



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 07:24 PM JST

PDB ID : 8JUJ
EMDB ID : EMD-36664
Title : rat megalin
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 : 3.80 Å (reported)
Based on initial model : .

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:

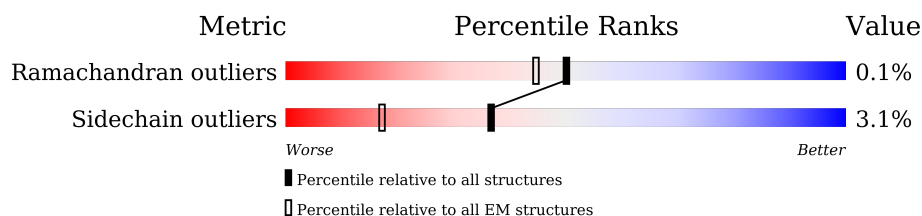
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (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 3.80 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)
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>25%</div> <div>90%</div> <div>8%</div> </div>
1	B	4660	<div> <div>25%</div> <div>90%</div> <div>8%</div> </div>
2	C	6	<div> <div>100%</div> </div>
2	I	6	<div> <div>100%</div> </div>
3	D	3	<div> <div>33%</div> <div>100%</div> </div>
3	J	3	<div> <div>33%</div> <div>100%</div> </div>
4	G	5	<div> <div>20%</div> <div>100%</div> </div>
4	K	5	<div> <div>100%</div> </div>
5	H	5	<div> <div>20%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
5	L	5	100%
5	O	5	100%
5	R	5	100%
6	M	6	83% 100%
6	P	6	67% 100%
7	N	5	100%
7	Q	5	100%
8	E	3	67% 67% 33%
8	T	3	67% 100%
8	b	3	100%
8	c	3	100%
8	l	3	33% 100%
8	o	3	100%
8	w	3	67% 100%
8	x	3	67% 33% 67%
9	0	2	100%
9	3	2	100%
9	5	2	100%
9	F	2	100%
9	S	2	50% 50%
9	U	2	100%
9	V	2	50% 100%
9	X	2	50% 100%
9	Z	2	50% 50%
9	a	2	50% 100%

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Mol	Chain	Length	Quality of chain
9	e	2	100% 100%
9	f	2	50% 100%
9	i	2	100% 100%
9	k	2	100% 100%
9	m	2	50% 50%
9	n	2	50% 100%
9	p	2	50% 50%
9	q	2	100% 100%
9	s	2	50% 100%
9	u	2	50% 100%
9	v	2	50% 100%
9	z	2	100% 100%
10	1	5	100% 20% 80%
10	2	5	80% 100%
10	W	5	60% 80% 20%
10	Y	5	100%
10	d	5	60% 80% 20%
10	g	5	100% 60% 40%
10	h	5	80% 60% 40%
10	r	5	80% 40% 60%
10	t	5	100%
10	y	5	40% 80% 20%
11	4	3	100% 67% 33%
11	j	3	100% 100%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 70018 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
			33638	20708	5950	6605	375		

- Molecule 2 is a protein called unclear peptide.

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

- Molecule 3 is a protein called unclear peptide.

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

- Molecule 4 is a protein called unclear peptide.

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

- Molecule 5 is a protein called unclear peptide.

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

- Molecule 6 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	6	Total 30	C 18	N 6	O 6	0	0
6	P	6	Total 30	C 18	N 6	O 6	0	0

- Molecule 7 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	5	Total 28	C 16	N 6	O 6	0	0
7	Q	5	Total 28	C 16	N 6	O 6	0	0

- Molecule 8 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
8	E	3	Total 39	C 22	N 2	O 15	0	0
8	T	3	Total 39	C 22	N 2	O 15	0	0
8	b	3	Total 39	C 22	N 2	O 15	0	0
8	c	3	Total 39	C 22	N 2	O 15	0	0
8	l	3	Total 39	C 22	N 2	O 15	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	o	3	Total	C	N	O	0	0
			39	22	2	15		
8	w	3	Total	C	N	O	0	0
			39	22	2	15		
8	x	3	Total	C	N	O	0	0
			39	22	2	15		

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



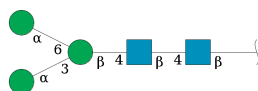
Mol	Chain	Residues	Atoms				AltConf	Trace
9	F	2	Total	C	N	O	0	0
			28	16	2	10		
9	S	2	Total	C	N	O	0	0
			28	16	2	10		
9	U	2	Total	C	N	O	0	0
			28	16	2	10		
9	V	2	Total	C	N	O	0	0
			28	16	2	10		
9	X	2	Total	C	N	O	0	0
			28	16	2	10		
9	Z	2	Total	C	N	O	0	0
			28	16	2	10		
9	a	2	Total	C	N	O	0	0
			28	16	2	10		
9	e	2	Total	C	N	O	0	0
			28	16	2	10		
9	f	2	Total	C	N	O	0	0
			28	16	2	10		
9	i	2	Total	C	N	O	0	0
			28	16	2	10		
9	k	2	Total	C	N	O	0	0
			28	16	2	10		
9	m	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	p	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
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	u	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	z	2	Total	C	N	O	0	0
			28	16	2	10		
9	0	2	Total	C	N	O	0	0
			28	16	2	10		
9	3	2	Total	C	N	O	0	0
			28	16	2	10		
9	5	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	W	5	Total	C	N	O	0	0
			61	34	2	25		
10	Y	5	Total	C	N	O	0	0
			61	34	2	25		
10	d	5	Total	C	N	O	0	0
			61	34	2	25		
10	g	5	Total	C	N	O	0	0
			61	34	2	25		
10	h	5	Total	C	N	O	0	0
			61	34	2	25		
10	r	5	Total	C	N	O	0	0
			61	34	2	25		
10	t	5	Total	C	N	O	0	0
			61	34	2	25		
10	y	5	Total	C	N	O	0	0
			61	34	2	25		

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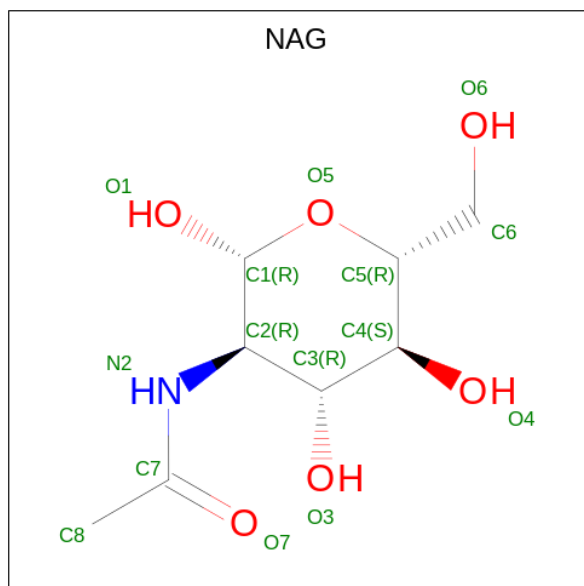
Mol	Chain	Residues	Atoms				AltConf	Trace
10	1	5	Total	C	N	O	0	0
			61	34	2	25		
10	2	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 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
11	j	3	Total	C	N	O	0	0
			39	22	2	15		
11	4	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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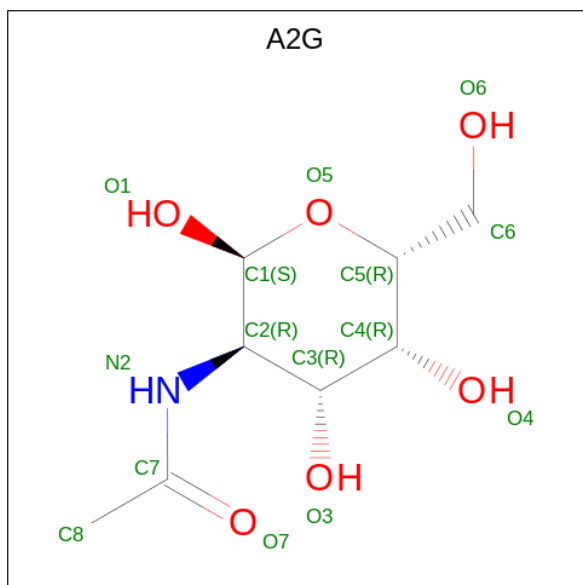
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O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

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

- Molecule 13 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 14 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

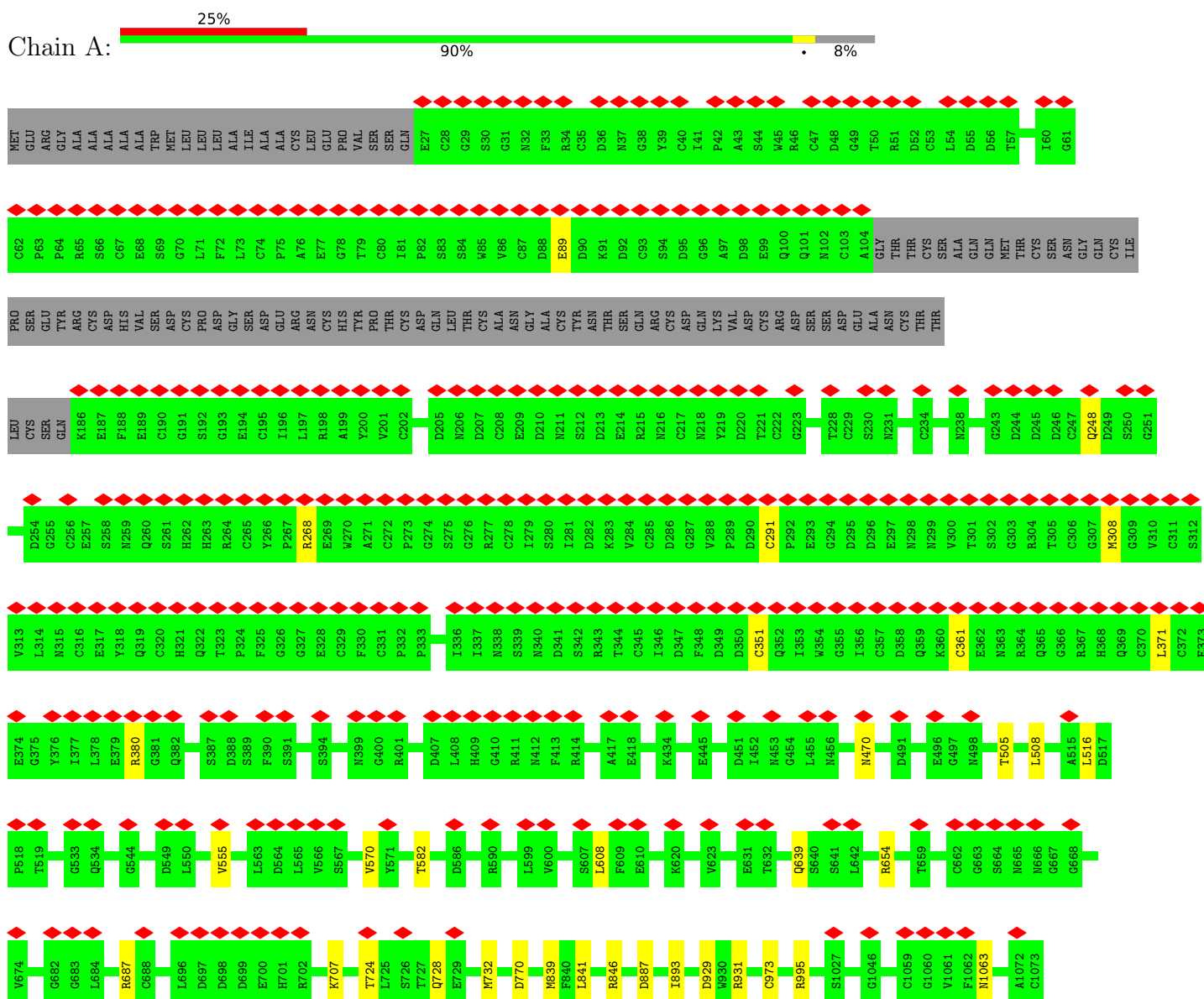
- Molecule 15 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

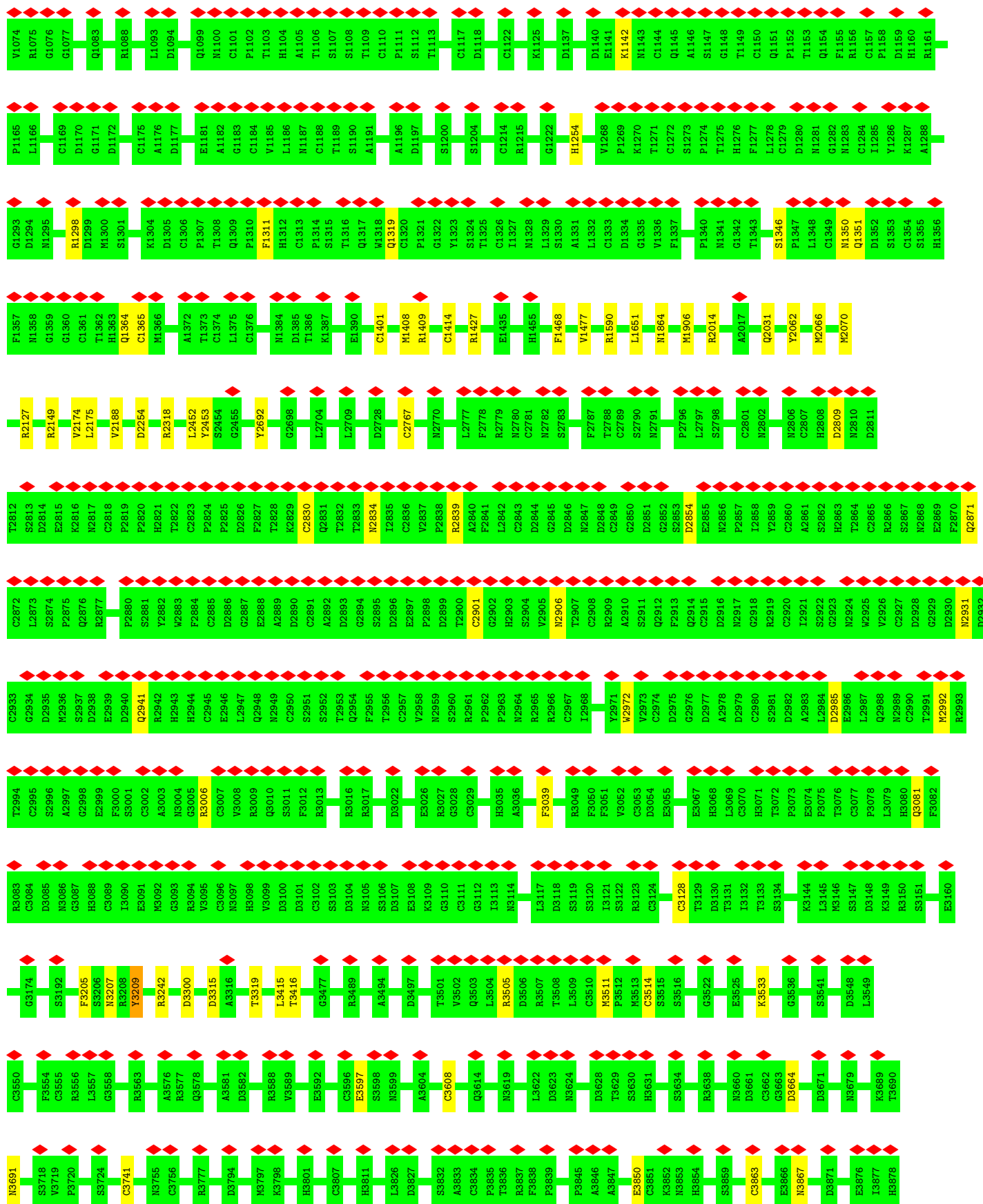
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Ni	0
			1	1	
15	B	1	Total	Ni	0
			1	1	

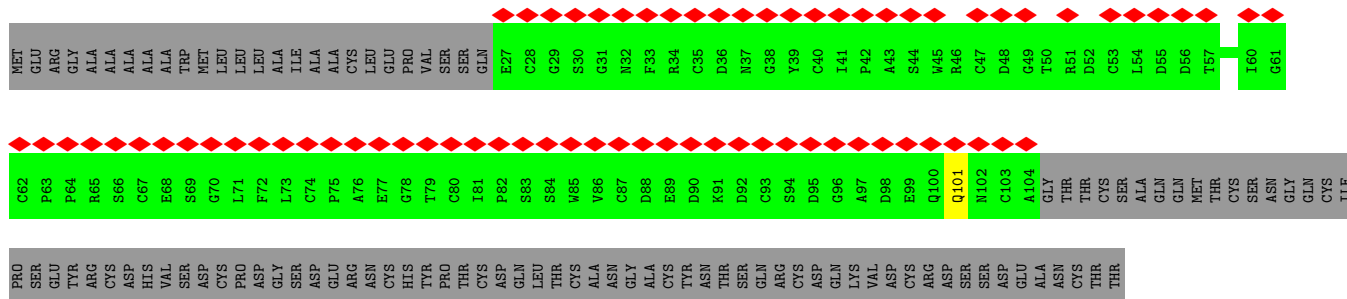
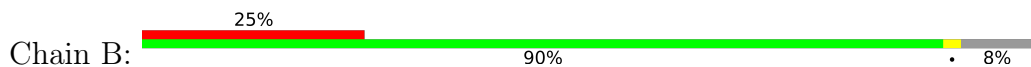
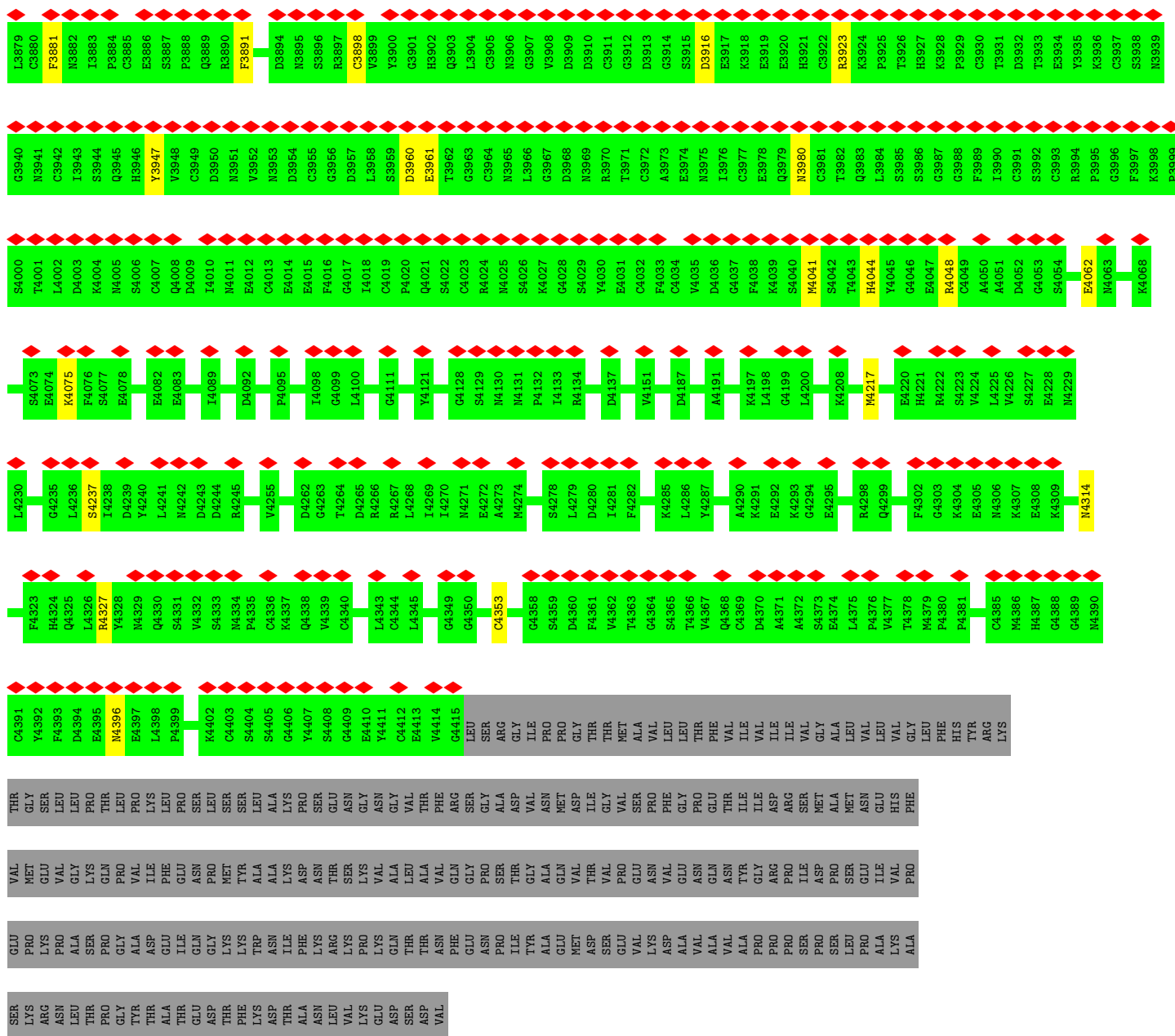
3 Residue-property plots

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: LDL receptor related protein 2







LEU	CYS	SER	GLN
K186	E187	F188	E189
C190	G191	S192	G193
E194	C195	I196	L197
L198	A199	Y200	V201
C202	D203	H204	D205
N206	D207	S208	C209
D210	N211	S212	D213
E214	R215	N216	C217
N218	Y219	D220	T221
C222	G223	H224	H225
Q226	F227	T228	C229
S230	N231	V232	Q233
G234	G243	D244	D245
C247	Q248		
D249	S250	G251	D254
G255	C256		
N259	Q260	G261	H262
H263	R264	C265	Y266
P267	R268	E269	V270
A271	C272	P273	G274
S275	G276	I277	C278
I279	S280	I281	C282
R283	V284	C285	C286
G287	D288	D289	D290
C291	P292	E293	G294
H295	D296	E297	I298
N299	V300	T301	S302
G303	R304	Q305	G306
G307	M308	Q309	V310
C311	S312	V313	L314
N315	G316	E317	Y318
Q319	R320	H321	Q322
T323	P324	F325	G326
G327	E328	C329	F330
C331	P332	P333	G334
H335	I336	I337	N338
I339	S339	N340	D341
S342	R343	T344	C345
G346	D347	F348	D349
D350	C351	Q352	I353
G354	H355	I356	C357
D358	Q359	K360	N361
S362	T363	S364	Q365
G366	R367	H368	Q369
C370			
L371	C372	E373	E374
G375	Y376	I377	L378
E379	R380	G381	Q382
D383	F384	G385	H386
S387	V388	I389	D390
E391	F392	G393	H394
I395	N396	D397	E398
C399	V400	T401	S402
G403	R404	Q405	G406
G407	M408	Q409	V410
C411	P412	E413	H414
S415	I416	C417	D418
N419	S420	I421	C422
D423	P424	E425	G426
H427	N428	D429	E430
C431	V432	T433	S434
G435	I436	C437	D438
D439	E440	F441	G442
H443	N444	S445	H446
C447	V448	T449	S450
G451	I452	C453	H454
D455	N456	D457	E458
C459	V460	T461	S462
G463	H464	Q465	G466
H467	N468	D469	E470
C471	V472	T473	S474
G475	I476	C477	D478
D479	E480	F481	G482
H483	N484	S485	H486
C487	V488	T489	S490
G491	F492	G493	H494
I495	N496	D497	E498
C499	V500	T501	S502
G503	R504	Q505	G506
G507	M508	Q509	V510
C511	P512	E513	H514
S515	I516	C517	D518
N519	S520	I521	C522
D523	P524	E525	G526
H527	N528	D529	E530
C531	V532	T533	S534
G535	I536	C537	D538
D539	E540	F541	G542
H543	N544	S545	H546
C547	V548	T549	S550
G551	I552	C553	H554
D555	N556	D557	E558
C559	V560	T561	S562
G563	H564	Q565	G566
H567	N568	D569	E570
C571	V572	T573	S574
G575	I576	C577	D578
D579	E580	F581	G582
H583	N584	S585	H586
C587	V588	T589	S590
G591	F592	G593	H594
I595	N596	D597	E598
C599	V600	T601	S602
G603	R604	Q605	G606
G607	M608	Q609	V610
C611	P612	E613	H614
S615	I616	C617	D618
N619	S620	I621	C622
D623	P624	E625	G626
H627	N628	D629	E630
C631	V632	T633	S634
G635	I636	C637	D638
D639	E640	F641	G642
H643	N644	S645	H646
C647	V648	T649	S650
G651	I652	C653	H654
D655	N656	D657	E658
C659	V660	T661	S662
G663	H664	Q665	G666
H667	N668	D669	E670
C671	V672	T673	S674
G675	I676	C677	D678
D679	E680	F681	G682
H683	N684	S685	H686
C687	V688	T689	S690
G691	F692	G693	H694
I695	N696	D697	E698
C699	V700	T701	S702
G703	R704	Q705	G706
G707	M708	Q709	V710
C711	P712	E713	H714
S715	I716	C717	D718
N719	S720	I721	C722
D723	P724	E725	G726
H727	N728	D729	E730
C731	V732	T733	S734
G735	I736	C737	D738
D739	E740	F741	G742
H743	N744	S745	H746
C747	V748	T749	S750
G751	I752	C753	H754
D755	N756	D757	E758
C759	V760	T761	S762
G763	H764	Q765	G766
H767	N768	D769	E770
C771	V772	T773	S774
G775	I776	C777	D778
D779	E780	F781	G782
H783	N784	S785	H786
C787	V788	T789	S790
G791	F792	G793	H794
I795	N796	D797	E798
C799	V800	T801	S802
G803	R804	Q805	G806
G807	M808	Q809	V810
C811	P812	E813	H814
S815	I816	C817	D818
N819	S820	I821	C822
D823	P824	E825	G826
H827	N828	D829	E830
C831	V832	T833	S834
G835	I836	C837	D838
D839	E840	F841	G842
H843	N844	S845	H846
C847	V848	T849	S850
G851	I852	C853	H854
D855	N856	D857	E858
C859	V860	T861	S862
G863	H864	Q865	G866
H867	N868	D869	E870
C871	V872	T873	S874
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D879	E880	F881	G882
H883	N884	S885	H886
C887	V888	T889	S890
G891	F892	G893	H894
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C899	V900	T901	S902
G903	R904	Q905	G906
G907	M908	Q909	V910
C911	P912	E913	H914
S915	I916	C917	D918
N919	S920	I921	C922
D923	P924	E925	G926
H927	N928	D929	E930
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G975	I976	C977	D978
D979	E980	F981	G982
H983	N984	S985	H986
C987	V988	T989	S990
G991	F992	G993	H994
I995	N996	D997	E998
C999	V1000	T1001	S1002
G1003	R1004	Q1005	G1006
G1007	M1008	Q1009	V1010
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S1015	I1016	C1017	D1018
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D1023	P1024	E1025	G1026
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C1031	V1032	T1033	S1034
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I1095	N1096	D1097	E1098
C1099	V1100	T1101	S1102
G1103	H1104	Q1105	G1106
H1107	N1108	D1109	E1110
C1111	P1112	E1113	H1114
S1115	I1116	C1117	D1118
N1119	S1120	I1121	C1122
D1123	P1124	E1125	G1126
H1127	N1128	D1129	E1130
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G1135	I1136	C1137	D1138
D1139	E1140	F1141	G1142
H1143	N1144	S1145	H1146
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D1155	N1156	D1157	E1158
C1159	V1160	T1161	S1162
G1163	H1164	Q1165	G1166
H1167	N1168	D1169	E1170
C1171	V1172	T1173	S1174
G1175	I1176	C1177	D1178
D1179	E1180	F1181	G1182
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C1187	V1188	T1189	S1190
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I1195	N1196	D1197	E1198
C1199	V1200	T1201	S1202
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G1207	M1208	Q1209	V1210
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G1307	M1308	Q1309	V1310
C1311	P1312	E1313	H1314
S1315	I1316	C1317	D1318
N1319	S1320	I1321	C1322
D1323	P1324	E1325	G1326
H1327	N1328	D1329	E1330
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G1335	I1336	C1337	D1338
D1339	E1340	F1341	G1342
H1343	N1344	S1345	H1346
C1347	V1348	T1349	S1350
G1351	I1352	C1353	H1354
D1355	N1356	D1357	E1358
C1359	V1360	T1361	S1362
G1363	H1364	Q1365	G1366
H1367	N1368	D1369	E1370
C1371	V1372	T1373	S1374
G1375	I1376	C1377	D1378
D1379	E1380	F1381	G1382
H1383	N1384	S1385	H1386
C1387	V1388	T1389	S1390
G1391	F1392	G1393	H1394
I1395	N1396	D1397	E1398
C1399	V1400	T1401	S1402
G1403	R1404	Q1405	G1406
G1407	M1408	Q1409	V1410
C1411	P1412	E1413	H1414
S1415	I1416	C1417	D1418
N1419	S1420	I1421	C1422
D1423	P1424	E1425	G1426
H1427	N1428	D1429	E1430
C1431	V1432	T1433	S1434
G1435	I1436	C1437	D1438
D1439	E1440	F1441	G1442
H1443	N1444	S1445	H1446
C1447	V1448	T1449	S1450
G1451	I1452	C1453	H1454
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D1479	E1480	F1481	G1482
H1483	N1484	S1485	H1486
C1487	V1488	T1489	S1490
G1			



TYR	ALA	GLU	NET	ASP	SER	GLU	VAL	LYS	ASP	ALA	VAL	ALA	ALA	VAL	PRO	PRO	PRO	SER	PRO	SER	LEU	LEU	PRO	PRO	GLY	TYR	THR	THR	ALA	ALA	GLU	ASP	THR	THR	PHI	ASP	LYS	ASP	ALA	ALA	ASN	LEU	VAL	LYS	GLU	ASP	SER	ASP	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



- Molecule 5: unclear peptide

Chain L: 100%

There are no outlier residues recorded for this chain.

- Molecule 5: unclear peptide

Chain O: 100%

There are no outlier residues recorded for this chain.

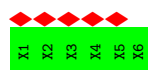
- Molecule 5: unclear peptide

Chain R: 100%

There are no outlier residues recorded for this chain.

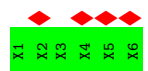
- Molecule 6: unclear peptide

Chain M: 83%
100%



- Molecule 6: unclear peptide

Chain P: 67%
100%



- Molecule 7: unclear peptide

Chain N: 100%

There are no outlier residues recorded for this chain.

- Molecule 7: unclear peptide

Chain Q: 100%

There are no outlier residues recorded for this chain.

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 67%
67% 33%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-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



- 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



- 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



- 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

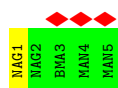
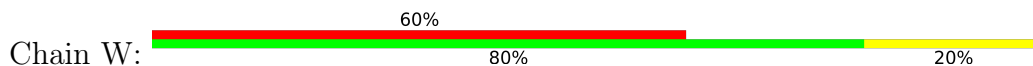


- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





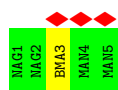
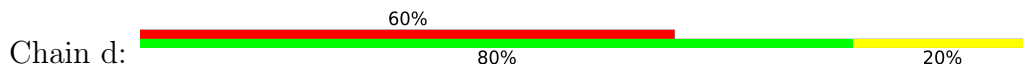
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



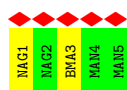
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



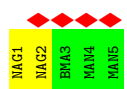
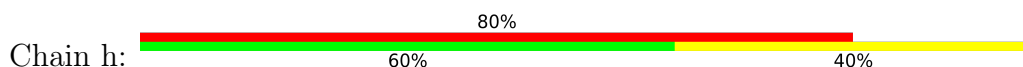
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



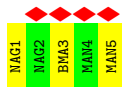
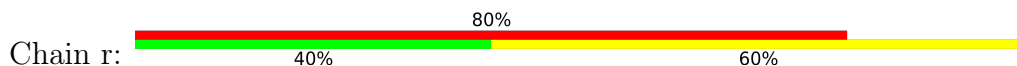
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



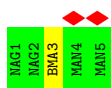
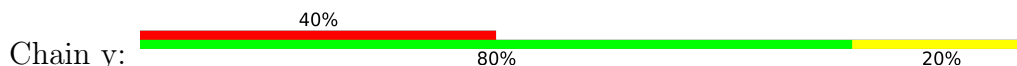
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



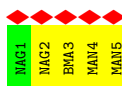
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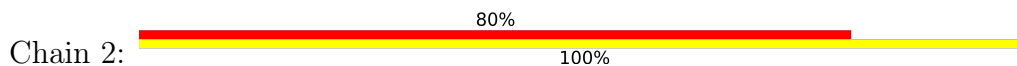
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- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 11: 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	101096	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)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.214	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/34456	0.58	0/46804
1	B	0.64	0/34456	0.66	0/46804
2	C	0.61	0/7	0.76	0/8
2	I	0.65	0/7	0.99	0/8
3	D	1.22	0/5	0.59	0/5
3	J	0.98	0/5	0.46	0/5
4	G	0.79	0/17	0.54	0/21
4	K	0.86	0/17	0.58	0/21
5	H	0.93	0/7	0.64	0/8
5	L	0.92	0/7	0.79	0/8
5	O	0.75	0/7	0.76	0/8
5	R	0.73	0/7	0.62	0/8
7	N	1.04	0/7	1.32	0/8
7	Q	0.46	0/7	1.79	0/8
All	All	0.51	0/69012	0.62	0/93724

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	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3242	ARG	Sidechain
1	B	2839	ARG	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	3970 (92%)	332 (8%)	2 (0%)	100	100
1	B	4304/4660 (92%)	3979 (92%)	322 (8%)	3 (0%)	48	79
2	C	1/6 (17%)	1 (100%)	0	0	100	100
2	I	1/6 (17%)	1 (100%)	0	0	100	100
3	D	1/3 (33%)	1 (100%)	0	0	100	100
3	J	1/3 (33%)	0	1 (100%)	0	100	100
4	G	2/5 (40%)	0	2 (100%)	0	100	100
4	K	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
5	H	1/5 (20%)	1 (100%)	0	0	100	100
5	L	1/5 (20%)	1 (100%)	0	0	100	100
5	O	1/5 (20%)	0	1 (100%)	0	100	100
5	R	1/5 (20%)	1 (100%)	0	0	100	100
7	N	1/5 (20%)	1 (100%)	0	0	100	100
7	Q	1/5 (20%)	1 (100%)	0	0	100	100
All	All	8622/9378 (92%)	7958 (92%)	659 (8%)	5 (0%)	50	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2840	ALA
1	B	2860	CYS
1	A	3209	TYR
1	A	846	ARG
1	B	1152	PRO

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%)	3663 (97%)	128 (3%)	32	55
1	B	3791/4089 (93%)	3684 (97%)	107 (3%)	38	59
2	C	1/1 (100%)	1 (100%)	0	100	100
2	I	1/1 (100%)	1 (100%)	0	100	100
3	D	1/1 (100%)	1 (100%)	0	100	100
3	J	1/1 (100%)	1 (100%)	0	100	100
4	G	2/2 (100%)	2 (100%)	0	100	100
4	K	2/2 (100%)	2 (100%)	0	100	100
5	H	1/1 (100%)	1 (100%)	0	100	100
5	L	1/1 (100%)	1 (100%)	0	100	100
5	O	1/1 (100%)	1 (100%)	0	100	100
5	R	1/1 (100%)	1 (100%)	0	100	100
7	N	1/1 (100%)	1 (100%)	0	100	100
7	Q	1/1 (100%)	1 (100%)	0	100	100
All	All	7596/8192 (93%)	7361 (97%)	235 (3%)	37	56

5 of 235 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3961	GLU
1	B	4044	HIS
1	B	489	ARG

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Mol	Chain	Res	Type
1	B	4008	GLN
1	B	3108	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4390	ASN
1	B	4131	ASN
1	B	1367	GLN
1	B	4390	ASN
1	B	3066	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

124 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	$\# Z > 2$
9	NAG	0	1	1,9	14,14,15	0.40	0	17,19,21	0.51	0
9	NAG	0	2	9	14,14,15	0.40	0	17,19,21	0.58	0
10	NAG	1	1	10,1	14,14,15	0.45	0	17,19,21	0.73	0
10	NAG	1	2	10	14,14,15	0.57	0	17,19,21	0.97	1 (5%)
10	BMA	1	3	10	11,11,12	1.00	1 (9%)	15,15,17	1.11	1 (6%)
10	MAN	1	4	10	11,11,12	0.95	1 (9%)	15,15,17	1.00	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	1	5	10	11,11,12	0.80	0	15,15,17	0.88	1 (6%)
10	NAG	2	1	10,1	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
10	NAG	2	2	10	14,14,15	0.58	0	17,19,21	0.81	1 (5%)
10	BMA	2	3	10	11,11,12	1.14	1 (9%)	15,15,17	1.30	2 (13%)
10	MAN	2	4	10	11,11,12	0.89	1 (9%)	15,15,17	0.86	1 (6%)
10	MAN	2	5	10	11,11,12	0.82	0	15,15,17	1.27	2 (13%)
9	NAG	3	1	1,9	14,14,15	0.41	0	17,19,21	0.51	0
9	NAG	3	2	9	14,14,15	0.39	0	17,19,21	0.55	0
11	NAG	4	1	11,1	14,14,15	0.43	0	17,19,21	0.41	0
11	NAG	4	2	11	14,14,15	0.39	0	17,19,21	0.45	0
11	BMA	4	3	11	11,11,12	0.80	1 (9%)	15,15,17	0.82	1 (6%)
9	NAG	5	1	1,9	14,14,15	0.55	0	17,19,21	0.81	1 (5%)
9	NAG	5	2	9	14,14,15	0.56	0	17,19,21	0.89	1 (5%)
8	NAG	E	1	1,8	14,14,15	0.40	0	17,19,21	0.48	0
8	NAG	E	2	8	14,14,15	0.41	0	17,19,21	0.82	1 (5%)
8	BMA	E	3	8	11,11,12	0.21	0	15,15,17	0.56	0
9	NAG	F	1	1,9	14,14,15	0.40	0	17,19,21	0.41	0
9	NAG	F	2	9	14,14,15	0.40	0	17,19,21	0.35	0
9	NAG	S	1	1,9	14,14,15	0.42	0	17,19,21	0.55	0
9	NAG	S	2	9	14,14,15	0.41	0	17,19,21	0.81	1 (5%)
8	NAG	T	1	1,8	14,14,15	0.36	0	17,19,21	0.66	0
8	NAG	T	2	8	14,14,15	0.50	0	17,19,21	0.75	0
8	BMA	T	3	8	11,11,12	0.25	0	15,15,17	0.62	0
9	NAG	U	1	1,9	14,14,15	0.41	0	17,19,21	0.45	0
9	NAG	U	2	9	14,14,15	0.39	0	17,19,21	0.42	0
9	NAG	V	1	1,9	14,14,15	0.63	0	17,19,21	1.10	2 (11%)
9	NAG	V	2	9	14,14,15	0.61	0	17,19,21	1.08	1 (5%)
10	NAG	W	1	10,1	14,14,15	0.40	0	17,19,21	0.99	2 (11%)
10	NAG	W	2	10	14,14,15	0.39	0	17,19,21	0.54	0
10	BMA	W	3	10	11,11,12	0.27	0	15,15,17	0.76	0
10	MAN	W	4	10	11,11,12	0.24	0	15,15,17	0.52	0
10	MAN	W	5	10	11,11,12	0.29	0	15,15,17	0.59	0
9	NAG	X	1	1,9	14,14,15	0.39	0	17,19,21	0.44	0
9	NAG	X	2	9	14,14,15	0.40	0	17,19,21	0.75	0
10	NAG	Y	1	10,1	14,14,15	0.47	0	17,19,21	0.63	0
10	NAG	Y	2	10	14,14,15	0.41	0	17,19,21	0.61	0
10	BMA	Y	3	10	11,11,12	0.38	0	15,15,17	0.62	0
10	MAN	Y	4	10	11,11,12	0.21	0	15,15,17	0.58	0
10	MAN	Y	5	10	11,11,12	0.30	0	15,15,17	0.58	0
9	NAG	Z	1	1,9	14,14,15	0.41	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	Z	2	9	14,14,15	0.41	0	17,19,21	0.75	1 (5%)
9	NAG	a	1	1,9	14,14,15	0.38	0	17,19,21	0.42	0
9	NAG	a	2	9	14,14,15	0.39	0	17,19,21	0.49	0
8	NAG	b	1	1,8	14,14,15	0.44	0	17,19,21	0.44	0
8	NAG	b	2	8	14,14,15	0.39	0	17,19,21	0.40	0
8	BMA	b	3	8	11,11,12	0.20	0	15,15,17	0.56	0
8	NAG	c	1	1,8	14,14,15	0.46	0	17,19,21	0.56	0
8	NAG	c	2	8	14,14,15	0.43	0	17,19,21	0.57	0
8	BMA	c	3	8	11,11,12	0.28	0	15,15,17	0.61	0
10	NAG	d	1	10,1	14,14,15	0.44	0	17,19,21	0.42	0
10	NAG	d	2	10	14,14,15	0.39	0	17,19,21	0.42	0
10	BMA	d	3	10	11,11,12	0.27	0	15,15,17	0.75	1 (6%)
10	MAN	d	4	10	11,11,12	0.26	0	15,15,17	0.62	0
10	MAN	d	5	10	11,11,12	0.27	0	15,15,17	0.53	0
9	NAG	e	1	1,9	14,14,15	0.59	0	17,19,21	1.26	2 (11%)
9	NAG	e	2	9	14,14,15	0.55	0	17,19,21	0.93	1 (5%)
9	NAG	f	1	1,9	14,14,15	0.43	0	17,19,21	0.40	0
9	NAG	f	2	9	14,14,15	0.41	0	17,19,21	0.49	0
10	NAG	g	1	10,1	14,14,15	0.50	0	17,19,21	1.40	2 (11%)
10	NAG	g	2	10	14,14,15	0.43	0	17,19,21	0.43	0
10	BMA	g	3	10	11,11,12	0.24	0	15,15,17	0.71	1 (6%)
10	MAN	g	4	10	11,11,12	0.29	0	15,15,17	0.53	0
10	MAN	g	5	10	11,11,12	0.29	0	15,15,17	0.52	0
10	NAG	h	1	10,1	14,14,15	0.45	0	17,19,21	1.16	1 (5%)
10	NAG	h	2	10	14,14,15	0.49	0	17,19,21	0.77	1 (5%)
10	BMA	h	3	10	11,11,12	0.37	0	15,15,17	0.72	0
10	MAN	h	4	10	11,11,12	0.30	0	15,15,17	0.60	0
10	MAN	h	5	10	11,11,12	0.31	0	15,15,17	0.54	0
9	NAG	i	1	1,9	14,14,15	0.41	0	17,19,21	0.55	0
9	NAG	i	2	9	14,14,15	0.41	0	17,19,21	0.55	0
11	NAG	j	1	11,1	14,14,15	0.41	0	17,19,21	0.39	0
11	NAG	j	2	11	14,14,15	0.40	0	17,19,21	0.46	0
11	BMA	j	3	11	11,11,12	0.27	0	15,15,17	0.53	0
9	NAG	k	1	1,9	14,14,15	0.64	0	17,19,21	1.10	1 (5%)
9	NAG	k	2	9	14,14,15	0.67	0	17,19,21	1.30	1 (5%)
8	NAG	l	1	1,8	14,14,15	0.50	0	17,19,21	1.00	1 (5%)
8	NAG	l	2	8	14,14,15	0.57	0	17,19,21	0.75	1 (5%)
8	BMA	l	3	8	11,11,12	0.84	1 (9%)	15,15,17	1.03	2 (13%)
9	NAG	m	1	1,9	14,14,15	0.47	0	17,19,21	0.85	0
9	NAG	m	2	9	14,14,15	0.53	0	17,19,21	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	n	1	1,9	14,14,15	0.55	0	17,19,21	0.93	1 (5%)
9	NAG	n	2	9	14,14,15	0.56	0	17,19,21	0.92	1 (5%)
8	NAG	o	1	1,8	14,14,15	0.43	0	17,19,21	0.54	0
8	NAG	o	2	8	14,14,15	0.42	0	17,19,21	0.41	0
8	BMA	o	3	8	11,11,12	0.28	0	15,15,17	0.64	0
9	NAG	p	1	1,9	14,14,15	0.38	0	17,19,21	0.79	1 (5%)
9	NAG	p	2	9	14,14,15	0.42	0	17,19,21	0.54	0
9	NAG	q	1	1,9	14,14,15	0.40	0	17,19,21	0.59	0
9	NAG	q	2	9	14,14,15	0.40	0	17,19,21	0.38	0
10	NAG	r	1	10,1	14,14,15	0.48	0	17,19,21	0.90	1 (5%)
10	NAG	r	2	10	14,14,15	0.42	0	17,19,21	0.66	0
10	BMA	r	3	10	11,11,12	0.28	0	15,15,17	0.73	1 (6%)
10	MAN	r	4	10	11,11,12	0.26	0	15,15,17	0.59	0
10	MAN	r	5	10	11,11,12	0.95	1 (9%)	15,15,17	0.92	1 (6%)
9	NAG	s	1	1,9	14,14,15	0.45	0	17,19,21	0.70	0
9	NAG	s	2	9	14,14,15	0.40	0	17,19,21	0.49	0
10	NAG	t	1	10,1	14,14,15	0.44	0	17,19,21	0.98	0
10	NAG	t	2	10	14,14,15	0.41	0	17,19,21	0.70	0
10	BMA	t	3	10	11,11,12	0.28	0	15,15,17	0.45	0
10	MAN	t	4	10	11,11,12	0.31	0	15,15,17	0.57	0
10	MAN	t	5	10	11,11,12	0.27	0	15,15,17	0.57	0
9	NAG	u	1	1,9	14,14,15	0.59	0	17,19,21	0.83	1 (5%)
9	NAG	u	2	9	14,14,15	0.57	0	17,19,21	1.00	1 (5%)
9	NAG	v	1	1,9	14,14,15	0.42	0	17,19,21	0.60	0
9	NAG	v	2	9	14,14,15	0.39	0	17,19,21	0.42	0
8	NAG	w	1	1,8	14,14,15	0.52	0	17,19,21	1.04	1 (5%)
8	NAG	w	2	8	14,14,15	0.38	0	17,19,21	0.66	0
8	BMA	w	3	8	11,11,12	0.22	0	15,15,17	0.63	0
8	NAG	x	1	1,8	14,14,15	0.48	0	17,19,21	0.74	0
8	NAG	x	2	8	14,14,15	0.40	0	17,19,21	0.99	1 (5%)
8	BMA	x	3	8	11,11,12	0.30	0	15,15,17	0.57	0
10	NAG	y	1	10,1	14,14,15	0.46	0	17,19,21	0.50	0
10	NAG	y	2	10	14,14,15	0.44	0	17,19,21	0.53	0
10	BMA	y	3	10	11,11,12	0.29	0	15,15,17	0.80	1 (6%)
10	MAN	y	4	10	11,11,12	0.28	0	15,15,17	0.52	0
10	MAN	y	5	10	11,11,12	0.27	0	15,15,17	0.52	0
9	NAG	z	1	1,9	14,14,15	0.54	0	17,19,21	1.14	1 (5%)
9	NAG	z	2	9	14,14,15	0.63	0	17,19,21	1.00	1 (5%)

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
9	NAG	0	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	0	2	9	-	2/6/23/26	0/1/1/1
10	NAG	1	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	1	2	10	-	0/6/23/26	0/1/1/1
10	BMA	1	3	10	-	0/2/19/22	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
10	NAG	2	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	2	2	10	-	0/6/23/26	0/1/1/1
10	BMA	2	3	10	-	2/2/19/22	0/1/1/1
10	MAN	2	4	10	-	0/2/19/22	0/1/1/1
10	MAN	2	5	10	-	0/2/19/22	0/1/1/1
9	NAG	3	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	3	2	9	-	3/6/23/26	0/1/1/1
11	NAG	4	1	11,1	-	0/6/23/26	0/1/1/1
11	NAG	4	2	11	-	2/6/23/26	0/1/1/1
11	BMA	4	3	11	-	0/2/19/22	0/1/1/1
9	NAG	5	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	5	2	9	-	0/6/23/26	0/1/1/1
8	NAG	E	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	E	2	8	-	3/6/23/26	0/1/1/1
8	BMA	E	3	8	-	0/2/19/22	0/1/1/1
9	NAG	F	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	3/6/23/26	0/1/1/1
9	NAG	S	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	S	2	9	-	3/6/23/26	0/1/1/1
8	NAG	T	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	T	2	8	-	0/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
9	NAG	U	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	U	2	9	-	0/6/23/26	0/1/1/1
9	NAG	V	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	V	2	9	-	1/6/23/26	0/1/1/1
10	NAG	W	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	W	2	10	-	0/6/23/26	0/1/1/1
10	BMA	W	3	10	-	0/2/19/22	0/1/1/1
10	MAN	W	4	10	-	0/2/19/22	0/1/1/1
10	MAN	W	5	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	X	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
10	NAG	Y	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	1/6/23/26	0/1/1/1
10	BMA	Y	3	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	4	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	5	10	-	0/2/19/22	0/1/1/1
9	NAG	Z	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	1/6/23/26	0/1/1/1
9	NAG	a	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	a	2	9	-	0/6/23/26	0/1/1/1
8	NAG	b	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	0/6/23/26	0/1/1/1
8	BMA	b	3	8	-	0/2/19/22	0/1/1/1
8	NAG	c	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	c	2	8	-	0/6/23/26	0/1/1/1
8	BMA	c	3	8	-	0/2/19/22	0/1/1/1
10	NAG	d	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	d	2	10	-	0/6/23/26	0/1/1/1
10	BMA	d	3	10	-	0/2/19/22	0/1/1/1
10	MAN	d	4	10	-	0/2/19/22	0/1/1/1
10	MAN	d	5	10	-	0/2/19/22	0/1/1/1
9	NAG	e	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	e	2	9	-	0/6/23/26	0/1/1/1
9	NAG	f	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	f	2	9	-	0/6/23/26	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	-	1/2/19/22	0/1/1/1
10	MAN	g	4	10	-	0/2/19/22	0/1/1/1
10	MAN	g	5	10	-	0/2/19/22	0/1/1/1
10	NAG	h	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	h	2	10	-	0/6/23/26	0/1/1/1
10	BMA	h	3	10	-	0/2/19/22	0/1/1/1
10	MAN	h	4	10	-	0/2/19/22	0/1/1/1
10	MAN	h	5	10	-	1/2/19/22	0/1/1/1
9	NAG	i	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	i	2	9	-	3/6/23/26	0/1/1/1
11	NAG	j	1	11,1	-	0/6/23/26	0/1/1/1
11	NAG	j	2	11	-	2/6/23/26	0/1/1/1
11	BMA	j	3	11	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	k	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	k	2	9	-	1/6/23/26	0/1/1/1
8	NAG	l	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	l	2	8	-	0/6/23/26	0/1/1/1
8	BMA	l	3	8	-	0/2/19/22	0/1/1/1
9	NAG	m	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	m	2	9	-	1/6/23/26	0/1/1/1
9	NAG	n	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	n	2	9	-	0/6/23/26	0/1/1/1
8	NAG	o	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	o	2	8	-	0/6/23/26	0/1/1/1
8	BMA	o	3	8	-	0/2/19/22	0/1/1/1
9	NAG	p	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	p	2	9	-	1/6/23/26	0/1/1/1
9	NAG	q	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	q	2	9	-	2/6/23/26	0/1/1/1
10	NAG	r	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	r	2	10	-	1/6/23/26	0/1/1/1
10	BMA	r	3	10	-	2/2/19/22	0/1/1/1
10	MAN	r	4	10	-	0/2/19/22	0/1/1/1
10	MAN	r	5	10	-	0/2/19/22	0/1/1/1
9	NAG	s	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	s	2	9	-	0/6/23/26	0/1/1/1
10	NAG	t	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	t	2	10	-	0/6/23/26	0/1/1/1
10	BMA	t	3	10	-	0/2/19/22	0/1/1/1
10	MAN	t	4	10	-	0/2/19/22	0/1/1/1
10	MAN	t	5	10	-	0/2/19/22	0/1/1/1
9	NAG	u	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	u	2	9	-	0/6/23/26	0/1/1/1
9	NAG	v	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	v	2	9	-	2/6/23/26	0/1/1/1
8	NAG	w	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	w	2	8	-	4/6/23/26	0/1/1/1
8	BMA	w	3	8	-	0/2/19/22	0/1/1/1
8	NAG	x	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	x	2	8	-	0/6/23/26	0/1/1/1
8	BMA	x	3	8	-	0/2/19/22	0/1/1/1
10	NAG	y	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	y	2	10	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	y	3	10	-	0/2/19/22	0/1/1/1
10	MAN	y	4	10	-	0/2/19/22	0/1/1/1
10	MAN	y	5	10	-	0/2/19/22	0/1/1/1
9	NAG	z	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	z	2	9	-	3/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1	3	BMA	O5-C5	2.42	1.48	1.43
10	1	4	MAN	O5-C5	2.24	1.48	1.43
10	2	3	BMA	O5-C5	2.24	1.48	1.43
10	r	5	MAN	O5-C5	2.24	1.48	1.43
10	2	4	MAN	O5-C5	2.14	1.47	1.43

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	k	2	NAG	C1-O5-C5	4.06	117.69	112.19
9	e	1	NAG	C1-O5-C5	3.69	117.20	112.19
10	2	1	NAG	C1-O5-C5	3.68	117.18	112.19
10	1	3	BMA	C1-O5-C5	3.62	117.10	112.19
9	V	2	NAG	C1-O5-C5	3.57	117.03	112.19

There are no chirality outliers.

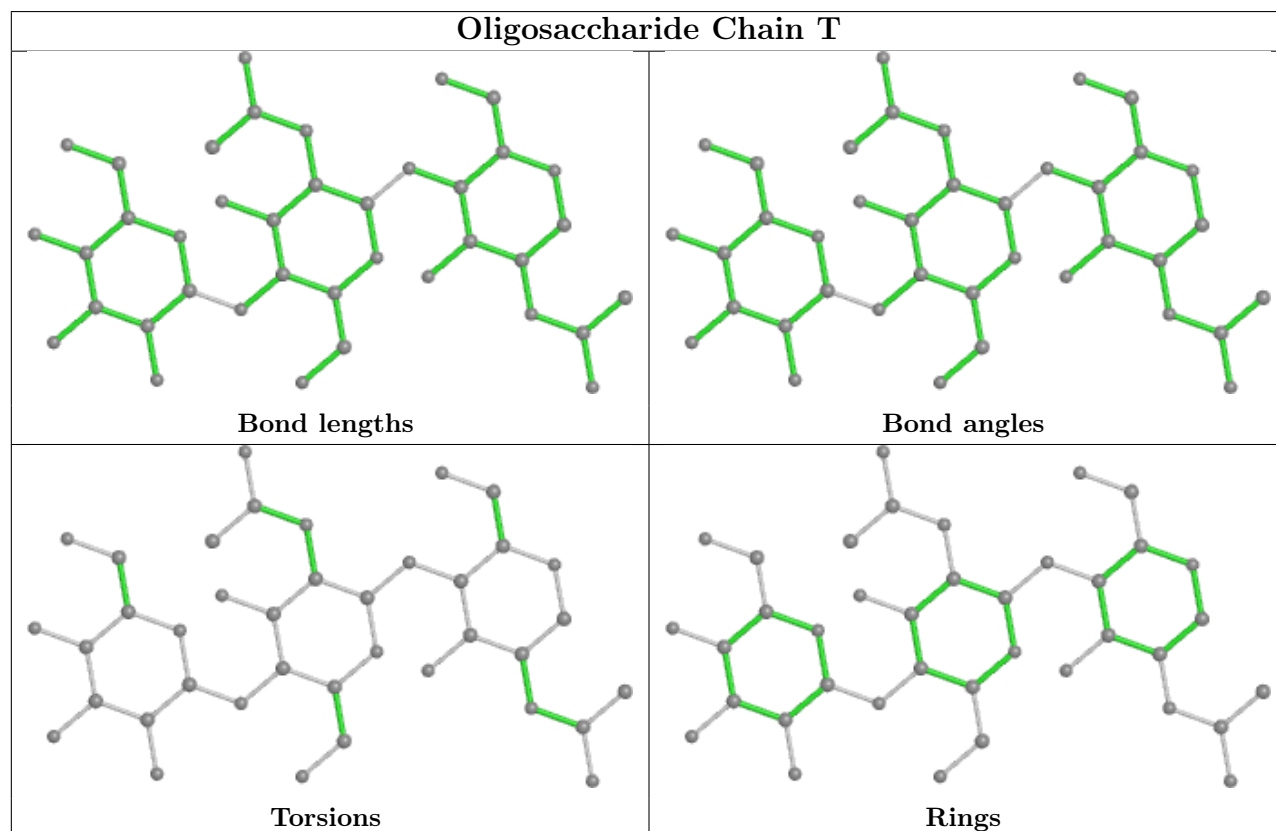
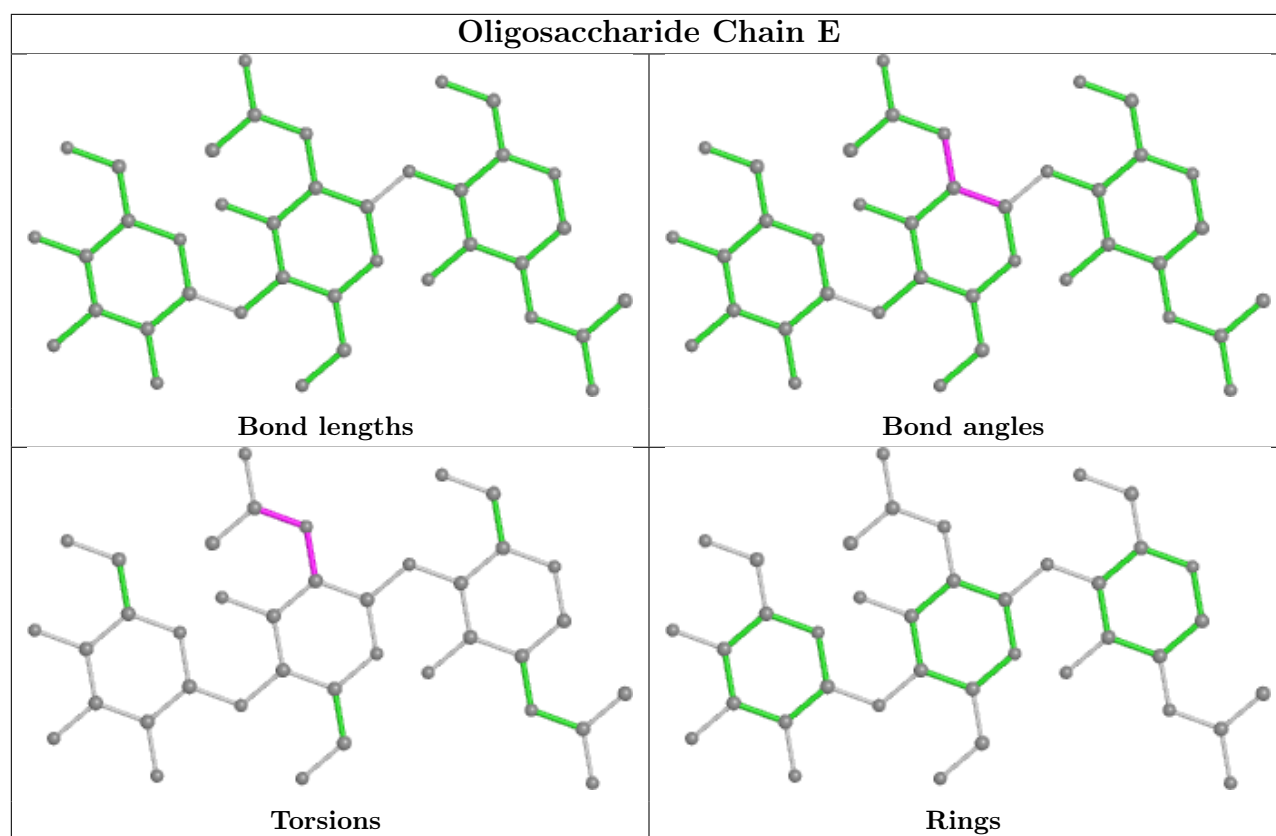
5 of 78 torsion outliers are listed below:

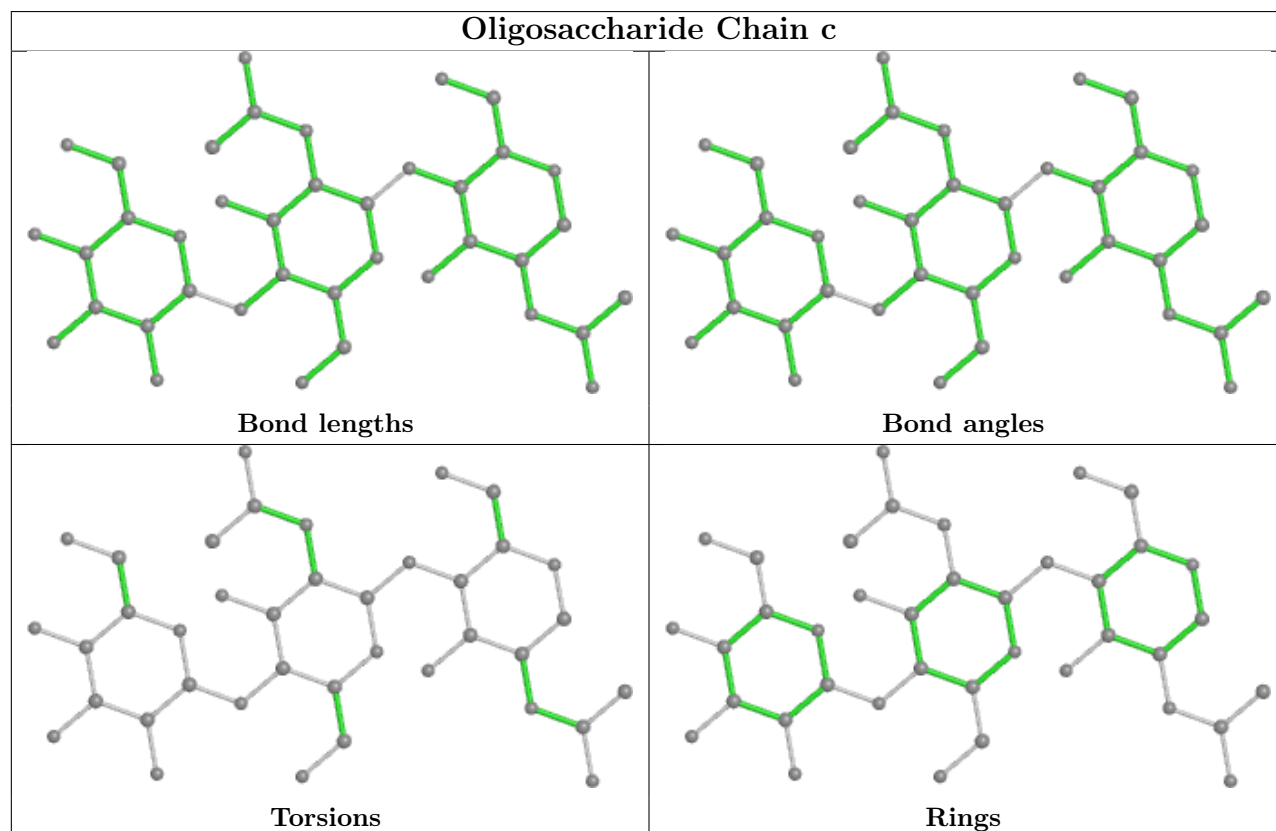
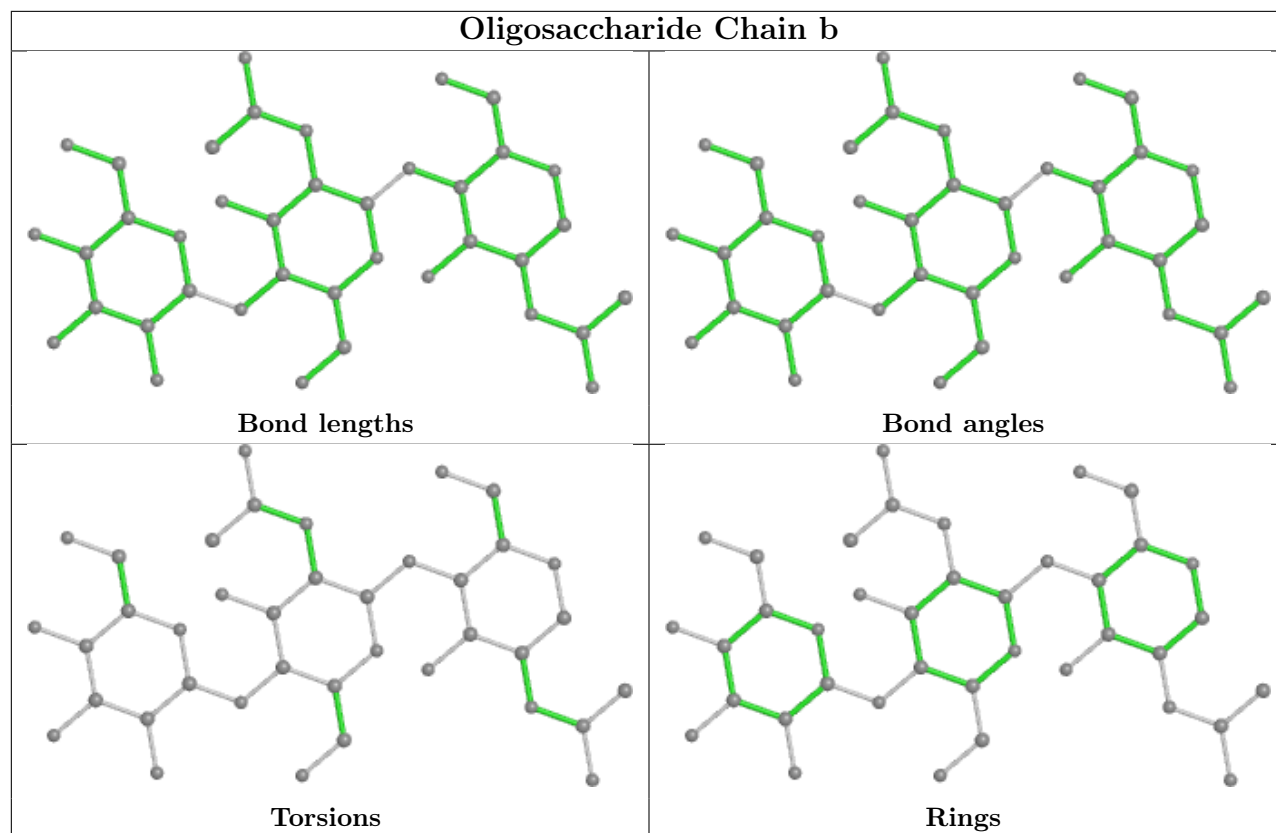
Mol	Chain	Res	Type	Atoms
9	F	2	NAG	C3-C2-N2-C7
9	F	2	NAG	C8-C7-N2-C2
9	F	2	NAG	O7-C7-N2-C2
10	y	2	NAG	C8-C7-N2-C2
10	y	2	NAG	O7-C7-N2-C2

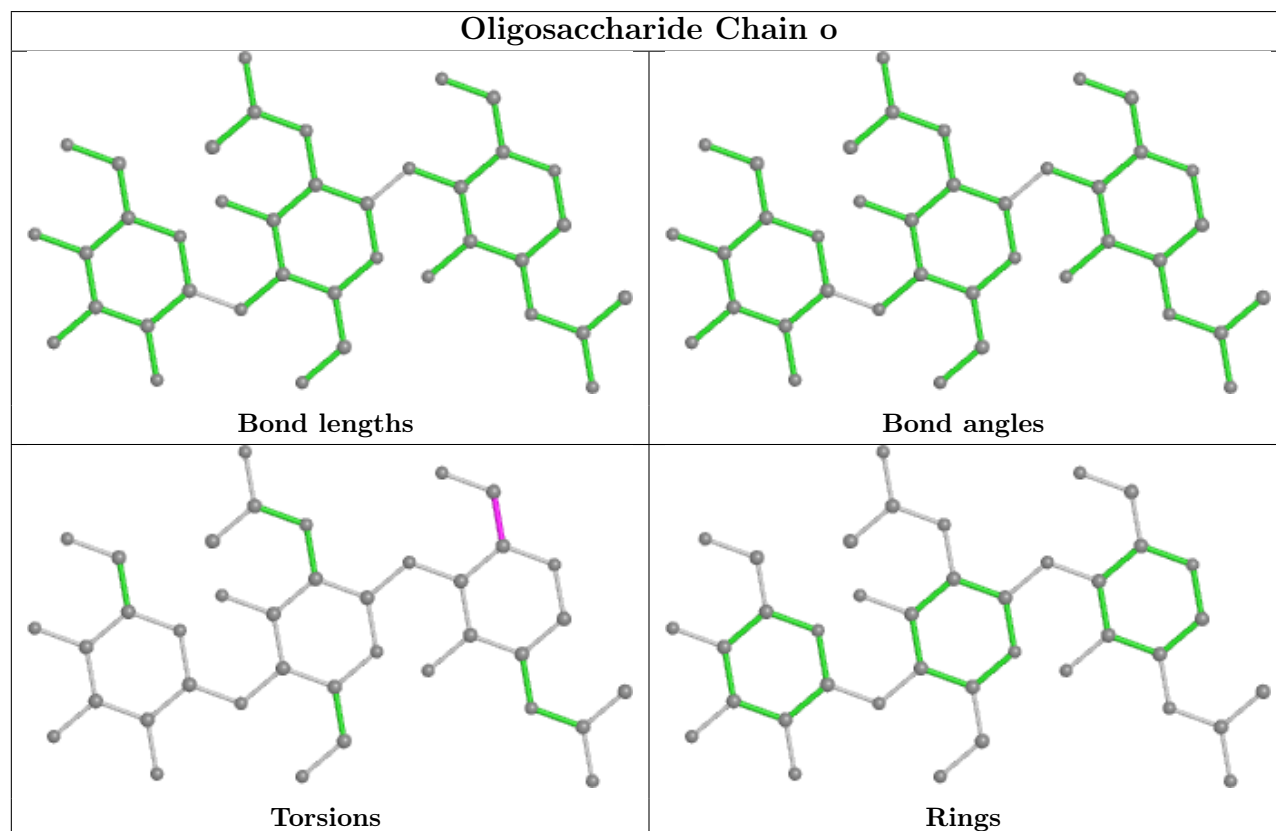
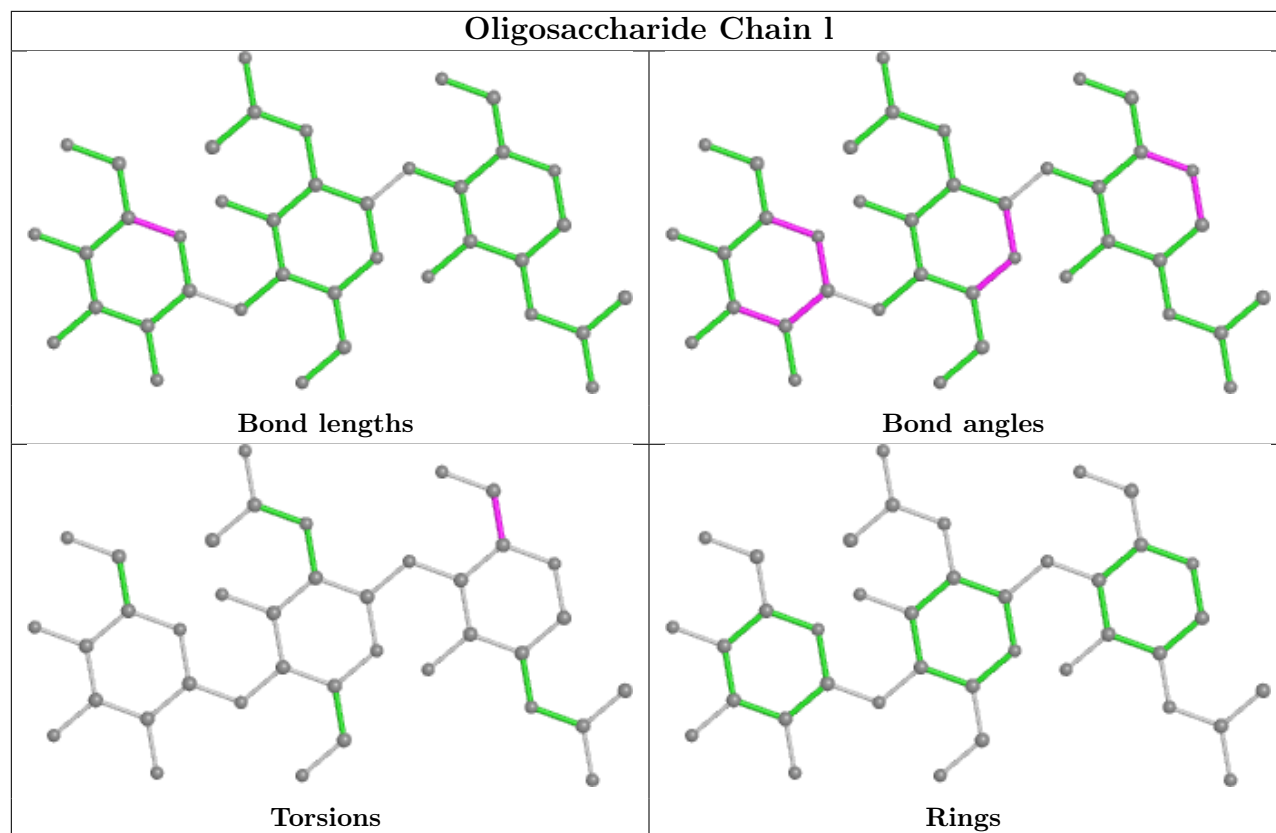
There are no ring outliers.

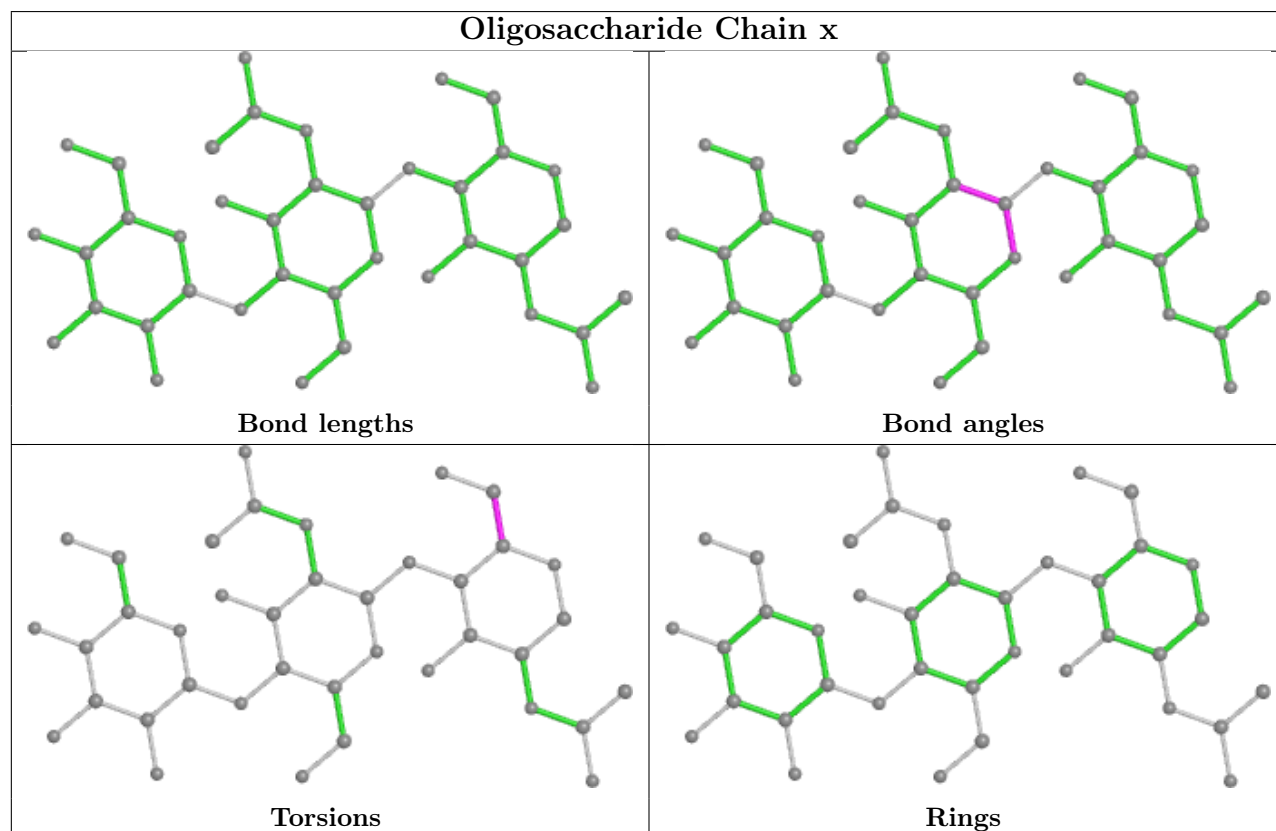
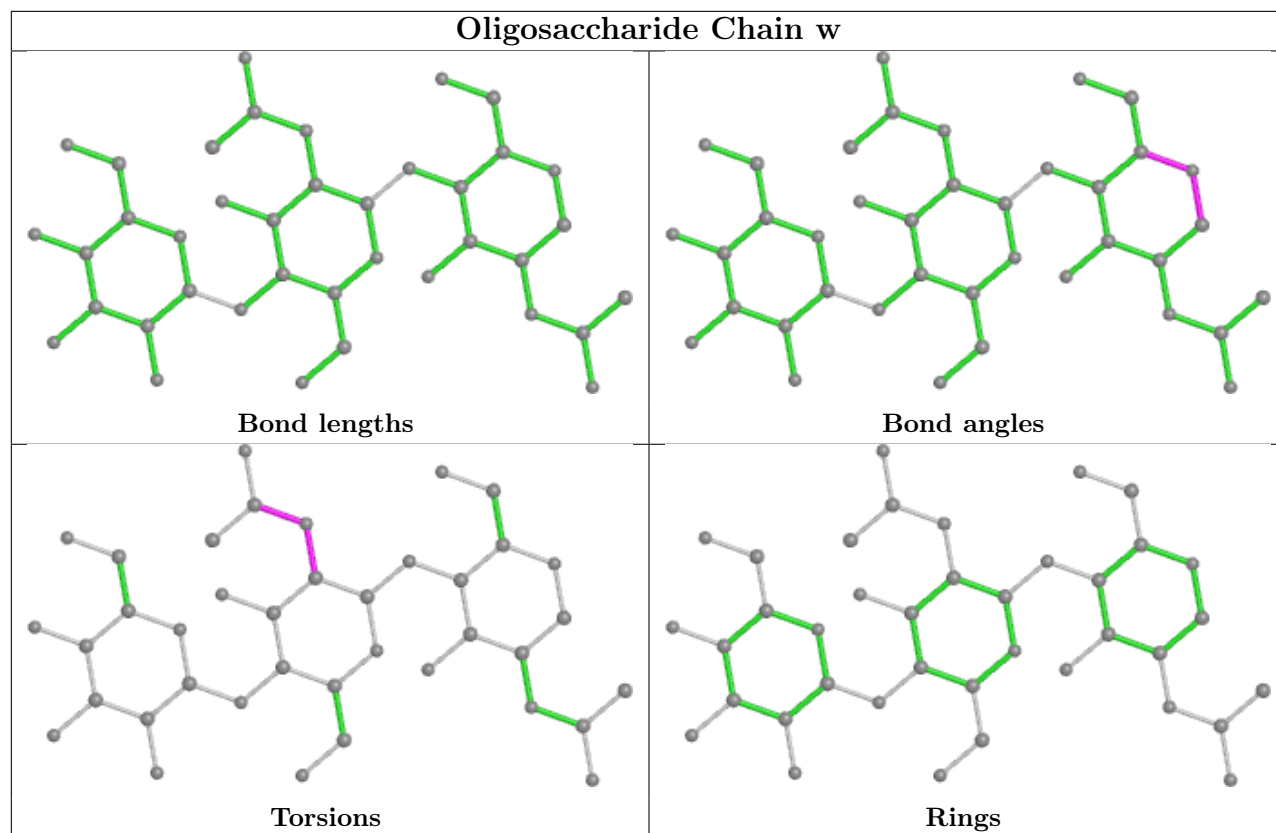
No monomer is involved in short contacts.

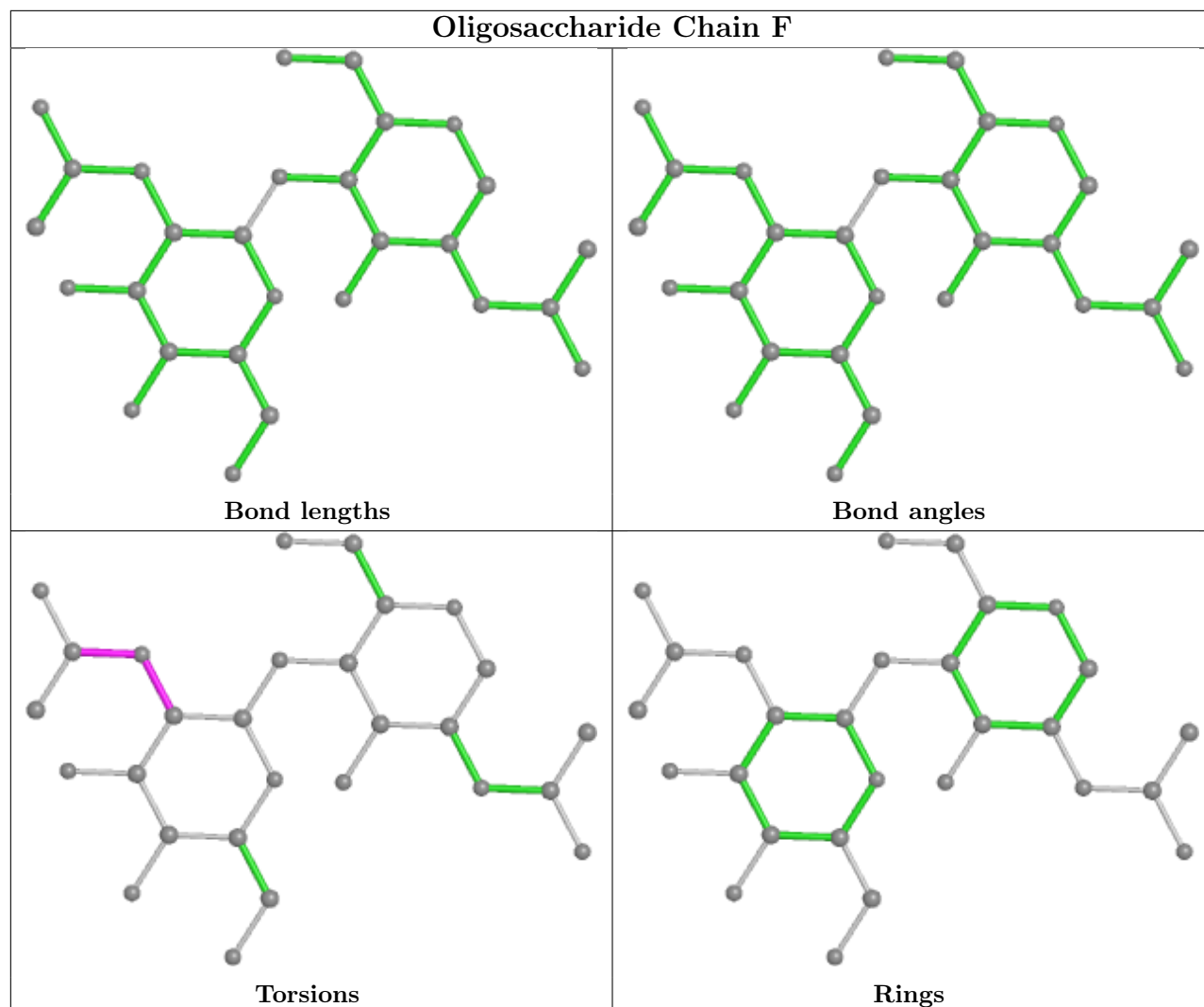
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

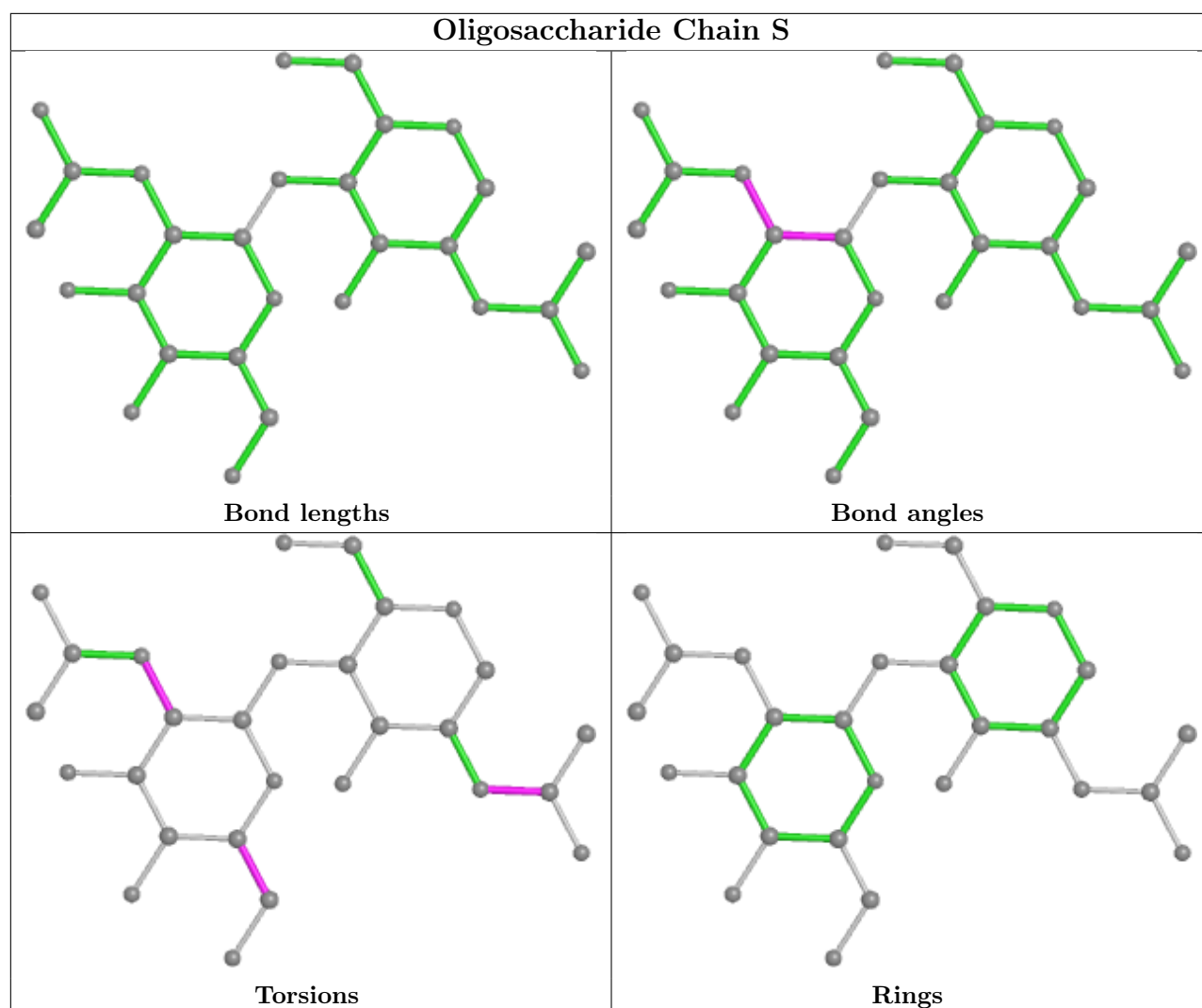


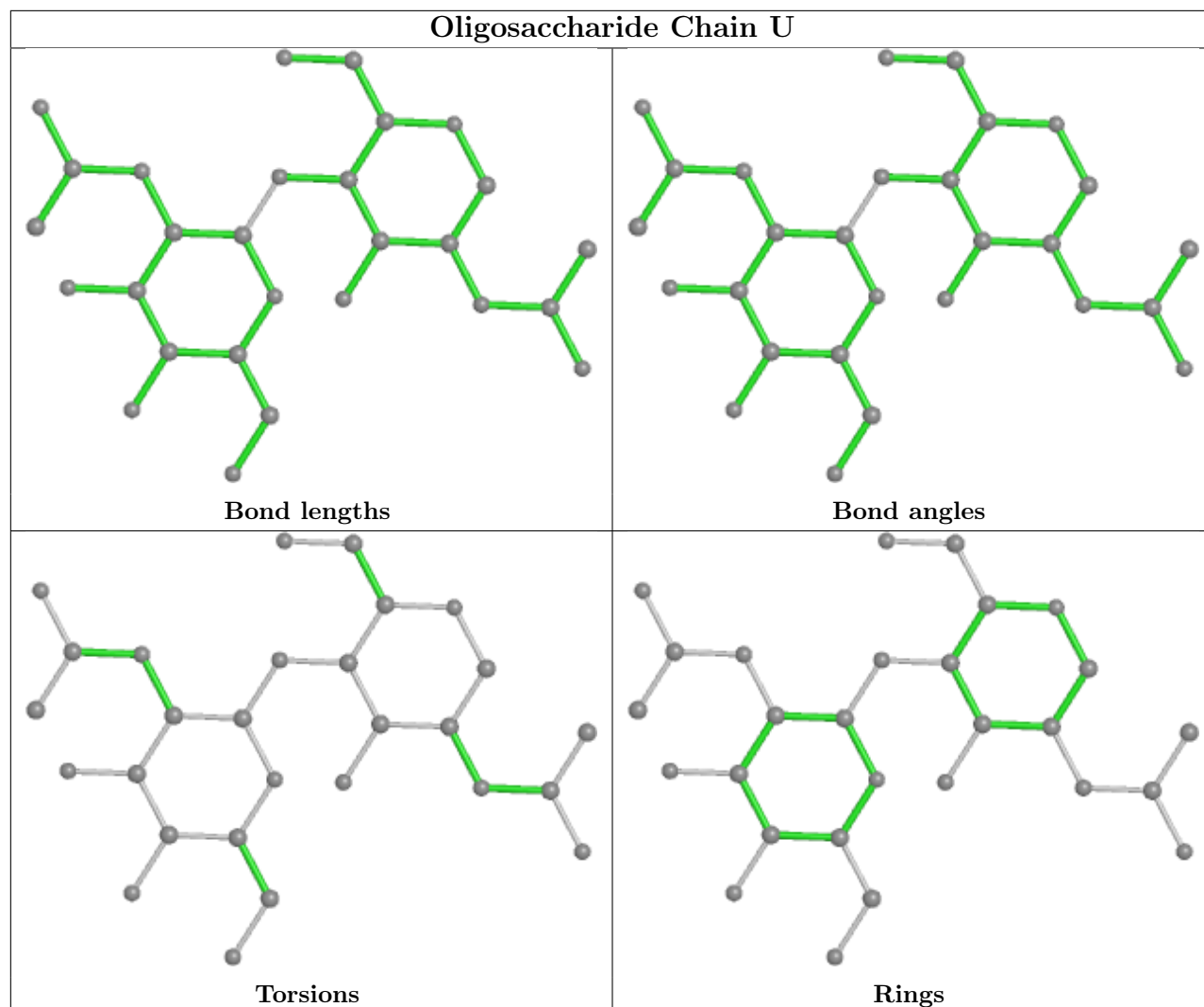


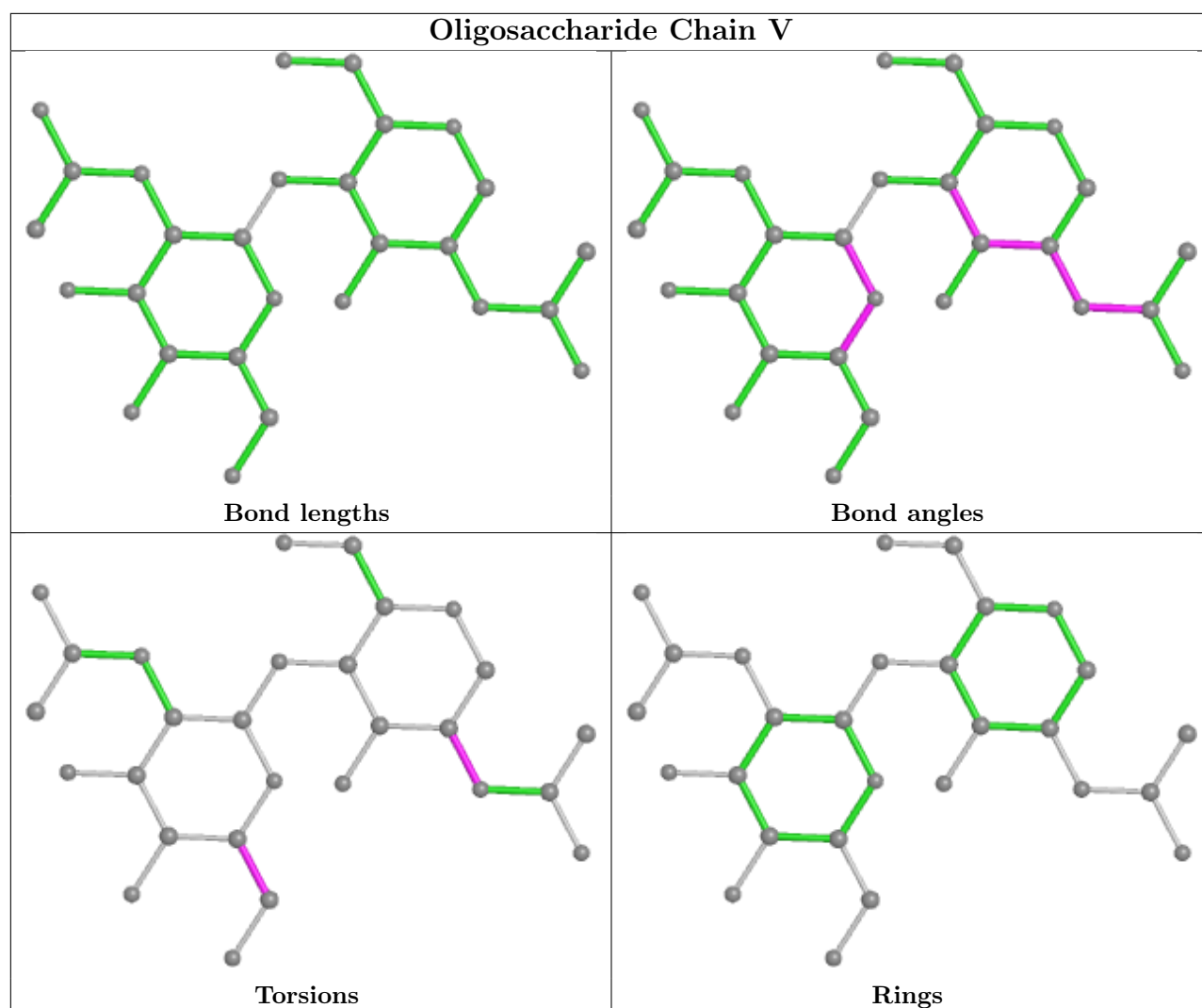


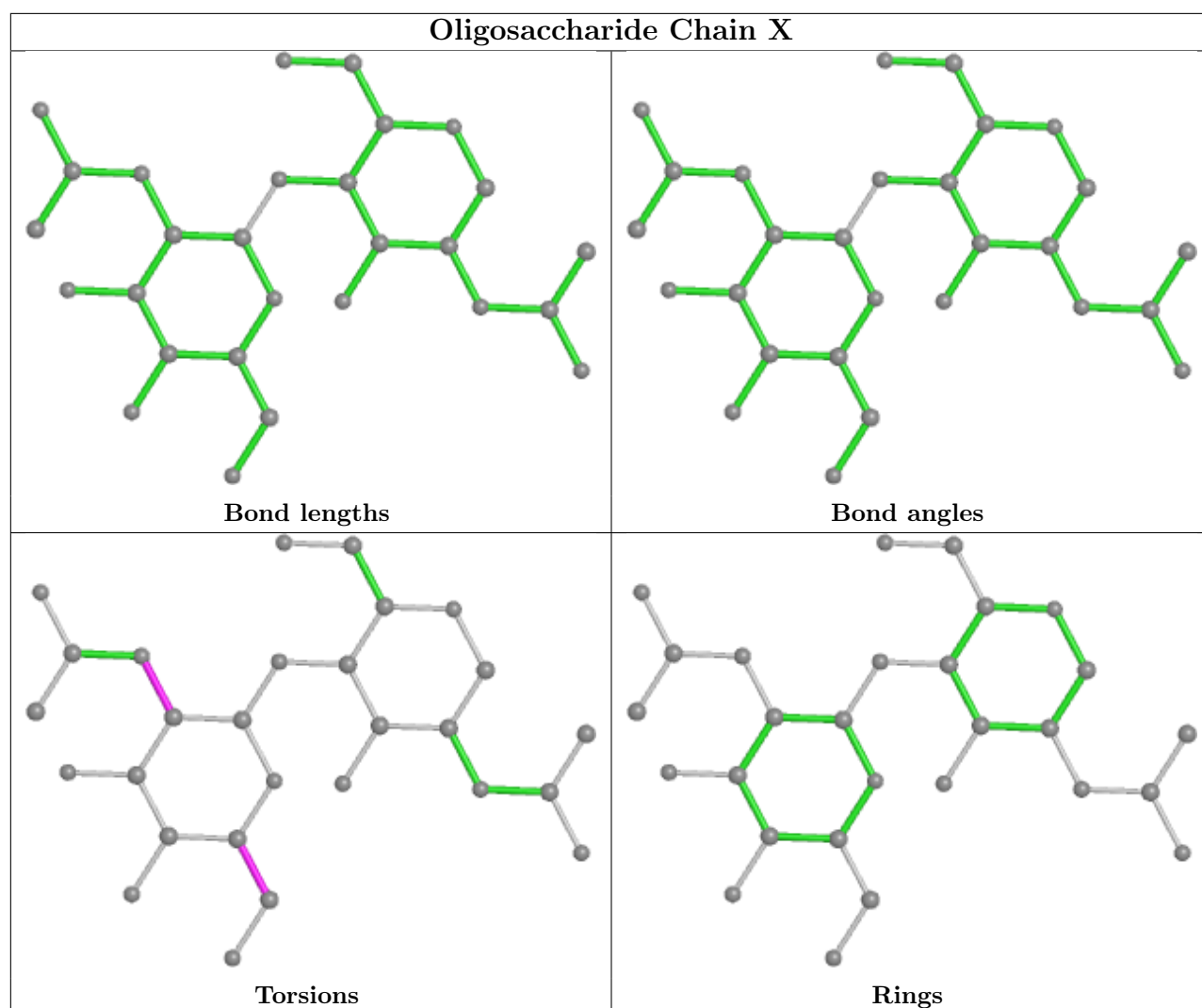


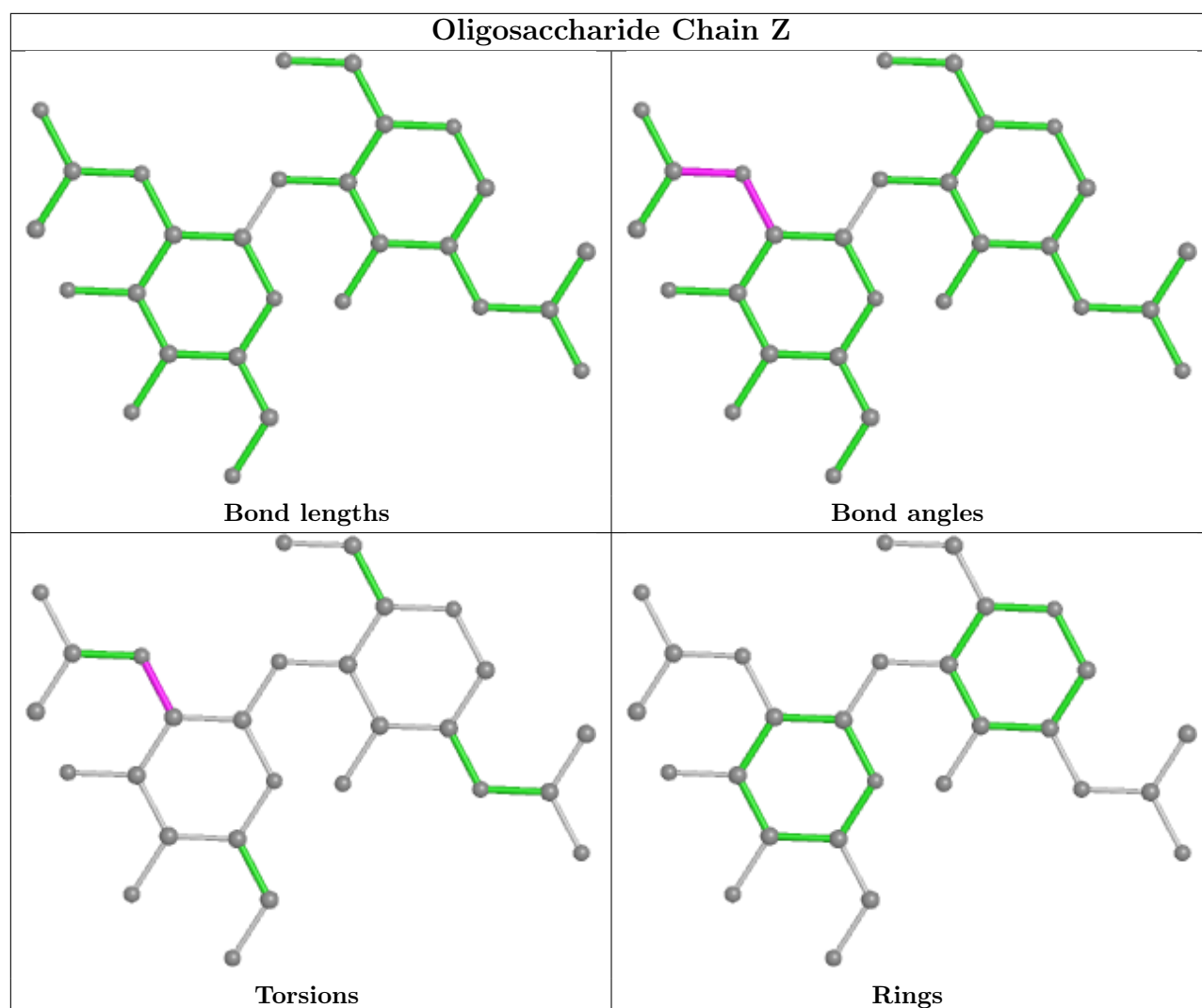


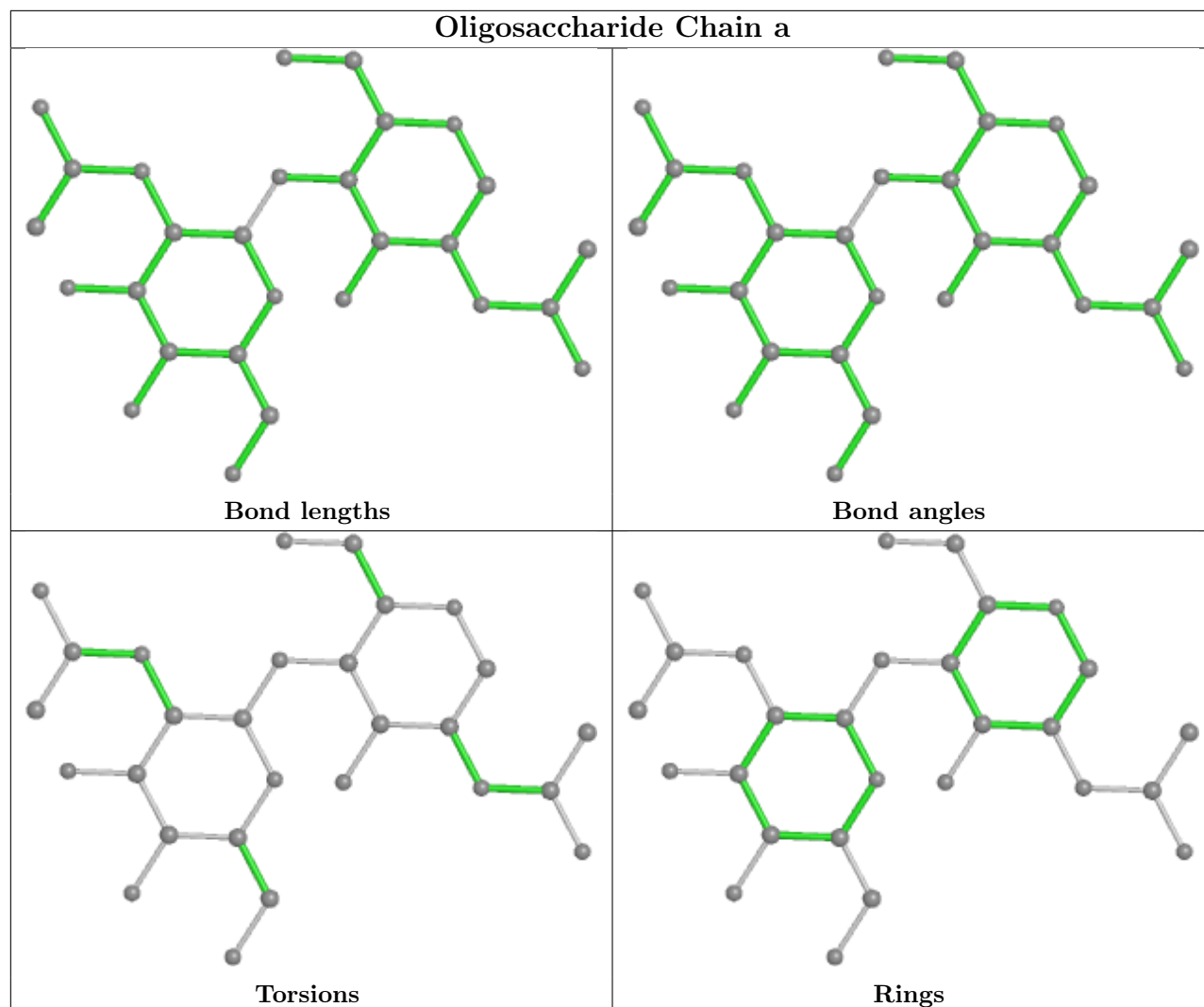


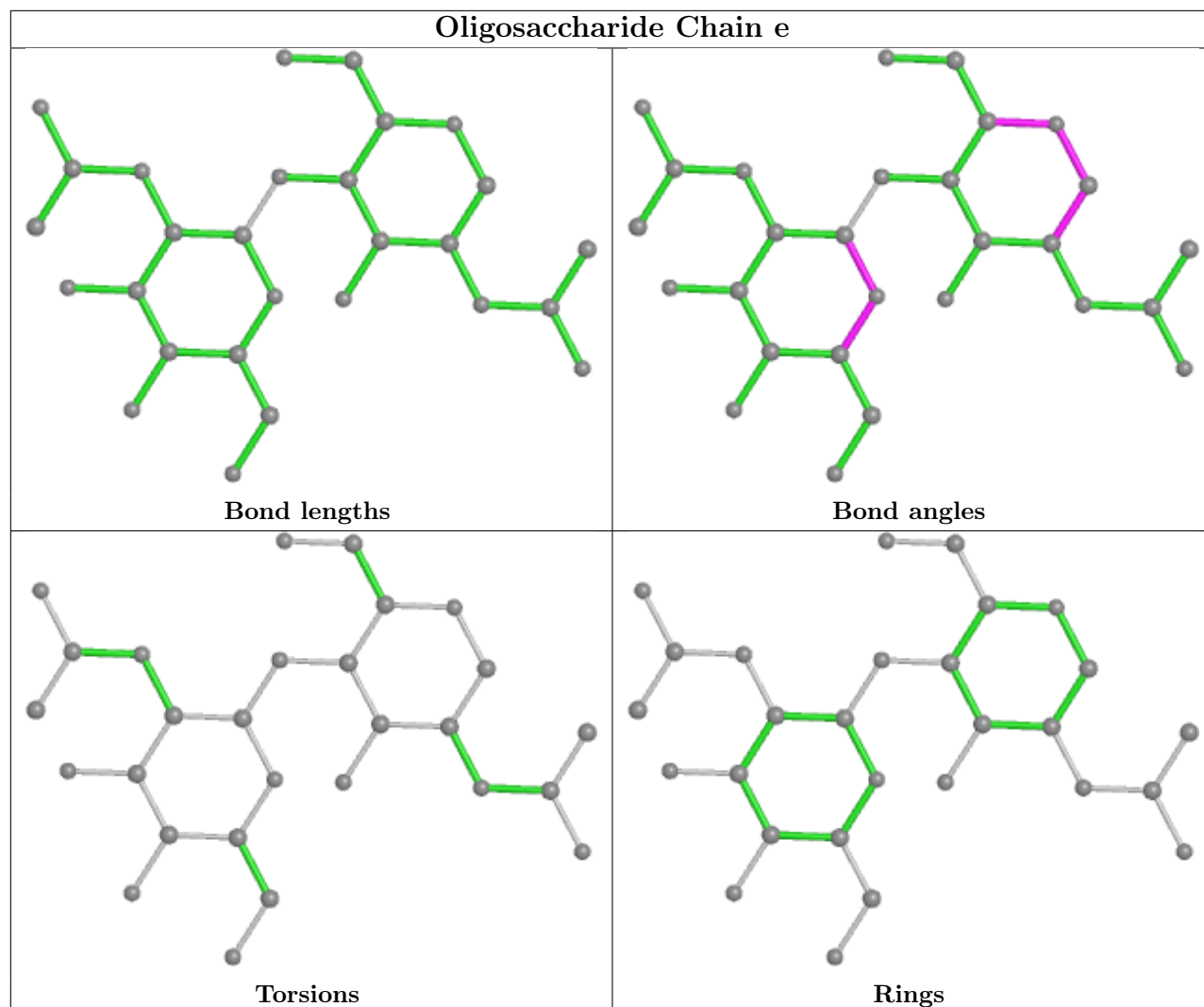


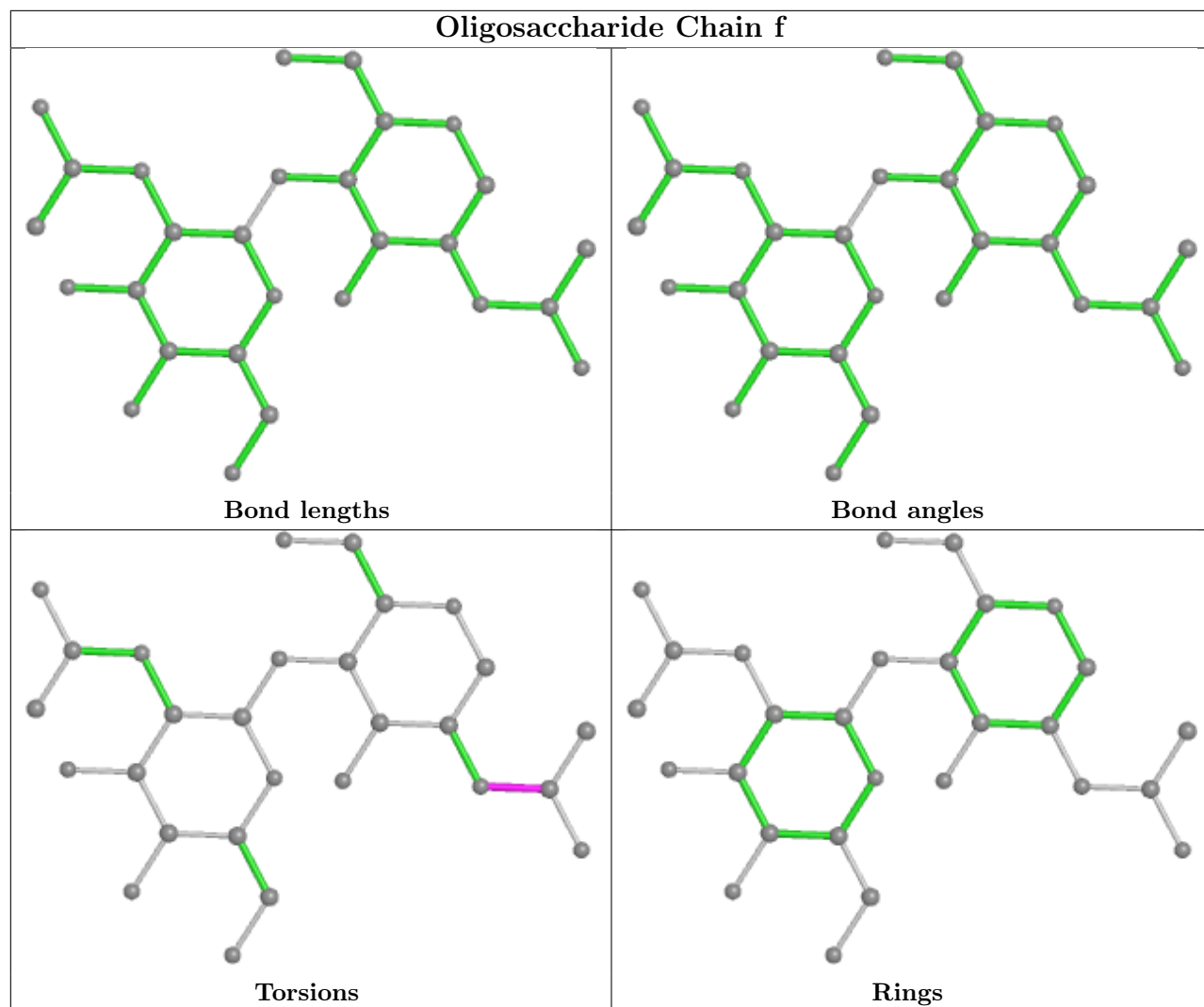


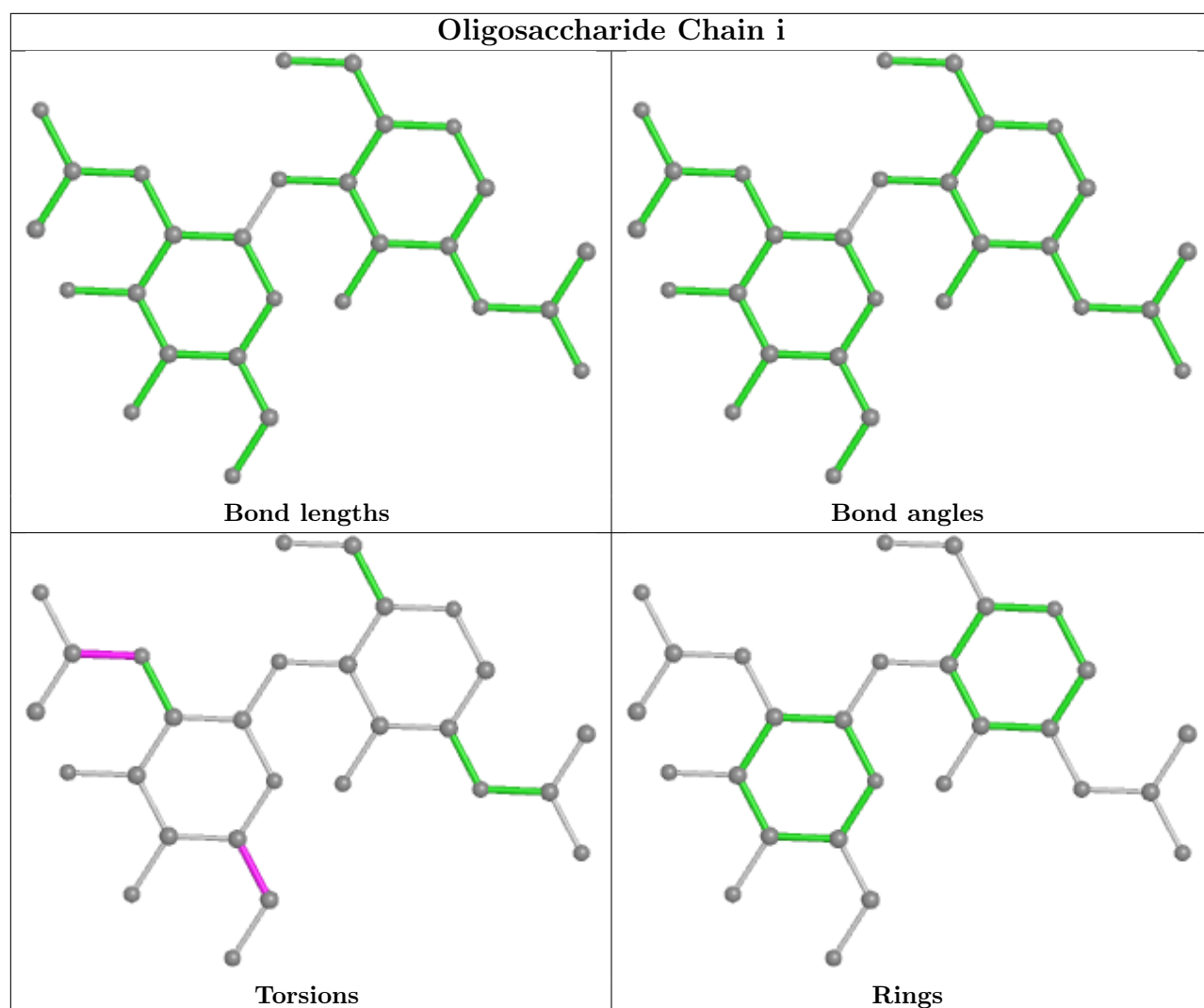


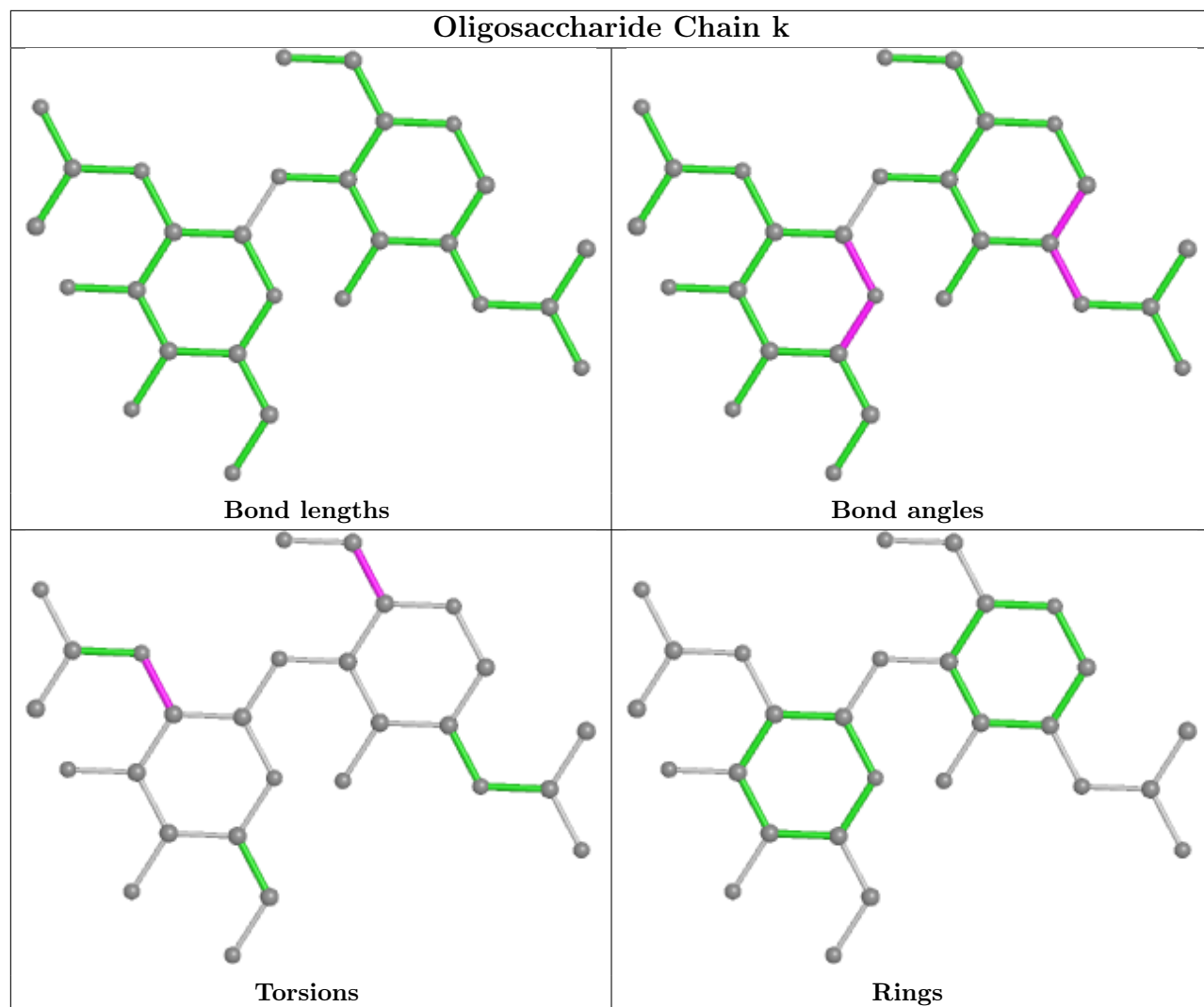


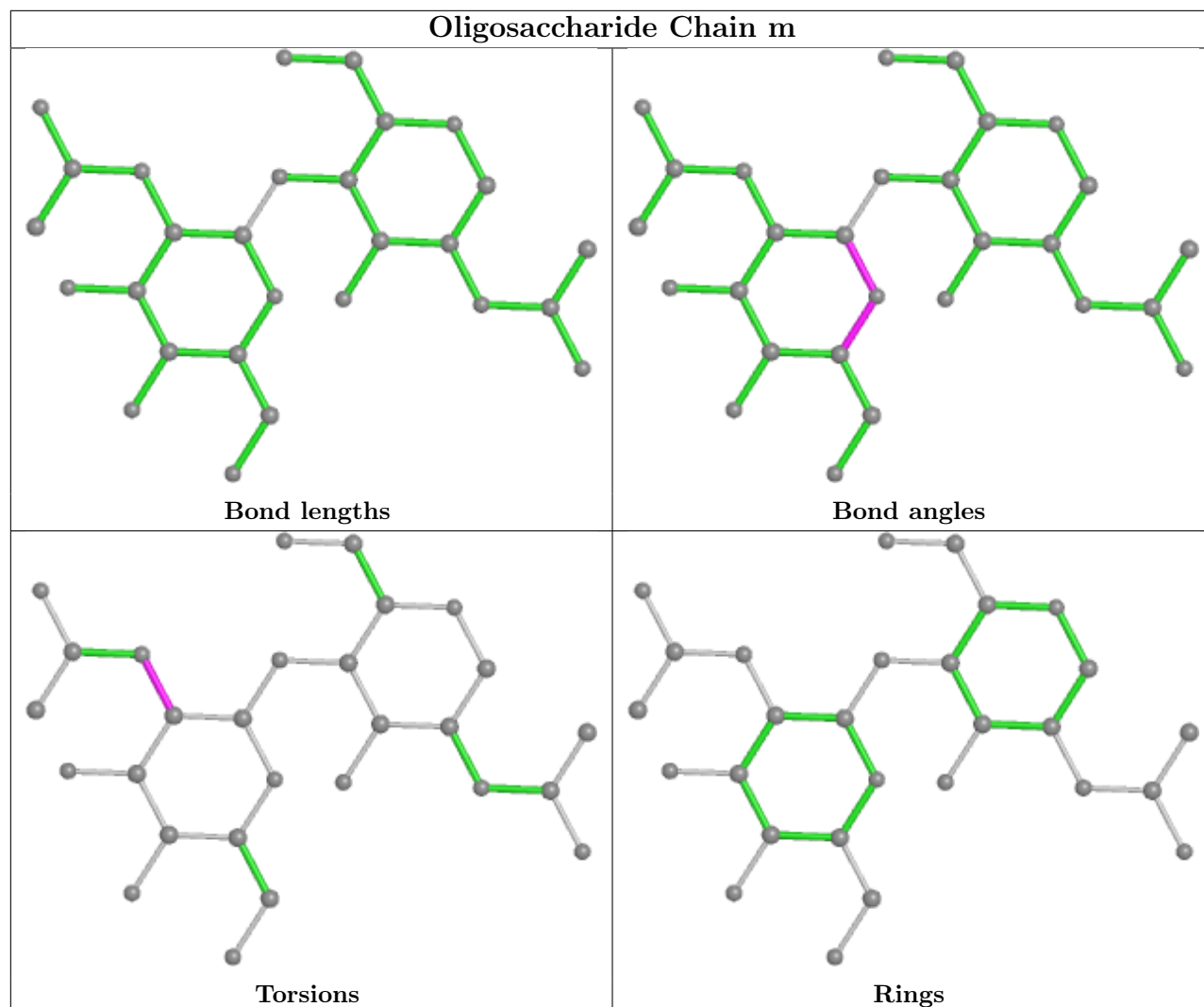


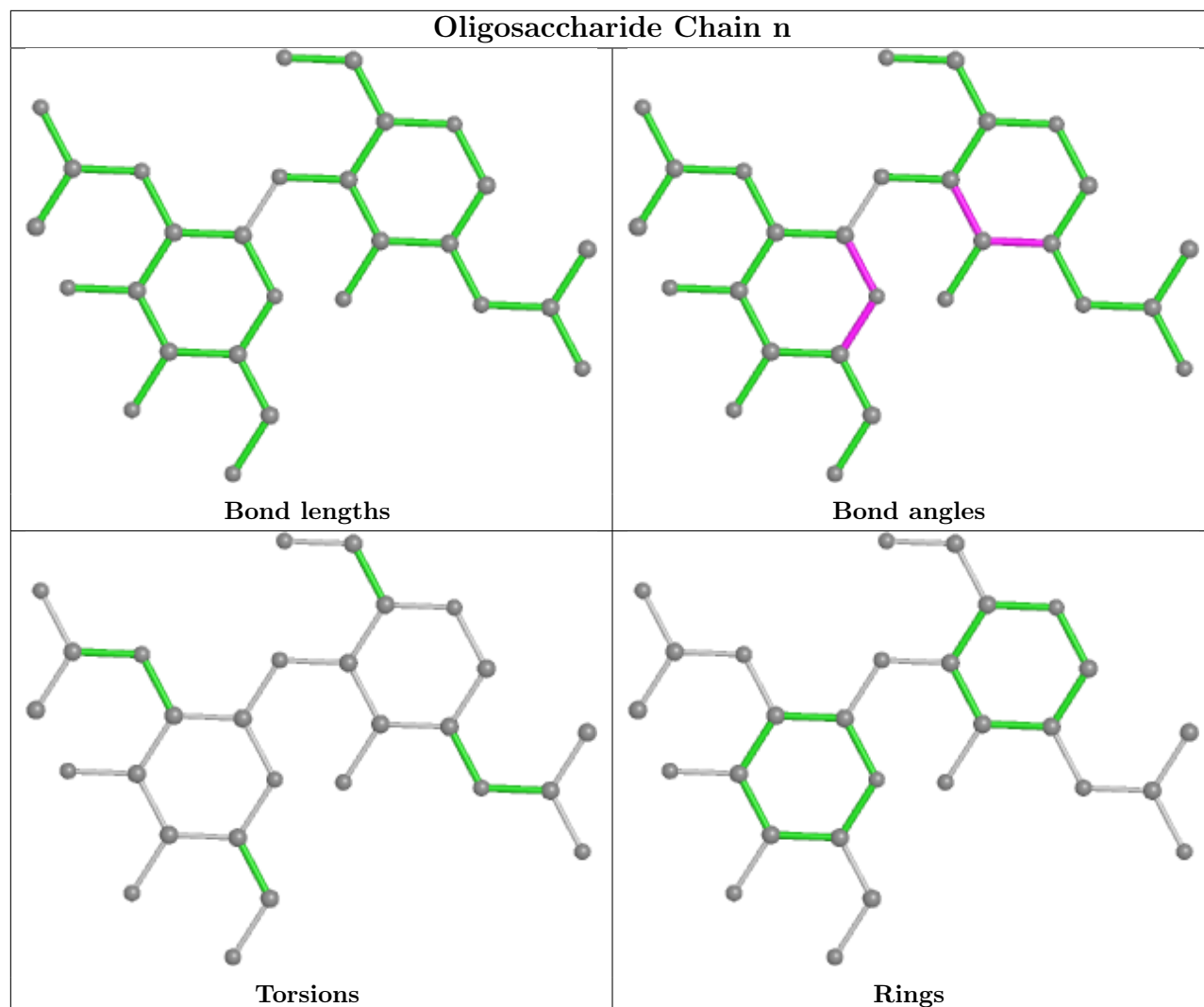


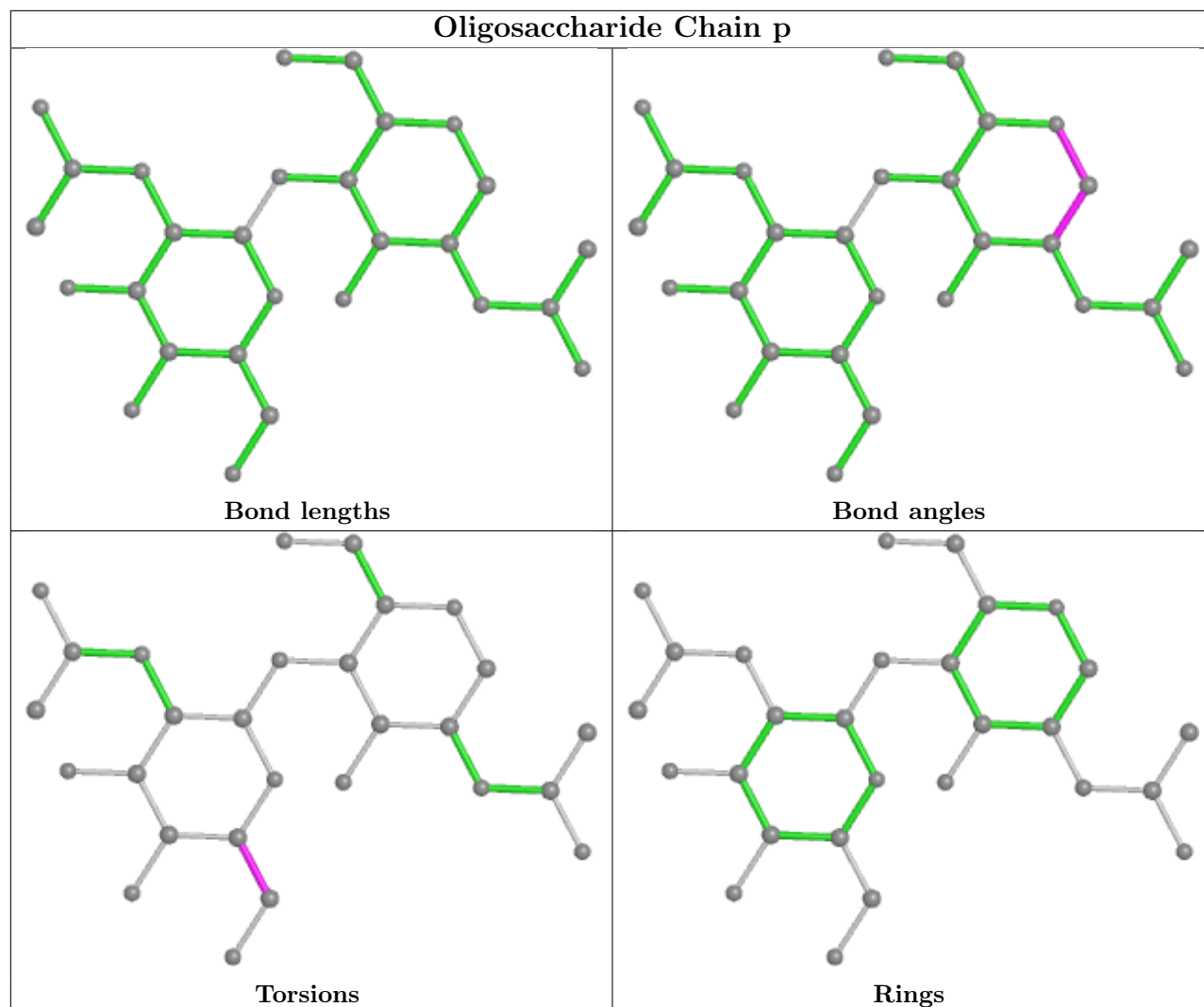


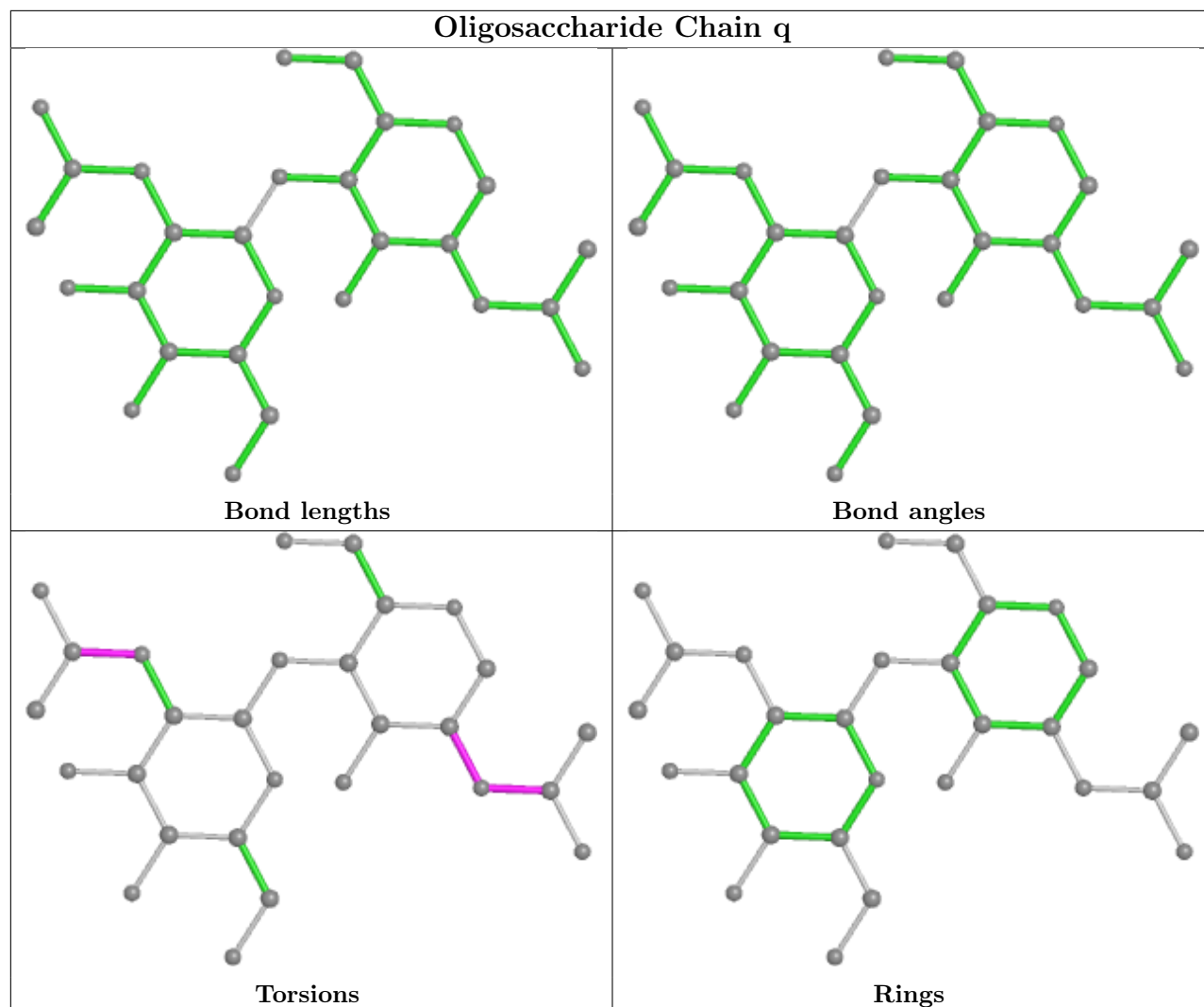


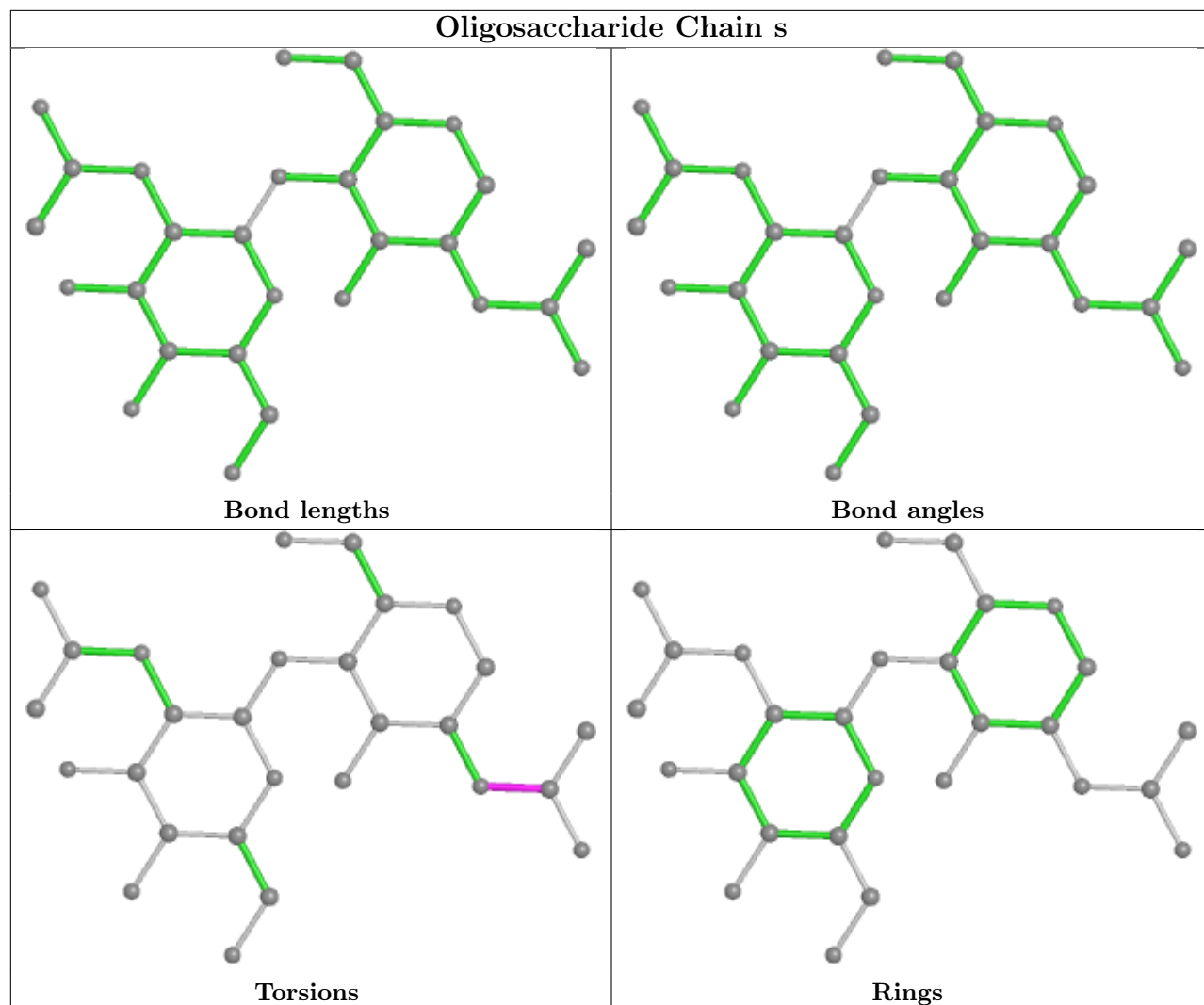


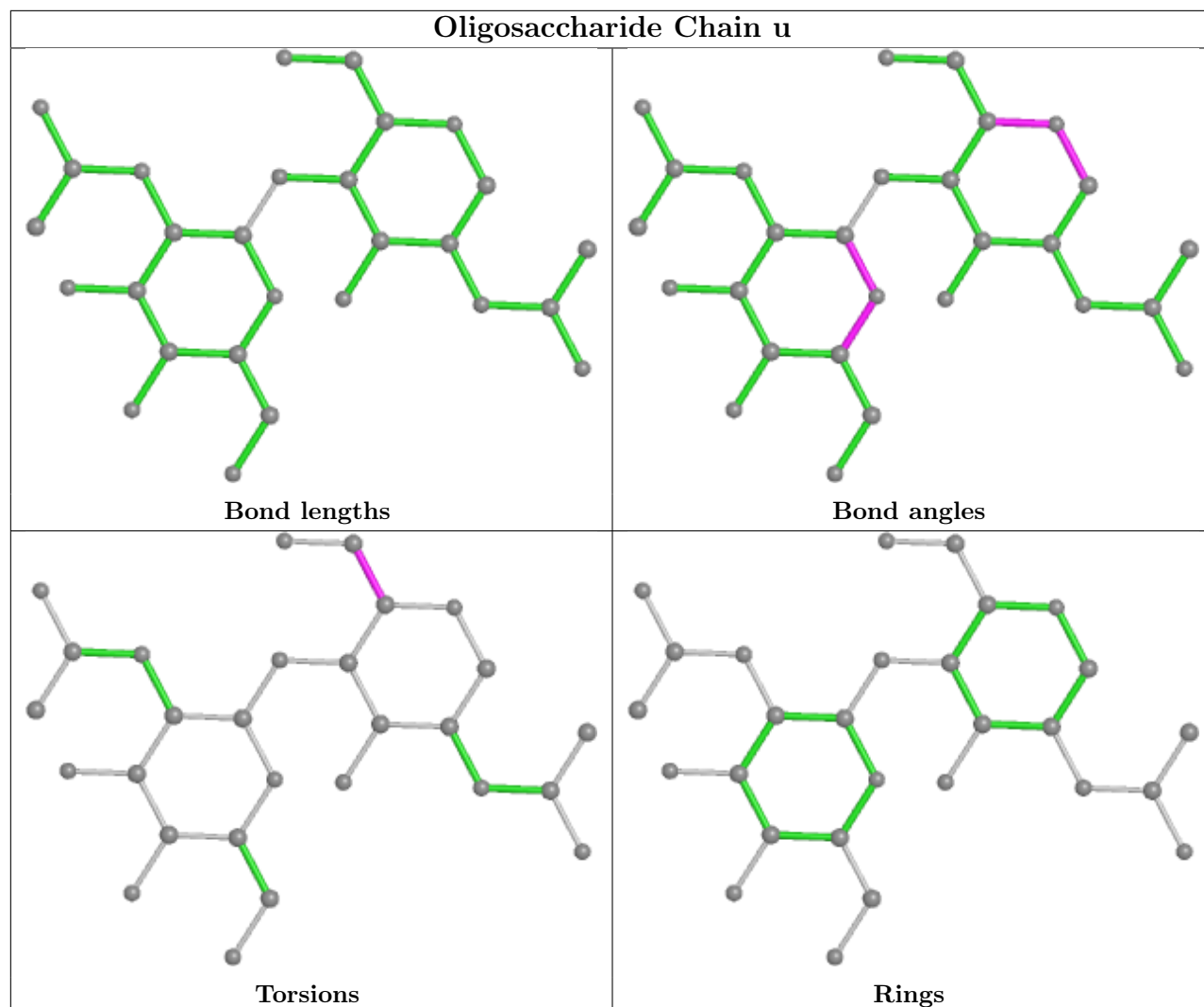


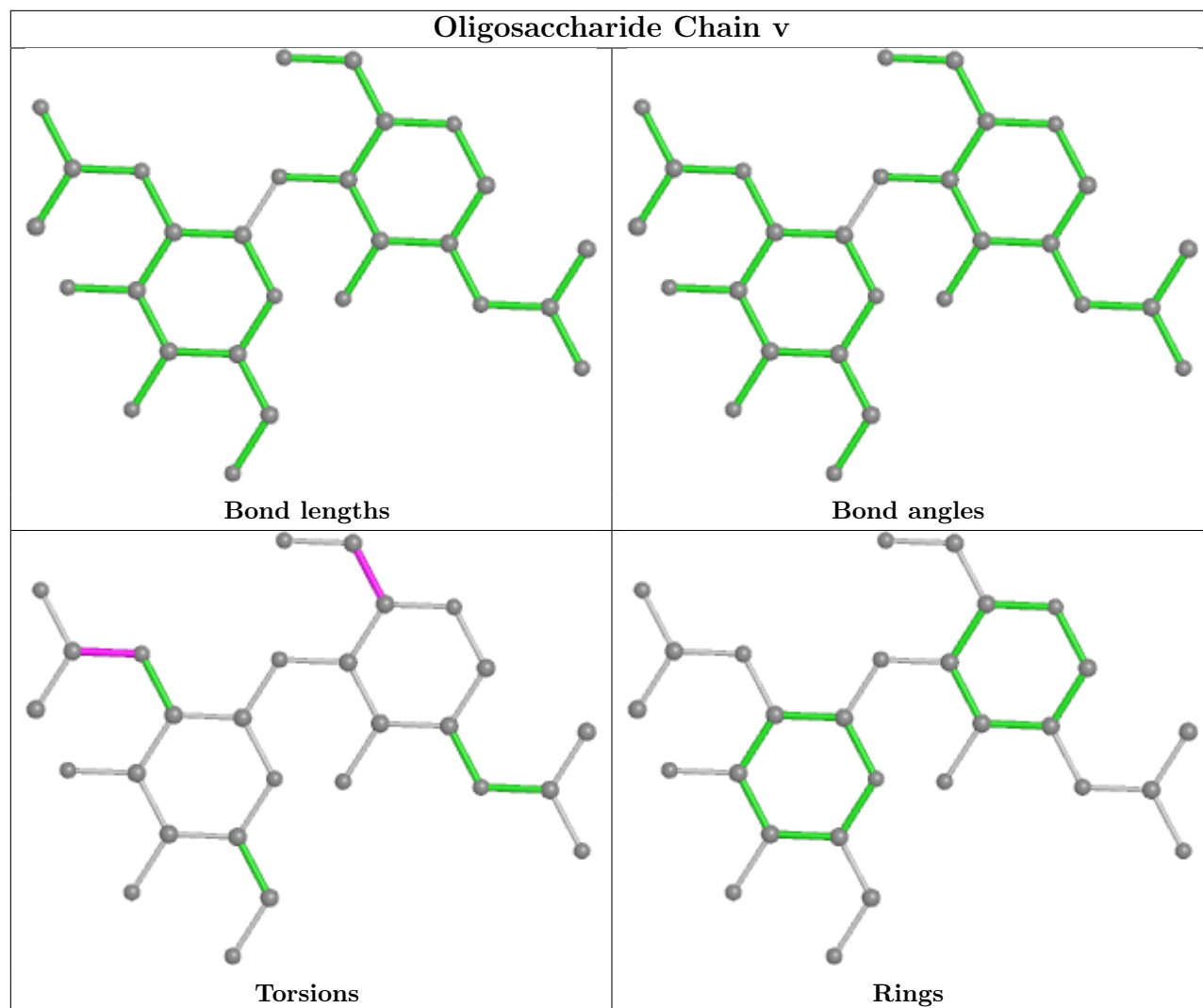


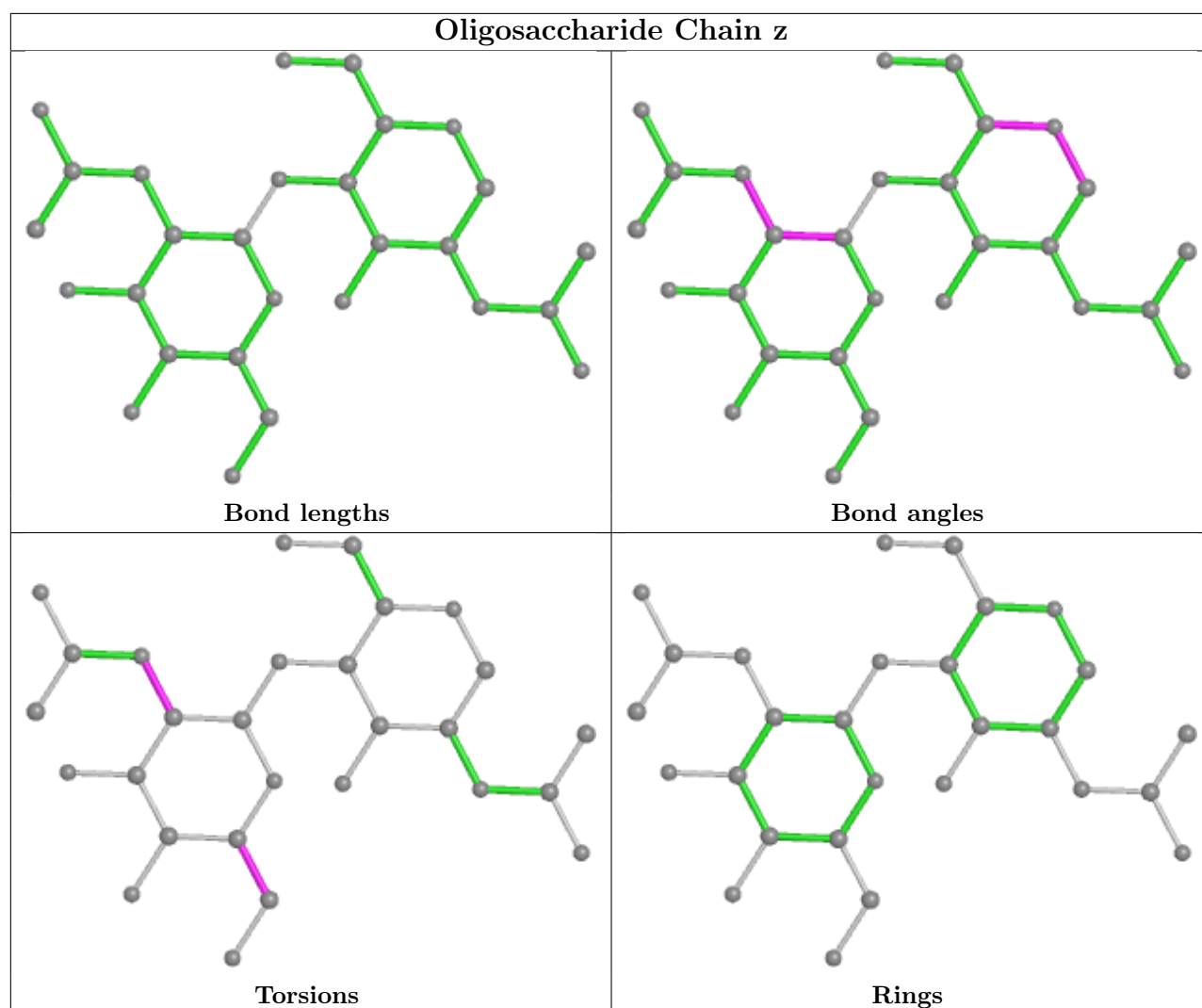


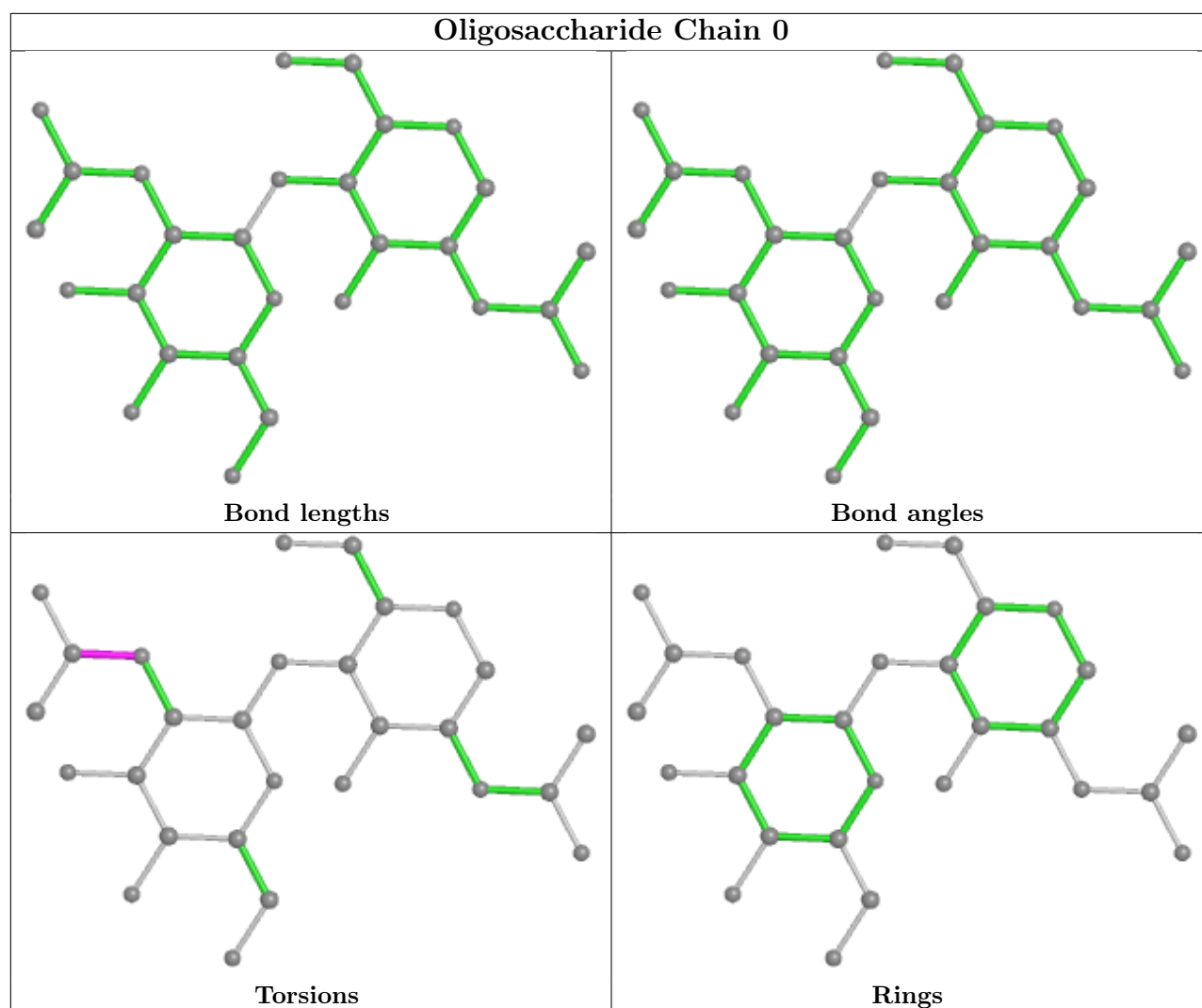


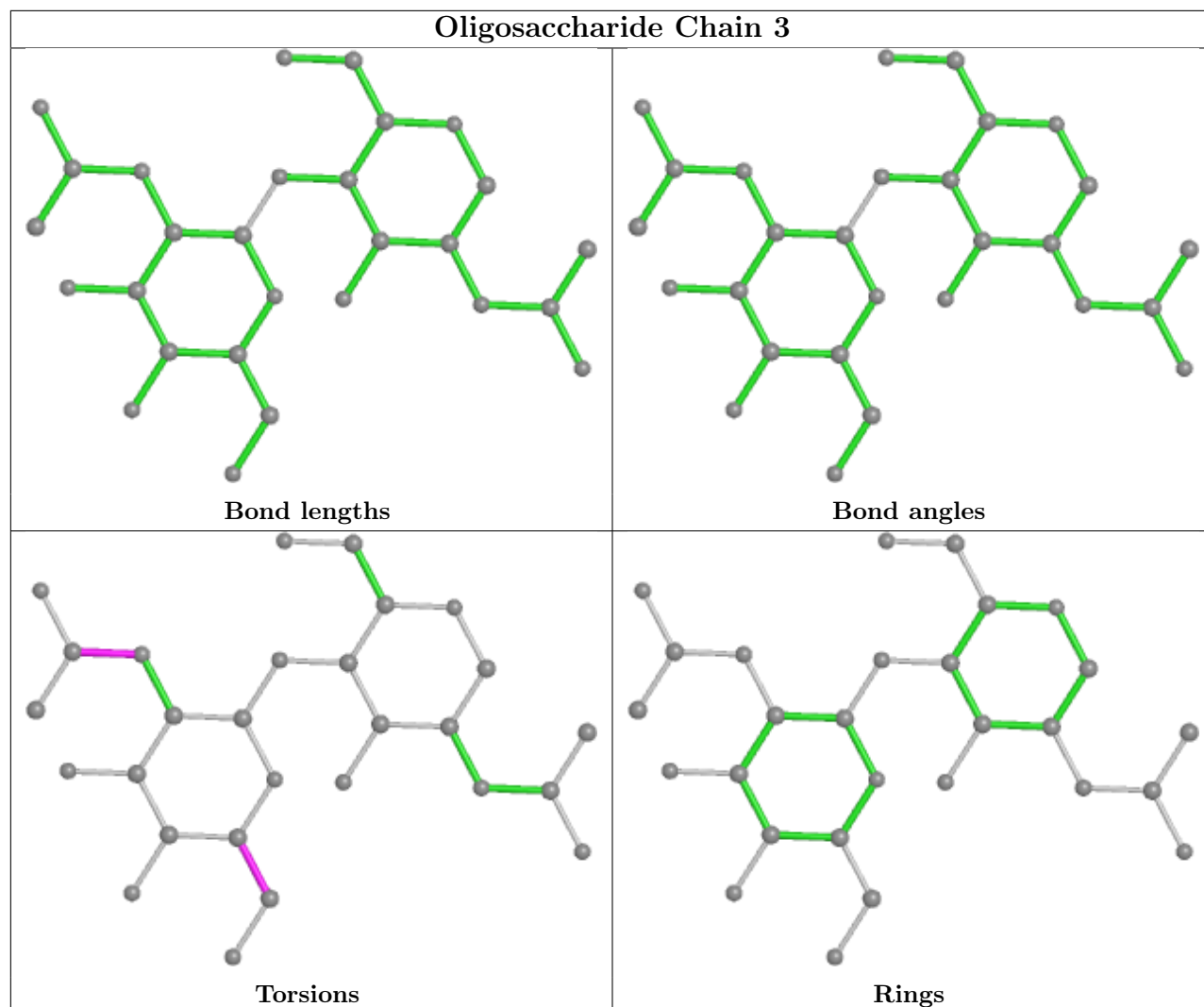


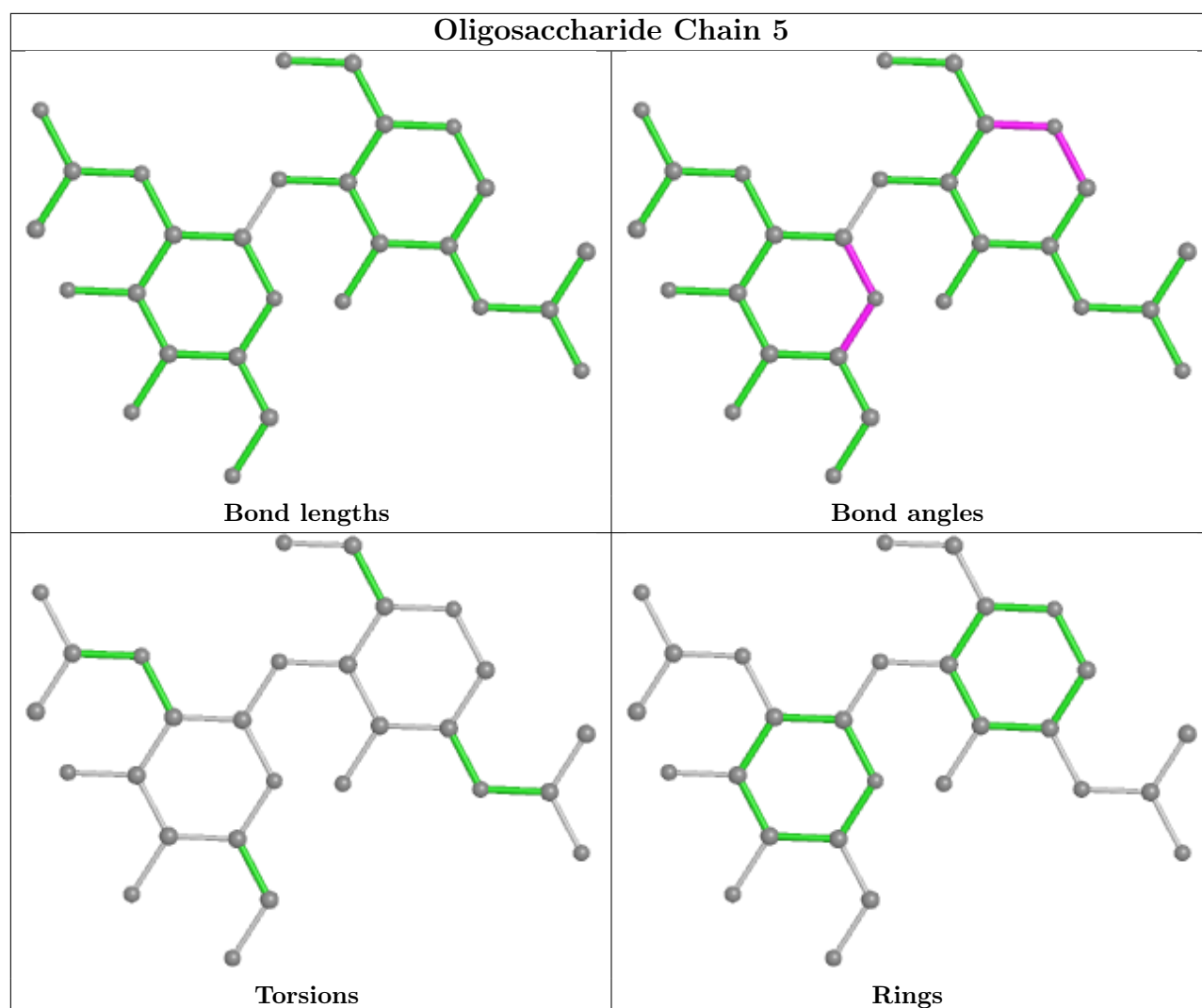


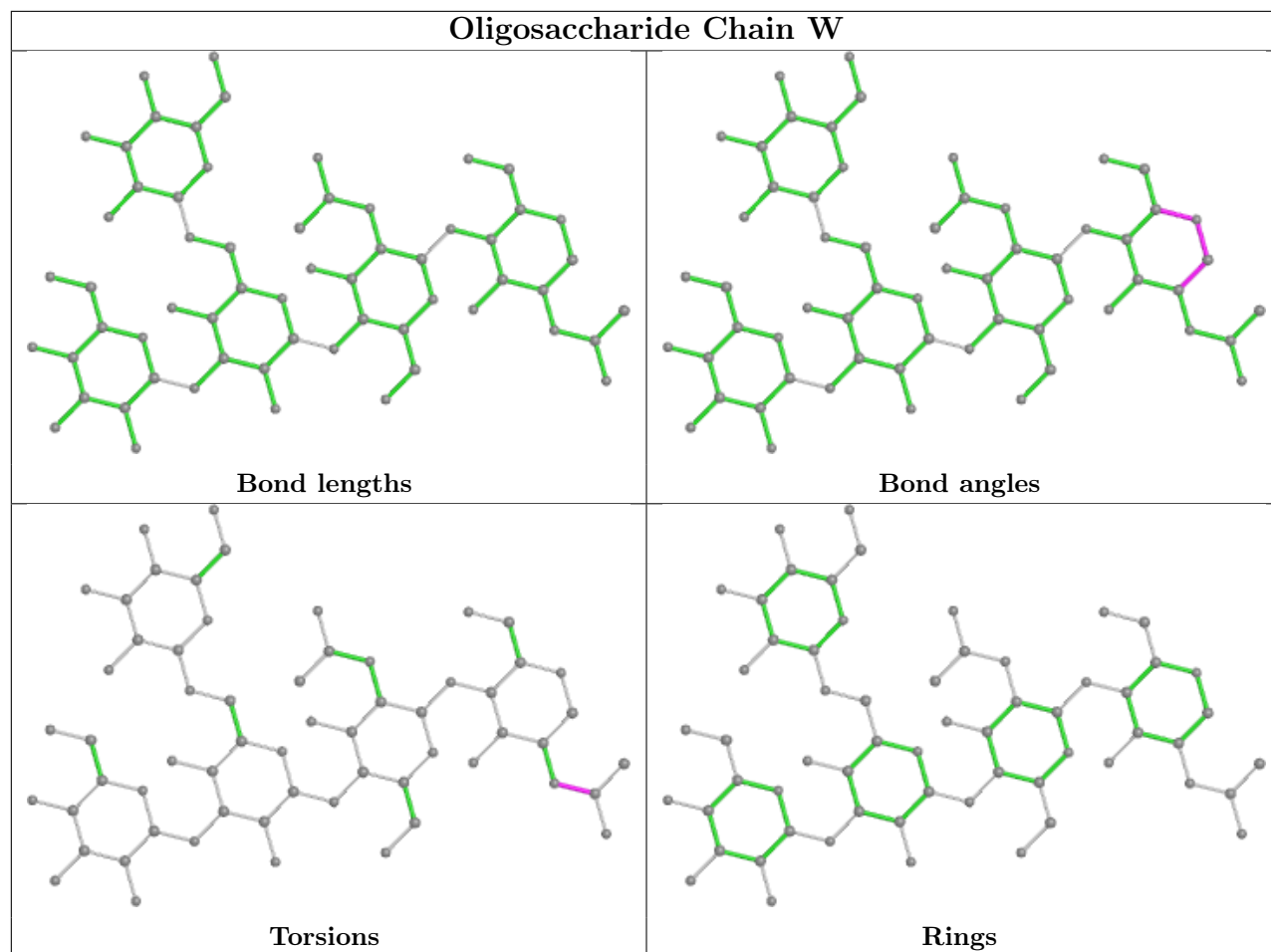


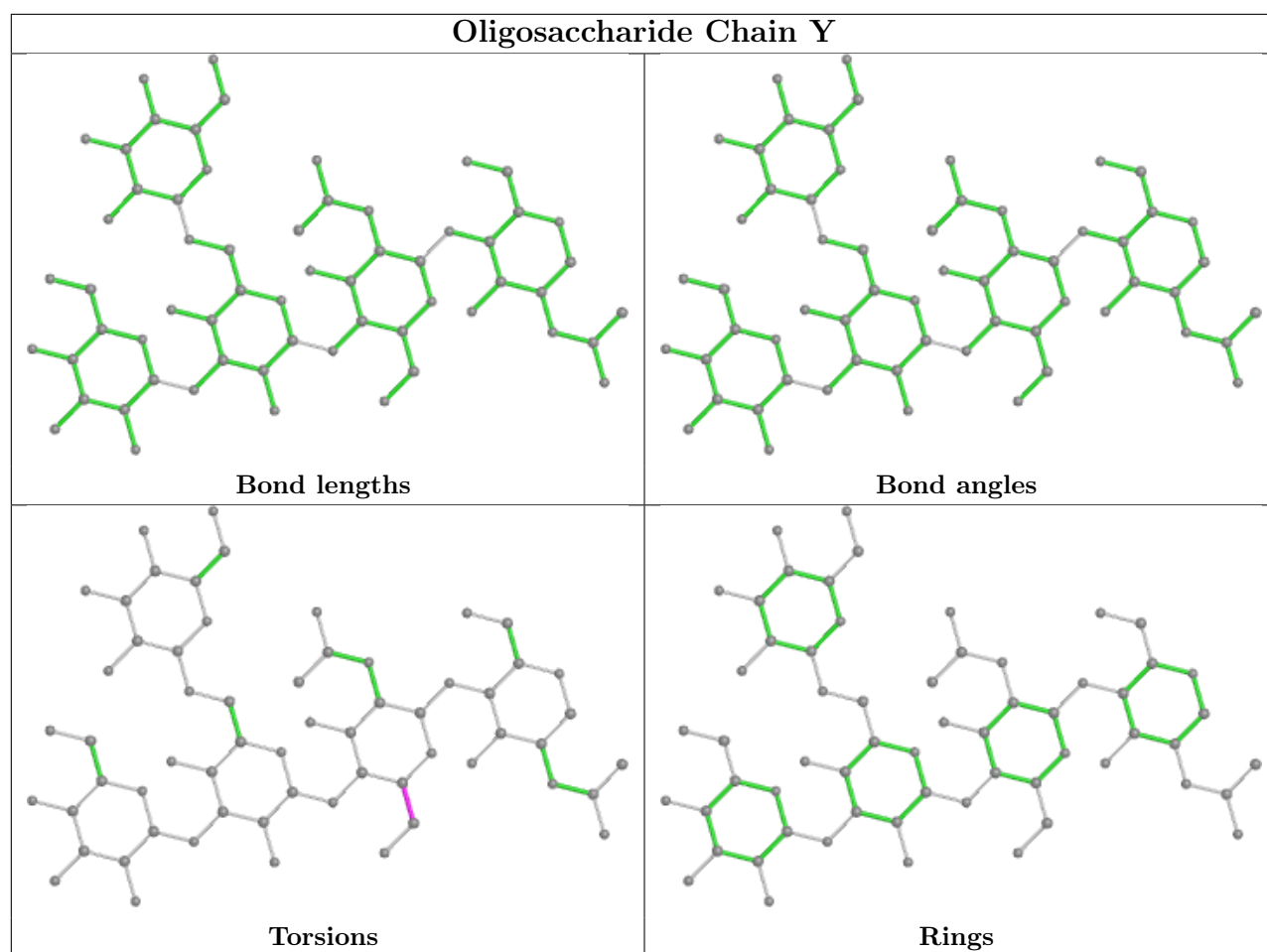


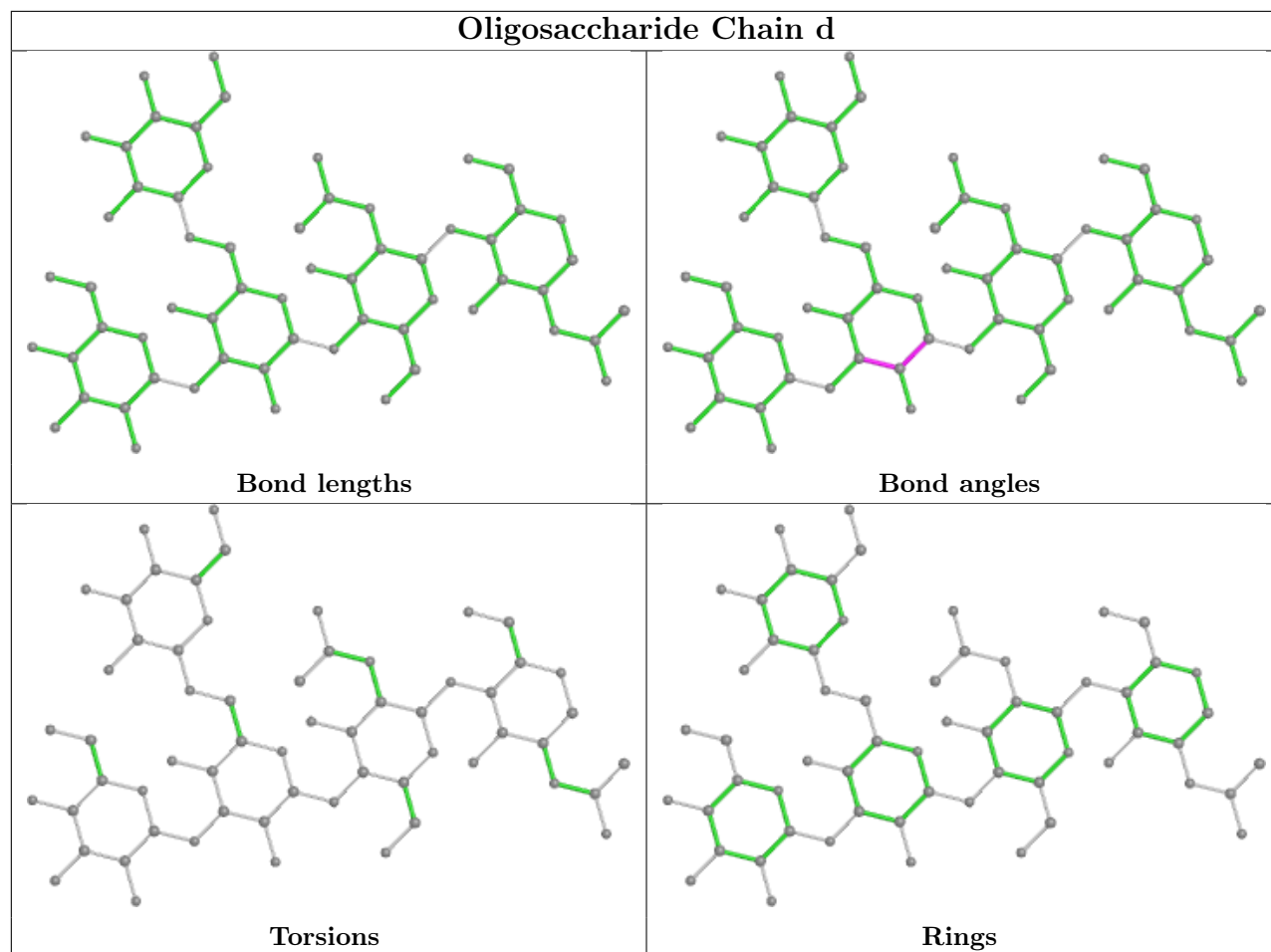


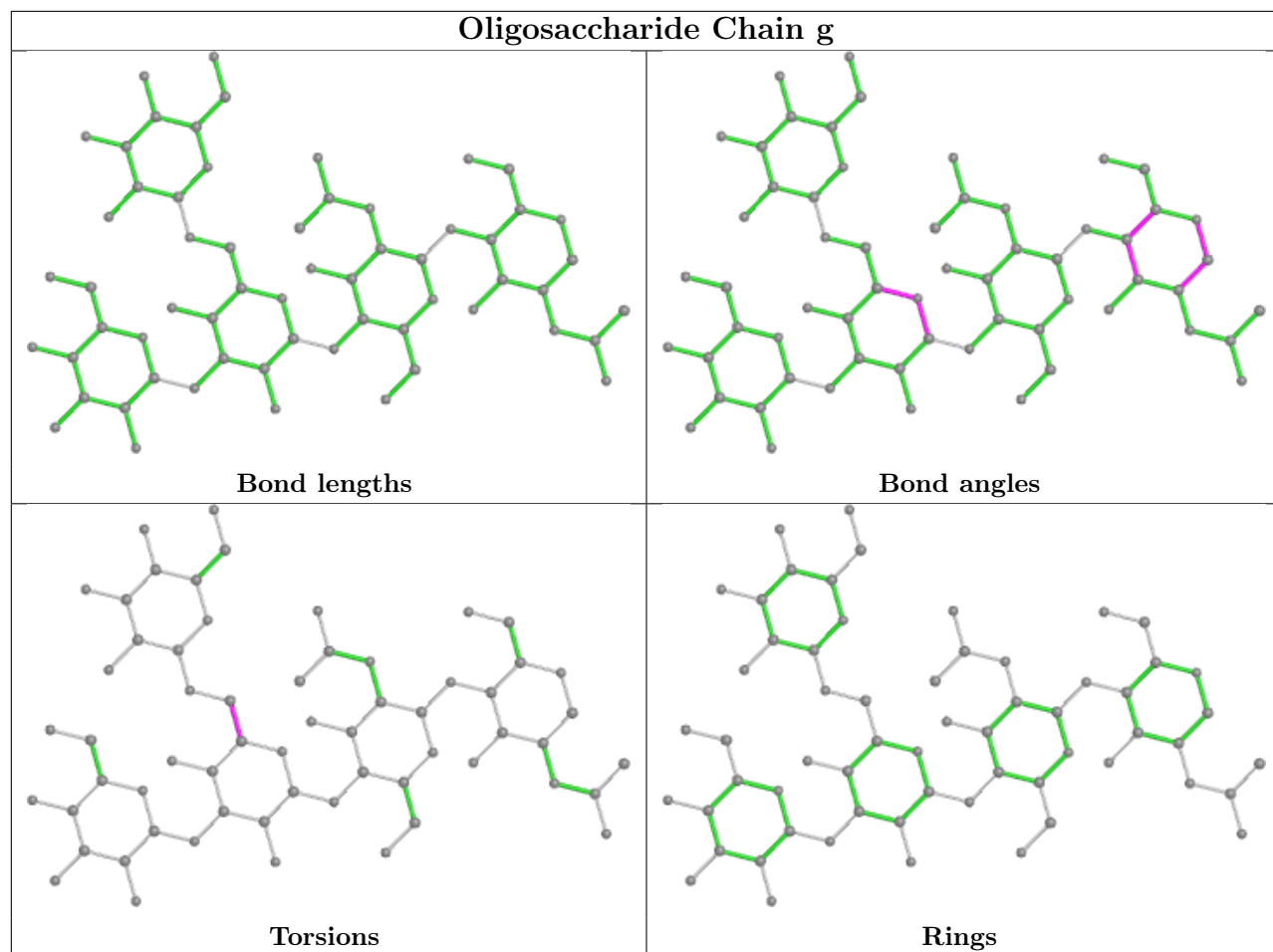


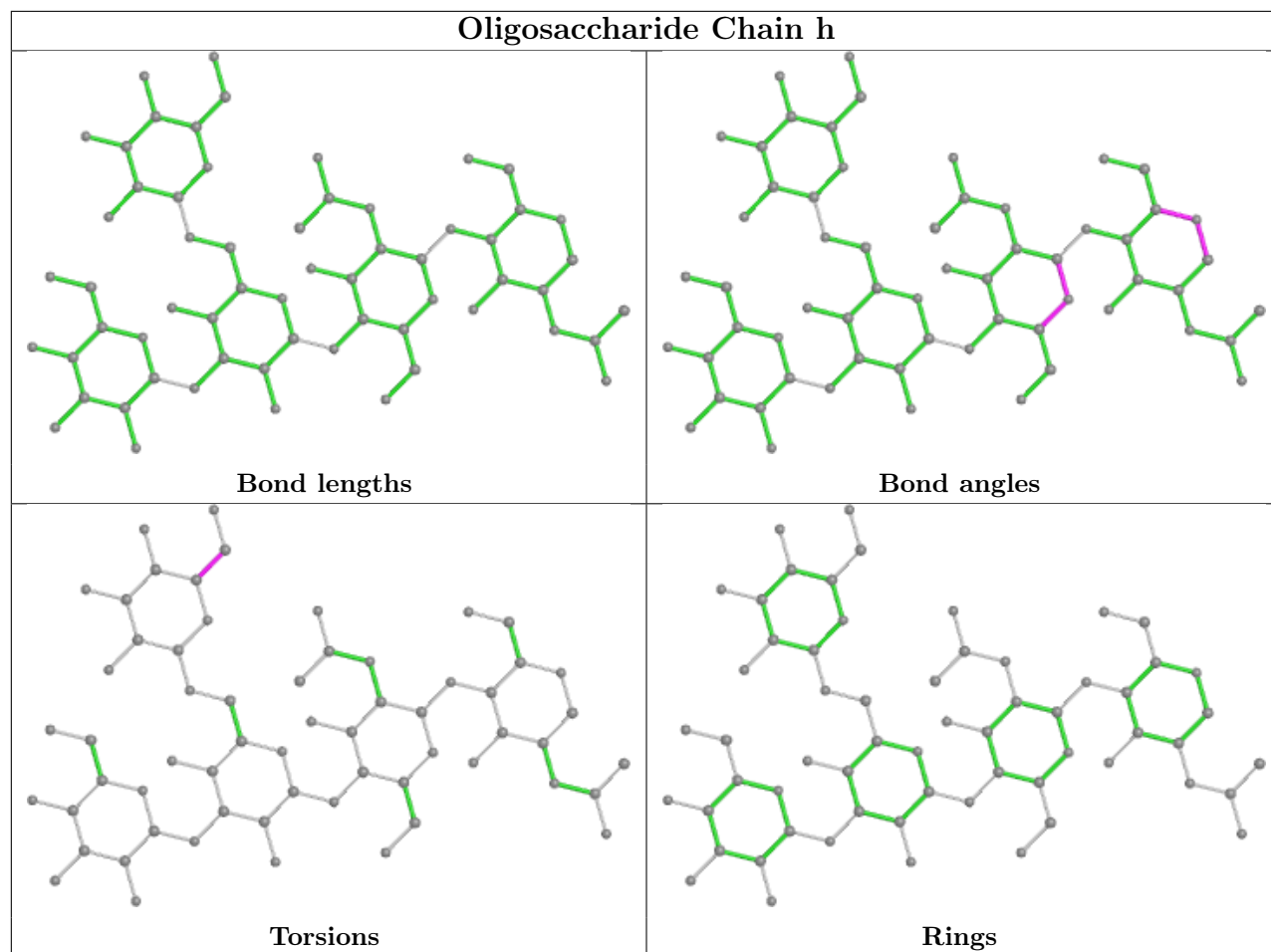


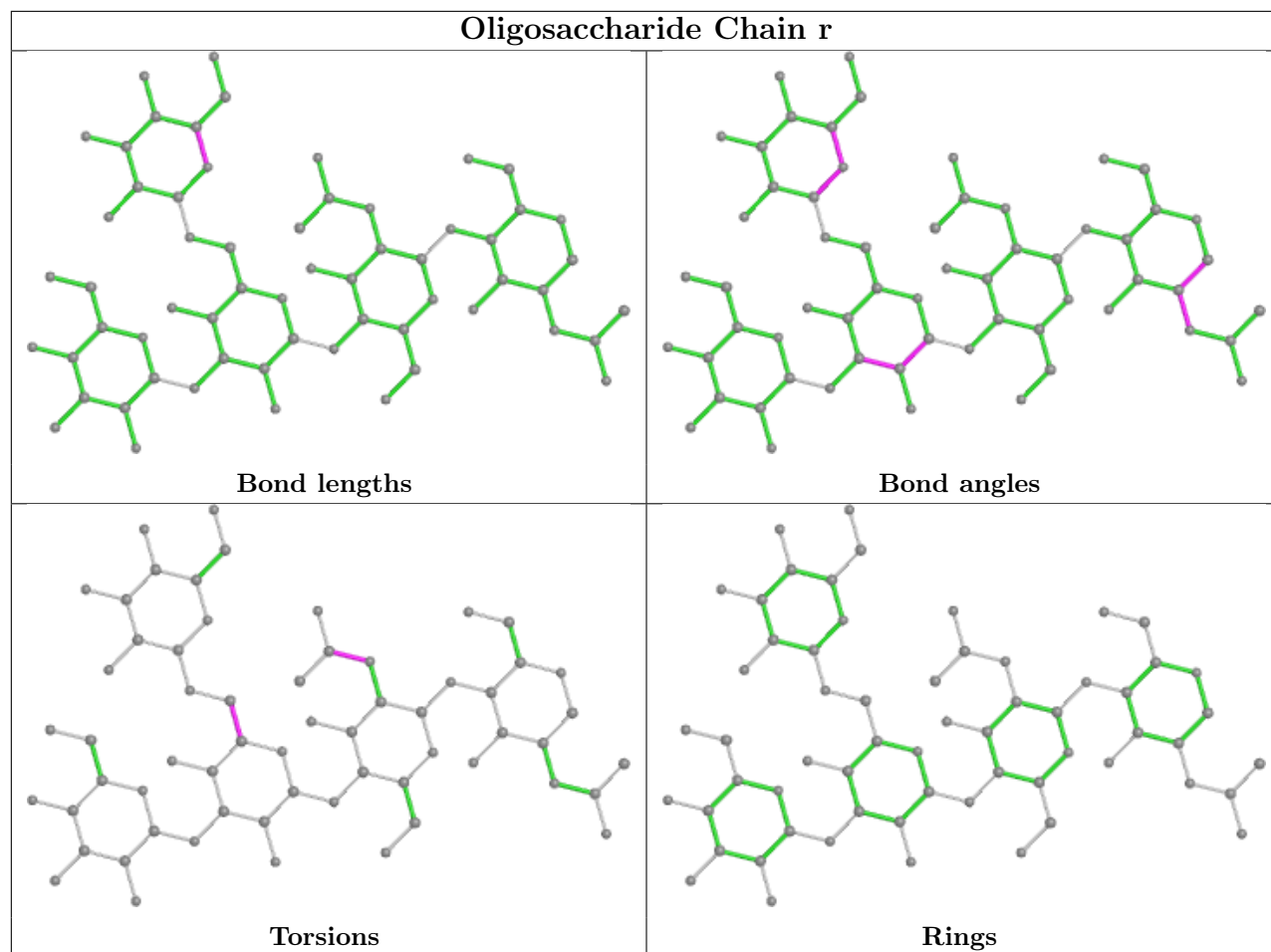


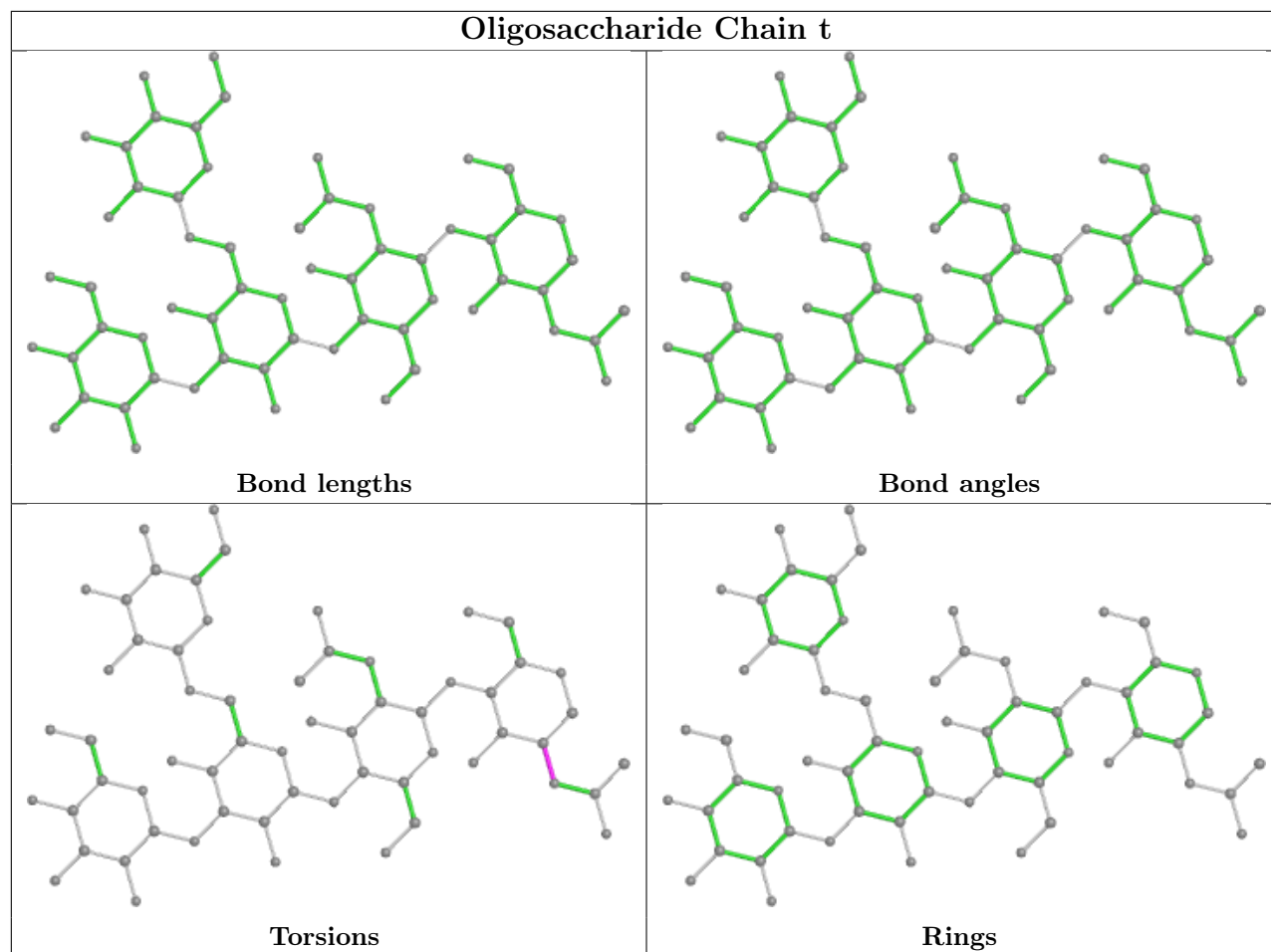


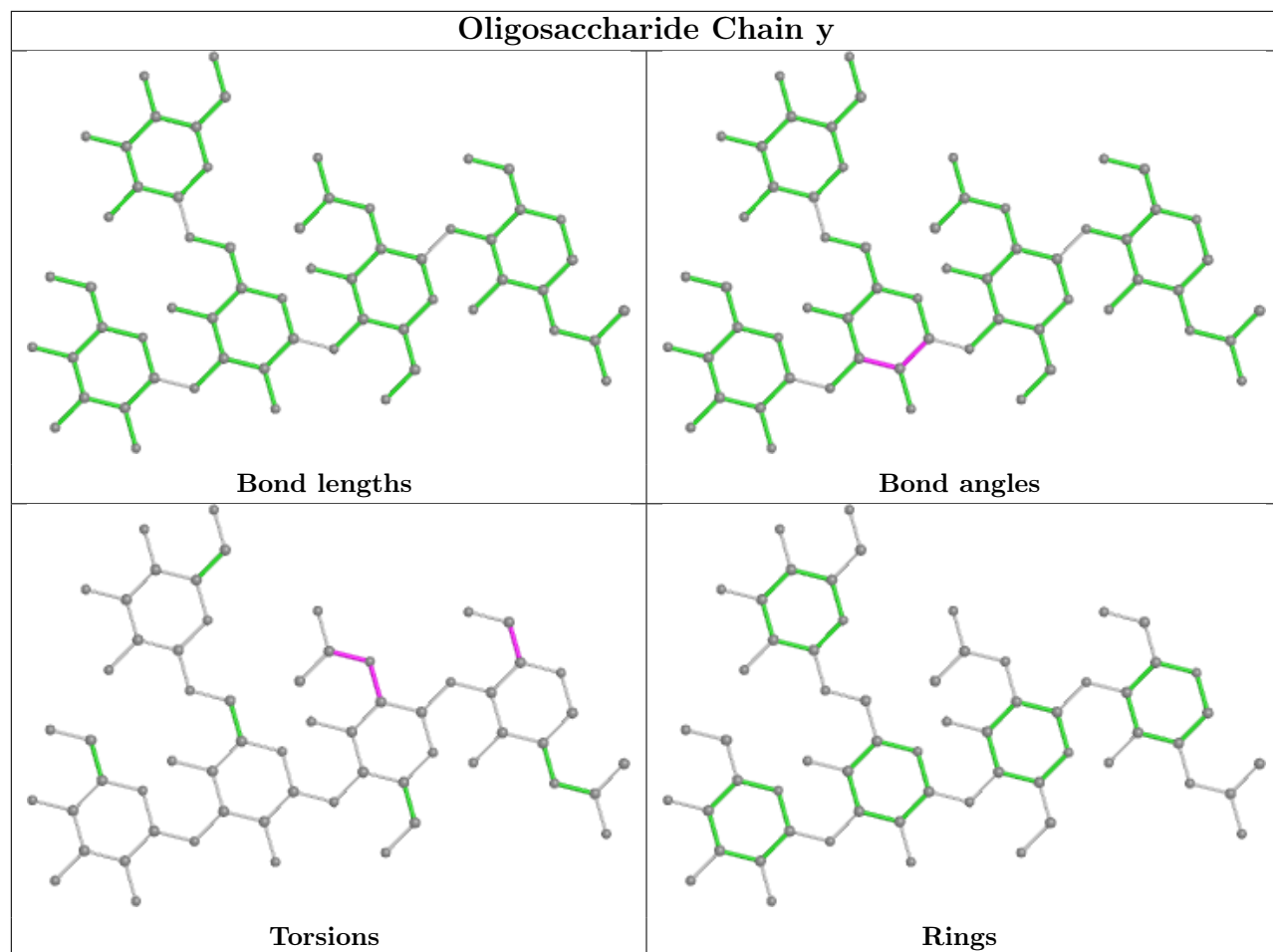


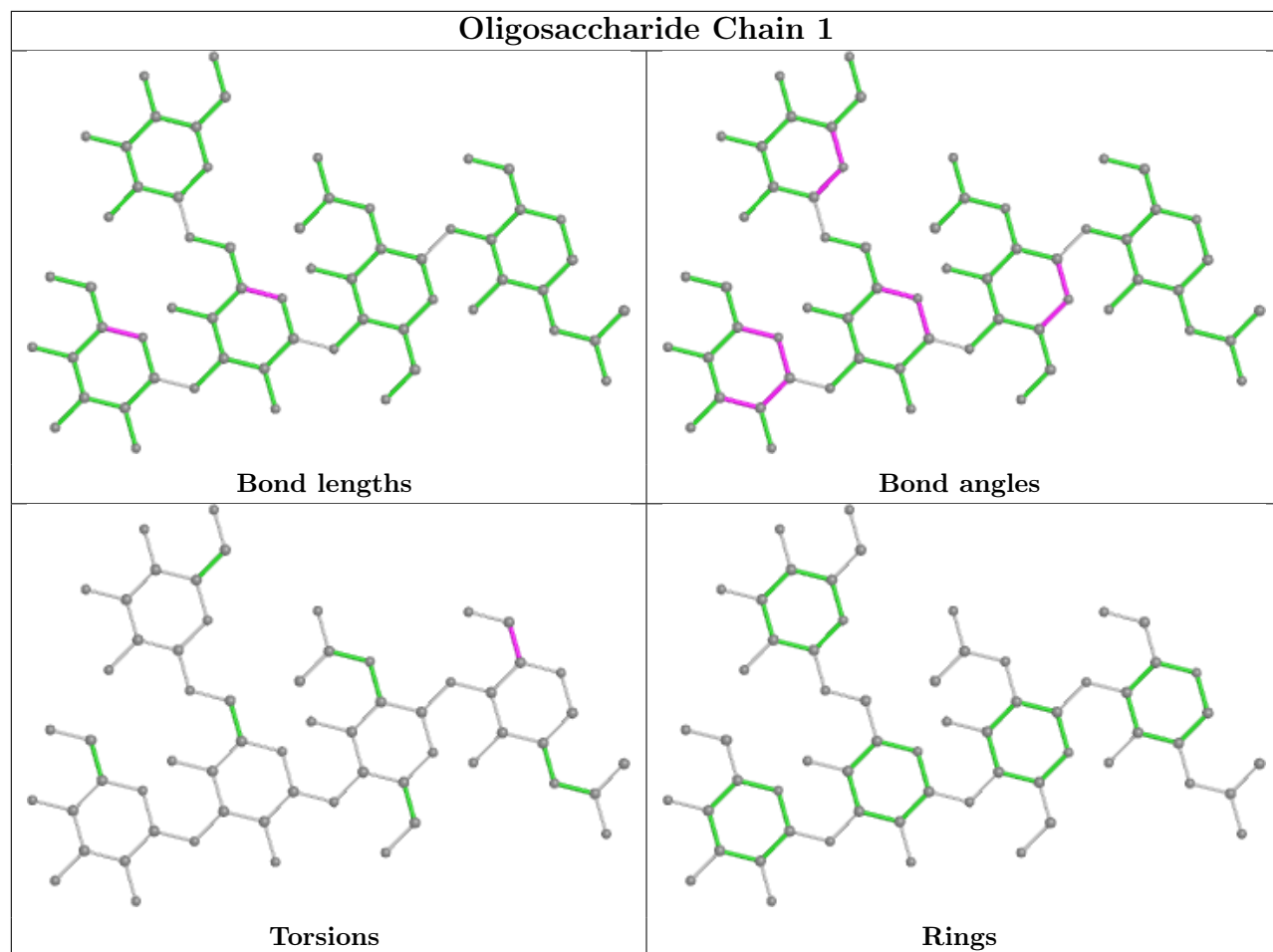


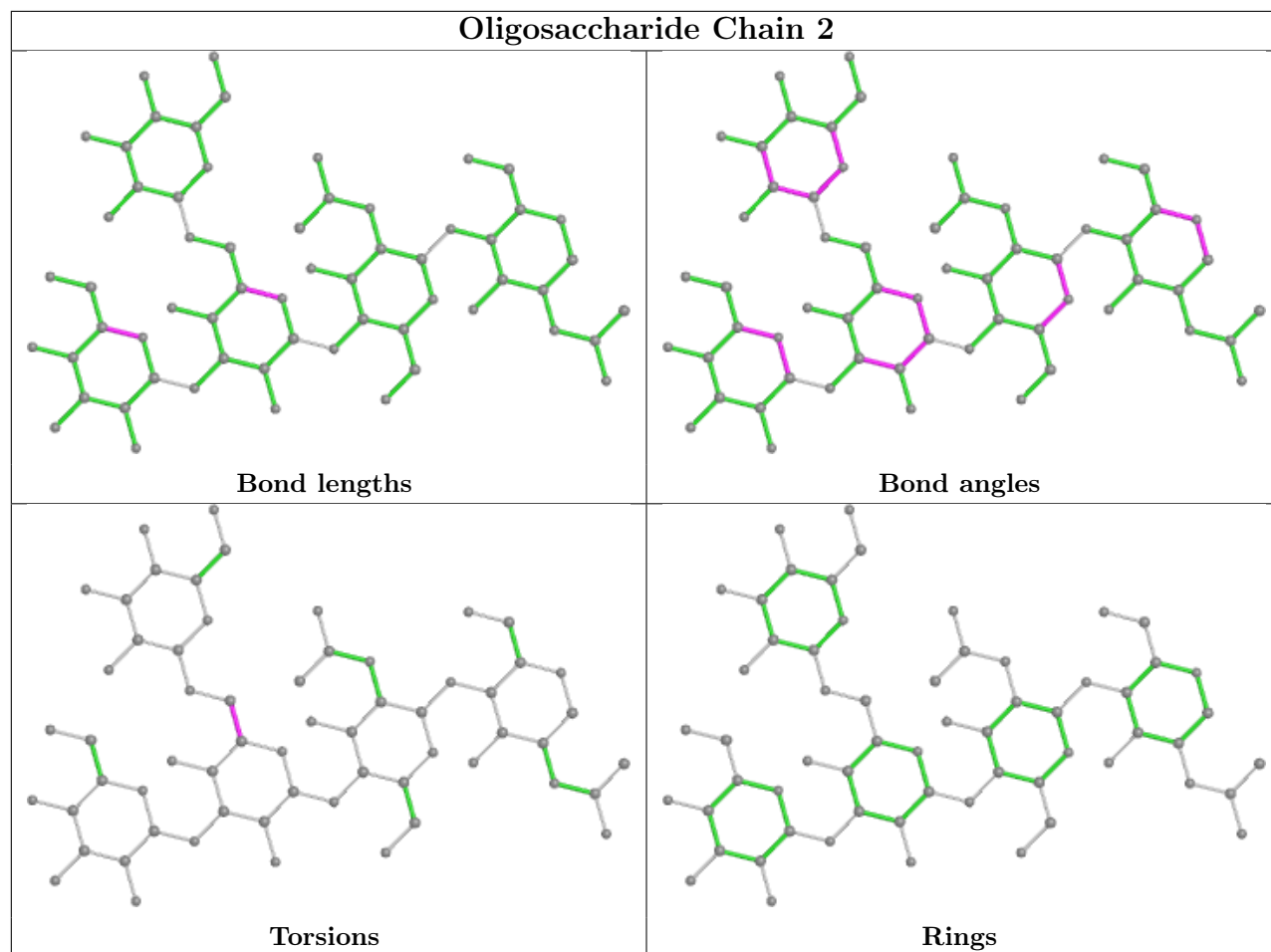


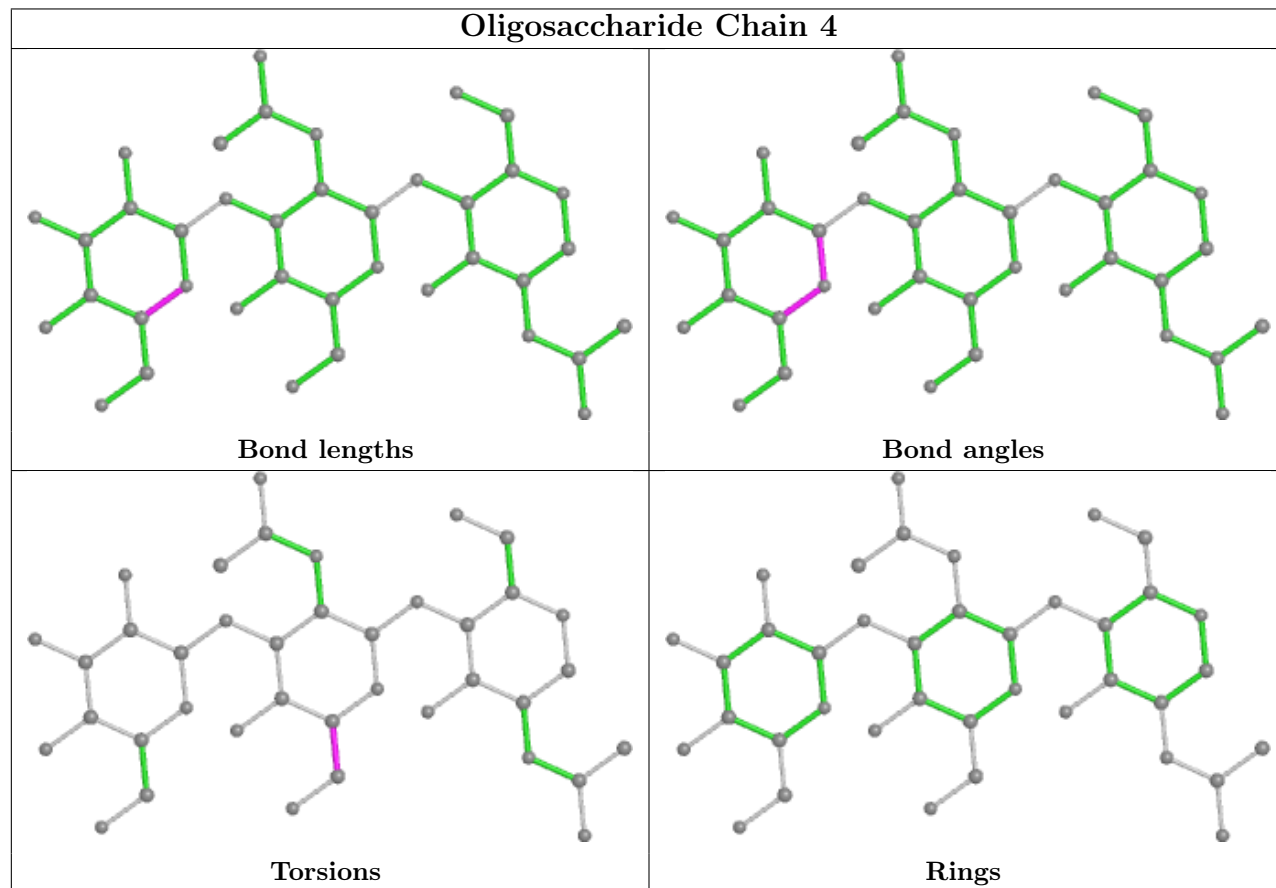
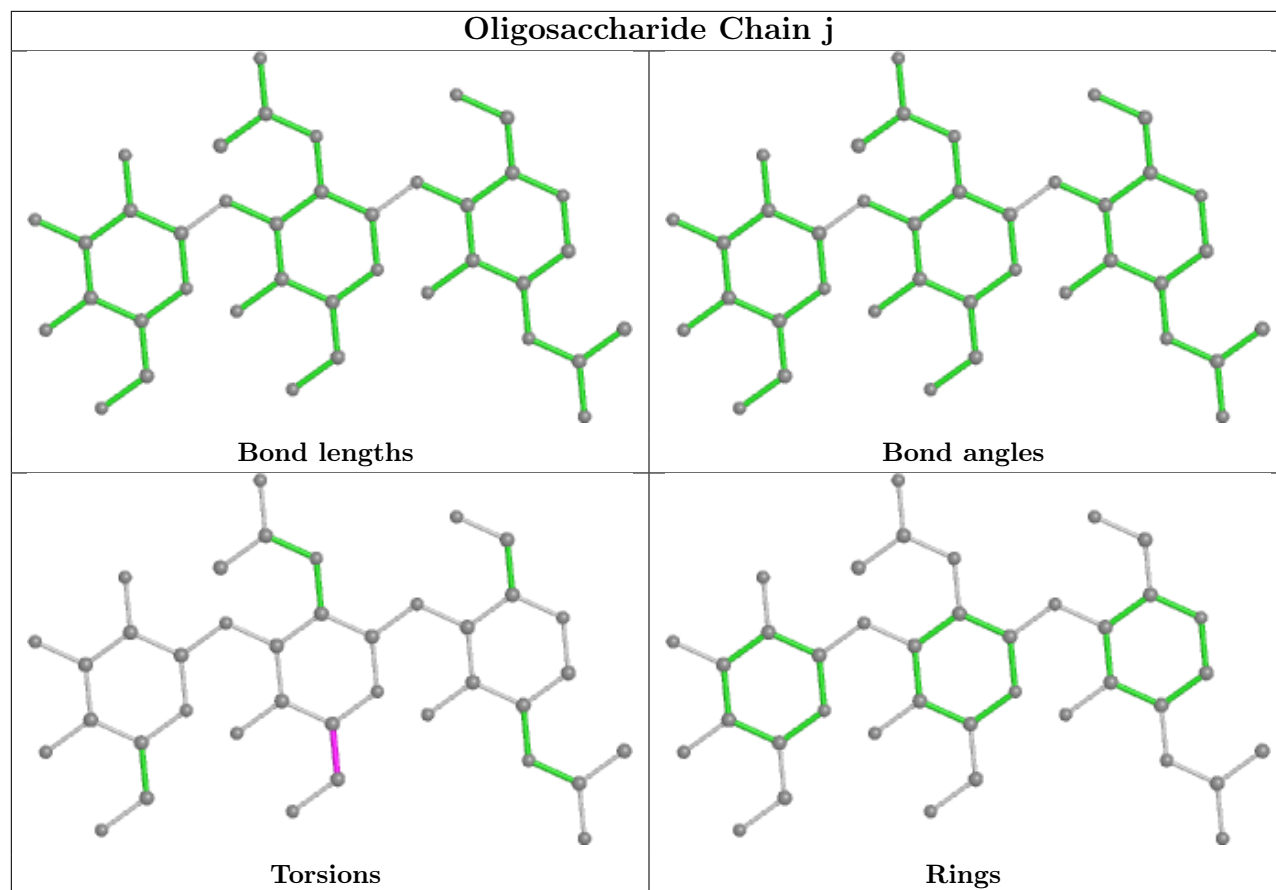












5.6 Ligand geometry

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
13	A2G	A	4714	1	14,14,15	0.62	0	17,19,21	0.66	0
12	NAG	B	4703	1	14,14,15	0.62	0	17,19,21	1.15	2 (11%)
13	A2G	B	4722	1	14,14,15	0.56	0	17,19,21	0.77	0
12	NAG	A	4704	1	14,14,15	0.42	0	17,19,21	0.78	1 (5%)
12	NAG	A	4702	1	14,14,15	0.39	0	17,19,21	0.51	0
13	A2G	A	4720	1	14,14,15	0.55	0	17,19,21	1.30	1 (5%)
12	NAG	B	4704	1	14,14,15	0.55	0	17,19,21	1.03	1 (5%)
12	NAG	B	4706	1	14,14,15	0.60	0	17,19,21	1.04	1 (5%)
12	NAG	B	4710	1	14,14,15	0.69	0	17,19,21	0.90	1 (5%)
13	A2G	A	4717	1	14,14,15	0.62	1 (7%)	17,19,21	1.58	4 (23%)
13	A2G	B	4720	1	14,14,15	0.58	0	17,19,21	1.35	2 (11%)
12	NAG	A	4710	1	14,14,15	0.38	0	17,19,21	0.53	0
13	A2G	B	4715	1	14,14,15	0.44	0	17,19,21	1.18	2 (11%)
12	NAG	A	4712	1	14,14,15	0.54	0	17,19,21	1.39	2 (11%)
12	NAG	B	4708	1	14,14,15	0.59	0	17,19,21	1.06	2 (11%)
13	A2G	B	4714	1	14,14,15	0.46	0	17,19,21	0.74	0
13	A2G	B	4723	1	14,14,15	0.47	0	17,19,21	0.65	0
12	NAG	A	4711	1	14,14,15	0.54	0	17,19,21	0.77	0
13	A2G	A	4723	1	14,14,15	0.48	0	17,19,21	1.06	2 (11%)
13	A2G	B	4718	1	14,14,15	0.59	0	17,19,21	1.05	2 (11%)
13	A2G	A	4713	1	14,14,15	0.50	0	17,19,21	1.11	1 (5%)
12	NAG	A	4705	1	14,14,15	0.61	0	17,19,21	1.05	1 (5%)
12	NAG	B	4712	1	14,14,15	0.40	0	17,19,21	0.53	0
13	A2G	B	4713	1	14,14,15	0.60	0	17,19,21	1.44	3 (17%)
13	A2G	B	4716	1	14,14,15	0.54	0	17,19,21	1.05	1 (5%)
13	A2G	A	4716	1	14,14,15	0.46	0	17,19,21	1.04	2 (11%)
12	NAG	B	4705	1	14,14,15	0.40	0	17,19,21	0.63	0
13	A2G	A	4718	1	14,14,15	0.63	0	17,19,21	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	A	4703	1	14,14,15	0.59	0	17,19,21	0.99	1 (5%)
12	NAG	B	4702	1	14,14,15	0.42	0	17,19,21	0.51	0
13	A2G	A	4721	1	14,14,15	0.45	0	17,19,21	1.13	2 (11%)
12	NAG	A	4709	1	14,14,15	0.53	0	17,19,21	0.92	1 (5%)
12	NAG	A	4701	1	14,14,15	0.40	0	17,19,21	0.38	0
12	NAG	B	4711	1	14,14,15	0.63	0	17,19,21	1.14	2 (11%)
13	A2G	B	4717	1	14,14,15	0.53	0	17,19,21	1.00	2 (11%)
13	A2G	A	4722	1	14,14,15	0.60	0	17,19,21	1.32	2 (11%)
13	A2G	B	4721	1	14,14,15	1.18	1 (7%)	17,19,21	1.60	6 (35%)
12	NAG	B	4701	1	14,14,15	0.41	0	17,19,21	0.41	0
12	NAG	B	4707	1	14,14,15	0.40	0	17,19,21	0.46	0
12	NAG	B	4709	1	14,14,15	0.62	0	17,19,21	0.96	1 (5%)
12	NAG	A	4706	1	14,14,15	0.46	0	17,19,21	1.18	1 (5%)
13	A2G	B	4719	1	14,14,15	0.50	0	17,19,21	0.91	0
13	A2G	A	4715	1	14,14,15	0.61	0	17,19,21	1.51	2 (11%)
13	A2G	A	4719	1	14,14,15	0.49	0	17,19,21	1.01	1 (5%)
12	NAG	A	4708	1	14,14,15	0.41	0	17,19,21	0.53	0
12	NAG	A	4707	1	14,14,15	0.57	0	17,19,21	1.06	1 (5%)

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
13	A2G	A	4714	1	-	0/6/23/26	0/1/1/1
12	NAG	B	4703	1	-	0/6/23/26	0/1/1/1
13	A2G	B	4722	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4704	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4702	1	-	0/6/23/26	0/1/1/1
13	A2G	A	4720	1	-	0/6/23/26	0/1/1/1
12	NAG	B	4704	1	-	1/6/23/26	0/1/1/1
12	NAG	B	4706	1	-	3/6/23/26	0/1/1/1
12	NAG	B	4710	1	-	1/6/23/26	0/1/1/1
13	A2G	A	4717	1	-	2/6/23/26	0/1/1/1
13	A2G	B	4720	1	-	2/6/23/26	0/1/1/1
12	NAG	A	4710	1	-	3/6/23/26	0/1/1/1
13	A2G	B	4715	1	-	2/6/23/26	0/1/1/1
12	NAG	A	4712	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	B	4708	1	-	0/6/23/26	0/1/1/1
13	A2G	B	4714	1	-	0/6/23/26	0/1/1/1
13	A2G	B	4723	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4711	1	-	2/6/23/26	0/1/1/1
13	A2G	A	4723	1	-	1/6/23/26	0/1/1/1
13	A2G	B	4718	1	-	0/6/23/26	0/1/1/1
13	A2G	A	4713	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4705	1	-	1/6/23/26	0/1/1/1
12	NAG	B	4712	1	-	3/6/23/26	0/1/1/1
13	A2G	B	4713	1	-	1/6/23/26	0/1/1/1
13	A2G	B	4716	1	-	0/6/23/26	0/1/1/1
13	A2G	A	4716	1	-	0/6/23/26	0/1/1/1
12	NAG	B	4705	1	-	3/6/23/26	0/1/1/1
13	A2G	A	4718	1	-	1/6/23/26	0/1/1/1
12	NAG	A	4703	1	-	0/6/23/26	0/1/1/1
12	NAG	B	4702	1	-	3/6/23/26	0/1/1/1
13	A2G	A	4721	1	-	1/6/23/26	0/1/1/1
12	NAG	A	4709	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4701	1	-	1/6/23/26	0/1/1/1
12	NAG	B	4711	1	-	0/6/23/26	0/1/1/1
13	A2G	B	4717	1	-	0/6/23/26	0/1/1/1
13	A2G	A	4722	1	-	0/6/23/26	0/1/1/1
13	A2G	B	4721	1	-	1/6/23/26	0/1/1/1
12	NAG	B	4701	1	-	0/6/23/26	0/1/1/1
12	NAG	B	4707	1	-	0/6/23/26	0/1/1/1
12	NAG	B	4709	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4706	1	-	2/6/23/26	0/1/1/1
13	A2G	B	4719	1	-	0/6/23/26	0/1/1/1
13	A2G	A	4715	1	-	2/6/23/26	0/1/1/1
13	A2G	A	4719	1	-	1/6/23/26	0/1/1/1
12	NAG	A	4708	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4707	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	4721	A2G	O5-C1	-2.83	1.39	1.43
13	A	4717	A2G	O5-C1	-2.05	1.40	1.43

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	4717	A2G	C1-O5-C5	-4.68	105.85	112.19
13	A	4715	A2G	C2-N2-C7	4.65	129.52	122.90
13	A	4722	A2G	C1-O5-C5	-4.38	106.25	112.19
13	B	4720	A2G	C1-O5-C5	-4.14	106.58	112.19
12	A	4706	NAG	C1-O5-C5	4.04	117.66	112.19

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	4710	NAG	C8-C7-N2-C2
12	A	4710	NAG	O7-C7-N2-C2
12	B	4702	NAG	C8-C7-N2-C2
12	B	4702	NAG	O7-C7-N2-C2
12	B	4706	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

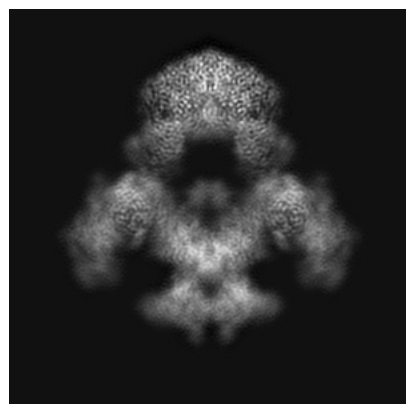
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36664. These allow visual inspection of the internal detail of the map and identification of artifacts.

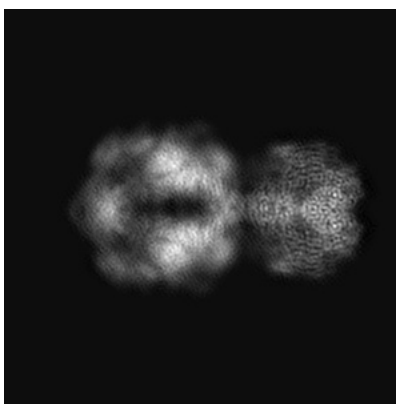
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

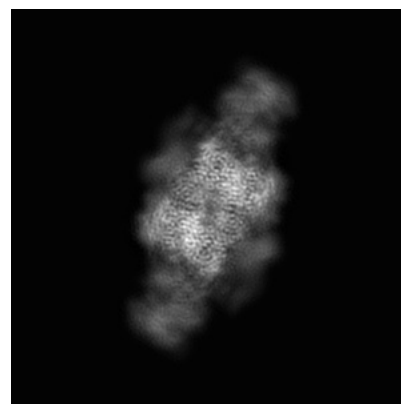
6.1.1 Primary map



X

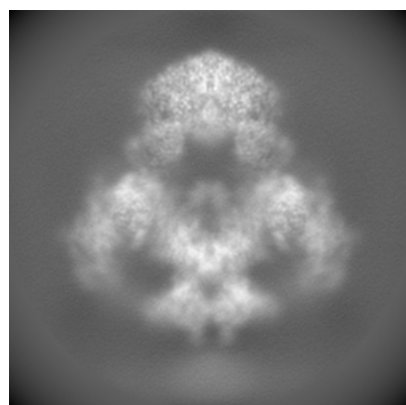


Y

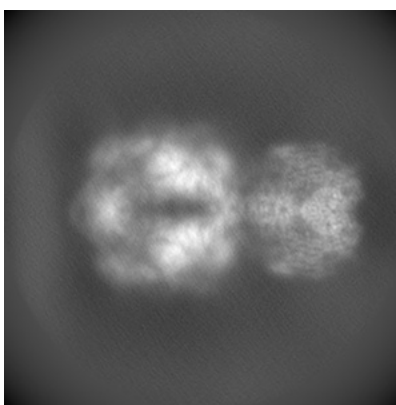


Z

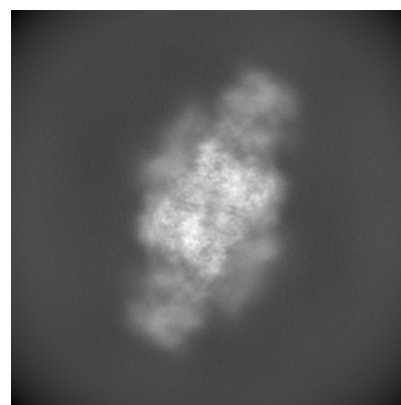
6.1.2 Raw map



X



Y

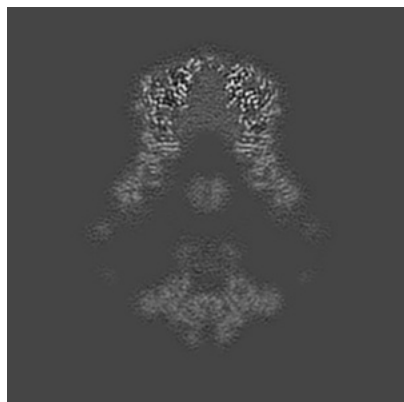


Z

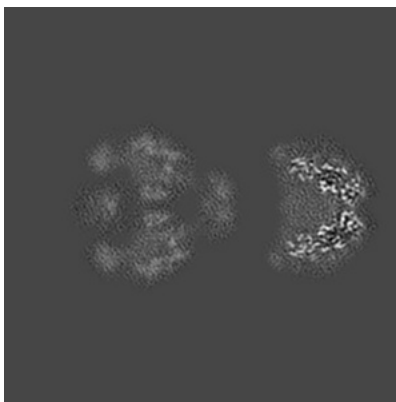
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 130

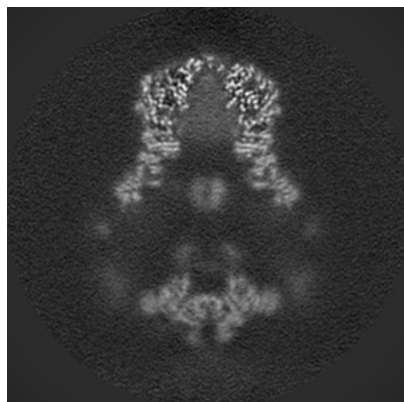


Y Index: 130

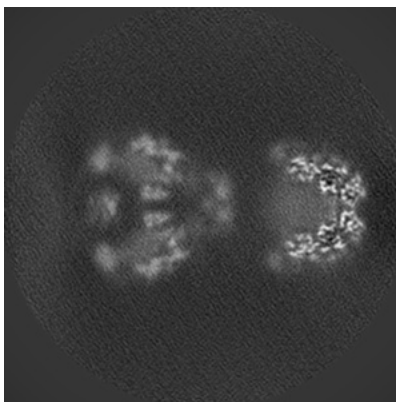


Z Index: 130

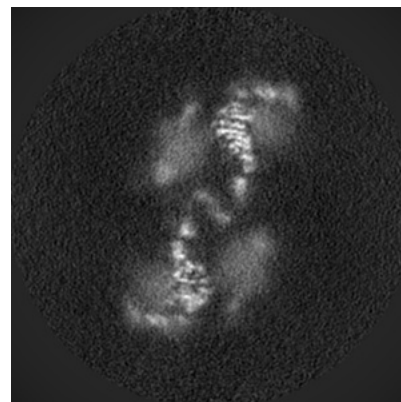
6.2.2 Raw map



X Index: 130



Y Index: 130

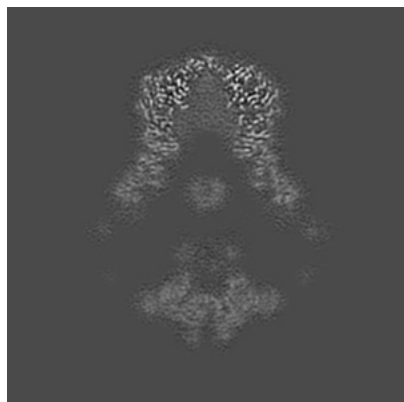


Z Index: 130

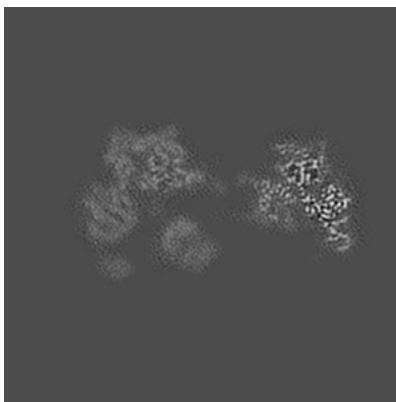
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

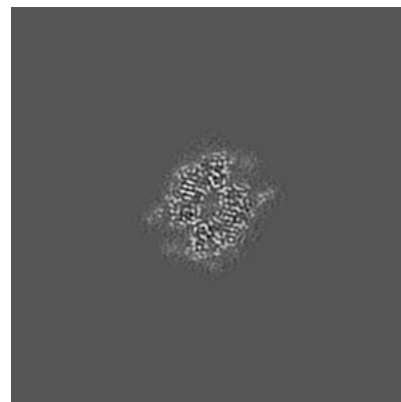
6.3.1 Primary map



X Index: 131

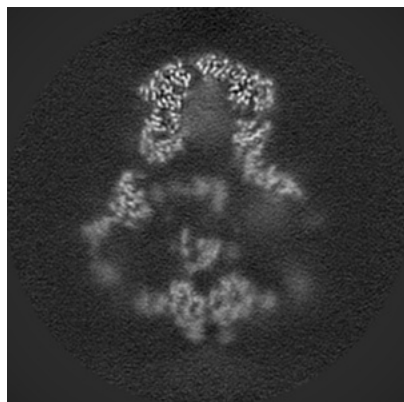


Y Index: 149

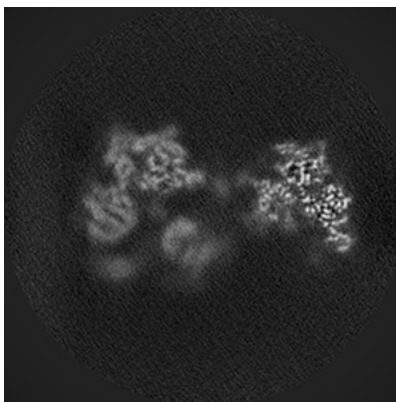


Z Index: 215

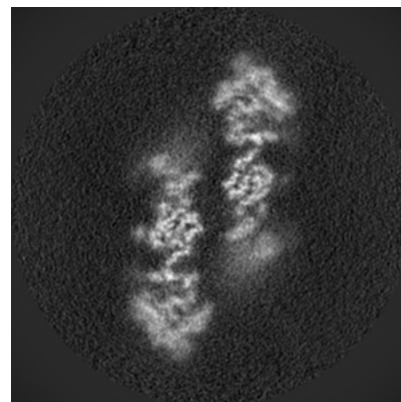
6.3.2 Raw map



X Index: 124



Y Index: 149

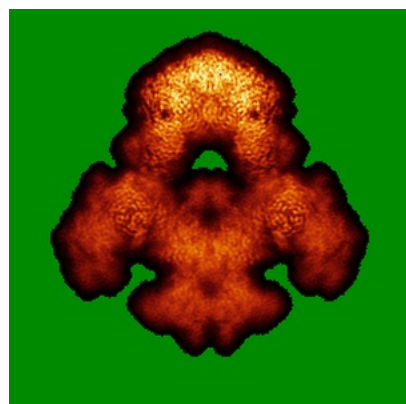


Z Index: 113

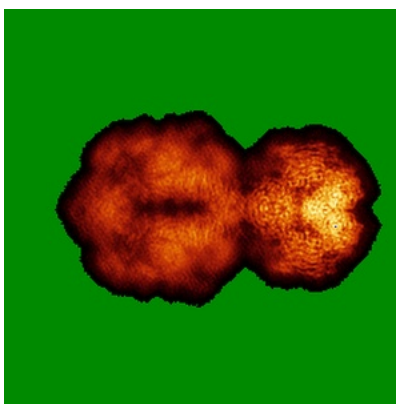
The images above show the largest variance slices of the map in three orthogonal directions.

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

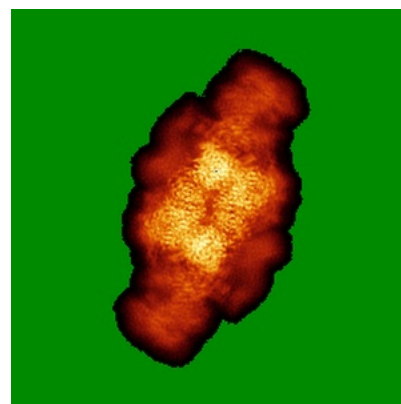
6.4.1 Primary map



X

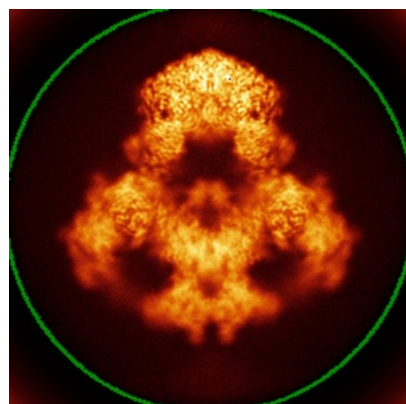


Y

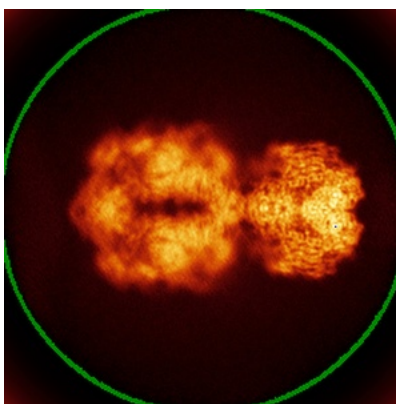


Z

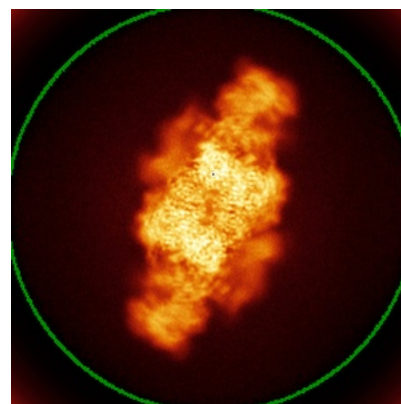
6.4.2 Raw map



X



Y

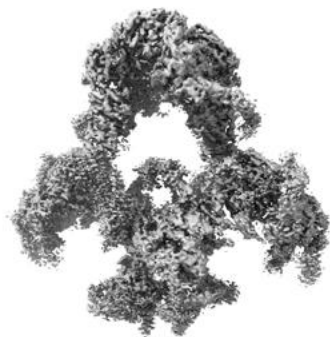


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



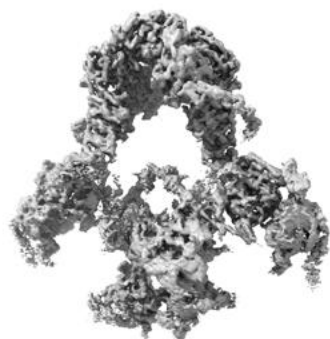
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

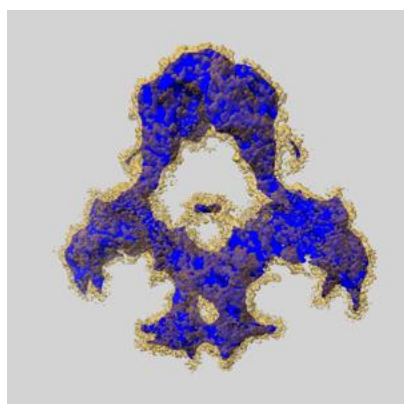
6.6 Mask visualisation [i](#)

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

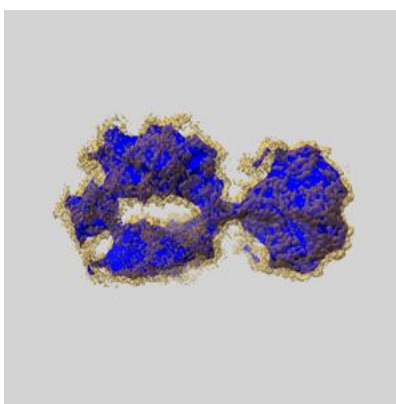
A mask typically either:

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

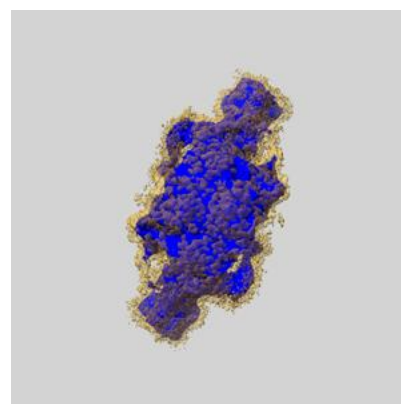
6.6.1 emd_36664_msk_1.map [i](#)



X



Y

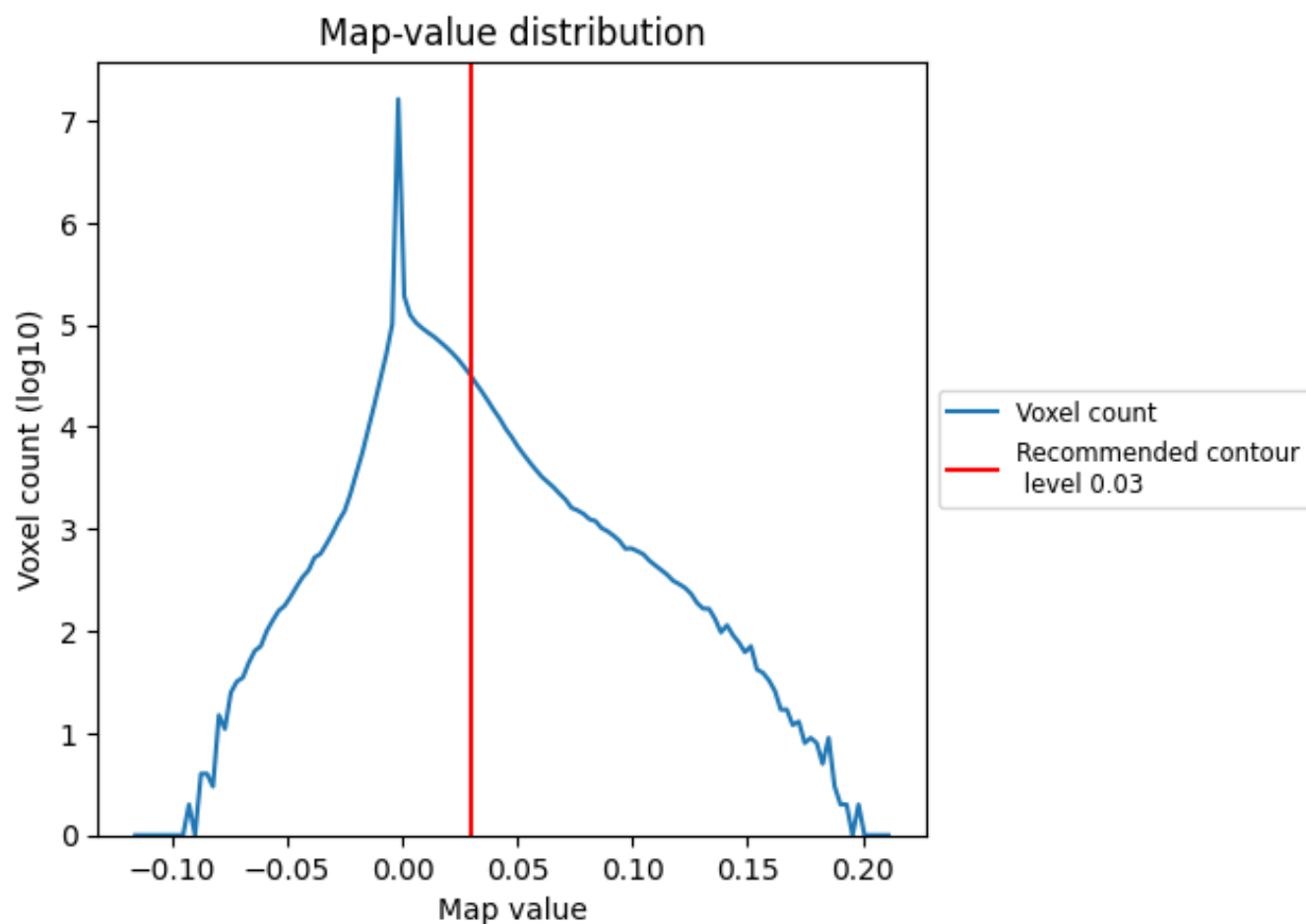


Z

7 Map analysis [i](#)

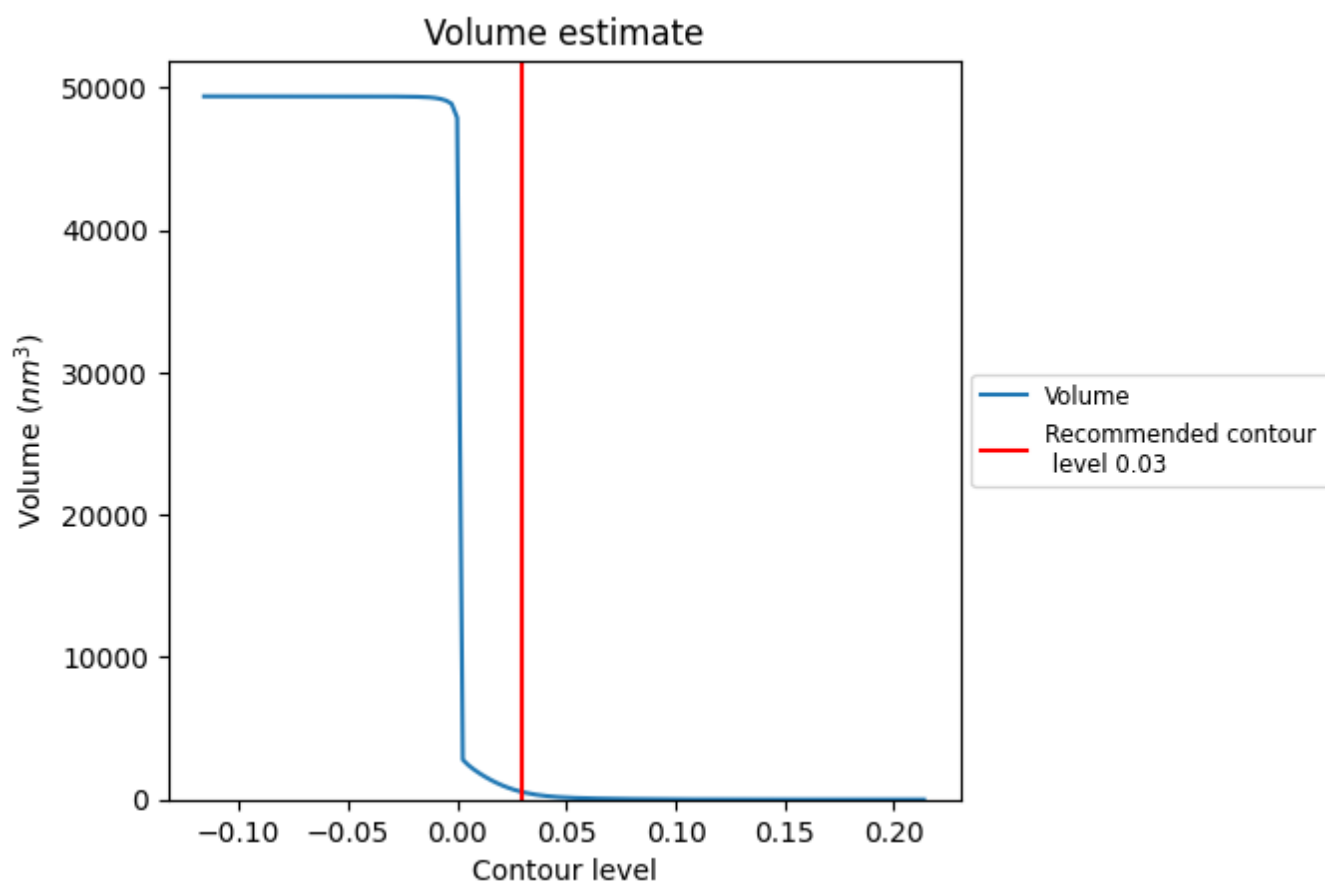
This section contains the results of statistical analysis of the map.

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.

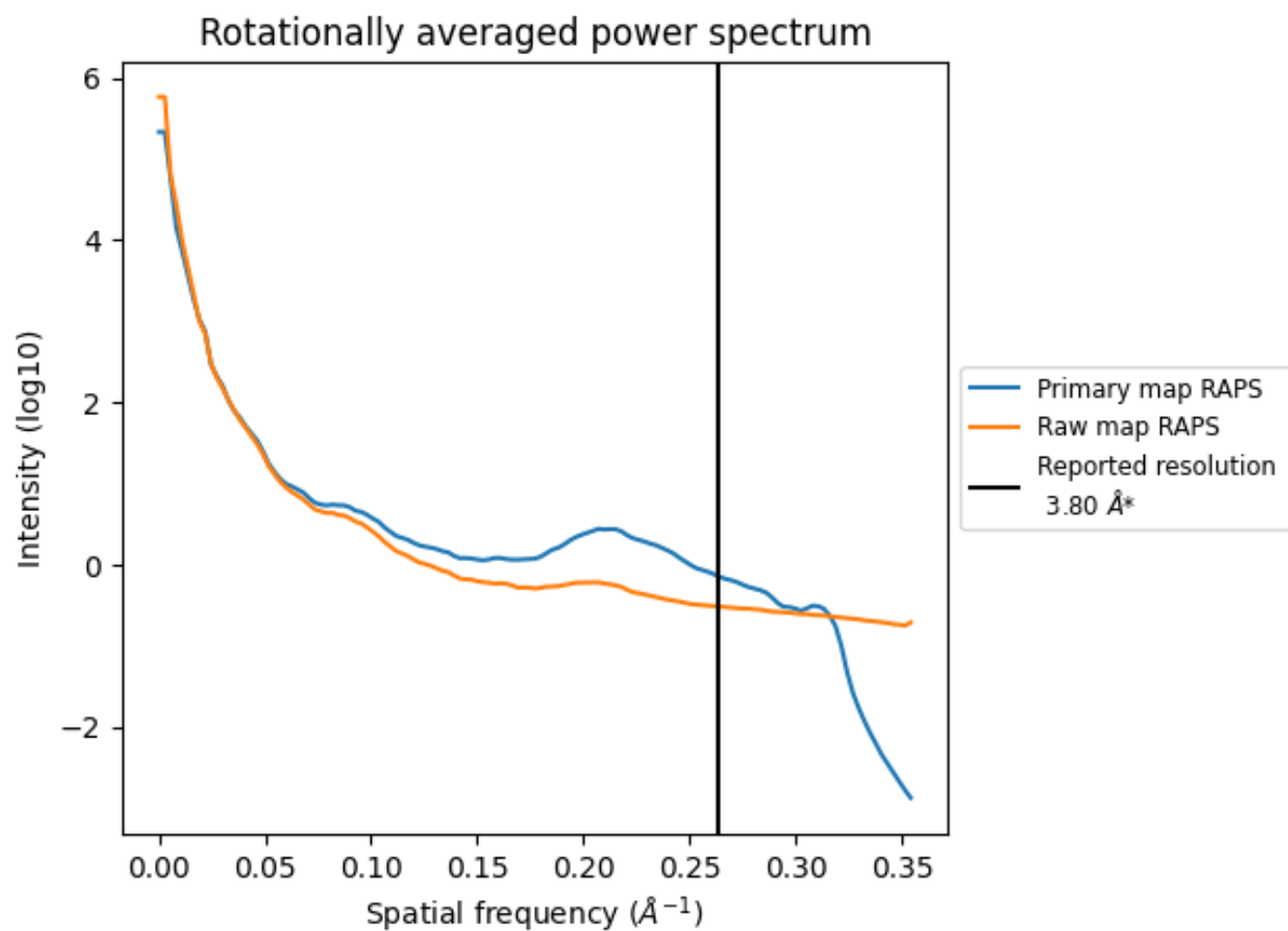
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 525 nm³; this corresponds to an approximate mass of 474 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 ⓘ

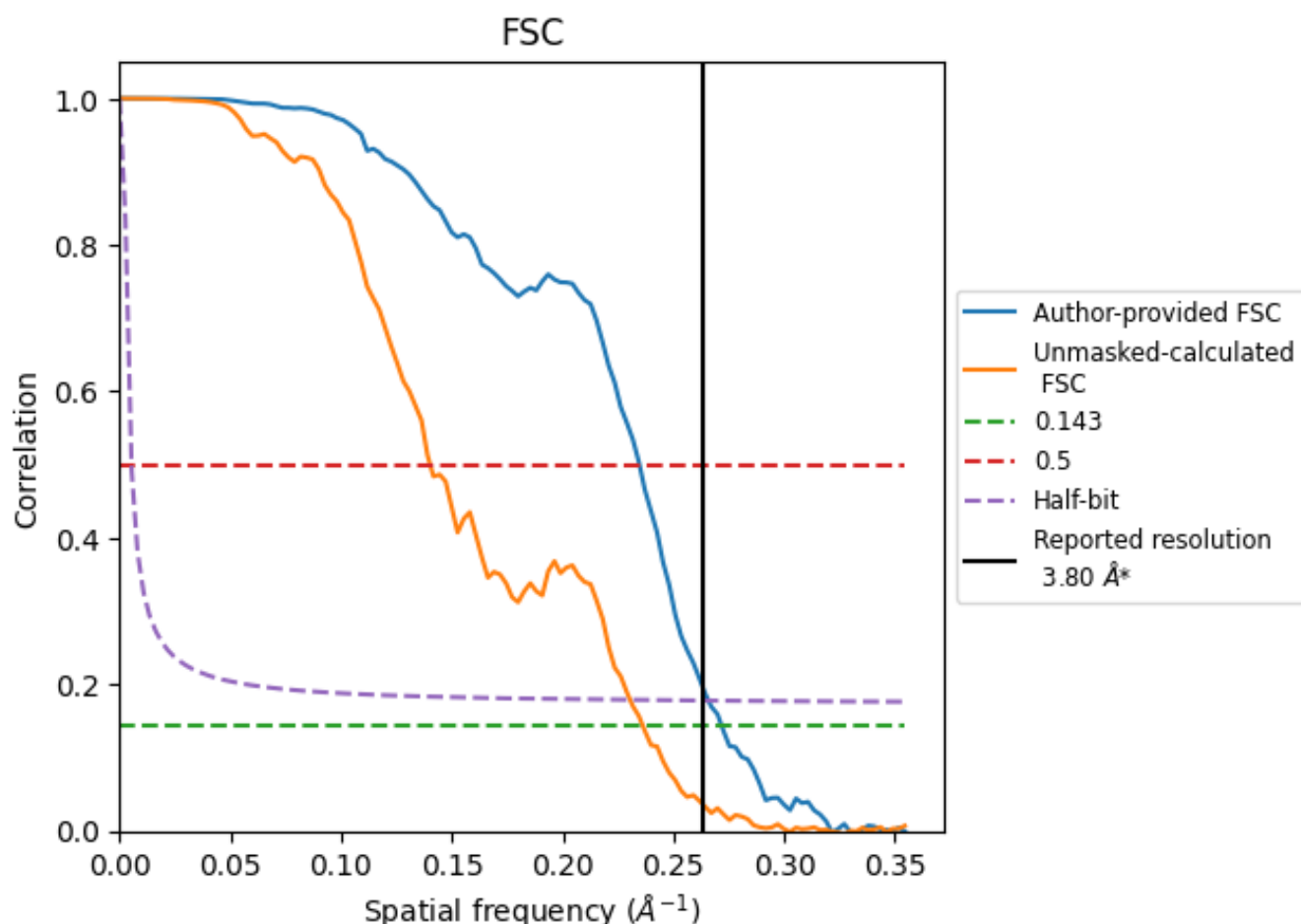


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

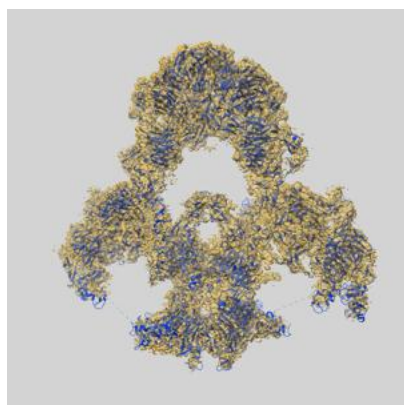
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.68	4.26	3.76
Unmasked-calculated*	4.23	7.13	4.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.23 differs from the reported value 3.8 by more than 10 %

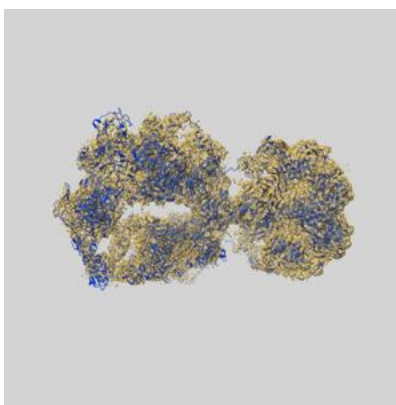
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36664 and PDB model 8JUU. Per-residue inclusion information can be found in section [3](#) on page [13](#).

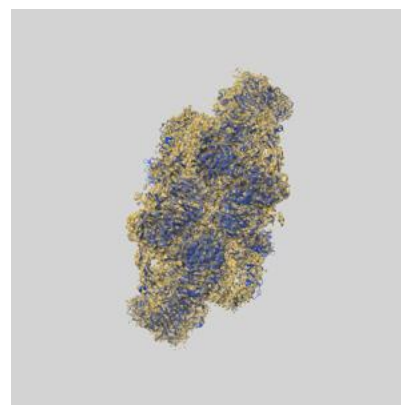
9.1 Map-model overlay [i](#)



X



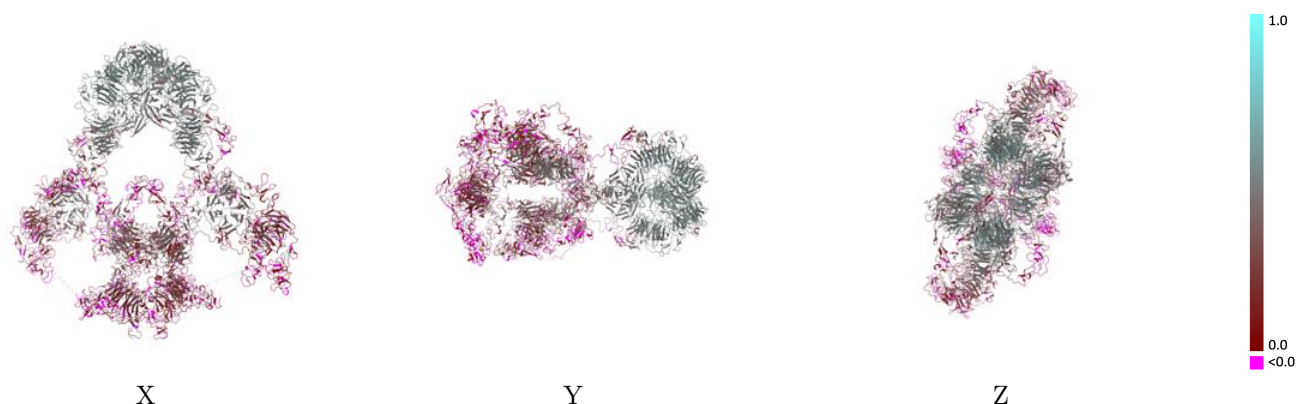
Y



Z

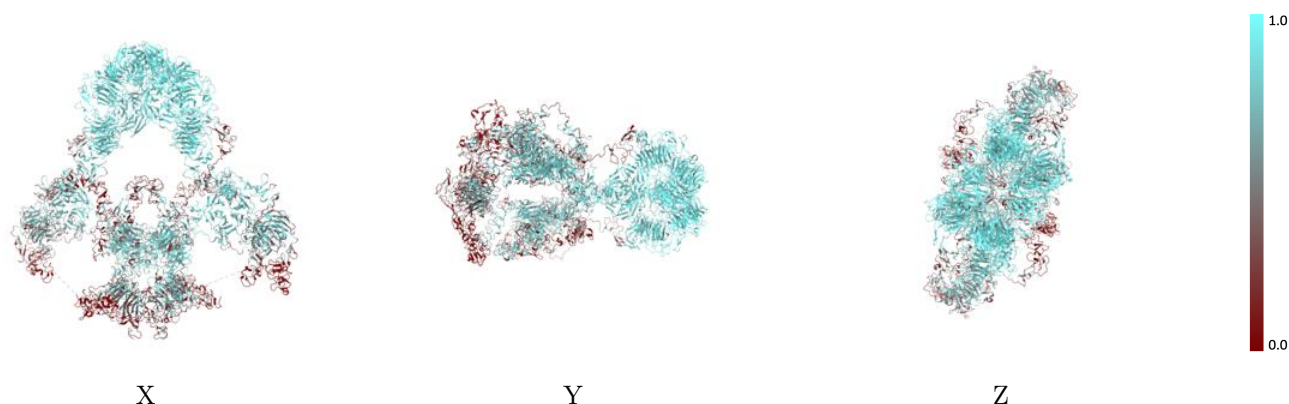
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



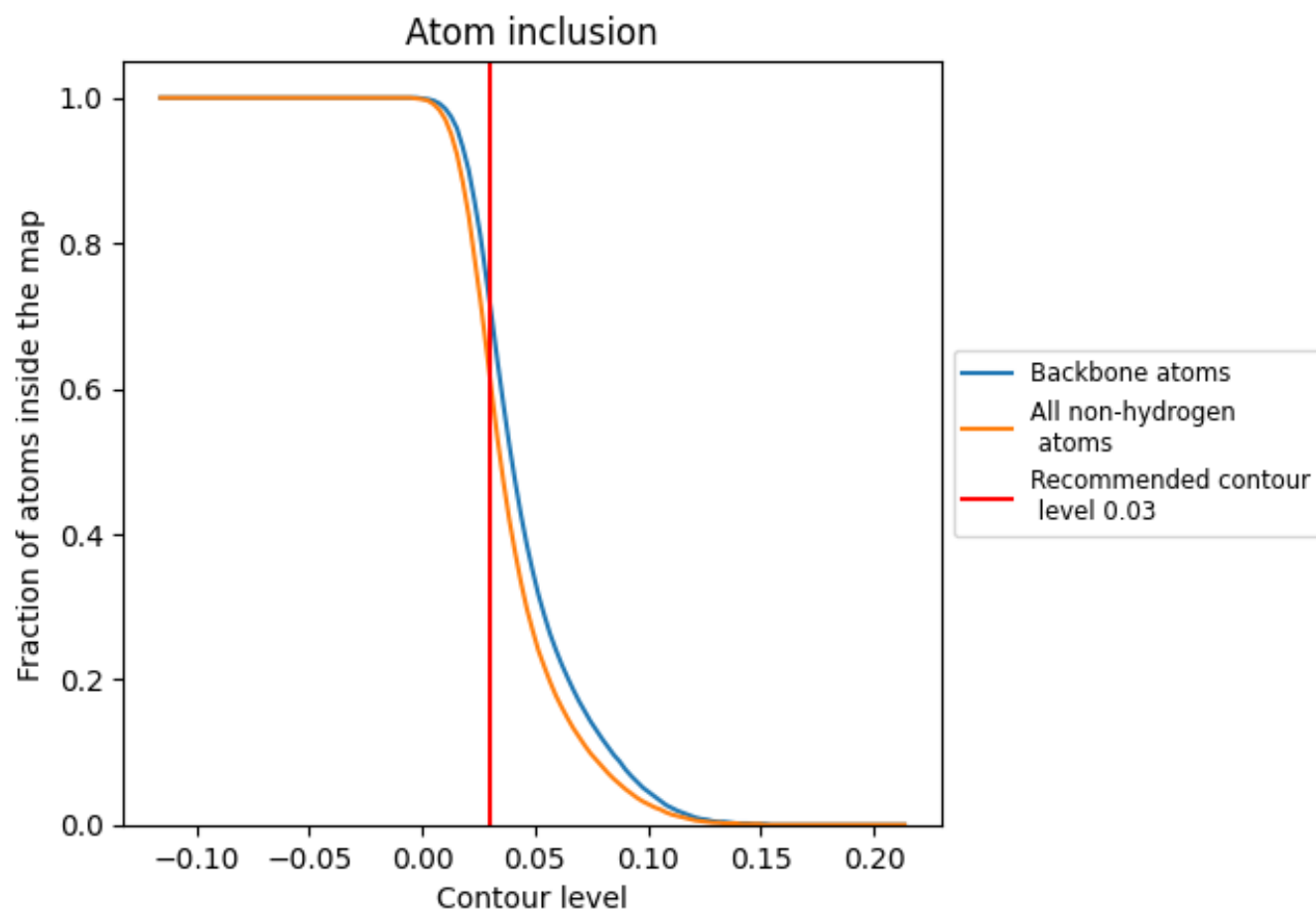
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 62% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6160	 0.2910
0	 0.1790	 0.1980
1	 0.1470	 0.0530
2	 0.2130	 0.1250
3	 0.0000	 0.0110
4	 0.1280	 0.0760
5	 0.1430	 0.2140
A	 0.6200	 0.2900
B	 0.6210	 0.2940
C	 0.9090	 0.4680
D	 0.7500	 0.3370
E	 0.1540	 0.0630
F	 0.7500	 0.3140
G	 0.8180	 0.4800
H	 0.7140	 0.3330
I	 0.9090	 0.4880
J	 0.7500	 0.3780
K	 0.7580	 0.3720
L	 0.7860	 0.4220
M	 0.3330	 0.1600
N	 0.8930	 0.4140
O	 0.9640	 0.4720
P	 0.4670	 0.1510
Q	 1.0000	 0.4880
R	 0.9290	 0.3910
S	 0.2500	 0.1690
T	 0.5130	 0.2980
U	 0.6430	 0.3810
V	 0.4290	 0.2320
W	 0.4430	 0.3610
X	 0.5000	 0.2450
Y	 0.8690	 0.4650
Z	 0.5360	 0.3450
a	 0.5000	 0.3060
b	 0.1790	 0.2150



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Continued from previous page...

Chain	Atom inclusion	Q-score
c	 0.4620	 0.2950
d	 0.4590	 0.2960
e	 0.1790	 0.2740
f	 0.3930	 0.2000
g	 0.0980	 0.1360
h	 0.2460	 0.1010
i	 0.1430	 0.1490
j	 0.1280	 0.1430
k	 0.1430	 0.1040
l	 0.1280	 0.0670
m	 0.6790	 0.3170
n	 0.3210	 0.2720
o	 0.4360	 0.3370
p	 0.6790	 0.3510
q	 0.2140	 0.2240
r	 0.3280	 0.3190
s	 0.5360	 0.3350
t	 0.8850	 0.4900
u	 0.5000	 0.3300
v	 0.3930	 0.3380
w	 0.1540	 0.1440
x	 0.5380	 0.2900
y	 0.4750	 0.2590
z	 0.0710	 0.0560