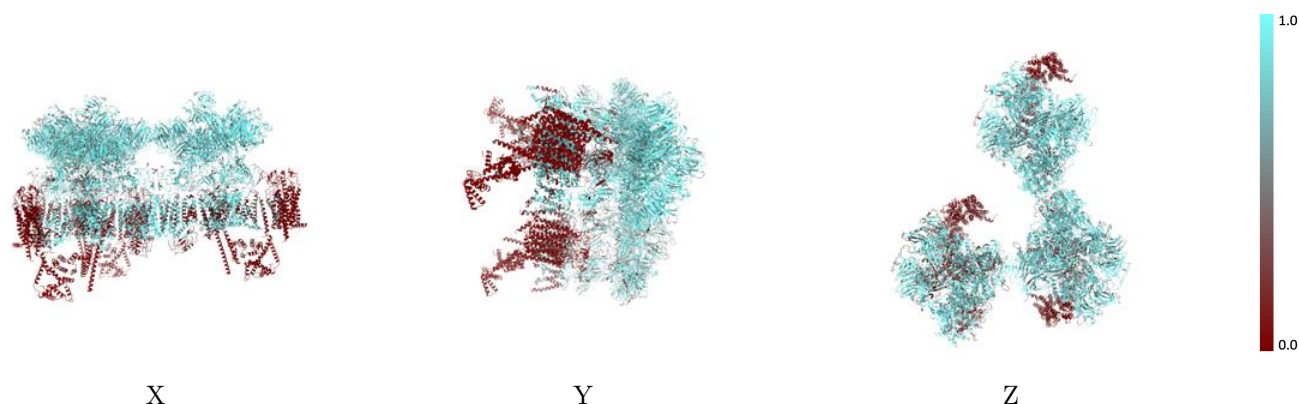
The images above show the 3D surface view of the map at the recommended contour level 0.245 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



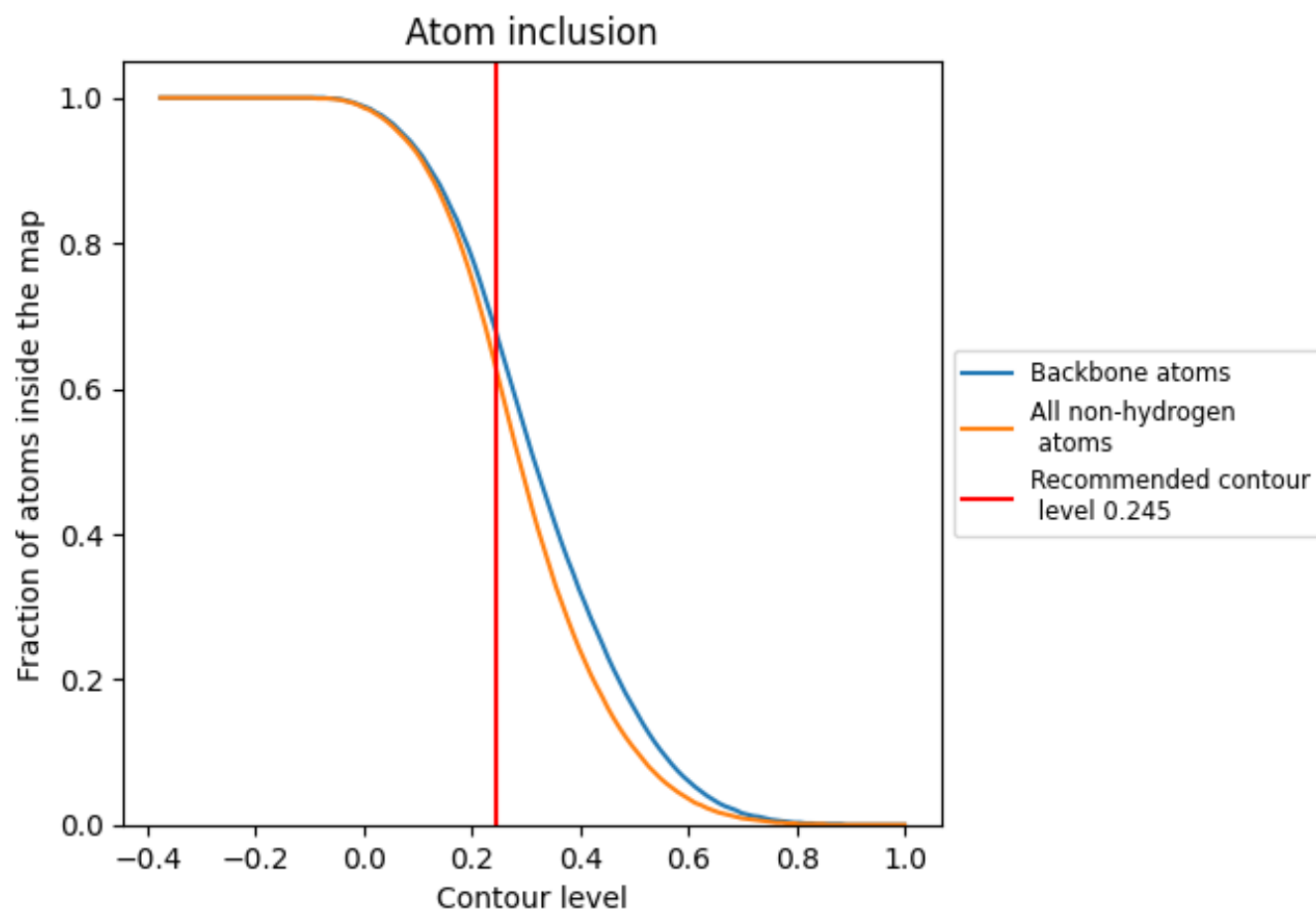
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.245).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 63% 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 (0.245) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6260	 0.0850
0	 0.8430	 0.1000
1	 0.7180	 0.1810
2	 0.3590	 -0.0370
3	 0.6430	 0.1290
4	 0.4100	 0.0940
5	 0.7690	 0.0740
6	 0.7180	 0.0380
7	 0.5420	 0.2150
8	 0.5710	 0.1510
9	 0.3930	 0.1070
A	 0.6480	 0.0480
AA	 0.7110	 0.0370
B	 0.5300	 0.0430
BA	 0.7180	 0.2270
C	 0.5340	 0.0250
CA	 0.0260	 -0.0510
D	 0.4930	 0.0630
DA	 0.4290	 0.1440
E	 0.8640	 0.1390
EA	 0.4100	 -0.0300
F	 0.8790	 0.1310
FA	 0.0260	 -0.0190
G	 0.8080	 0.1060
GA	 0.6150	 0.1540
H	 0.8350	 0.1090
HA	 0.4700	 0.2130
I	 0.0430	 0.0180
IA	 0.0360	 0.0840
J	 0.4970	 0.0680
JA	 0.5080	 0.0980
K	 0.0030	 -0.0020
L	 0.0500	 0.0180
M	 0.7660	 0.0900
N	 0.7640	 0.0950



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
O	 0.2360	 0.0340
P	 0.9290	 0.1270
Q	 0.0450	 -0.0090
R	 0.9160	 0.1630
S	 0.9230	 0.1790
T	 0.8970	 0.2060
U	 0.4290	 0.1290
V	 0.3850	 0.0240
W	 0.5380	 0.1940
X	 0.9490	 0.2130
Y	 0.6870	 0.1980
Z	 0.6790	 0.0650
a	 0.2860	 0.0330
b	 0.3040	 0.0160
c	 0.3600	 0.0230
d	 0.3630	 0.0320
e	 0.7540	 0.0870
f	 0.8100	 0.1340
g	 0.6760	 0.0650
h	 0.7030	 0.0680
i	 0.0360	 -0.0130
j	 0.0490	 0.0060
k	 0.0010	 0.0300
l	 0.0110	 0.0120
m	 0.2060	 0.0190
n	 0.6200	 0.0730
o	 0.6200	 0.0590
p	 0.6000	 0.0690
q	 0.6330	 0.0660
r	 0.8620	 0.1400
s	 0.7570	 0.1270
t	 0.8030	 0.1250
u	 0.8230	 0.1160
v	 0.6560	 0.1210
w	 0.4930	 0.0840
x	 0.0160	 0.0170
y	 0.0420	 0.0060
z	 0.8200	 0.0850