



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:22 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 Full wwPDB EM Validation 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

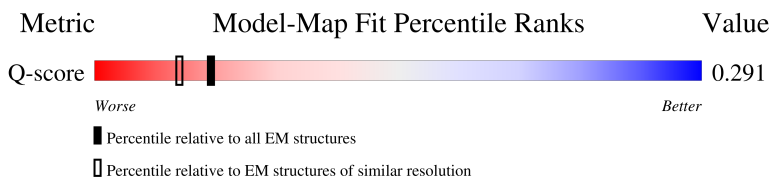
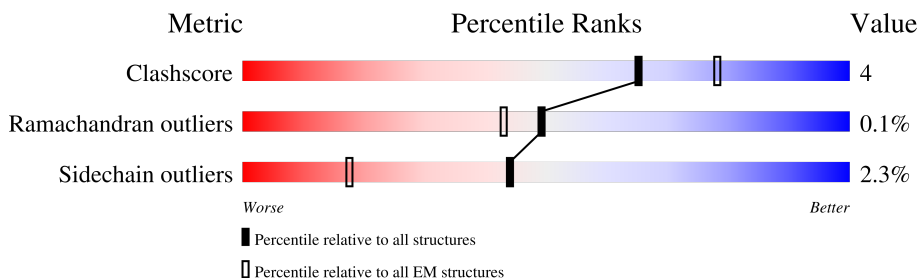
1 Overall quality at a glance

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	
9	V	2	
9	X	2	
9	Z	2	
9	a	2	
9	e	2	
9	f	2	
9	i	2	
9	k	2	
9	m	2	
9	n	2	
9	p	2	
9	q	2	
9	s	2	
9	u	2	
9	v	2	
9	z	2	
10	1	5	
10	2	5	
10	W	5	
10	Y	5	
10	d	5	
10	g	5	
10	h	5	
10	r	5	

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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		

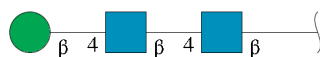
- Molecule 6 is a protein called unclear peptide.

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.



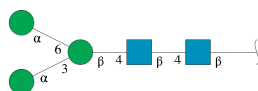
Mol	Chain	Residues	Atoms				AltConf	Trace
9	F	2	Total	C	N	O	0	0
			28	16	2	10		
9	S	2	Total	C	N	O	0	0
			28	16	2	10		
9	U	2	Total	C	N	O	0	0
			28	16	2	10		
9	V	2	Total	C	N	O	0	0
			28	16	2	10		
9	X	2	Total	C	N	O	0	0
			28	16	2	10		
9	Z	2	Total	C	N	O	0	0
			28	16	2	10		
9	a	2	Total	C	N	O	0	0
			28	16	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.



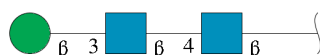
Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	5	Total	C	N	O	0	0
			61	34	2	25		
10	Y	5	Total	C	N	O	0	0
			61	34	2	25		
10	d	5	Total	C	N	O	0	0
			61	34	2	25		
10	g	5	Total	C	N	O	0	0
			61	34	2	25		
10	h	5	Total	C	N	O	0	0
			61	34	2	25		
10	r	5	Total	C	N	O	0	0
			61	34	2	25		
10	t	5	Total	C	N	O	0	0
	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

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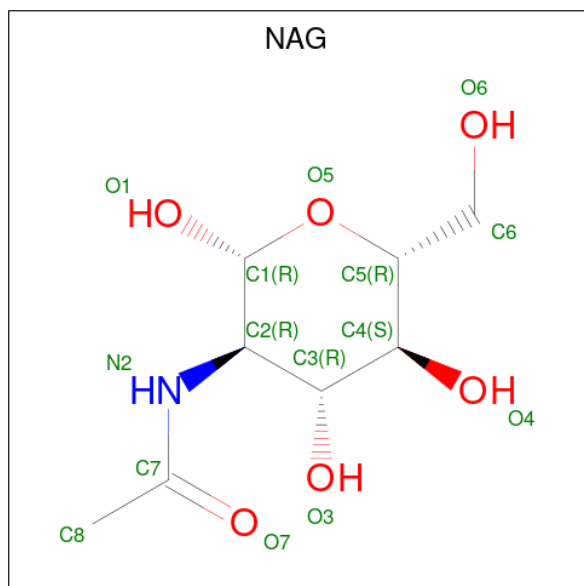
Mol	Chain	Residues	Atoms				AltConf	Trace
10	1	5	Total	C	N	O	0	0
			61	34	2	25		
10	2	5	Total	C	N	O	0	0
			61	34	2	25		

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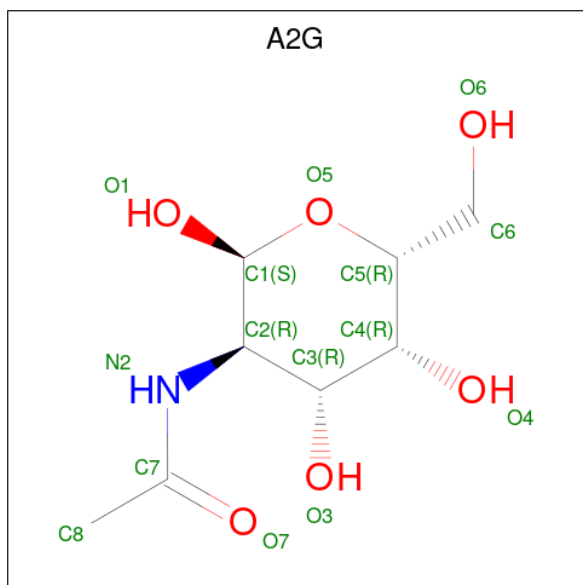
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O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

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

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



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

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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	

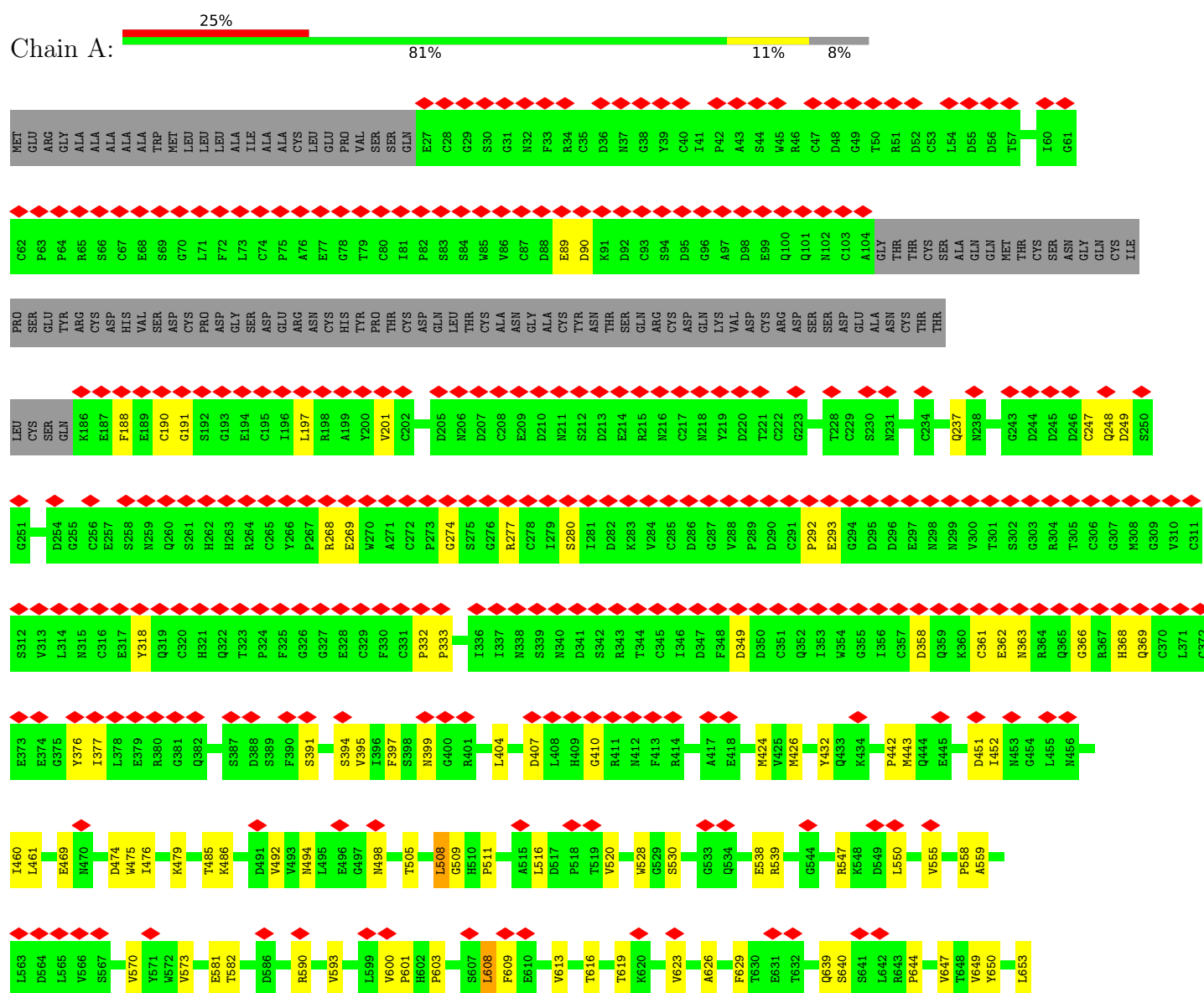
- Molecule 15 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

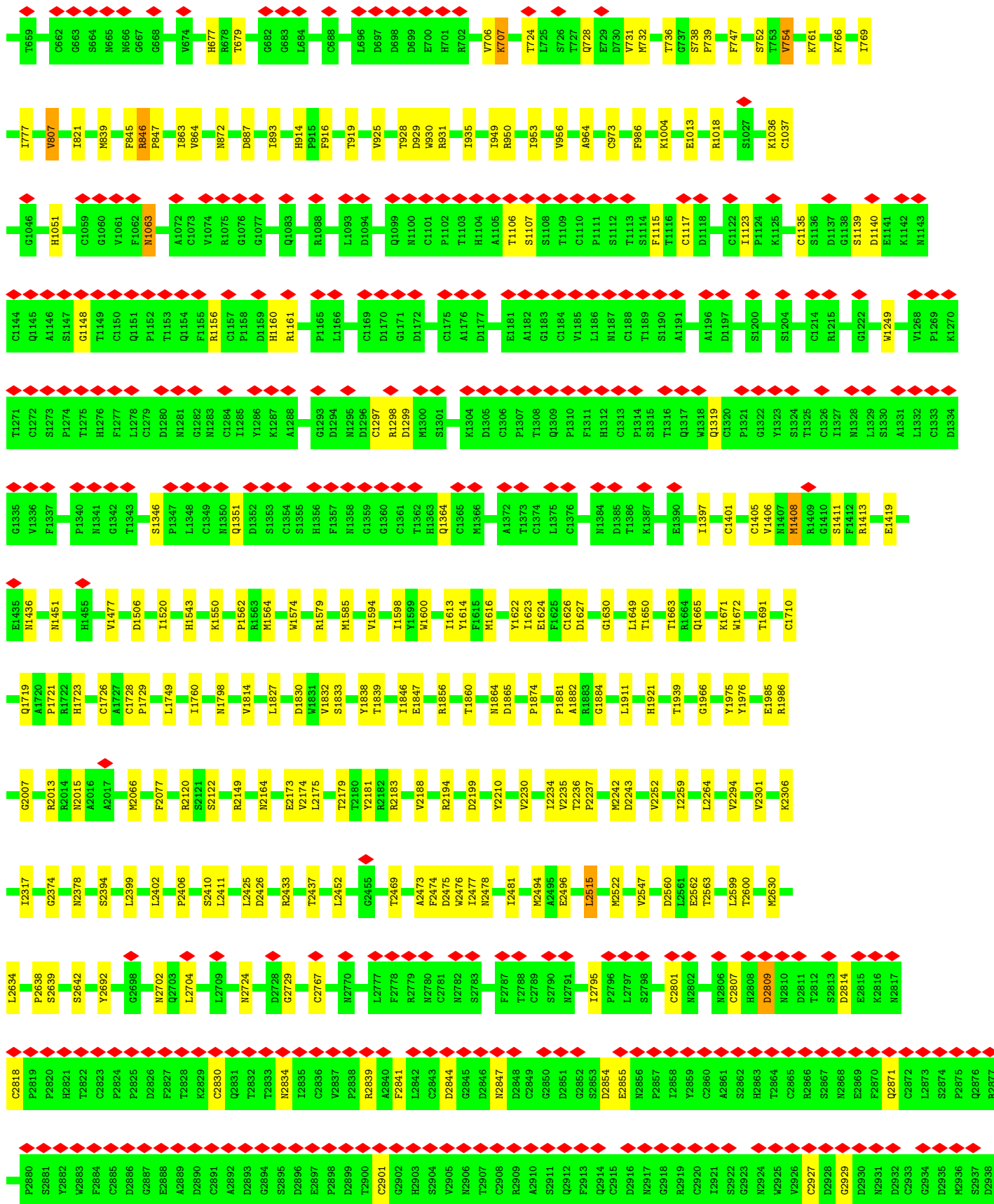
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Ni	0
			1	1	
15	B	1	Total	Ni	0
			1	1	

3 Residue-property plots

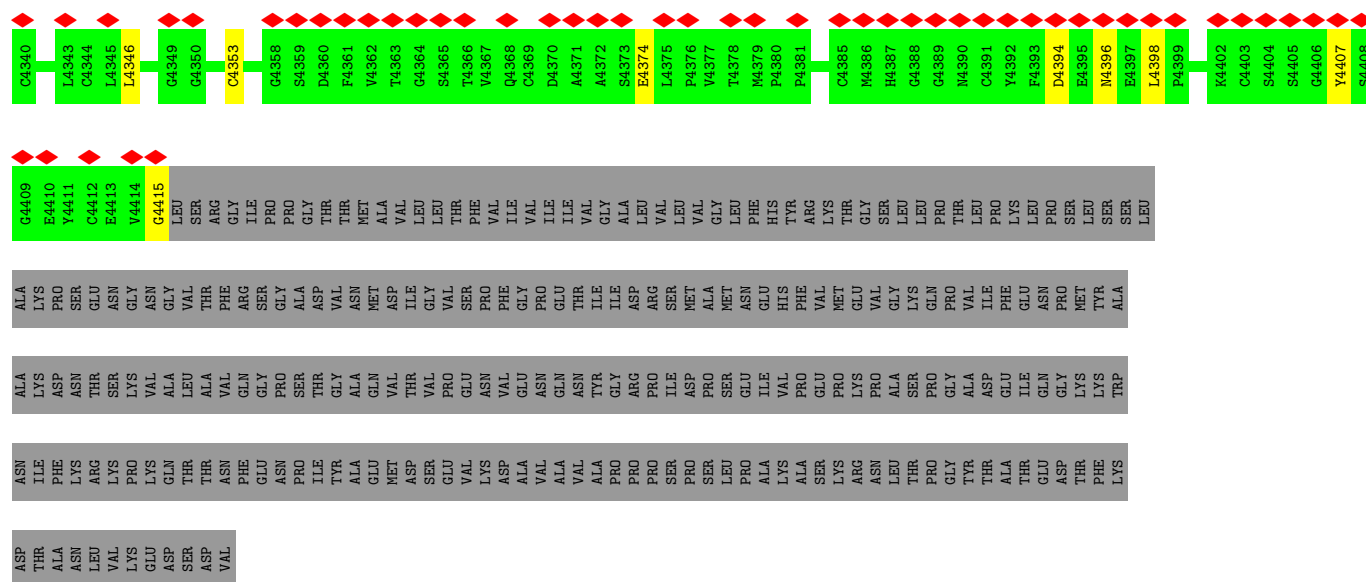
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

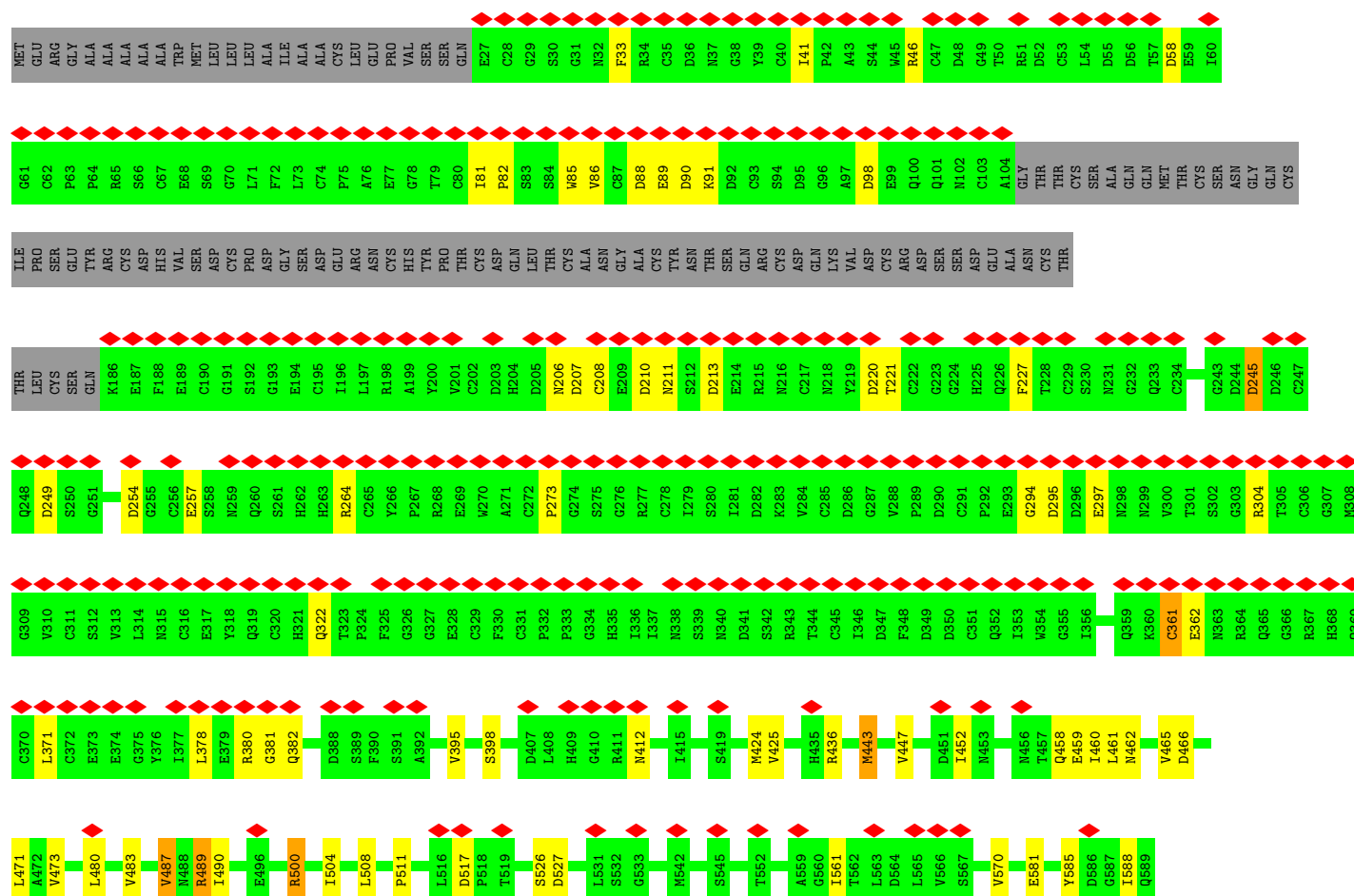
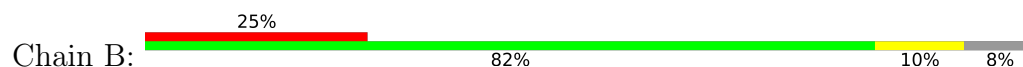


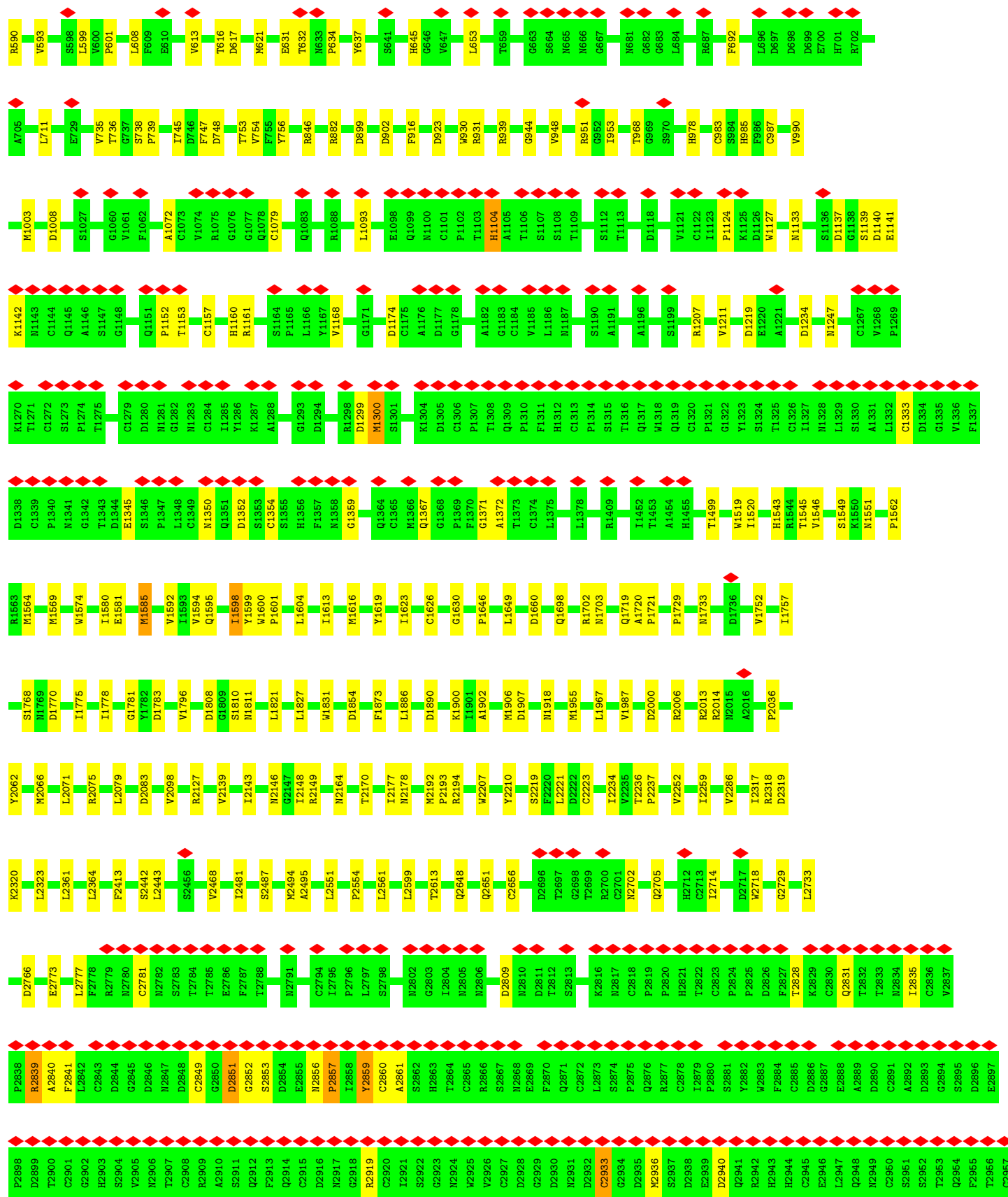


E2939	E2999	F3082	R3150	D3497	C3591	P3720	C3863	F3929	F3989	A4049	A4193	E4272
D2940	F3000	R3083	S3151	D3498	E3592	S3724	E3866	C3930	I3990	A4050	V4194	A4273
Q2941	S3001	C3084	E3160	F3499	C3596	C3741	N3867	T3931	C3991	A4051	K4197	N4274
R2942	A3002	D3085	G3174	Q3500	E3597	N3755	D3871	D3932	S3992	D4052	L4198	K4275
H2943	A3003	N3086	G3174	T3501	S3598	C3756	E3876	T3933	C3993	S4054	R4276	F4277
H2944	N3004	G3087	S3192	V3502	N3599	C3756	E3877	E3934	C3994	N4063	L4200	S4278
C2945	R3005	H3088	F3205	Q3503	A3604	S3764	E3878	Y3935	F3995	K4068	W4203	L4279
E2946	R3006	C3089	N3206	L3504	N3605	E3765	I3877	K3936	G3996	K4068	T4204	D4280
L2947	V3008	I3090	N3207	D3506	R3607	F3766	H3878	C3937	F3997	E4074	K4208	L4281
Q2948	R3009	E3091	R3208	D3507	R3607	F3766	I3879	S3938	C3998	S4073	E4208	F4282
H2949	Q3010	M3092	Y3209	T3507	Q3614	I3774	L3879	G3940	F3999	E4074	E4212	L4286
C2950	S3011	G3093	Y3210	T3508	Q3614	I3774	C3880	N3941	S4000	F4076	M4217	L4286
S2951	F3012	R3094	L3509	T3509	N3619	R3777	C3881	C3942	T4001	K4075	E4217	L4286
S2952	R3013	V3095	M3511	C3510	D3620	C3780	F3882	N3943	L4002	E4078	E4220	L4286
T2953	C3014	C3096	Q3226	M3512	C3621	Q3781	I3883	I3943	D4003	E4078	H4221	L4286
Q2954	D3015	N3097	G3227	P3512	D3781	Q3782	P3884	S3944	K4004	E4078	S4223	L4286
F2955	R3016	H3098	L3228	M3513	L3622	Q3782	C3885	H3945	M4005	E4082	V4224	L4286
T2956	R3017	D3100	R3242	S3516	D3623	D3791	E3886	H3946	S4006	E4083	L4225	L4286
C2957	C3020	D3101	H3269	L3520	N3624	E3792	S3887	Y3947	C4007	I4089	S4227	L4286
V2958	G3021	C3102	H3269	C3521	D3628	R3793	P3888	C3949	Q4008	D4092	E4228	L4286
N2959	D3022	S3103	L3277	G3522	T3629	D3794	Q3889	N3950	D4009	W4093	S4227	L4286
S2960	E3026	D3104	L3277	G3522	S3630	M3797	R3890	N3951	M4011	P4095	N4229	L4286
R2961	R3027	N3105	D3300	E3525	H3631	K3798	F3991	V3952	E4012	P4095	L4230	L4286
F2962	G3028	S3106	D3315	K3526	S3634	H3801	D3894	D3954	E4013	I4098	L4230	L4286
T2963	C3029	D3107	A3316	C3527	R3635	P3802	N3895	N3954	E4014	G4099	G4231	L4286
N2964	H3035	E3108	N3317	W3532	R3635	E3803	S3896	C3955	E4015	L4100	W4232	L4286
R2965	A3036	K3109	T3319	D3535	F3638	C3807	C3897	G3956	F4016	L4111	E4233	L4286
R2966	F3039	G3110	V3329	G3536	G3647	H3811	V3999	D3957	G4017	E4111	L4236	L4286
C2967	R3049	C3112	T3373	S3541	R3648	D3657	I3900	L3958	I4018	E4121	E4237	L4286
T2968	F3050	I3113	D3385	D3548	C3647	C3825	C3901	S3959	C4019	G4128	I4238	L4286
Q2970	F3051	N3114	L3388	L3549	D3660	L3826	H3902	D3960	Q4020	S4129	D4239	L4286
T2971	V3052	D3118	L3388	C3550	D3661	D3827	Q3903	E3961	Q4021	E4129	L4240	L4286
V2973	C3053	S3119	F3413	R3553	C3662	C3832	C3905	T3962	S4022	N4130	L4241	L4286
C2974	D3054	S3120	A3414	R3554	D3671	A3833	N3906	G3963	C4023	P4132	N4242	L4286
D2975	E3055	I3121	L3415	C3555	N3679	C3834	C3907	C3964	R4024	N4131	D4243	L4286
D2976	D3064	S3122	T3416	R3556	N3679	A3833	V3908	N3965	M4025	E4133	D4244	L4286
D2977	E3065	R3123	T3425	L3557	K3689	C3834	D3909	L3966	S4026	L4133	R4245	L4286
A2978	E3066	C3124	D3426	G3558	T3690	T3836	D3909	G3967	K4027	R4134	D4250	L4286
D2979	E3067	T3129	W3427	R3558	N3691	T3837	C3910	D3968	G4028	D4137	V4255	L4286
C2980	H3068	D3130	P3453	P3578	N3692	F3838	C3911	N3969	S4029	E4137	L4259	L4286
S2981	L3071	T3131	A3494	A3576	R3693	P3839	D3912	R3970	E4031	A4149	D4262	L4286
D2982	C3070	T3132	G3477	A3577	C3707	P3845	D3913	C3972	C4032	A4150	G4263	L4286
L2983	T3072	T3133	R3459	Q3578	R3708	A3846	C3914	A3973	C4033	V4151	T4264	L4286
L2984	E3074	S3134	A3494	A3581	R3710	A3847	N3915	N3975	C4034	I4168	R4266	L4286
D2985	P3073	S3140	A3494	D3582	Q3714	K3852	E3917	I3976	D4036	R4176	R4267	L4286
E2986	P3075	P3141	A3494	D3587	S3718	N3853	C3918	C3977	F4037	L4181	L4268	L4286
L2987	C3076	K3144	A3494	R3588	V3719	H3854	K3918	C3978	P4038	D4187	I4269	L4286
Q2988	P3078	L3145	A3494	V3589	S3718	H3854	E3920	E3978	K4039	A4191	N4270	L4286
N2989	P3076	M3146	A3494	L3590	V3719	S3859	E3921	Q3979	L4041	I4192	N4271	L4286
C2990	C3077	S3147	A3494	L3590	V3719	S3859	C3922	N3980	M4041	E4192	L4271	L4286
T2991	P3077	D3148	A3494	L3590	V3719	S3859	C3923	C3981	S4042	L4192	L4271	L4286
H2992	P3078	K3144	A3494	L3590	V3719	S3859	K3924	T3982	T4043	L4192	L4271	L4286
R2993	P3078	L3145	A3494	L3590	V3719	S3859	P3925	Q3983	H4044	L4192	L4271	L4286
T2994	P3078	M3146	A3494	L3590	V3719	S3859	T3926	L3984	Y4045	L4192	L4271	L4286
C2995	H3080	S3147	A3494	L3590	V3719	S3859	H3927	S3985	G4046	L4192	L4271	L4286
S2996	Q3081	D3148	A3494	L3590	V3719	S3859	K3927	S3986	E4047	L4192	L4271	L4286
A2997		K3149	A3494	L3590	V3719	S3859	K3928	C3987	R4048	L4192	L4271	L4286
Q2998			A3494	L3590	V3719	S3859				L4192	L4271	L4286

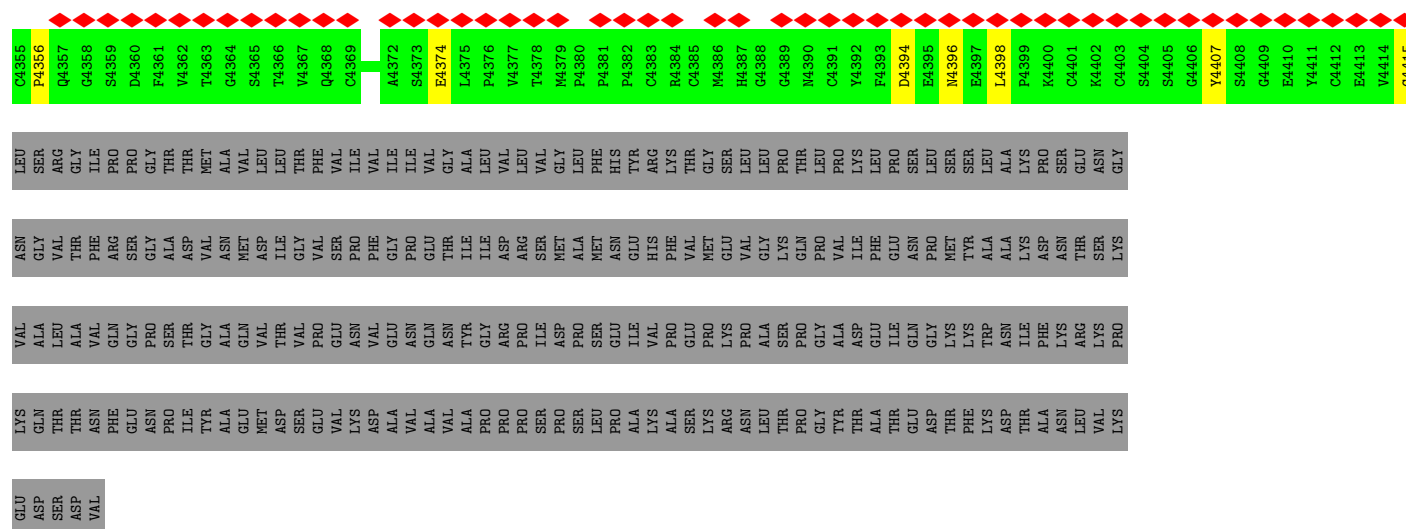


• Molecule 1: LDL receptor related protein 2

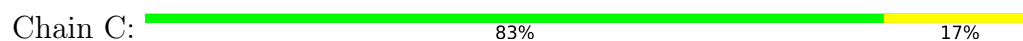




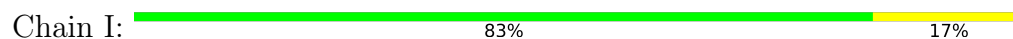




- Molecule 2: unclear peptide



- Molecule 2: unclear peptide



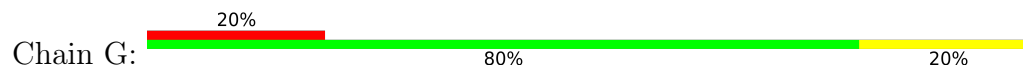
- Molecule 3: unclear peptide



- 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.

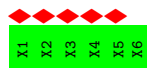
- Molecule 5: unclear peptide

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%

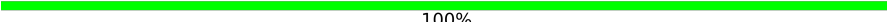


- Molecule 7: unclear peptide

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



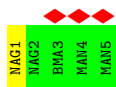
- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



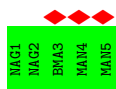
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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

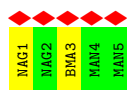


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

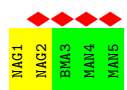
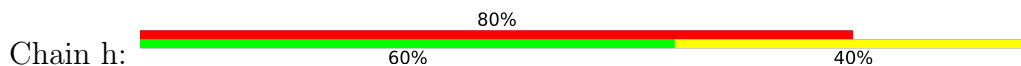


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

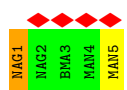
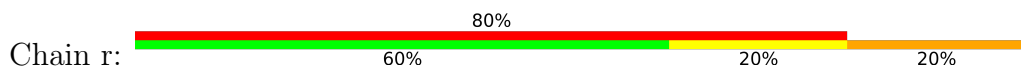




- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



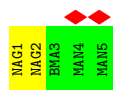
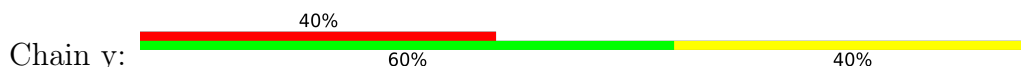
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



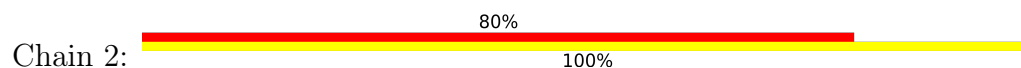
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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.

All (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
1	B	2809	ASP	CA-CB-CG	6.66	119.26	112.60
1	B	2851	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	1063	ASN	CA-CB-CG	6.21	118.81	112.60
1	A	1506	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	2841	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	1864	ASN	CA-CB-CG	5.56	118.16	112.60
1	B	3937	CYS	CA-C-N	5.50	127.92	120.38
1	B	3937	CYS	C-N-CA	5.50	127.92	120.38
1	B	2000	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	3148	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	3318	ASN	CA-CB-CG	5.44	118.04	112.60
1	B	3207	ASN	CA-CB-CG	5.42	118.02	112.60
1	B	3999	PRO	CA-C-N	5.41	129.35	120.63
1	B	3999	PRO	C-N-CA	5.41	129.35	120.63
1	B	2413	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	90	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	1008	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	1865	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	2857	PRO	N-CA-C	-5.26	107.28	113.86
1	A	2847	ASN	CA-CB-CG	5.16	117.76	112.60
1	B	220	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	3960	ASP	CA-CB-CG	5.05	117.65	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 ⓘ

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:A:3425:THR:HB	1:A:3453:PRO:HB2	1.68	0.73
1:A:1574:TRP:CE3	2:I:3:LEU:HD13	2.23	0.73
10:y:1:NAG:H61	10:y:2:NAG:HN2	1.53	0.73
1:A:4269:ILE:HG22	1:A:4270:ILE:HG23	1.71	0.72
1:A:1436:ASN:ND2	1:A:1451:ASN:OD1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4269:ILE:HG22	1:B:4270:ILE:HG23	1.74	0.69
1:A:3525:GLU:N	1:A:3525:GLU:OE1	2.26	0.68
1:A:4204:THR:HG22	1:A:4212:ILE:HG12	1.74	0.68
1:B:4204:THR:HG22	1:B:4212:ILE:HG12	1.75	0.67
1:A:2600:THR:HG21	1:A:2642:SER:HA	1.75	0.67
1:B:380:ARG:HE	1:B:382:GLN:HB3	1.59	0.67
1:B:2149:ARG:HG2	1:B:2194:ARG:HD2	1.75	0.67
1:B:3959:SER:HA	1:B:3962:THR:HG23	1.76	0.66
1:A:1408:MET:HE2	1:A:1411:SER:HB3	1.76	0.66
1:B:3852:LYS:CE	1:B:3871:ASP:OD2	2.45	0.65
1:B:2936:MET:SD	1:B:2940:ASP:HB3	2.37	0.65
1:B:3009:ARG:HG2	1:B:3011:SER:H	1.61	0.65
1:B:1595:GLN:HA	1:B:1598:ILE:HD11	1.79	0.65
1:A:2801:CYS:SG	1:A:2818:CYS:N	2.69	0.65
1:B:1574:TRP:CE3	2:C:3:LEU:HD23	2.32	0.64
1:B:504:ILE:HG22	1:B:508:LEU:HD11	1.78	0.64
1:A:1839:THR:HG22	1:A:1846:ILE:HG12	1.80	0.64
1:A:1719:GLN:HG3	1:A:1721:PRO:HD2	1.80	0.63
1:B:1811:ASN:OD1	9:s:1:NAG:N2	2.32	0.63
1:B:3852:LYS:HE3	1:B:3871:ASP:OD2	1.99	0.62
1:A:4407:TYR:HA	1:A:4415:GLY:HA3	1.81	0.62
1:B:4407:TYR:HA	1:B:4415:GLY:HA3	1.81	0.62
1:B:91:LYS:HE2	1:B:91:LYS:HA	1.80	0.62
1:A:846:ARG:HB3	1:A:847:PRO:HD3	1.82	0.62
1:A:613:VAL:HG23	1:A:626:ALA:HB3	1.81	0.61
1:A:863:ILE:HG13	1:A:864:VAL:HG23	1.82	0.61
1:B:4274:MET:HE1	1:B:4297:TRP:CE2	2.35	0.61
1:A:1520:ILE:HD12	1:A:1562:PRO:HB2	1.83	0.61
1:B:1519:TRP:HB3	1:B:1698:GLN:HE21	1.65	0.61
1:A:1600:TRP:CD2	2:I:3:LEU:HD12	2.36	0.61
1:A:2179:THR:HG22	1:A:2181:TYR:H	1.65	0.61
1:A:2235:VAL:HG12	1:A:2236:THR:HG23	1.83	0.61
1:A:509:GLY:HA3	1:A:530:SER:HA	1.82	0.61
1:B:2210:TYR:HB2	1:B:2236:THR:HA	1.81	0.61
1:B:1234:ASP:HA	1:B:1247:ASN:ND2	2.16	0.60
1:A:2961:ARG:HG2	1:A:2963:PRO:HD2	1.83	0.60
1:B:2859:TYR:O	1:B:2861:ALA:N	2.35	0.60
1:A:2433:ARG:NH2	1:A:2496:GLU:OE2	2.33	0.60
1:A:1106:THR:HG22	1:A:1107:SER:H	1.66	0.60
1:B:297:GLU:O	1:B:304:ARG:NH1	2.34	0.60
1:A:1543:HIS:HB3	1:A:1729:PRO:HG3	1.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLN:OE1	1:A:539:ARG:NH1	2.33	0.59
1:A:2013:ARG:NH2	1:A:2015:ASN:OD1	2.33	0.59
1:A:4274:MET:HE1	1:A:4297:TRP:CE2	2.37	0.59
1:B:4038:PHE:HB3	1:B:4049:CYS:HB3	1.85	0.59
1:A:639:GLN:NE2	1:A:640:SER:O	2.36	0.59
1:B:1569:MET:HE2	1:B:1585:MET:HA	1.85	0.59
1:A:2953:THR:O	1:A:2970:GLN:NE2	2.36	0.58
1:B:1616:MET:CE	1:B:1646:PRO:HB2	2.33	0.58
1:A:4008:GLN:HB2	1:B:90:ASP:HB3	1.86	0.58
1:A:4038:PHE:HB3	1:A:4049:CYS:HB3	1.85	0.58
1:B:3344:VAL:HG11	1:B:3653:SER:HB2	1.85	0.58
1:A:475:TRP:CD1	1:A:476:ILE:HG23	2.39	0.58
1:A:4006:SER:OG	1:B:89:GLU:OE2	2.21	0.58
1:B:608:LEU:HB3	1:B:613:VAL:HG12	1.86	0.58
1:B:4093:TRP:CE2	1:B:4325:GLN:HB3	2.39	0.58
1:B:4228:GLU:N	1:B:4228:GLU:OE1	2.37	0.58
1:A:600:VAL:HG23	1:A:600:VAL:O	2.04	0.57
1:A:1397:ILE:HD12	1:A:1397:ILE:H	1.69	0.57
1:A:3965:ASN:O	1:A:3970:ARG:NH1	2.37	0.57
1:B:3210:TYR:OH	1:B:3764:SER:N	2.34	0.57
1:B:86:VAL:HG23	1:B:98:ASP:HB2	1.86	0.57
1:B:1616:MET:HG2	1:B:1623:ILE:HG12	1.86	0.57
1:A:4093:TRP:CE2	1:A:4325:GLN:HB3	2.38	0.57
1:B:3605:ASN:ND2	1:B:3623:ASP:OD2	2.36	0.57
1:B:711:LEU:HD22	1:B:745:ILE:HD13	1.85	0.57
1:A:2066:MET:HE2	1:A:2077:PHE:HB2	1.87	0.57
1:A:4394:ASP:OD1	1:A:4398:LEU:N	2.37	0.57
1:A:1579:ARG:HA	1:A:1598:ILE:HD11	1.87	0.56
1:B:846:ARG:O	1:B:846:ARG:NH2	2.38	0.56
1:B:4394:ASP:OD1	1:B:4398:LEU:N	2.36	0.56
1:A:4228:GLU:OE1	1:A:4228:GLU:N	2.38	0.56
1:A:3055:GLU:N	1:A:3065:GLU:OE1	2.38	0.56
1:B:735:VAL:HG11	1:B:756:TYR:CZ	2.41	0.56
1:B:254:ASP:HB3	1:B:588:ILE:CG2	2.36	0.56
1:B:1733:ASN:OD1	10:r:1:NAG:N2	2.39	0.55
1:B:3016:ARG:N	1:B:3026:GLU:OE1	2.39	0.55
1:A:3766:PHE:HD2	1:A:3774:ILE:HD11	1.70	0.55
1:B:3025:ASP:OD1	1:B:3025:ASP:N	2.39	0.55
1:B:2146:ASN:O	1:B:2149:ARG:NH2	2.39	0.55
1:B:294:GLY:O	1:B:304:ARG:NH1	2.40	0.55
1:B:1352:ASP:O	1:B:1367:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2170:THR:HG21	1:B:2192:MET:HA	1.89	0.55
1:B:1821:LEU:HD13	1:B:2075:ARG:HD2	1.89	0.55
1:B:3963:GLY:H	1:B:4004:LYS:HD2	1.72	0.55
1:B:1600:TRP:CD2	2:C:3:LEU:HD22	2.42	0.55
1:A:2956:THR:OG1	1:A:2965:ARG:NH2	2.40	0.55
1:A:3657:ASP:OD1	1:A:3693:ARG:NH1	2.35	0.55
1:A:3385:ASP:OD1	1:A:3388:LEU:N	2.40	0.54
1:A:4000:SER:HA	1:A:4008:GLN:HE22	1.71	0.54
1:B:378:LEU:HD21	1:B:381:GLY:HA2	1.88	0.54
1:A:2149:ARG:HG2	1:A:2194:ARG:HD2	1.90	0.54
1:A:3413:PHE:CD2	1:A:3427:TRP:CZ2	2.95	0.54
1:B:2919:ARG:HD3	1:B:2933:CYS:O	2.08	0.54
1:A:3974:GLU:HB2	1:A:3976:ILE:HD11	1.89	0.54
1:A:559:ALA:HB3	1:A:573:VAL:HG23	1.89	0.54
1:B:3238:ARG:NH2	1:B:3464:GLN:O	2.41	0.53
1:A:3520:LEU:HD23	1:A:3527:CYS:SG	2.49	0.53
1:A:4313:VAL:HG22	1:A:4314:ASN:H	1.73	0.53
1:A:1838:TYR:CZ	1:A:1847:GLU:HG3	2.44	0.53
1:B:2702:ASN:HB3	1:B:2705:GLN:HG3	1.91	0.53
1:A:486:LYS:HG2	1:A:736:THR:HG21	1.90	0.53
1:A:1663:THR:HG23	1:A:1665:GLN:HG2	1.90	0.53
1:B:2852:GLY:O	1:B:2856:ASN:N	2.41	0.53
1:A:3791:ASP:OD1	1:A:3791:ASP:N	2.42	0.53
1:B:2839:ARG:O	1:B:2841:PHE:N	2.42	0.53
1:B:3289:LEU:HD21	1:B:3339:TRP:HB2	1.90	0.53
1:A:277:ARG:HH21	1:A:292:PRO:HD3	1.74	0.52
1:B:527:ASP:N	1:B:527:ASP:OD1	2.41	0.52
1:B:2831:GLN:H	1:B:2853:SER:HB2	1.74	0.52
1:A:363:ASN:HA	1:A:368:HIS:HA	1.91	0.52
1:B:2361:LEU:HD12	1:B:2364:LEU:HD12	1.91	0.52
1:A:2210:TYR:HB2	1:A:2236:THR:HA	1.90	0.52
1:B:526:SER:HB3	1:B:561:ILE:HD11	1.92	0.52
1:A:845:PHE:O	1:A:846:ARG:C	2.52	0.52
1:B:257:GLU:N	1:B:257:GLU:OE1	2.43	0.52
1:A:3592:GLU:O	1:A:3606:LYS:NZ	2.43	0.52
1:B:1564:MET:HE2	1:B:1702:ARG:HG2	1.92	0.52
1:A:1117:CYS:HB3	1:A:1139:SER:HB3	1.92	0.52
1:B:1918:ASN:OD1	1:B:1918:ASN:N	2.43	0.52
1:B:3038:GLN:HG2	1:B:3046:CYS:HB3	1.92	0.52
1:A:706:VAL:HG21	1:A:731:VAL:HG11	1.92	0.52
1:A:1594:VAL:HG12	1:A:1598:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2374:GLY:N	1:A:2411:LEU:O	2.42	0.52
1:B:2219:SER:OG	1:B:2223:CYS:HA	2.10	0.52
1:B:361:CYS:SG	1:B:362:GLU:N	2.82	0.52
1:A:274:GLY:HA3	1:A:293:GLU:HG3	1.92	0.51
1:A:3576:ALA:HB1	1:A:3622:LEU:HD21	1.91	0.51
1:B:1139:SER:O	1:B:1142:LYS:NZ	2.38	0.51
1:B:1752:VAL:HG23	1:B:1757:ILE:HG12	1.92	0.51
1:B:483:VAL:HG22	1:B:490:ILE:HG12	1.92	0.51
1:B:2148:ILE:HD13	1:B:2164:ASN:HB3	1.92	0.51
1:B:1520:ILE:O	1:B:1703:ASN:ND2	2.44	0.51
1:A:4276:PRO:HB3	1:A:4288:TRP:CD1	2.46	0.51
1:A:1650:THR:HG21	1:A:1691:THR:HA	1.93	0.51
1:A:3635:ARG:NH2	1:A:3647:GLY:O	2.43	0.51
1:B:2062:TYR:OH	1:B:2083:ASP:OD2	2.26	0.51
1:A:2426:ASP:OD2	1:A:2473:ALA:HA	2.11	0.51
1:A:2970:GLN:HG2	1:A:2973:VAL:HB	1.93	0.51
1:A:3520:LEU:HD13	1:A:3521:CYS:O	2.11	0.51
1:B:4232:TRP:N	1:B:4250:ASP:OD1	2.44	0.51
1:A:2066:MET:HE1	1:A:2317:ILE:HG21	1.92	0.51
1:A:3966:LEU:HD22	1:A:3987:GLY:HA3	1.93	0.51
1:A:1004:LYS:HD3	1:A:1018:ARG:HH11	1.76	0.51
1:A:2956:THR:O	1:A:2965:ARG:NH2	2.44	0.51
1:A:539:ARG:HD3	1:A:550:LEU:HD13	1.93	0.50
1:A:4234:ASN:HD21	1:A:4277:PHE:HA	1.75	0.50
1:B:1604:LEU:HD22	1:B:1613:ILE:HD11	1.93	0.50
12:B:4704:NAG:H82	10:t:2:NAG:H82	1.94	0.50
1:A:4279:LEU:HD12	1:A:4286:LEU:HD11	1.92	0.50
1:A:616:THR:HG23	1:A:644:PRO:HB2	1.93	0.50
1:A:1832:VAL:HG22	1:A:1881:PRO:HB3	1.93	0.50
1:A:3500:GLN:HB3	1:A:3511:MET:SD	2.52	0.50
1:A:2406:PRO:HG3	1:A:2630:MET:HE1	1.93	0.50
1:B:245:ASP:OD1	1:B:245:ASP:N	2.45	0.50
1:A:707:LYS:HE3	1:A:964:ALA:HB3	1.94	0.50
1:A:3210:TYR:HE2	1:A:3764:SER:HB2	1.77	0.49
1:B:254:ASP:HB3	1:B:588:ILE:HG23	1.94	0.49
1:B:1157:CYS:HB2	1:B:1160:HIS:HB3	1.93	0.49
1:B:3416:THR:HG21	1:B:3457:HIS:HA	1.93	0.49
1:A:1616:MET:HG2	1:A:1623:ILE:HG12	1.92	0.49
1:A:2959:ASN:HD22	1:A:2964:ASN:ND2	2.09	0.49
1:B:581:GLU:CD	1:B:590:ARG:HE	2.21	0.49
1:B:2013:ARG:HH21	1:B:2013:ARG:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3671:ASP:OD1	1:B:3671:ASP:N	2.45	0.49
1:B:2149:ARG:NH1	4:G:2:GLU:HB2	2.28	0.49
1:A:2986:GLU:HG3	1:A:3006:ARG:HD2	1.95	0.49
1:B:1886:LEU:HB2	1:B:1906:MET:HG3	1.94	0.49
1:A:3782:GLN:HE22	1:A:3825:CYS:HA	1.78	0.49
1:A:1966:GLY:HA3	1:A:2007:GLY:HA2	1.93	0.49
1:A:2394:SER:OG	1:A:2639:SER:O	2.27	0.49
1:A:4232:TRP:N	1:A:4250:ASP:OD1	2.45	0.49
1:A:2242:MET:HE1	1:A:2264:LEU:HD11	1.95	0.49
1:A:399:ASN:HB2	1:A:404:LEU:HD13	1.95	0.49
1:A:3891:PHE:N	1:A:3899:VAL:O	2.44	0.49
1:B:1907:ASP:OD1	1:B:1907:ASP:C	2.56	0.49
1:A:738:SER:HB2	1:A:739:PRO:HD3	1.94	0.49
1:A:3140:LEU:HG	1:A:3141:PRO:HD2	1.94	0.49
1:A:4300:ASN:ND2	1:A:4305:GLU:OE2	2.41	0.49
1:B:953:ILE:O	1:B:953:ILE:HG13	2.12	0.49
1:B:1616:MET:SD	1:B:1649:LEU:HB3	2.53	0.49
1:A:1626:CYS:SG	1:A:1627:ASP:N	2.86	0.48
1:A:1600:TRP:CG	2:I:3:LEU:HD12	2.48	0.48
1:A:3005:GLY:HA3	1:A:3020:CYS:HB3	1.95	0.48
1:B:81:ILE:HD12	1:B:81:ILE:O	2.13	0.48
1:A:407:ASP:OD1	1:A:410:GLY:N	2.45	0.48
1:A:1160:HIS:CD2	1:A:1161:ARG:HG2	2.48	0.48
1:A:2929:GLY:HA2	1:A:2966:ARG:HB3	1.95	0.48
1:A:2973:VAL:HG23	1:A:2985:ASP:HB2	1.95	0.48
1:A:494:ASN:OD1	1:A:498:ASN:N	2.38	0.48
1:A:872:ASN:HD21	7:N:2:ASN:HD21	1.61	0.48
1:A:1749:LEU:HD23	1:A:1760:ILE:HD11	1.94	0.48
1:A:2210:TYR:CB	1:A:2236:THR:HA	2.44	0.48
1:B:1574:TRP:CZ3	2:C:3:LEU:HD23	2.49	0.48
1:B:1581:GLU:HG2	1:B:1592:VAL:HG22	1.94	0.48
1:A:528:TRP:HA	1:A:558:PRO:HD2	1.95	0.48
1:A:4287:TYR:CD2	1:A:4322:ILE:HD11	2.49	0.48
1:B:1354:CYS:HA	1:B:1359:GLY:HA3	1.96	0.48
1:B:2319:ASP:OD1	1:B:2320:LYS:N	2.47	0.48
1:B:3000:PHE:N	1:B:3008:VAL:O	2.47	0.48
1:A:2634:LEU:HD12	1:A:2638:PRO:HG3	1.96	0.48
1:B:1299:ASP:O	1:B:1300:MET:HG2	2.13	0.48
1:A:1798:ASN:C	1:A:1798:ASN:OD1	2.57	0.48
1:B:1873:PHE:N	1:B:1890:ASP:OD1	2.39	0.48
1:B:3887:SER:OG	1:B:3888:PRO:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:SER:O	1:A:650:TYR:N	2.43	0.48
1:A:2475:ASP:OD1	1:A:2477:ILE:HG13	2.13	0.48
1:B:1350:ASN:H	1:B:1371:GLY:HA3	1.79	0.48
1:B:1775:ILE:HG22	1:B:1778:ILE:HD11	1.95	0.48
1:B:3291:ALA:HA	1:B:3325:PRO:HD2	1.96	0.48
1:B:4271:ASN:OD1	1:B:4271:ASN:N	2.47	0.48
1:B:4300:ASN:ND2	1:B:4305:GLU:OE2	2.41	0.48
1:A:2809:ASP:N	1:A:2809:ASP:OD1	2.36	0.47
1:B:33:PHE:N	1:B:41:ILE:O	2.46	0.47
1:B:2849:CYS:SG	1:B:2853:SER:HB3	2.54	0.47
1:B:4099:GLY:O	1:B:4100:LEU:HD23	2.14	0.47
1:B:500:ARG:HD3	1:B:692:PHE:HE2	1.80	0.47
1:A:846:ARG:NH1	1:A:1249:TRP:CD2	2.82	0.47
1:A:1975:TYR:CE2	1:A:1986:ARG:HD3	2.49	0.47
1:A:3064:ASP:N	1:A:3064:ASP:OD1	2.48	0.47
1:B:227:PHE:CE1	1:B:588:ILE:HD11	2.49	0.47
1:B:2714:ILE:HD13	1:B:2718:TRP:HB2	1.97	0.47
1:A:3691:ASN:ND2	1:A:3707:CYS:O	2.48	0.47
1:A:3887:SER:N	1:A:3888:PRO:HD2	2.30	0.47
1:B:2835:ILE:HD12	1:B:2835:ILE:H	1.79	0.47
1:B:3015:ASP:N	1:B:3026:GLU:OE1	2.42	0.47
1:B:3662:CYS:SG	1:B:3667:ASP:HB3	2.55	0.47
1:B:3984:LEU:HD22	1:B:3990:ILE:HG13	1.97	0.47
1:A:3597:GLU:HG3	1:A:3598:SER:H	1.80	0.47
1:B:1140:ASP:OD1	1:B:1141:GLU:HG2	2.14	0.47
1:B:2139:VAL:HG12	1:B:2143:ILE:HD11	1.97	0.47
1:A:508:LEU:HD22	1:A:511:PRO:HB3	1.96	0.47
1:A:949:ILE:O	1:A:950:ARG:HD2	2.14	0.47
1:A:1004:LYS:HD3	1:A:1018:ARG:NH1	2.29	0.47
1:B:985:HIS:CE1	1:B:1003:MET:HE1	2.49	0.47
1:B:2442:SER:C	1:B:2443:LEU:HD23	2.40	0.47
1:B:3258:LEU:HD23	1:B:3258:LEU:HA	1.69	0.47
1:A:766:LYS:HD2	1:A:777:ILE:HD11	1.95	0.47
1:A:2234:ILE:HD11	1:A:2237:PRO:HB3	1.96	0.47
1:B:82:PRO:HD2	1:B:85:TRP:CD1	2.50	0.47
1:B:1207:ARG:NH2	1:B:1219:ASP:O	2.44	0.47
1:B:2494:MET:HG3	1:B:2495:ALA:O	2.15	0.47
1:A:3535:ASP:HA	1:A:3553:ARG:HD2	1.96	0.47
1:B:1551:ASN:HD22	9:p:1:NAG:C7	2.27	0.47
1:A:451:ASP:OD1	1:A:452:ILE:N	2.48	0.46
1:A:1830:ASP:OD2	1:A:1833:SER:OG	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2560:ASP:OD2	1:A:2563:THR:OG1	2.28	0.46
1:A:3576:ALA:CB	1:A:3622:LEU:HD21	2.44	0.46
1:B:1906:MET:HE3	1:B:2036:PRO:HG2	1.96	0.46
1:A:1106:THR:HG22	1:A:1107:SER:N	2.30	0.46
1:A:3498:ASP:OD2	1:A:3527:CYS:HB2	2.16	0.46
1:A:3607:ARG:NH1	1:A:3620:ASP:O	2.48	0.46
1:B:621:MET:HE1	1:B:1133:ASN:HD21	1.80	0.46
1:A:845:PHE:CZ	1:A:1298:ARG:HG2	2.51	0.46
1:A:2562:GLU:N	1:A:2562:GLU:OE1	2.48	0.46
1:A:3209:TYR:HA	1:A:3228:LEU:HB2	1.97	0.46
1:A:3513:MET:CG	1:A:3513:MET:O	2.64	0.46
1:A:4287:TYR:HD2	1:A:4322:ILE:HD11	1.81	0.46
1:B:1900:LYS:HE2	1:B:1902:ALA:HB2	1.96	0.46
1:B:3210:TYR:HH	1:B:3764:SER:H	1.62	0.46
1:A:3648:ARG:NH2	1:A:3661:ASP:O	2.49	0.46
1:A:4099:GLY:O	1:A:4100:LEU:HD23	2.14	0.46
1:B:1580:ILE:HB	1:B:1594:VAL:HB	1.97	0.46
1:B:1752:VAL:HG11	1:B:1783:ASP:HA	1.98	0.46
1:A:807:VAL:HG13	1:A:821:ILE:HB	1.96	0.46
1:A:2844:ASP:H	1:A:2855:GLU:HB3	1.81	0.46
1:A:4000:SER:C	1:A:4002:LEU:H	2.23	0.46
1:A:928:THR:HG22	1:A:935:ILE:HG12	1.97	0.46
1:A:2474:PHE:HD1	1:A:2481:ILE:HG12	1.81	0.46
1:B:398:SER:OG	1:B:425:VAL:O	2.24	0.46
1:B:939:ARG:CZ	1:B:944:GLY:HA2	2.46	0.46
1:B:1104:HIS:ND1	1:B:1104:HIS:C	2.73	0.46
1:B:2468:VAL:HG22	1:B:2487:SER:HB3	1.98	0.46
1:A:2437:THR:HB	1:A:2469:THR:HG23	1.98	0.46
1:B:460:ILE:HG22	1:B:461:LEU:HG	1.97	0.46
1:B:3039:PHE:HD2	1:B:3047:ILE:HD11	1.81	0.46
1:A:1036:LYS:HG2	1:A:1037:CYS:H	1.80	0.46
1:A:2183:ARG:NH1	1:A:2410:SER:OG	2.49	0.46
1:A:4271:ASN:OD1	1:A:4271:ASN:N	2.47	0.46
1:B:88:ASP:O	1:B:89:GLU:HG2	2.16	0.46
1:B:1333:CYS:HA	1:B:1345:GLU:HG3	1.98	0.46
1:B:1545:THR:HB	1:B:1729:PRO:HA	1.98	0.46
1:A:1115:PHE:N	1:A:1123:ILE:O	2.49	0.45
1:A:366:GLY:C	1:A:368:HIS:H	2.24	0.45
1:A:469:GLU:HG3	1:A:485:THR:HG21	1.98	0.45
1:A:2970:GLN:HG2	1:A:2970:GLN:O	2.16	0.45
1:B:601:PRO:HD2	1:B:617:ASP:OD2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3417:ILE:HD12	1:B:3417:ILE:N	2.31	0.45
1:B:3919:GLU:HG2	1:B:3923:ARG:CZ	2.46	0.45
1:A:2630:MET:HE2	1:A:2630:MET:HA	1.98	0.45
1:A:3886:GLU:OE1	1:A:3889:GLN:NE2	2.30	0.45
1:B:2969:PRO:HD2	1:B:2972:TRP:HE1	1.81	0.45
1:B:599:LEU:HG	1:B:634:PRO:HD3	1.97	0.45
1:A:3009:ARG:HD2	1:A:3011:SER:HB3	1.98	0.45
1:B:2958:VAL:HA	1:B:2966:ARG:HD2	1.97	0.45
1:B:1562:PRO:HA	1:B:1585:MET:HE2	1.98	0.45
1:B:2252:VAL:HG12	1:B:2259:ILE:HG12	1.99	0.45
1:B:3016:ARG:NH1	1:B:3044:GLY:O	2.46	0.45
1:A:1600:TRP:CE2	2:I:3:LEU:HD12	2.52	0.45
1:A:3329:VAL:HG11	1:A:3373:THR:HA	1.99	0.45
1:A:4306:ASN:N	1:A:4306:ASN:OD1	2.50	0.45
1:B:424:MET:HG2	1:B:443:MET:HG3	1.99	0.45
1:B:2177:ILE:HG22	1:B:2178:ASN:OD1	2.17	0.45
1:A:1976:TYR:OH	1:A:1985:GLU:OE1	2.28	0.45
1:A:2394:SER:HB3	1:A:2425:LEU:HD11	1.99	0.45
1:B:2551:LEU:HD13	1:B:2554:PRO:HB3	1.98	0.45
1:A:358:ASP:HA	1:A:629:PHE:HZ	1.82	0.45
1:B:249:ASP:OD1	1:B:249:ASP:C	2.59	0.45
1:B:4306:ASN:OD1	1:B:4306:ASN:N	2.50	0.45
1:A:4027:LYS:NZ	1:B:90:ASP:OD2	2.50	0.45
1:B:273:PRO:HD2	1:B:295:ASP:HB3	1.99	0.45
1:B:3744:THR:OG1	1:B:3746:ASP:OD1	2.34	0.45
1:B:4020:PRO:HD2	1:B:4032:CYS:HB3	1.99	0.45
1:A:1408:MET:SD	1:A:1413:ARG:NH2	2.89	0.44
1:B:1702:ARG:HH21	1:B:1702:ARG:HB2	1.80	0.44
1:B:3736:PRO:HD2	1:B:3739:TRP:CE3	2.51	0.44
1:B:4177:TYR:HA	1:B:4356:PRO:HG3	1.98	0.44
1:A:3016:ARG:N	1:A:3026:GLU:OE2	2.50	0.44
1:B:2071:LEU:HD12	1:B:2323:LEU:HD22	2.00	0.44
1:B:46:ARG:HD2	1:B:58:ASP:O	2.17	0.44
1:B:1499:THR:HG21	8:o:1:NAG:H82	2.00	0.44
1:B:1519:TRP:CD2	1:B:1698:GLN:HG3	2.52	0.44
1:B:4234:ASN:HD21	1:B:4277:PHE:HA	1.81	0.44
1:B:4272:GLU:O	1:B:4307:LYS:NZ	2.50	0.44
1:A:269:GLU:HA	1:A:280:SER:HA	2.00	0.44
1:A:474:ASP:HB3	1:A:479:LYS:HB2	1.99	0.44
1:A:953:ILE:HG23	1:A:956:VAL:HB	2.00	0.44
1:A:4078:GLU:HB3	1:A:4129:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ASP:OD2	1:B:585:TYR:OH	2.26	0.44
1:B:916:PHE:CD2	1:B:930:TRP:CZ2	3.06	0.44
1:B:3976:ILE:HD13	1:B:3989:PHE:CE2	2.52	0.44
1:A:397:PHE:CD2	1:A:623:VAL:HG21	2.53	0.44
1:A:2927:CYS:SG	1:A:2939:GLU:HA	2.58	0.44
1:A:4272:GLU:O	1:A:4307:LYS:NZ	2.50	0.44
1:B:2194:ARG:HG3	1:B:2210:TYR:CZ	2.52	0.44
1:B:4194:VAL:HB	1:B:4217:MET:HE3	2.00	0.44
1:A:4130:ASN:C	1:A:4131:ASN:HD22	2.26	0.44
1:B:3049:ARG:HD3	1:B:3049:ARG:O	2.18	0.44
1:A:362:GLU:O	1:A:369:GLN:N	2.50	0.44
1:A:3009:ARG:HG3	1:A:3011:SER:H	1.82	0.44
1:A:4274:MET:HE1	1:A:4297:TRP:NE1	2.33	0.44
1:B:473:VAL:HG12	1:B:480:LEU:HD12	2.00	0.44
1:B:931:ARG:HH11	1:B:1211:VAL:HB	1.82	0.44
1:A:4149:LEU:HD23	1:A:4150:ALA:N	2.33	0.44
1:B:1543:HIS:HB3	1:B:1729:PRO:HG3	2.00	0.44
1:B:3170:GLU:HB3	1:B:3177:ILE:HG23	2.00	0.44
1:B:4259:ILE:HG22	1:B:4266:ARG:HA	1.99	0.44
1:A:916:PHE:CD1	1:A:930:TRP:CZ2	3.05	0.43
1:A:4194:VAL:HB	1:A:4217:MET:HE3	1.99	0.43
1:B:1626:CYS:HB3	1:B:1630:GLY:HA2	1.98	0.43
1:A:2294:VAL:HG12	1:A:2301:VAL:HG22	2.00	0.43
1:B:465:VAL:HG23	1:B:465:VAL:O	2.18	0.43
1:B:1808:ASP:OD2	1:B:1810:SER:OG	2.36	0.43
1:B:2965:ARG:HH22	1:B:2966:ARG:NH1	2.16	0.43
1:B:3621:CYS:SG	1:B:3626:ASP:HB3	2.59	0.43
1:A:1419:GLU:OE1	1:A:1419:GLU:N	2.43	0.43
1:A:3013:ARG:HG3	1:A:3014:CYS:SG	2.58	0.43
1:A:4020:PRO:HD2	1:A:4032:CYS:HB3	2.00	0.43
1:B:637:TYR:CD1	1:B:637:TYR:C	2.95	0.43
1:A:376:TYR:CZ	1:A:653:LEU:HD13	2.53	0.43
1:A:609:PHE:HB2	1:A:649:VAL:HG11	2.01	0.43
1:A:1004:LYS:NZ	1:A:1013:GLU:OE2	2.52	0.43
1:A:3277:LEU:HD12	1:A:3277:LEU:C	2.43	0.43
1:B:508:LEU:HD23	1:B:511:PRO:HB3	2.01	0.43
1:A:1614:TYR:HB3	1:A:1649:LEU:HD21	1.99	0.43
1:A:3780:CYS:HA	1:A:3792:GLU:OE1	2.18	0.43
1:B:2143:ILE:HD12	1:B:2148:ILE:HD11	2.01	0.43
1:A:608:LEU:HD23	1:A:608:LEU:HA	1.89	0.43
1:A:1626:CYS:SG	1:A:1630:GLY:HA2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4285:LYS:HD2	1:A:4298:ARG:HD2	2.00	0.43
1:B:459:GLU:OE2	1:B:462:ASN:ND2	2.44	0.43
1:B:3831:GLU:HG3	1:B:3855:VAL:HG12	2.00	0.43
1:A:600:VAL:HB	1:A:603:PRO:HG3	2.01	0.43
1:A:914:HIS:CE1	7:N:2:ASN:HD22	2.37	0.43
1:A:2481:ILE:HD12	1:A:2494:MET:HE3	2.01	0.43
1:A:3983:GLN:HA	1:A:3989:PHE:HA	2.00	0.43
1:B:436:ARG:NH1	1:B:458:GLN:OE1	2.52	0.43
1:B:1796:VAL:HG13	1:B:1827:LEU:HD22	2.01	0.43
1:B:2839:ARG:C	1:B:2841:PHE:H	2.26	0.43
1:B:2857:PRO:HA	1:B:2861:ALA:HB3	2.00	0.43
1:A:3205:PHE:CD2	1:A:3212:ARG:HB2	2.54	0.43
1:A:391:SER:OG	1:A:432:TYR:OH	2.36	0.43
1:A:1148:GLY:HA2	1:A:1156:ARG:CZ	2.49	0.43
1:A:1397:ILE:HD12	1:A:1397:ILE:N	2.33	0.43
1:A:2940:ASP:HB3	1:A:2943:HIS:HD2	1.84	0.43
1:A:1564:MET:HE2	1:A:1723:HIS:HD2	1.84	0.42
1:A:1827:LEU:HD23	1:A:1838:TYR:HB3	2.00	0.42
1:A:1839:THR:HG21	1:A:1874:PRO:HB2	2.00	0.42
1:A:1856:ARG:HA	1:A:1856:ARG:HH21	1.84	0.42
1:A:3587:ASP:HB2	1:A:3590:LEU:HD13	2.00	0.42
1:A:3622:LEU:C	1:A:3622:LEU:HD12	2.44	0.42
1:A:3803:GLU:OE1	1:A:3803:GLU:N	2.42	0.42
1:B:398:SER:HB3	1:B:645:HIS:HB2	2.01	0.42
1:B:948:VAL:HG21	1:B:951:ARG:HH11	1.84	0.42
8:c:1:NAG:H61	8:c:2:NAG:C7	2.50	0.42
1:A:247:CYS:C	1:A:249:ASP:H	2.27	0.42
1:A:4259:ILE:HG22	1:A:4266:ARG:HA	2.01	0.42
1:B:85:TRP:HA	1:B:85:TRP:CE3	2.54	0.42
1:B:1367:GLN:HA	1:B:1372:ALA:HA	2.01	0.42
1:B:3659:ASP:OD2	1:B:3708:ARG:NE	2.53	0.42
1:A:268:ARG:NH2	1:A:333:PRO:HA	2.33	0.42
1:A:1622:TYR:CD1	1:A:1624:GLU:HG3	2.55	0.42
1:A:3891:PHE:CD1	1:A:3891:PHE:C	2.97	0.42
1:B:1831:TRP:CD2	1:B:2014:ARG:HD2	2.55	0.42
1:B:2729:GLY:O	1:B:2733:LEU:N	2.53	0.42
1:B:4181:LEU:HD12	1:B:4181:LEU:HA	1.84	0.42
1:A:761:LYS:HG2	1:A:1051:HIS:CE1	2.54	0.42
1:A:1847:GLU:HB3	1:A:1860:THR:HA	2.00	0.42
1:B:747:PHE:HA	1:B:754:VAL:HA	2.01	0.42
1:A:1882:ALA:C	1:A:1884:GLY:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1574:TRP:HB3	1:B:1601:PRO:HD2	2.02	0.42
1:B:1781:GLY:O	1:B:2006:ARG:HG2	2.19	0.42
1:B:2831:GLN:N	1:B:2853:SER:HB2	2.33	0.42
1:B:3296:LEU:HD22	1:B:3309:ILE:HD11	2.00	0.42
1:A:2954:GLN:HA	1:A:2969:PRO:HA	2.02	0.42
1:A:3690:THR:OG1	1:A:3709:ASP:OD2	2.28	0.42
1:A:4176:ARG:NH2	1:A:4374:GLU:O	2.52	0.42
1:A:4228:GLU:O	1:A:4266:ARG:NH2	2.36	0.42
1:B:1768:SER:HB3	1:B:1770:ASP:OD2	2.19	0.42
1:B:2988:GLN:NE2	1:B:2989:ASN:OD1	2.47	0.42
1:B:4176:ARG:NH2	1:B:4374:GLU:O	2.52	0.42
1:B:4274:MET:HE1	1:B:4297:TRP:NE1	2.34	0.42
1:A:1405:CYS:SG	1:A:1406:VAL:N	2.93	0.42
1:A:2961:ARG:NH2	1:A:3671:ASP:OD2	2.52	0.42
1:A:846:ARG:CB	1:A:847:PRO:HD3	2.49	0.42
1:A:2402:LEU:HD21	1:A:2630:MET:HB3	2.02	0.42
1:A:2475:ASP:OD2	1:A:2478:ASN:HB3	2.18	0.42
1:A:2515:LEU:HA	1:A:2522:MET:HA	2.02	0.42
1:A:2807:CYS:SG	1:A:2814:ASP:HB2	2.59	0.42
1:A:3796:GLU:OE1	1:A:3796:GLU:HA	2.19	0.42
1:B:1519:TRP:CE3	1:B:1698:GLN:NE2	2.88	0.42
1:B:471:LEU:HD21	1:B:480:LEU:HD11	2.02	0.42
1:B:1546:VAL:CG1	1:B:1549:SER:HB2	2.50	0.42
1:A:1550:LYS:HE2	9:U:1:NAG:H82	2.01	0.42
1:A:1585:MET:HE3	1:A:1585:MET:HB3	1.84	0.42
1:A:3205:PHE:HE1	1:A:3453:PRO:HA	1.85	0.42
1:B:412:ASN:OD1	1:B:412:ASN:N	2.53	0.42
1:B:1139:SER:HA	1:B:1142:LYS:HE3	2.01	0.42
1:A:538:GLU:CD	1:A:547:ARG:HH11	2.28	0.41
1:A:752:SER:HB3	1:A:769:ILE:HD12	2.01	0.41
1:A:3948:VAL:HG13	1:A:3960:ASP:O	2.21	0.41
1:A:4278:SER:HB3	1:A:4319:GLN:HA	2.02	0.41
1:B:487:VAL:HG23	1:B:489:ARG:HE	1.85	0.41
1:B:1093:LEU:HA	1:B:1093:LEU:HD12	1.81	0.41
1:B:1854:ASP:OD1	1:B:1854:ASP:N	2.47	0.41
1:A:1413:ARG:NH2	1:A:1413:ARG:HB2	2.35	0.41
1:A:2243:ASP:OD2	1:A:2306:LYS:NZ	2.39	0.41
1:A:2724:ASN:OD1	1:A:2729:GLY:N	2.51	0.41
1:A:4181:LEU:HD12	1:A:4181:LEU:HA	1.88	0.41
1:B:3720:PRO:HA	1:B:3728:ARG:HH22	1.84	0.41
1:B:2960:SER:HB3	1:B:2966:ARG:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4228:GLU:O	1:B:4266:ARG:NH2	2.36	0.41
1:A:188:PHE:HB3	1:A:201:VAL:HG21	2.02	0.41
1:A:397:PHE:HB3	1:A:647:VAL:HG13	2.01	0.41
1:B:206:ASN:C	1:B:208:CYS:H	2.27	0.41
1:B:210:ASP:OD1	1:B:211:ASN:N	2.54	0.41
1:B:1827:LEU:HD12	1:B:1827:LEU:HA	1.78	0.41
1:A:581:GLU:OE1	1:A:590:ARG:NE	2.42	0.41
1:B:1072:ALA:HA	1:B:1079:CYS:HB2	2.02	0.41
1:B:2318:ARG:HG2	1:B:2318:ARG:HH21	1.85	0.41
1:B:3289:LEU:CD1	1:B:3328:ILE:HD12	2.50	0.41
1:B:4273:ALA:C	1:B:4274:MET:HG3	2.46	0.41
1:A:349:ASP:CG	1:A:363:ASN:HD22	2.29	0.41
1:A:1710:CYS:HB3	1:A:1726:CYS:HB3	1.98	0.41
1:B:466:ASP:OD1	1:B:736:THR:OG1	2.24	0.41
1:B:2066:MET:HE1	1:B:2317:ILE:HD13	2.03	0.41
1:A:318:TYR:HB2	1:A:332:PRO:HD3	2.03	0.41
1:A:1921:HIS:CG	1:A:1939:THR:HB	2.56	0.41
1:A:2476:TRP:CD1	1:A:2477:ILE:HG23	2.55	0.41
1:A:3207:ASN:HD22	1:A:3207:ASN:HA	1.53	0.41
1:B:3883:ILE:HD12	1:B:3883:ILE:C	2.46	0.41
1:A:3208:ARG:C	1:A:3210:TYR:H	2.29	0.41
1:A:3209:TYR:O	1:A:3226:GLN:HA	2.20	0.41
1:B:882:ARG:NH1	1:B:902:ASP:OD2	2.54	0.41
1:B:2839:ARG:C	1:B:2841:PHE:N	2.79	0.41
10:Y:1:NAG:H62	10:Y:2:NAG:H82	2.03	0.41
1:A:424:MET:HB2	1:A:443:MET:HG3	2.03	0.41
1:A:677:HIS:CE1	1:A:679:THR:HG23	2.56	0.41
1:A:1135:CYS:SG	1:A:1140:ASP:HB3	2.61	0.41
1:A:1297:CYS:C	1:A:1299:ASP:H	2.27	0.41
1:A:1671:LYS:HE3	1:A:1672:TRP:CZ2	2.55	0.41
1:A:2120:ARG:C	1:A:2122:SER:H	2.29	0.41
1:A:3269:HIS:HB2	1:A:3532:TRP:CZ2	2.56	0.41
1:B:380:ARG:HG2	1:B:382:GLN:H	1.86	0.41
1:B:738:SER:OG	1:B:739:PRO:HD3	2.21	0.41
1:B:1124:PRO:HD2	1:B:1127:TRP:CE3	2.56	0.41
1:B:1161:ARG:NH1	1:B:1174:ASP:O	2.49	0.41
1:B:2234:ILE:HD11	1:B:2237:PRO:HB3	2.03	0.41
1:B:3009:ARG:H	1:B:3009:ARG:HE	1.68	0.41
1:B:3245:TRP:CE2	1:B:3254:GLU:HB2	2.55	0.41
1:A:601:PRO:HB2	1:A:619:THR:HB	2.02	0.41
1:A:3897:ARG:H	1:A:3897:ARG:HG2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:ASP:N	1:B:753:THR:O	2.51	0.41
1:B:1599:TYR:HB3	1:B:1619:TYR:HB3	2.03	0.41
1:B:1719:GLN:HG3	1:B:1721:PRO:HD2	2.02	0.41
1:B:2648:GLN:NE2	1:B:2651:GLN:OE1	2.54	0.41
1:B:4276:PRO:HB3	1:B:4288:TRP:CD1	2.56	0.41
1:A:197:LEU:O	1:A:201:VAL:HG23	2.20	0.40
1:A:4192:ILE:HG22	1:A:4203:TRP:HB2	2.04	0.40
1:A:4262:ASP:OD1	1:A:4264:THR:HG22	2.22	0.40
1:B:3637:CYS:SG	1:B:3643:LYS:HA	2.61	0.40
1:A:2164:ASN:ND2	1:A:2173:GLU:OE2	2.54	0.40
1:A:2199:ASP:CG	1:A:2242:MET:HE2	2.46	0.40
1:B:452:ILE:N	1:B:452:ILE:HD12	2.36	0.40
1:B:2481:ILE:HB	1:B:2494:MET:HG2	2.03	0.40
1:B:3618:VAL:N	1:B:3627:GLU:OE1	2.54	0.40
1:A:2399:LEU:HD22	1:A:2425:LEU:HD21	2.04	0.40
1:B:2149:ARG:HG2	1:B:2194:ARG:CD	2.47	0.40
1:B:4180:TRP:N	1:B:4180:TRP:CD1	2.89	0.40
1:A:872:ASN:ND2	7:N:2:ASN:HD21	2.19	0.40
1:A:2378:ASN:OD1	1:A:2378:ASN:N	2.44	0.40
1:A:2702:ASN:HB3	1:A:2704:LEU:CD2	2.52	0.40
1:A:3710:ASN:O	1:A:3714:GLN:HG2	2.21	0.40
1:B:3966:LEU:HD23	1:B:3966:LEU:HA	1.89	0.40
1:A:190:CYS:SG	1:A:191:GLY:N	2.94	0.40
1:A:747:PHE:HA	1:A:754:VAL:HA	2.04	0.40
1:A:2252:VAL:HG12	1:A:2259:ILE:HG12	2.03	0.40
1:B:983:CYS:SG	1:B:987:CYS:HB3	2.62	0.40
1:B:1720:ALA:N	1:B:1721:PRO:HD2	2.36	0.40
1:B:2193:PRO:HB3	1:B:2207:TRP:CD1	2.57	0.40
1:B:2936:MET:HE3	1:B:2936:MET:HB3	1.94	0.40
1:B:3670:ILE:HA	1:B:3673:CYS:HB2	2.03	0.40
1:B:4079:TYR:CG	1:B:4080:LEU:N	2.88	0.40
1:B:4262:ASP:OD1	1:B:4264:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

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

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	248	GLN
1	A	361	CYS
1	A	377	ILE
1	A	395	VAL
1	A	492	VAL
1	A	505	THR
1	A	508	LEU
1	A	516	LEU
1	A	520	VAL
1	A	555	VAL
1	A	570	VAL
1	A	582	THR
1	A	593	VAL
1	A	608	LEU
1	A	707	LYS
1	A	724	THR
1	A	728	GLN
1	A	732	MET

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Mol	Chain	Res	Type
1	A	754	VAL
1	A	807	VAL
1	A	839	MET
1	A	887	ASP
1	A	893	ILE
1	A	919	THR
1	A	925	VAL
1	A	929	ASP
1	A	931	ARG
1	A	973	CYS
1	A	1063	ASN
1	A	1319	GLN
1	A	1346	SER
1	A	1351	GLN
1	A	1364	GLN
1	A	1401	CYS
1	A	1408	MET
1	A	1477	VAL
1	A	1613	ILE
1	A	1728	CYS
1	A	1814	VAL
1	A	1911	LEU
1	A	2174	VAL
1	A	2175	LEU
1	A	2188	VAL
1	A	2230	VAL
1	A	2452	LEU
1	A	2515	LEU
1	A	2547	VAL
1	A	2599	LEU
1	A	2692	TYR
1	A	2767	CYS
1	A	2795	ILE
1	A	2809	ASP
1	A	2830	CYS
1	A	2834	ASN
1	A	2839	ARG
1	A	2854	ASP
1	A	2871	GLN
1	A	2901	CYS
1	A	2968	ILE
1	A	3081	GLN

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Mol	Chain	Res	Type
1	A	3128	CYS
1	A	3205	PHE
1	A	3207	ASN
1	A	3209	TYR
1	A	3226	GLN
1	A	3300	ASP
1	A	3315	ASP
1	A	3318	ASN
1	A	3319	THR
1	A	3373	THR
1	A	3415	LEU
1	A	3416	THR
1	A	3511	MET
1	A	3541	SER
1	A	3661	ASP
1	A	3741	CYS
1	A	3774	ILE
1	A	3867	ASN
1	A	3898	CYS
1	A	3916	ASP
1	A	3960	ASP
1	A	3961	GLU
1	A	3980	ASN
1	A	4041	MET
1	A	4168	ILE
1	A	4217	MET
1	A	4237	SER
1	A	4314	ASN
1	A	4339	VAL
1	A	4346	LEU
1	A	4353	CYS
1	A	4396	ASN
1	B	207	ASP
1	B	213	ASP
1	B	221	THR
1	B	245	ASP
1	B	264	ARG
1	B	322	GLN
1	B	361	CYS
1	B	371	LEU
1	B	395	VAL
1	B	443	MET

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Mol	Chain	Res	Type
1	B	447	VAL
1	B	487	VAL
1	B	489	ARG
1	B	500	ARG
1	B	570	VAL
1	B	593	VAL
1	B	616	THR
1	B	631	GLU
1	B	632	THR
1	B	653	LEU
1	B	899	ASP
1	B	968	THR
1	B	978	HIS
1	B	990	VAL
1	B	1104	HIS
1	B	1137	ASP
1	B	1153	THR
1	B	1168	VAL
1	B	1300	MET
1	B	1585	MET
1	B	1598	ILE
1	B	1660	ASP
1	B	1955	MET
1	B	1967	LEU
1	B	1987	VAL
1	B	2079	LEU
1	B	2098	VAL
1	B	2127	ARG
1	B	2221	LEU
1	B	2286	VAL
1	B	2561	LEU
1	B	2599	LEU
1	B	2613	THR
1	B	2656	CYS
1	B	2766	ASP
1	B	2773	GLU
1	B	2777	LEU
1	B	2781	CYS
1	B	2828	THR
1	B	2851	ASP
1	B	2859	TYR
1	B	2933	CYS

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Mol	Chain	Res	Type
1	B	2992	MET
1	B	3091	GLU
1	B	3108	GLU
1	B	3130	ASP
1	B	3172	VAL
1	B	3207	ASN
1	B	3235	ASP
1	B	3373	THR
1	B	3416	THR
1	B	3515	SER
1	B	3534	CYS
1	B	3744	THR
1	B	3822	ARG
1	B	3897	ARG
1	B	3974	GLU
1	B	3982	THR
1	B	4041	MET
1	B	4062	GLU
1	B	4065	ARG
1	B	4078	GLU
1	B	4168	ILE
1	B	4217	MET
1	B	4313	VAL
1	B	4314	ASN
1	B	4319	GLN
1	B	4339	VAL
1	B	4346	LEU
1	B	4353	CYS
1	B	4396	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	GLN
1	A	368	HIS
1	A	638	HIS
1	A	660	ASN
1	A	1009	GLN
1	A	1053	ASN
1	A	1283	ASN
1	A	1317	GLN
1	A	1350	ASN

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Mol	Chain	Res	Type
1	A	1458	ASN
1	A	1523	ASN
1	A	1610	ASN
1	A	1670	ASN
1	A	1780	HIS
1	A	1803	HIS
1	A	1920	GLN
1	A	1921	HIS
1	A	2026	ASN
1	A	2322	ASN
1	A	2349	GLN
1	A	2351	ASN
1	A	2356	HIS
1	A	2431	ASN
1	A	2446	GLN
1	A	2604	GLN
1	A	2677	GLN
1	A	2758	HIS
1	A	2770	ASN
1	A	2903	HIS
1	A	2931	ASN
1	A	2941	GLN
1	A	2943	HIS
1	A	2959	ASN
1	A	3081	GLN
1	A	3318	ASN
1	A	3400	HIS
1	A	3402	HIS
1	A	3518	GLN
1	A	3552	HIS
1	A	3714	GLN
1	A	3854	HIS
1	A	3921	HIS
1	A	4011	ASN
1	A	4131	ASN
1	A	4234	ASN
1	A	4390	ASN
1	B	100	GLN
1	B	226	GLN
1	B	259	ASN
1	B	431	HIS
1	B	478	ASN

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Mol	Chain	Res	Type
1	B	612	HIS
1	B	633	ASN
1	B	665	ASN
1	B	751	HIS
1	B	980	ASN
1	B	1051	HIS
1	B	1133	ASN
1	B	1317	GLN
1	B	1543	HIS
1	B	1576	HIS
1	B	1698	GLN
1	B	1719	GLN
1	B	1746	GLN
1	B	1798	ASN
1	B	2026	ASN
1	B	2084	HIS
1	B	2100	HIS
1	B	2107	ASN
1	B	2431	ASN
1	B	2465	ASN
1	B	2595	HIS
1	B	2648	GLN
1	B	2650	GLN
1	B	2722	ASN
1	B	2954	GLN
1	B	2970	GLN
1	B	3057	ASN
1	B	3066	GLN
1	B	3086	ASN
1	B	3318	ASN
1	B	3387	HIS
1	B	3500	GLN
1	B	3614	GLN
1	B	3691	ASN
1	B	3714	GLN
1	B	3722	HIS
1	B	3732	HIS
1	B	3733	HIS
1	B	3789	ASN
1	B	3806	GLN
1	B	3965	ASN
1	B	4130	ASN

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Mol	Chain	Res	Type
1	B	4234	ASN
1	B	4390	ASN
7	N	2	ASN

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
8	1	3	BMA	O5-C5	2.13	1.47	1.43
11	4	3	BMA	O5-C5	2.09	1.47	1.43
10	1	5	MAN	O5-C5	2.08	1.47	1.43

All (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
8	w	1	NAG	C1-O5-C5	3.54	116.94	112.19
8	x	2	NAG	O5-C1-C2	-3.27	106.23	111.29
9	z	1	NAG	C1-O5-C5	3.20	116.48	112.19
10	g	1	NAG	O5-C1-C2	3.19	116.22	111.29
10	h	1	NAG	C1-O5-C5	3.15	116.41	112.19
10	1	2	NAG	C1-O5-C5	3.08	116.32	112.19
10	r	1	NAG	C1-C2-N2	3.05	115.23	110.43
9	V	1	NAG	C4-C3-C2	3.00	115.42	111.02
9	k	1	NAG	C1-C2-N2	2.98	115.13	110.43
9	u	2	NAG	C1-O5-C5	2.94	116.13	112.19
9	n	2	NAG	C1-O5-C5	2.93	116.11	112.19
8	l	3	BMA	C1-O5-C5	2.91	116.08	112.19
10	2	3	BMA	C1-O5-C5	2.88	116.04	112.19
9	e	2	NAG	C1-O5-C5	2.81	115.95	112.19
10	W	1	NAG	C1-O5-C5	2.78	115.91	112.19
10	2	5	MAN	C1-O5-C5	2.74	115.85	112.19
10	2	5	MAN	C1-C2-C3	2.70	113.58	109.64
10	W	1	NAG	O5-C1-C2	-2.66	107.18	111.29
8	E	2	NAG	C1-C2-N2	2.58	114.50	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	5	2	NAG	C1-O5-C5	2.55	115.61	112.19
10	g	1	NAG	C3-C4-C5	-2.48	105.73	110.23
9	5	1	NAG	C1-O5-C5	2.48	115.51	112.19
10	2	2	NAG	C1-O5-C5	2.46	115.49	112.19
9	n	1	NAG	C4-C3-C2	2.45	114.61	111.02
8	l	2	NAG	C1-O5-C5	2.45	115.47	112.19
10	1	4	MAN	C1-O5-C5	2.38	115.38	112.19
9	V	1	NAG	C2-N2-C7	2.35	126.06	122.90
9	m	2	NAG	C1-O5-C5	2.34	115.32	112.19
9	p	1	NAG	O5-C1-C2	-2.32	107.70	111.29
9	e	1	NAG	O5-C1-C2	2.32	114.88	111.29
10	r	5	MAN	C1-O5-C5	2.31	115.29	112.19
9	z	2	NAG	C1-C2-N2	2.30	114.05	110.43
10	2	3	BMA	C1-C2-C3	2.24	112.91	109.64
9	S	2	NAG	C1-C2-N2	2.23	113.95	110.43
11	4	3	BMA	C1-O5-C5	2.18	115.11	112.19
9	u	1	NAG	C1-O5-C5	2.18	115.10	112.19
9	Z	2	NAG	C2-N2-C7	2.15	125.78	122.90
10	2	4	MAN	C1-O5-C5	2.15	115.06	112.19
10	1	4	MAN	C1-C2-C3	2.13	112.75	109.64
9	X	2	NAG	C2-N2-C7	2.11	125.73	122.90
10	1	5	MAN	C1-O5-C5	2.11	115.01	112.19
10	t	1	NAG	C1-C2-N2	2.09	113.72	110.43
10	g	3	BMA	C1-O5-C5	2.08	114.98	112.19
9	X	2	NAG	C1-C2-N2	2.07	113.69	110.43
8	l	1	NAG	C1-O5-C5	2.06	114.94	112.19
9	k	2	NAG	C1-C2-N2	2.06	113.67	110.43
9	s	1	NAG	C1-C2-N2	2.04	113.65	110.43
10	h	2	NAG	C1-O5-C5	2.04	114.92	112.19
8	T	2	NAG	C1-O5-C5	2.02	114.89	112.19
9	n	1	NAG	C1-O5-C5	2.02	114.89	112.19
9	k	1	NAG	C1-O5-C5	2.01	114.88	112.19
8	x	1	NAG	O5-C1-C2	-2.01	108.18	111.29

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Atoms
9	X	2	NAG	C1-C2-N2-C7
10	t	1	NAG	C1-C2-N2-C7
10	y	2	NAG	C8-C7-N2-C2
10	y	2	NAG	O7-C7-N2-C2
11	j	2	NAG	O5-C5-C6-O6
11	4	2	NAG	O5-C5-C6-O6
10	1	1	NAG	O5-C5-C6-O6
10	2	3	BMA	O5-C5-C6-O6
9	S	1	NAG	C8-C7-N2-C2
9	q	1	NAG	C8-C7-N2-C2
9	q	1	NAG	O7-C7-N2-C2
10	2	3	BMA	C4-C5-C6-O6
10	r	3	BMA	O5-C5-C6-O6
9	S	1	NAG	O7-C7-N2-C2
9	s	1	NAG	C8-C7-N2-C2
8	w	2	NAG	C8-C7-N2-C2
8	w	2	NAG	O7-C7-N2-C2
9	v	2	NAG	C8-C7-N2-C2
10	1	1	NAG	C4-C5-C6-O6
9	f	1	NAG	C8-C7-N2-C2
9	s	1	NAG	O7-C7-N2-C2
9	v	2	NAG	O7-C7-N2-C2
9	0	2	NAG	C8-C7-N2-C2
9	3	2	NAG	C8-C7-N2-C2
8	l	1	NAG	O5-C5-C6-O6
10	r	3	BMA	C4-C5-C6-O6
9	u	1	NAG	O5-C5-C6-O6
9	i	2	NAG	C8-C7-N2-C2
11	4	2	NAG	C4-C5-C6-O6
10	y	1	NAG	O5-C5-C6-O6
8	x	1	NAG	C4-C5-C6-O6
9	f	1	NAG	O7-C7-N2-C2
10	W	1	NAG	C8-C7-N2-C2
11	j	2	NAG	C4-C5-C6-O6
10	y	1	NAG	C4-C5-C6-O6
8	x	1	NAG	O5-C5-C6-O6
9	z	2	NAG	O5-C5-C6-O6
9	p	2	NAG	O5-C5-C6-O6
10	h	5	MAN	O5-C5-C6-O6
9	3	2	NAG	O7-C7-N2-C2
9	S	2	NAG	O5-C5-C6-O6
9	v	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	Y	2	NAG	O5-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
8	o	1	NAG	O5-C5-C6-O6
9	X	2	NAG	O5-C5-C6-O6
9	i	2	NAG	O7-C7-N2-C2
9	0	2	NAG	O7-C7-N2-C2
9	3	2	NAG	O5-C5-C6-O6
9	i	2	NAG	O5-C5-C6-O6
9	q	1	NAG	C3-C2-N2-C7
10	g	3	BMA	O5-C5-C6-O6
9	S	2	NAG	C1-C2-N2-C7
9	z	2	NAG	C1-C2-N2-C7
10	W	1	NAG	O7-C7-N2-C2
9	q	2	NAG	C8-C7-N2-C2
8	w	2	NAG	C3-C2-N2-C7
9	Z	2	NAG	C3-C2-N2-C7
9	k	2	NAG	C3-C2-N2-C7
10	y	2	NAG	C3-C2-N2-C7
8	E	2	NAG	C8-C7-N2-C2
9	u	1	NAG	C4-C5-C6-O6
9	q	2	NAG	O7-C7-N2-C2
8	c	2	NAG	C1-C2-N2-C7
9	Z	2	NAG	C1-C2-N2-C7
9	m	2	NAG	C1-C2-N2-C7
10	h	2	NAG	C1-C2-N2-C7
11	j	1	NAG	C1-C2-N2-C7
11	j	2	NAG	C1-C2-N2-C7
11	4	2	NAG	C1-C2-N2-C7
8	E	2	NAG	O7-C7-N2-C2
9	S	2	NAG	C3-C2-N2-C7
9	m	2	NAG	C3-C2-N2-C7
9	z	2	NAG	C3-C2-N2-C7
9	k	1	NAG	C4-C5-C6-O6
8	l	1	NAG	C4-C5-C6-O6
10	r	2	NAG	C8-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 9 short contacts:

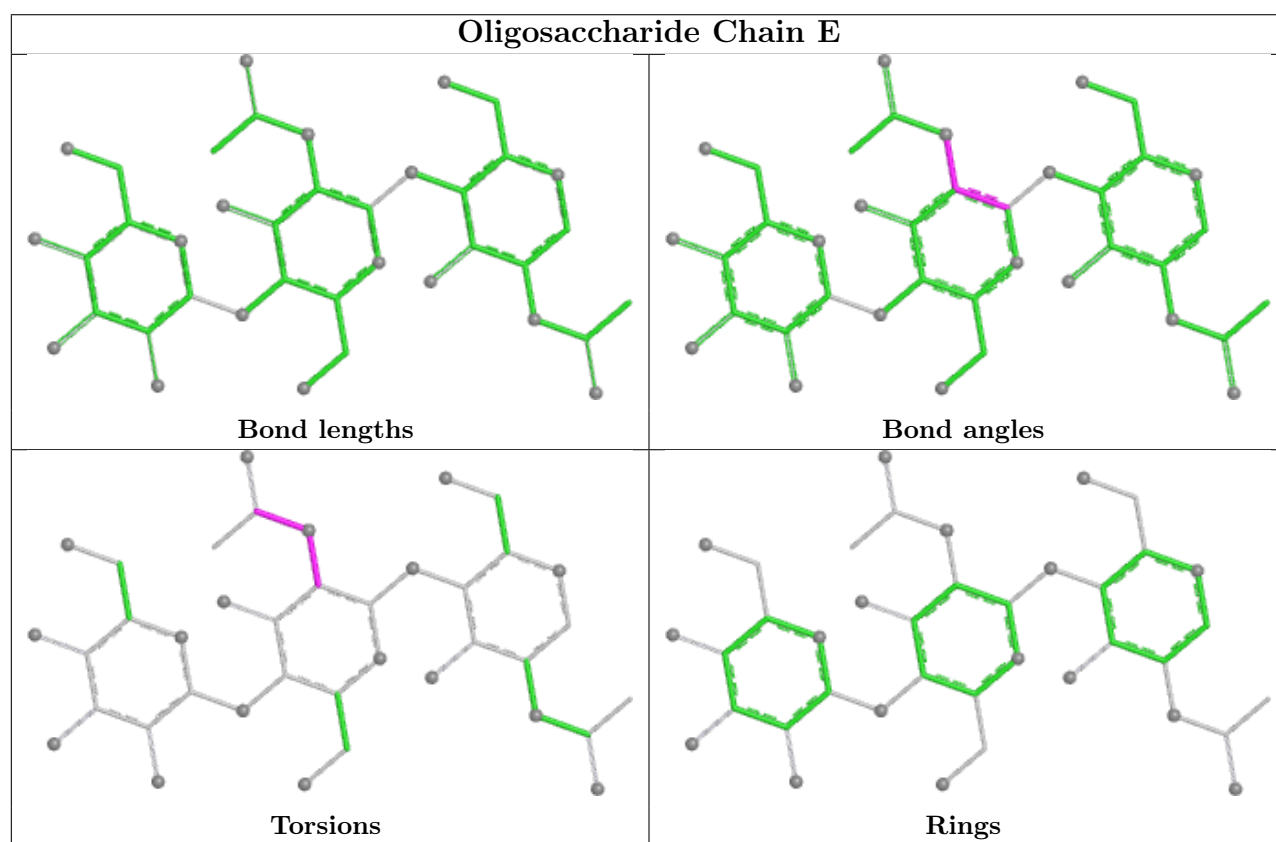
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	t	2	NAG	1	0
8	c	1	NAG	1	0

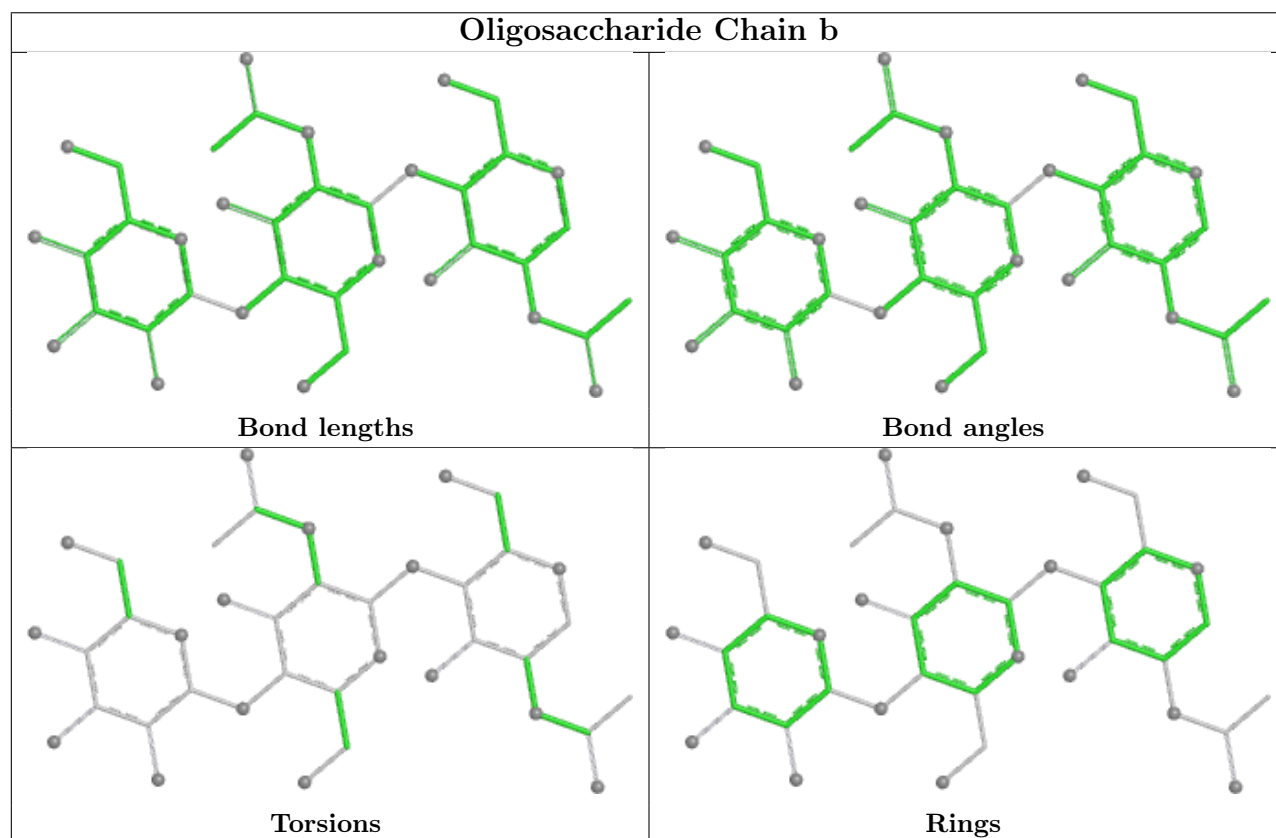
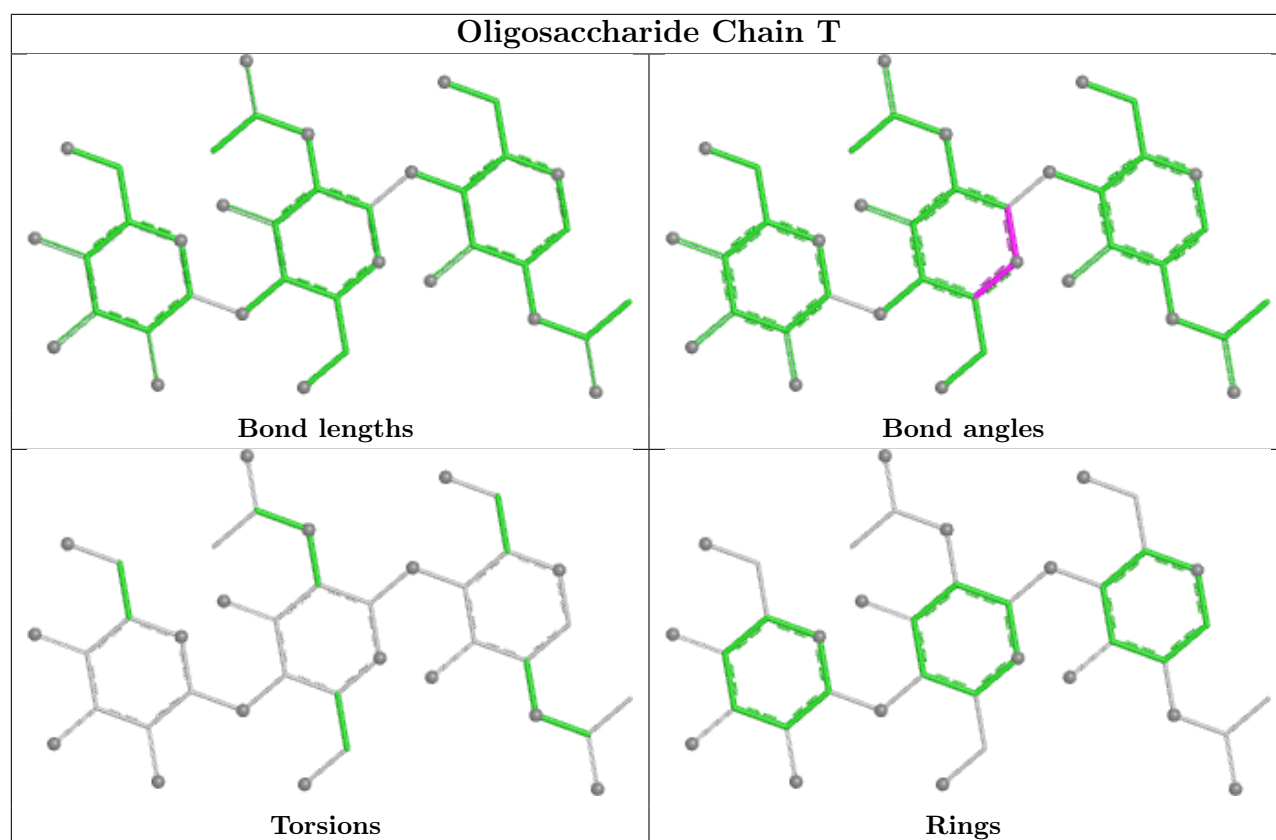
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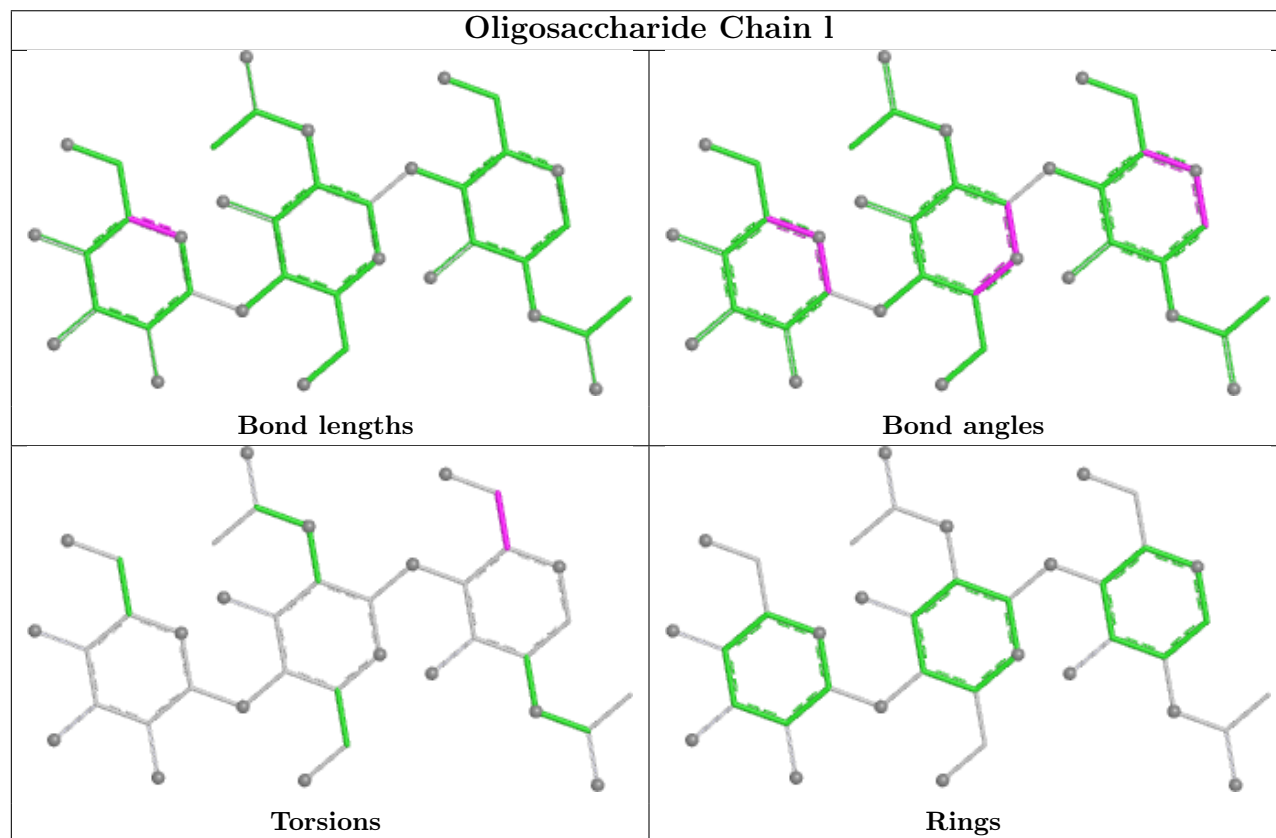
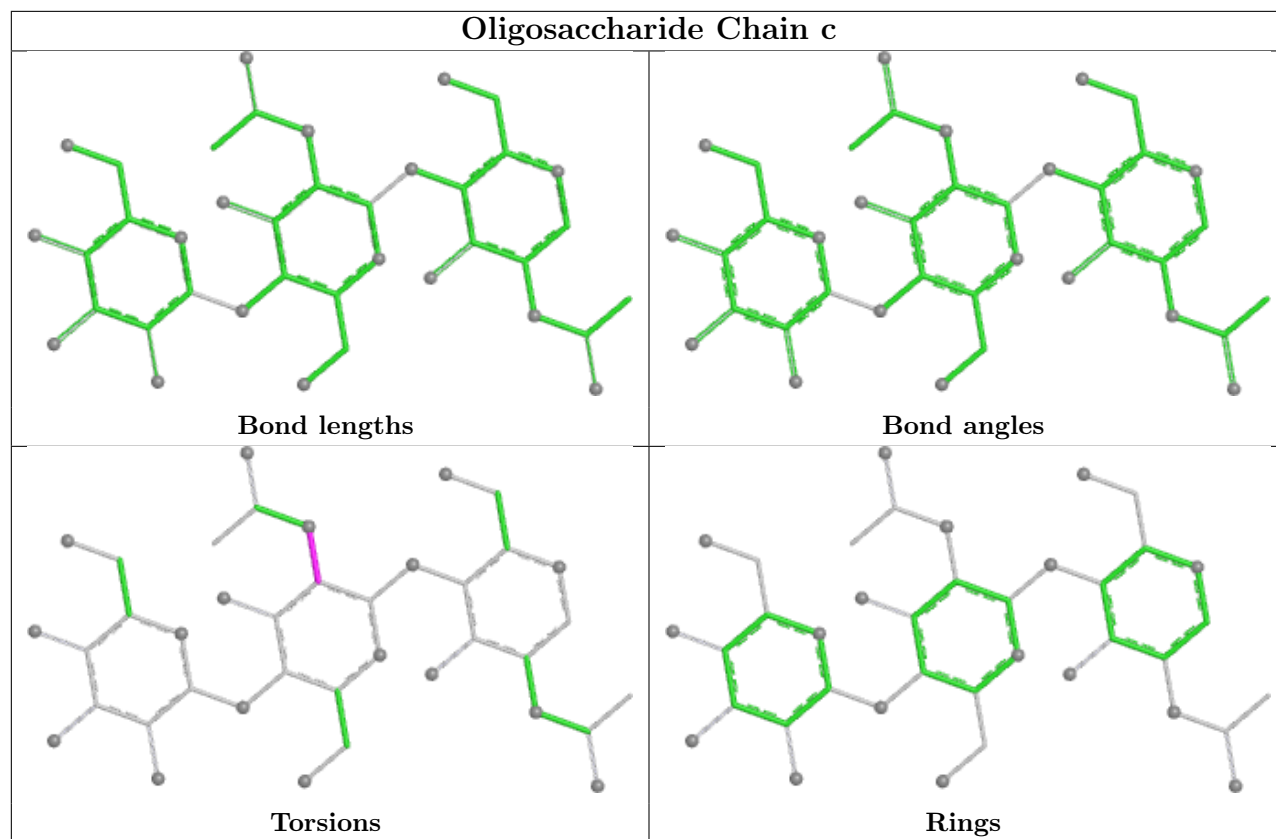
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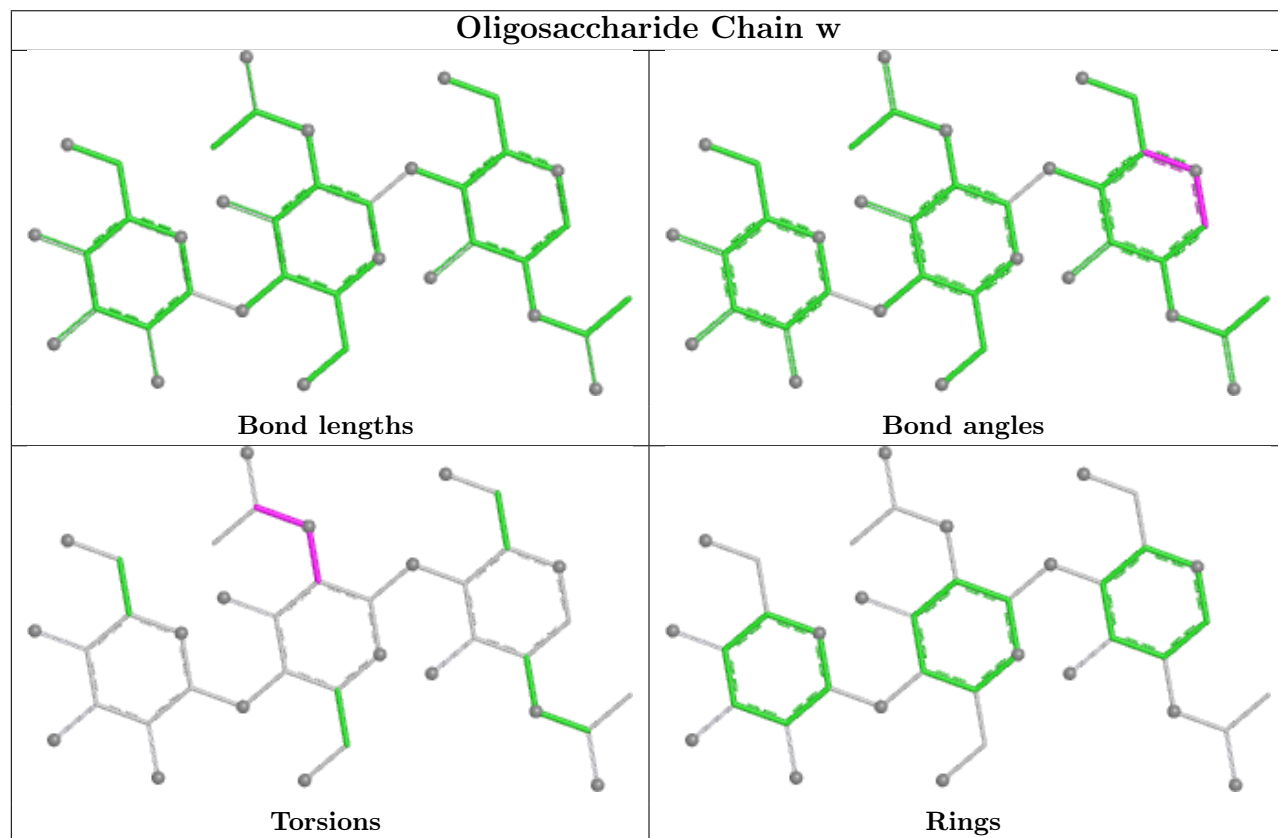
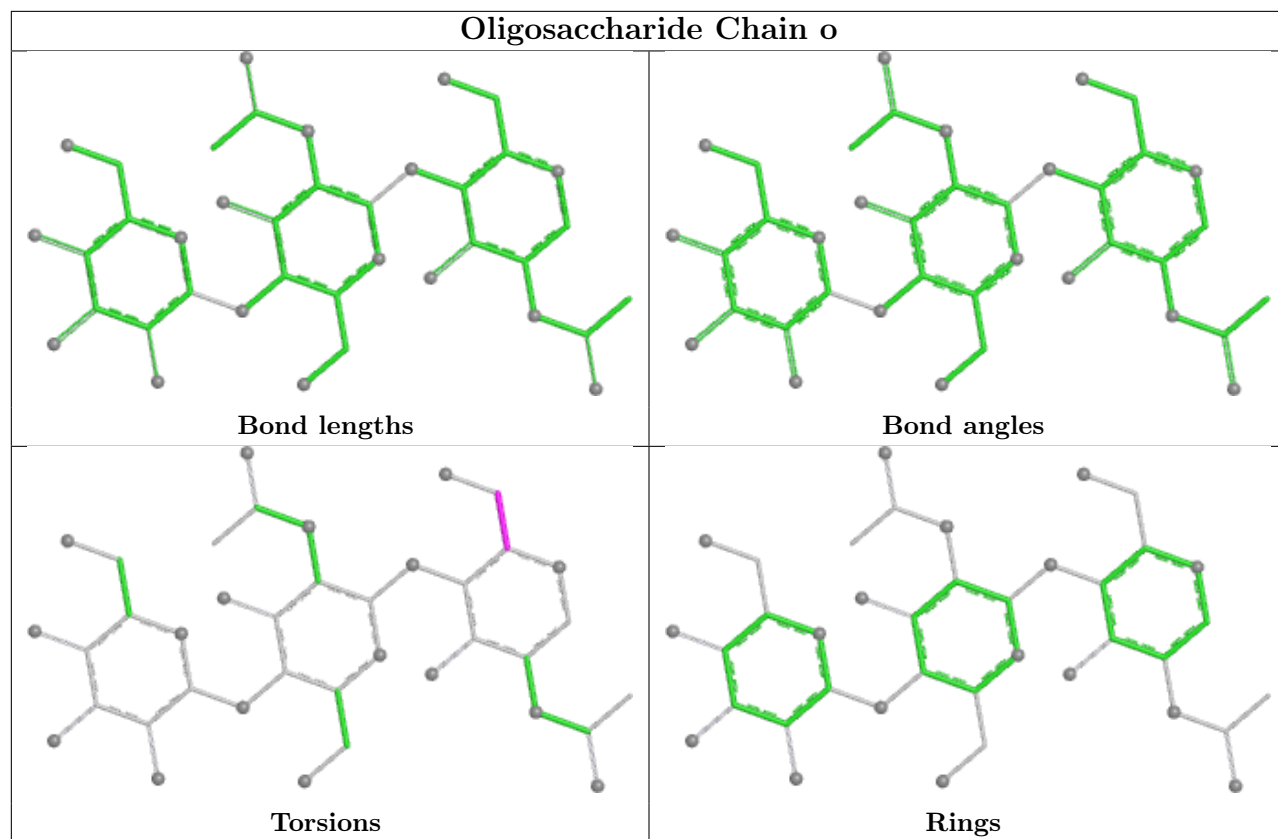
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	U	1	NAG	1	0
8	c	2	NAG	1	0
8	o	1	NAG	1	0
10	y	1	NAG	1	0
10	Y	1	NAG	1	0
10	r	1	NAG	1	0
9	p	1	NAG	1	0
10	Y	2	NAG	1	0
9	s	1	NAG	1	0
10	y	2	NAG	1	0

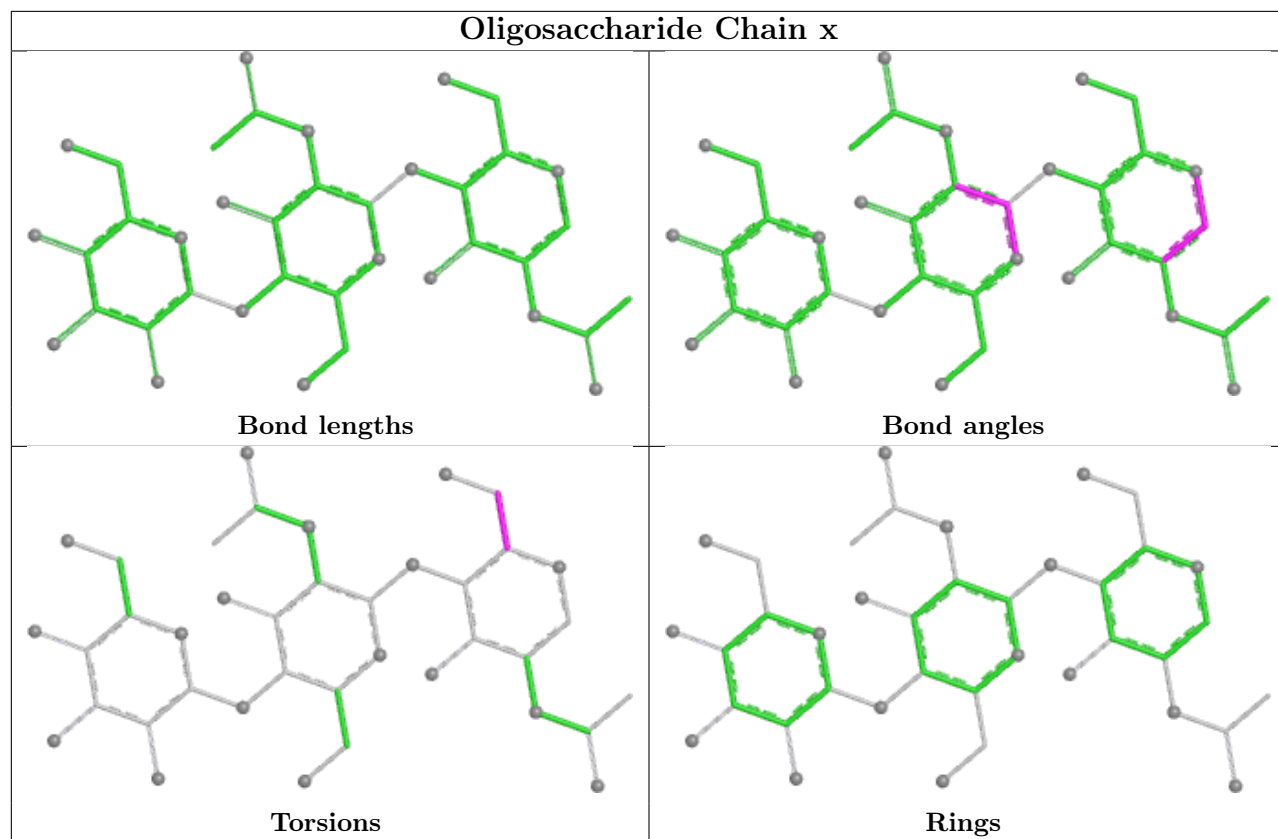
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

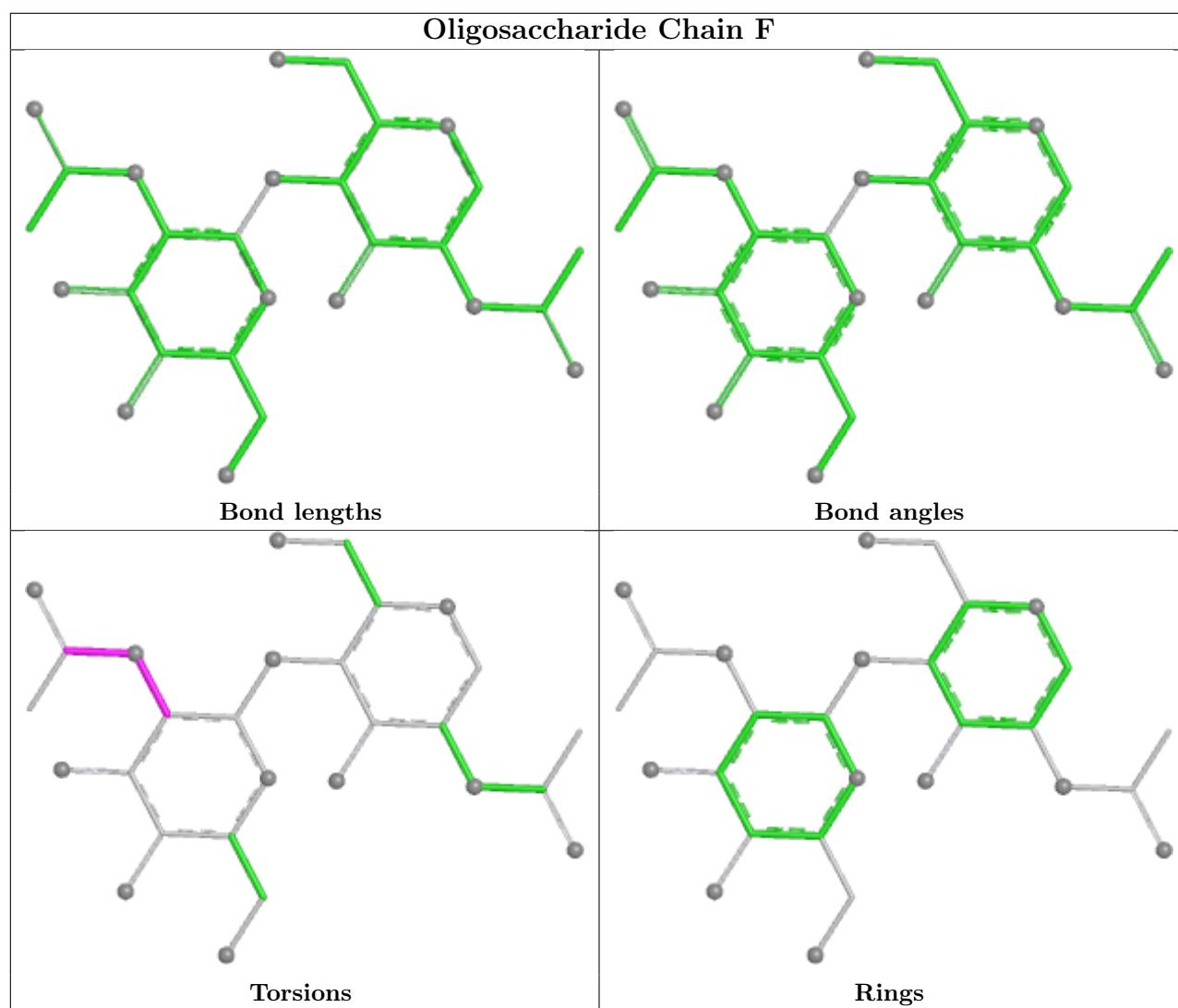


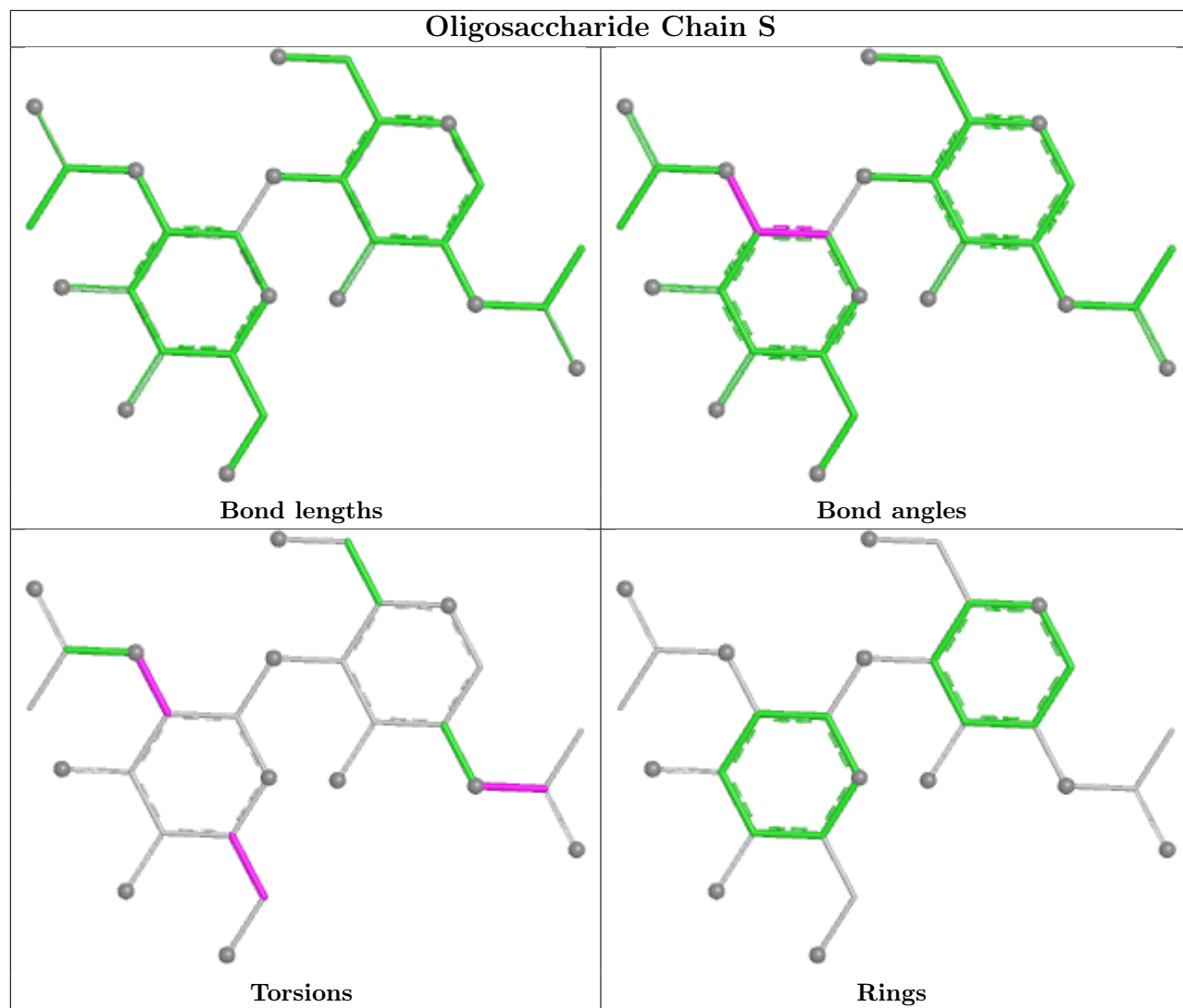


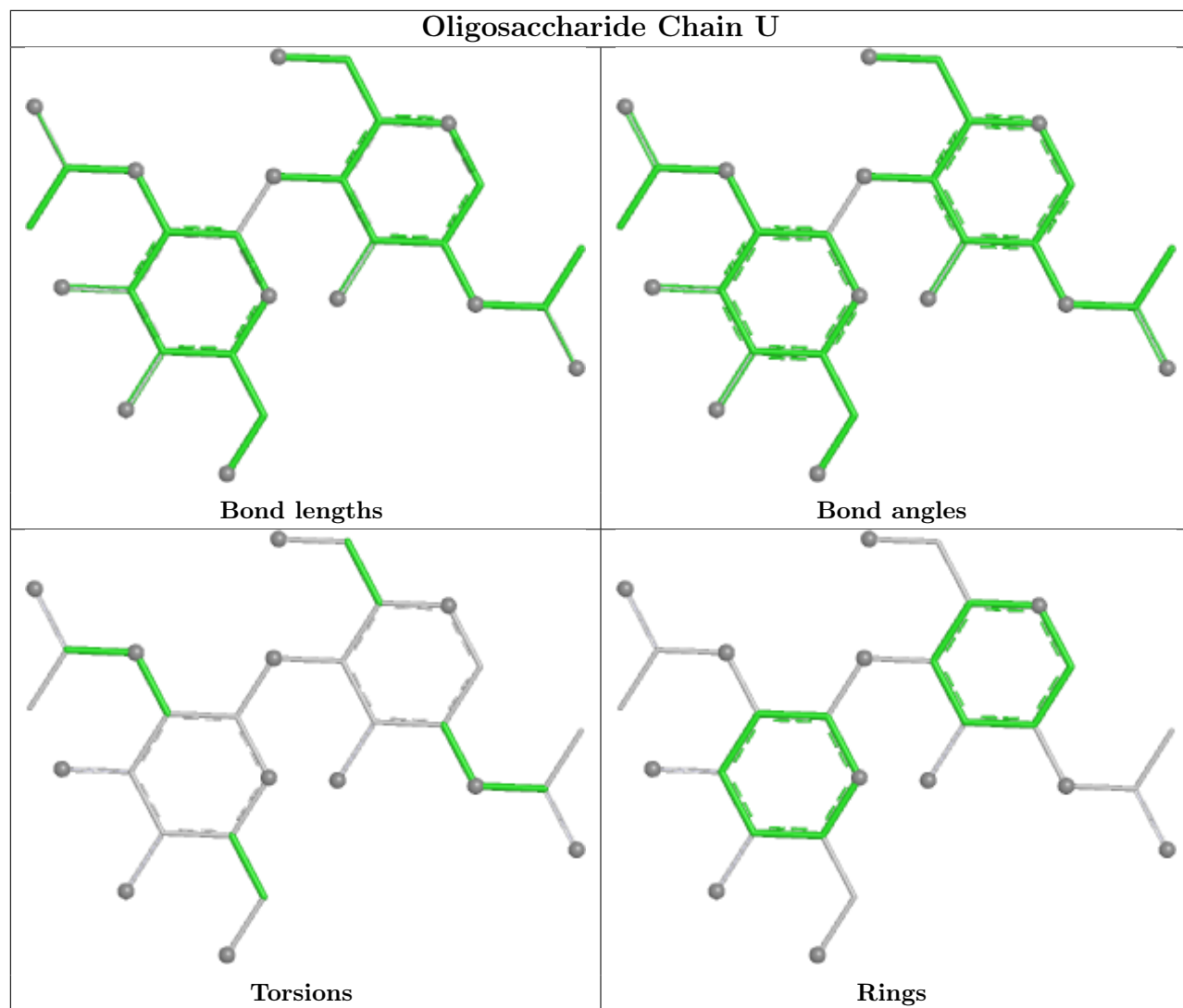


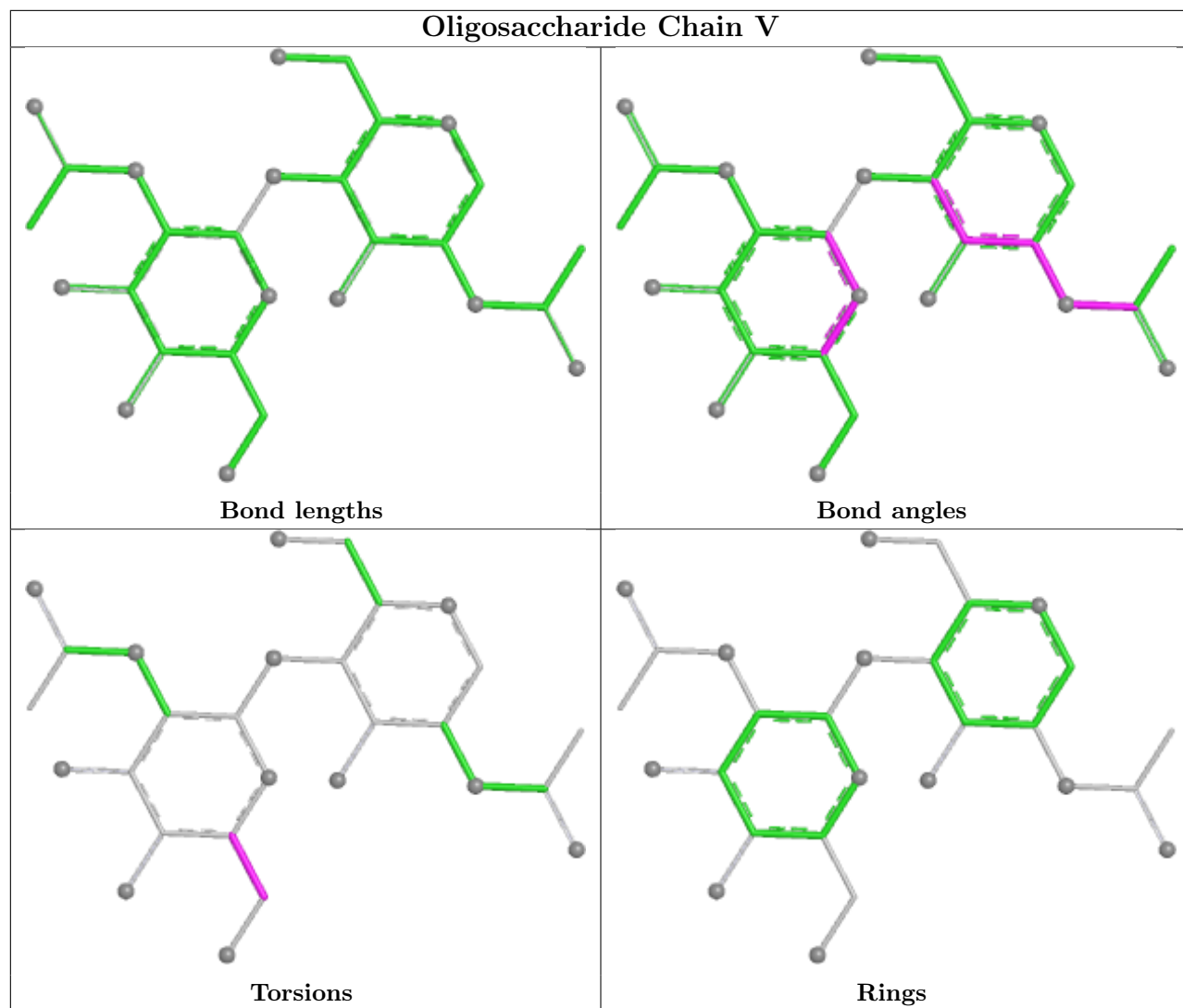


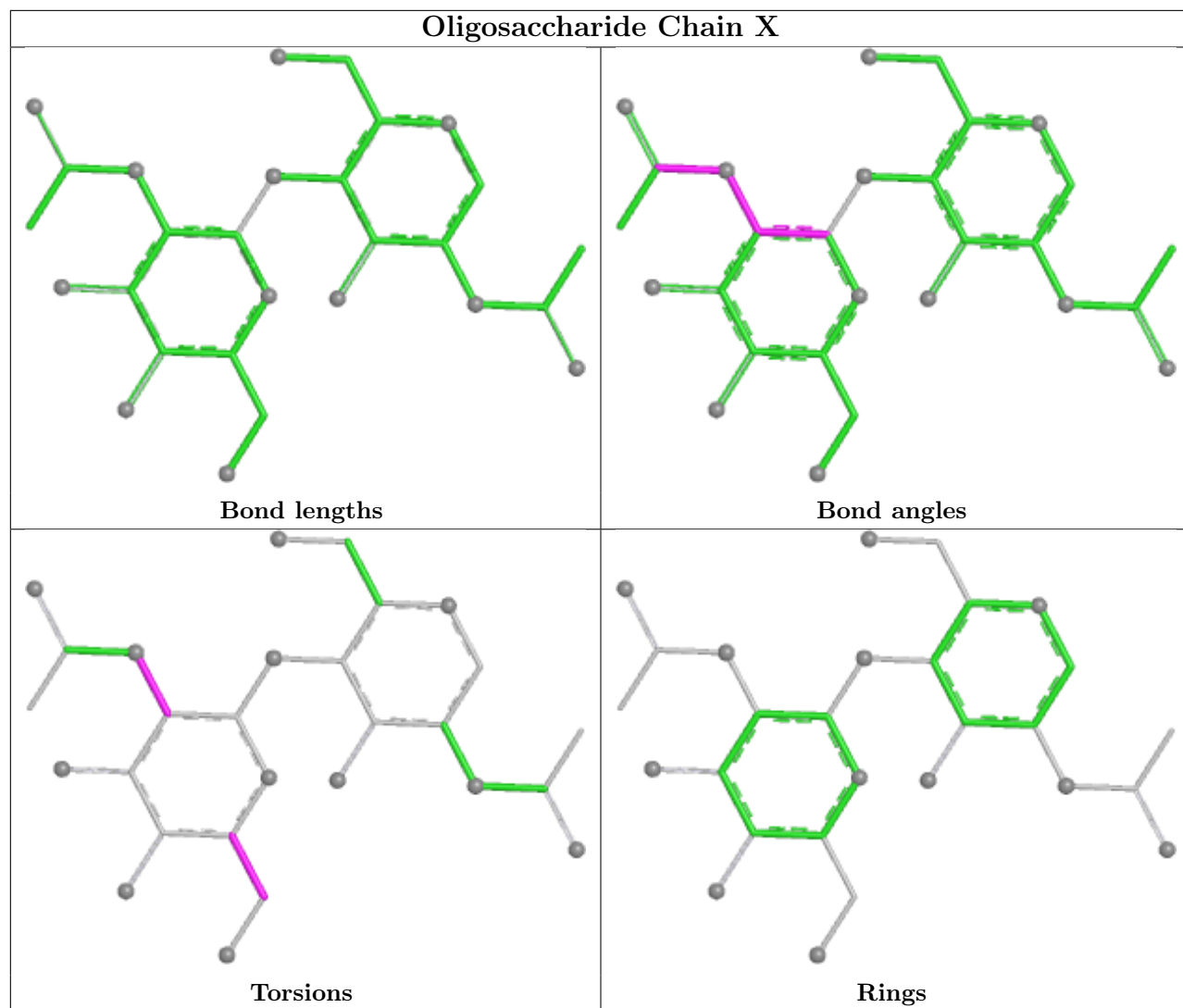


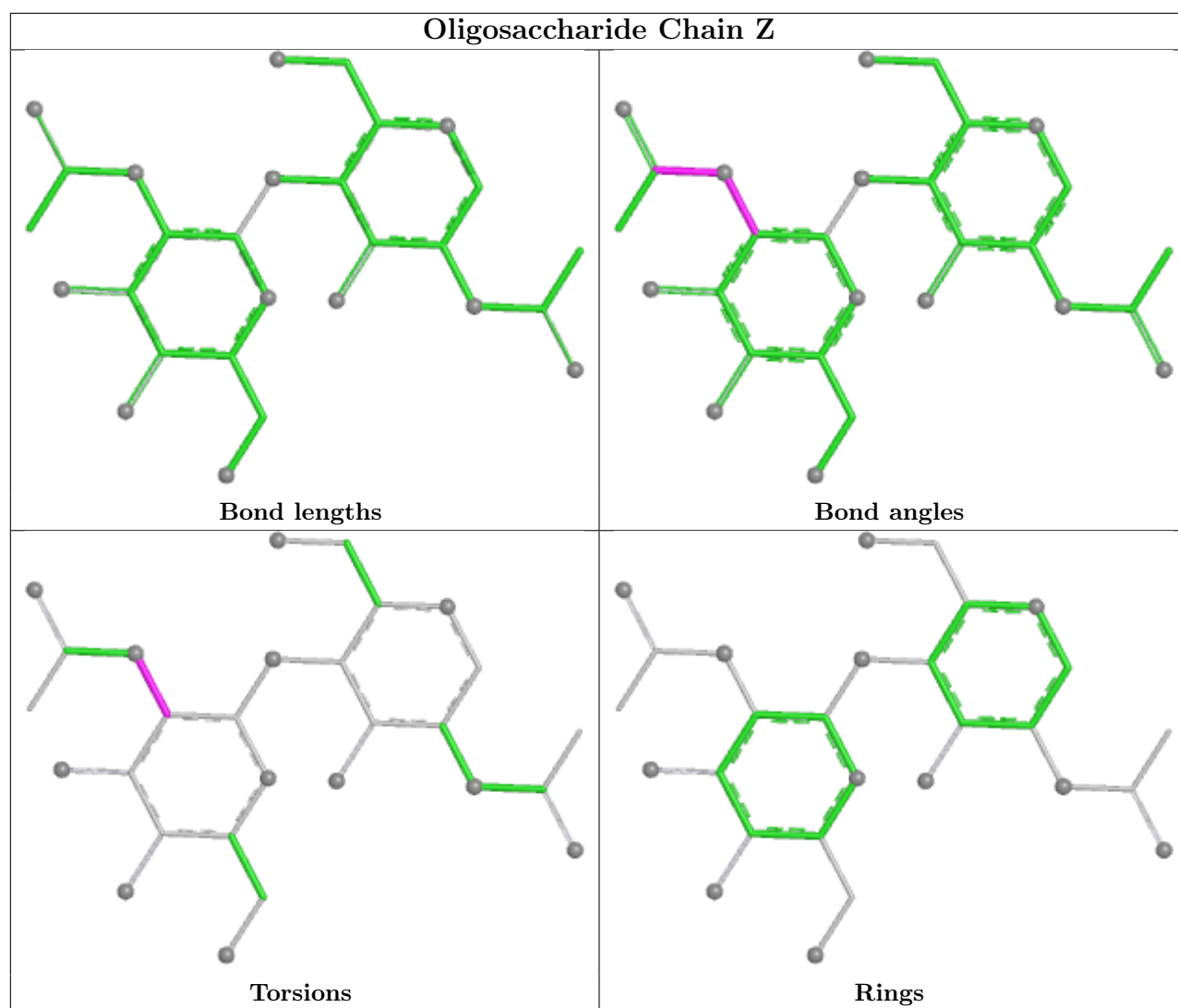


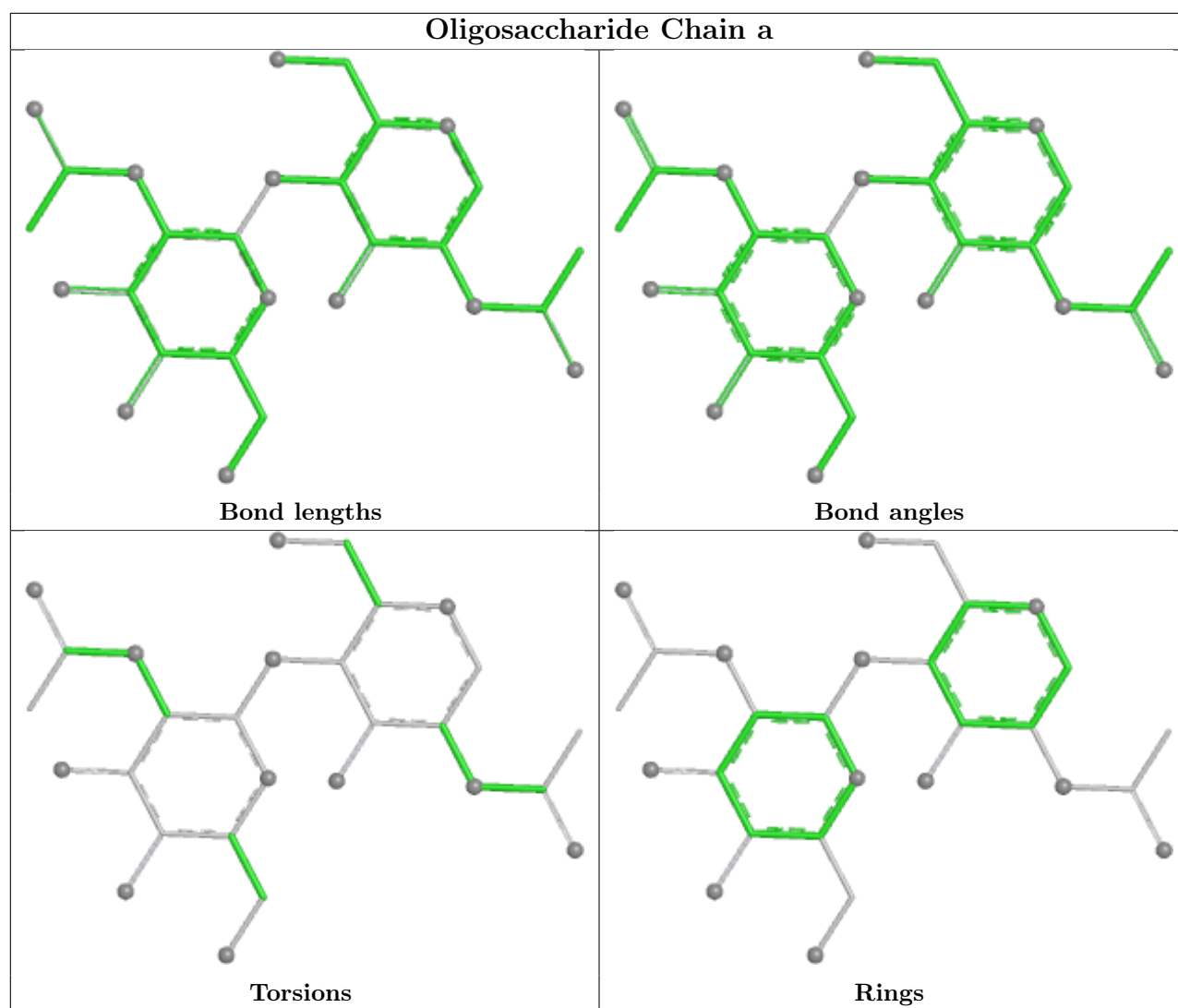


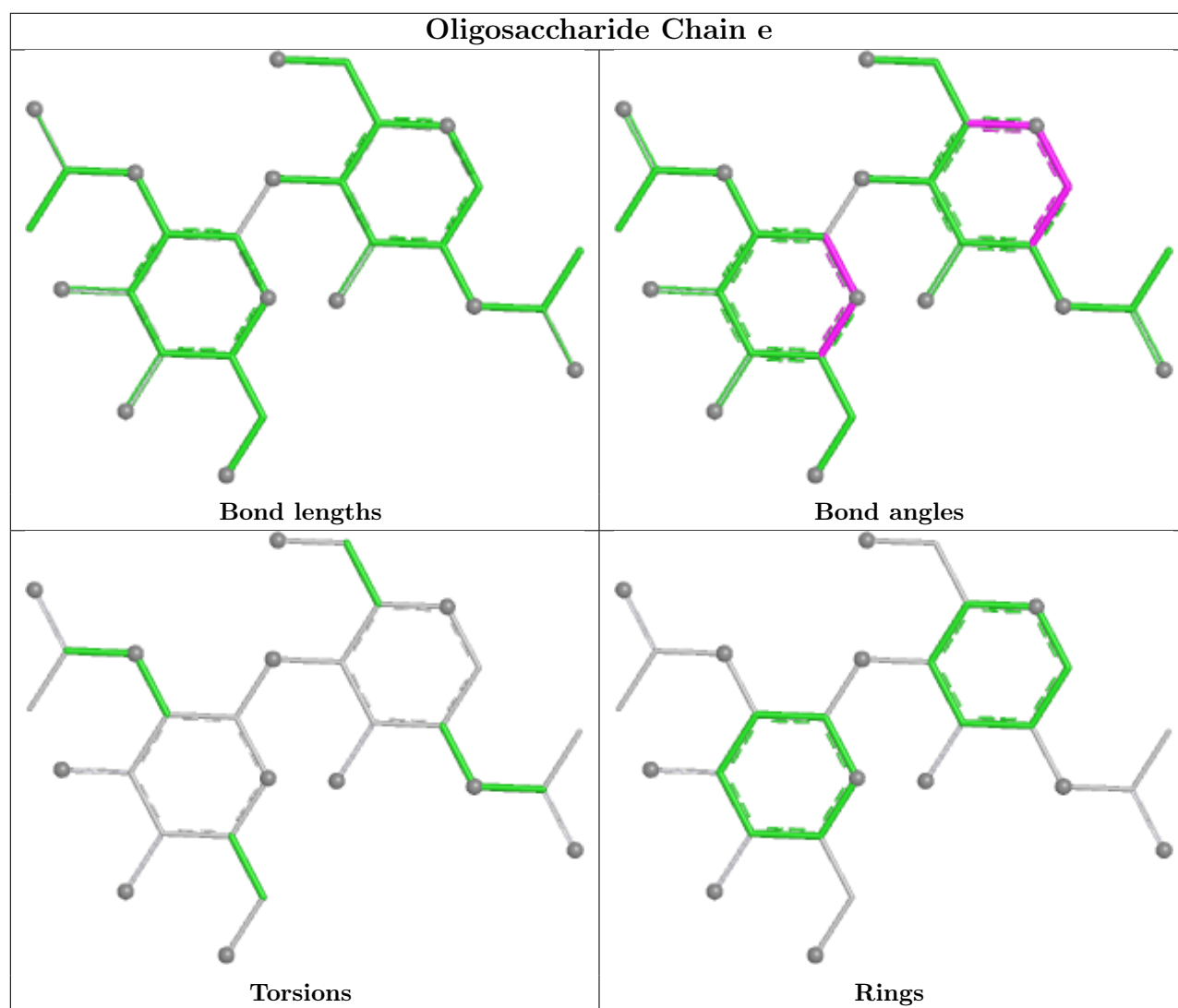


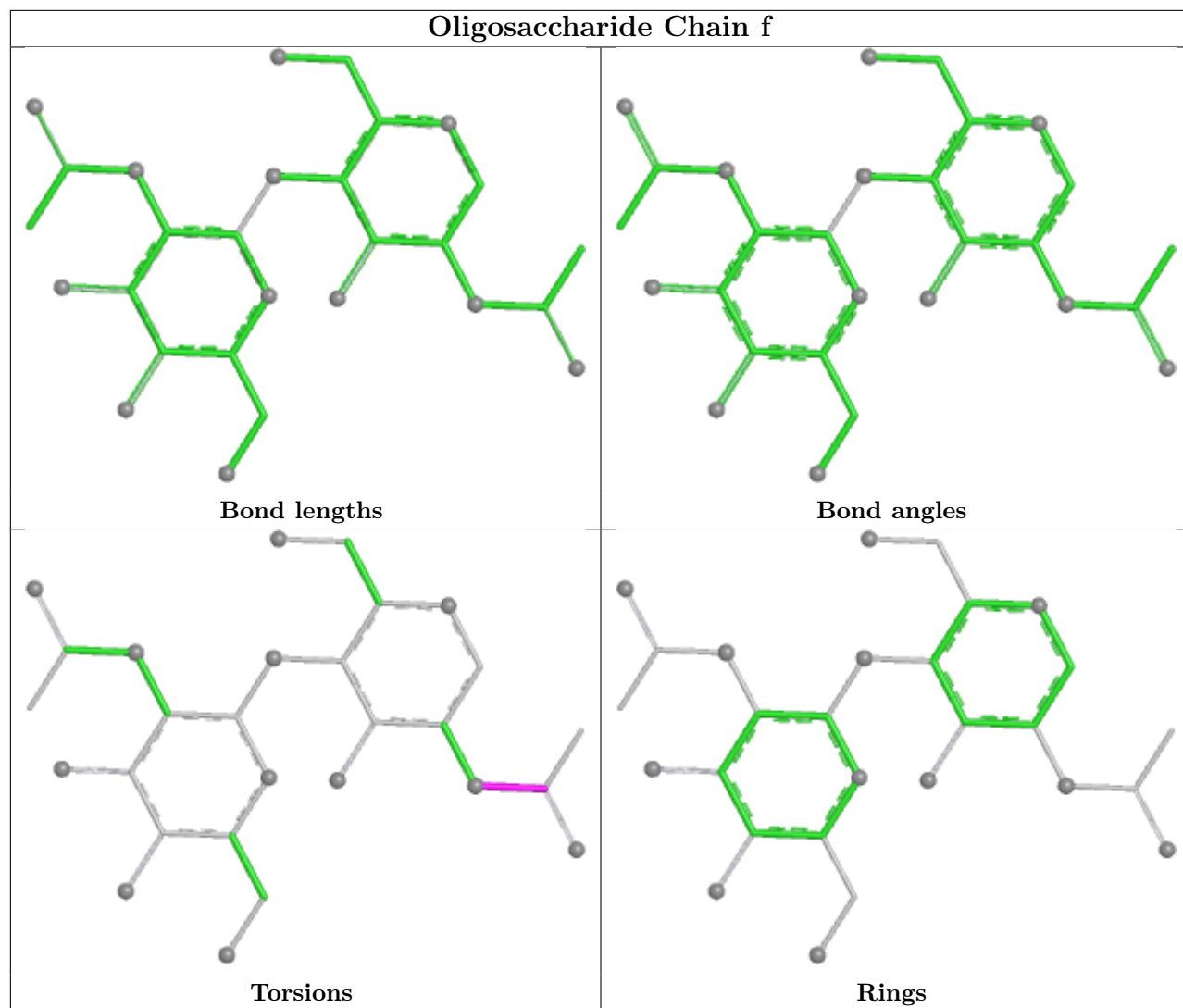


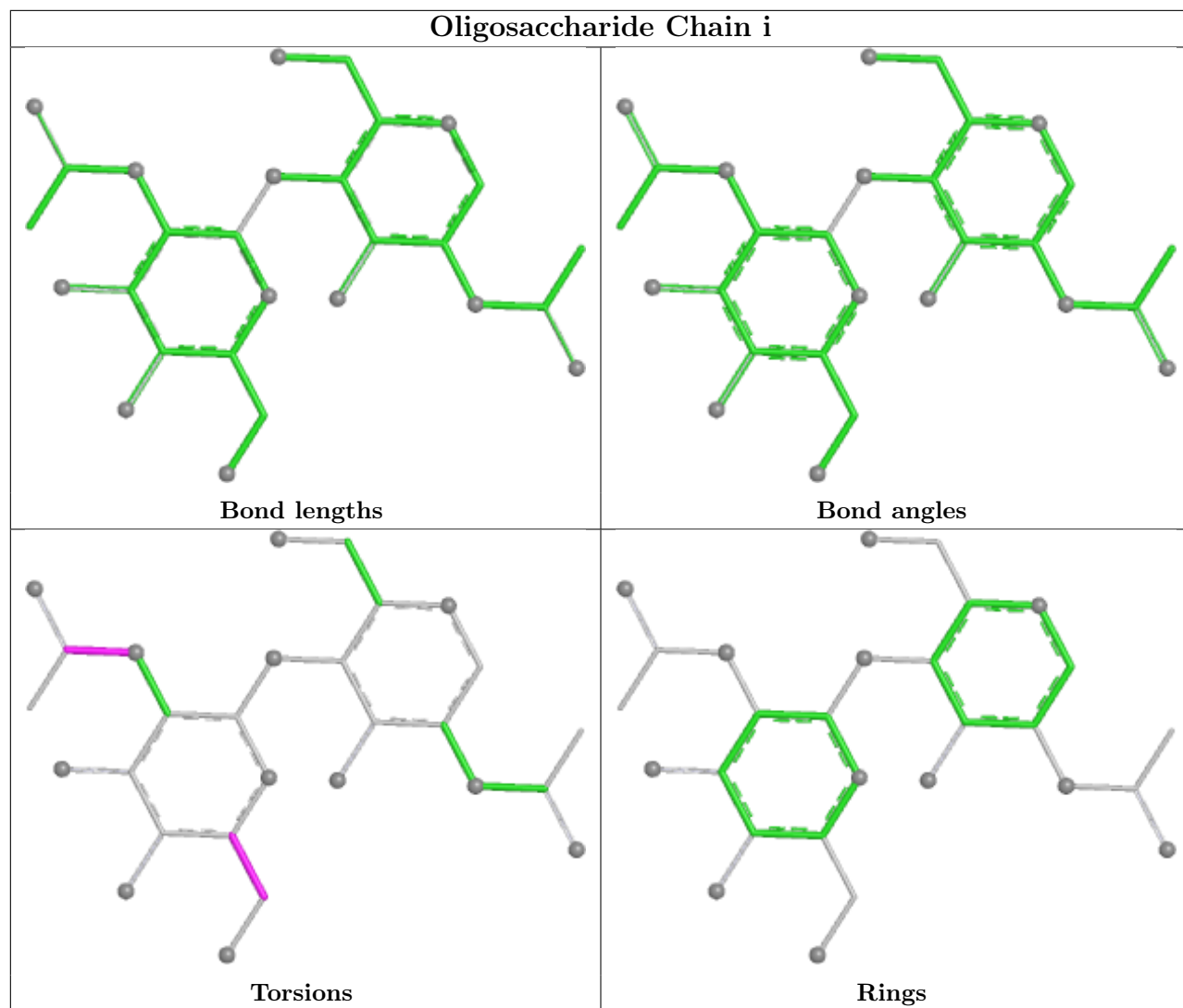


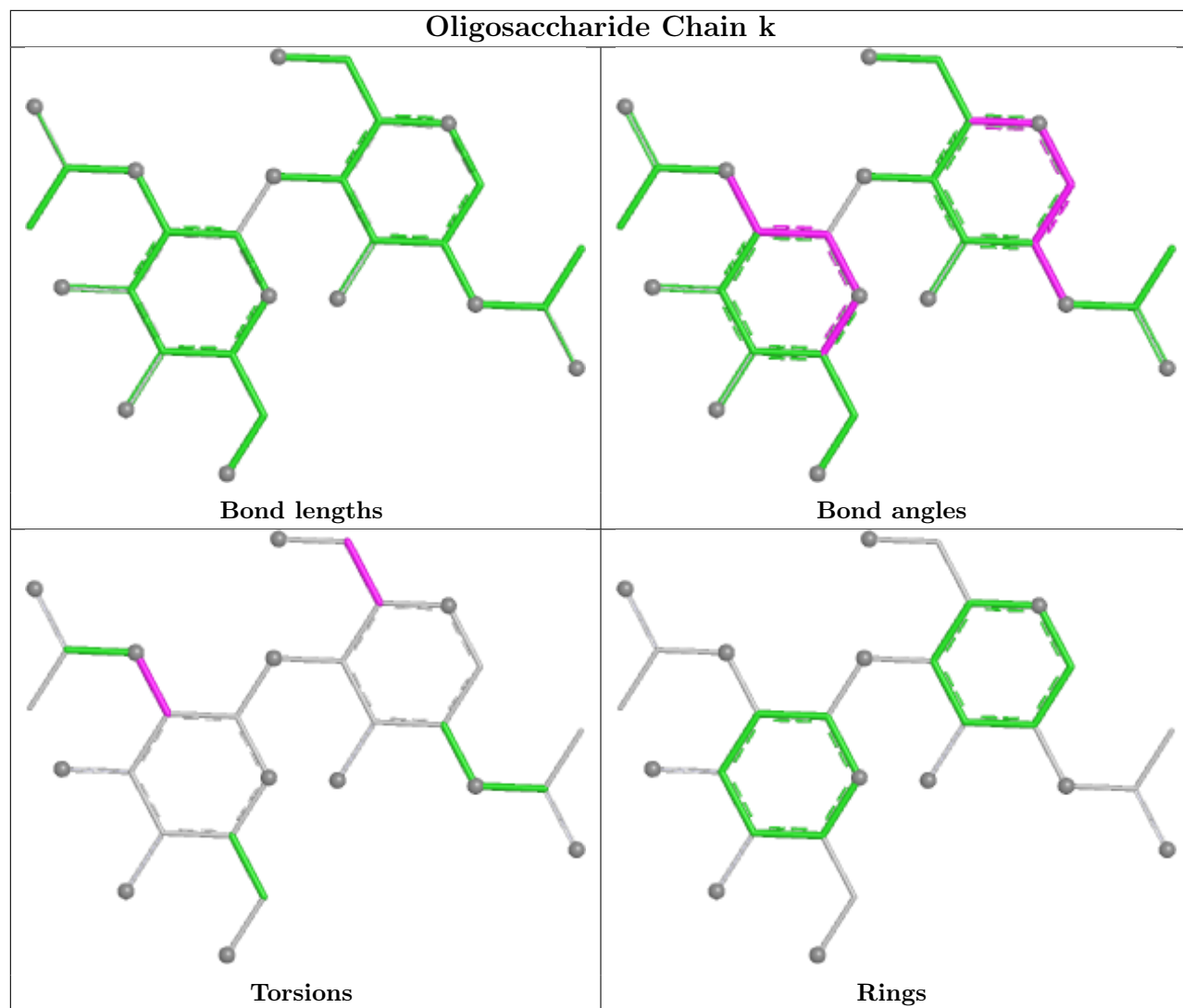


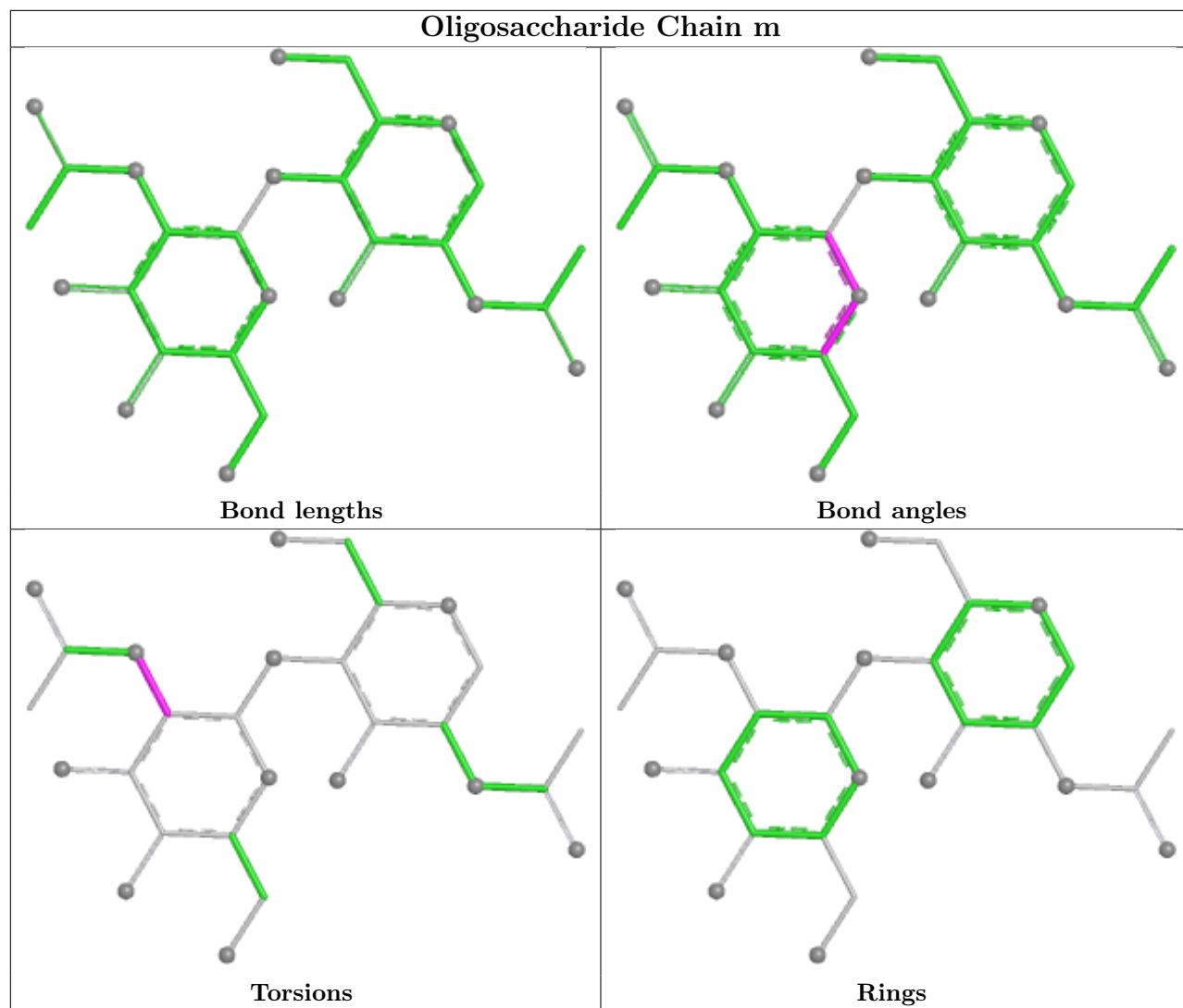


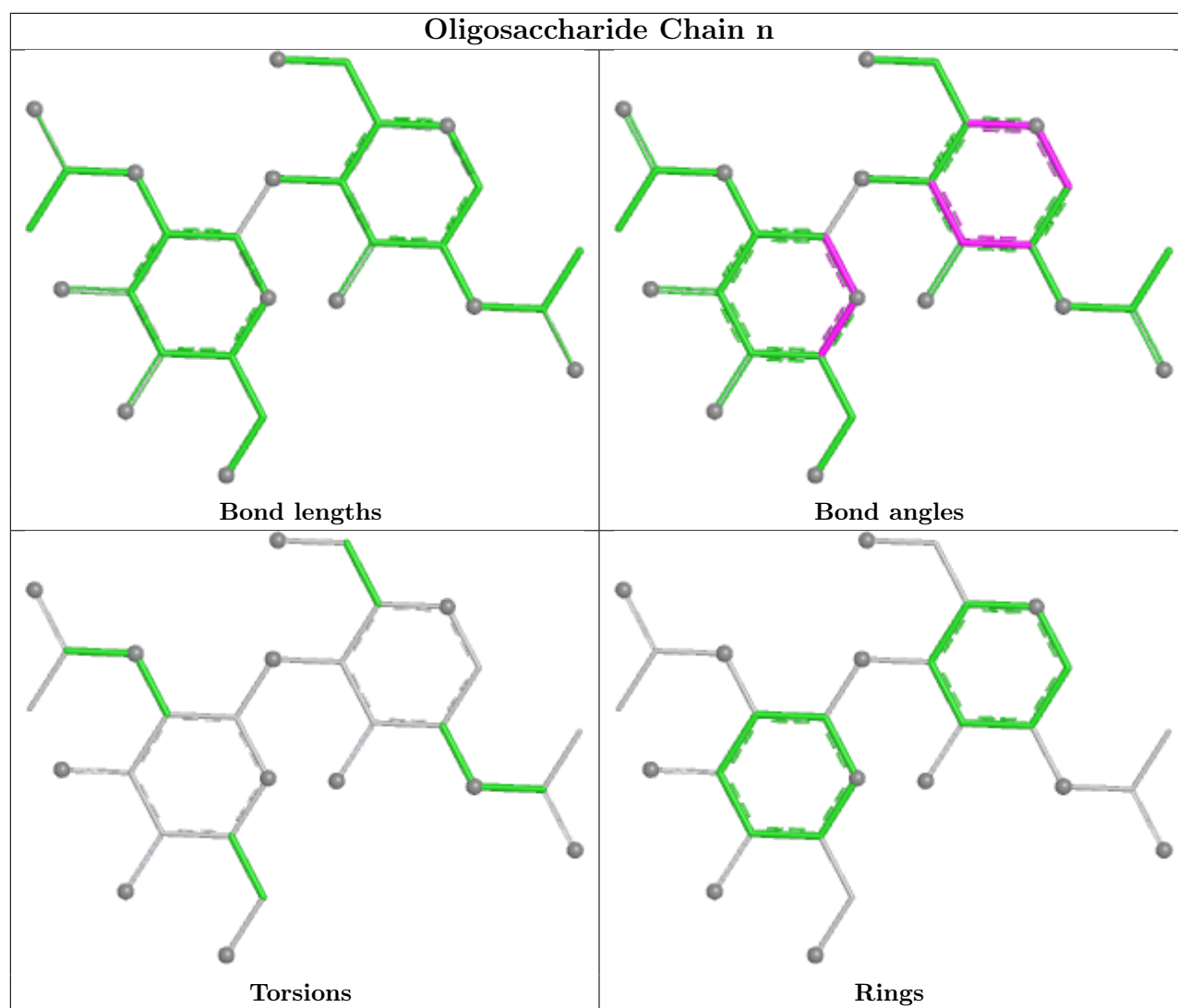


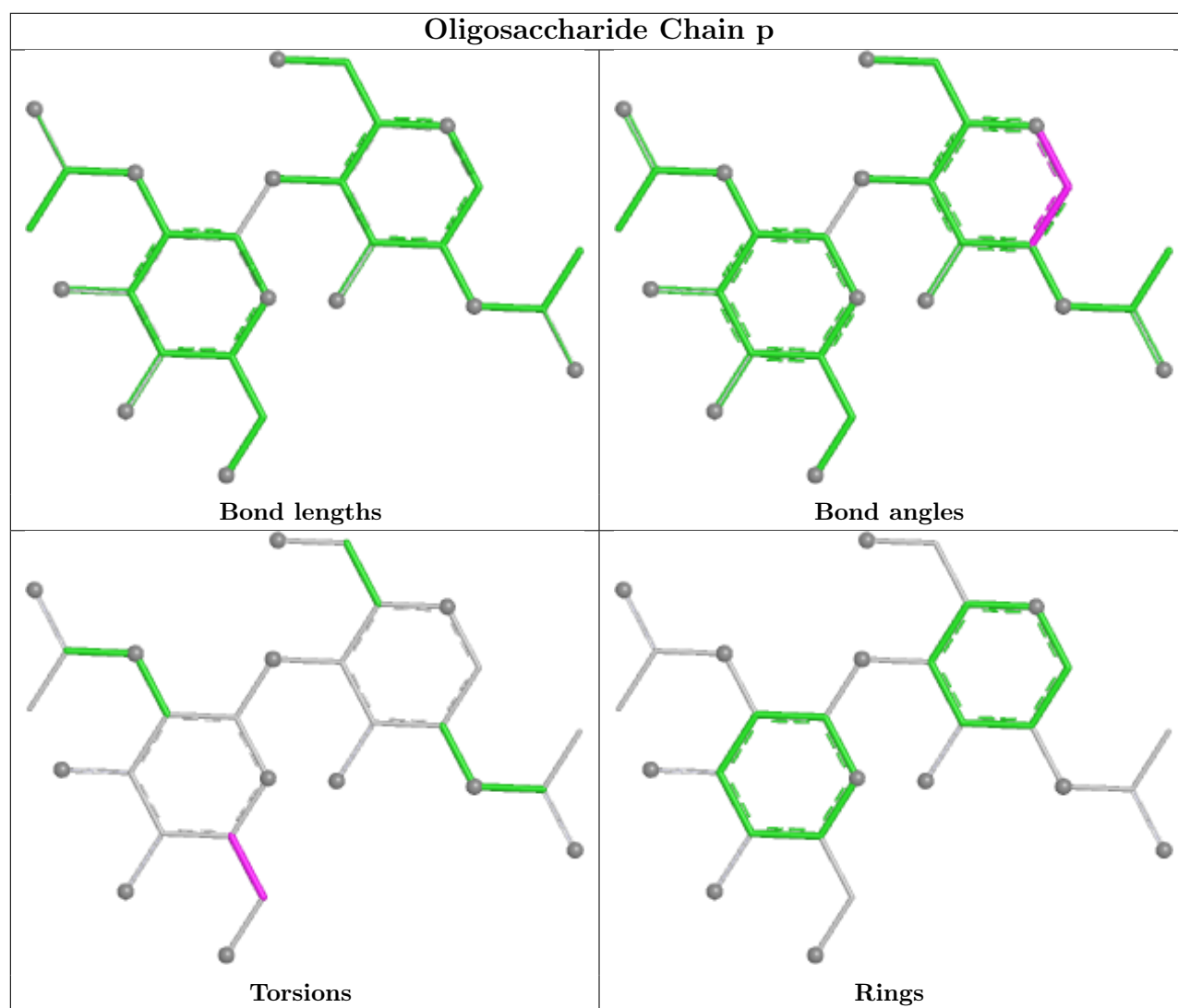


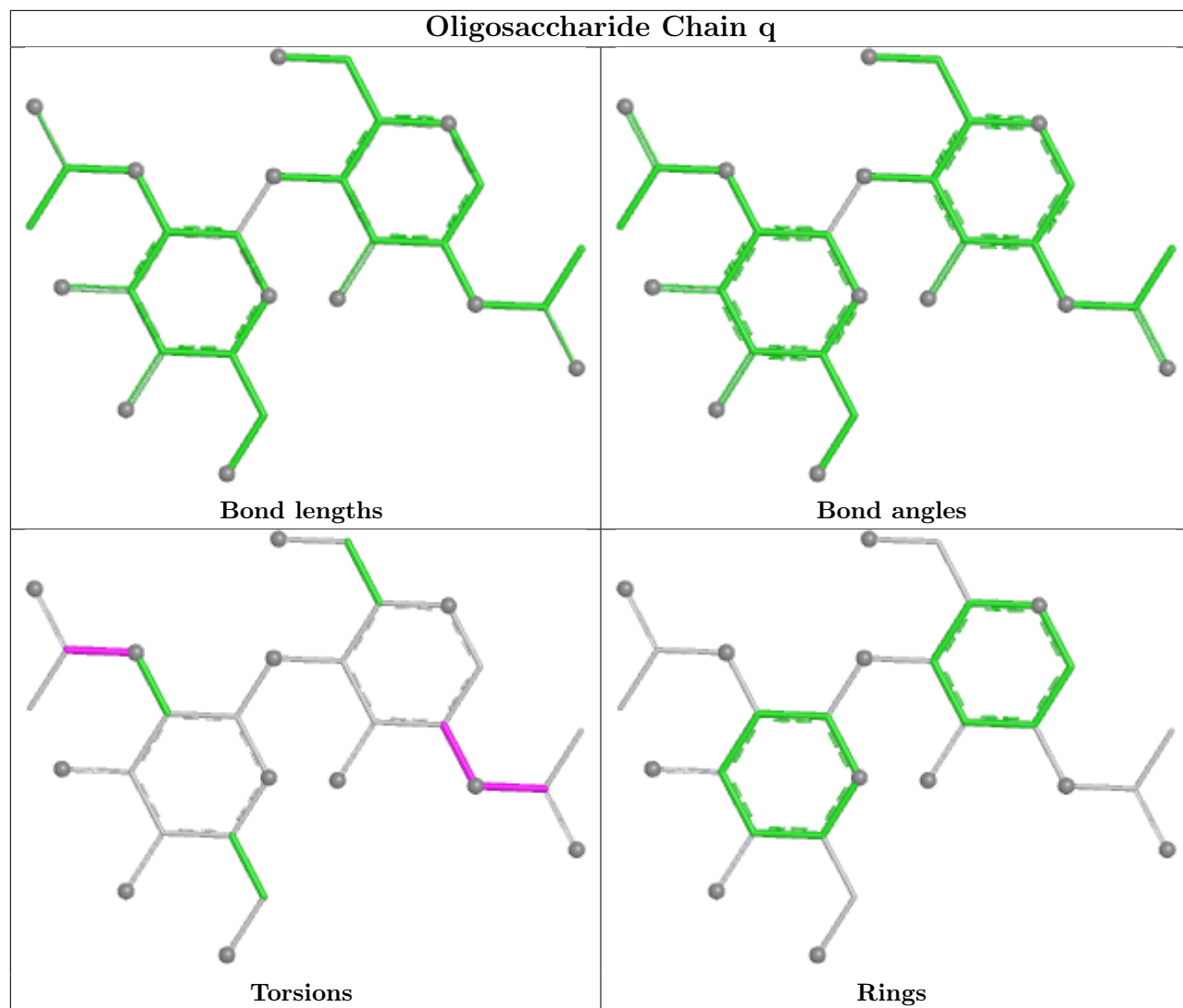


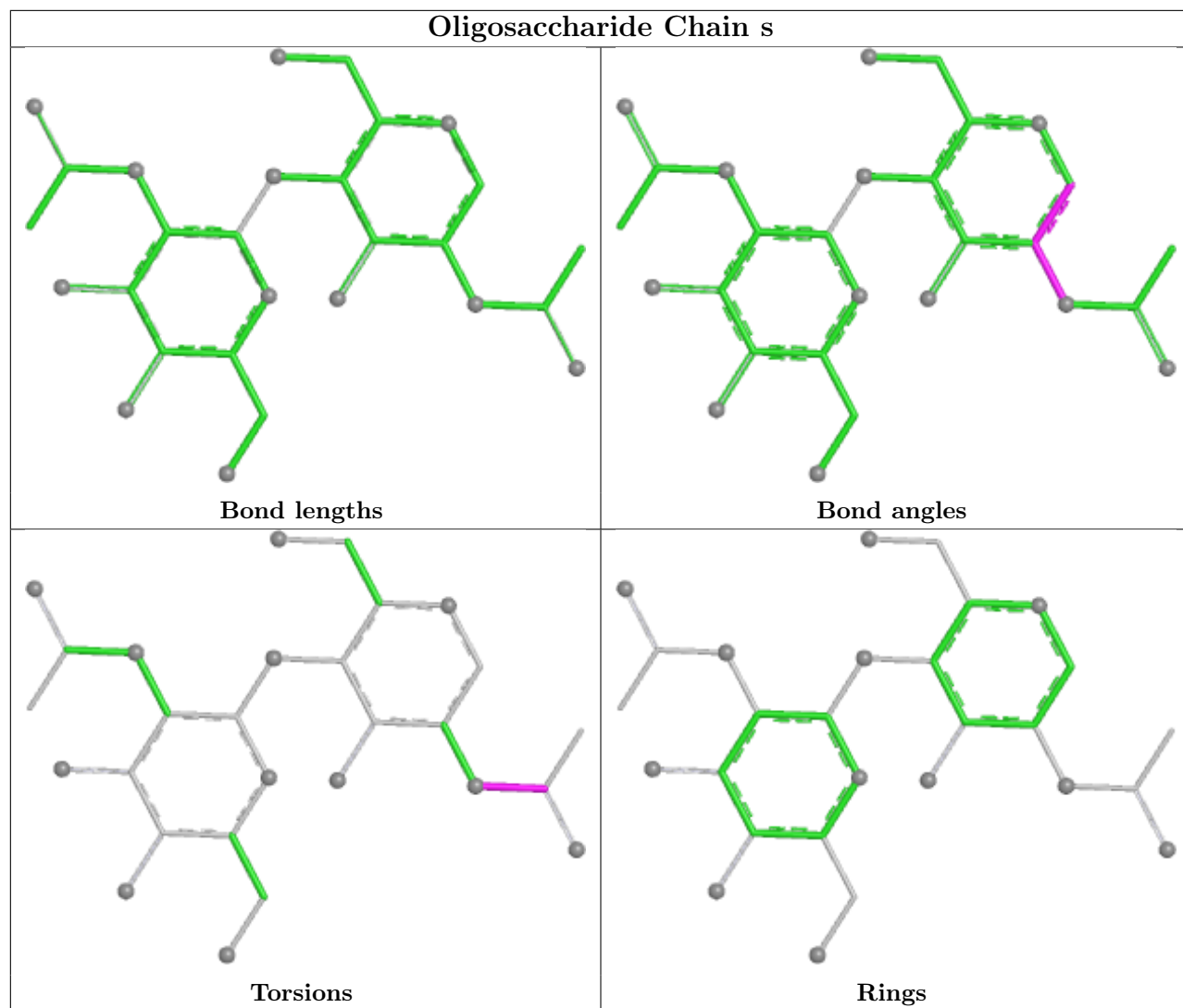


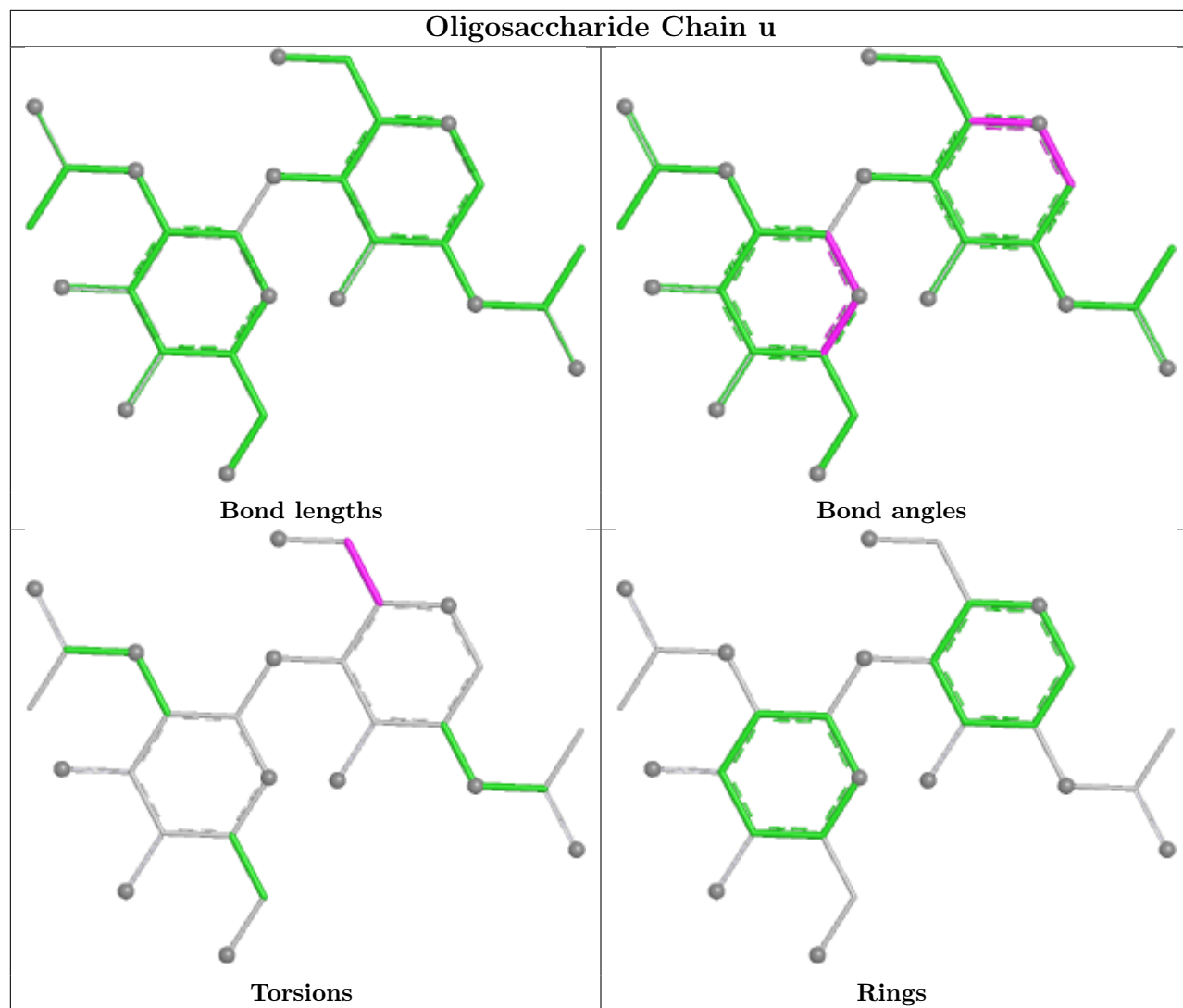


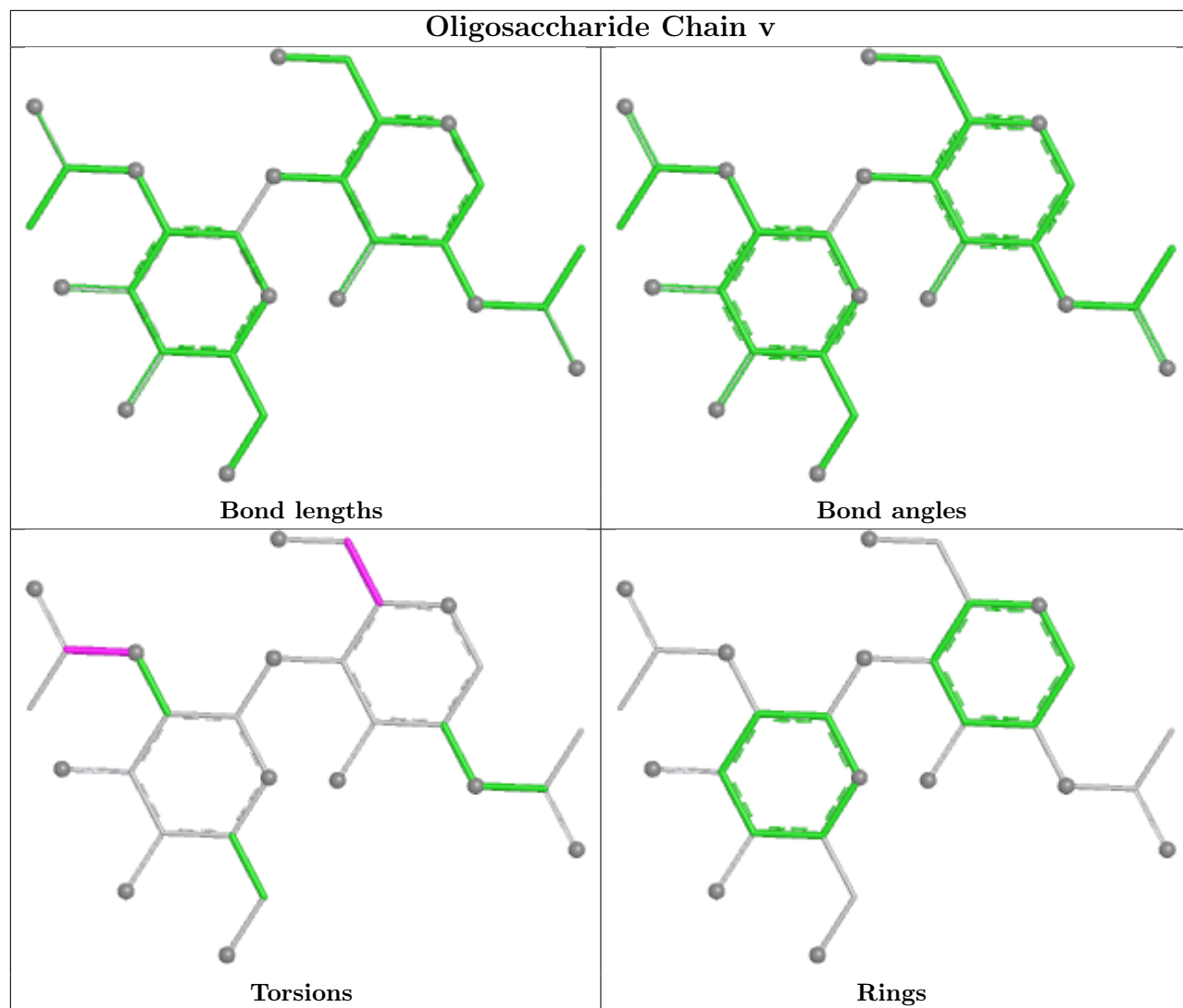


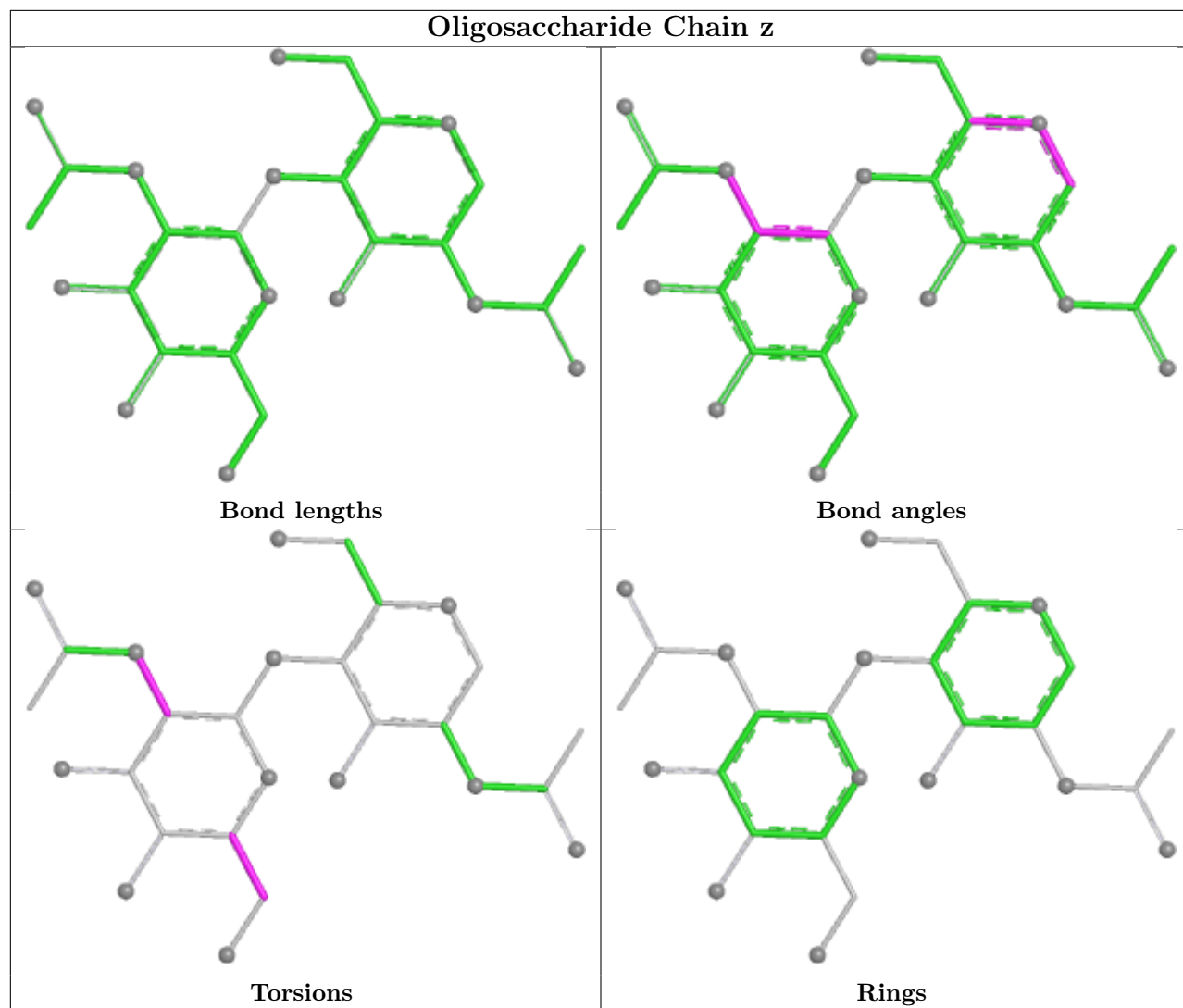


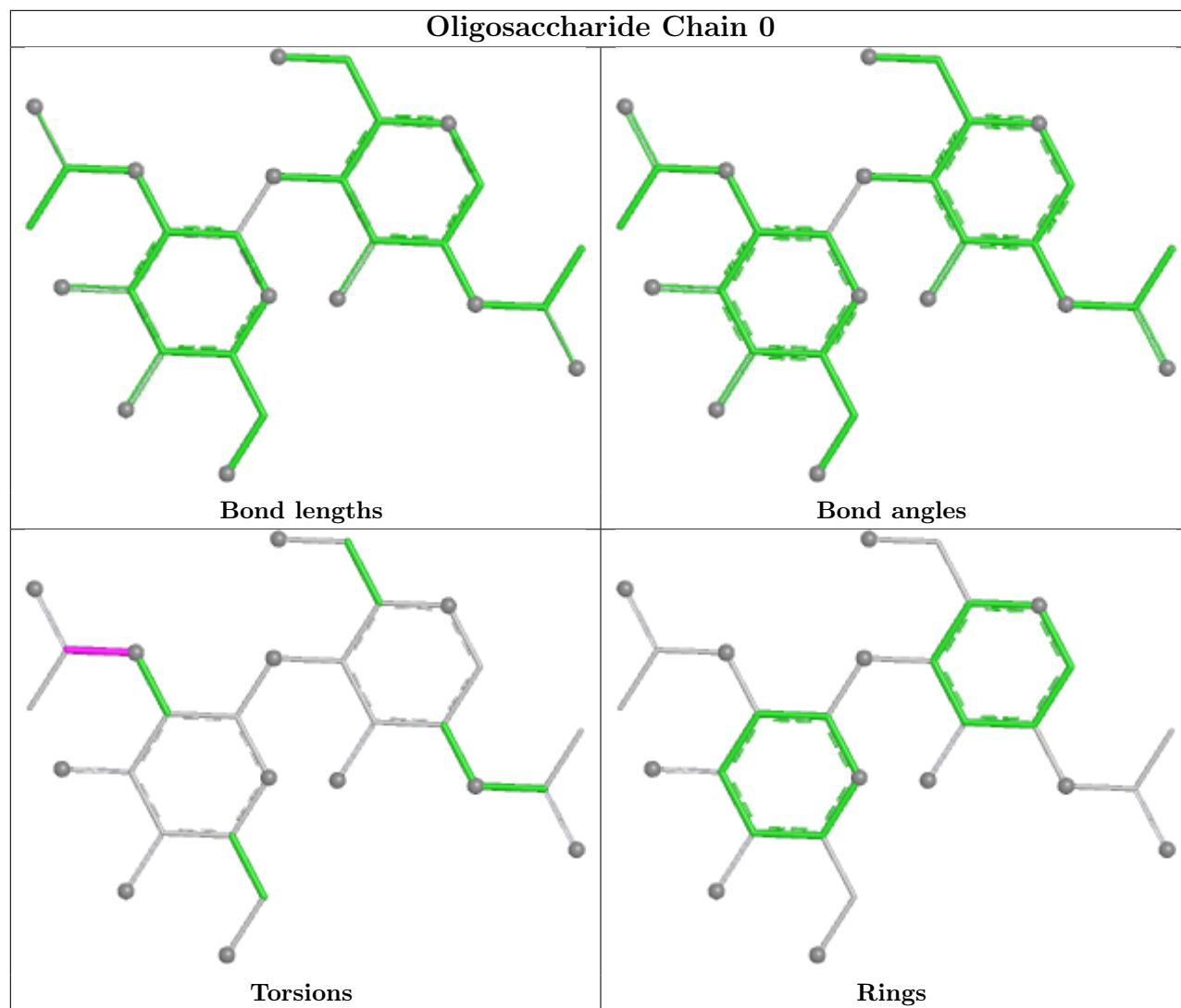


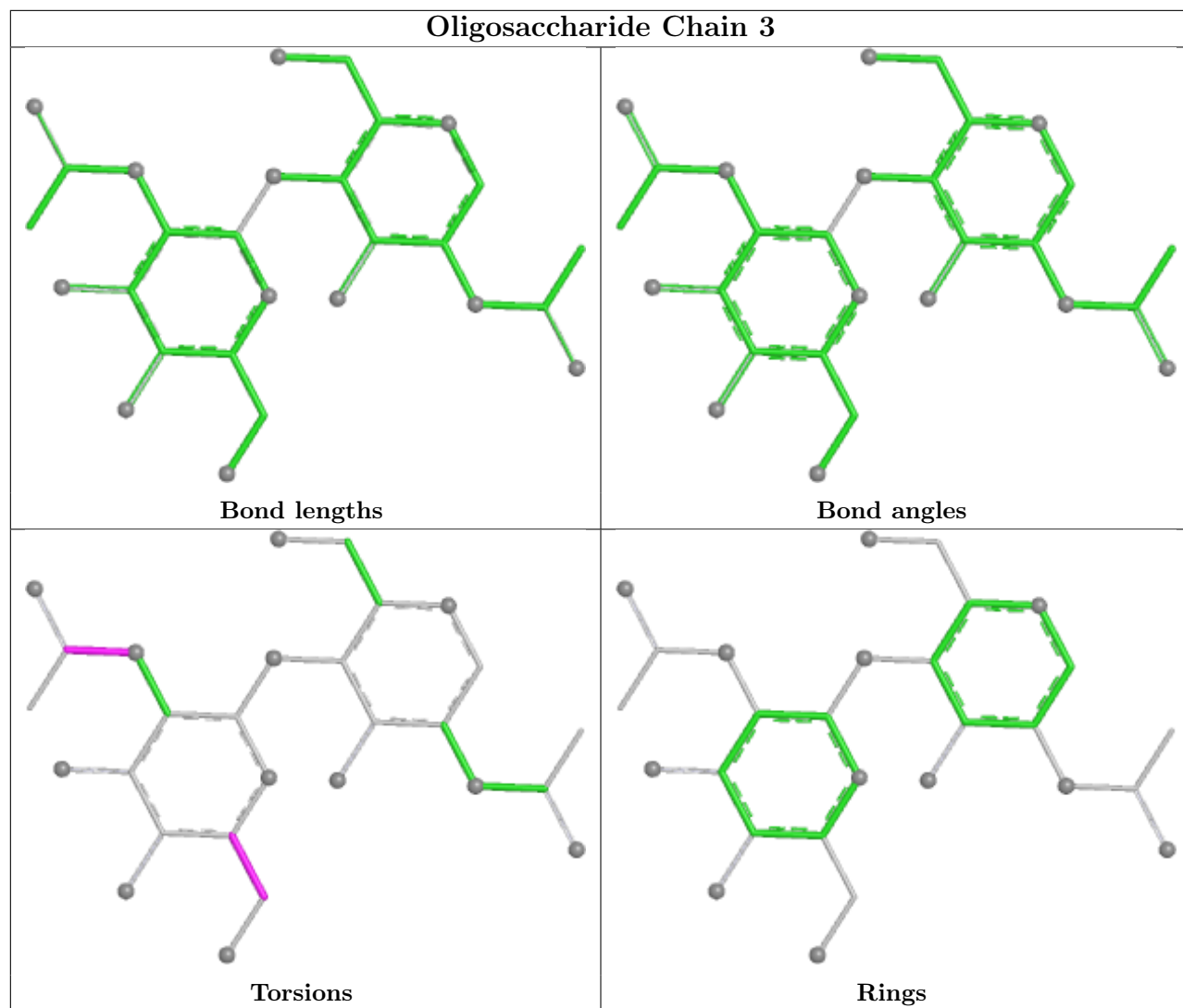


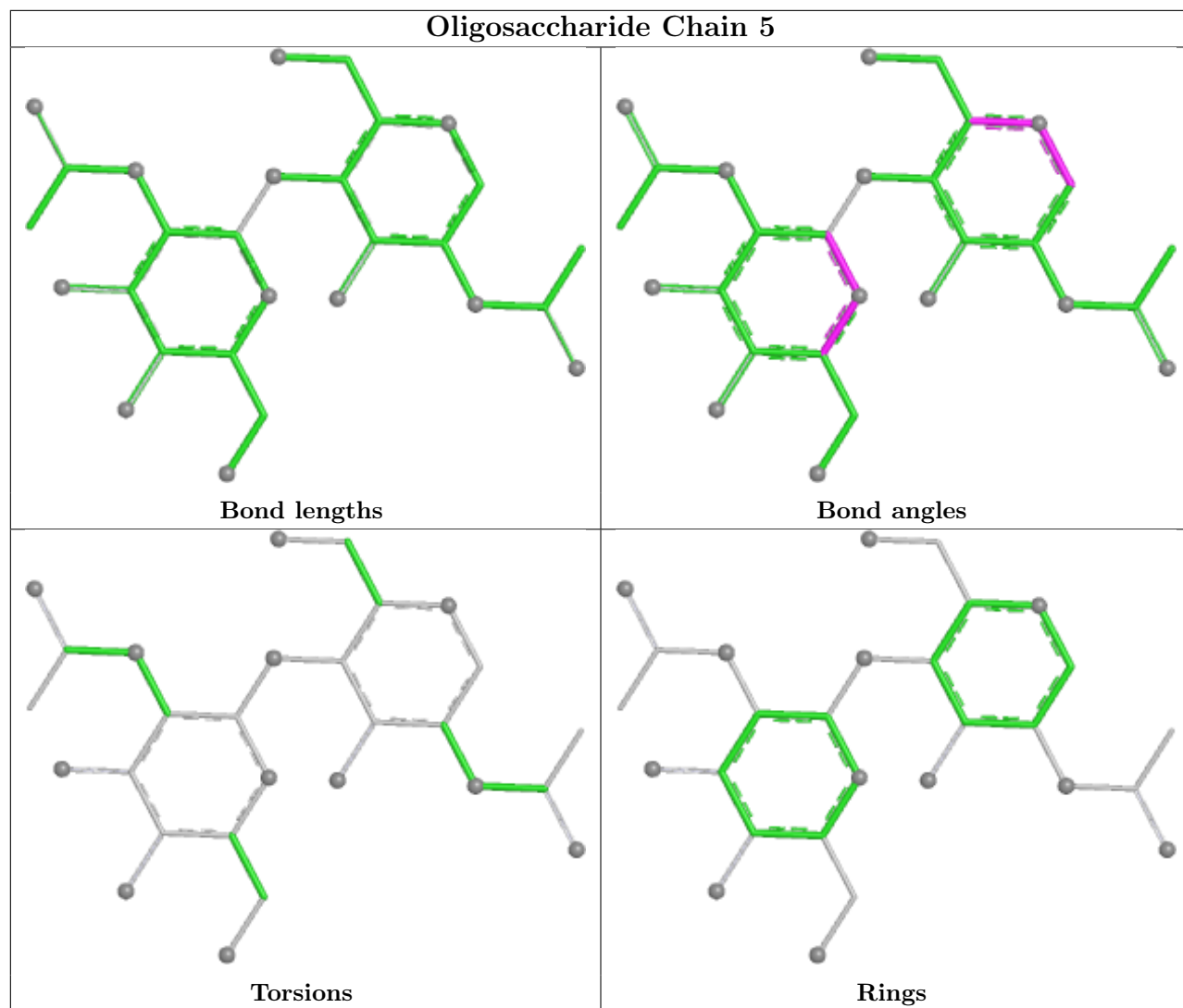


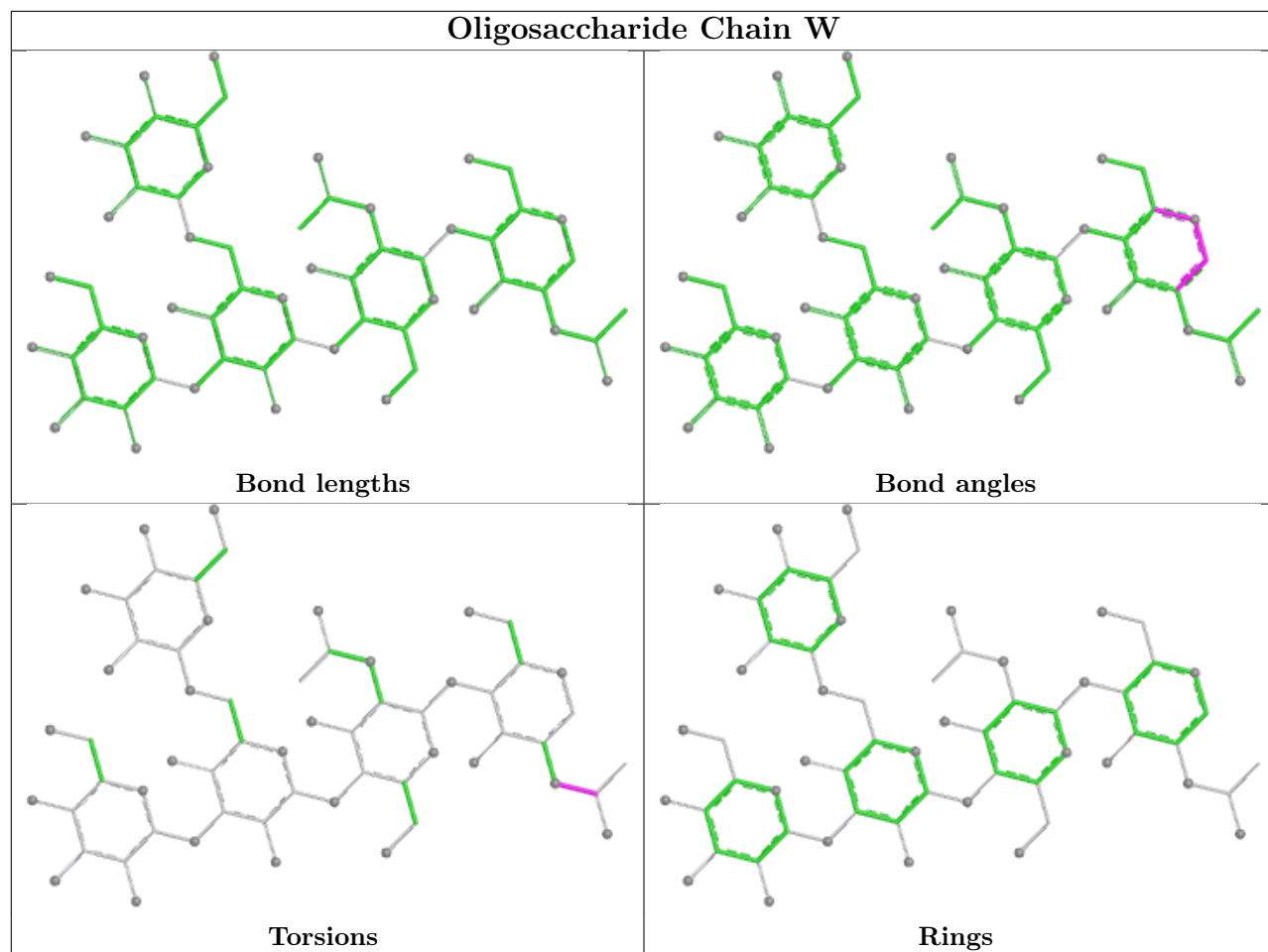


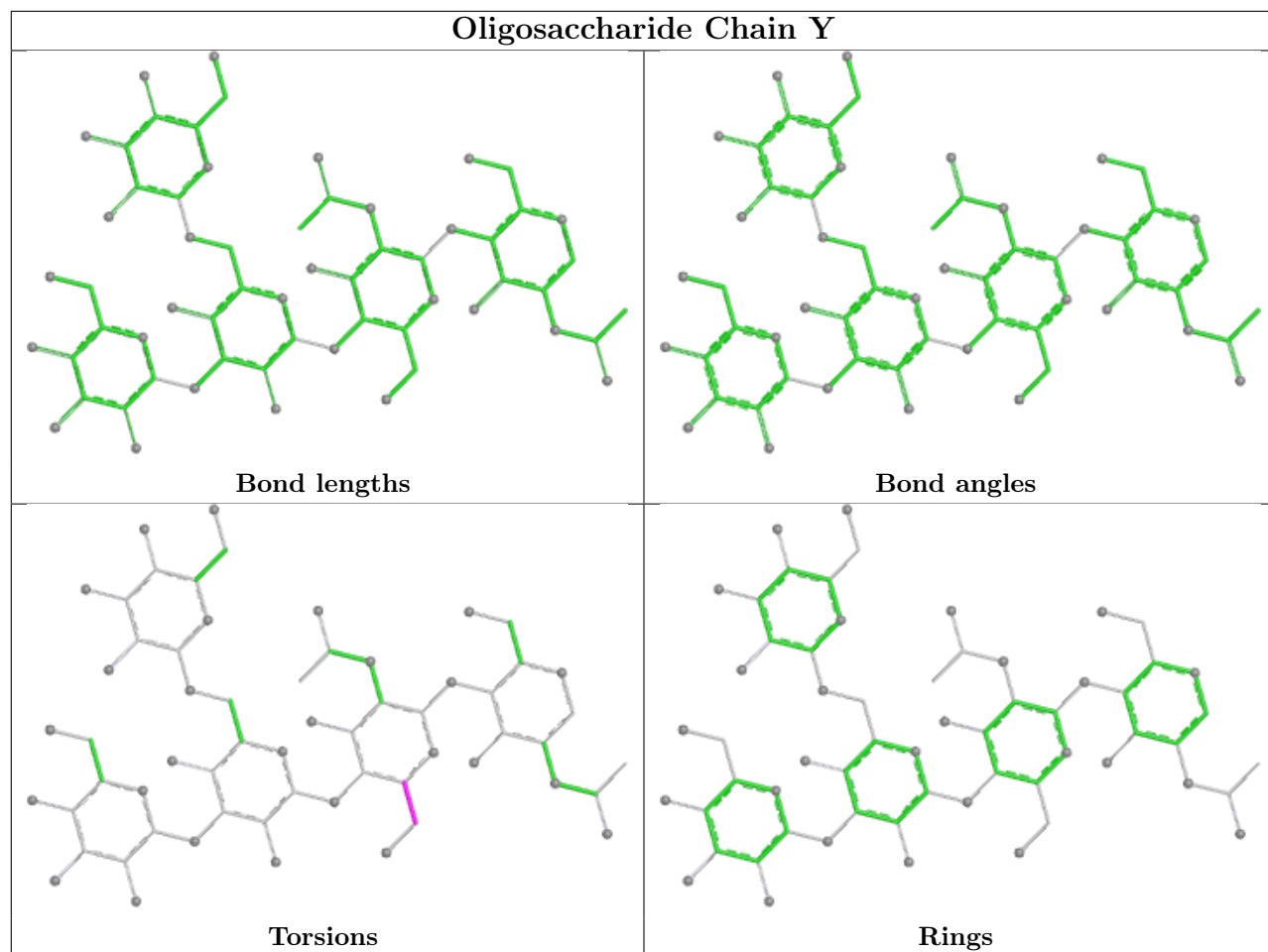


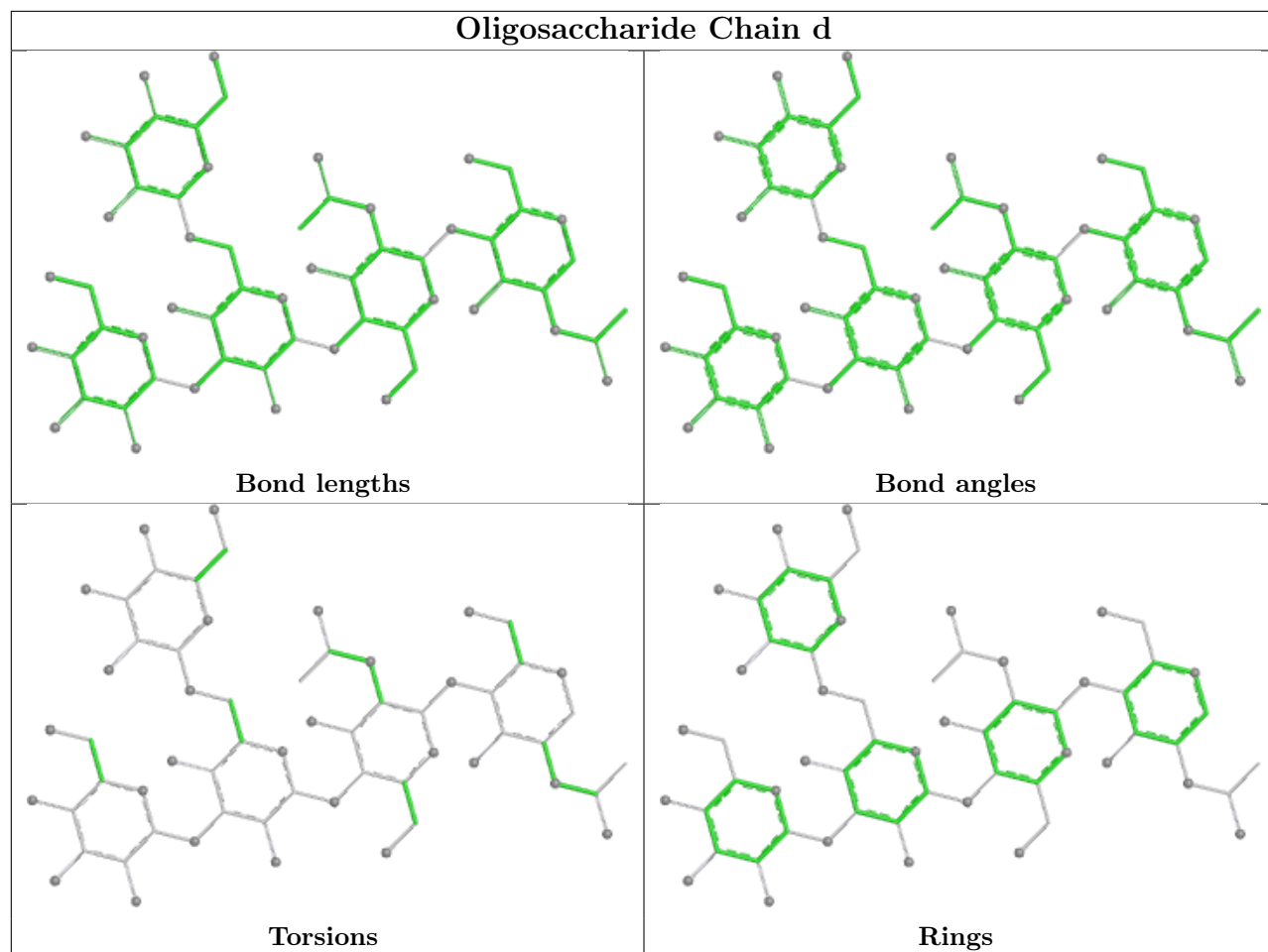


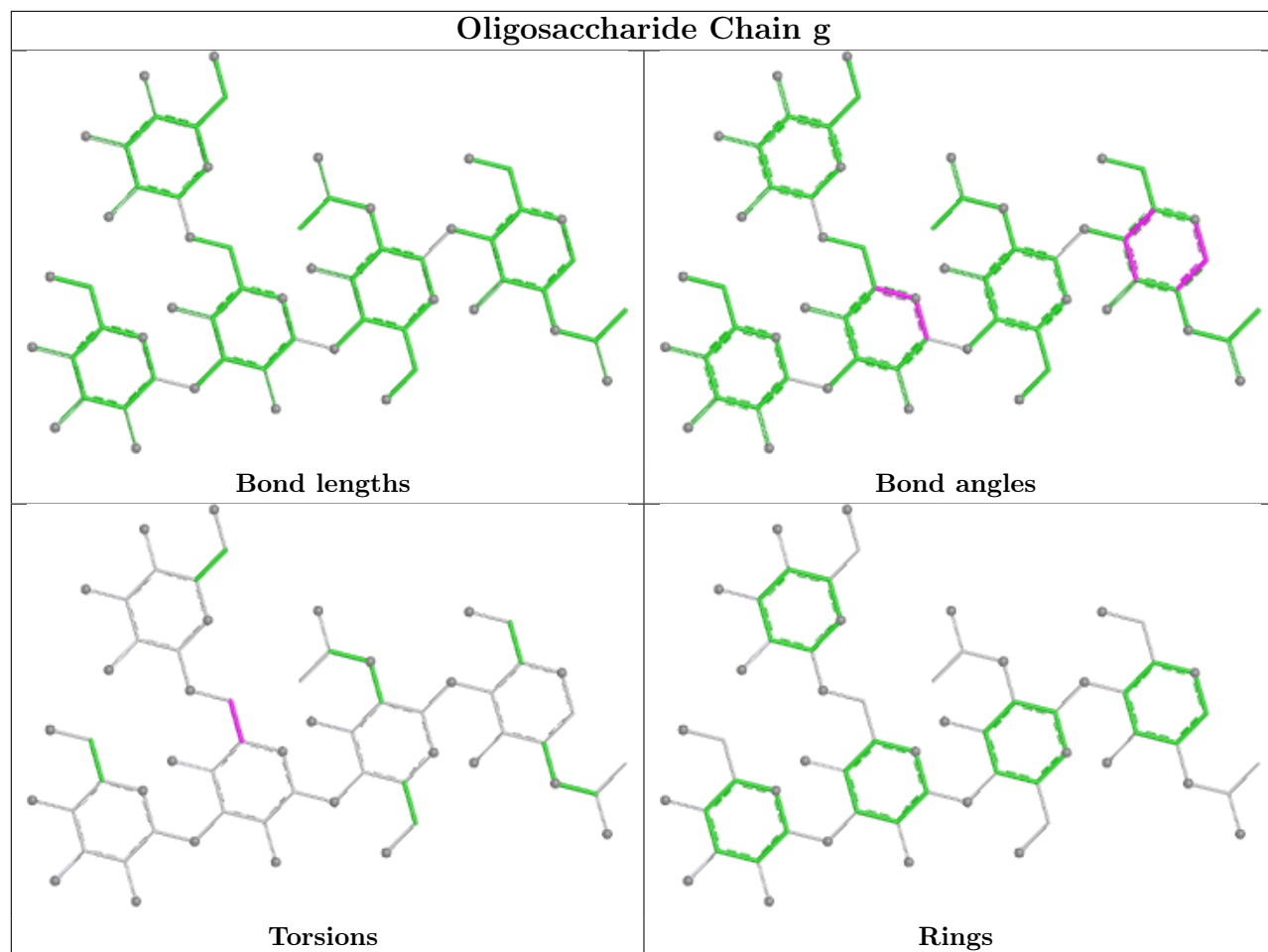


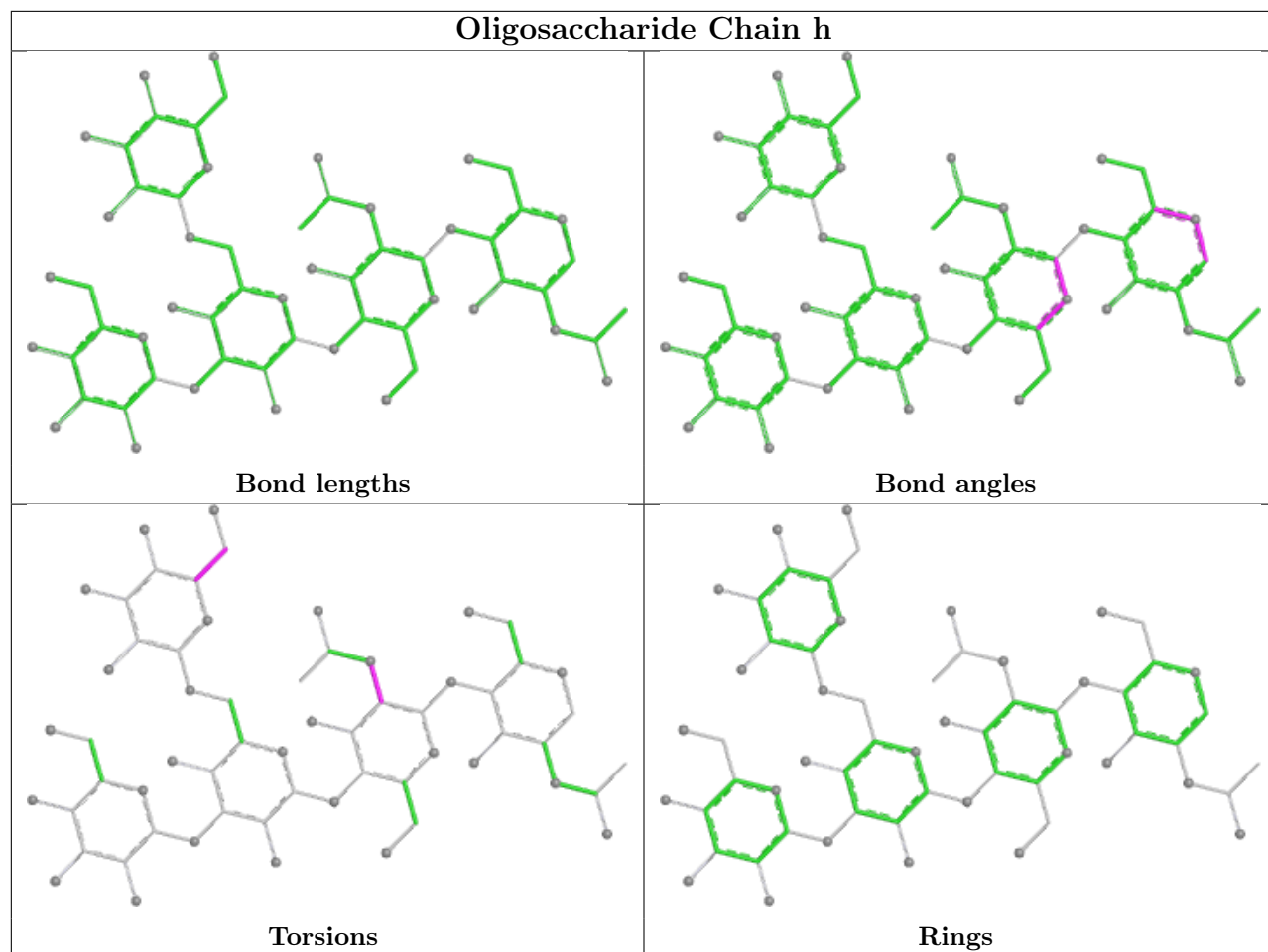


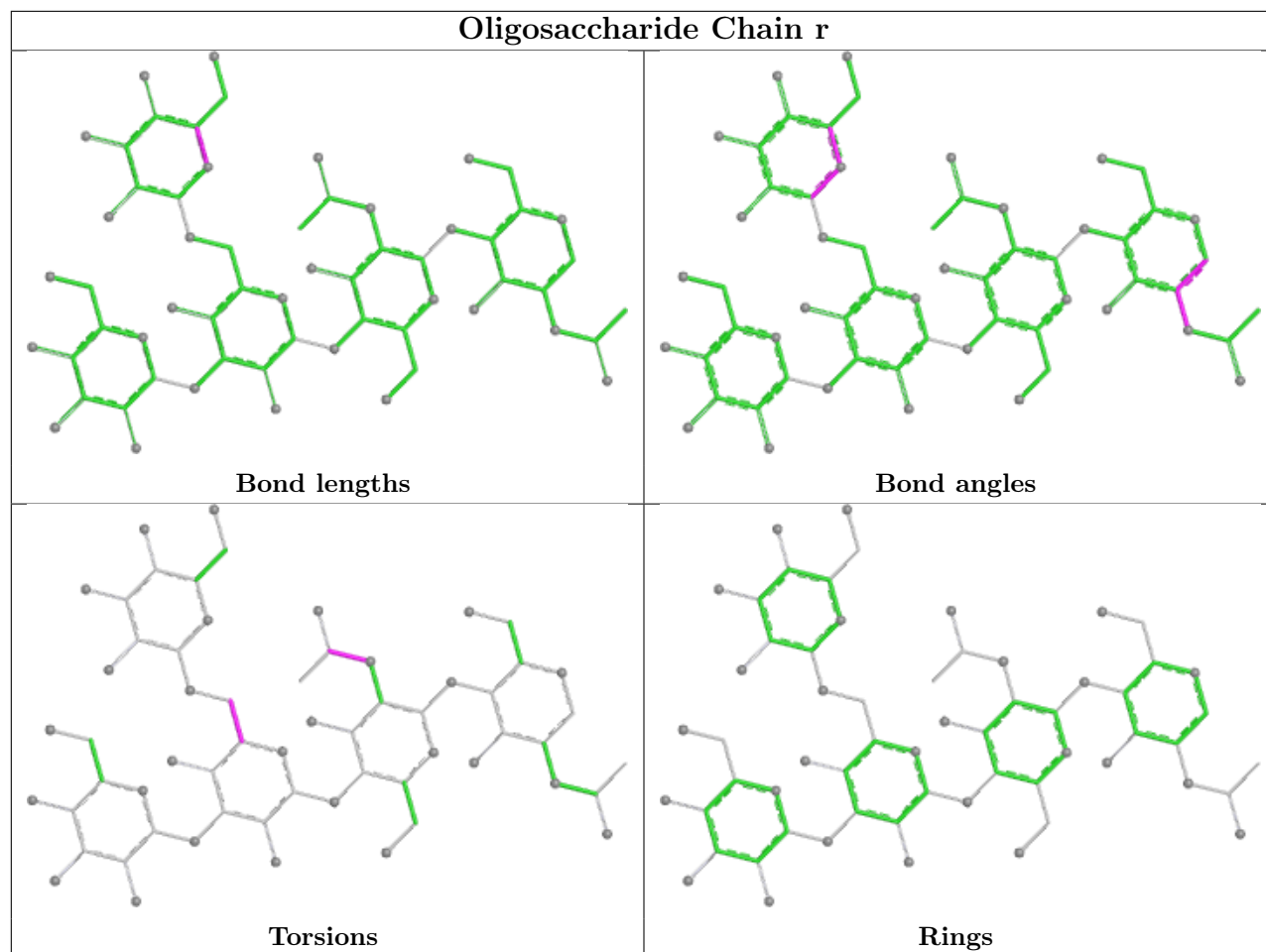


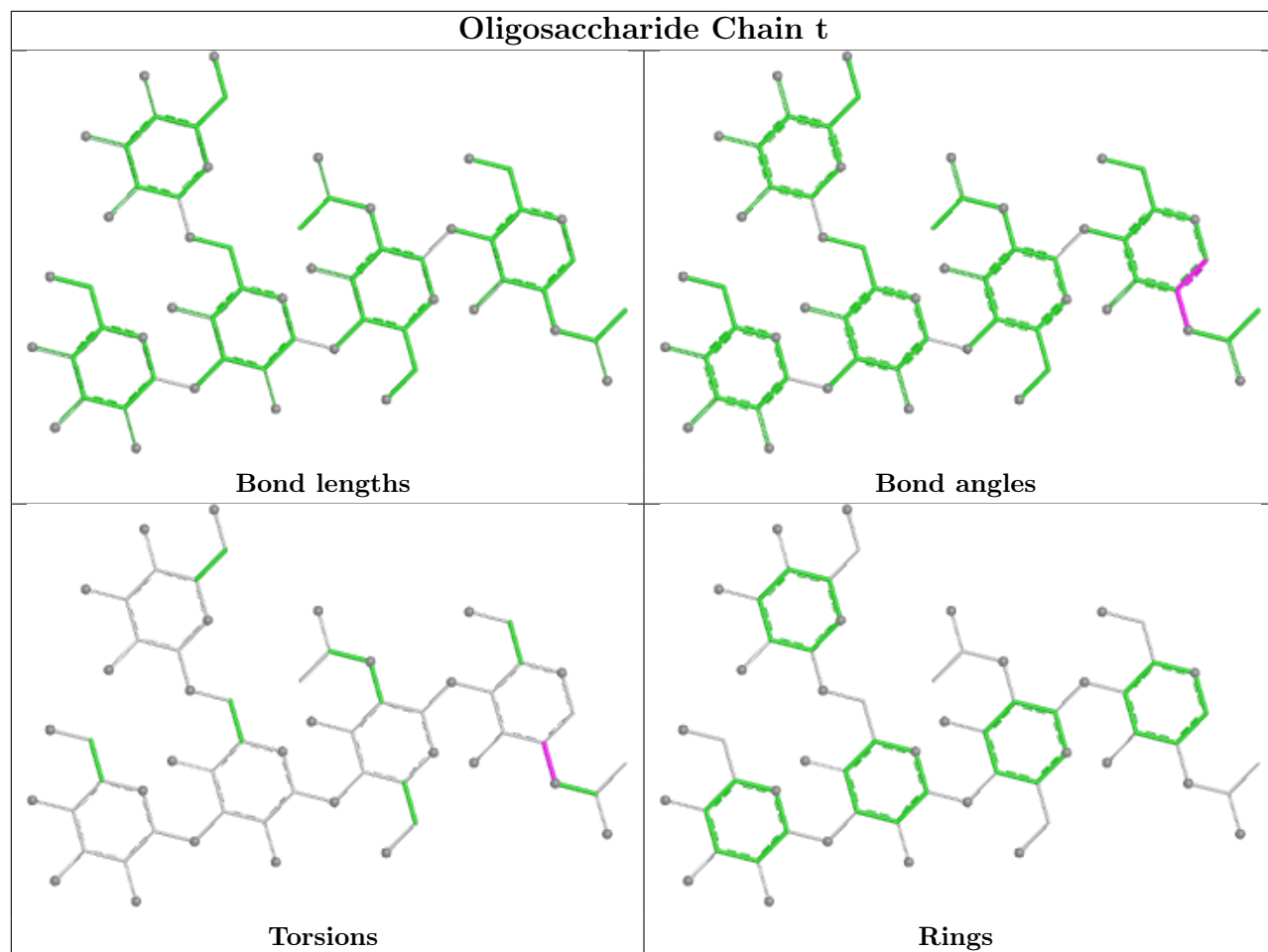


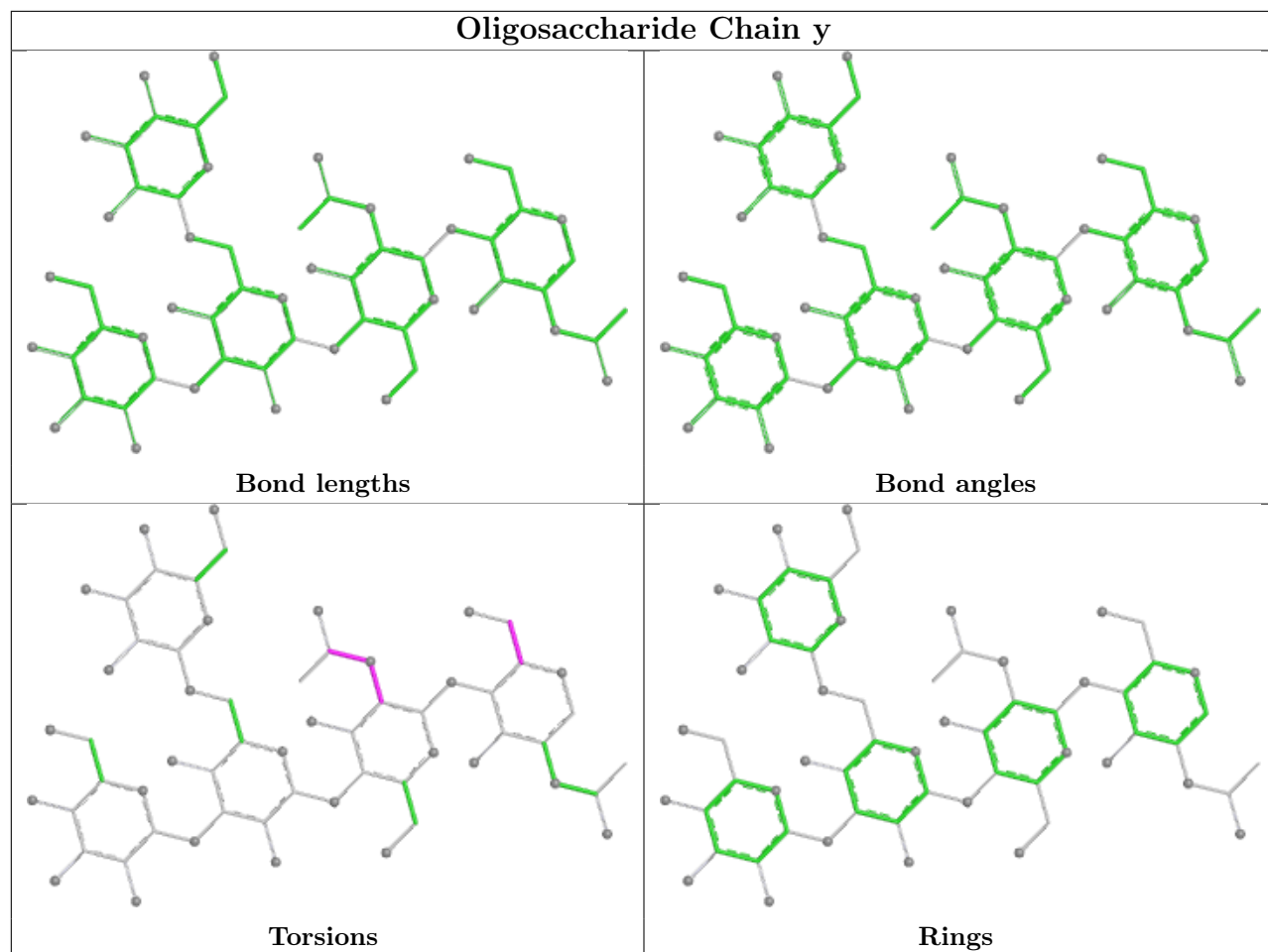


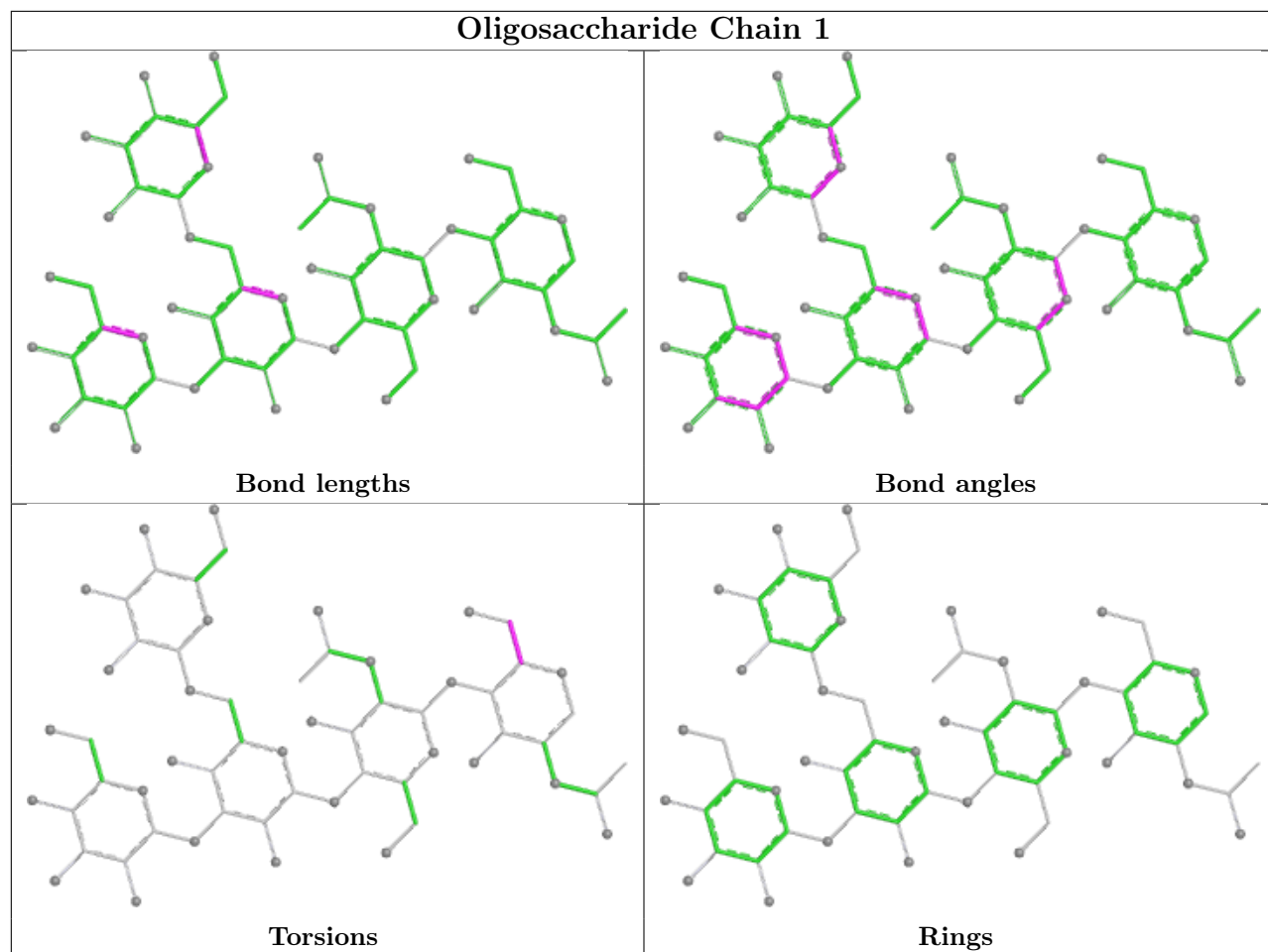


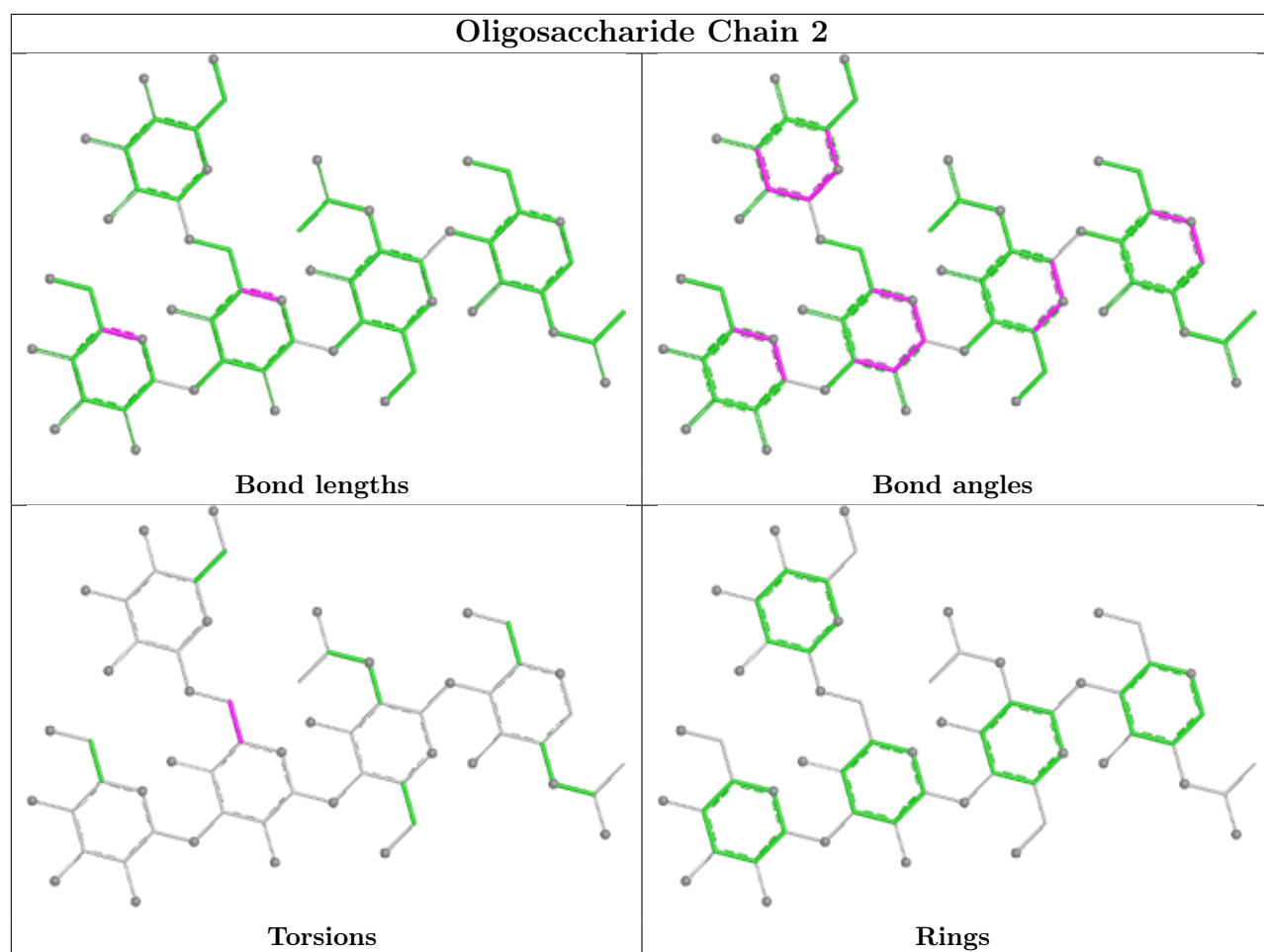


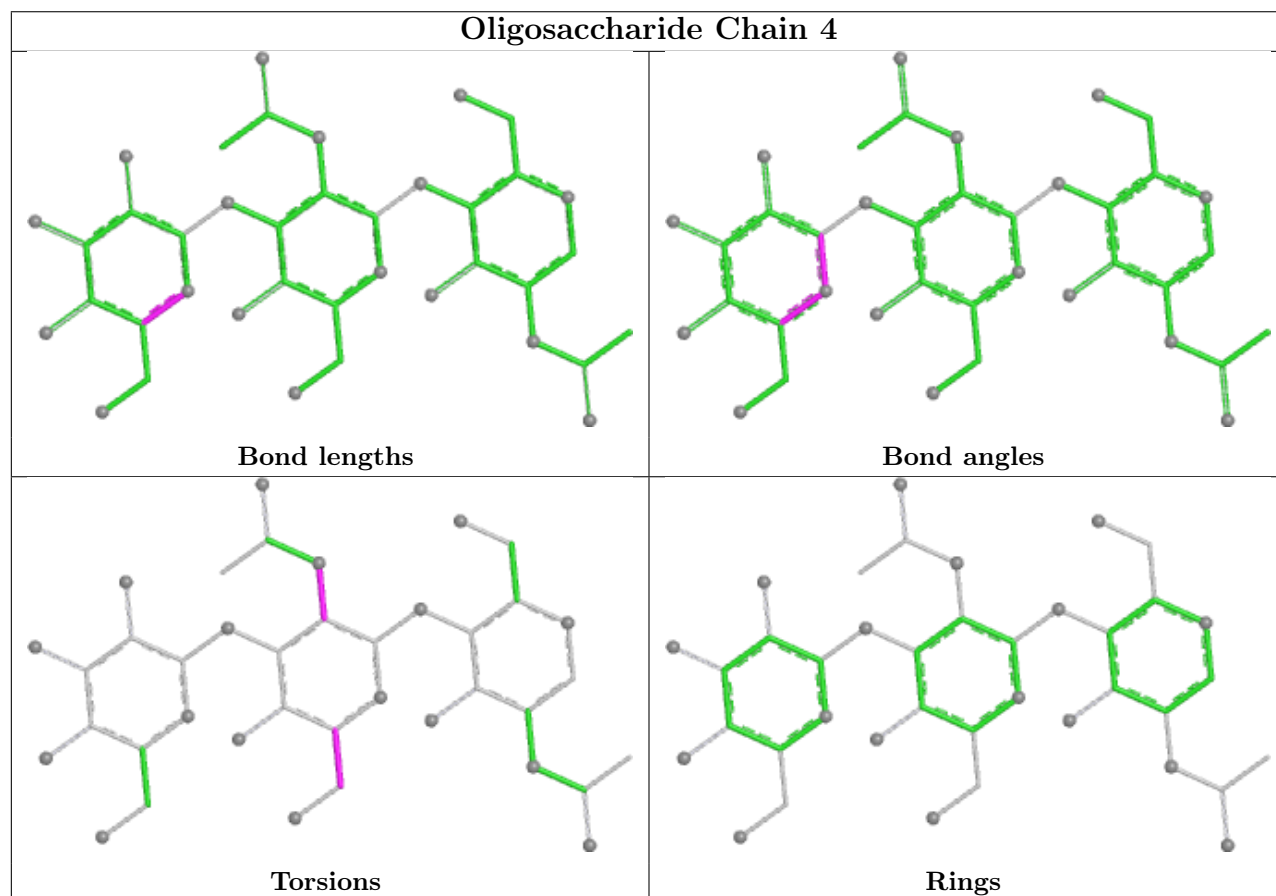
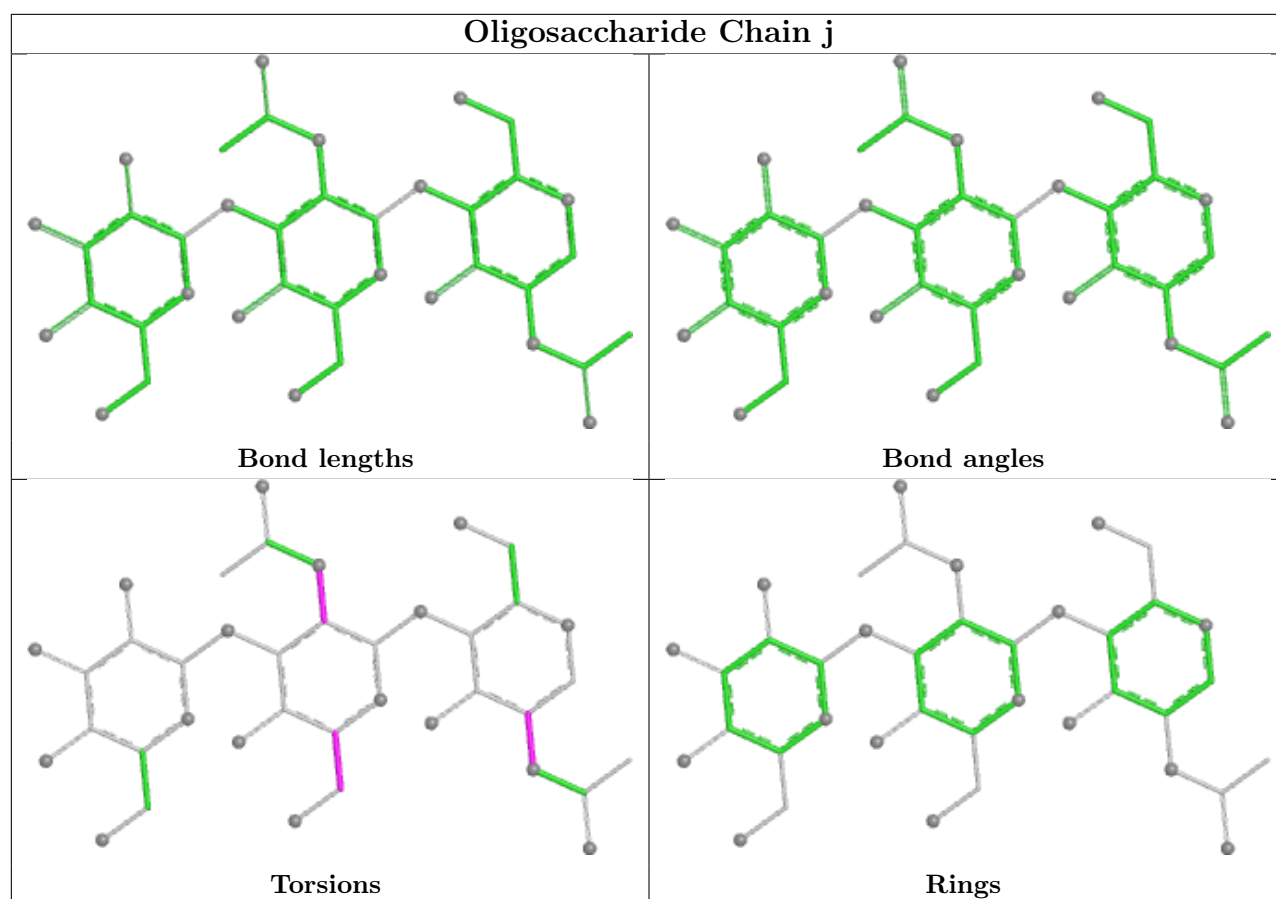












5.6 Ligand geometry

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

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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

All (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
13	A	4713	A2G	C1-O5-C5	-4.02	106.79	112.19
12	A	4712	NAG	C1-O5-C5	4.01	117.56	112.19
13	B	4713	A2G	C1-C2-N2	3.71	116.29	110.43
12	A	4707	NAG	C1-O5-C5	3.70	117.14	112.19
12	A	4712	NAG	O5-C1-C2	3.63	116.91	111.29
13	B	4716	A2G	C1-O5-C5	-3.48	107.52	112.19
12	B	4703	NAG	C1-O5-C5	3.36	116.69	112.19
13	B	4721	A2G	C1-C2-N2	3.36	115.72	110.43
13	A	4716	A2G	C1-O5-C5	-3.17	107.94	112.19
12	B	4704	NAG	C1-O5-C5	3.05	116.27	112.19
12	A	4705	NAG	C1-O5-C5	3.04	116.26	112.19
13	B	4721	A2G	C2-N2-C7	3.03	126.95	122.90
13	B	4718	A2G	C1-O5-C5	-2.97	108.20	112.19
12	B	4711	NAG	C1-O5-C5	2.93	116.11	112.19
12	A	4709	NAG	C1-O5-C5	2.90	116.08	112.19
13	B	4720	A2G	O5-C1-C2	2.87	115.74	111.29
13	B	4718	A2G	O5-C1-C2	2.83	115.66	111.29
13	A	4717	A2G	C1-C2-N2	2.82	114.87	110.43
12	B	4709	NAG	C1-O5-C5	2.80	115.94	112.19
13	B	4717	A2G	C1-C2-N2	2.71	114.71	110.43
13	A	4722	A2G	O5-C1-C2	2.70	115.47	111.29
12	B	4706	NAG	C2-N2-C7	2.65	126.45	122.90
13	B	4713	A2G	O5-C1-C2	2.62	115.34	111.29
13	A	4721	A2G	C2-N2-C7	2.59	126.37	122.90
12	B	4710	NAG	C2-N2-C7	2.54	126.30	122.90
13	A	4717	A2G	O5-C1-C2	2.47	115.11	111.29
12	A	4703	NAG	C1-O5-C5	2.46	115.48	112.19
12	B	4708	NAG	C1-O5-C5	2.45	115.47	112.19
13	A	4720	A2G	O5-C5-C6	2.44	112.41	107.66
13	A	4717	A2G	C2-N2-C7	2.43	126.16	122.90
13	B	4721	A2G	O3-C3-C2	-2.36	104.50	109.40
13	B	4713	A2G	C1-O5-C5	-2.32	109.08	112.19
12	A	4704	NAG	O5-C1-C2	2.28	114.82	111.29
13	A	4716	A2G	O5-C1-C2	2.28	114.82	111.29
12	B	4708	NAG	O5-C1-C2	2.19	114.69	111.29
13	B	4715	A2G	O5-C1-C2	2.15	114.62	111.29
12	B	4711	NAG	O5-C1-C2	2.14	114.61	111.29
13	B	4721	A2G	O5-C5-C4	-2.14	105.63	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	4721	A2G	O7-C7-N2	2.13	125.75	121.98
12	B	4703	NAG	O5-C1-C2	2.13	114.58	111.29
13	A	4723	A2G	C1-O5-C5	-2.13	109.33	112.19
13	A	4723	A2G	O5-C5-C6	2.12	111.79	107.66
13	B	4721	A2G	O4-C4-C3	-2.08	105.47	110.38
13	A	4718	A2G	C1-C2-N2	2.02	113.61	110.43

There are no chirality outliers.

All (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
12	B	4702	NAG	O7-C7-N2-C2
12	B	4706	NAG	C3-C2-N2-C7
12	B	4706	NAG	C8-C7-N2-C2
12	B	4706	NAG	O7-C7-N2-C2
12	B	4712	NAG	C1-C2-N2-C7
13	A	4715	A2G	C3-C2-N2-C7
12	B	4712	NAG	C8-C7-N2-C2
12	B	4712	NAG	O7-C7-N2-C2
12	B	4705	NAG	C8-C7-N2-C2
12	B	4705	NAG	O7-C7-N2-C2
12	A	4711	NAG	O5-C5-C6-O6
13	A	4723	A2G	O5-C5-C6-O6
13	A	4718	A2G	O5-C5-C6-O6
12	B	4704	NAG	O5-C5-C6-O6
13	A	4717	A2G	O5-C5-C6-O6
12	A	4707	NAG	O5-C5-C6-O6
13	B	4721	A2G	O5-C5-C6-O6
12	A	4701	NAG	O5-C5-C6-O6
13	A	4715	A2G	O5-C5-C6-O6
12	A	4706	NAG	O5-C5-C6-O6
13	B	4715	A2G	O5-C5-C6-O6
12	B	4705	NAG	C3-C2-N2-C7
12	B	4710	NAG	O5-C5-C6-O6
12	A	4705	NAG	C1-C2-N2-C7
13	A	4717	A2G	C1-C2-N2-C7
12	A	4705	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
12	A	4706	NAG	C3-C2-N2-C7
13	A	4717	A2G	C3-C2-N2-C7
12	A	4711	NAG	C4-C5-C6-O6
12	A	4701	NAG	C1-C2-N2-C7
12	A	4706	NAG	C1-C2-N2-C7
12	B	4701	NAG	C1-C2-N2-C7
13	B	4713	A2G	C1-C2-N2-C7
13	B	4720	A2G	C1-C2-N2-C7
13	B	4720	A2G	C3-C2-N2-C7

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.

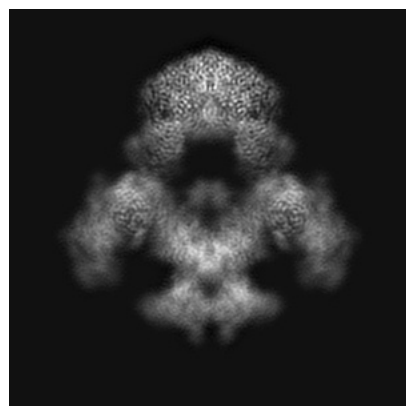
6 Map visualisation [i](#)

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.

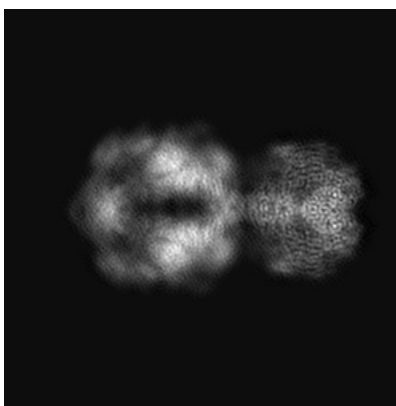
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

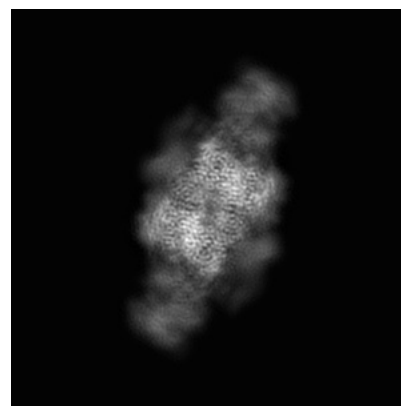
6.1.1 Primary map



X

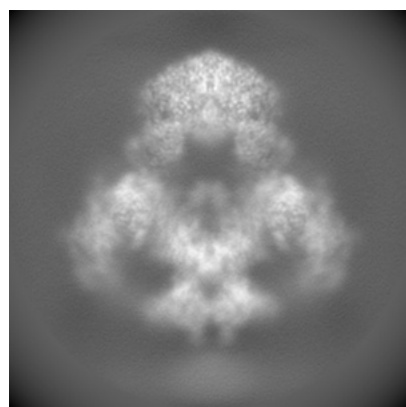


Y

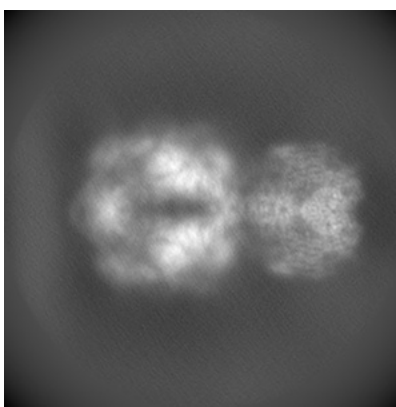


Z

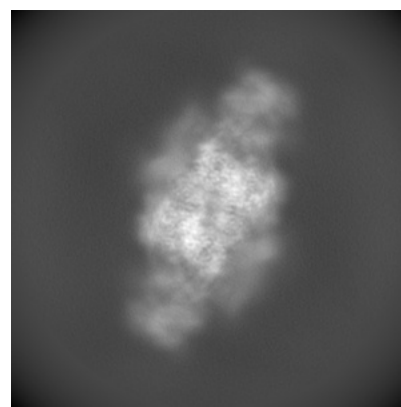
6.1.2 Raw map



X



Y

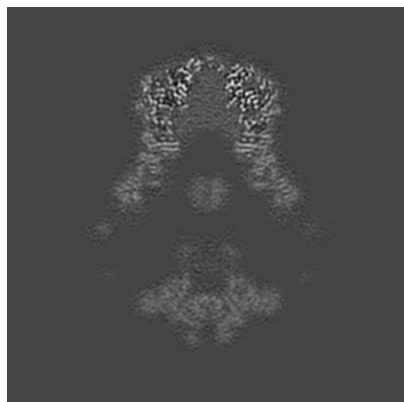


Z

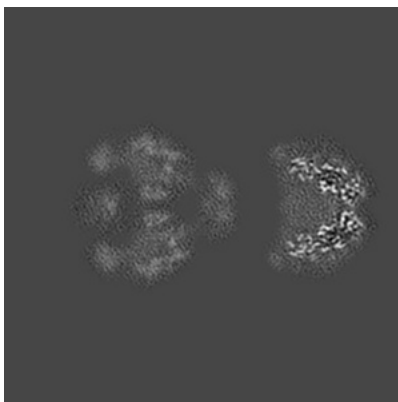
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 130

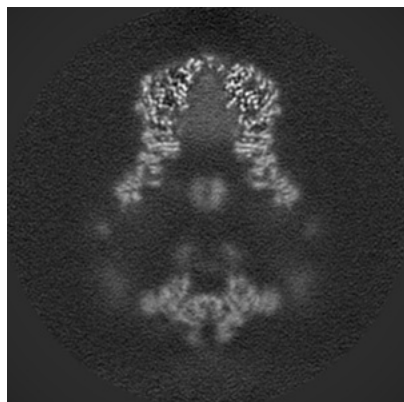


Y Index: 130

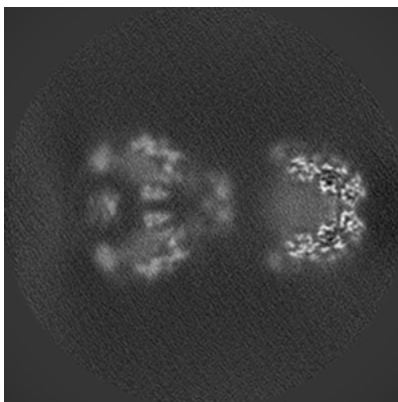


Z Index: 130

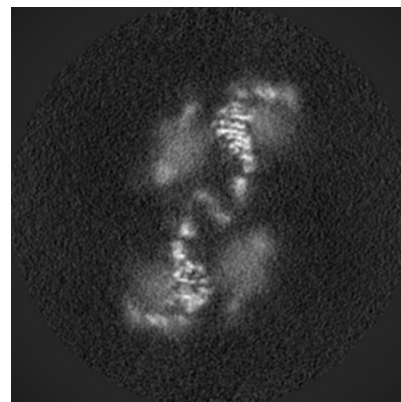
6.2.2 Raw map



X Index: 130



Y Index: 130

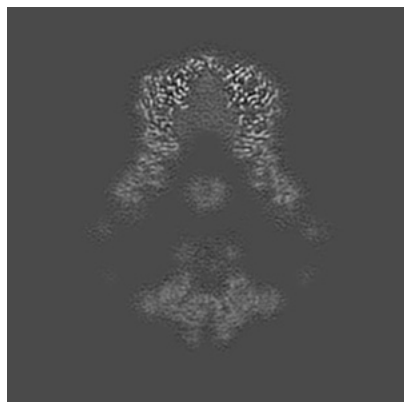


Z Index: 130

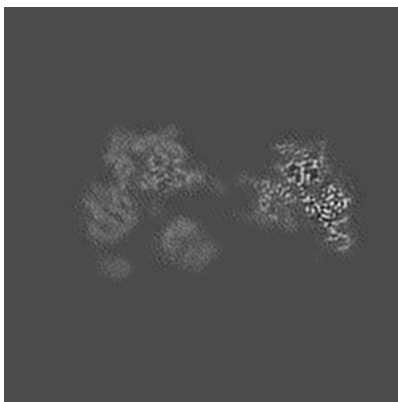
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

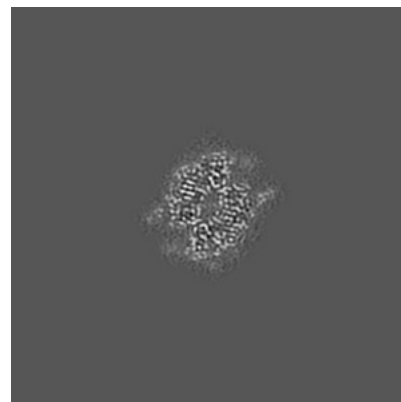
6.3.1 Primary map



X Index: 131

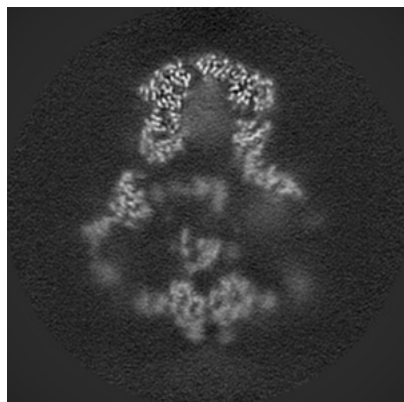


Y Index: 149

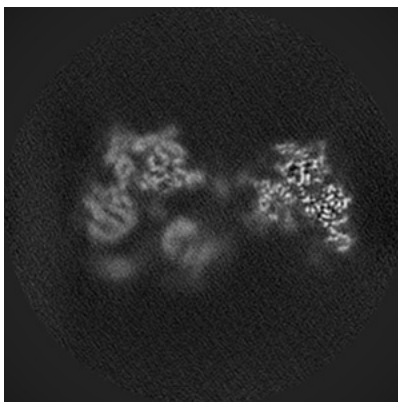


Z Index: 215

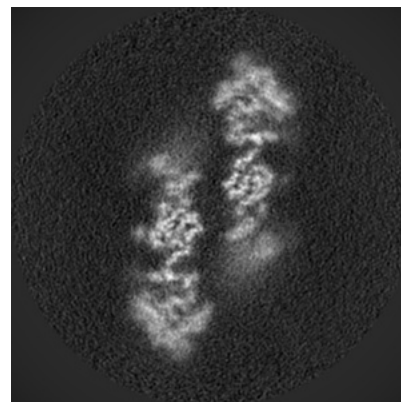
6.3.2 Raw map



X Index: 124



Y Index: 149

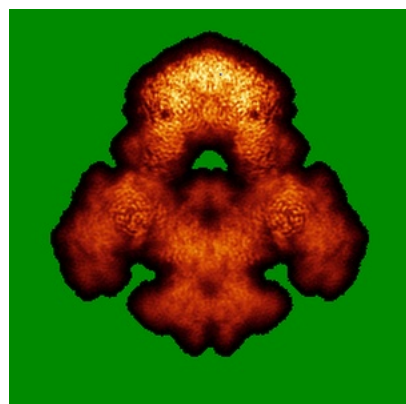


Z Index: 113

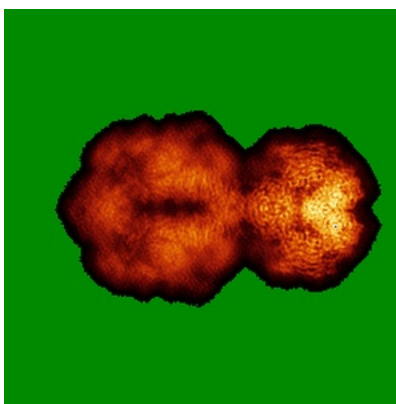
The images above show the largest variance slices of the map in three orthogonal directions.

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

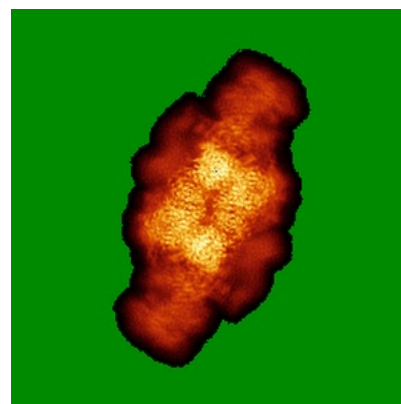
6.4.1 Primary map



X

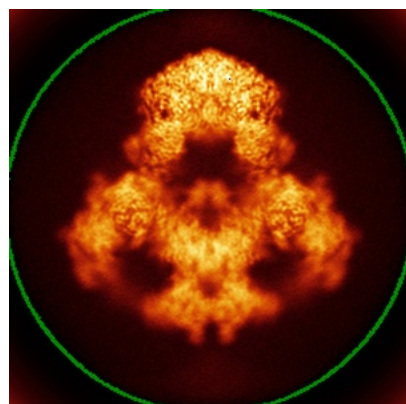


Y

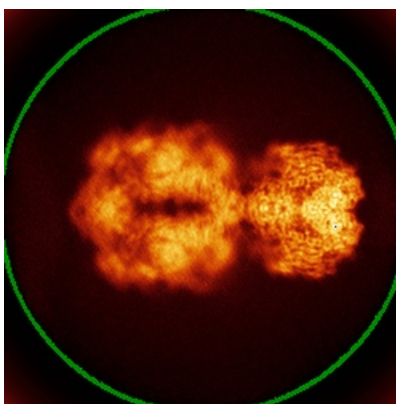


Z

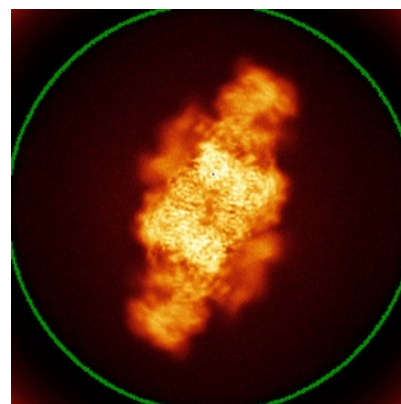
6.4.2 Raw map



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.

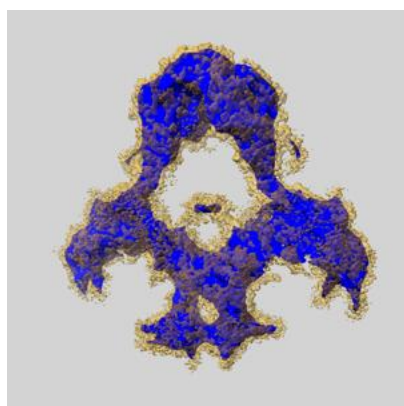
6.6 Mask visualisation [i](#)

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

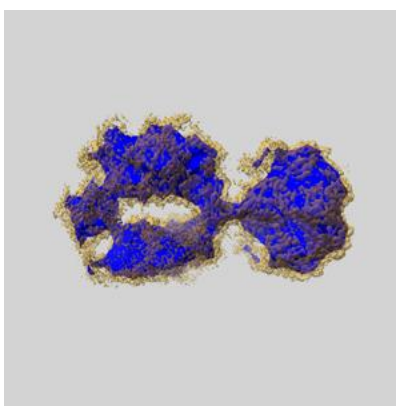
A mask typically either:

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

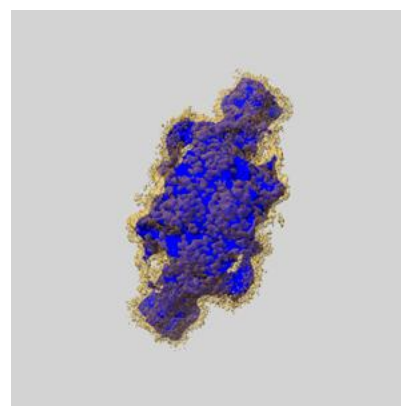
6.6.1 emd_36664_msk_1.map [i](#)



X



Y

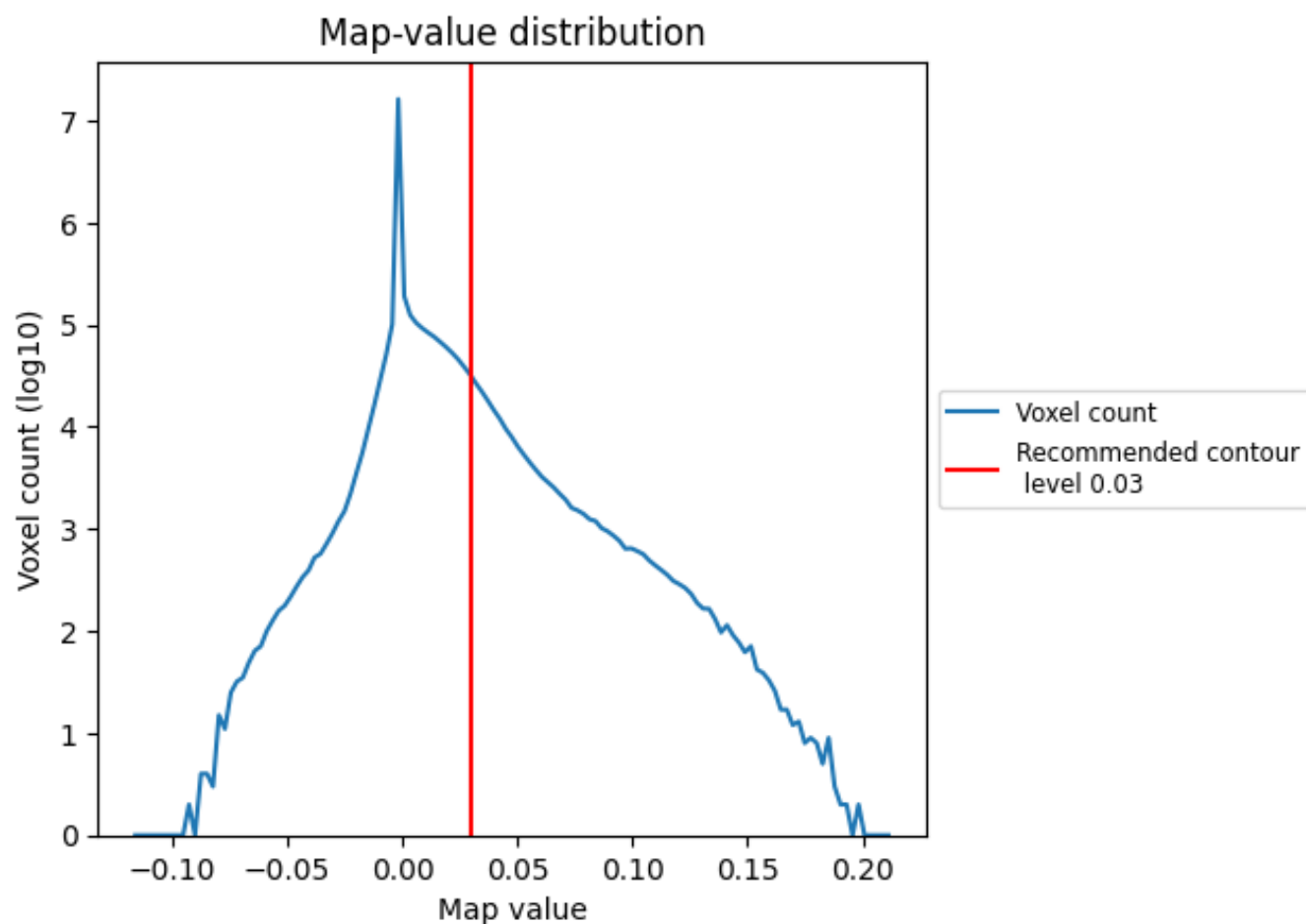


Z

7 Map analysis [i](#)

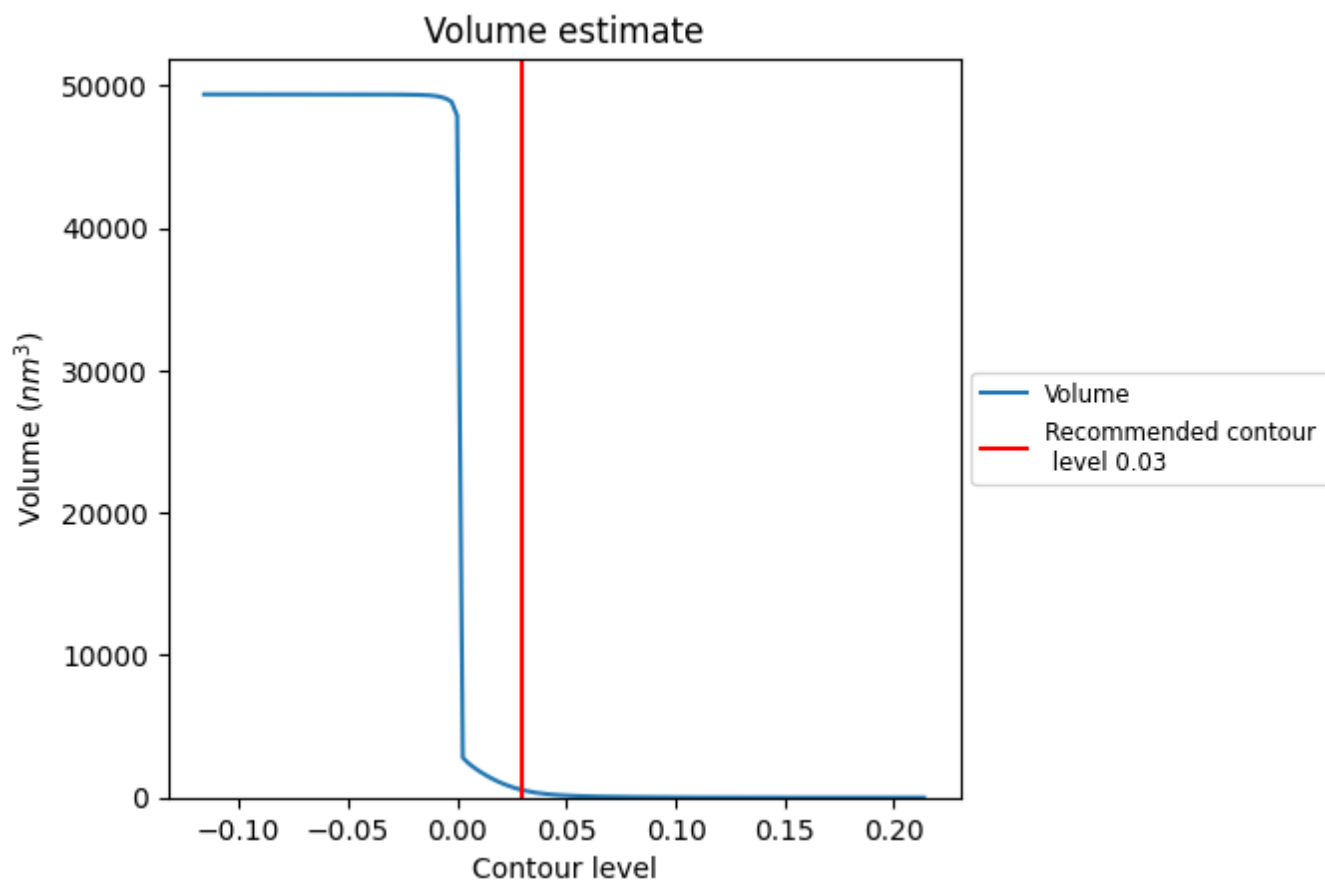
This section contains the results of statistical analysis of the map.

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.

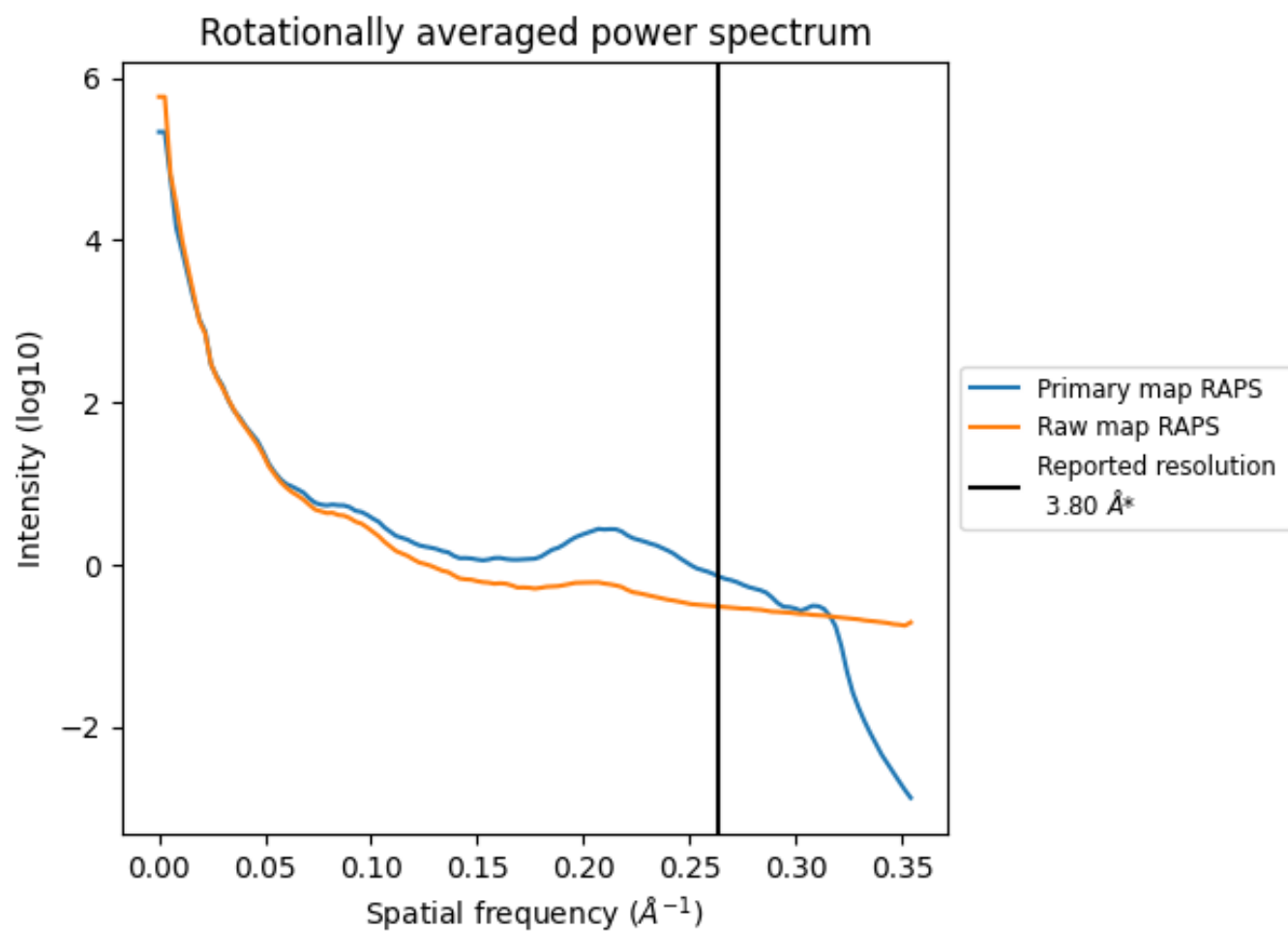
7.2 Volume estimate [i](#)



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 ⓘ

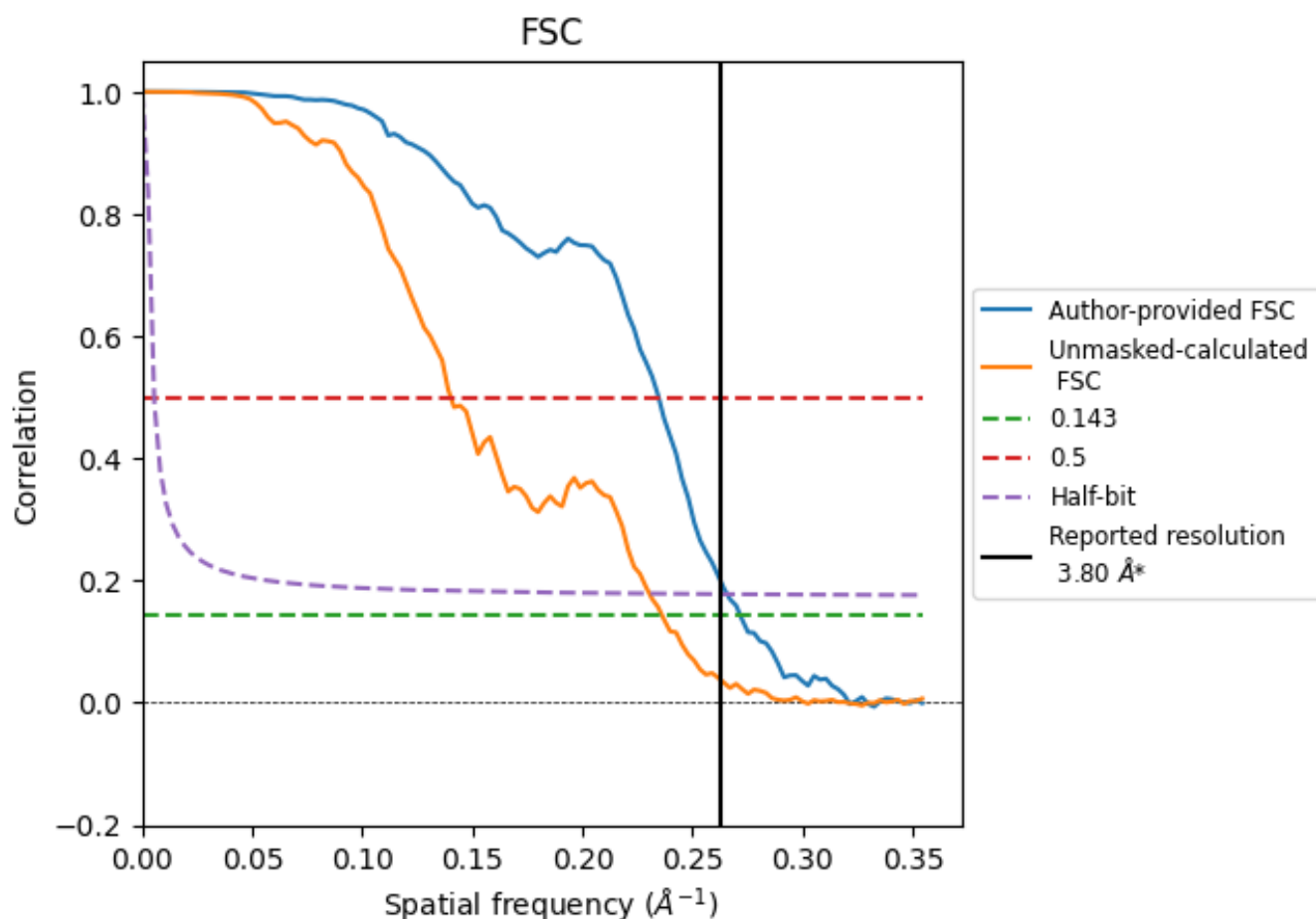


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

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 %

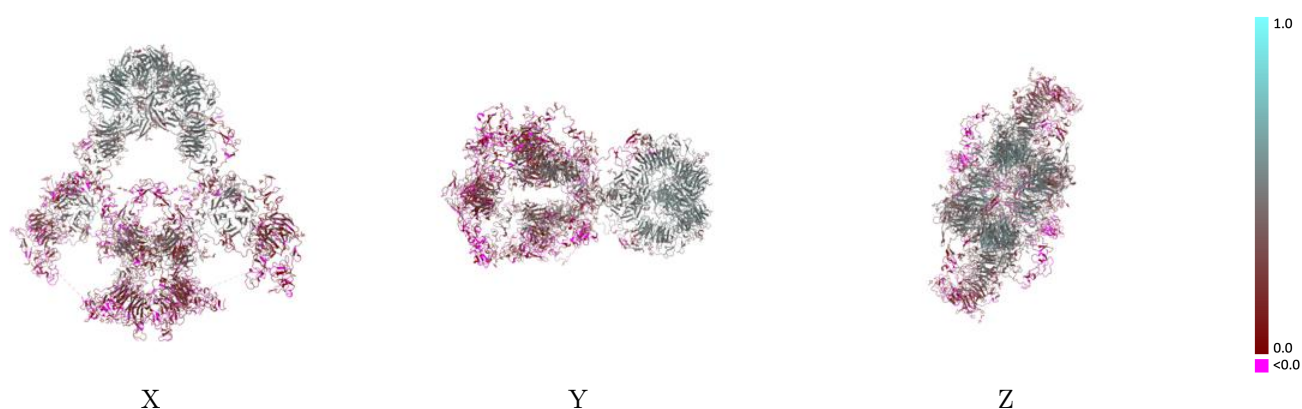
9 Map-model fit [i](#)

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

9.1 Map-model overlay [i](#)

This section was not generated.

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

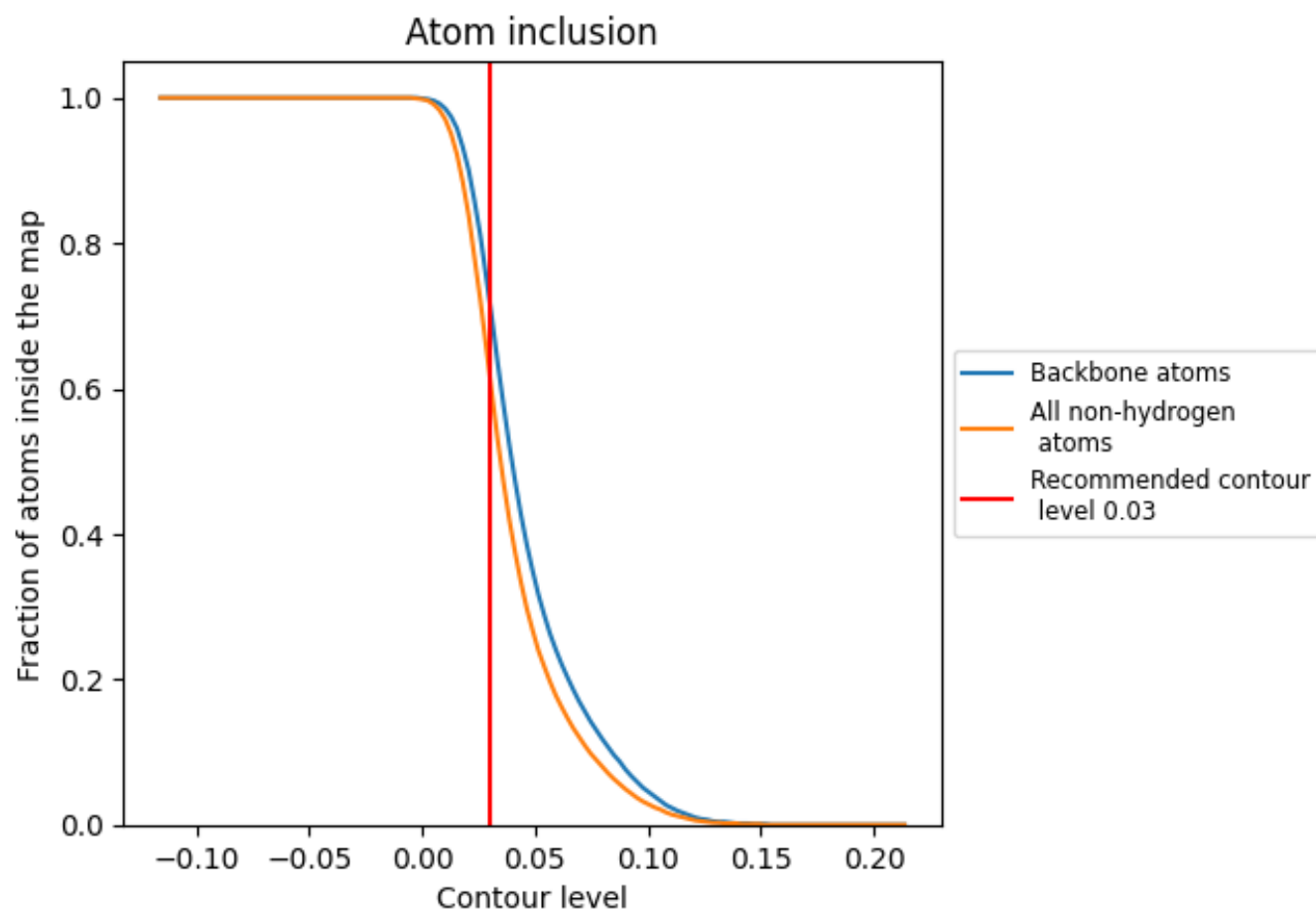


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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