



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:20 PM UTC

PDB ID : 8JUT / pdb_00008jut
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:

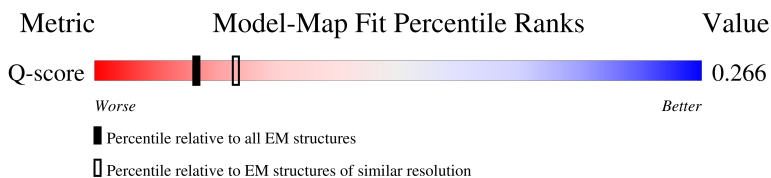
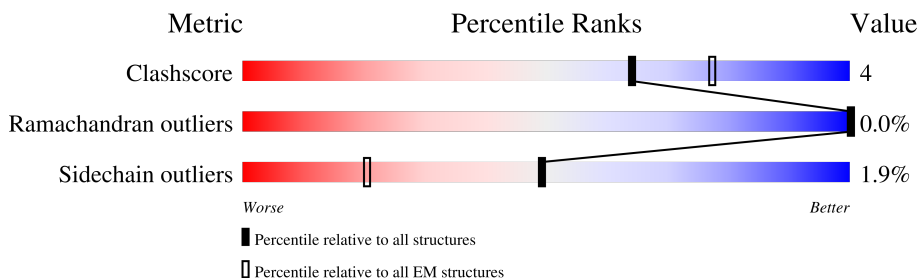
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	<p>34% (Poor fit), 82% (0 outliers), 10% (1 outlier), 8% (2 outliers), 0% (3+ outliers)</p>
1	B	4660	<p>32% (Poor fit), 82% (0 outliers), 10% (1 outlier), 8% (2 outliers), 0% (3+ outliers)</p>
2	C	360	<p>47% (Poor fit), 39% (0 outliers), 11% (1 outlier), 51% (2+ outliers)</p>
2	D	360	<p>48% (Poor fit), 38% (0 outliers), 11% (1 outlier), 51% (2+ outliers)</p>

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Mol	Chain	Length	Quality of chain
3	G	6	100%
3	N	6	100%
4	H	5	20%
4	O	5	100%
5	I	6	83%
5	P	6	83%
6	J	3	67%
6	Q	3	33%
7	K	5	20%
7	R	5	20%
8	L	5	40%
8	M	5	100%
8	S	5	60%
8	T	5	100%
9	E	2	50%
9	V	2	50%
9	X	2	50%
9	Y	2	50%
9	a	2	50%
9	d	2	50%
9	n	2	50%
9	q	2	50%
9	s	2	50%
9	t	2	50%
9	v	2	50%

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Mol	Chain	Length	Quality of chain
9	x	2	50% 100%
9	y	2	50% 50%
10	1	5	60% 40%
10	4	5	100% 40% 20% 40%
10	5	5	80% 80% 20%
10	9	5	100% 80% 20%
10	F	5	100% 100%
10	Z	5	60% 40% 60%
10	b	5	20% 100%
10	g	5	60% 80% 20%
10	j	5	80% 60% 20% 20%
10	k	5	80% 40% 60%
10	l	5	100% 60% 20% 20%
10	u	5	80% 60% 40%
11	U	5	60% 40% 60%
12	2	3	67% 100%
12	3	3	67% 67% 33%
12	W	3	33% 33% 33% 33%
12	e	3	100% 67% 33%
12	f	3	67% 100%
12	h	3	100% 100%
12	i	3	67% 33% 67%
12	m	3	100% 33% 67%
12	p	3	33% 67% 33%
12	r	3	33% 67% 33%

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Mol	Chain	Length	Quality of chain
13	8	2	100%
13	c	2	50%
13	o	2	100%
14	6	5	100%
14	w	5	60%
15	z	3	100%
16	0	3	67%
16	7	3	100%

2 Entry composition [i](#)

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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O		
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
			Total	C	N	O		
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.



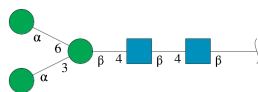
Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	2	Total	C	N	O	0	0
			28	16	2	10		

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

- 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.



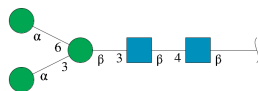
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	F	5	61	34	2	25	0	0
10	Z	5	61	34	2	25	0	0
10	b	5	61	34	2	25	0	0
10	g	5	61	34	2	25	0	0

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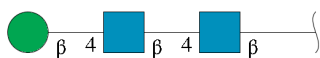
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	j	5	61	34	2	25	0	0
10	k	5	61	34	2	25	0	0
10	l	5	61	34	2	25	0	0
10	u	5	61	34	2	25	0	0
10	1	5	61	34	2	25	0	0
10	4	5	61	34	2	25	0	0
10	5	5	61	34	2	25	0	0
10	9	5	61	34	2	25	0	0

- 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
			Total	C	N	O		
11	U	5	61	34	2	25	0	0

- 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.



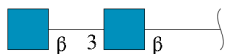
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	W	3	39	22	2	15	0	0
12	e	3	39	22	2	15	0	0

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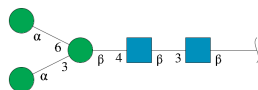
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	f	3	Total 39	C 22	N 2	O 15	0	0
12	h	3	Total 39	C 22	N 2	O 15	0	0
12	i	3	Total 39	C 22	N 2	O 15	0	0
12	m	3	Total 39	C 22	N 2	O 15	0	0
12	p	3	Total 39	C 22	N 2	O 15	0	0
12	r	3	Total 39	C 22	N 2	O 15	0	0
12	2	3	Total 39	C 22	N 2	O 15	0	0
12	3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

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



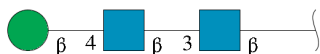
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	c	2	Total 28	C 16	N 2	O 10	0	0
13	o	2	Total 28	C 16	N 2	O 10	0	0
13	8	2	Total 28	C 16	N 2	O 10	0	0

- 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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



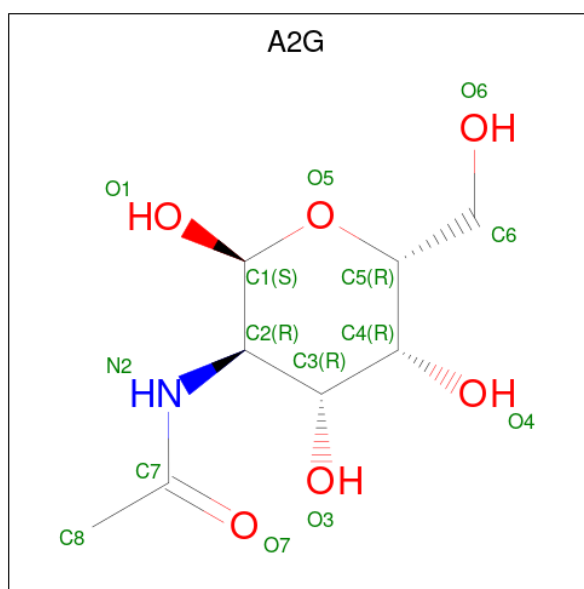
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total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

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
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 (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



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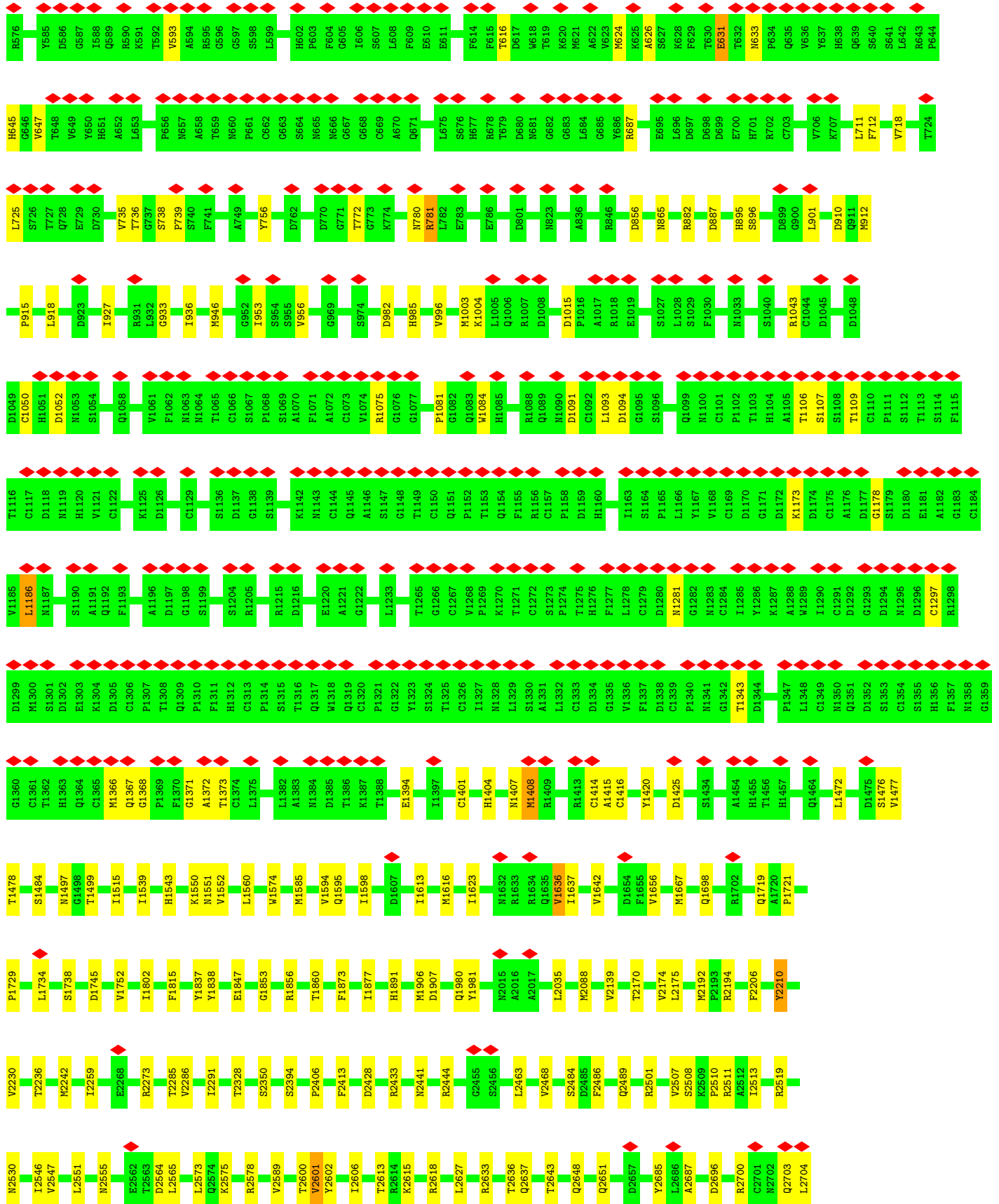
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
18	A	1	Total 14	C 8	N 1	O 5	0
18	A	1	Total 14	C 8	N 1	O 5	0
18	A	1	Total 14	C 8	N 1	O 5	0
18	A	1	Total 14	C 8	N 1	O 5	0
18	A	1	Total 14	C 8	N 1	O 5	0
18	A	1	Total 14	C 8	N 1	O 5	0
18	A	1	Total 14	C 8	N 1	O 5	0
18	A	1	Total 14	C 8	N 1	O 5	0
18	A	1	Total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

- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

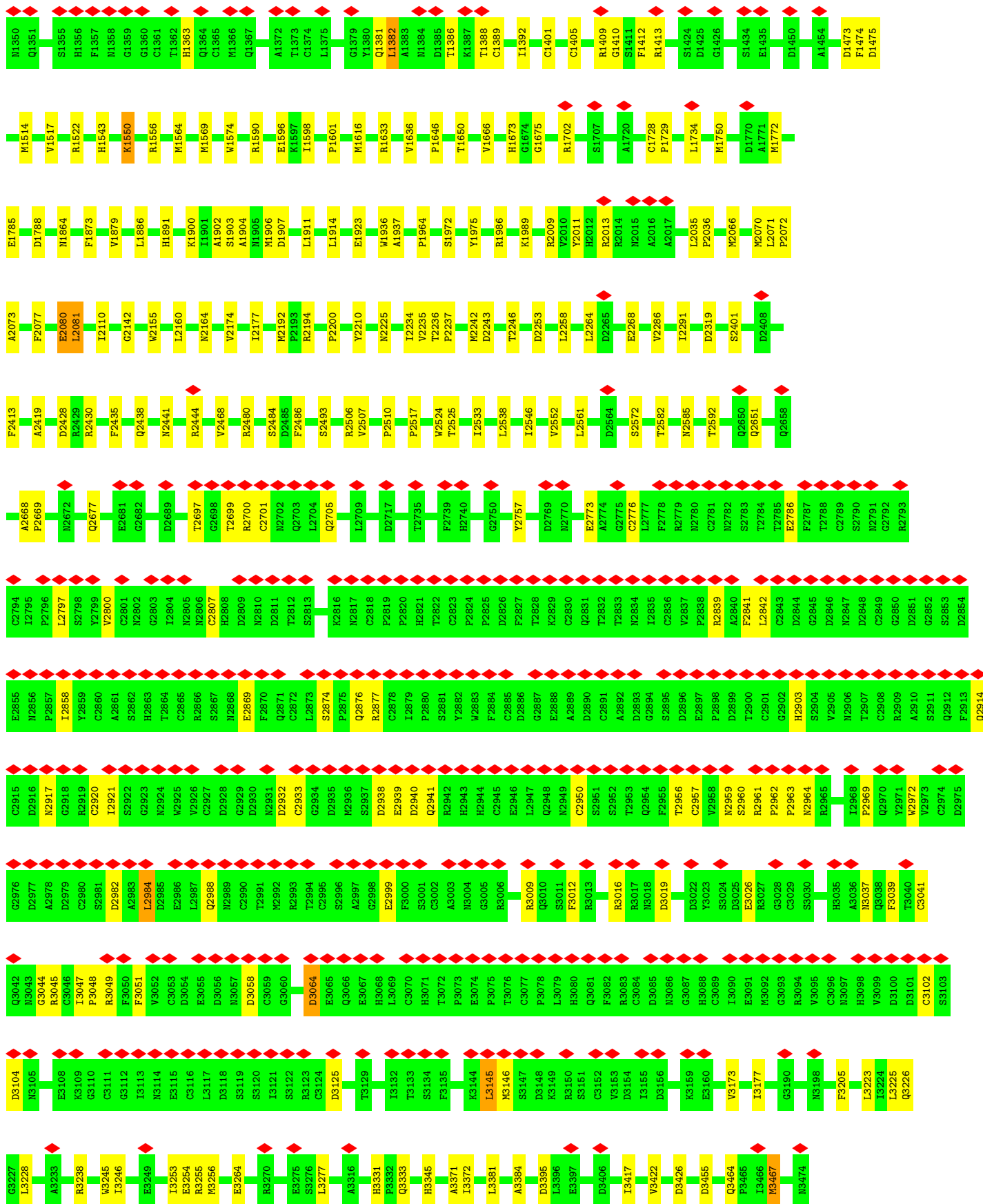
- Molecule 20 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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



E3886	C3812	R3693	L3509	M3308	Y3136	T3076	G3005	Q2941	R2877	N2817	Q2705
S3887	V3813	C3694	M3513	H3312	C3137	C3077	R3006	R2942	C2878	C2818	C2708
P3888	P3814	I3695	S3516	D3315	K3144	F3078	R3009	H2943	I2879	P2819	L2709
I3889	L3817	D3705	S3598	D3316	L3145	L3079	Q3010	H2944	P2880	P2820	I2710
R3890	A3818	R3708	N3523	A3316	M3146	H3081	Q3011	C2945	S2881	H2821	G2711
F3891	C3819	R3708	N3524	R3326	S3147	F3082	F3012	E2946	W2882	T2822	H2712
R3892	D3820	R3708	E3525	H3345	D3148	R3083	R3013	L2947	W2883	C2823	C2713
C3893	G3821	Q3714	E3525	H3345	K3149	C3084	C3014	H2949	F2884	P2824	Q2716
D3894	L3826	I3714	I3530	D3375	R3150	D3085	D3015	C2950	D2885	P2825	I2722
S3896	C3834	S3718	C3534	C3151	S3151	D3086	R3016	C2952	G2887	D2828	I2722
R3897	P3835	V3719	C3534	N3378	C3152	G3087	R3017	S2952	E2887	F2827	G2727
C3898	L3836	F3720	K3538	D3406	I3155	H3088	D3022	A2889	A2888	K2829	S2730
F3899	R3837	V3722	V3618	L3415	C3158	C3089	Y3023	Q2954	A2889	C2829	S2730
Y3900	F3838	P3723	N3619	L3415	K3159	E3091	E3026	F2955	C2891	Q2831	F2739
G3901	P3839	H3722	D3620	T3416	E3160	N3092	R3027	V2958	A2892	T2832	F2747
H3902	N3840	P3723	G3543	I3417	E3160	G3093	G3028	N2959	D2893	T2833	F2747
G3841	G3841	D3726	S3544	L3421	V3173	G3094	C3029	S2960	G2894	N2834	F2747
C3844	D3623	A3730	D3545	T3421	G3189	R3095	S3030	R2961	I2835	I2835	G2775
C3905	D3626	H3732	E3546	V3422	D3189	C3096	S3032	P2962	C2836	C2836	R2779
P3845	E3627	N3731	P3547	T3425	K3191	N3097	P3032	P2962	D2899	W2837	I2780
A3846	D3628	T3425	D3548	T3425	K3191	H3098	N3037	P2963	T2900	C2781	C2781
V3908	T3629	D3426	L3549	D3426	S3206	V3099	Q3038	N2964	R2839	I2782	I2782
D3909	S3630	T3431	C3550	T3431	R3212	H3099	F3039	R2965	A2840	A2840	S2783
C3905	F3551	N3448	H3552	N3448	T3215	D3100	F3042	S2904	L2842	L2842	T2784
P3845	H3552	T3449	H3552	T3449	T3215	D3101	Q3042	S2904	C2843	C2843	T2784
A3846	R3553	F3450	F3554	F3450	S3220	S3103	N3043	V2905	D2844	D2844	E2786
M3848	C3637	H3451	C3555	H3451	S3220	D3104	G3044	Q2970	G2845	G2845	F2787
F3849	R3638	R3452	R3556	R3452	L3228	H3105	R3045	V2972	D2846	D2846	T2788
E3850	K3643	C3756	L3557	P3453	V3231	S3106	C3046	W2972	N2847	N2847	C2789
C3851	C3644	V3757	G3558	T3473	V3231	D3107	I3047	V2973	D2848	D2848	S2790
D3913	C3644	P3758	Q3559	N3474	E3249	E3108	P3048	G2976	C2849	C2849	I2791
G3912	R3637	R3746	C3562	N3474	E3249	I3109	R3049	D2977	G2850	G2850	G2792
C3914	K3655	G3748	R3563	G3476	M3256	K3110	R3052	D2977	D2851	D2851	R2793
S3915	K3655	E3765	G3565	G3477	M3256	G3111	V3052	C2980	Q2912	Q2912	C2794
I3916	N3660	E3765	G3565	C3478	K3260	G3111	C3053	C2980	Q2913	Q2913	I2795
E3917	S3666	A3769	Q3571	S3479	R3270	I3113	D3064	S2981	C2915	C2915	F2796
K3918	D3671	N3784	A3572	H3480	L3271	I3113	E3055	D2982	D2916	D2916	L2797
C3922	E3672	G3787	L3572	L3481	R3271	G3115	D3056	A2983	N2917	N2917	S2798
R3923	T3675	T3675	L3573	L3483	R3272	E3115	N3057	L2984	N2856	N2856	Y2799
K3924	T3675	T3675	A3576	L3483	E3275	C3116	C3059	L2987	P2857	P2857	Y2800
T3926	A3676	A3676	R3577	D3497	E3275	L3117	G3060	Q2988	I2858	I2858	C2801
H3927	A3677	A3677	R3577	D3497	L3277	D3118	S3063	Q2988	Y2859	Y2859	C2801
K3928	Y3678	Y3678	Q3578	D3498	L3277	S3119	D3064	N2989	C2860	C2860	G2803
F3929	N3679	N3679	D3579	D3498	D3280	S3120	S3063	C2990	A2861	A2861	G2803
C3930	C3680	C3680	A3580	T3501	D2800	I3121	E3065	C2990	A2861	A2861	I2804
T3931	N3682	N3682	A3581	V3502	S3283	S3122	Q3066	G2923	S2922	S2922	I2804
I3932	H3683	H3683	L3504	L3296	S3283	C3124	D3068	N2924	N2924	N2924	I2804
E3934	R3683	R3683	R3506	L3296	S3283	H3125	H3068	C2929	C2929	C2929	I2804
Y3935	S3687	S3687	A3507	A3507	G3303	D3126	L3069	D2929	D2929	D2929	I2804
K3936	S3687	S3687	R3507	T3508	G3303	H3127	L3069	D2929	D2929	D2929	I2804
C3937	S3688	S3688	R3507	T3508	G3303	C3128	S3070	D2929	D2929	D2929	I2804
S3938	K3689	K3689	H3592	H3592	G3303	C3128	H3071	D2929	D2929	D2929	I2804
I3939	S3809	S3809	L3590	L3590	G3303	C3129	H3071	D2929	D2929	D2929	I2804
G3940	G3810	G3810	C3591	C3591	G3303	T3072	T3072	D2929	D2929	D2929	I2804
N3941	H3811	H3811	E3592	E3592	G3303	P3073	P3073	D2929	D2929	D2929	I2804
C3942	N3882	N3882	H3593	H3593	G3303	F3000	F3000	D2929	D2929	D2929	I2804
I3943	I3883	I3883	H3593	H3593	G3303	S3001	S3001	D2929	D2929	D2929	I2804
S3944	C3884	C3884	H3593	H3593	G3303	A3002	A3002	D2929	D2929	D2929	I2804
I3945	C3885	C3885	H3593	H3593	G3303	A3003	A3003	D2929	D2929	D2929	I2804

THR	LEU	CYS	SER	GLN	K186	E187	F188	E189	C190	G191	S192	G193	E194	C195	I196	L197	R198	A199	R200	Y201	H204	D205	N206	D207	C208	E209	D210	N211	S212	D213	E214	N216	C217	N218	Y219	D220	C221	G222	G223	H224	G225	Q226	F227	T228	C229	S230	Q233	C234	N238	W239	V240	G243	D244	D245						
D246	C247	Q248	D249	S250	Q251	D252	E253	D254	G255	C256	E257	S258	N259	Q260	S261	H262	H263	R264	C265	Y266	P267	R268	E269	W270	A271	C272	P273	G274	S275	G276	R277	I279	S280	I281	D282	K283	V284	C285	G286	G287	V288	P289	D290	C291	P292	E293	G294	D295	D296	E297	N298	N299	V300	T301	G303	R304	T305			
C306	G307	M308	G309	V310	C311	S312	V313	L314	G315	C316	E317	Q318	Q319	C320	H321	Q322	T323	P324	F325	G326	G327	E328	C329	F330	C331	P332	P333	G334	H335	I336	I337	N338	S339	N340	D341	S342	R343	T344	C345	I346	D347	F348	D349	D350	C351	Q352	I353	W354	G355	D356	I356	C357	D358	Q359	K360	C361	E362	N363	R364	Q365
G366	R367	H368	Q369	C370	L371	C372	E373	E374	G375	Y376	I377	L378	E379	R380	G381	Q382	H383	C384	K385	S386	S387	D388	S389	F390	S391	A392	A393	S394	S395	G396	F397	S398	R401	D402	L403	L404	V405	D407	L408	H409	G410	R411	N412	D3949	D350	R414	I415	L416	A417	E418	W421	G427	V428	D429	F430	H431				
Y432	Q433	K434	F438	W439	T440	D441	P442	M443	Q444	E445	V446	V447	F448	S449	T450	D451	T452	M453	G454	L455	M456	T457	Q458	L461	S464	V465	D466	T467	P468	E469	M470	A472	V473	D474	W475	I476	M477	M478	K479	L480	Y481	K486	V487	M488	R489	I490	D491	V492	V493	E496	G497	M498	Q499							
R500	L503	I504	T505	L508	R512	G513	L514	A515	L516	D517	P518	T519	F525	S526	D527	S530	L531	S532	G533	V537	M542	D543	G544	D549	L550	V551	T552	T553	K554	A559	G560	I561	T562	L563	D564	L565	V566	S567	K568	T571	D574	Y577	L580	D586	G587															
I588	Q589	T592	W593	A594	R595	S596	L599	V600	F604	G605	T606	S607	L608	F609	E610	E611	H612	V613	F614	T615	T616	T619	K620	V623	M624	K625	A626	S627	K628	F629	T630	E631	T632	N633	P634	Q635	V636	V637	H638	D639	S640	S641	L642	P643	P644	H645	G646	T646	V649	R654	T659									
R661	C662	G663	S664	R665	N666	G667	C669	A670	D671	L675	R676	T679	D680	M681	G682	G683	L684	R687	F615	C688	K689	C690	E691	E695	L696	D697	D698	D699	E700	H701	R702	C703	W704	A705	V706	K707	L725	V735	T736	S738	F739	S740	F741	F742	Y756	S757	K766	G771												
I777	M1003	K1004	M1010	T1011	C1012	A1017	Q1023	L1028	N1033	F1041	H1051	H1057	Q1058	C1059	G1060	F1062	N1063	C1066	S1069	A1072	C1073	V1074	R1075	G1076	Q1077	Q1078	C1079	I1080	P1081	V1084	H1085	C1086	D1087	R1088	D1091	C1092	L1093	Q1099	N1100	C1101	P1102	T1103																		
H1104	A1105	T1106	S1107	S1108	T1109	C1110	P1111	T1112	S1113	S1114	F1115	D1118	M1119	H1120	V1121	C1122	I1123	P1124	K1125	D1126	C1129	D1134	C1135	S1136	L1137	G1138	S1139	D1140	E1141	K1142	M1143	C1144	Q1145	S1146	G1148	T1149	C1150	Q1151	P1152	T1153	Q1154	F1155	R1156	C1157	P1158	D1159	H1160	C1161	L1162	I1163	S1164	P1165	L1166	C1169						
D1170	G1171	D1172	K1173	A1176	D1177	G1178	S1179	D1180	E1181	A1182	G1183	C1184	V1185	L1186	M1187	C1188	T1189	S1190	A1191	K1194	C1195	A1196	D1197	G1198	S1199	S1200	C1201	R1215	D1216	N1217	C1223	L1233	E1250	T1265	G1266	C1267	K1270	T1271	C1272	S1273	P1274	T1275	H1276	F1277	L1278	C1279	D1280	M1281	G1282	N1283	C1284									
I1285	Y1286	K1287	D1292	G1293	D1294	N1295	R1298	D1299	M1300	S1301	D1302	E1303	K1304	D1305	C1306	P1307	T1308	Q1309	P1310	F1311	H1312	C1313	P1314	S1315	T1316	Q1317	M1318	C1320	Q1319	D1216	N1217	C1223	L1233	E1250	T1265	G1266	C1267	K1270	T1271	C1272	S1273	P1274	T1275	H1276	F1277	L1278	C1279	D1280	M1281	G1282	N1283	C1284								
S1346	P1347	L1348	C1349																																																									



LEU	T4366	K4301	M4234	M4011	N3951	R3890	E3792	D3671	T3568	G3477
THR	V4367	F4302	G4235	E4012	V3952	F3891	R3793	E3672	A3572	C3478
PHE		G4303	L4236	C4013	N3953		D3794	G3680	L3573	S3479
VAL		K4304	S4237	E4014	D3954	D3894	C3684	C3574	C3574	H3480
ILE		E4305	I4238	E4015	C3955	N3895	A3816	T3684	G3578	L3481
ILE		M4306	D4239	F4016	C3956	S3896	L3817	T3685		
VAL	S4373	K4307	Y4240	F4017	D3957	R3897	A3818	F3686		
GLY	E4374	E4308	L4241	I4018	L3958	C3898	G3821	K3689		
ALA	L4375	K4309	L4242	C4019	S3959	V3899	R3822	A3581		
LEU	P4376	V4310	D4243	P4020	S3960	Y3900	A3823	R3582		
VAL	V4377	L4311	D4244	Q4021	G3901	G3901	L3826	D3587		
LEU	T4378	V4312	R4245	S4022	H3902	H3902	D3827	R3588		
VAL		V4313	Y4246	C4023	Q3903	Q3903	D3827	V3589		
LEU	P4381	M4314	Y4247	R4023	L3904	L3904	Q3714	T3501		
PHE		P4315	S4251	R4024	C3905	C3905	G3715	V3502		
HIS		M4316	K4252	M4025	N3906	N3906	A3730	T3503		
TYR		Q4319	E4253	S4026	L3966	L3966	A3730	Q3503		
ARG		F4323	V4255	K4027	G3967	G3967	S3718	L3504		
LYS	H4387	H4324	I4256	G4028	D3968	D3968	V3719	R3506		
THR	G4388	H4324	Q4325	S4029	N3969	N3969	R3720	D3506		
GLY	G4389	Q4325	E4257	E4030	R3970	R3970	C3721	P3506		
SER	M4390	L4326	E4257	Y4030	R3970	R3970	D3726	R3507		
LEU	C4391	L4326	A4258	E4031	T3971	T3971	F3727	T3508		
LEU		R4327	I4259	C4032	C3972	C3972	F3727	L3509		
PRO	Y4392	Y4328	K4260	F4033	A3973	A3973	A3730	S3516		
THR	F4393	Y4328	K4260	F4033	A3973	A3973	A3730	S3516		
LEU	D4394	M4329	Y4261	C4034	E3974	E3974	A3847	Q3602		
PRO	D4394	M4329	Y4261	C4034	E3974	E3974	A3847	C3603		
LYS	E4395	Q4330	D4262	Y4035	N3975	N3975	A3847	A3604		
LEU	M4396	S4331	Q4263	D4036	R3976	R3976	H3848	N3605		
LEU	E4397	V4332	Y4264	G4037	C3977	C3977	F3849	K3606		
PRO	E4397	V4332	Y4264	G4037	C3977	C3977	F3849	K3606		
SER	L4398	S4333	M4195	F4038	E3978	E3978	K3852	P3610		
LEU	P4399	M4334	D4265	F4038	E3978	E3978	K3852	P3610		
SER	L4400	P4335	R4266	K4039	Q3979	Q3979	L3857	Q3611		
SER	K4400	P4335	R4266	K4039	Q3979	Q3979	L3857	Q3611		
LEU	C4401	C4336	L4268	S4040	N3980	N3980	N3750	V3613		
ALA	K4402	K4337	I4269	M4041	C3981	C3981	N3750	V3613		
LYS	C4403	Q4338	I4270	S4042	T3982	T3982	N3750	V3613		
PRO	C4403	Q4338	I4270	S4042	T3982	T3982	N3750	V3613		
SER	S4404	V4339	M4271	T4043	Q3983	Q3983	C3862	Q3614		
GLU	S4405	C4340	M4271	T4043	Q3983	Q3983	C3862	Q3614		
ASN	S4405	C4340	M4271	T4043	Q3983	Q3983	C3862	Q3614		
GLY	G4406	S4341	A4273	H4044	S3985	S3985	D3864	S3617		
ASN	G4406	S4341	A4273	H4044	S3985	S3985	D3864	S3617		
GLY	Y4407	H4342	M4274	Y4045	S3986	S3986	G3866	D3620		
GLY	Y4407	H4342	M4274	Y4045	S3986	S3986	G3866	D3620		
VAL	S4408	L4343	D4205	E4047	S3987	S3987	N3867	C3621		
THR	S4408	L4343	D4205	E4047	S3987	S3987	N3867	C3621		
VAL	G4409	C4344	K4208	C4048	G3988	G3988	D3868	L3622		
PHE	G4409	C4344	K4208	C4048	G3988	G3988	D3868	L3622		
ARG	Y4411	L4345	I4212	A4051	F3989	F3989	C3869	D3623		
ARG	Y4411	L4345	I4212	A4051	F3989	F3989	C3869	D3623		
SER	C4412	L4346	E4213	A4051	C3991	C3991	V3870	D3626		
SER	C4412	L4346	E4213	A4051	C3991	C3991	V3870	D3626		
GLY	E4413	P4348	E4126	D4052	C3993	C3993	E3875	T3629		
ALA	E4413	P4348	E4126	D4052	C3993	C3993	E3875	T3629		
ASP	G4414	G4349	S4127	G4053	C3993	C3993	E3875	T3629		
ASP	G4414	G4349	S4127	G4053	C3993	C3993	E3875	T3629		
VAL	G4414	G4350	G4128	S4054	C3994	C3994	E3876	S3630		
VAL	G4414	G4350	G4128	S4054	C3994	C3994	E3876	S3630		
ASN	G4415	C4353	S4129	A4054	C3995	C3995	I3877	H3631		
ASN	G4415	C4353	S4129	A4054	C3995	C3995	I3877	H3631		
MET	LEU	A4354	Y4224	L4057	F3995	F3995	C3768	C3632		
MET	LEU	A4354	Y4224	L4057	F3995	F3995	C3768	C3632		
ARG	ARG	A4354	L4225	L4058	K3936	K3936	D3770	A3633		
GLY	GLY	A4354	L4225	L4058	K3936	K3936	D3770	A3633		
ILE	ILE	Q4357	K4290	L4059	C3937	C3937	Q3771	A3633		
ILE	ILE	Q4357	K4290	L4059	C3937	C3937	Q3771	A3633		
PRO	PRO	G4358	K4291	L4060	S3938	S3938	Q3772	R3635		
PRO	PRO	G4358	K4291	L4060	S3938	S3938	Q3772	R3635		
LEU	LEU	S4359	K4292	P4061	N3939	N3939	R3777	N3645		
LEU	LEU	S4359	K4292	P4061	N3939	N3939	R3777	N3645		
GLY	THR	D4360	K4293	E4062	G3940	G3940	G3787	G3663		
GLY	THR	D4360	K4293	E4062	G3940	G3940	G3787	G3663		
THR	THR	L4230	G4294	R4066	N3941	N3941	I3943	D3664		
THR	THR	L4230	G4294	R4066	N3941	N3941	I3943	D3664		
THR	THR	G4361	G4231	R4067	C3942	C3942	I3943	D3664		
THR	THR	G4361	G4231	R4067	C3942	C3942	I3943	D3664		
MET	MET	V4362	K4232	I4066	D4003	D4003	G3787	I3670		
MET	MET	V4362	K4232	I4066	D4003	D4003	G3787	I3670		
ALA	ALA	T4363	P4233	R4067	L4002	L4002	D3791			
ALA	ALA	T4363	P4233	R4067	L4002	L4002	D3791			
VAL	VAL	G4364	R4295	K4068	D4003	D4003	D3791			
VAL	VAL	G4364	R4295	K4068	D4003	D4003	D3791			
LEU	LEU	S4365	Y4299	Y4070	C4007	C4007				
LEU	LEU	S4365	Y4299	Y4070	C4007	C4007				
LEU	LEU	S4365	M4300	S4073	D4009	D4009				
LEU	LEU	S4365	M4300	S4073	D4009	D4009				



• Molecule 3: unclear peptide



• Molecule 3: unclear peptide



• Molecule 4: unclear peptide

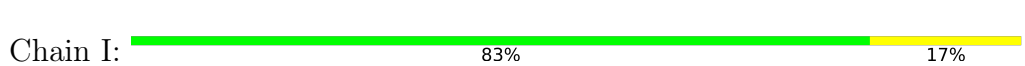


• Molecule 4: unclear peptide

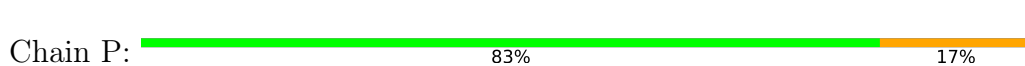


There are no outlier residues recorded for this chain.

• Molecule 5: unclear peptide



• Molecule 5: unclear peptide



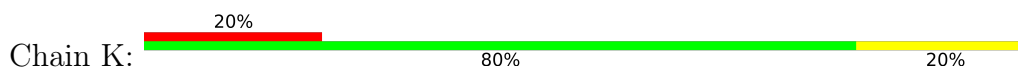
• Molecule 6: unclear peptide



- 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%



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

Chain V:  100%



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

Chain X:  100%



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

Chain Y:  100%



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

Chain a:  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



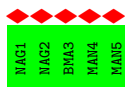
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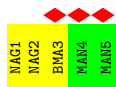
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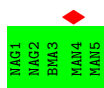
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



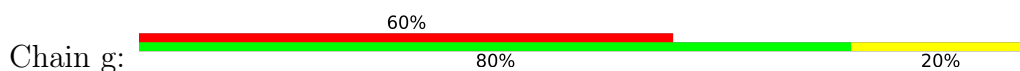
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

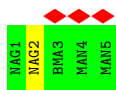


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

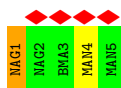
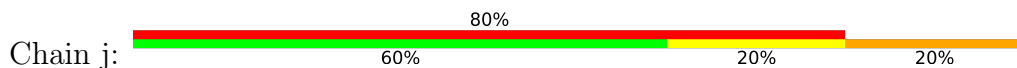


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

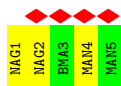
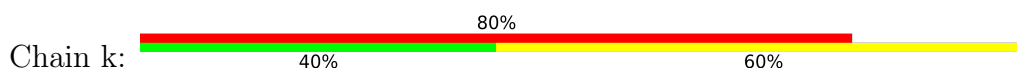




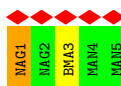
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



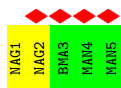
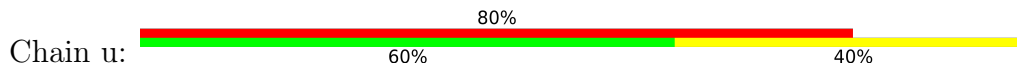
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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

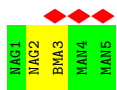


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

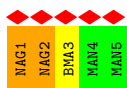


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

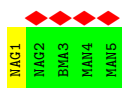




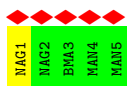
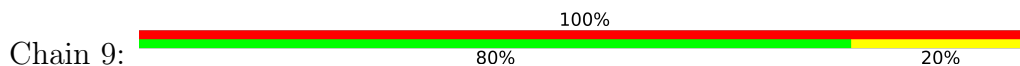
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



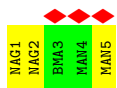
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



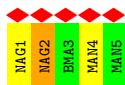
- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/34456	0.79	19/46804 (0.0%)
1	B	0.92	0/34454	0.97	9/46801 (0.0%)
2	C	0.92	0/1521	1.17	0/2033
2	D	0.89	0/1521	1.16	0/2033
4	H	0.68	0/7	0.67	0/8
4	O	0.81	0/7	0.91	0/8
5	I	0.66	0/7	0.79	0/8
5	P	0.67	0/7	1.01	0/8
6	J	1.05	0/5	0.78	0/5
6	Q	1.04	0/5	0.60	0/5
7	K	0.98	0/17	0.94	0/21
7	R	0.66	0/17	0.73	0/21
8	L	0.62	0/7	0.66	0/8
8	M	0.67	0/7	0.70	0/8
8	S	0.94	0/7	0.74	0/8
8	T	0.60	0/7	0.71	0/8
All	All	0.75	0/72052	0.90	28/97787 (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 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2938	ASP	CA-CB-CG	9.92	122.52	112.60
1	A	4243	ASP	CA-CB-CG	8.24	120.84	112.60
1	A	2810	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	A	2819	PRO	N-CA-C	7.41	119.74	110.70
1	A	4284	ASP	CA-CB-CG	6.50	119.11	112.60

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	266	0
1	B	33636	0	31021	264	0
2	C	1494	0	1505	24	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	13	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	1	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	2	0
10	k	61	0	52	0	0
10	l	61	0	52	2	0
10	u	61	0	52	1	0
11	U	61	0	52	1	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	2	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	67424	574	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 574 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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3791/4089 (93%)	3709 (98%)	82 (2%)	45	64
1	B	3790/4089 (93%)	3727 (98%)	63 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	163/326 (50%)	159 (98%)	4 (2%)	42	62
2	D	163/326 (50%)	161 (99%)	2 (1%)	63	73
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%)	2 (100%)	0	100	100
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%)	7769 (98%)	152 (2%)	49	66

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1772	MET
1	B	3971	THR
1	B	2081	LEU
1	B	3064	ASP
2	D	337	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3941	ASN
1	B	3854	HIS
1	B	826	ASN
1	B	3755	ASN
2	C	83	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	1.44	1 (5%)
16	NAG	0	2	16	14,14,15	0.38	0	17,19,21	1.43	3 (17%)
16	BMA	0	3	16	11,11,12	0.32	0	15,15,17	0.46	0
10	NAG	1	1	10,1	14,14,15	0.48	0	17,19,21	0.90	0
10	NAG	1	2	10	14,14,15	0.43	0	17,19,21	0.67	1 (5%)
10	BMA	1	3	10	11,11,12	0.27	0	15,15,17	0.80	1 (6%)
10	MAN	1	4	10	11,11,12	0.31	0	15,15,17	0.61	0
10	MAN	1	5	10	11,11,12	0.28	0	15,15,17	0.51	0
12	NAG	2	1	12,1	14,14,15	0.91	0	17,19,21	1.55	5 (29%)
12	NAG	2	2	12	14,14,15	1.20	2 (14%)	17,19,21	1.02	1 (5%)
12	BMA	2	3	12	11,11,12	1.06	1 (9%)	15,15,17	0.94	1 (6%)
12	NAG	3	1	12,1	14,14,15	0.44	0	17,19,21	0.55	0
12	NAG	3	2	12	14,14,15	0.50	0	17,19,21	0.58	0
12	BMA	3	3	12	11,11,12	0.80	0	15,15,17	0.80	1 (6%)
10	NAG	4	1	10,1	14,14,15	0.41	0	17,19,21	1.02	1 (5%)
10	NAG	4	2	10	14,14,15	0.47	0	17,19,21	1.08	1 (5%)
10	BMA	4	3	10	11,11,12	0.30	0	15,15,17	0.97	2 (13%)
10	MAN	4	4	10	11,11,12	0.30	0	15,15,17	0.44	0
10	MAN	4	5	10	11,11,12	0.34	0	15,15,17	0.42	0
10	NAG	5	1	10,1	14,14,15	0.51	0	17,19,21	0.92	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	0.47	0	17,19,21	0.38	0
10	BMA	5	3	10	11,11,12	0.34	0	15,15,17	0.61	0
10	MAN	5	4	10	11,11,12	0.27	0	15,15,17	0.58	0
10	MAN	5	5	10	11,11,12	0.21	0	15,15,17	0.60	0
14	NAG	6	1	1,14	14,14,15	0.44	0	17,19,21	0.78	0
14	NAG	6	2	14	14,14,15	0.46	0	17,19,21	0.88	1 (5%)
14	BMA	6	3	14	11,11,12	0.38	0	15,15,17	0.98	0
14	MAN	6	4	14	11,11,12	0.27	0	15,15,17	0.83	1 (6%)
14	MAN	6	5	14	11,11,12	0.31	0	15,15,17	0.57	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	0.42	0
16	BMA	7	3	16	11,11,12	0.23	0	15,15,17	0.62	0
13	NAG	8	1	1,13	14,14,15	0.72	1 (7%)	17,19,21	1.38	2 (11%)
13	NAG	8	2	13	14,14,15	0.62	0	17,19,21	0.97	1 (5%)
10	NAG	9	1	10,1	14,14,15	0.39	0	17,19,21	0.86	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	0.28	0	15,15,17	0.61	0
10	MAN	9	4	10	11,11,12	0.28	0	15,15,17	0.60	0
10	MAN	9	5	10	11,11,12	0.26	0	15,15,17	0.47	0
9	NAG	E	1	9,1	14,14,15	0.40	0	17,19,21	1.02	1 (5%)
9	NAG	E	2	9	14,14,15	0.39	0	17,19,21	0.55	0
10	NAG	F	1	10,1	14,14,15	0.40	0	17,19,21	0.54	0
10	NAG	F	2	10	14,14,15	0.40	0	17,19,21	0.37	0
10	BMA	F	3	10	11,11,12	0.27	0	15,15,17	0.63	0
10	MAN	F	4	10	11,11,12	0.34	0	15,15,17	0.51	0
10	MAN	F	5	10	11,11,12	0.22	0	15,15,17	0.55	0
11	NAG	U	1	11,1	14,14,15	0.41	0	17,19,21	0.57	0
11	NAG	U	2	11	14,14,15	0.48	0	17,19,21	1.77	4 (23%)
11	BMA	U	3	11	11,11,12	0.59	0	15,15,17	0.85	0
11	MAN	U	4	11	11,11,12	0.31	0	15,15,17	0.65	0
11	MAN	U	5	11	11,11,12	0.37	0	15,15,17	0.74	1 (6%)
9	NAG	V	1	9,1	14,14,15	0.53	0	17,19,21	1.30	2 (11%)
9	NAG	V	2	9	14,14,15	0.55	0	17,19,21	0.89	1 (5%)
12	NAG	W	1	12,1	14,14,15	0.43	0	17,19,21	0.75	1 (5%)
12	NAG	W	2	12	14,14,15	0.41	0	17,19,21	0.86	1 (5%)
12	BMA	W	3	12	11,11,12	0.36	0	15,15,17	0.65	0
9	NAG	X	1	9,1	14,14,15	0.43	0	17,19,21	0.62	0
9	NAG	X	2	9	14,14,15	0.42	0	17,19,21	0.62	0
9	NAG	Y	1	9,1	14,14,15	0.40	0	17,19,21	0.42	0
9	NAG	Y	2	9	14,14,15	0.41	0	17,19,21	0.74	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	1.34	1 (5%)
10	NAG	Z	2	10	14,14,15	0.39	0	17,19,21	1.21	3 (17%)
10	BMA	Z	3	10	11,11,12	0.33	0	15,15,17	0.64	1 (6%)
10	MAN	Z	4	10	11,11,12	0.28	0	15,15,17	0.43	0
10	MAN	Z	5	10	11,11,12	0.25	0	15,15,17	0.46	0
9	NAG	a	1	9,1	14,14,15	0.39	0	17,19,21	0.72	0
9	NAG	a	2	9	14,14,15	0.40	0	17,19,21	0.36	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	0.44	0
10	BMA	b	3	10	11,11,12	0.33	0	15,15,17	0.75	0
10	MAN	b	4	10	11,11,12	0.28	0	15,15,17	0.54	0
10	MAN	b	5	10	11,11,12	0.23	0	15,15,17	0.49	0
13	NAG	c	1	1,13	14,14,15	0.52	0	17,19,21	0.83	1 (5%)
13	NAG	c	2	13	14,14,15	0.56	0	17,19,21	1.10	1 (5%)
9	NAG	d	1	9,1	14,14,15	0.40	0	17,19,21	0.65	0
9	NAG	d	2	9	14,14,15	0.40	0	17,19,21	0.50	0
12	NAG	e	1	12,1	14,14,15	0.42	0	17,19,21	0.40	0
12	NAG	e	2	12	14,14,15	0.42	0	17,19,21	0.59	0
12	BMA	e	3	12	11,11,12	0.33	0	15,15,17	0.72	1 (6%)
12	NAG	f	1	12,1	14,14,15	0.42	0	17,19,21	0.46	0
12	NAG	f	2	12	14,14,15	0.42	0	17,19,21	0.56	0
12	BMA	f	3	12	11,11,12	0.23	0	15,15,17	0.56	0
10	NAG	g	1	10,1	14,14,15	0.46	0	17,19,21	0.40	0
10	NAG	g	2	10	14,14,15	0.39	0	17,19,21	0.73	1 (5%)
10	BMA	g	3	10	11,11,12	0.41	0	15,15,17	0.73	0
10	MAN	g	4	10	11,11,12	0.30	0	15,15,17	0.47	0
10	MAN	g	5	10	11,11,12	0.28	0	15,15,17	0.58	0
12	NAG	h	1	12,1	14,14,15	0.41	0	17,19,21	0.71	0
12	NAG	h	2	12	14,14,15	0.44	0	17,19,21	0.51	0
12	BMA	h	3	12	11,11,12	0.30	0	15,15,17	0.51	0
12	NAG	i	1	12,1	14,14,15	0.48	0	17,19,21	0.82	0
12	NAG	i	2	12	14,14,15	0.49	0	17,19,21	0.97	2 (11%)
12	BMA	i	3	12	11,11,12	0.64	0	15,15,17	0.80	1 (6%)
10	NAG	j	1	10,1	14,14,15	0.39	0	17,19,21	1.32	3 (17%)
10	NAG	j	2	10	14,14,15	0.41	0	17,19,21	0.39	0
10	BMA	j	3	10	11,11,12	0.56	0	15,15,17	0.73	0
10	MAN	j	4	10	11,11,12	0.50	0	15,15,17	0.86	1 (6%)
10	MAN	j	5	10	11,11,12	0.38	0	15,15,17	0.61	0
10	NAG	k	1	10,1	14,14,15	0.46	0	17,19,21	0.90	1 (5%)
10	NAG	k	2	10	14,14,15	0.50	0	17,19,21	1.13	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BMA	k	3	10	11,11,12	0.26	0	15,15,17	0.61	0
10	MAN	k	4	10	11,11,12	0.32	0	15,15,17	0.85	2 (13%)
10	MAN	k	5	10	11,11,12	0.32	0	15,15,17	0.50	0
10	NAG	l	1	10,1	14,14,15	0.40	0	17,19,21	0.73	1 (5%)
10	NAG	l	2	10	14,14,15	0.44	0	17,19,21	0.37	0
10	BMA	l	3	10	11,11,12	0.33	0	15,15,17	1.10	2 (13%)
10	MAN	l	4	10	11,11,12	0.30	0	15,15,17	0.65	0
10	MAN	l	5	10	11,11,12	0.33	0	15,15,17	0.44	0
12	NAG	m	1	12,1	14,14,15	1.09	1 (7%)	17,19,21	1.21	1 (5%)
12	NAG	m	2	12	14,14,15	0.43	0	17,19,21	0.73	1 (5%)
12	BMA	m	3	12	11,11,12	0.29	0	15,15,17	0.56	0
9	NAG	n	1	9,1	14,14,15	0.54	0	17,19,21	1.07	1 (5%)
9	NAG	n	2	9	14,14,15	0.58	0	17,19,21	0.93	2 (11%)
13	NAG	o	1	1,13	14,14,15	0.41	0	17,19,21	0.84	0
13	NAG	o	2	13	14,14,15	0.41	0	17,19,21	0.42	0
12	NAG	p	1	12,1	14,14,15	0.42	0	17,19,21	0.73	0
12	NAG	p	2	12	14,14,15	0.40	0	17,19,21	0.86	1 (5%)
12	BMA	p	3	12	11,11,12	0.27	0	15,15,17	0.62	0
9	NAG	q	1	9,1	14,14,15	1.15	2 (14%)	17,19,21	1.12	1 (5%)
9	NAG	q	2	9	14,14,15	0.94	1 (7%)	17,19,21	1.08	1 (5%)
12	NAG	r	1	12,1	14,14,15	0.42	0	17,19,21	0.84	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	0.31	0	15,15,17	0.61	0
9	NAG	s	1	9,1	14,14,15	0.46	0	17,19,21	1.06	3 (17%)
9	NAG	s	2	9	14,14,15	0.41	0	17,19,21	0.63	0
9	NAG	t	1	9,1	14,14,15	1.00	0	17,19,21	1.58	3 (17%)
9	NAG	t	2	9	14,14,15	1.11	1 (7%)	17,19,21	1.52	1 (5%)
10	NAG	u	1	10,1	14,14,15	0.50	0	17,19,21	0.59	0
10	NAG	u	2	10	14,14,15	0.45	0	17,19,21	0.72	0
10	BMA	u	3	10	11,11,12	0.42	0	15,15,17	0.64	0
10	MAN	u	4	10	11,11,12	0.24	0	15,15,17	0.49	0
10	MAN	u	5	10	11,11,12	0.26	0	15,15,17	0.53	0
9	NAG	v	1	9,1	14,14,15	0.45	0	17,19,21	0.51	0
9	NAG	v	2	9	14,14,15	0.40	0	17,19,21	0.41	0
14	NAG	w	1	1,14	14,14,15	0.53	0	17,19,21	1.20	2 (11%)
14	NAG	w	2	14	14,14,15	0.46	0	17,19,21	1.36	3 (17%)
14	BMA	w	3	14	11,11,12	0.42	0	15,15,17	0.58	0
14	MAN	w	4	14	11,11,12	0.29	0	15,15,17	0.47	0
14	MAN	w	5	14	11,11,12	0.27	0	15,15,17	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	x	1	9,1	14,14,15	0.53	0	17,19,21	0.85	0
9	NAG	x	2	9	14,14,15	0.41	0	17,19,21	0.73	0
9	NAG	y	1	9,1	14,14,15	0.42	0	17,19,21	0.72	1 (5%)
9	NAG	y	2	9	14,14,15	0.42	0	17,19,21	0.44	0
15	NAG	z	1	15,1	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	1.34	2 (11%)
15	BMA	z	3	15	11,11,12	0.37	0	15,15,17	0.63	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	-	3/6/23/26	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	-	2/6/23/26	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	1,14	-	2/6/23/26	0/1/1/1
14	NAG	6	2	14	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,13	-	2/6/23/26	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
9	NAG	a	1	9,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,13	-	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	-	3/6/23/26	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	-	2/6/23/26	0/1/1/1
10	NAG	j	2	10	-	3/6/23/26	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
10	BMA	l	3	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,13	-	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	-	2/6/23/26	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	-	1/6/23/26	0/1/1/1
14	NAG	w	1	1,14	-	4/6/23/26	0/1/1/1
14	NAG	w	2	14	-	2/6/23/26	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	-	2/6/23/26	0/1/1/1
15	NAG	z	1	15,1	-	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	-	2/6/23/26	0/1/1/1
15	BMA	z	3	15	-	1/2/19/22	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	1	NAG	O5-C5	2.68	1.48	1.43
9	t	2	NAG	C1-C2	2.58	1.55	1.52
9	q	1	NAG	O5-C5	2.56	1.48	1.43
12	2	2	NAG	O5-C5	2.40	1.48	1.43
9	q	2	NAG	O5-C5	2.33	1.48	1.43

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	0	1	NAG	C1-O5-C5	5.07	118.98	112.19
9	t	2	NAG	C1-O5-C5	4.94	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	-4.25	104.72	111.29

There are no chirality outliers.

5 of 126 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	Y	2	NAG	C1-C2-N2-C7
9	n	2	NAG	C1-C2-N2-C7
9	x	2	NAG	C1-C2-N2-C7
9	y	1	NAG	C1-C2-N2-C7
12	h	1	NAG	C3-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 12 short contacts:

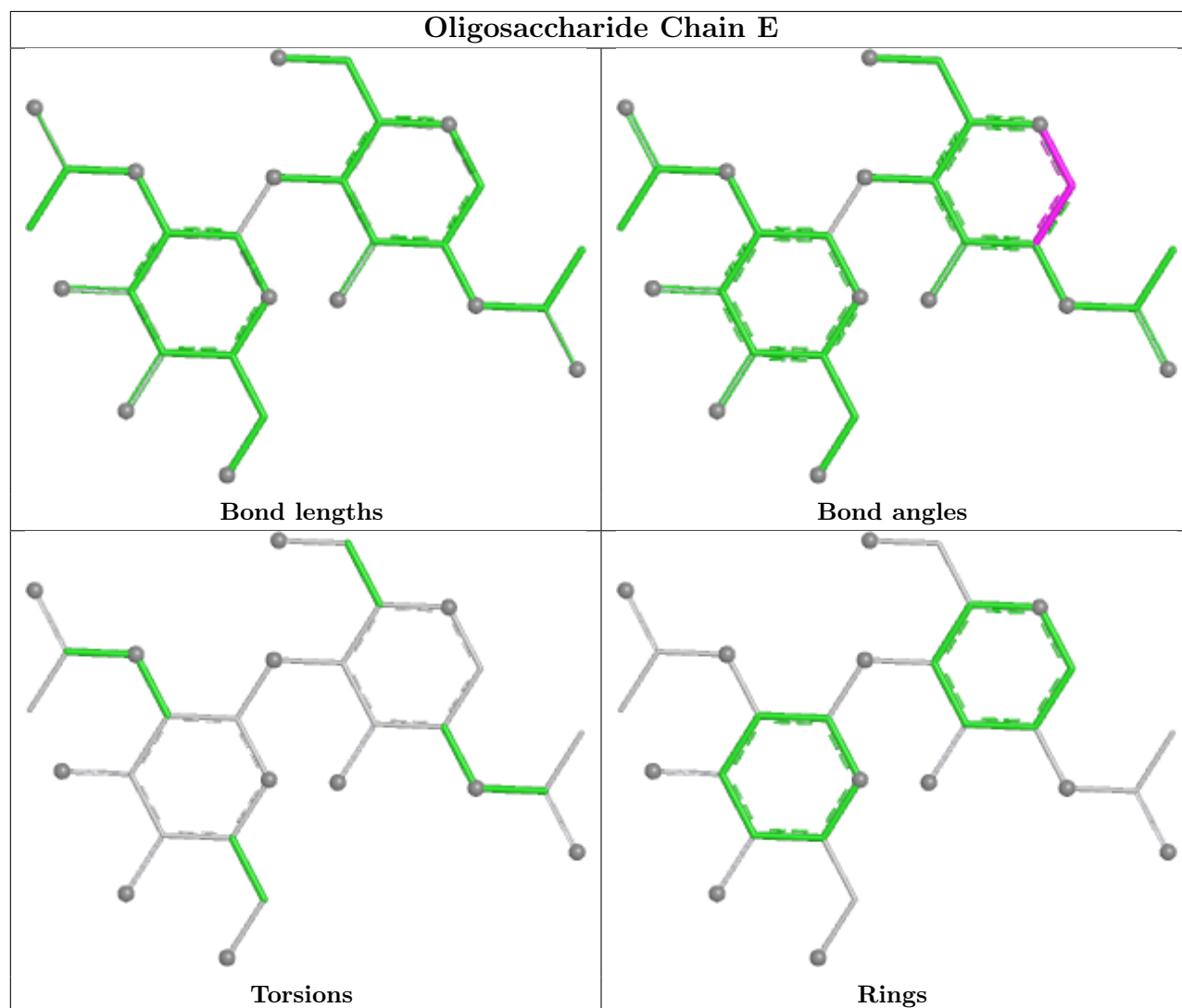
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	X	1	NAG	1	0
14	6	2	NAG	2	0
10	4	1	NAG	1	0
10	u	2	NAG	1	0
10	4	2	NAG	1	0
11	U	1	NAG	1	0

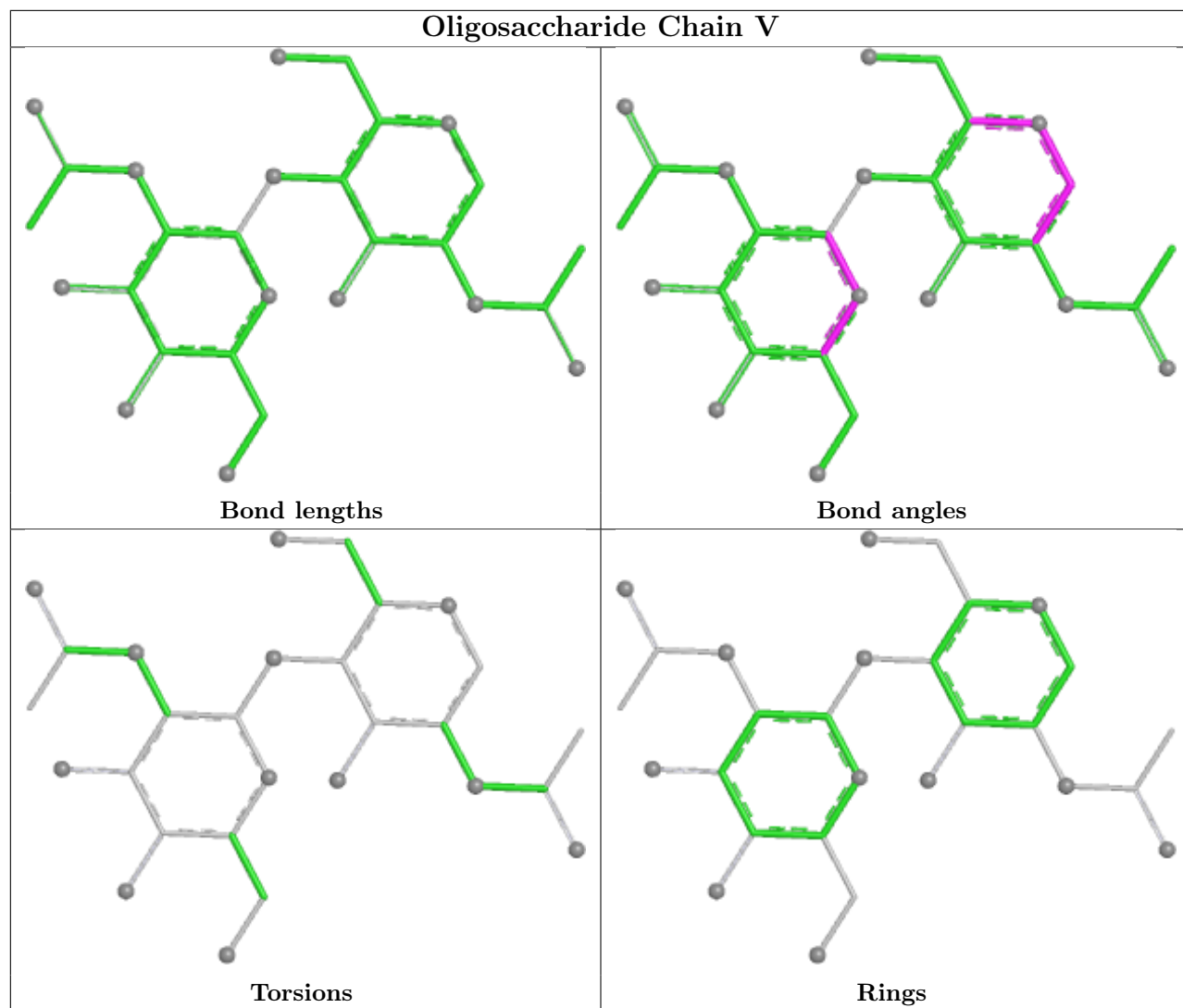
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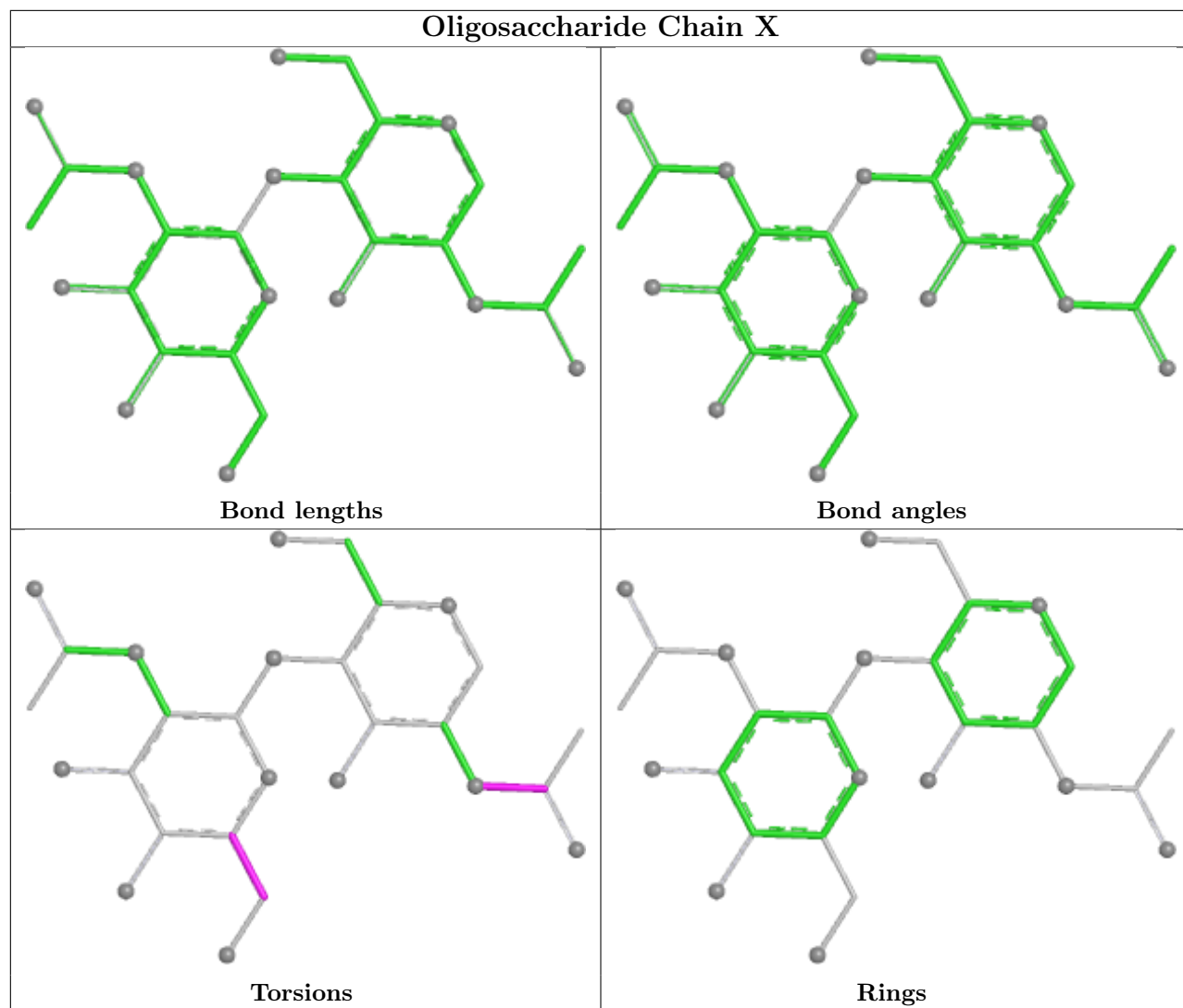
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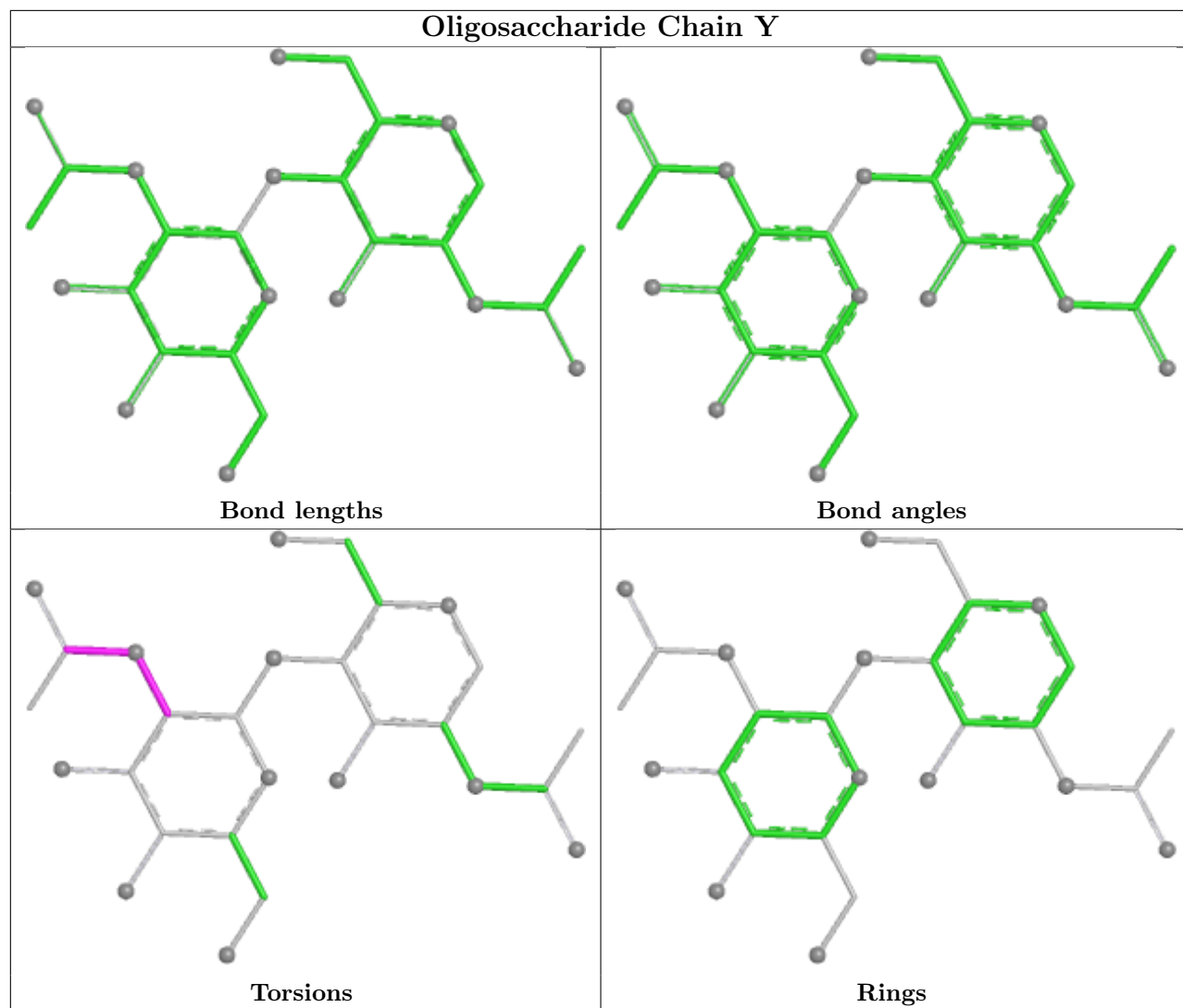
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	u	1	NAG	1	0
14	6	1	NAG	2	0
10	j	1	NAG	2	0
9	t	1	NAG	1	0
10	l	1	NAG	2	0
12	W	1	NAG	1	0

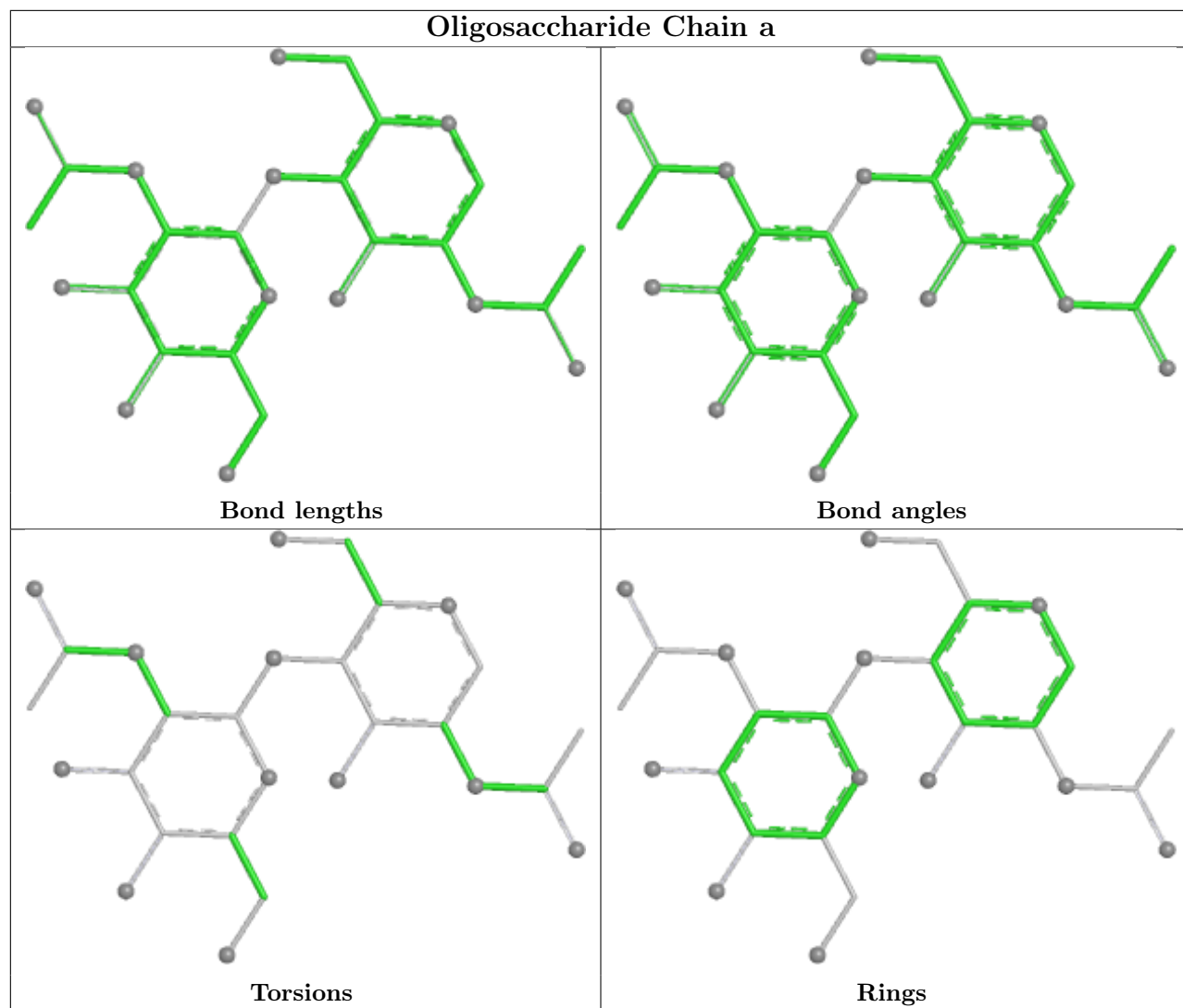
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

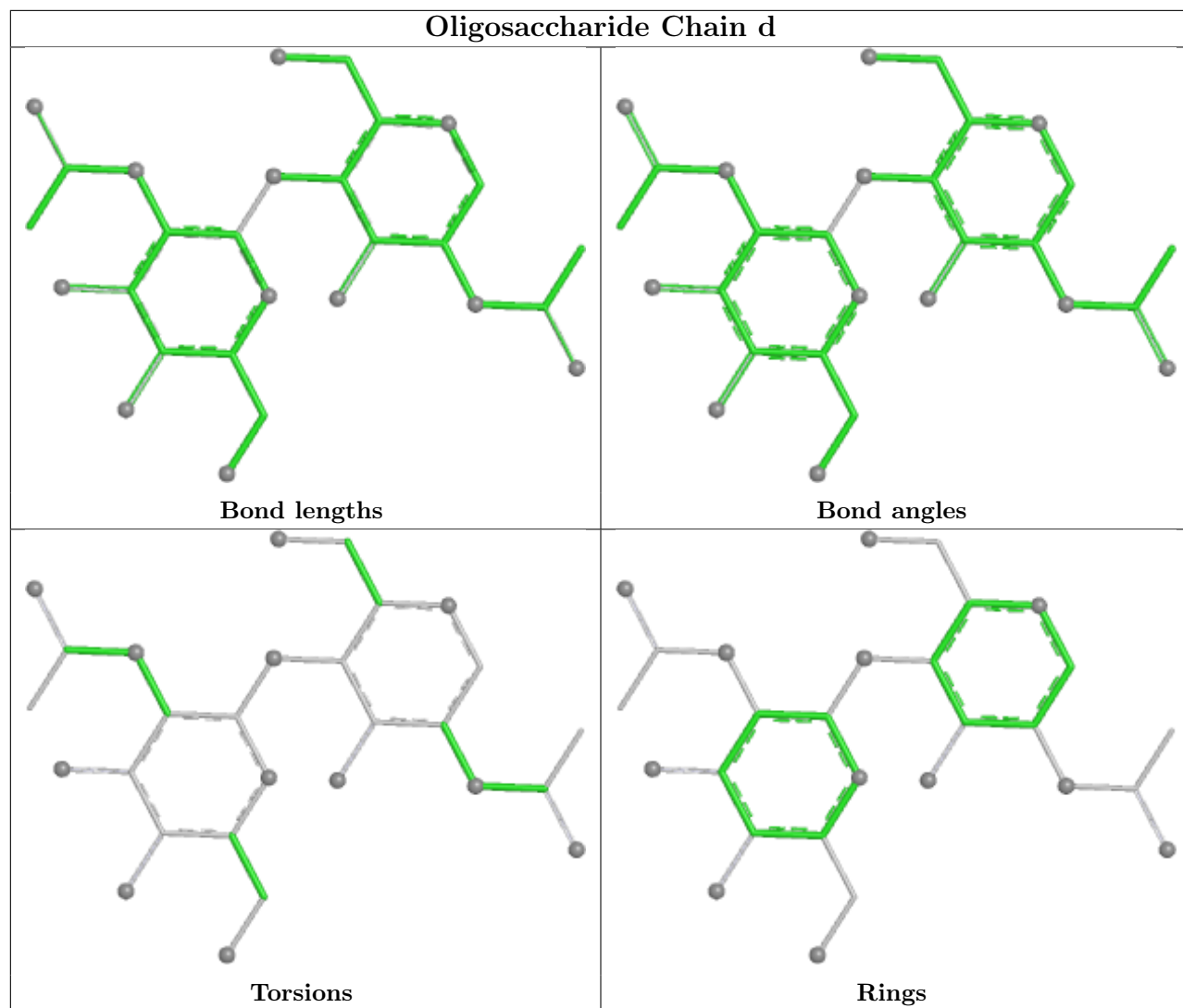


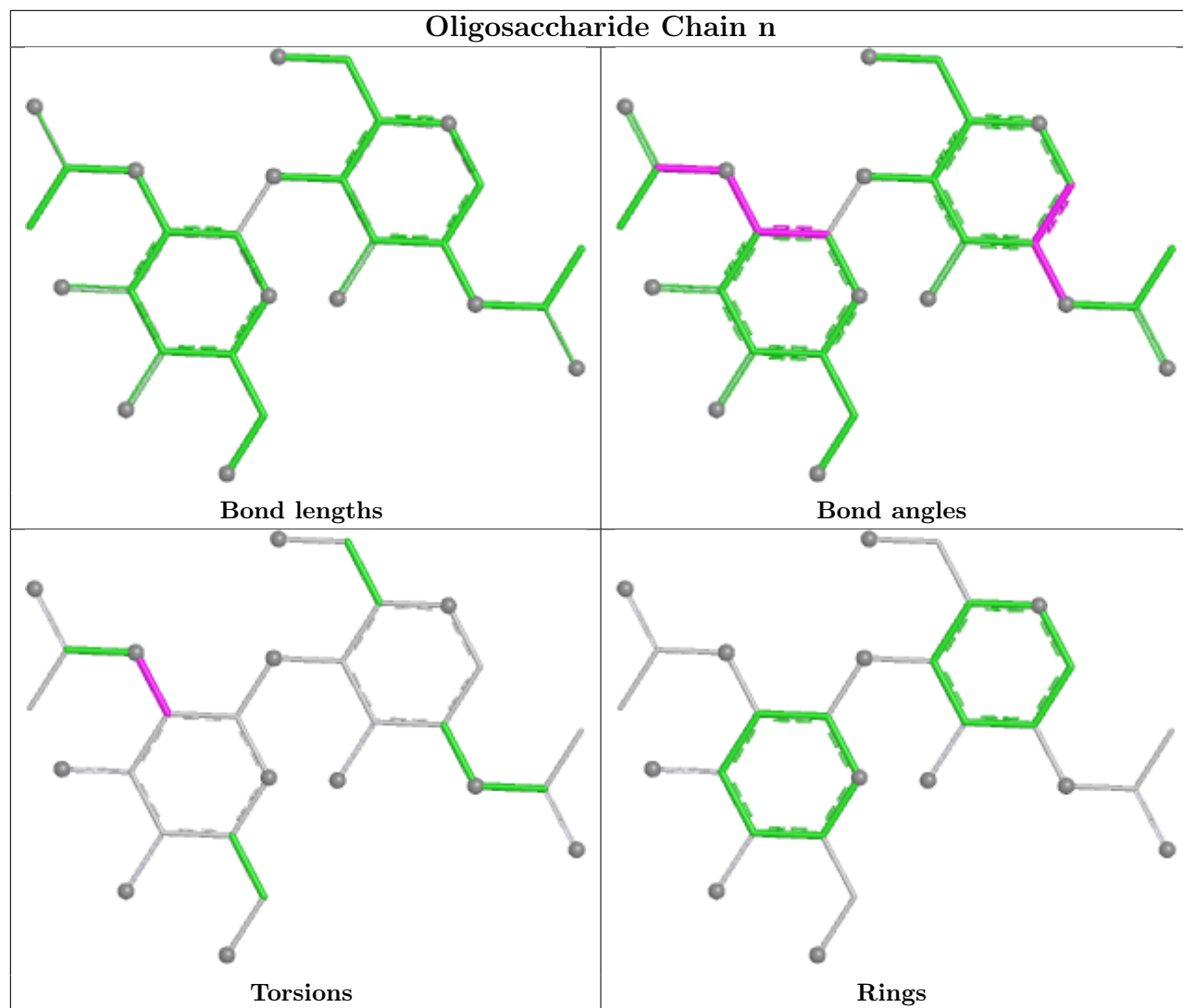


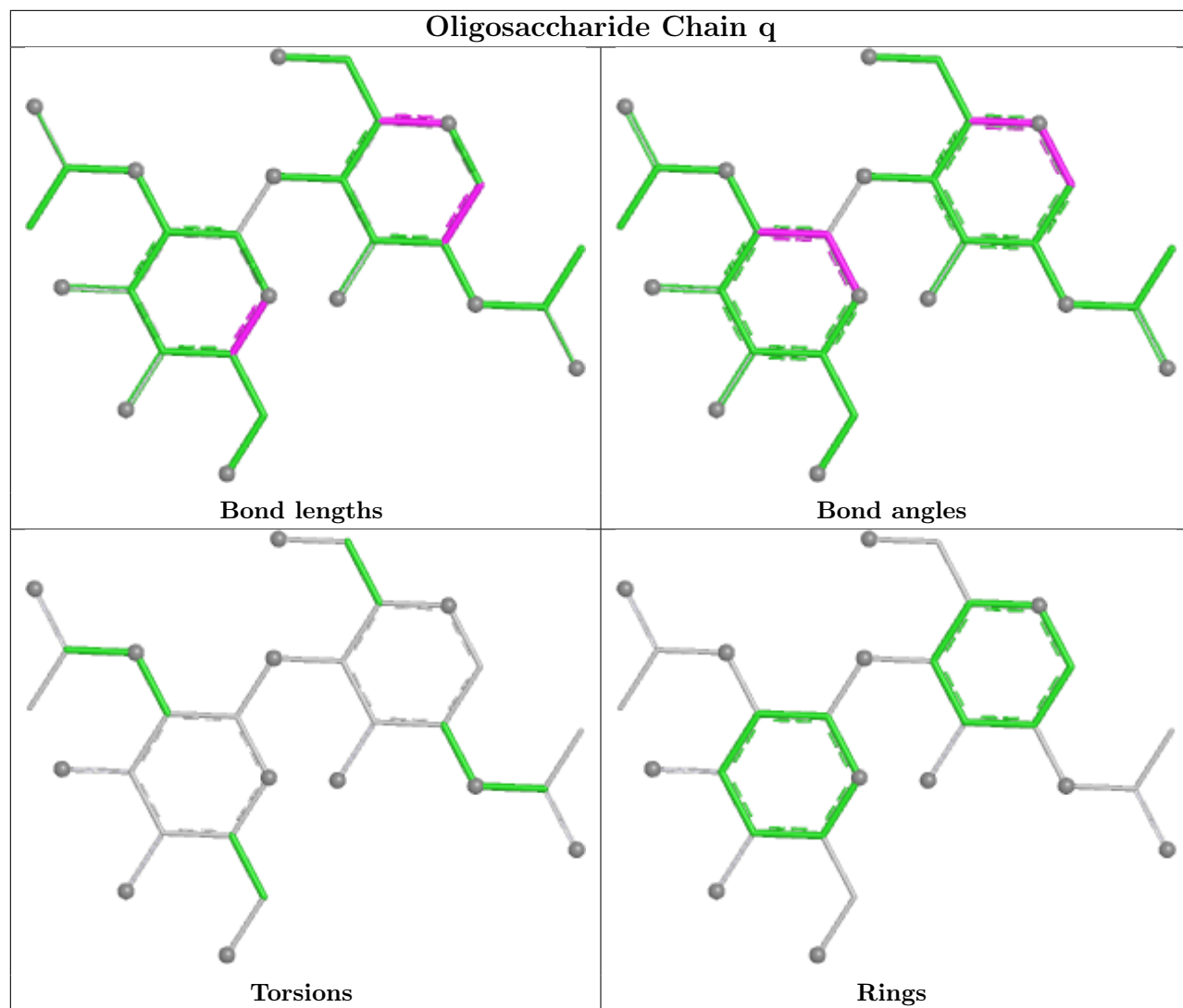


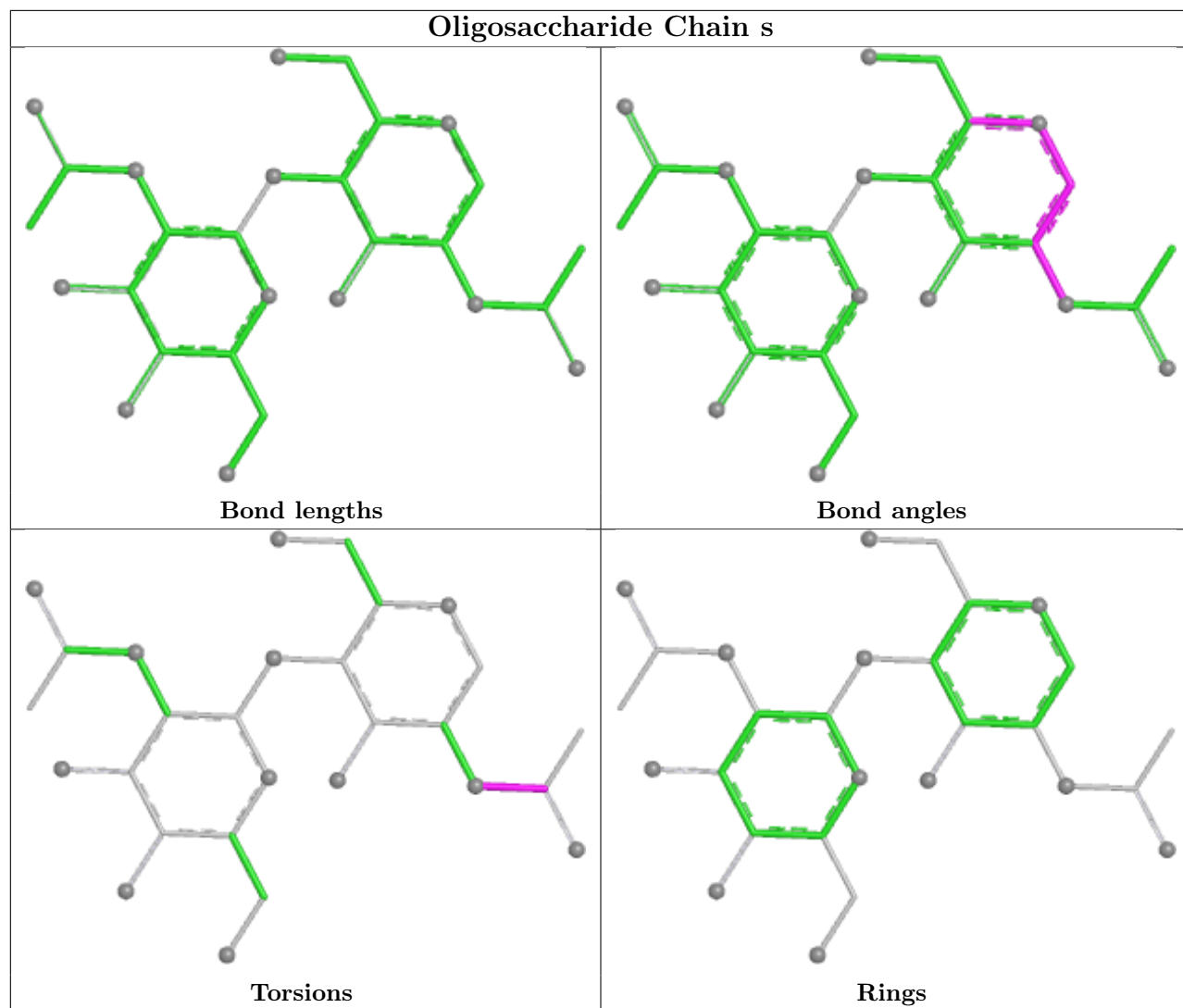


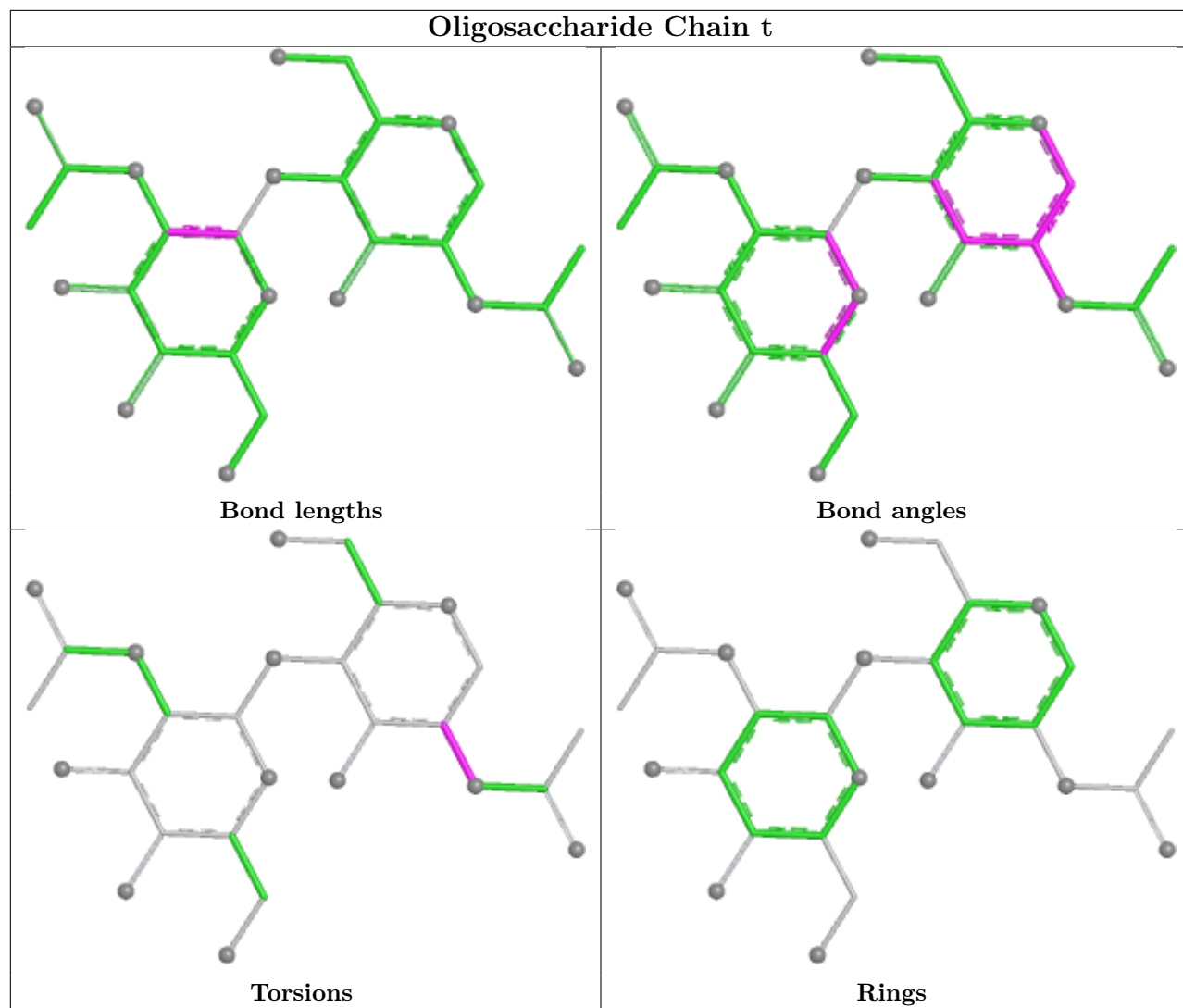


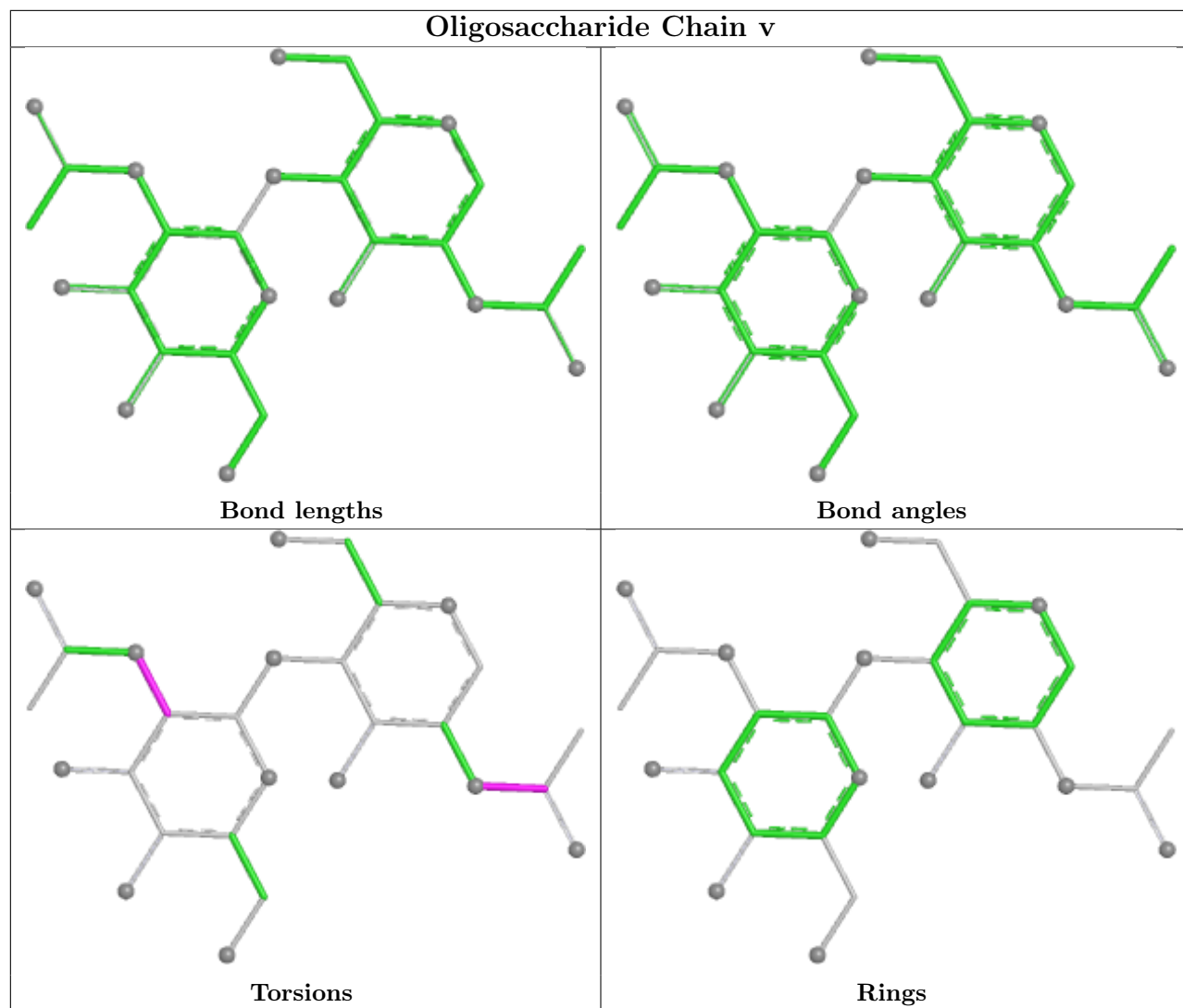


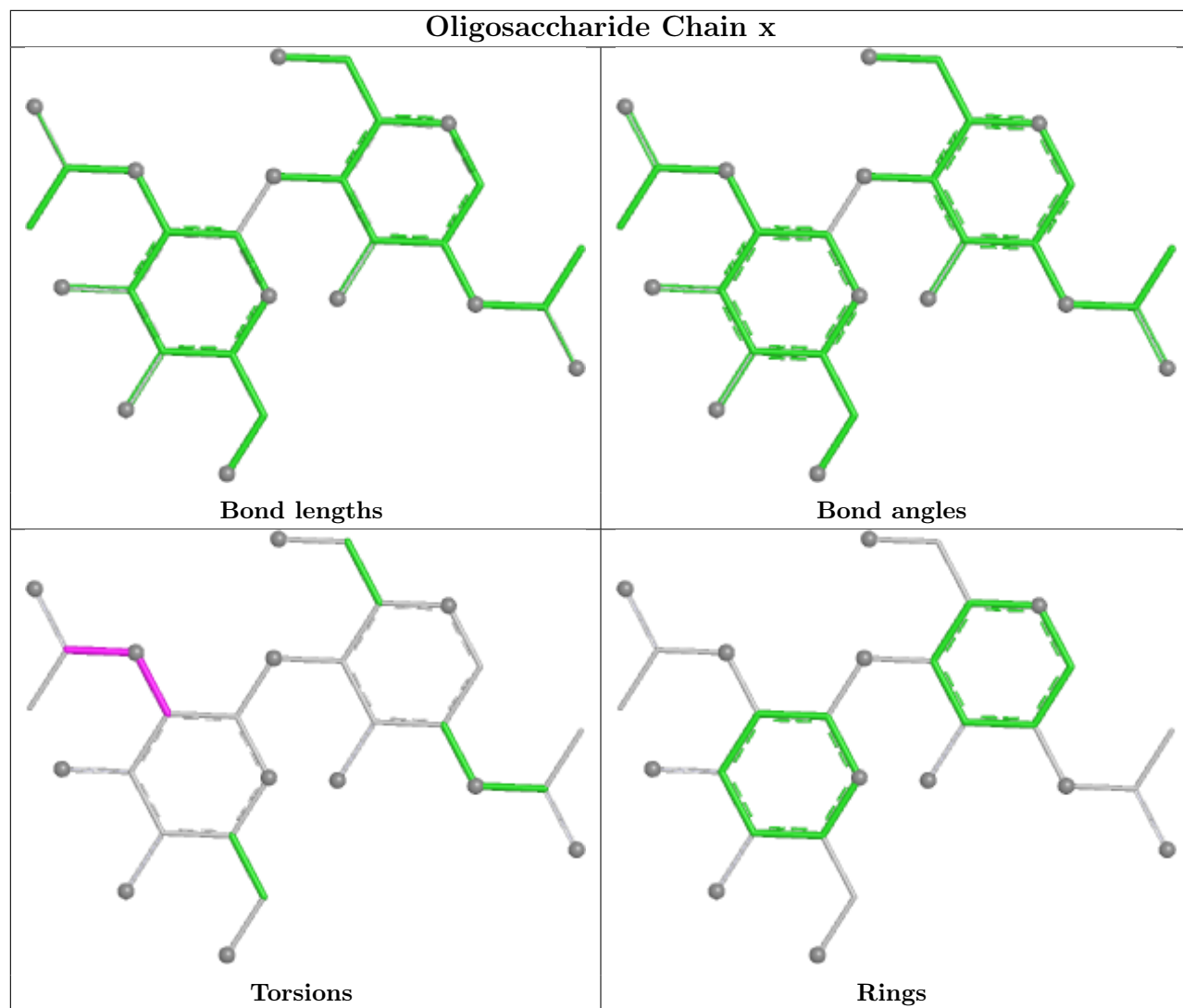


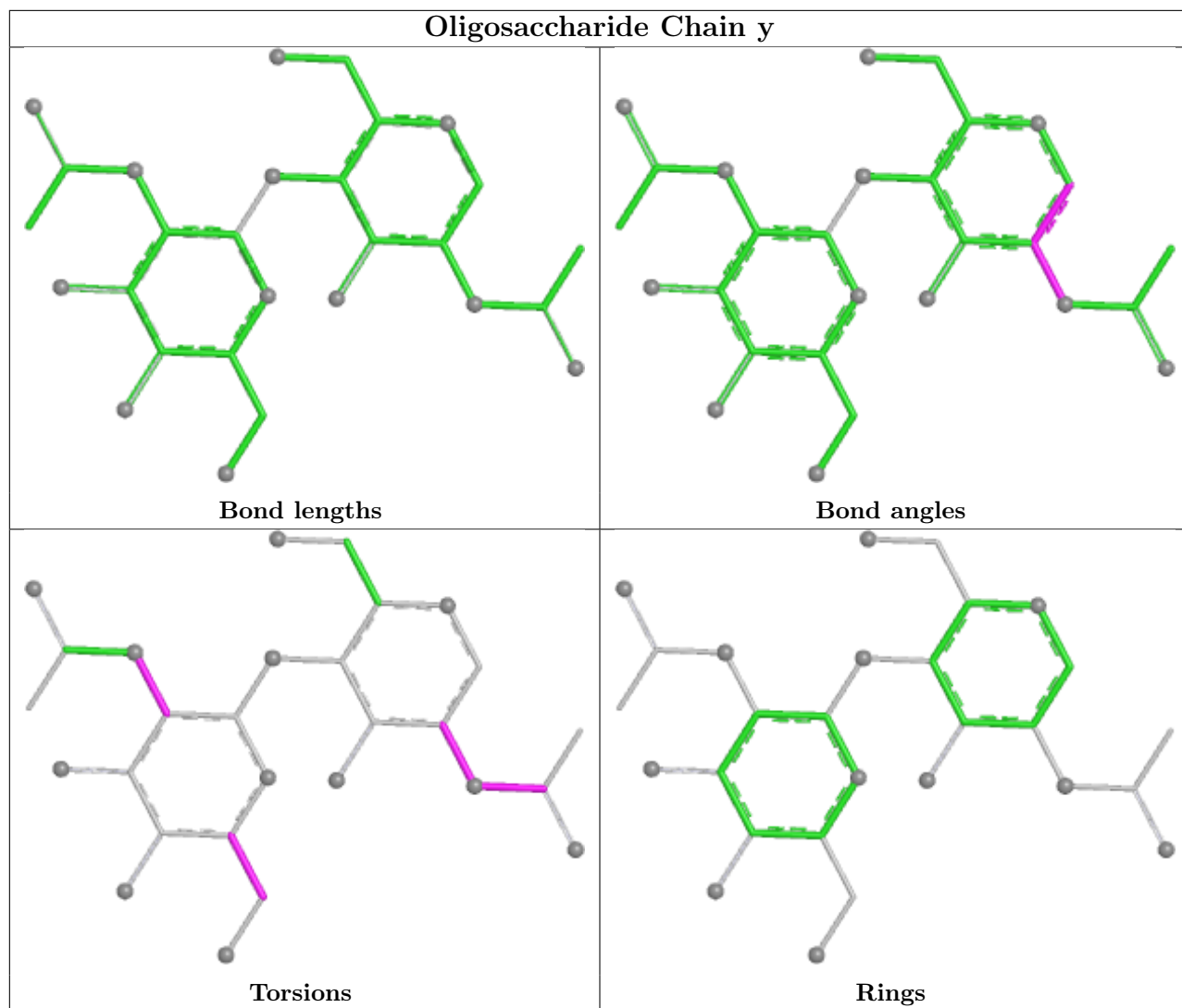


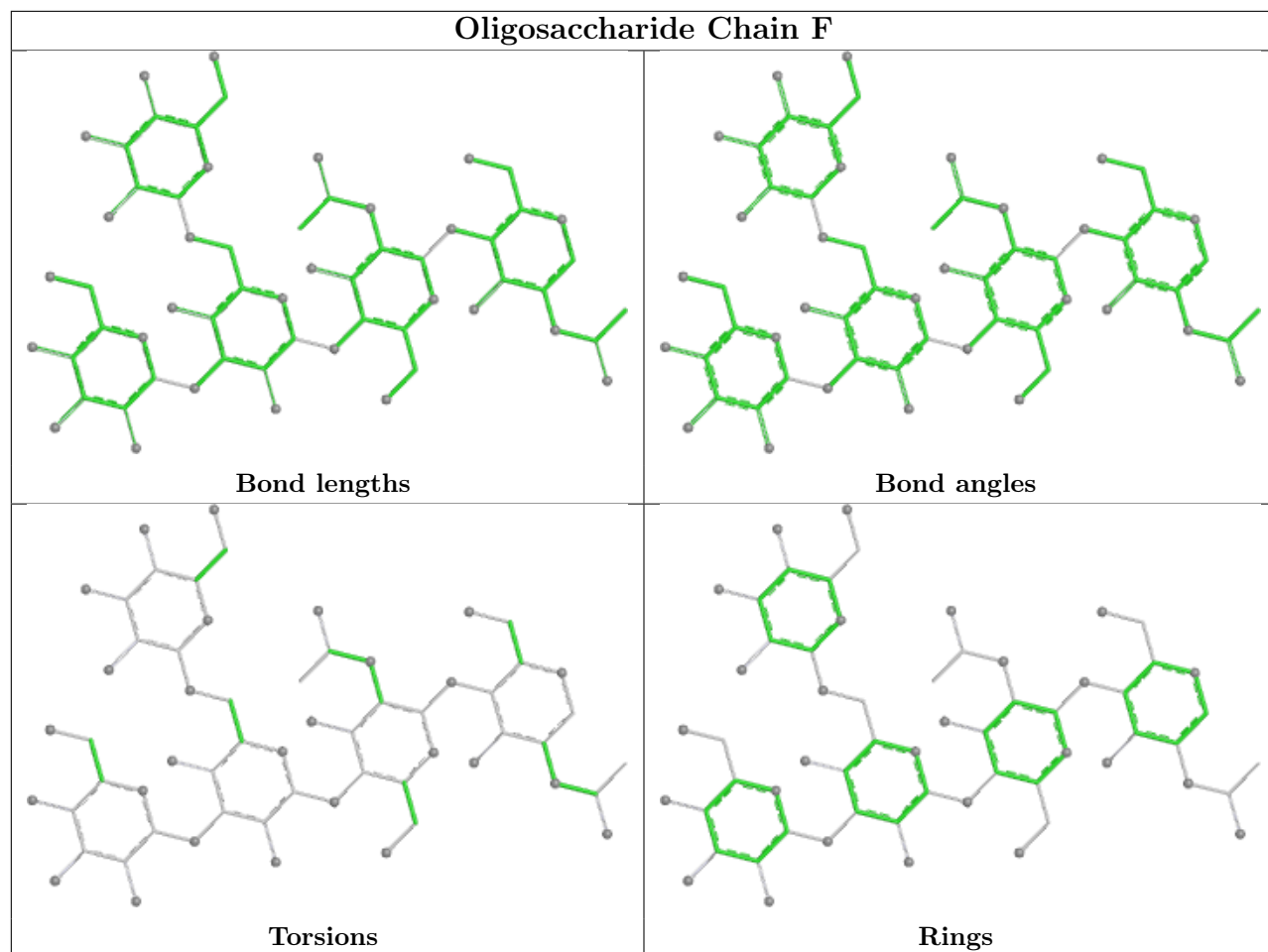


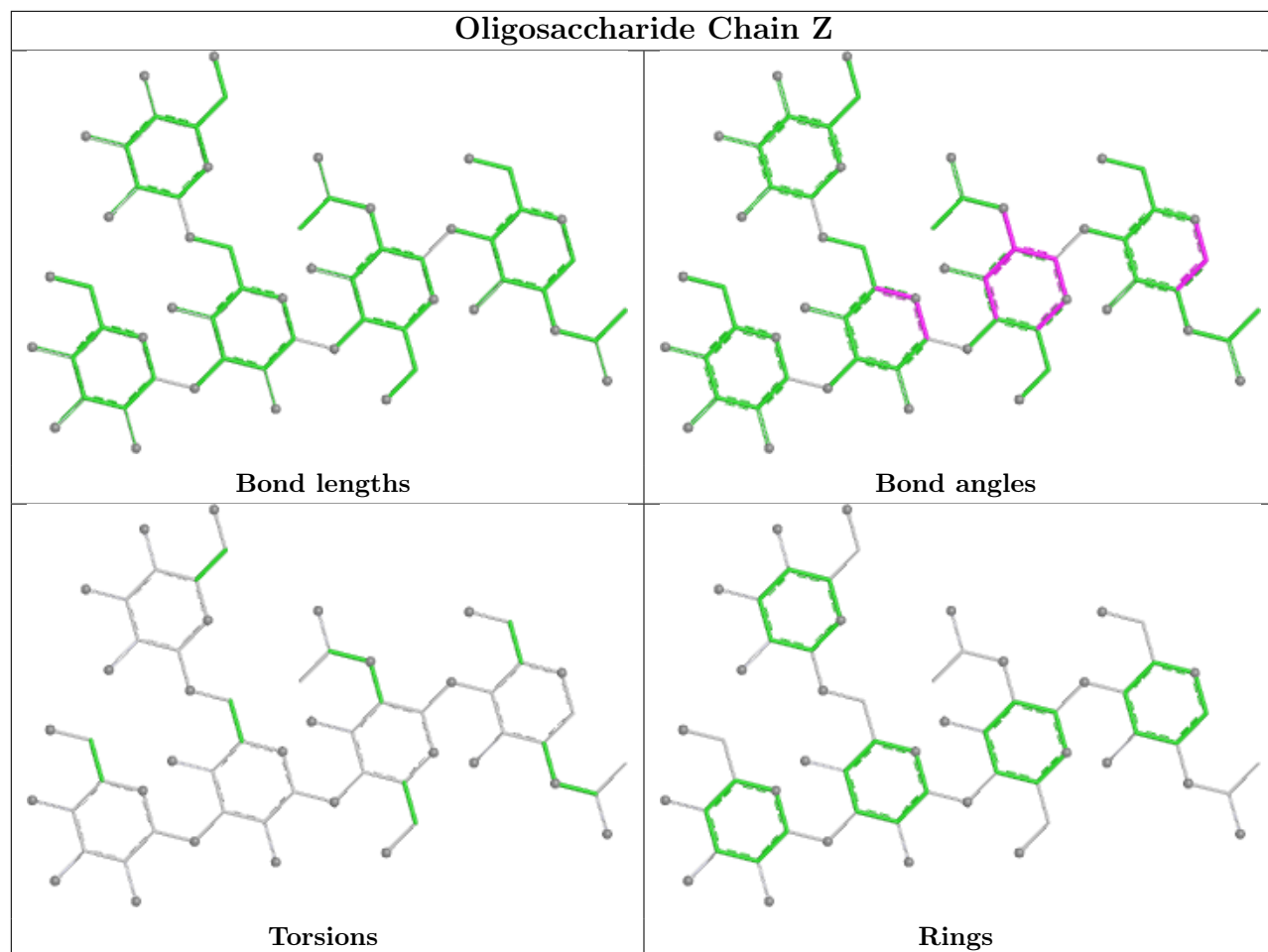


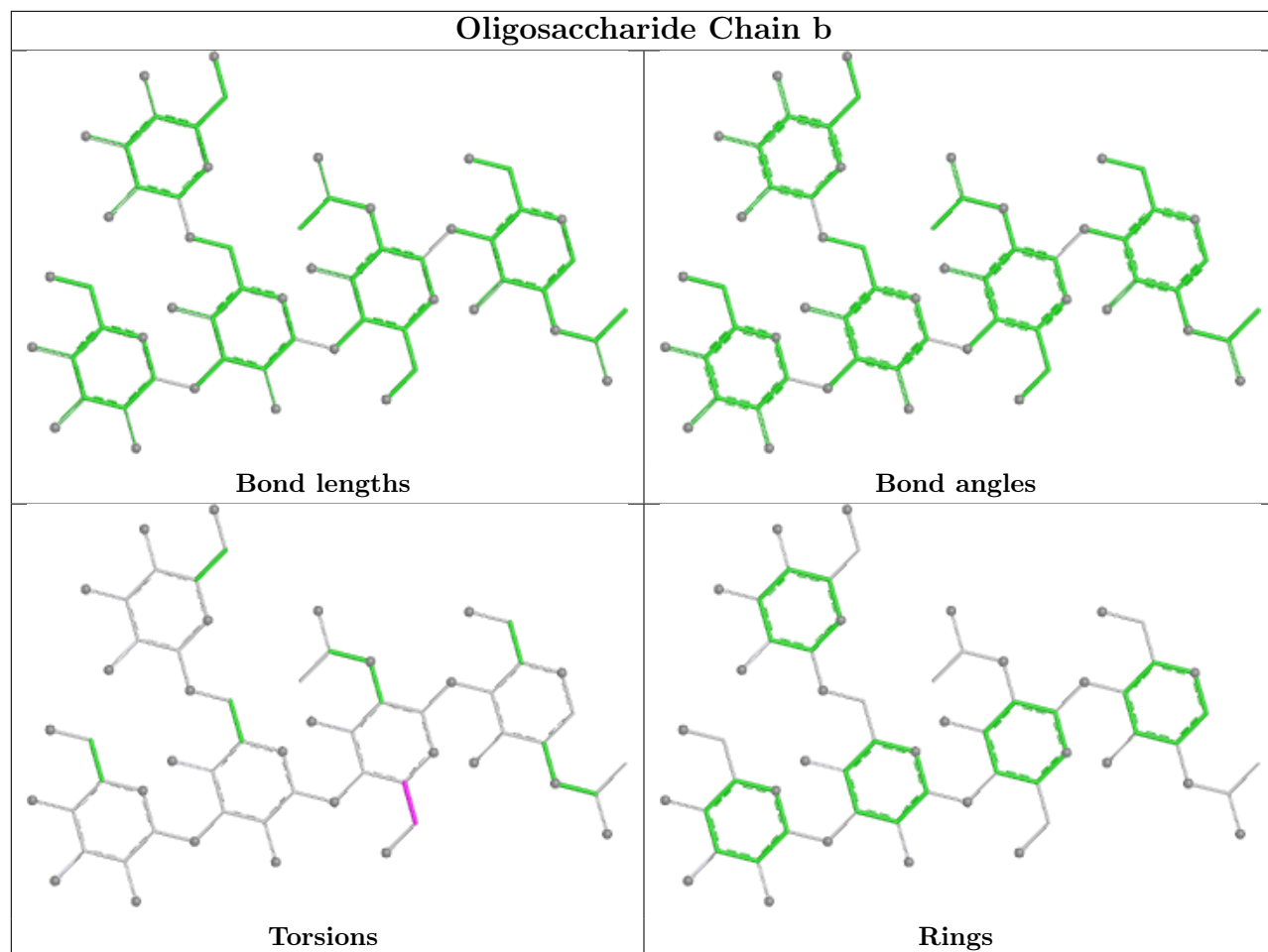


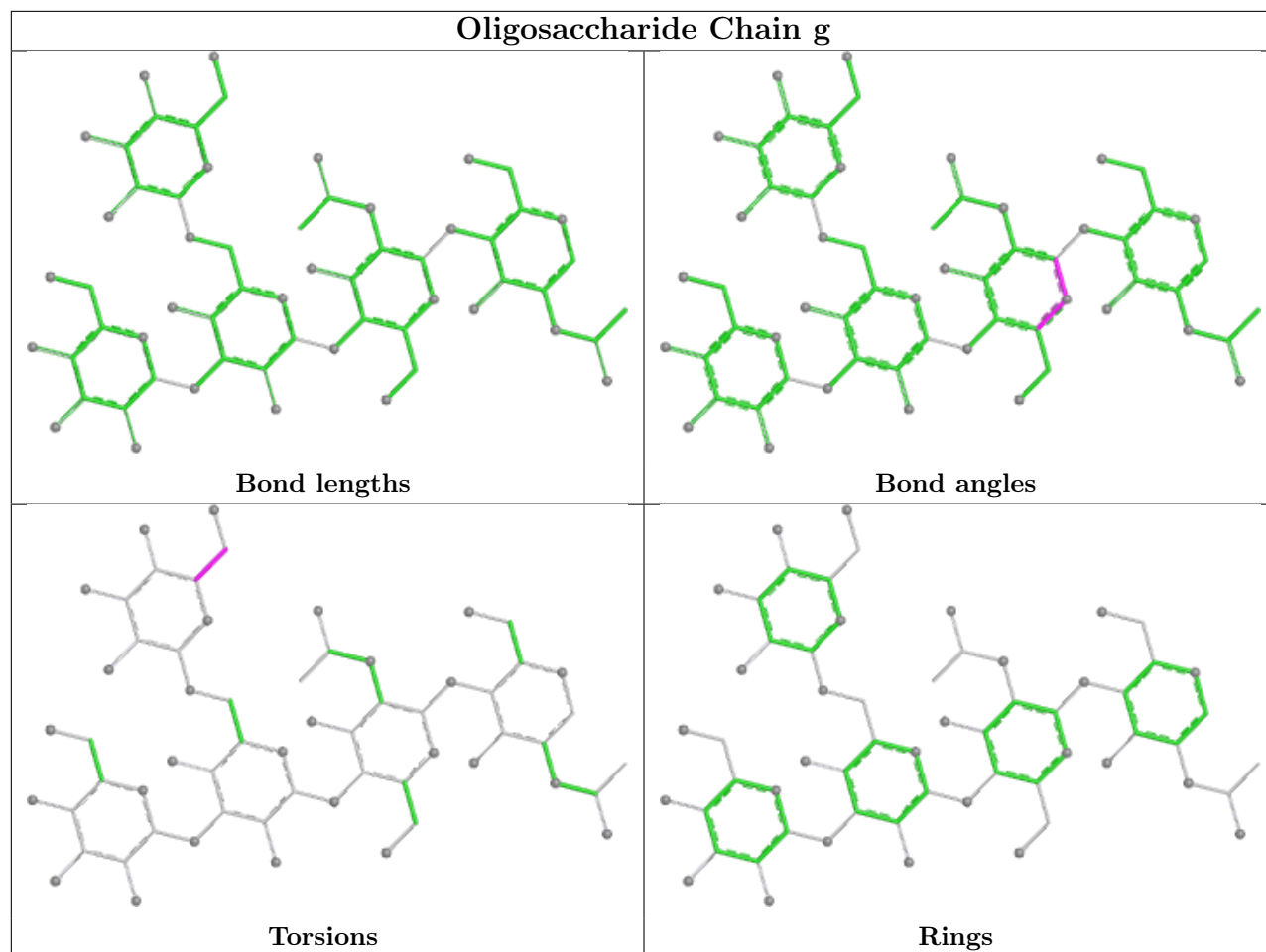


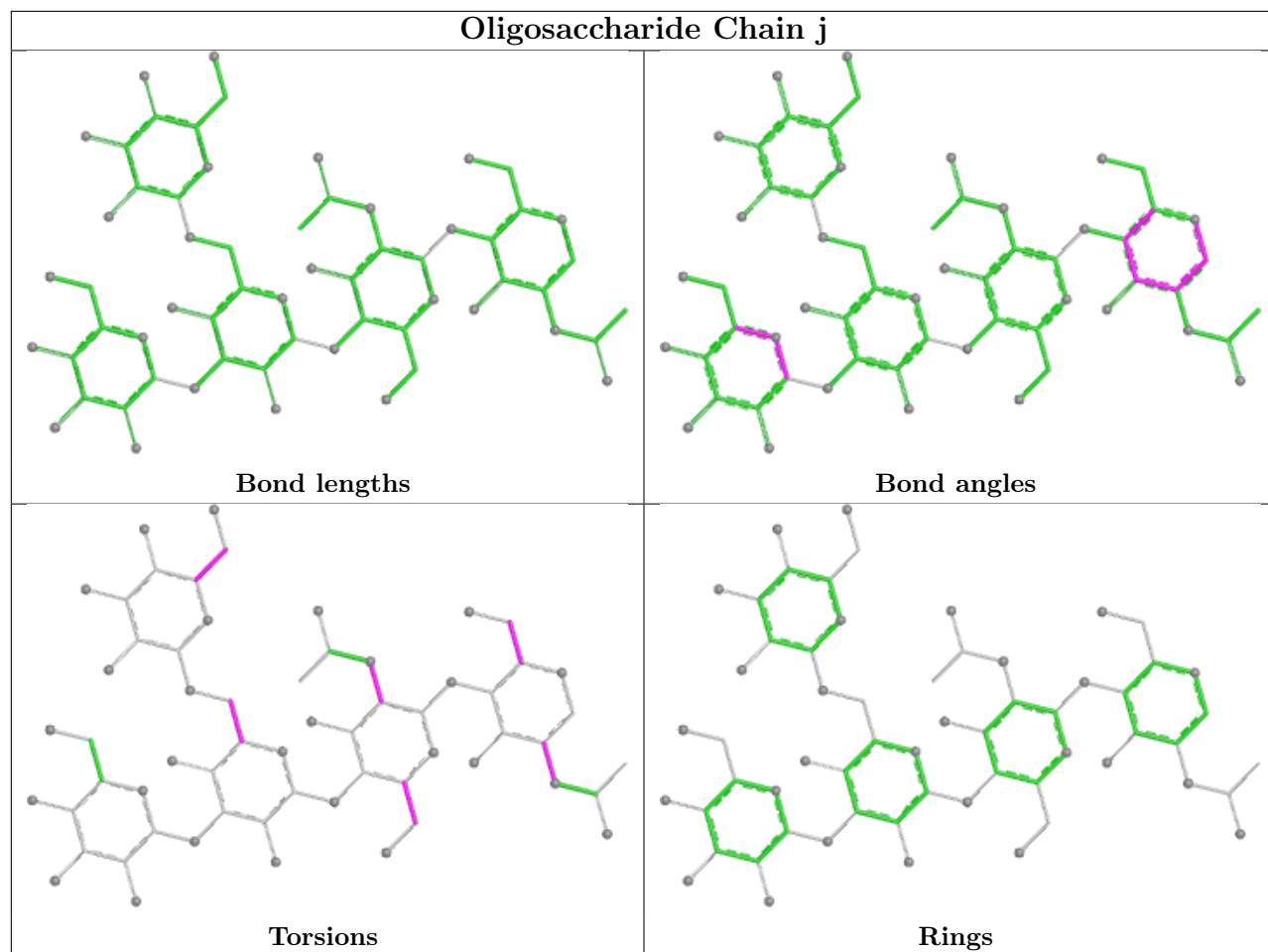


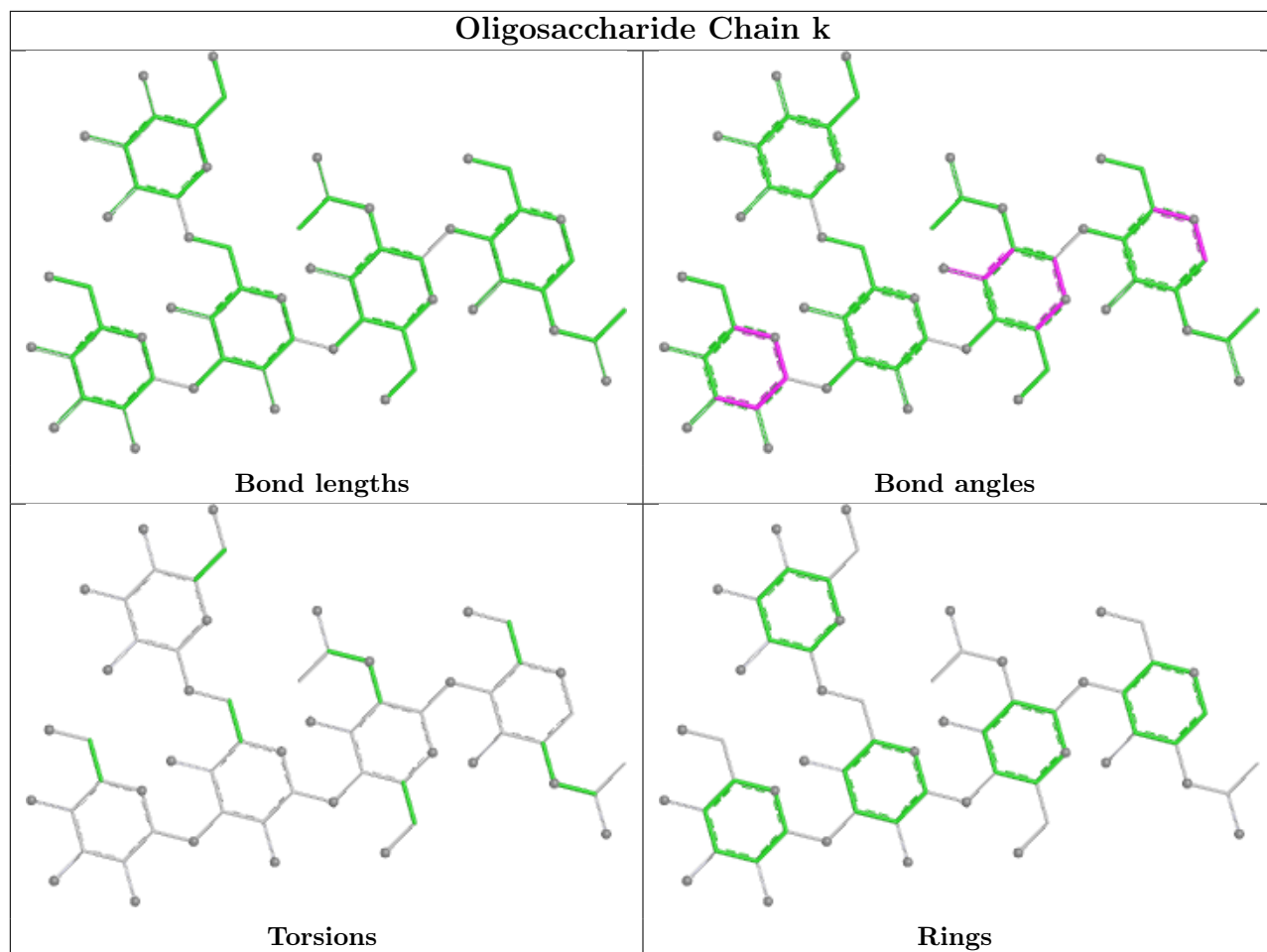


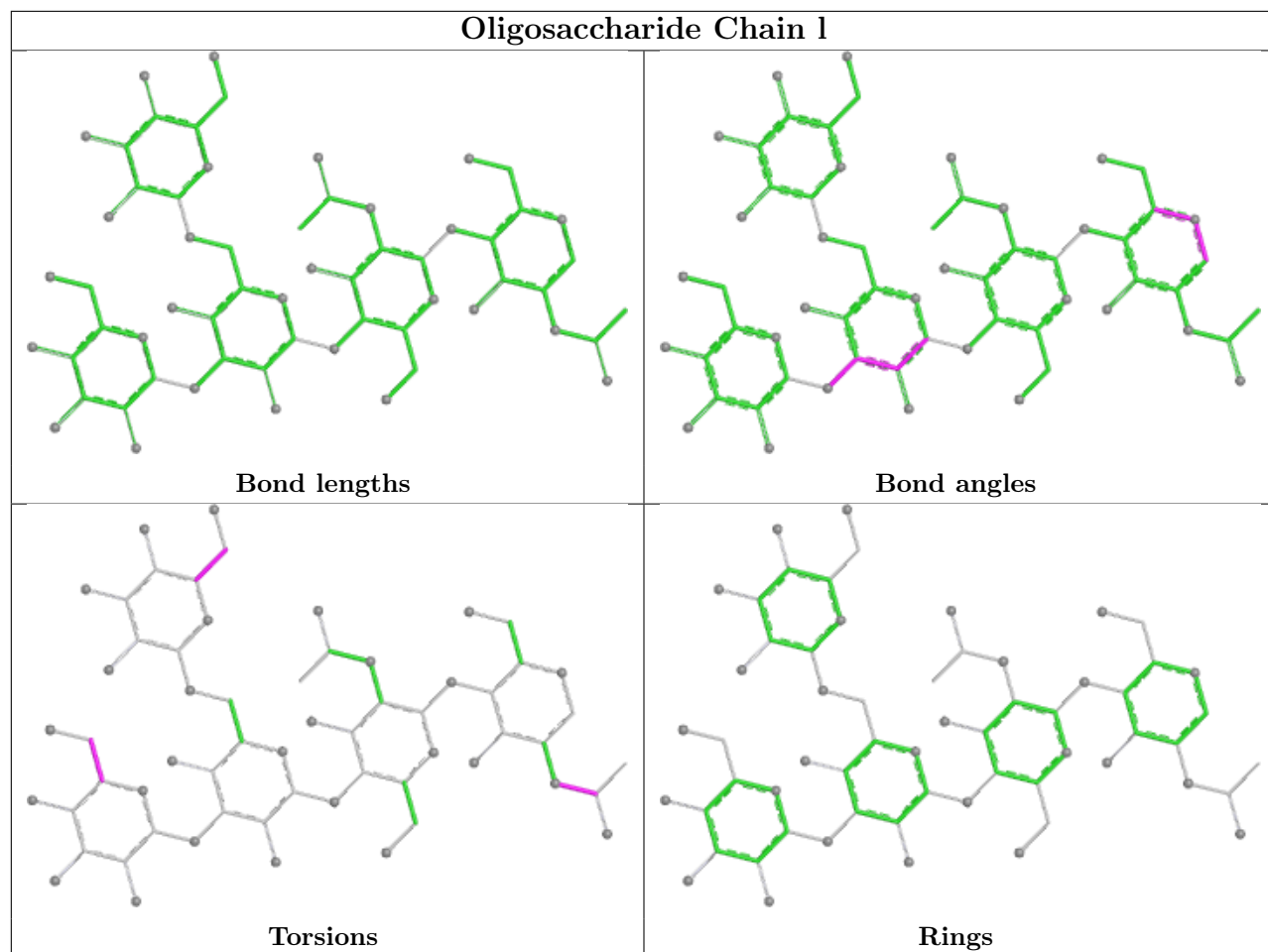


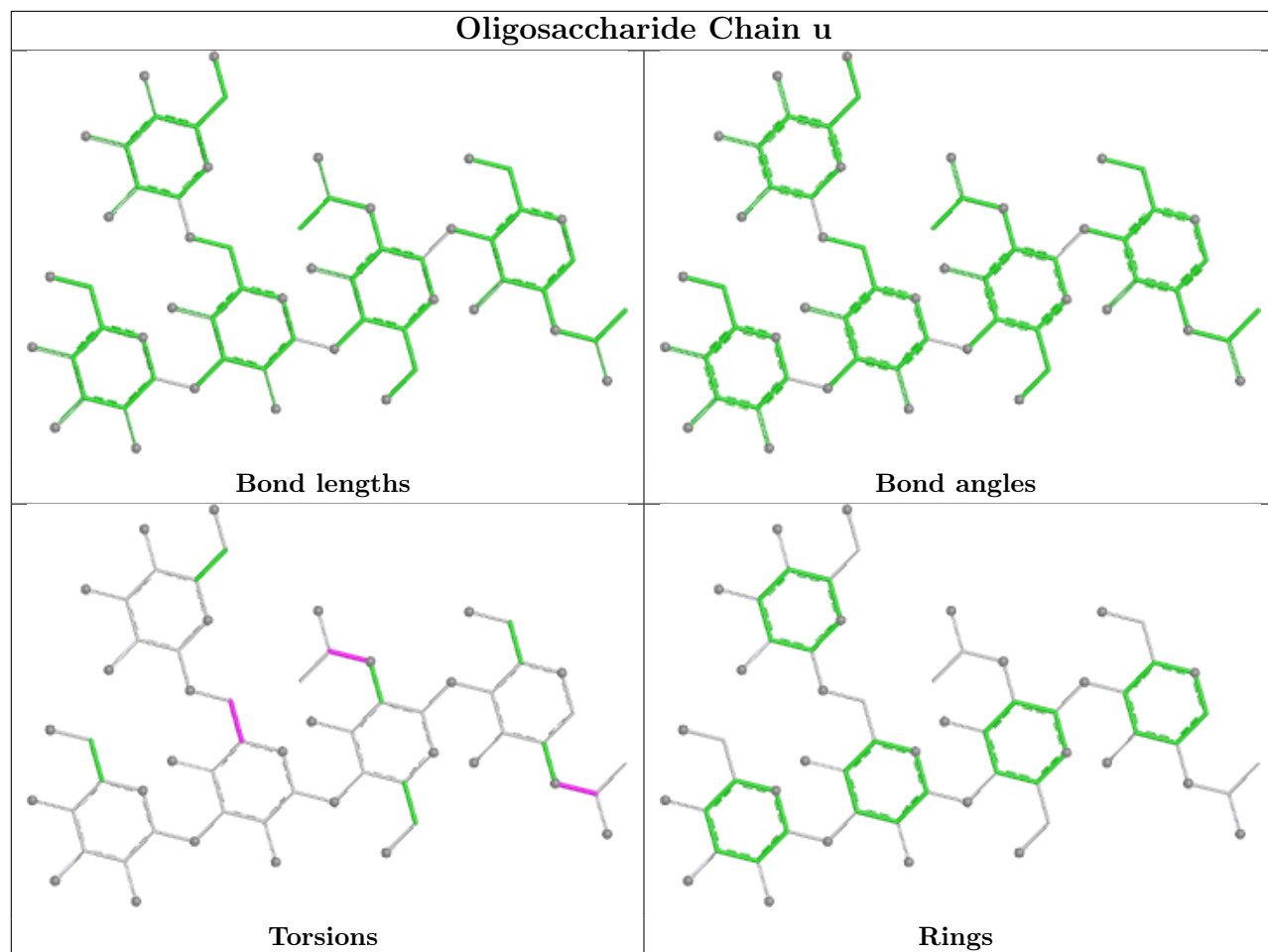


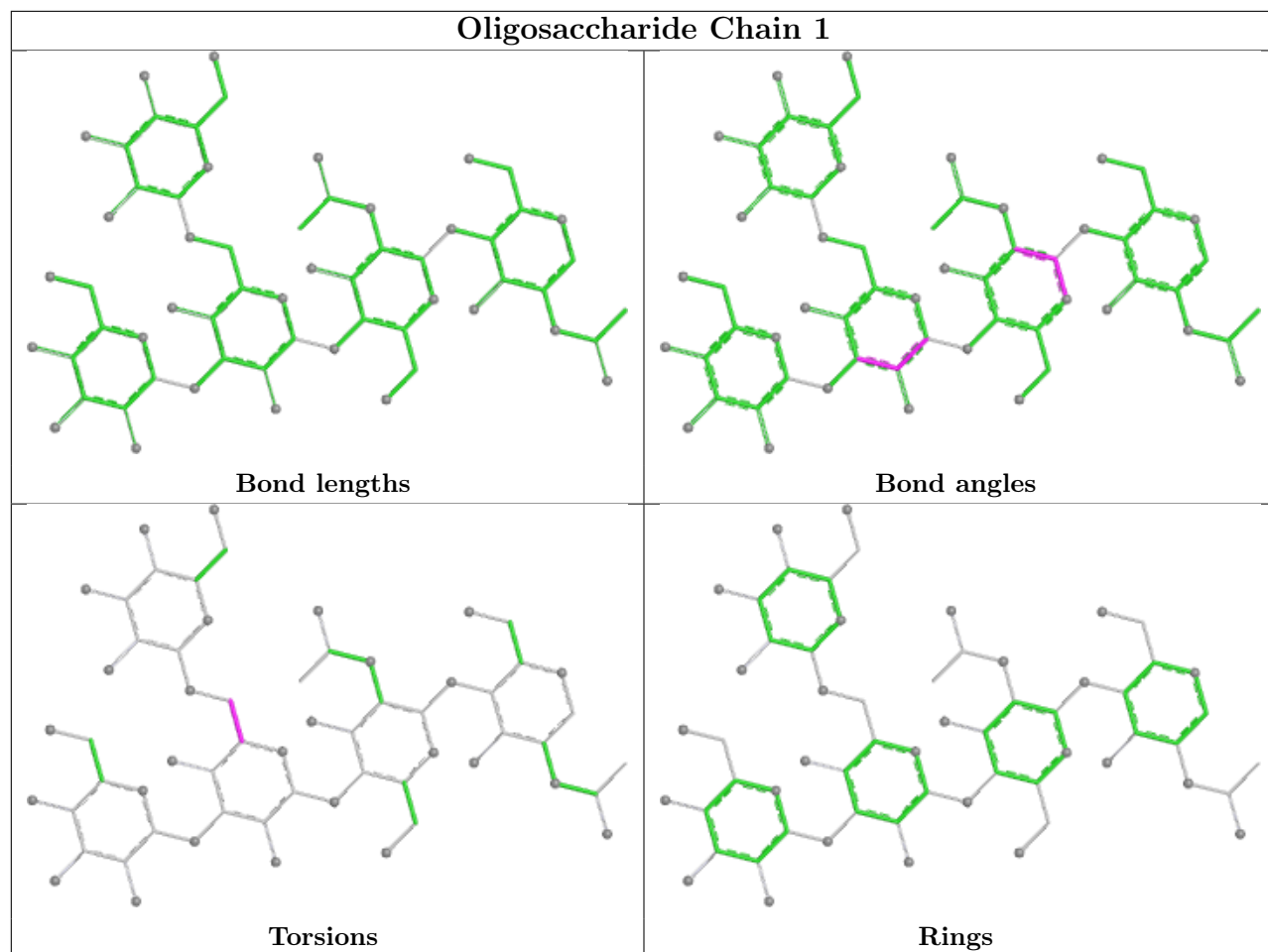


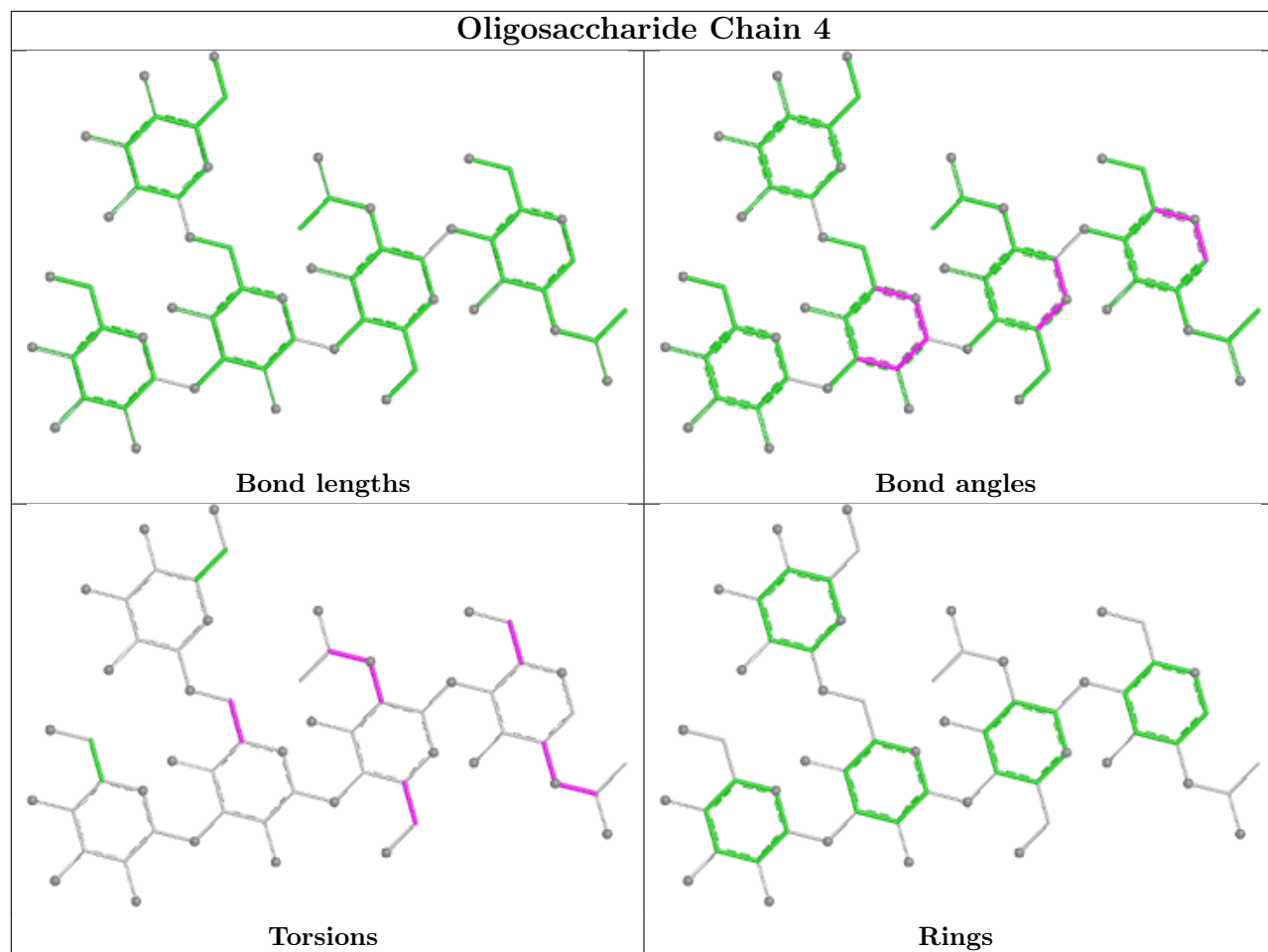


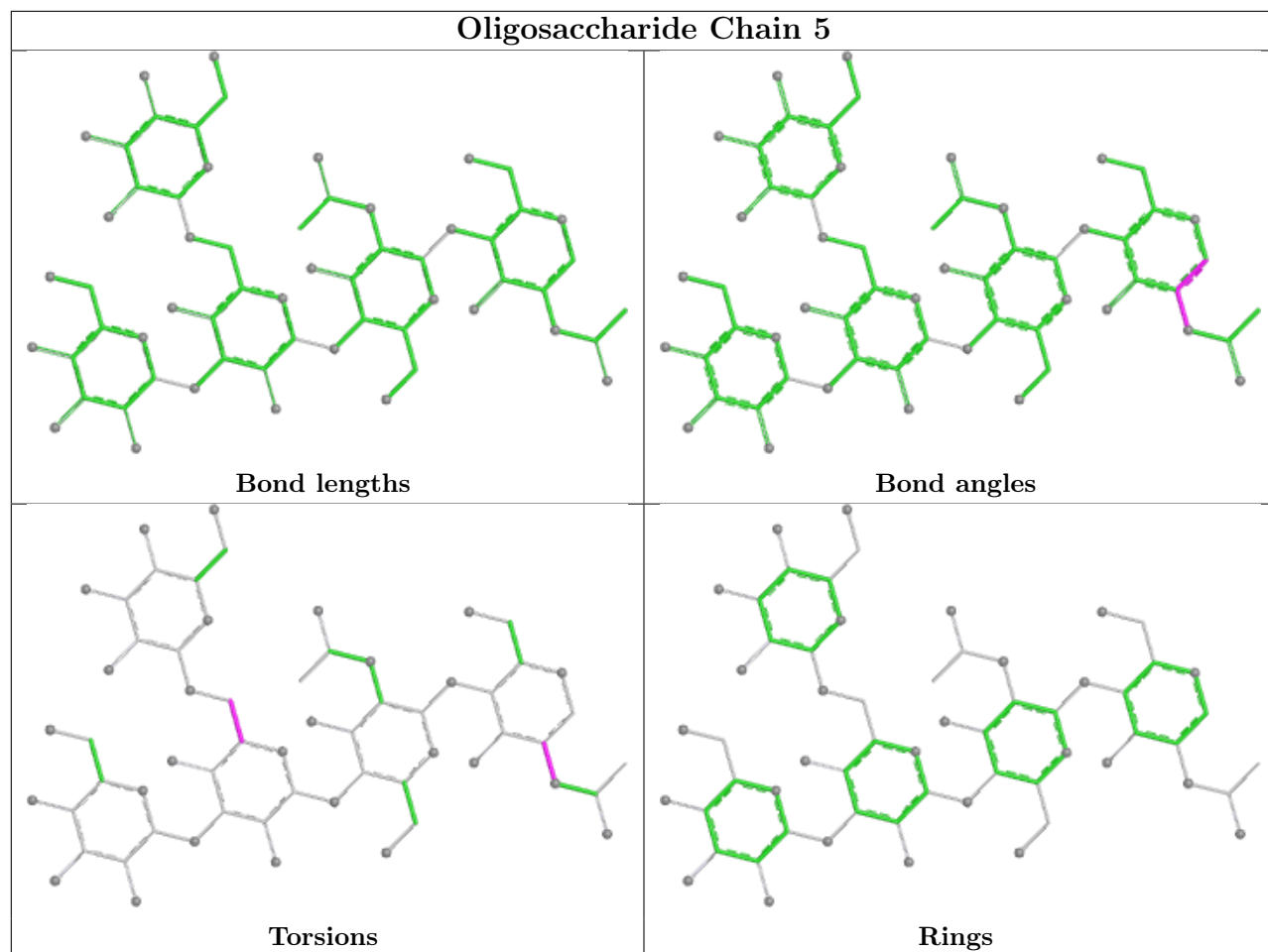


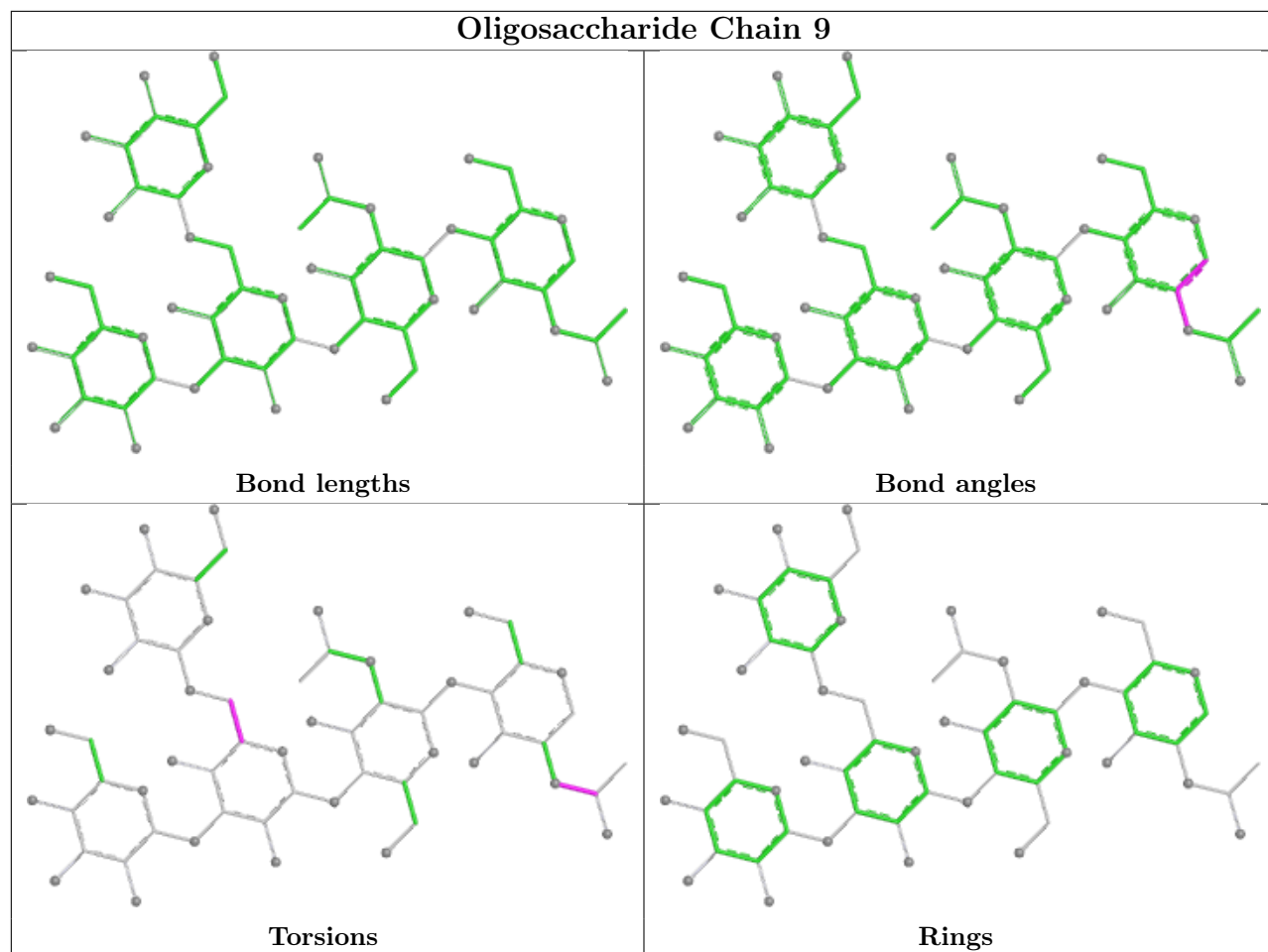


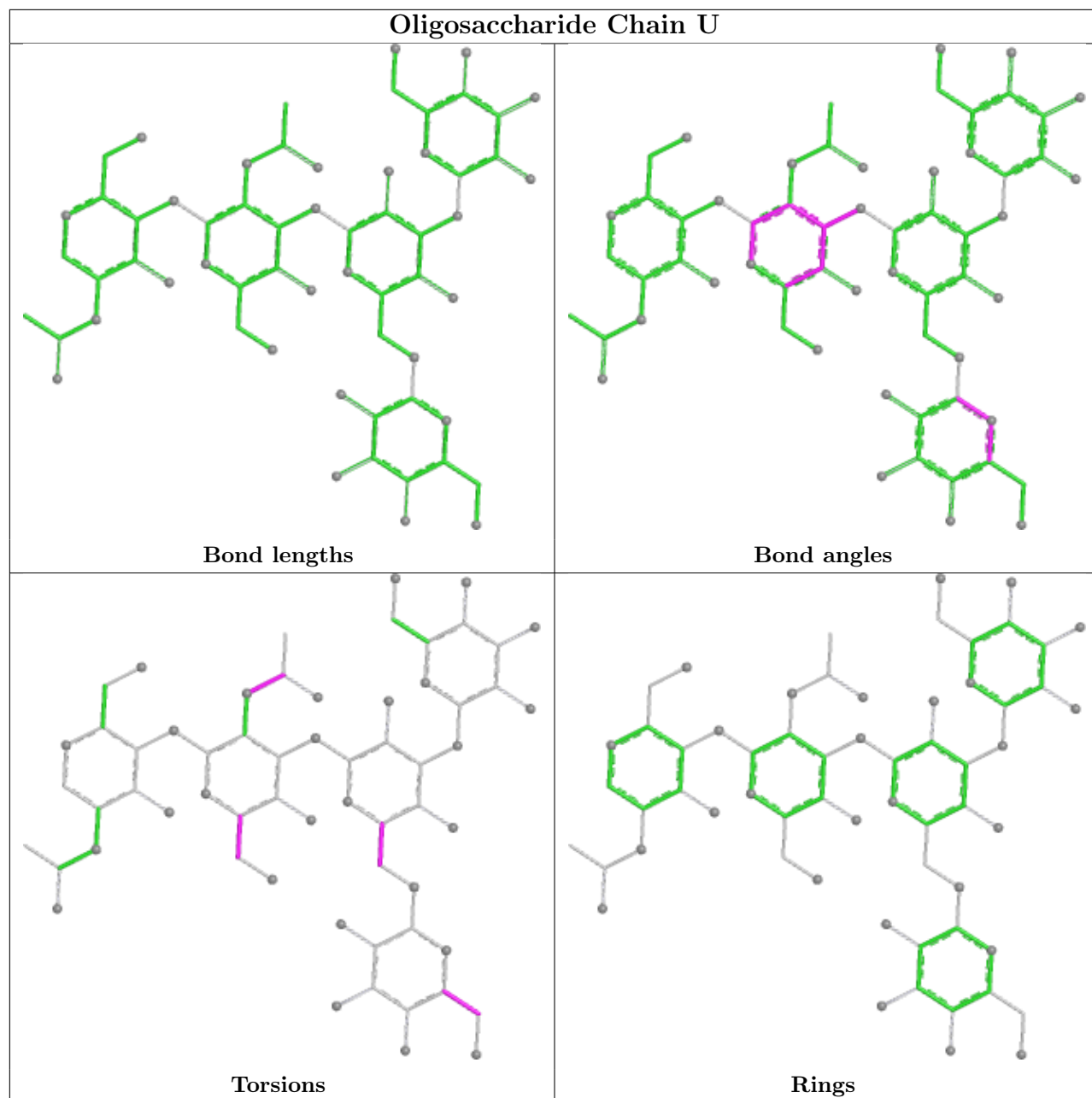


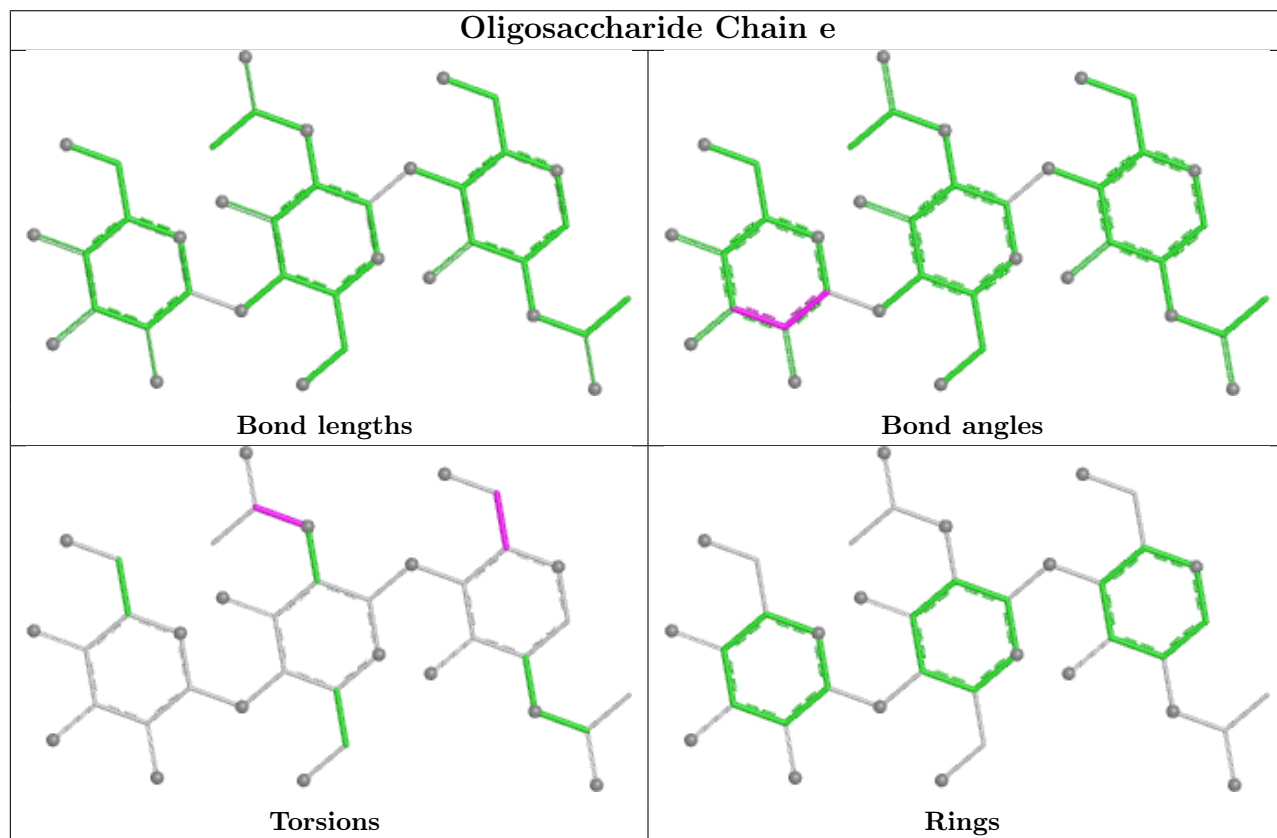
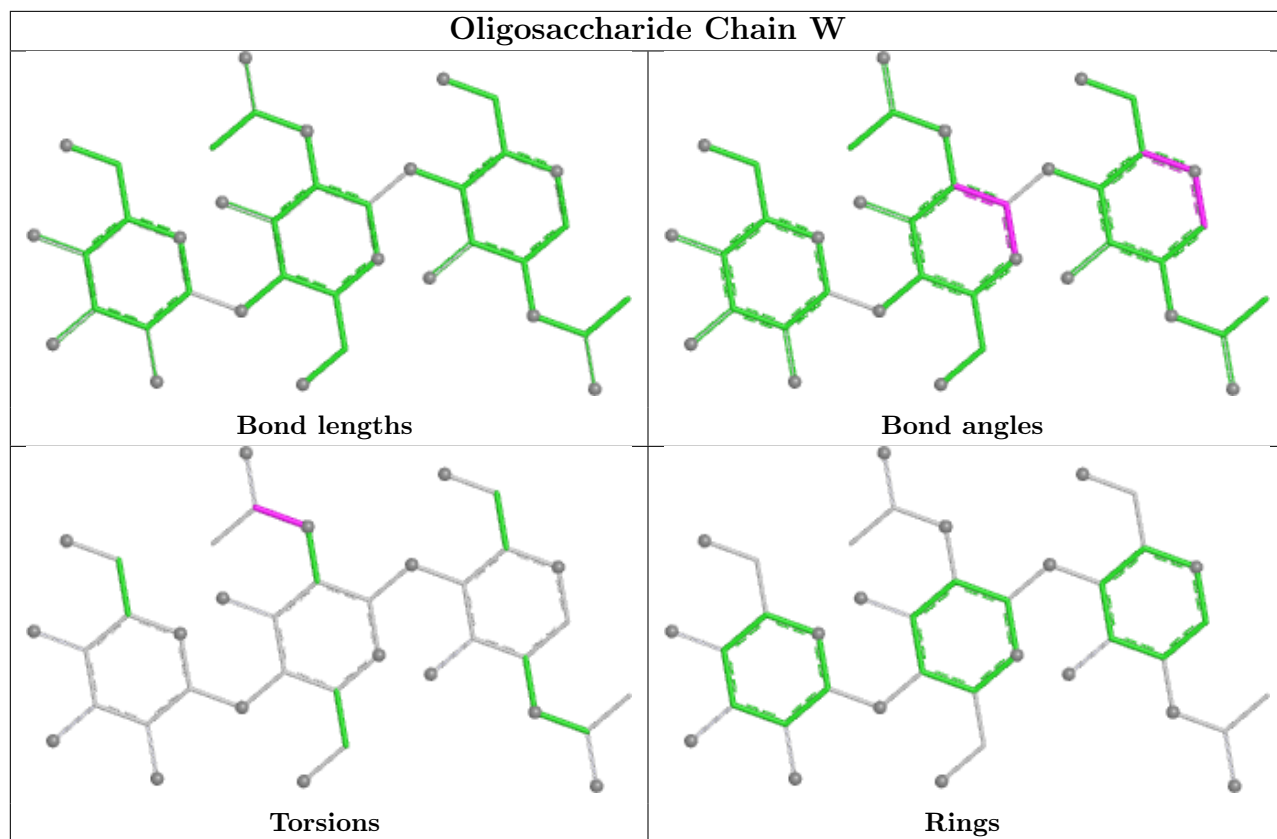


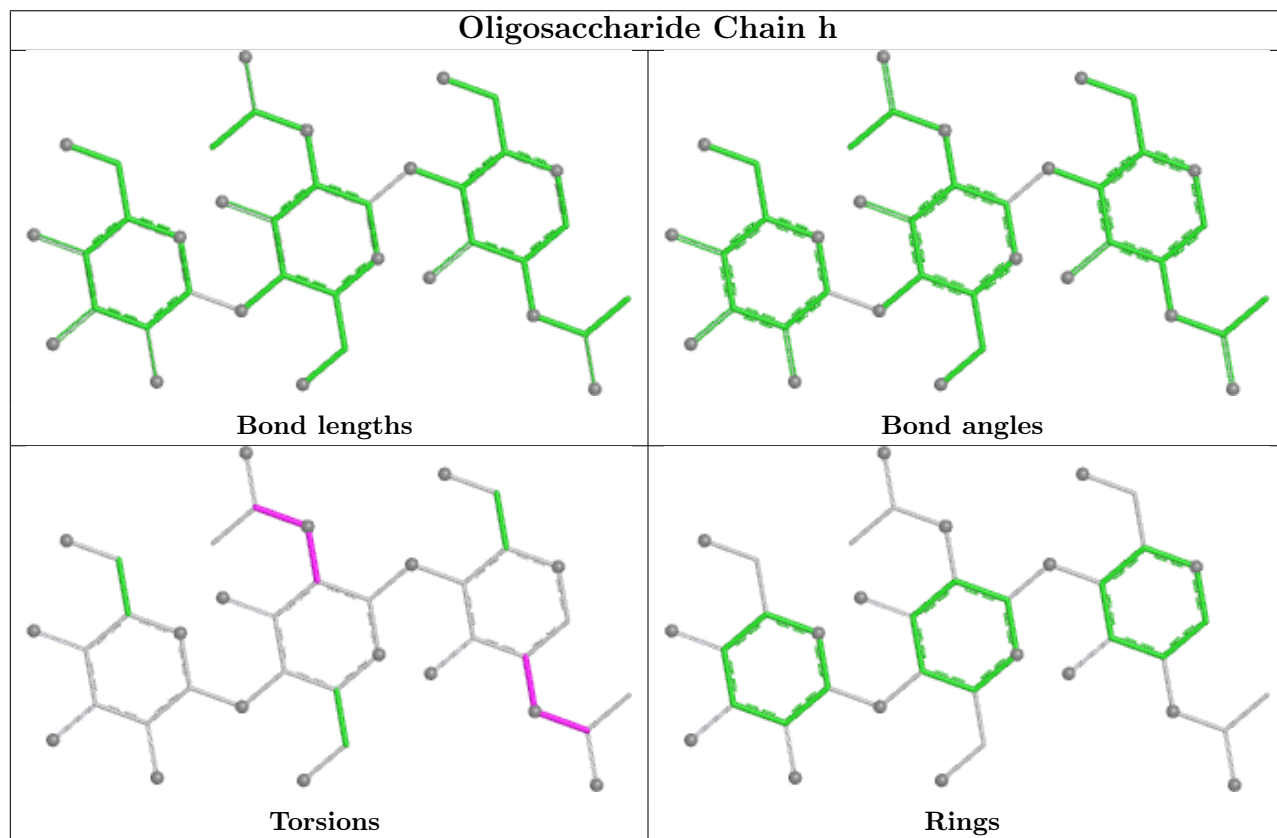
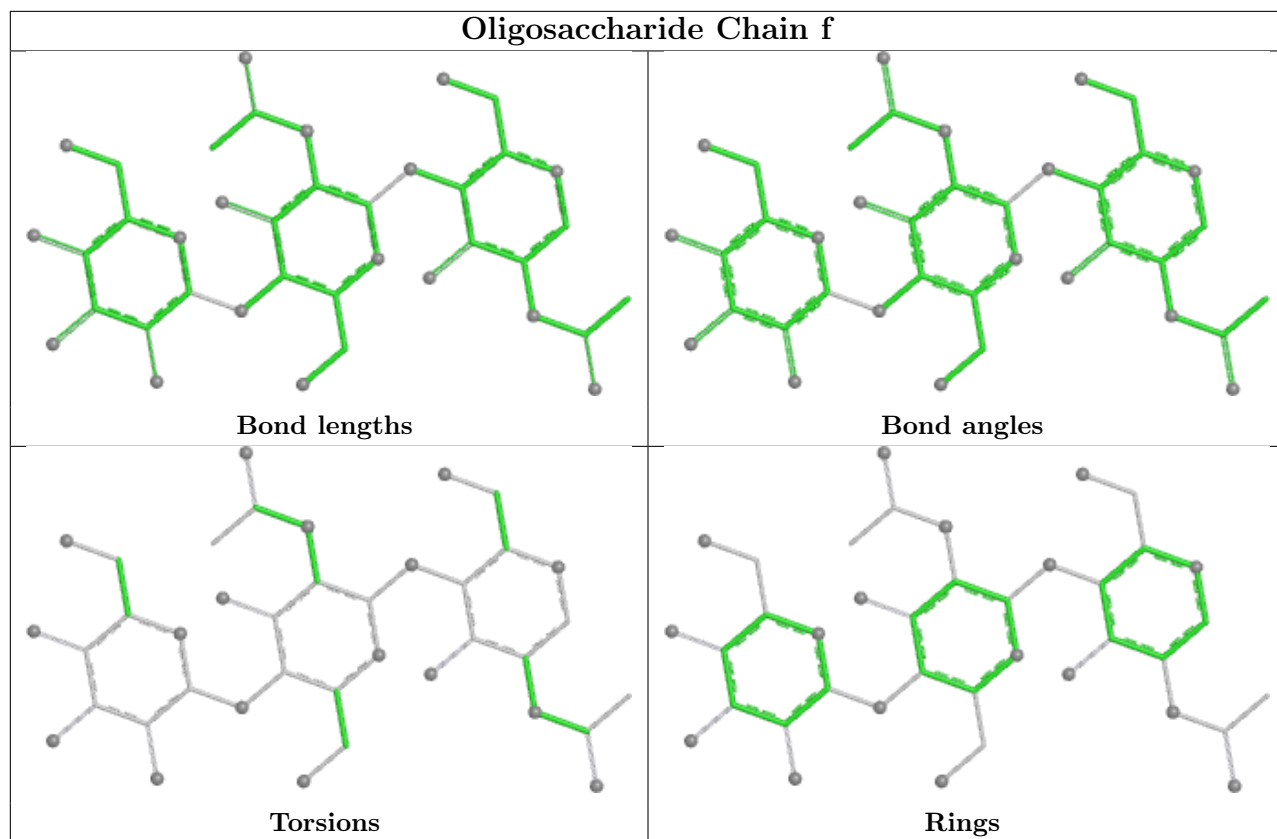


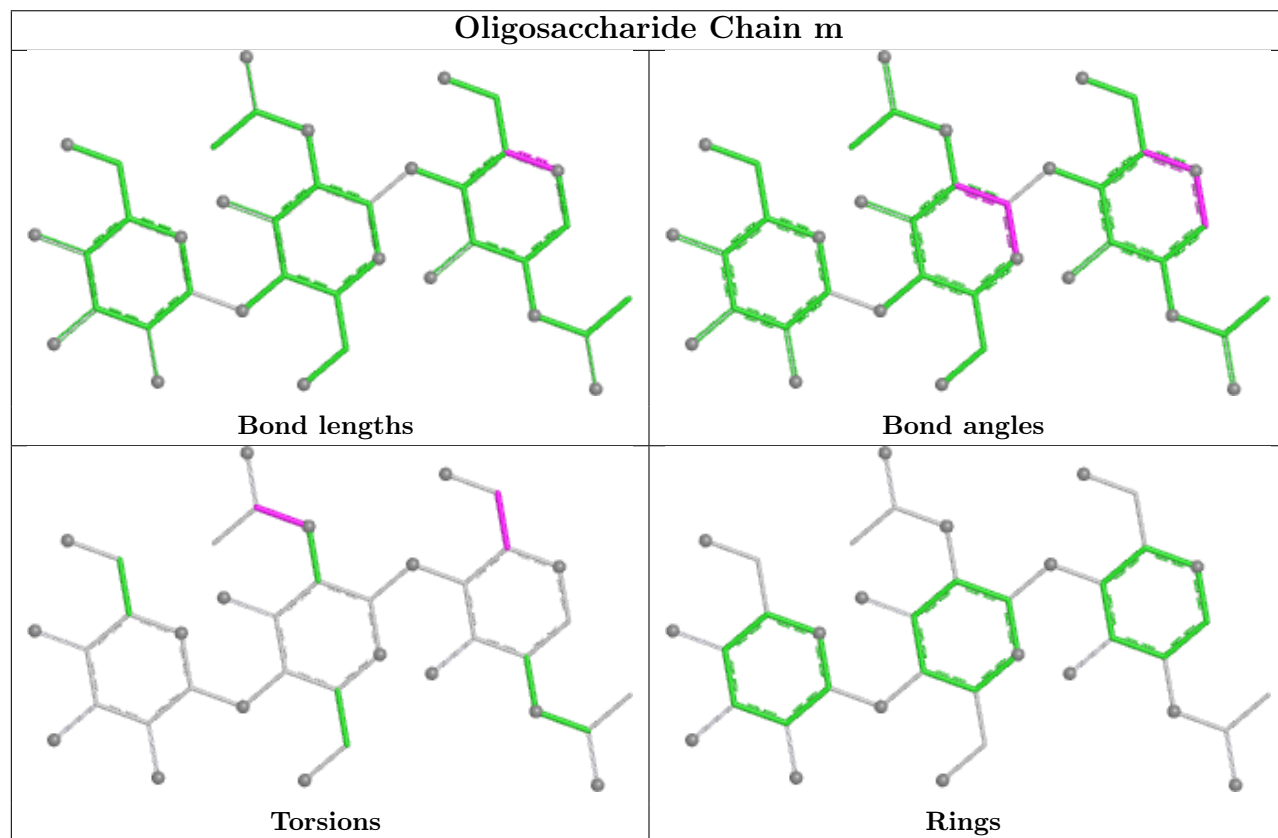
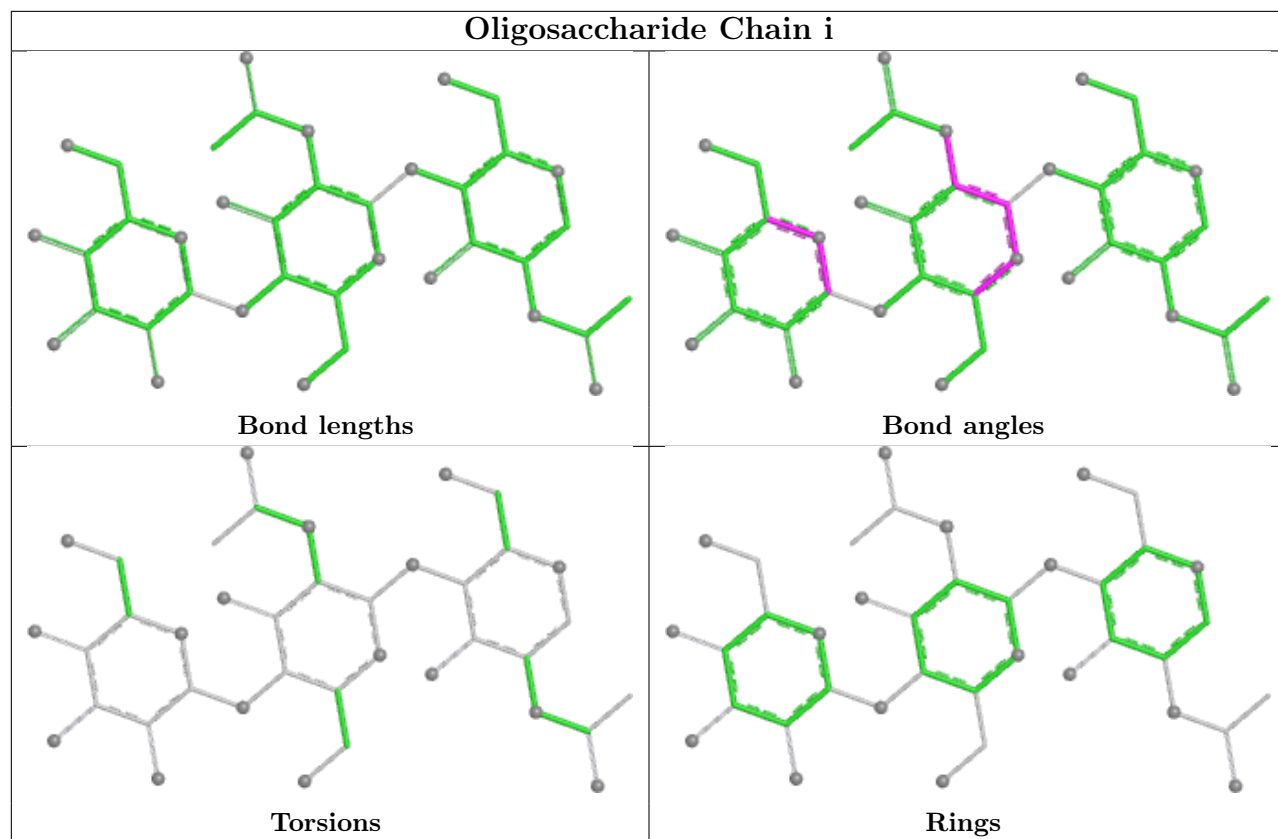


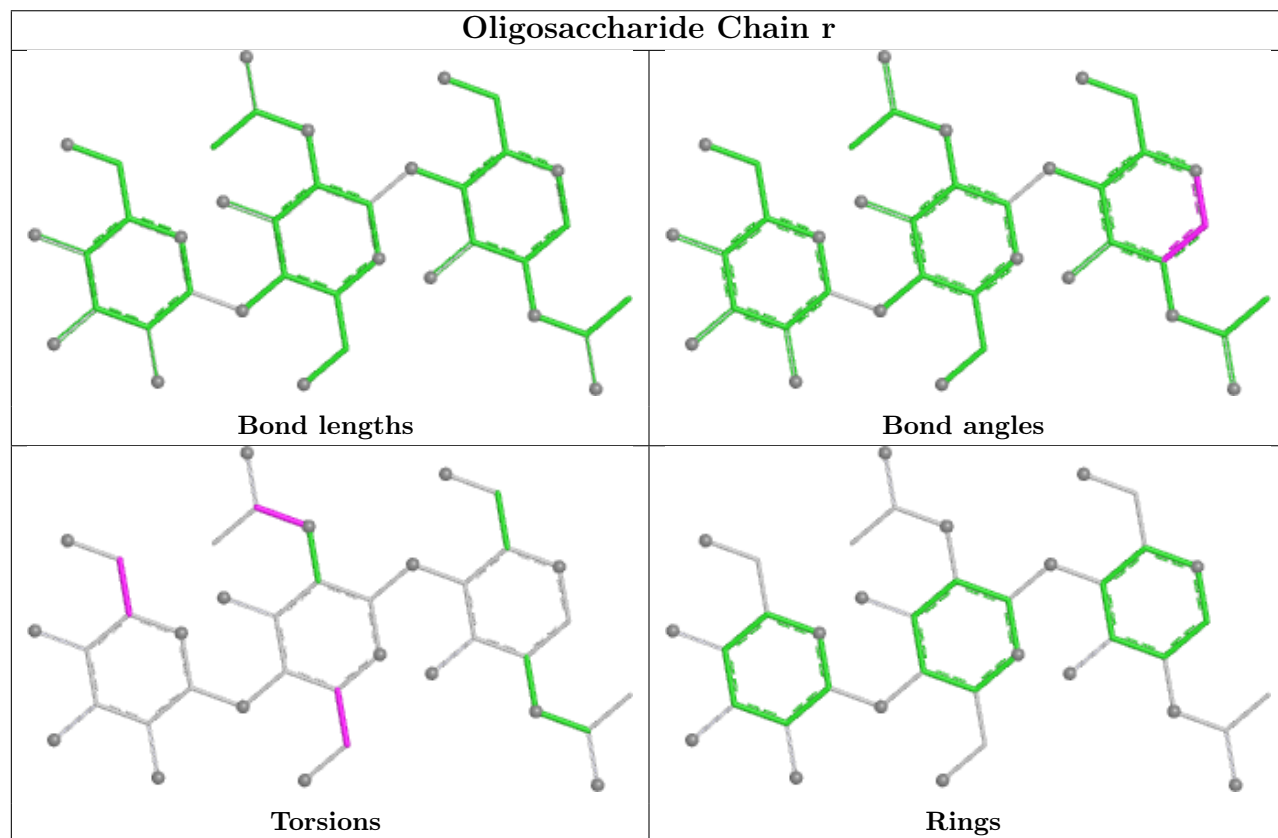
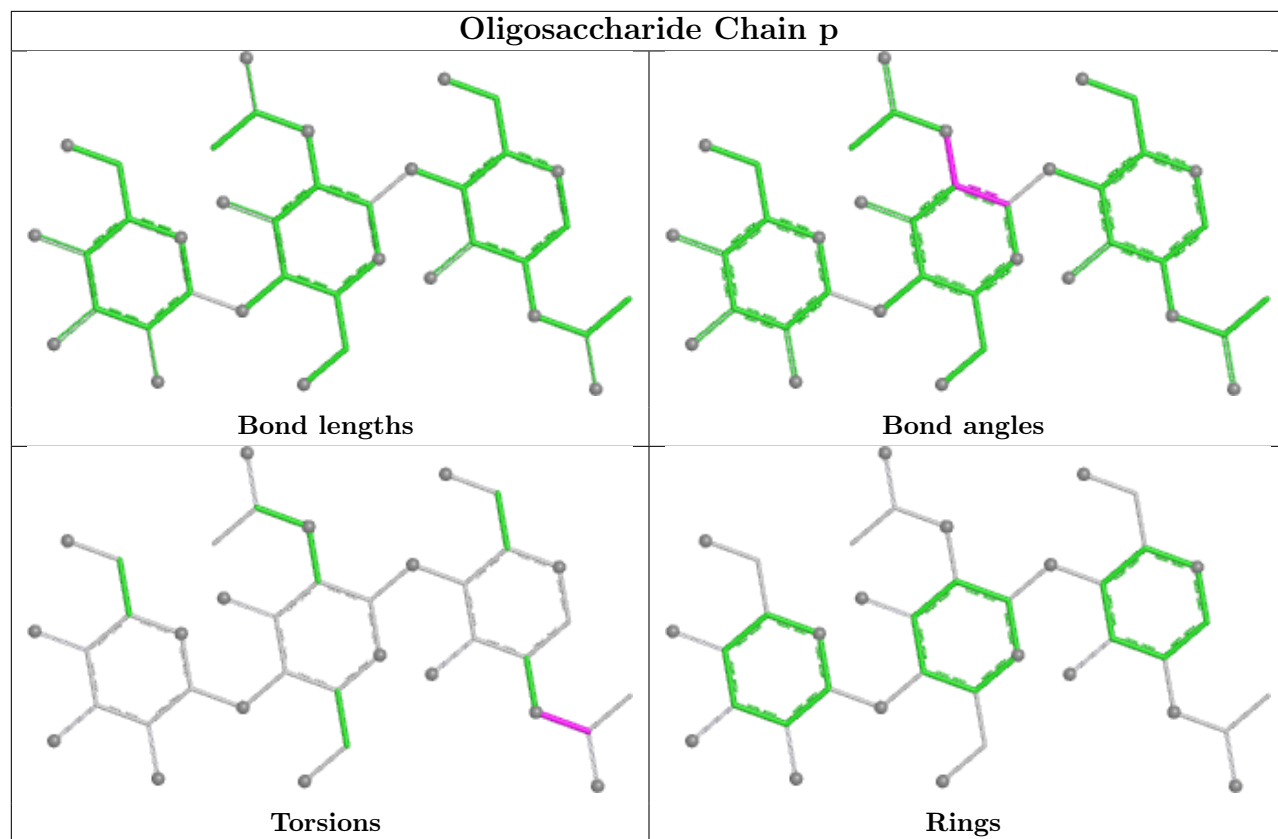


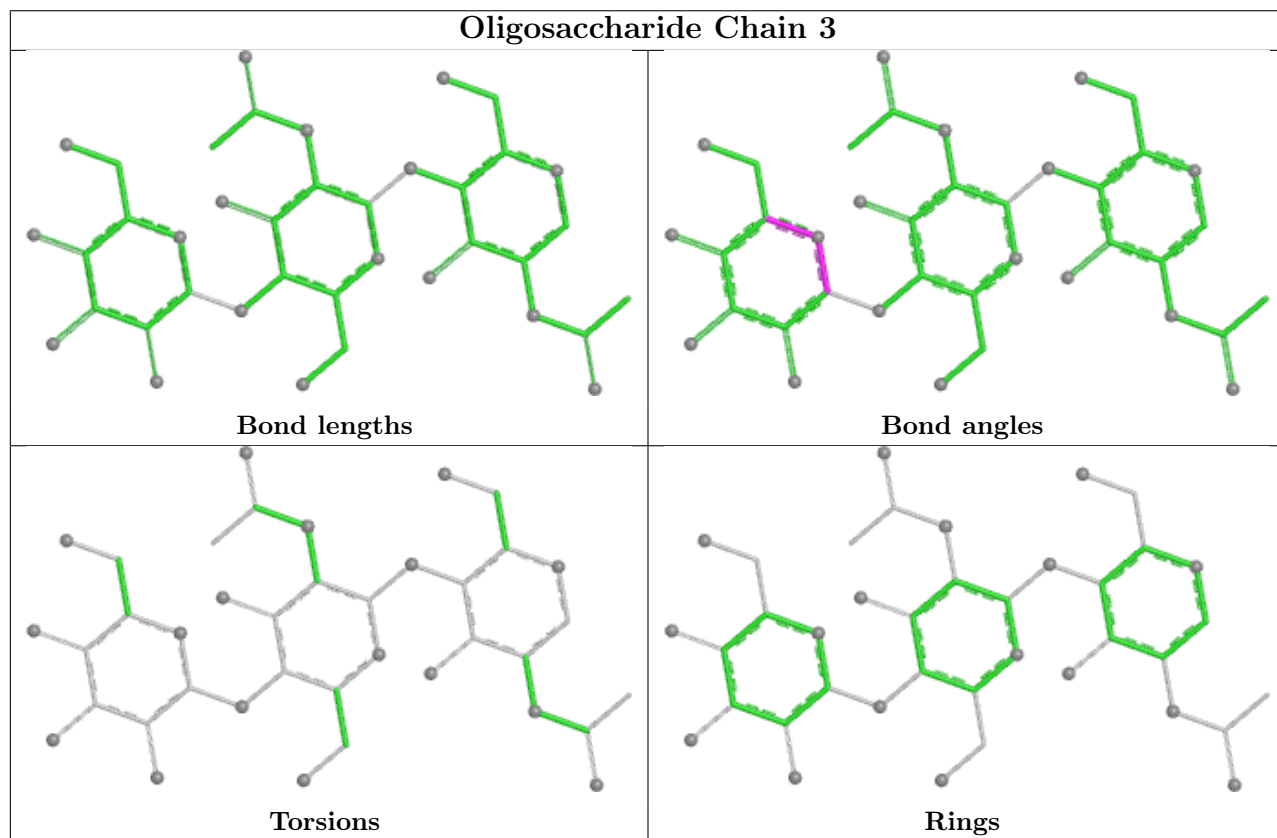
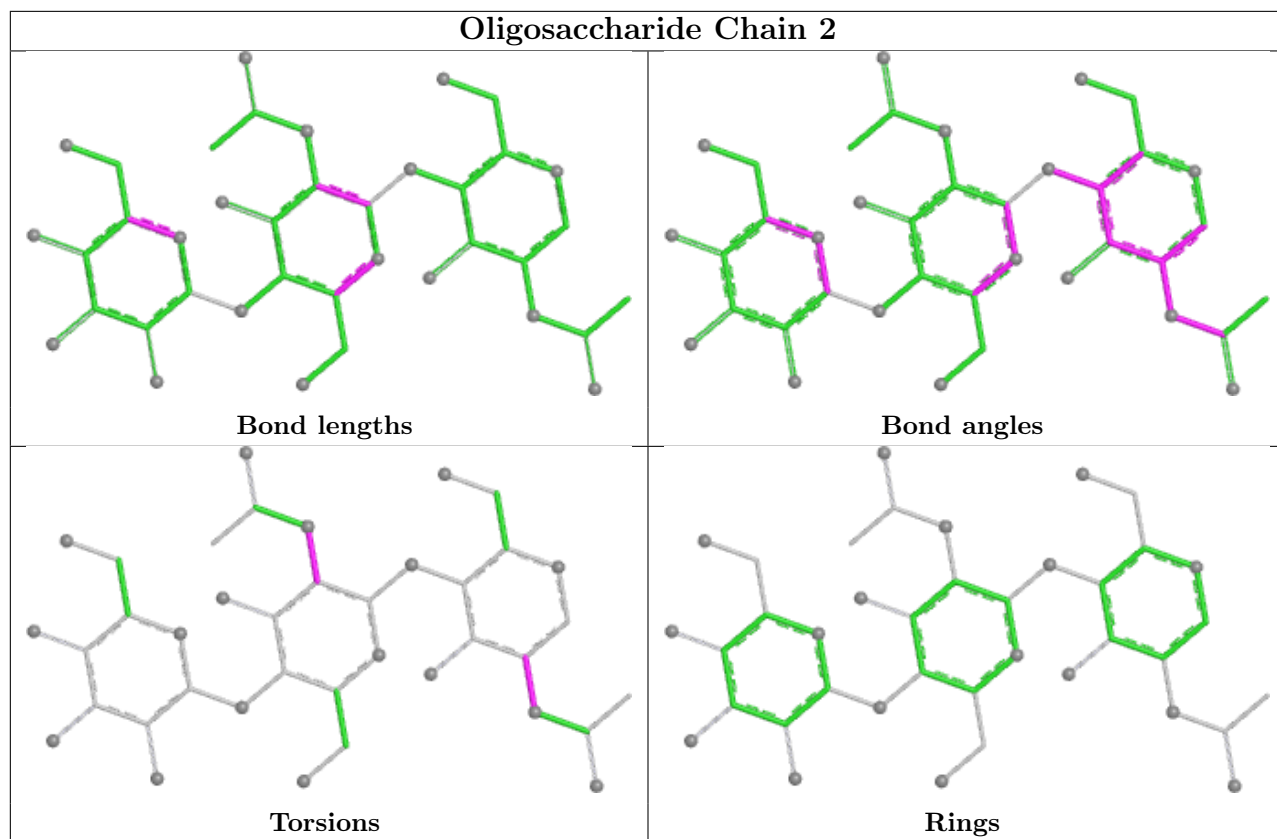


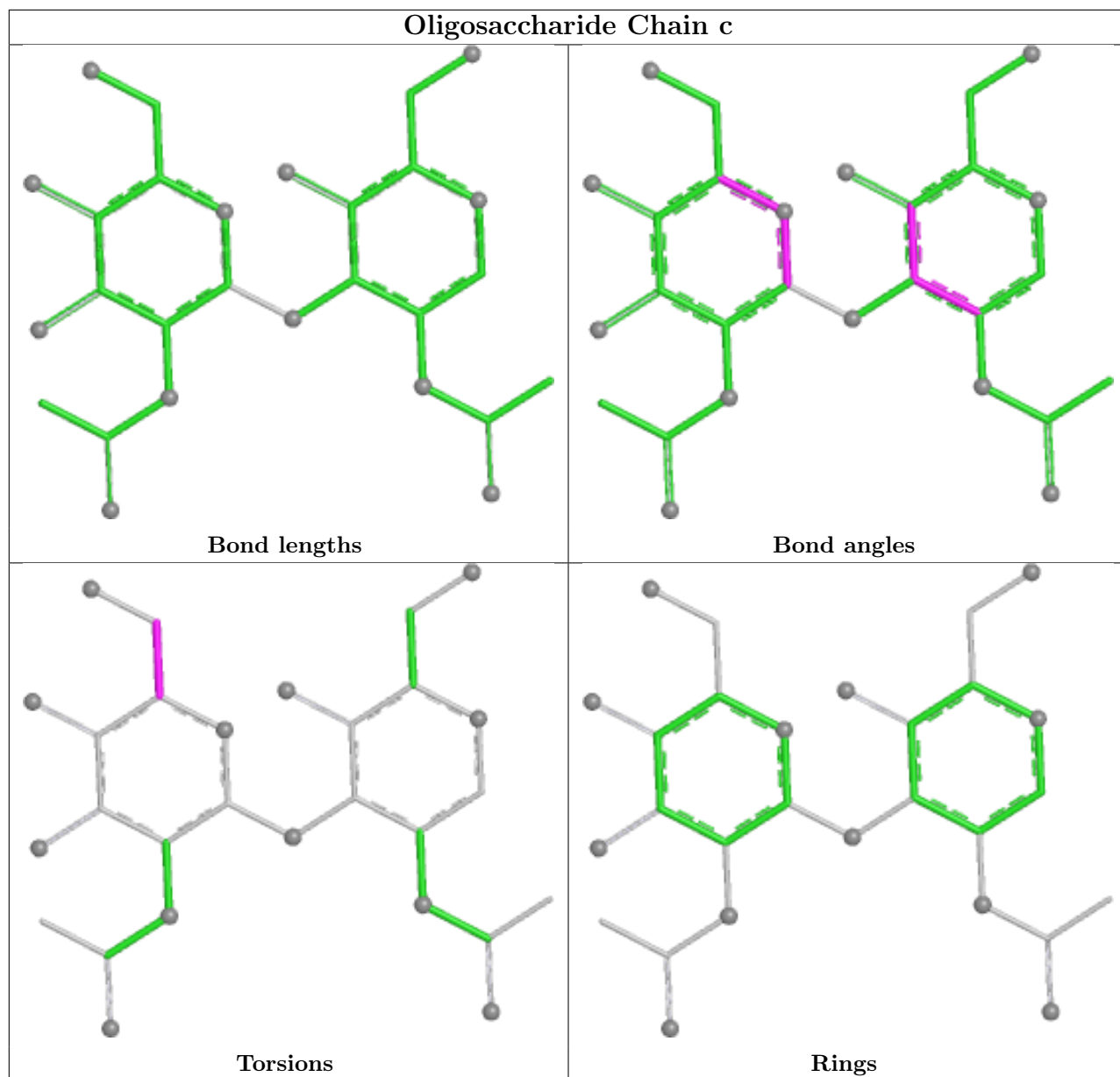


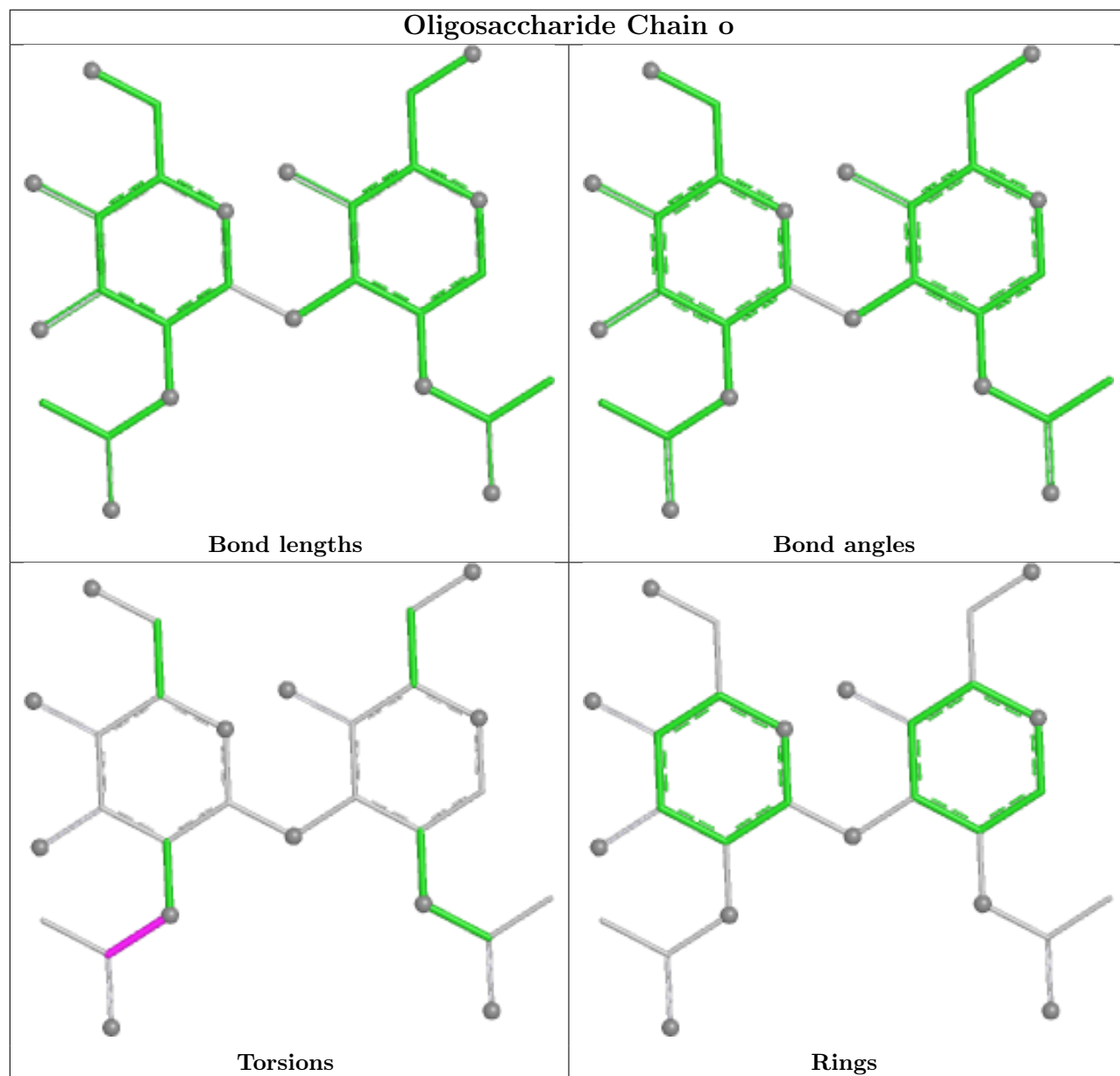


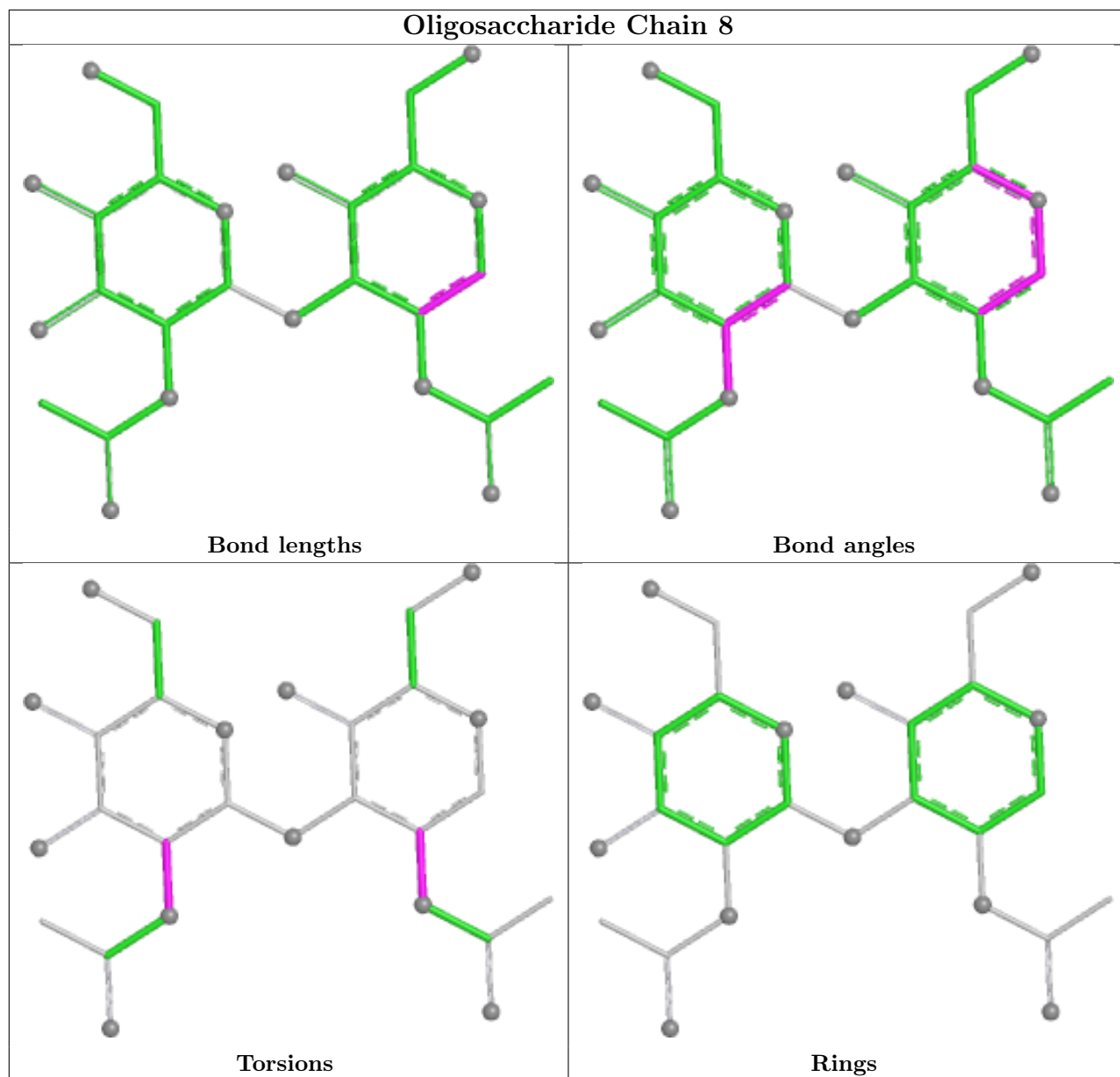


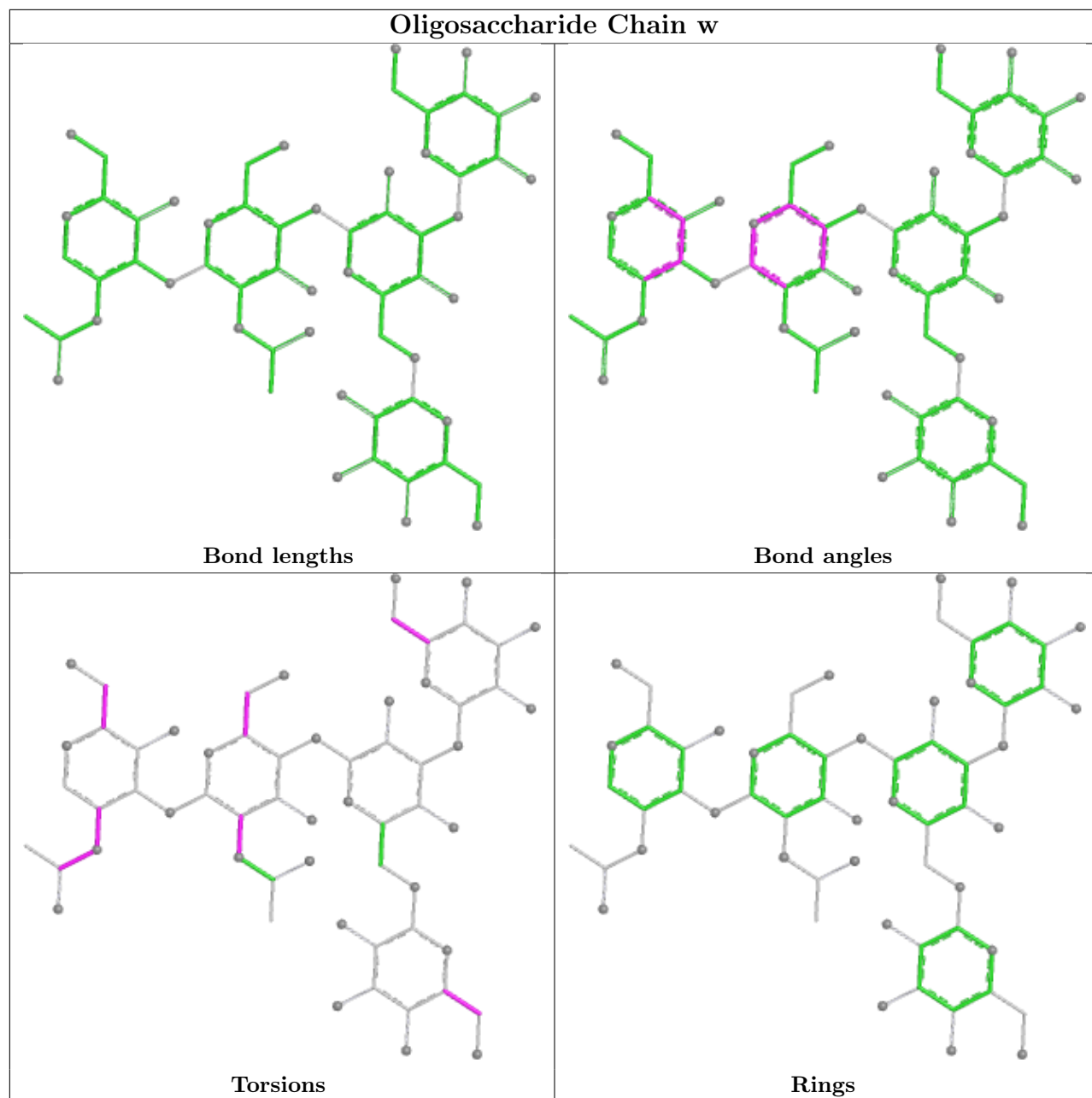


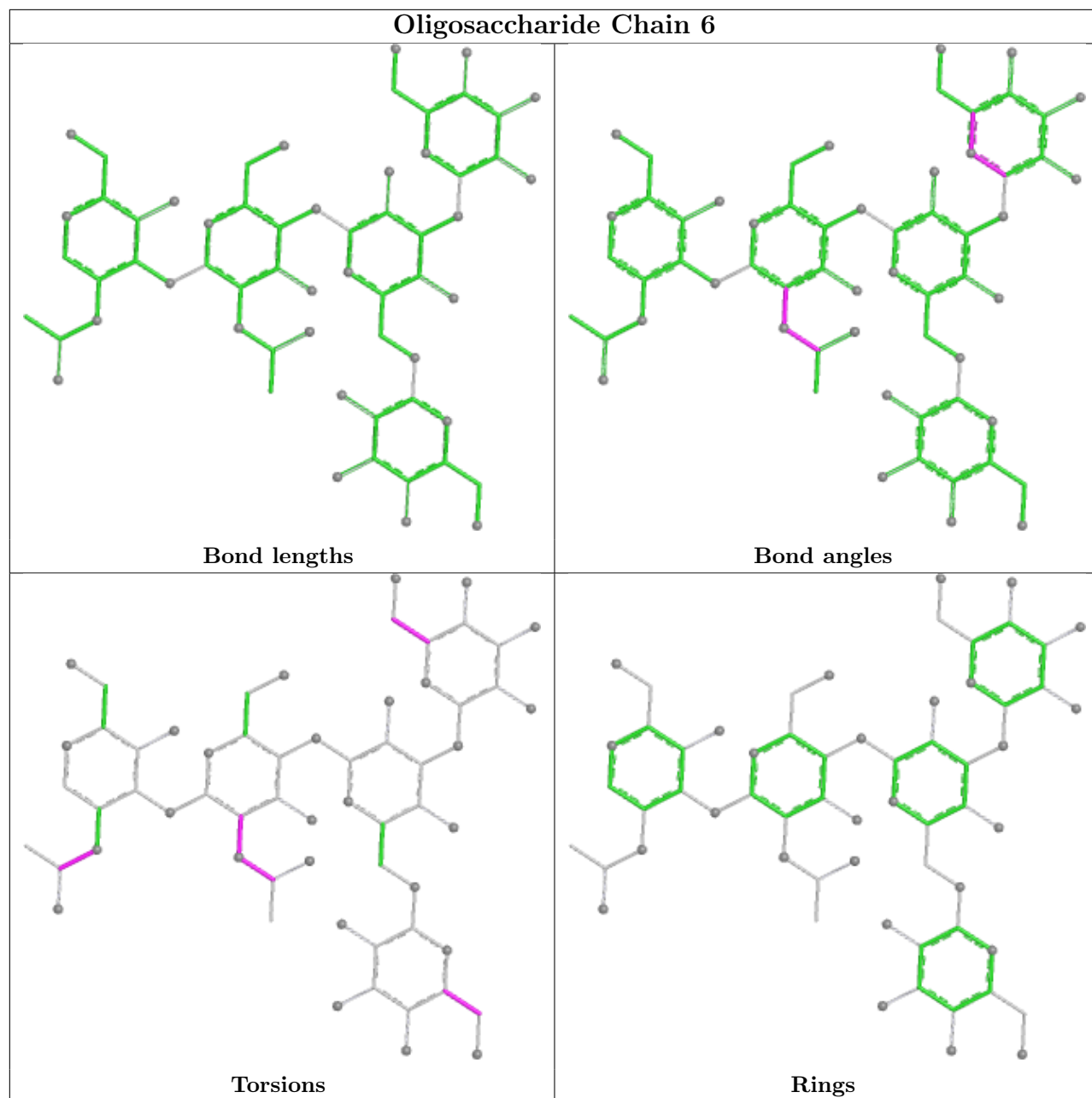


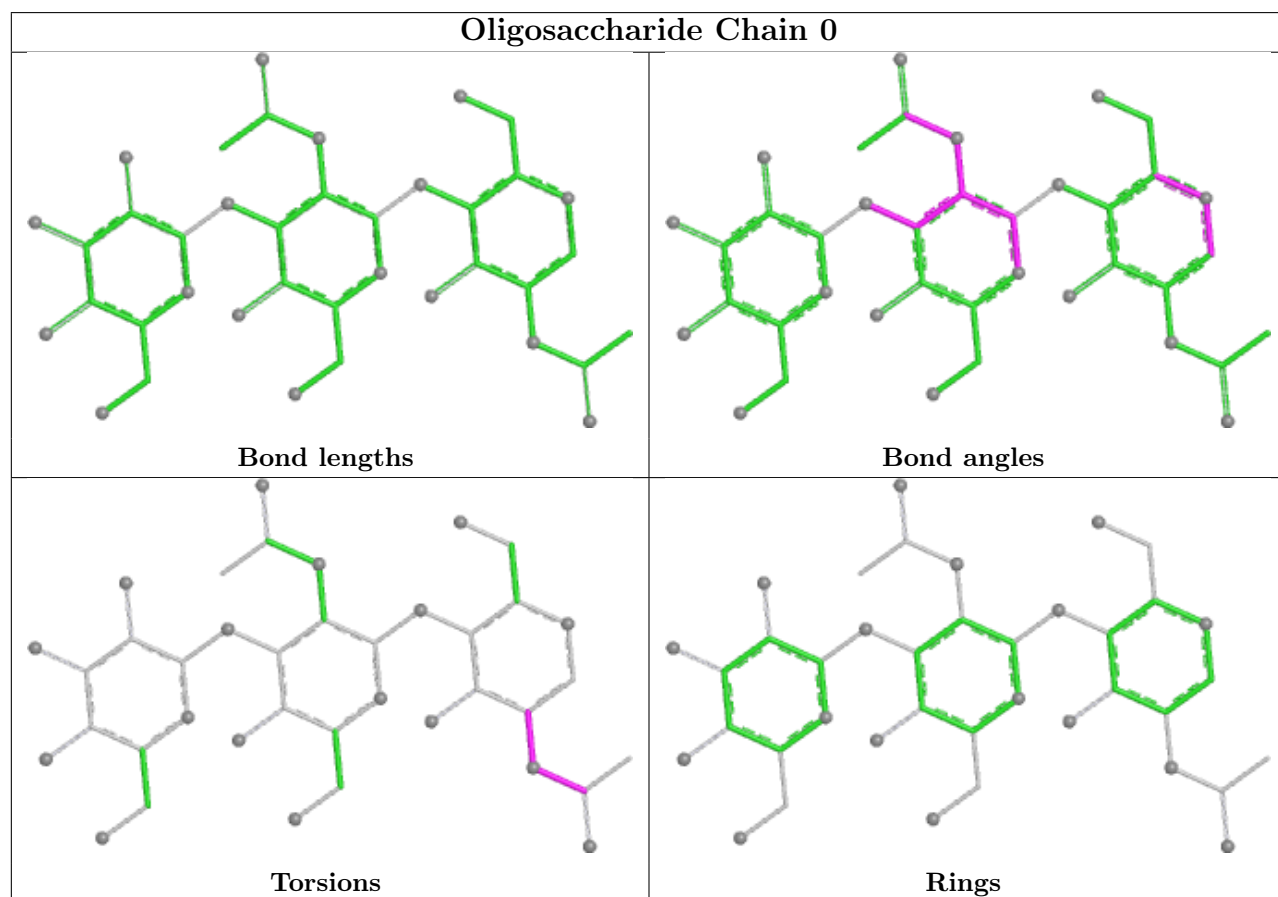
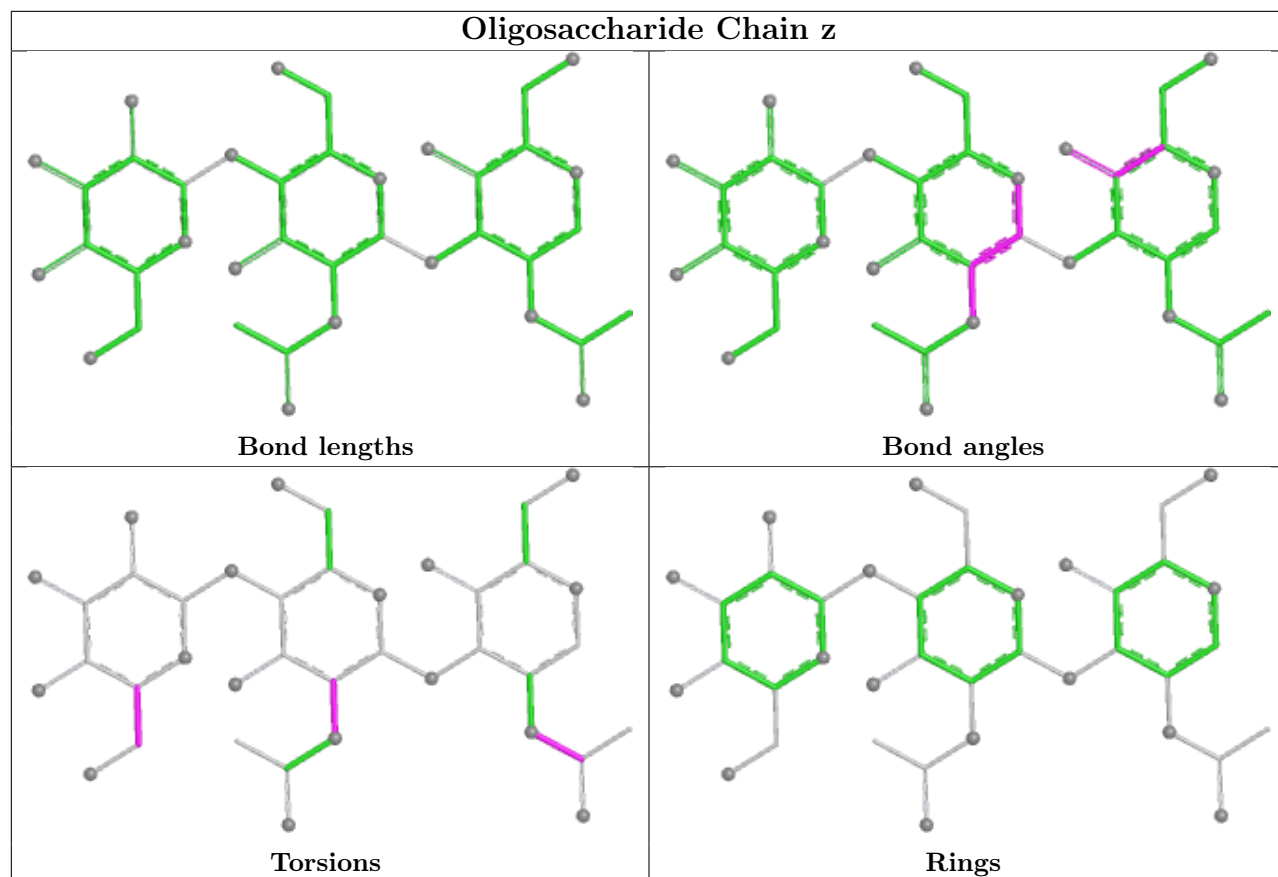


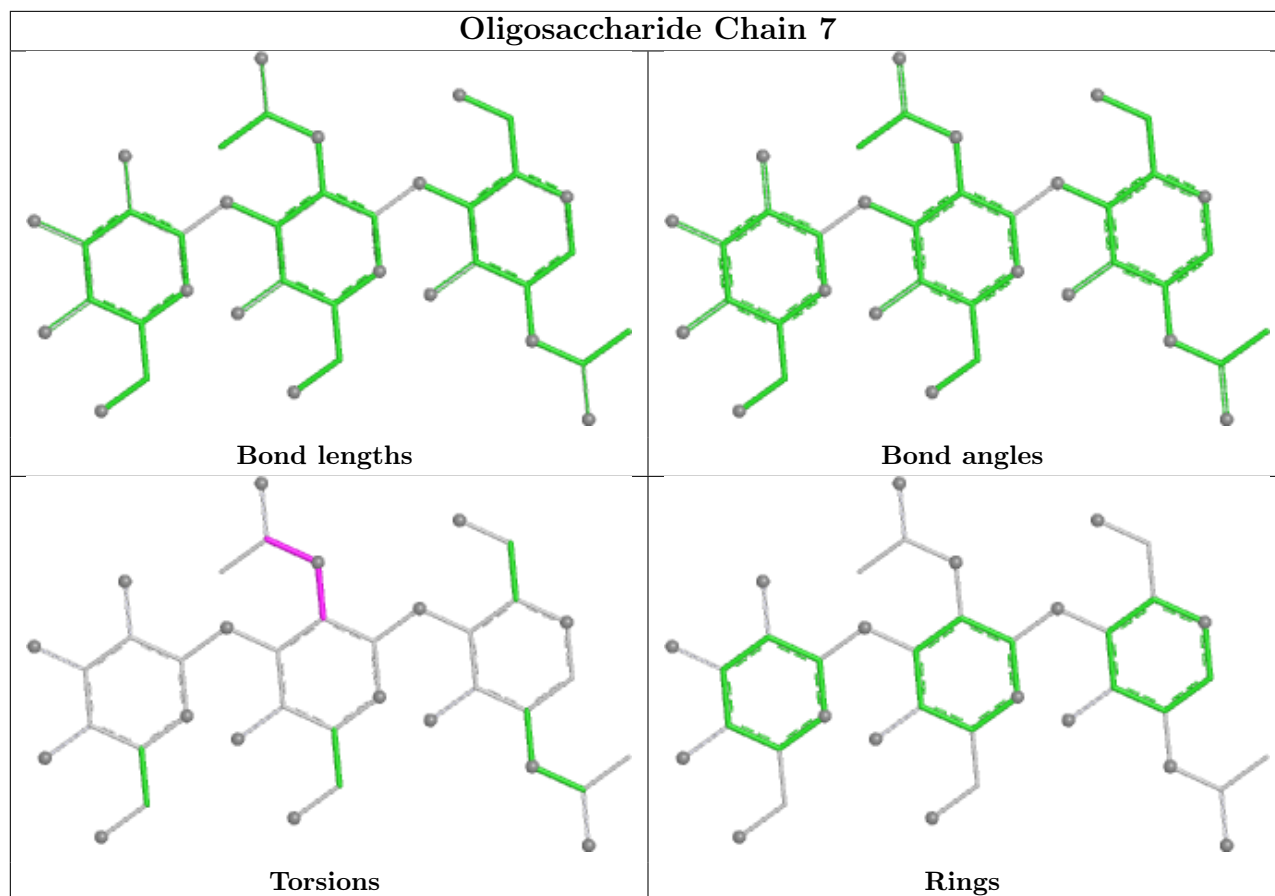












5.6 Ligand geometry [i](#)

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
18	A2G	A	4715	1	14,14,15	0.49	0	17,19,21	1.42	1 (5%)
18	A2G	B	4712	1	14,14,15	0.45	0	17,19,21	1.37	3 (17%)
18	A2G	B	4723	1	14,14,15	0.52	0	17,19,21	0.97	1 (5%)
17	NAG	A	4707	1	14,14,15	0.40	0	17,19,21	1.33	3 (17%)
18	A2G	A	4720	1	14,14,15	0.45	0	17,19,21	0.50	0
18	A2G	B	4714	1	14,14,15	0.91	1 (7%)	17,19,21	0.86	1 (5%)
17	NAG	A	4701	1	14,14,15	0.41	0	17,19,21	0.67	0

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	0.39	0	17,19,21	0.84	2 (11%)
17	NAG	B	4708	1	14,14,15	0.53	0	17,19,21	1.02	1 (5%)
18	A2G	B	4713	1	14,14,15	0.53	0	17,19,21	0.62	0
17	NAG	B	4706	1	14,14,15	0.40	0	17,19,21	0.40	0
18	A2G	B	4722	1	14,14,15	0.51	0	17,19,21	1.58	3 (17%)
18	A2G	A	4721	1	14,14,15	0.52	0	17,19,21	1.03	1 (5%)
17	NAG	A	4710	1	14,14,15	0.41	0	17,19,21	0.64	1 (5%)
18	A2G	B	4716	1	14,14,15	0.50	0	17,19,21	1.05	1 (5%)
17	NAG	B	4703	1	14,14,15	0.40	0	17,19,21	0.43	0
17	NAG	B	4711	1	14,14,15	0.45	0	17,19,21	0.67	0
17	NAG	B	4705	1	14,14,15	0.41	0	17,19,21	0.72	0
18	A2G	A	4717	1	14,14,15	0.40	0	17,19,21	0.60	0
18	A2G	A	4719	1	14,14,15	0.49	0	17,19,21	1.10	2 (11%)
18	A2G	A	4723	1	14,14,15	0.53	0	17,19,21	1.14	1 (5%)
17	NAG	B	4704	1	14,14,15	0.93	1 (7%)	17,19,21	0.95	0
18	A2G	B	4717	1	14,14,15	0.37	0	17,19,21	0.71	0
17	NAG	B	4701	1	14,14,15	0.41	0	17,19,21	0.67	0
17	NAG	A	4711	1	14,14,15	0.40	0	17,19,21	1.21	2 (11%)
17	NAG	A	4705	1	14,14,15	0.54	0	17,19,21	2.17	2 (11%)
17	NAG	A	4702	1	14,14,15	0.40	0	17,19,21	1.02	1 (5%)
17	NAG	A	4704	1	14,14,15	0.56	0	17,19,21	1.15	1 (5%)
17	NAG	B	4702	1	14,14,15	0.40	0	17,19,21	0.48	0
18	A2G	A	4712	1	14,14,15	0.47	0	17,19,21	1.81	3 (17%)
17	NAG	A	4709	1	14,14,15	0.41	0	17,19,21	0.33	0
18	A2G	B	4721	1	14,14,15	0.53	0	17,19,21	1.00	1 (5%)
18	A2G	A	4714	1	14,14,15	0.48	0	17,19,21	0.90	1 (5%)
18	A2G	B	4719	1	14,14,15	0.38	0	17,19,21	1.06	1 (5%)
17	NAG	B	4710	1	14,14,15	0.45	0	17,19,21	0.72	0
18	A2G	A	4718	1	14,14,15	0.52	0	17,19,21	1.63	3 (17%)
17	NAG	A	4708	1	14,14,15	0.41	0	17,19,21	0.33	0
17	NAG	A	4703	1	14,14,15	0.39	0	17,19,21	0.43	0
18	A2G	B	4718	1	14,14,15	0.49	0	17,19,21	0.84	0
18	A2G	A	4713	1	14,14,15	0.56	0	17,19,21	0.59	0
18	A2G	A	4722	1	14,14,15	0.51	0	17,19,21	1.61	3 (17%)
17	NAG	B	4709	1	14,14,15	1.01	1 (7%)	17,19,21	0.92	1 (5%)
18	A2G	A	4716	1	14,14,15	1.01	1 (7%)	17,19,21	1.31	2 (11%)
18	A2G	B	4720	1	14,14,15	0.48	0	17,19,21	0.84	1 (5%)
18	A2G	B	4715	1	14,14,15	0.45	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NAG	B	4707	1	14,14,15	0.48	0	17,19,21	0.95	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
18	A2G	A	4715	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4712	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	4707	1	-	2/6/23/26	0/1/1/1
18	A2G	A	4720	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4714	1	-	1/6/23/26	0/1/1/1
17	NAG	A	4701	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4706	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4708	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4713	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4706	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4722	1	-	1/6/23/26	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	B	4716	1	-	1/6/23/26	0/1/1/1
17	NAG	B	4703	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4711	1	-	4/6/23/26	0/1/1/1
17	NAG	B	4705	1	-	3/6/23/26	0/1/1/1
18	A2G	A	4717	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4719	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4723	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	4717	1	-	1/6/23/26	0/1/1/1
17	NAG	B	4701	1	-	3/6/23/26	0/1/1/1
17	NAG	A	4711	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4705	1	-	3/6/23/26	0/1/1/1
17	NAG	A	4702	1	-	0/6/23/26	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
18	A2G	A	4712	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4709	1	-	2/6/23/26	0/1/1/1
18	A2G	B	4721	1	-	1/6/23/26	0/1/1/1

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	A2G	A	4714	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4719	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	4718	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4708	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4703	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4718	1	-	1/6/23/26	0/1/1/1
18	A2G	A	4713	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4722	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4709	1	-	1/6/23/26	0/1/1/1
18	A2G	A	4716	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	4715	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4707	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	4709	NAG	O5-C5	2.53	1.48	1.43
18	A	4716	A2G	O5-C5	2.21	1.47	1.43
18	B	4714	A2G	O5-C5	2.15	1.47	1.43
17	B	4704	NAG	C1-C2	2.12	1.55	1.52

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	4705	NAG	O5-C1-C2	6.45	121.26	111.29
17	A	4705	NAG	C1-O5-C5	5.81	119.97	112.19
18	A	4712	A2G	C1-C2-N2	4.92	118.19	110.43
18	A	4715	A2G	C1-C2-N2	4.59	117.67	110.43
18	A	4718	A2G	C2-N2-C7	4.26	128.61	122.90

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	4704	NAG	C1-C2-N2-C7
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

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.

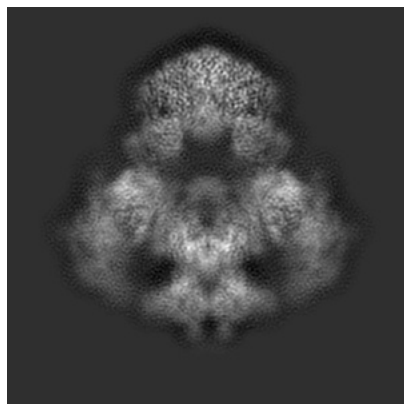
6 Map visualisation [i](#)

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.

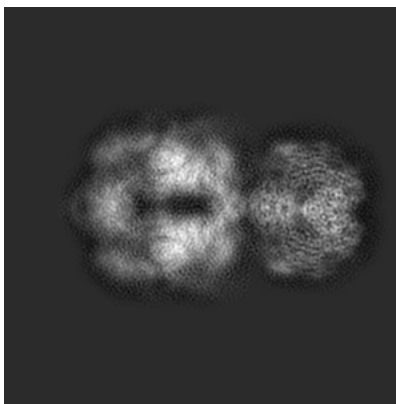
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

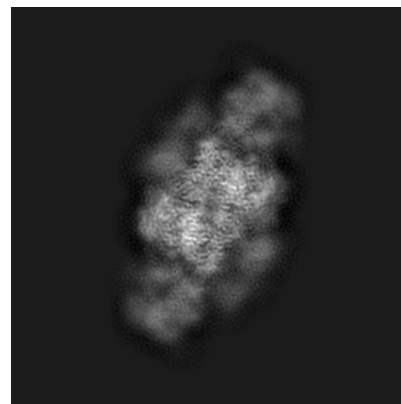
6.1.1 Primary map



X

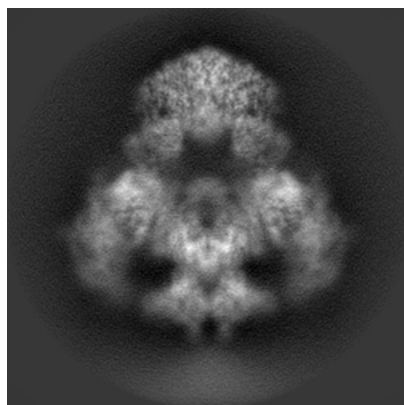


Y

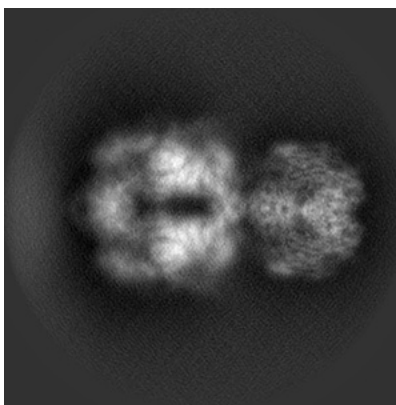


Z

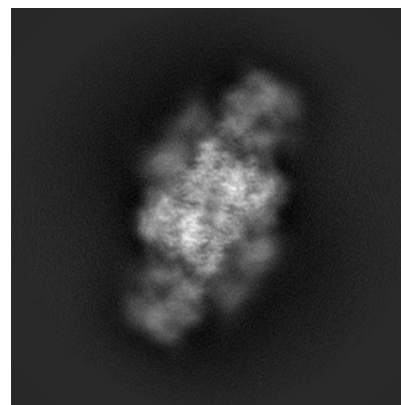
6.1.2 Raw map



X



Y

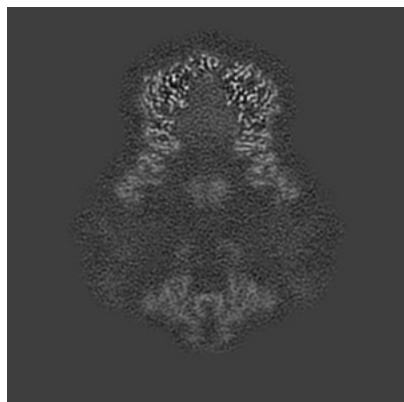


Z

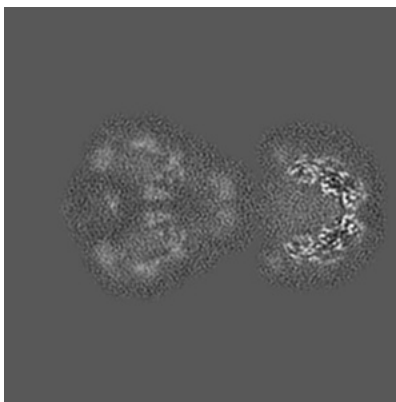
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

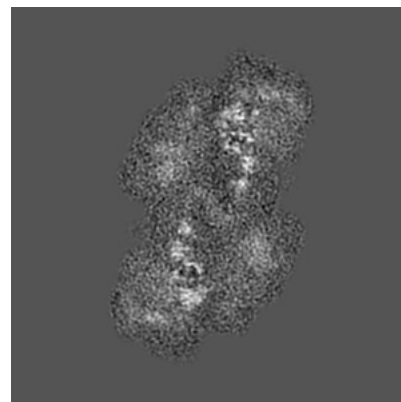
6.2.1 Primary map



X Index: 130

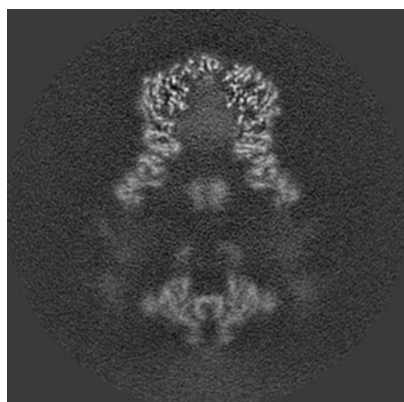


Y Index: 130

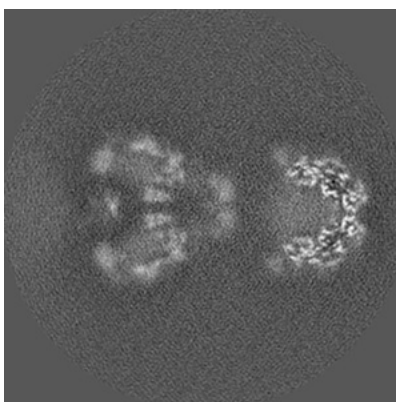


Z Index: 130

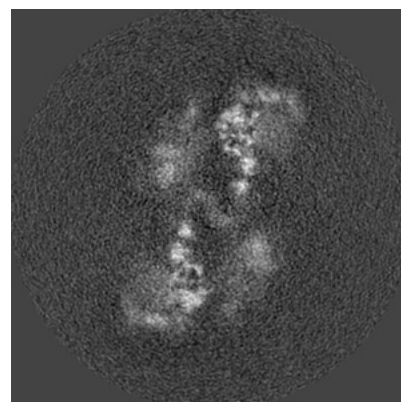
6.2.2 Raw map



X Index: 130



Y Index: 130

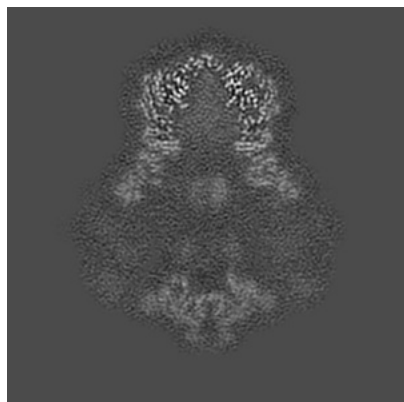


Z Index: 130

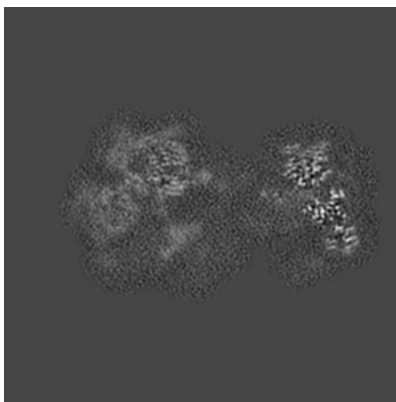
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

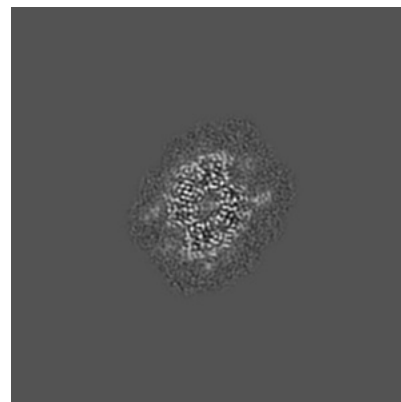
6.3.1 Primary map



X Index: 129

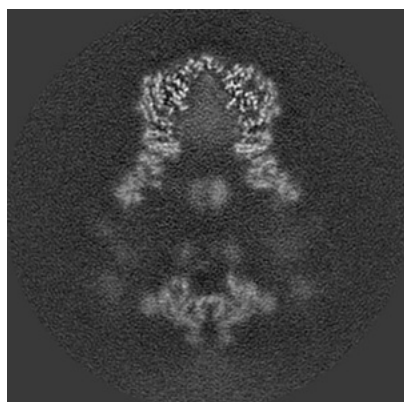


Y Index: 145

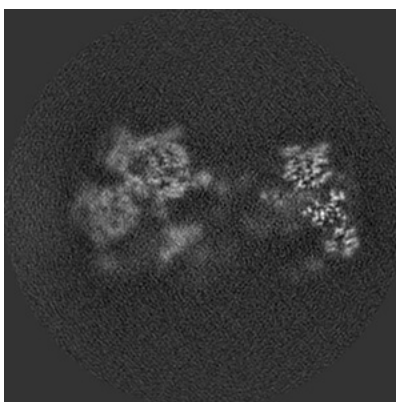


Z Index: 215

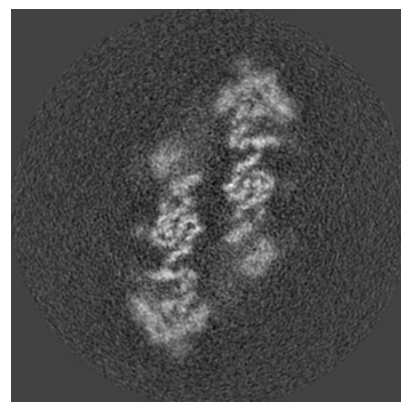
6.3.2 Raw map



X Index: 129



Y Index: 145

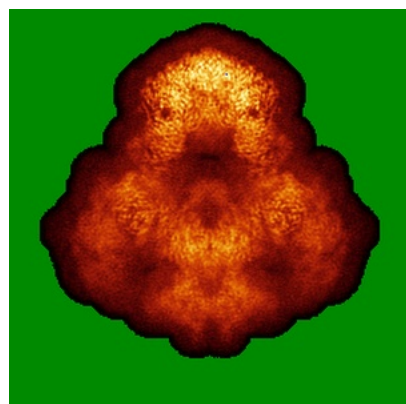


Z Index: 115

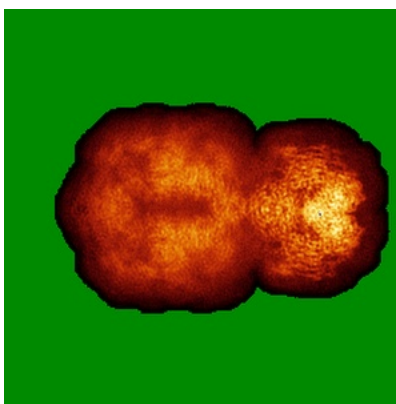
The images above show the largest variance slices of the map in three orthogonal directions.

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

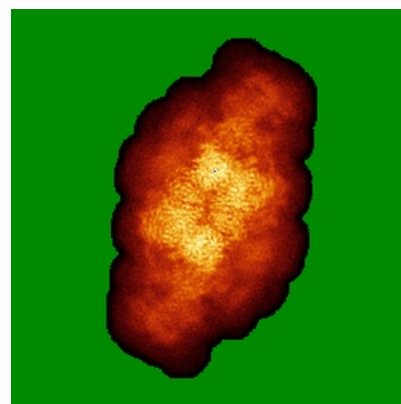
6.4.1 Primary map



X

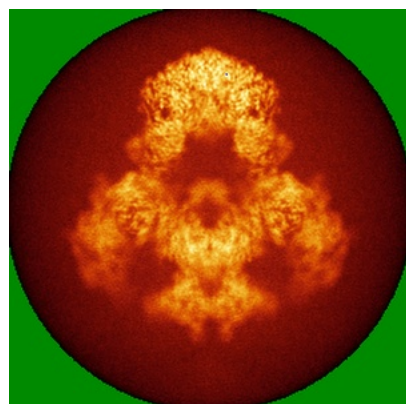


Y

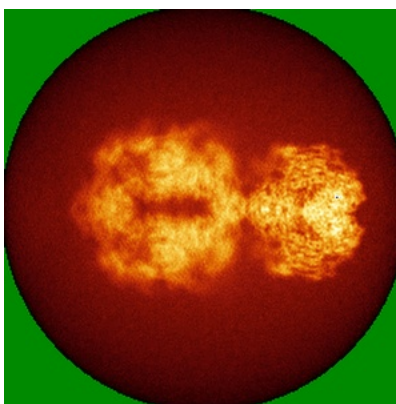


Z

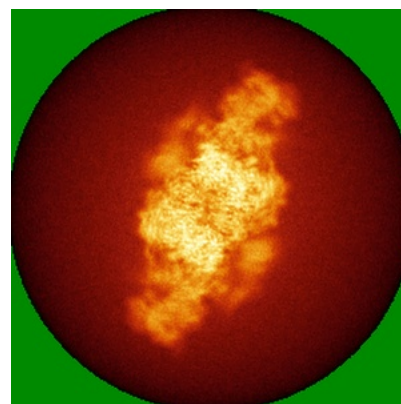
6.4.2 Raw map



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](#)

This section was not generated.

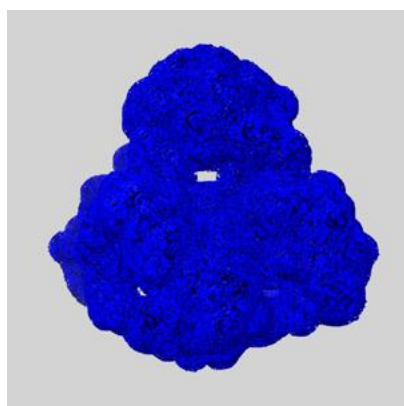
6.6 Mask visualisation [i](#)

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

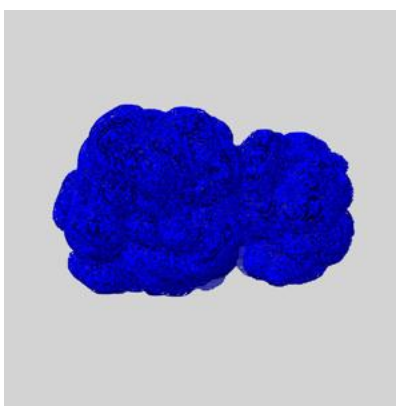
A mask typically either:

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

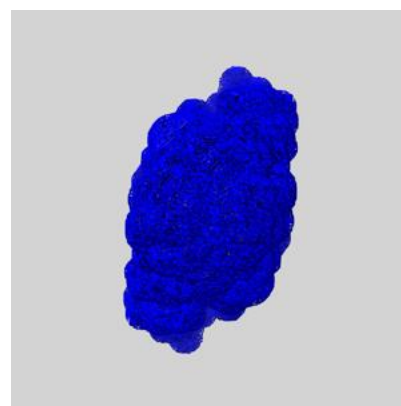
6.6.1 emd_36663_msk_1.map [i](#)



X



Y

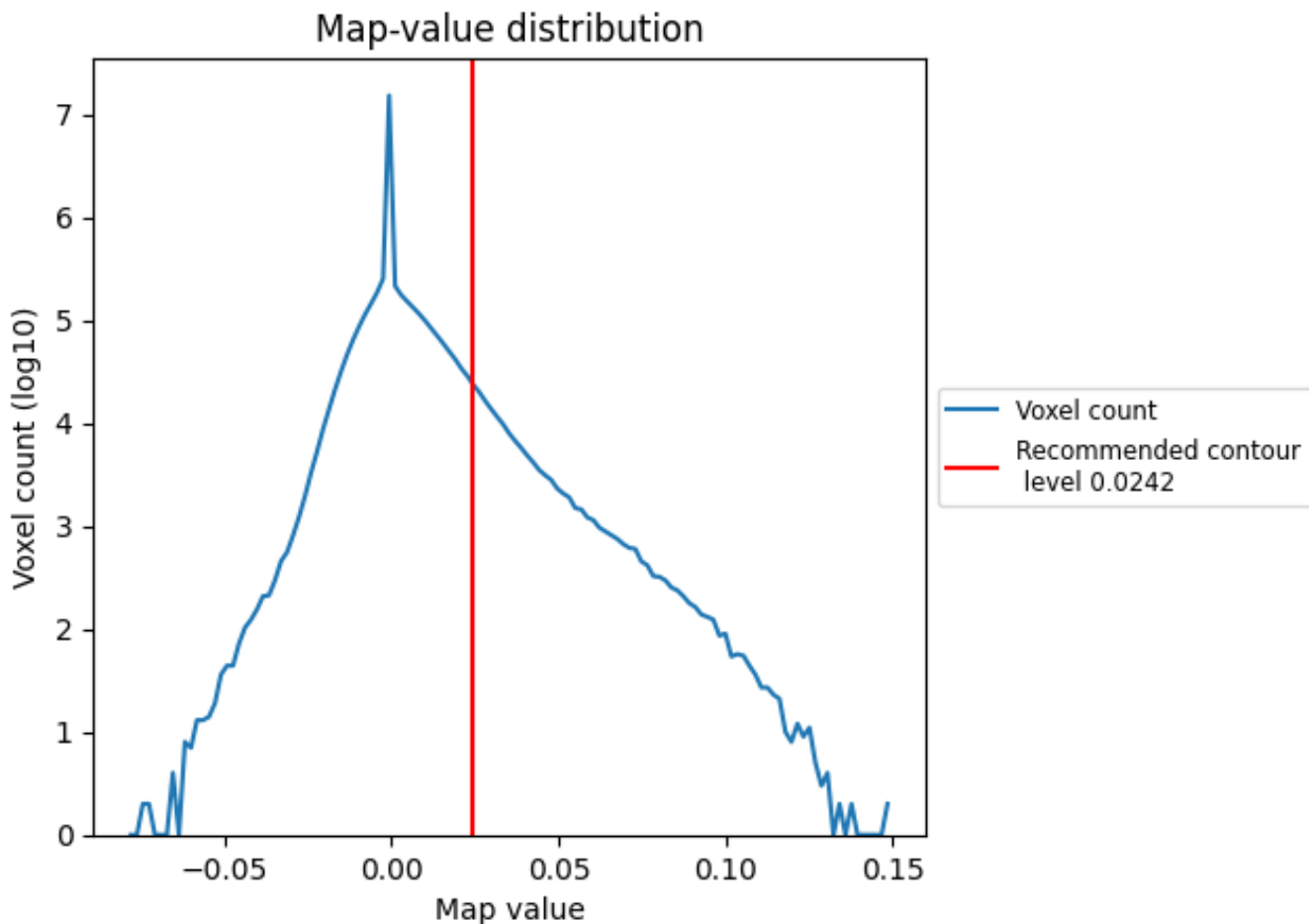


Z

7 Map analysis [i](#)

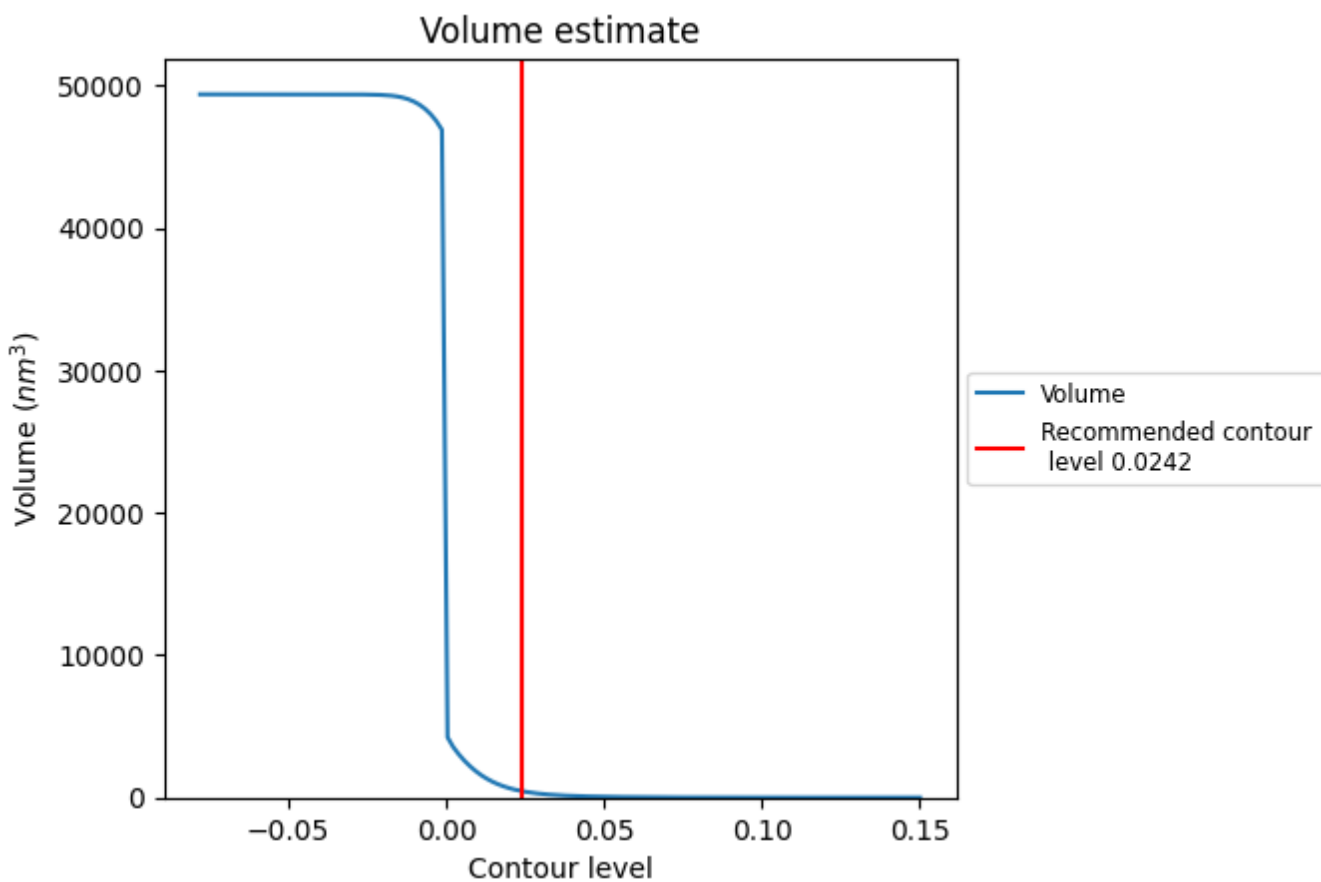
This section contains the results of statistical analysis of the map.

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.

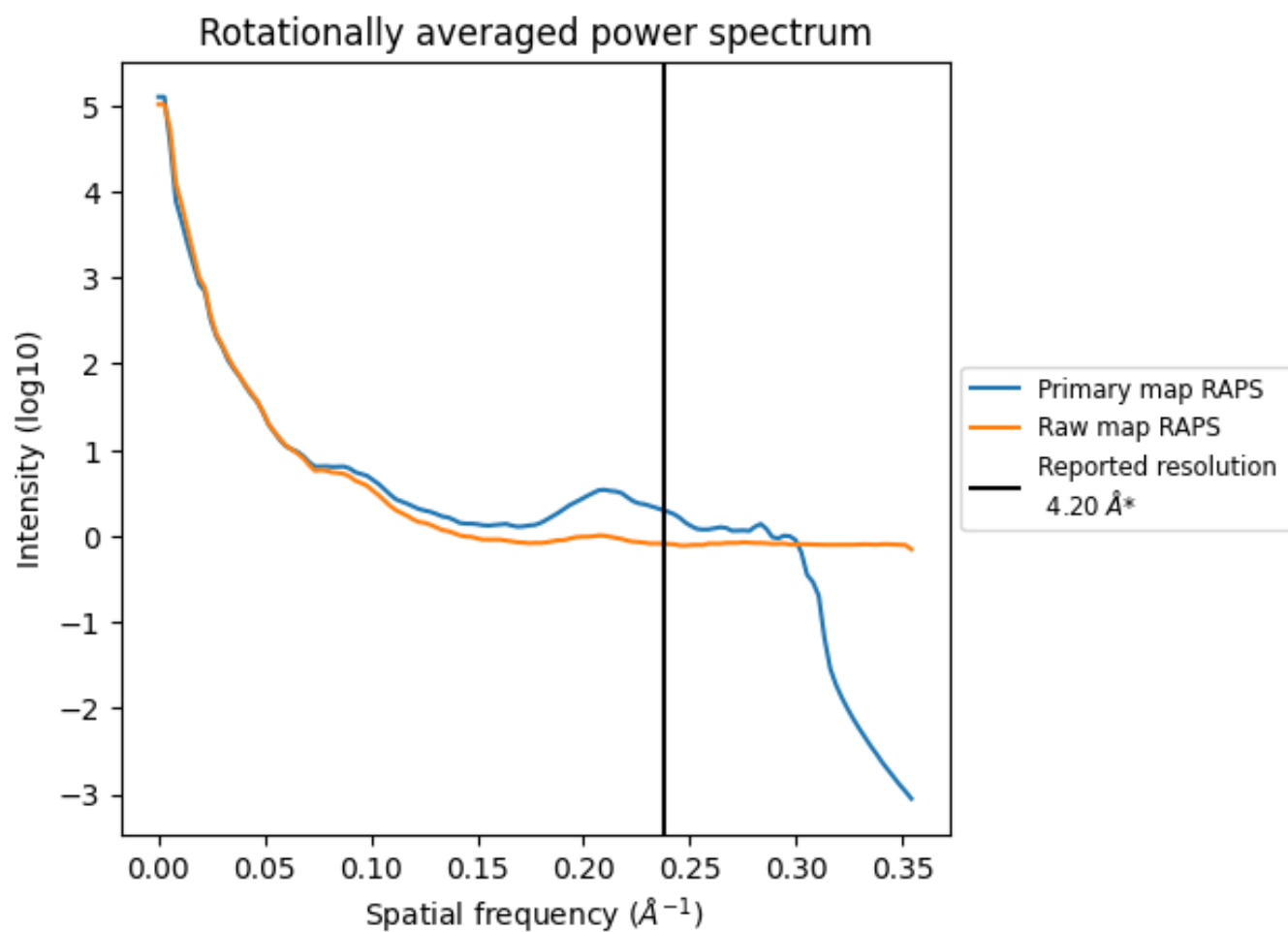
7.2 Volume estimate [\(i\)](#)



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 i

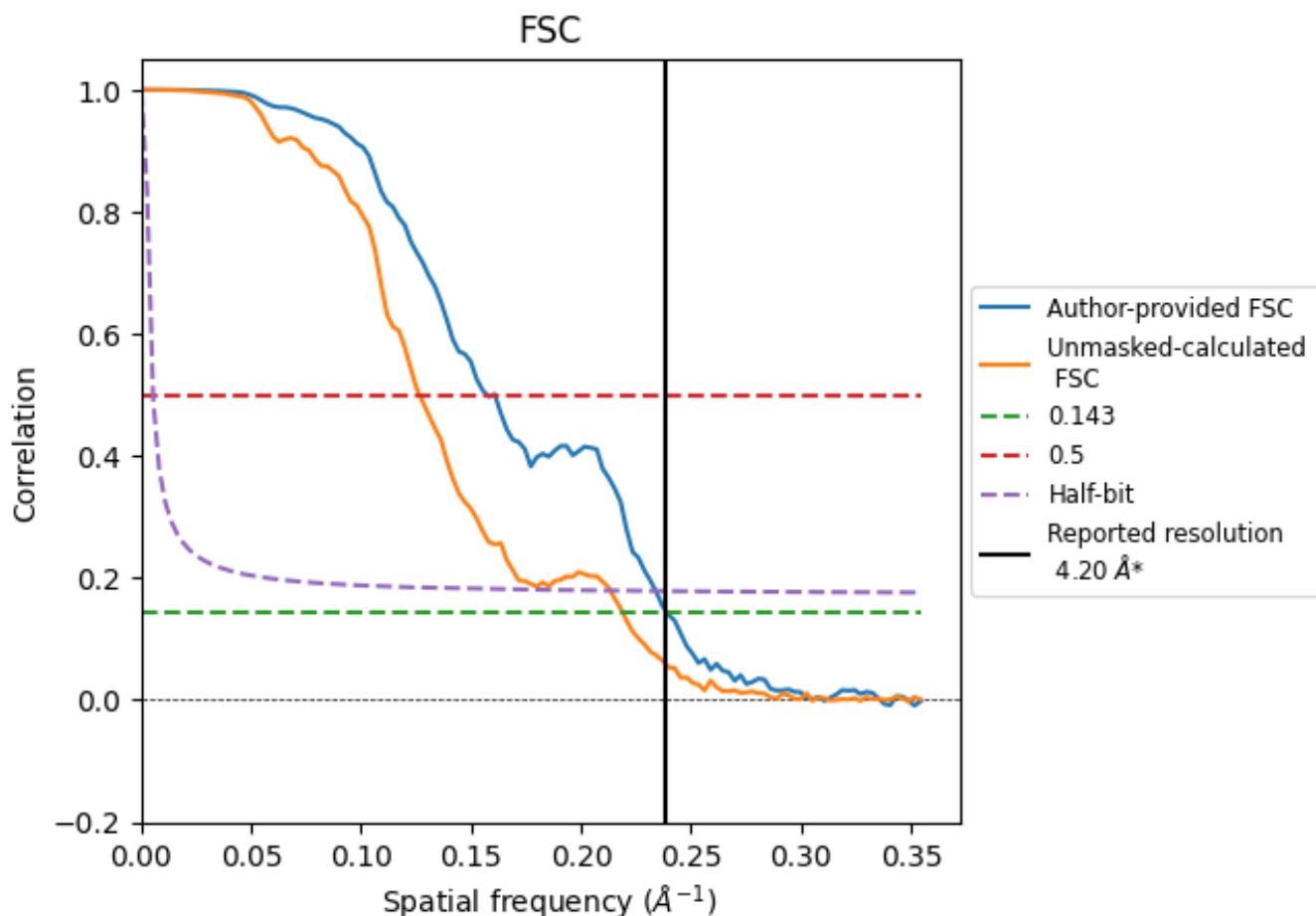


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

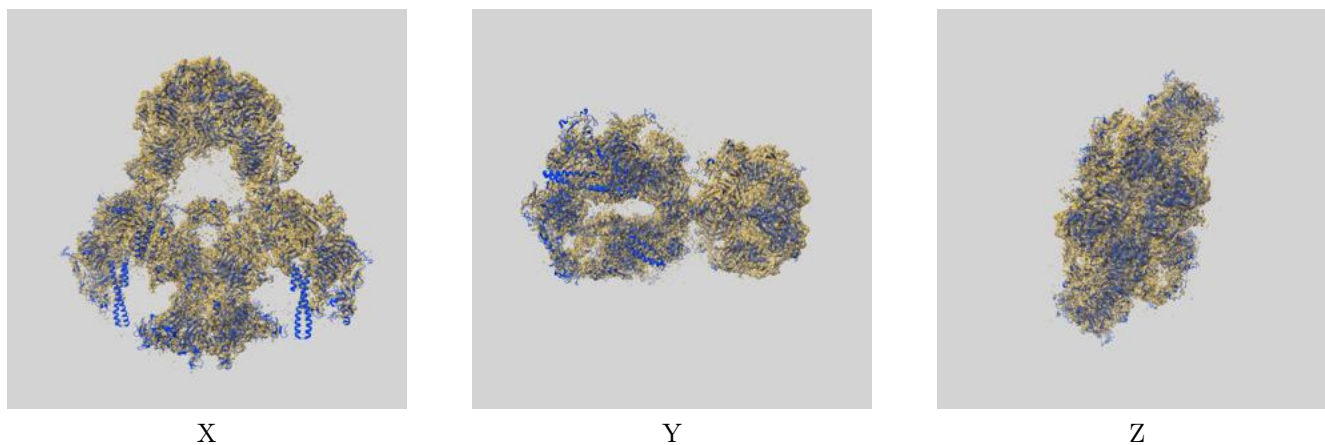
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	6.36	4.27
Unmasked-calculated*	4.57	7.90	4.69

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

9 Map-model fit [i](#)

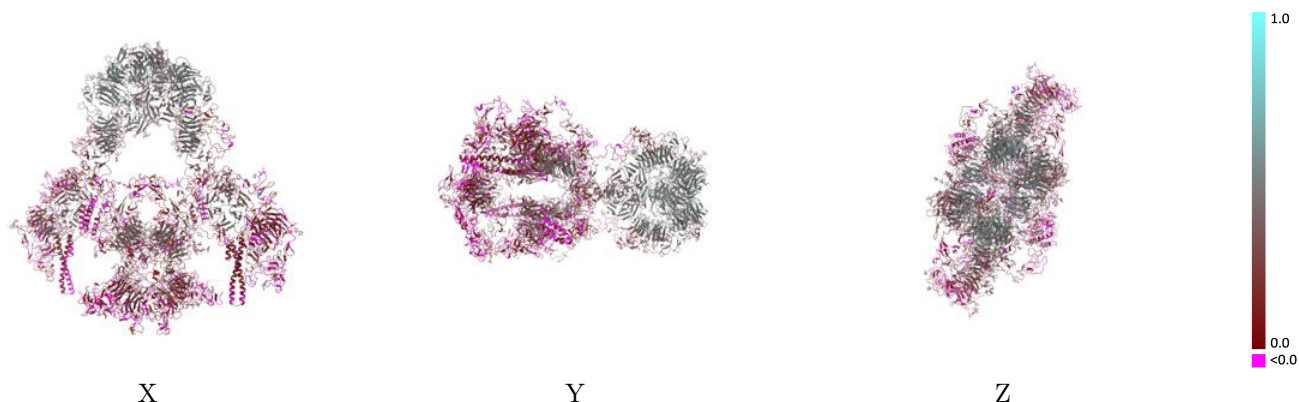
This section contains information regarding the fit between EMDB map EMD-36663 and PDB model 8JUT. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



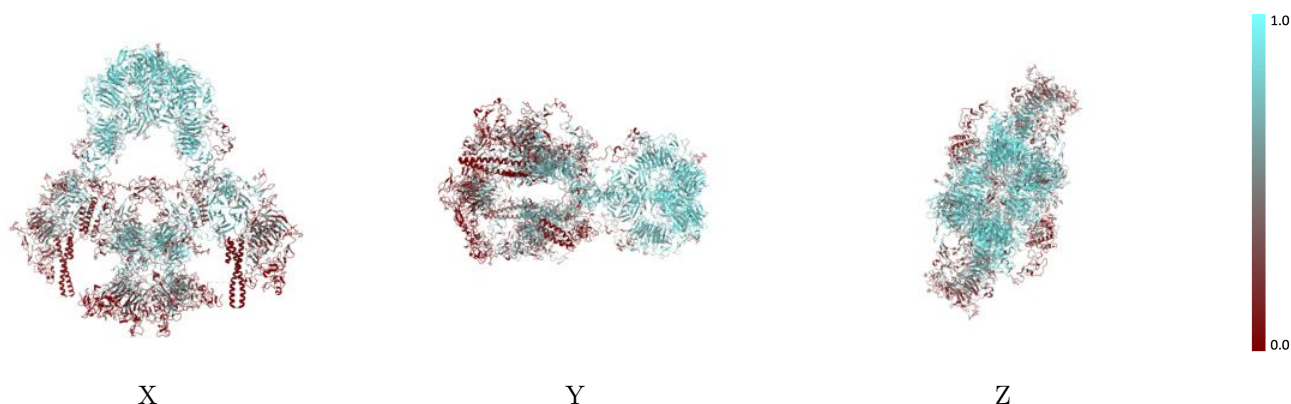
The images above show the 3D surface view of the map at the recommended contour level 0.0242 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



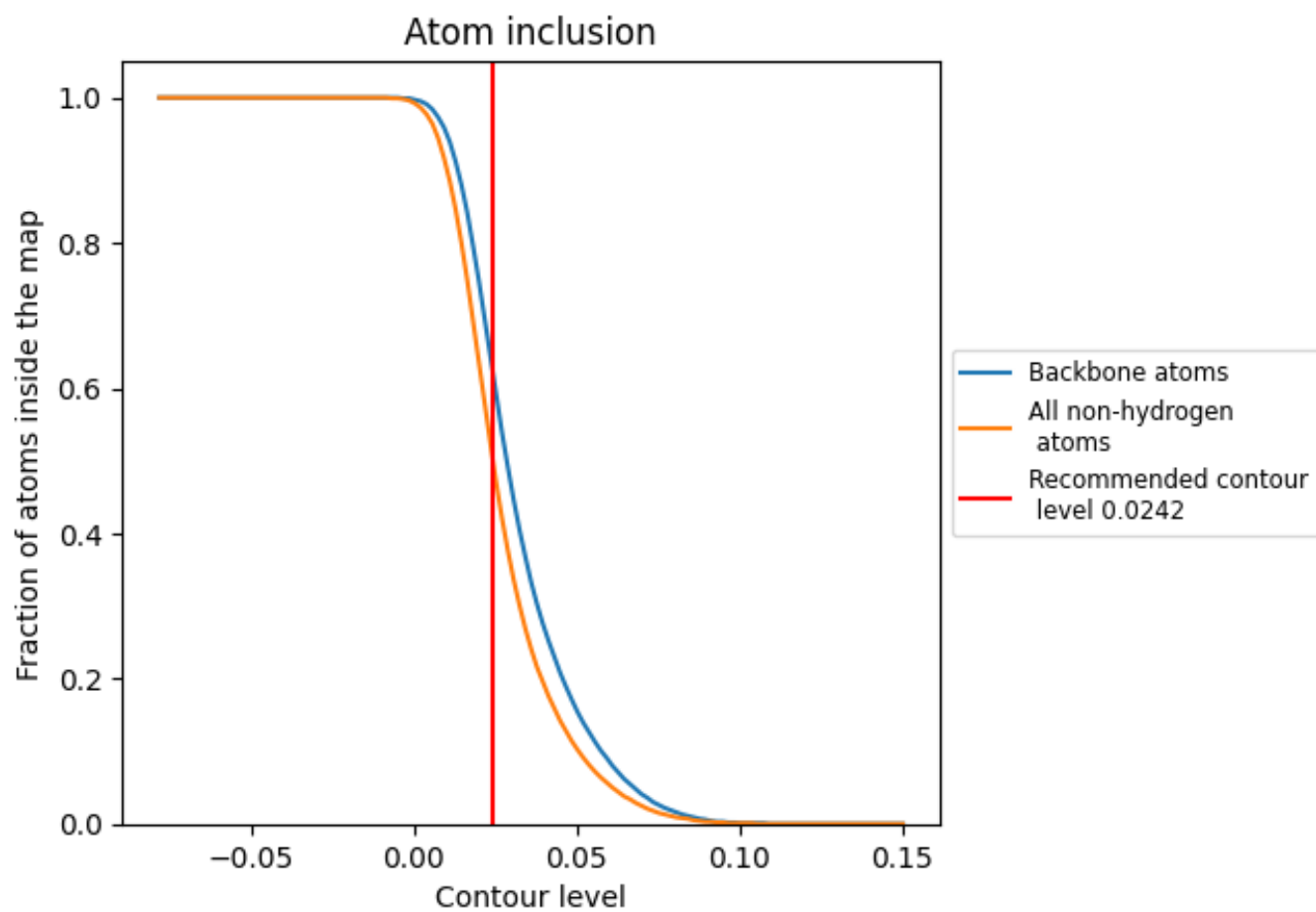
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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