



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:14 AM UTC

PDB ID : 8JUJ / pdb_00008juj
EMDB ID : EMD-36664
Title : rat megalin
Authors : Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.
Deposited on : 2023-06-27
Resolution : 3.80 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

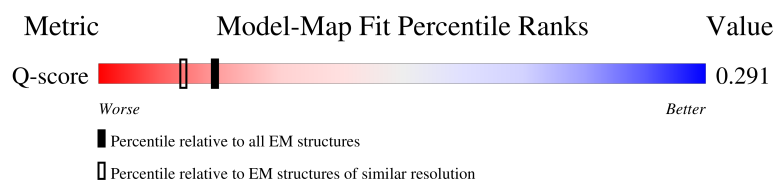
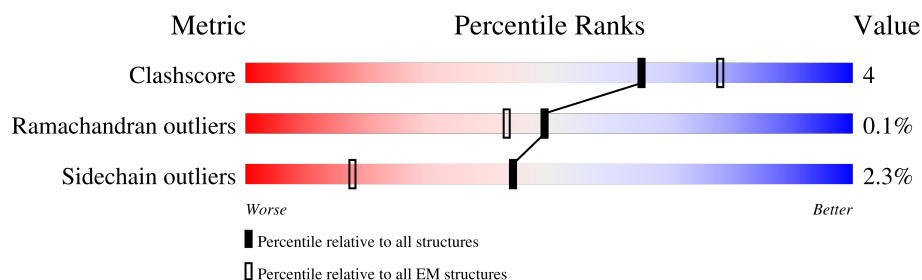
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	A	4660	25% 81% 11% 8%
1	B	4660	25% 82% 10% 8%
2	C	6	83% 17%
2	I	6	83% 17%

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Mol	Chain	Length	Quality of chain
3	D	3	33% 100%
3	J	3	33% 100%
4	G	5	20% 80% 20%
4	K	5	100%
5	H	5	20% 100%
5	L	5	100%
5	O	5	100%
5	R	5	100%
6	M	6	83% 100%
6	P	6	67% 100%
7	N	5	80% 20%
7	Q	5	100%
8	E	3	67% 67% 33%
8	T	3	67% 67% 33%
8	b	3	100% 100%
8	c	3	33% 33% 67%
8	l	3	100% 100%
8	o	3	67% 67% 33%
8	w	3	67% 67% 33%
8	x	3	33% 33% 67%
9	0	2	100% 100%
9	3	2	100% 100%
9	5	2	100% 100%
9	F	2	100%
9	S	2	50% 50% 50%

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Mol	Chain	Length	Quality of chain
9	U	2	50% 50%
9	V	2	50% 100%
9	X	2	50% 50%
9	Z	2	50% 50%
9	a	2	50% 100%
9	e	2	100% 100%
9	f	2	50% 100%
9	i	2	100% 100%
9	k	2	100% 100%
9	m	2	50% 50%
9	n	2	50% 100%
9	p	2	50% 50%
9	q	2	100% 100%
9	s	2	50% 50%
9	u	2	50% 100%
9	v	2	50% 100%
9	z	2	100% 100%
10	1	5	20% 80% 80%
10	2	5	80% 100%
10	W	5	60% 80% 20%
10	Y	5	60% 40%
10	d	5	60% 100%
10	g	5	100% 60% 40%
10	h	5	80% 60% 40%
10	r	5	80% 60% 20% 20%

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Mol	Chain	Length	Quality of chain
10	t	5	60% 40%
10	y	5	40% 60% 40%
11	4	3	100% 67% 33%
11	j	3	100% 100%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 70018 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called LDL receptor related protein 2.

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

- Molecule 2 is a protein called unclear peptide.

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

- Molecule 3 is a protein called unclear peptide.

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

- Molecule 4 is a protein called unclear peptide.

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

- Molecule 5 is a protein called unclear peptide.

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

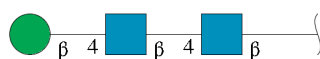
- Molecule 6 is a protein called unclear peptide.

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

- Molecule 7 is a protein called unclear peptide.

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

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	3	Total	C	N	O	0	0
			39	22	2	15		
8	T	3	Total	C	N	O	0	0
			39	22	2	15		
8	b	3	Total	C	N	O	0	0
			39	22	2	15		
8	c	3	Total	C	N	O	0	0
			39	22	2	15		
8	l	3	Total	C	N	O	0	0
			39	22	2	15		

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

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



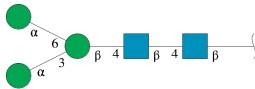
Mol	Chain	Residues	Atoms				AltConf	Trace
9	F	2	Total	C	N	O	0	0
			28	16	2	10		
9	S	2	Total	C	N	O	0	0
			28	16	2	10		
9	U	2	Total	C	N	O	0	0
			28	16	2	10		
9	V	2	Total	C	N	O	0	0
			28	16	2	10		
9	X	2	Total	C	N	O	0	0
			28	16	2	10		
9	Z	2	Total	C	N	O	0	0
			28	16	2	10		
9	a	2	Total	C	N	O	0	0
			28	16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

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	q	2	Total	C	N	O	0	0
			28	16	2	10		
9	s	2	Total	C	N	O	0	0
			28	16	2	10		
9	u	2	Total	C	N	O	0	0
			28	16	2	10		
9	v	2	Total	C	N	O	0	0
			28	16	2	10		
9	z	2	Total	C	N	O	0	0
			28	16	2	10		
9	0	2	Total	C	N	O	0	0
			28	16	2	10		
9	3	2	Total	C	N	O	0	0
			28	16	2	10		
9	5	2	Total	C	N	O	0	0
			28	16	2	10		

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



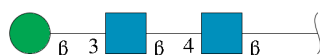
Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	5	Total	C	N	O	0	0
			61	34	2	25		
10	Y	5	Total	C	N	O	0	0
			61	34	2	25		
10	d	5	Total	C	N	O	0	0
			61	34	2	25		
10	g	5	Total	C	N	O	0	0
			61	34	2	25		
10	h	5	Total	C	N	O	0	0
			61	34	2	25		
10	r	5	Total	C	N	O	0	0
			61	34	2	25		
10	t	5	Total	C	N	O	0	0
	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

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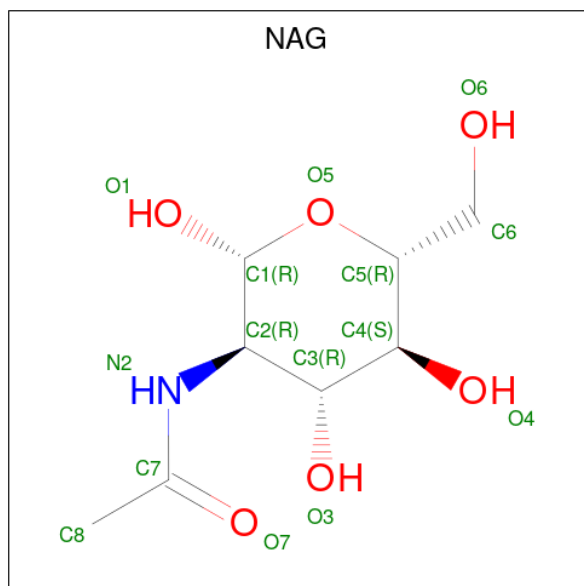
Mol	Chain	Residues	Atoms				AltConf	Trace
10	1	5	Total	C	N	O	0	0
			61	34	2	25		
10	2	5	Total	C	N	O	0	0
			61	34	2	25		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
11	j	3	Total	C	N	O	0	0
			39	22	2	15		
11	4	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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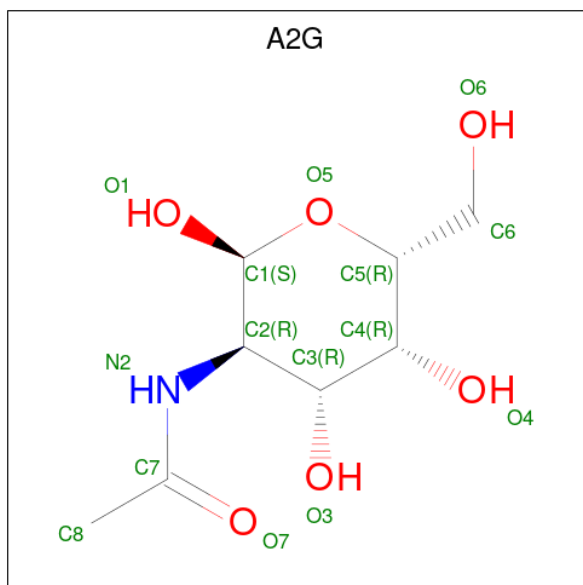
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O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

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

- Molecule 13 is 2-acetamido-2-deoxy- α -D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 14 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

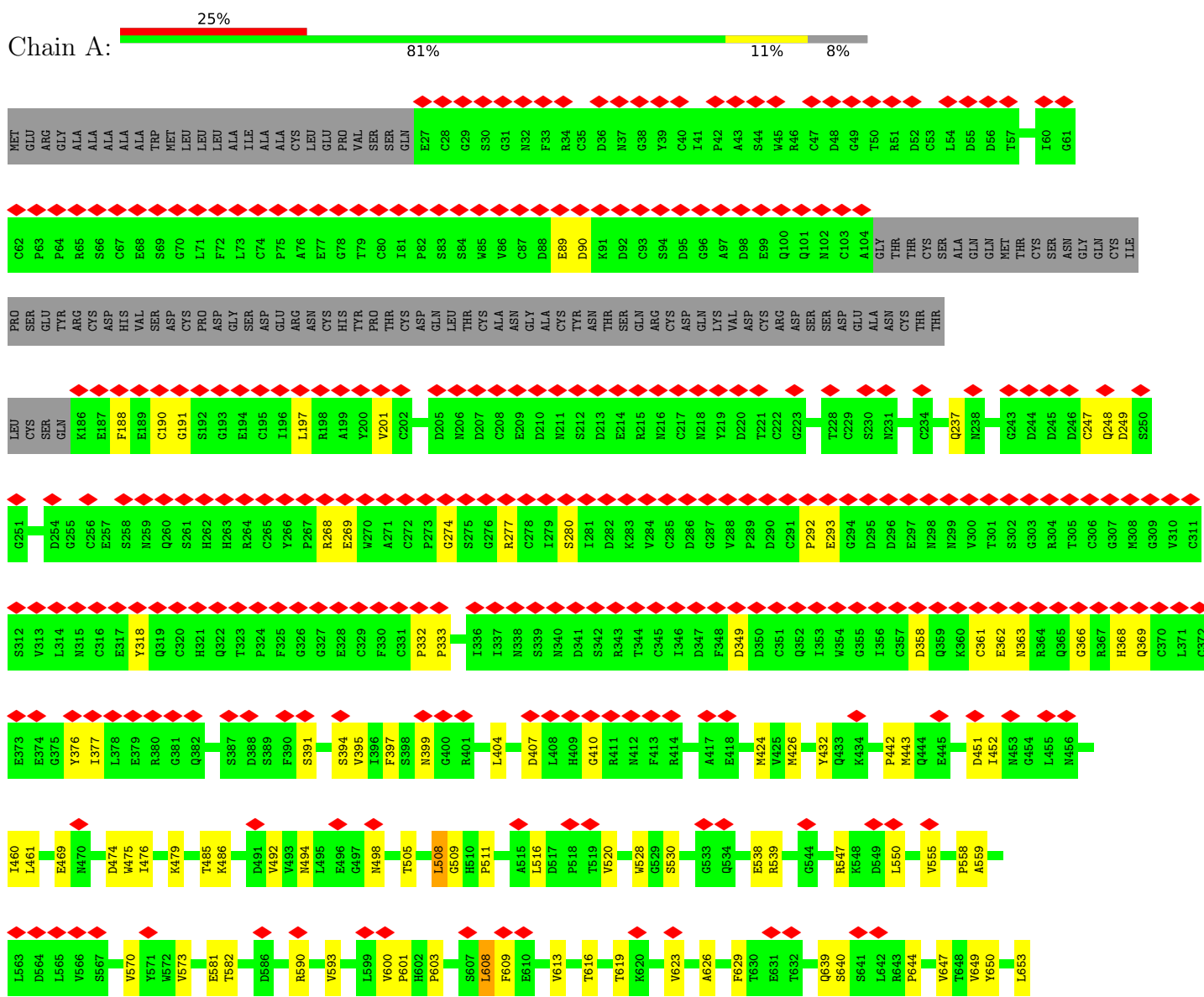
- Molecule 15 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

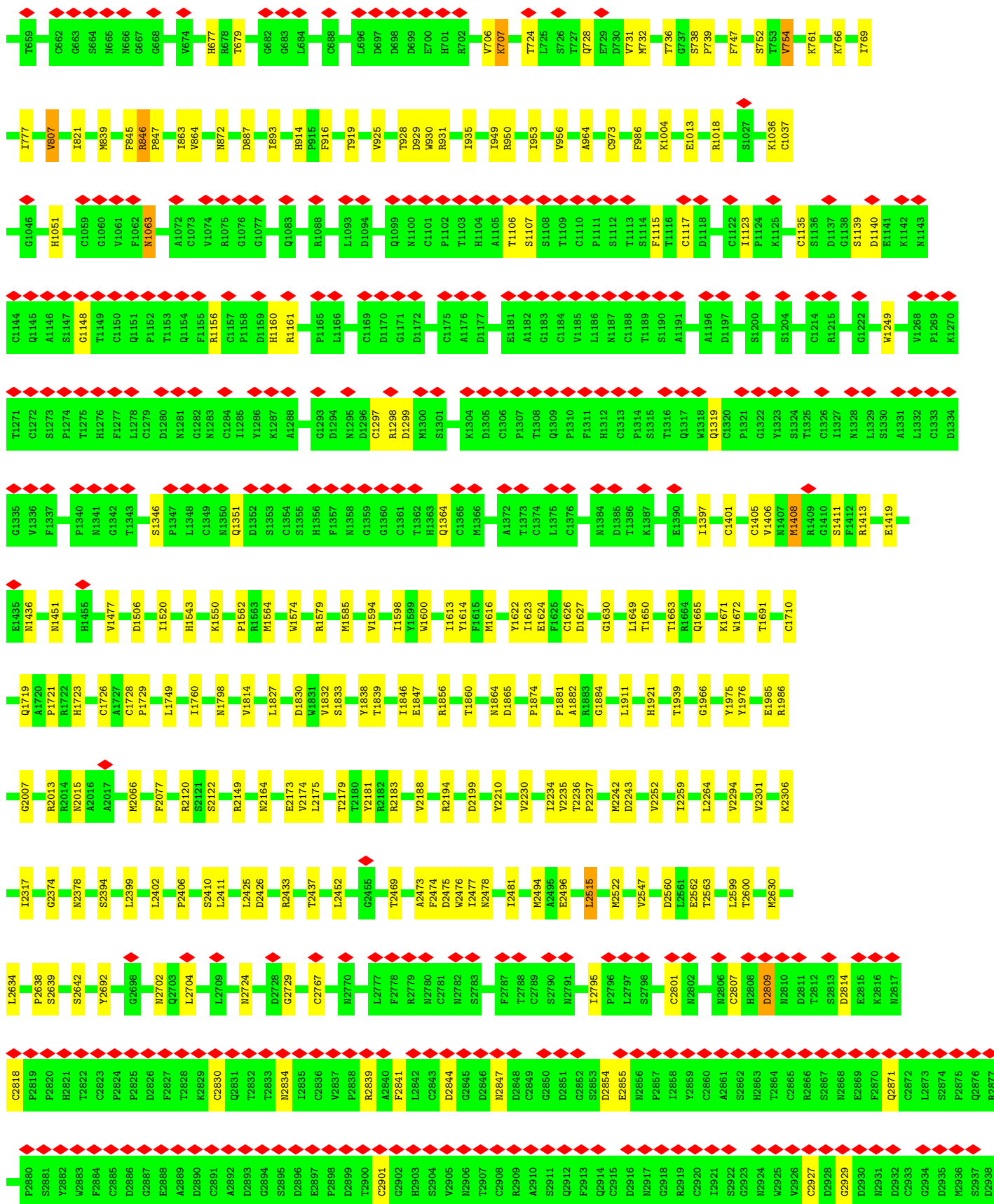
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Ni	0
			1	1	
15	B	1	Total	Ni	0
			1	1	

3 Residue-property plots

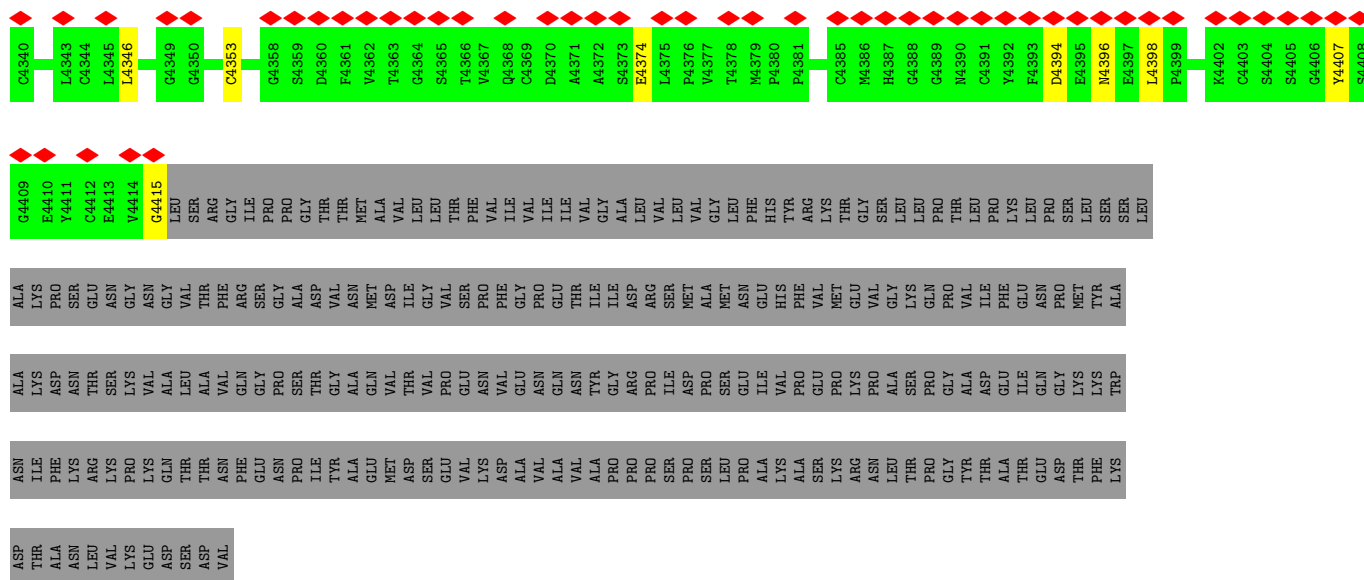
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: LDL receptor related protein 2

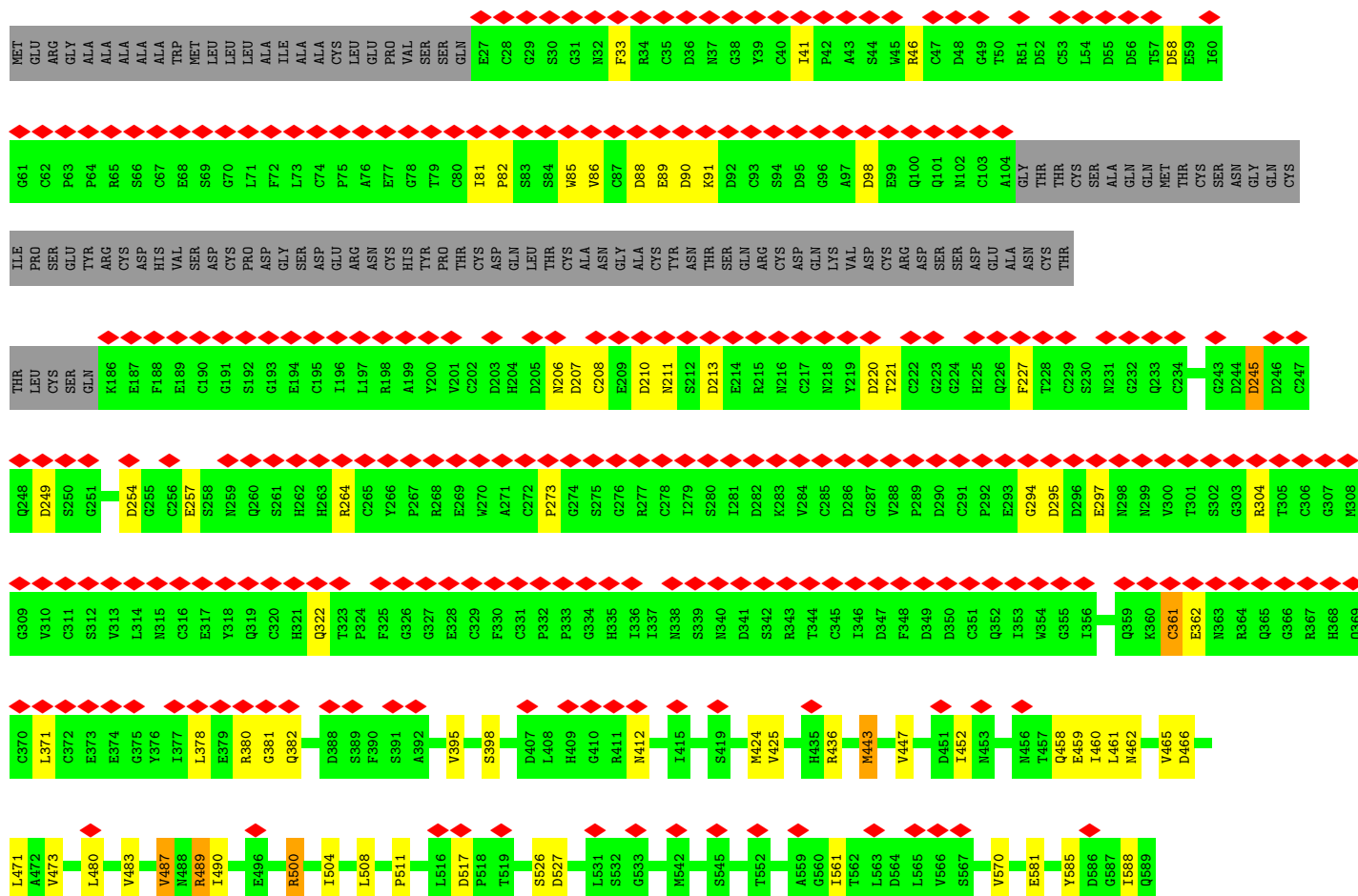
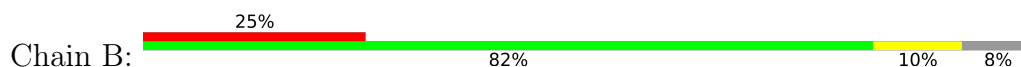


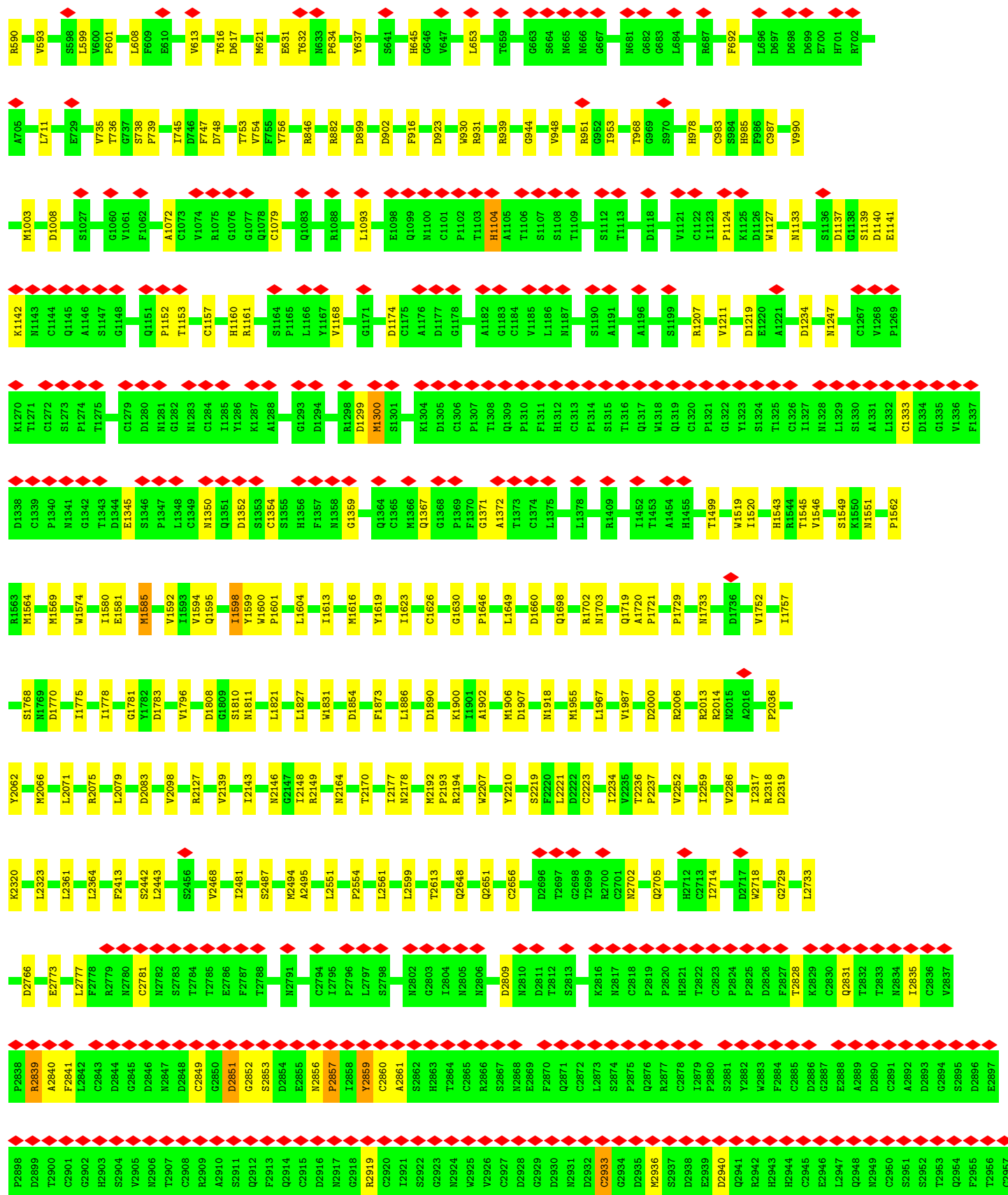


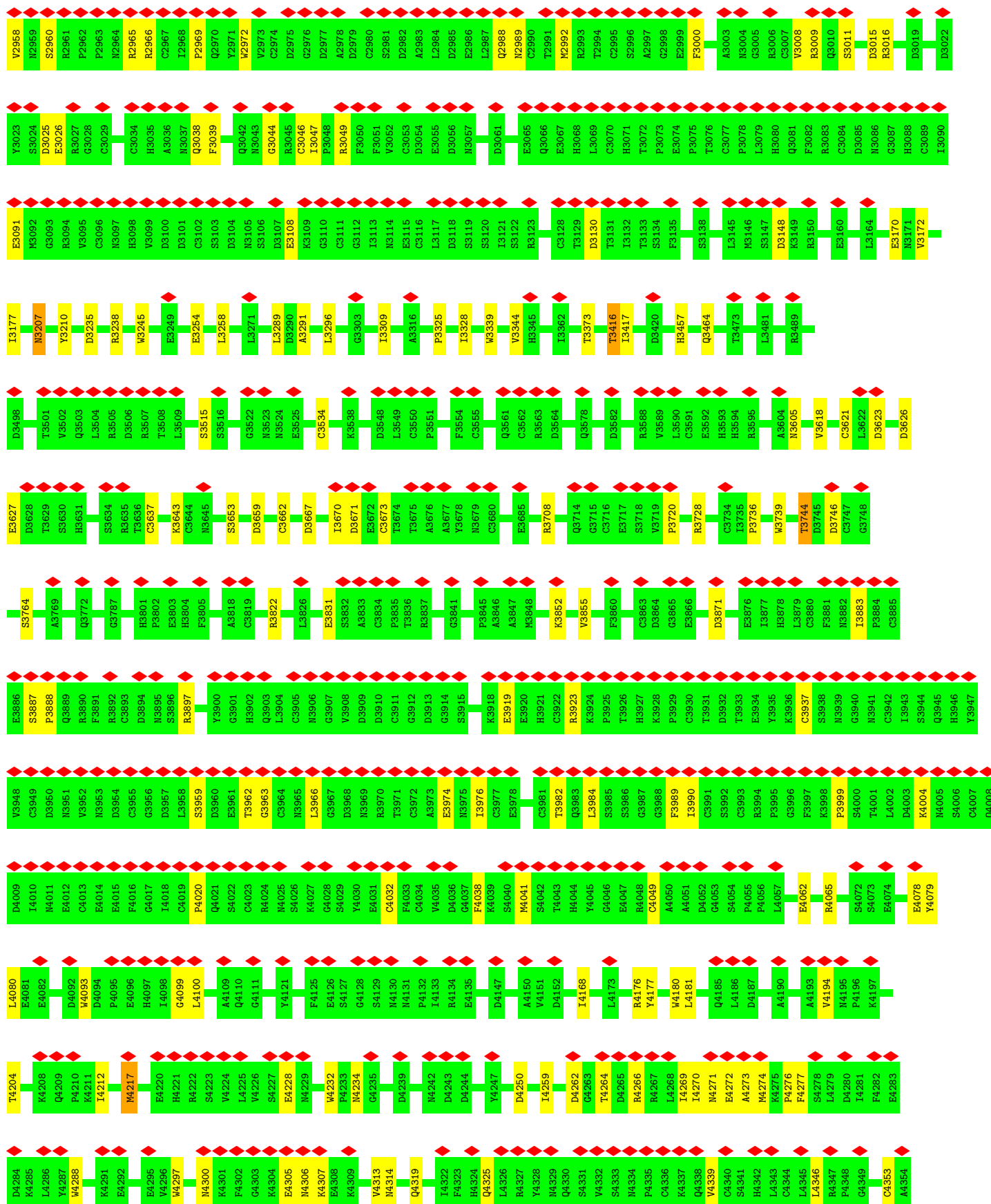
E2939	E2999	F3082	R3150	D3497	C3591	P3720	C3863	F3929	F3989	A4049	A4193	E4272
D2940	F3000	R3083	S3151	D3498	E3592	S3724	E3866	C3930	I3990	A4050	V4194	A4273
Q2941	S3001	C3084	E3160	F3499	C3596	C3741	N3867	T3931	C3991	A4051	K4197	N4274
R2942	A3002	D3085	G3174	Q3500	E3597	N3755	D3871	D3932	S3992	D4052	L4198	K4275
H2943	A3003	N3086	G3174	T3501	S3598	C3756	D3871	T3933	C3993	S4053	G4199	F4277
H2944	N3004	G3087	S3192	V3502	N3599	N3755	D3871	E3934	C3994	N4054	L4200	S4278
C2945	R3005	H3088	F3205	Q3503	A3604	C3766	E3876	Y3935	F3995	N4063	L4203	S4279
E2946	C3007	C3089	F3206	L3504	N3605	S3764	F3877	K3936	G3996	K4068	T4204	D4280
L2947	V3008	I3090	N3206	R3505	R3606	E3765	H3878	C3937	F3997	K4068	K4206	L4281
Q2948	R3009	E3091	N3207	D3506	R3607	F3766	I3879	S3938	C3998	S4073	K4206	F4282
H2949	Q3010	M3092	R3208	R3507	R3607	F3766	L3879	N3939	F3999	E4074	E4286	L4286
C2950	S3011	G3093	Y3209	T3508	Q3614	I3774	C3880	G3940	S4000	F4076	L4286	L4286
S2951	F3012	R3094	Y3210	R3509	Q3614	I3774	C3881	C3941	T4001	K4075	E4286	L4286
S2952	R3013	V3095	I3211	C3510	Q3614	I3774	F3881	N3942	L4002	F4076	E4286	L4286
T2953	R3014	C3096	R3212	M3511	N3619	R3777	N3882	C3943	D4003	E4078	E4286	L4286
Q2954	C3015	N3097	Q3226	R3512	D3620	C3780	I3883	I3943	K4004	E4078	E4286	L4286
F2955	R3016	H3098	G3227	M3513	C3621	Q3781	P3884	S3944	M4005	E4082	E4286	L4286
T2956	R3017	D3100	L3228	M3513	D3623	Q3782	C3885	H3946	S4006	E4083	E4286	L4286
C2957	C3020	D3101	R3242	S3516	N3624	D3791	S3887	Y3947	C4007	I4089	E4286	L4286
V2958	G3021	C3102	H3269	L3520	D3628	E3792	P3888	C3949	Q4008	I4089	E4286	L4286
N2959	D3022	S3103	L3277	C3521	T3629	D3794	Q3889	C3950	D4009	D4092	E4286	L4286
S2960	E3026	D3104	L3277	G3522	S3630	C3795	R3890	N3951	M4011	Y4093	E4286	L4286
R2961	R3027	N3105	D3300	E3525	H3631	M3797	F3991	C3952	E4012	D4094	E4286	L4286
F2962	G3028	S3106	D3315	K3526	S3634	K3798	D3894	D3953	E4013	P4095	E4286	L4286
T2963	C3029	D3107	A3316	C3527	R3635	H3801	N3895	N3954	E4014	E4098	E4286	L4286
N2964	H3035	E3108	N3317	W3532	R3635	P3802	S3896	C3955	E4015	G4099	E4286	L4286
R2965	A3036	K3109	T3319	D3535	F3638	E3803	C3897	G3956	F4016	L4100	E4286	L4286
R2966	F3039	G3111	V3329	G3536	G3647	C3807	C3898	D3957	G4017	G4111	E4286	L4286
C2967	R3049	C3112	T3373	S3541	R3648	H3811	V3900	L3958	C4019	Y4121	E4286	L4286
T2968	F3050	I3113	D3385	D3548	D3667	C3825	H3902	S3959	Q4020	Y4121	E4286	L4286
P2969	F3051	D3118	L3388	L3549	N3660	L3826	Q3903	D3960	Q4021	G4128	E4286	L4286
D2970	V3052	S3119	L3388	C3550	D3661	D3827	C3905	E3961	S4022	S4129	E4286	L4286
C2974	C3053	S3120	F3413	R3553	C3662	S3832	N3906	T3962	C4023	N4130	E4286	L4286
D2975	D3054	I3121	A3414	F3554	D3671	A3833	C3907	C3963	R4024	N4131	E4286	L4286
D2976	E3055	S3122	L3415	C3555	N3679	C3834	V3908	C3964	M4025	P4132	E4286	L4286
A2978	D3064	R3123	T3416	R3556	N3679	A3833	D3909	N3965	S4026	I4133	E4286	L4286
D2979	E3065	C3124	T3425	L3557	K3689	T3836	D3909	L3966	K4027	R4134	E4286	L4286
C2980	E3067	T3129	D3426	G3558	T3690	T3836	D3910	G3967	G4028	D4137	E4286	L4286
S2981	H3068	D3130	W3427	P3453	N3691	R3837	C3911	D3968	S4029	E4137	E4286	L4286
D2982	L3069	T3131	P3453	A3576	R3692	P3839	D3913	N3969	E4031	A4149	E4286	L4286
L2983	H3071	T3132	G3477	A3576	R3693	P3839	C3914	T3970	F4032	A4150	E4286	L4286
D2985	C3070	T3133	R3459	R3577	R3693	P3839	S3915	C3972	F4033	V4151	E4286	L4286
E2986	P3073	S3134	A3494	Q3578	N3710	A3847	D3916	A3973	C4034	I4168	E4286	L4286
L2987	E3074	S3134	A3494	A3581	Q3714	K3852	E3917	N3975	D4036	R4176	E4286	L4286
Q2988	P3075	L3140	A3494	D3582	S3718	N3853	C3918	I3976	F4037	L4181	E4286	L4286
N2989	C3076	P3141	A3494	D3582	S3718	H3854	K3918	C3977	P4038	D4187	E4286	L4286
C2990	P3078	L3145	A3494	R3588	V3719	H3854	E3920	C3978	K4039	N4187	E4286	L4286
T2991	P3078	M3146	A3494	V3589	S3719	H3854	E3921	Q3979	S4040	A4191	E4286	L4286
H2992	H3080	S3147	A3494	L3590	S3719	H3854	C3922	N3980	M4041	I4192	E4286	L4286
C2995	Q3081	D3148	A3494	L3590	S3719	H3854	C3923	T3981	S4042	T4043	E4286	L4286
A2997		K3149	A3494	L3590	S3719	H3854	K3924	C3983	H4044	L4192	E4286	L4286
Q2998			A3494	L3590	S3719	H3854	T3926	L3984	Y4045		E4286	L4286

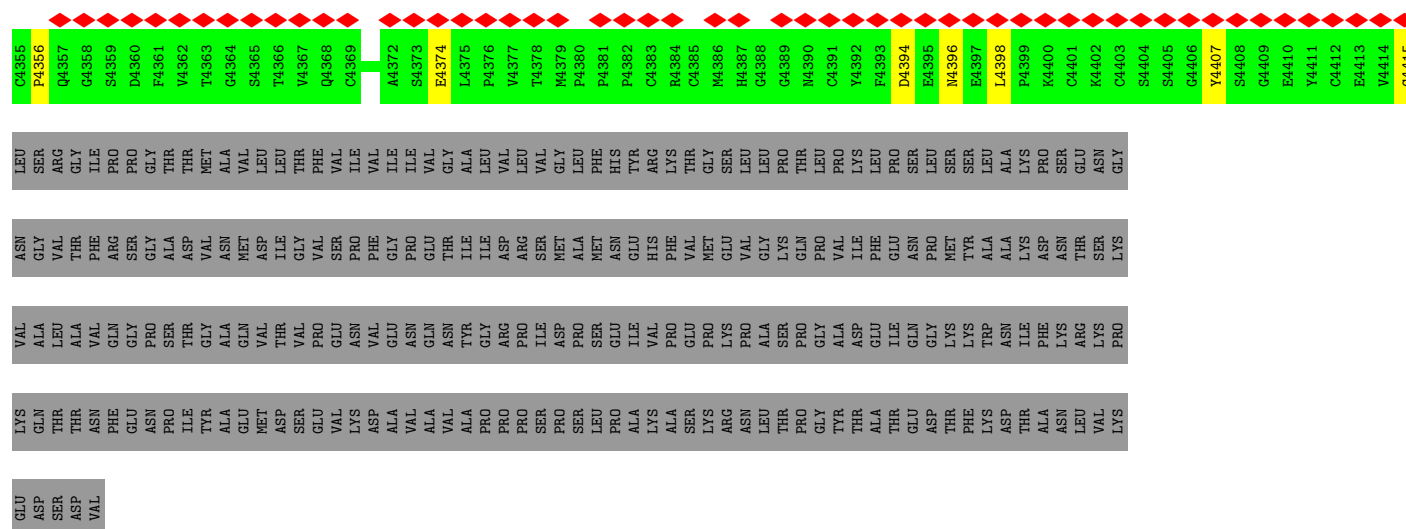


• Molecule 1: LDL receptor related protein 2

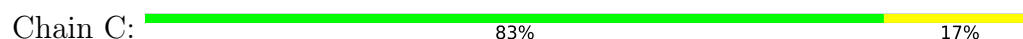




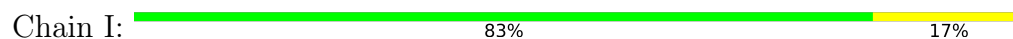




- Molecule 2: unclear peptide



- Molecule 2: unclear peptide



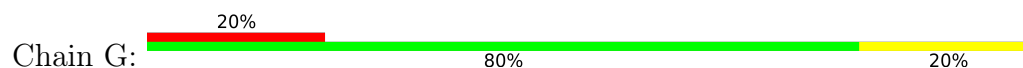
- Molecule 3: unclear peptide



- Molecule 3: unclear peptide



- Molecule 4: unclear peptide





- Molecule 4: unclear peptide

Chain K: 100%

There are no outlier residues recorded for this chain.

- Molecule 5: unclear peptide

Chain H: 20% 100%



- Molecule 5: unclear peptide

Chain L: 100%

There are no outlier residues recorded for this chain.

- Molecule 5: unclear peptide

Chain O: 100%

There are no outlier residues recorded for this chain.

- Molecule 5: unclear peptide

Chain R: 100%

There are no outlier residues recorded for this chain.

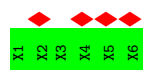
- Molecule 6: unclear peptide

Chain M: 83% 100%



- Molecule 6: unclear peptide

Chain P: 67% 100%

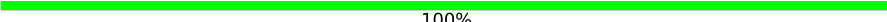


- Molecule 7: unclear peptide

Chain N:  80% 20%



- Molecule 7: unclear peptide

Chain Q:  100%

There are no outlier residues recorded for this chain.

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

Chain E:  67% 67% 33%



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

Chain T:  67% 67% 33%



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

Chain b:  100% 100%

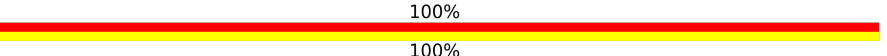


- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  33% 33% 67%



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

Chain l:  100% 100%



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



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



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



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



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



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





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



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



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



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



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



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





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



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



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



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



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



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





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



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



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



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



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



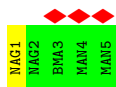
- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



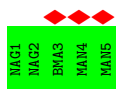
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

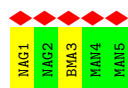


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

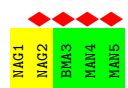
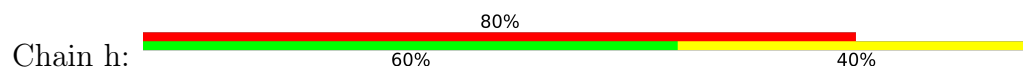


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

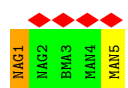




- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



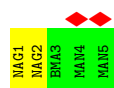
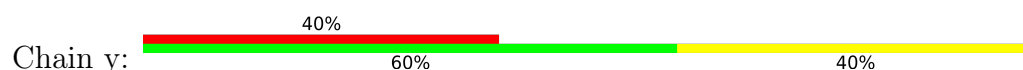
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



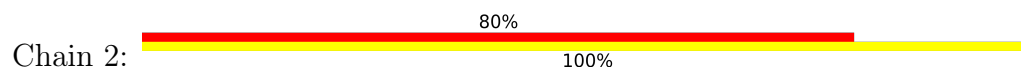
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	101096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.214	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	1.411, 1.411, 1.411	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/34456	0.80	13/46804 (0.0%)
1	B	0.94	0/34456	0.96	14/46804 (0.0%)
2	C	0.63	0/7	0.91	0/8
2	I	0.64	0/7	1.15	0/8
3	D	1.27	0/5	0.88	0/5
3	J	1.00	0/5	0.70	0/5
4	G	0.79	0/17	0.83	0/21
4	K	0.86	0/17	0.85	0/21
5	H	0.91	0/7	0.74	0/8
5	L	0.90	0/7	1.01	0/8
5	O	0.78	0/7	0.85	0/8
5	R	0.71	0/7	0.81	0/8
7	N	1.00	0/7	1.84	0/8
7	Q	0.54	0/7	1.94	0/8
All	All	0.76	0/69012	0.88	27/93724 (0.0%)

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

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

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3916	ASP	CA-CB-CG	8.63	121.23	112.60
1	A	3300	ASP	CA-CB-CG	7.96	120.56	112.60
1	A	3315	ASP	CA-CB-CG	7.83	120.43	112.60
1	A	986	PHE	CA-CB-CG	7.32	121.12	113.80
1	B	923	ASP	CA-CB-CG	6.67	119.27	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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	31027	279	0
1	B	33638	0	31025	254	0
2	C	33	0	18	3	0
2	I	33	0	18	4	0
3	D	16	0	8	0	0
3	J	16	0	8	0	0
4	G	33	0	19	1	0
4	K	33	0	18	0	0
5	H	28	0	13	0	0
5	L	28	0	12	0	0
5	O	28	0	12	0	0
5	R	28	0	12	0	0
6	M	30	0	8	0	0
6	P	30	0	8	0	0
7	N	28	0	12	3	0
7	Q	28	0	12	0	0
8	E	39	0	34	0	0
8	T	39	0	34	0	0
8	b	39	0	34	0	0
8	c	39	0	34	1	0
8	l	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	o	39	0	34	1	0
8	w	39	0	34	0	0
8	x	39	0	34	0	0
9	0	28	0	25	0	0
9	3	28	0	25	0	0
9	5	28	0	25	0	0
9	F	28	0	25	0	0
9	S	28	0	25	0	0
9	U	28	0	25	1	0
9	V	28	0	25	0	0
9	X	28	0	25	0	0
9	Z	28	0	25	0	0
9	a	28	0	25	0	0
9	e	28	0	25	0	0
9	f	28	0	25	0	0
9	i	28	0	25	0	0
9	k	28	0	25	0	0
9	m	28	0	25	0	0
9	n	28	0	25	0	0
9	p	28	0	25	1	0
9	q	28	0	25	0	0
9	s	28	0	25	1	0
9	u	28	0	25	0	0
9	v	28	0	25	0	0
9	z	28	0	25	0	0
10	1	61	0	52	0	0
10	2	61	0	52	0	0
10	W	61	0	52	0	0
10	Y	61	0	52	1	0
10	d	61	0	52	0	0
10	g	61	0	52	0	0
10	h	61	0	52	0	0
10	r	61	0	52	1	0
10	t	61	0	52	1	0
10	y	61	0	52	1	0
11	4	39	0	34	0	0
11	j	39	0	34	0	0
12	A	168	0	156	0	0
12	B	168	0	156	1	0
13	A	154	0	132	0	0
13	B	154	0	132	0	0
14	A	44	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	B	44	0	0	0	0
15	A	1	0	0	0	0
15	B	1	0	0	0	0
All	All	70018	0	64216	534	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 534 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:3852:LYS:NZ	1:B:3871:ASP:OD2	2.15	0.80
1:B:1616:MET:HE3	1:B:1646:PRO:HB2	1.65	0.78
1:A:426:MET:HB2	1:A:442:PRO:HD3	1.66	0.77
1:A:3621:CYS:O	1:A:3622:LEU:HG	1.86	0.75
1:A:460:ILE:HG22	1:A:461:LEU:HG	1.69	0.74

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%)	3970 (92%)	332 (8%)	2 (0%)	100	100
1	B	4304/4660 (92%)	3979 (92%)	322 (8%)	3 (0%)	48	79
2	C	1/6 (17%)	1 (100%)	0	0	100	100
2	I	1/6 (17%)	1 (100%)	0	0	100	100
3	D	1/3 (33%)	1 (100%)	0	0	100	100
3	J	1/3 (33%)	0	1 (100%)	0	100	100
4	G	2/5 (40%)	0	2 (100%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
5	H	1/5 (20%)	1 (100%)	0	0	100	100
5	L	1/5 (20%)	1 (100%)	0	0	100	100
5	O	1/5 (20%)	0	1 (100%)	0	100	100
5	R	1/5 (20%)	1 (100%)	0	0	100	100
7	N	1/5 (20%)	1 (100%)	0	0	100	100
7	Q	1/5 (20%)	1 (100%)	0	0	100	100
All	All	8622/9378 (92%)	7958 (92%)	659 (8%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3791/4089 (93%)	3698 (98%)	93 (2%)	42	61
1	B	3791/4089 (93%)	3710 (98%)	81 (2%)	47	64
2	C	1/1 (100%)	1 (100%)	0	100	100
2	I	1/1 (100%)	1 (100%)	0	100	100
3	D	1/1 (100%)	1 (100%)	0	100	100
3	J	1/1 (100%)	1 (100%)	0	100	100
4	G	2/2 (100%)	2 (100%)	0	100	100
4	K	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	H	1/1 (100%)	1 (100%)	0	100	100
5	L	1/1 (100%)	1 (100%)	0	100	100
5	O	1/1 (100%)	1 (100%)	0	100	100
5	R	1/1 (100%)	1 (100%)	0	100	100
7	N	1/1 (100%)	1 (100%)	0	100	100
7	Q	1/1 (100%)	1 (100%)	0	100	100
All	All	7596/8192 (93%)	7422 (98%)	174 (2%)	44	63

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	978	HIS
1	B	2859	TYR
1	B	1153	THR
1	B	2127	ARG
1	B	3207	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1133	ASN
1	B	2595	HIS
1	B	1543	HIS
1	B	2026	ASN
1	B	2954	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

124 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	NAG	0	1	9,1	14,14,15	0.40	0	17,19,21	0.54	0
9	NAG	0	2	9	14,14,15	0.41	0	17,19,21	0.60	0
10	NAG	1	1	10,1	14,14,15	0.47	0	17,19,21	0.69	0
10	NAG	1	2	10	14,14,15	0.59	0	17,19,21	0.98	1 (5%)
10	BMA	1	3	10	11,11,12	1.01	1 (9%)	15,15,17	1.07	1 (6%)
10	MAN	1	4	10	11,11,12	0.95	1 (9%)	15,15,17	0.93	2 (13%)
10	MAN	1	5	10	11,11,12	0.81	1 (9%)	15,15,17	0.80	1 (6%)
10	NAG	2	1	10,1	14,14,15	0.53	0	17,19,21	1.04	1 (5%)
10	NAG	2	2	10	14,14,15	0.60	0	17,19,21	0.80	1 (5%)
10	BMA	2	3	10	11,11,12	1.13	1 (9%)	15,15,17	1.17	2 (13%)
10	MAN	2	4	10	11,11,12	0.90	1 (9%)	15,15,17	0.80	1 (6%)
10	MAN	2	5	10	11,11,12	0.81	0	15,15,17	1.17	2 (13%)
9	NAG	3	1	9,1	14,14,15	0.41	0	17,19,21	0.53	0
9	NAG	3	2	9	14,14,15	0.40	0	17,19,21	0.55	0
11	NAG	4	1	11,1	14,14,15	0.42	0	17,19,21	0.42	0
11	NAG	4	2	11	14,14,15	0.40	0	17,19,21	0.46	0
11	BMA	4	3	11	11,11,12	0.81	1 (9%)	15,15,17	0.75	1 (6%)
9	NAG	5	1	9,1	14,14,15	0.57	0	17,19,21	0.82	1 (5%)
9	NAG	5	2	9	14,14,15	0.59	0	17,19,21	0.89	1 (5%)
8	NAG	E	1	1,8	14,14,15	0.39	0	17,19,21	0.49	0
8	NAG	E	2	8	14,14,15	0.42	0	17,19,21	0.88	1 (5%)
8	BMA	E	3	8	11,11,12	0.22	0	15,15,17	0.51	0
9	NAG	F	1	9,1	14,14,15	0.40	0	17,19,21	0.40	0
9	NAG	F	2	9	14,14,15	0.40	0	17,19,21	0.36	0
9	NAG	S	1	9,1	14,14,15	0.42	0	17,19,21	0.56	0
9	NAG	S	2	9	14,14,15	0.42	0	17,19,21	0.86	1 (5%)
8	NAG	T	1	1,8	14,14,15	0.37	0	17,19,21	0.65	0
8	NAG	T	2	8	14,14,15	0.51	0	17,19,21	0.75	1 (5%)
8	BMA	T	3	8	11,11,12	0.26	0	15,15,17	0.56	0
9	NAG	U	1	9,1	14,14,15	0.42	0	17,19,21	0.45	0
9	NAG	U	2	9	14,14,15	0.39	0	17,19,21	0.43	0
9	NAG	V	1	9,1	14,14,15	0.64	0	17,19,21	1.11	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	V	2	9	14,14,15	0.65	0	17,19,21	1.10	1 (5%)
10	NAG	W	1	10,1	14,14,15	0.40	0	17,19,21	1.01	2 (11%)
10	NAG	W	2	10	14,14,15	0.40	0	17,19,21	0.55	0
10	BMA	W	3	10	11,11,12	0.28	0	15,15,17	0.72	0
10	MAN	W	4	10	11,11,12	0.23	0	15,15,17	0.45	0
10	MAN	W	5	10	11,11,12	0.29	0	15,15,17	0.47	0
9	NAG	X	1	9,1	14,14,15	0.38	0	17,19,21	0.46	0
9	NAG	X	2	9	14,14,15	0.40	0	17,19,21	0.80	2 (11%)
10	NAG	Y	1	10,1	14,14,15	0.46	0	17,19,21	0.66	0
10	NAG	Y	2	10	14,14,15	0.41	0	17,19,21	0.64	0
10	BMA	Y	3	10	11,11,12	0.37	0	15,15,17	0.53	0
10	MAN	Y	4	10	11,11,12	0.21	0	15,15,17	0.48	0
10	MAN	Y	5	10	11,11,12	0.30	0	15,15,17	0.48	0
9	NAG	Z	1	9,1	14,14,15	0.40	0	17,19,21	0.51	0
9	NAG	Z	2	9	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
9	NAG	a	1	9,1	14,14,15	0.38	0	17,19,21	0.44	0
9	NAG	a	2	9	14,14,15	0.40	0	17,19,21	0.51	0
8	NAG	b	1	1,8	14,14,15	0.43	0	17,19,21	0.46	0
8	NAG	b	2	8	14,14,15	0.39	0	17,19,21	0.40	0
8	BMA	b	3	8	11,11,12	0.21	0	15,15,17	0.52	0
8	NAG	c	1	1,8	14,14,15	0.46	0	17,19,21	0.59	0
8	NAG	c	2	8	14,14,15	0.43	0	17,19,21	0.60	0
8	BMA	c	3	8	11,11,12	0.28	0	15,15,17	0.51	0
10	NAG	d	1	10,1	14,14,15	0.44	0	17,19,21	0.44	0
10	NAG	d	2	10	14,14,15	0.39	0	17,19,21	0.43	0
10	BMA	d	3	10	11,11,12	0.27	0	15,15,17	0.67	0
10	MAN	d	4	10	11,11,12	0.25	0	15,15,17	0.51	0
10	MAN	d	5	10	11,11,12	0.27	0	15,15,17	0.47	0
9	NAG	e	1	9,1	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
9	NAG	e	2	9	14,14,15	0.58	0	17,19,21	0.94	1 (5%)
9	NAG	f	1	9,1	14,14,15	0.43	0	17,19,21	0.40	0
9	NAG	f	2	9	14,14,15	0.41	0	17,19,21	0.50	0
10	NAG	g	1	10,1	14,14,15	0.52	0	17,19,21	1.36	2 (11%)
10	NAG	g	2	10	14,14,15	0.44	0	17,19,21	0.42	0
10	BMA	g	3	10	11,11,12	0.25	0	15,15,17	0.68	1 (6%)
10	MAN	g	4	10	11,11,12	0.28	0	15,15,17	0.47	0
10	MAN	g	5	10	11,11,12	0.30	0	15,15,17	0.42	0
10	NAG	h	1	10,1	14,14,15	0.48	0	17,19,21	1.16	1 (5%)
10	NAG	h	2	10	14,14,15	0.51	0	17,19,21	0.77	1 (5%)
10	BMA	h	3	10	11,11,12	0.38	0	15,15,17	0.66	0
10	MAN	h	4	10	11,11,12	0.31	0	15,15,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	h	5	10	11,11,12	0.31	0	15,15,17	0.46	0
9	NAG	i	1	9,1	14,14,15	0.41	0	17,19,21	0.57	0
9	NAG	i	2	9	14,14,15	0.42	0	17,19,21	0.55	0
11	NAG	j	1	11,1	14,14,15	0.40	0	17,19,21	0.39	0
11	NAG	j	2	11	14,14,15	0.41	0	17,19,21	0.46	0
11	BMA	j	3	11	11,11,12	0.28	0	15,15,17	0.46	0
9	NAG	k	1	9,1	14,14,15	0.65	0	17,19,21	1.15	2 (11%)
9	NAG	k	2	9	14,14,15	0.71	0	17,19,21	1.33	2 (11%)
8	NAG	l	1	1,8	14,14,15	0.52	0	17,19,21	1.01	1 (5%)
8	NAG	l	2	8	14,14,15	0.59	0	17,19,21	0.75	1 (5%)
8	BMA	l	3	8	11,11,12	0.85	1 (9%)	15,15,17	0.96	1 (6%)
9	NAG	m	1	9,1	14,14,15	0.49	0	17,19,21	0.85	0
9	NAG	m	2	9	14,14,15	0.56	0	17,19,21	0.88	1 (5%)
9	NAG	n	1	9,1	14,14,15	0.56	0	17,19,21	0.93	2 (11%)
9	NAG	n	2	9	14,14,15	0.59	0	17,19,21	0.90	1 (5%)
8	NAG	o	1	1,8	14,14,15	0.43	0	17,19,21	0.56	0
8	NAG	o	2	8	14,14,15	0.42	0	17,19,21	0.42	0
8	BMA	o	3	8	11,11,12	0.28	0	15,15,17	0.60	0
9	NAG	p	1	9,1	14,14,15	0.38	0	17,19,21	0.82	1 (5%)
9	NAG	p	2	9	14,14,15	0.42	0	17,19,21	0.55	0
9	NAG	q	1	9,1	14,14,15	0.40	0	17,19,21	0.59	0
9	NAG	q	2	9	14,14,15	0.41	0	17,19,21	0.38	0
10	NAG	r	1	10,1	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
10	NAG	r	2	10	14,14,15	0.43	0	17,19,21	0.67	0
10	BMA	r	3	10	11,11,12	0.29	0	15,15,17	0.63	0
10	MAN	r	4	10	11,11,12	0.27	0	15,15,17	0.52	0
10	MAN	r	5	10	11,11,12	0.96	1 (9%)	15,15,17	0.86	1 (6%)
9	NAG	s	1	9,1	14,14,15	0.46	0	17,19,21	0.74	1 (5%)
9	NAG	s	2	9	14,14,15	0.40	0	17,19,21	0.51	0
10	NAG	t	1	10,1	14,14,15	0.45	0	17,19,21	1.01	1 (5%)
10	NAG	t	2	10	14,14,15	0.43	0	17,19,21	0.67	0
10	BMA	t	3	10	11,11,12	0.28	0	15,15,17	0.38	0
10	MAN	t	4	10	11,11,12	0.30	0	15,15,17	0.49	0
10	MAN	t	5	10	11,11,12	0.27	0	15,15,17	0.48	0
9	NAG	u	1	9,1	14,14,15	0.61	0	17,19,21	0.83	1 (5%)
9	NAG	u	2	9	14,14,15	0.60	0	17,19,21	0.99	1 (5%)
9	NAG	v	1	9,1	14,14,15	0.42	0	17,19,21	0.63	0
9	NAG	v	2	9	14,14,15	0.39	0	17,19,21	0.44	0
8	NAG	w	1	1,8	14,14,15	0.54	0	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	w	2	8	14,14,15	0.39	0	17,19,21	0.69	0
8	BMA	w	3	8	11,11,12	0.23	0	15,15,17	0.58	0
8	NAG	x	1	1,8	14,14,15	0.48	0	17,19,21	0.76	1 (5%)
8	NAG	x	2	8	14,14,15	0.40	0	17,19,21	1.02	1 (5%)
8	BMA	x	3	8	11,11,12	0.31	0	15,15,17	0.50	0
10	NAG	y	1	10,1	14,14,15	0.45	0	17,19,21	0.51	0
10	NAG	y	2	10	14,14,15	0.43	0	17,19,21	0.55	0
10	BMA	y	3	10	11,11,12	0.29	0	15,15,17	0.71	0
10	MAN	y	4	10	11,11,12	0.28	0	15,15,17	0.46	0
10	MAN	y	5	10	11,11,12	0.27	0	15,15,17	0.45	0
9	NAG	z	1	9,1	14,14,15	0.55	0	17,19,21	1.15	1 (5%)
9	NAG	z	2	9	14,14,15	0.66	0	17,19,21	1.04	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	0	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	0	2	9	-	2/6/23/26	0/1/1/1
10	NAG	1	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	1	2	10	-	0/6/23/26	0/1/1/1
10	BMA	1	3	10	-	0/2/19/22	0/1/1/1
10	MAN	1	4	10	-	0/2/19/22	0/1/1/1
10	MAN	1	5	10	-	0/2/19/22	0/1/1/1
10	NAG	2	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	2	2	10	-	0/6/23/26	0/1/1/1
10	BMA	2	3	10	-	2/2/19/22	0/1/1/1
10	MAN	2	4	10	-	0/2/19/22	0/1/1/1
10	MAN	2	5	10	-	0/2/19/22	0/1/1/1
9	NAG	3	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	3	2	9	-	3/6/23/26	0/1/1/1
11	NAG	4	1	11,1	-	0/6/23/26	0/1/1/1
11	NAG	4	2	11	-	3/6/23/26	0/1/1/1
11	BMA	4	3	11	-	0/2/19/22	0/1/1/1
9	NAG	5	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	5	2	9	-	0/6/23/26	0/1/1/1
8	NAG	E	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	E	2	8	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	E	3	8	-	0/2/19/22	0/1/1/1
9	NAG	F	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	3/6/23/26	0/1/1/1
9	NAG	S	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	S	2	9	-	3/6/23/26	0/1/1/1
8	NAG	T	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	T	2	8	-	0/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
9	NAG	U	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	U	2	9	-	0/6/23/26	0/1/1/1
9	NAG	V	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	1/6/23/26	0/1/1/1
10	NAG	W	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	W	2	10	-	0/6/23/26	0/1/1/1
10	BMA	W	3	10	-	0/2/19/22	0/1/1/1
10	MAN	W	4	10	-	0/2/19/22	0/1/1/1
10	MAN	W	5	10	-	0/2/19/22	0/1/1/1
9	NAG	X	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
10	NAG	Y	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	1/6/23/26	0/1/1/1
10	BMA	Y	3	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	4	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	5	10	-	0/2/19/22	0/1/1/1
9	NAG	Z	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	2/6/23/26	0/1/1/1
9	NAG	a	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	a	2	9	-	0/6/23/26	0/1/1/1
8	NAG	b	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	0/6/23/26	0/1/1/1
8	BMA	b	3	8	-	0/2/19/22	0/1/1/1
8	NAG	c	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	c	2	8	-	1/6/23/26	0/1/1/1
8	BMA	c	3	8	-	0/2/19/22	0/1/1/1
10	NAG	d	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	d	2	10	-	0/6/23/26	0/1/1/1
10	BMA	d	3	10	-	0/2/19/22	0/1/1/1
10	MAN	d	4	10	-	0/2/19/22	0/1/1/1
10	MAN	d	5	10	-	0/2/19/22	0/1/1/1
9	NAG	e	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	e	2	9	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	f	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	f	2	9	-	0/6/23/26	0/1/1/1
10	NAG	g	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	g	2	10	-	0/6/23/26	0/1/1/1
10	BMA	g	3	10	-	1/2/19/22	0/1/1/1
10	MAN	g	4	10	-	0/2/19/22	0/1/1/1
10	MAN	g	5	10	-	0/2/19/22	0/1/1/1
10	NAG	h	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	h	2	10	-	1/6/23/26	0/1/1/1
10	BMA	h	3	10	-	0/2/19/22	0/1/1/1
10	MAN	h	4	10	-	0/2/19/22	0/1/1/1
10	MAN	h	5	10	-	1/2/19/22	0/1/1/1
9	NAG	i	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	i	2	9	-	3/6/23/26	0/1/1/1
11	NAG	j	1	11,1	-	1/6/23/26	0/1/1/1
11	NAG	j	2	11	-	3/6/23/26	0/1/1/1
11	BMA	j	3	11	-	0/2/19/22	0/1/1/1
9	NAG	k	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	k	2	9	-	1/6/23/26	0/1/1/1
8	NAG	l	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	l	2	8	-	0/6/23/26	0/1/1/1
8	BMA	l	3	8	-	0/2/19/22	0/1/1/1
9	NAG	m	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	m	2	9	-	2/6/23/26	0/1/1/1
9	NAG	n	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	n	2	9	-	0/6/23/26	0/1/1/1
8	NAG	o	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	o	2	8	-	0/6/23/26	0/1/1/1
8	BMA	o	3	8	-	0/2/19/22	0/1/1/1
9	NAG	p	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	p	2	9	-	1/6/23/26	0/1/1/1
9	NAG	q	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	q	2	9	-	2/6/23/26	0/1/1/1
10	NAG	r	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	r	2	10	-	1/6/23/26	0/1/1/1
10	BMA	r	3	10	-	2/2/19/22	0/1/1/1
10	MAN	r	4	10	-	0/2/19/22	0/1/1/1
10	MAN	r	5	10	-	0/2/19/22	0/1/1/1
9	NAG	s	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	s	2	9	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	t	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	t	2	10	-	0/6/23/26	0/1/1/1
10	BMA	t	3	10	-	0/2/19/22	0/1/1/1
10	MAN	t	4	10	-	0/2/19/22	0/1/1/1
10	MAN	t	5	10	-	0/2/19/22	0/1/1/1
9	NAG	u	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	u	2	9	-	0/6/23/26	0/1/1/1
9	NAG	v	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	v	2	9	-	2/6/23/26	0/1/1/1
8	NAG	w	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	w	2	8	-	3/6/23/26	0/1/1/1
8	BMA	w	3	8	-	0/2/19/22	0/1/1/1
8	NAG	x	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	x	2	8	-	0/6/23/26	0/1/1/1
8	BMA	x	3	8	-	0/2/19/22	0/1/1/1
10	NAG	y	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	y	2	10	-	3/6/23/26	0/1/1/1
10	BMA	y	3	10	-	0/2/19/22	0/1/1/1
10	MAN	y	4	10	-	0/2/19/22	0/1/1/1
10	MAN	y	5	10	-	0/2/19/22	0/1/1/1
9	NAG	z	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	z	2	9	-	3/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1	3	BMA	O5-C5	2.52	1.48	1.43
10	1	4	MAN	O5-C5	2.34	1.48	1.43
10	2	3	BMA	O5-C5	2.34	1.48	1.43
10	r	5	MAN	O5-C5	2.33	1.48	1.43
10	2	4	MAN	O5-C5	2.23	1.47	1.43

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	k	2	NAG	C1-O5-C5	4.10	117.69	112.19
9	e	1	NAG	C1-O5-C5	3.74	117.20	112.19
10	2	1	NAG	C1-O5-C5	3.72	117.18	112.19
10	1	3	BMA	C1-O5-C5	3.67	117.10	112.19
9	V	2	NAG	C1-O5-C5	3.61	117.03	112.19

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

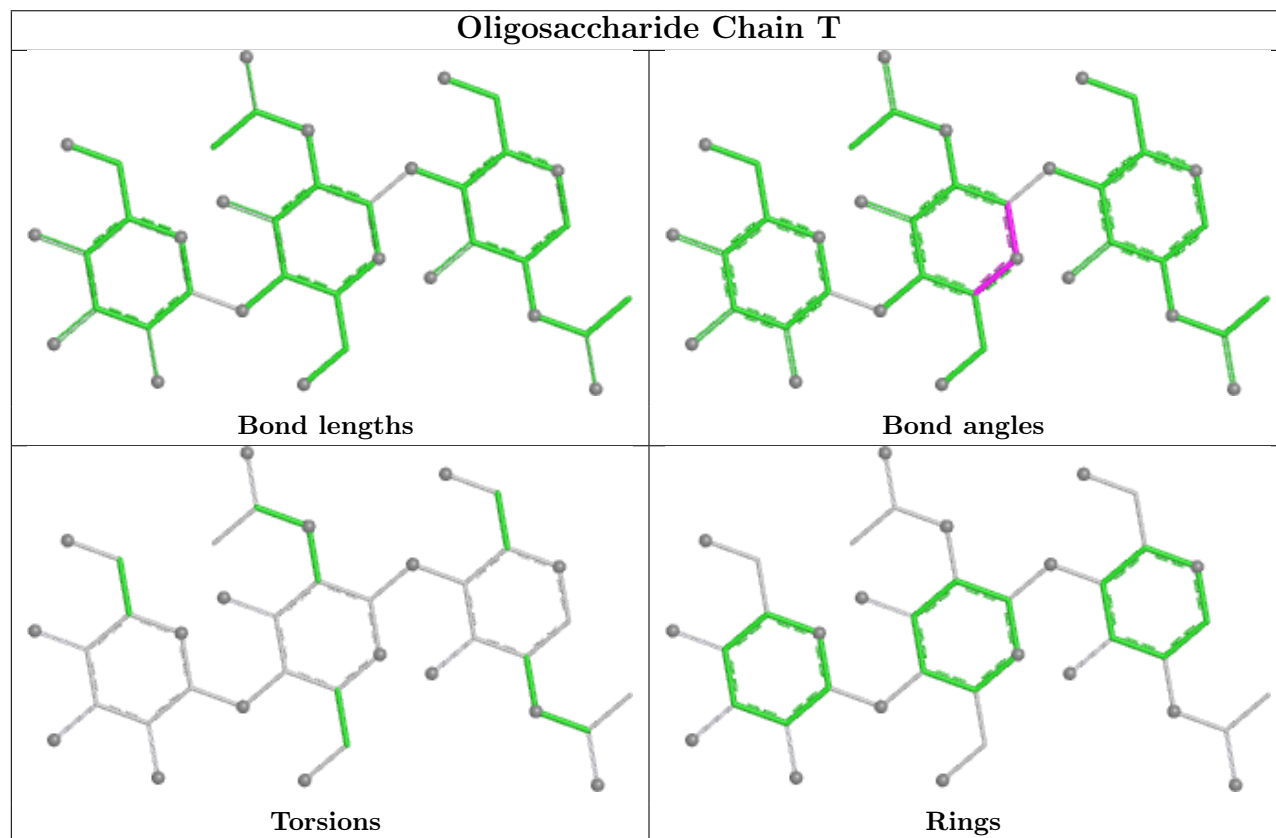
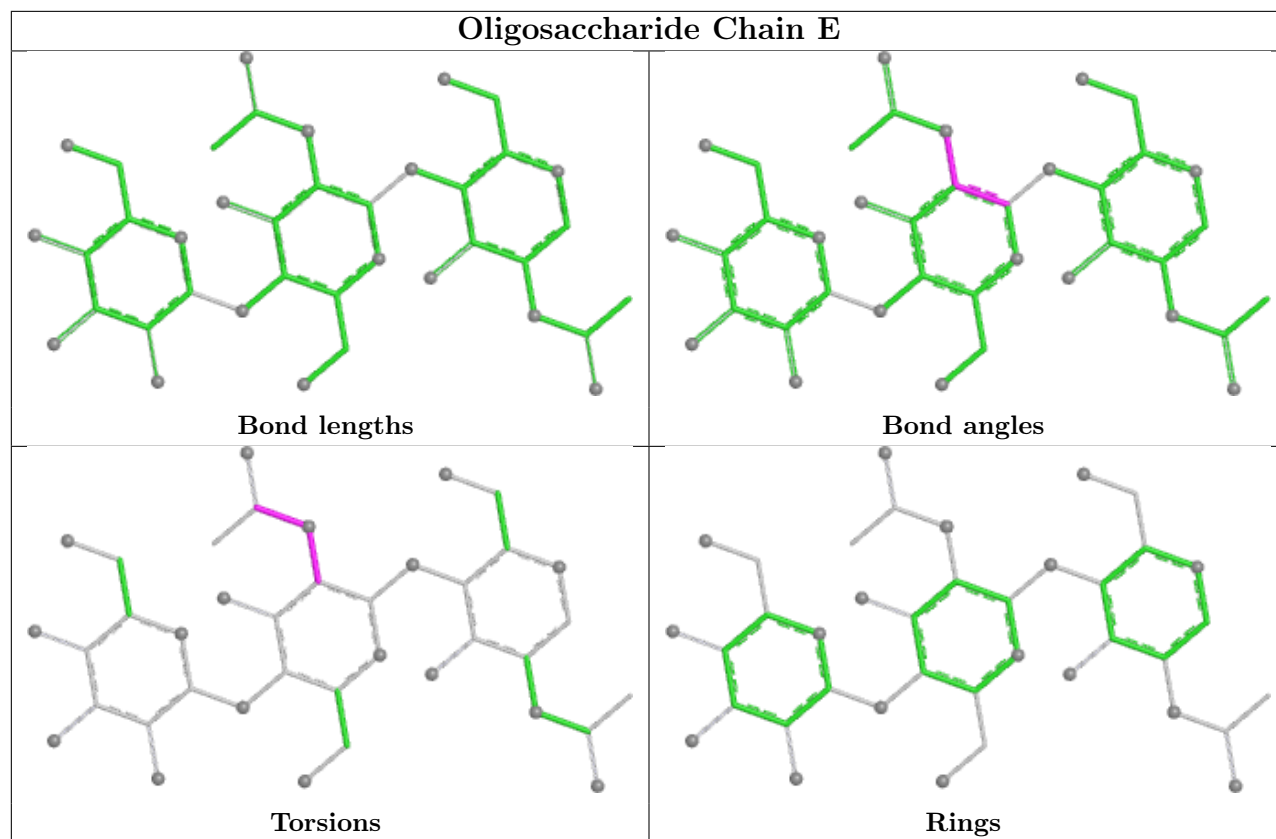
Mol	Chain	Res	Type	Atoms
8	E	2	NAG	C1-C2-N2-C7
9	F	2	NAG	C3-C2-N2-C7
9	F	2	NAG	C8-C7-N2-C2
9	F	2	NAG	O7-C7-N2-C2
9	X	2	NAG	C1-C2-N2-C7

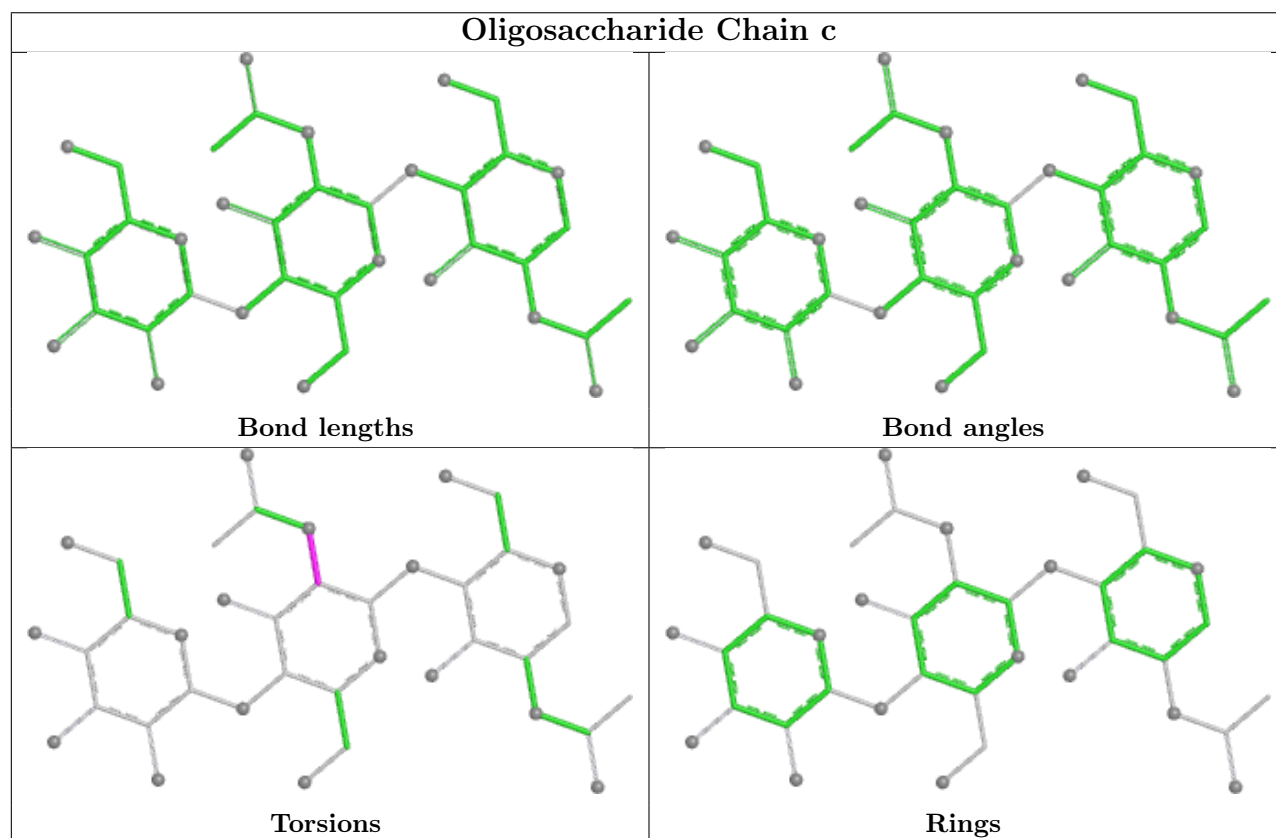
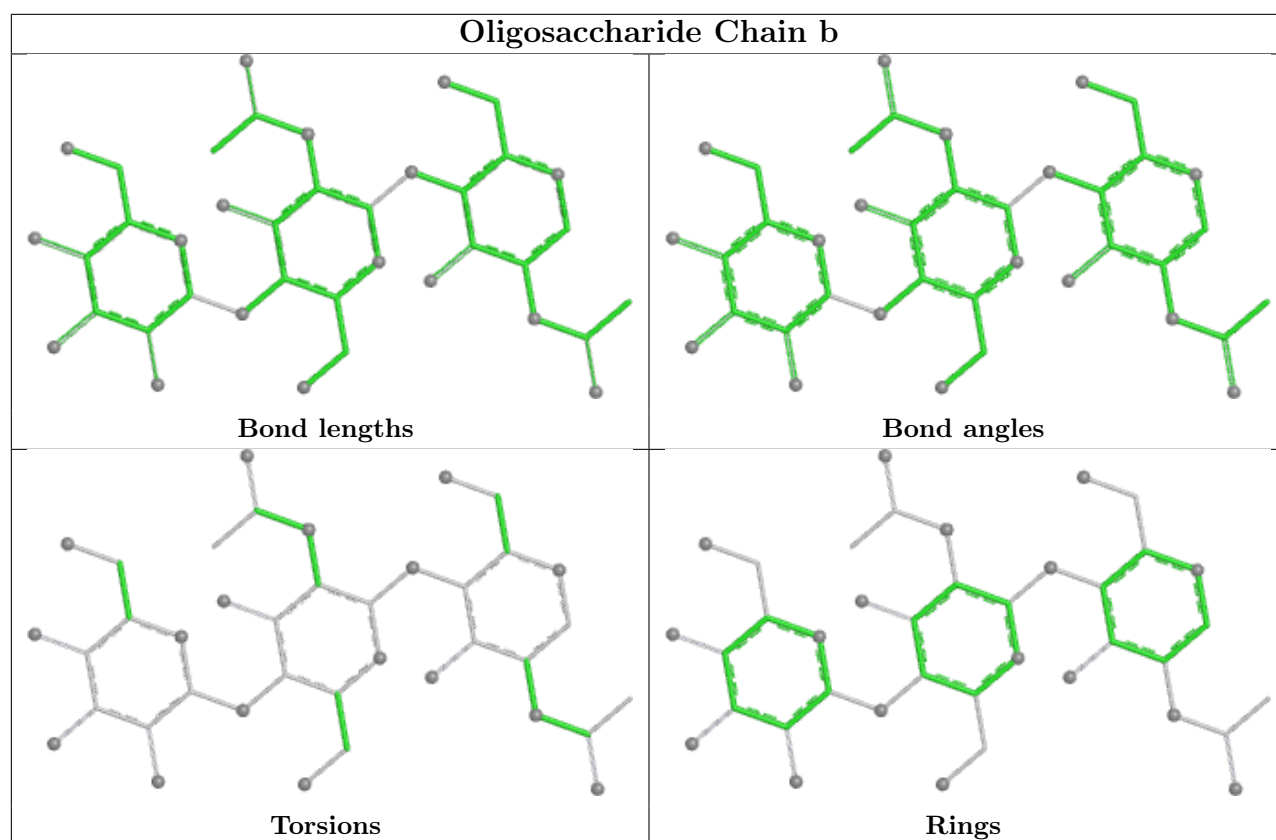
There are no ring outliers.

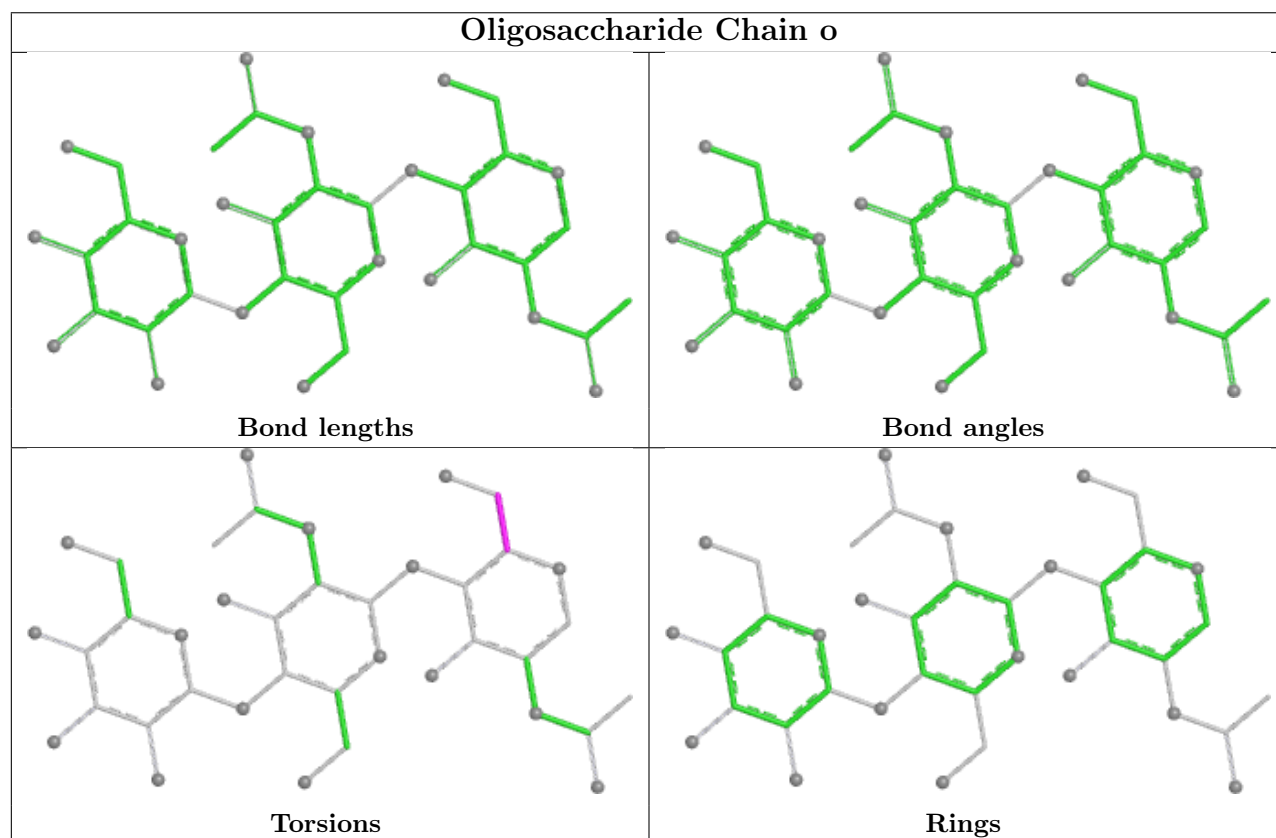
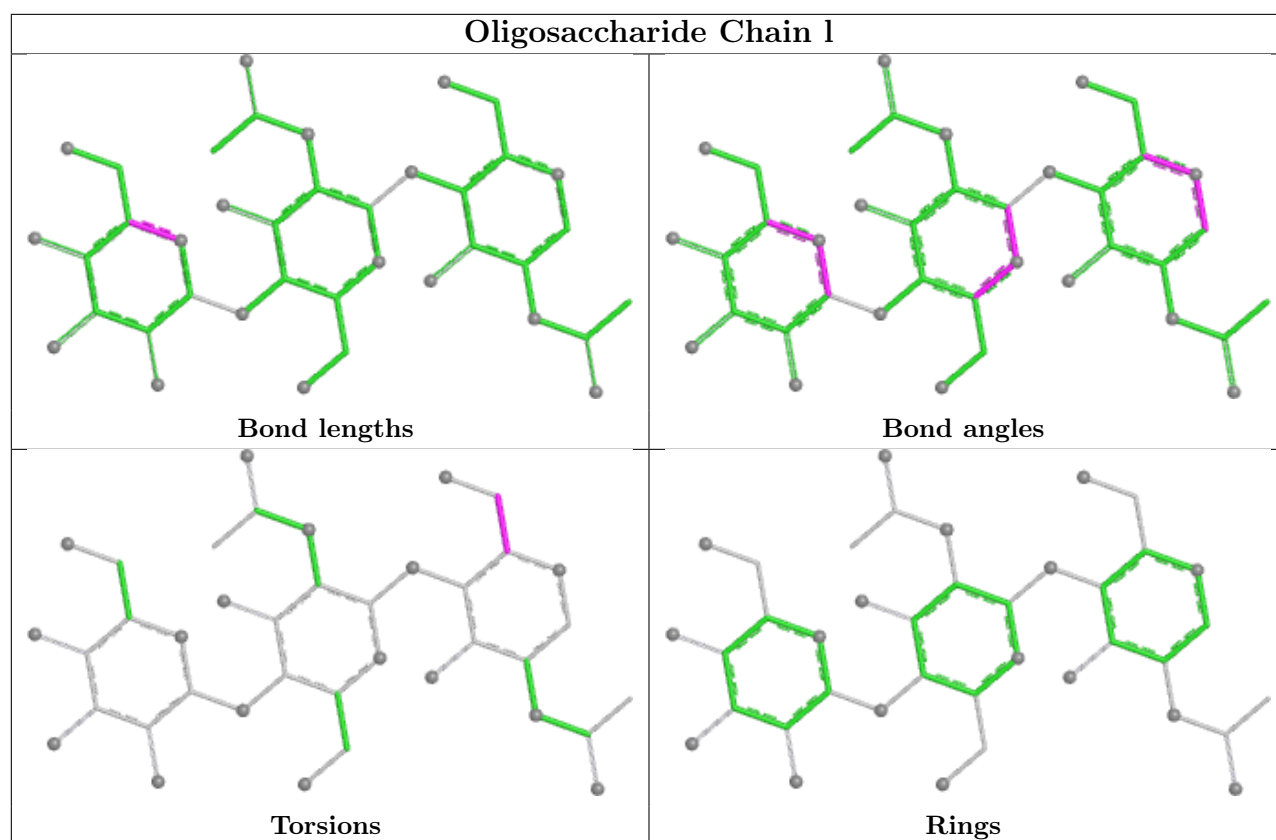
12 monomers are involved in 9 short contacts:

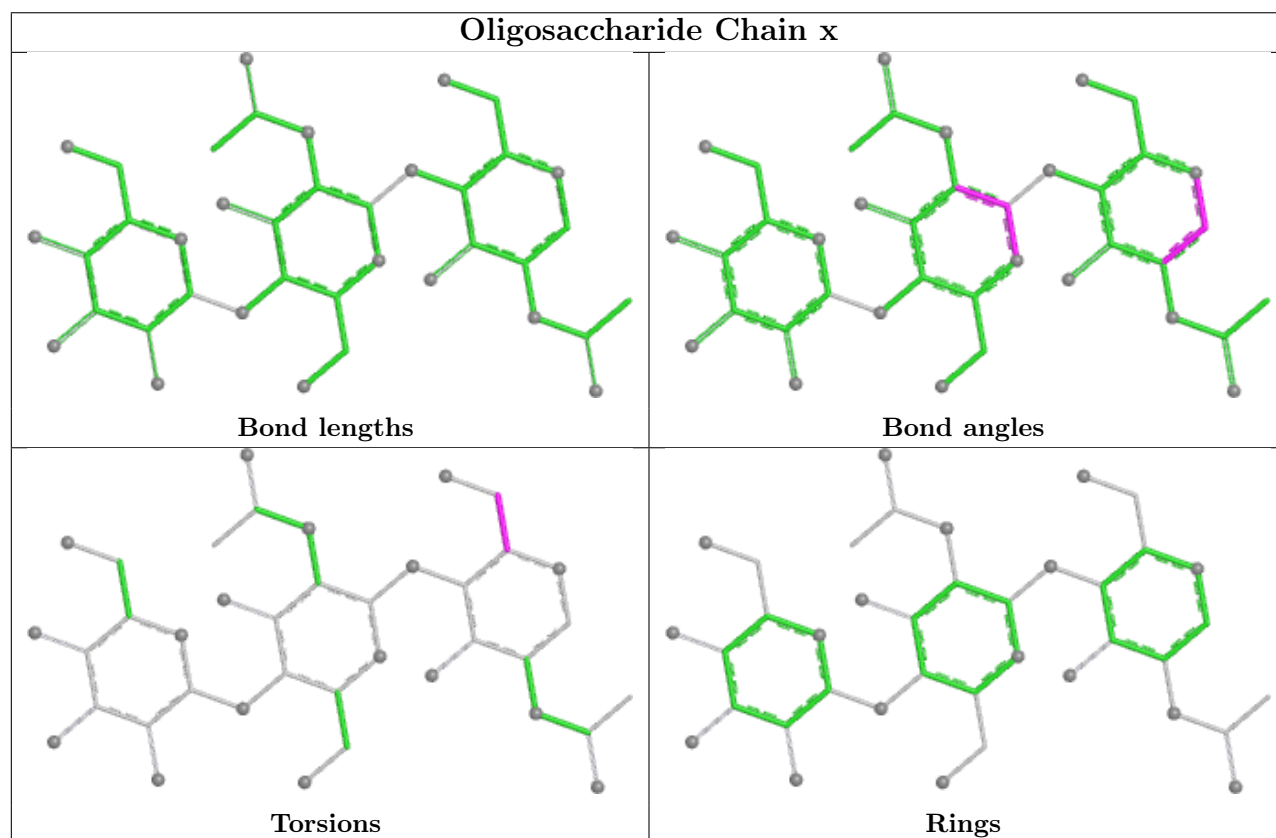
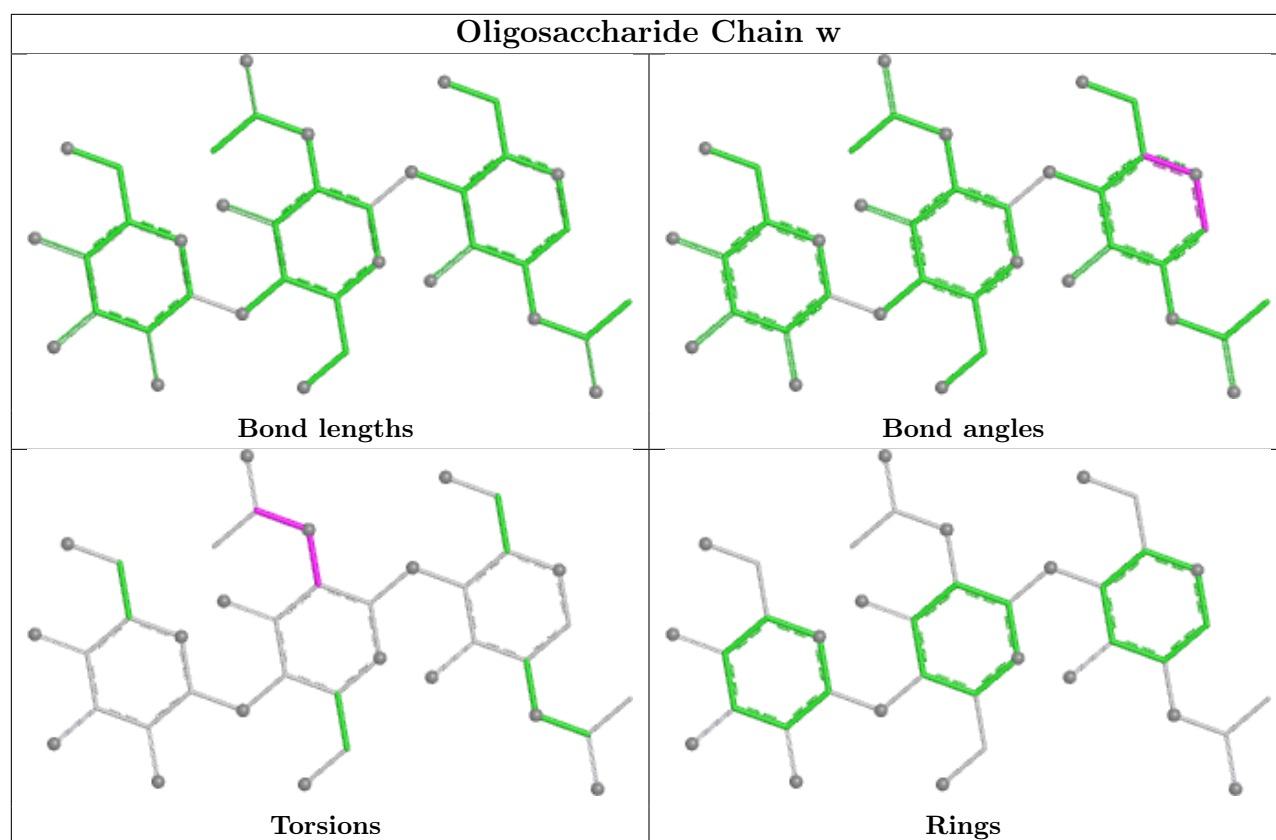
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	t	2	NAG	1	0
8	c	1	NAG	1	0
9	U	1	NAG	1	0
8	c	2	NAG	1	0
8	o	1	NAG	1	0
10	y	1	NAG	1	0
10	Y	1	NAG	1	0
10	r	1	NAG	1	0
9	p	1	NAG	1	0
10	Y	2	NAG	1	0
9	s	1	NAG	1	0
10	y	2	NAG	1	0

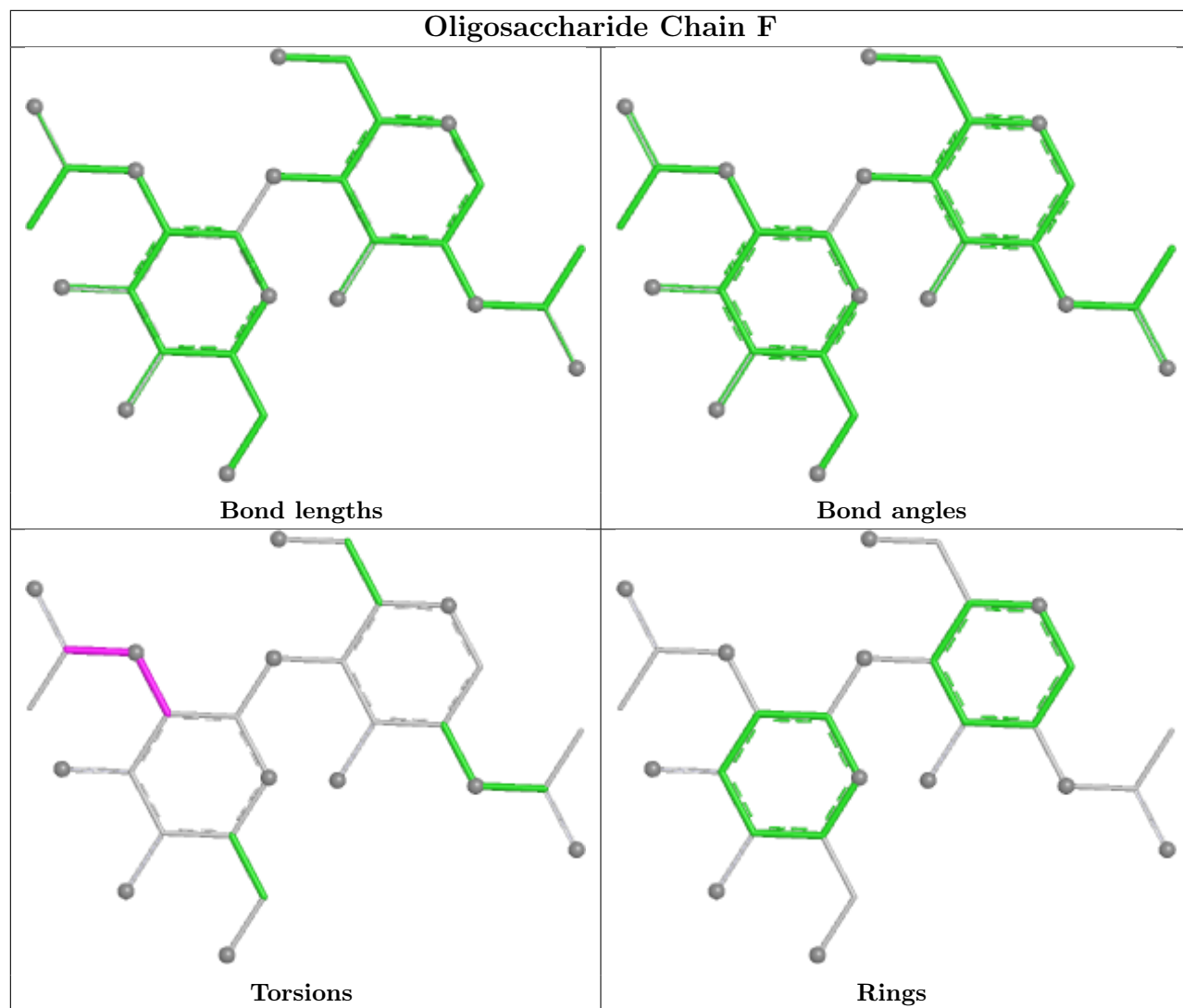
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

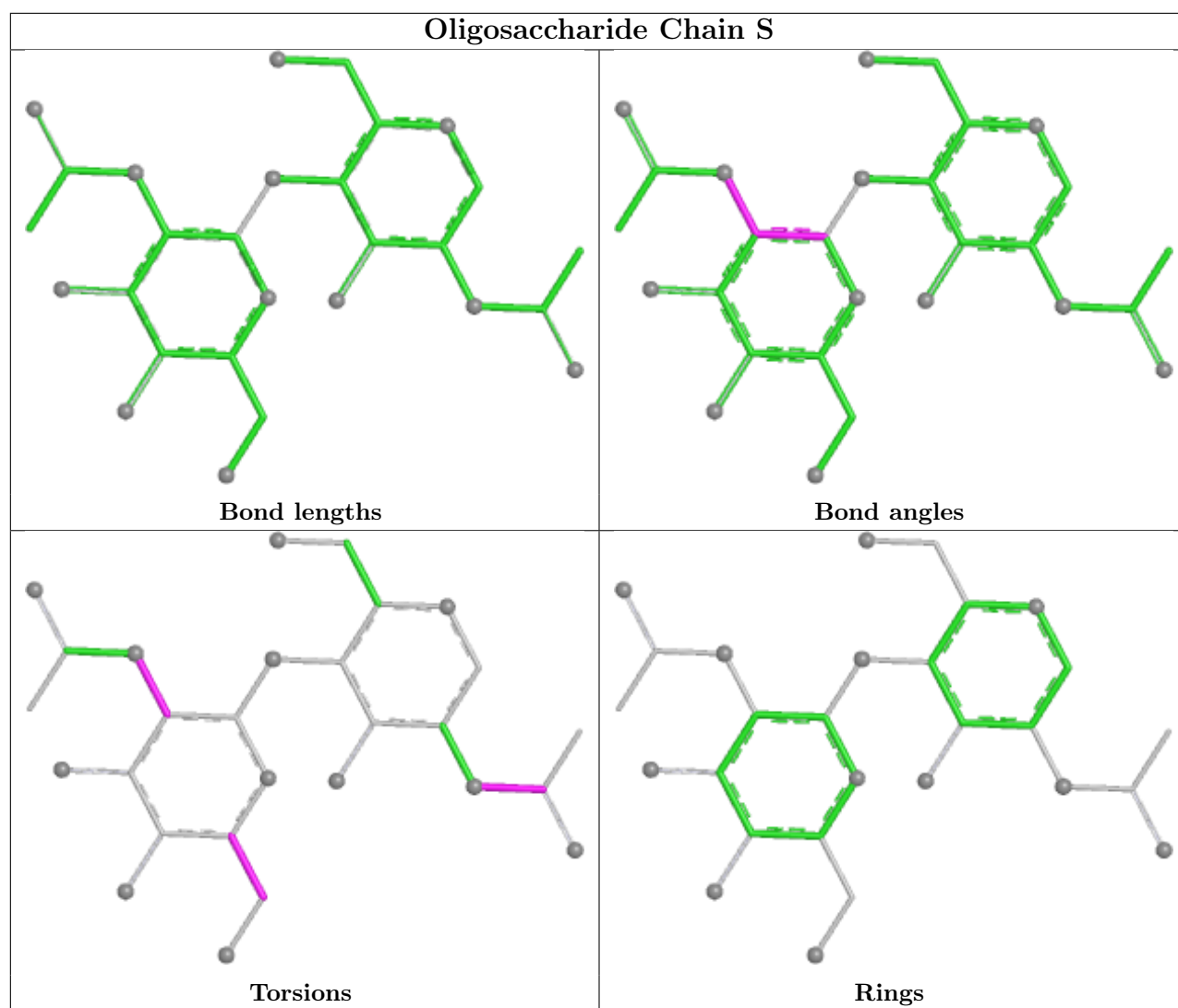


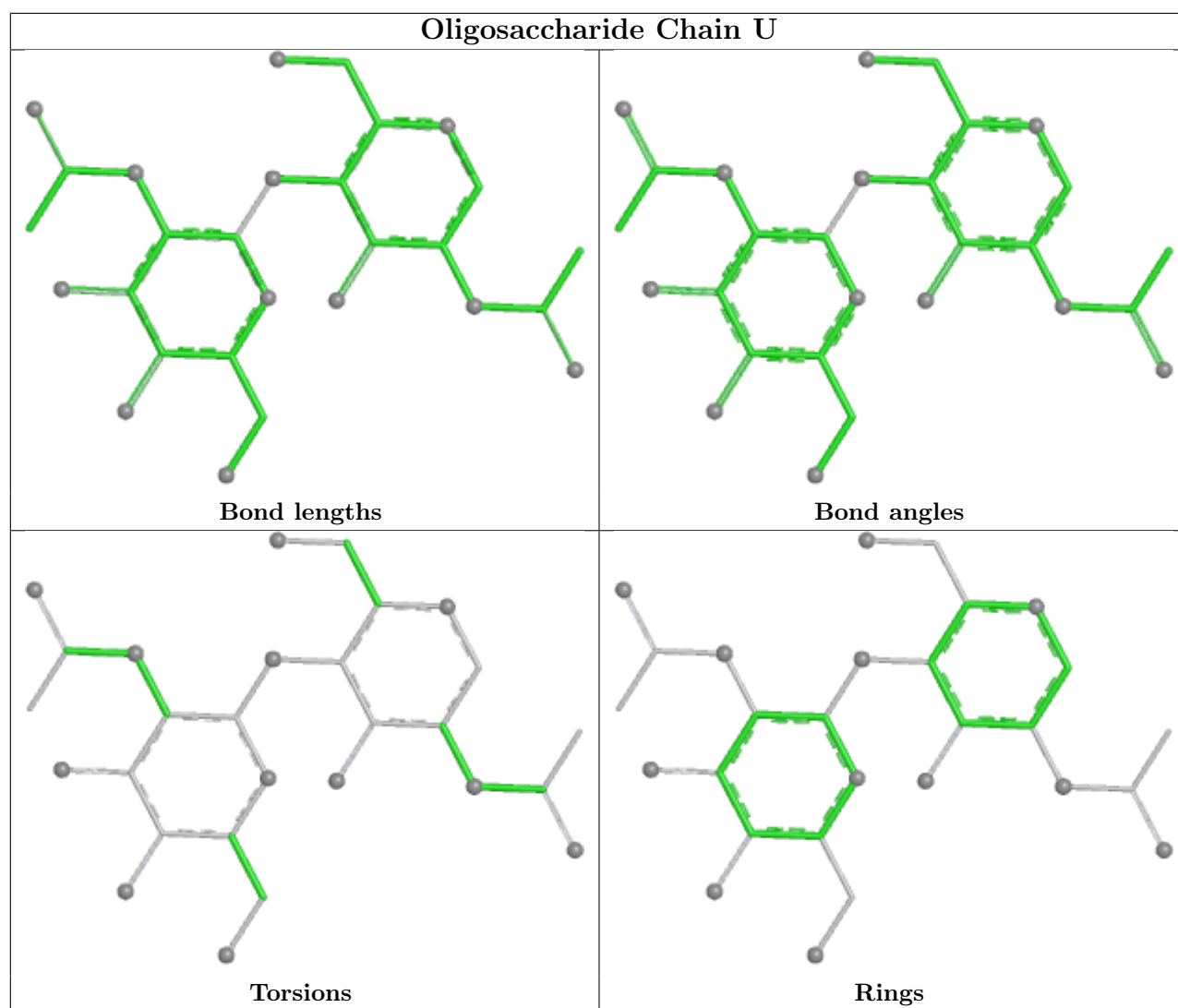


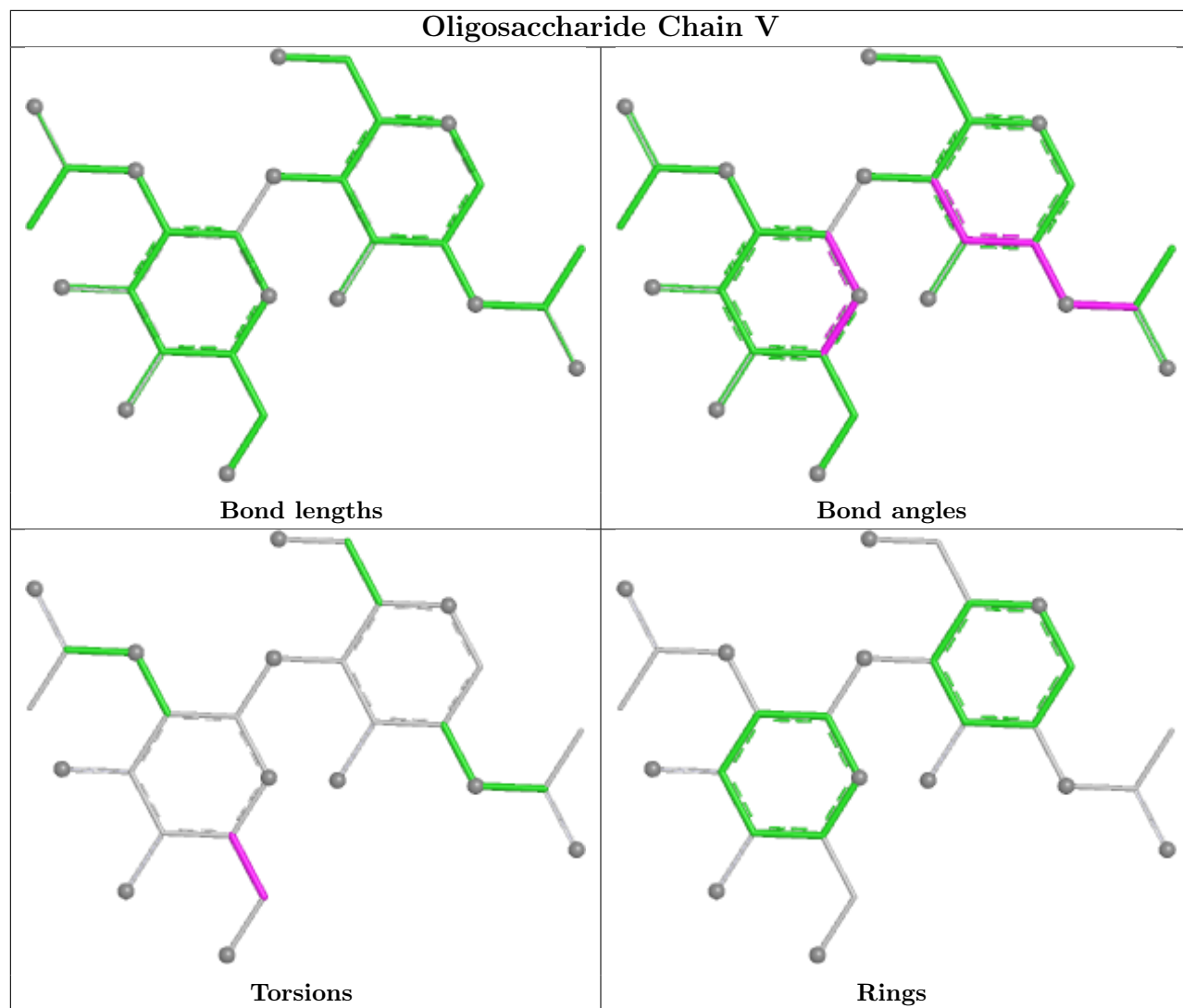


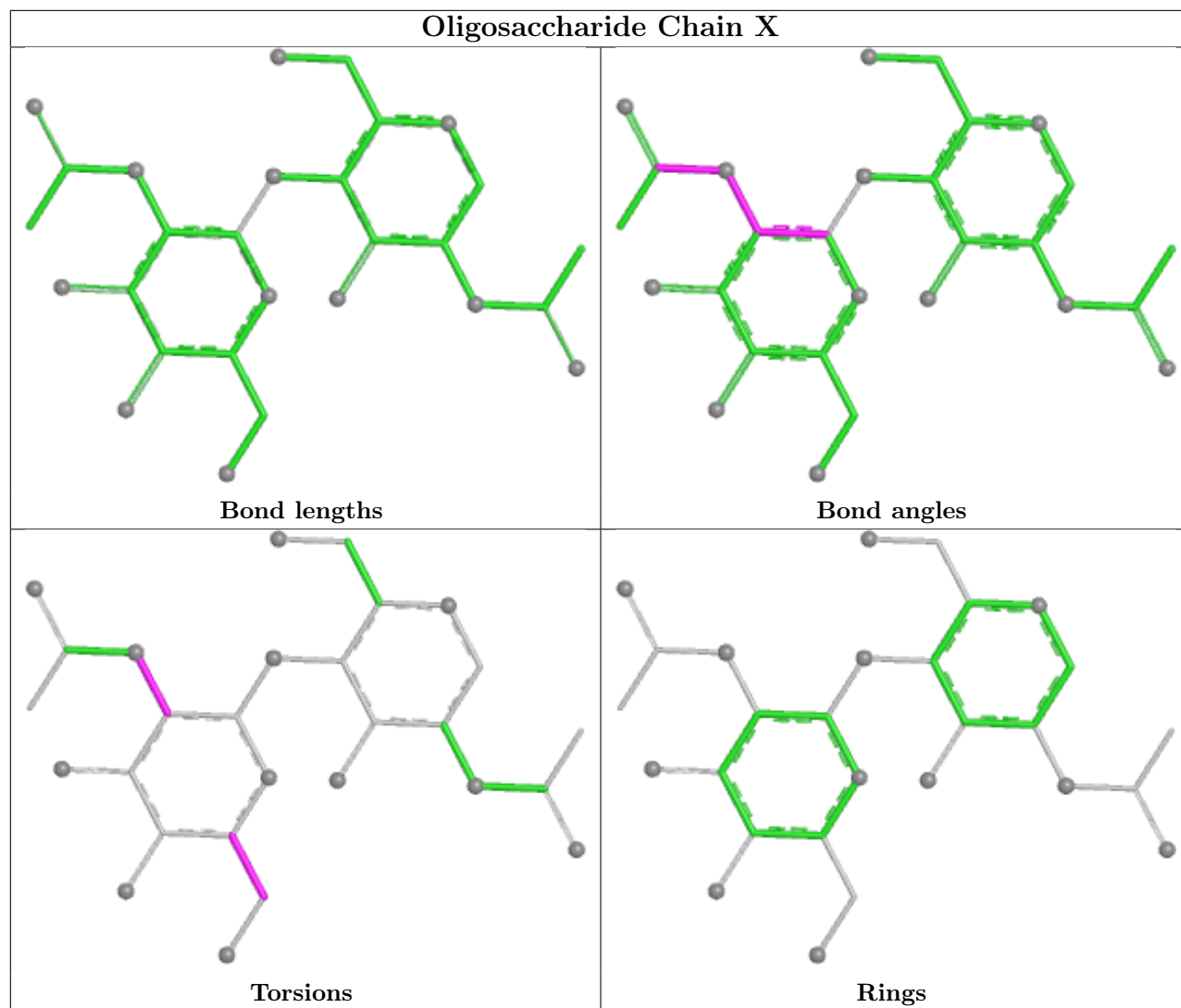


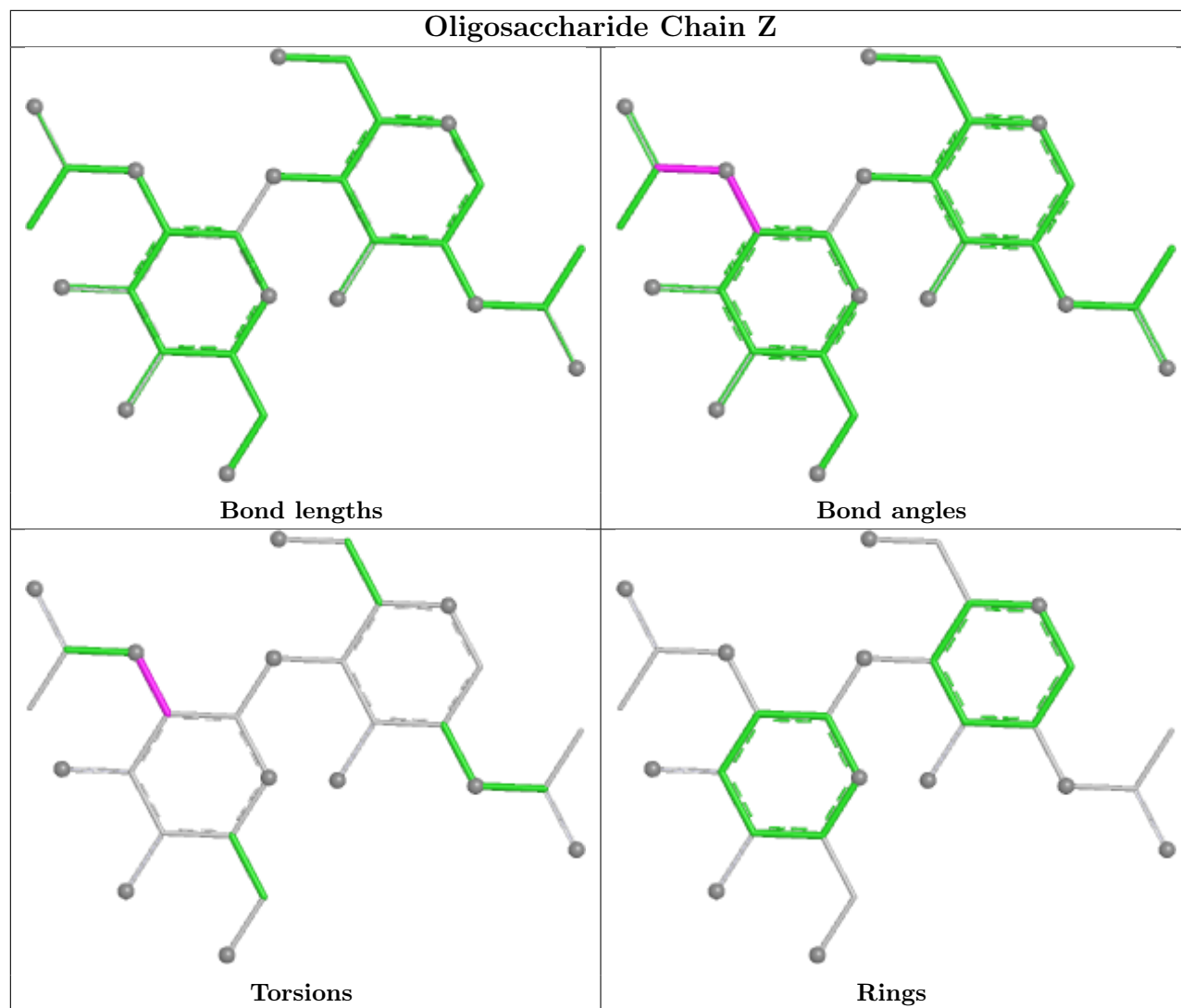


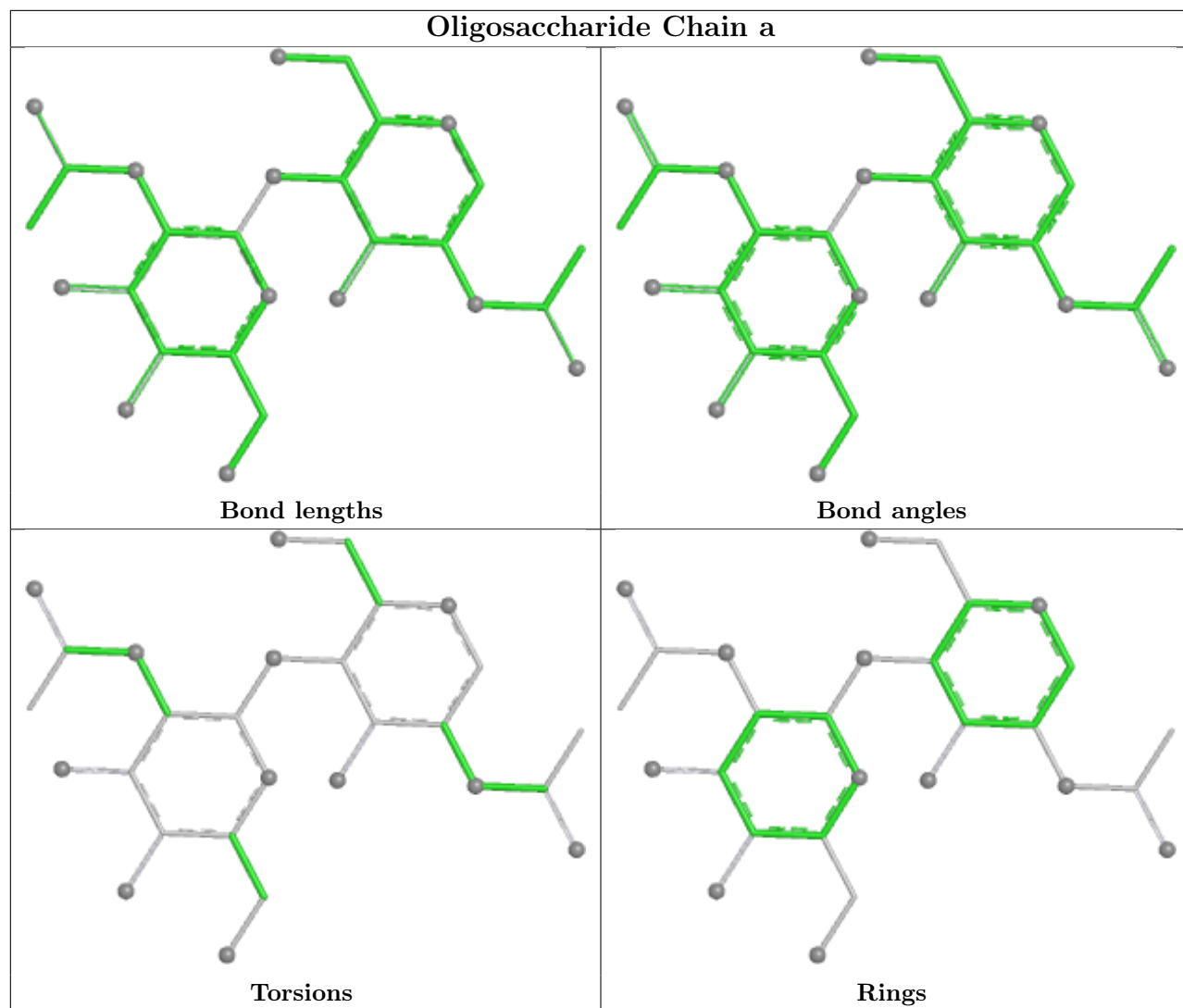


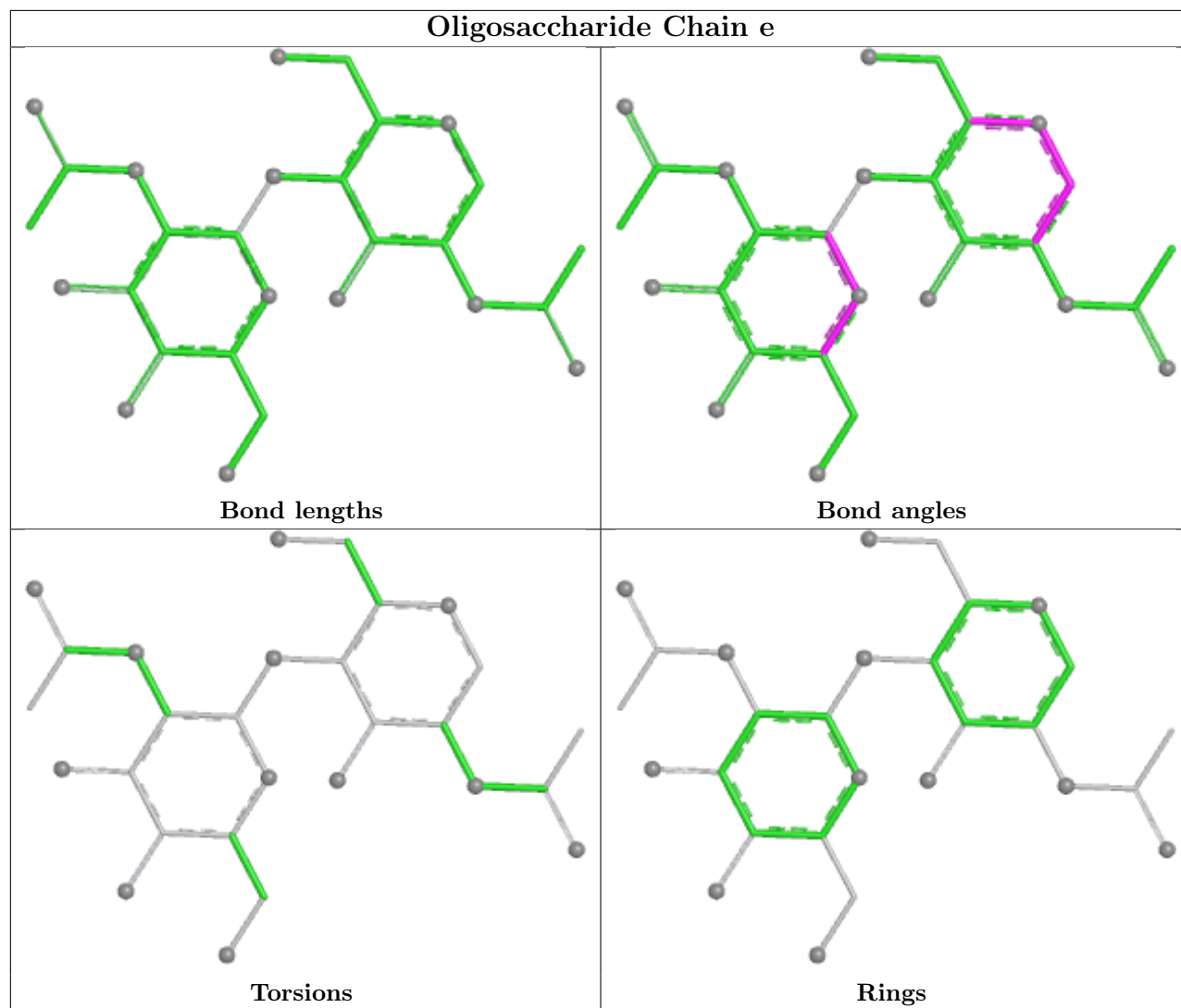


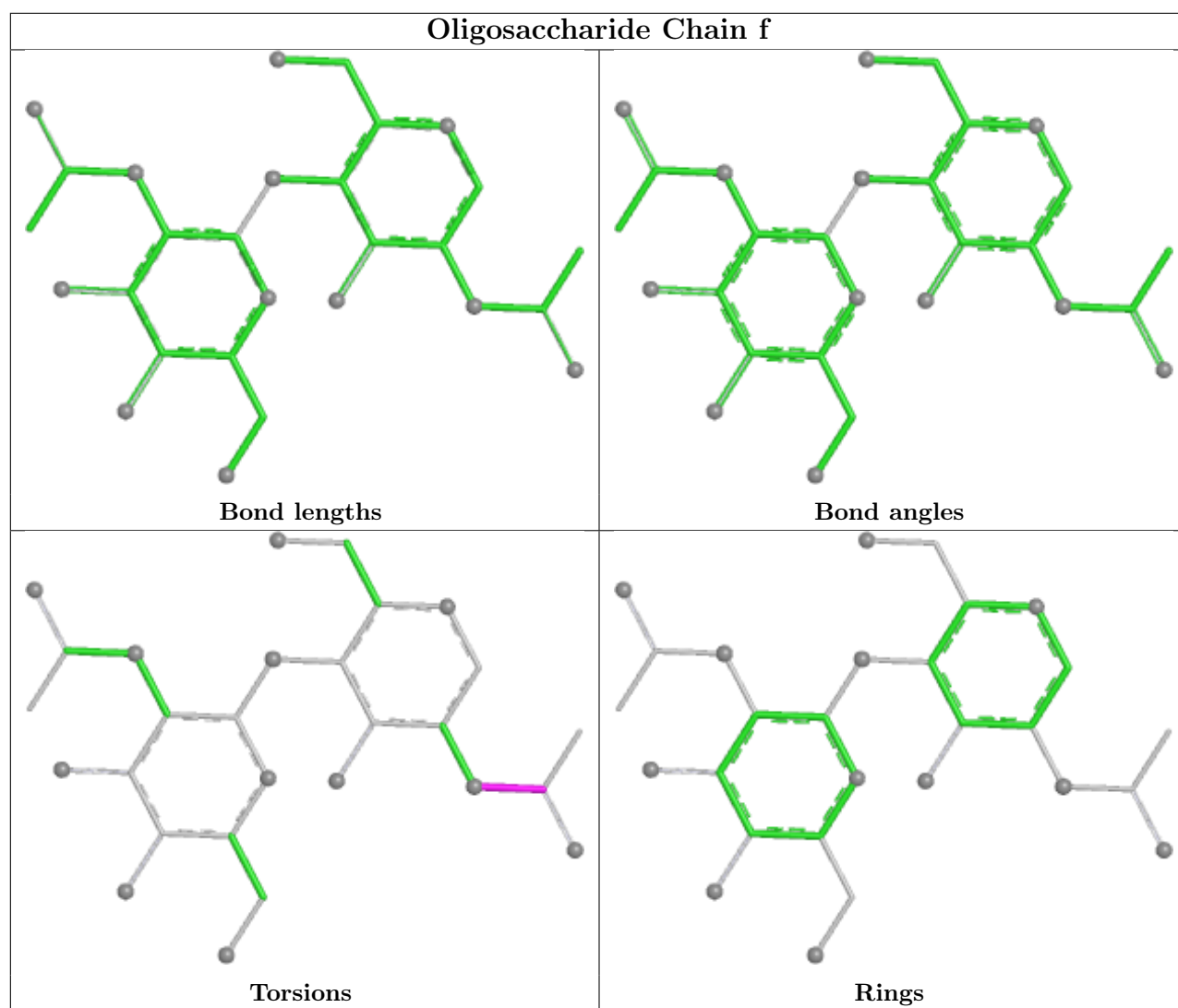


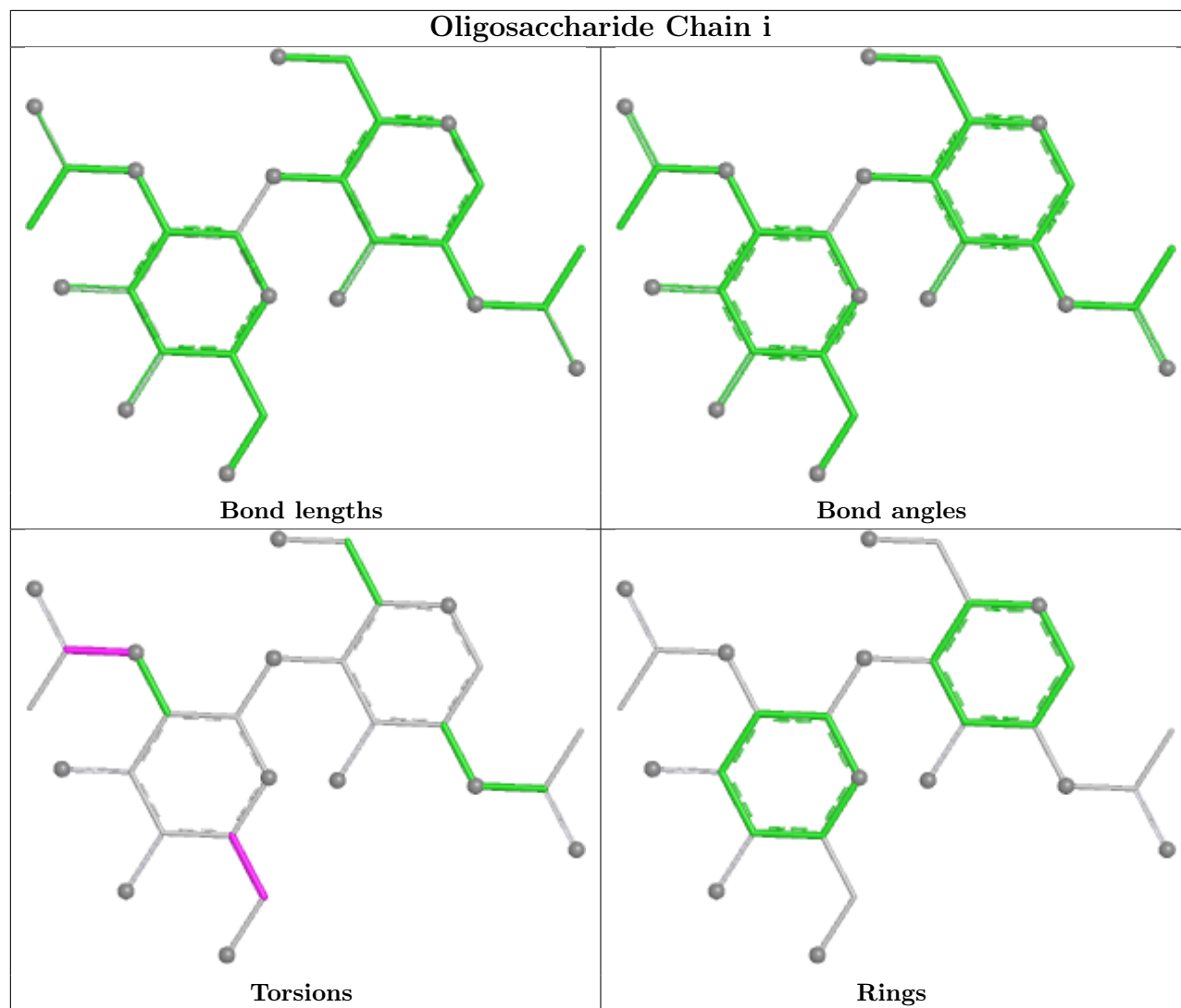


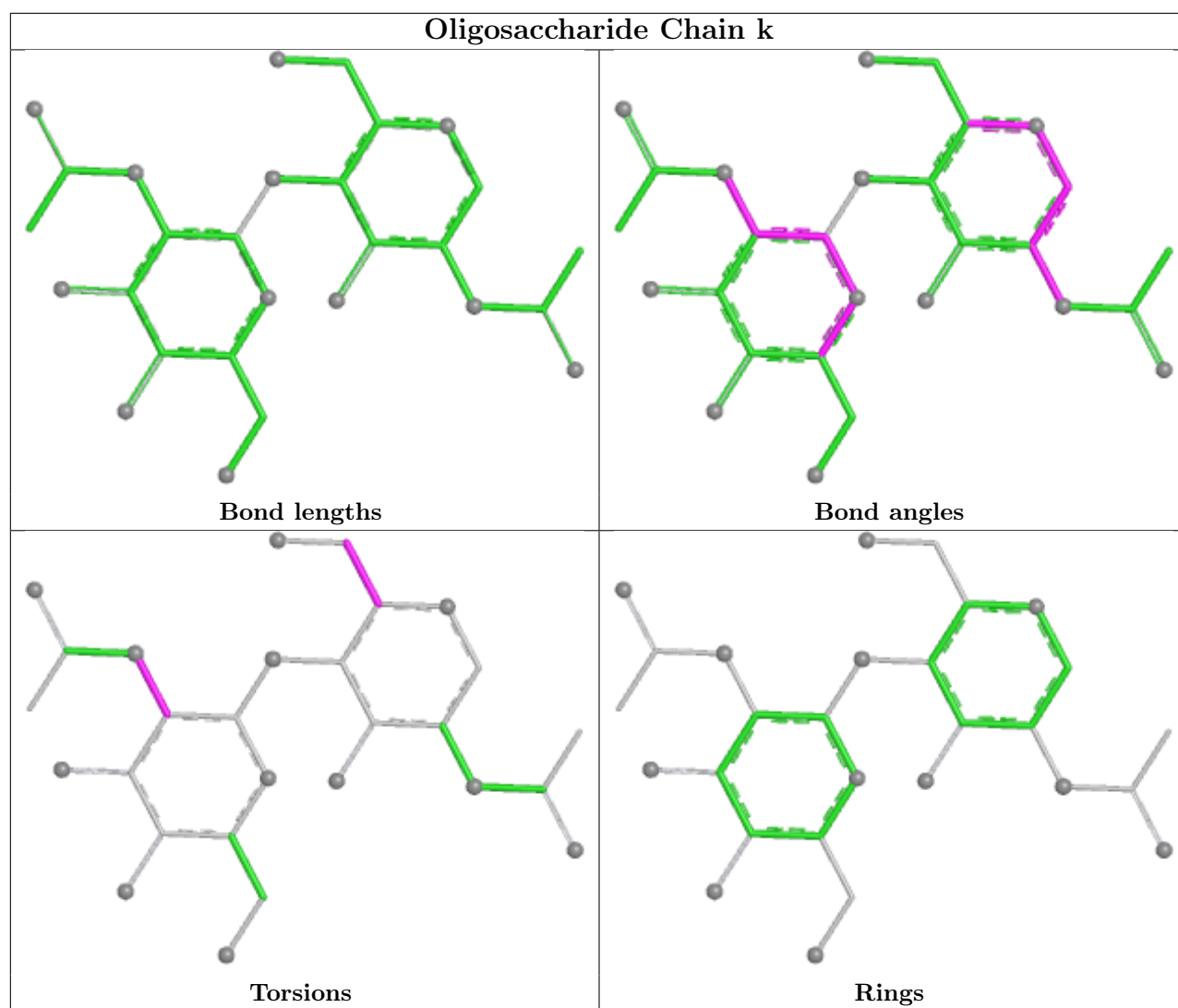


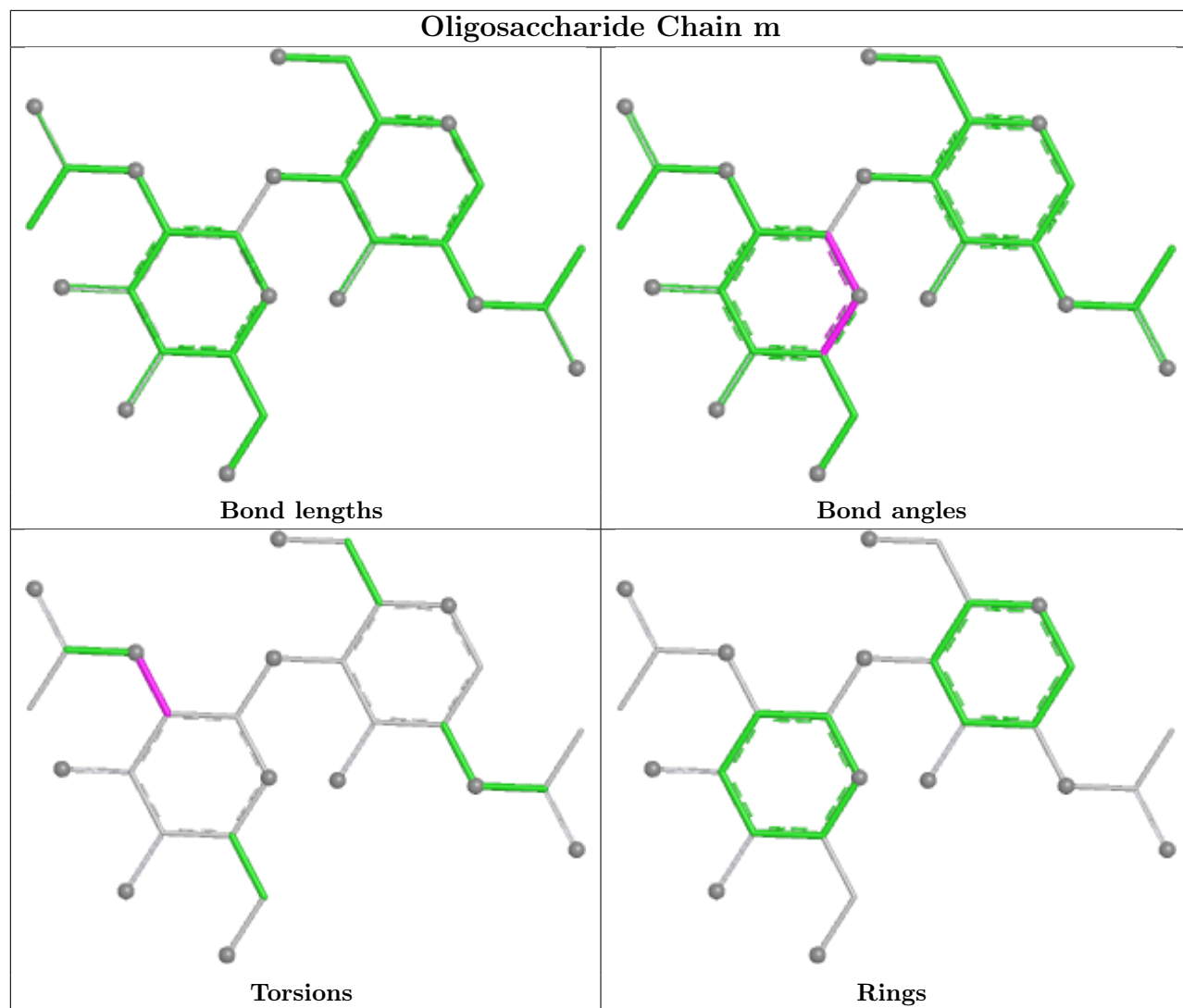


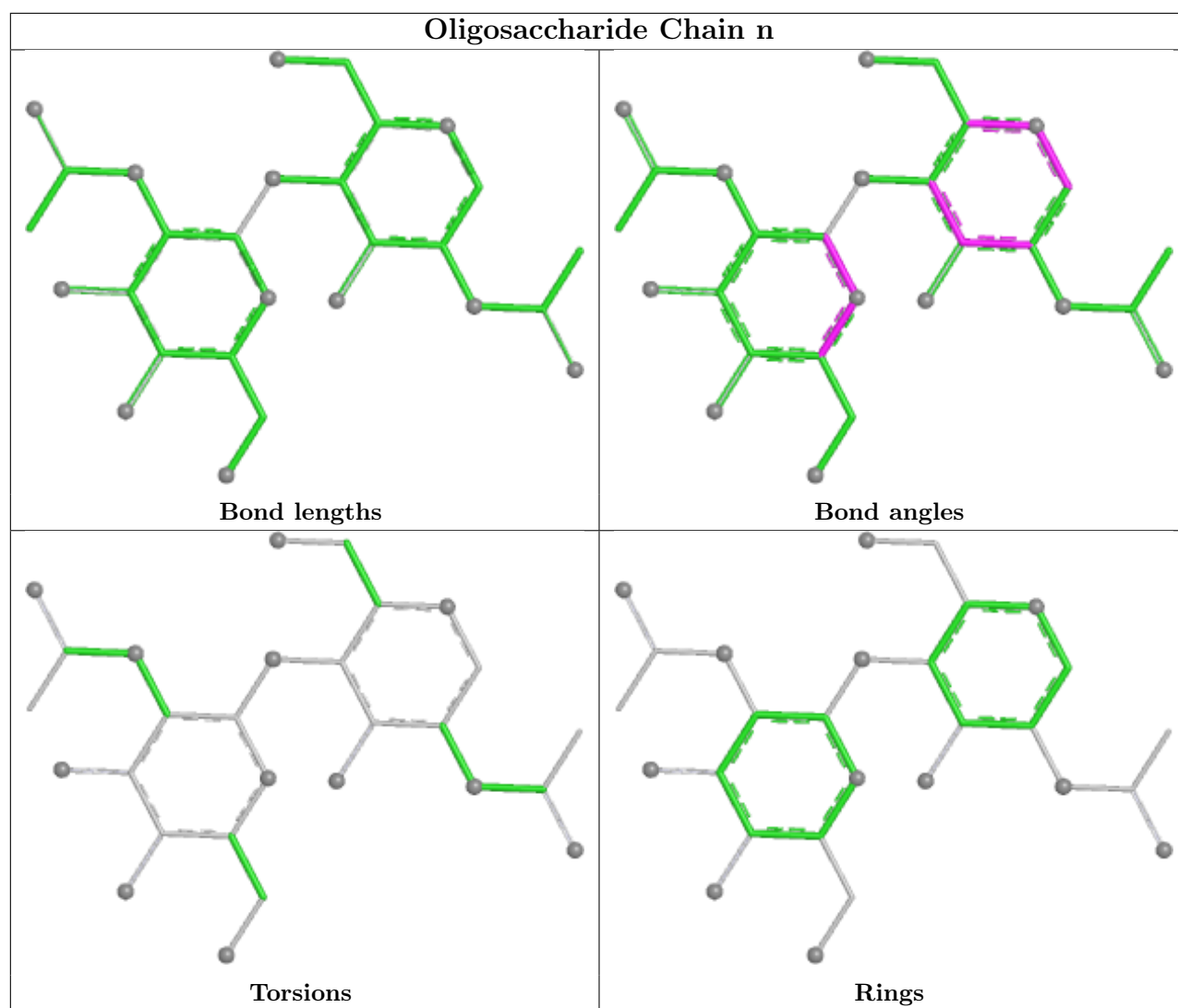


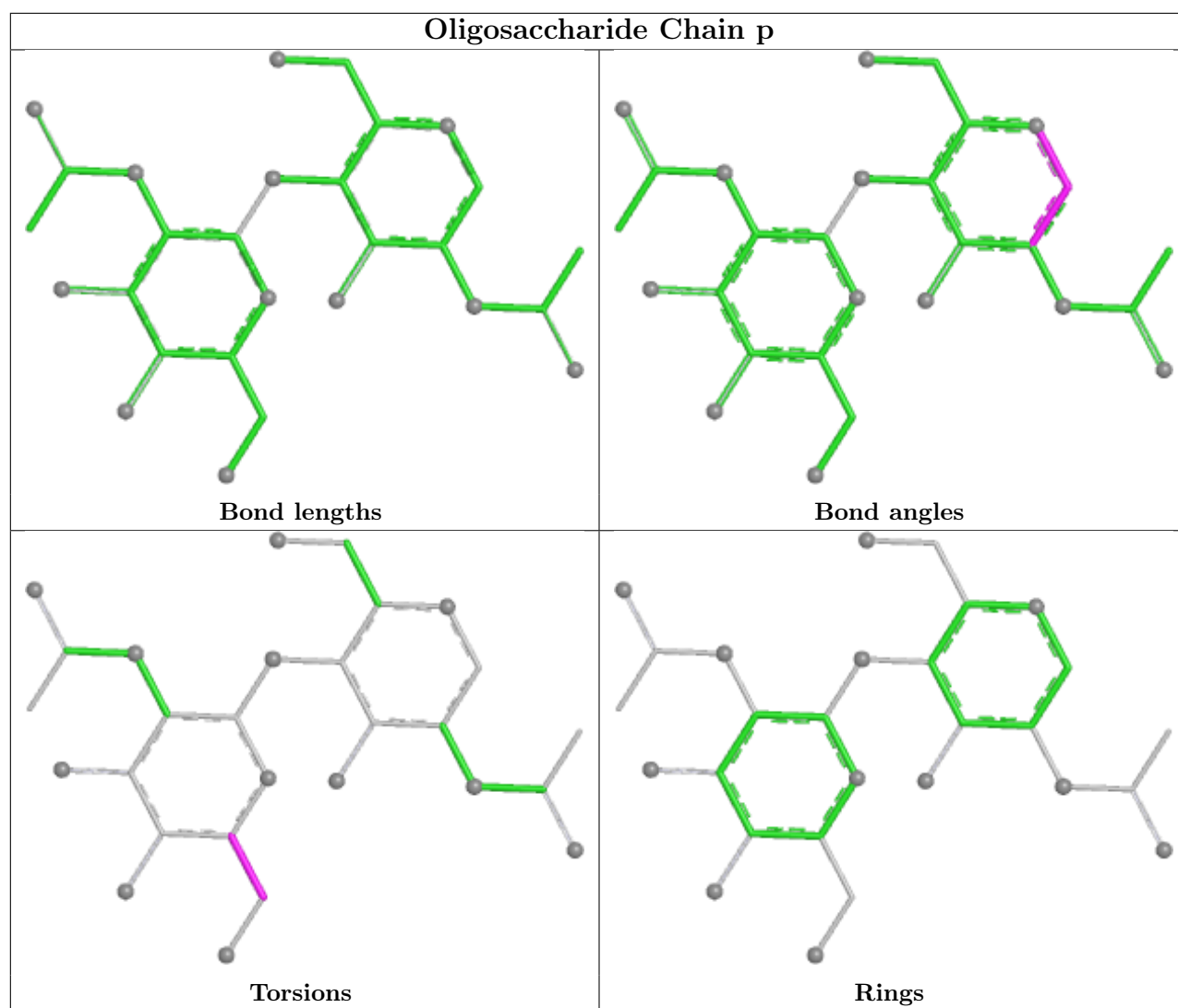


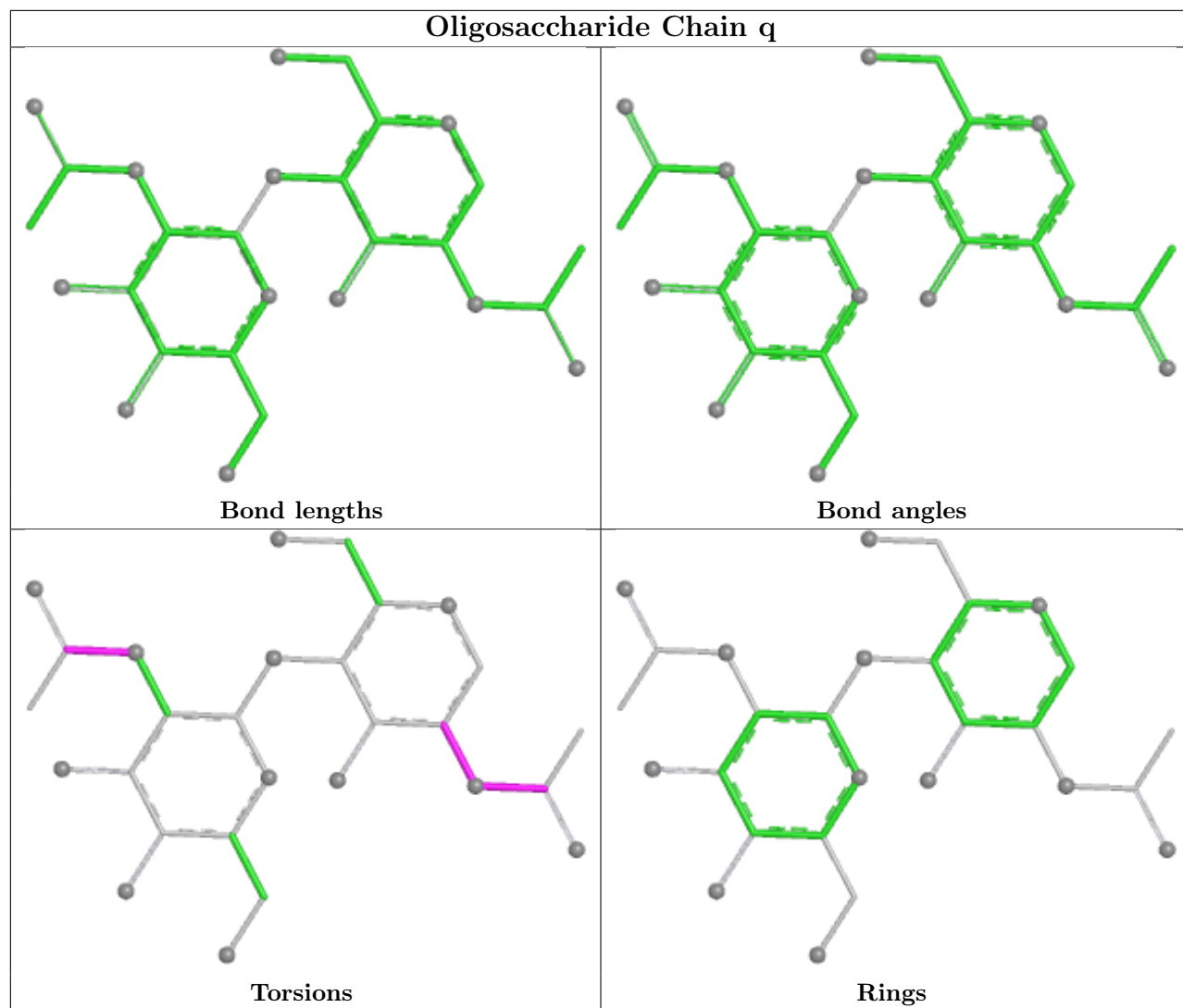


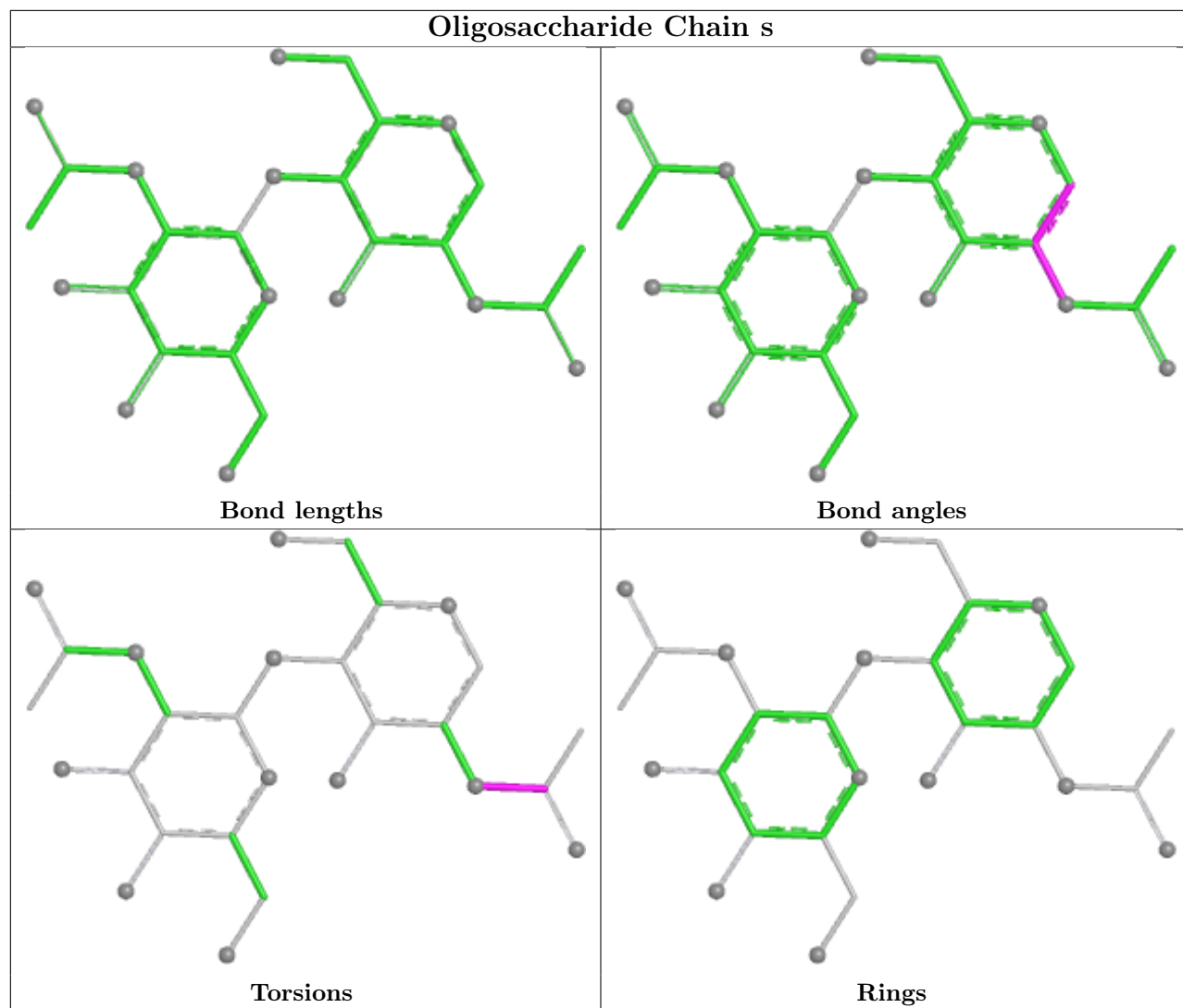


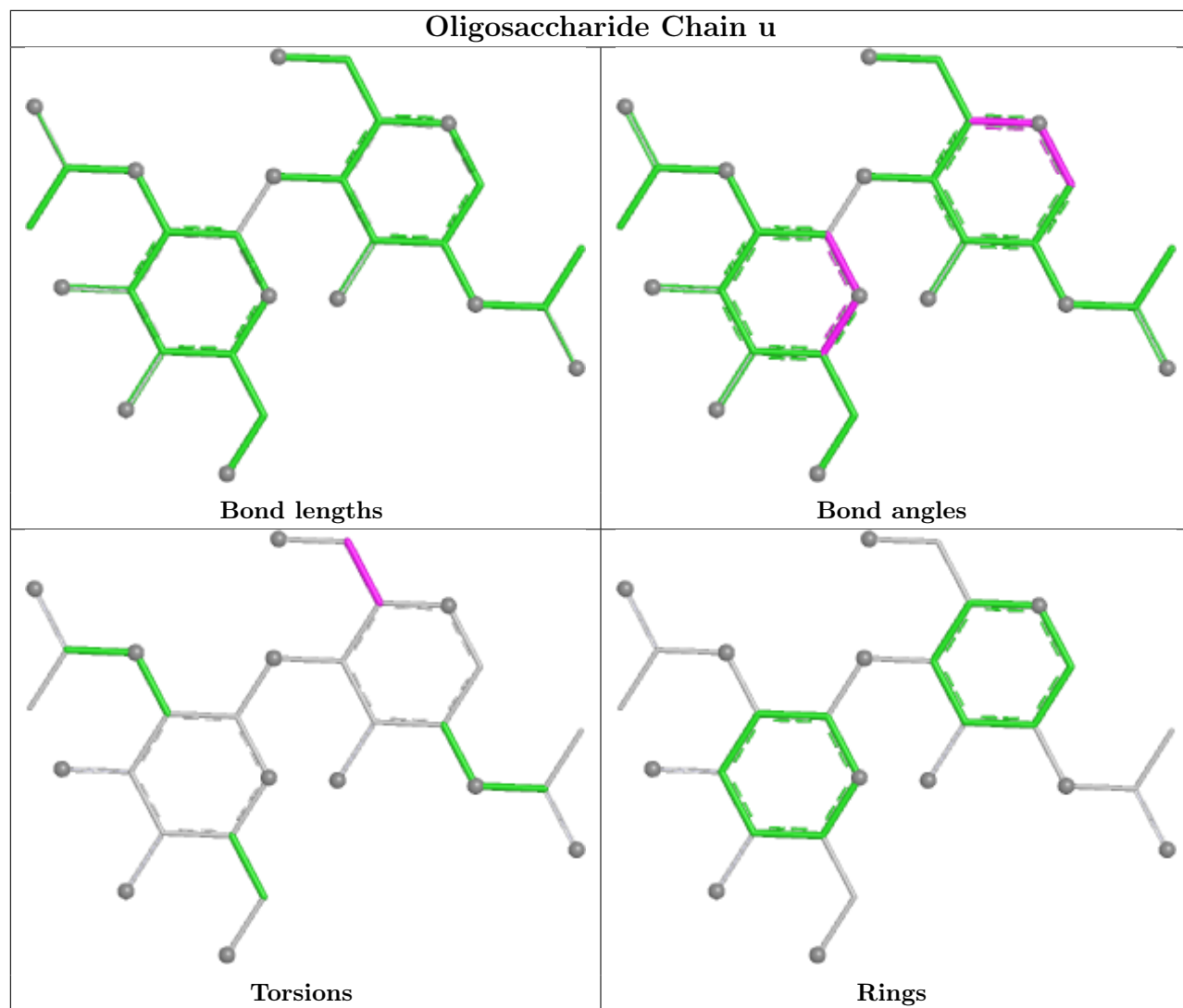


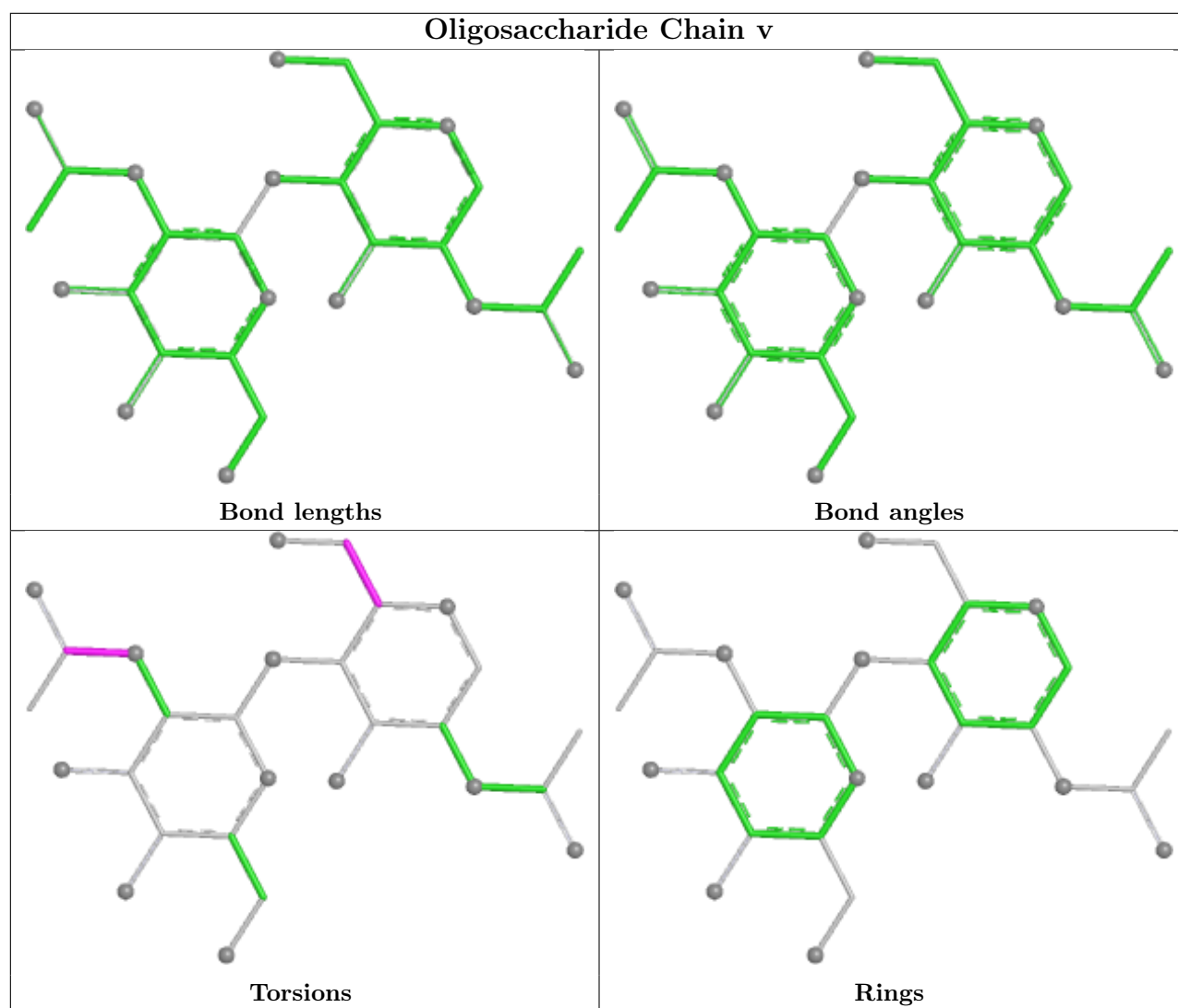


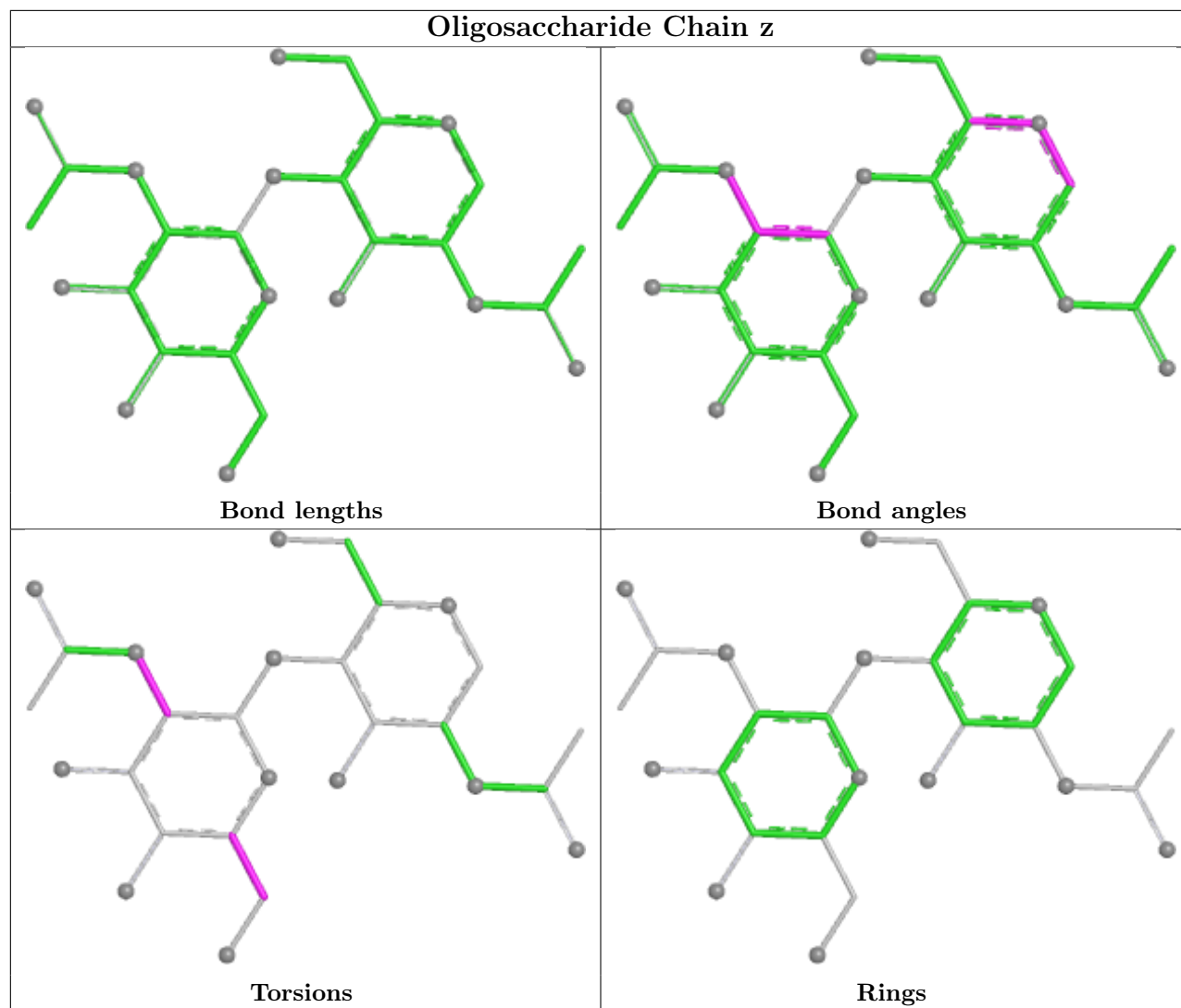


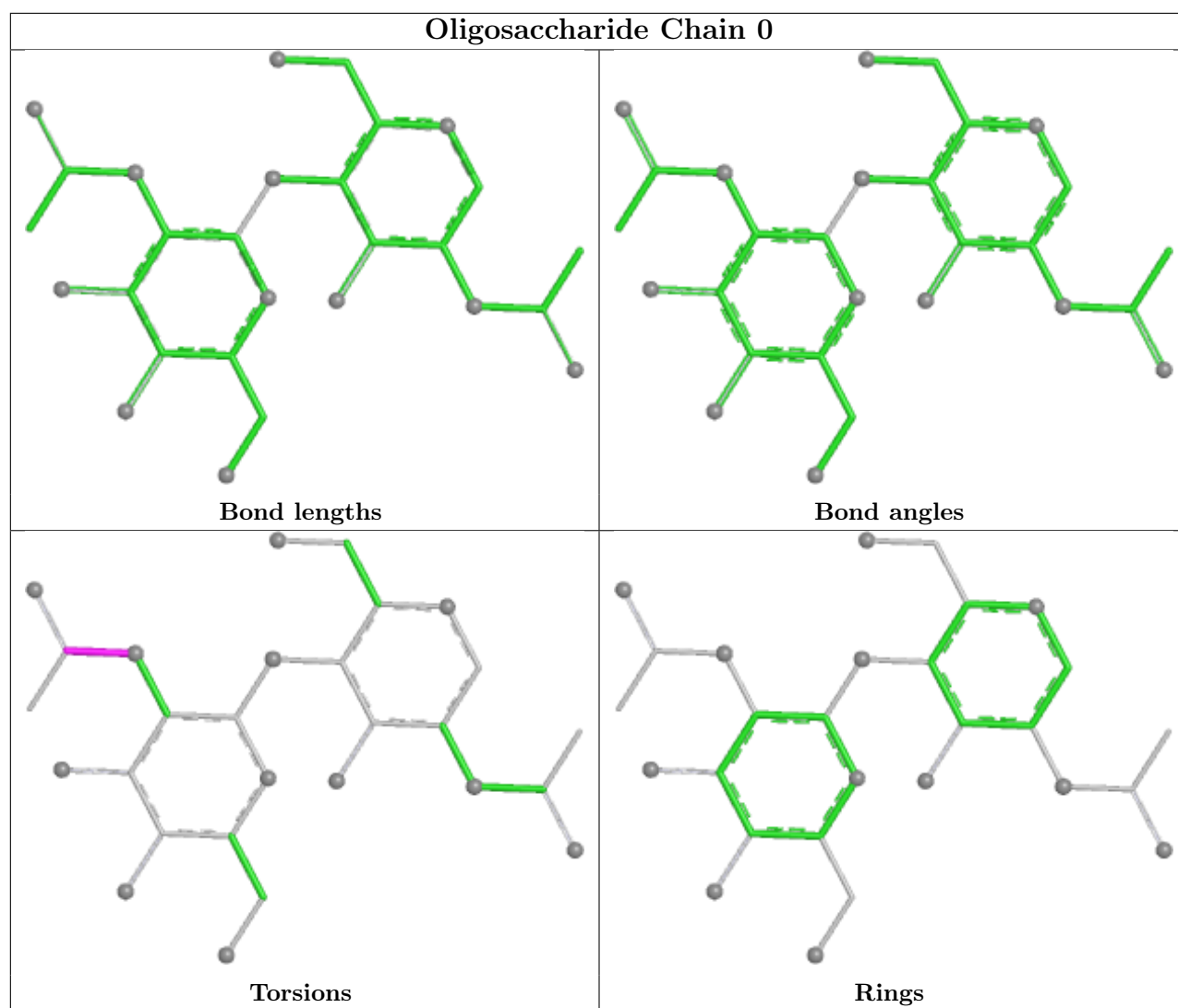


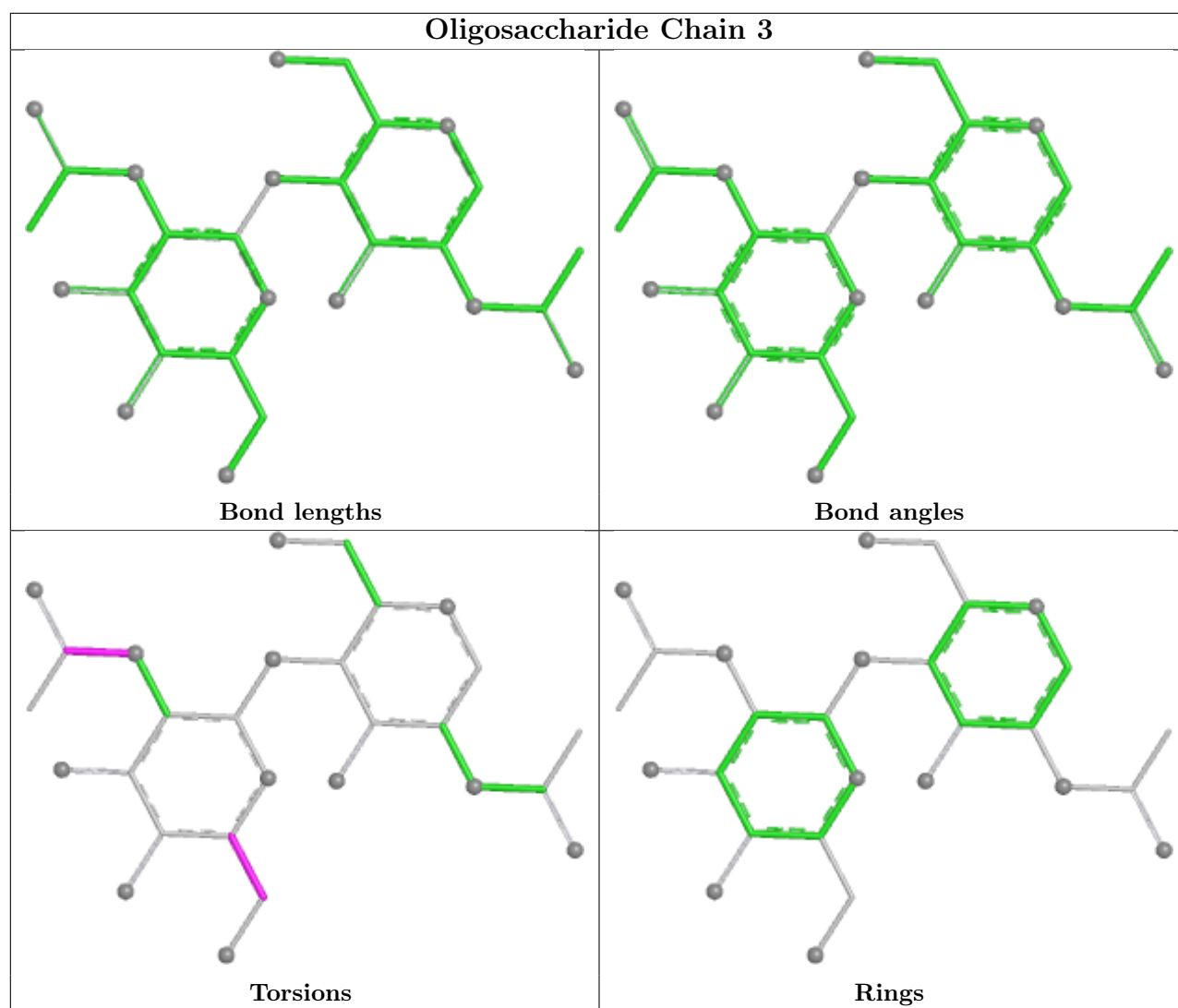


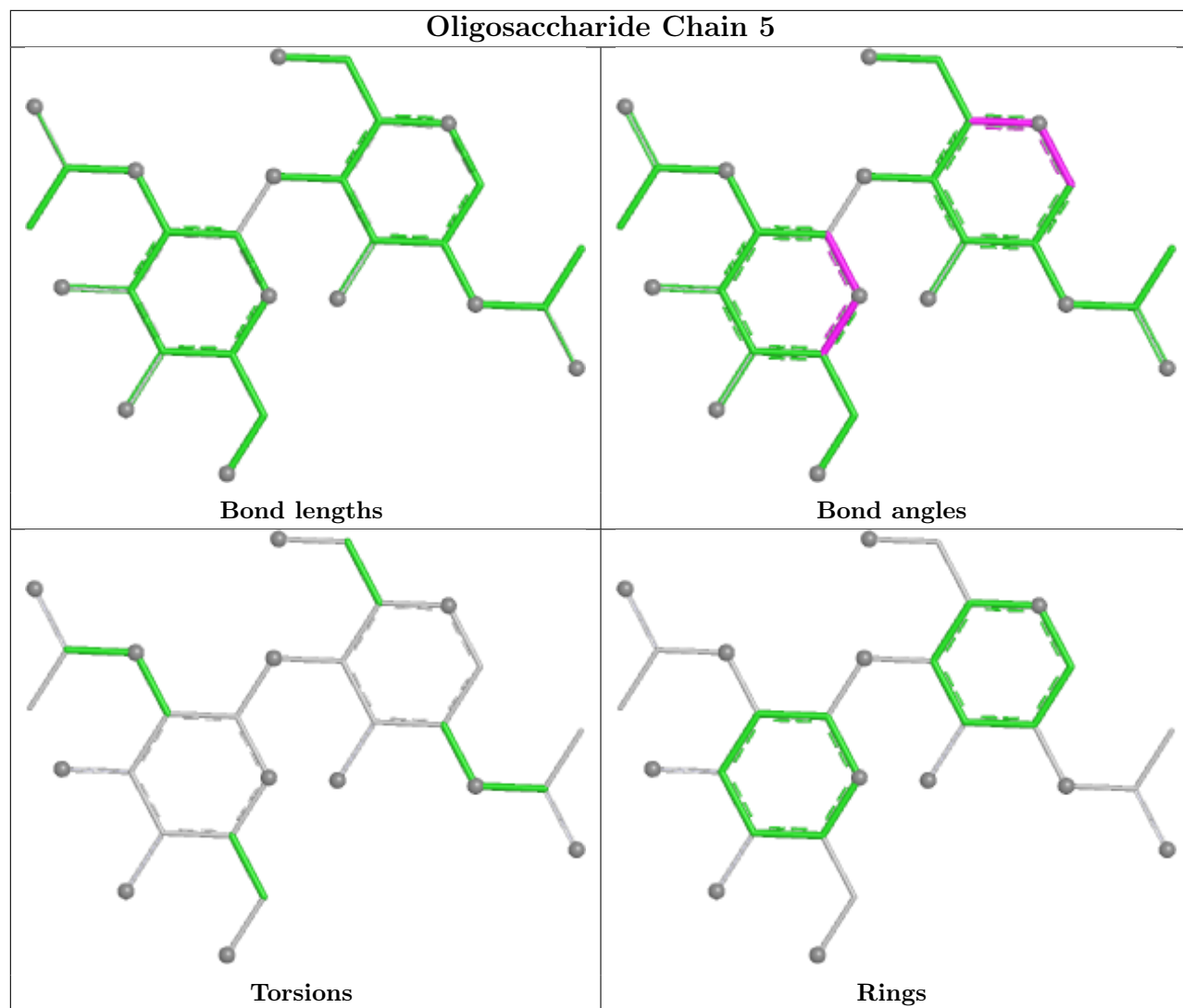


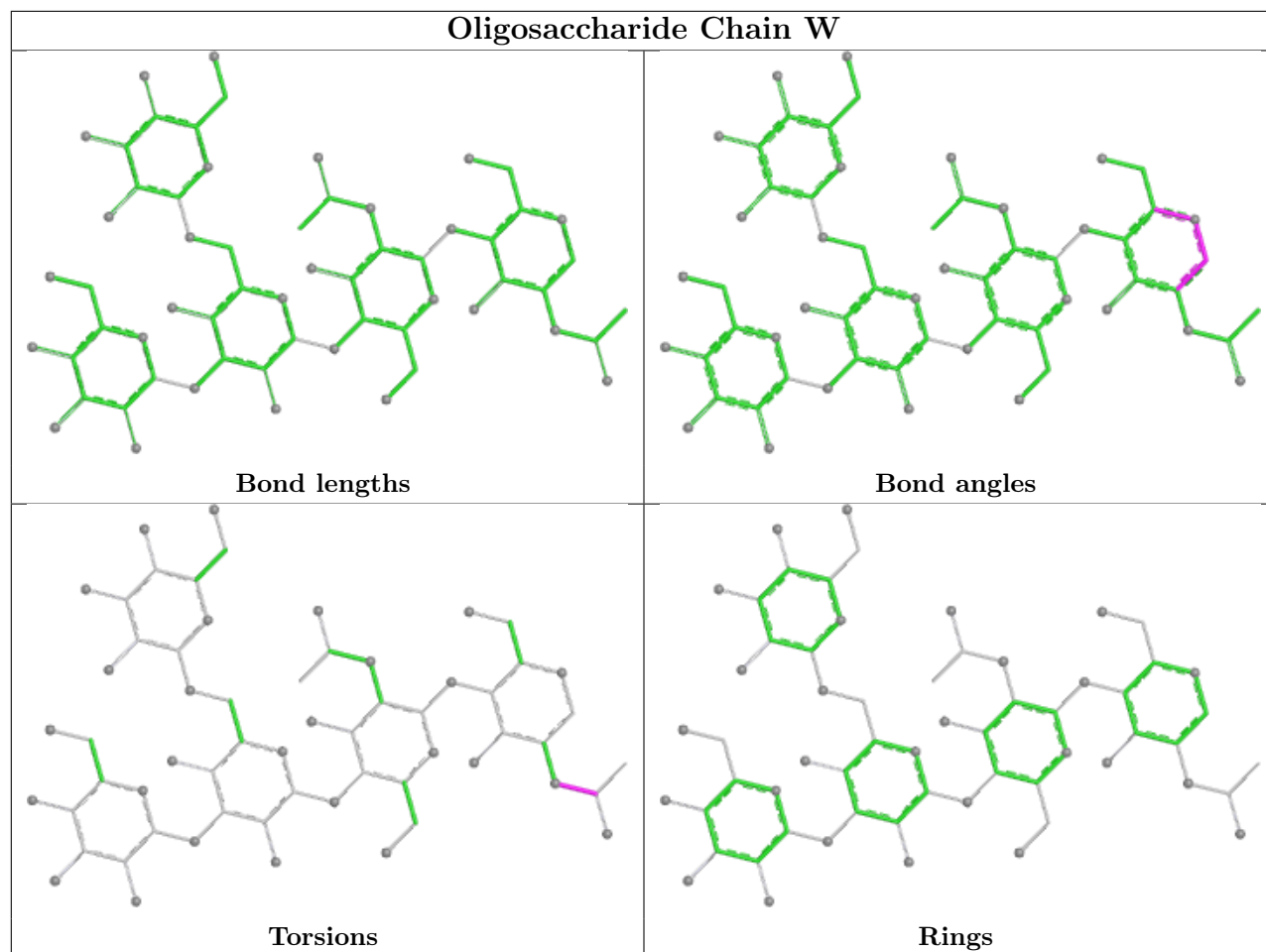


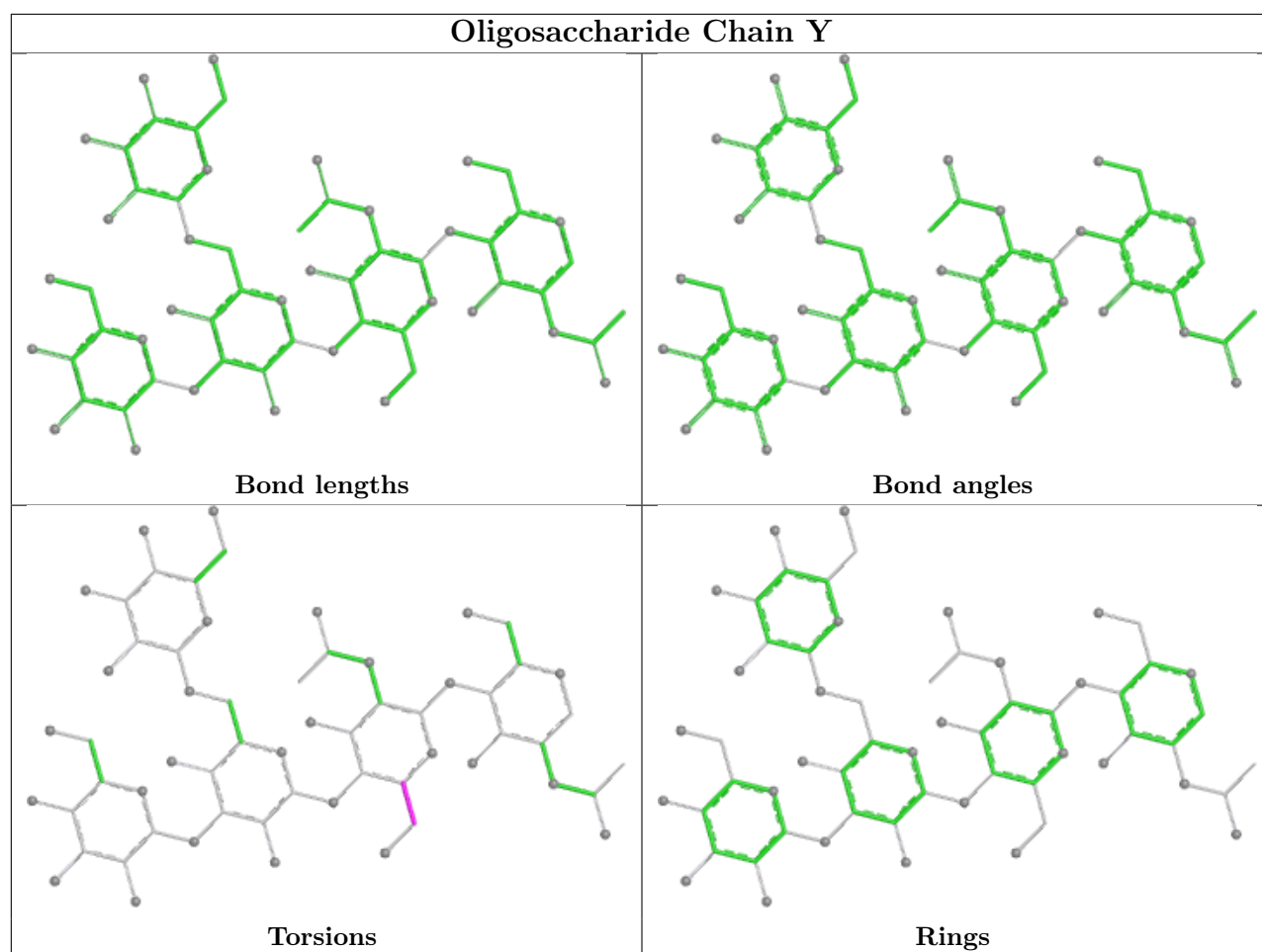


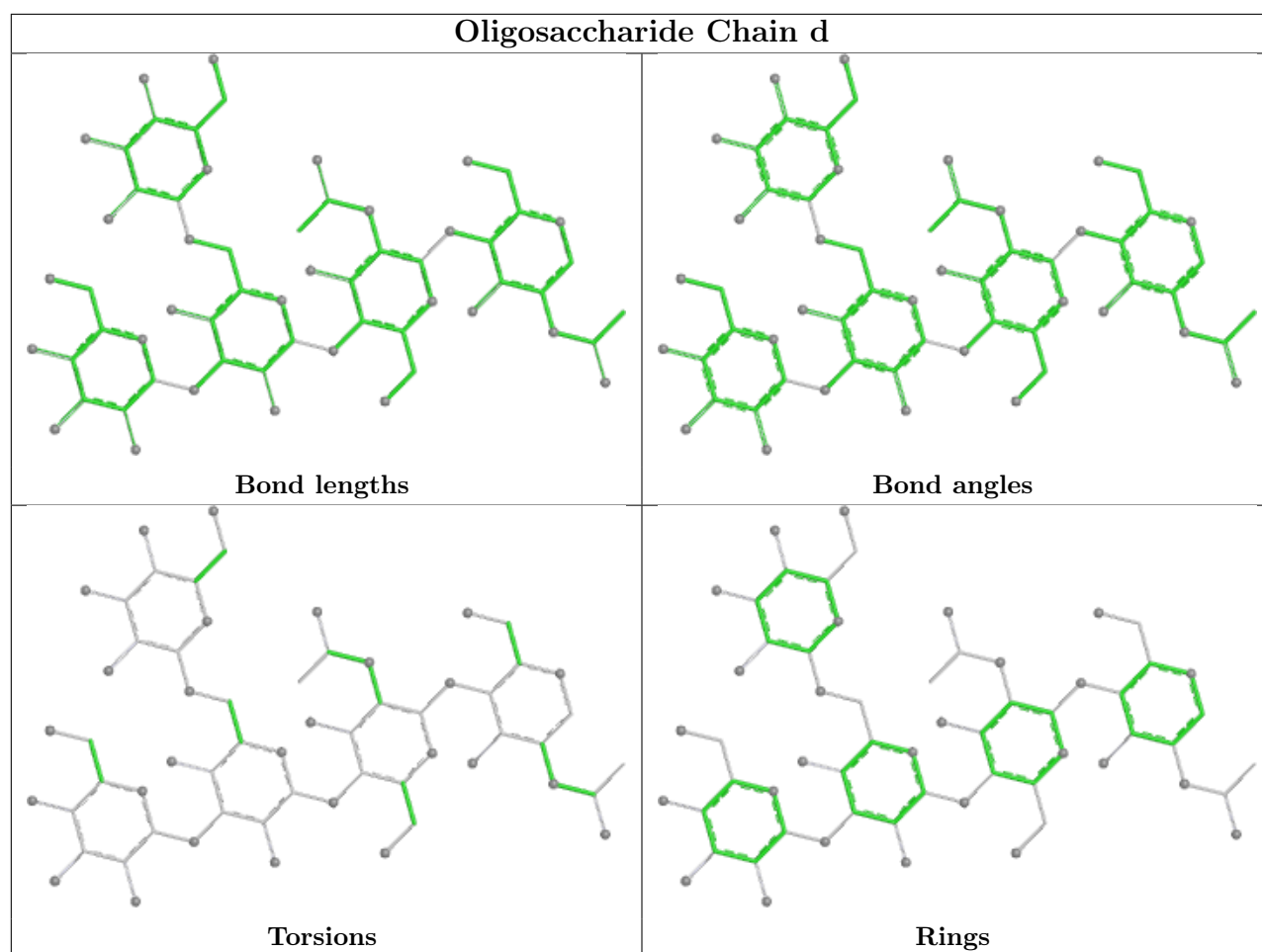


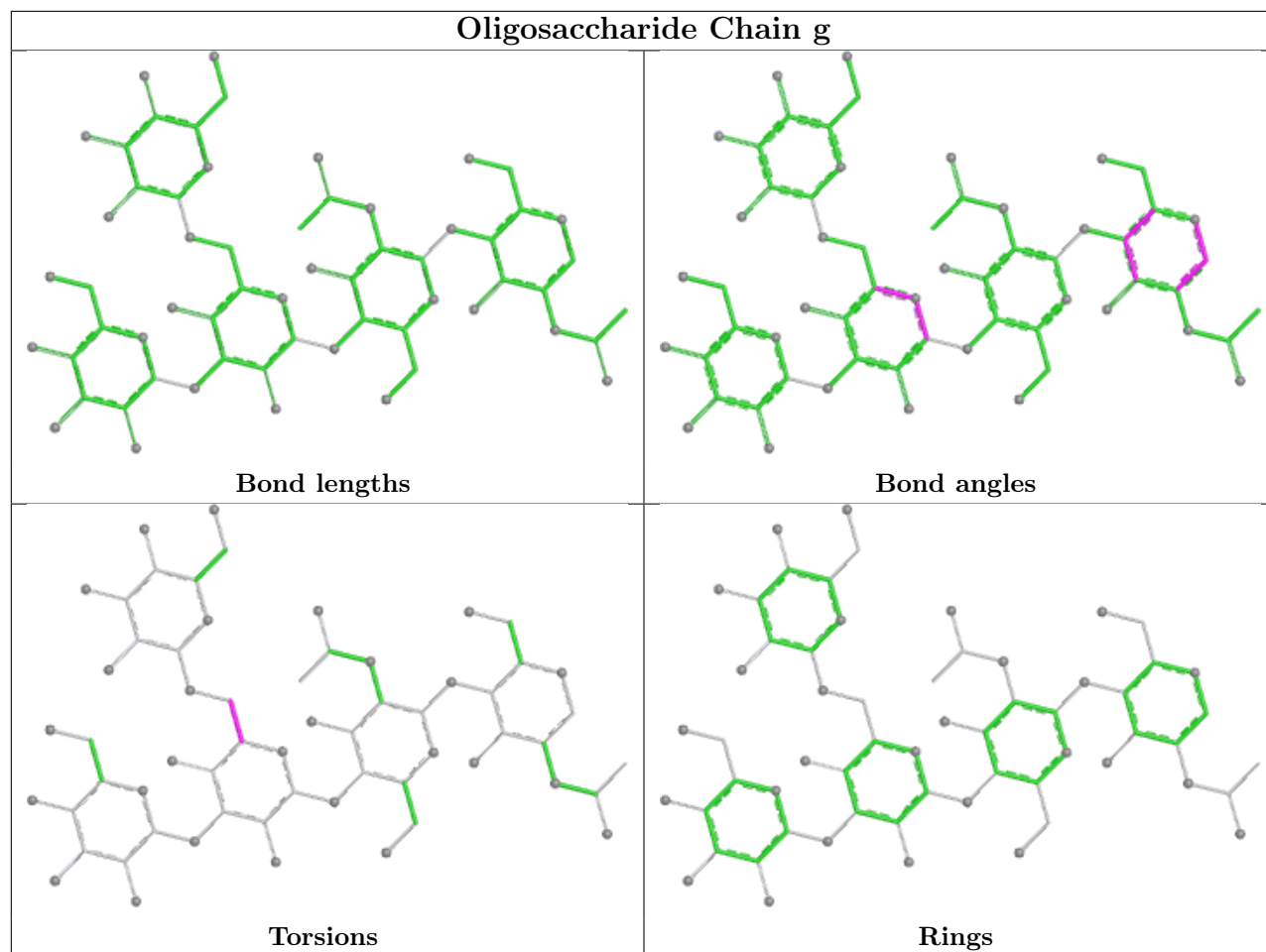


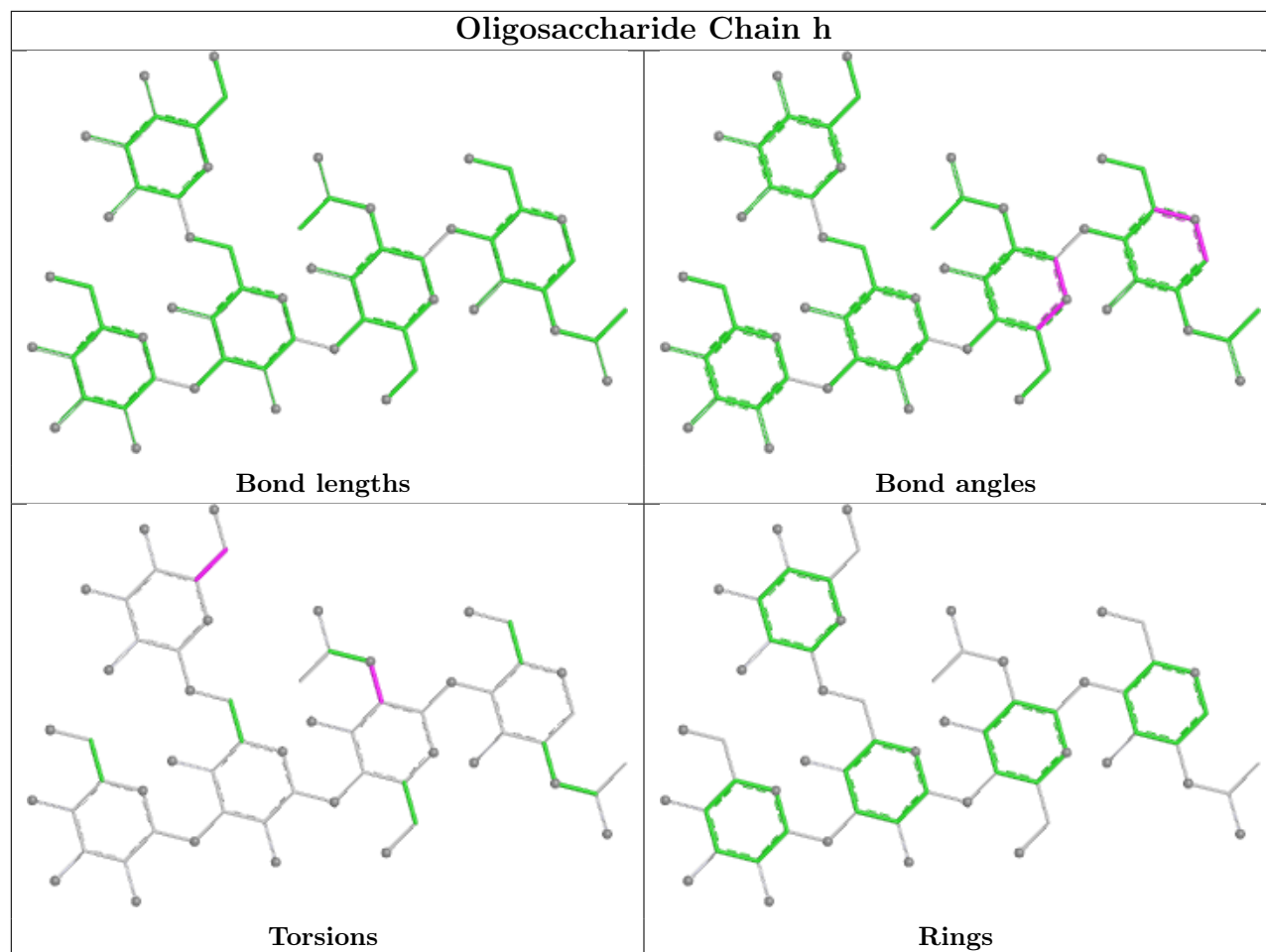


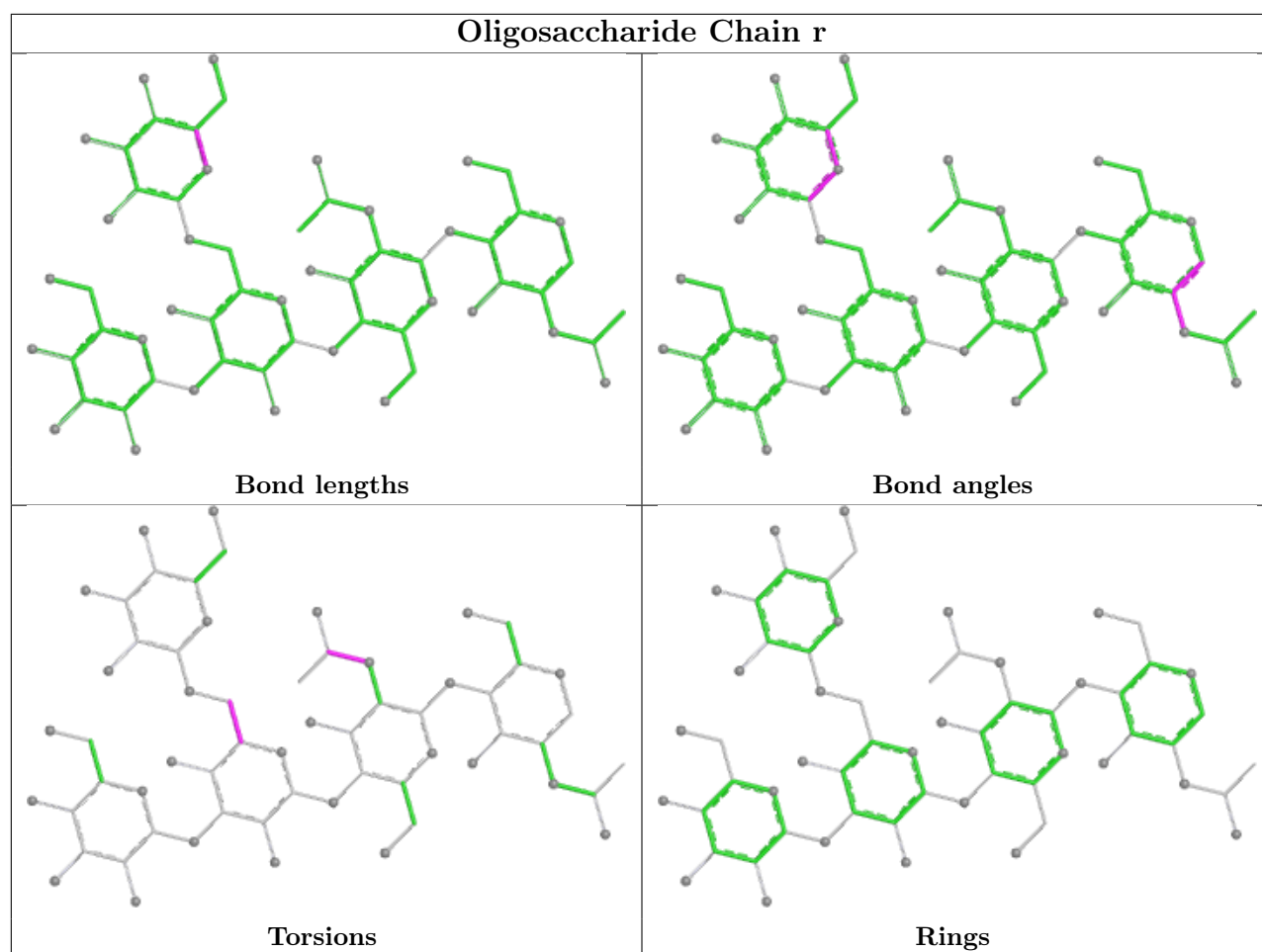


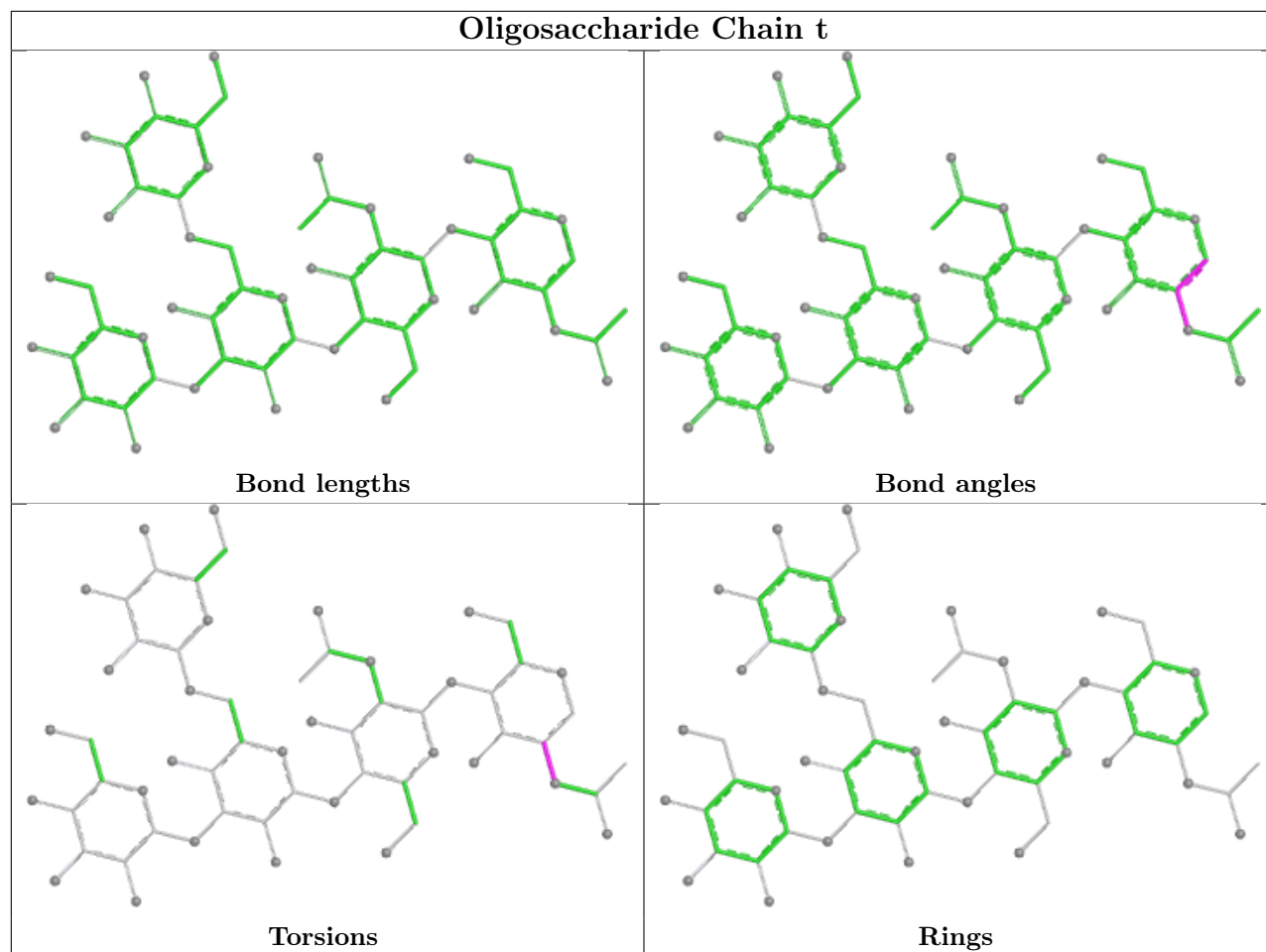


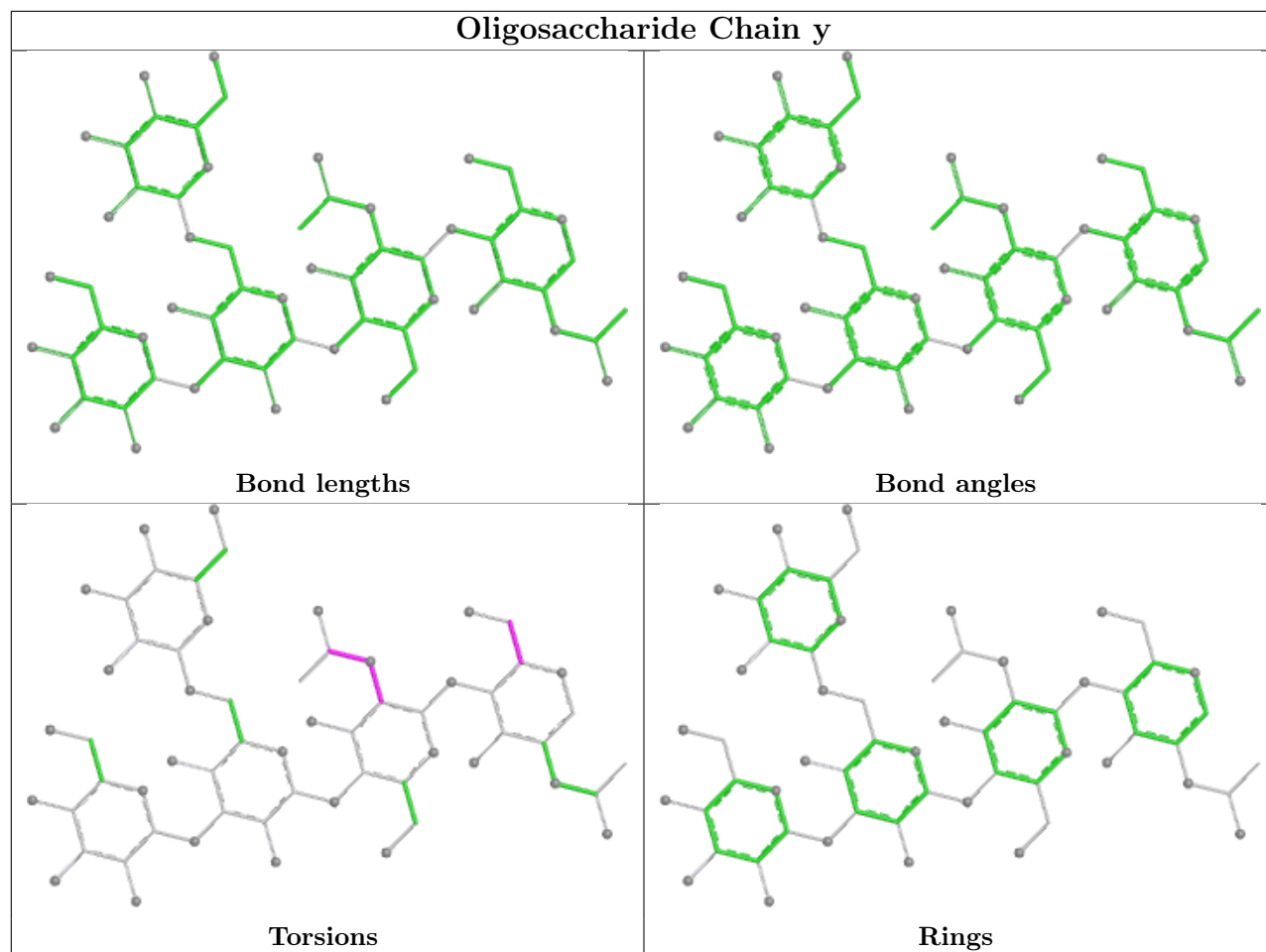


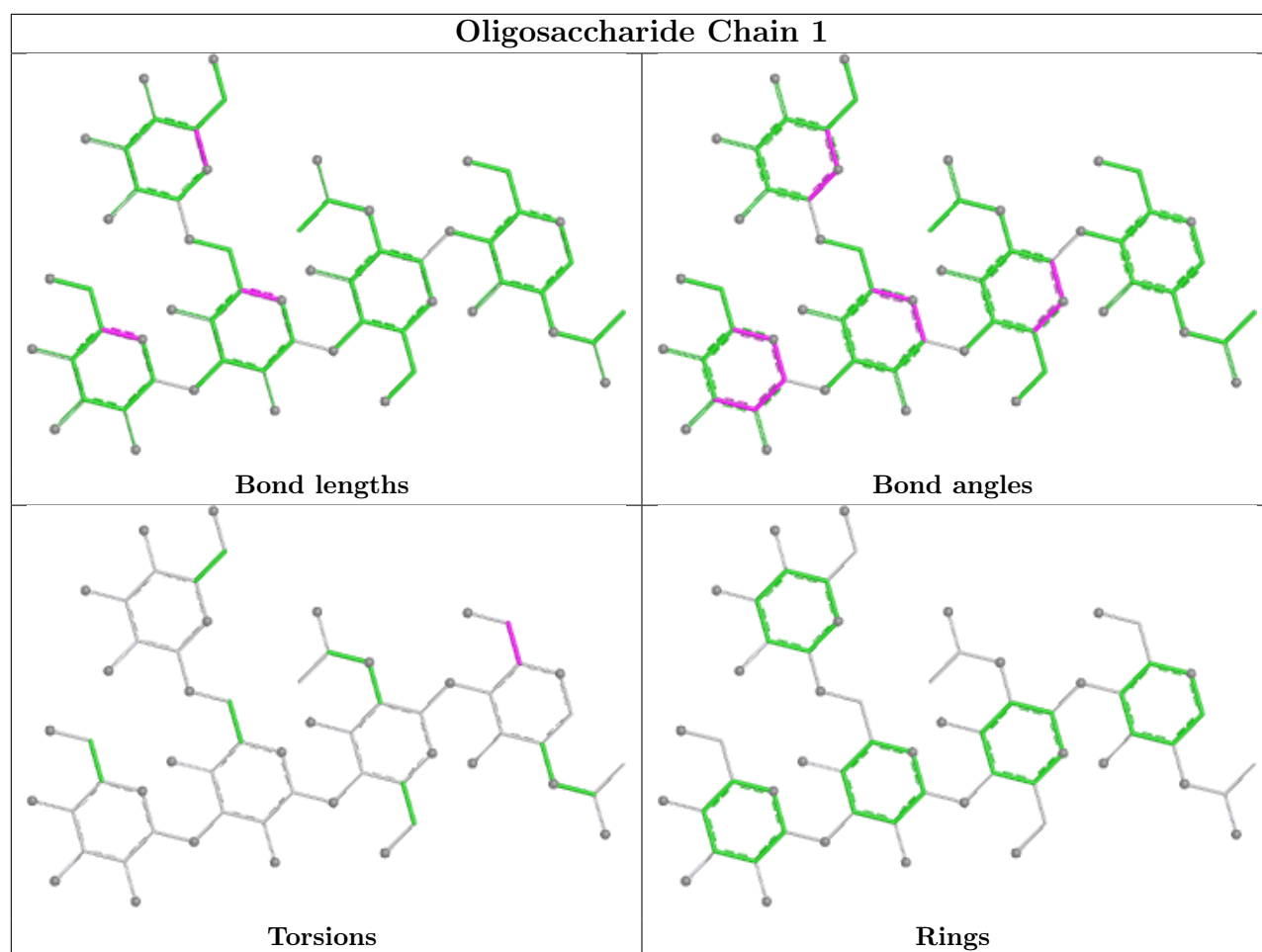


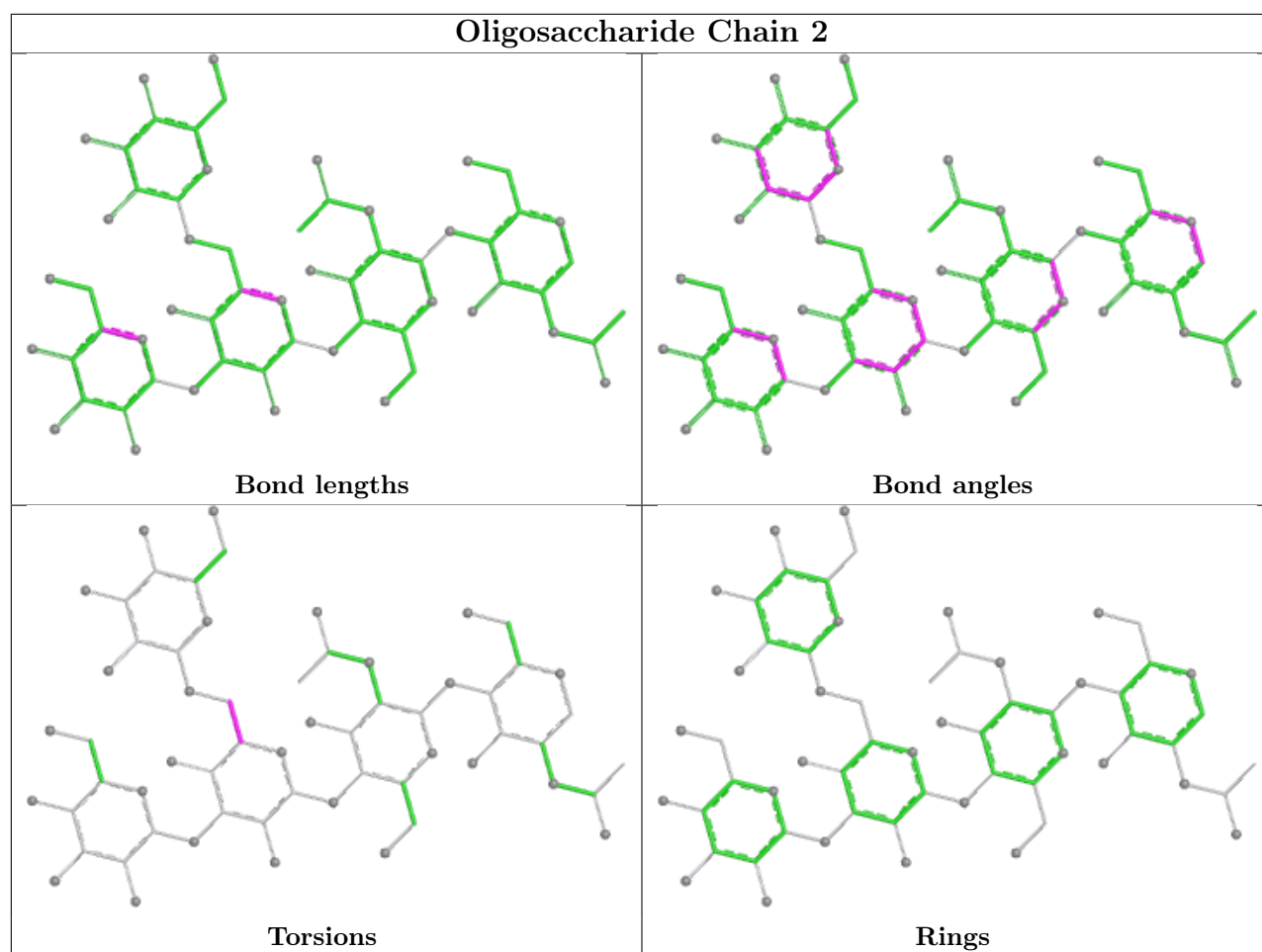


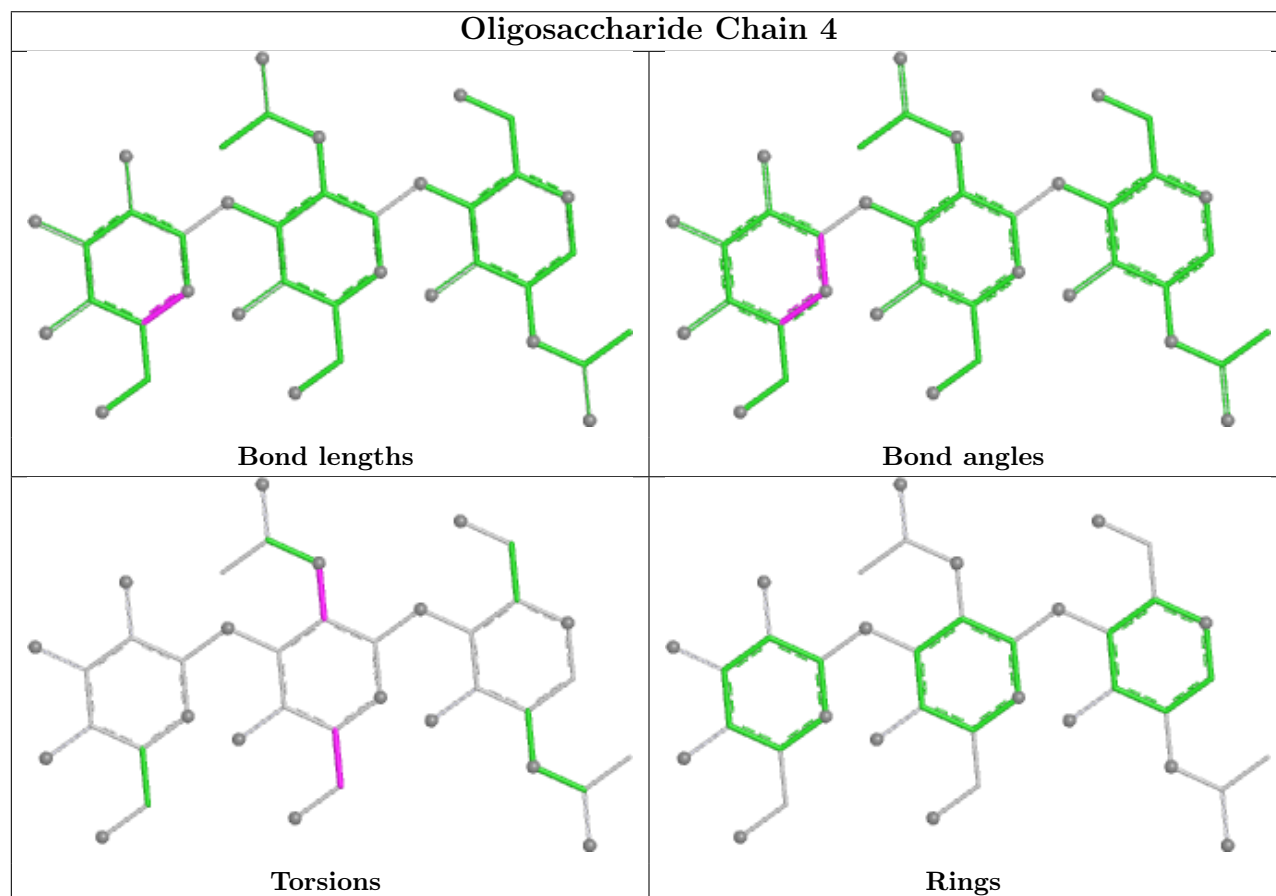
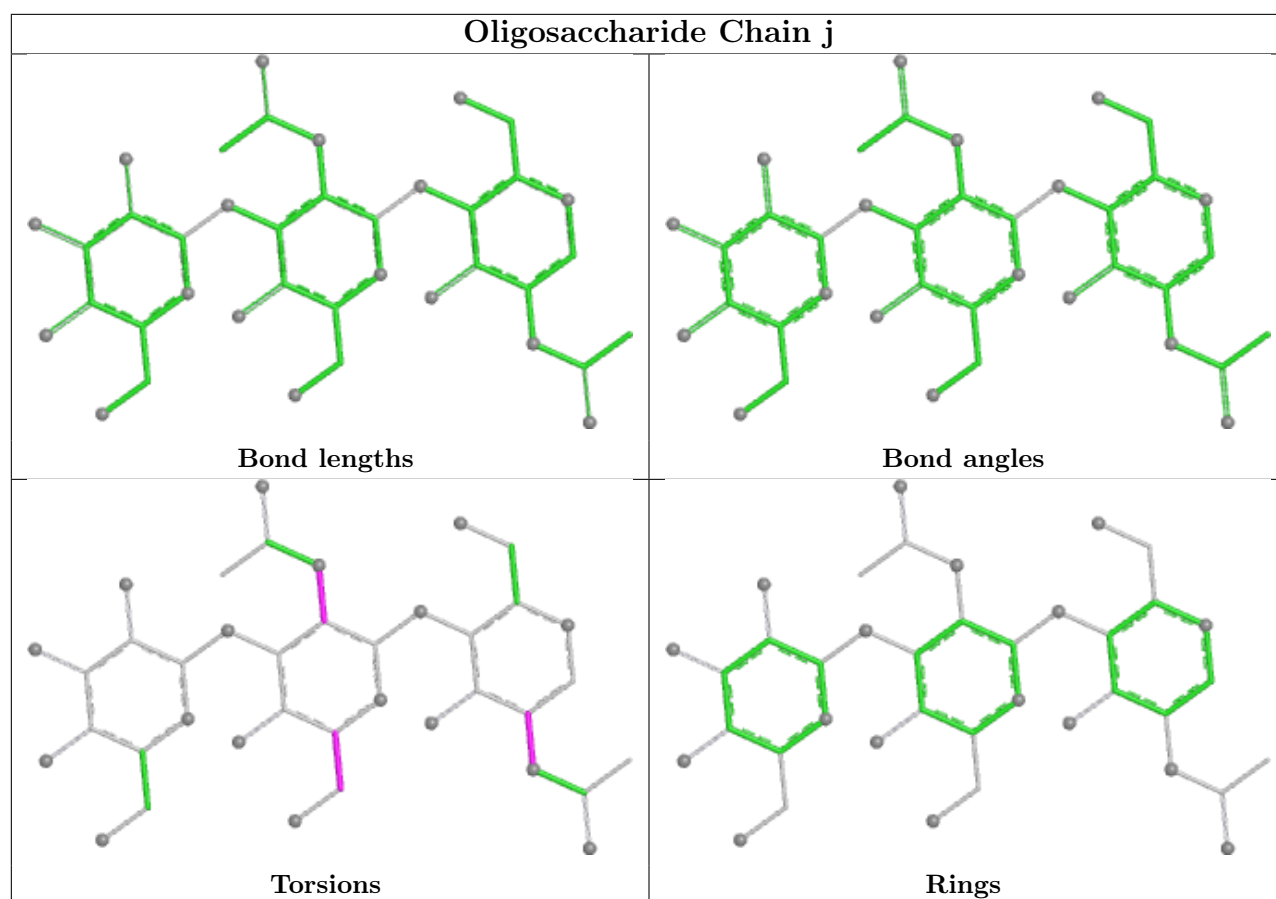












5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	A2G	A	4715	1	14,14,15	0.62	0	17,19,21	1.52	1 (5%)
12	NAG	B	4702	1	14,14,15	0.42	0	17,19,21	0.52	0
13	A2G	B	4722	1	14,14,15	0.56	0	17,19,21	0.73	0
13	A2G	B	4714	1	14,14,15	0.47	0	17,19,21	0.73	0
12	NAG	A	4701	1	14,14,15	0.40	0	17,19,21	0.39	0
13	A2G	A	4719	1	14,14,15	0.49	0	17,19,21	0.95	0
13	A2G	A	4722	1	14,14,15	0.58	0	17,19,21	1.33	2 (11%)
12	NAG	A	4711	1	14,14,15	0.56	0	17,19,21	0.79	0
12	NAG	A	4710	1	14,14,15	0.39	0	17,19,21	0.57	0
13	A2G	A	4714	1	14,14,15	0.62	0	17,19,21	0.66	0
12	NAG	A	4707	1	14,14,15	0.59	0	17,19,21	1.07	1 (5%)
12	NAG	B	4708	1	14,14,15	0.62	0	17,19,21	1.07	2 (11%)
12	NAG	B	4709	1	14,14,15	0.65	0	17,19,21	0.97	1 (5%)
13	A2G	B	4716	1	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
13	A2G	A	4713	1	14,14,15	0.48	0	17,19,21	1.13	1 (5%)
13	A2G	B	4718	1	14,14,15	0.57	0	17,19,21	1.07	2 (11%)
13	A2G	B	4721	1	14,14,15	1.17	1 (7%)	17,19,21	1.64	6 (35%)
12	NAG	B	4704	1	14,14,15	0.58	0	17,19,21	1.06	1 (5%)
12	NAG	B	4707	1	14,14,15	0.41	0	17,19,21	0.47	0
12	NAG	B	4701	1	14,14,15	0.41	0	17,19,21	0.43	0
13	A2G	B	4715	1	14,14,15	0.45	0	17,19,21	1.10	1 (5%)
12	NAG	A	4706	1	14,14,15	0.46	0	17,19,21	1.21	1 (5%)
12	NAG	A	4703	1	14,14,15	0.62	0	17,19,21	1.00	1 (5%)
13	A2G	B	4719	1	14,14,15	0.50	0	17,19,21	0.89	0
13	A2G	A	4720	1	14,14,15	0.56	0	17,19,21	1.19	1 (5%)
12	NAG	A	4705	1	14,14,15	0.64	0	17,19,21	1.06	1 (5%)
13	A2G	B	4723	1	14,14,15	0.48	0	17,19,21	0.60	0
13	A2G	B	4713	1	14,14,15	0.60	0	17,19,21	1.46	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	A2G	A	4723	1	14,14,15	0.48	0	17,19,21	0.97	2 (11%)
13	A2G	A	4717	1	14,14,15	0.60	0	17,19,21	1.63	4 (23%)
12	NAG	B	4710	1	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
12	NAG	A	4712	1	14,14,15	0.57	0	17,19,21	1.40	2 (11%)
12	NAG	B	4706	1	14,14,15	0.61	0	17,19,21	1.08	1 (5%)
13	A2G	B	4720	1	14,14,15	0.57	0	17,19,21	1.37	2 (11%)
12	NAG	A	4709	1	14,14,15	0.55	0	17,19,21	0.92	1 (5%)
12	NAG	A	4702	1	14,14,15	0.39	0	17,19,21	0.53	0
12	NAG	B	4705	1	14,14,15	0.41	0	17,19,21	0.66	0
13	A2G	B	4717	1	14,14,15	0.54	0	17,19,21	0.95	1 (5%)
12	NAG	A	4704	1	14,14,15	0.42	0	17,19,21	0.80	1 (5%)
12	NAG	A	4708	1	14,14,15	0.41	0	17,19,21	0.55	0
12	NAG	B	4711	1	14,14,15	0.67	0	17,19,21	1.16	2 (11%)
13	A2G	A	4721	1	14,14,15	0.45	0	17,19,21	1.09	1 (5%)
12	NAG	B	4712	1	14,14,15	0.41	0	17,19,21	0.56	0
13	A2G	A	4716	1	14,14,15	0.45	0	17,19,21	1.05	2 (11%)
13	A2G	A	4718	1	14,14,15	0.62	0	17,19,21	0.99	1 (5%)
12	NAG	B	4703	1	14,14,15	0.65	0	17,19,21	1.16	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	A2G	A	4715	1	-	2/6/23/26	0/1/1/1
12	NAG	B	4702	1	-	3/6/23/26	0/1/1/1
13	A2G	B	4722	1	-	0/6/23/26	0/1/1/1
13	A2G	B	4714	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4701	1	-	2/6/23/26	0/1/1/1
13	A2G	A	4719	1	-	0/6/23/26	0/1/1/1
13	A2G	A	4722	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4711	1	-	2/6/23/26	0/1/1/1
12	NAG	A	4710	1	-	3/6/23/26	0/1/1/1
13	A2G	A	4714	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4707	1	-	1/6/23/26	0/1/1/1
12	NAG	B	4708	1	-	0/6/23/26	0/1/1/1
12	NAG	B	4709	1	-	0/6/23/26	0/1/1/1

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	A2G	B	4716	1	-	0/6/23/26	0/1/1/1
13	A2G	A	4713	1	-	0/6/23/26	0/1/1/1
13	A2G	B	4718	1	-	0/6/23/26	0/1/1/1
13	A2G	B	4721	1	-	1/6/23/26	0/1/1/1
12	NAG	B	4704	1	-	1/6/23/26	0/1/1/1
12	NAG	B	4707	1	-	0/6/23/26	0/1/1/1
12	NAG	B	4701	1	-	1/6/23/26	0/1/1/1
13	A2G	B	4715	1	-	1/6/23/26	0/1/1/1
12	NAG	A	4706	1	-	3/6/23/26	0/1/1/1
12	NAG	A	4703	1	-	0/6/23/26	0/1/1/1
13	A2G	B	4719	1	-	0/6/23/26	0/1/1/1
13	A2G	A	4720	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4705	1	-	2/6/23/26	0/1/1/1
13	A2G	B	4723	1	-	0/6/23/26	0/1/1/1
13	A2G	B	4713	1	-	1/6/23/26	0/1/1/1
13	A2G	A	4723	1	-	1/6/23/26	0/1/1/1
13	A2G	A	4717	1	-	3/6/23/26	0/1/1/1
12	NAG	B	4710	1	-	1/6/23/26	0/1/1/1
12	NAG	A	4712	1	-	0/6/23/26	0/1/1/1
12	NAG	B	4706	1	-	3/6/23/26	0/1/1/1
13	A2G	B	4720	1	-	2/6/23/26	0/1/1/1
12	NAG	A	4709	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4702	1	-	0/6/23/26	0/1/1/1
12	NAG	B	4705	1	-	3/6/23/26	0/1/1/1
13	A2G	B	4717	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4704	1	-	0/6/23/26	0/1/1/1
12	NAG	A	4708	1	-	0/6/23/26	0/1/1/1
12	NAG	B	4711	1	-	0/6/23/26	0/1/1/1
13	A2G	A	4721	1	-	0/6/23/26	0/1/1/1
12	NAG	B	4712	1	-	3/6/23/26	0/1/1/1
13	A2G	A	4716	1	-	0/6/23/26	0/1/1/1
13	A2G	A	4718	1	-	1/6/23/26	0/1/1/1
12	NAG	B	4703	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	4721	A2G	O5-C1	-2.68	1.39	1.43

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	4715	A2G	C2-N2-C7	4.94	129.52	122.90
13	A	4717	A2G	C1-O5-C5	-4.73	105.85	112.19
13	A	4722	A2G	C1-O5-C5	-4.43	106.25	112.19
13	B	4720	A2G	C1-O5-C5	-4.18	106.58	112.19
12	A	4706	NAG	C1-O5-C5	4.09	117.66	112.19

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	4710	NAG	C1-C2-N2-C7
12	A	4710	NAG	C8-C7-N2-C2
12	A	4710	NAG	O7-C7-N2-C2
12	B	4702	NAG	C1-C2-N2-C7
12	B	4702	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	4704	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.

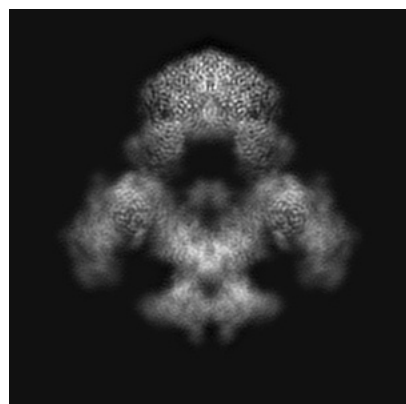
6 Map visualisation [i](#)

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

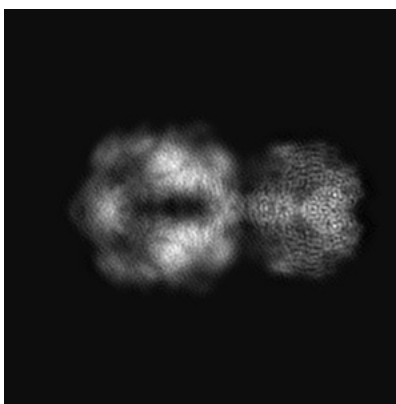
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

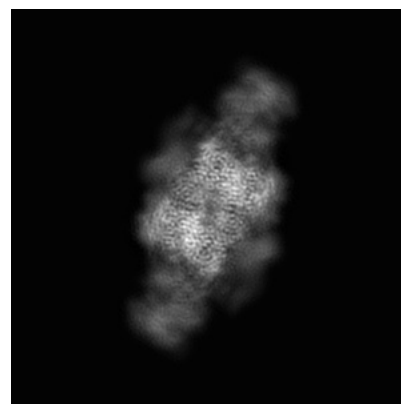
6.1.1 Primary map



X

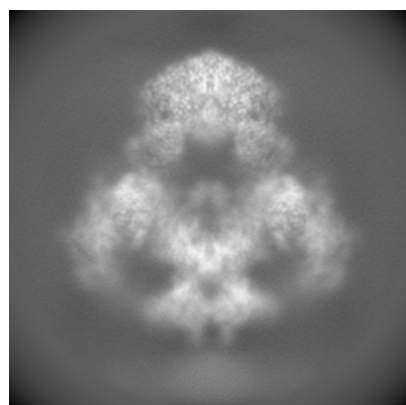


Y

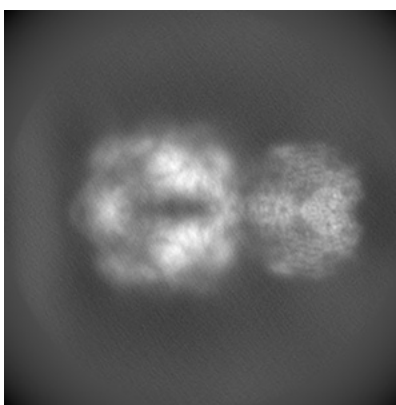


Z

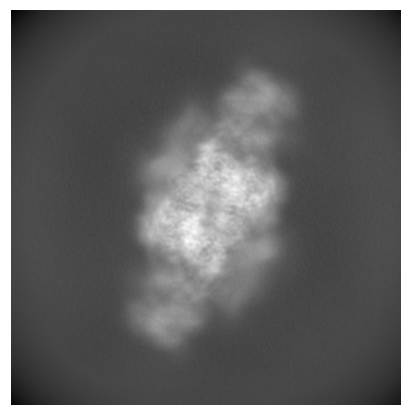
6.1.2 Raw map



X



Y

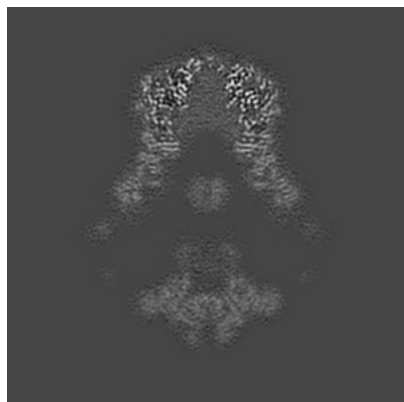


Z

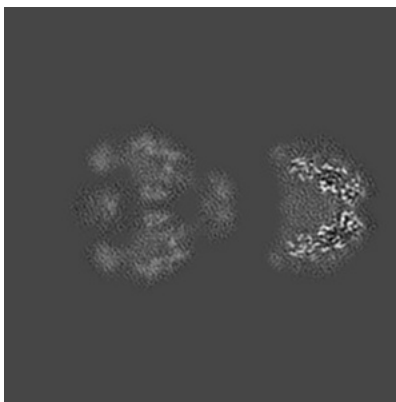
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 130

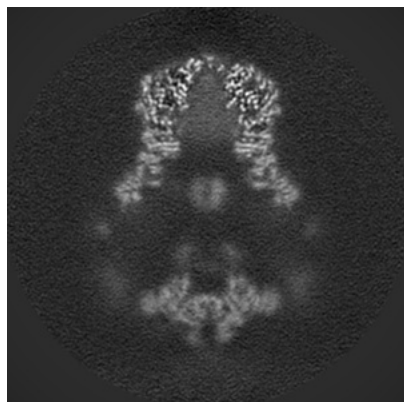


Y Index: 130

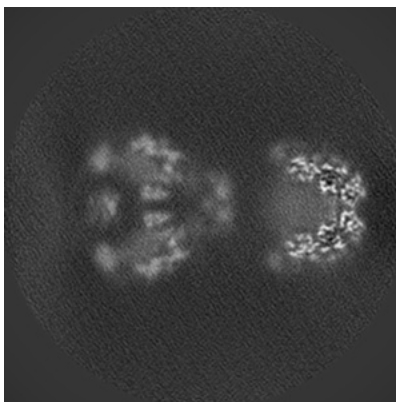


Z Index: 130

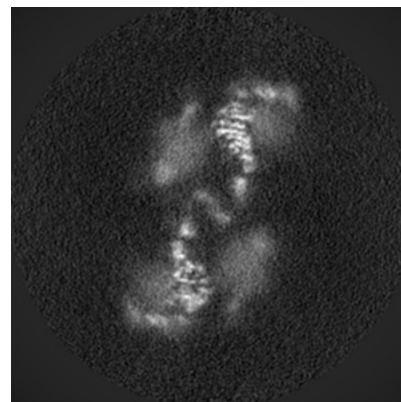
6.2.2 Raw map



X Index: 130



Y Index: 130

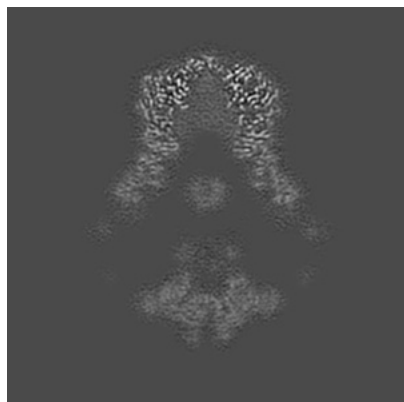


Z Index: 130

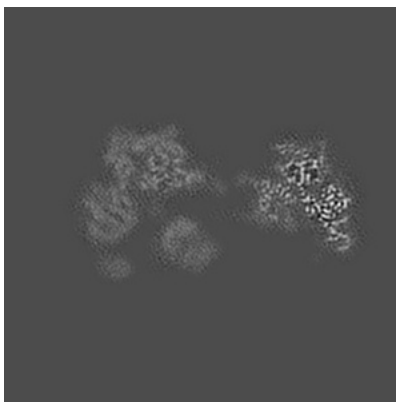
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

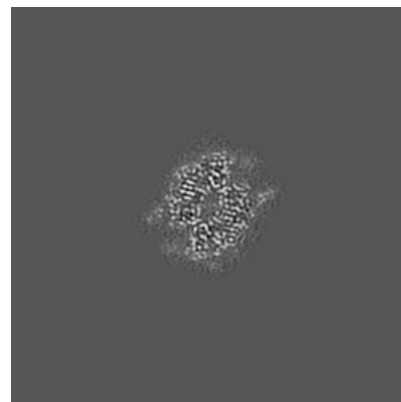
6.3.1 Primary map



X Index: 131

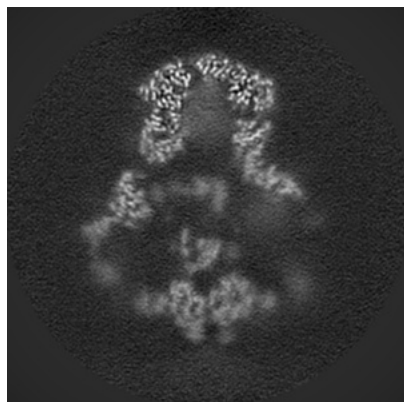


Y Index: 149

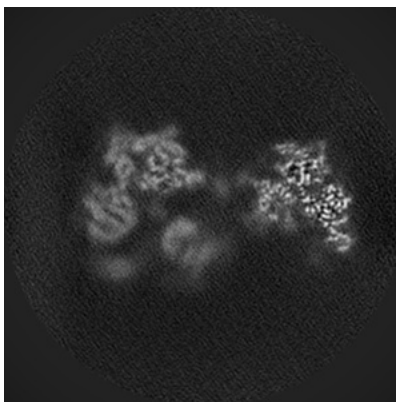


Z Index: 215

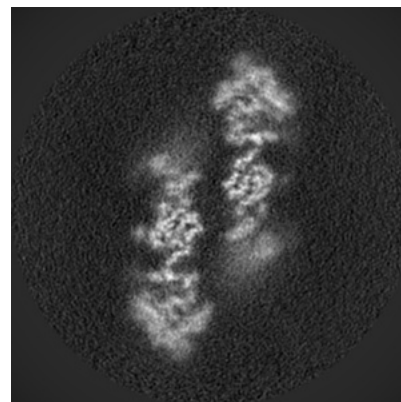
6.3.2 Raw map



X Index: 124



Y Index: 149

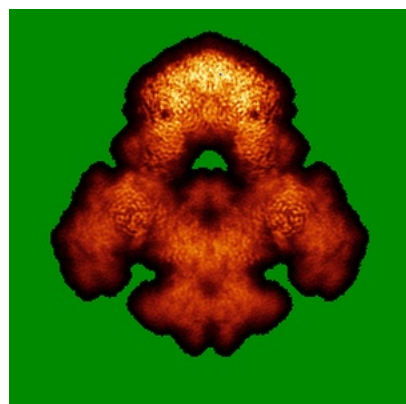


Z Index: 113

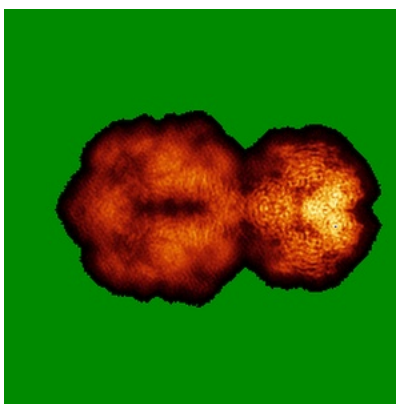
The images above show the largest variance slices of the map in three orthogonal directions.

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

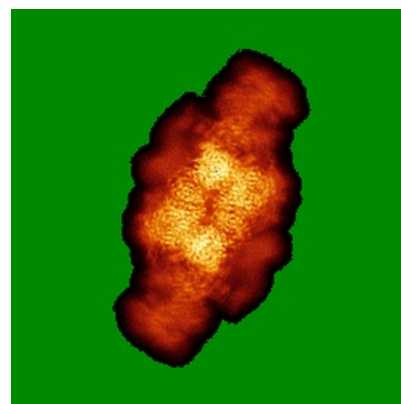
6.4.1 Primary map



X

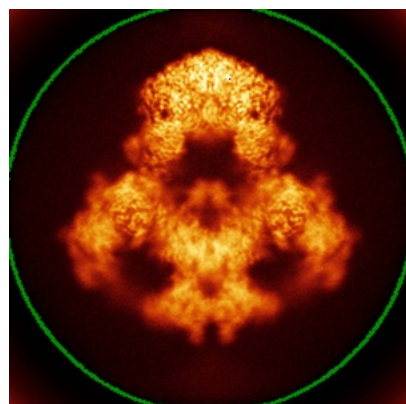


Y

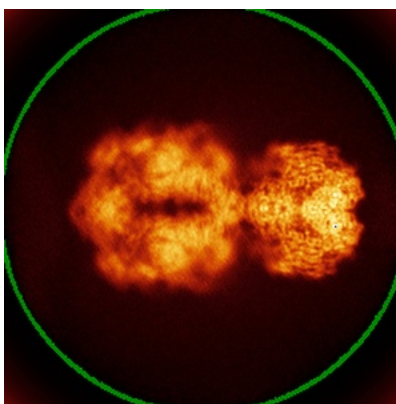


Z

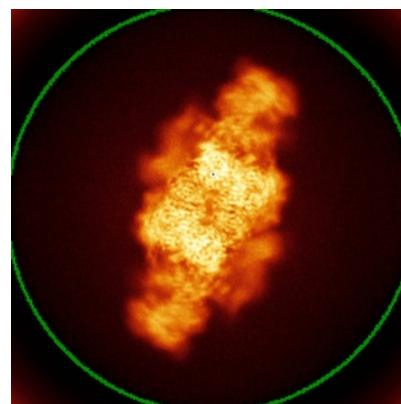
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

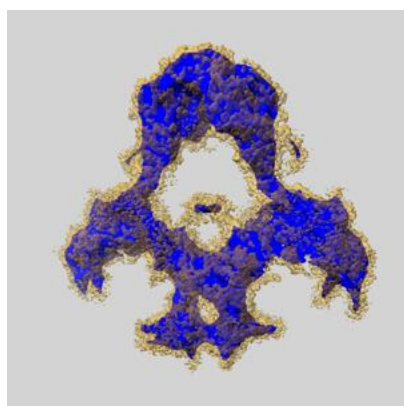
6.6 Mask visualisation [i](#)

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

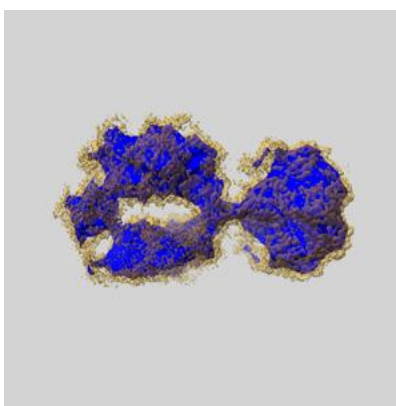
A mask typically either:

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

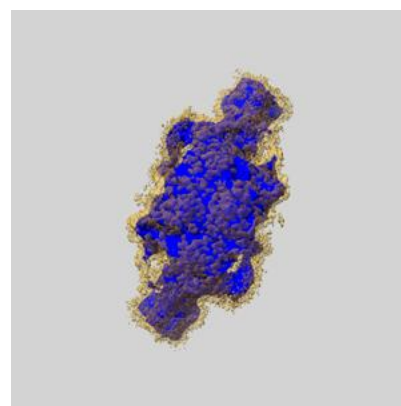
6.6.1 emd_36664_msk_1.map [i](#)



X



Y

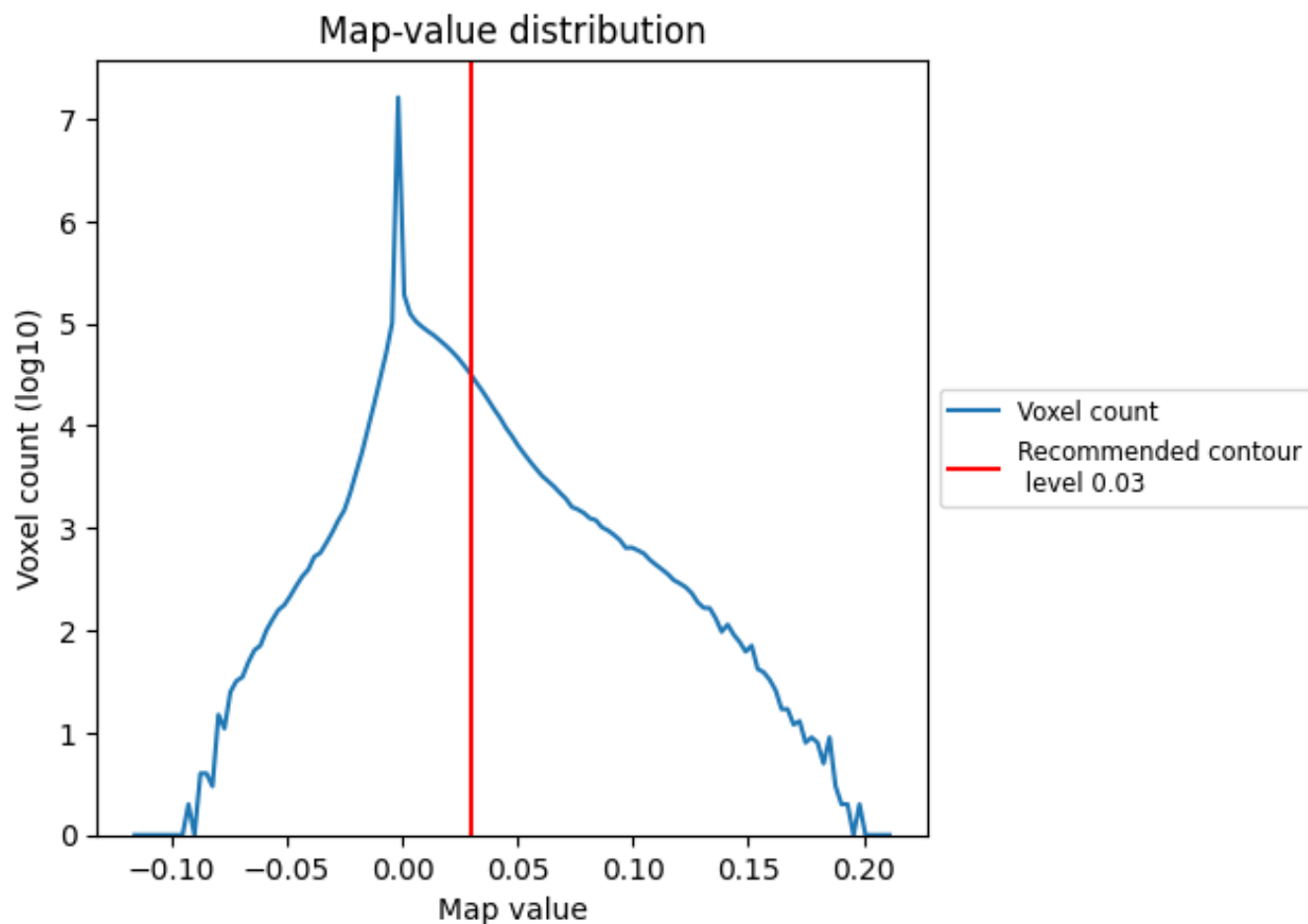


Z

7 Map analysis [i](#)

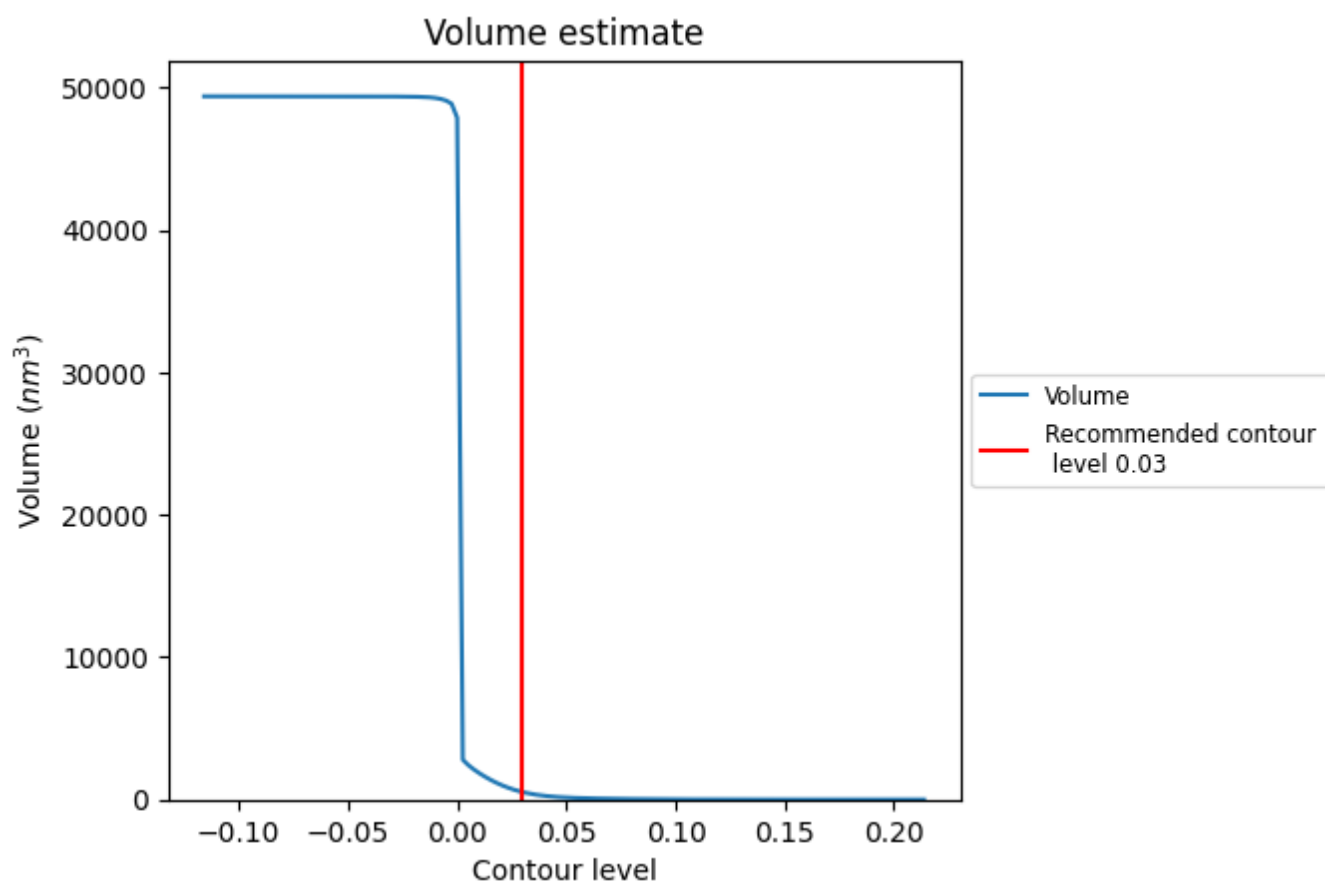
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

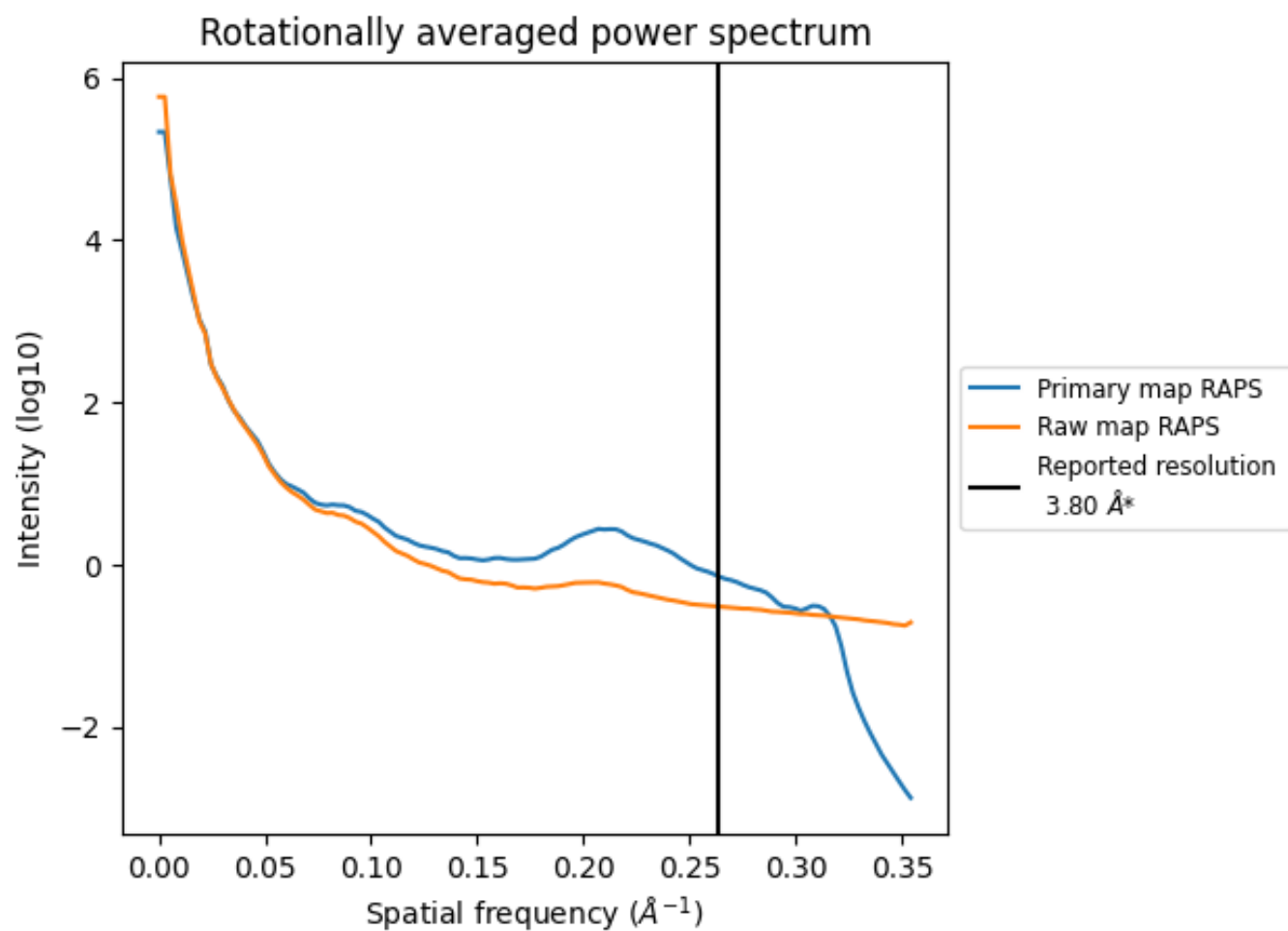
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

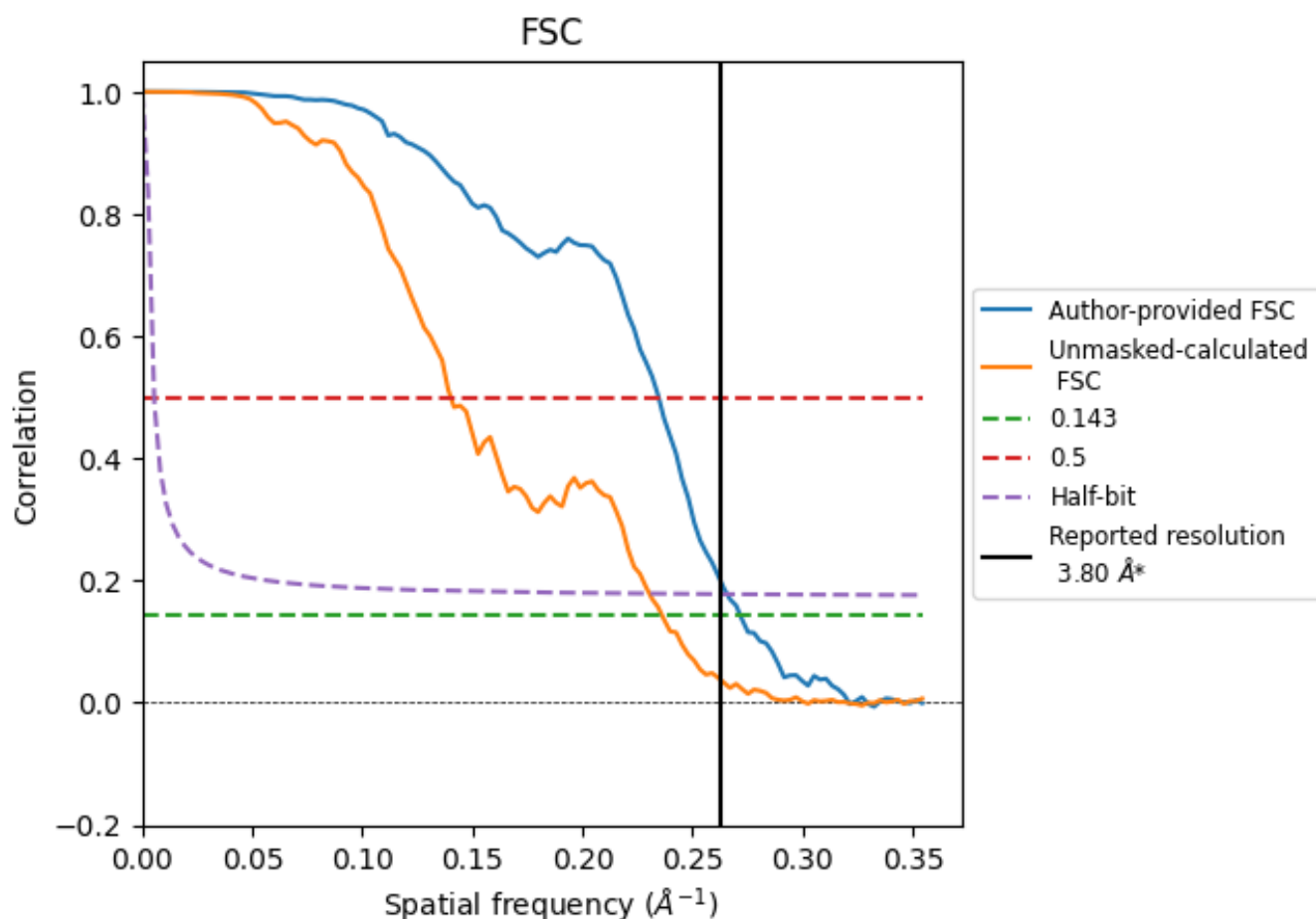


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

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

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

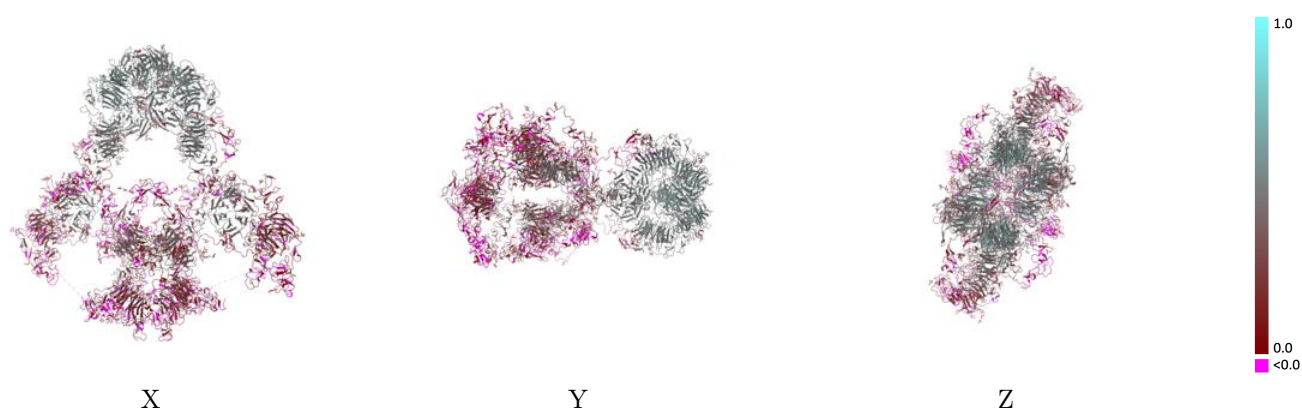
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-36664 and PDB model 8JUU. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay ⓘ

This section was not generated.

9.2 Q-score mapped to coordinate model ⓘ

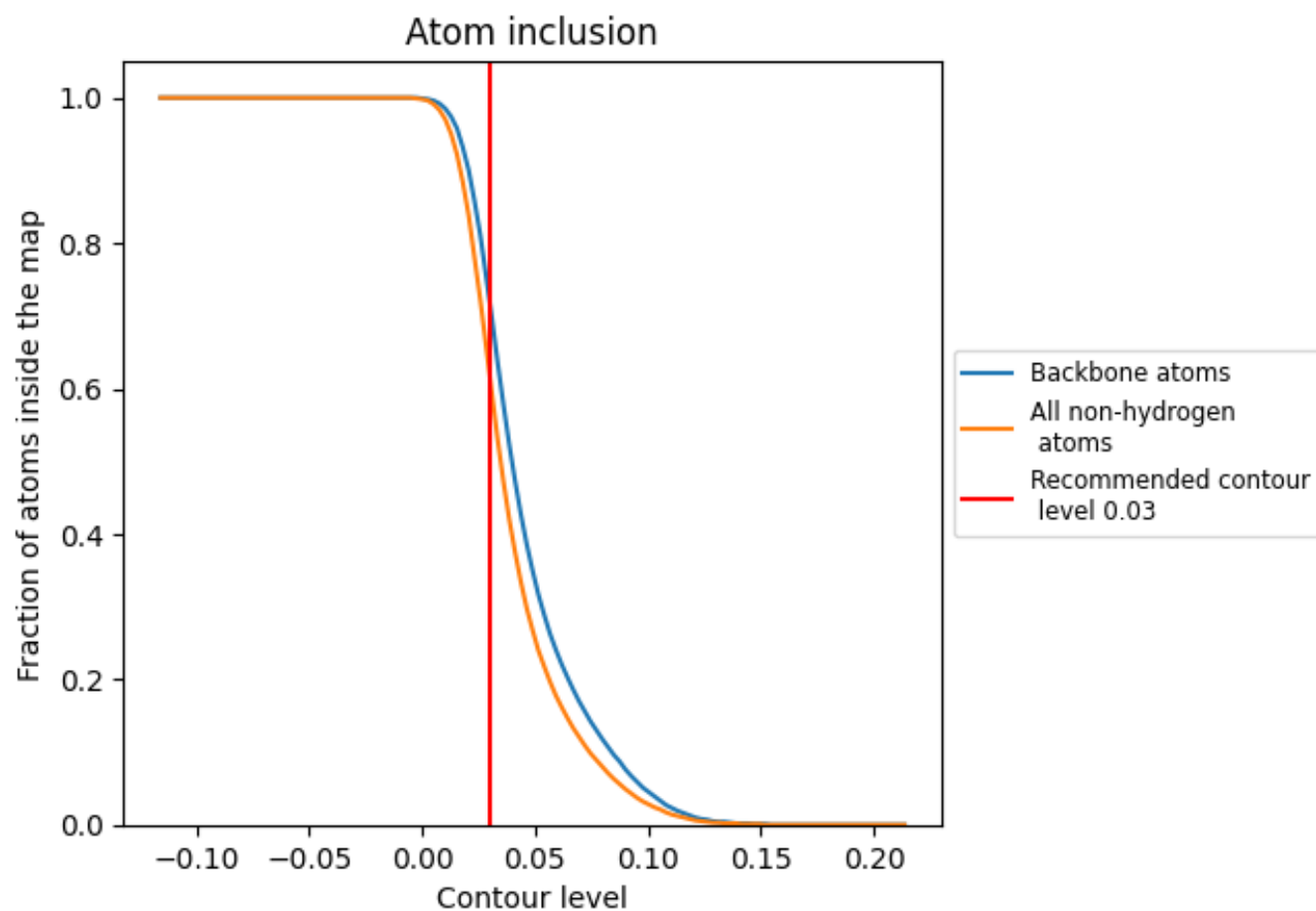


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

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



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