



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 04:01 AM JST

PDB ID : 8JUT
EMDB ID : EMD-36663
Title : rat megalin RAP complex
Authors : Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.
Deposited on : 2023-06-27
Resolution : 4.20 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

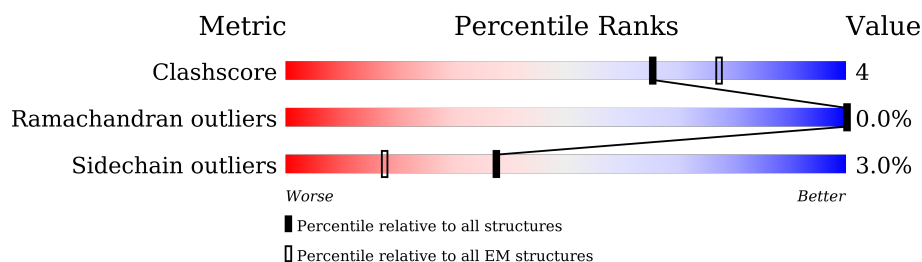
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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









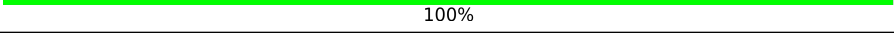
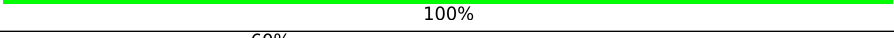
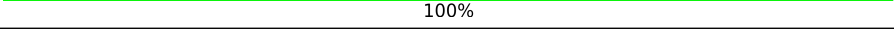
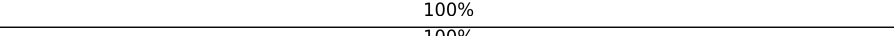
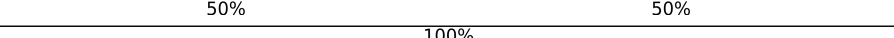
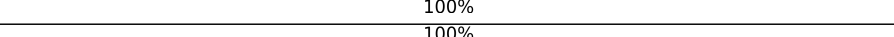

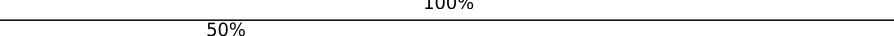
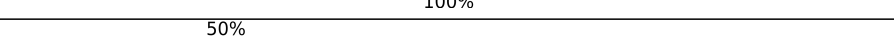
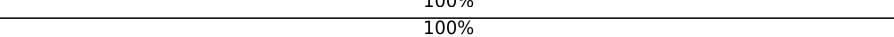
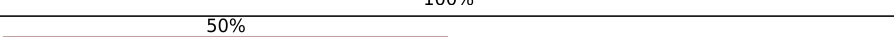
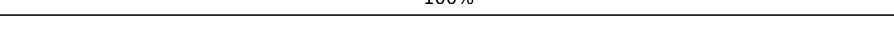







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	4660	<div> <div>34%</div> <div>82% 10% 8%</div> </div>
1	B	4660	<div> <div>32%</div> <div>82% 10% 8%</div> </div>
2	C	360	<div> <div>47%</div> <div>39% 10% 51%</div> </div>
2	D	360	<div> <div>48%</div> <div>38% 11% 51%</div> </div>
3	G	6	<div> <div>100%</div> <div>100%</div> </div>
3	N	6	<div> <div>100%</div> <div>100%</div> </div>
4	H	5	<div> <div>20%</div> <div>100%</div> </div>
4	O	5	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
5	I	6	
5	P	6	
6	J	3	
6	Q	3	
7	K	5	
7	R	5	
8	L	5	
8	M	5	
8	S	5	
8	T	5	
9	E	2	
9	V	2	
9	X	2	
9	Y	2	
9	a	2	
9	d	2	
9	n	2	
9	q	2	
9	s	2	
9	t	2	
9	v	2	
9	x	2	
9	y	2	
10	1	5	
10	4	5	

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Mol	Chain	Length	Quality of chain
10	5	5	<div>80%</div> <div>60% 40%</div>
10	9	5	<div>100%</div> <div>80% 20%</div>
10	F	5	<div>100%</div> <div>80% 20%</div>
10	Z	5	<div>60%</div> <div>60% 40%</div>
10	b	5	<div>20%</div> <div>80% 20%</div>
10	g	5	<div>60%</div> <div>60% 40%</div>
10	j	5	<div>80%</div> <div>60% 40%</div>
10	k	5	<div>80%</div> <div>40% 60%</div>
10	l	5	<div>100%</div> <div>60% 40%</div>
10	u	5	<div>80%</div> <div>80% 20%</div>
11	U	5	<div>60%</div> <div>20% 60% 20%</div>
12	2	3	<div>67%</div> <div>100%</div>
12	3	3	<div>67%</div> <div>67% 33%</div>
12	W	3	<div>33%</div> <div>33% 33% 33%</div>
12	e	3	<div>100%</div> <div>67% 33%</div>
12	f	3	<div>67%</div> <div>67% 33%</div>
12	h	3	<div>100%</div> <div>100%</div>
12	i	3	<div>67%</div> <div>33% 67%</div>
12	m	3	<div>100%</div> <div>33% 67%</div>
12	p	3	<div>33%</div> <div>67% 33%</div>
12	r	3	<div>33%</div> <div>67% 33%</div>
13	8	2	<div>100%</div> <div>100%</div>
13	c	2	<div>50%</div> <div>100%</div>
13	o	2	<div>100%</div> <div>100%</div>
14	6	5	<div>100%</div> <div>40% 60%</div>

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Mol	Chain	Length	Quality of chain
14	w	5	<div><div></div><div>60%40%</div></div>
15	z	3	<div><div></div><div>33%100%67%</div></div>
16	0	3	<div><div></div><div>33%67%67%</div></div>
16	7	3	<div><div></div><div>100%100%</div></div>

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 73258 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 LDL receptor related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4308	Total	C	N	O	S	0	0
			33638	20708	5950	6605	375		
1	B	4308	Total	C	N	O	S	0	0
			33636	20706	5950	6605	375		

- Molecule 2 is a protein called Alpha-2-macroglobulin receptor-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	177	Total	C	N	O	S	0	0
			1494	944	273	276	1		
2	D	177	Total	C	N	O	S	0	0
			1494	944	273	276	1		

- Molecule 3 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	6	Total	C	N	O	0	0
			30	18	6	6		
3	N	6	Total	C	N	O	0	0
			30	18	6	6		

- Molecule 4 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	5	Total	C	N	O	0	0
			28	16	6	6		
4	O	5	Total	C	N	O	0	0
			28	16	6	6		

- Molecule 5 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	6	Total	C	N	O	0	0
			33	21	6	6		
5	P	6	Total	C	N	O	0	0
			33	21	6	6		

- Molecule 6 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	3	Total	C	N	O	S	0	0
			16	9	3	3	1		
6	Q	3	Total	C	N	O	S	0	0
			16	9	3	3	1		

- Molecule 7 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	K	5	Total	C	N	O	0	0
			33	19	5	9		
7	R	5	Total	C	N	O	0	0
			33	19	5	9		

- Molecule 8 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	5	Total	C	N	O	0	0
			28	16	6	6		
8	M	5	Total	C	N	O	0	0
			28	16	6	6		
8	S	5	Total	C	N	O	0	0
			28	16	6	6		
8	T	5	Total	C	N	O	0	0
			28	16	6	6		

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



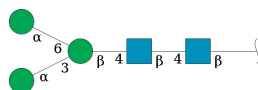
Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	V	2	Total	C	N	O	0	0
			28	16	2	10		
9	X	2	Total	C	N	O	0	0
			28	16	2	10		
9	Y	2	Total	C	N	O	0	0
			28	16	2	10		
9	a	2	Total	C	N	O	0	0
			28	16	2	10		
9	d	2	Total	C	N	O	0	0
			28	16	2	10		
9	n	2	Total	C	N	O	0	0
			28	16	2	10		
9	q	2	Total	C	N	O	0	0
			28	16	2	10		
9	s	2	Total	C	N	O	0	0
			28	16	2	10		
9	t	2	Total	C	N	O	0	0
			28	16	2	10		
9	v	2	Total	C	N	O	0	0
			28	16	2	10		
9	x	2	Total	C	N	O	0	0
			28	16	2	10		
9	y	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



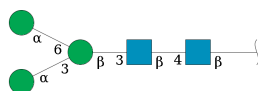
Mol	Chain	Residues	Atoms				AltConf	Trace
10	F	5	Total	C	N	O	0	0
			61	34	2	25		
10	Z	5	Total	C	N	O	0	0
			61	34	2	25		
10	b	5	Total	C	N	O	0	0
			61	34	2	25		
10	g	5	Total	C	N	O	0	0
			61	34	2	25		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	5	Total	C	N	O	0	0
			61	34	2	25		
10	k	5	Total	C	N	O	0	0
			61	34	2	25		
10	l	5	Total	C	N	O	0	0
			61	34	2	25		
10	u	5	Total	C	N	O	0	0
			61	34	2	25		
10	1	5	Total	C	N	O	0	0
			61	34	2	25		
10	4	5	Total	C	N	O	0	0
			61	34	2	25		
10	5	5	Total	C	N	O	0	0
			61	34	2	25		
10	9	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	U	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 12 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
12	W	3	Total	C	N	O	0	0
			39	22	2	15		
12	e	3	Total	C	N	O	0	0
			39	22	2	15		

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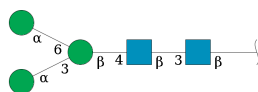
Mol	Chain	Residues	Atoms				AltConf	Trace
12	f	3	Total	C	N	O	0	0
			39	22	2	15		
12	h	3	Total	C	N	O	0	0
			39	22	2	15		
12	i	3	Total	C	N	O	0	0
			39	22	2	15		
12	m	3	Total	C	N	O	0	0
			39	22	2	15		
12	p	3	Total	C	N	O	0	0
			39	22	2	15		
12	r	3	Total	C	N	O	0	0
			39	22	2	15		
12	2	3	Total	C	N	O	0	0
			39	22	2	15		
12	3	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 13 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
13	c	2	Total	C	N	O	0	0
			28	16	2	10		
13	o	2	Total	C	N	O	0	0
			28	16	2	10		
13	8	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
14	w	5	Total	C	N	O	0	0
			61	34	2	25		
14	6	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 15 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
15	z	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 16 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
16	0	3	Total	C	N	O	0	0
			39	22	2	15		
16	7	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



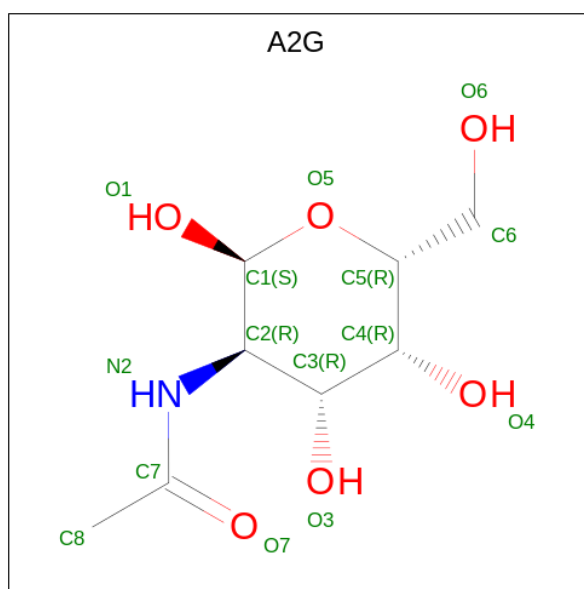
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
17	A	1	14	8	1	5	0
17	A	1	14	8	1	5	0
17	A	1	14	8	1	5	0
17	A	1	14	8	1	5	0
17	A	1	14	8	1	5	0
17	A	1	14	8	1	5	0
17	A	1	14	8	1	5	0
17	A	1	14	8	1	5	0
17	A	1	14	8	1	5	0
17	A	1	14	8	1	5	0
17	B	1	14	8	1	5	0
17	B	1	14	8	1	5	0
17	B	1	14	8	1	5	0

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

- Molecule 18 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
19	A	44	Total 44	Ca 44	0
19	B	44	Total 44	Ca 44	0

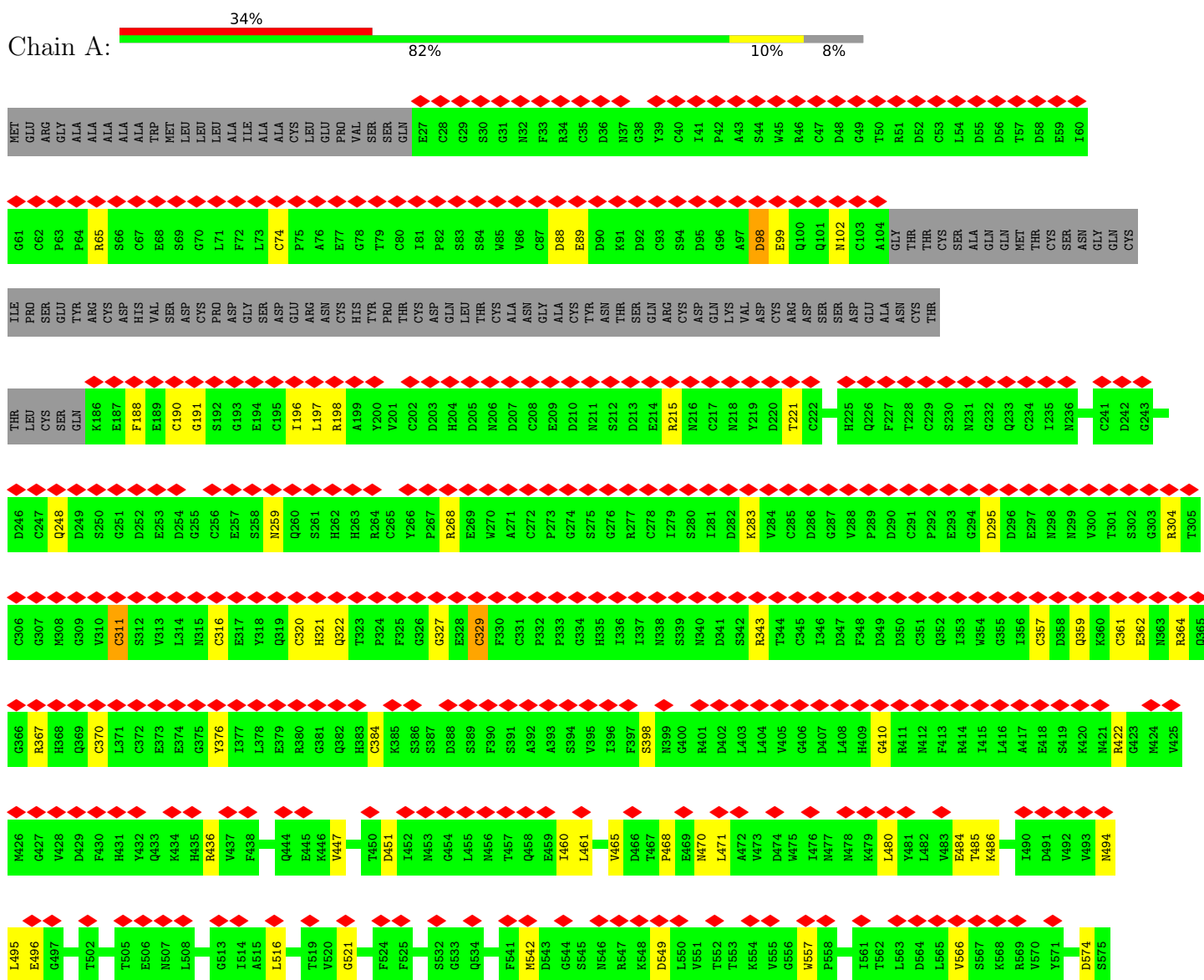
- Molecule 20 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

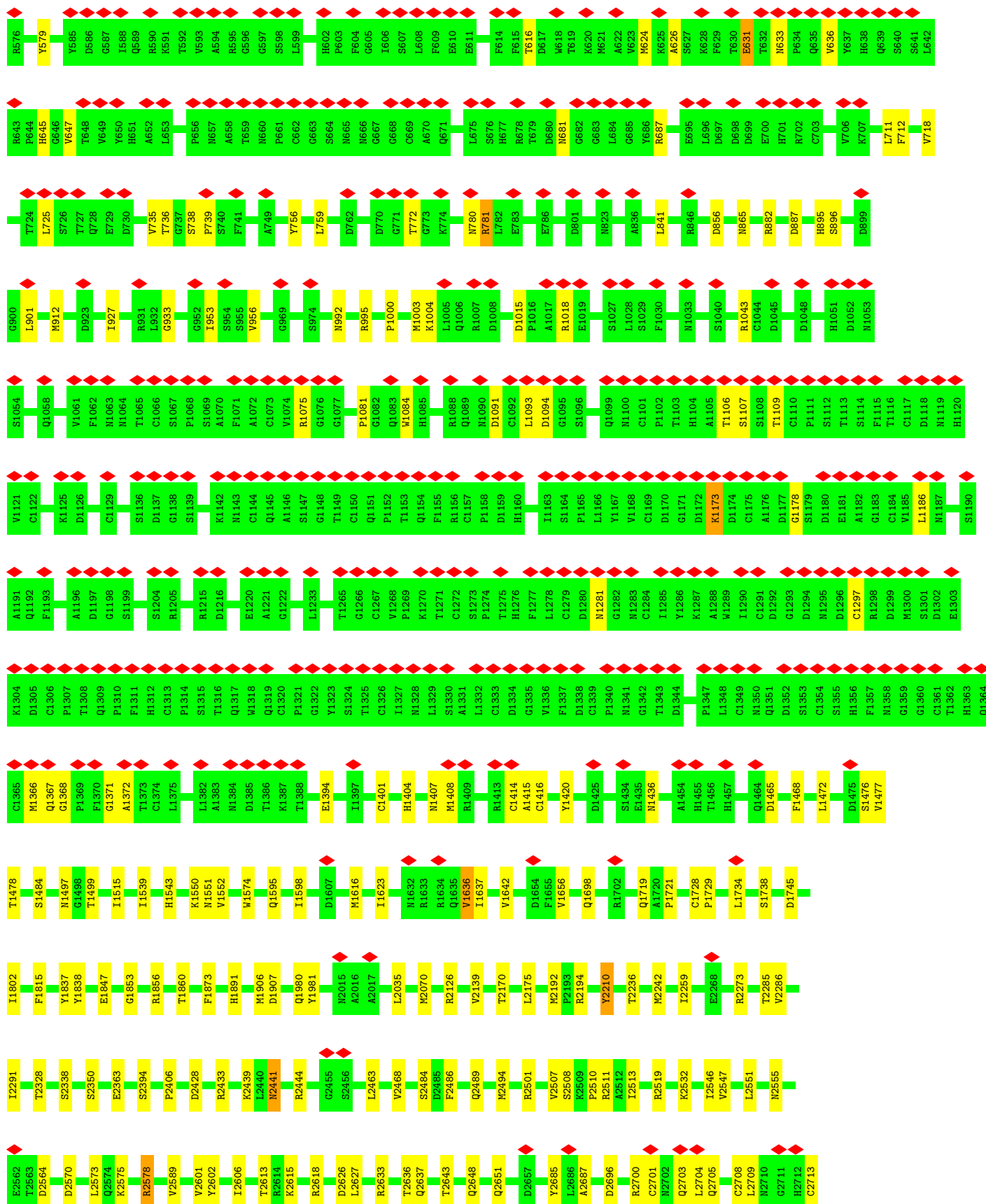
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total 1	Ni 1	0
20	B	1	Total 1	Ni 1	0

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: LDL receptor related protein 2





G3901	H3902	Q3903	L3904	C3905	N3906	G3907	V3908	D3909	D3910	C3911	G3912	D3913	G3914	S3915	D3916	E3917	K3918	E3919	E3920	H3921	C3922	R3923	K3924	P3925	D3926	H3927	H3928	P3929	C3930	T3931	D3932	T3933	E3934	Y3935	K3936	C3937	S3938	N3939	G3940	N3941	T3942	T3943	S3944	Q3945	H3946	Q3947	V3948	C3949	D3950	N3951	V3952	N3953	S3954	C3955	C3956	D3957	S3959	D3960
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THR	LEU	CYS	SER	GLN	K186	E187	F188	E189	C190	G191	S192	G193	E194	C195	I196	L197	R198	A199	Y200	V201	H204	D205	N206	D207	C208	E209	D210	N211	S212	D213	E214	R215	N216	C217	N218	Y219	D220	T221	C222	G223	G224	H225	Q226	F227	T228	C229	S230	Q233	C234	N238	W239	V240	G243	D244	D245				
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L503	I504	L508	R512	G513	I514	A515	L516	D517	P518	T519	F525	S526	D527	S530	L531	S532	C588	G533	Q534	V537	G544	D549	L550	V551	T552	T553	K554	A559	G560	I561	T562	L563	D564	L565	V566	S567	K568	Y571	D574	Y577	I580	S586	G587	I588	Q589														
T592	V593	A594	R595	S598	L599	V600	F604	G605	I606	S607	L608	F609	E610	F611	H612	V613	F614	F615	T616	T619	K620	V623	M624	K625	A626	D627	K628	F629	T630	E631	T632	N633	P634	Q635	V636	V637	H638	Q639	S640	S641	L642	R643	P644	H645	G646	V647	T648	V649	R654	T659	N660	P661	C662						
G663	S664	N665	N666	G667	C668	A670	Q671	L675	R678	T679	D680	N681	G682	G683	L684	R687	C688	K689	C690	E691	E695	L696	D697	D698	D699	E700	H701	R702	C703	V704	A705	V706	K707	L725	V735	T736	G737	S738	F739	S740	F741	F742	D746	Y756	S757	K766	G771												
I777	E783	L788	I793	W799	V807	R811	L812	A813	D814	T821	N825	N826	W844	R845	R846	P847	A848	K849	D856	T863	V864	W870	H895	D899	L932	D945	R951	S954	D963	L966	G969	S970	N971	A979	R995																								
M1003	C1012	A1017	Q1023	L1028	N1033	F1041	H1051	H1057	Q1058	C1059	G1060	F1062	N1063	C1066	S1069	A1072	C1073	V1074	R1075	G1076	G1077	Q1078	C1079	I1080	P1081	W1084	H1085	C1086	D1087	R1088	D1091	C1092	Q1099	N1100	C1101	P1102	T1103	H1104	A1105	T1106	S1107	S1108	T1109																
C1110	P1111	S1112	T1113	S1114	F1115	D1118	N1119	H1120	V1121	C1122	I1123	P1124	K1125	D1126	C1129	D1134	C1135	R1136	D1137	G1138	S1139	D1140	E1141	K1142	N1143	C1144	Q1145	A1146	S1147	G1148	T1149	C1150	Q1151	P1152	T1153	Q1154	F1155	R1156	C1157	P1158	D1159	H1160	R1161	C1162	I1163	S1164	P1165	L1166	C1169	D1170	G1171	D1172	K1173	A1176					
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D1294	N1295	R1298	D1299	M1300	S1301	K1304	D1305	C1306	P1307	T1308	Q1309	P1310	F1311	H1312	C1313	P1314	S1315	T1316	Q1317	W1318	Q1319	C1320	P1321	G1322	Y1323	S1324	T1325	C1326	I1327	N1328	L1329	S1330	A1331	L1332	C1333	D1334	G1335	V1336	F1337	D1338	C1339	P1340	N1341	G1342	T1343	S1346	P1347	L1348	C1349	N1350	Q1351	D1352	S1355	H1356	F1357				





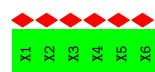




- Molecule 3: unclear peptide



- Molecule 3: unclear peptide



- Molecule 4: unclear peptide

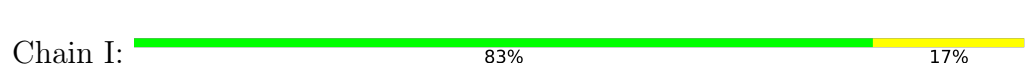


- Molecule 4: unclear peptide

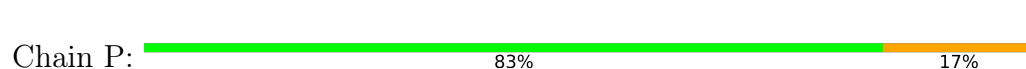


There are no outlier residues recorded for this chain.

- Molecule 5: unclear peptide



- Molecule 5: unclear peptide



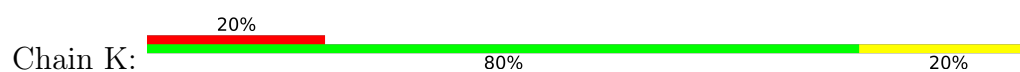
- Molecule 6: unclear peptide



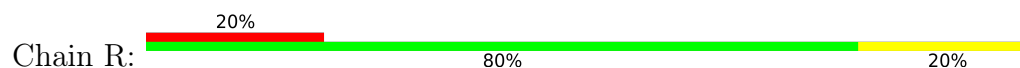
- Molecule 6: unclear peptide



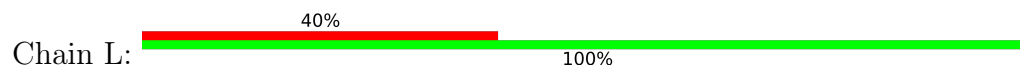
- Molecule 7: unclear peptide



- Molecule 7: unclear peptide



- Molecule 8: unclear peptide



- Molecule 8: unclear peptide

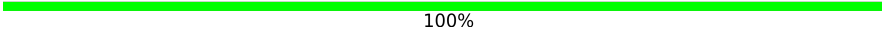


There are no outlier residues recorded for this chain.

- Molecule 8: unclear peptide



- Molecule 8: unclear peptide

Chain T:  100%

There are no outlier residues recorded for this chain.

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

Chain E:  100%
50% 50%



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

Chain V:  100%
100%



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

Chain X:  100%
50% 50%



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

Chain Y:  50%
100%



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

Chain a:  50%
100%



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



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



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



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



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



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



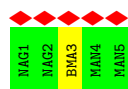
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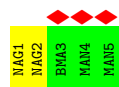
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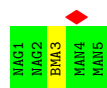
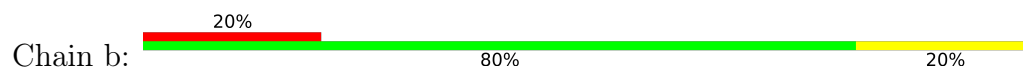
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

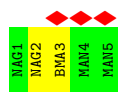


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

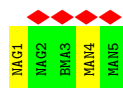
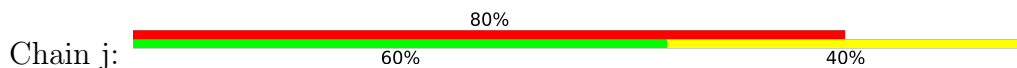


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

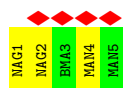
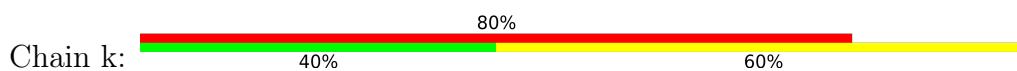




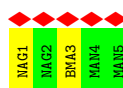
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



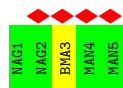
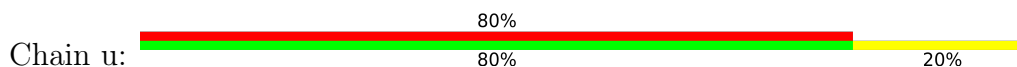
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

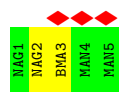


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

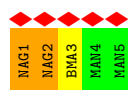


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

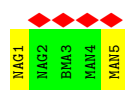
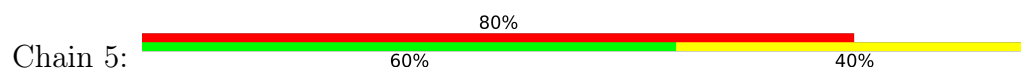




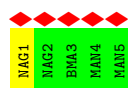
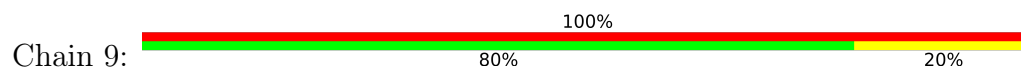
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



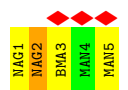
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 14: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 14: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 16: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 16: beta-D-mannopyranose-(1-3)-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, C1	Depositor
Number of particles used	67775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0242	Depositor
Map size (\AA)	366.86002, 366.86002, 366.86002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.411, 1.411, 1.411	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NI, BMA, NAG, MAN, A2G

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	0.32	0/34456	0.58	5/46804 (0.0%)
1	B	0.63	0/34454	0.67	5/46801 (0.0%)
2	C	0.64	0/1521	0.60	0/2033
2	D	0.63	0/1521	0.62	0/2033
4	H	0.68	0/7	0.49	0/8
4	O	0.82	0/7	0.68	0/8
5	I	0.67	0/7	0.63	0/8
5	P	0.68	0/7	0.88	0/8
6	J	1.03	0/5	0.57	0/5
6	Q	1.03	0/5	0.38	0/5
7	K	0.95	0/17	0.64	0/21
7	R	0.65	0/17	0.48	0/21
8	L	0.57	0/7	0.62	0/8
8	M	0.64	0/7	0.52	0/8
8	S	0.93	0/7	0.59	0/8
8	T	0.58	0/7	0.54	0/8
All	All	0.51	0/72052	0.63	10/97787 (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	4
1	B	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4327	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	B	3693	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	B	2218	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	B	364	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	B	2919	ARG	NE-CZ-NH2	6.32	123.46	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1043	ARG	Sidechain
1	A	3212	ARG	Sidechain
1	A	4321	ARG	Sidechain
1	A	781	ARG	Sidechain
1	B	2877	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33638	0	31021	237	0
1	B	33636	0	31021	245	0
2	C	1494	0	1505	22	0
2	D	1494	0	1505	26	0
3	G	30	0	8	0	0
3	N	30	0	8	0	0
4	H	28	0	12	0	0
4	O	28	0	12	0	0
5	I	33	0	18	5	0
5	P	33	0	18	1	0
6	J	16	0	8	0	0
6	Q	16	0	8	0	0
7	K	33	0	18	1	0
7	R	33	0	17	0	0
8	L	28	0	12	0	0
8	M	28	0	12	0	0
8	S	28	0	12	0	0
8	T	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	28	0	25	0	0
9	V	28	0	25	0	0
9	X	28	0	25	1	0
9	Y	28	0	25	0	0
9	a	28	0	25	0	0
9	d	28	0	25	0	0
9	n	28	0	25	0	0
9	q	28	0	25	0	0
9	s	28	0	25	0	0
9	t	28	0	25	0	0
9	v	28	0	25	0	0
9	x	28	0	25	0	0
9	y	28	0	25	0	0
10	1	61	0	52	0	0
10	4	61	0	52	1	0
10	5	61	0	52	0	0
10	9	61	0	52	0	0
10	F	61	0	52	0	0
10	Z	61	0	52	0	0
10	b	61	0	52	0	0
10	g	61	0	52	0	0
10	j	61	0	52	0	0
10	k	61	0	52	0	0
10	l	61	0	52	0	0
10	u	61	0	52	0	0
11	U	61	0	52	2	0
12	2	39	0	34	0	0
12	3	39	0	34	0	0
12	W	39	0	34	1	0
12	e	39	0	34	0	0
12	f	39	0	34	0	0
12	h	39	0	34	0	0
12	i	39	0	34	0	0
12	m	39	0	34	0	0
12	p	39	0	34	0	0
12	r	39	0	34	0	0
13	8	28	0	25	0	0
13	c	28	0	25	0	0
13	o	28	0	25	0	0
14	6	61	0	52	1	0
14	w	61	0	52	0	0
15	z	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	0	39	0	34	0	0
16	7	39	0	34	0	0
17	A	154	0	143	2	0
17	B	154	0	143	0	0
18	A	168	0	144	0	0
18	B	168	0	144	0	0
19	A	44	0	0	0	0
19	B	44	0	0	0	0
20	A	1	0	0	0	0
20	B	1	0	0	0	0
All	All	73258	0	67423	526	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 4.

The worst 5 of 526 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3505:ARG:H	1:B:3505:ARG:HD3	1.38	0.90
1:A:3015:ASP:HB2	1:A:3017:ARG:NH2	1.90	0.87
1:A:2786:GLU:HG2	1:A:2788:THR:H	1.43	0.82
1:A:2708:CYS:SG	1:A:2730:SER:OG	2.40	0.79
1:A:3963:GLY:HA2	1:A:4004:LYS:HE2	1.65	0.79

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4304/4660 (92%)	3983 (92%)	319 (7%)	2 (0%)	100	100
1	B	4304/4660 (92%)	3994 (93%)	308 (7%)	2 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	173/360 (48%)	170 (98%)	3 (2%)	0	100	100
2	D	173/360 (48%)	171 (99%)	2 (1%)	0	100	100
4	H	1/5 (20%)	1 (100%)	0	0	100	100
4	O	1/5 (20%)	1 (100%)	0	0	100	100
5	I	1/6 (17%)	1 (100%)	0	0	100	100
5	P	1/6 (17%)	1 (100%)	0	0	100	100
6	J	1/3 (33%)	0	1 (100%)	0	100	100
6	Q	1/3 (33%)	1 (100%)	0	0	100	100
7	K	2/5 (40%)	0	2 (100%)	0	100	100
7	R	2/5 (40%)	2 (100%)	0	0	100	100
8	L	1/5 (20%)	0	1 (100%)	0	100	100
8	M	1/5 (20%)	1 (100%)	0	0	100	100
8	S	1/5 (20%)	0	1 (100%)	0	100	100
8	T	1/5 (20%)	1 (100%)	0	0	100	100
All	All	8968/10098 (89%)	8327 (93%)	637 (7%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2874	SER
1	A	2874	SER
1	B	2858	ILE
1	A	410	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3791/4089 (93%)	3672 (97%)	119 (3%)	35	56
1	B	3790/4089 (93%)	3688 (97%)	102 (3%)	40	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	163/326 (50%)	156 (96%)	7 (4%)	25	48
2	D	163/326 (50%)	159 (98%)	4 (2%)	42	62
4	H	1/1 (100%)	1 (100%)	0	100	100
4	O	1/1 (100%)	1 (100%)	0	100	100
5	I	1/1 (100%)	1 (100%)	0	100	100
5	P	1/1 (100%)	0	1 (100%)	0	0
6	J	1/1 (100%)	1 (100%)	0	100	100
6	Q	1/1 (100%)	1 (100%)	0	100	100
7	K	2/2 (100%)	2 (100%)	0	100	100
7	R	2/2 (100%)	1 (50%)	1 (50%)	0	0
8	L	1/1 (100%)	1 (100%)	0	100	100
8	M	1/1 (100%)	1 (100%)	0	100	100
8	S	1/1 (100%)	1 (100%)	0	100	100
8	T	1/1 (100%)	1 (100%)	0	100	100
All	All	7921/8844 (90%)	7687 (97%)	234 (3%)	37	57

5 of 234 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4366	THR
2	C	259	ARG
1	B	895	HIS
1	B	4274	MET
1	B	3467	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3941	ASN
1	B	1033	ASN
2	D	294	HIS
1	B	4008	GLN
1	A	4221	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

146 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	$\# Z > 2$
16	NAG	0	1	16,1	14,14,15	0.49	0	17,19,21	1.42	1 (5%)
16	NAG	0	2	16	14,14,15	0.38	0	17,19,21	1.41	3 (17%)
16	BMA	0	3	16	11,11,12	0.32	0	15,15,17	0.54	0
10	NAG	1	1	10,1	14,14,15	0.49	0	17,19,21	0.86	0
10	NAG	1	2	10	14,14,15	0.43	0	17,19,21	0.66	1 (5%)
10	BMA	1	3	10	11,11,12	0.27	0	15,15,17	0.90	1 (6%)
10	MAN	1	4	10	11,11,12	0.30	0	15,15,17	0.69	0
10	MAN	1	5	10	11,11,12	0.29	0	15,15,17	0.60	0
12	NAG	2	1	12,1	14,14,15	0.89	0	17,19,21	1.52	5 (29%)
12	NAG	2	2	12	14,14,15	1.18	2 (14%)	17,19,21	1.04	1 (5%)
12	BMA	2	3	12	11,11,12	1.07	2 (18%)	15,15,17	1.00	1 (6%)
12	NAG	3	1	12,1	14,14,15	0.44	0	17,19,21	0.53	0
12	NAG	3	2	12	14,14,15	0.47	0	17,19,21	0.59	0
12	BMA	3	3	12	11,11,12	0.79	0	15,15,17	0.85	1 (6%)
10	NAG	4	1	10,1	14,14,15	0.41	0	17,19,21	0.99	1 (5%)
10	NAG	4	2	10	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
10	BMA	4	3	10	11,11,12	0.31	0	15,15,17	1.04	2 (13%)
10	MAN	4	4	10	11,11,12	0.30	0	15,15,17	0.54	0
10	MAN	4	5	10	11,11,12	0.34	0	15,15,17	0.55	0
10	NAG	5	1	10,1	14,14,15	0.49	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	5	2	10	14,14,15	0.46	0	17,19,21	0.38	0
10	BMA	5	3	10	11,11,12	0.34	0	15,15,17	0.69	0
10	MAN	5	4	10	11,11,12	0.27	0	15,15,17	0.62	0
10	MAN	5	5	10	11,11,12	0.22	0	15,15,17	0.66	1 (6%)
14	NAG	6	1	14,1	14,14,15	0.44	0	17,19,21	0.77	0
14	NAG	6	2	14	14,14,15	0.44	0	17,19,21	0.86	0
14	BMA	6	3	14	11,11,12	0.39	0	15,15,17	1.04	0
14	MAN	6	4	14	11,11,12	0.27	0	15,15,17	0.88	2 (13%)
14	MAN	6	5	14	11,11,12	0.31	0	15,15,17	0.62	0
16	NAG	7	1	16,1	14,14,15	0.43	0	17,19,21	0.50	0
16	NAG	7	2	16	14,14,15	0.44	0	17,19,21	0.41	0
16	BMA	7	3	16	11,11,12	0.23	0	15,15,17	0.66	0
13	NAG	8	1	13,1	14,14,15	0.68	0	17,19,21	1.36	2 (11%)
13	NAG	8	2	13	14,14,15	0.58	0	17,19,21	0.94	1 (5%)
10	NAG	9	1	10,1	14,14,15	0.39	0	17,19,21	0.82	1 (5%)
10	NAG	9	2	10	14,14,15	0.40	0	17,19,21	0.47	0
10	BMA	9	3	10	11,11,12	0.27	0	15,15,17	0.71	0
10	MAN	9	4	10	11,11,12	0.27	0	15,15,17	0.65	0
10	MAN	9	5	10	11,11,12	0.26	0	15,15,17	0.54	0
9	NAG	E	1	9,1	14,14,15	0.40	0	17,19,21	0.99	1 (5%)
9	NAG	E	2	9	14,14,15	0.38	0	17,19,21	0.53	0
10	NAG	F	1	10,1	14,14,15	0.40	0	17,19,21	0.53	0
10	NAG	F	2	10	14,14,15	0.40	0	17,19,21	0.36	0
10	BMA	F	3	10	11,11,12	0.27	0	15,15,17	0.70	1 (6%)
10	MAN	F	4	10	11,11,12	0.34	0	15,15,17	0.58	0
10	MAN	F	5	10	11,11,12	0.22	0	15,15,17	0.62	0
11	NAG	U	1	11,1	14,14,15	0.41	0	17,19,21	0.56	0
11	NAG	U	2	11	14,14,15	0.49	0	17,19,21	1.77	4 (23%)
11	BMA	U	3	11	11,11,12	0.59	0	15,15,17	1.02	1 (6%)
11	MAN	U	4	11	11,11,12	0.30	0	15,15,17	0.69	0
11	MAN	U	5	11	11,11,12	0.36	0	15,15,17	0.79	2 (13%)
9	NAG	V	1	9,1	14,14,15	0.51	0	17,19,21	1.29	2 (11%)
9	NAG	V	2	9	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
12	NAG	W	1	12,1	14,14,15	0.42	0	17,19,21	0.72	1 (5%)
12	NAG	W	2	12	14,14,15	0.41	0	17,19,21	0.83	1 (5%)
12	BMA	W	3	12	11,11,12	0.35	0	15,15,17	0.70	0
9	NAG	X	1	9,1	14,14,15	0.42	0	17,19,21	0.60	0
9	NAG	X	2	9	14,14,15	0.42	0	17,19,21	0.60	0
9	NAG	Y	1	9,1	14,14,15	0.39	0	17,19,21	0.41	0
9	NAG	Y	2	9	14,14,15	0.40	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	Z	1	10,1	14,14,15	0.46	0	17,19,21	1.32	1 (5%)
10	NAG	Z	2	10	14,14,15	0.38	0	17,19,21	1.18	2 (11%)
10	BMA	Z	3	10	11,11,12	0.33	0	15,15,17	0.66	0
10	MAN	Z	4	10	11,11,12	0.28	0	15,15,17	0.50	0
10	MAN	Z	5	10	11,11,12	0.24	0	15,15,17	0.56	0
9	NAG	a	1	9,1	14,14,15	0.40	0	17,19,21	0.71	0
9	NAG	a	2	9	14,14,15	0.40	0	17,19,21	0.35	0
10	NAG	b	1	10,1	14,14,15	0.41	0	17,19,21	0.41	0
10	NAG	b	2	10	14,14,15	0.40	0	17,19,21	0.42	0
10	BMA	b	3	10	11,11,12	0.34	0	15,15,17	0.83	1 (6%)
10	MAN	b	4	10	11,11,12	0.28	0	15,15,17	0.67	0
10	MAN	b	5	10	11,11,12	0.23	0	15,15,17	0.54	0
13	NAG	c	1	13,1	14,14,15	0.51	0	17,19,21	0.85	1 (5%)
13	NAG	c	2	13	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
9	NAG	d	1	9,1	14,14,15	0.40	0	17,19,21	0.62	0
9	NAG	d	2	9	14,14,15	0.39	0	17,19,21	0.50	0
12	NAG	e	1	12,1	14,14,15	0.41	0	17,19,21	0.39	0
12	NAG	e	2	12	14,14,15	0.42	0	17,19,21	0.58	0
12	BMA	e	3	12	11,11,12	0.32	0	15,15,17	0.79	1 (6%)
12	NAG	f	1	12,1	14,14,15	0.42	0	17,19,21	0.45	0
12	NAG	f	2	12	14,14,15	0.42	0	17,19,21	0.54	0
12	BMA	f	3	12	11,11,12	0.22	0	15,15,17	0.63	1 (6%)
10	NAG	g	1	10,1	14,14,15	0.46	0	17,19,21	0.39	0
10	NAG	g	2	10	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
10	BMA	g	3	10	11,11,12	0.40	0	15,15,17	0.79	1 (6%)
10	MAN	g	4	10	11,11,12	0.30	0	15,15,17	0.58	0
10	MAN	g	5	10	11,11,12	0.27	0	15,15,17	0.64	0
12	NAG	h	1	12,1	14,14,15	0.41	0	17,19,21	0.70	0
12	NAG	h	2	12	14,14,15	0.43	0	17,19,21	0.49	0
12	BMA	h	3	12	11,11,12	0.29	0	15,15,17	0.57	0
12	NAG	i	1	12,1	14,14,15	0.47	0	17,19,21	0.80	0
12	NAG	i	2	12	14,14,15	0.47	0	17,19,21	0.95	1 (5%)
12	BMA	i	3	12	11,11,12	0.62	0	15,15,17	0.84	1 (6%)
10	NAG	j	1	10,1	14,14,15	0.40	0	17,19,21	1.30	3 (17%)
10	NAG	j	2	10	14,14,15	0.41	0	17,19,21	0.38	0
10	BMA	j	3	10	11,11,12	0.55	0	15,15,17	0.79	0
10	MAN	j	4	10	11,11,12	0.50	0	15,15,17	0.88	1 (6%)
10	MAN	j	5	10	11,11,12	0.38	0	15,15,17	0.65	0
10	NAG	k	1	10,1	14,14,15	0.44	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	k	2	10	14,14,15	0.49	0	17,19,21	1.11	2 (11%)
10	BMA	k	3	10	11,11,12	0.26	0	15,15,17	0.64	0
10	MAN	k	4	10	11,11,12	0.31	0	15,15,17	0.93	2 (13%)
10	MAN	k	5	10	11,11,12	0.33	0	15,15,17	0.56	0
10	NAG	l	1	10,1	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
10	NAG	l	2	10	14,14,15	0.43	0	17,19,21	0.37	0
10	BMA	l	3	10	11,11,12	0.34	0	15,15,17	1.21	2 (13%)
10	MAN	l	4	10	11,11,12	0.29	0	15,15,17	0.70	0
10	MAN	l	5	10	11,11,12	0.33	0	15,15,17	0.53	0
12	NAG	m	1	12,1	14,14,15	1.07	1 (7%)	17,19,21	1.19	1 (5%)
12	NAG	m	2	12	14,14,15	0.42	0	17,19,21	0.70	1 (5%)
12	BMA	m	3	12	11,11,12	0.28	0	15,15,17	0.61	0
9	NAG	n	1	9,1	14,14,15	0.53	0	17,19,21	1.01	1 (5%)
9	NAG	n	2	9	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
13	NAG	o	1	13,1	14,14,15	0.40	0	17,19,21	0.82	0
13	NAG	o	2	13	14,14,15	0.41	0	17,19,21	0.41	0
12	NAG	p	1	12,1	14,14,15	0.42	0	17,19,21	0.71	0
12	NAG	p	2	12	14,14,15	0.40	0	17,19,21	0.82	1 (5%)
12	BMA	p	3	12	11,11,12	0.26	0	15,15,17	0.67	0
9	NAG	q	1	9,1	14,14,15	1.13	1 (7%)	17,19,21	1.14	1 (5%)
9	NAG	q	2	9	14,14,15	0.92	1 (7%)	17,19,21	1.07	1 (5%)
12	NAG	r	1	12,1	14,14,15	0.42	0	17,19,21	0.82	1 (5%)
12	NAG	r	2	12	14,14,15	0.41	0	17,19,21	0.57	0
12	BMA	r	3	12	11,11,12	0.30	0	15,15,17	0.66	0
9	NAG	s	1	9,1	14,14,15	0.44	0	17,19,21	1.02	2 (11%)
9	NAG	s	2	9	14,14,15	0.40	0	17,19,21	0.61	0
9	NAG	t	1	9,1	14,14,15	0.98	0	17,19,21	1.55	3 (17%)
9	NAG	t	2	9	14,14,15	1.08	1 (7%)	17,19,21	1.53	1 (5%)
10	NAG	u	1	10,1	14,14,15	0.48	0	17,19,21	0.56	0
10	NAG	u	2	10	14,14,15	0.45	0	17,19,21	0.70	0
10	BMA	u	3	10	11,11,12	0.40	0	15,15,17	0.72	1 (6%)
10	MAN	u	4	10	11,11,12	0.24	0	15,15,17	0.60	0
10	MAN	u	5	10	11,11,12	0.27	0	15,15,17	0.64	0
9	NAG	v	1	9,1	14,14,15	0.45	0	17,19,21	0.49	0
9	NAG	v	2	9	14,14,15	0.39	0	17,19,21	0.39	0
14	NAG	w	1	14,1	14,14,15	0.52	0	17,19,21	1.20	2 (11%)
14	NAG	w	2	14	14,14,15	0.46	0	17,19,21	1.34	3 (17%)
14	BMA	w	3	14	11,11,12	0.42	0	15,15,17	0.66	0
14	MAN	w	4	14	11,11,12	0.29	0	15,15,17	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	MAN	w	5	14	11,11,12	0.27	0	15,15,17	0.57	0
9	NAG	x	1	9,1	14,14,15	0.51	0	17,19,21	0.85	0
9	NAG	x	2	9	14,14,15	0.40	0	17,19,21	0.69	0
9	NAG	y	1	9,1	14,14,15	0.41	0	17,19,21	0.67	1 (5%)
9	NAG	y	2	9	14,14,15	0.41	0	17,19,21	0.43	0
15	NAG	z	1	1,15	14,14,15	0.54	0	17,19,21	0.82	1 (5%)
15	NAG	z	2	15	14,14,15	0.39	0	17,19,21	1.29	2 (11%)
15	BMA	z	3	15	11,11,12	0.37	0	15,15,17	0.69	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
16	NAG	0	1	16,1	-	2/6/23/26	0/1/1/1
16	NAG	0	2	16	-	0/6/23/26	0/1/1/1
16	BMA	0	3	16	-	0/2/19/22	0/1/1/1
10	NAG	1	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	1	2	10	-	0/6/23/26	0/1/1/1
10	BMA	1	3	10	-	2/2/19/22	0/1/1/1
10	MAN	1	4	10	-	0/2/19/22	0/1/1/1
10	MAN	1	5	10	-	0/2/19/22	0/1/1/1
12	NAG	2	1	12,1	-	1/6/23/26	0/1/1/1
12	NAG	2	2	12	-	1/6/23/26	0/1/1/1
12	BMA	2	3	12	-	0/2/19/22	0/1/1/1
12	NAG	3	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	3	2	12	-	0/6/23/26	0/1/1/1
12	BMA	3	3	12	-	0/2/19/22	0/1/1/1
10	NAG	4	1	10,1	-	6/6/23/26	0/1/1/1
10	NAG	4	2	10	-	5/6/23/26	0/1/1/1
10	BMA	4	3	10	-	2/2/19/22	0/1/1/1
10	MAN	4	4	10	-	0/2/19/22	0/1/1/1
10	MAN	4	5	10	-	0/2/19/22	0/1/1/1
10	NAG	5	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	5	2	10	-	0/6/23/26	0/1/1/1
10	BMA	5	3	10	-	2/2/19/22	0/1/1/1
10	MAN	5	4	10	-	0/2/19/22	0/1/1/1
10	MAN	5	5	10	-	0/2/19/22	0/1/1/1
14	NAG	6	1	14,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	6	2	14	-	4/6/23/26	0/1/1/1
14	BMA	6	3	14	-	0/2/19/22	0/1/1/1
14	MAN	6	4	14	-	1/2/19/22	0/1/1/1
14	MAN	6	5	14	-	1/2/19/22	0/1/1/1
16	NAG	7	1	16,1	-	0/6/23/26	0/1/1/1
16	NAG	7	2	16	-	3/6/23/26	0/1/1/1
16	BMA	7	3	16	-	0/2/19/22	0/1/1/1
13	NAG	8	1	13,1	-	1/6/23/26	0/1/1/1
13	NAG	8	2	13	-	2/6/23/26	0/1/1/1
10	NAG	9	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	9	2	10	-	0/6/23/26	0/1/1/1
10	BMA	9	3	10	-	2/2/19/22	0/1/1/1
10	MAN	9	4	10	-	0/2/19/22	0/1/1/1
10	MAN	9	5	10	-	0/2/19/22	0/1/1/1
9	NAG	E	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	E	2	9	-	0/6/23/26	0/1/1/1
10	NAG	F	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	F	2	10	-	0/6/23/26	0/1/1/1
10	BMA	F	3	10	-	0/2/19/22	0/1/1/1
10	MAN	F	4	10	-	0/2/19/22	0/1/1/1
10	MAN	F	5	10	-	0/2/19/22	0/1/1/1
11	NAG	U	1	11,1	-	0/6/23/26	0/1/1/1
11	NAG	U	2	11	-	4/6/23/26	0/1/1/1
11	BMA	U	3	11	-	1/2/19/22	0/1/1/1
11	MAN	U	4	11	-	0/2/19/22	0/1/1/1
11	MAN	U	5	11	-	1/2/19/22	0/1/1/1
9	NAG	V	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	0/6/23/26	0/1/1/1
12	NAG	W	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	W	2	12	-	2/6/23/26	0/1/1/1
12	BMA	W	3	12	-	0/2/19/22	0/1/1/1
9	NAG	X	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	X	2	9	-	1/6/23/26	0/1/1/1
9	NAG	Y	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	3/6/23/26	0/1/1/1
10	NAG	Z	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	0/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	4	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	5	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	a	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	a	2	9	-	0/6/23/26	0/1/1/1
10	NAG	b	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	b	2	10	-	1/6/23/26	0/1/1/1
10	BMA	b	3	10	-	0/2/19/22	0/1/1/1
10	MAN	b	4	10	-	0/2/19/22	0/1/1/1
10	MAN	b	5	10	-	0/2/19/22	0/1/1/1
13	NAG	c	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	c	2	13	-	1/6/23/26	0/1/1/1
9	NAG	d	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	d	2	9	-	0/6/23/26	0/1/1/1
12	NAG	e	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	e	2	12	-	2/6/23/26	0/1/1/1
12	BMA	e	3	12	-	0/2/19/22	0/1/1/1
12	NAG	f	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	f	2	12	-	0/6/23/26	0/1/1/1
12	BMA	f	3	12	-	0/2/19/22	0/1/1/1
10	NAG	g	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	g	2	10	-	0/6/23/26	0/1/1/1
10	BMA	g	3	10	-	0/2/19/22	0/1/1/1
10	MAN	g	4	10	-	0/2/19/22	0/1/1/1
10	MAN	g	5	10	-	1/2/19/22	0/1/1/1
12	NAG	h	1	12,1	-	3/6/23/26	0/1/1/1
12	NAG	h	2	12	-	4/6/23/26	0/1/1/1
12	BMA	h	3	12	-	0/2/19/22	0/1/1/1
12	NAG	i	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	i	2	12	-	0/6/23/26	0/1/1/1
12	BMA	i	3	12	-	0/2/19/22	0/1/1/1
10	NAG	j	1	10,1	-	3/6/23/26	0/1/1/1
10	NAG	j	2	10	-	4/6/23/26	0/1/1/1
10	BMA	j	3	10	-	2/2/19/22	0/1/1/1
10	MAN	j	4	10	-	0/2/19/22	0/1/1/1
10	MAN	j	5	10	-	1/2/19/22	0/1/1/1
10	NAG	k	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	k	2	10	-	0/6/23/26	0/1/1/1
10	BMA	k	3	10	-	0/2/19/22	0/1/1/1
10	MAN	k	4	10	-	0/2/19/22	0/1/1/1
10	MAN	k	5	10	-	0/2/19/22	0/1/1/1
10	NAG	l	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	l	2	10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	l	3	10	-	0/2/19/22	0/1/1/1
10	MAN	l	4	10	-	1/2/19/22	0/1/1/1
10	MAN	l	5	10	-	1/2/19/22	0/1/1/1
12	NAG	m	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	m	2	12	-	2/6/23/26	0/1/1/1
12	BMA	m	3	12	-	0/2/19/22	0/1/1/1
9	NAG	n	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	n	2	9	-	1/6/23/26	0/1/1/1
13	NAG	o	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	o	2	13	-	2/6/23/26	0/1/1/1
12	NAG	p	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	p	2	12	-	0/6/23/26	0/1/1/1
12	BMA	p	3	12	-	0/2/19/22	0/1/1/1
9	NAG	q	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	q	2	9	-	0/6/23/26	0/1/1/1
12	NAG	r	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	r	2	12	-	3/6/23/26	0/1/1/1
12	BMA	r	3	12	-	1/2/19/22	0/1/1/1
9	NAG	s	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	s	2	9	-	0/6/23/26	0/1/1/1
9	NAG	t	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	t	2	9	-	0/6/23/26	0/1/1/1
10	NAG	u	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	u	2	10	-	2/6/23/26	0/1/1/1
10	BMA	u	3	10	-	2/2/19/22	0/1/1/1
10	MAN	u	4	10	-	0/2/19/22	0/1/1/1
10	MAN	u	5	10	-	0/2/19/22	0/1/1/1
9	NAG	v	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	v	2	9	-	0/6/23/26	0/1/1/1
14	NAG	w	1	14,1	-	4/6/23/26	0/1/1/1
14	NAG	w	2	14	-	3/6/23/26	0/1/1/1
14	BMA	w	3	14	-	0/2/19/22	0/1/1/1
14	MAN	w	4	14	-	1/2/19/22	0/1/1/1
14	MAN	w	5	14	-	1/2/19/22	0/1/1/1
9	NAG	x	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	x	2	9	-	3/6/23/26	0/1/1/1
9	NAG	y	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	y	2	9	-	1/6/23/26	0/1/1/1
15	NAG	z	1	1,15	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	z	2	15	-	1/6/23/26	0/1/1/1
15	BMA	z	3	15	-	1/2/19/22	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	1	NAG	O5-C5	2.57	1.48	1.43
9	q	1	NAG	O5-C5	2.45	1.48	1.43
9	t	2	NAG	C1-C2	2.36	1.55	1.52
12	2	2	NAG	O5-C5	2.31	1.48	1.43
9	q	2	NAG	O5-C5	2.23	1.48	1.43

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	0	1	NAG	C1-O5-C5	5.01	118.98	112.19
9	t	2	NAG	C1-O5-C5	4.88	118.80	112.19
11	U	2	NAG	C4-C3-C2	4.72	117.93	111.02
9	t	1	NAG	C4-C3-C2	4.47	117.57	111.02
15	z	2	NAG	O5-C1-C2	-4.16	104.72	111.29

There are no chirality outliers.

5 of 124 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	4	1	NAG	C1-C2-N2-C7
12	h	1	NAG	C3-C2-N2-C7
12	h	1	NAG	C8-C7-N2-C2
12	h	1	NAG	O7-C7-N2-C2
14	w	1	NAG	C1-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 6 short contacts:

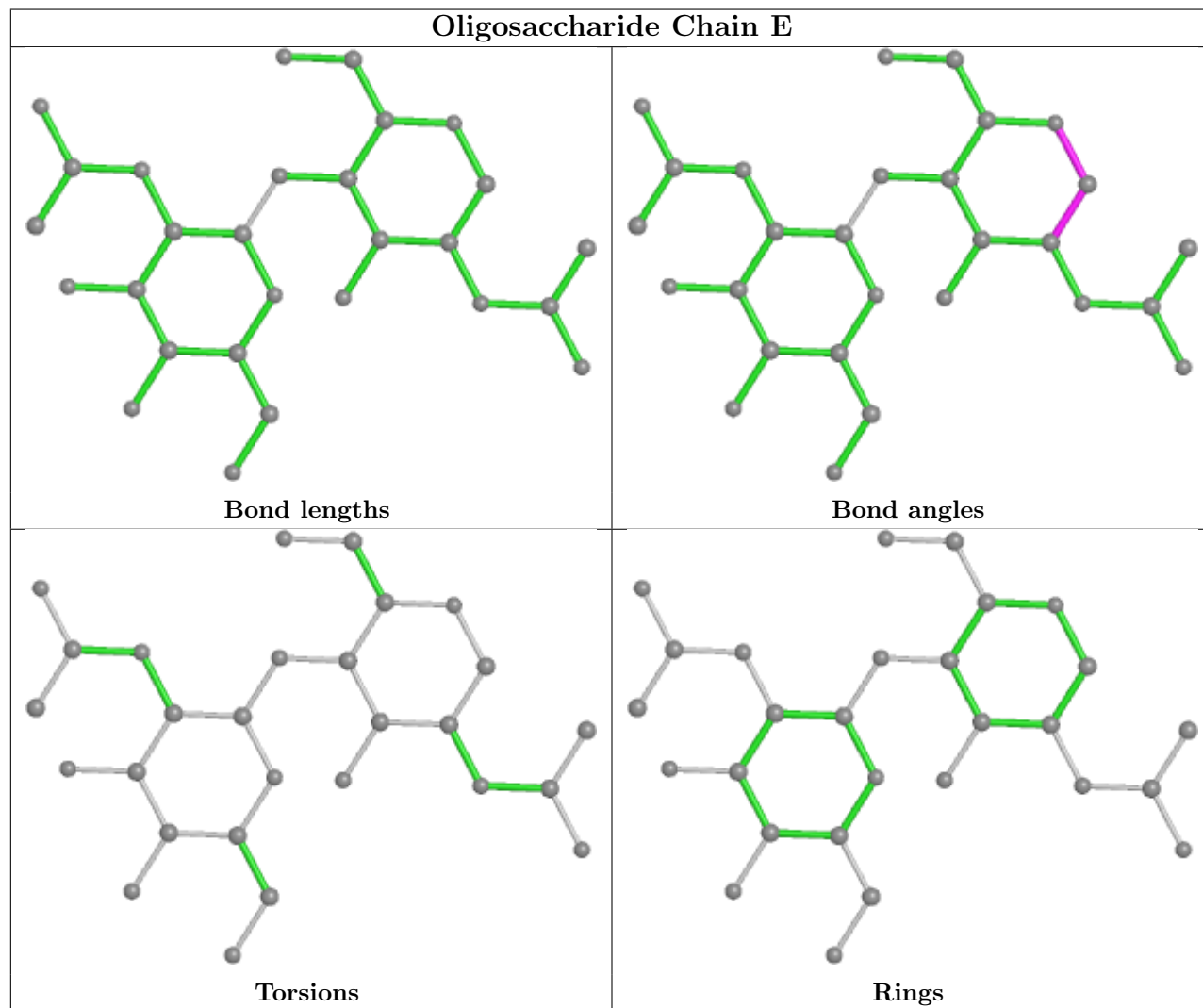
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	X	1	NAG	1	0
14	6	1	NAG	1	0
12	W	1	NAG	1	0
10	4	1	NAG	1	0
14	6	2	NAG	1	0
11	U	1	NAG	2	0

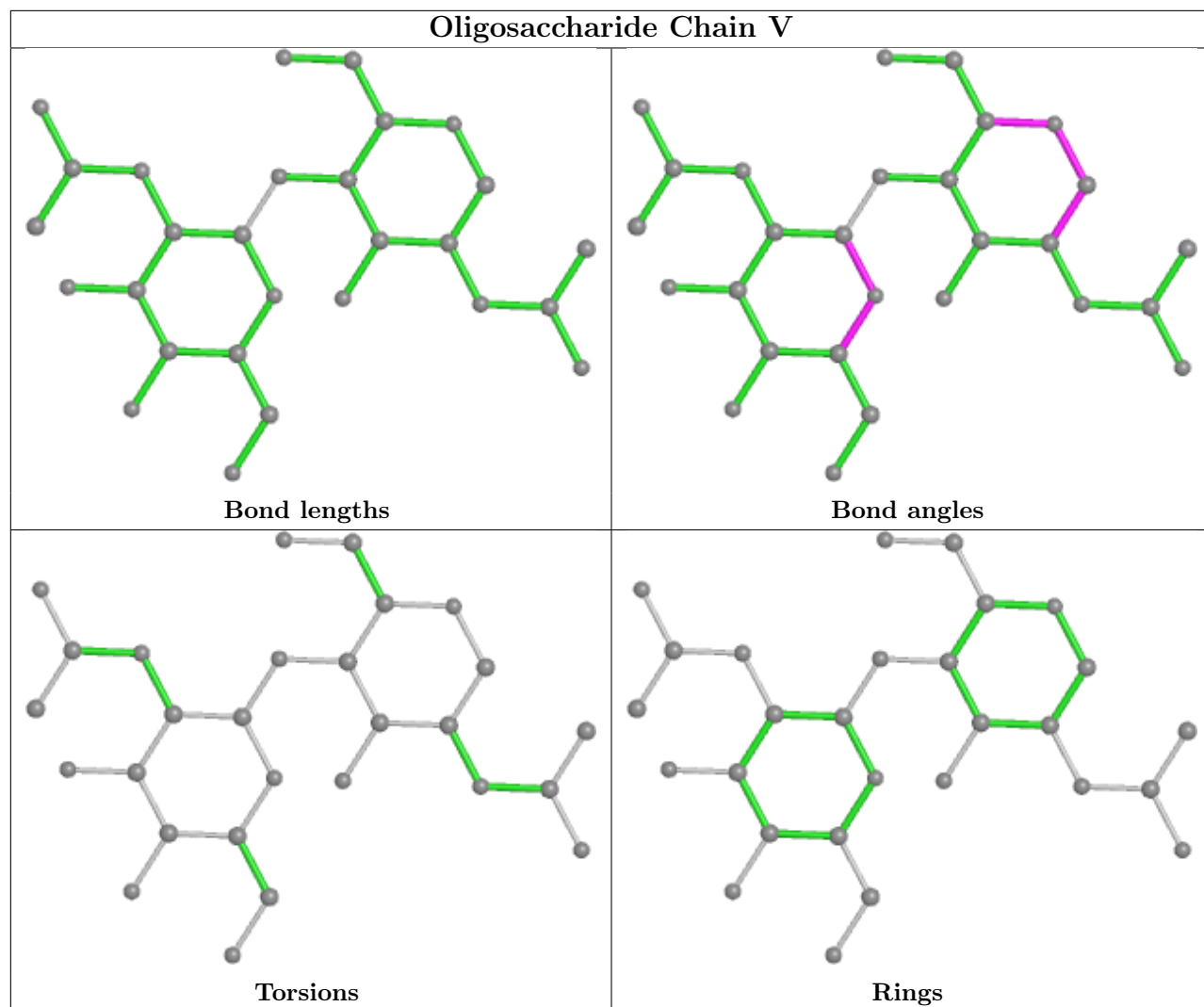
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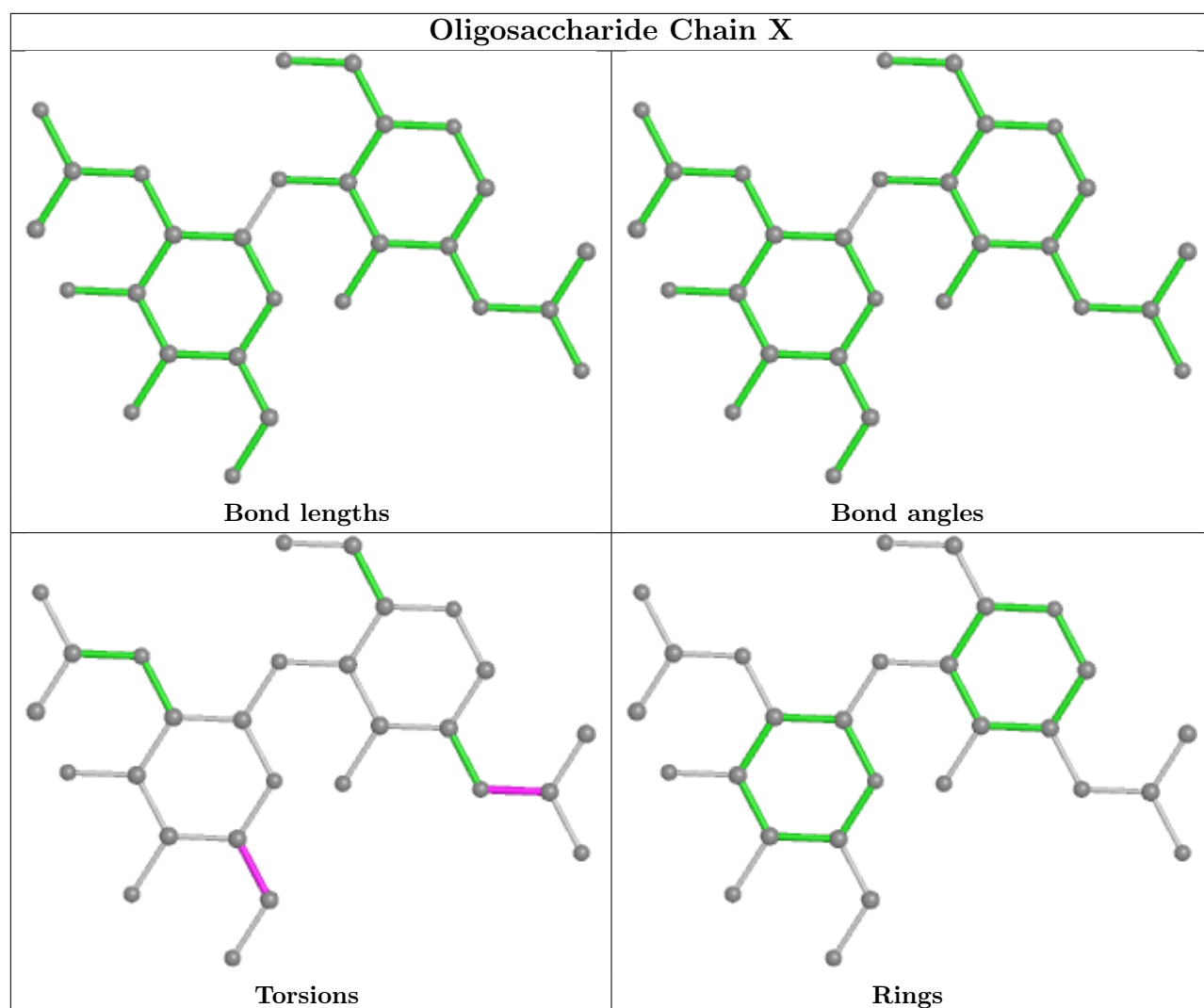
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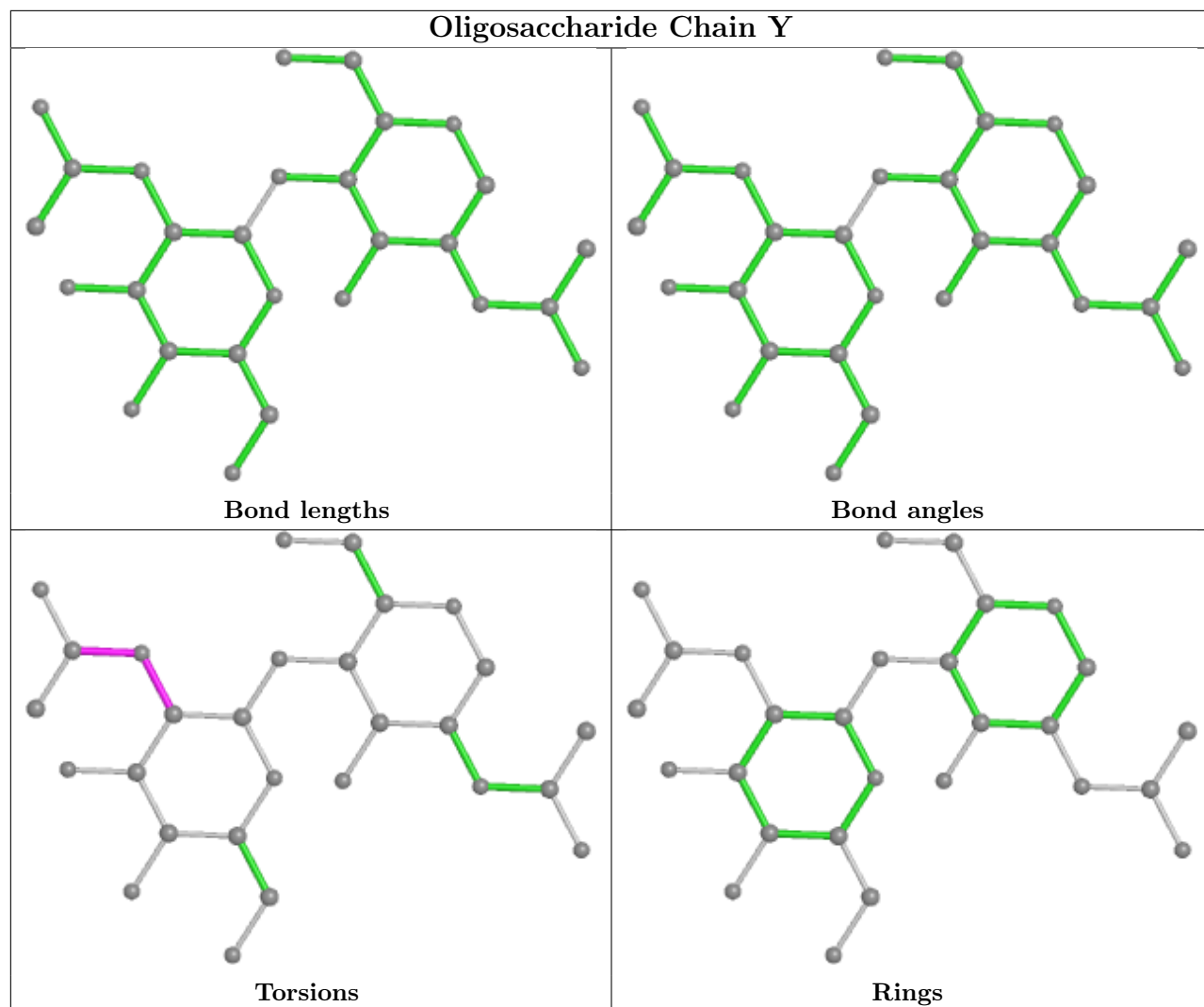
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	U	2	NAG	1	0
10	4	2	NAG	1	0

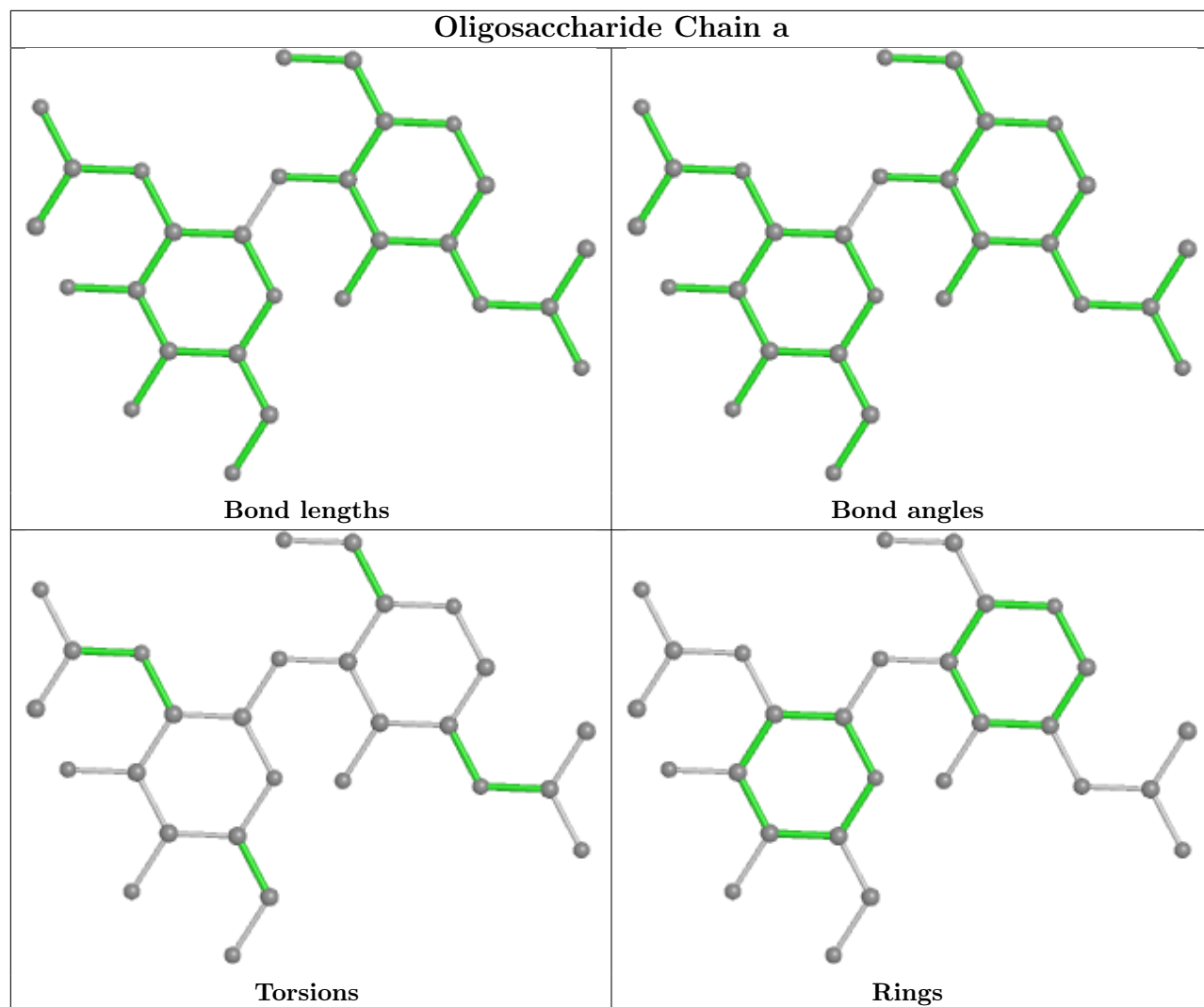
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

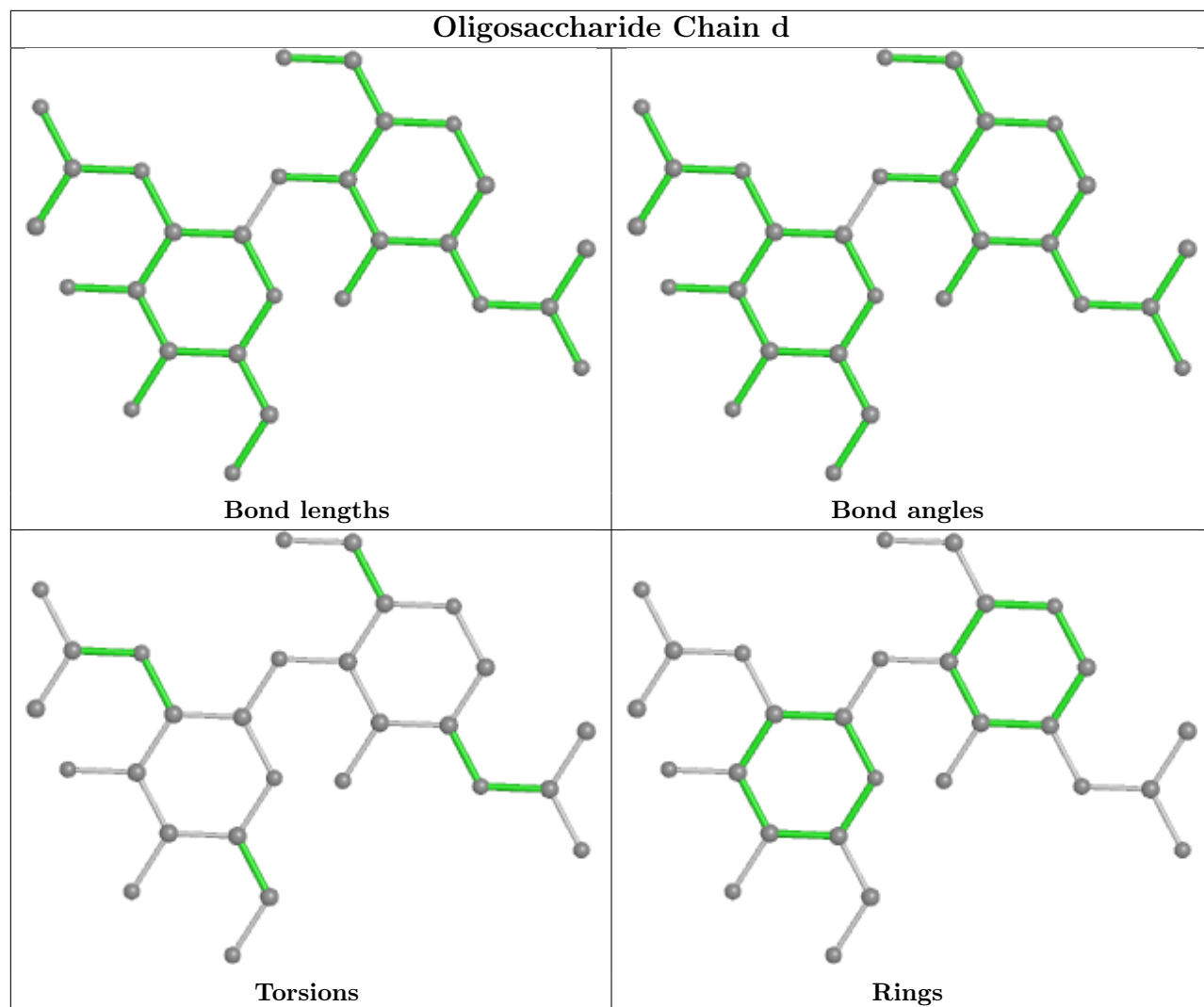


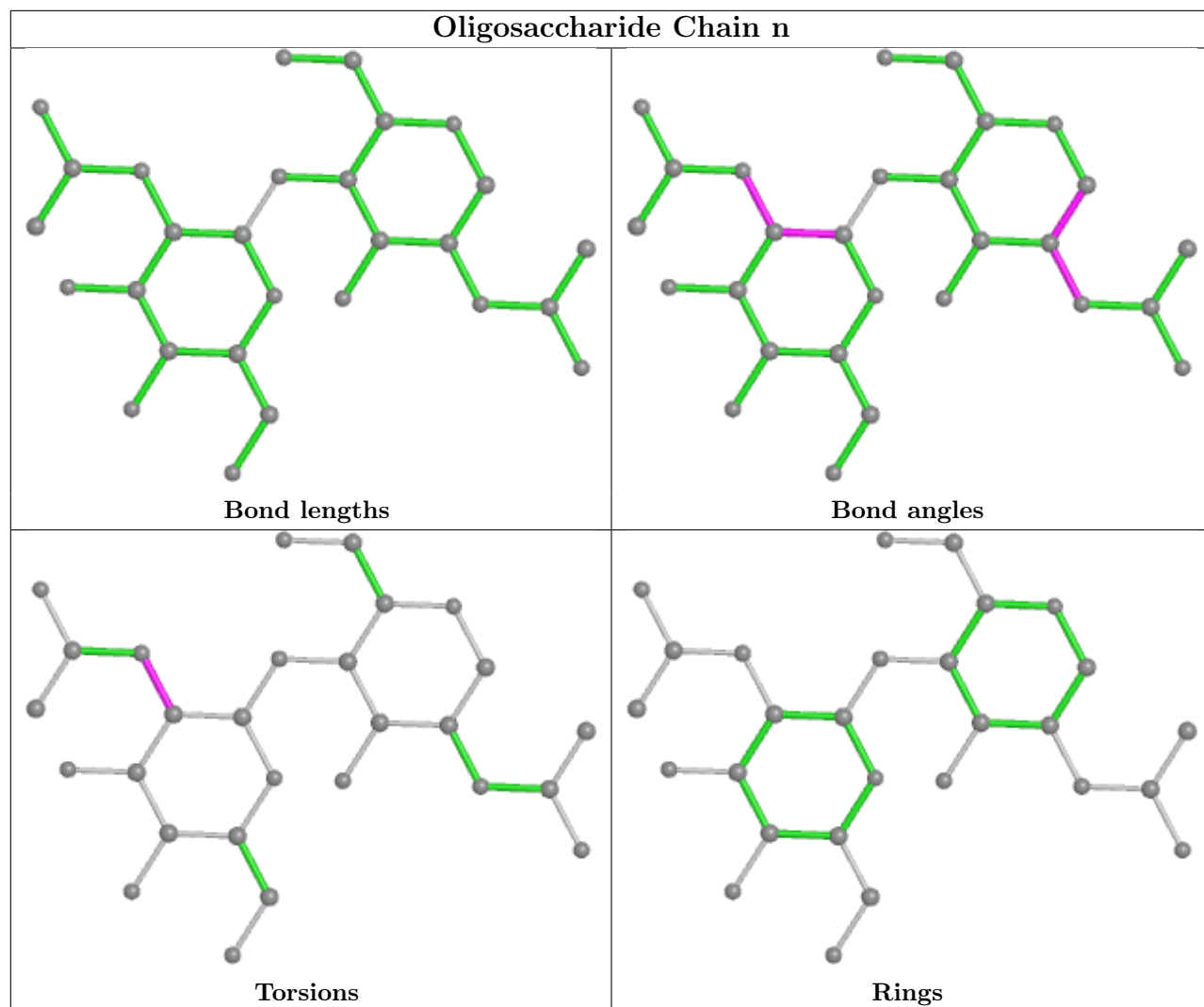


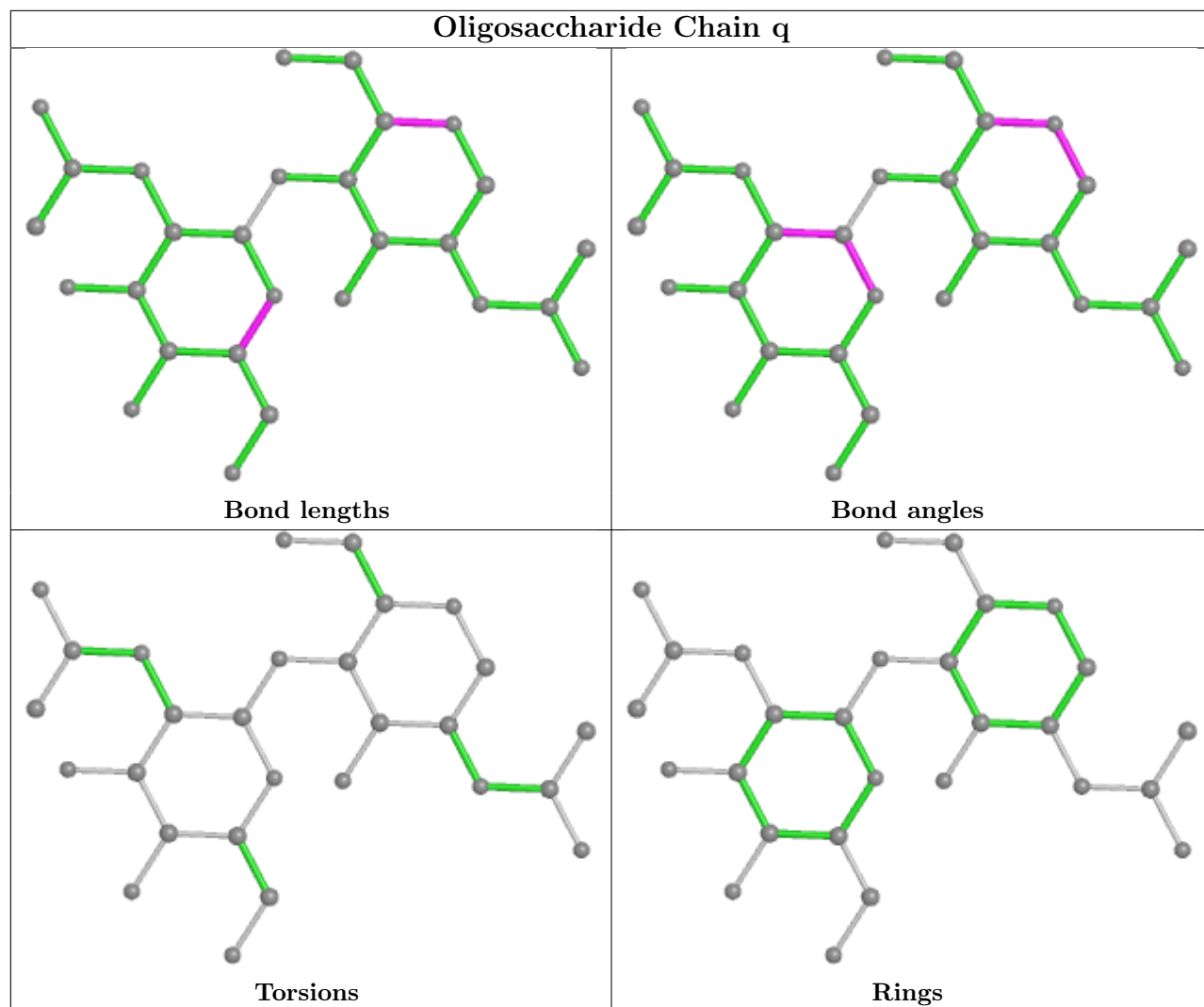


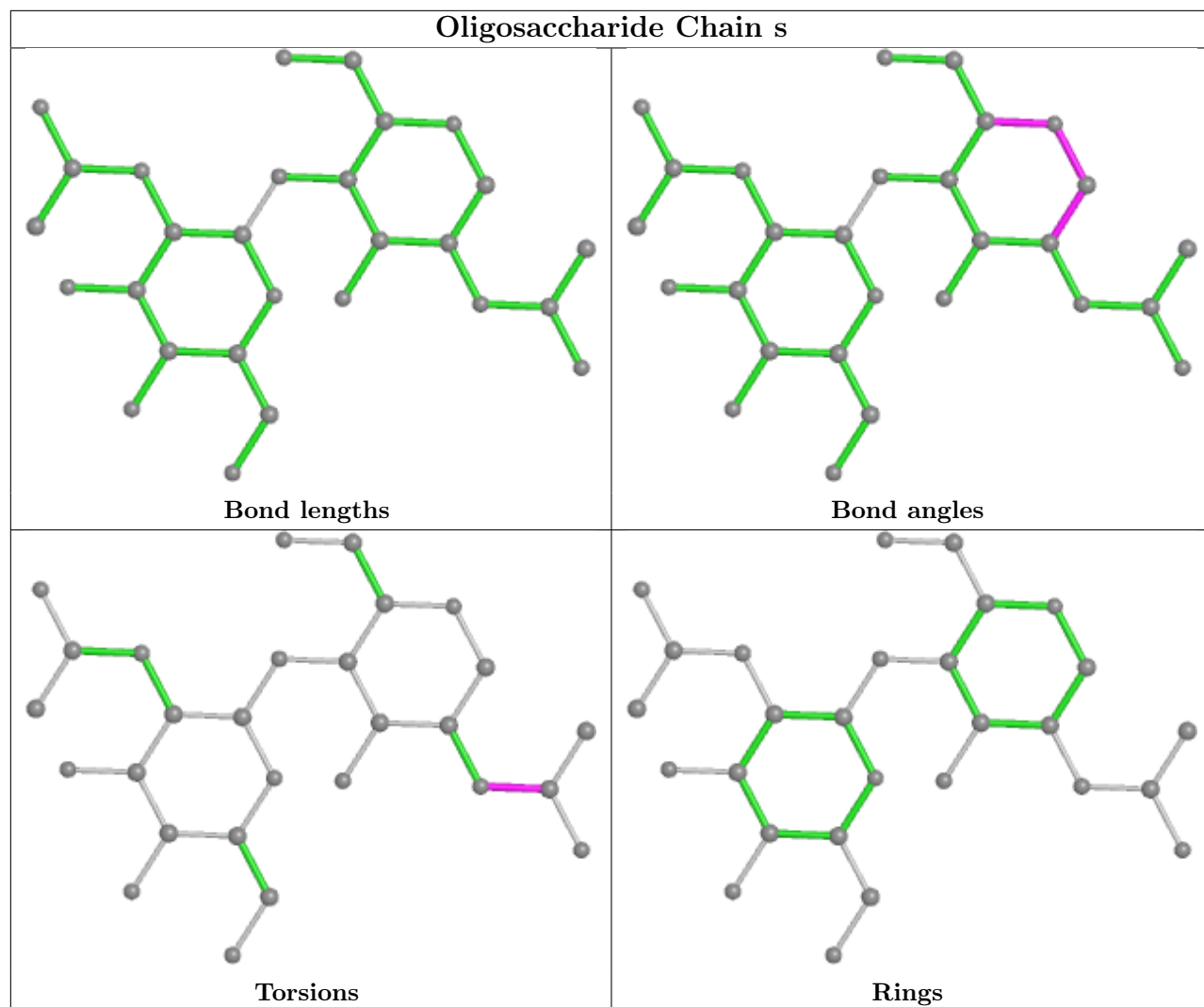


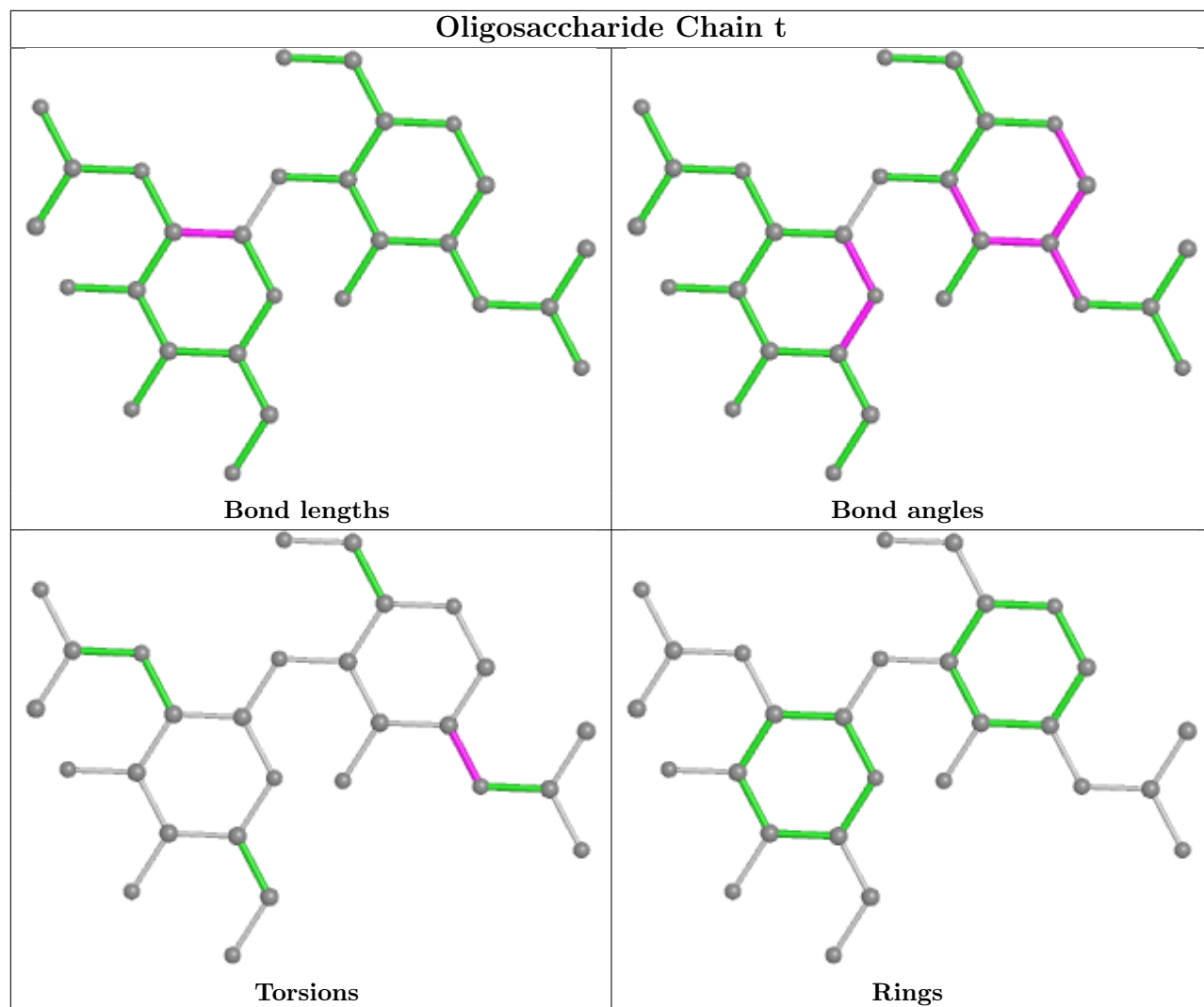


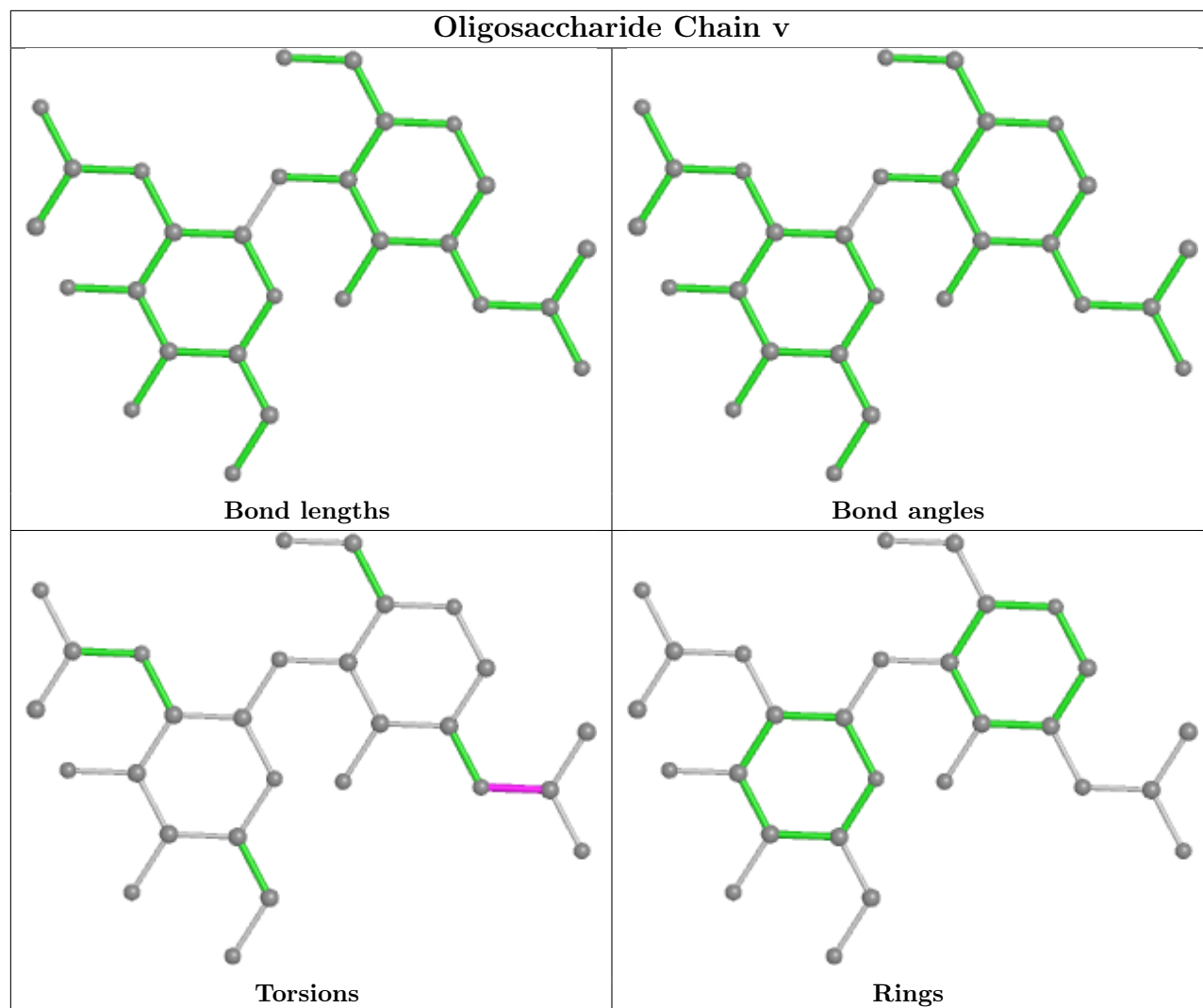


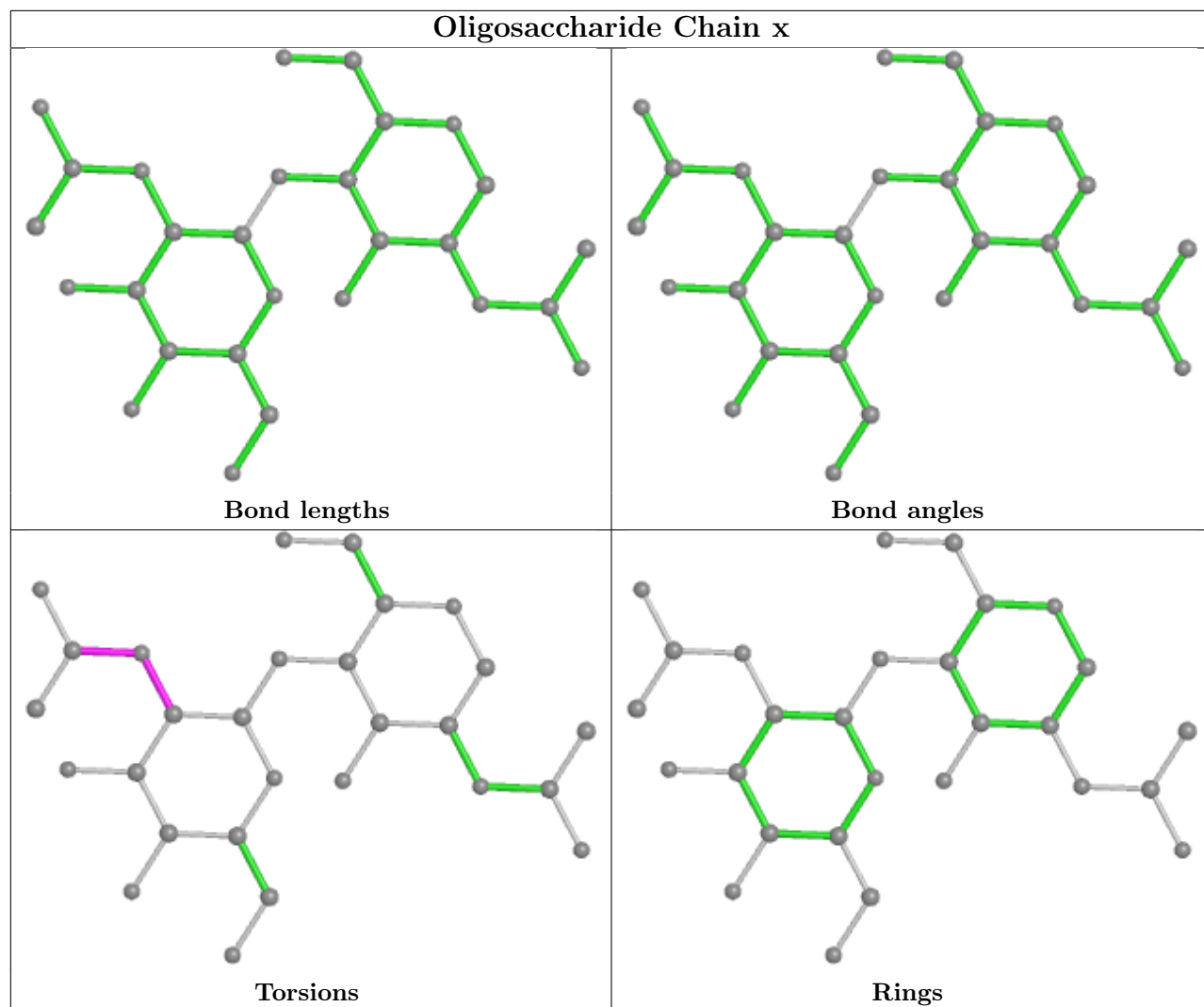


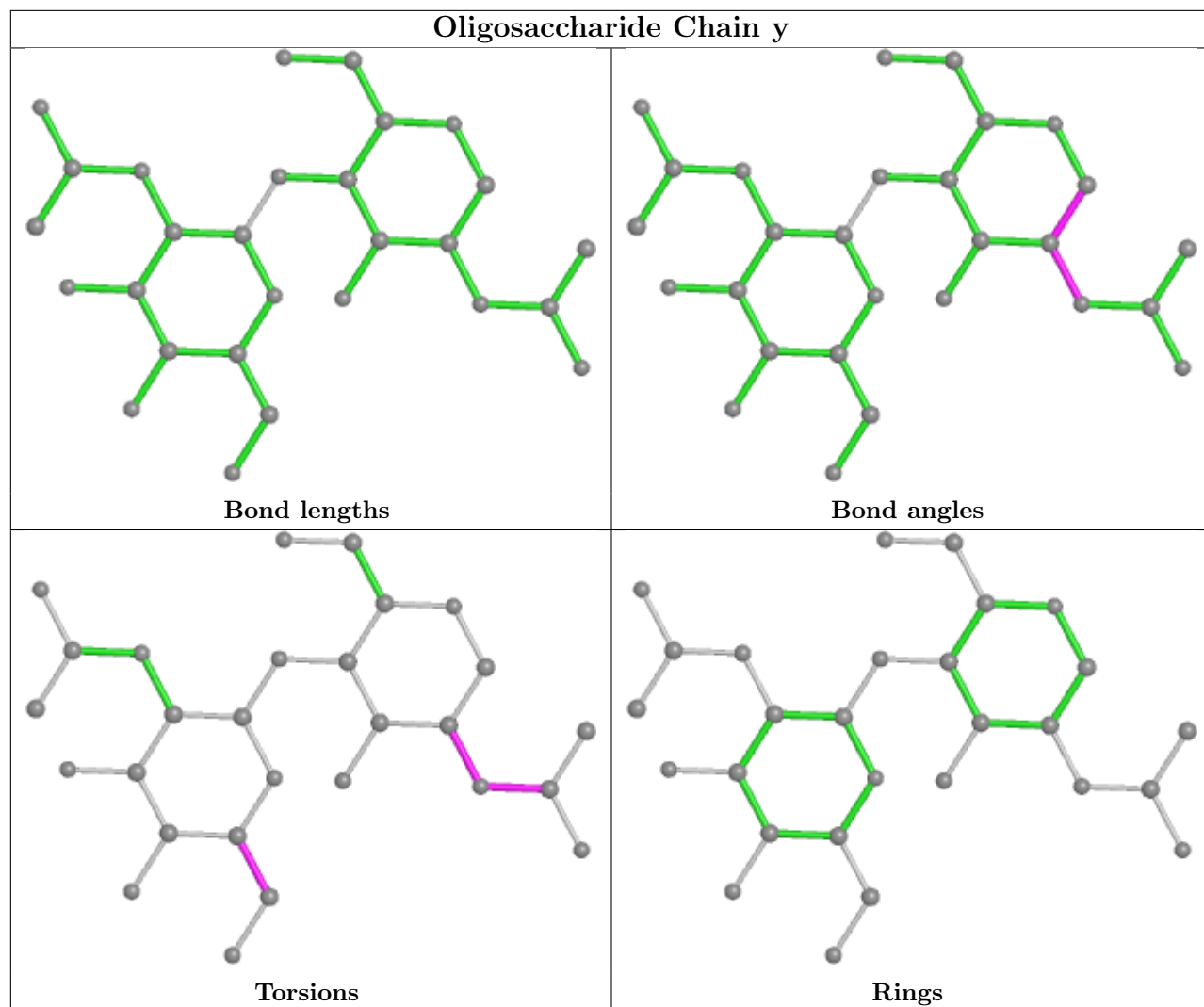


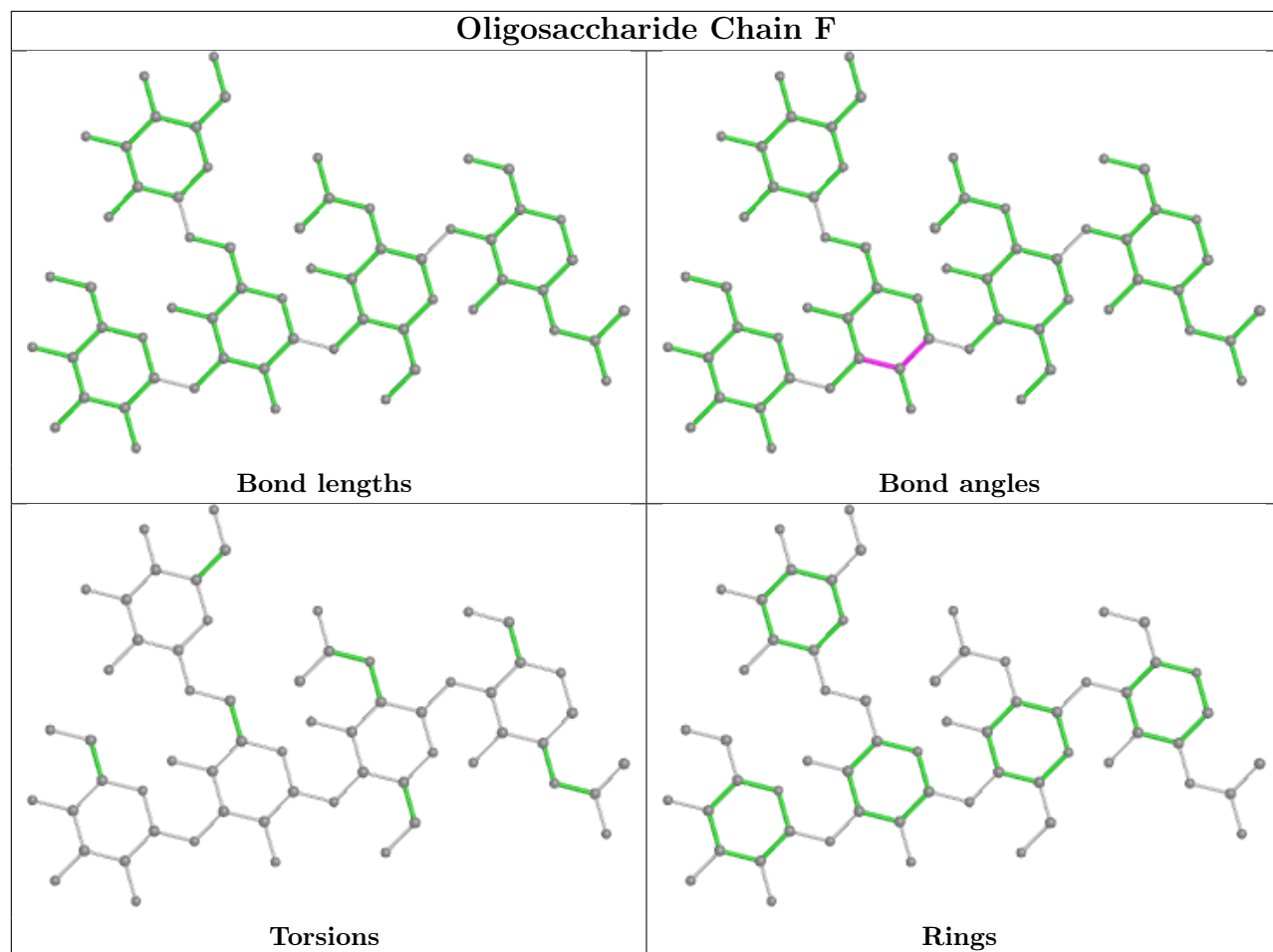


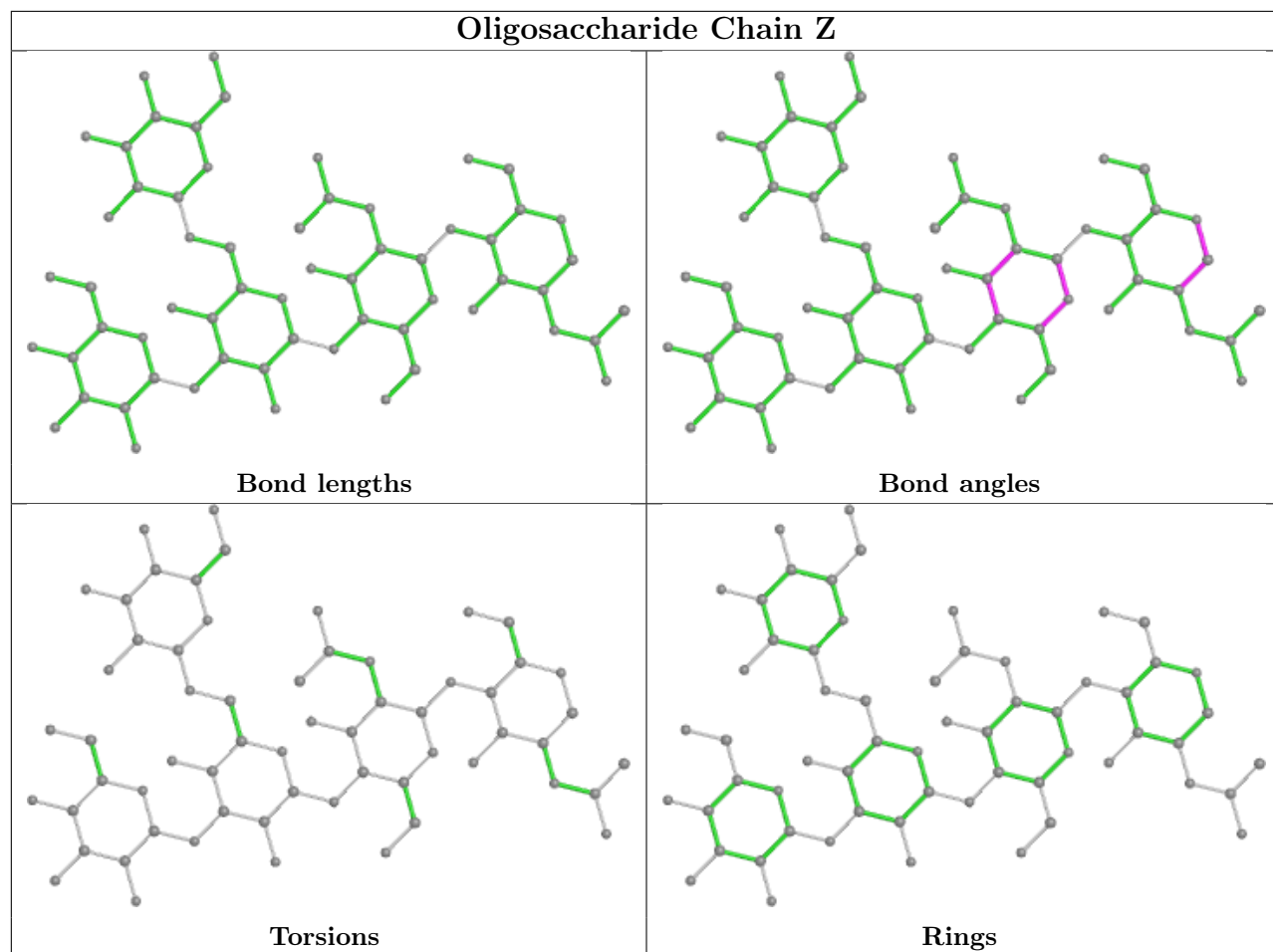


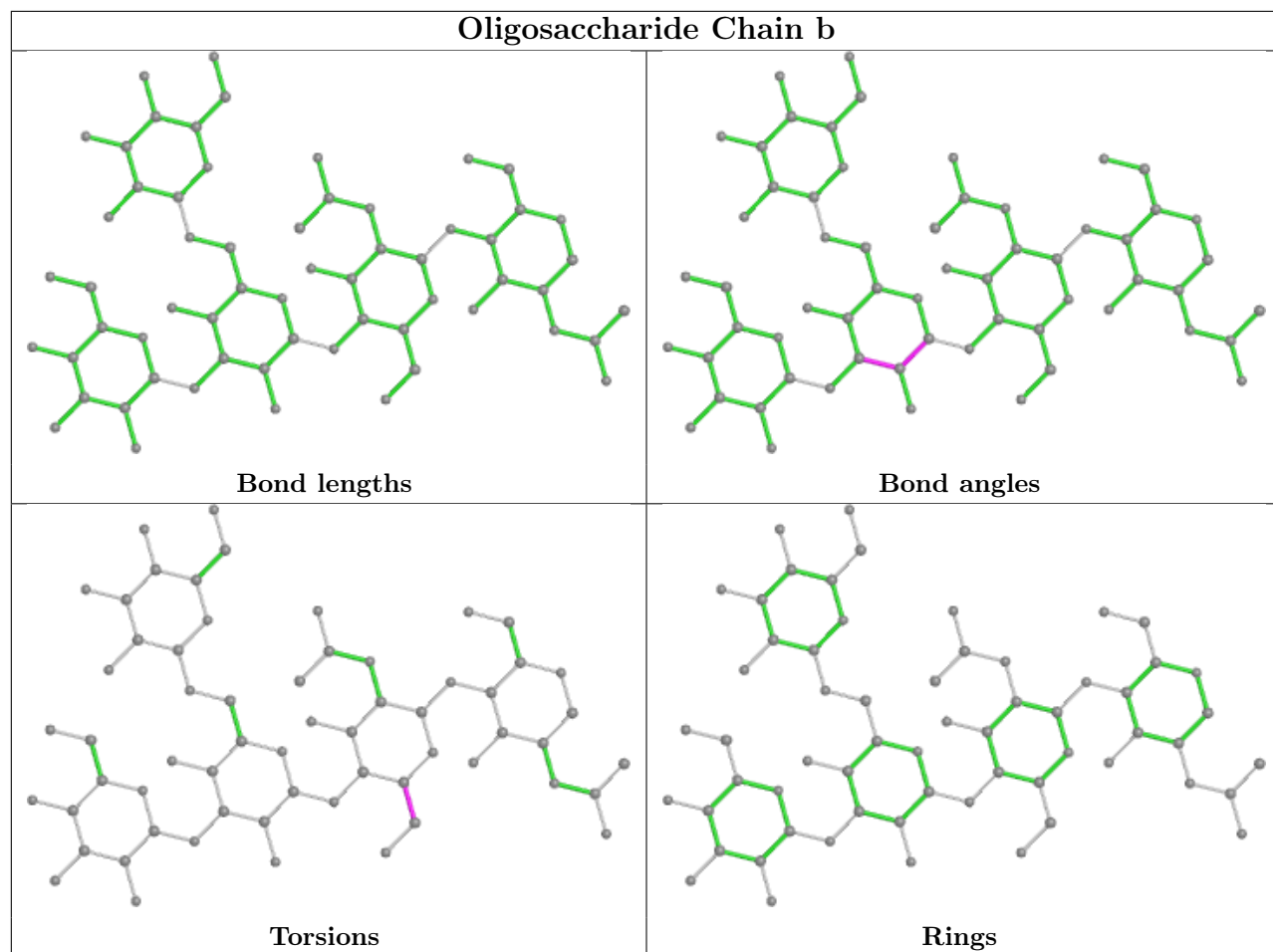


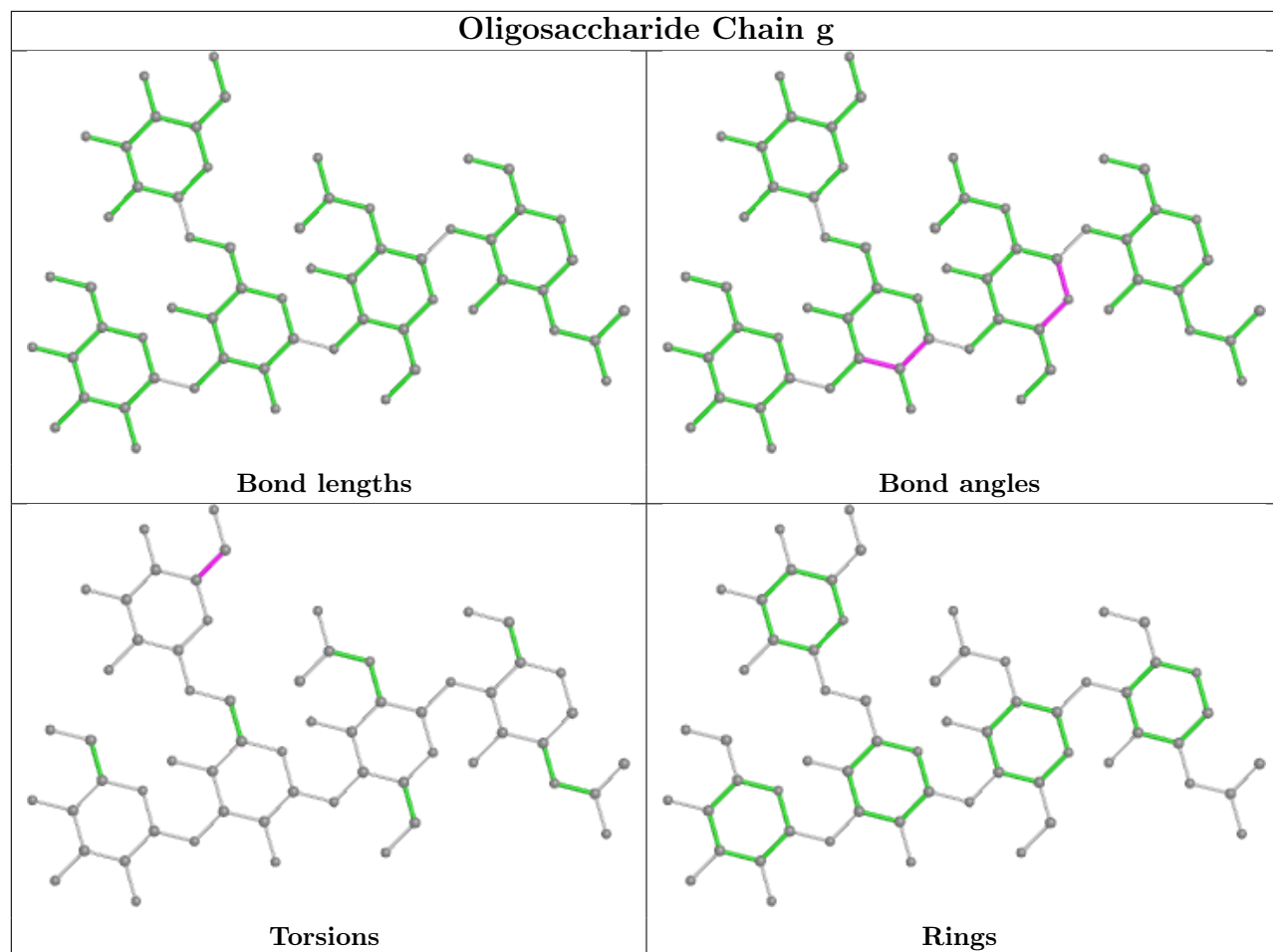


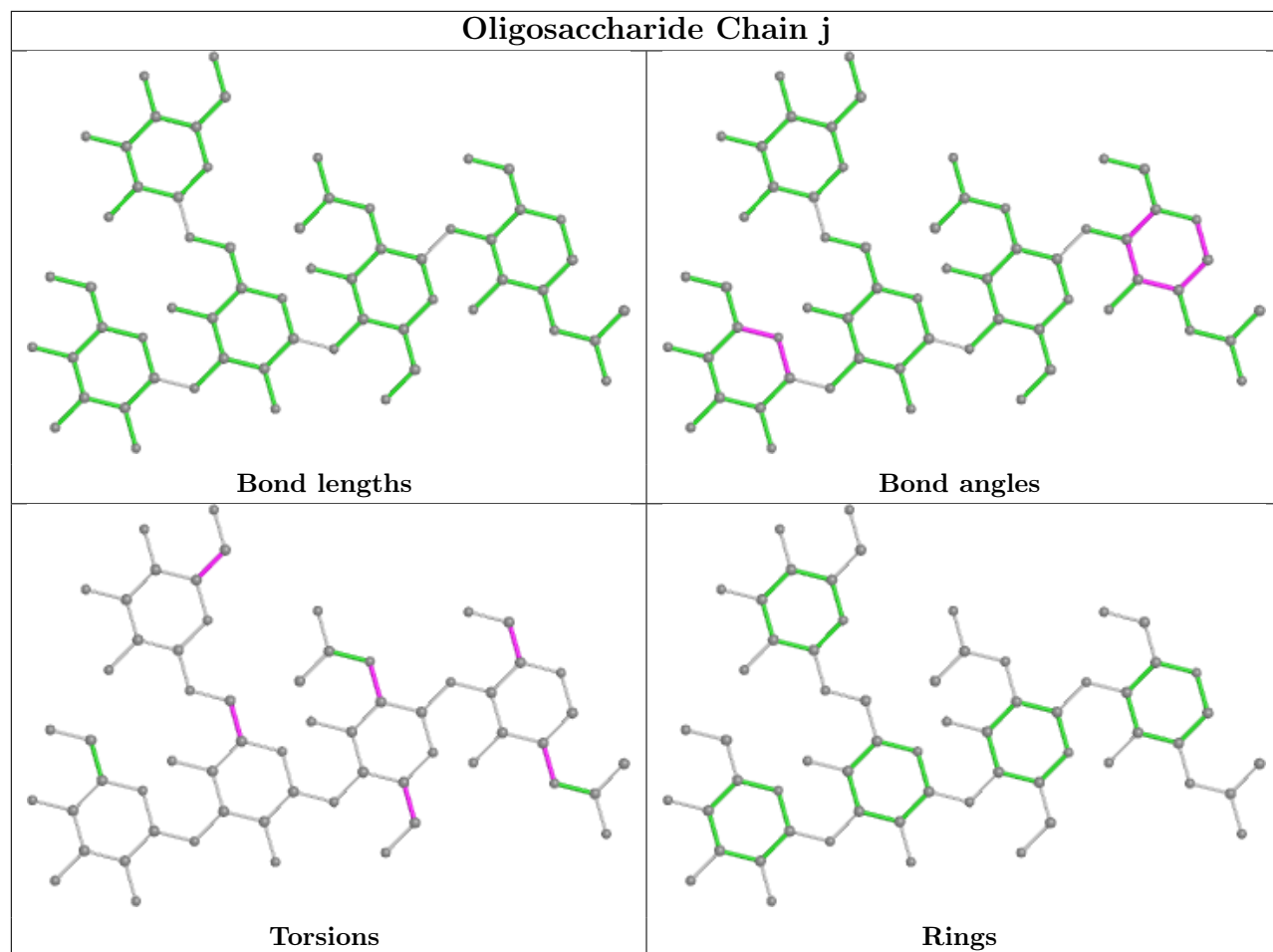


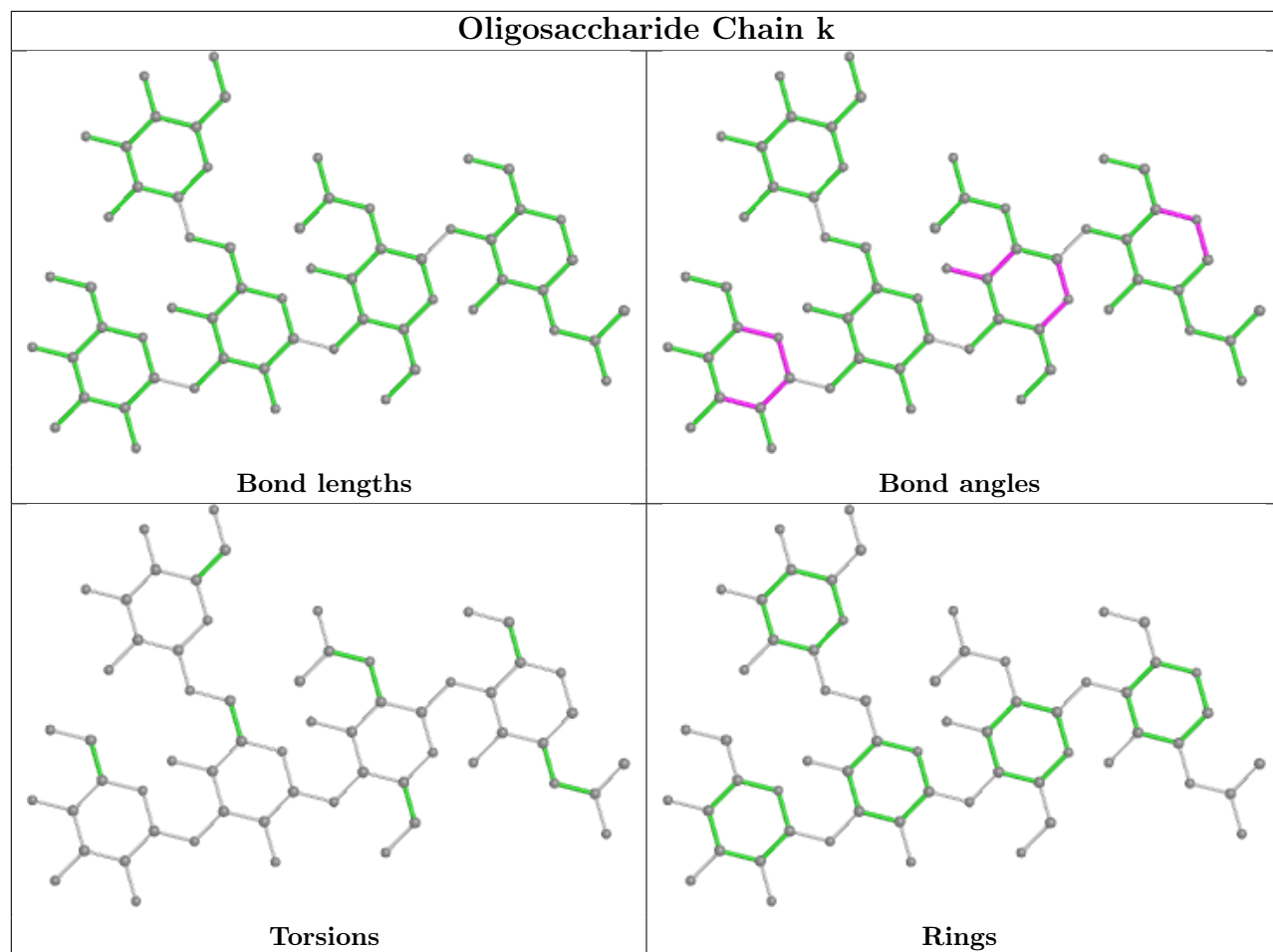


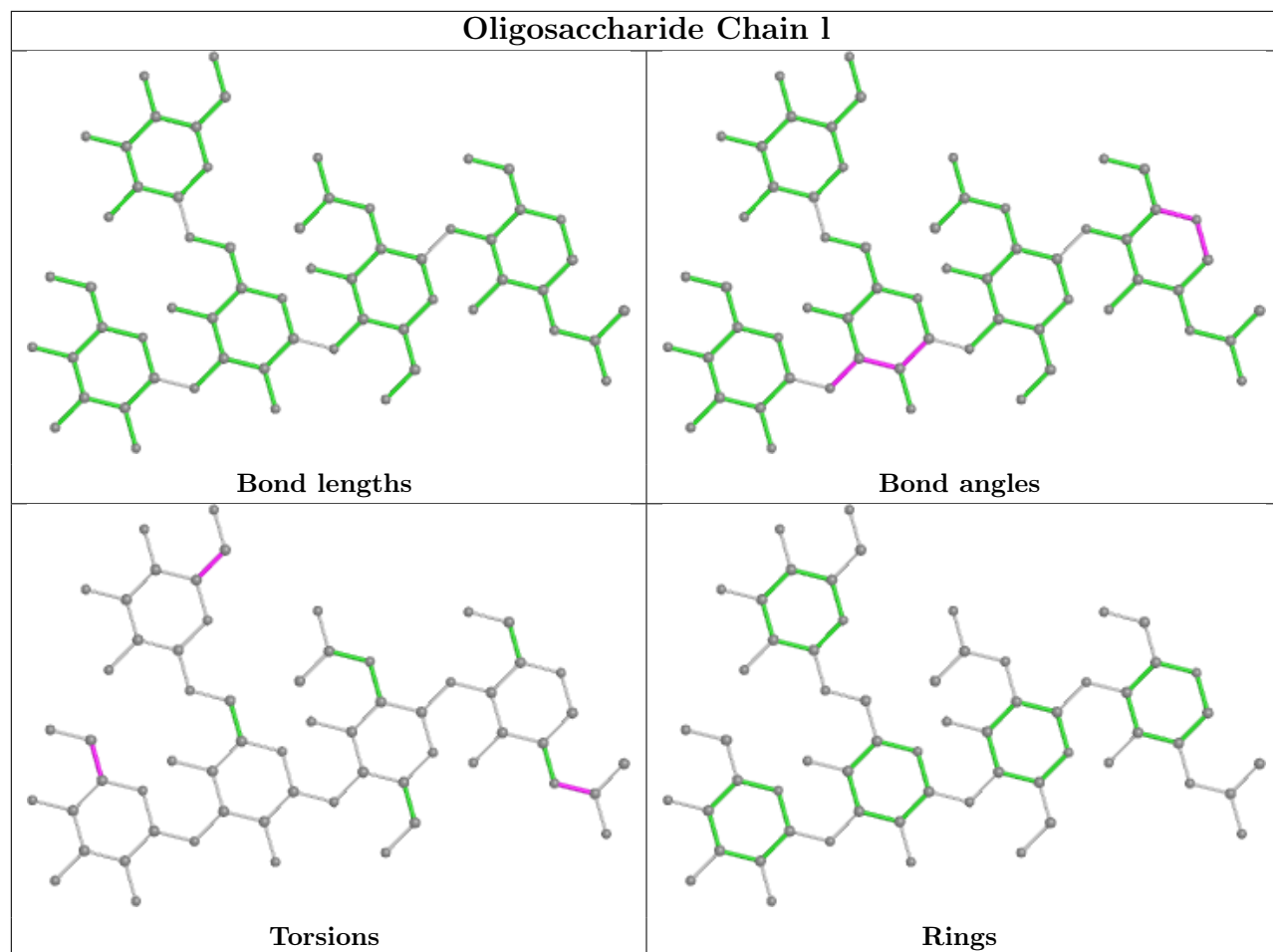


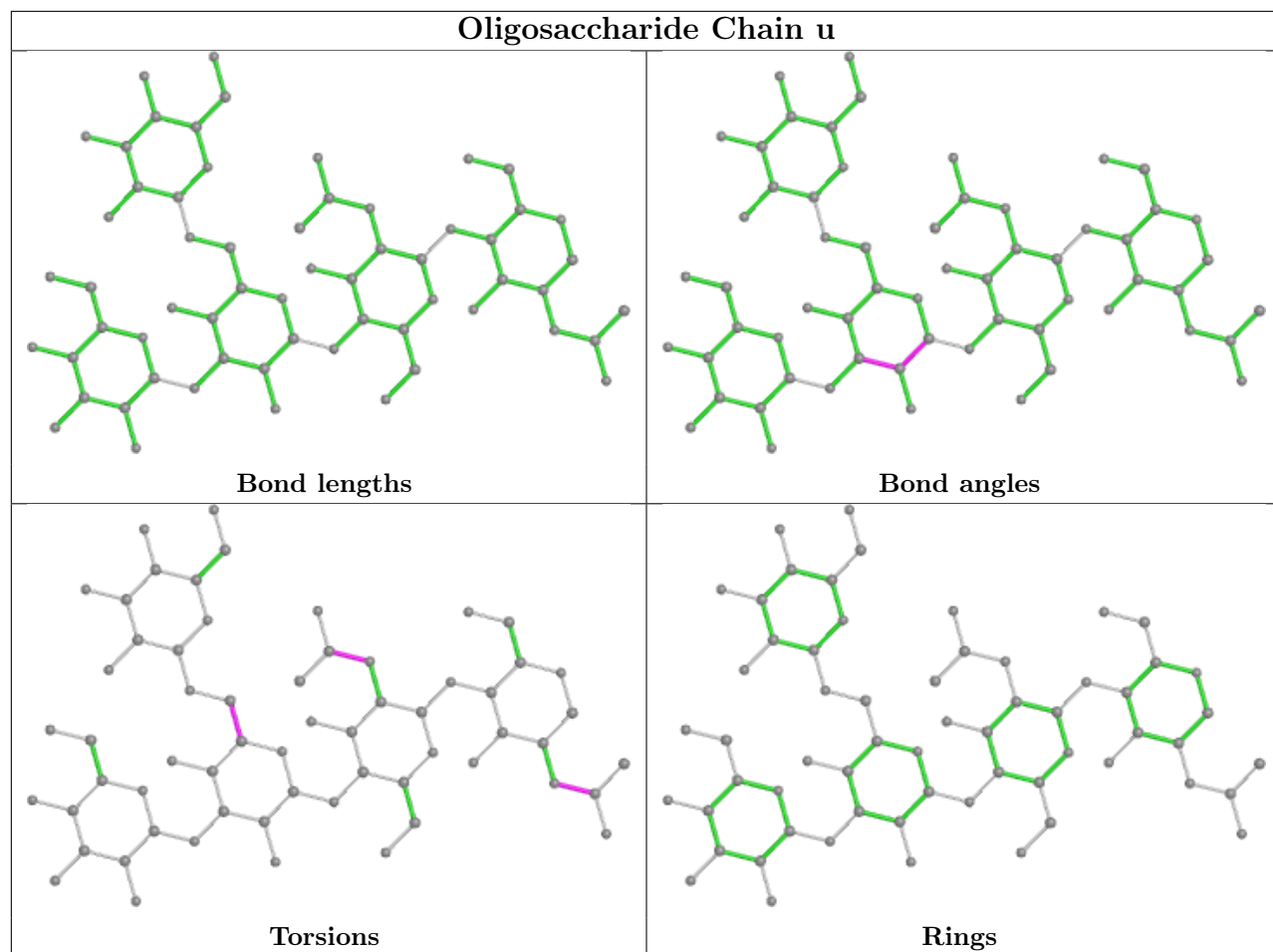


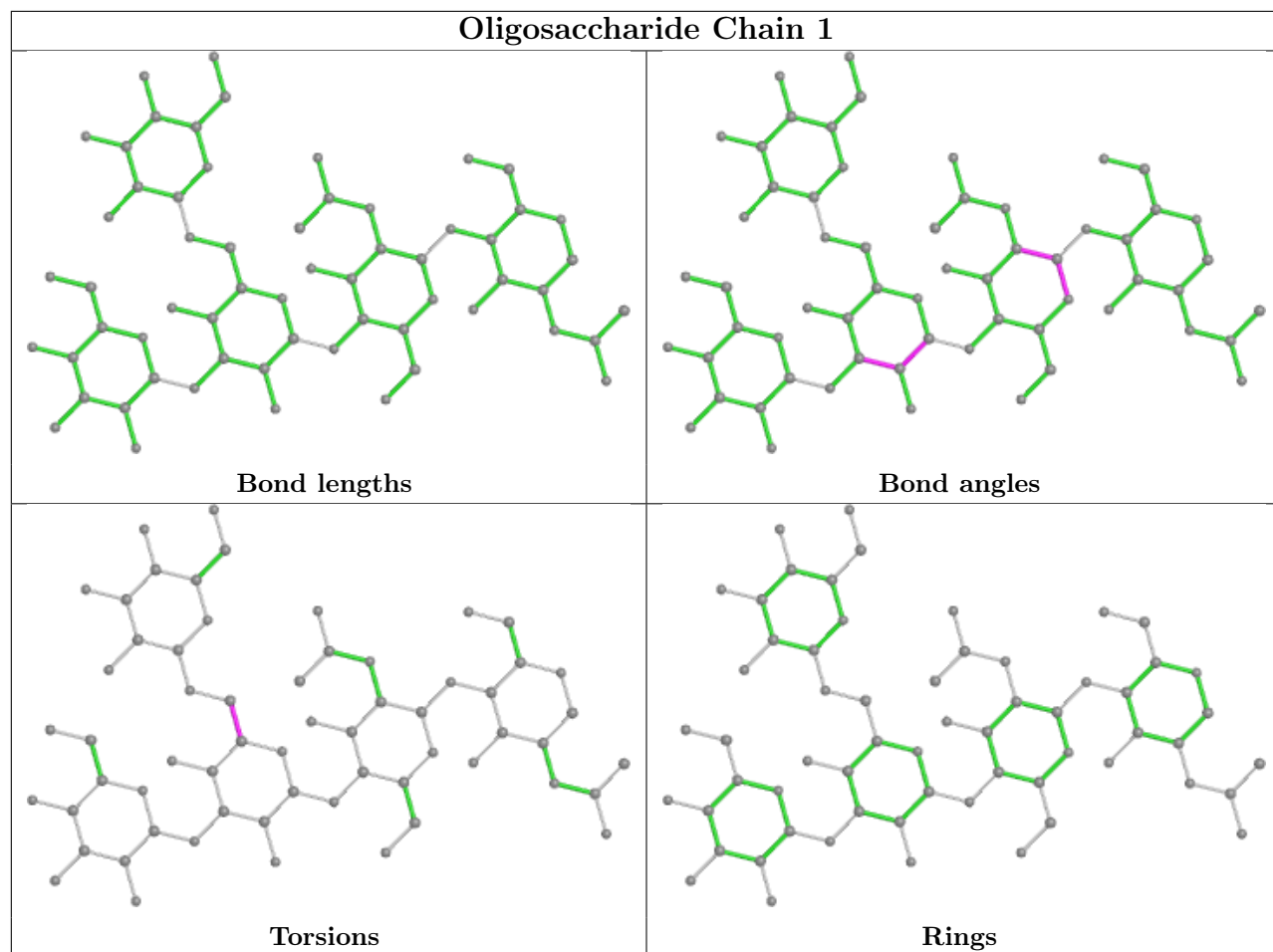


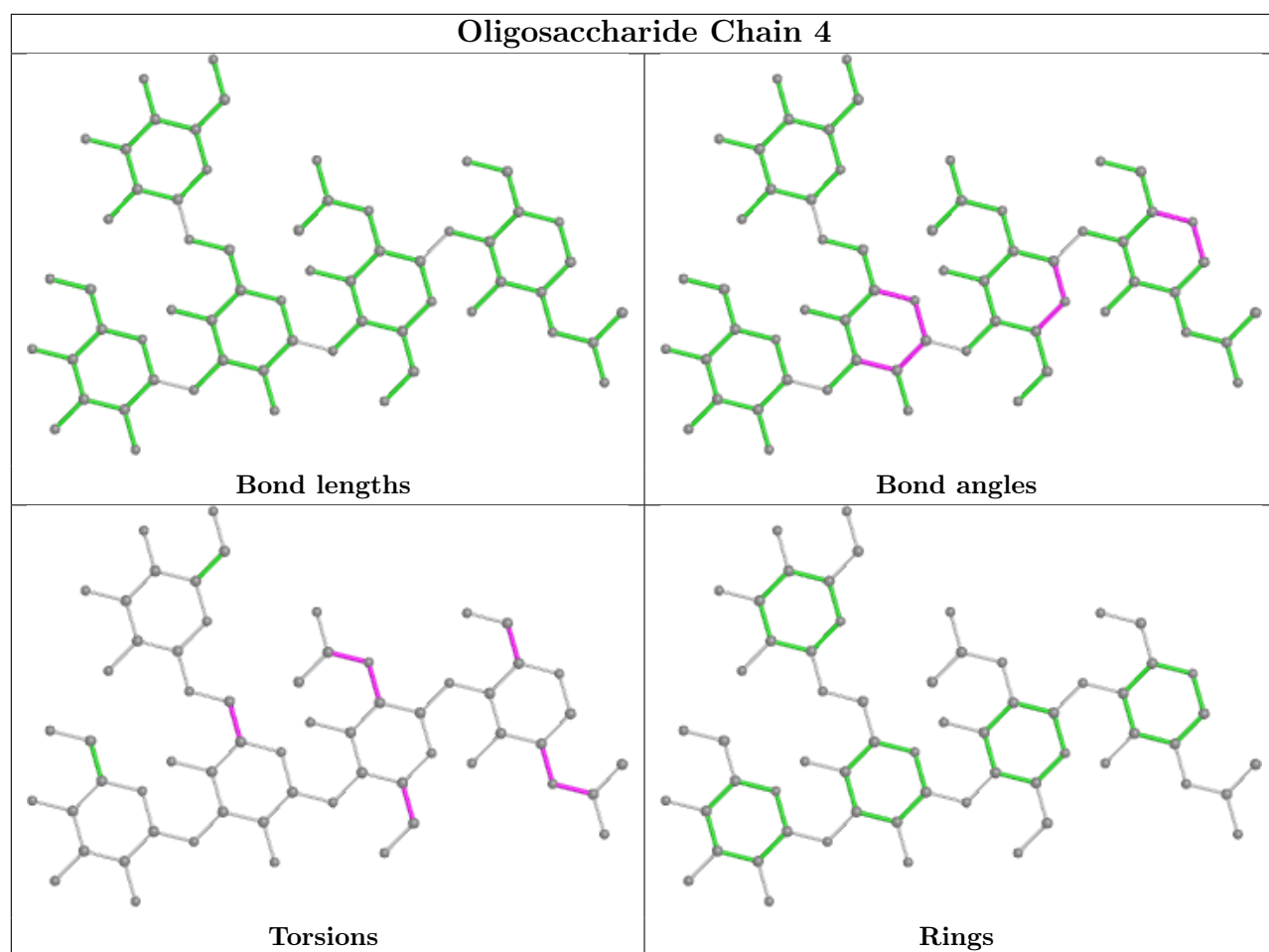


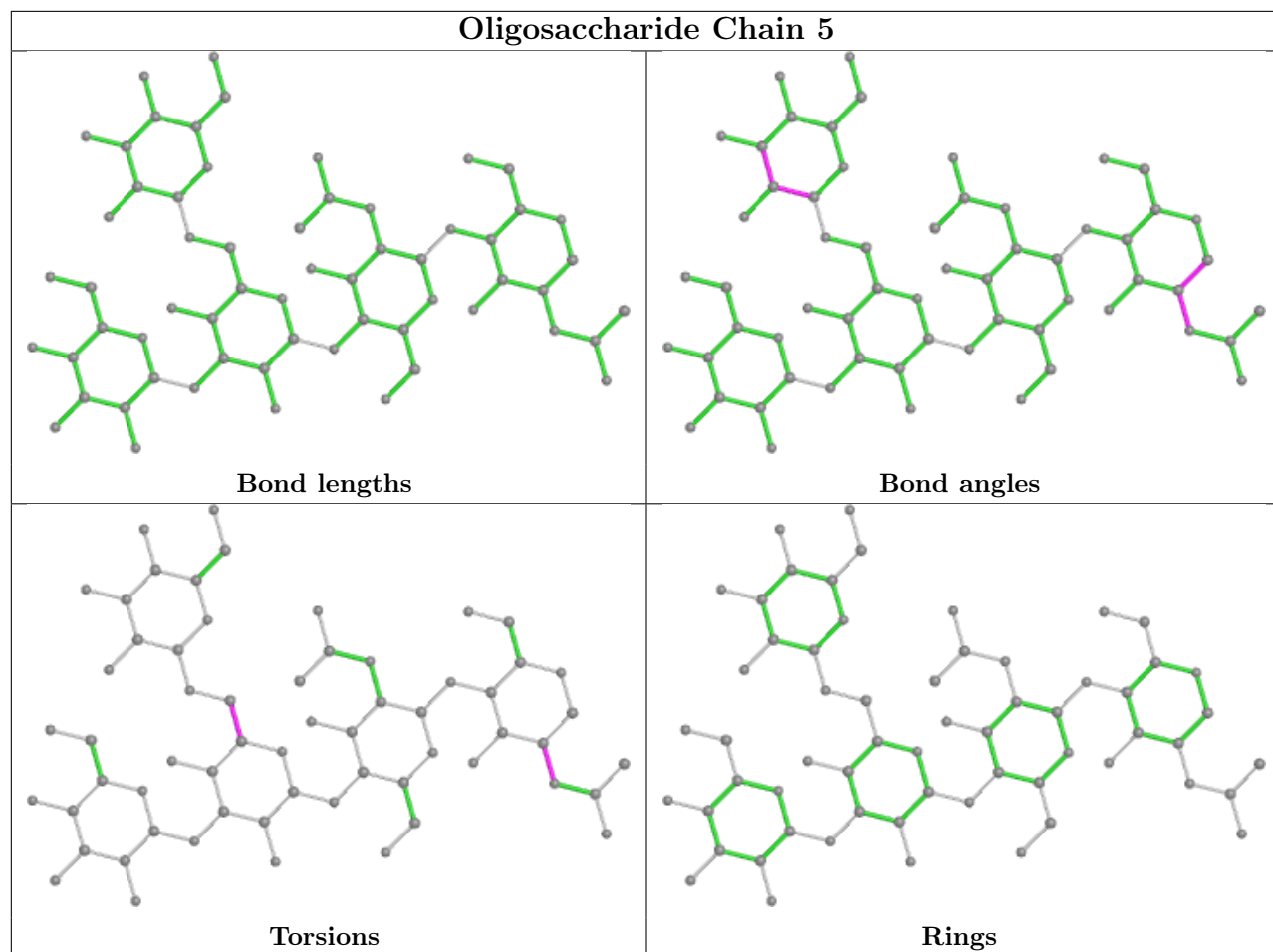


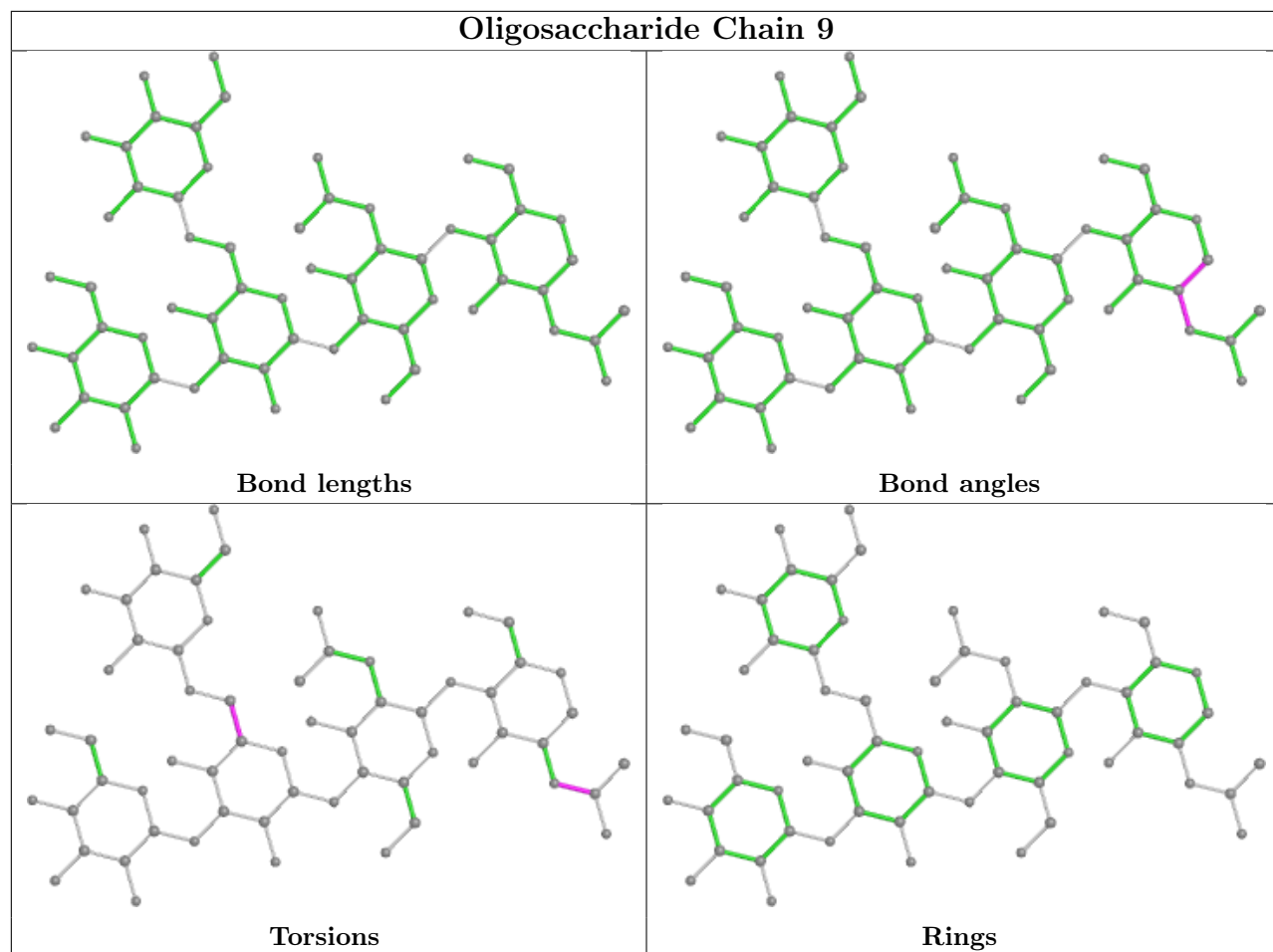


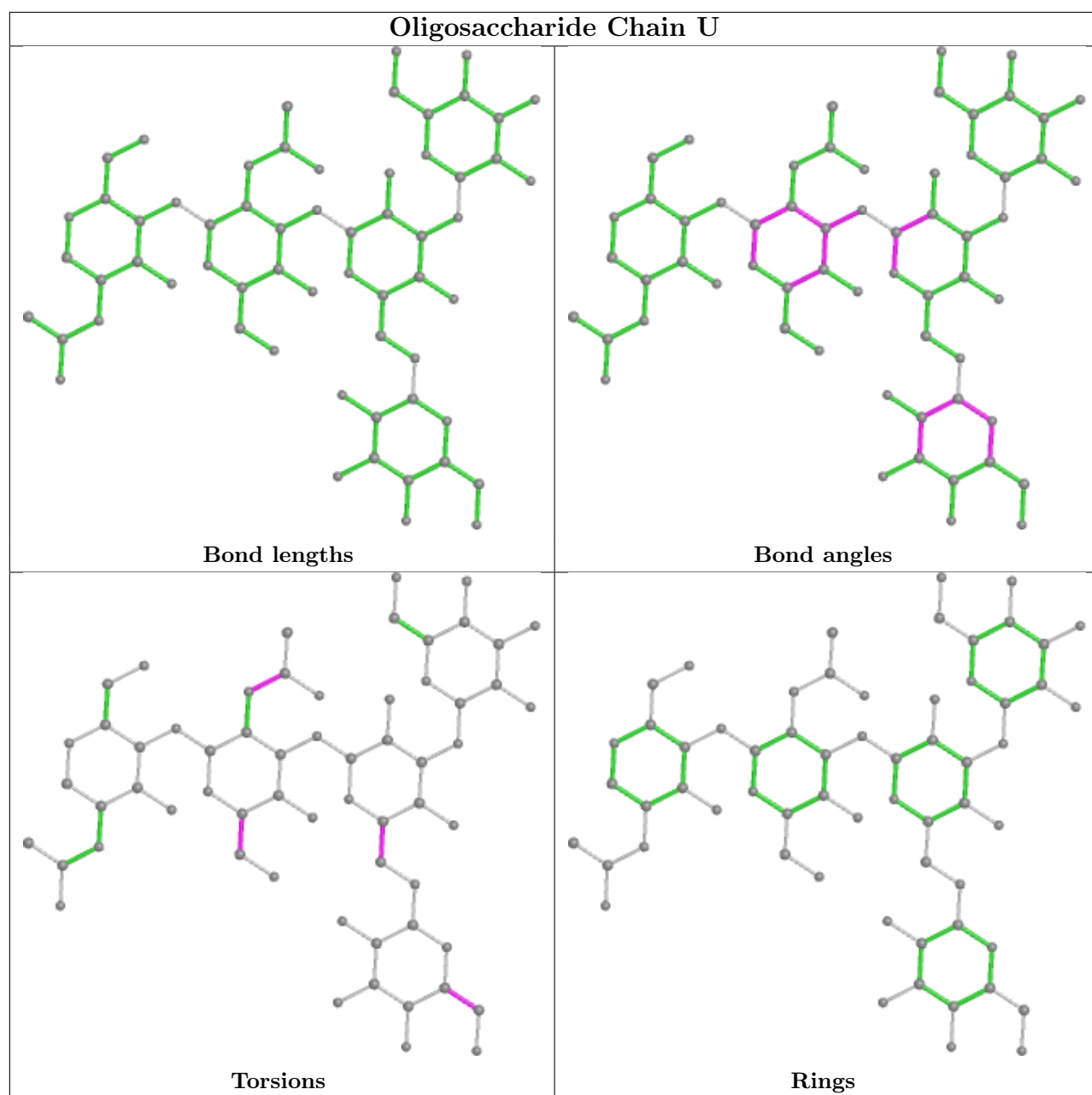


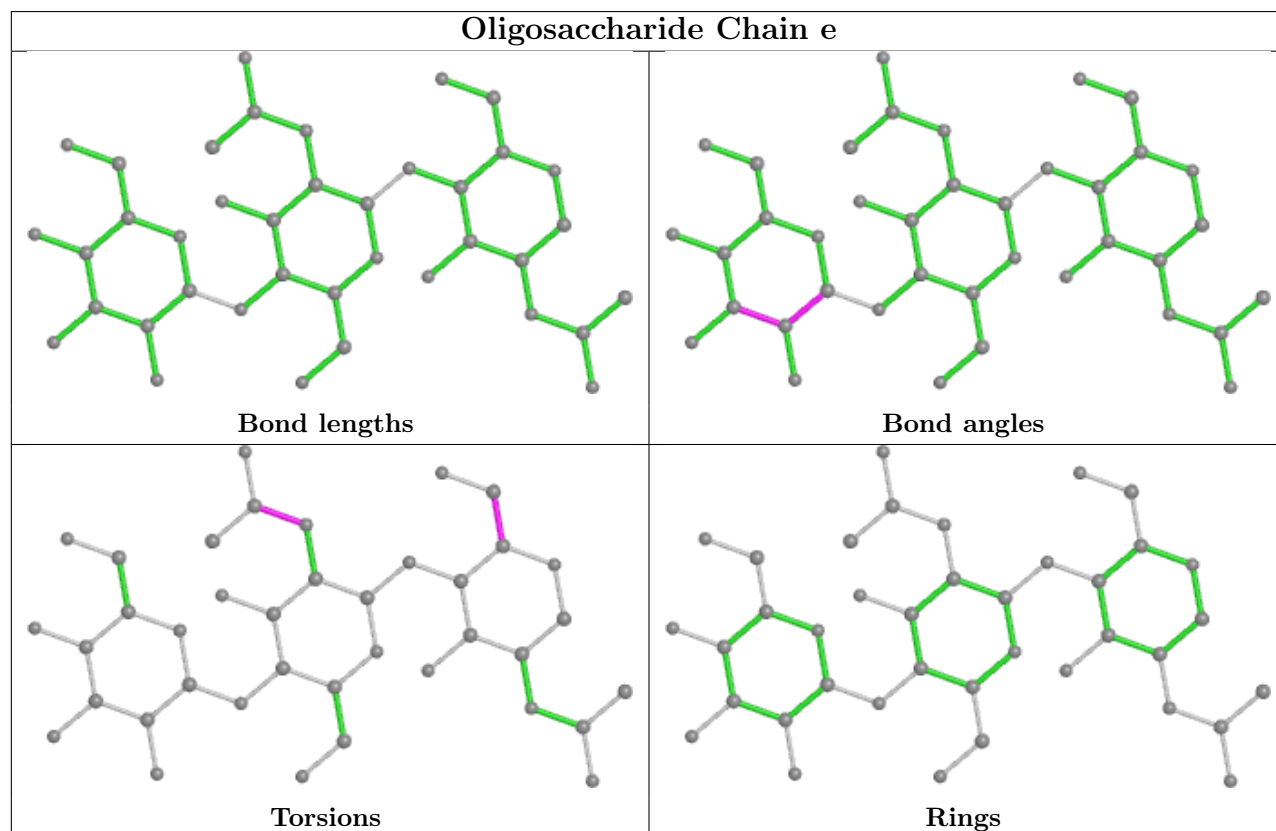
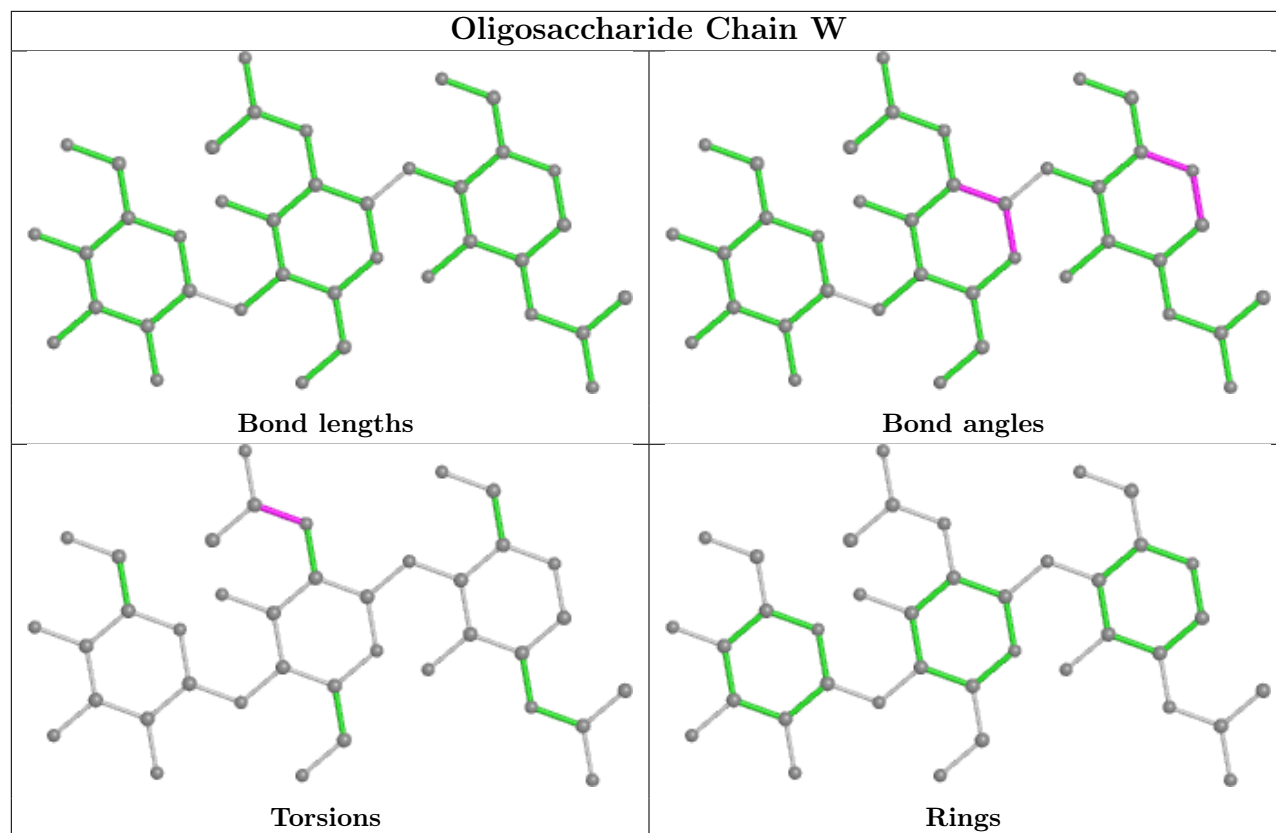


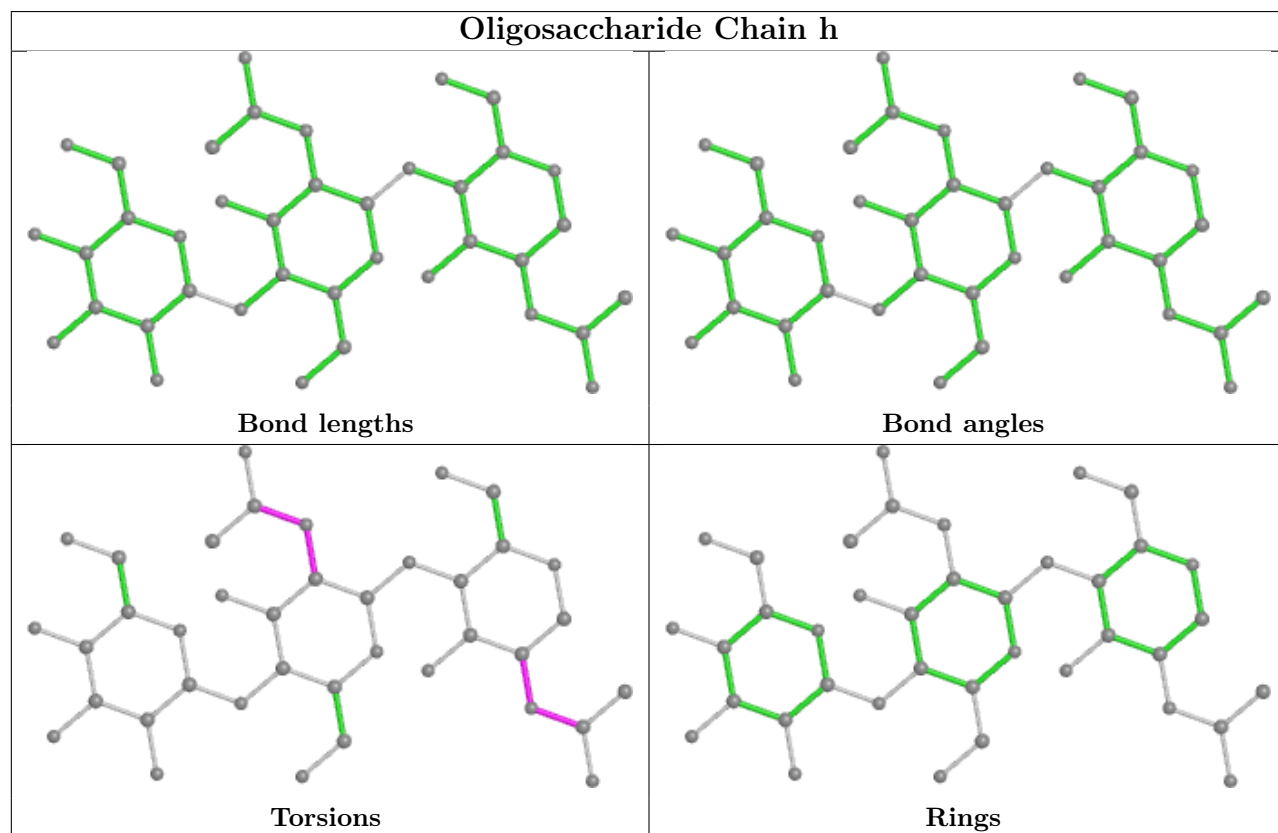
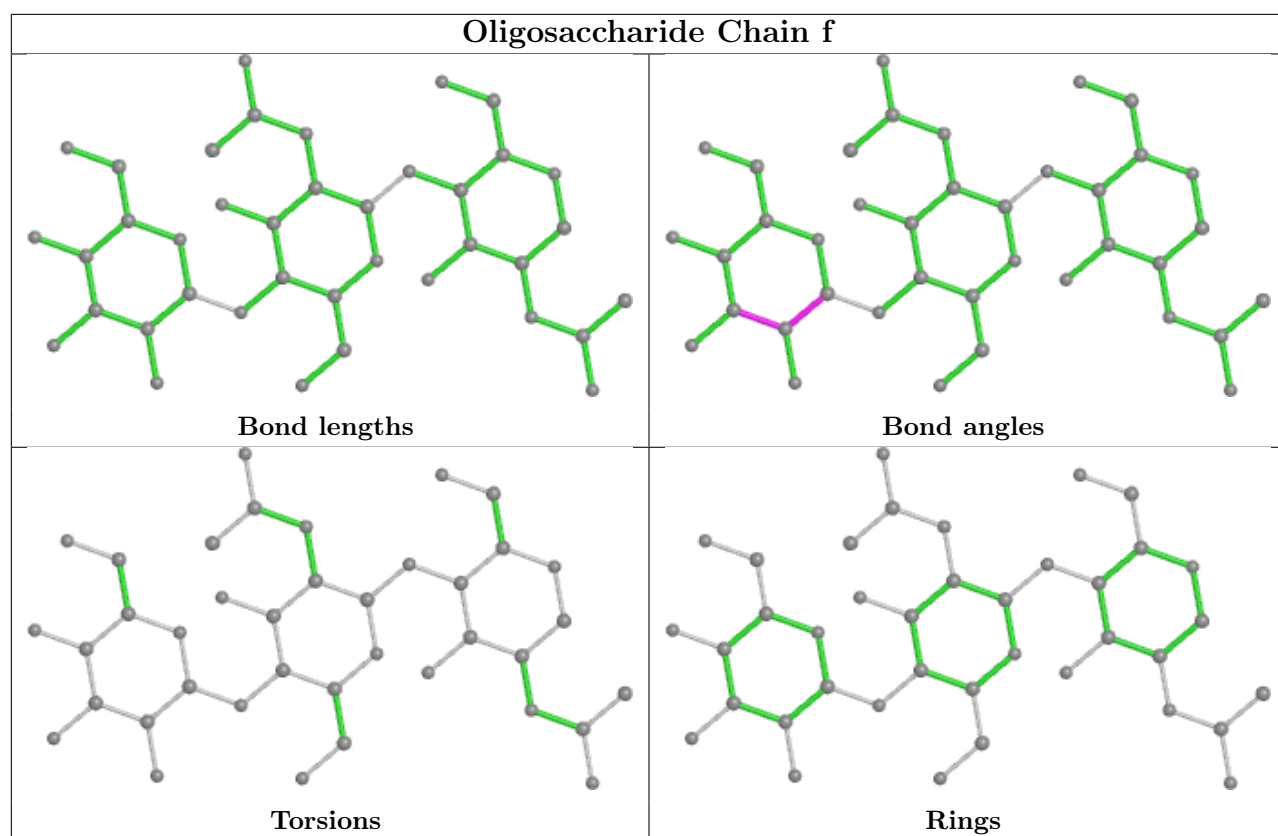


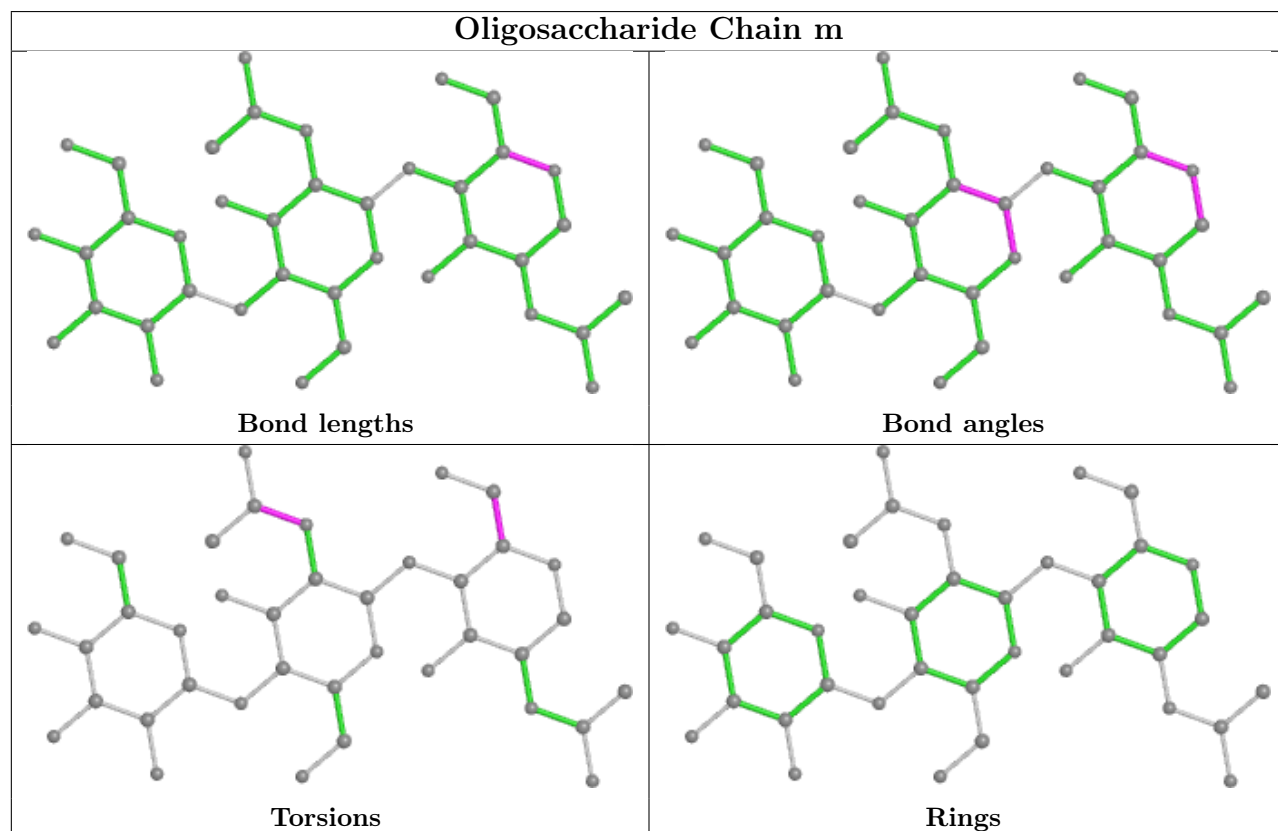
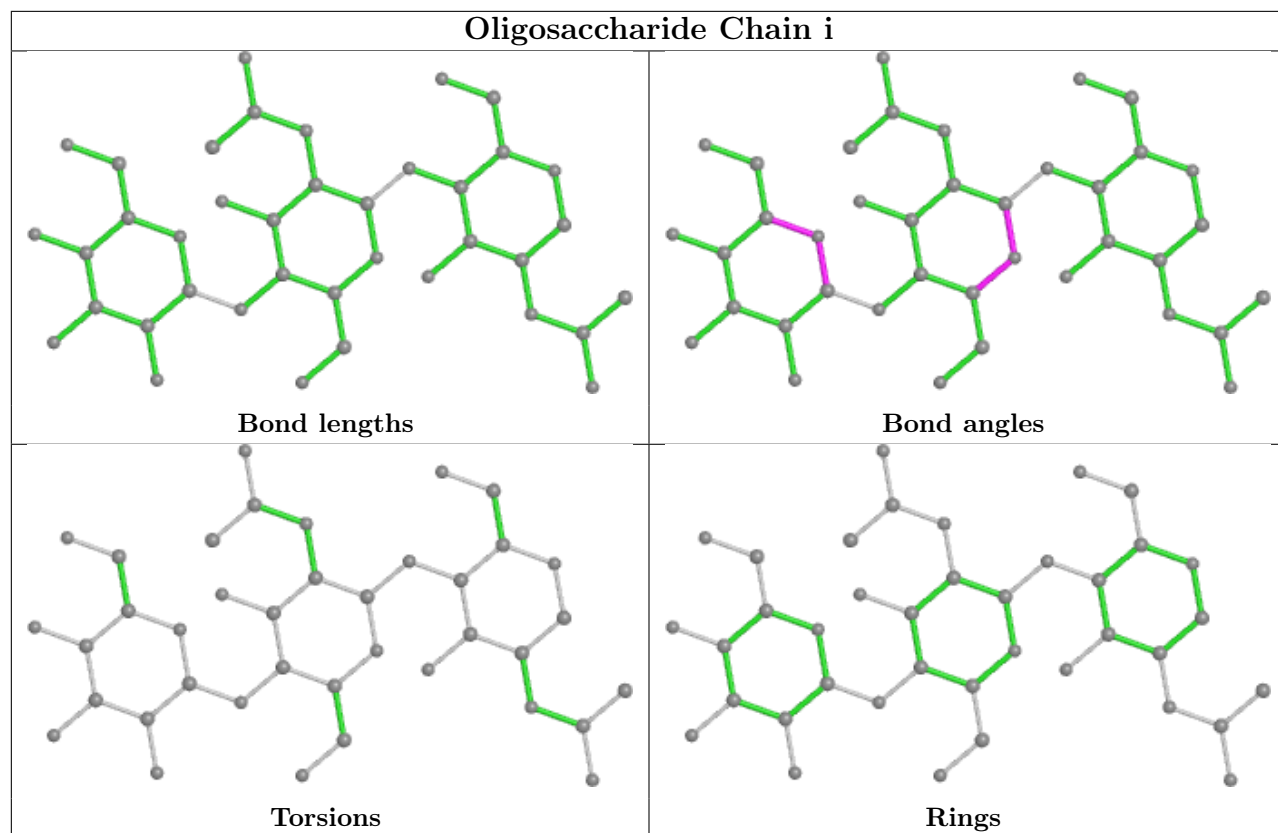


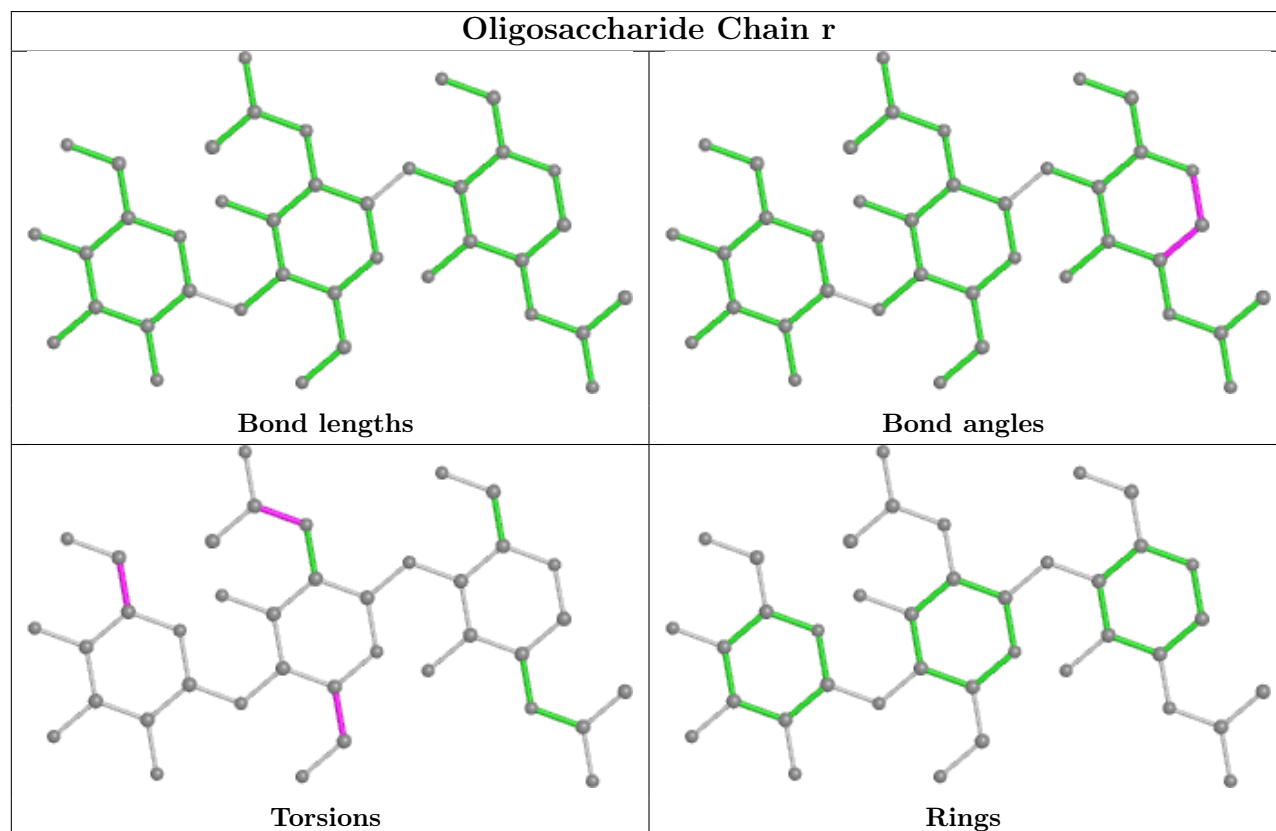
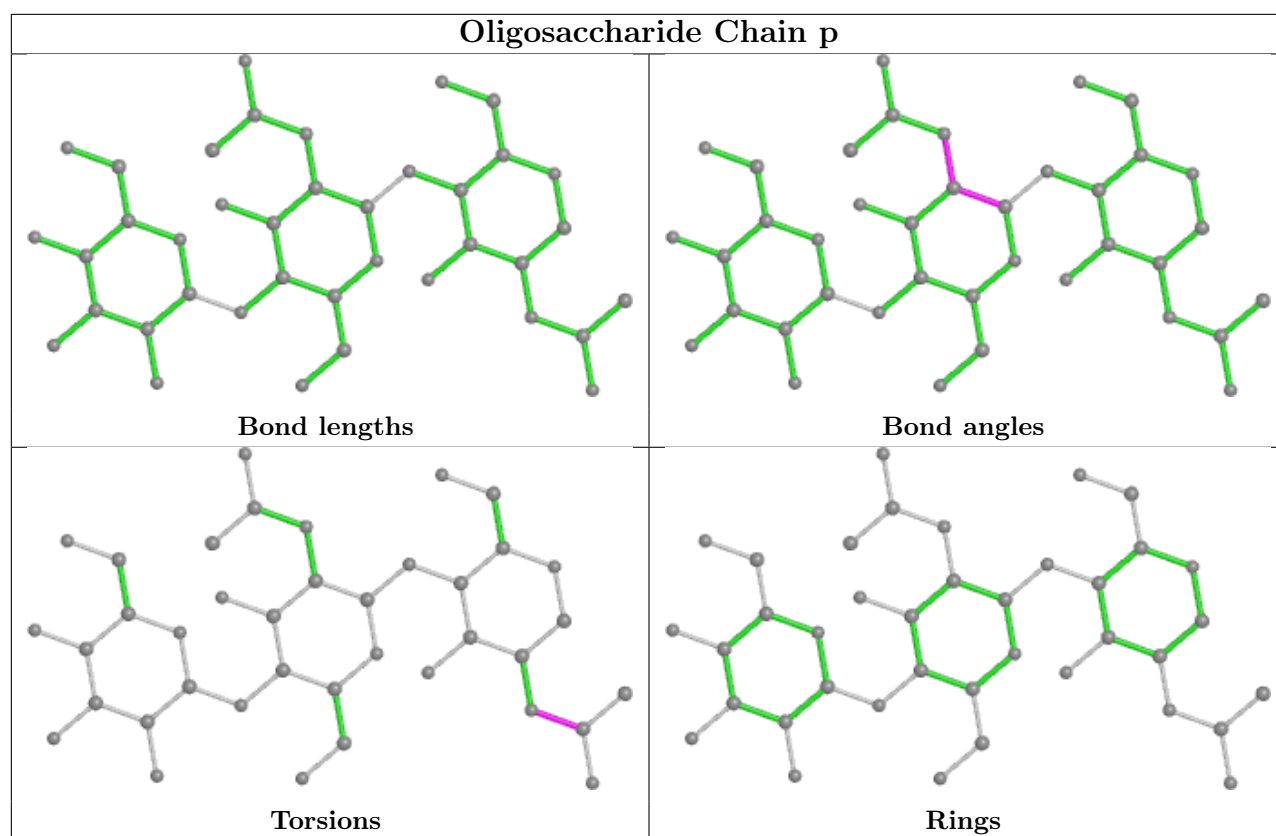


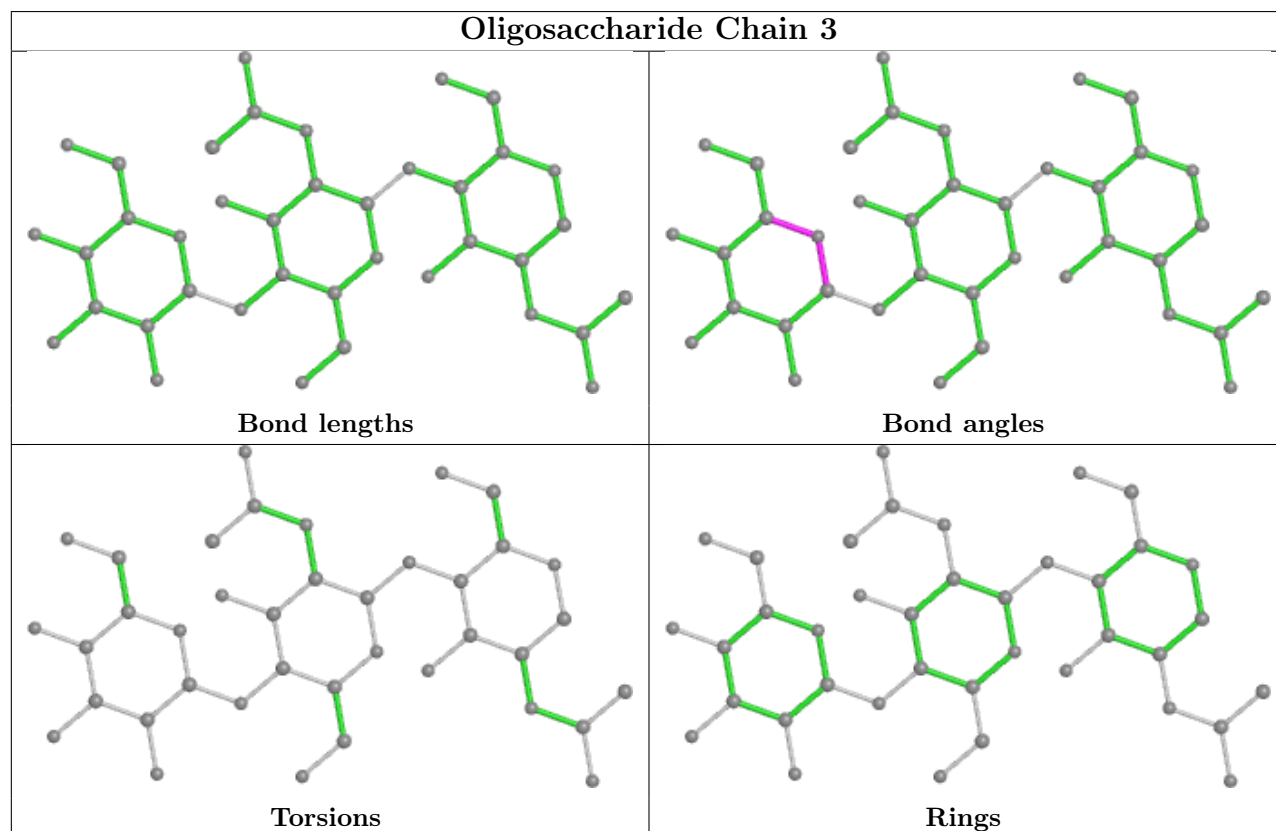
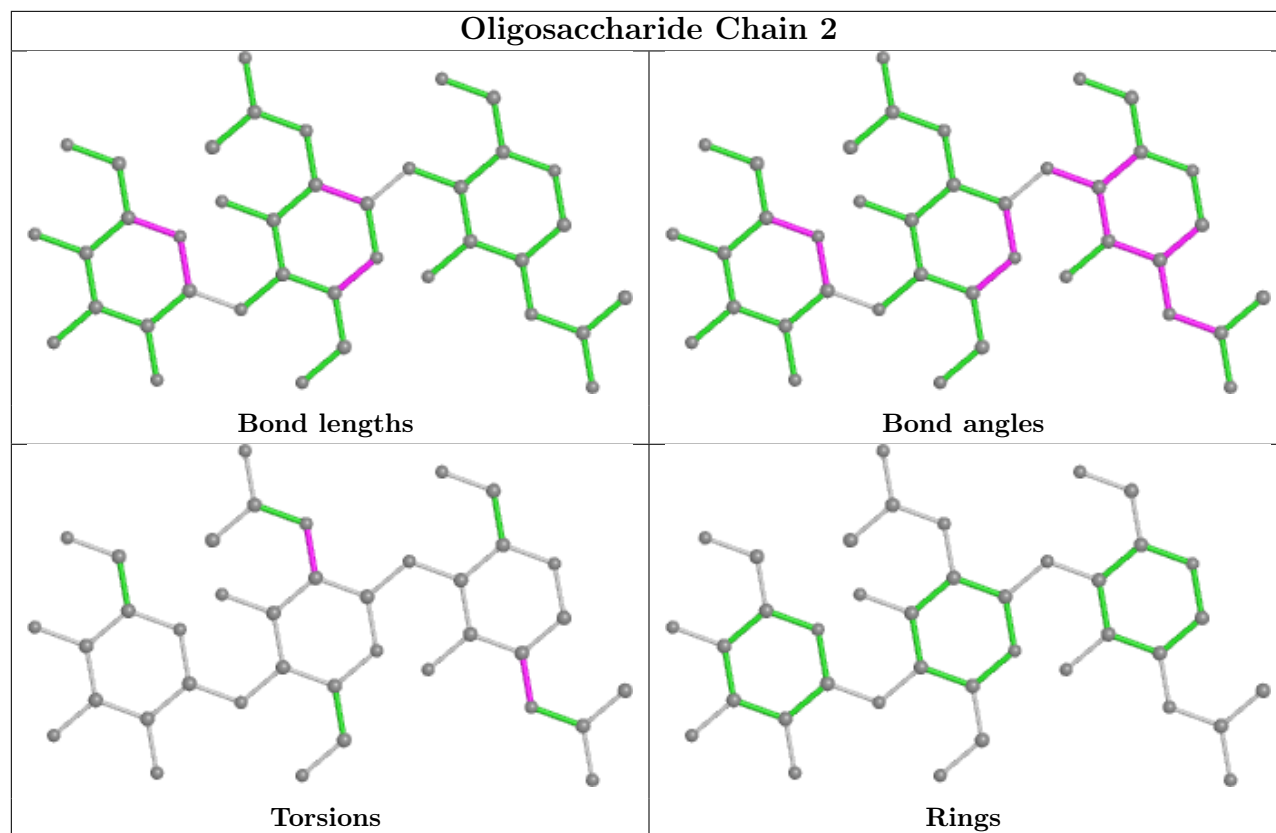


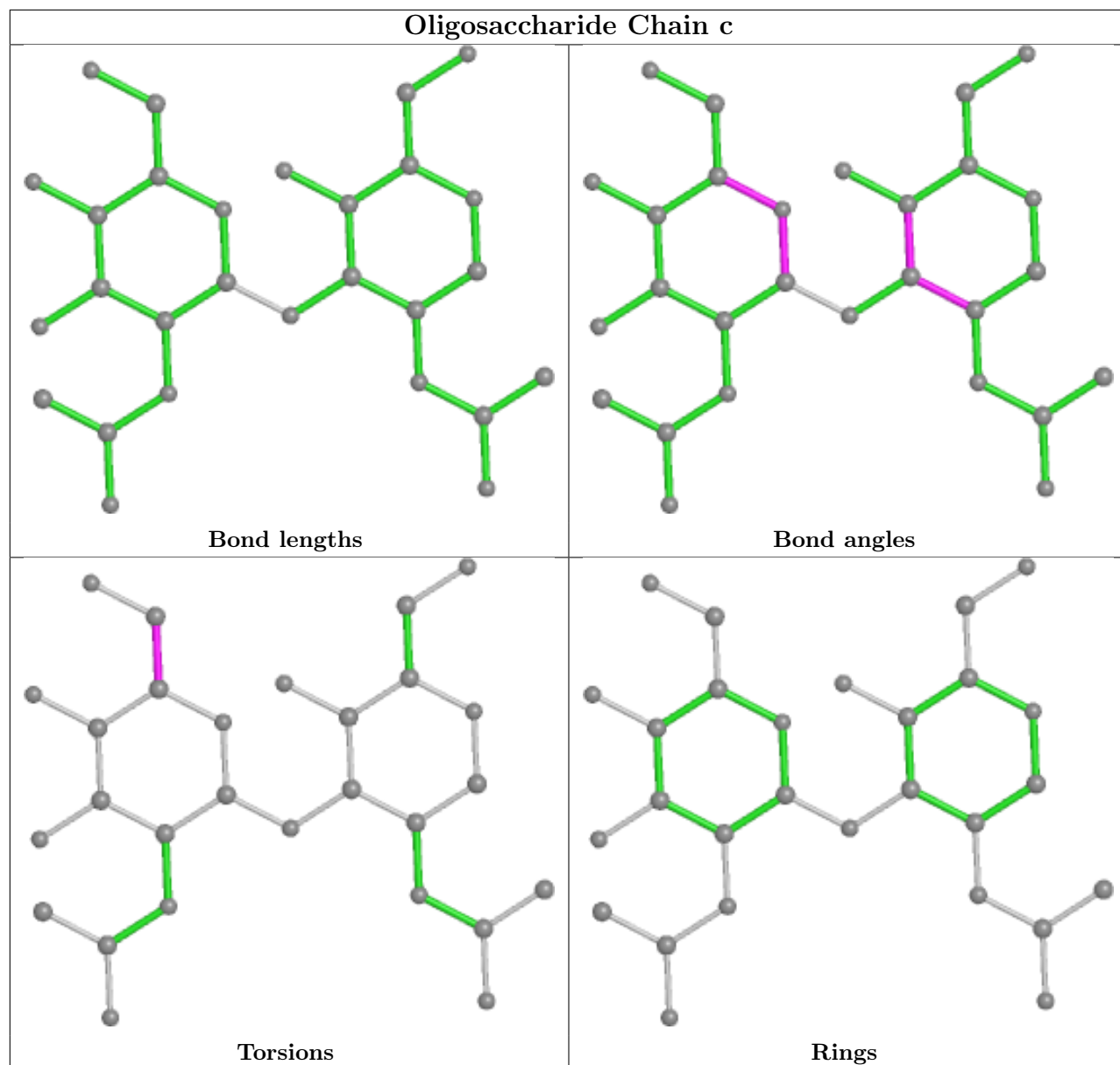


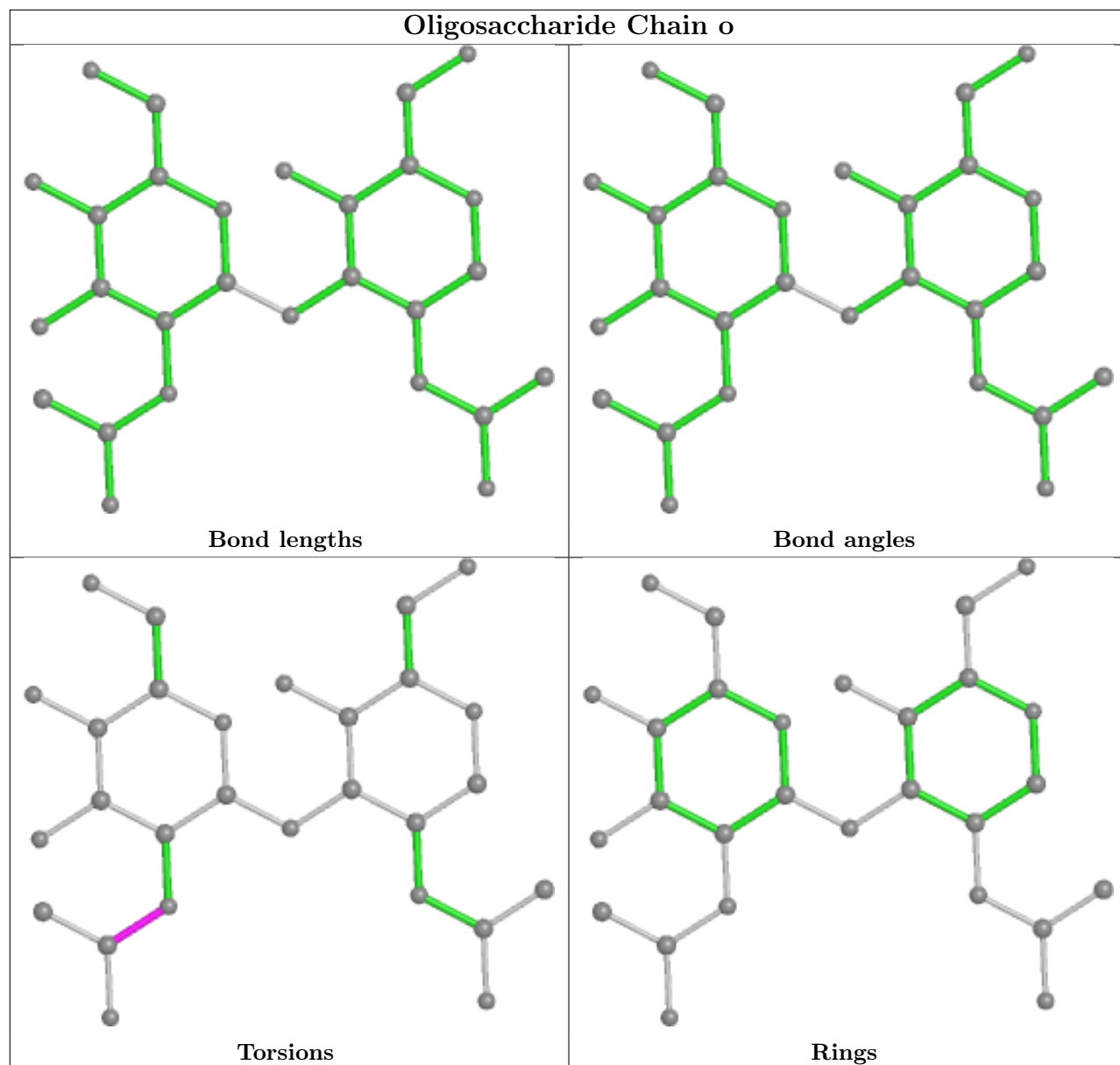


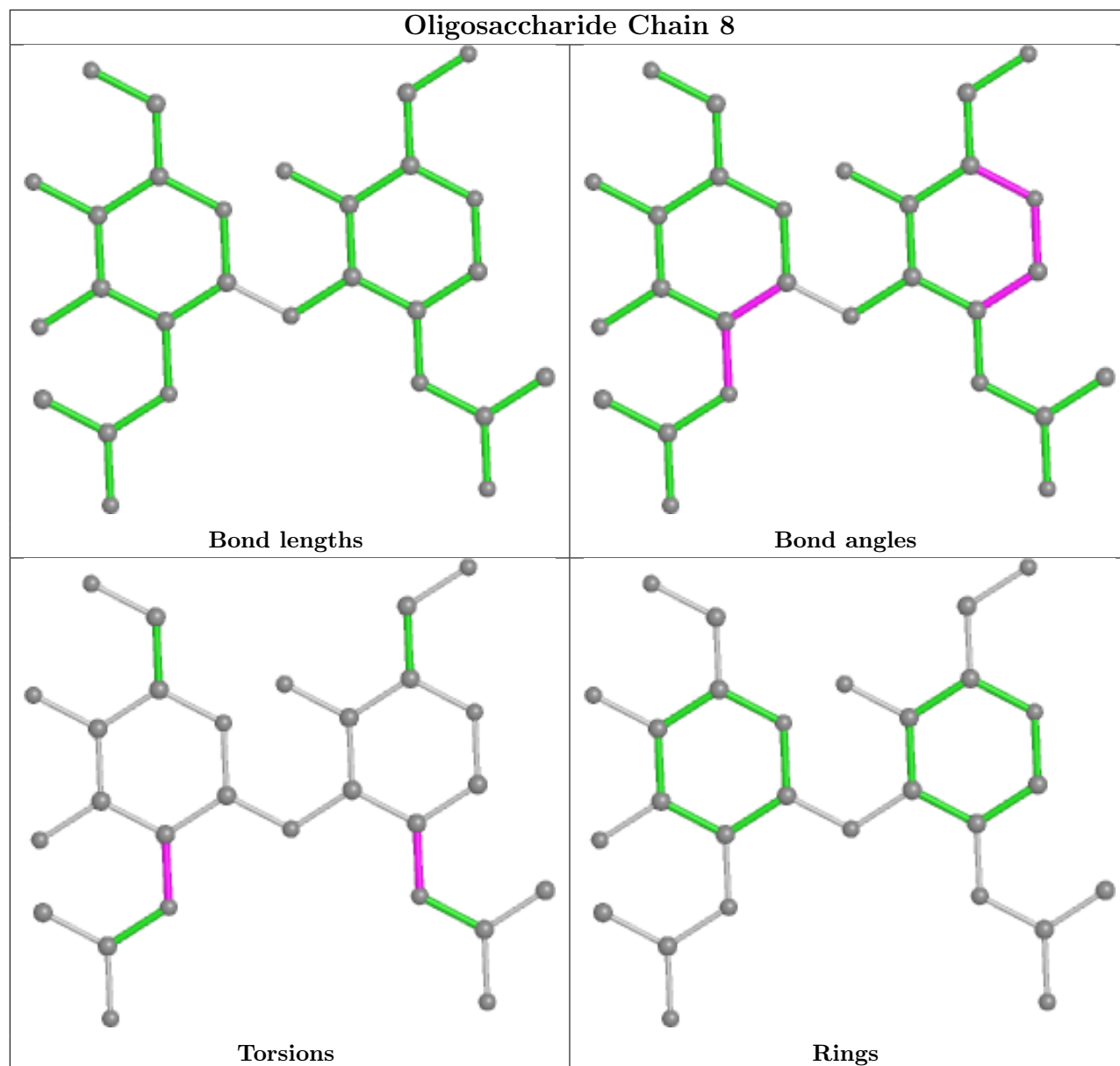


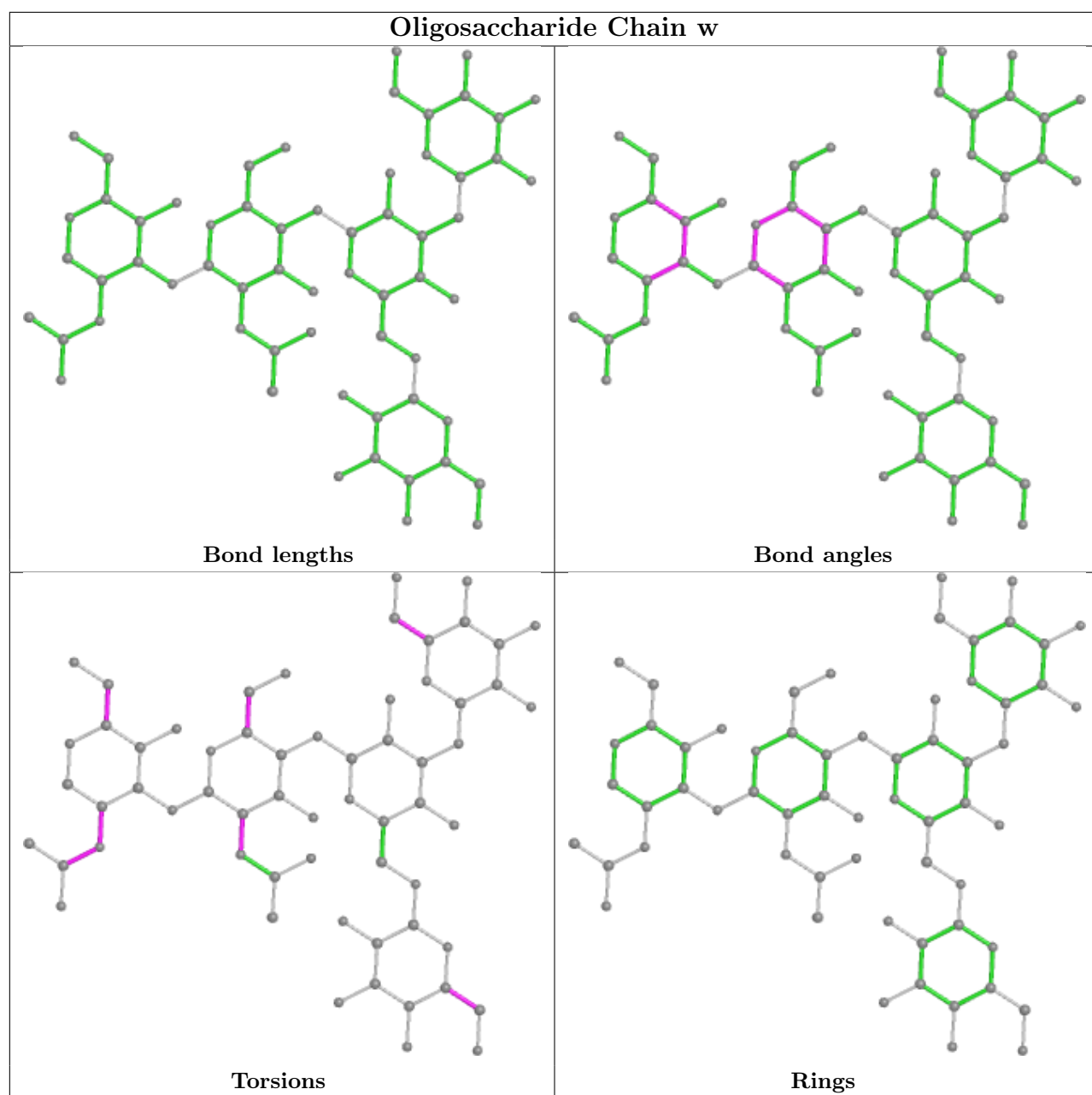


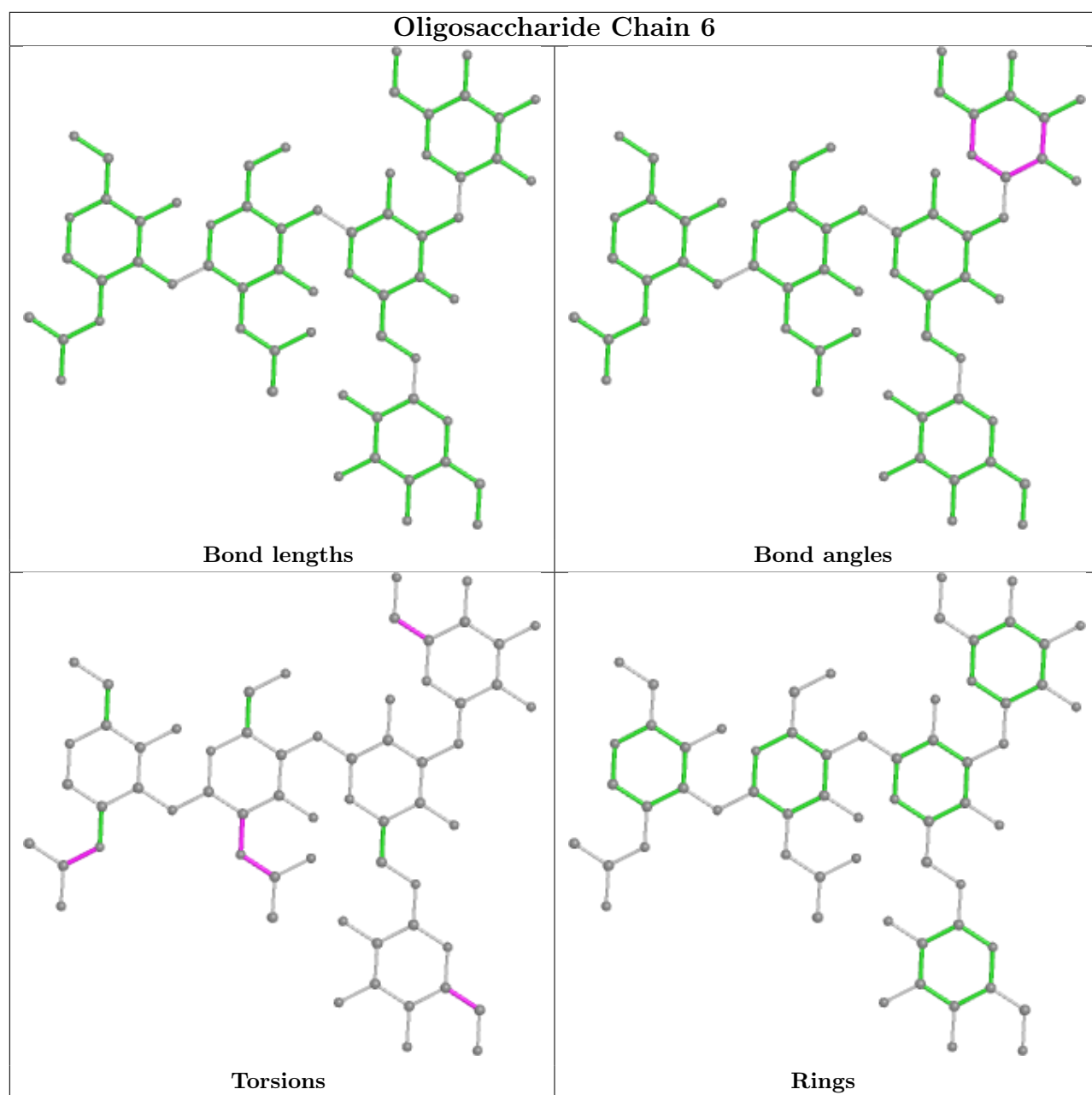


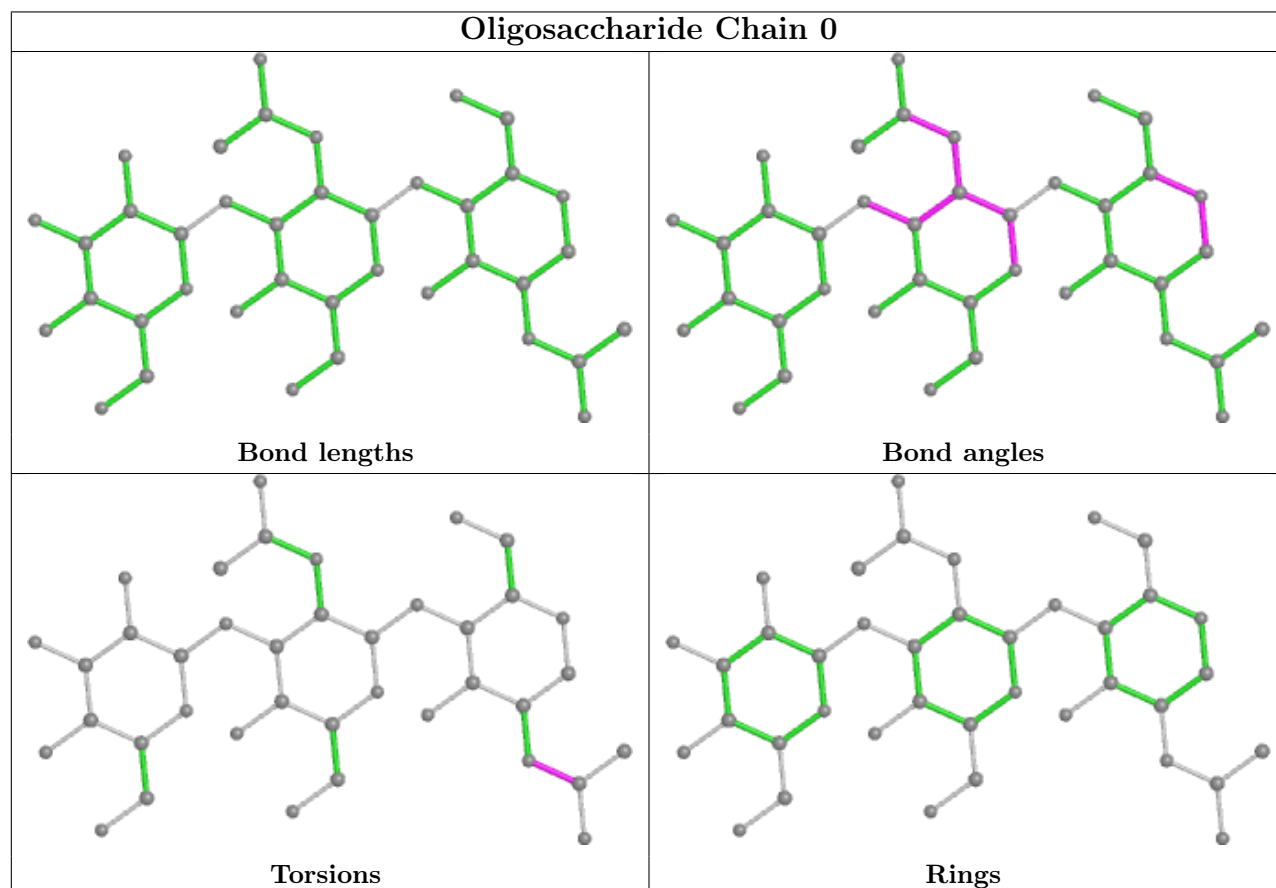
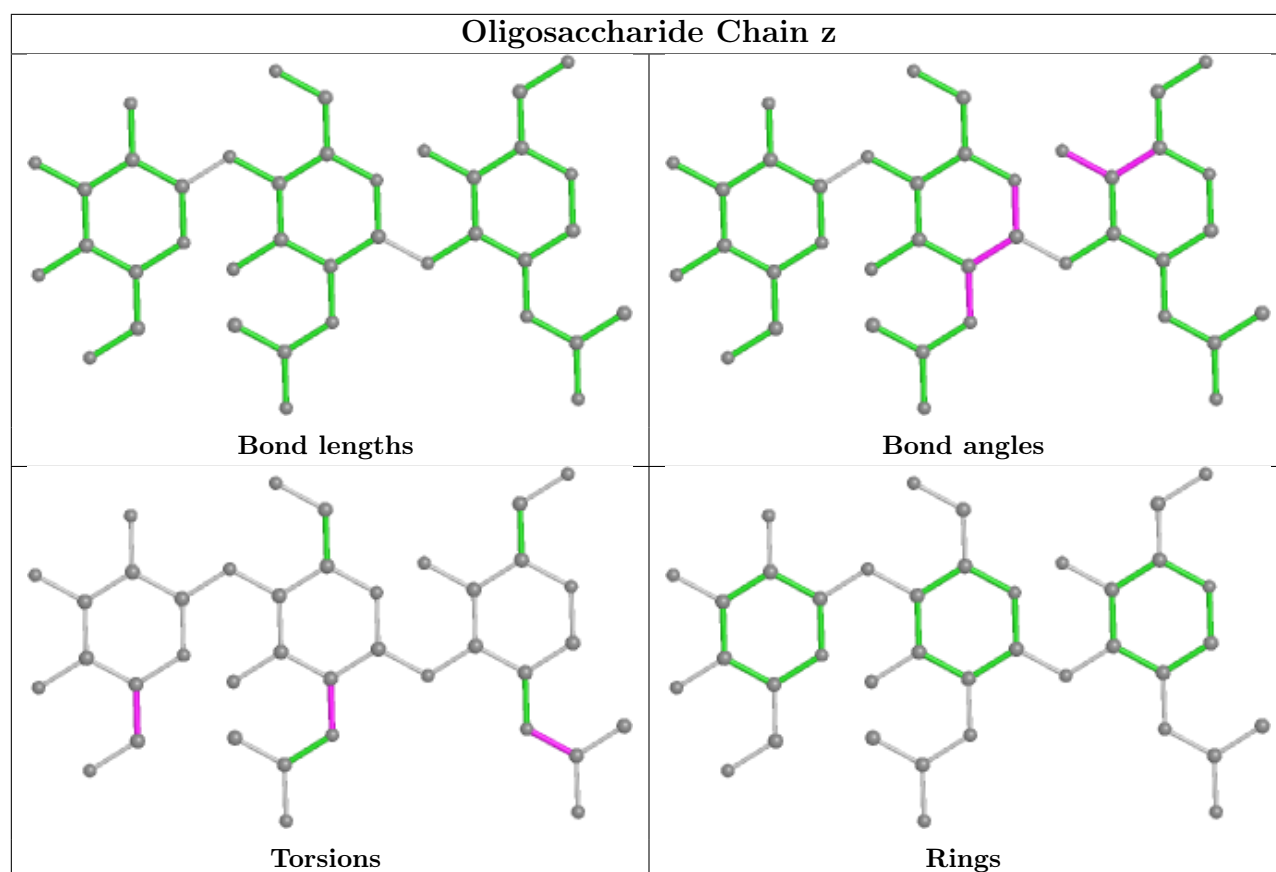


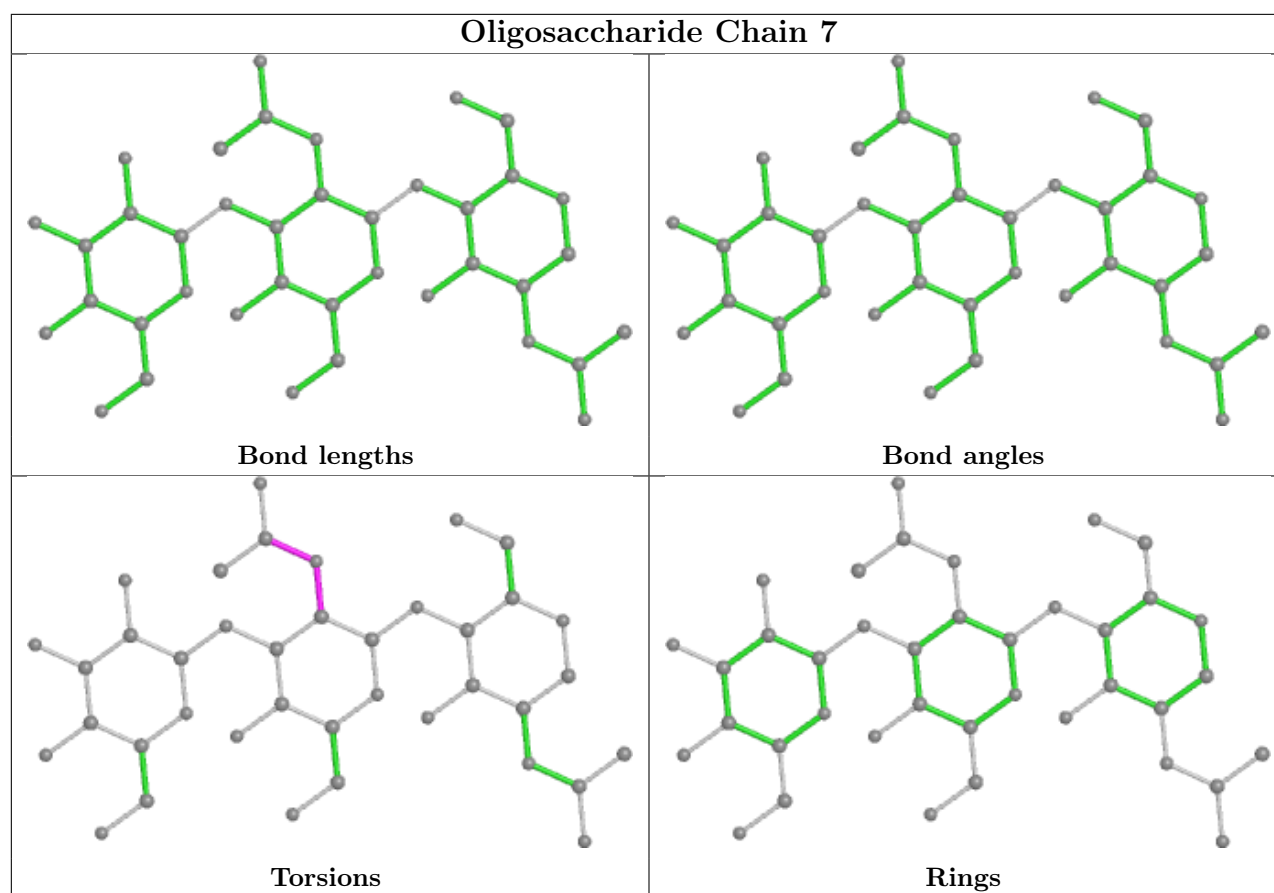












5.6 Ligand geometry [i](#)

Of 136 ligands modelled in this entry, 90 are monoatomic - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	NAG	A	4703	1	14,14,15	0.39	0	17,19,21	0.42	0
17	NAG	B	4704	1	14,14,15	0.90	0	17,19,21	0.98	0
18	A2G	B	4715	1	14,14,15	0.45	0	17,19,21	0.68	0
17	NAG	A	4702	1	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
18	A2G	B	4712	1	14,14,15	0.46	0	17,19,21	1.41	4 (23%)
17	NAG	B	4708	1	14,14,15	0.50	0	17,19,21	1.01	1 (5%)
18	A2G	A	4719	1	14,14,15	0.50	0	17,19,21	1.14	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NAG	A	4706	1	14,14,15	0.38	0	17,19,21	0.79	1 (5%)
17	NAG	A	4711	1	14,14,15	0.39	0	17,19,21	1.19	2 (11%)
18	A2G	A	4712	1	14,14,15	0.47	0	17,19,21	1.73	3 (17%)
17	NAG	A	4705	1	14,14,15	0.51	0	17,19,21	2.13	2 (11%)
17	NAG	A	4707	1	14,14,15	0.40	0	17,19,21	1.36	4 (23%)
18	A2G	B	4716	1	14,14,15	0.51	0	17,19,21	1.11	2 (11%)
18	A2G	A	4720	1	14,14,15	0.46	0	17,19,21	0.51	0
18	A2G	A	4718	1	14,14,15	0.52	0	17,19,21	1.56	3 (17%)
17	NAG	B	4707	1	14,14,15	0.46	0	17,19,21	0.93	1 (5%)
17	NAG	B	4710	1	14,14,15	0.43	0	17,19,21	0.80	0
18	A2G	A	4713	1	14,14,15	0.56	0	17,19,21	0.58	0
17	NAG	B	4703	1	14,14,15	0.40	0	17,19,21	0.41	0
17	NAG	A	4708	1	14,14,15	0.41	0	17,19,21	0.31	0
17	NAG	A	4701	1	14,14,15	0.41	0	17,19,21	0.65	0
18	A2G	A	4716	1	14,14,15	0.99	1 (7%)	17,19,21	1.33	2 (11%)
18	A2G	B	4723	1	14,14,15	0.53	0	17,19,21	0.99	1 (5%)
17	NAG	A	4704	1	14,14,15	0.53	0	17,19,21	1.13	1 (5%)
17	NAG	B	4702	1	14,14,15	0.40	0	17,19,21	0.47	0
17	NAG	B	4701	1	14,14,15	0.40	0	17,19,21	0.63	0
17	NAG	B	4711	1	14,14,15	0.43	0	17,19,21	0.67	0
18	A2G	A	4721	1	14,14,15	0.52	0	17,19,21	1.02	1 (5%)
17	NAG	A	4710	1	14,14,15	0.40	0	17,19,21	0.59	0
18	A2G	A	4723	1	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
18	A2G	B	4722	1	14,14,15	0.51	0	17,19,21	1.53	3 (17%)
18	A2G	B	4719	1	14,14,15	0.39	0	17,19,21	1.07	1 (5%)
17	NAG	B	4706	1	14,14,15	0.40	0	17,19,21	0.39	0
18	A2G	B	4713	1	14,14,15	0.52	0	17,19,21	0.65	0
18	A2G	A	4714	1	14,14,15	0.48	0	17,19,21	0.91	1 (5%)
18	A2G	A	4715	1	14,14,15	0.50	0	17,19,21	1.37	1 (5%)
17	NAG	B	4705	1	14,14,15	0.40	0	17,19,21	0.69	0
18	A2G	B	4714	1	14,14,15	0.89	1 (7%)	17,19,21	0.86	1 (5%)
18	A2G	B	4718	1	14,14,15	0.50	0	17,19,21	0.88	0
18	A2G	B	4721	1	14,14,15	0.53	0	17,19,21	1.07	2 (11%)
18	A2G	B	4720	1	14,14,15	0.49	0	17,19,21	0.85	1 (5%)
18	A2G	B	4717	1	14,14,15	0.38	0	17,19,21	0.76	0
17	NAG	B	4709	1	14,14,15	0.98	1 (7%)	17,19,21	0.92	1 (5%)
18	A2G	A	4717	1	14,14,15	0.40	0	17,19,21	0.64	0
18	A2G	A	4722	1	14,14,15	0.51	0	17,19,21	1.55	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NAG	A	4709	1	14,14,15	0.41	0	17,19,21	0.30	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
17	NAG	A	4703	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4704	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4715	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4702	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4712	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4708	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4719	1	-	1/6/23/26	0/1/1/1
17	NAG	A	4706	1	-	1/6/23/26	0/1/1/1
17	NAG	A	4711	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4712	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4705	1	-	3/6/23/26	0/1/1/1
17	NAG	A	4707	1	-	2/6/23/26	0/1/1/1
18	A2G	B	4716	1	-	1/6/23/26	0/1/1/1
18	A2G	A	4720	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4718	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4707	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4710	1	-	2/6/23/26	0/1/1/1
18	A2G	A	4713	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4703	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4708	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4701	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4716	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4723	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4704	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4702	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4701	1	-	3/6/23/26	0/1/1/1
17	NAG	B	4711	1	-	4/6/23/26	0/1/1/1
18	A2G	A	4721	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4710	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4723	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4722	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4719	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	NAG	B	4706	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4713	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4714	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4715	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4705	1	-	3/6/23/26	0/1/1/1
18	A2G	B	4714	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4718	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4721	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4720	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4717	1	-	1/6/23/26	0/1/1/1
17	NAG	B	4709	1	-	1/6/23/26	0/1/1/1
18	A2G	A	4717	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4722	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4709	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	4709	NAG	O5-C5	2.43	1.48	1.43
18	A	4716	A2G	O5-C5	2.12	1.47	1.43
18	B	4714	A2G	O5-C5	2.07	1.47	1.43

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	4705	NAG	O5-C1-C2	6.32	121.26	111.29
17	A	4705	NAG	C1-O5-C5	5.74	119.97	112.19
18	A	4712	A2G	C1-C2-N2	4.51	118.19	110.49
18	A	4715	A2G	C1-C2-N2	4.21	117.67	110.49
18	A	4718	A2G	C2-N2-C7	4.01	128.61	122.90

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	4705	NAG	C3-C2-N2-C7
17	A	4705	NAG	C8-C7-N2-C2
17	A	4705	NAG	O7-C7-N2-C2
17	A	4708	NAG	C8-C7-N2-C2
17	A	4708	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	4707	NAG	1	0
17	A	4710	NAG	1	0

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.

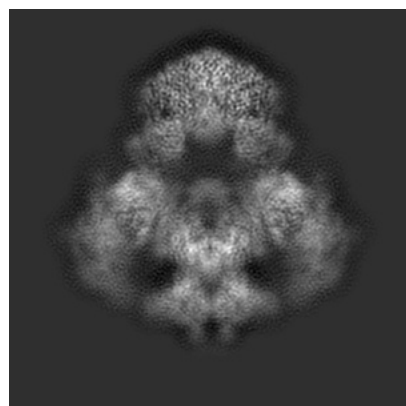
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36663. These allow visual inspection of the internal detail of the map and identification of artifacts.

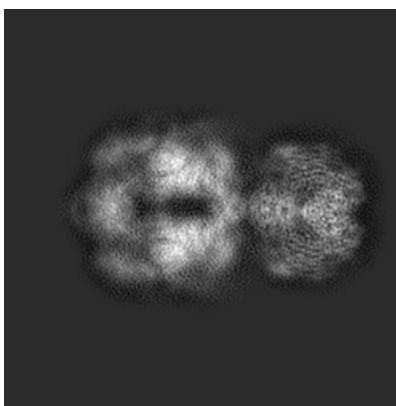
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

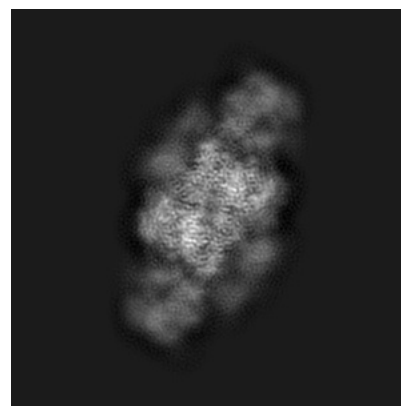
6.1.1 Primary map



X

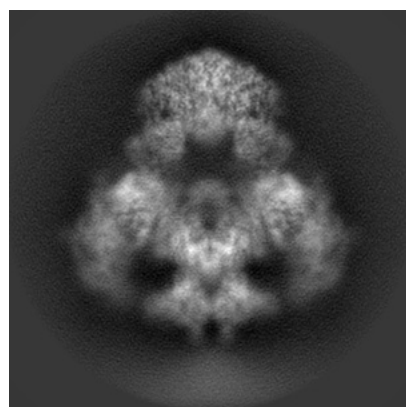


Y

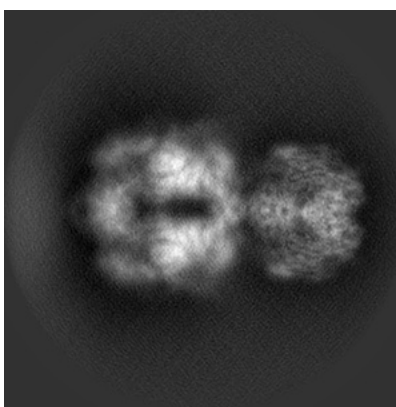


Z

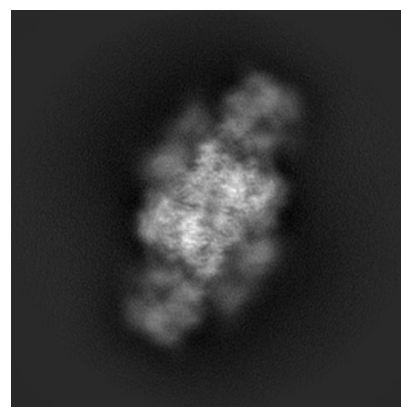
6.1.2 Raw map



X



Y

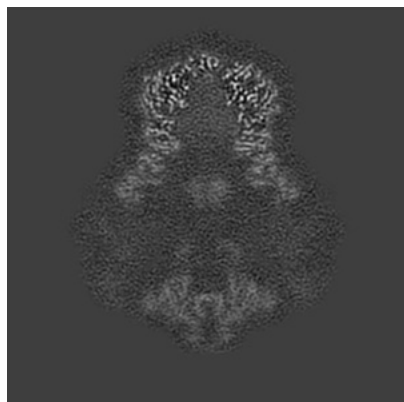


Z

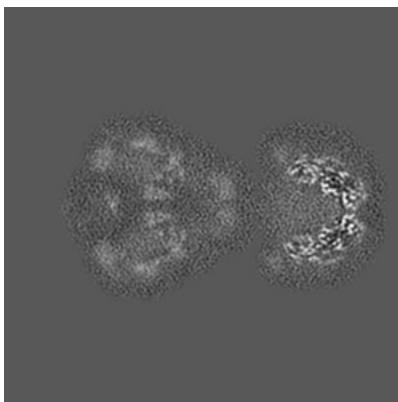
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

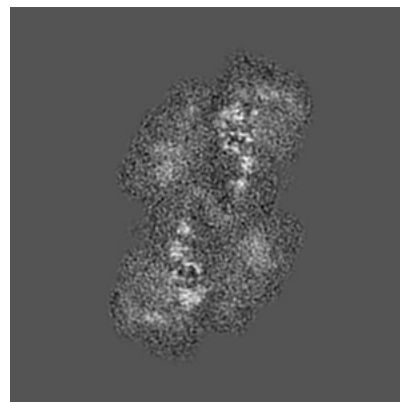
6.2.1 Primary map



X Index: 130

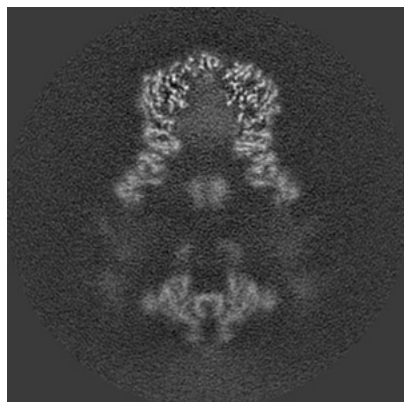


Y Index: 130

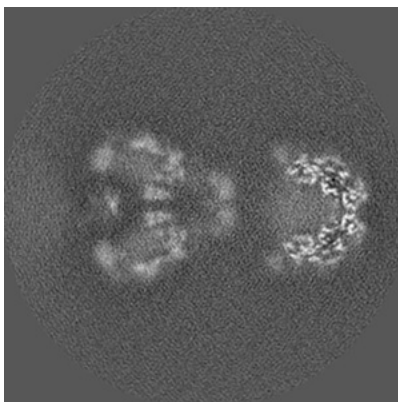


Z Index: 130

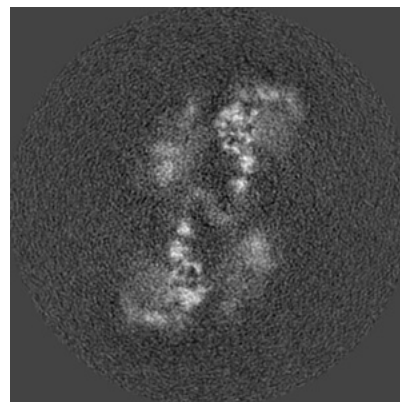
6.2.2 Raw map



X Index: 130



Y Index: 130

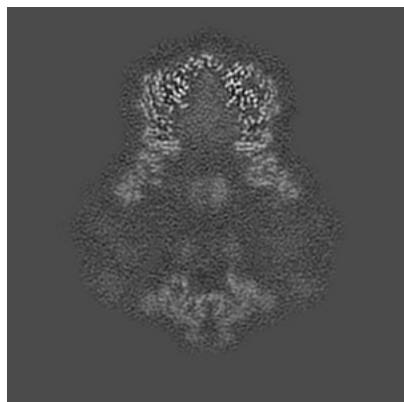


Z Index: 130

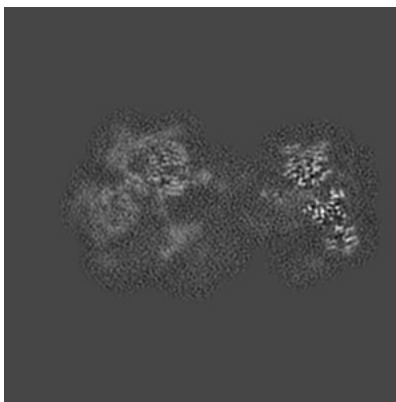
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

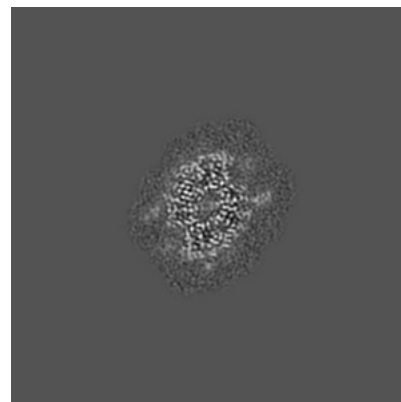
6.3.1 Primary map



X Index: 129

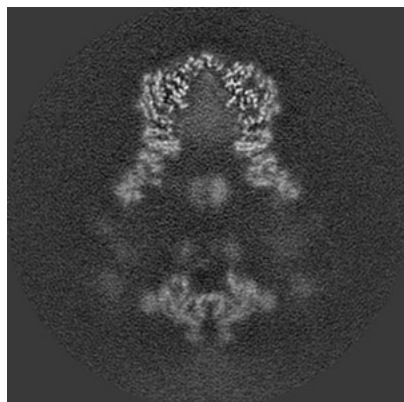


Y Index: 145

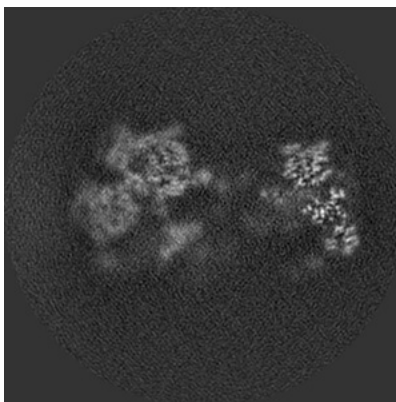


Z Index: 215

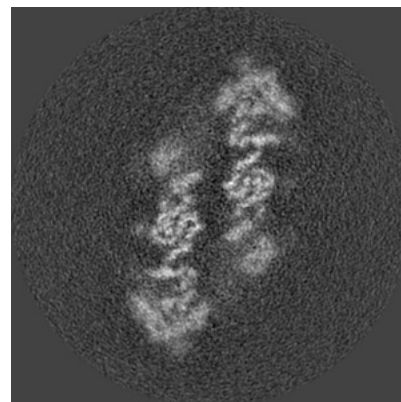
6.3.2 Raw map



X Index: 129



Y Index: 145

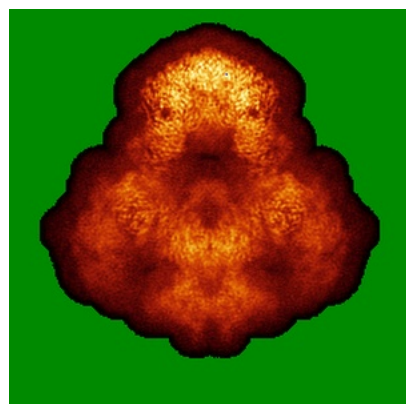


Z Index: 115

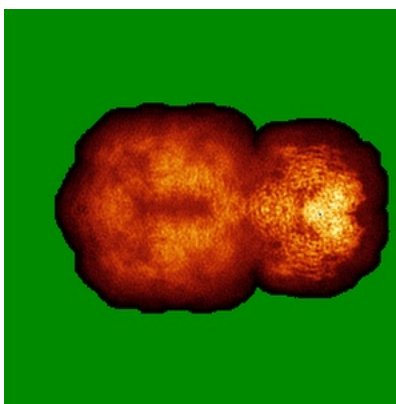
The images above show the largest variance slices of the map in three orthogonal directions.

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

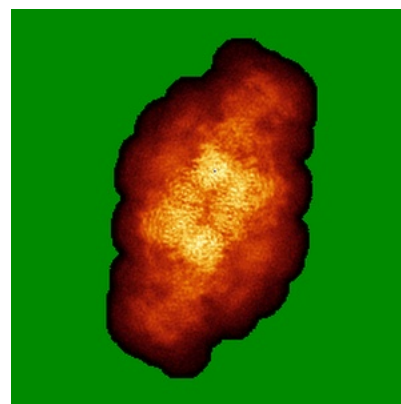
6.4.1 Primary map



X

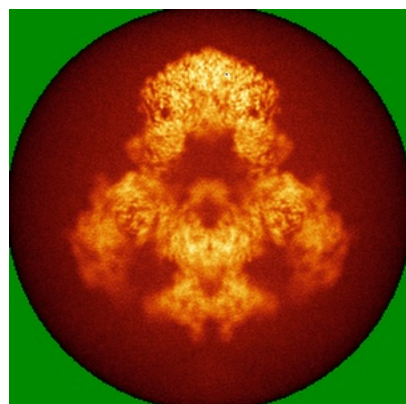


Y

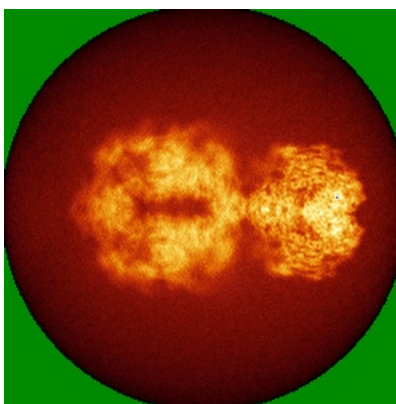


Z

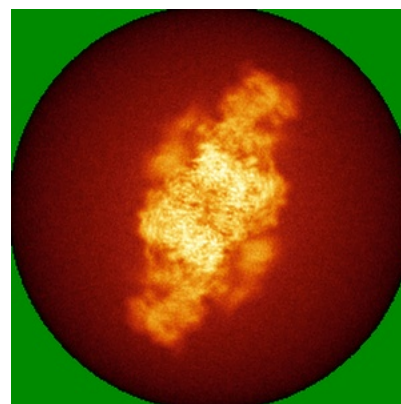
6.4.2 Raw map



X



Y

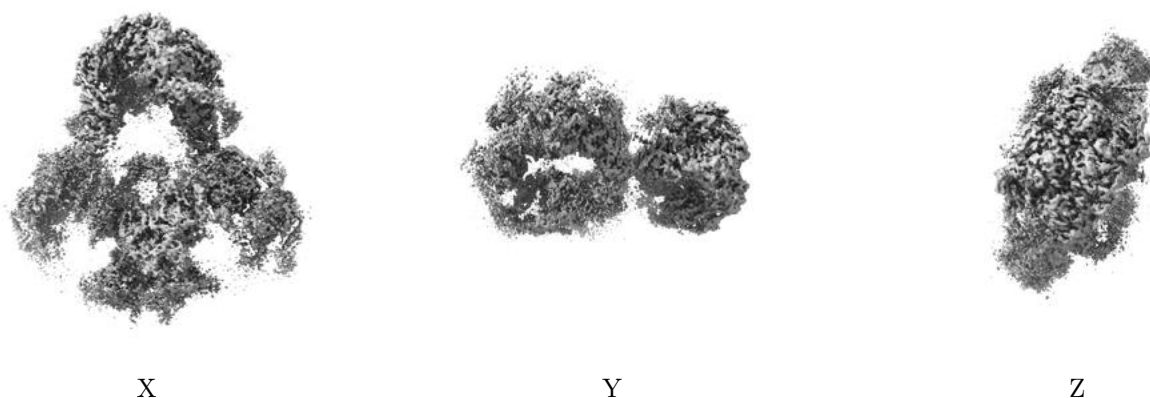


Z

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.

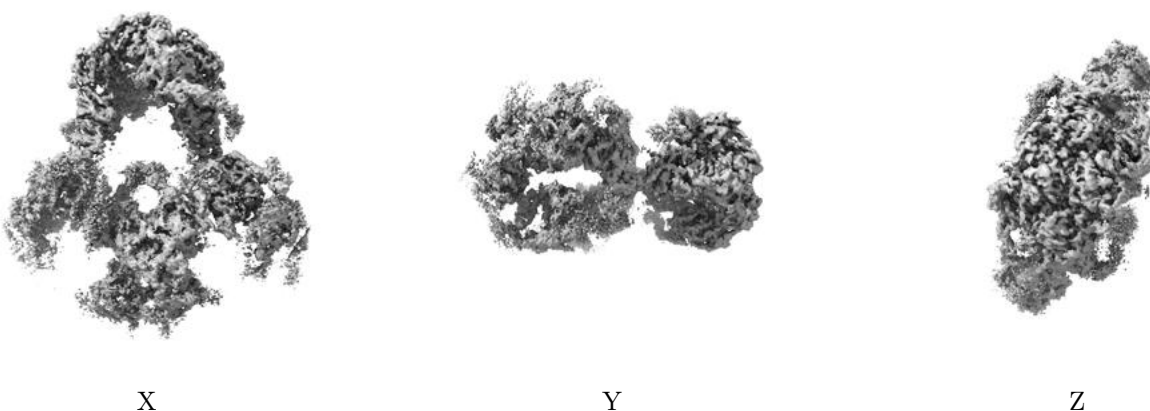
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0242. 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.

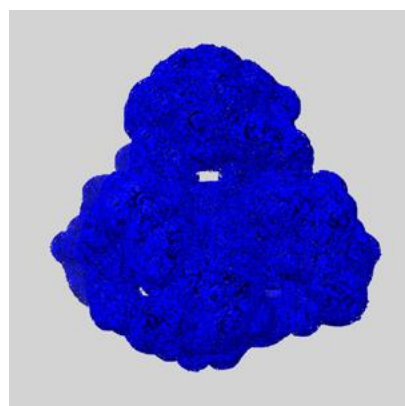
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

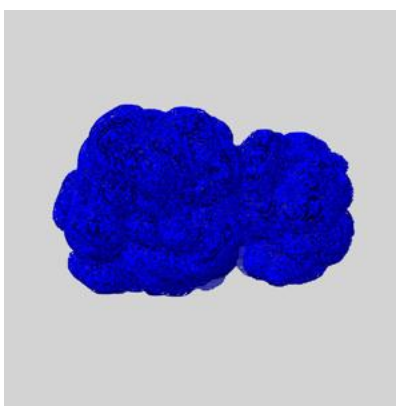
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

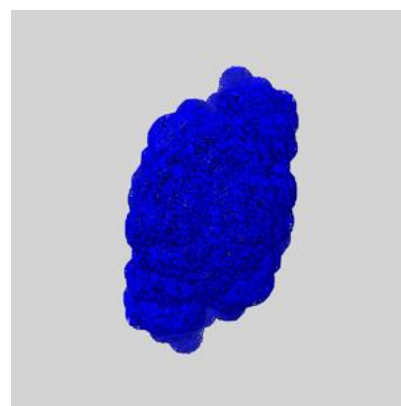
6.6.1 emd_36663_msk_1.map [i](#)



X



Y

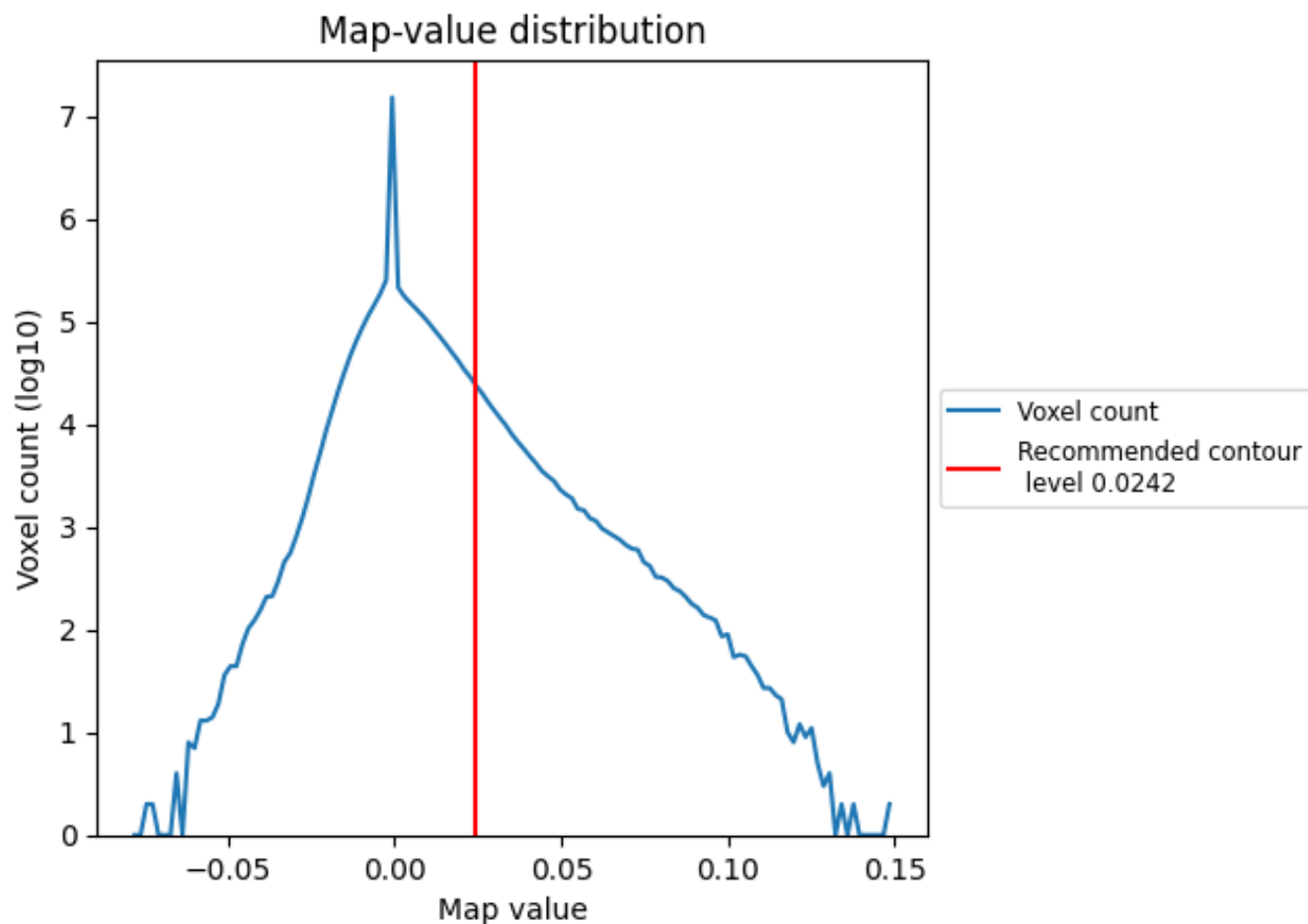


Z

7 Map analysis [i](#)

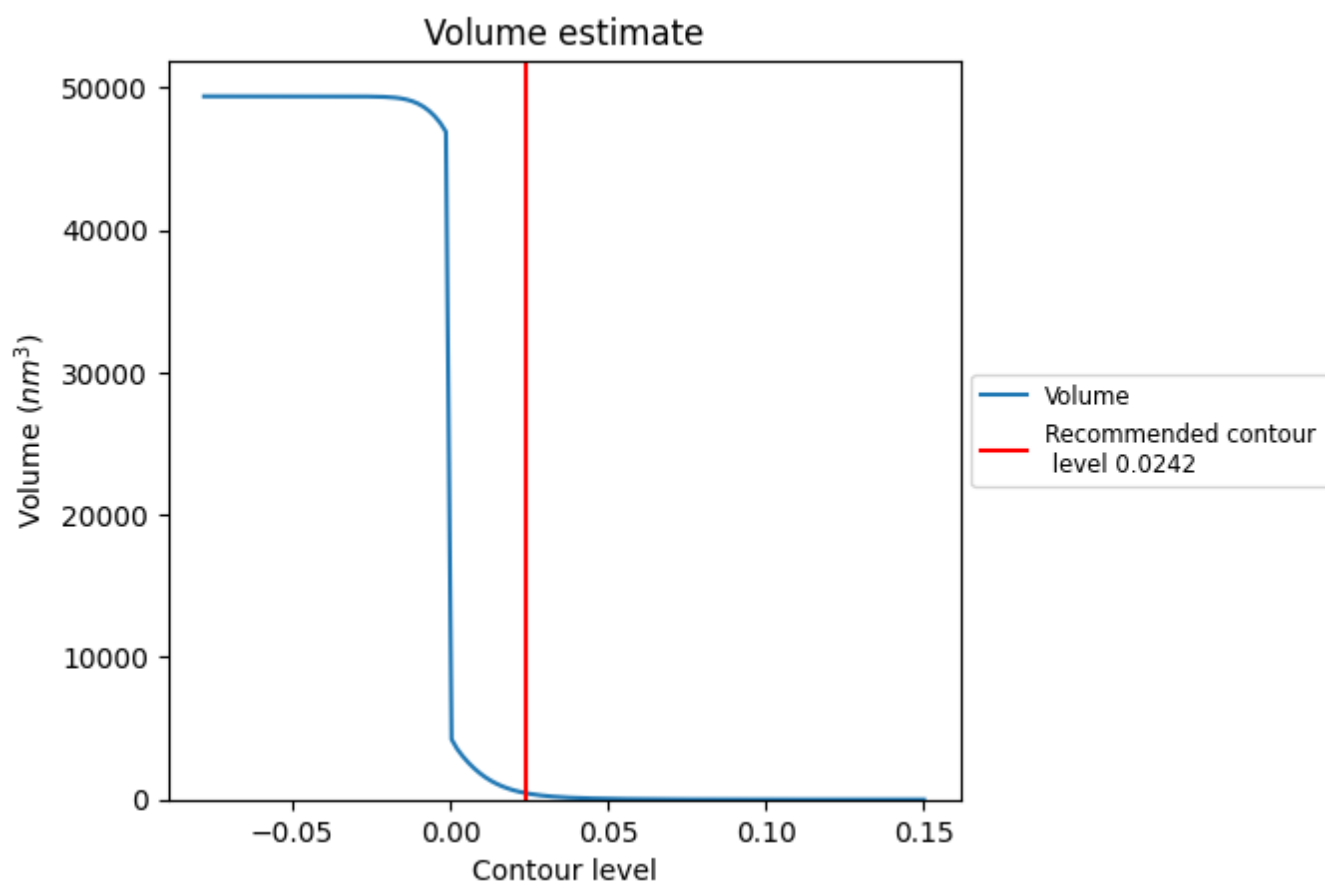
This section contains the results of statistical analysis of the map.

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.

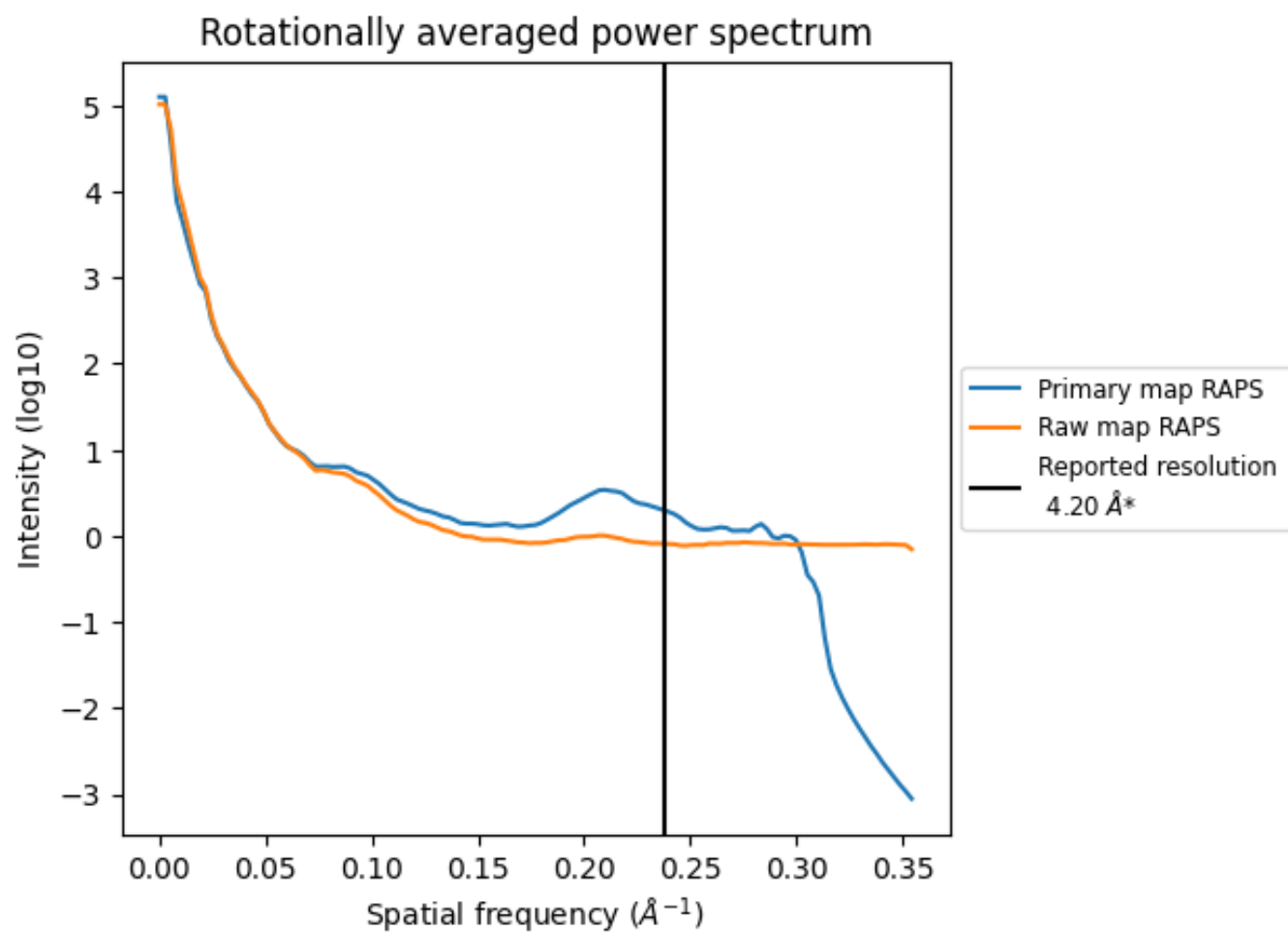
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 445 nm³; this corresponds to an approximate mass of 402 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 ⓘ

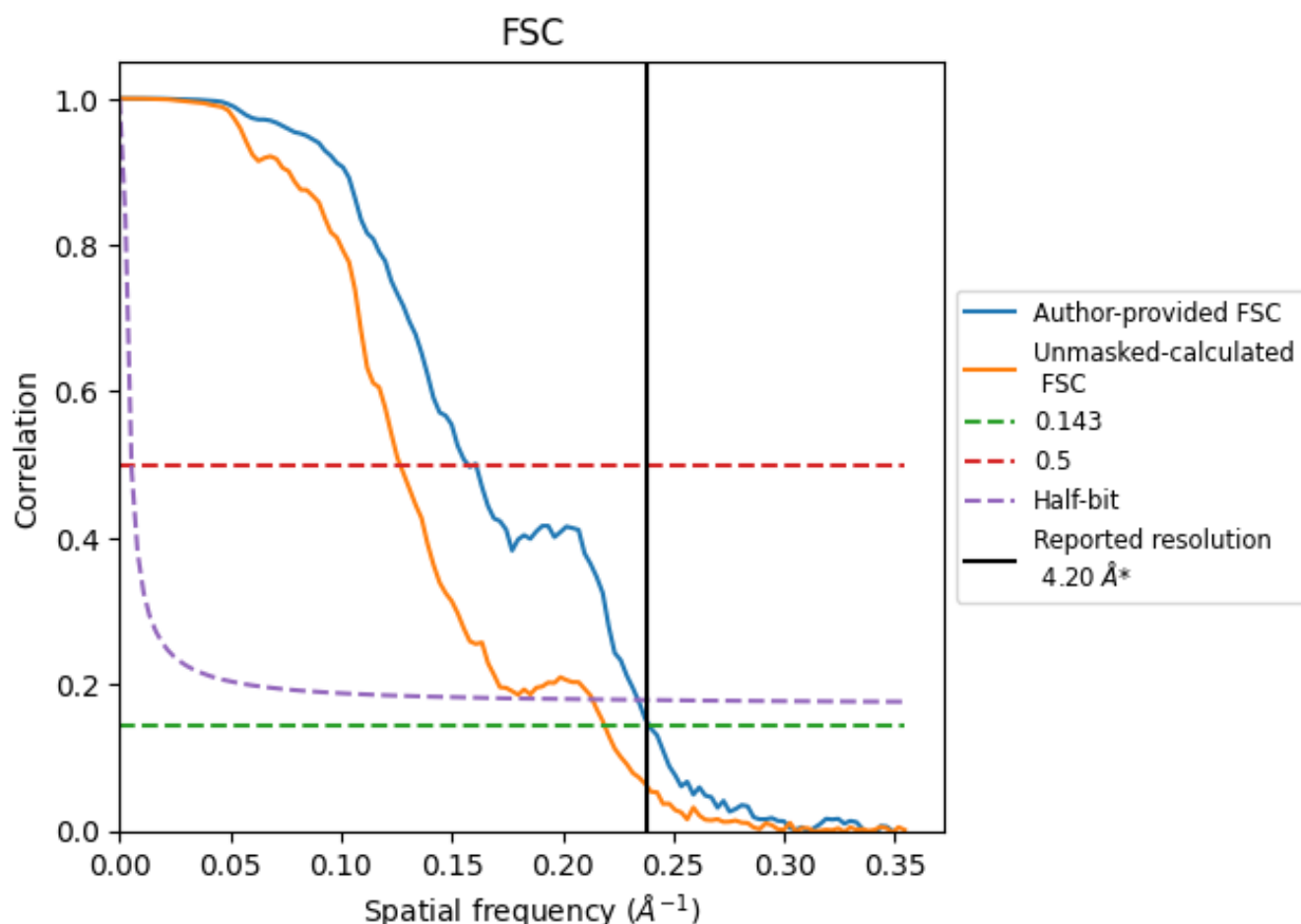


*Reported resolution corresponds to spatial frequency of 0.238 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

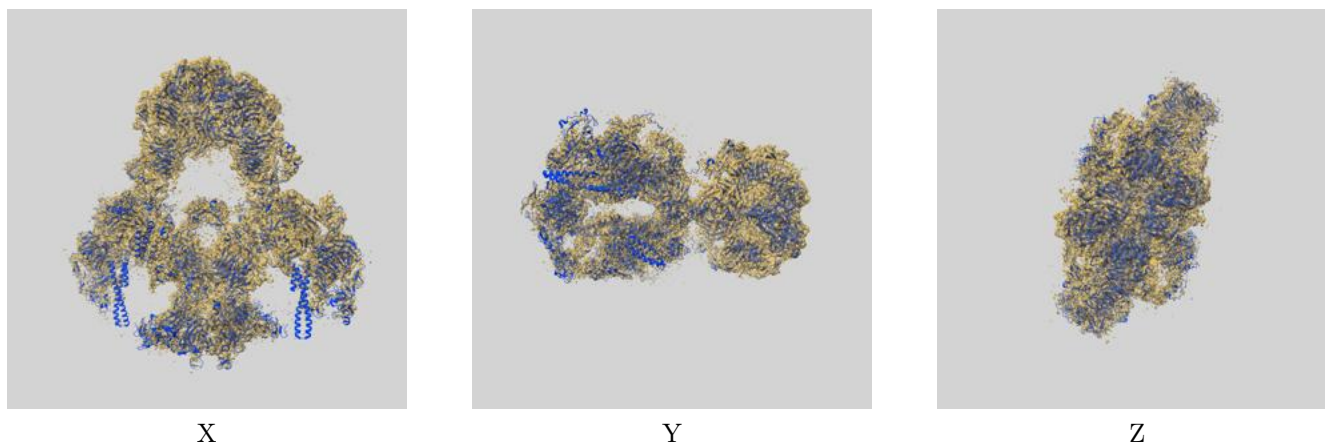
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	6.36	4.27
Unmasked-calculated*	4.57	7.90	4.69

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

9 Map-model fit [i](#)

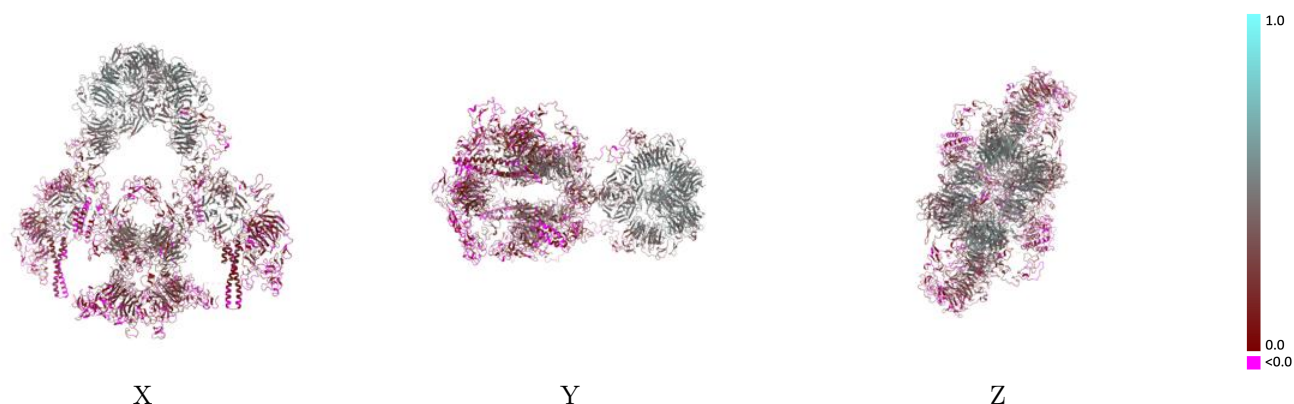
This section contains information regarding the fit between EMDB map EMD-36663 and PDB model 8JUT. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



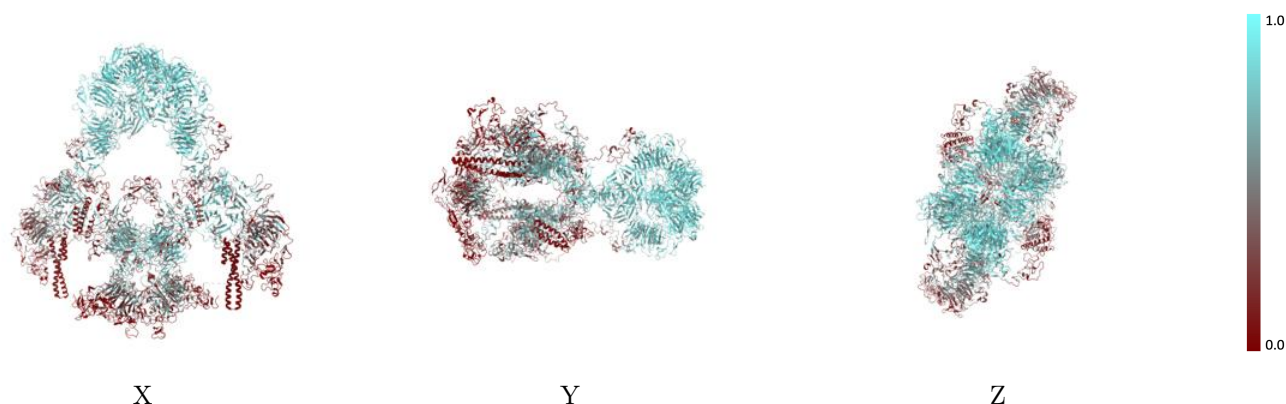
The images above show the 3D surface view of the map at the recommended contour level 0.0242 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



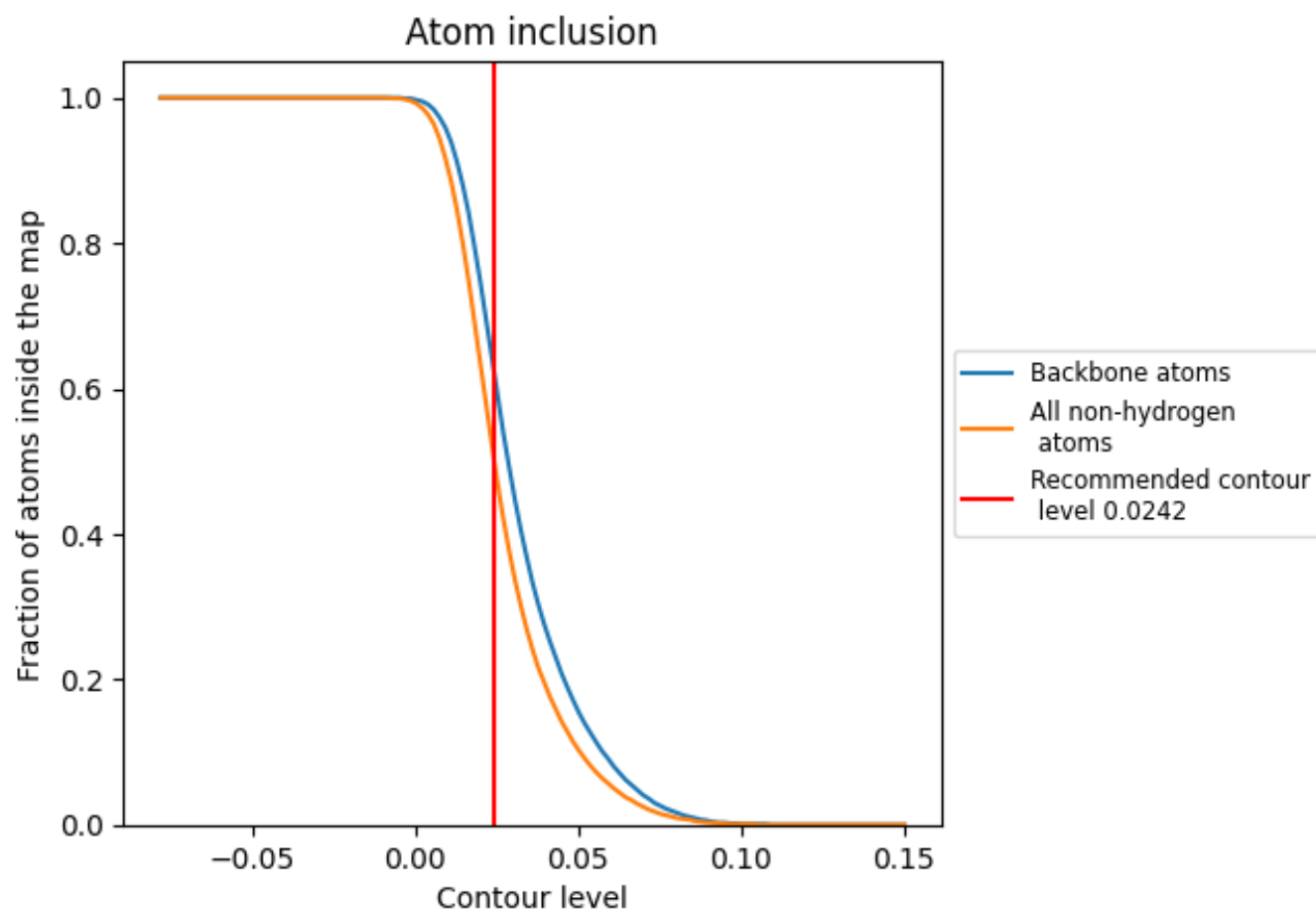
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0242).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 50% 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 (0.0242) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5050	 0.2660
0	 0.3850	 0.2180
1	 0.3440	 0.2710
2	 0.1540	 0.3230
3	 0.2050	 0.1120
4	 0.0820	 0.1020
5	 0.1640	 0.1380
6	 0.0000	 0.0090
7	 0.0260	 0.1010
8	 0.0000	 -0.0760
9	 0.0160	 0.0770
A	 0.5220	 0.2700
B	 0.5360	 0.2830
C	 0.1000	 0.0690
D	 0.0830	 0.0740
E	 0.0360	 0.0950
F	 0.0330	 0.1270
G	 0.1670	 0.0860
H	 0.6790	 0.3580
I	 0.8790	 0.4280
J	 0.4380	 0.2380
K	 0.5450	 0.3920
L	 0.5000	 0.3310
M	 0.7500	 0.4240
N	 0.2000	 0.2410
O	 0.8210	 0.4120
P	 0.8490	 0.4680
Q	 0.6250	 0.2130
R	 0.6360	 0.4410
S	 0.5360	 0.3240
T	 0.8570	 0.4090
U	 0.3610	 0.2860
V	 0.1790	 0.0880
W	 0.5130	 0.3470
X	 0.3570	 0.1840



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Chain	Atom inclusion	Q-score
Y	 0.3570	 0.2610
Z	 0.3440	 0.2510
a	 0.3570	 0.1800
b	 0.7210	 0.4070
c	 0.4290	 0.2360
d	 0.3930	 0.2950
e	 0.2050	 0.1320
f	 0.4100	 0.3070
g	 0.3770	 0.2160
h	 0.1280	 0.0990
i	 0.2050	 0.1630
j	 0.1310	 -0.0180
k	 0.1310	 0.1450
l	 0.0160	 0.0730
m	 0.0260	 0.1920
n	 0.0710	 -0.0280
o	 0.0710	 0.0970
p	 0.5130	 0.3370
q	 0.4290	 0.4120
r	 0.5640	 0.3000
s	 0.6070	 0.4470
t	 0.4640	 0.3800
u	 0.2460	 0.2960
v	 0.3930	 0.3110
w	 0.7210	 0.3990
x	 0.4290	 0.2300
y	 0.4290	 0.2700
z	 0.1030	 0.0360