



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:29 PM UTC

PDB ID : 8JUT / pdb_00008jut
EMDB ID : EMD-36663
Title : rat megalin RAP complex
Authors : Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.
Deposited on : 2023-06-27
Resolution : 4.20 Å(reported)

This is a 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:

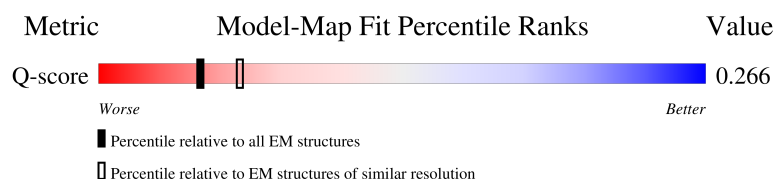
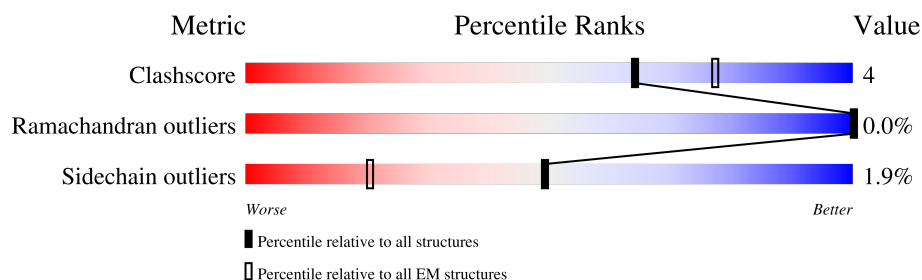
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

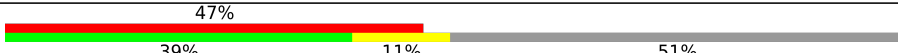
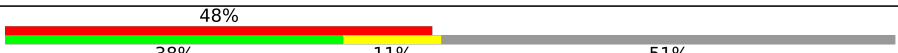
The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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

Mol	Chain	Length	Quality of chain
1	A	4660	
1	B	4660	
2	C	360	
2	D	360	

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

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

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Mol	Chain	Length	Quality of chain
13	8	2	100%
13	c	2	50% 100%
13	o	2	100%
14	6	5	100%
14	w	5	40% 40% 20%
14	w	5	60% 40%
15	z	3	100%
15	z	3	33% 67%
16	0	3	67% 33% 67%
16	7	3	100%
16	7	3	100%

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 73258 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a protein called unclear peptide.

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

- Molecule 4 is a protein called unclear peptide.

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

- Molecule 5 is a protein called unclear peptide.

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

- Molecule 6 is a protein called unclear peptide.

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

- Molecule 7 is a protein called unclear peptide.

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

- Molecule 8 is a protein called unclear peptide.

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

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



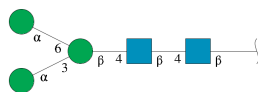
Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	2	Total	C	N	O	0	0
			28	16	2	10		

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

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



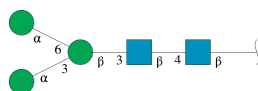
Mol	Chain	Residues	Atoms				AltConf	Trace
10	F	5	Total	C	N	O	0	0
			61	34	2	25		
10	Z	5	Total	C	N	O	0	0
			61	34	2	25		
10	b	5	Total	C	N	O	0	0
			61	34	2	25		
10	g	5	Total	C	N	O	0	0
			61	34	2	25		

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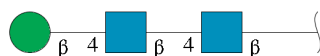
Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	5	Total	C	N	O	0	0
			61	34	2	25		
10	k	5	Total	C	N	O	0	0
			61	34	2	25		
10	l	5	Total	C	N	O	0	0
			61	34	2	25		
10	u	5	Total	C	N	O	0	0
			61	34	2	25		
10	1	5	Total	C	N	O	0	0
			61	34	2	25		
10	4	5	Total	C	N	O	0	0
			61	34	2	25		
10	5	5	Total	C	N	O	0	0
	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

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



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

- Molecule 12 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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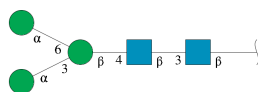
Mol	Chain	Residues	Atoms				AltConf	Trace
12	f	3	Total	C	N	O	0	0
			39	22	2	15		
12	h	3	Total	C	N	O	0	0
			39	22	2	15		
12	i	3	Total	C	N	O	0	0
			39	22	2	15		
12	m	3	Total	C	N	O	0	0
			39	22	2	15		
12	p	3	Total	C	N	O	0	0
			39	22	2	15		
12	r	3	Total	C	N	O	0	0
			39	22	2	15		
12	2	3	Total	C	N	O	0	0
	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

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



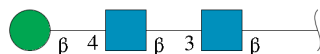
Mol	Chain	Residues	Atoms				AltConf	Trace
13	c	2	Total	C	N	O	0	0
			28	16	2	10		
13	o	2	Total	C	N	O	0	0
			28	16	2	10		
13	8	2	Total	C	N	O	0	0
			28	16	2	10		

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



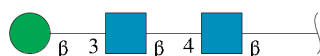
Mol	Chain	Residues	Atoms				AltConf	Trace
14	w	5	Total	C	N	O	0	0
			61	34	2	25		
14	6	5	Total	C	N	O	0	0
			61	34	2	25		

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



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

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



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

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



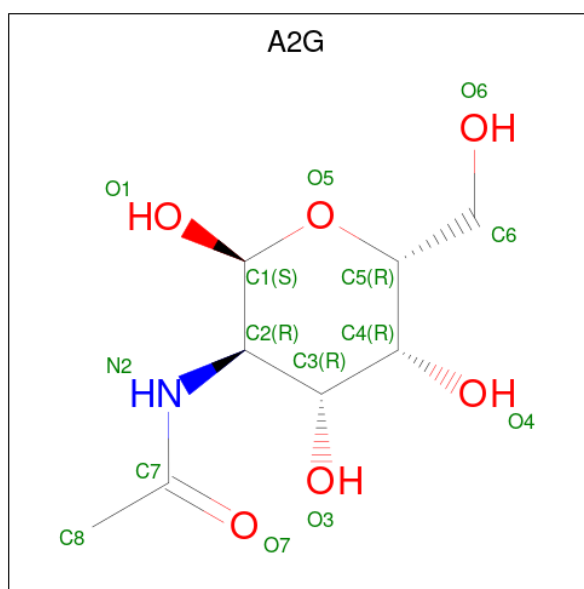
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14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

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

- Molecule 18 is 2-acetamido-2-deoxy- α -D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



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

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

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

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

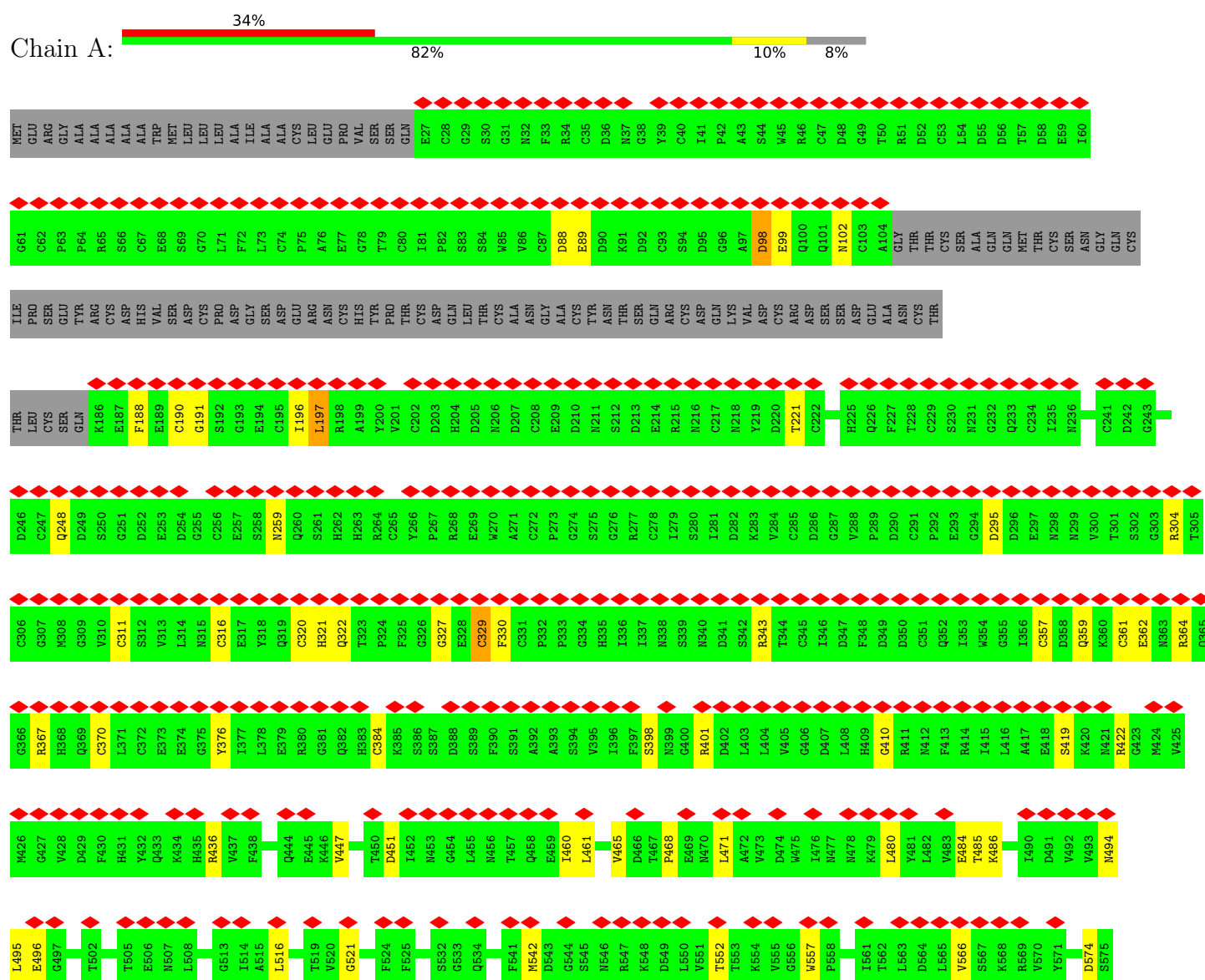
- Molecule 20 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

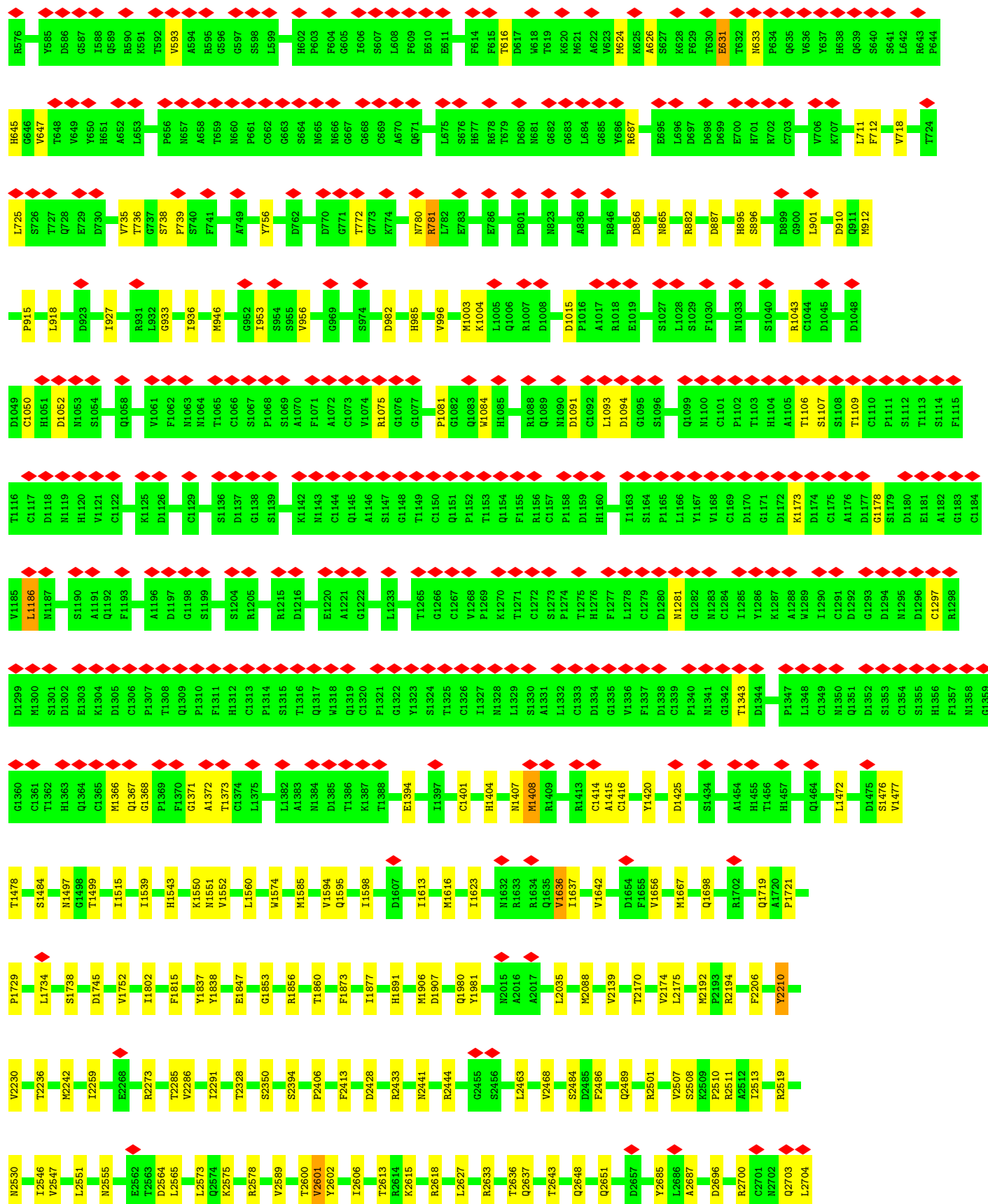
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total 1	Ni 1	0
20	B	1	Total 1	Ni 1	0

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





E3886	Q2705	N2817	R2877	Q2941	G3005	T3076	Y3136	M3308	L3509	H3594	R3693	C3812	E3886
S3887	C2708	C2818	C2878	R2942	R3006	C3077	C3137	H3312	M3513	R3595	C3694	V3813	S3887
P3888	L2709	P2819	I2879	H2943	R3009	F3078	K3144	G3312	S3516	C3596	I3695	P3814	P3888
Q3889	N2710	P2820	P2880	H2944	Q3010	L3079	L3145	D3315	S3523	S3597	D3705	L3817	Q3889
R3890	G2711	P2821	S2881	C2945	F3011	H3080	M3146	A3316	N3524	S3598	R3708	A3818	R3890
F3891	H2712	T2822	Y2882	E2946	F3012	F3082	S3147	R3326	E3525	M3599	Q3708	D3820	F3891
C3892	C2713	C2823	W2883	L2947	R3013	R3083	D3148	R3345	E3525	A3604	Q3714	G3821	C3892
C3893	Q2716	P2824	F2884	Q2948	R3014	C3084	K3149	D3375	I3530	I3609	S3718	L3826	C3893
C3894	N2722	P2825	D2885	N2949	D3015	D3085	R3150	D3378	C3534	Q3614	V3719	C3826	C3894
N3895	N2727	F2827	C2887	C2950	R3016	N3086	S3151	D3378	K3538	C3615	V3720	C3834	N3895
S3896	G2727	K2828	E2888	T2953	R3017	G3087	I3155	D3406	K3538	D3616	C3721	P3835	S3896
R3897	S2730	C2829	F2888	Q2954	D3022	H3088	C3158	D3406	S3541	S3617	S3719	R3836	R3897
C3898	F2739	Q2831	A2889	F2955	Y3023	C3089	K3159	L3415	D3542	V3618	V3720	F3837	C3898
F2747	F2747	T2832	C2891	C2955	E3026	E3091	E3160	T3416	G3543	N3619	C3721	F3838	F2747
G2775	G2775	N2834	G2894	S2960	R3026	N3092	G3093	I3417	S3544	D3620	H3722	N3839	G2775
R2779	R2779	I2835	S2995	R2961	G3029	G3094	V3173	D3420	E3546	L3622	D3726	N3840	R2779
N2780	N2780	C2836	D2896	P2962	S3030	C3096	D3189	V3422	P3547	D3623	A3730	G3841	N2780
C2781	C2781	P2838	T2900	P2963	Y3031	N3097	K3191	T3425	D3548	E3627	H3732	C3844	C2781
N2782	N2782	R2839	C2901	N2964	G3032	H3098	S3206	D3426	C3550	D3628	P3736	P3845	N2782
S2783	S2783	A2840	C2902	R2965	F3039	V3099	R3212	T3431	H3552	T3629	N3739	A3846	S2783
T2784	T2784	F2841	C2907	I2968	N3037	D3100	T3215	N3448	F3553	S3630	D3745	C3849	T2784
T2785	T2785	L2842	H2903	P2969	Q3038	D3101	S3220	T3449	F3554	S3634	D3746	E3850	T2785
E2786	E2786	C2843	W2905	Q2970	Q3039	C3102	G3215	T3450	C3555	C3637	C3747	C3851	E2786
F2787	F2787	G2845	N2906	Y2971	F3044	S3103	S3220	H3451	R3556	R3638	G3748	C3852	F2787
T2788	T2788	D2846	T2907	Y2972	R3045	N3105	L3228	P3452	L3557	K3643	N3755	N3853	T2788
C2789	C2789	N2847	C2908	Y2972	G3046	S3106	V3231	P3453	G3558	C3644	C3756	H3854	C2789
S2790	S2790	D2848	R2909	Y2973	I3047	D3107	G3231	T3473	Q3559	N3645	V3757	I3857	S2790
N2791	N2791	C2849	A2910	G2976	R3048	C3108	E3249	N3474	C3562	N3645	R3758	F3860	N2791
Q2792	Q2792	G2850	S2911	D2977	F3049	K3109	M3256	N3475	R3563	K3655	P3759	V3861	Q2792
R2793	R2793	G2852	Q2912	C2980	V3052	G3110	K3260	G3476	D3564	N3660	E3760	C3862	R2793
C2794	C2794	S2853	Q2913	S2981	C3053	G3111	G3260	C3477	G3565	S3666	E3765	C3863	C2794
I2795	I2795	E2855	C2915	D2982	D3054	G3112	R3270	N3479	N3566	S3666	A3769	E3866	I2795
F2796	F2796	N2856	D2916	D2983	E3055	G3113	L3271	G3482	C3567	D3671	N3784	N3867	F2796
S2798	S2798	C2857	N2917	L2984	D3056	E3115	R3272	L3481	Q3571	E3672	G3787	C3869	S2798
Y2799	Y2799	P2857	Q2918	L2987	N3057	C3116	E3275	L3483	L3572	D3672	C3787	V3870	Y2799
Y2800	Y2800	I2858	Q2918	Q2987	C3058	L3117	E3276	L3484	C3573	T3675	R3793	C3871	Y2800
C2801	C2801	Y2859	Q2918	Q2988	G3059	L3117	S3276	H3480	A3576	A3676	D3794	D3872	C2801
N2802	N2802	C2860	Q2918	N2989	G3060	L3118	L3277	G3482	R3577	A3677	C3795	C3873	N2802
Q2803	Q2803	A2861	C2923	C2990	S3063	S3119	D3280	D3497	Q3578	S3678	C3796	N3874	Q2803
I2804	I2804	S2862	G2923	C2990	D3064	S3120	D3280	D3498	Q3578	N3679	N3797	E3875	I2804
N2805	N2805	H2863	N2923	T2991	E3065	T3121	S3283	T3501	D3579	C3680	K3798	C3876	N2805
N2806	N2806	C2865	Q2923	T2992	Q3066	S3122	S3283	V3502	C3580	D3681	K3798	I3877	N2806
C2807	C2807	P2866	D2929	T2994	E3067	S3123	C3295	L3504	A3591	N3682	H3801	H3878	C2807
H2808	H2808	S2867	Q2930	C2995	H3068	C3124	L3296	R3505	D3592	H3683	T3808	L3879	H2808
D2809	D2809	C2868	N2931	S2996	L3069	H3125	G3303	C3506	R3588	I3683	S3809	C3880	D2809
N2810	N2810	S2867	Q2931	A2997	C3070	H3126	G3303	R3507	V3599	S3687	G3810	F3881	N2810
D2811	D2811	C2869	D2932	K2999	H3071	N3127	G3303	T3508	C3592	K3688	H3811	N3882	D2811
D2814	D2814	F2870	C2933	F3000	T3072	C3128	G3303	T3508	C3592	K3688	H3811	I3883	D2814
E2815	E2815	Q2871	G2934	S3001	P3073	T3129	G3303	T3508	C3592	K3688	H3811	P3884	E2815
N2816	N2816	C2872	D2935	A3003	E3074	T3131	G3303	T3508	C3592	K3688	H3811	N3941	N2816
		L2873	D2938	A3003	P3075	T3132	G3303	T3508	C3592	K3688	H3811	C3942	
		S2874	D2938	A3003	P3075	T3133	G3303	T3508	C3592	K3688	H3811	I3943	
		P2875	D2938	A3003	P3075	T3133	G3303	T3508	C3592	K3688	H3811	S3944	
		Q2876	D2938	A3003	P3075	T3133	G3303	T3508	C3592	K3688	H3811	I3945	

THR	LEU	CYS	SER	GLN	K186	E187	F188	E189	C190	G191	S192	G193	E194	C195	I196	L197	A198	A199	Y200	V201	H204	D205	N206	D207	C208	E209	D210	N211	S212	D213	E214	N215	N216	C217	N218	Y219	D220	T221	C222	G223	G224	H225	Q226	F227	T228	C229	S230	Q233	C234	N238	W239	V240	G243	D244	D245				
D246	C247	Q248	D249	S250	D251	D252	D253	D254	G255	C256	E257	S258	N259	Q260	S261	H262	H263	R264	C265	Y266	P267	R268	E269	W270	A271	C272	P273	G274	S275	G276	R277	C278	I279	S280	I281	D282	K283	V284	C285	G287	V288	P289	D290	C291	P292	E293	W294	D296	E297	N298	N299	V300	T301	S302	G303	R304	T305		
C306	G307	M308	G309	V310	C311	S312	V313	L314	N315	C316	E317	Y318	Q319	C320	H321	Q322	T323	P324	F325	G326	G327	E328	C329	F330	C331	P332	P333	G334	H335	I336	I337	N338	S339	N340	D341	G342	R343	T344	C345	I346	G347	F348	D349	S350	C351	Q352	I353	W354	G355	I356	C357	D358	Q359	K360	C361	E362	N363	R364	Q365
G366	R367	H368	Q369	C370	L371	C372	E373	E374	G375	Y376	I377	L378	E379	R380	Q381	Q382	H383	C384	K385	S386	S387	D388	S389	F390	S391	A392	A393	S394	V395	I396	F397	S398	R401	D402	L403	L404	V405	G406	D407	L408	H409	G410	R411	N412	F413	R414	I415	L416	A417	E418	W421	G427	V428	D429	F430	H431			
Y432	Q433	K434	F438	A439	T440	D441	P442	N443	Q444	E445	Y446	Y447	F448	S449	T450	D451	T452	N453	G454	L455	N456	T457	Q458	L461	S464	V465	D466	T467	P468	E469	N470	L471	A472	V473	D474	Y475	L476	N477	N478	K479	L480	Y481	K486	V487	N488	R489	I490	D491	V492	V493	E496	G497	N498	Q499					
R500	L503	Y504	T505	L508	R512	G513	E514	A515	L516	D517	P518	T519	F525	S526	D527	S530	L531	S532	G533	V537	N542	D543	G544	D549	L550	V551	T552	T553	K554	A559	G560	I561	T562	L563	D564	L565	V566	S567	K568	Y571	D574	Y577	E496	G497	N498	D586	G587												
I588	Q589	T592	V593	A594	R595	S596	L599	V600	F604	G605	T606	S607	L608	F609	E610	E611	H612	V613	F614	F615	T616	T619	K620	V623	N624	K625	A626	S627	K628	F629	T630	E631	T632	N633	P634	Q635	V636	V637	H638	Q639	S640	S641	L642	P644	H645	G646	V647	T648	V649	R654	T659								
N660	P661	C662	G663	S664	N665	N666	G667	C668	A670	D671	L675	R676	T679	D680	N681	G682	G683	L684	R687	C688	K689	C690	E691	E695	L696	D697	N698	D699	E700	H701	R702	C703	V704	A705	V706	K707	L725	V735	T736	G737	S738	P739	R740	F741	F742	Y756	S757	K766	G771										
I777	E783	L788	T793	W799	V807	R811	L812	A813	D814	T821	N825	N826	T830	N839	W844	F845	R846	P847	D856	T863	V864	W870	T927	L932	D945	R951	S954	N957	D963	L966	G969	S970	N971	A979	V1084	H1085	C1086	D1087	R1088	D1091	C1092	L1093	Q1099	N1100	C1101	P1102	T1103												
V990	M1003	K1004	M1010	T1011	C1012	A1017	Q1023	L1028	N1033	F1041	H1051	H1057	Q1058	C1059	G1060	F1062	N1063	C1066	S1069	A1072	C1073	V1074	R1075	G1076	Q1077	Q1078	C1079	I1080	P1081	V1084	H1085	C1086	D1087	R1088	D1091	C1092	L1093	Q1099	N1100	C1101	P1102	T1103																	
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D1170	G1171	D1172	K1173	A1176	D1177	G1178	S1179	D1180	E1181	A1182	G1183	C1184	V1185	L1186	N1187	C1188	P1189	S1190	A1191	K1194	C1195	A1196	D1197	G1198	S1199	S1200	C1201	R1215	D1216	N1217	C1223	L1233	E1250	T1265	G1266	C1267	K1270	T1271	C1272	S1273	P1274	T1275	H1276	F1277	L1278	C1279	D1280	N1281	G1282	N1283	C1284								
I1285	Y1286	K1287	D1292	G1293	D1294	N1295	R1298	D1299	M1300	S1301	D1302	E1303	K1304	D1305	C1306	P1307	T1308	Q1309	P1310	F1311	H1312	C1313	P1314	S1315	T1316	Q1317	N1318	Q1319	C1320	P1321	Y1323	S1324	T1325	C1326	I1327	N1328	L1329	S1330	A1331	L1332	C1333	D1334	G1335	V1336	F1337	D1338	C1339	N1341	G1342	T1343	S1346	P1347	L1348	C1349					

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D3104	N3105	E3108	K3109	G3110	G3111	G3112	I3113	N3114	E3115	G3116	L3117	D3118	S3119	S3120	I3121	S3122	R3123	C3124	D3125	T3129	I3132	T3133	S3134	F3135	K3144	L3145	M3146	S3147	D3148	K3149	R3150	S3151	C3152	V3153	C3154	I3155	D3156	K3159	E3160	V3173	I3177	G3190	N3198	F3205	L3223	L3224	L3225	Q3226												
E1785	D1788	N1864	F1873	V1879	L1886	H1891	K1900	I1901	A1902	S1903	A1904	N1905	M1906	D1907	L1911	L1914	E1923	W1936	A1937	P1964	S1972	Y1975	R1986	K1989	R2009	V2010	Y2011	R2012	R2013	R2014	N2015	A2016	A2017	L2035	P2036	M2066	N2070	L2071	P2072																					
A2073	F2077	E2080	L2081	T2110	G2142	W2155	L2160	N2164	V2174	T2177	M2192	P2193	R2194	P2200	Y2210	N2225	T2234	V2235	T2236	P2237	N2242	D2243	T2246	D2253	L2258	L2264	D2265	E2268	V2286	L2291	L2035	P2036	M2066	N2070	L2071	P2072																								
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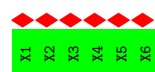
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- Molecule 3: unclear peptide



- Molecule 3: unclear peptide



- Molecule 4: unclear peptide

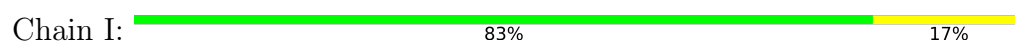


- Molecule 4: unclear peptide

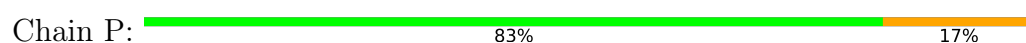


There are no outlier residues recorded for this chain.

- Molecule 5: unclear peptide



- Molecule 5: unclear peptide



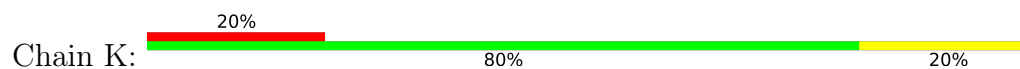
- Molecule 6: unclear peptide



- Molecule 6: unclear peptide



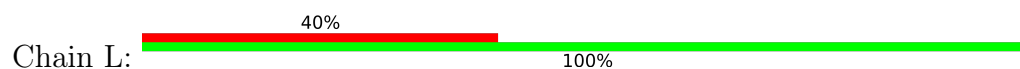
- Molecule 7: unclear peptide



- Molecule 7: unclear peptide



- Molecule 8: unclear peptide



- Molecule 8: unclear peptide



There are no outlier residues recorded for this chain.

- Molecule 8: unclear peptide

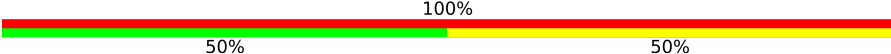


- Molecule 8: unclear peptide

Chain T:  100%

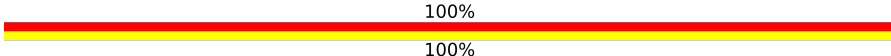
There are no outlier residues recorded for this chain.

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

Chain E:  100%
50% 50%

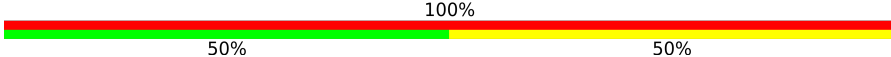


- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%
100%



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

Chain X:  100%
50% 50%



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

Chain Y:  50%
100%



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

Chain a:  50%
100%



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



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



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



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



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



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



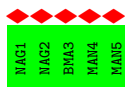
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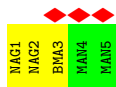
- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



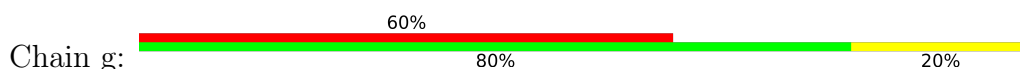
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

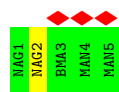


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

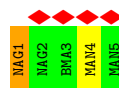
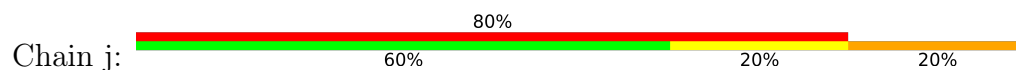


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

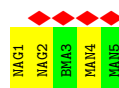
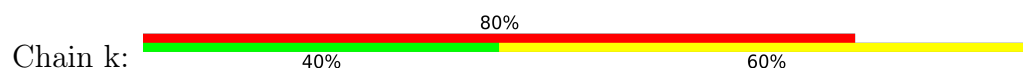




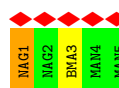
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



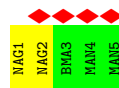
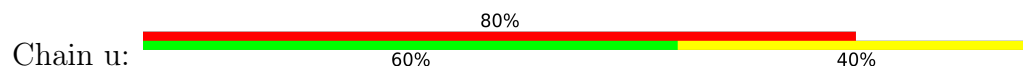
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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

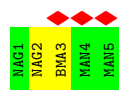


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

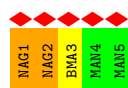


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

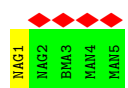
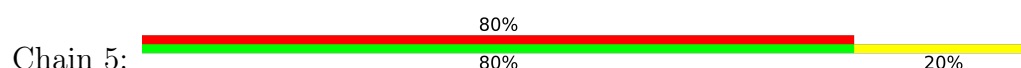




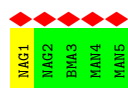
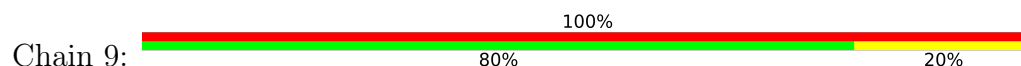
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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



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



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



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



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





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



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



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



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



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



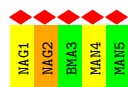
- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0242	Depositor
Map size ($\text{\AA}$)	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

5.1 Standard geometry

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2938	ASP	CA-CB-CG	9.92	122.52	112.60
1	A	4243	ASP	CA-CB-CG	8.24	120.84	112.60
1	A	2810	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	A	2819	PRO	N-CA-C	7.41	119.74	110.70
1	A	4284	ASP	CA-CB-CG	6.50	119.11	112.60
1	A	2413	PHE	CA-CB-CG	6.42	120.22	113.80
1	A	2943	HIS	CA-CB-CG	6.15	119.95	113.80
1	A	3794	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	2810	ASN	CB-CG-ND2	6.02	125.43	116.40
1	B	990	VAL	CB-CA-C	5.95	115.16	109.33
1	A	2924	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	330	PHE	CA-CB-CG	5.72	119.52	113.80
1	B	3709	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	2930	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	957	MET	N-CA-C	5.50	116.67	108.31
1	A	2903	HIS	O-C-N	5.44	127.67	122.07
1	B	2585	ASN	CA-CB-CG	5.33	117.93	112.60
1	B	3395	ASP	CA-CB-CG	5.30	117.91	112.60
1	B	3791	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	3784	ASN	CA-CB-CG	5.18	117.78	112.60
1	A	2839	ARG	CA-C-N	5.12	129.28	120.72
1	A	2839	ARG	C-N-CA	5.12	129.28	120.72
1	A	2944	HIS	CA-C-N	5.12	130.00	122.63
1	A	2944	HIS	C-N-CA	5.12	130.00	122.63
1	B	252	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	4327	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	3345	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	B	3693	ARG	NE-CZ-NH2	5.03	123.73	119.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1043	ARG	Sidechain
1	A	3212	ARG	Sidechain
1	A	4321	ARG	Sidechain
1	A	781	ARG	Sidechain
1	B	2877	ARG	Sidechain
1	B	3693	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	31021	266	0
1	B	33636	0	31021	264	0
2	C	1494	0	1505	24	0
2	D	1494	0	1505	26	0
3	G	30	0	8	0	0
3	N	30	0	8	0	0
4	H	28	0	12	0	0
4	O	28	0	12	0	0
5	I	33	0	18	5	0
5	P	33	0	18	1	0
6	J	16	0	8	0	0
6	Q	16	0	8	0	0
7	K	33	0	18	1	0
7	R	33	0	17	0	0
8	L	28	0	12	0	0
8	M	28	0	12	0	0
8	S	28	0	13	0	0
8	T	28	0	12	0	0
9	E	28	0	25	0	0
9	V	28	0	25	0	0
9	X	28	0	25	1	0
9	Y	28	0	25	0	0
9	a	28	0	25	0	0
9	d	28	0	25	0	0
9	n	28	0	25	0	0
9	q	28	0	25	0	0
9	s	28	0	25	0	0
9	t	28	0	25	1	0
9	v	28	0	25	0	0
9	x	28	0	25	0	0
9	y	28	0	25	0	0
10	1	61	0	52	0	0
10	4	61	0	52	1	0
10	5	61	0	52	0	0
10	9	61	0	52	0	0
10	F	61	0	52	0	0
10	Z	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	b	61	0	52	0	0
10	g	61	0	52	0	0
10	j	61	0	52	2	0
10	k	61	0	52	0	0
10	l	61	0	52	2	0
10	u	61	0	52	1	0
11	U	61	0	52	1	0
12	2	39	0	34	0	0
12	3	39	0	34	0	0
12	W	39	0	34	1	0
12	e	39	0	34	0	0
12	f	39	0	34	0	0
12	h	39	0	34	0	0
12	i	39	0	34	0	0
12	m	39	0	34	0	0
12	p	39	0	34	0	0
12	r	39	0	34	0	0
13	8	28	0	25	0	0
13	c	28	0	25	0	0
13	o	28	0	25	0	0
14	6	61	0	52	2	0
14	w	61	0	52	0	0
15	z	39	0	34	0	0
16	0	39	0	34	0	0
16	7	39	0	34	0	0
17	A	154	0	143	2	0
17	B	154	0	143	0	0
18	A	168	0	144	0	0
18	B	168	0	144	0	0
19	A	44	0	0	0	0
19	B	44	0	0	0	0
20	A	1	0	0	0	0
20	B	1	0	0	0	0
All	All	73258	0	67424	574	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (574) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3505:ARG:H	1:B:3505:ARG:HD3	1.38	0.90
1:A:3015:ASP:HB2	1:A:3017:ARG:NH2	1.90	0.87
1:A:2786:GLU:HG2	1:A:2788:THR:H	1.43	0.82
1:A:2708:CYS:SG	1:A:2730:SER:OG	2.40	0.79
1:A:3963:GLY:HA2	1:A:4004:LYS:HE2	1.65	0.79
1:B:4073:SER:HB3	1:B:4075:LYS:HG3	1.64	0.79
2:C:59:MET:HE3	2:C:61:LYS:HG2	1.63	0.78
1:A:1574:TRP:CE3	5:I:3:LEU:HD23	2.20	0.77
1:A:1173:LYS:HD2	1:A:1178:GLY:HA2	1.69	0.74
1:A:3860:PHE:CE2	10:j:1:NAG:H2	2.22	0.74
1:A:3860:PHE:HE2	10:j:1:NAG:H2	1.54	0.73
1:A:4131:ASN:HD21	1:A:4385:CYS:HB2	1.54	0.73
1:A:912:MET:HE1	1:A:927:ILE:HD13	1.70	0.72
1:B:1900:LYS:HE2	1:B:1902:ALA:HB2	1.70	0.72
1:B:518:PRO:HA	1:B:542:MET:HE1	1.71	0.72
1:B:3983:GLN:NE2	1:B:3988:GLY:O	2.23	0.71
1:A:3431:THR:HG22	1:A:3448:ASN:HB3	1.72	0.71
1:B:4282:PHE:O	1:B:4283:GLU:HG3	1.91	0.70
1:B:4041:MET:SD	1:B:4042:SER:N	2.65	0.70
1:A:4313:VAL:O	1:A:4314:ASN:ND2	2.24	0.69
1:A:3937:CYS:SG	1:A:3938:SER:N	2.65	0.69
1:B:2507:VAL:HG21	1:B:2524:TRP:HE1	1.57	0.69
1:A:3675:THR:HG23	1:A:3677:ALA:H	1.57	0.69
1:B:1003:MET:HG2	1:B:1012:CYS:HB3	1.74	0.69
1:B:2959:ASN:ND2	1:B:2982:ASP:OD2	2.26	0.68
1:A:320:CYS:HA	1:A:329:CYS:HB2	1.75	0.68
1:A:4398:LEU:O	1:A:4400:LYS:NZ	2.23	0.68
1:B:2651:GLN:N	1:B:2651:GLN:OE1	2.27	0.68
14:6:1:NAG:O4	14:6:2:NAG:N2	2.25	0.67
1:B:2242:MET:HE1	1:B:2264:LEU:HD21	1.76	0.67
1:B:3943:ILE:HG13	1:B:3955:CYS:HB3	1.75	0.67
1:A:912:MET:HE3	1:A:936:ILE:HD11	1.76	0.67
2:C:99:LEU:O	2:C:103:GLY:N	2.29	0.66
1:A:1574:TRP:CE3	5:I:3:LEU:CD2	2.79	0.66
1:A:3814:PRO:HG2	1:A:3817:LEU:HD13	1.76	0.66
1:B:4269:ILE:HG22	1:B:4270:ILE:HG12	1.76	0.66
1:B:2939:GLU:HG2	1:B:2941:GLN:H	1.60	0.65
1:B:3372:ILE:HD11	1:B:3381:LEU:HD11	1.80	0.64
2:D:96:TRP:HB2	2:D:110:LYS:HG3	1.79	0.64
1:B:1382:LEU:HD12	1:B:1386:THR:HA	1.79	0.64
1:A:2463:LEU:HD11	1:A:2501:ARG:HD2	1.79	0.64
1:A:3876:GLU:OE1	1:A:3876:GLU:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4100:LEU:HD11	1:A:4384:ARG:HG2	1.79	0.63
1:B:574:ASP:OD1	1:B:577:TYR:N	2.23	0.63
2:D:122:LEU:HD22	2:D:127:LEU:HD22	1.79	0.63
1:B:4204:THR:HG22	1:B:4212:ILE:HG12	1.79	0.63
1:A:1719:GLN:HG3	1:A:1721:PRO:HD2	1.81	0.63
1:A:1574:TRP:CZ3	5:I:3:LEU:HD23	2.34	0.63
2:D:282:GLU:HA	2:D:285:LYS:HZ3	1.64	0.63
1:A:2954:GLN:HA	1:A:2969:PRO:HA	1.79	0.63
1:B:811:ARG:NH2	1:B:814:ASP:OD1	2.31	0.63
2:D:79:LEU:HA	2:D:82:LEU:HD12	1.81	0.63
1:A:882:ARG:HE	1:A:895:HIS:HD2	1.46	0.62
1:A:1366:MET:HE3	1:A:1373:THR:HB	1.79	0.62
1:A:3295:CYS:SG	1:A:3296:LEU:N	2.72	0.62
1:A:4126:GLU:OE2	10:I:1:NAG:O3	2.10	0.62
1:A:2705:GLN:HB3	1:A:2713:CYS:HB3	1.80	0.62
1:A:1550:LYS:O	1:A:1552:VAL:HG23	2.00	0.61
1:A:1281:ASN:ND2	1:A:1297:CYS:O	2.32	0.61
1:A:1595:GLN:HA	1:A:1598:ILE:HD11	1.82	0.61
1:B:863:ILE:HG22	1:B:864:VAL:HG23	1.82	0.60
1:B:616:THR:HG22	1:B:623:VAL:HG22	1.83	0.60
1:A:2795:ILE:HD11	1:A:2800:VAL:HG12	1.84	0.60
1:A:2546:ILE:HG22	1:A:2547:VAL:HG13	1.82	0.60
1:A:1574:TRP:CD2	5:I:3:LEU:HD23	2.37	0.60
1:A:3554:PHE:CD1	1:A:3848:MET:HE1	2.37	0.60
1:A:4068:LYS:HB2	1:A:4077:SER:HB2	1.82	0.60
1:B:3862:ILE:HG13	1:B:3863:CYS:SG	2.41	0.60
2:C:291:ILE:O	2:C:295:ASN:ND2	2.35	0.60
1:B:2933:CYS:HB2	1:B:2938:ASP:HB3	1.83	0.60
1:A:3017:ARG:HD3	1:A:3017:ARG:N	2.17	0.60
1:B:465:VAL:HG12	1:B:465:VAL:O	2.02	0.59
1:B:4295:GLU:N	1:B:4295:GLU:OE1	2.35	0.59
1:A:1551:ASN:OD1	9:X:1:NAG:N2	2.35	0.59
1:A:2809:ASP:OD1	1:A:2811:ASP:N	2.35	0.59
1:A:2648:GLN:HB3	1:A:2651:GLN:HE21	1.68	0.59
1:B:1088:ARG:HB3	1:B:1088:ARG:HH21	1.67	0.59
2:C:56:GLU:OE1	2:C:66:TRP:NE1	2.36	0.59
1:B:451:ASP:OD2	1:B:453:ASN:ND2	2.36	0.59
1:B:36:ASP:HB2	1:B:57:THR:HG21	1.84	0.58
1:B:4100:LEU:HD11	1:B:4384:ARG:HG2	1.83	0.58
2:D:111:GLU:O	2:D:114:LEU:HG	2.01	0.58
1:A:3082:PHE:CD2	1:A:3095:VAL:HG21	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:HIS:HD2	1:B:434:LYS:H	1.50	0.58
1:B:2210:TYR:HB2	1:B:2236:THR:HA	1.85	0.58
1:A:1367:GLN:NE2	1:A:1371:GLY:O	2.31	0.58
2:C:59:MET:O	2:C:63:ASN:ND2	2.26	0.58
1:B:830:ILE:HD11	1:B:839:MET:HE2	1.86	0.58
1:B:3016:ARG:HD3	1:B:3045:ARG:HD2	1.85	0.58
2:D:72:LEU:O	2:D:73:HIS:ND1	2.37	0.58
1:A:3982:THR:HB	1:A:3990:ILE:HG23	1.86	0.58
1:A:3984:LEU:HD13	1:A:3987:GLY:HA3	1.85	0.58
1:A:4119:ARG:NH2	1:A:4173:LEU:O	2.36	0.58
1:B:766:LYS:HD3	1:B:777:ILE:HD11	1.86	0.58
1:B:2525:THR:HG22	1:B:2533:ILE:HD12	1.86	0.58
1:A:912:MET:HE2	1:A:915:PRO:HB3	1.86	0.58
1:A:1497:ASN:OD1	12:W:1:NAG:N2	2.37	0.58
1:A:1574:TRP:CD2	5:I:3:LEU:CD2	2.86	0.58
1:A:738:SER:OG	1:A:739:PRO:HD3	2.03	0.57
1:A:2972:TRP:CZ2	2:D:127:LEU:HD21	2.39	0.57
1:B:268:ARG:HG3	1:B:281:ILE:HG12	1.86	0.57
1:B:1564:MET:HE1	1:B:1702:ARG:HE	1.67	0.57
1:B:2070:MET:HG3	1:B:2072:PRO:HD2	1.86	0.57
1:B:3064:ASP:OD1	1:B:3064:ASP:N	2.33	0.57
1:B:1923:GLU:HB2	1:B:1937:ALA:HB3	1.86	0.57
10:4:1:NAG:H83	10:4:2:NAG:H83	1.85	0.57
1:B:1864:ASN:ND2	1:B:2319:ASP:OD1	2.37	0.57
2:C:281:ARG:O	2:C:285:LYS:HG2	2.05	0.57
1:A:3144:LYS:HB3	1:A:3155:ILE:HD11	1.86	0.57
1:B:2950:CYS:HB3	1:B:2956:THR:HB	1.86	0.57
2:C:281:ARG:HA	2:C:284:LEU:HD12	1.87	0.57
1:A:321:HIS:CD2	1:A:322:GLN:H	2.22	0.56
1:B:1937:ALA:HB1	1:B:1964:PRO:HG2	1.87	0.56
1:A:2192:MET:HG3	1:A:2192:MET:O	2.04	0.56
1:A:2484:SER:HB3	1:A:2513:ILE:HD11	1.86	0.56
1:A:3295:CYS:SG	1:A:3308:MET:HG2	2.45	0.56
1:A:4254:ASP:HB2	1:A:4275:LYS:H	1.71	0.56
1:B:486:LYS:HG2	1:B:736:THR:HG21	1.87	0.56
1:B:616:THR:HB	1:B:644:PRO:HB2	1.88	0.56
1:B:3225:LEU:HD13	1:B:3256:MET:HE1	1.86	0.56
1:B:4295:GLU:HG3	1:B:4312:VAL:HG13	1.87	0.56
1:A:295:ASP:OD1	1:A:304:ARG:NH1	2.38	0.56
1:B:3016:ARG:NE	1:B:3044:GLY:O	2.38	0.56
1:B:2959:ASN:O	1:B:2961:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4098:ILE:O	1:B:4384:ARG:NH1	2.38	0.56
1:A:3066:GLN:HE21	1:A:3069:LEU:H	1.54	0.56
1:B:4398:LEU:HD23	1:B:4399:PRO:HD2	1.88	0.56
1:A:1853:GLY:O	1:A:1856:ARG:NH1	2.30	0.56
1:B:3981:CYS:SG	1:B:3982:THR:N	2.78	0.56
1:A:3693:ARG:HH22	1:A:3708:ARG:HG2	1.70	0.55
1:B:272:CYS:HB2	1:B:295:ASP:HB3	1.88	0.55
1:B:3976:ILE:HG12	1:B:3989:PHE:HE2	1.70	0.55
1:B:3048:PRO:HD2	1:B:3051:PHE:HE1	1.71	0.55
1:A:486:LYS:HG2	1:A:736:THR:HG21	1.87	0.55
1:B:3026:GLU:HA	1:B:3026:GLU:OE1	2.07	0.55
1:A:712:PHE:CE1	1:A:953:ILE:HD11	2.41	0.55
1:A:3617:SER:N	1:A:3627:GLU:OE1	2.39	0.55
1:A:3425:THR:HB	1:A:3453:PRO:HG2	1.88	0.55
1:A:2285:THR:HG21	1:A:2328:THR:HA	1.89	0.54
1:B:1473:ASP:OD1	1:B:1474:PHE:N	2.40	0.54
1:B:4204:THR:HG23	1:B:4236:LEU:HD22	1.88	0.54
1:A:616:THR:HG23	1:A:647:VAL:HG23	1.89	0.54
1:A:2139:VAL:HG22	1:A:2175:LEU:HD13	1.88	0.54
1:B:2081:LEU:H	1:B:2081:LEU:HD22	1.72	0.54
1:B:4256:ILE:HB	1:B:4270:ILE:HB	1.89	0.54
1:B:3146:MET:SD	1:B:3146:MET:N	2.80	0.54
1:B:190:CYS:SG	1:B:191:GLY:N	2.81	0.54
1:B:1088:ARG:HB3	1:B:1088:ARG:NH2	2.22	0.54
1:B:2999:GLU:HA	1:B:3009:ARG:HA	1.89	0.54
2:D:283:GLU:HG2	2:D:348:LEU:HD21	1.88	0.54
1:A:1560:LEU:HD22	1:A:1585:MET:HE2	1.89	0.54
1:B:4390:ASN:O	1:B:4401:CYS:HB2	2.08	0.54
1:A:3760:GLU:OE1	1:A:3760:GLU:N	2.41	0.54
1:A:4130:ASN:HB2	1:A:4389:GLY:O	2.08	0.54
1:A:1636:VAL:HG23	1:A:1637:ILE:HG13	1.90	0.54
1:B:2192:MET:O	1:B:2192:MET:HG3	2.08	0.54
1:A:557:TRP:N	1:A:574:ASP:OD1	2.41	0.53
1:A:3949:CYS:SG	1:A:3990:ILE:HB	2.48	0.53
1:B:1750:MET:HE2	1:B:2011:TYR:HB2	1.89	0.53
1:B:3145:LEU:HD22	1:B:3146:MET:H	1.73	0.53
2:D:113:LYS:HA	2:D:116:HIS:CD2	2.42	0.53
1:B:2080:GLU:O	1:B:2080:GLU:HG3	2.08	0.53
1:A:321:HIS:HD2	1:A:322:GLN:H	1.57	0.53
1:A:3090:ILE:HG12	1:A:3094:ARG:HG3	1.91	0.53
2:C:62:LEU:HG	2:C:86:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2468:VAL:HG12	1:A:2486:PHE:HB3	1.90	0.53
1:B:1598:ILE:HD11	1:B:1601:PRO:HB3	1.88	0.53
1:B:1550:LYS:O	1:B:1590:ARG:NH2	2.38	0.53
1:B:4391:CYS:HA	1:B:4401:CYS:HB2	1.90	0.53
1:A:1497:ASN:OD1	1:A:1499:THR:OG1	2.22	0.53
1:A:2484:SER:HB2	1:A:2510:PRO:HB2	1.90	0.53
1:A:1394:GLU:OE1	1:A:1407:ASN:ND2	2.35	0.53
1:A:4131:ASN:ND2	1:A:4385:CYS:HB2	2.20	0.53
1:A:3504:LEU:HG	1:A:3505:ARG:H	1.74	0.52
1:B:2903:HIS:CD2	1:B:2917:ASN:HD22	2.27	0.52
1:B:4314:ASN:OD1	1:B:4314:ASN:N	2.41	0.52
1:A:2954:GLN:HG2	1:A:2969:PRO:HA	1.91	0.52
1:B:3238:ARG:NH2	1:B:3464:GLN:O	2.43	0.52
1:A:2601:VAL:HB	1:A:2606:ILE:HG22	1.90	0.52
1:A:4024:ARG:N	1:A:4031:GLU:O	2.41	0.52
1:A:4228:GLU:O	1:A:4266:ARG:NH2	2.29	0.52
1:A:1004:LYS:HD2	1:A:1015:ASP:HB2	1.92	0.52
1:B:2697:THR:HG23	1:B:2699:THR:H	1.74	0.52
1:A:3564:ASP:OD2	1:A:3582:ASP:HB2	2.09	0.52
1:A:2194:ARG:HG3	1:A:2210:TYR:CZ	2.45	0.52
1:B:1543:HIS:HB3	1:B:1729:PRO:HG3	1.91	0.52
1:B:3371:ALA:HB3	1:B:3384:ALA:HB3	1.92	0.52
1:A:616:THR:HG23	1:A:647:VAL:CG2	2.39	0.52
1:A:1416:CYS:SG	1:A:1420:TYR:HB2	2.50	0.52
1:B:3978:GLU:OE1	1:B:3978:GLU:N	2.43	0.52
1:B:4299:GLN:NE2	1:B:4307:LYS:HG3	2.25	0.52
1:A:359:GLN:HE21	1:A:566:VAL:HG21	1.73	0.52
1:B:963:ASP:HB3	1:B:966:LEU:HD23	1.92	0.52
1:B:3915:SER:HA	1:B:3918:LYS:HG3	1.92	0.52
1:A:2797:LEU:O	1:A:2798:SER:HB3	2.11	0.51
1:B:807:VAL:HG13	1:B:821:ILE:HB	1.93	0.51
1:B:2468:VAL:HG23	1:B:2486:PHE:HB3	1.92	0.51
1:A:3597:GLU:OE1	1:A:3597:GLU:N	2.37	0.51
1:A:3886:GLU:HG3	1:A:3888:PRO:HD2	1.91	0.51
1:A:3135:PHE:CD1	1:A:3135:PHE:C	2.88	0.51
1:A:1980:GLN:O	1:A:1981:TYR:HB2	2.10	0.51
1:A:4274:MET:HE1	1:A:4297:TRP:CE2	2.46	0.51
1:B:735:VAL:HG11	1:B:756:TYR:CZ	2.45	0.51
1:B:825:ASN:O	1:B:826:ASN:ND2	2.43	0.51
1:A:1802:ILE:HG23	1:A:1815:PHE:HB3	1.93	0.51
1:A:2955:PHE:HB2	1:A:2970:GLN:HE22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3246:ILE:HG12	1:B:3253:ILE:HG12	1.92	0.51
1:B:3671:ASP:OD1	1:B:3672:GLU:N	2.43	0.51
2:D:64:GLN:HG2	2:D:68:LYS:HD2	1.92	0.51
1:B:1081:PRO:HD2	1:B:1084:TRP:CE3	2.45	0.51
1:B:1574:TRP:CD2	5:P:3:LEU:HD13	2.46	0.51
1:A:2960:SER:O	1:A:2961:ARG:NH2	2.43	0.51
1:A:3966:LEU:O	1:A:3970:ARG:NH1	2.44	0.51
1:B:2210:TYR:CB	1:B:2236:THR:HA	2.41	0.51
1:A:3015:ASP:HB2	1:A:3017:ARG:HH22	1.72	0.50
1:B:2441:ASN:OD1	1:B:2444:ARG:N	2.41	0.50
1:B:3039:PHE:N	1:B:3047:ILE:O	2.44	0.50
1:B:407:ASP:OD1	1:B:407:ASP:N	2.44	0.50
1:B:4299:GLN:HE21	1:B:4307:LYS:HG3	1.75	0.50
1:B:2932:ASP:HB2	1:B:2938:ASP:CG	2.35	0.50
1:A:2547:VAL:HG23	1:A:2551:LEU:HD11	1.93	0.50
1:B:3125:ASP:OD1	1:B:3125:ASP:N	2.45	0.50
1:B:3331:HIS:CE1	1:B:3333:GLN:HB3	2.46	0.50
1:A:422:ARG:HH11	1:A:1091:ASP:CG	2.20	0.50
1:A:624:MET:HE3	1:A:624:MET:HA	1.94	0.50
1:A:2441:ASN:HD21	1:A:2444:ARG:HD3	1.75	0.50
1:B:4234:ASN:HD21	1:B:4251:SER:HB3	1.77	0.50
1:A:471:LEU:HD11	1:A:480:LEU:HD21	1.94	0.50
1:A:1404:HIS:HB2	1:A:1415:ALA:HB3	1.93	0.50
1:B:4078:GLU:OE1	1:B:4078:GLU:HA	2.12	0.50
1:A:447:VAL:O	1:A:460:ILE:N	2.41	0.49
1:B:461:LEU:HB3	1:B:465:VAL:HG21	1.95	0.49
1:B:1363:HIS:ND1	1:B:1389:CYS:SG	2.86	0.49
1:A:436:ARG:NH2	1:A:451:ASP:OD1	2.43	0.49
1:A:460:ILE:HD12	1:A:496:GLU:HA	1.95	0.49
1:A:4079:TYR:HD2	1:A:4080:LEU:H	1.61	0.49
2:C:113:LYS:HG2	2:C:114:LEU:HD23	1.93	0.49
2:D:99:LEU:HB3	2:D:105:ASP:HB2	1.95	0.49
1:A:2519:ARG:NH1	1:A:2564:ASP:OD1	2.46	0.49
1:B:1140:ASP:OD1	1:B:1140:ASP:N	2.46	0.49
1:A:190:CYS:SG	1:A:191:GLY:N	2.86	0.49
1:A:953:ILE:HG23	1:A:956:VAL:HB	1.94	0.49
1:A:3849:PHE:HB3	1:A:3857:ILE:HG23	1.94	0.49
1:A:3863:CYS:O	1:A:3890:ARG:NH1	2.45	0.49
1:A:3128:CYS:SG	1:A:3129:THR:N	2.85	0.49
1:A:3616:ASP:N	1:A:3627:GLU:OE1	2.46	0.49
1:A:4055:PRO:HD2	10:I:1:NAG:H3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2480:ARG:NH2	1:B:2493:SER:OG	2.46	0.49
2:D:78:ARG:HG3	2:D:125:TYR:HD1	1.78	0.49
1:A:1907:ASP:HA	1:A:2035:LEU:HD13	1.94	0.49
1:A:4337:LYS:NZ	1:B:48:ASP:OD2	2.33	0.49
1:B:2268:GLU:HA	1:B:2268:GLU:OE1	2.13	0.49
1:B:4098:ILE:HG23	1:B:4384:ARG:HH11	1.76	0.49
1:B:4314:ASN:ND2	1:B:4316:TRP:HB2	2.28	0.49
1:A:1075:ARG:HD2	1:A:1094:ASP:CB	2.43	0.48
1:A:321:HIS:HD2	1:A:322:GLN:HG2	1.78	0.48
1:B:2194:ARG:HG3	1:B:2210:TYR:CZ	2.48	0.48
1:B:3333:GLN:HA	1:B:3467:MET:HE1	1.95	0.48
1:A:2511:ARG:NH2	1:A:2555:ASN:OD1	2.45	0.48
1:A:484:GLU:OE1	1:A:486:LYS:N	2.46	0.48
1:A:2210:TYR:OH	7:K:2:GLU:OE2	2.28	0.48
1:B:91:LYS:HD2	1:B:96:GLY:HA3	1.95	0.48
1:B:396:ILE:HG22	1:B:405:VAL:HG22	1.94	0.48
1:B:2969:PRO:HD2	1:B:2972:TRP:CD2	2.48	0.48
1:B:3671:ASP:OD1	1:B:3671:ASP:C	2.57	0.48
1:B:4043:THR:HG22	1:B:4044:HIS:H	1.77	0.48
1:A:494:ASN:OD1	1:A:495:LEU:N	2.47	0.48
1:B:2070:MET:HG2	1:B:2073:ALA:O	2.14	0.48
1:B:2234:ILE:HD11	1:B:2237:PRO:HG3	1.96	0.48
1:B:2921:ILE:HD11	1:B:2938:ASP:HB2	1.96	0.48
1:B:1903:SER:HB3	1:B:1914:LEU:HD11	1.95	0.48
1:B:2957:CYS:HB3	1:B:2984:LEU:HD11	1.96	0.48
1:A:1477:VAL:HG23	1:A:1478:THR:HG23	1.96	0.48
1:B:1514:MET:HG3	1:B:1556:ARG:O	2.14	0.48
1:B:793:ILE:HG21	1:B:971:ASN:OD1	2.14	0.47
1:B:3048:PRO:HD2	1:B:3051:PHE:CE1	2.49	0.47
1:A:197:LEU:H	1:A:197:LEU:HD22	1.79	0.47
1:B:3051:PHE:HB3	1:B:3058:ASP:OD2	2.14	0.47
1:A:98:ASP:OD1	1:A:98:ASP:N	2.42	0.47
1:B:788:LEU:HD13	1:B:799:TRP:HB3	1.95	0.47
1:B:1879:VAL:HB	1:B:1906:MET:HE3	1.95	0.47
1:A:1543:HIS:HB3	1:A:1729:PRO:HG3	1.95	0.47
1:A:1873:PHE:HB3	1:A:1891:HIS:HB2	1.96	0.47
1:A:4394:ASP:N	1:A:4400:LYS:HZ1	2.12	0.47
1:B:846:ARG:HB3	1:B:847:PRO:HD3	1.97	0.47
1:B:2984:LEU:O	1:B:2988:GLN:HG2	2.13	0.47
2:D:110:LYS:O	2:D:114:LEU:HD23	2.14	0.47
1:A:311:CYS:HB2	1:A:327:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3417:ILE:CD1	1:A:3422:VAL:HG12	2.45	0.47
1:B:699:ASP:OD2	1:B:702:ARG:NH2	2.47	0.47
1:B:1300:MET:HE3	1:B:1303:GLU:HG3	1.96	0.47
1:B:1596:GLU:O	1:B:1633:ARG:NH2	2.32	0.47
1:B:299:ASN:OD1	1:B:301:THR:OG1	2.31	0.47
1:B:1381:GLN:HB3	1:B:1392:ILE:HD11	1.96	0.47
1:B:4247:TYR:CD2	1:B:4258:ALA:HB2	2.49	0.47
1:A:2972:TRP:CH2	2:D:127:LEU:HD21	2.50	0.47
1:B:1188:CYS:HB2	1:B:1194:LYS:HE2	1.97	0.47
1:B:1412:PHE:O	1:B:1413:ARG:NH2	2.48	0.47
1:B:1616:MET:CE	1:B:1646:PRO:HB2	2.45	0.47
1:B:3758:PRO:HB2	1:B:3767:ARG:NH1	2.30	0.47
1:B:4068:LYS:HB2	1:B:4077:SER:OG	2.15	0.47
1:B:4070:ASN:HD22	1:B:4073:SER:HB2	1.79	0.47
1:B:2160:LEU:HB2	1:B:2177:ILE:HD11	1.96	0.47
1:A:521:GLY:C	1:A:542:MET:HG3	2.40	0.47
1:A:2519:ARG:HH21	1:A:2519:ARG:HG3	1.80	0.47
1:B:1785:GLU:OE2	1:B:2009:ARG:NH2	2.48	0.47
1:A:460:ILE:HG22	1:A:461:LEU:HG	1.97	0.46
1:A:484:GLU:OE1	1:A:485:THR:N	2.49	0.46
1:A:2602:TYR:HB2	1:A:2643:THR:HG21	1.96	0.46
1:B:34:ARG:NE	1:B:38:GLY:HA2	2.30	0.46
1:B:3553:ARG:NH2	1:B:3555:CYS:HB2	2.30	0.46
1:B:3758:PRO:HB2	1:B:3767:ARG:HH11	1.80	0.46
1:A:2747:PHE:CE1	1:B:1010:MET:HE1	2.50	0.46
1:A:3930:CYS:N	1:A:3942:CYS:SG	2.89	0.46
1:A:4080:LEU:HD21	1:A:4083:GLU:HG3	1.96	0.46
1:A:3949:CYS:HA	1:A:3961:GLU:HG3	1.97	0.46
1:A:4022:SER:O	1:A:4032:CYS:HB2	2.15	0.46
1:A:4142:TYR:HB3	1:B:3793:ARG:HB2	1.96	0.46
1:A:4301:LYS:HE3	1:A:4302:PHE:CZ	2.51	0.46
1:B:1907:ASP:HA	1:B:2035:LEU:HD13	1.97	0.46
1:B:3102:CYS:HB3	1:B:3104:ASP:OD1	2.16	0.46
1:A:3146:MET:HE1	1:A:3151:SER:HB3	1.97	0.46
1:B:1734:LEU:HD12	1:B:1734:LEU:HA	1.82	0.46
1:A:982:ASP:OD2	1:B:2757:TYR:OH	2.31	0.46
1:A:2703:GLN:HE21	1:A:2704:LEU:HG	1.80	0.46
1:A:3759:ARG:HH22	1:A:3765:GLU:CD	2.24	0.46
1:A:735:VAL:HG11	1:A:756:TYR:CZ	2.51	0.46
1:A:1476:SER:HB3	1:A:1698:GLN:HG3	1.97	0.46
1:A:2573:LEU:HB3	1:A:2575:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3721:CYS:HB3	1:A:3726:ASP:HB2	1.98	0.46
1:B:1409:ARG:HG3	1:B:1410:GLY:N	2.30	0.46
1:B:2419:ALA:O	1:B:2438:GLN:NE2	2.45	0.46
1:A:465:VAL:O	1:A:468:PRO:HD3	2.15	0.46
1:A:2286:VAL:HG22	1:A:2291:ILE:HG22	1.97	0.46
1:B:33:PHE:CD2	1:B:46:ARG:HG3	2.51	0.46
1:B:3041:CYS:SG	1:B:3045:ARG:HB2	2.56	0.46
1:A:316:CYS:HB3	1:A:343:ARG:HA	1.98	0.45
1:A:3280:ASP:OD2	1:A:3283:SER:N	2.36	0.45
1:A:3449:THR:OG1	1:A:3451:HIS:O	2.34	0.45
1:B:844:TRP:HB2	1:B:870:TRP:HA	1.98	0.45
1:B:1596:GLU:HA	1:B:1596:GLU:OE1	2.16	0.45
1:B:3417:ILE:CD1	1:B:3422:VAL:HG12	2.46	0.45
1:A:1734:LEU:HD11	1:A:1738:SER:HA	1.98	0.45
1:A:2685:TYR:CE2	1:A:2687:ALA:HB2	2.51	0.45
1:A:3125:ASP:HB2	1:A:3151:SER:HA	1.98	0.45
1:B:4018:ILE:HG22	1:B:4019:CYS:SG	2.56	0.45
1:B:4065:ARG:HD2	1:B:4067:ARG:HD3	1.98	0.45
1:A:3984:LEU:HB3	1:A:3988:GLY:N	2.32	0.45
1:B:1788:ASP:OD2	1:B:2013:ARG:HA	2.16	0.45
1:A:1847:GLU:HB3	1:A:1860:THR:HA	1.99	0.45
1:A:2210:TYR:HB2	1:A:2236:THR:HA	1.98	0.45
1:A:2613:THR:O	1:A:2615:LYS:N	2.50	0.45
1:B:2253:ASP:HB3	1:B:2258:LEU:HD23	1.99	0.45
1:B:757:SER:HB3	1:B:788:LEU:HD21	1.98	0.45
2:D:311:VAL:HA	2:D:314:ILE:HD12	1.97	0.45
1:A:1837:TYR:CZ	1:A:1906:MET:HG2	2.52	0.45
1:B:318:TYR:CD2	1:B:319:GLN:HG2	2.52	0.45
1:B:2797:LEU:O	1:B:2800:VAL:HG22	2.17	0.45
1:B:4119:ARG:HH11	1:B:4173:LEU:C	2.23	0.45
1:B:4384:ARG:HD3	1:B:4411:TYR:CE2	2.52	0.45
1:A:1075:ARG:HD2	1:A:1094:ASP:HB2	1.98	0.45
1:A:1408:MET:HE3	1:A:1408:MET:HB2	1.68	0.45
1:B:266:TYR:HB3	1:B:267:PRO:HD2	1.99	0.45
1:A:321:HIS:CD2	1:A:322:GLN:HG2	2.53	0.45
1:A:1106:THR:HG22	1:A:1107:SER:H	1.81	0.45
1:B:2592:THR:HG22	1:B:2592:THR:O	2.16	0.45
1:B:4295:GLU:HG2	1:B:4309:LYS:HE2	1.99	0.45
2:D:85:ASP:HB3	2:D:121:ILE:HD11	1.99	0.45
1:A:1539:ILE:HD12	1:A:1539:ILE:HA	1.86	0.44
1:B:440:THR:HB	1:B:468:PRO:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1091:ASP:OD1	1:B:1091:ASP:N	2.50	0.44
1:B:2506:ARG:HH21	1:B:2506:ARG:HB3	1.81	0.44
1:B:3916:ASP:OD1	1:B:3916:ASP:N	2.50	0.44
2:C:58:ARG:N	2:C:90:GLU:OE1	2.50	0.44
1:A:89:GLU:N	1:A:99:GLU:OE1	2.50	0.44
1:A:461:LEU:HB3	1:A:465:VAL:HG21	2.00	0.44
1:A:910:ASP:HB3	1:A:946:MET:HE3	1.99	0.44
1:A:1368:GLY:H	1:A:1372:ALA:HA	1.82	0.44
1:A:3562:CYS:SG	1:A:3566:ASN:HB2	2.57	0.44
1:B:4079:TYR:CG	1:B:4080:LEU:N	2.85	0.44
1:A:1484:SER:HB3	1:A:1515:ILE:HD11	1.99	0.44
1:A:2406:PRO:HG2	1:A:2618:ARG:HH11	1.82	0.44
1:A:2489:GLN:NE2	1:A:2508:SER:O	2.49	0.44
1:A:3146:MET:HG2	1:A:3147:SER:N	2.32	0.44
1:B:474:ASP:HB3	1:B:479:LYS:HB2	1.99	0.44
2:D:118:LEU:O	2:D:122:LEU:HG	2.18	0.44
1:A:687:ARG:HH22	2:C:275:LYS:HE3	1.82	0.44
1:A:985:HIS:CE1	1:A:1003:MET:HE1	2.53	0.44
1:A:3228:LEU:HD13	1:A:3231:VAL:HG21	2.00	0.44
1:B:4100:LEU:HD23	1:B:4123:PRO:HA	1.99	0.44
2:D:273:THR:HG22	2:D:275:LYS:H	1.82	0.44
1:A:3115:GLU:HB2	1:A:3135:PHE:HD2	1.81	0.44
1:A:98:ASP:HA	1:A:102:ASN:ND2	2.33	0.44
1:A:1109:THR:HG23	1:A:1109:THR:O	2.17	0.44
1:B:3223:LEU:HD11	1:B:3226:GLN:HB3	1.99	0.44
1:B:4019:CYS:HB3	1:B:4032:CYS:HB3	1.94	0.44
1:A:3626:ASP:OD1	1:A:3626:ASP:N	2.51	0.44
1:A:3887:SER:N	1:A:3888:PRO:HD2	2.33	0.44
2:D:66:TRP:CZ2	2:D:70:LYS:NZ	2.84	0.44
1:B:308:MET:HG3	1:B:322:GLN:HB3	2.00	0.44
1:B:2962:PRO:N	1:B:2963:PRO:HD2	2.32	0.44
1:B:3626:ASP:OD1	1:B:3626:ASP:N	2.50	0.44
1:B:3962:THR:N	1:B:3990:ILE:HD11	2.32	0.44
1:B:270:TRP:CH2	1:B:272:CYS:HA	2.53	0.43
1:B:1972:SER:HA	1:B:1989:LYS:HD2	2.00	0.43
1:B:2286:VAL:HG22	1:B:2291:ILE:HG22	2.00	0.43
1:A:718:VAL:HB	1:A:735:VAL:HB	2.00	0.43
1:A:2787:PHE:CZ	1:A:2814:ASP:HA	2.53	0.43
1:A:4394:ASP:CG	1:A:4400:LYS:HZ2	2.26	0.43
1:A:3081:GLN:HB3	1:A:3089:CYS:SG	2.58	0.43
1:B:1616:MET:HE3	1:B:1646:PRO:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:76:PRO:HA	2:C:79:LEU:HB3	2.01	0.43
2:C:82:LEU:HD13	2:C:125:TYR:CE2	2.53	0.43
1:A:626:ALA:HB1	1:A:631:GLU:HG2	2.00	0.43
1:B:3012:PHE:HB3	1:B:3019:ASP:CG	2.43	0.43
2:C:316:ASP:HB3	2:C:319:HIS:HB2	2.00	0.43
1:A:364:ARG:O	1:A:367:ARG:HD3	2.19	0.43
1:A:1616:MET:HG2	1:A:1623:ILE:HG12	2.00	0.43
1:B:1873:PHE:HB3	1:B:1891:HIS:HB2	1.99	0.43
1:B:2507:VAL:HG21	1:B:2524:TRP:NE1	2.30	0.43
1:B:2773:GLU:HA	1:B:2776:CYS:SG	2.59	0.43
1:A:188:PHE:O	1:A:196:ILE:N	2.52	0.43
1:A:780:ASN:OD1	1:A:781:ARG:HG2	2.19	0.43
1:A:1734:LEU:CD1	1:A:1738:SER:HA	2.49	0.43
1:A:3793:ARG:NH1	1:B:4142:TYR:O	2.52	0.43
1:A:4273:ALA:C	1:A:4274:MET:HG3	2.44	0.43
1:B:1564:MET:HE1	1:B:1702:ARG:NE	2.34	0.43
1:B:2484:SER:HB2	1:B:2510:PRO:HG2	2.01	0.43
1:B:2561:LEU:HD12	1:B:2561:LEU:HA	1.87	0.43
1:B:3037:ASN:O	1:B:3049:ARG:HG2	2.18	0.43
1:B:3225:LEU:HD23	1:B:3228:LEU:HD11	2.01	0.43
1:B:3255:ARG:NE	1:B:3264:GLU:OE2	2.36	0.43
1:B:3857:ILE:HD12	1:B:3857:ILE:O	2.17	0.43
2:D:96:TRP:HE3	2:D:110:LYS:HB3	1.84	0.43
1:A:1186:LEU:HD12	1:A:1186:LEU:O	2.19	0.43
1:A:2636:THR:HG22	1:A:2637:GLN:N	2.33	0.43
1:A:2787:PHE:O	1:A:2788:THR:OG1	2.29	0.43
1:B:1265:THR:HG21	1:B:3177:ILE:HD11	2.00	0.43
1:B:1475:ASP:CG	1:B:1522:ARG:HH12	2.27	0.43
1:B:3610:PRO:HG2	1:B:3613:TRP:CD2	2.54	0.43
2:C:95:ASN:C	2:C:95:ASN:OD1	2.61	0.43
2:C:97:LYS:O	2:C:100:LYS:N	2.50	0.43
1:A:1623:ILE:HD12	1:A:1637:ILE:HD12	2.00	0.43
1:B:451:ASP:HB3	1:B:454:GLY:O	2.19	0.43
2:C:59:MET:SD	2:C:60:GLU:N	2.91	0.43
1:A:3722:HIS:CG	1:A:3723:PRO:HD2	2.54	0.43
1:B:461:LEU:HD11	1:B:493:VAL:HG11	2.00	0.43
1:A:3980:ASN:OD1	17:A:4710:NAG:N2	2.52	0.43
1:B:2401:SER:HB2	1:B:2413:PHE:CZ	2.54	0.43
1:B:2939:GLU:HG2	1:B:2940:ASP:N	2.33	0.43
1:B:3016:ARG:HB2	1:B:3016:ARG:NH2	2.33	0.43
2:D:80:ALA:O	2:D:83:HIS:ND1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:303:ILE:HD13	2:D:303:ILE:HA	1.95	0.43
1:A:865:ASN:N	1:A:865:ASN:OD1	2.50	0.42
1:A:1667:MET:HE2	1:A:1667:MET:HB3	1.82	0.42
1:A:2578:ARG:HD2	1:A:2589:VAL:HG22	2.00	0.42
1:B:2960:SER:HB3	1:B:2964:ASN:HB3	2.01	0.42
1:B:3904:LEU:HD12	1:B:3916:ASP:HA	2.00	0.42
1:A:2428:ASP:HB3	1:A:2433:ARG:HG2	2.01	0.42
1:B:2546:ILE:HD12	1:B:2582:THR:HA	2.01	0.42
1:A:865:ASN:HD22	11:U:1:NAG:C7	2.32	0.42
1:A:1050:CYS:C	1:A:1052:ASP:H	2.27	0.42
1:A:1838:TYR:CZ	1:A:1847:GLU:HG3	2.54	0.42
1:A:2259:ILE:HB	1:A:2273:ARG:HB2	2.01	0.42
1:A:3052:VAL:HG12	1:A:3053:CYS:SG	2.59	0.42
1:B:1189:THR:OG1	1:B:1190:SER:N	2.52	0.42
1:B:4065:ARG:HD3	1:B:4081:GLU:OE2	2.19	0.42
1:A:2810:ASN:HB2	17:A:4707:NAG:O5	2.19	0.42
1:B:740:SER:HB2	1:B:742:PHE:CE2	2.55	0.42
2:D:96:TRP:CH2	2:D:111:GLU:HB2	2.54	0.42
1:B:1906:MET:SD	1:B:2036:PRO:HG2	2.59	0.42
1:B:4284:ASP:HA	1:B:4301:LYS:HE2	2.01	0.42
2:C:96:TRP:HA	2:C:110:LYS:NZ	2.35	0.42
1:B:1886:LEU:N	1:B:1904:ALA:O	2.45	0.42
1:B:2235:VAL:HG12	1:B:2236:THR:HG23	2.02	0.42
1:B:2699:THR:O	1:B:2700:ARG:HD3	2.20	0.42
1:B:2914:GLN:HA	1:B:2920:CYS:HB3	2.02	0.42
2:C:97:LYS:O	2:C:97:LYS:HD2	2.20	0.42
2:D:262:ASP:OD1	2:D:263:LEU:N	2.53	0.42
1:A:376:TYR:HB3	1:A:384:CYS:HB3	2.02	0.42
1:A:3015:ASP:HB2	1:A:3017:ARG:CZ	2.46	0.42
1:B:2668:ALA:HB2	1:B:2677:GLN:HE22	1.84	0.42
1:A:2242:MET:HE2	1:A:2242:MET:HB2	1.80	0.42
1:A:3275:GLU:OE1	1:A:3326:ARG:NE	2.45	0.42
1:A:3997:PHE:HB3	1:A:4007:CYS:HB3	2.02	0.42
1:B:431:HIS:CD2	1:B:434:LYS:H	2.33	0.42
1:B:2517:PRO:HA	1:B:2538:LEU:HD11	2.01	0.42
1:B:4061:PRO:HD2	1:B:4319:GLN:O	2.20	0.42
2:D:324:LYS:O	2:D:328:VAL:HG13	2.20	0.42
1:B:445:GLU:OE2	1:B:738:SER:OG	2.28	0.42
1:B:4213:GLU:HG2	1:B:4224:VAL:HG12	2.02	0.42
1:B:4234:ASN:HD21	1:B:4251:SER:CB	2.32	0.42
1:A:361:CYS:SG	1:A:362:GLU:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4076:PHE:HZ	1:A:4311:LEU:HD13	1.85	0.41
1:B:2538:LEU:HD12	1:B:2669:PRO:O	2.20	0.41
1:B:2701:CYS:SG	1:B:2705:GLN:HB2	2.60	0.41
1:B:3245:TRP:CE2	1:B:3254:GLU:HB2	2.55	0.41
1:B:3981:CYS:HA	1:B:3991:CYS:HA	2.00	0.41
2:C:82:LEU:HD22	2:C:125:TYR:CD1	2.55	0.41
1:A:1081:PRO:HD2	1:A:1084:TRP:CE3	2.55	0.41
1:A:2206:PHE:CE1	1:A:2242:MET:HE1	2.55	0.41
1:A:3256:MET:HE2	1:A:3260:LYS:HA	2.02	0.41
1:A:4121:TYR:CD2	1:A:4382:PRO:HB3	2.55	0.41
1:B:72:PHE:CD1	1:B:72:PHE:C	2.97	0.41
1:B:3998:LYS:O	1:B:4008:GLN:HG3	2.19	0.41
1:A:1401:CYS:HB3	1:A:1414:CYS:HB3	1.98	0.41
1:A:3609:ILE:HD12	1:A:3609:ILE:O	2.18	0.41
1:B:3205:PHE:HA	1:B:3455:ASP:O	2.21	0.41
1:A:882:ARG:HE	1:A:895:HIS:CD2	2.32	0.41
1:A:896:SER:OG	1:A:901:LEU:O	2.23	0.41
1:A:2350:SER:O	1:A:2350:SER:OG	2.34	0.41
1:A:3736:PRO:HD2	1:A:3739:TRP:CE3	2.55	0.41
1:B:3601:TRP:CD2	1:B:3614:GLN:NE2	2.89	0.41
1:A:357:CYS:HB3	1:A:370:CYS:HB3	1.89	0.41
1:A:398:SER:HB3	1:A:645:HIS:O	2.20	0.41
1:A:1642:VAL:HA	1:B:2592:THR:HG21	2.02	0.41
1:A:3135:PHE:C	1:A:3135:PHE:HD1	2.27	0.41
1:B:1675:GLY:HA3	9:t:1:NAG:H83	2.03	0.41
1:B:4314:ASN:HD22	1:B:4316:TRP:HB2	1.84	0.41
1:A:88:ASP:N	1:A:99:GLU:OE1	2.50	0.41
1:A:631:GLU:OE1	1:A:633:ASN:N	2.49	0.41
1:A:933:GLY:O	1:A:953:ILE:HG22	2.20	0.41
1:A:2530:ASN:O	1:A:2530:ASN:CG	2.63	0.41
1:B:2155:TRP:CH2	1:B:2200:PRO:HD2	2.55	0.41
1:B:2428:ASP:HB2	1:B:2435:PHE:HE2	1.85	0.41
1:A:2696:ASP:HA	1:A:2700:ARG:HH12	1.86	0.41
1:B:1975:TYR:CE2	1:B:1986:ARG:HD3	2.56	0.41
2:C:97:LYS:HD2	2:C:100:LYS:HB2	2.03	0.41
1:A:401:ARG:O	1:A:419:SER:OG	2.37	0.41
1:A:3672:GLU:O	1:A:3675:THR:HG22	2.21	0.41
1:A:3860:PHE:CE1	1:A:3861:TRP:CD1	3.09	0.41
1:B:476:ILE:HG22	1:B:660:ASN:HB3	2.02	0.41
1:B:1134:ASP:OD1	1:B:1134:ASP:N	2.54	0.41
1:B:2552:VAL:HB	1:B:2572:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2841:PHE:C	1:B:2842:LEU:HD22	2.46	0.41
1:B:4413:GLU:OE1	1:B:4413:GLU:N	2.54	0.41
2:C:100:LYS:NZ	2:C:105:ASP:HB3	2.36	0.41
1:A:3417:ILE:HD13	1:A:3422:VAL:HG12	2.03	0.41
1:A:4019:CYS:SG	1:A:4020:PRO:HD2	2.60	0.41
1:B:54:LEU:HD13	1:B:54:LEU:HA	1.95	0.41
1:B:4232:TRP:N	1:B:4232:TRP:CD1	2.88	0.41
2:C:283:GLU:CD	2:C:344:HIS:HE2	2.27	0.41
1:A:2618:ARG:O	1:A:2627:LEU:HA	2.21	0.40
1:A:2709:LEU:HD12	1:A:2730:SER:HB2	2.03	0.40
1:A:2970:GLN:NE2	1:A:2973:VAL:HG21	2.35	0.40
1:A:3479:SER:HG	1:A:3480:HIS:CE1	2.34	0.40
1:A:3984:LEU:HD13	1:A:3987:GLY:CA	2.52	0.40
1:B:2066:MET:HG2	1:B:2077:PHE:O	2.20	0.40
1:B:2142:GLY:O	1:B:2164:ASN:ND2	2.54	0.40
1:B:3970:ARG:CZ	1:B:3976:ILE:HD13	2.51	0.40
2:D:283:GLU:OE2	2:D:344:HIS:NE2	2.40	0.40
10:u:1:NAG:H61	10:u:2:NAG:H82	2.02	0.40
14:6:1:NAG:HO4	14:6:2:NAG:HN2	1.63	0.40
1:B:856:ASP:C	1:B:856:ASP:OD1	2.64	0.40
1:B:1401:CYS:HB3	1:B:1405:CYS:HB2	2.04	0.40
1:B:2243:ASP:OD2	1:B:2246:THR:OG1	2.31	0.40
1:B:3246:ILE:HD11	1:B:3277:LEU:HB3	2.04	0.40
1:B:3934:GLU:HA	1:B:3944:SER:HA	2.02	0.40
1:B:4413:GLU:HG2	1:B:4414:VAL:HG13	2.03	0.40
2:C:97:LYS:HA	2:C:100:LYS:HG2	2.04	0.40
1:A:359:GLN:OE1	1:A:384:CYS:HB2	2.20	0.40
1:A:1425:ASP:OD1	1:A:1425:ASP:C	2.63	0.40
1:A:4401:CYS:HB2	1:A:4411:TYR:HA	2.03	0.40
1:B:72:PHE:C	1:B:72:PHE:HD1	2.29	0.40
1:B:2071:LEU:HB2	1:B:2072:PRO:HD3	2.02	0.40
1:B:4057:LEU:HD12	1:B:4323:PHE:HD2	1.87	0.40
1:A:2993:ARG:HD2	1:A:2993:ARG:C	2.46	0.40
1:A:3553:ARG:NH1	1:A:3559:GLN:O	2.53	0.40
1:A:4314:ASN:CG	1:B:4314:ASN:HB3	2.46	0.40
1:B:447:VAL:HG23	1:B:465:VAL:HG11	2.03	0.40
1:B:4273:ALA:O	1:B:4274:MET:HG2	2.21	0.40
1:A:1173:LYS:CD	1:A:1178:GLY:HA2	2.47	0.40
1:A:3015:ASP:H	1:A:3026:GLU:CD	2.30	0.40
1:B:4057:LEU:HB2	1:B:4323:PHE:HB3	2.03	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%)	3983 (92%)	319 (7%)	2 (0%)	100	100
1	B	4304/4660 (92%)	3994 (93%)	308 (7%)	2 (0%)	100	100
2	C	173/360 (48%)	170 (98%)	3 (2%)	0	100	100
2	D	173/360 (48%)	171 (99%)	2 (1%)	0	100	100
4	H	1/5 (20%)	1 (100%)	0	0	100	100
4	O	1/5 (20%)	1 (100%)	0	0	100	100
5	I	1/6 (17%)	1 (100%)	0	0	100	100
5	P	1/6 (17%)	1 (100%)	0	0	100	100
6	J	1/3 (33%)	0	1 (100%)	0	100	100
6	Q	1/3 (33%)	1 (100%)	0	0	100	100
7	K	2/5 (40%)	0	2 (100%)	0	100	100
7	R	2/5 (40%)	2 (100%)	0	0	100	100
8	L	1/5 (20%)	0	1 (100%)	0	100	100
8	M	1/5 (20%)	1 (100%)	0	0	100	100
8	S	1/5 (20%)	0	1 (100%)	0	100	100
8	T	1/5 (20%)	1 (100%)	0	0	100	100
All	All	8968/10098 (89%)	8327 (93%)	637 (7%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3791/4089 (93%)	3709 (98%)	82 (2%)	45	64
1	B	3790/4089 (93%)	3727 (98%)	63 (2%)	53	67
2	C	163/326 (50%)	159 (98%)	4 (2%)	42	62
2	D	163/326 (50%)	161 (99%)	2 (1%)	63	73
4	H	1/1 (100%)	1 (100%)	0	100	100
4	O	1/1 (100%)	1 (100%)	0	100	100
5	I	1/1 (100%)	1 (100%)	0	100	100
5	P	1/1 (100%)	0	1 (100%)	0	0
6	J	1/1 (100%)	1 (100%)	0	100	100
6	Q	1/1 (100%)	1 (100%)	0	100	100
7	K	2/2 (100%)	2 (100%)	0	100	100
7	R	2/2 (100%)	2 (100%)	0	100	100
8	L	1/1 (100%)	1 (100%)	0	100	100
8	M	1/1 (100%)	1 (100%)	0	100	100
8	S	1/1 (100%)	1 (100%)	0	100	100
8	T	1/1 (100%)	1 (100%)	0	100	100
All	All	7921/8844 (90%)	7769 (98%)	152 (2%)	49	66

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ASP
1	A	197	LEU
1	A	221	THR
1	A	248	GLN
1	A	259	ASN
1	A	329	CYS
1	A	516	LEU
1	A	552	THR

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Mol	Chain	Res	Type
1	A	593	VAL
1	A	631	GLU
1	A	711	LEU
1	A	725	LEU
1	A	772	THR
1	A	856	ASP
1	A	887	ASP
1	A	918	LEU
1	A	996	VAL
1	A	1093	LEU
1	A	1186	LEU
1	A	1343	THR
1	A	1408	MET
1	A	1472	LEU
1	A	1594	VAL
1	A	1613	ILE
1	A	1636	VAL
1	A	1656	VAL
1	A	1745	ASP
1	A	1752	VAL
1	A	1877	ILE
1	A	2088	MET
1	A	2170	THR
1	A	2174	VAL
1	A	2210	TYR
1	A	2230	VAL
1	A	2394	SER
1	A	2507	VAL
1	A	2565	LEU
1	A	2600	THR
1	A	2601	VAL
1	A	2633	ARG
1	A	2722	ASN
1	A	2835	ILE
1	A	2849	CYS
1	A	2856	ASN
1	A	2914	GLN
1	A	2919	ARG
1	A	2927	CYS
1	A	2938	ASP
1	A	2999	GLU
1	A	3047	ILE

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Mol	Chain	Res	Type
1	A	3096	CYS
1	A	3106	SER
1	A	3206	SER
1	A	3212	ARG
1	A	3215	THR
1	A	3220	SER
1	A	3277	LEU
1	A	3375	ASP
1	A	3378	ASN
1	A	3415	LEU
1	A	3449	THR
1	A	3450	THR
1	A	3509	LEU
1	A	3549	LEU
1	A	3757	VAL
1	A	3784	ASN
1	A	3793	ARG
1	A	3812	CYS
1	A	3826	LEU
1	A	3874	ASP
1	A	3922	CYS
1	A	3924	LYS
1	A	4032	CYS
1	A	4174	ASP
1	A	4201	MET
1	A	4217	MET
1	A	4236	LEU
1	A	4243	ASP
1	A	4284	ASP
1	A	4321	ARG
1	A	4366	THR
1	A	4377	VAL
1	B	54	LEU
1	B	58	ASP
1	B	247	CYS
1	B	278	CYS
1	B	335	HIS
1	B	359	GLN
1	B	365	GLN
1	B	505	THR
1	B	516	LEU
1	B	530	SER

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Mol	Chain	Res	Type
1	B	563	LEU
1	B	613	VAL
1	B	788	LEU
1	B	807	VAL
1	B	927	ILE
1	B	966	LEU
1	B	1004	LYS
1	B	1028	LEU
1	B	1074	VAL
1	B	1163	ILE
1	B	1201	CYS
1	B	1250	GLU
1	B	1271	THR
1	B	1382	LEU
1	B	1388	THR
1	B	1517	VAL
1	B	1550	LYS
1	B	1569	MET
1	B	1636	VAL
1	B	1650	THR
1	B	1666	VAL
1	B	1673	HIS
1	B	1728	CYS
1	B	1772	MET
1	B	1911	LEU
1	B	1936	TRP
1	B	2080	GLU
1	B	2081	LEU
1	B	2110	ILE
1	B	2174	VAL
1	B	2225	ASN
1	B	2430	ARG
1	B	2786	GLU
1	B	2807	CYS
1	B	2839	ARG
1	B	2869	GLU
1	B	2876	GLN
1	B	2984	LEU
1	B	3064	ASP
1	B	3145	LEU
1	B	3173	VAL
1	B	3426	ASP

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Mol	Chain	Res	Type
1	B	3467	MET
1	B	3500	GLN
1	B	3545	ASP
1	B	3568	THR
1	B	3635	ARG
1	B	3737	LEU
1	B	3793	ARG
1	B	3942	CYS
1	B	3962	THR
1	B	3971	THR
1	B	4274	MET
2	C	72	LEU
2	C	268	GLN
2	C	277	LEU
2	C	307	LYS
2	D	93	GLU
2	D	337	LEU
5	P	3	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	102	ASN
1	A	321	HIS
1	A	382	GLN
1	A	383	HIS
1	A	412	ASN
1	A	444	GLN
1	A	456	ASN
1	A	488	ASN
1	A	546	ASN
1	A	612	HIS
1	A	639	GLN
1	A	681	ASN
1	A	825	ASN
1	A	826	ASN
1	A	833	HIS
1	A	895	HIS
1	A	908	HIS
1	A	978	HIS
1	A	985	HIS

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Mol	Chain	Res	Type
1	A	992	ASN
1	A	1058	GLN
1	A	1089	GLN
1	A	1192	GLN
1	A	1254	HIS
1	A	1276	HIS
1	A	1283	ASN
1	A	1356	HIS
1	A	1496	GLN
1	A	1920	GLN
1	A	1921	HIS
1	A	1963	HIS
1	A	2333	HIS
1	A	2595	HIS
1	A	2651	GLN
1	A	2703	GLN
1	A	2722	ASN
1	A	2770	ASN
1	A	2831	GLN
1	A	2856	ASN
1	A	2906	ASN
1	A	2914	GLN
1	A	2924	ASN
1	A	2943	HIS
1	A	2964	ASN
1	A	3010	GLN
1	A	3035	HIS
1	A	3042	GLN
1	A	3066	GLN
1	A	3126	HIS
1	A	3262	ASN
1	A	3311	GLN
1	A	3451	HIS
1	A	3500	GLN
1	A	3523	ASN
1	A	3652	GLN
1	A	3878	HIS
1	A	3941	ASN
1	A	4011	ASN
1	A	4110	GLN
1	A	4206	GLN
1	A	4221	HIS

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Mol	Chain	Res	Type
1	A	4314	ASN
1	B	102	ASN
1	B	315	ASN
1	B	412	ASN
1	B	431	HIS
1	B	488	ASN
1	B	612	HIS
1	B	750	GLN
1	B	825	ASN
1	B	826	ASN
1	B	908	HIS
1	B	1058	GLN
1	B	1078	GLN
1	B	1083	GLN
1	B	1085	HIS
1	B	1281	ASN
1	B	1312	HIS
1	B	1458	ASN
1	B	1635	GLN
1	B	1921	HIS
1	B	1959	HIS
1	B	1980	GLN
1	B	2297	ASN
1	B	2303	GLN
1	B	2344	ASN
1	B	2378	ASN
1	B	2414	GLN
1	B	2431	ASN
1	B	2500	ASN
1	B	2677	GLN
1	B	2710	ASN
1	B	2805	ASN
1	B	2808	HIS
1	B	2831	GLN
1	B	2917	ASN
1	B	3105	ASN
1	B	3251	GLN
1	B	3312	HIS
1	B	3331	HIS
1	B	3336	HIS
1	B	3378	ASN
1	B	3503	GLN

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Mol	Chain	Res	Type
1	B	3624	ASN
1	B	3631	HIS
1	B	3679	ASN
1	B	3697	GLN
1	B	3750	ASN
1	B	3755	ASN
1	B	3854	HIS
1	B	3903	GLN
1	B	3951	ASN
1	B	4008	GLN
1	B	4131	ASN
1	B	4206	GLN
1	B	4234	ASN
2	C	73	HIS
2	C	83	HIS
2	C	271	ASN
2	C	296	HIS
2	D	63	ASN
2	D	268	GLN
2	D	296	HIS
2	D	300	GLN
2	D	305	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

146 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	NAG	0	1	16,1	14,14,15	0.49	0	17,19,21	1.44	1 (5%)
16	NAG	0	2	16	14,14,15	0.38	0	17,19,21	1.43	3 (17%)
16	BMA	0	3	16	11,11,12	0.32	0	15,15,17	0.46	0
10	NAG	1	1	10,1	14,14,15	0.48	0	17,19,21	0.90	0
10	NAG	1	2	10	14,14,15	0.43	0	17,19,21	0.67	1 (5%)
10	BMA	1	3	10	11,11,12	0.27	0	15,15,17	0.80	1 (6%)
10	MAN	1	4	10	11,11,12	0.31	0	15,15,17	0.61	0
10	MAN	1	5	10	11,11,12	0.28	0	15,15,17	0.51	0
12	NAG	2	1	12,1	14,14,15	0.91	0	17,19,21	1.55	5 (29%)
12	NAG	2	2	12	14,14,15	1.20	2 (14%)	17,19,21	1.02	1 (5%)
12	BMA	2	3	12	11,11,12	1.06	1 (9%)	15,15,17	0.94	1 (6%)
12	NAG	3	1	12,1	14,14,15	0.44	0	17,19,21	0.55	0
12	NAG	3	2	12	14,14,15	0.50	0	17,19,21	0.58	0
12	BMA	3	3	12	11,11,12	0.80	0	15,15,17	0.80	1 (6%)
10	NAG	4	1	10,1	14,14,15	0.41	0	17,19,21	1.02	1 (5%)
10	NAG	4	2	10	14,14,15	0.47	0	17,19,21	1.08	1 (5%)
10	BMA	4	3	10	11,11,12	0.30	0	15,15,17	0.97	2 (13%)
10	MAN	4	4	10	11,11,12	0.30	0	15,15,17	0.44	0
10	MAN	4	5	10	11,11,12	0.34	0	15,15,17	0.42	0
10	NAG	5	1	10,1	14,14,15	0.51	0	17,19,21	0.92	1 (5%)
10	NAG	5	2	10	14,14,15	0.47	0	17,19,21	0.38	0
10	BMA	5	3	10	11,11,12	0.34	0	15,15,17	0.61	0
10	MAN	5	4	10	11,11,12	0.27	0	15,15,17	0.58	0
10	MAN	5	5	10	11,11,12	0.21	0	15,15,17	0.60	0
14	NAG	6	1	1,14	14,14,15	0.44	0	17,19,21	0.78	0
14	NAG	6	2	14	14,14,15	0.46	0	17,19,21	0.88	1 (5%)
14	BMA	6	3	14	11,11,12	0.38	0	15,15,17	0.98	0
14	MAN	6	4	14	11,11,12	0.27	0	15,15,17	0.83	1 (6%)
14	MAN	6	5	14	11,11,12	0.31	0	15,15,17	0.57	0
16	NAG	7	1	16,1	14,14,15	0.43	0	17,19,21	0.50	0
16	NAG	7	2	16	14,14,15	0.44	0	17,19,21	0.42	0
16	BMA	7	3	16	11,11,12	0.23	0	15,15,17	0.62	0
13	NAG	8	1	1,13	14,14,15	0.72	1 (7%)	17,19,21	1.38	2 (11%)
13	NAG	8	2	13	14,14,15	0.62	0	17,19,21	0.97	1 (5%)
10	NAG	9	1	10,1	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
10	NAG	9	2	10	14,14,15	0.40	0	17,19,21	0.47	0
10	BMA	9	3	10	11,11,12	0.28	0	15,15,17	0.61	0
10	MAN	9	4	10	11,11,12	0.28	0	15,15,17	0.60	0
10	MAN	9	5	10	11,11,12	0.26	0	15,15,17	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	E	1	9,1	14,14,15	0.40	0	17,19,21	1.02	1 (5%)
9	NAG	E	2	9	14,14,15	0.39	0	17,19,21	0.55	0
10	NAG	F	1	10,1	14,14,15	0.40	0	17,19,21	0.54	0
10	NAG	F	2	10	14,14,15	0.40	0	17,19,21	0.37	0
10	BMA	F	3	10	11,11,12	0.27	0	15,15,17	0.63	0
10	MAN	F	4	10	11,11,12	0.34	0	15,15,17	0.51	0
10	MAN	F	5	10	11,11,12	0.22	0	15,15,17	0.55	0
11	NAG	U	1	11,1	14,14,15	0.41	0	17,19,21	0.57	0
11	NAG	U	2	11	14,14,15	0.48	0	17,19,21	1.77	4 (23%)
11	BMA	U	3	11	11,11,12	0.59	0	15,15,17	0.85	0
11	MAN	U	4	11	11,11,12	0.31	0	15,15,17	0.65	0
11	MAN	U	5	11	11,11,12	0.37	0	15,15,17	0.74	1 (6%)
9	NAG	V	1	9,1	14,14,15	0.53	0	17,19,21	1.30	2 (11%)
9	NAG	V	2	9	14,14,15	0.55	0	17,19,21	0.89	1 (5%)
12	NAG	W	1	12,1	14,14,15	0.43	0	17,19,21	0.75	1 (5%)
12	NAG	W	2	12	14,14,15	0.41	0	17,19,21	0.86	1 (5%)
12	BMA	W	3	12	11,11,12	0.36	0	15,15,17	0.65	0
9	NAG	X	1	9,1	14,14,15	0.43	0	17,19,21	0.62	0
9	NAG	X	2	9	14,14,15	0.42	0	17,19,21	0.62	0
9	NAG	Y	1	9,1	14,14,15	0.40	0	17,19,21	0.42	0
9	NAG	Y	2	9	14,14,15	0.41	0	17,19,21	0.74	0
10	NAG	Z	1	10,1	14,14,15	0.46	0	17,19,21	1.34	1 (5%)
10	NAG	Z	2	10	14,14,15	0.39	0	17,19,21	1.21	3 (17%)
10	BMA	Z	3	10	11,11,12	0.33	0	15,15,17	0.64	1 (6%)
10	MAN	Z	4	10	11,11,12	0.28	0	15,15,17	0.43	0
10	MAN	Z	5	10	11,11,12	0.25	0	15,15,17	0.46	0
9	NAG	a	1	9,1	14,14,15	0.39	0	17,19,21	0.72	0
9	NAG	a	2	9	14,14,15	0.40	0	17,19,21	0.36	0
10	NAG	b	1	10,1	14,14,15	0.41	0	17,19,21	0.41	0
10	NAG	b	2	10	14,14,15	0.40	0	17,19,21	0.44	0
10	BMA	b	3	10	11,11,12	0.33	0	15,15,17	0.75	0
10	MAN	b	4	10	11,11,12	0.28	0	15,15,17	0.54	0
10	MAN	b	5	10	11,11,12	0.23	0	15,15,17	0.49	0
13	NAG	c	1	1,13	14,14,15	0.52	0	17,19,21	0.83	1 (5%)
13	NAG	c	2	13	14,14,15	0.56	0	17,19,21	1.10	1 (5%)
9	NAG	d	1	9,1	14,14,15	0.40	0	17,19,21	0.65	0
9	NAG	d	2	9	14,14,15	0.40	0	17,19,21	0.50	0
12	NAG	e	1	12,1	14,14,15	0.42	0	17,19,21	0.40	0
12	NAG	e	2	12	14,14,15	0.42	0	17,19,21	0.59	0
12	BMA	e	3	12	11,11,12	0.33	0	15,15,17	0.72	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	f	1	12,1	14,14,15	0.42	0	17,19,21	0.46	0
12	NAG	f	2	12	14,14,15	0.42	0	17,19,21	0.56	0
12	BMA	f	3	12	11,11,12	0.23	0	15,15,17	0.56	0
10	NAG	g	1	10,1	14,14,15	0.46	0	17,19,21	0.40	0
10	NAG	g	2	10	14,14,15	0.39	0	17,19,21	0.73	1 (5%)
10	BMA	g	3	10	11,11,12	0.41	0	15,15,17	0.73	0
10	MAN	g	4	10	11,11,12	0.30	0	15,15,17	0.47	0
10	MAN	g	5	10	11,11,12	0.28	0	15,15,17	0.58	0
12	NAG	h	1	12,1	14,14,15	0.41	0	17,19,21	0.71	0
12	NAG	h	2	12	14,14,15	0.44	0	17,19,21	0.51	0
12	BMA	h	3	12	11,11,12	0.30	0	15,15,17	0.51	0
12	NAG	i	1	12,1	14,14,15	0.48	0	17,19,21	0.82	0
12	NAG	i	2	12	14,14,15	0.49	0	17,19,21	0.97	2 (11%)
12	BMA	i	3	12	11,11,12	0.64	0	15,15,17	0.80	1 (6%)
10	NAG	j	1	10,1	14,14,15	0.39	0	17,19,21	1.32	3 (17%)
10	NAG	j	2	10	14,14,15	0.41	0	17,19,21	0.39	0
10	BMA	j	3	10	11,11,12	0.56	0	15,15,17	0.73	0
10	MAN	j	4	10	11,11,12	0.50	0	15,15,17	0.86	1 (6%)
10	MAN	j	5	10	11,11,12	0.38	0	15,15,17	0.61	0
10	NAG	k	1	10,1	14,14,15	0.46	0	17,19,21	0.90	1 (5%)
10	NAG	k	2	10	14,14,15	0.50	0	17,19,21	1.13	2 (11%)
10	BMA	k	3	10	11,11,12	0.26	0	15,15,17	0.61	0
10	MAN	k	4	10	11,11,12	0.32	0	15,15,17	0.85	2 (13%)
10	MAN	k	5	10	11,11,12	0.32	0	15,15,17	0.50	0
10	NAG	l	1	10,1	14,14,15	0.40	0	17,19,21	0.73	1 (5%)
10	NAG	l	2	10	14,14,15	0.44	0	17,19,21	0.37	0
10	BMA	l	3	10	11,11,12	0.33	0	15,15,17	1.10	2 (13%)
10	MAN	l	4	10	11,11,12	0.30	0	15,15,17	0.65	0
10	MAN	l	5	10	11,11,12	0.33	0	15,15,17	0.44	0
12	NAG	m	1	12,1	14,14,15	1.09	1 (7%)	17,19,21	1.21	1 (5%)
12	NAG	m	2	12	14,14,15	0.43	0	17,19,21	0.73	1 (5%)
12	BMA	m	3	12	11,11,12	0.29	0	15,15,17	0.56	0
9	NAG	n	1	9,1	14,14,15	0.54	0	17,19,21	1.07	1 (5%)
9	NAG	n	2	9	14,14,15	0.58	0	17,19,21	0.93	2 (11%)
13	NAG	o	1	1,13	14,14,15	0.41	0	17,19,21	0.84	0
13	NAG	o	2	13	14,14,15	0.41	0	17,19,21	0.42	0
12	NAG	p	1	12,1	14,14,15	0.42	0	17,19,21	0.73	0
12	NAG	p	2	12	14,14,15	0.40	0	17,19,21	0.86	1 (5%)
12	BMA	p	3	12	11,11,12	0.27	0	15,15,17	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	q	1	9,1	14,14,15	1.15	2 (14%)	17,19,21	1.12	1 (5%)
9	NAG	q	2	9	14,14,15	0.94	1 (7%)	17,19,21	1.08	1 (5%)
12	NAG	r	1	12,1	14,14,15	0.42	0	17,19,21	0.84	1 (5%)
12	NAG	r	2	12	14,14,15	0.41	0	17,19,21	0.57	0
12	BMA	r	3	12	11,11,12	0.31	0	15,15,17	0.61	0
9	NAG	s	1	9,1	14,14,15	0.46	0	17,19,21	1.06	3 (17%)
9	NAG	s	2	9	14,14,15	0.41	0	17,19,21	0.63	0
9	NAG	t	1	9,1	14,14,15	1.00	0	17,19,21	1.58	3 (17%)
9	NAG	t	2	9	14,14,15	1.11	1 (7%)	17,19,21	1.52	1 (5%)
10	NAG	u	1	10,1	14,14,15	0.50	0	17,19,21	0.59	0
10	NAG	u	2	10	14,14,15	0.45	0	17,19,21	0.72	0
10	BMA	u	3	10	11,11,12	0.42	0	15,15,17	0.64	0
10	MAN	u	4	10	11,11,12	0.24	0	15,15,17	0.49	0
10	MAN	u	5	10	11,11,12	0.26	0	15,15,17	0.53	0
9	NAG	v	1	9,1	14,14,15	0.45	0	17,19,21	0.51	0
9	NAG	v	2	9	14,14,15	0.40	0	17,19,21	0.41	0
14	NAG	w	1	1,14	14,14,15	0.53	0	17,19,21	1.20	2 (11%)
14	NAG	w	2	14	14,14,15	0.46	0	17,19,21	1.36	3 (17%)
14	BMA	w	3	14	11,11,12	0.42	0	15,15,17	0.58	0
14	MAN	w	4	14	11,11,12	0.29	0	15,15,17	0.47	0
14	MAN	w	5	14	11,11,12	0.27	0	15,15,17	0.51	0
9	NAG	x	1	9,1	14,14,15	0.53	0	17,19,21	0.85	0
9	NAG	x	2	9	14,14,15	0.41	0	17,19,21	0.73	0
9	NAG	y	1	9,1	14,14,15	0.42	0	17,19,21	0.72	1 (5%)
9	NAG	y	2	9	14,14,15	0.42	0	17,19,21	0.44	0
15	NAG	z	1	15,1	14,14,15	0.54	0	17,19,21	0.82	1 (5%)
15	NAG	z	2	15	14,14,15	0.39	0	17,19,21	1.34	2 (11%)
15	BMA	z	3	15	11,11,12	0.37	0	15,15,17	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	NAG	0	1	16,1	-	3/6/23/26	0/1/1/1
16	NAG	0	2	16	-	0/6/23/26	0/1/1/1
16	BMA	0	3	16	-	0/2/19/22	0/1/1/1
10	NAG	1	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	1	2	10	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	F	4	10	-	0/2/19/22	0/1/1/1
10	MAN	F	5	10	-	0/2/19/22	0/1/1/1
11	NAG	U	1	11,1	-	0/6/23/26	0/1/1/1
11	NAG	U	2	11	-	4/6/23/26	0/1/1/1
11	BMA	U	3	11	-	1/2/19/22	0/1/1/1
11	MAN	U	4	11	-	0/2/19/22	0/1/1/1
11	MAN	U	5	11	-	1/2/19/22	0/1/1/1
9	NAG	V	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	0/6/23/26	0/1/1/1
12	NAG	W	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	W	2	12	-	2/6/23/26	0/1/1/1
12	BMA	W	3	12	-	0/2/19/22	0/1/1/1
9	NAG	X	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	X	2	9	-	1/6/23/26	0/1/1/1
9	NAG	Y	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	3/6/23/26	0/1/1/1
10	NAG	Z	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	0/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	4	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	5	10	-	0/2/19/22	0/1/1/1
9	NAG	a	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	a	2	9	-	0/6/23/26	0/1/1/1
10	NAG	b	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	b	2	10	-	1/6/23/26	0/1/1/1
10	BMA	b	3	10	-	0/2/19/22	0/1/1/1
10	MAN	b	4	10	-	0/2/19/22	0/1/1/1
10	MAN	b	5	10	-	0/2/19/22	0/1/1/1
13	NAG	c	1	1,13	-	0/6/23/26	0/1/1/1
13	NAG	c	2	13	-	1/6/23/26	0/1/1/1
9	NAG	d	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	d	2	9	-	0/6/23/26	0/1/1/1
12	NAG	e	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	e	2	12	-	2/6/23/26	0/1/1/1
12	BMA	e	3	12	-	0/2/19/22	0/1/1/1
12	NAG	f	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	f	2	12	-	0/6/23/26	0/1/1/1
12	BMA	f	3	12	-	0/2/19/22	0/1/1/1
10	NAG	g	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	g	2	10	-	0/6/23/26	0/1/1/1
10	BMA	g	3	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	g	4	10	-	0/2/19/22	0/1/1/1
10	MAN	g	5	10	-	1/2/19/22	0/1/1/1
12	NAG	h	1	12,1	-	3/6/23/26	0/1/1/1
12	NAG	h	2	12	-	3/6/23/26	0/1/1/1
12	BMA	h	3	12	-	0/2/19/22	0/1/1/1
12	NAG	i	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	i	2	12	-	0/6/23/26	0/1/1/1
12	BMA	i	3	12	-	0/2/19/22	0/1/1/1
10	NAG	j	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	j	2	10	-	3/6/23/26	0/1/1/1
10	BMA	j	3	10	-	2/2/19/22	0/1/1/1
10	MAN	j	4	10	-	0/2/19/22	0/1/1/1
10	MAN	j	5	10	-	1/2/19/22	0/1/1/1
10	NAG	k	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	k	2	10	-	0/6/23/26	0/1/1/1
10	BMA	k	3	10	-	0/2/19/22	0/1/1/1
10	MAN	k	4	10	-	0/2/19/22	0/1/1/1
10	MAN	k	5	10	-	0/2/19/22	0/1/1/1
10	NAG	l	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	l	2	10	-	0/6/23/26	0/1/1/1
10	BMA	l	3	10	-	0/2/19/22	0/1/1/1
10	MAN	l	4	10	-	1/2/19/22	0/1/1/1
10	MAN	l	5	10	-	1/2/19/22	0/1/1/1
12	NAG	m	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	m	2	12	-	2/6/23/26	0/1/1/1
12	BMA	m	3	12	-	0/2/19/22	0/1/1/1
9	NAG	n	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	n	2	9	-	1/6/23/26	0/1/1/1
13	NAG	o	1	1,13	-	0/6/23/26	0/1/1/1
13	NAG	o	2	13	-	2/6/23/26	0/1/1/1
12	NAG	p	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	p	2	12	-	0/6/23/26	0/1/1/1
12	BMA	p	3	12	-	0/2/19/22	0/1/1/1
9	NAG	q	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	q	2	9	-	0/6/23/26	0/1/1/1
12	NAG	r	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	r	2	12	-	3/6/23/26	0/1/1/1
12	BMA	r	3	12	-	1/2/19/22	0/1/1/1
9	NAG	s	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	s	2	9	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	t	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	t	2	9	-	0/6/23/26	0/1/1/1
10	NAG	u	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	u	2	10	-	2/6/23/26	0/1/1/1
10	BMA	u	3	10	-	2/2/19/22	0/1/1/1
10	MAN	u	4	10	-	0/2/19/22	0/1/1/1
10	MAN	u	5	10	-	0/2/19/22	0/1/1/1
9	NAG	v	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	v	2	9	-	1/6/23/26	0/1/1/1
14	NAG	w	1	1,14	-	4/6/23/26	0/1/1/1
14	NAG	w	2	14	-	2/6/23/26	0/1/1/1
14	BMA	w	3	14	-	0/2/19/22	0/1/1/1
14	MAN	w	4	14	-	1/2/19/22	0/1/1/1
14	MAN	w	5	14	-	1/2/19/22	0/1/1/1
9	NAG	x	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	x	2	9	-	3/6/23/26	0/1/1/1
9	NAG	y	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	y	2	9	-	2/6/23/26	0/1/1/1
15	NAG	z	1	15,1	-	2/6/23/26	0/1/1/1
15	NAG	z	2	15	-	2/6/23/26	0/1/1/1
15	BMA	z	3	15	-	1/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	1	NAG	O5-C5	2.68	1.48	1.43
9	t	2	NAG	C1-C2	2.58	1.55	1.52
9	q	1	NAG	O5-C5	2.56	1.48	1.43
12	2	2	NAG	O5-C5	2.40	1.48	1.43
9	q	2	NAG	O5-C5	2.33	1.48	1.43
12	2	3	BMA	O5-C5	2.28	1.47	1.43
12	2	2	NAG	C1-C2	2.25	1.55	1.52
13	8	1	NAG	C1-C2	2.18	1.55	1.52
9	q	1	NAG	C1-C2	2.13	1.55	1.52

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	0	1	NAG	C1-O5-C5	5.07	118.98	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	t	2	NAG	C1-O5-C5	4.94	118.80	112.19
11	U	2	NAG	C4-C3-C2	4.72	117.93	111.02
9	t	1	NAG	C4-C3-C2	4.47	117.57	111.02
15	z	2	NAG	O5-C1-C2	-4.25	104.72	111.29
13	8	1	NAG	O5-C1-C2	4.08	117.60	111.29
10	Z	1	NAG	O5-C1-C2	-3.84	105.36	111.29
14	w	2	NAG	O5-C1-C2	-3.75	105.49	111.29
9	n	1	NAG	C1-C2-N2	3.63	116.16	110.43
10	Z	2	NAG	C1-O5-C5	3.55	116.95	112.19
16	0	2	NAG	O5-C1-C2	3.50	116.70	111.29
9	V	1	NAG	C1-O5-C5	3.42	116.77	112.19
9	E	1	NAG	O5-C1-C2	-3.39	106.04	111.29
14	w	1	NAG	C4-C3-C2	3.33	115.89	111.02
10	j	1	NAG	O5-C1-C2	-3.22	106.30	111.29
13	c	2	NAG	C1-O5-C5	3.12	116.37	112.19
11	U	2	NAG	C3-C4-C5	3.10	115.86	110.23
9	q	2	NAG	O5-C1-C2	-3.09	106.51	111.29
12	m	1	NAG	C1-O5-C5	2.98	116.18	112.19
9	t	1	NAG	C1-C2-N2	2.96	115.10	110.43
11	U	2	NAG	O5-C1-C2	-2.94	106.74	111.29
10	j	4	MAN	C1-O5-C5	2.94	116.12	112.19
9	V	2	NAG	C1-O5-C5	2.92	116.11	112.19
12	2	1	NAG	C3-C4-C5	2.89	115.47	110.23
9	q	1	NAG	C1-O5-C5	2.88	116.05	112.19
9	V	1	NAG	O5-C1-C2	2.88	115.75	111.29
10	4	1	NAG	C1-O5-C5	2.82	115.96	112.19
12	i	2	NAG	C1-O5-C5	2.79	115.92	112.19
10	k	1	NAG	C1-O5-C5	2.78	115.91	112.19
13	8	2	NAG	C1-C2-N2	2.76	114.79	110.43
12	2	3	BMA	C1-O5-C5	2.74	115.85	112.19
12	2	1	NAG	C1-C2-N2	2.66	114.62	110.43
16	0	2	NAG	O3-C3-C2	-2.65	103.89	109.40
10	4	2	NAG	C1-O5-C5	2.63	115.71	112.19
10	l	3	BMA	C1-C2-C3	2.62	113.46	109.64
12	i	3	BMA	C1-O5-C5	2.59	115.66	112.19
12	2	1	NAG	C4-C3-C2	2.51	114.69	111.02
13	8	1	NAG	C1-O5-C5	2.49	115.52	112.19
9	s	1	NAG	O5-C1-C2	2.49	115.14	111.29
10	4	3	BMA	C1-O5-C5	2.49	115.52	112.19
10	1	3	BMA	C1-C2-C3	2.47	113.24	109.64
10	5	1	NAG	C1-C2-N2	2.46	114.32	110.43
10	l	1	NAG	C1-O5-C5	2.46	115.49	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	2	1	NAG	C2-N2-C7	2.46	126.19	122.90
10	9	1	NAG	C1-C2-N2	2.45	114.30	110.43
12	p	2	NAG	C1-C2-N2	2.41	114.23	110.43
12	3	3	BMA	C1-O5-C5	2.35	115.34	112.19
9	t	1	NAG	O5-C1-C2	-2.34	107.67	111.29
15	z	2	NAG	C1-C2-N2	2.34	114.12	110.43
11	U	2	NAG	O3-C3-C2	-2.34	104.55	109.40
10	k	2	NAG	C1-O5-C5	2.34	115.32	112.19
10	j	1	NAG	C3-C4-C5	2.33	114.45	110.23
12	2	2	NAG	C1-O5-C5	2.32	115.30	112.19
14	w	1	NAG	C3-C4-C5	2.32	114.43	110.23
9	n	2	NAG	C1-C2-N2	2.29	114.04	110.43
13	c	1	NAG	C4-C3-C2	2.29	114.37	111.02
14	6	4	MAN	C1-O5-C5	2.27	115.23	112.19
10	k	2	NAG	O3-C3-C2	2.27	114.11	109.40
12	r	1	NAG	O5-C1-C2	-2.24	107.82	111.29
9	y	1	NAG	C1-C2-N2	2.24	113.96	110.43
14	w	2	NAG	C1-O5-C5	-2.24	109.19	112.19
10	k	4	MAN	C1-C2-C3	2.23	112.89	109.64
10	4	3	BMA	C1-C2-C3	2.21	112.86	109.64
12	W	1	NAG	C1-O5-C5	2.21	115.15	112.19
9	s	1	NAG	C1-C2-N2	2.20	113.90	110.43
10	k	4	MAN	C1-O5-C5	2.19	115.13	112.19
16	0	2	NAG	C2-N2-C7	-2.17	119.99	122.90
12	2	1	NAG	O4-C4-C3	-2.16	105.28	110.38
12	m	2	NAG	O5-C1-C2	-2.16	107.94	111.29
10	Z	2	NAG	C1-C2-N2	2.14	113.81	110.43
12	W	2	NAG	O5-C1-C2	-2.14	107.98	111.29
11	U	5	MAN	C1-O5-C5	2.13	115.04	112.19
14	6	2	NAG	C2-N2-C7	2.13	125.75	122.90
15	z	1	NAG	O4-C4-C5	-2.12	104.10	109.32
10	Z	2	NAG	C4-C3-C2	-2.11	107.93	111.02
10	j	1	NAG	C4-C3-C2	2.08	114.07	111.02
10	l	3	BMA	O3-C3-C2	-2.08	105.81	110.05
10	g	2	NAG	C1-O5-C5	2.08	114.97	112.19
10	1	2	NAG	O5-C1-C2	-2.07	108.08	111.29
12	e	3	BMA	C1-C2-C3	2.07	112.66	109.64
14	w	2	NAG	C3-C4-C5	2.05	113.95	110.23
12	i	2	NAG	C1-C2-N2	2.04	113.65	110.43
9	s	1	NAG	C1-O5-C5	2.04	114.92	112.19
9	n	2	NAG	C2-N2-C7	2.01	125.60	122.90
10	Z	3	BMA	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	Y	2	NAG	C1-C2-N2-C7
9	n	2	NAG	C1-C2-N2-C7
9	x	2	NAG	C1-C2-N2-C7
9	y	1	NAG	C1-C2-N2-C7
12	h	1	NAG	C3-C2-N2-C7
12	h	1	NAG	C8-C7-N2-C2
12	h	1	NAG	O7-C7-N2-C2
12	2	1	NAG	C1-C2-N2-C7
12	2	2	NAG	C1-C2-N2-C7
14	w	1	NAG	C1-C2-N2-C7
14	w	1	NAG	C8-C7-N2-C2
14	w	1	NAG	O7-C7-N2-C2
14	6	2	NAG	C8-C7-N2-C2
14	6	2	NAG	O7-C7-N2-C2
16	7	2	NAG	C1-C2-N2-C7
16	7	2	NAG	C8-C7-N2-C2
16	7	2	NAG	O7-C7-N2-C2
10	4	1	NAG	C8-C7-N2-C2
14	6	1	NAG	C8-C7-N2-C2
14	6	1	NAG	O7-C7-N2-C2
9	y	1	NAG	O7-C7-N2-C2
10	4	1	NAG	O7-C7-N2-C2
10	u	3	BMA	O5-C5-C6-O6
10	j	2	NAG	O5-C5-C6-O6
9	x	2	NAG	C8-C7-N2-C2
9	y	1	NAG	C8-C7-N2-C2
10	9	1	NAG	C8-C7-N2-C2
13	o	2	NAG	C8-C7-N2-C2
15	z	1	NAG	C8-C7-N2-C2
15	z	1	NAG	O7-C7-N2-C2
11	U	2	NAG	O5-C5-C6-O6
11	U	2	NAG	C8-C7-N2-C2
10	u	3	BMA	C4-C5-C6-O6
11	U	2	NAG	C4-C5-C6-O6
9	x	2	NAG	O7-C7-N2-C2
10	l	1	NAG	C8-C7-N2-C2
10	9	1	NAG	O7-C7-N2-C2
11	U	2	NAG	O7-C7-N2-C2
12	W	2	NAG	C8-C7-N2-C2
12	h	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
13	o	2	NAG	O7-C7-N2-C2
12	h	2	NAG	O7-C7-N2-C2
10	4	3	BMA	O5-C5-C6-O6
10	j	2	NAG	C4-C5-C6-O6
10	l	1	NAG	O7-C7-N2-C2
12	p	1	NAG	C8-C7-N2-C2
16	0	1	NAG	C8-C7-N2-C2
10	j	1	NAG	O5-C5-C6-O6
14	w	1	NAG	O5-C5-C6-O6
10	4	3	BMA	C4-C5-C6-O6
12	m	1	NAG	O5-C5-C6-O6
10	4	2	NAG	C4-C5-C6-O6
10	b	2	NAG	O5-C5-C6-O6
11	U	3	BMA	O5-C5-C6-O6
10	9	3	BMA	O5-C5-C6-O6
14	6	4	MAN	O5-C5-C6-O6
12	m	2	NAG	C8-C7-N2-C2
12	W	2	NAG	O7-C7-N2-C2
12	p	1	NAG	O7-C7-N2-C2
14	w	4	MAN	O5-C5-C6-O6
12	r	3	BMA	O5-C5-C6-O6
9	Y	2	NAG	C8-C7-N2-C2
16	0	1	NAG	O7-C7-N2-C2
9	y	2	NAG	O5-C5-C6-O6
10	l	4	MAN	O5-C5-C6-O6
10	j	5	MAN	O5-C5-C6-O6
10	l	5	MAN	O5-C5-C6-O6
10	g	5	MAN	O5-C5-C6-O6
14	6	5	MAN	O5-C5-C6-O6
11	U	5	MAN	O5-C5-C6-O6
14	w	5	MAN	O5-C5-C6-O6
9	X	2	NAG	O5-C5-C6-O6
9	s	1	NAG	C8-C7-N2-C2
10	j	1	NAG	C3-C2-N2-C7
14	6	2	NAG	C3-C2-N2-C7
12	r	2	NAG	O5-C5-C6-O6
14	w	2	NAG	O5-C5-C6-O6
10	1	3	BMA	C4-C5-C6-O6
10	1	3	BMA	O5-C5-C6-O6
9	v	1	NAG	C8-C7-N2-C2
12	e	1	NAG	C4-C5-C6-O6
10	4	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	5	3	BMA	C4-C5-C6-O6
10	4	1	NAG	C1-C2-N2-C7
13	8	2	NAG	C1-C2-N2-C7
15	z	2	NAG	C1-C2-N2-C7
9	Y	2	NAG	O7-C7-N2-C2
12	m	2	NAG	O7-C7-N2-C2
12	r	2	NAG	C8-C7-N2-C2
12	e	2	NAG	C8-C7-N2-C2
15	z	3	BMA	O5-C5-C6-O6
10	u	2	NAG	C8-C7-N2-C2
9	v	1	NAG	O7-C7-N2-C2
10	5	3	BMA	O5-C5-C6-O6
9	t	1	NAG	C3-C2-N2-C7
10	4	1	NAG	C3-C2-N2-C7
10	4	2	NAG	C3-C2-N2-C7
12	h	2	NAG	C3-C2-N2-C7
12	e	1	NAG	O5-C5-C6-O6
10	j	3	BMA	C4-C5-C6-O6
10	u	2	NAG	O7-C7-N2-C2
12	e	2	NAG	O7-C7-N2-C2
9	X	1	NAG	C8-C7-N2-C2
12	r	2	NAG	O7-C7-N2-C2
10	u	1	NAG	C8-C7-N2-C2
9	v	2	NAG	C1-C2-N2-C7
9	y	2	NAG	C1-C2-N2-C7
10	5	1	NAG	C1-C2-N2-C7
13	8	1	NAG	C1-C2-N2-C7
16	0	1	NAG	C1-C2-N2-C7
10	9	3	BMA	C4-C5-C6-O6
10	j	3	BMA	O5-C5-C6-O6
10	j	2	NAG	C3-C2-N2-C7
10	5	1	NAG	C3-C2-N2-C7
13	8	1	NAG	C3-C2-N2-C7
13	8	2	NAG	C3-C2-N2-C7
14	w	2	NAG	C3-C2-N2-C7
15	z	2	NAG	C3-C2-N2-C7
10	4	2	NAG	O7-C7-N2-C2
12	m	1	NAG	C4-C5-C6-O6
10	4	2	NAG	C8-C7-N2-C2
9	X	1	NAG	O7-C7-N2-C2
10	4	1	NAG	O5-C5-C6-O6
10	4	1	NAG	C4-C5-C6-O6

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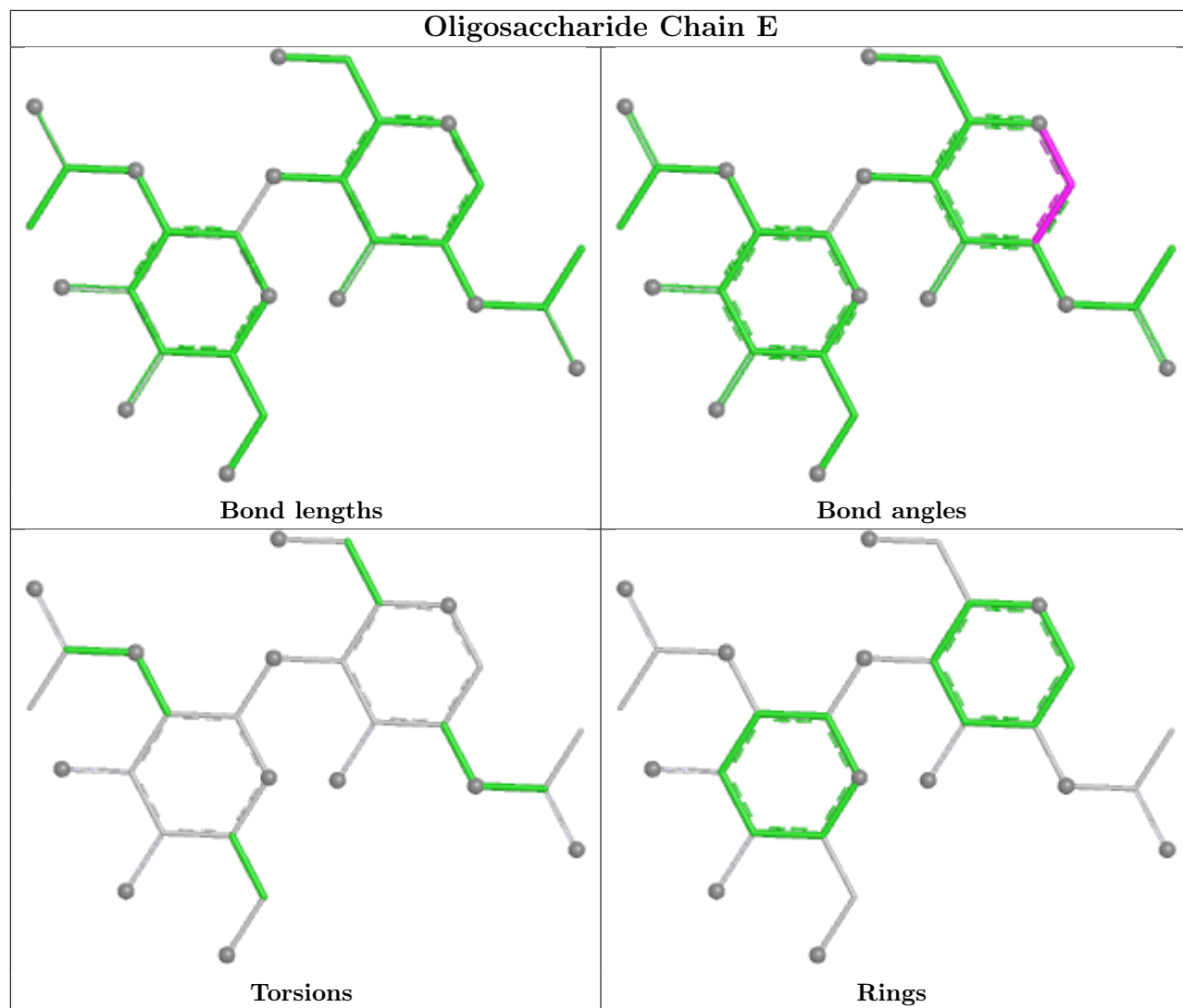
Mol	Chain	Res	Type	Atoms
13	c	2	NAG	C4-C5-C6-O6
10	u	1	NAG	O7-C7-N2-C2

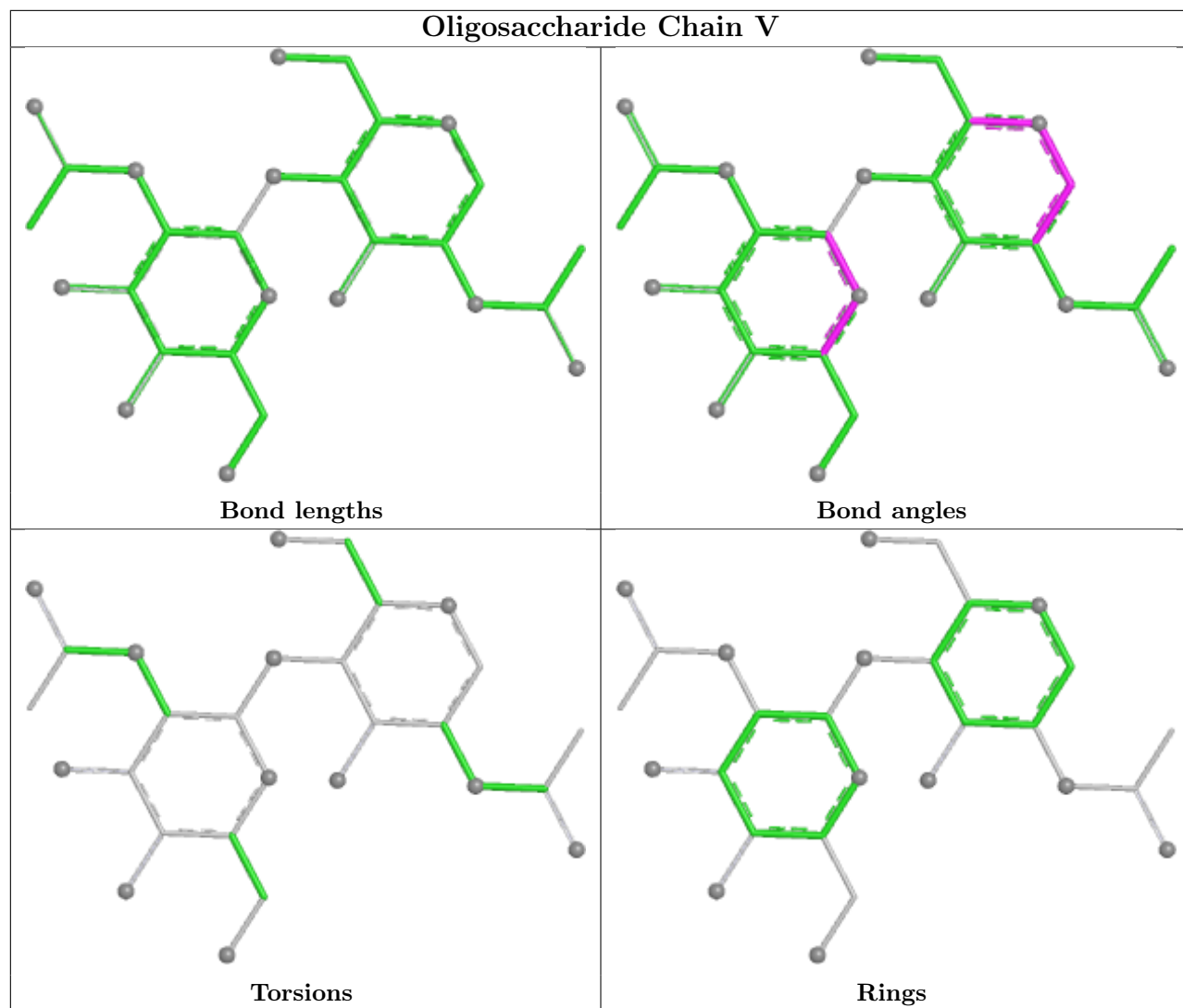
There are no ring outliers.

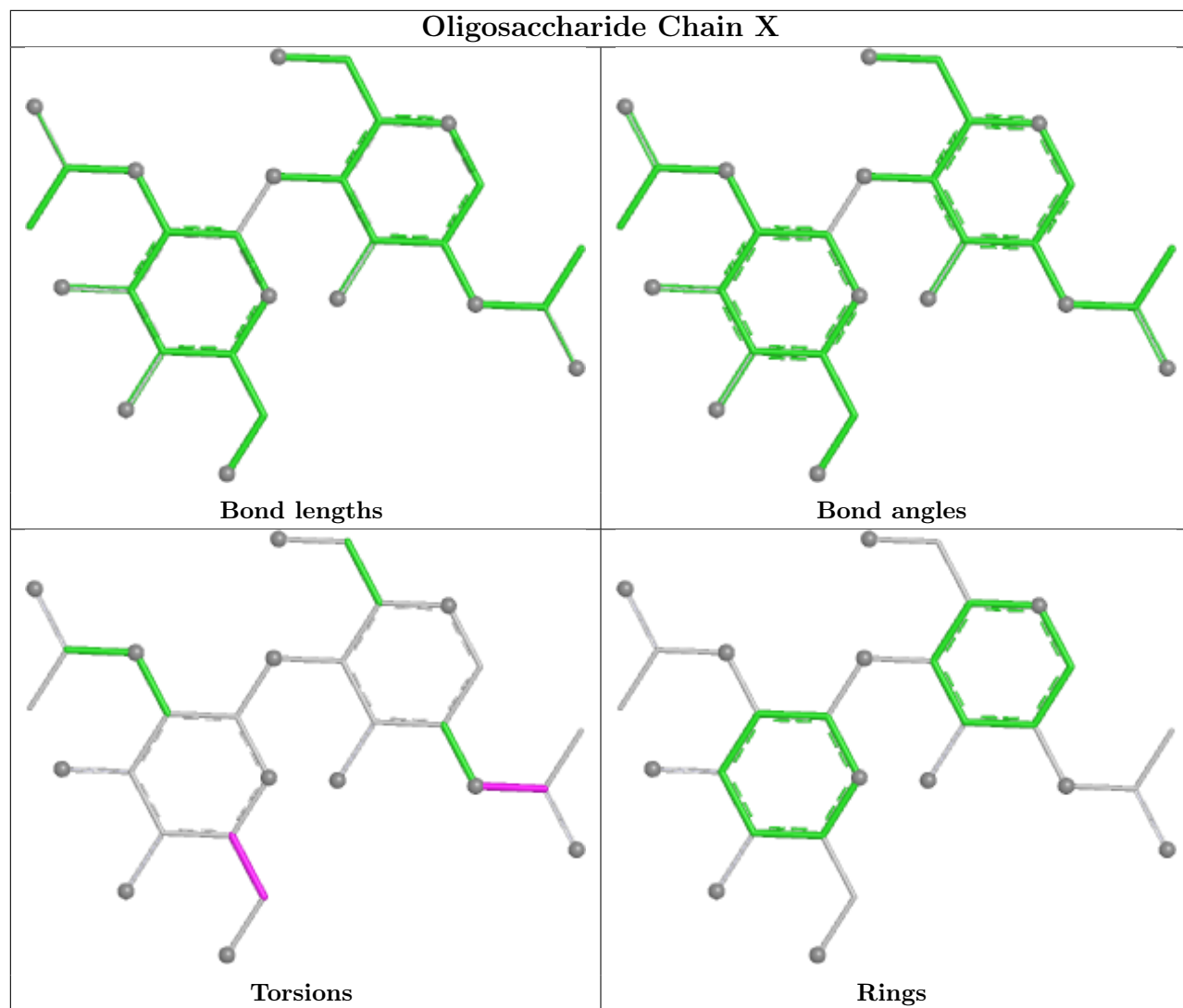
12 monomers are involved in 12 short contacts:

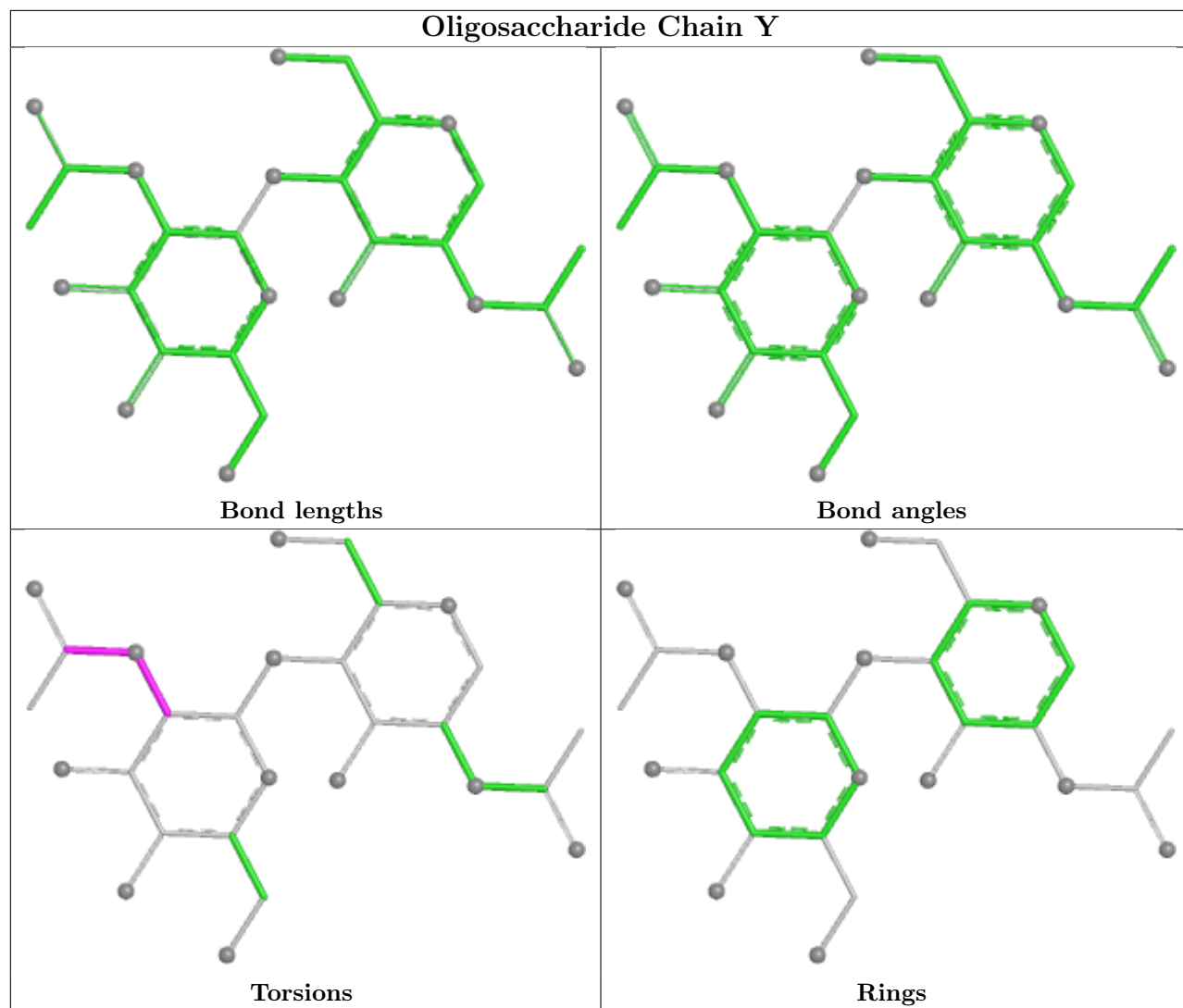
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	X	1	NAG	1	0
14	6	2	NAG	2	0
10	4	1	NAG	1	0
10	u	2	NAG	1	0
10	4	2	NAG	1	0
11	U	1	NAG	1	0
10	u	1	NAG	1	0
14	6	1	NAG	2	0
10	j	1	NAG	2	0
9	t	1	NAG	1	0
10	l	1	NAG	2	0
12	W	1	NAG	1	0

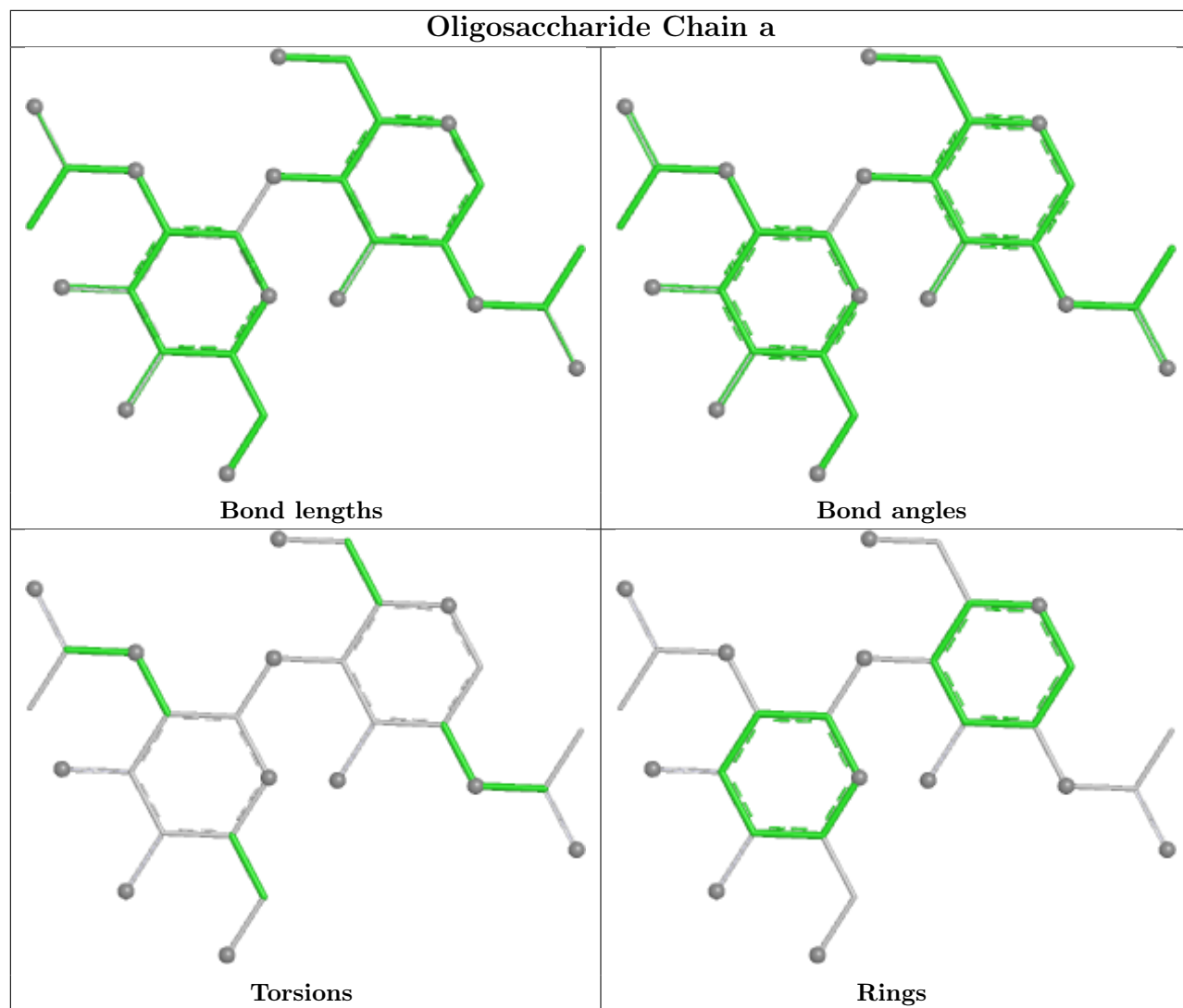
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

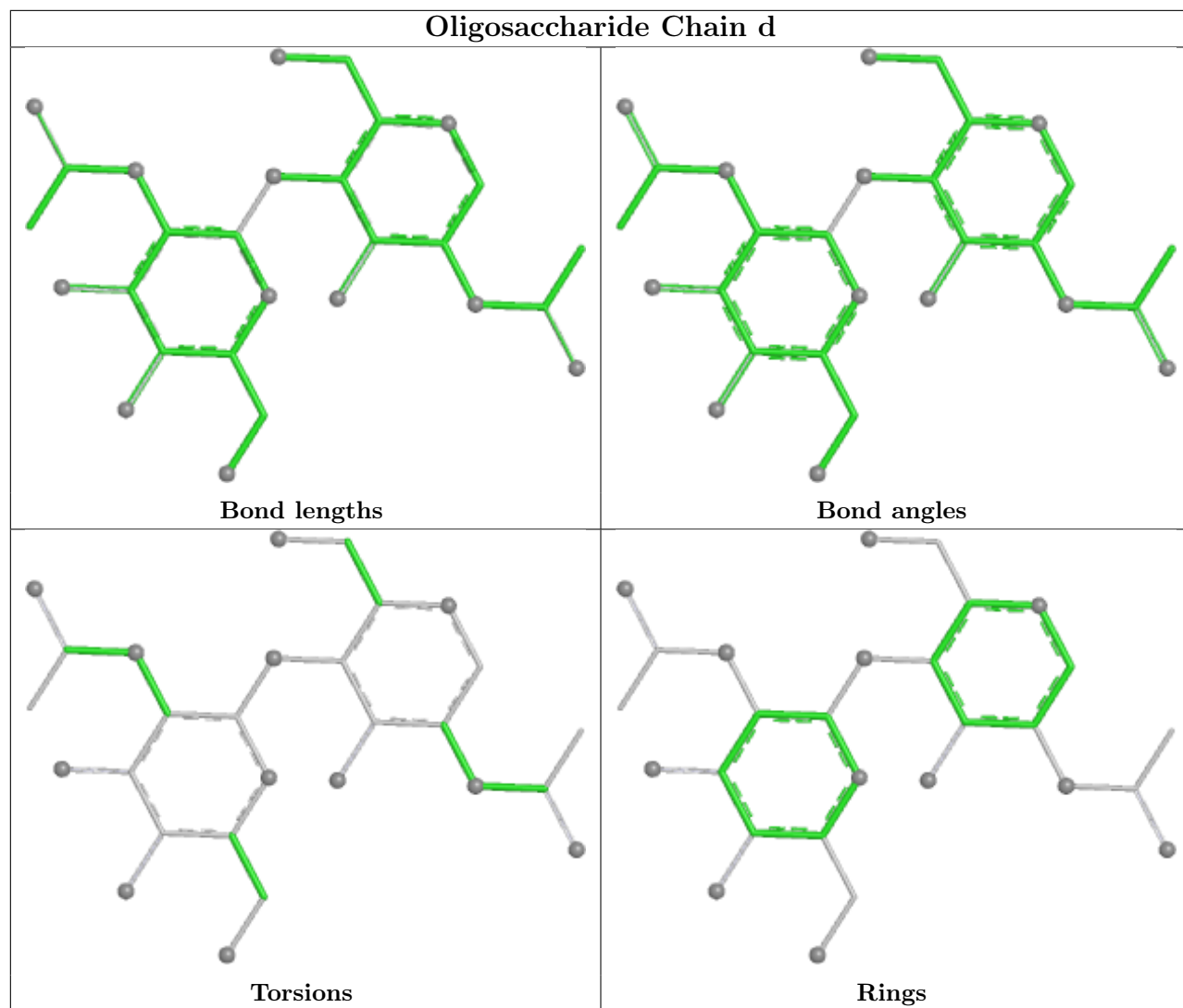


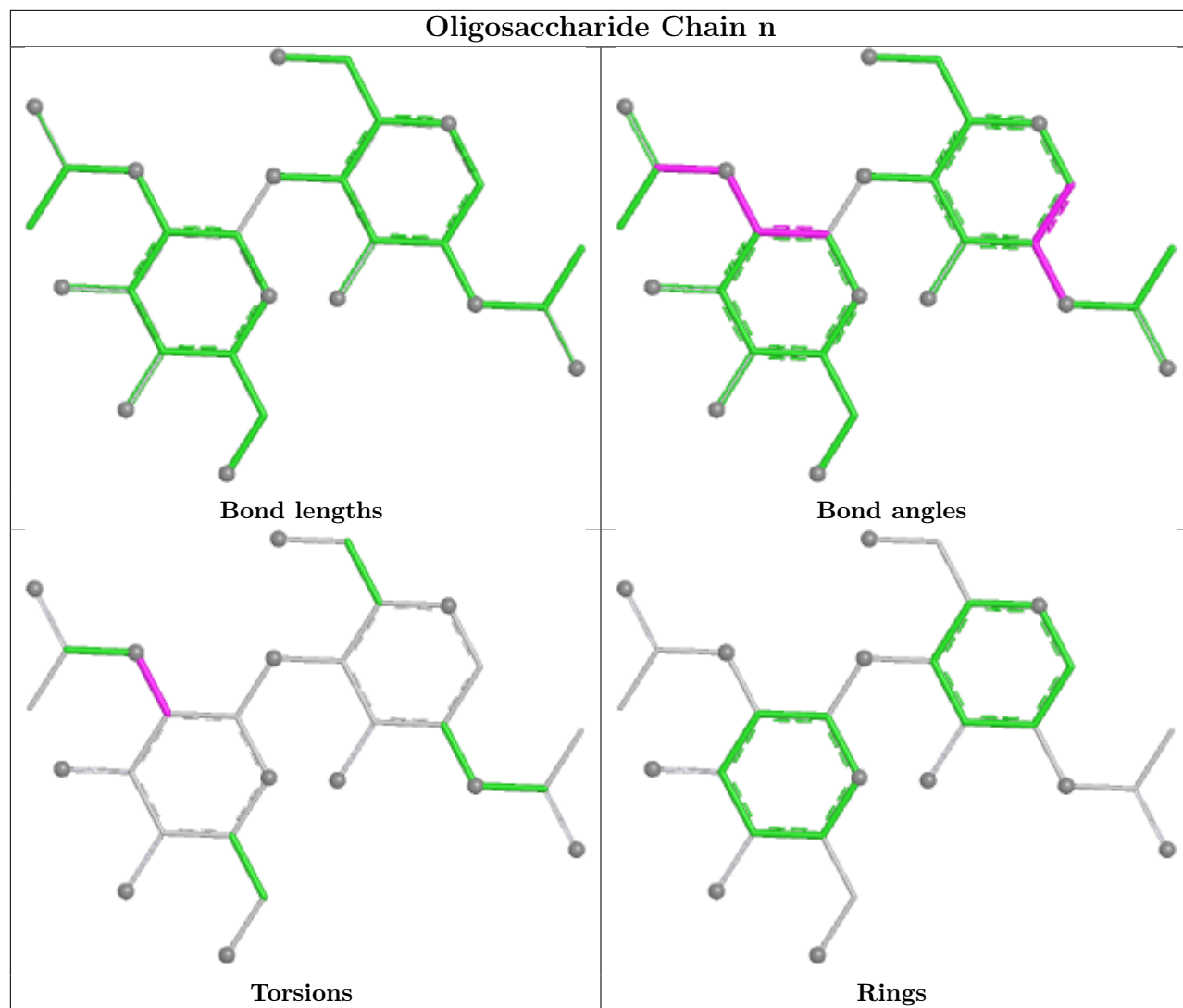


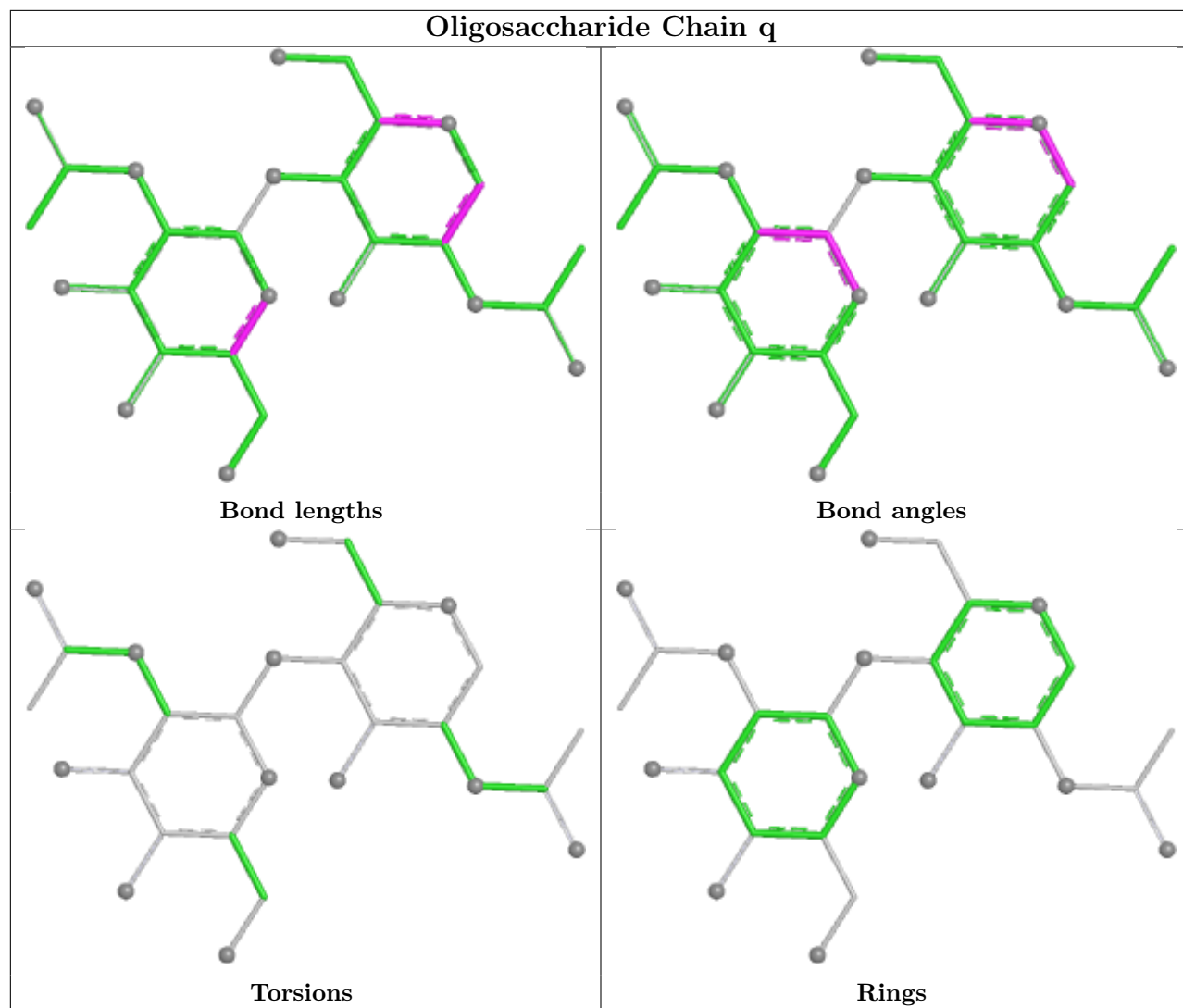


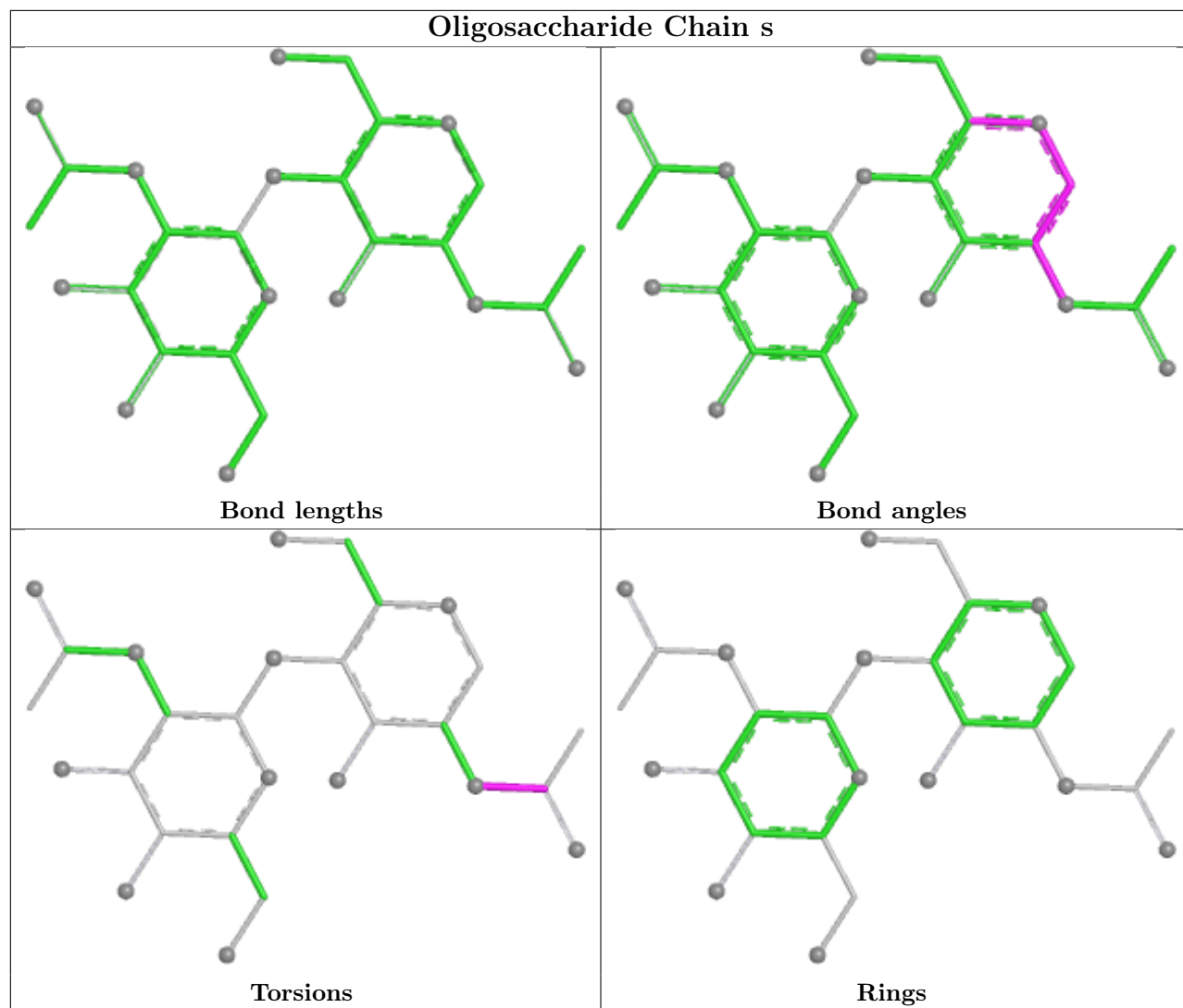


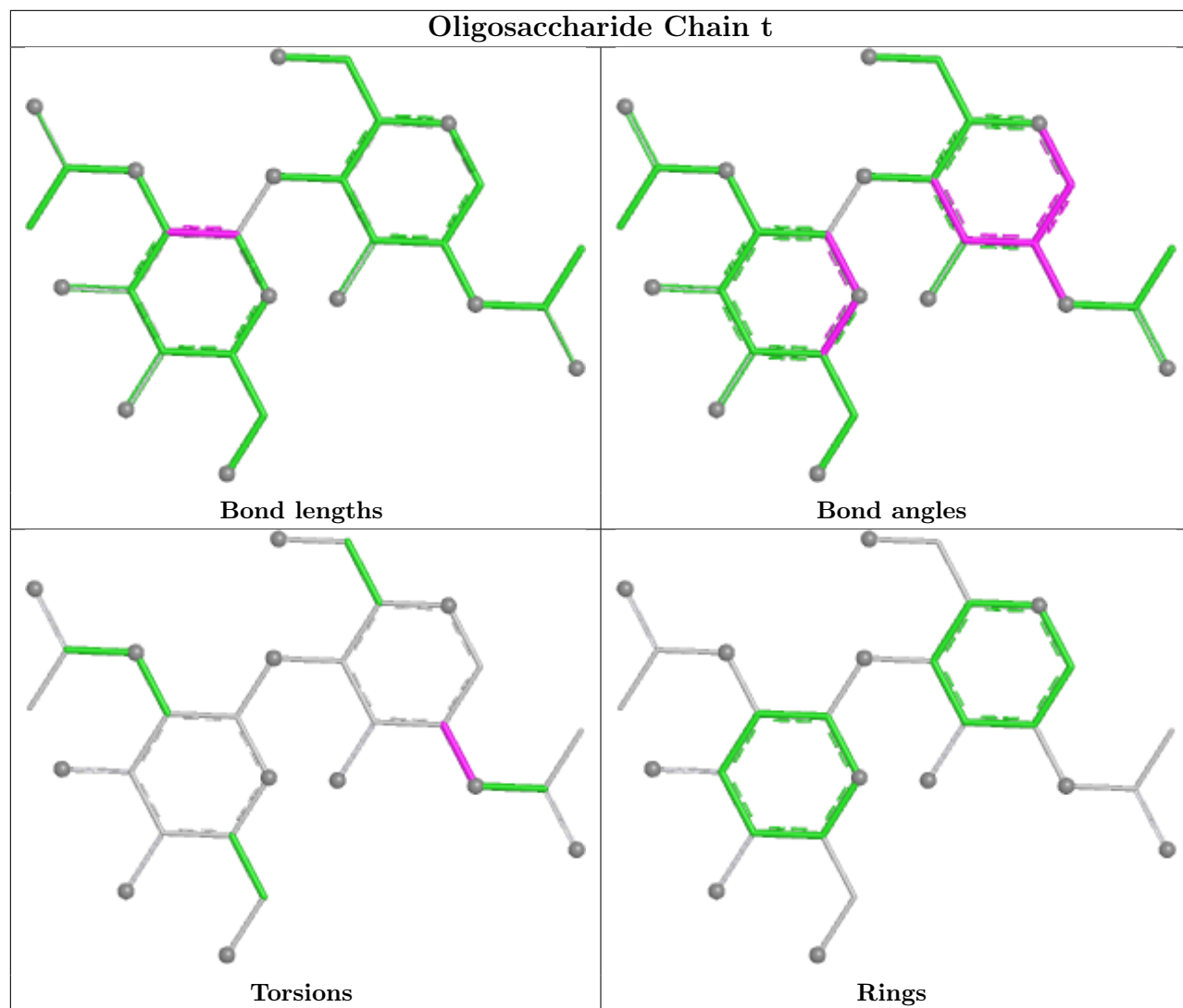


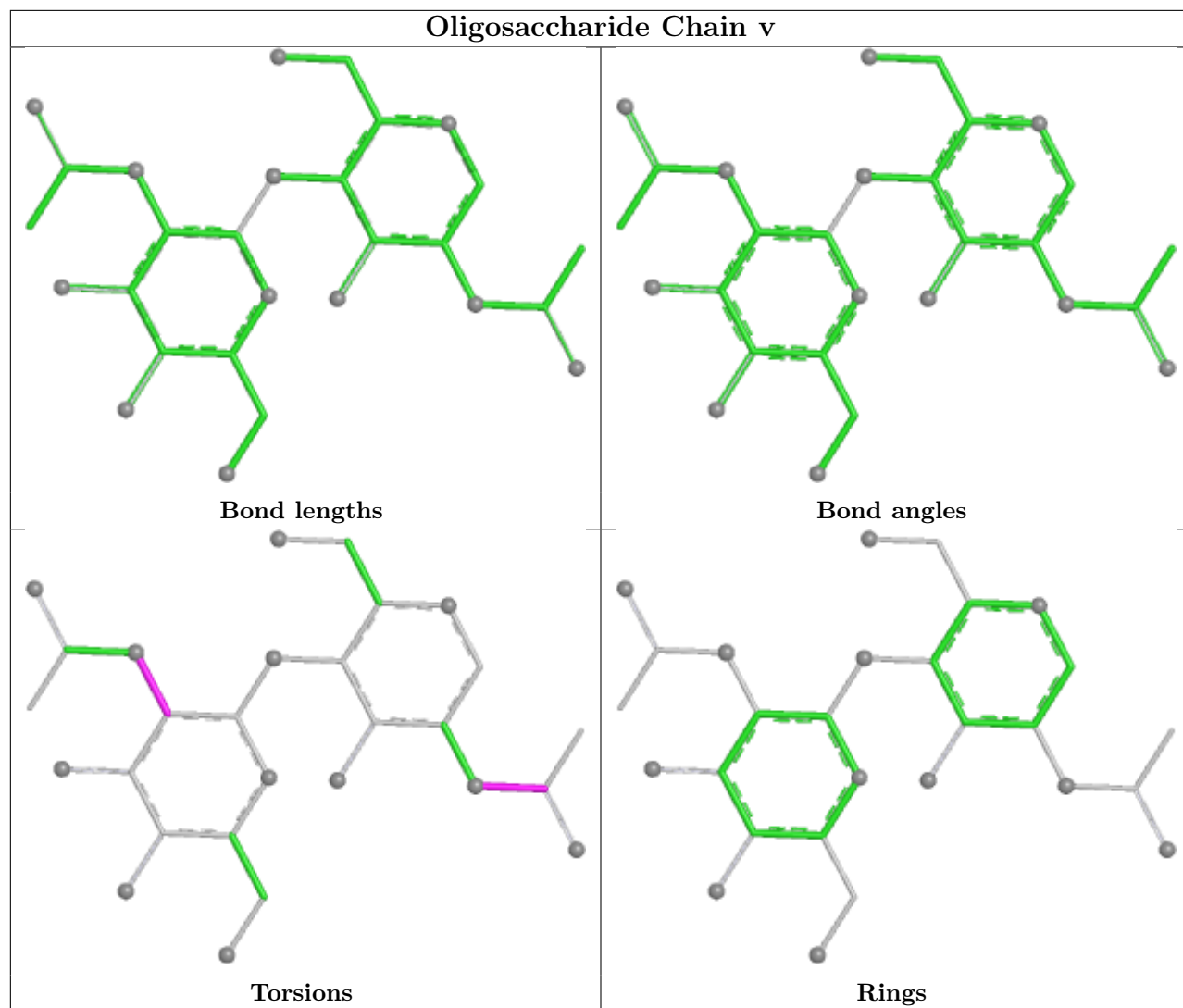


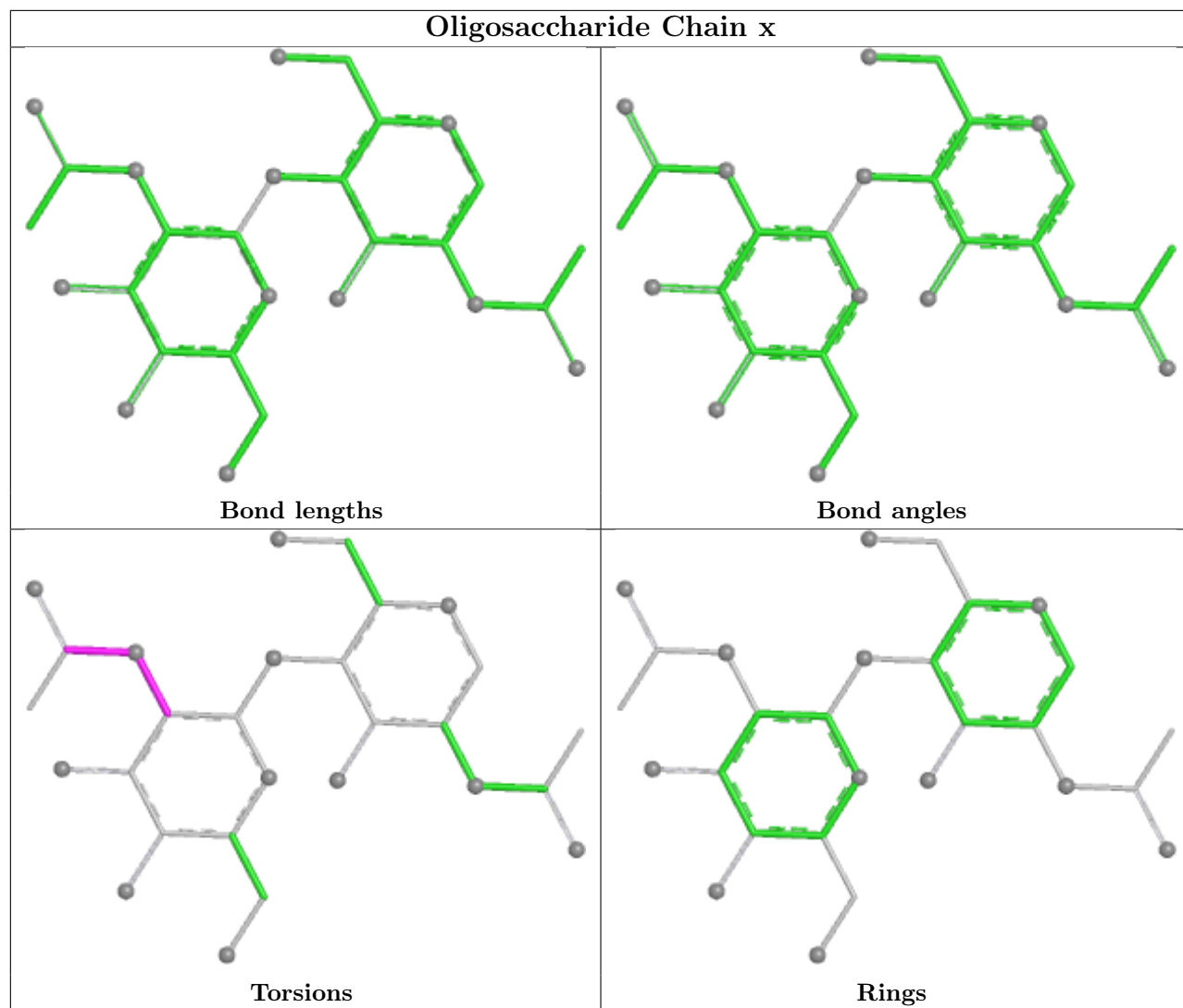


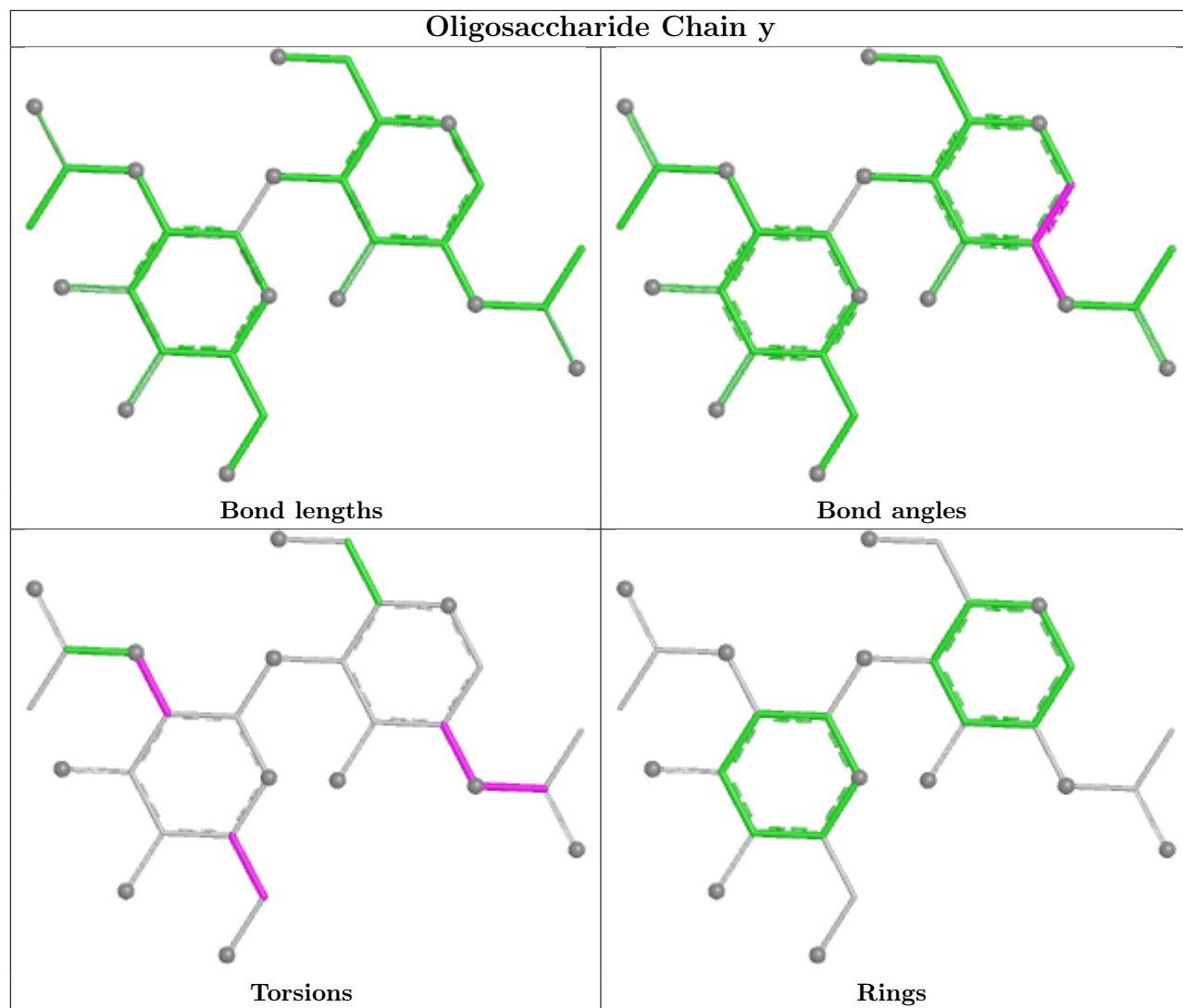


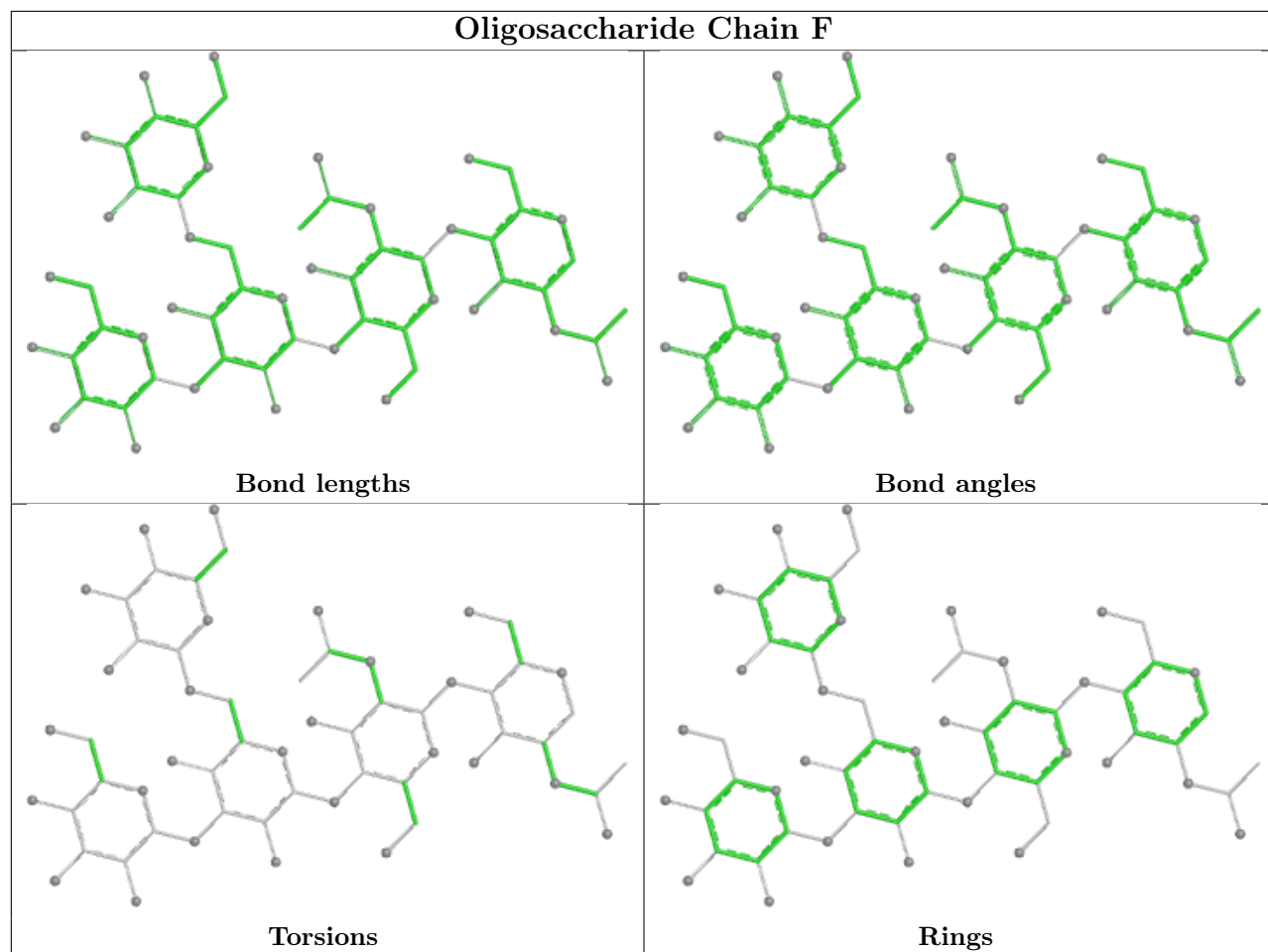


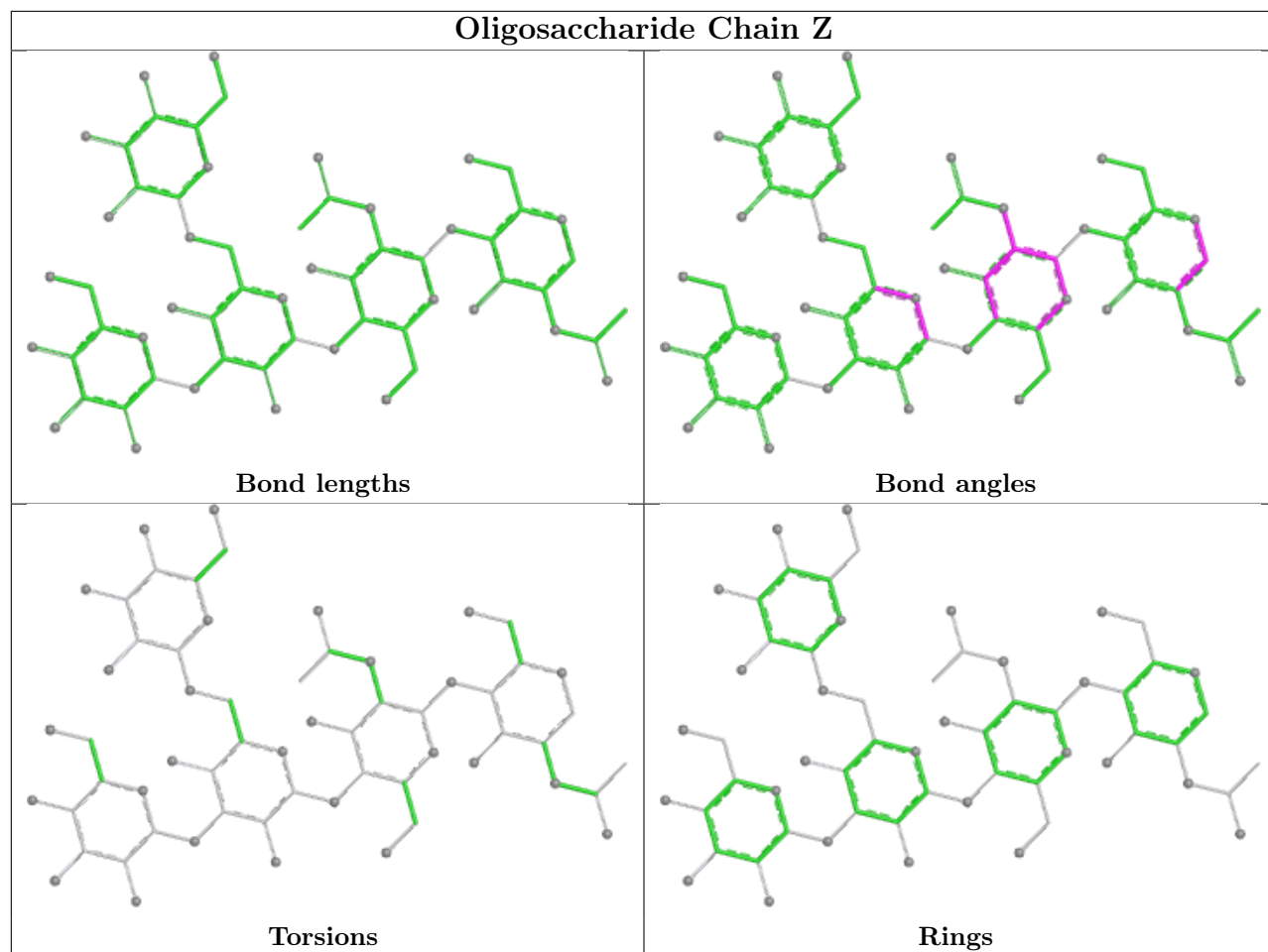


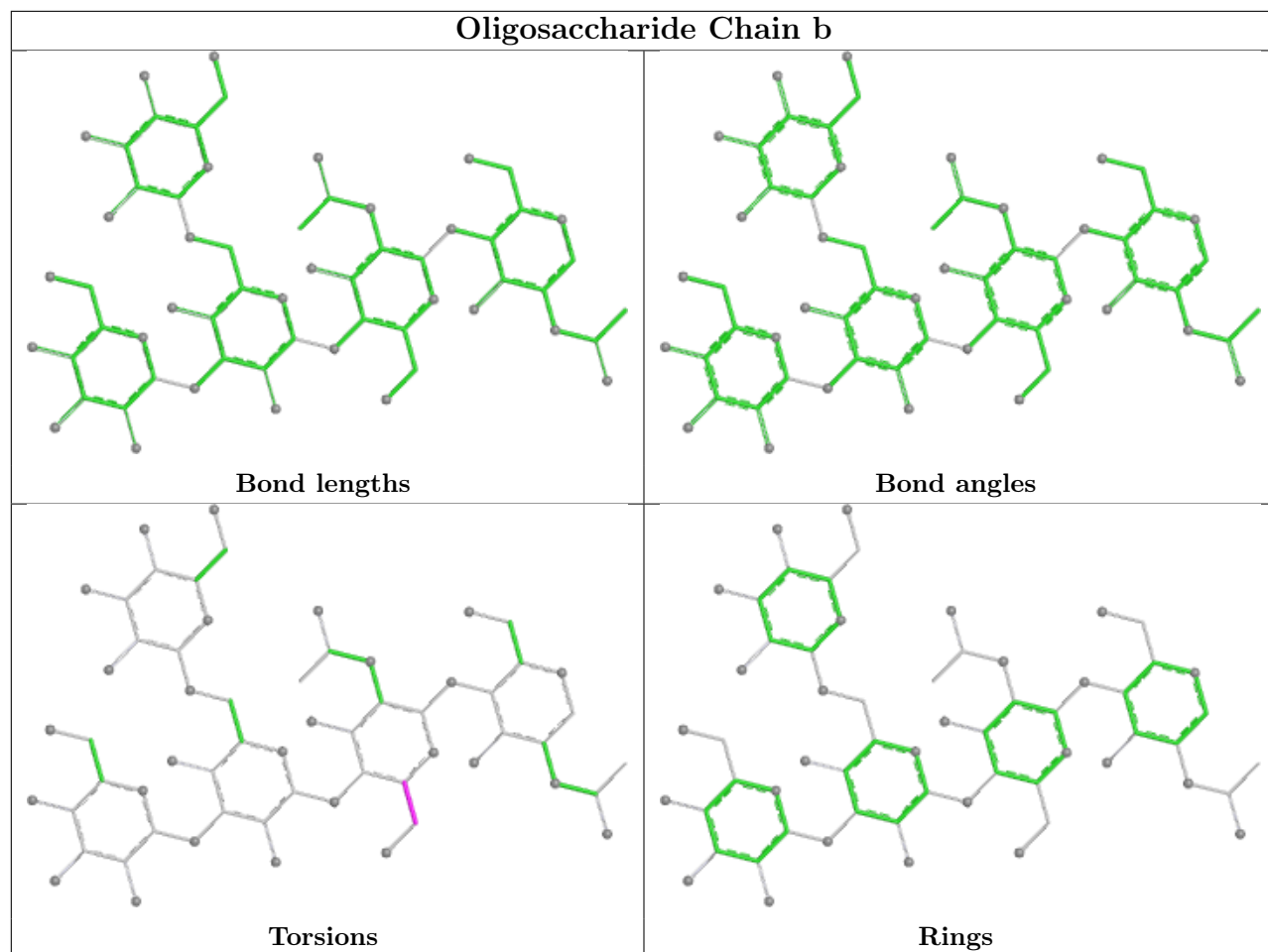


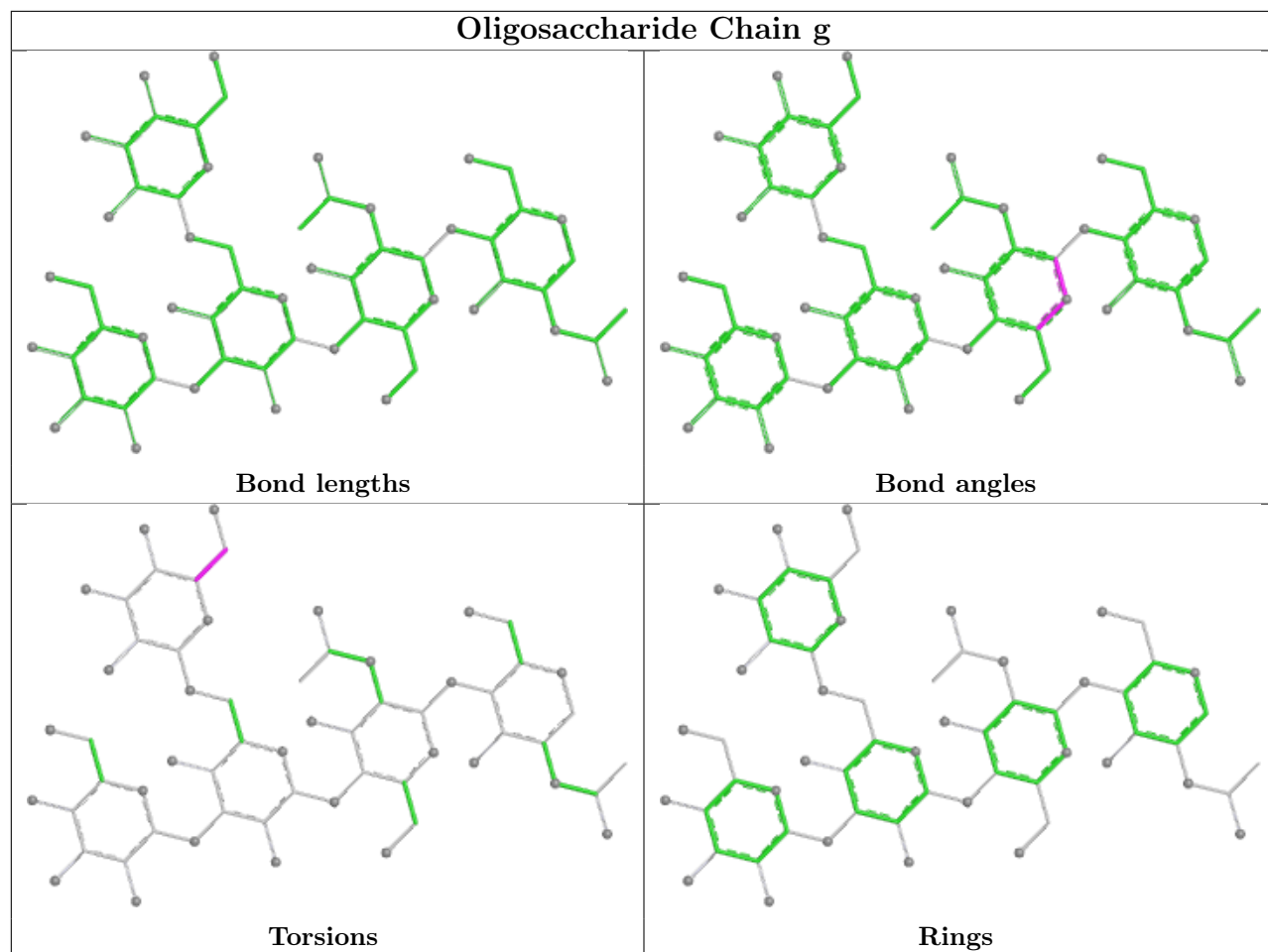


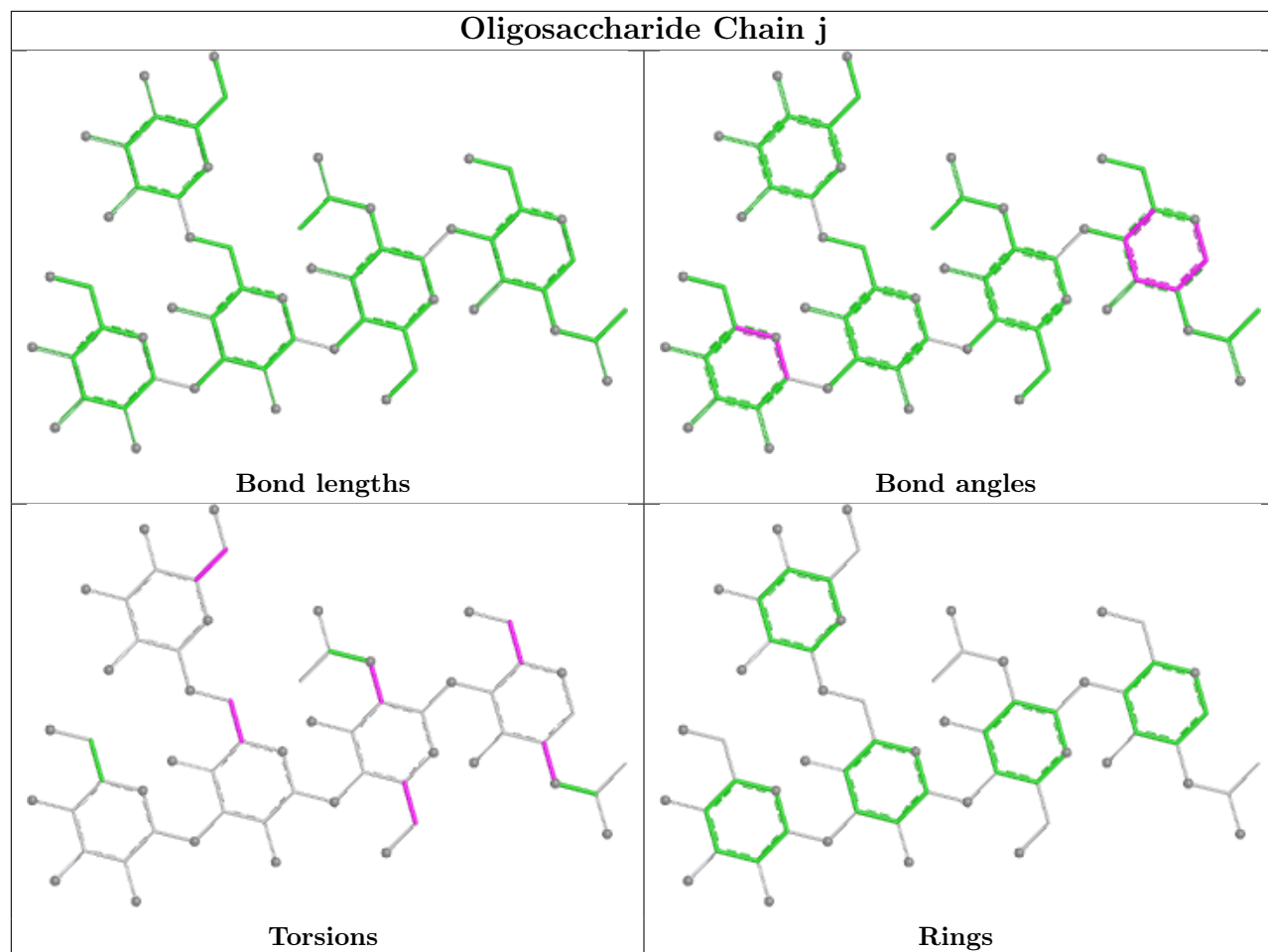


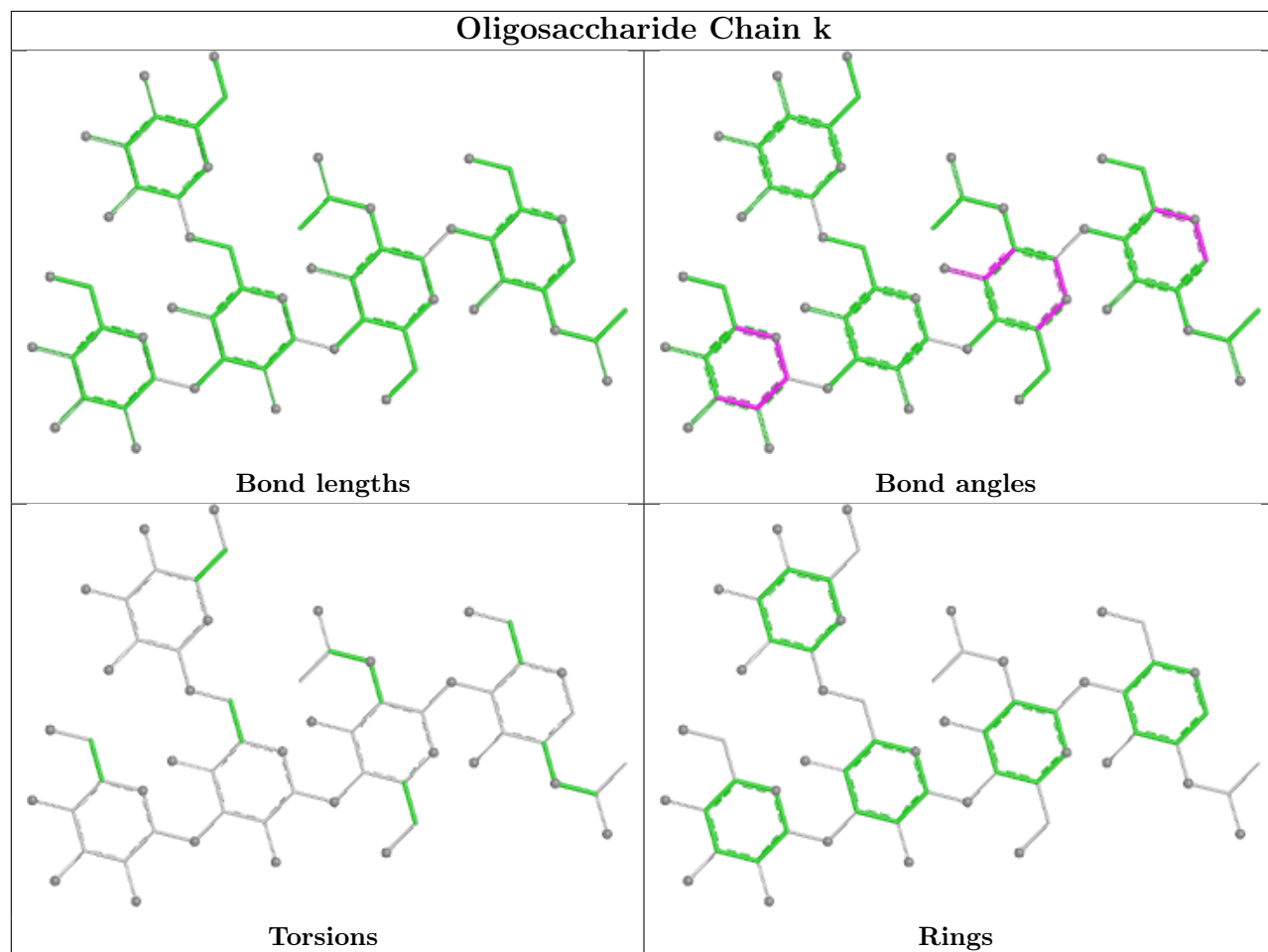


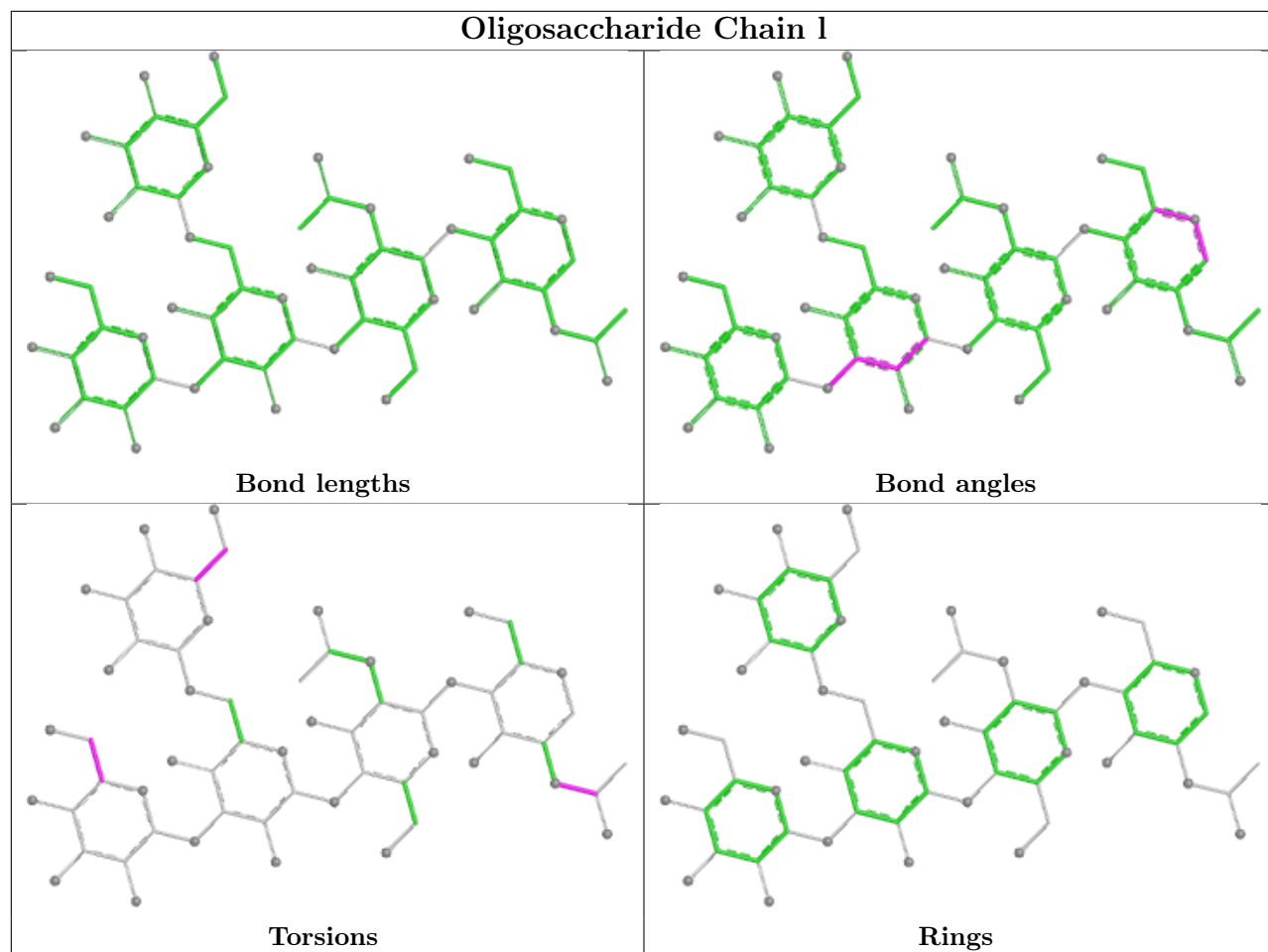


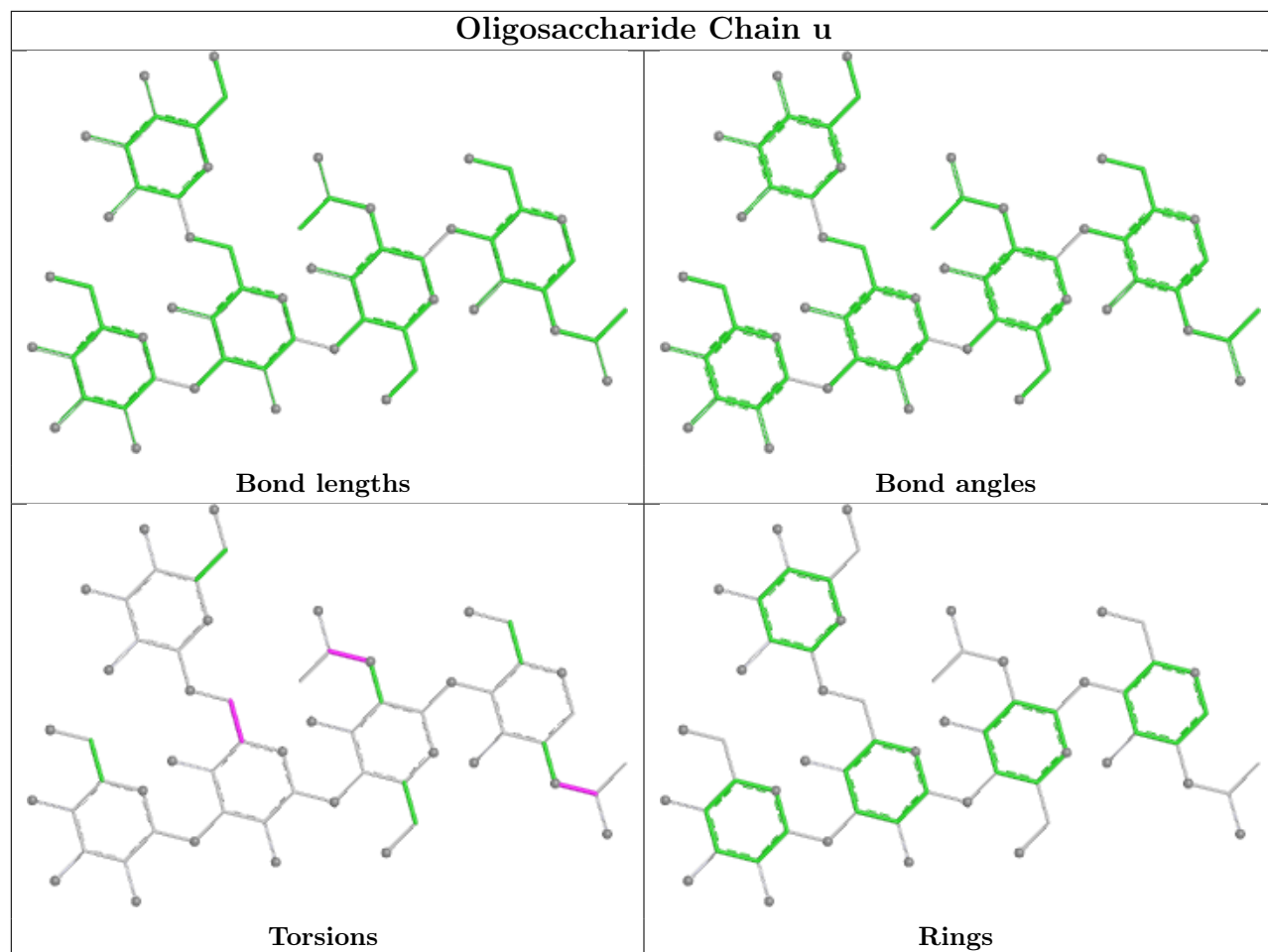


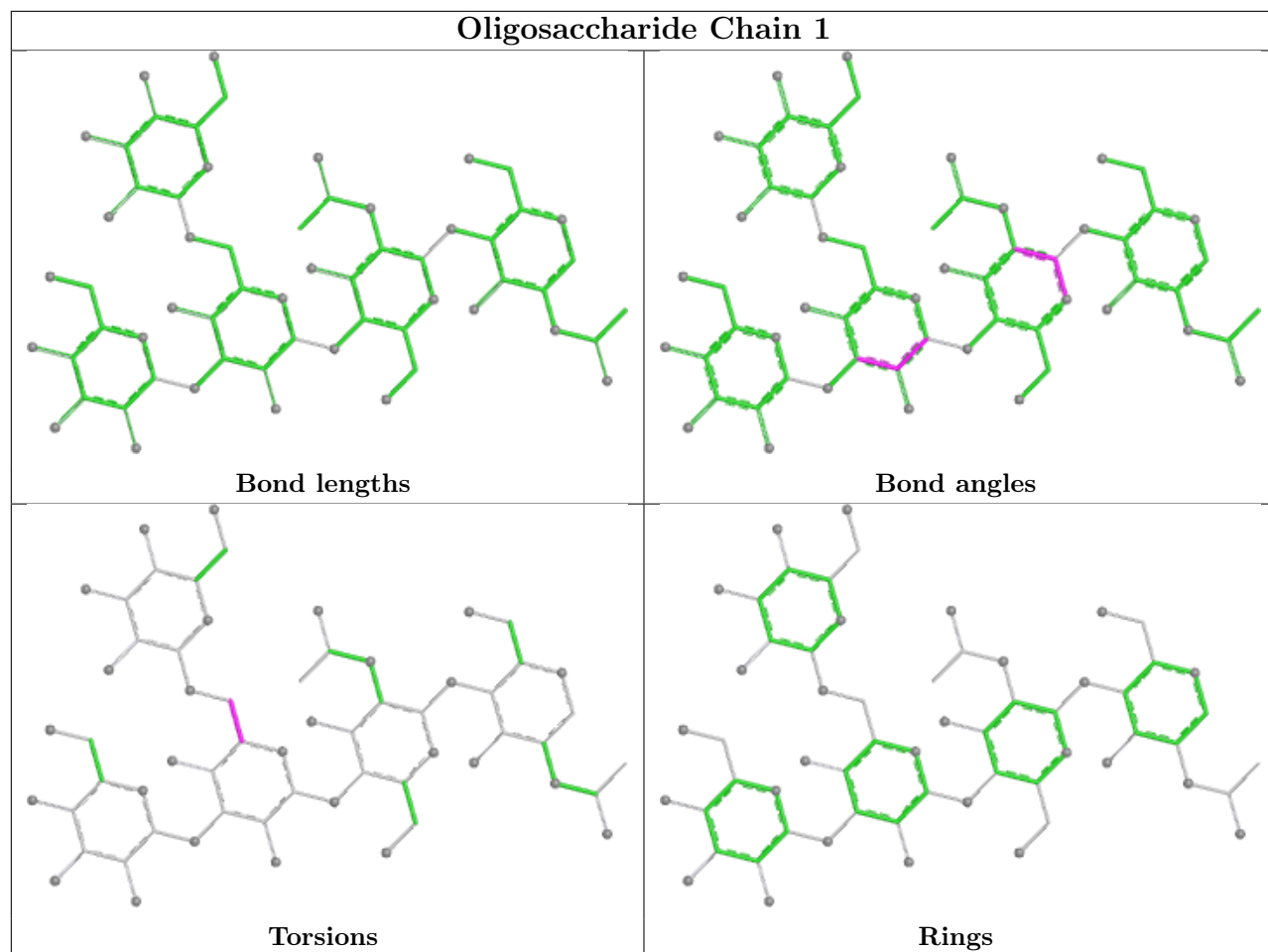


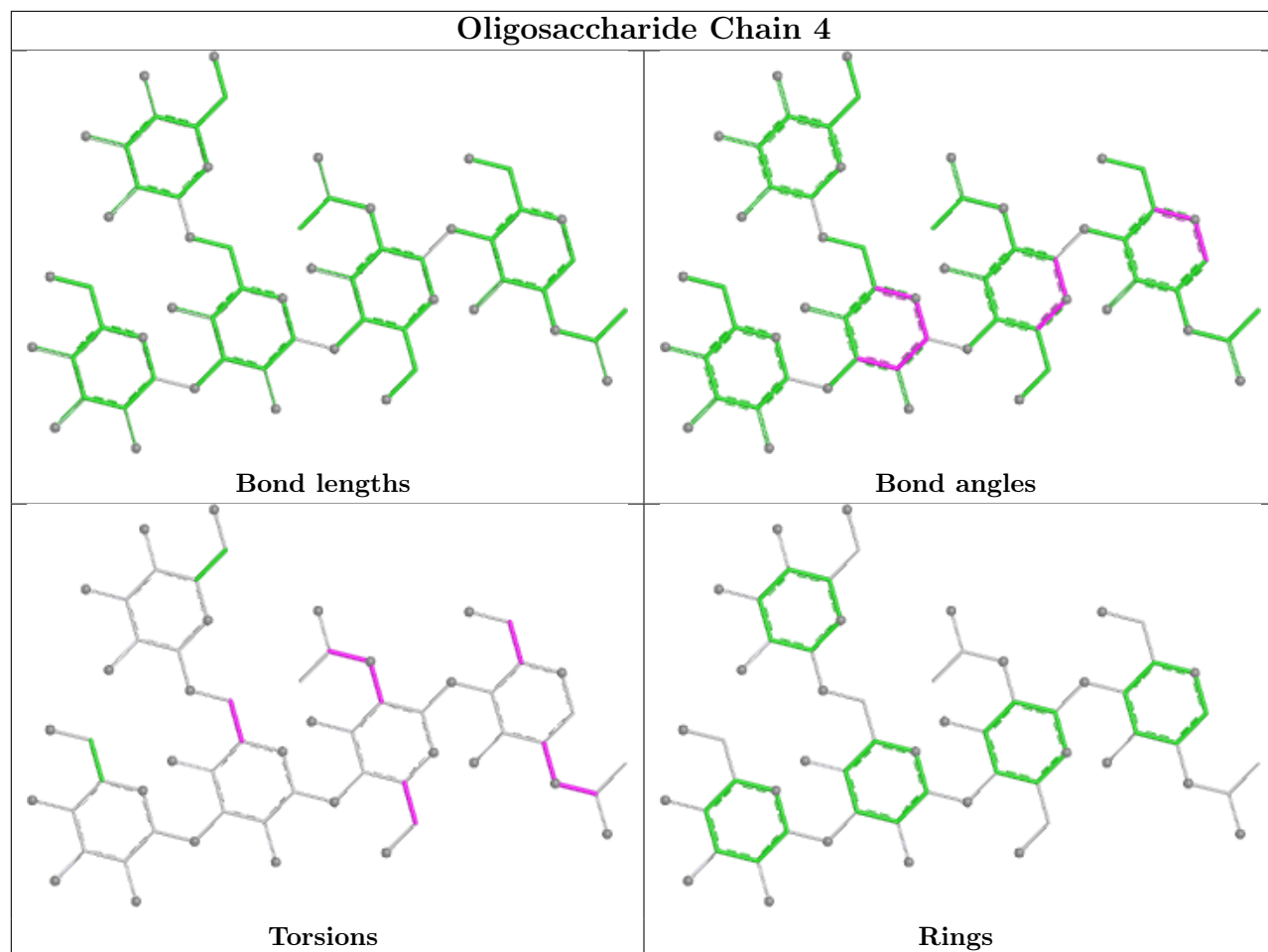


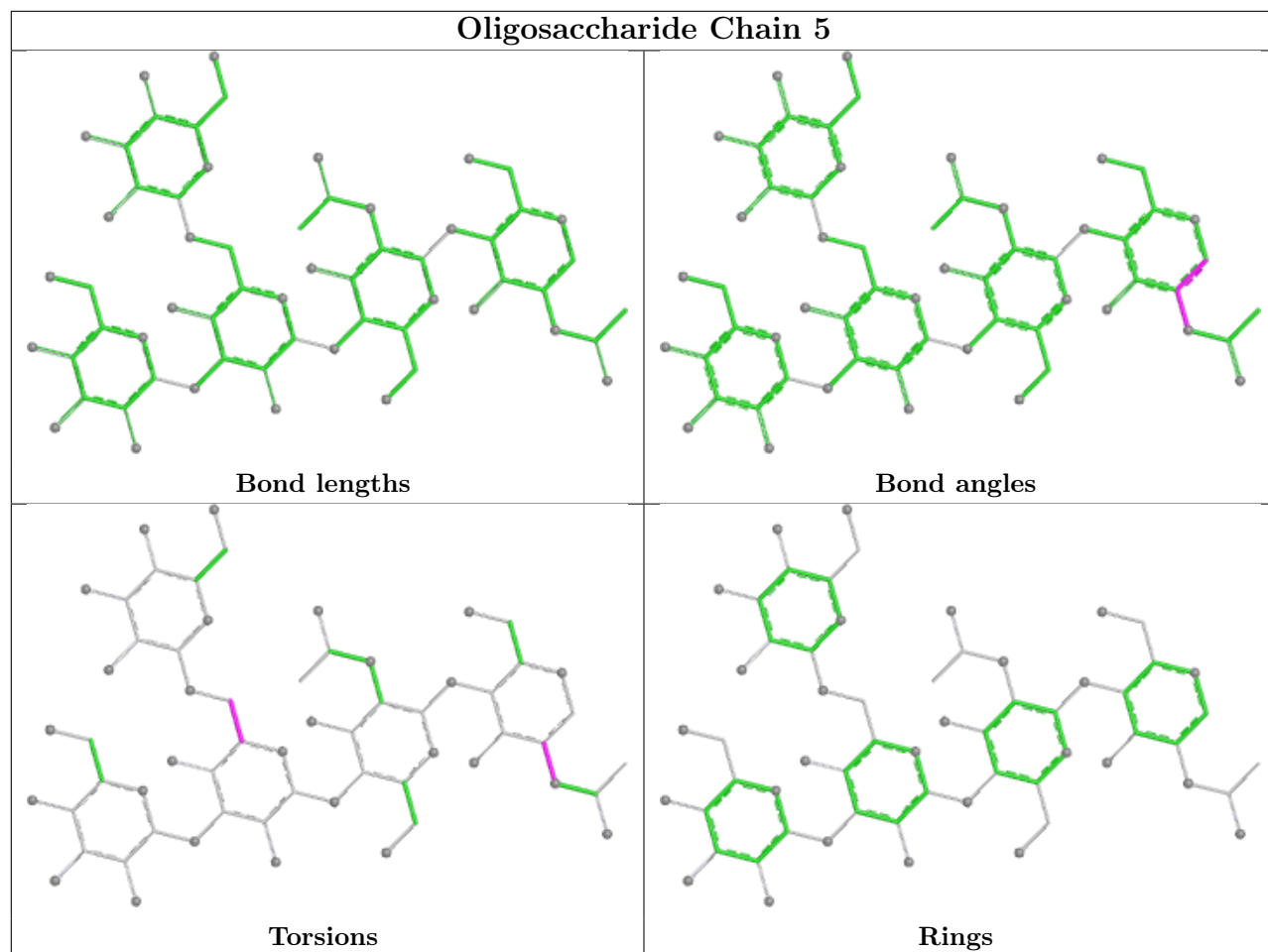


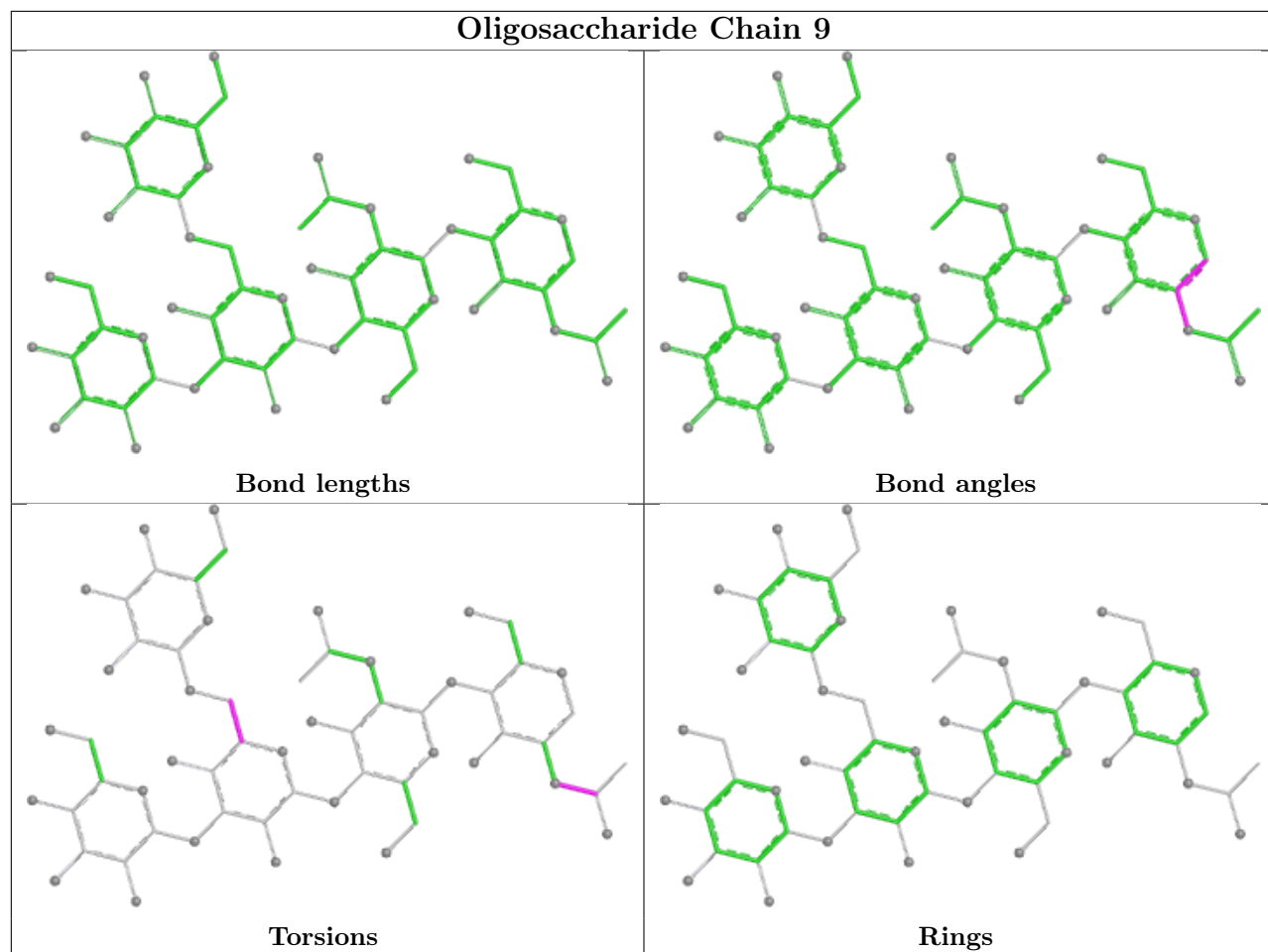


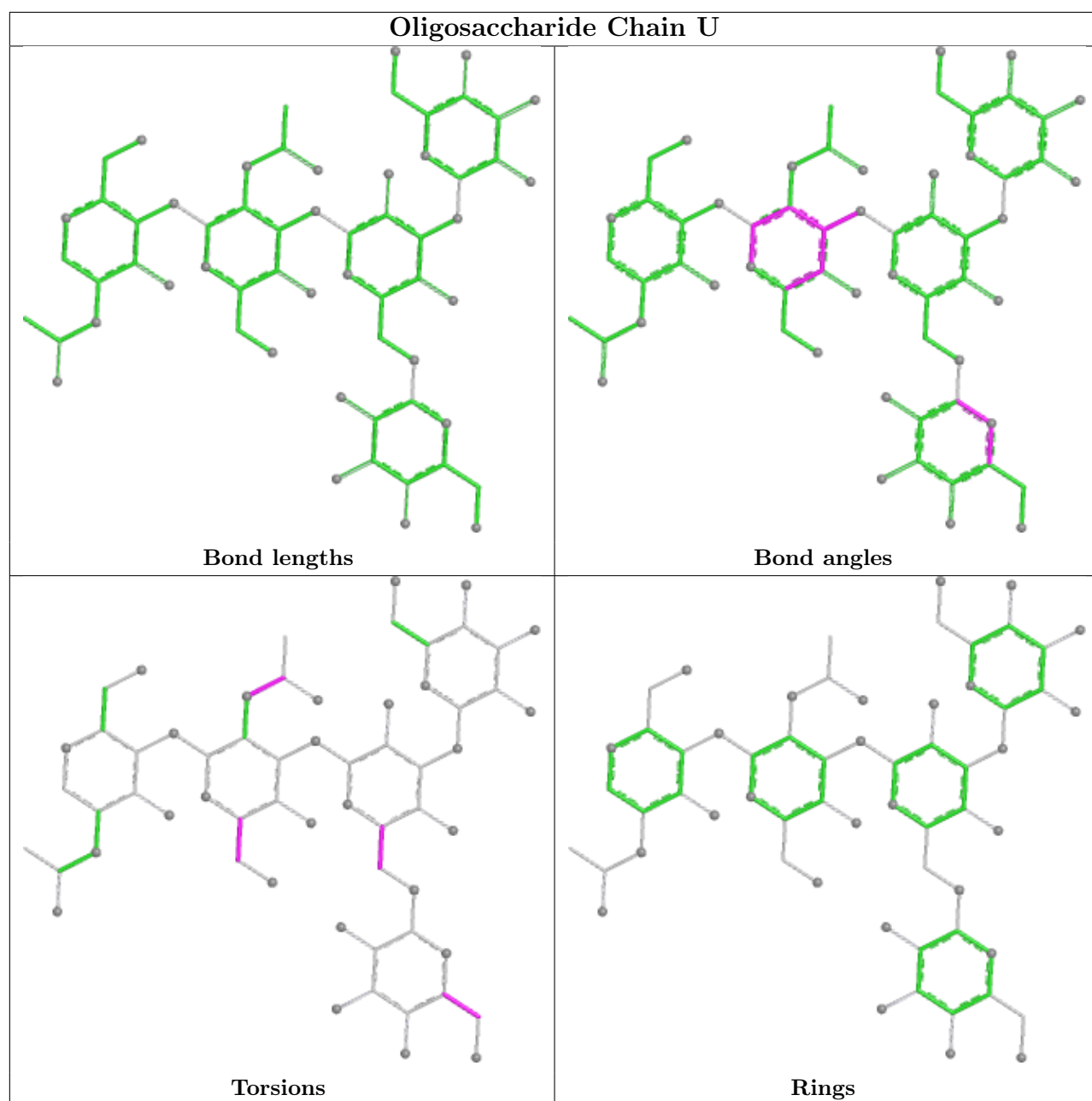


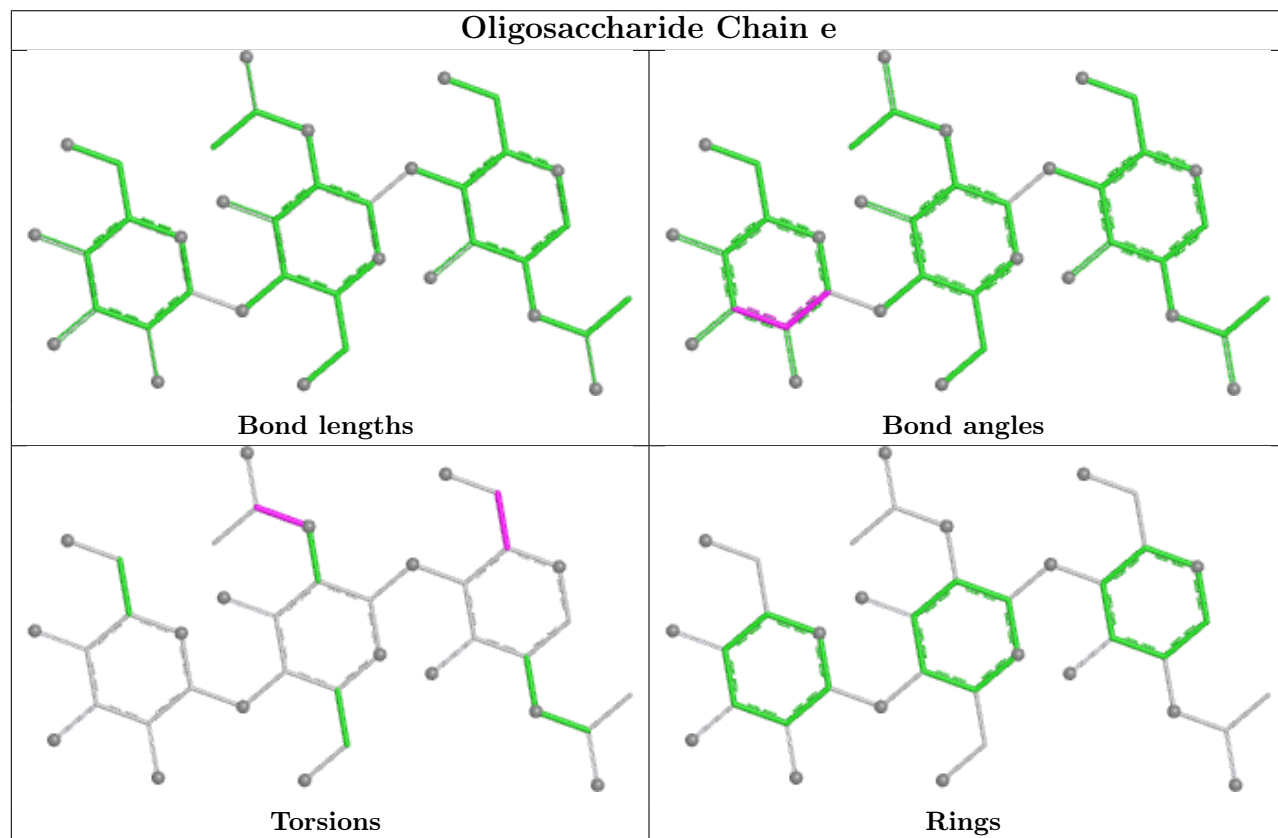
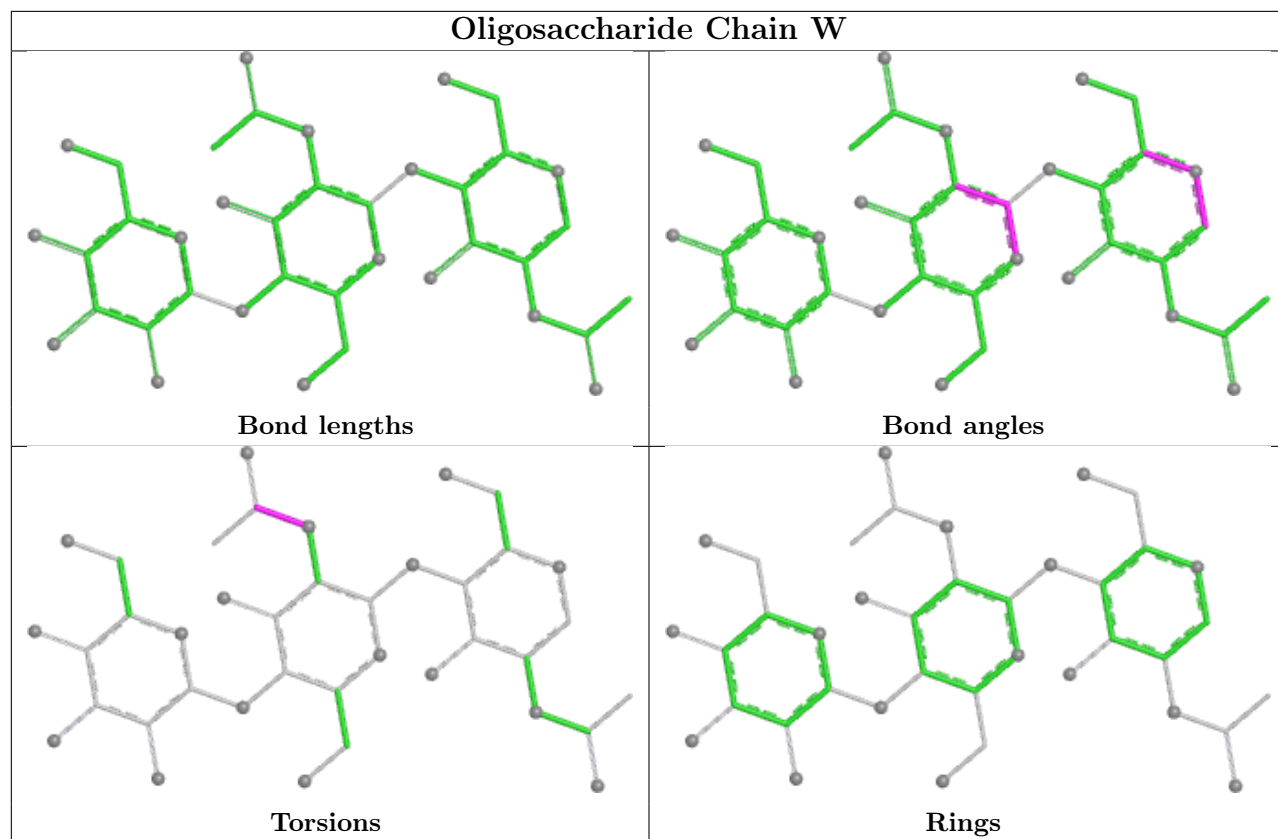


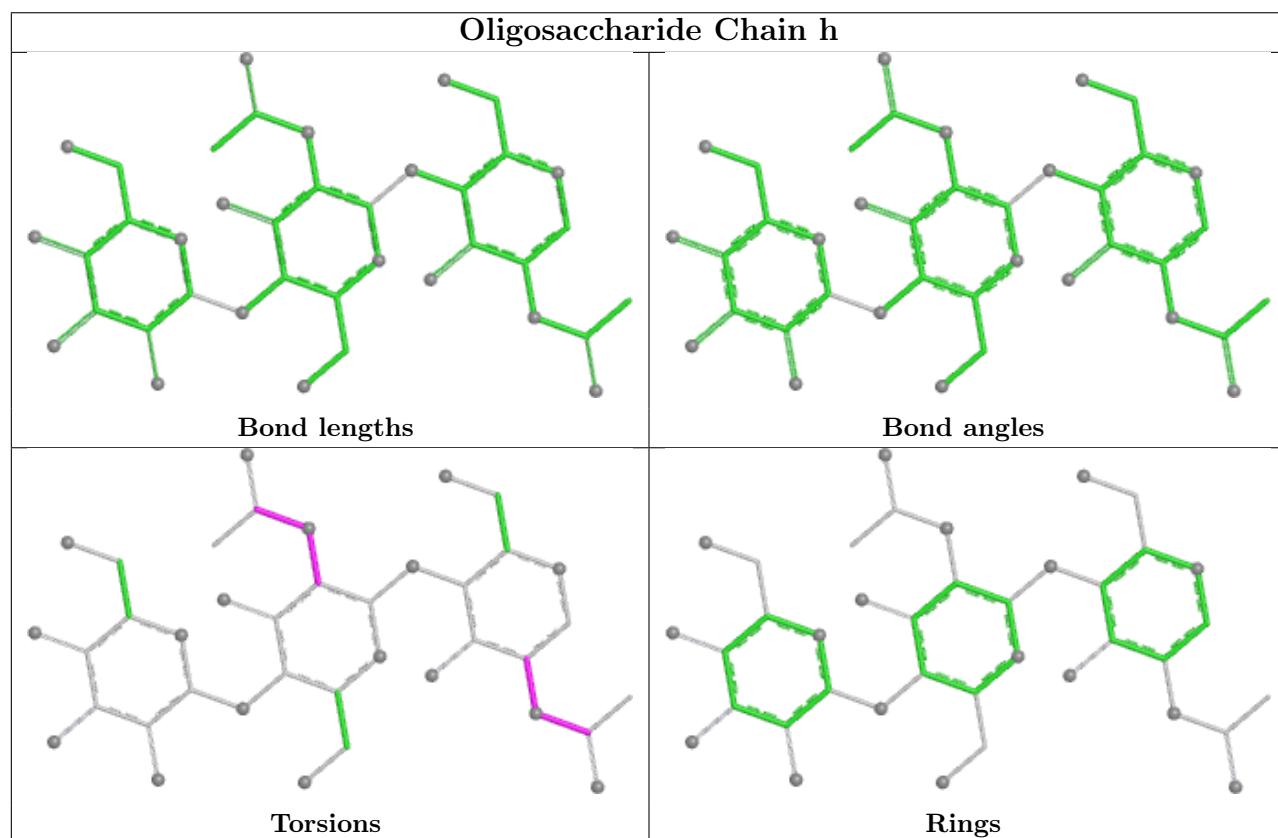
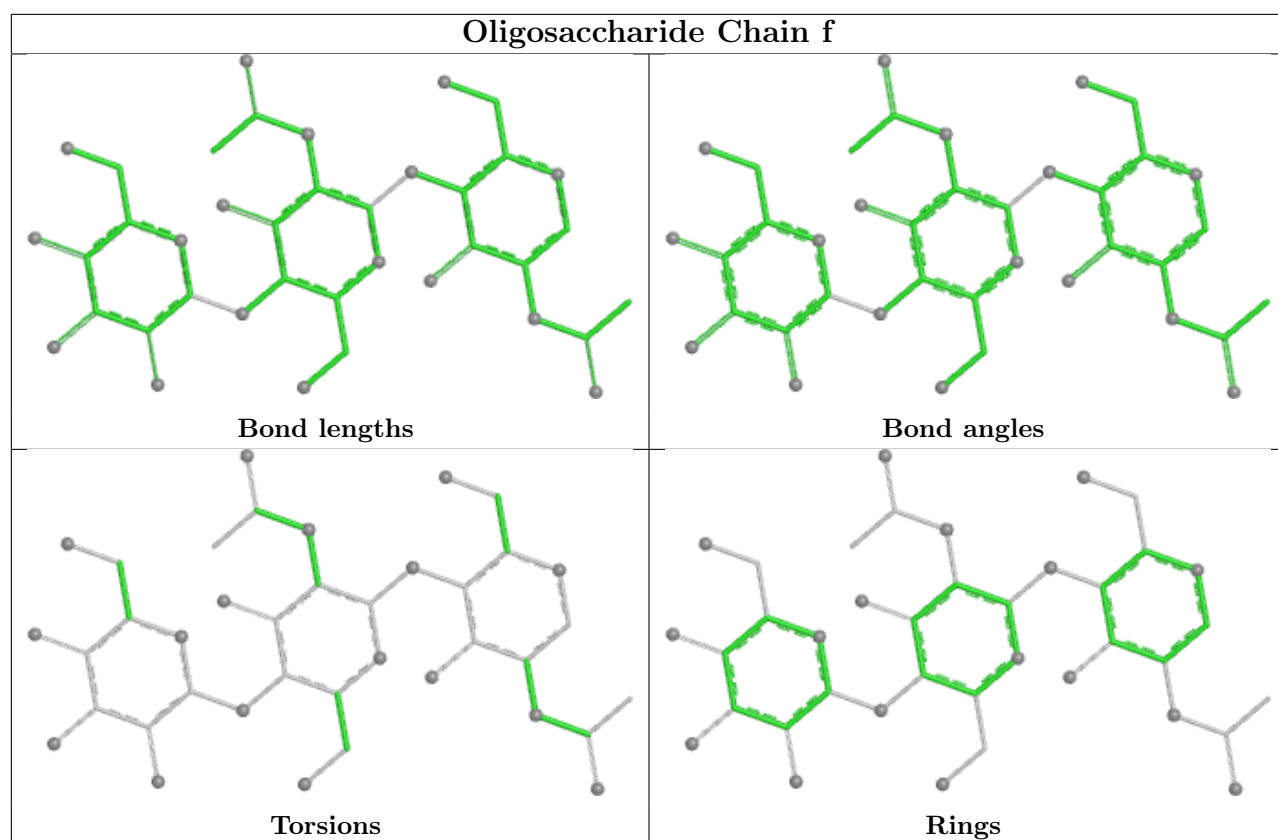


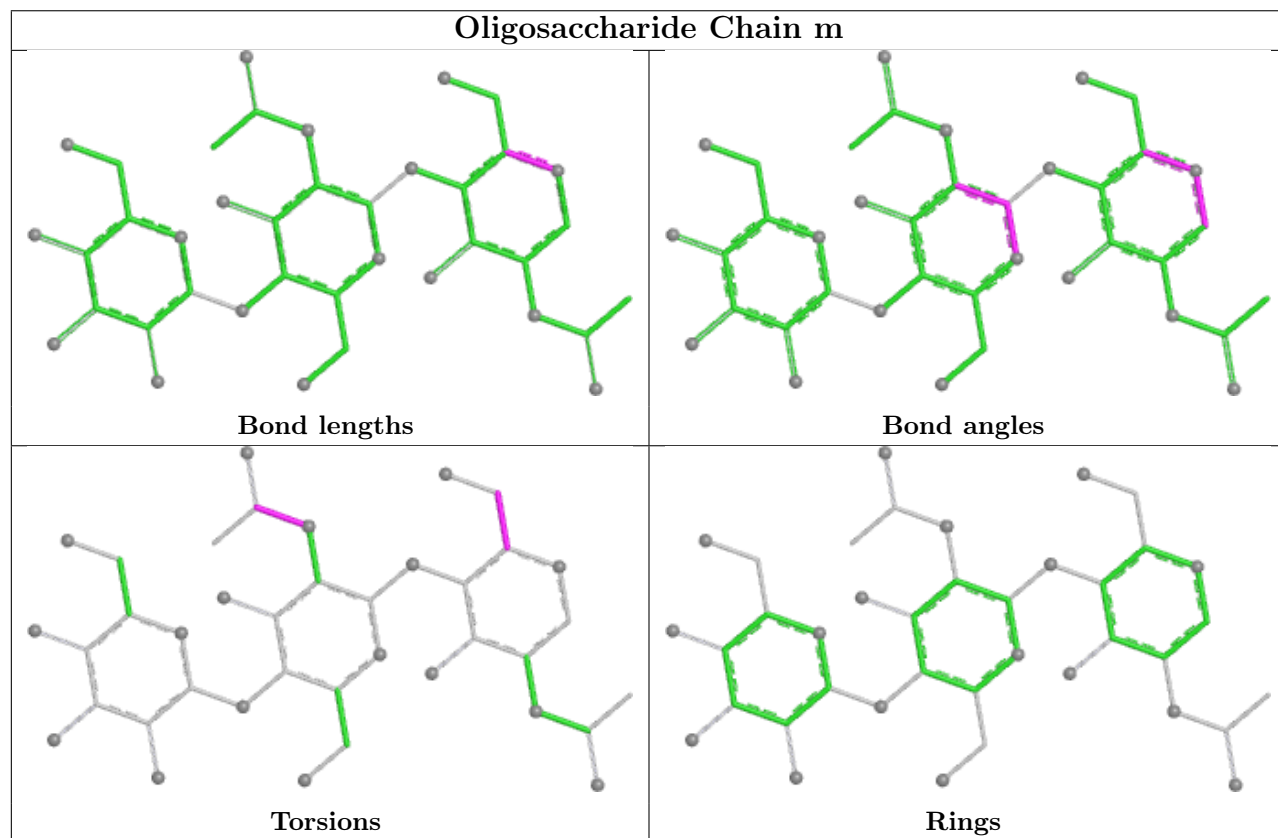
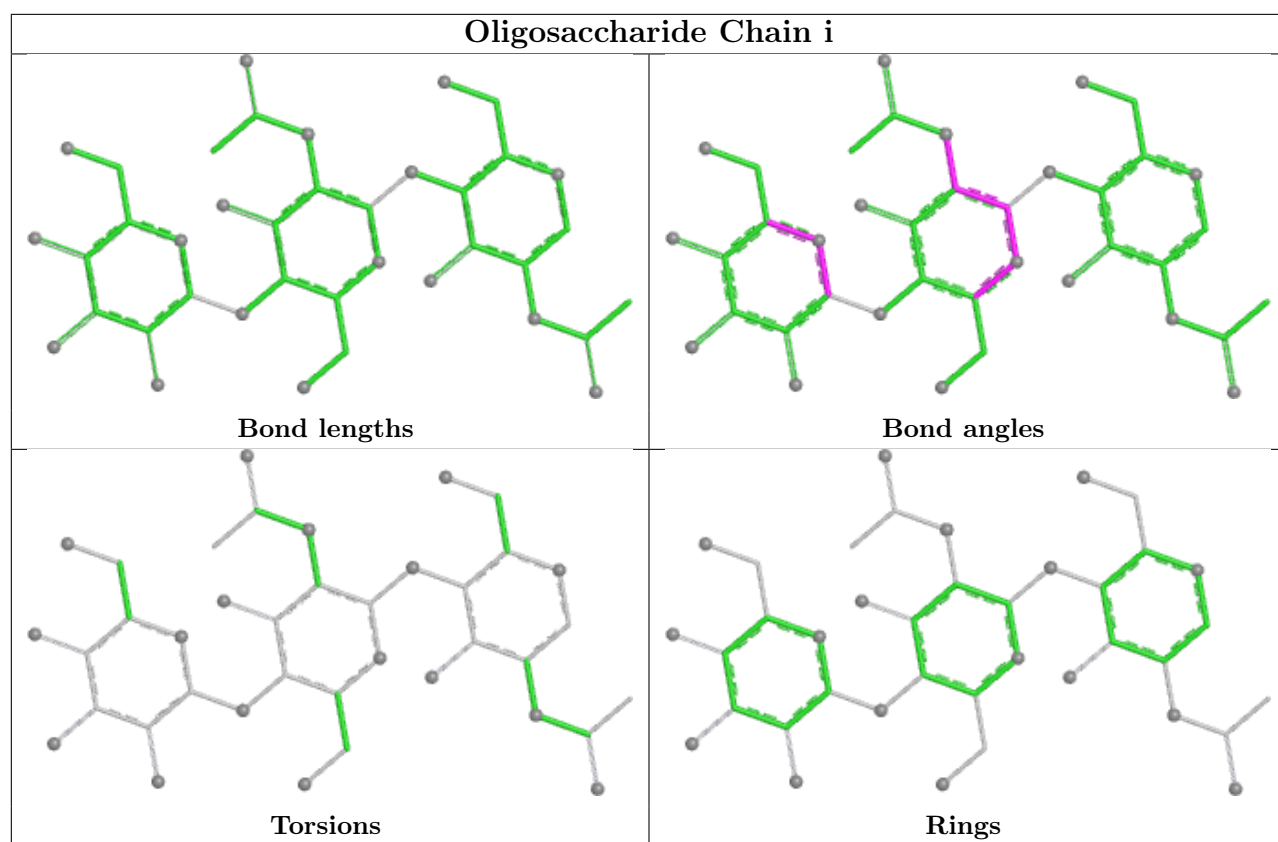


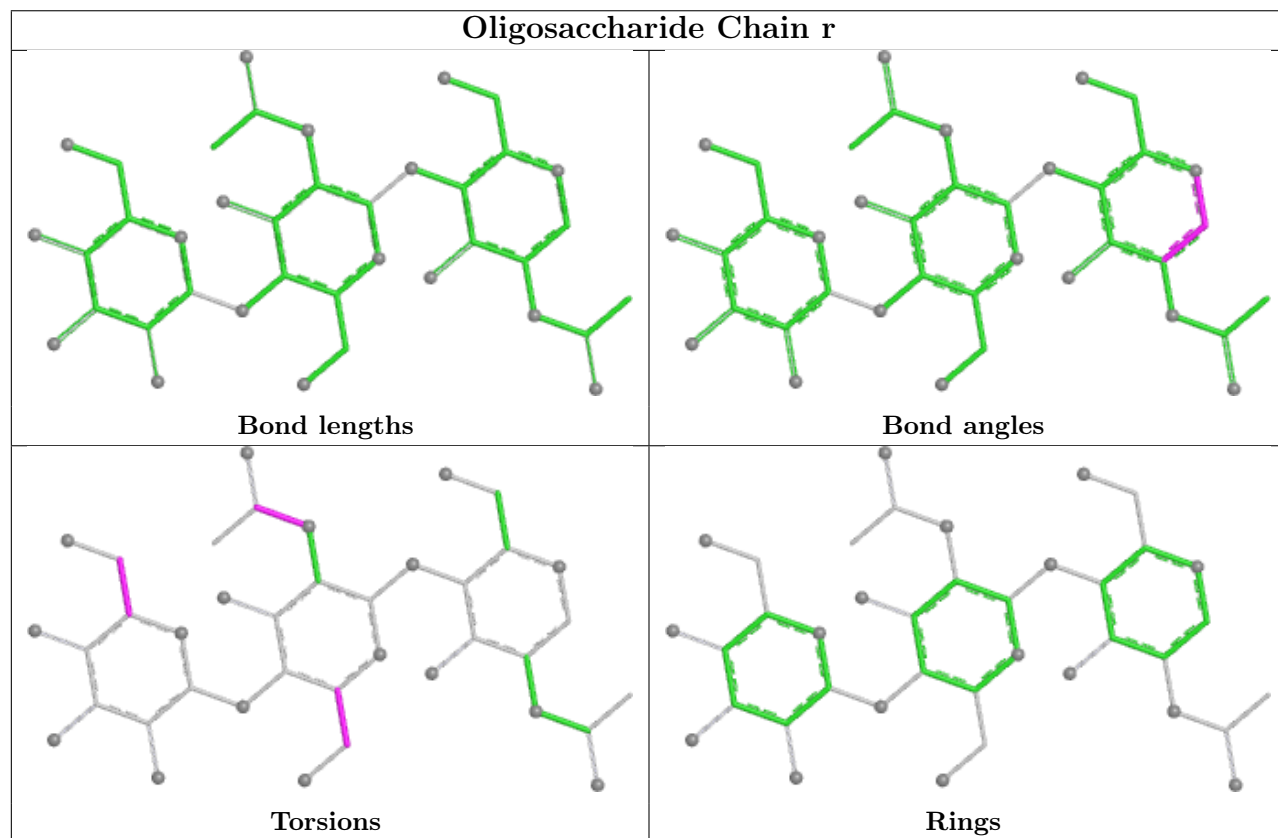
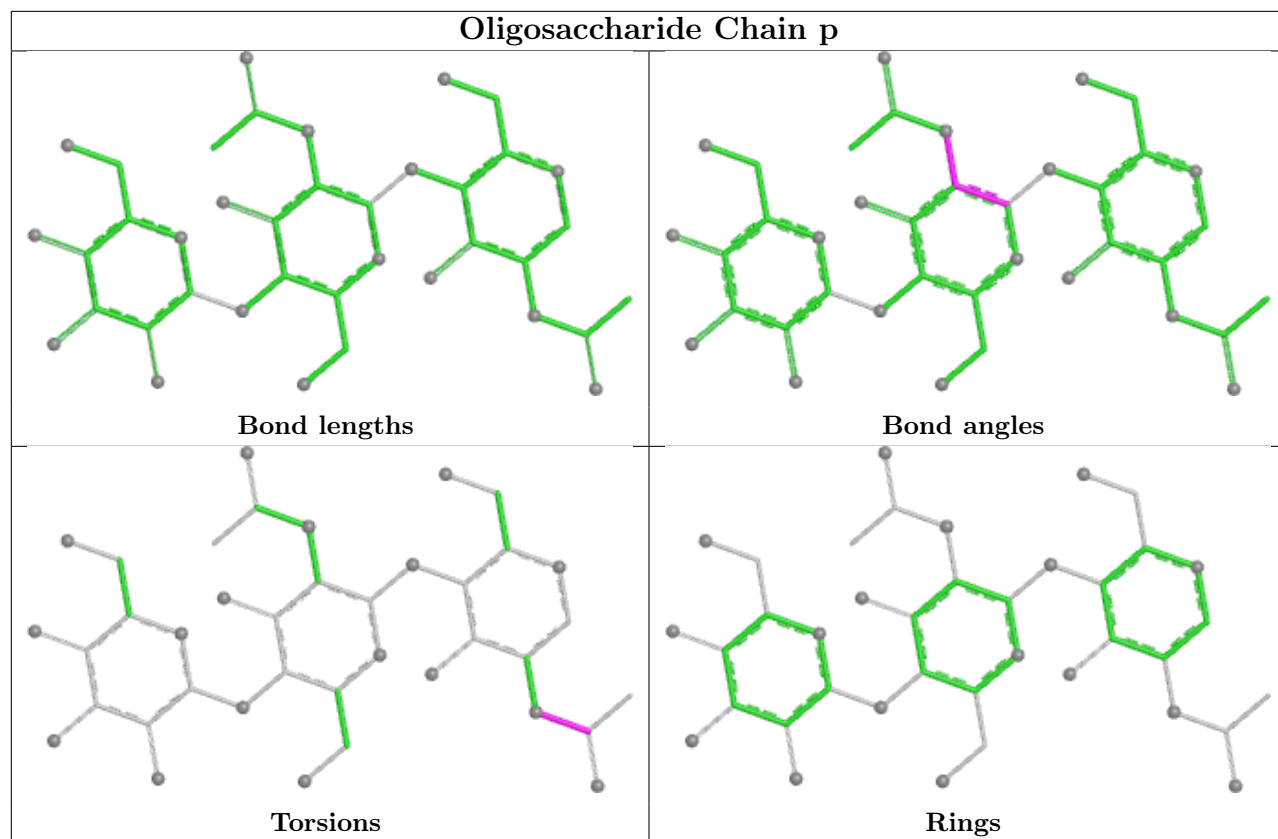


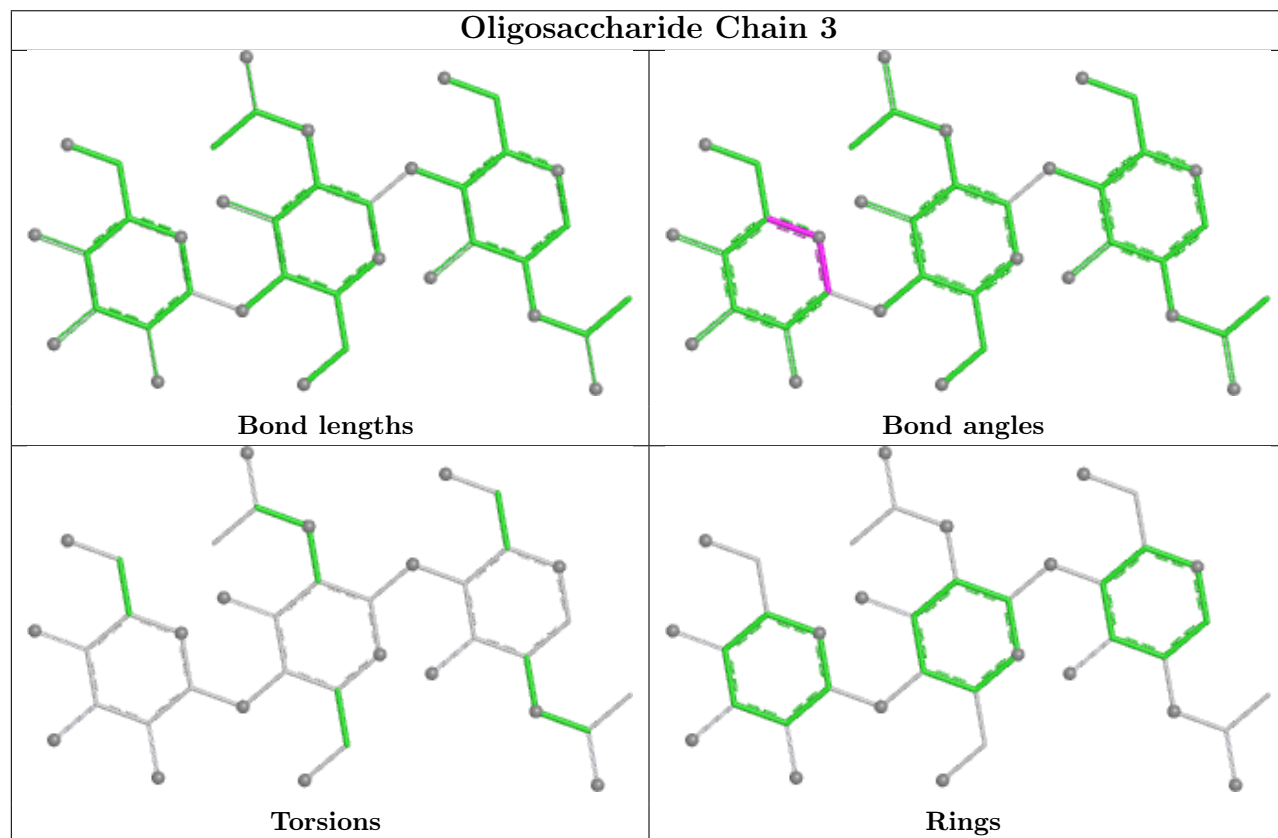
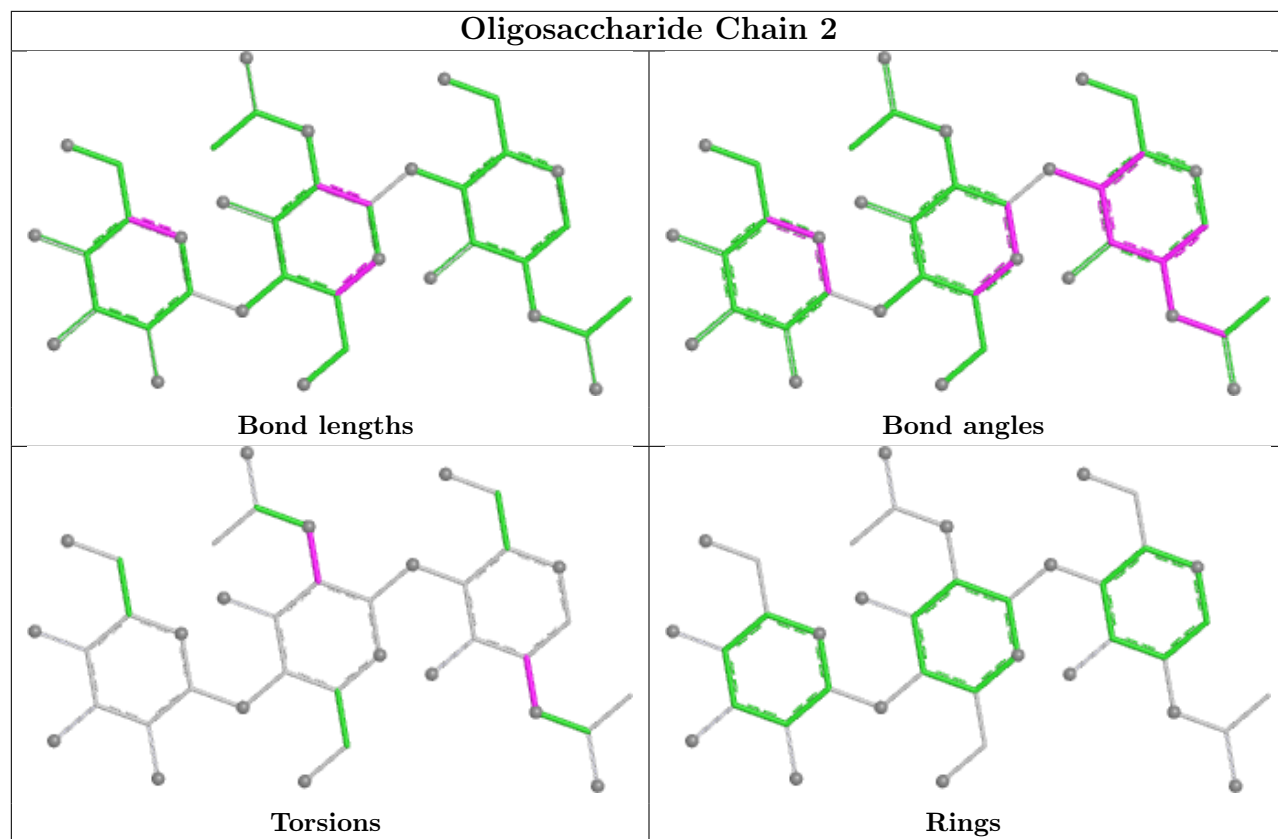


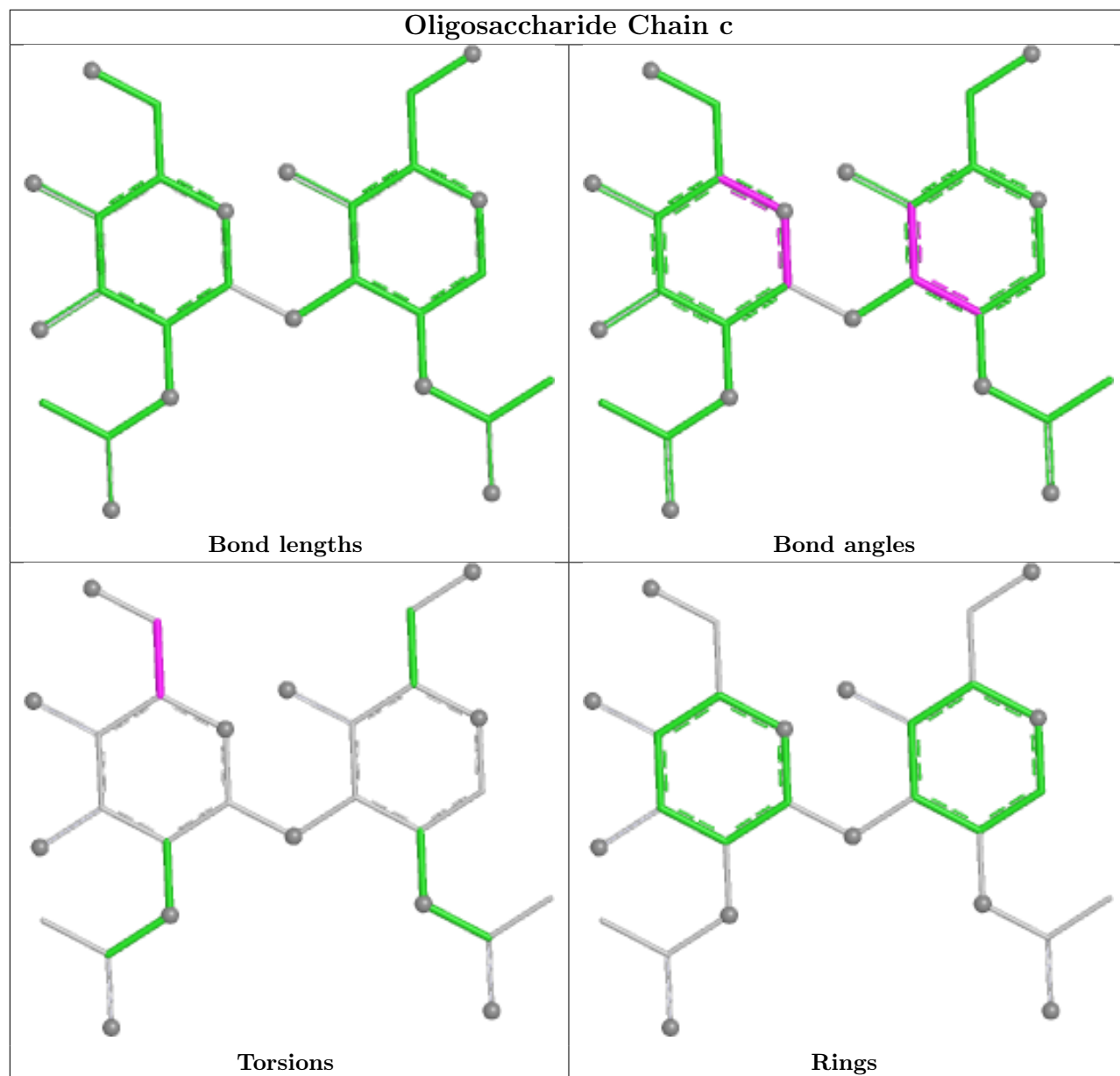


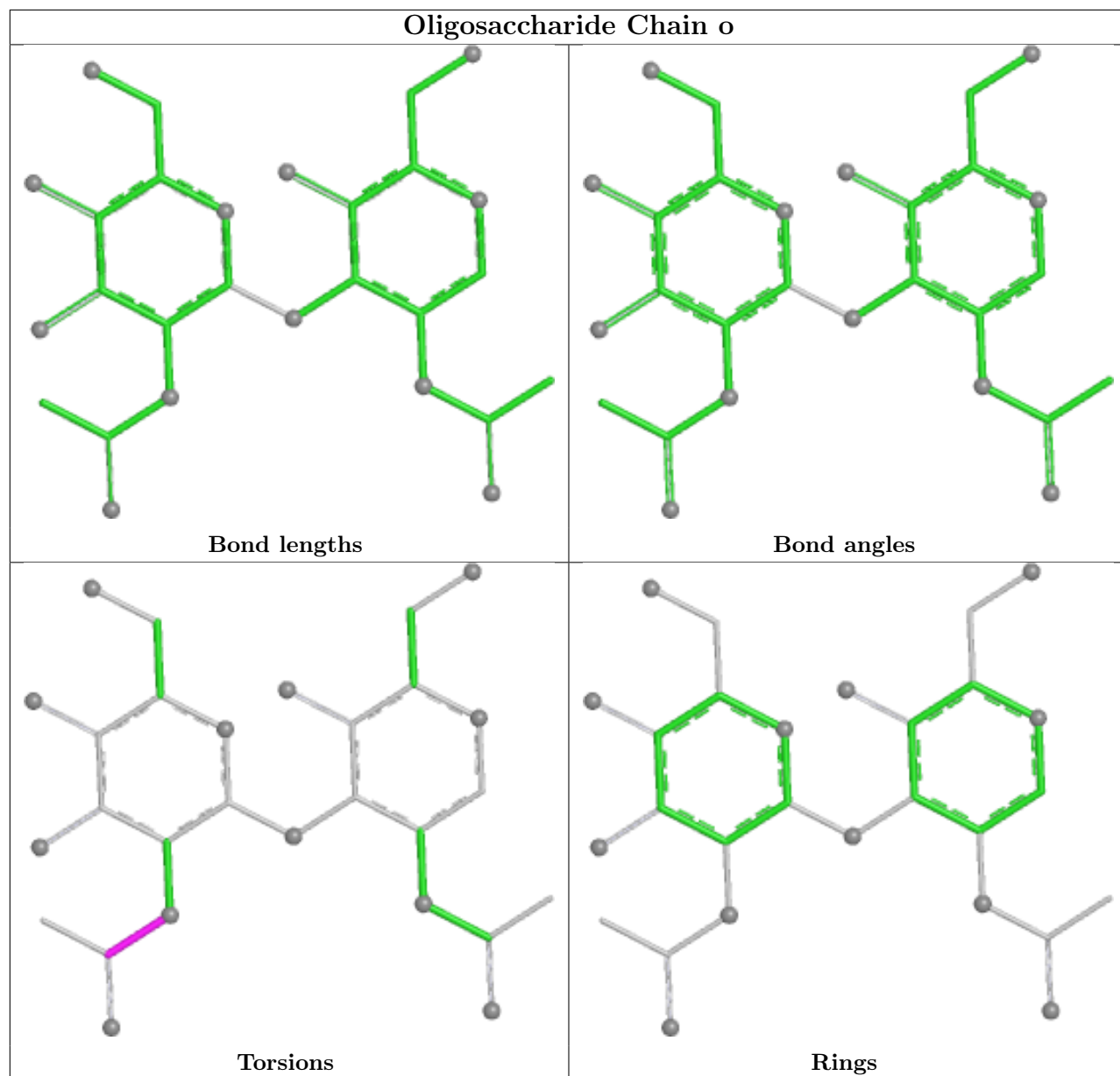


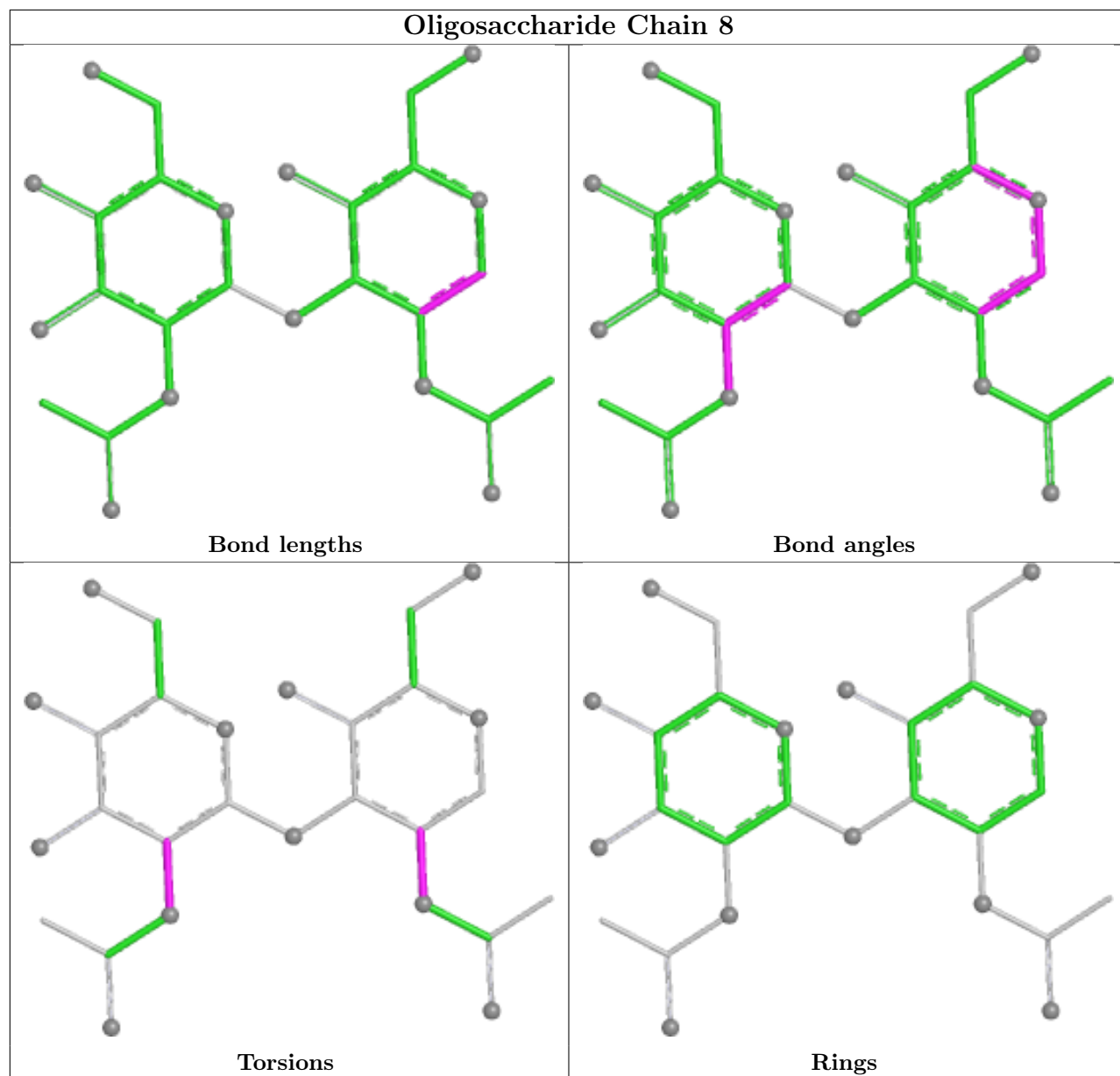


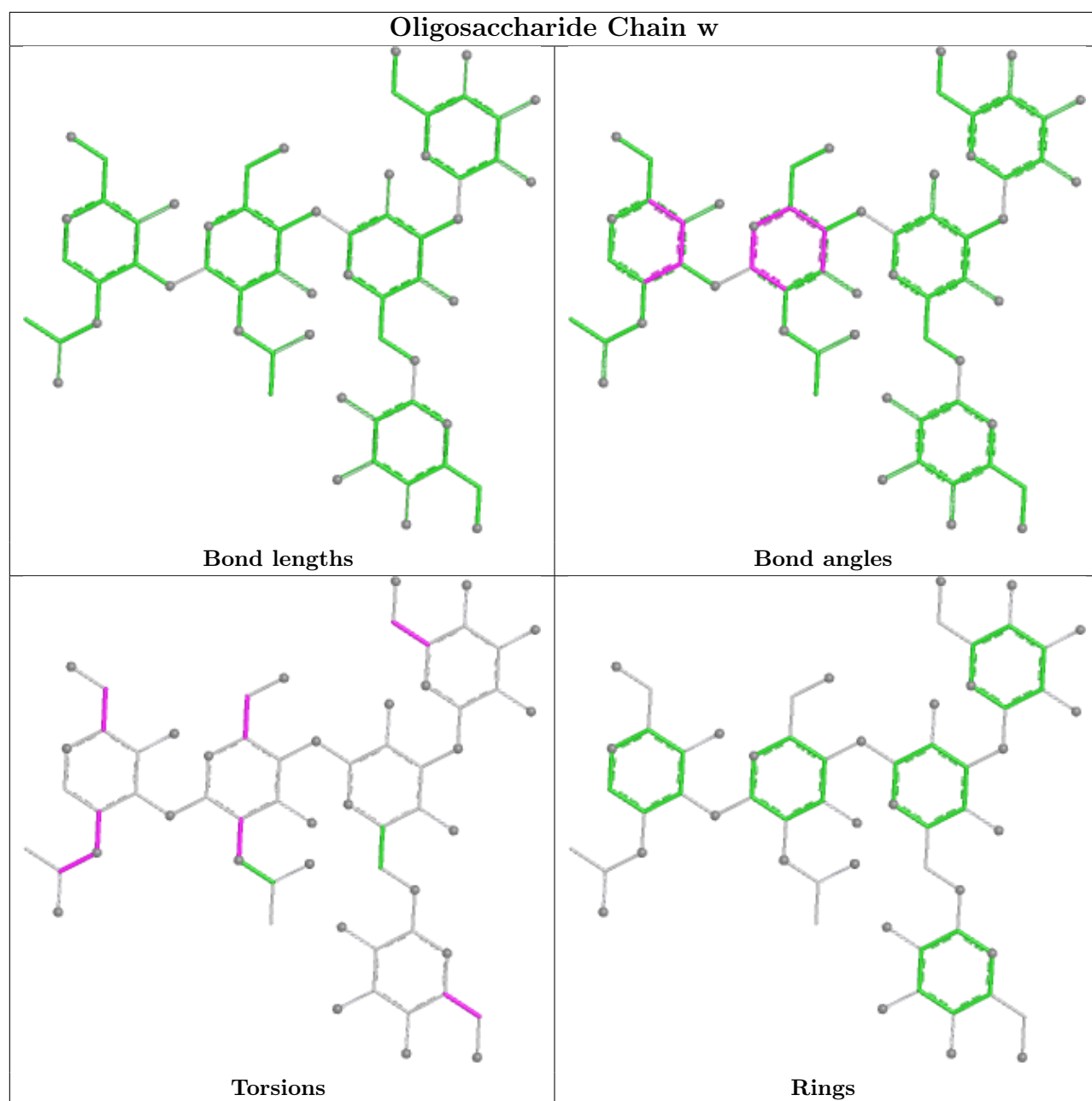


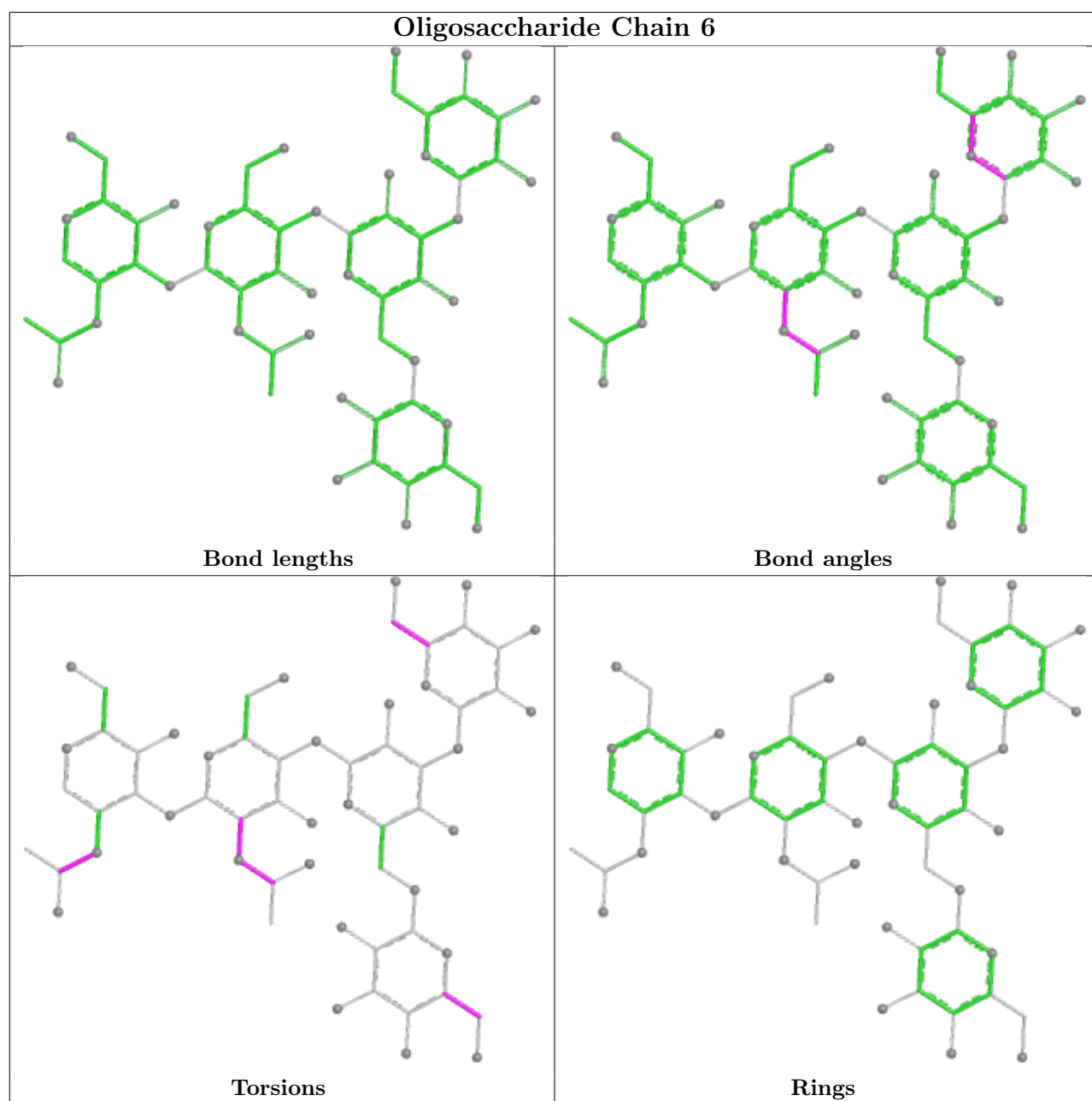


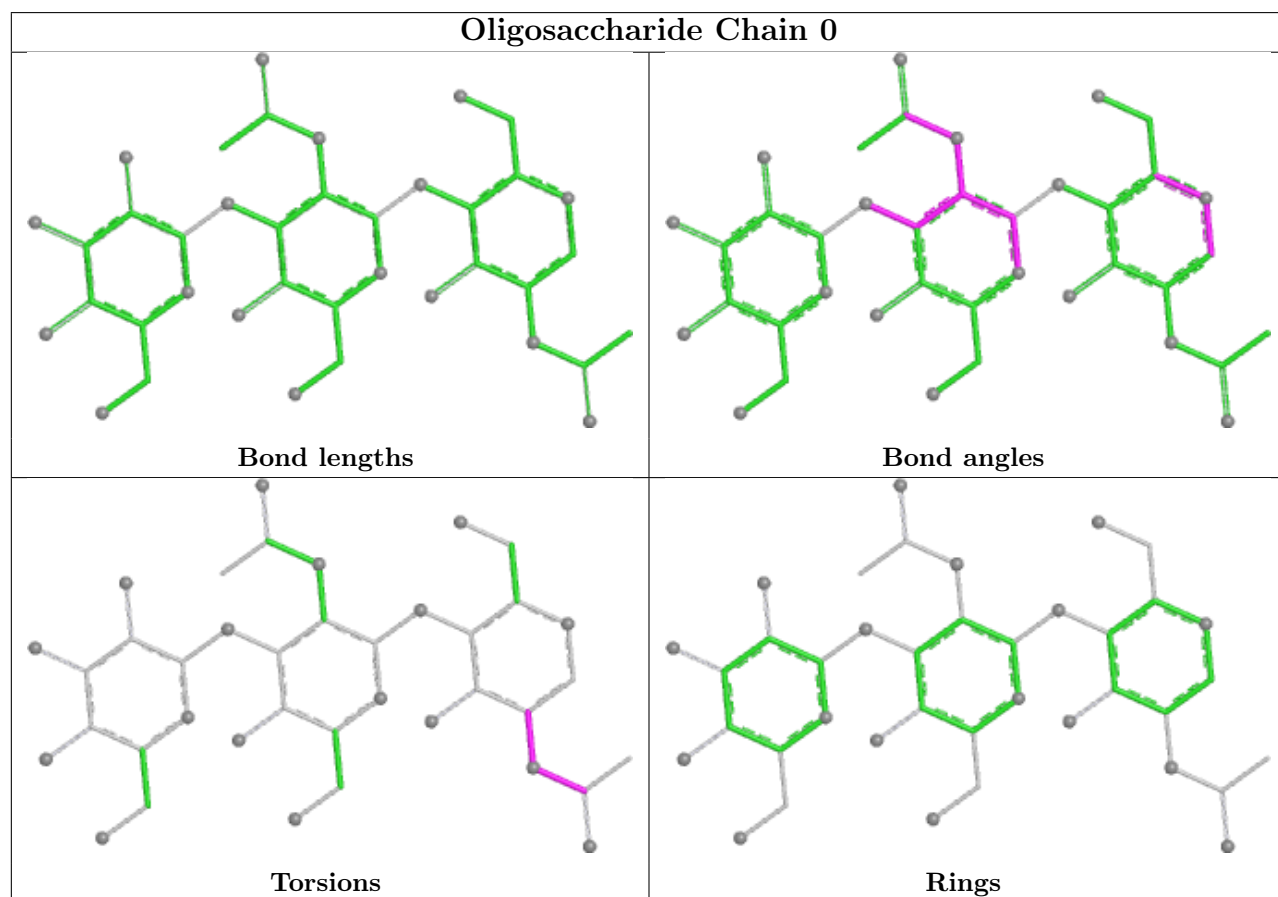
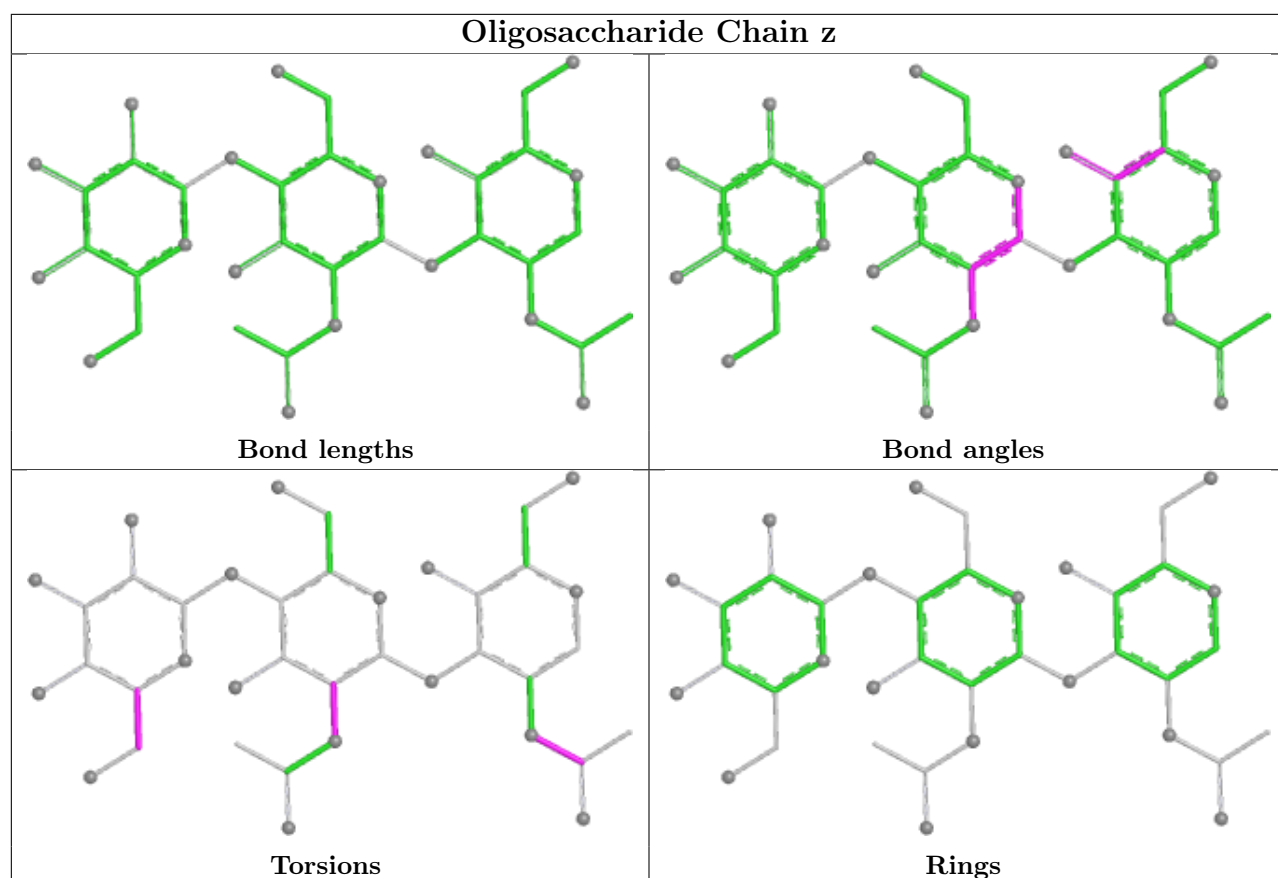


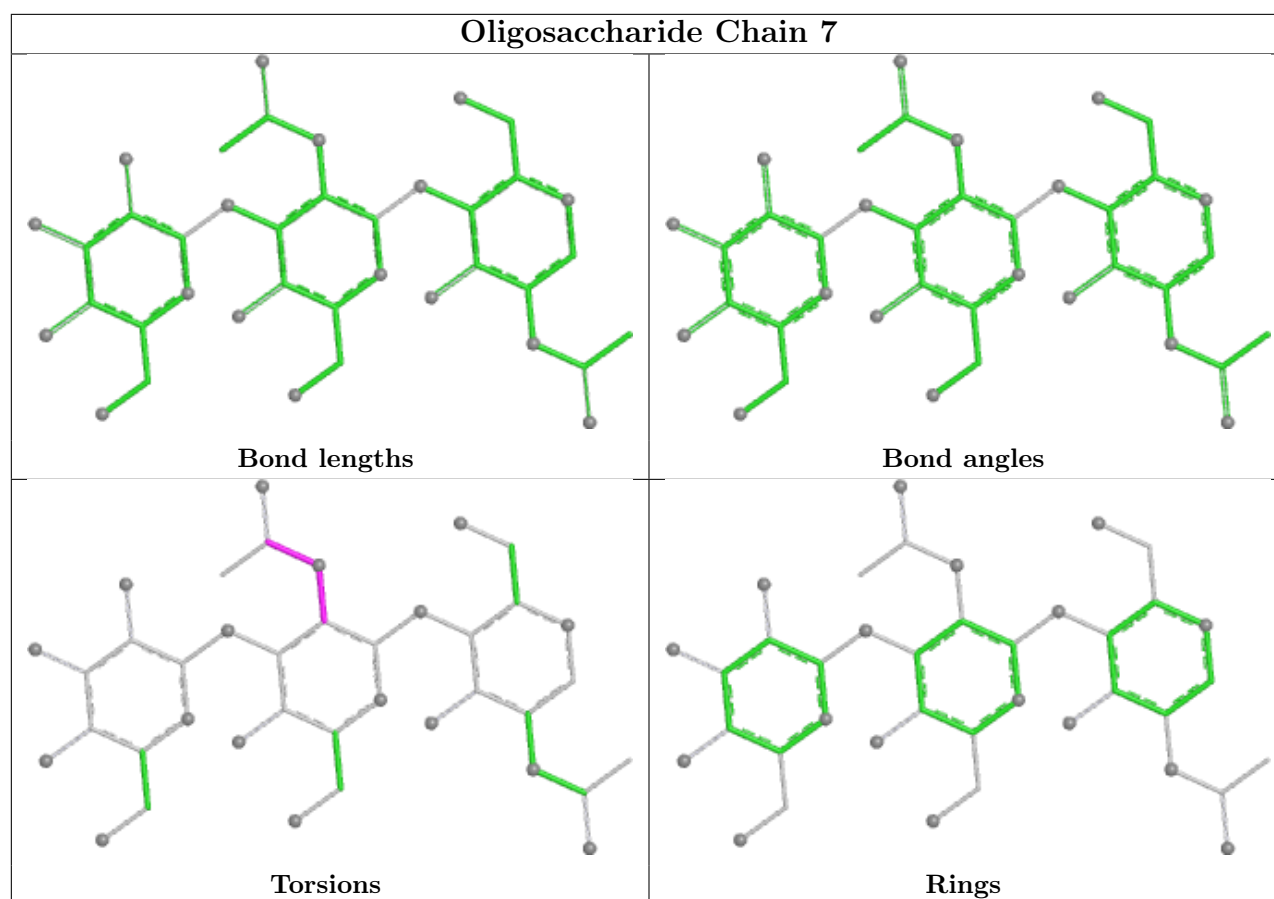












5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	A2G	A	4715	1	14,14,15	0.49	0	17,19,21	1.42	1 (5%)
18	A2G	B	4712	1	14,14,15	0.45	0	17,19,21	1.37	3 (17%)
18	A2G	B	4723	1	14,14,15	0.52	0	17,19,21	0.97	1 (5%)
17	NAG	A	4707	1	14,14,15	0.40	0	17,19,21	1.33	3 (17%)
18	A2G	A	4720	1	14,14,15	0.45	0	17,19,21	0.50	0
18	A2G	B	4714	1	14,14,15	0.91	1 (7%)	17,19,21	0.86	1 (5%)
17	NAG	A	4701	1	14,14,15	0.41	0	17,19,21	0.67	0

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NAG	B	4707	1	14,14,15	0.48	0	17,19,21	0.95	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	A2G	A	4715	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4712	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4723	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4707	1	-	2/6/23/26	0/1/1/1
18	A2G	A	4720	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4714	1	-	1/6/23/26	0/1/1/1
17	NAG	A	4701	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4706	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4708	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4713	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4706	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4722	1	-	1/6/23/26	0/1/1/1
18	A2G	A	4721	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4710	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4716	1	-	1/6/23/26	0/1/1/1
17	NAG	B	4703	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4711	1	-	4/6/23/26	0/1/1/1
17	NAG	B	4705	1	-	3/6/23/26	0/1/1/1
18	A2G	A	4717	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4719	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4723	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4704	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4717	1	-	1/6/23/26	0/1/1/1
17	NAG	B	4701	1	-	3/6/23/26	0/1/1/1
17	NAG	A	4711	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4705	1	-	3/6/23/26	0/1/1/1
17	NAG	A	4702	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4704	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4702	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4712	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4709	1	-	2/6/23/26	0/1/1/1
18	A2G	B	4721	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	A2G	A	4714	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4719	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4710	1	-	2/6/23/26	0/1/1/1
18	A2G	A	4718	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4708	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4703	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4718	1	-	1/6/23/26	0/1/1/1
18	A2G	A	4713	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4722	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4709	1	-	1/6/23/26	0/1/1/1
18	A2G	A	4716	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4720	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4715	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4707	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

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

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	4705	NAG	O5-C1-C2	6.45	121.26	111.29
17	A	4705	NAG	C1-O5-C5	5.81	119.97	112.19
18	A	4712	A2G	C1-C2-N2	4.92	118.19	110.43
18	A	4715	A2G	C1-C2-N2	4.59	117.67	110.43
18	A	4718	A2G	C2-N2-C7	4.26	128.61	122.90
18	B	4722	A2G	C2-N2-C7	4.12	128.43	122.90
18	A	4723	A2G	C1-C2-N2	4.12	116.92	110.43
18	A	4722	A2G	C1-C2-N2	4.10	116.89	110.43
18	A	4718	A2G	C1-C2-N2	4.09	116.88	110.43
18	A	4722	A2G	C2-N2-C7	4.02	128.29	122.90
17	A	4704	NAG	C1-O5-C5	3.79	117.26	112.19
18	A	4712	A2G	C2-N2-C7	3.64	127.77	122.90
18	B	4712	A2G	O5-C1-C2	3.55	116.79	111.29
17	A	4707	NAG	C1-O5-C5	3.47	116.84	112.19
18	A	4716	A2G	C2-N2-C7	3.42	127.48	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	4711	NAG	C1-O5-C5	3.36	116.69	112.19
18	B	4722	A2G	C1-C2-N2	3.14	115.38	110.43
17	A	4702	NAG	C1-O5-C5	3.07	116.30	112.19
17	B	4708	NAG	C1-O5-C5	3.03	116.24	112.19
18	A	4712	A2G	O5-C1-C2	2.94	115.84	111.29
18	B	4719	A2G	O5-C1-C2	2.93	115.82	111.29
18	B	4712	A2G	C1-O5-C5	-2.92	108.27	112.19
18	A	4719	A2G	O5-C1-C2	2.88	115.75	111.29
17	A	4711	NAG	O5-C1-C2	2.84	115.69	111.29
17	B	4709	NAG	C1-O5-C5	2.83	115.98	112.19
18	A	4721	A2G	C1-C2-N2	2.81	114.87	110.43
18	B	4716	A2G	C1-O5-C5	-2.80	108.43	112.19
18	A	4714	A2G	O5-C1-C2	2.76	115.57	111.29
17	B	4707	NAG	C1-O5-C5	2.44	115.45	112.19
17	A	4707	NAG	O5-C1-C2	2.41	115.03	111.29
18	B	4720	A2G	C1-O5-C5	-2.39	108.98	112.19
18	B	4723	A2G	C1-O5-C5	-2.34	109.05	112.19
18	B	4722	A2G	C1-O5-C5	-2.30	109.10	112.19
17	A	4706	NAG	C2-N2-C7	2.30	125.98	122.90
18	A	4718	A2G	O3-C3-C2	2.19	113.94	109.40
18	A	4716	A2G	C1-C2-N2	2.16	113.84	110.43
18	A	4722	A2G	O3-C3-C2	2.16	113.89	109.40
18	B	4721	A2G	C1-O5-C5	-2.13	109.33	112.19
17	A	4707	NAG	C2-N2-C7	-2.13	120.05	122.90
17	A	4710	NAG	C1-C2-N2	2.05	113.66	110.43
18	B	4714	A2G	C1-O5-C5	2.05	114.93	112.19
18	B	4712	A2G	O3-C3-C2	2.04	113.64	109.40
18	A	4719	A2G	C1-O5-C5	-2.04	109.46	112.19
17	A	4706	NAG	C1-C2-N2	2.00	113.59	110.43

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	4704	NAG	C1-C2-N2-C7
17	A	4705	NAG	C3-C2-N2-C7
17	A	4705	NAG	C8-C7-N2-C2
17	A	4705	NAG	O7-C7-N2-C2
17	A	4708	NAG	C8-C7-N2-C2
17	A	4708	NAG	O7-C7-N2-C2
17	B	4701	NAG	C1-C2-N2-C7
17	B	4705	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
17	B	4711	NAG	C1-C2-N2-C7
17	B	4711	NAG	C8-C7-N2-C2
17	B	4711	NAG	O7-C7-N2-C2
18	A	4718	A2G	C3-C2-N2-C7
18	A	4722	A2G	C3-C2-N2-C7
17	A	4709	NAG	C8-C7-N2-C2
17	A	4709	NAG	O7-C7-N2-C2
17	B	4701	NAG	C8-C7-N2-C2
17	B	4705	NAG	C8-C7-N2-C2
17	A	4707	NAG	O5-C5-C6-O6
17	B	4701	NAG	O7-C7-N2-C2
17	B	4705	NAG	O7-C7-N2-C2
18	B	4723	A2G	O5-C5-C6-O6
18	B	4716	A2G	O5-C5-C6-O6
17	B	4710	NAG	C4-C5-C6-O6
17	B	4711	NAG	O5-C5-C6-O6
17	A	4707	NAG	C4-C5-C6-O6
18	A	4722	A2G	O5-C5-C6-O6
18	B	4721	A2G	O5-C5-C6-O6
18	B	4714	A2G	O5-C5-C6-O6
18	B	4718	A2G	O5-C5-C6-O6
18	A	4712	A2G	C3-C2-N2-C7
18	B	4722	A2G	C3-C2-N2-C7
18	B	4712	A2G	O5-C5-C6-O6
17	B	4710	NAG	O5-C5-C6-O6
17	A	4706	NAG	C3-C2-N2-C7
18	A	4716	A2G	C3-C2-N2-C7
17	B	4709	NAG	O5-C5-C6-O6
17	A	4706	NAG	C1-C2-N2-C7
17	A	4704	NAG	C3-C2-N2-C7
18	B	4723	A2G	C4-C5-C6-O6
18	A	4712	A2G	C4-C5-C6-O6
18	B	4717	A2G	C4-C5-C6-O6
18	A	4718	A2G	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

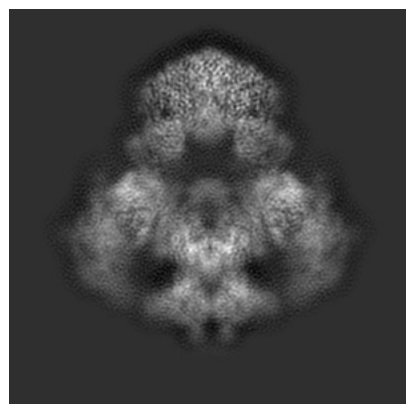
6 Map visualisation [i](#)

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

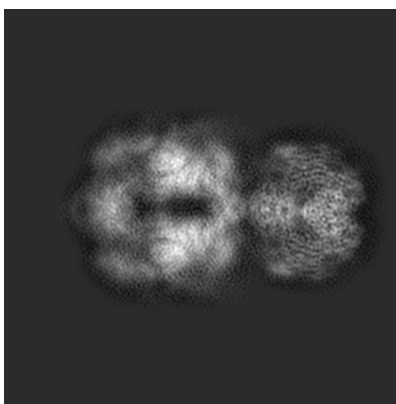
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

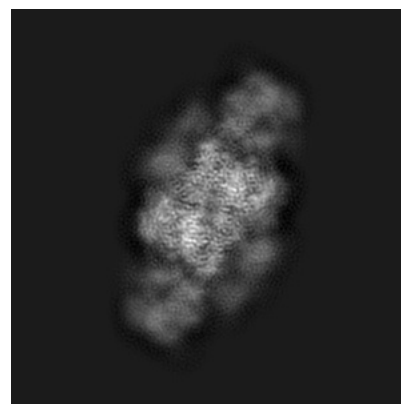
6.1.1 Primary map



X

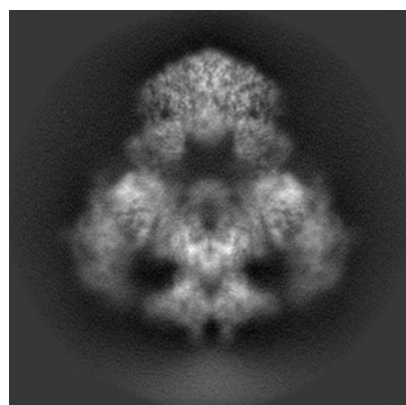


Y

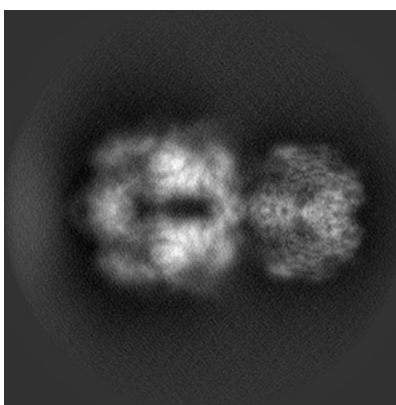


Z

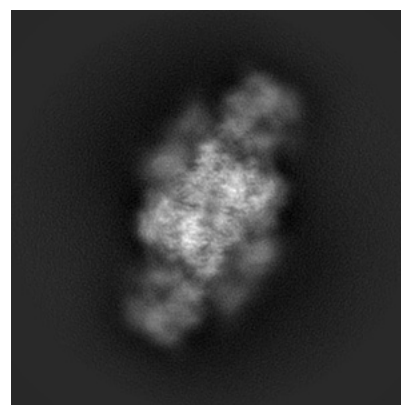
6.1.2 Raw map



X



Y

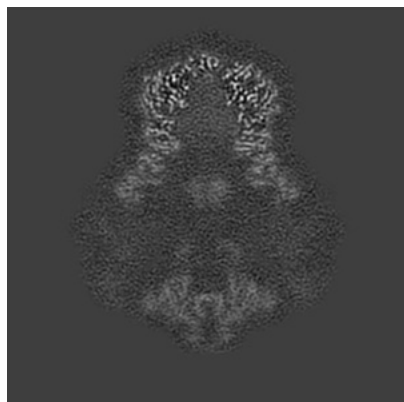


Z

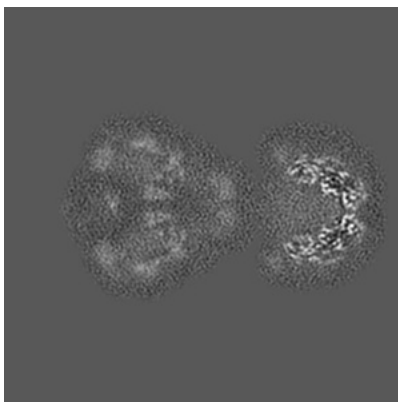
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

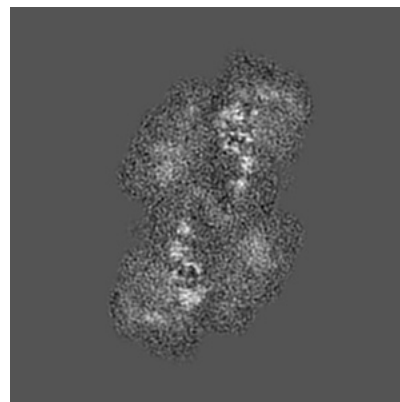
6.2.1 Primary map



X Index: 130

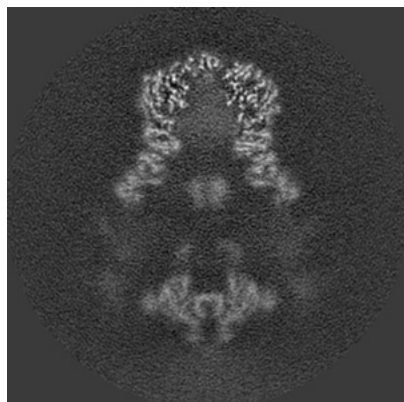


Y Index: 130

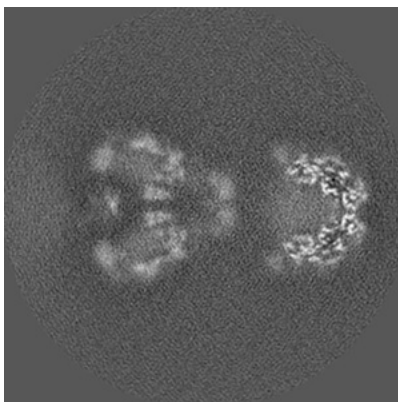


Z Index: 130

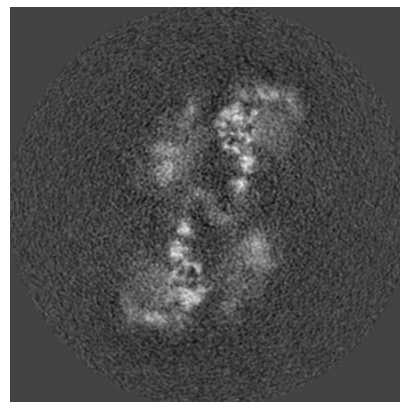
6.2.2 Raw map



X Index: 130



Y Index: 130

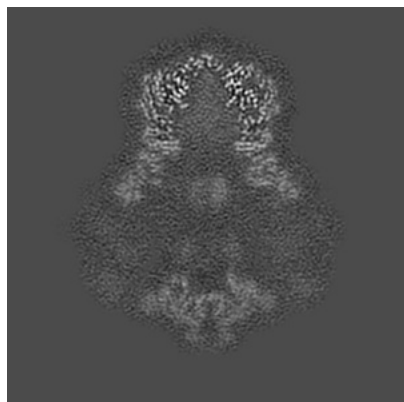


Z Index: 130

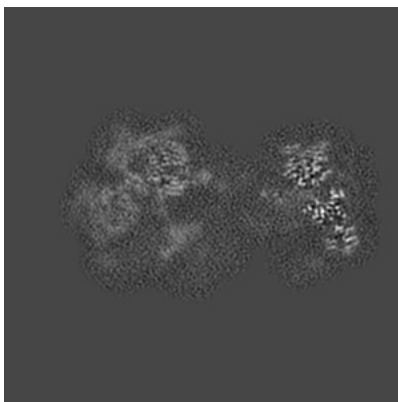
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

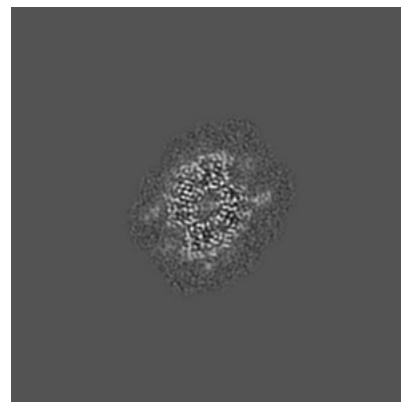
6.3.1 Primary map



X Index: 129

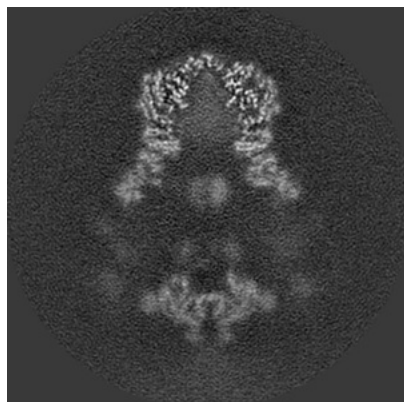


Y Index: 145

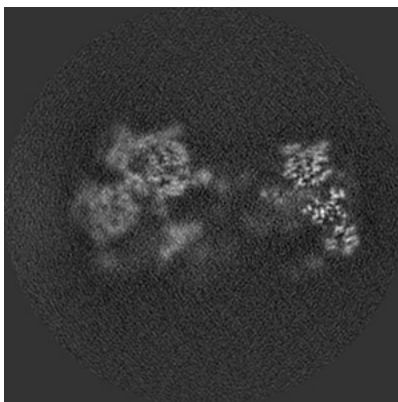


Z Index: 215

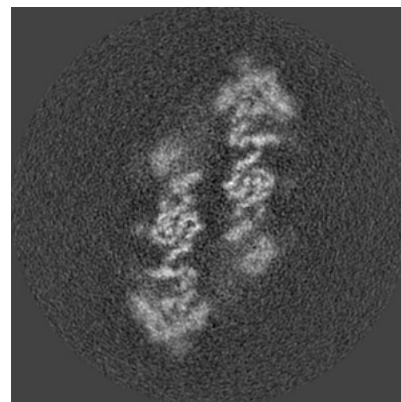
6.3.2 Raw map



X Index: 129



Y Index: 145

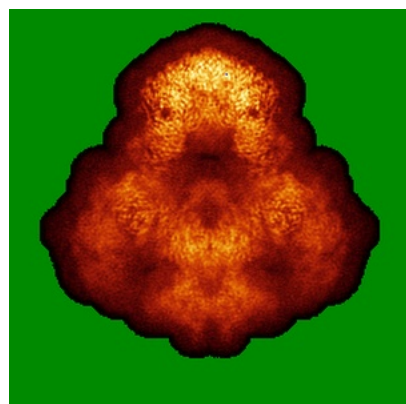


Z Index: 115

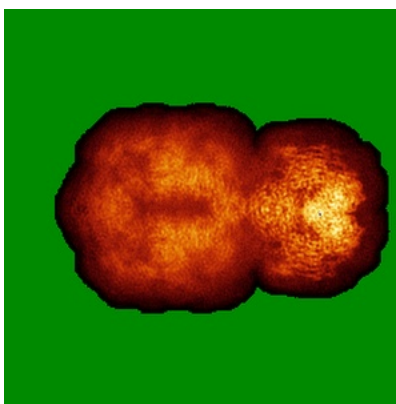
The images above show the largest variance slices of the map in three orthogonal directions.

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

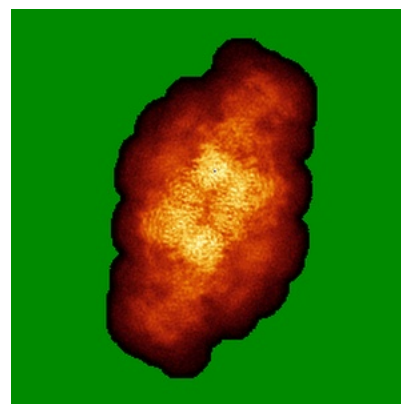
6.4.1 Primary map



X

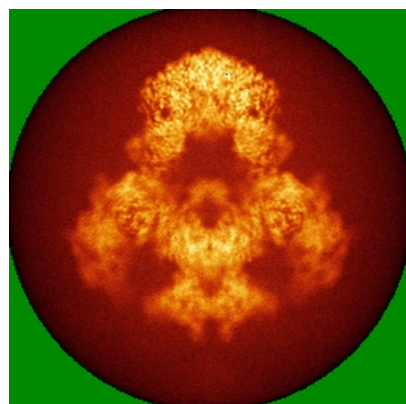


Y

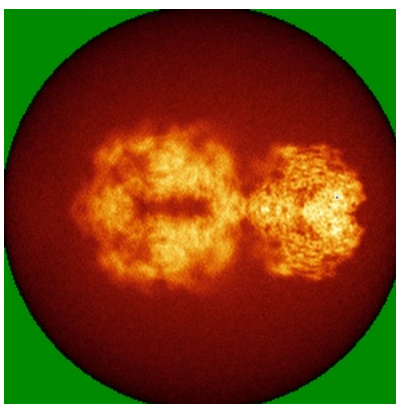


Z

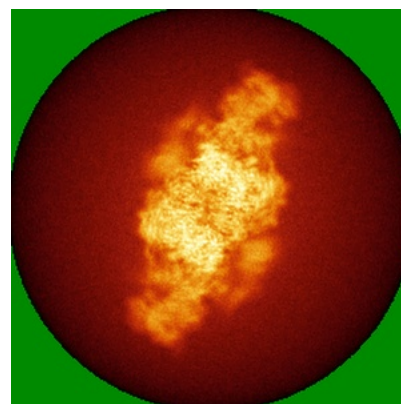
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

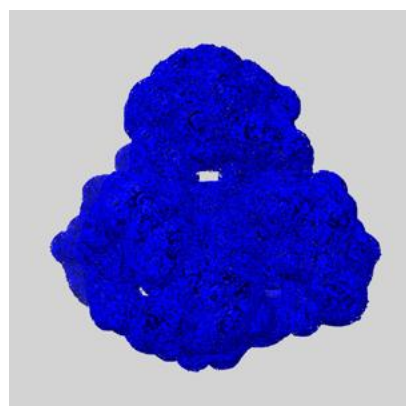
6.6 Mask visualisation [i](#)

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

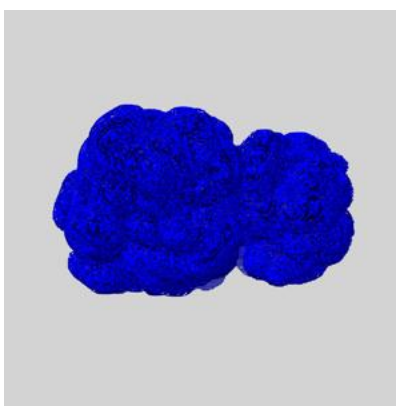
A mask typically either:

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

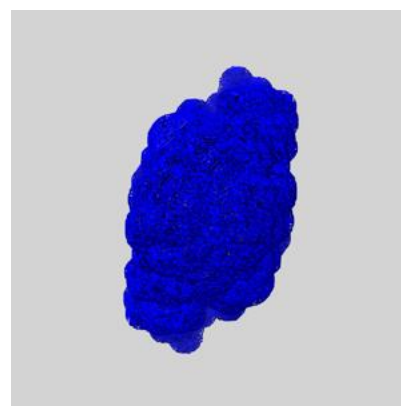
6.6.1 emd_36663_msk_1.map [i](#)



X



Y

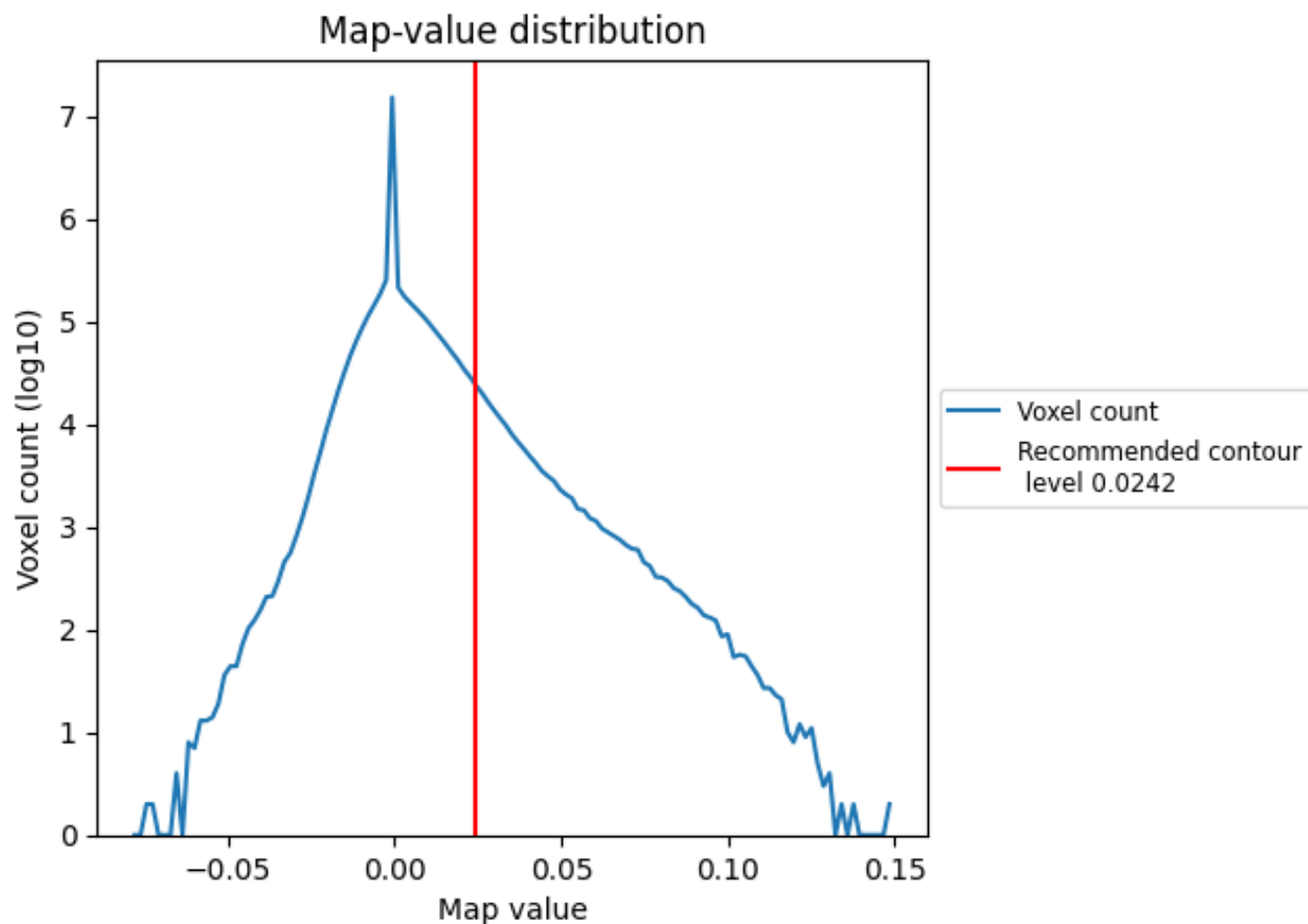


Z

7 Map analysis [i](#)

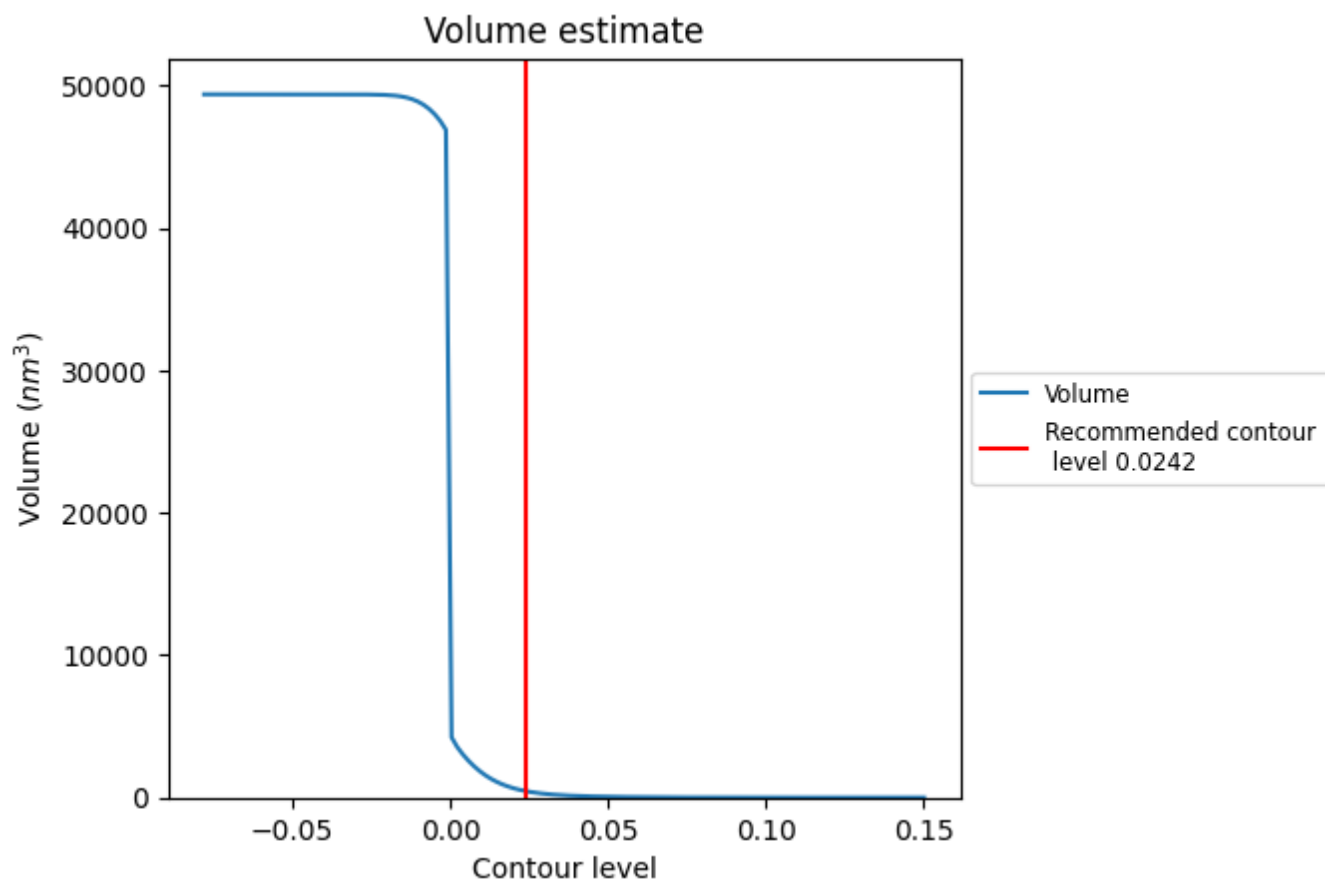
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

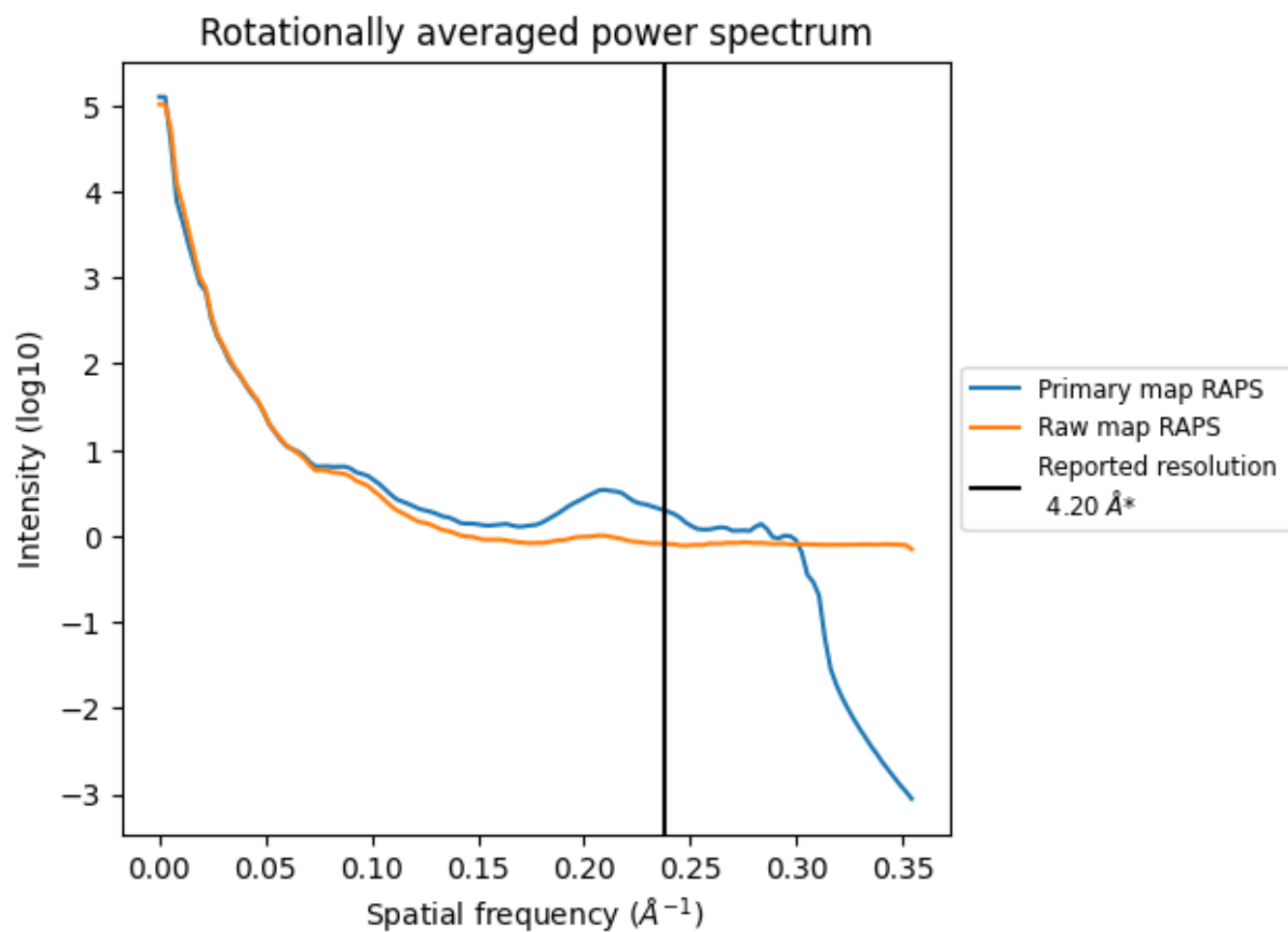
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

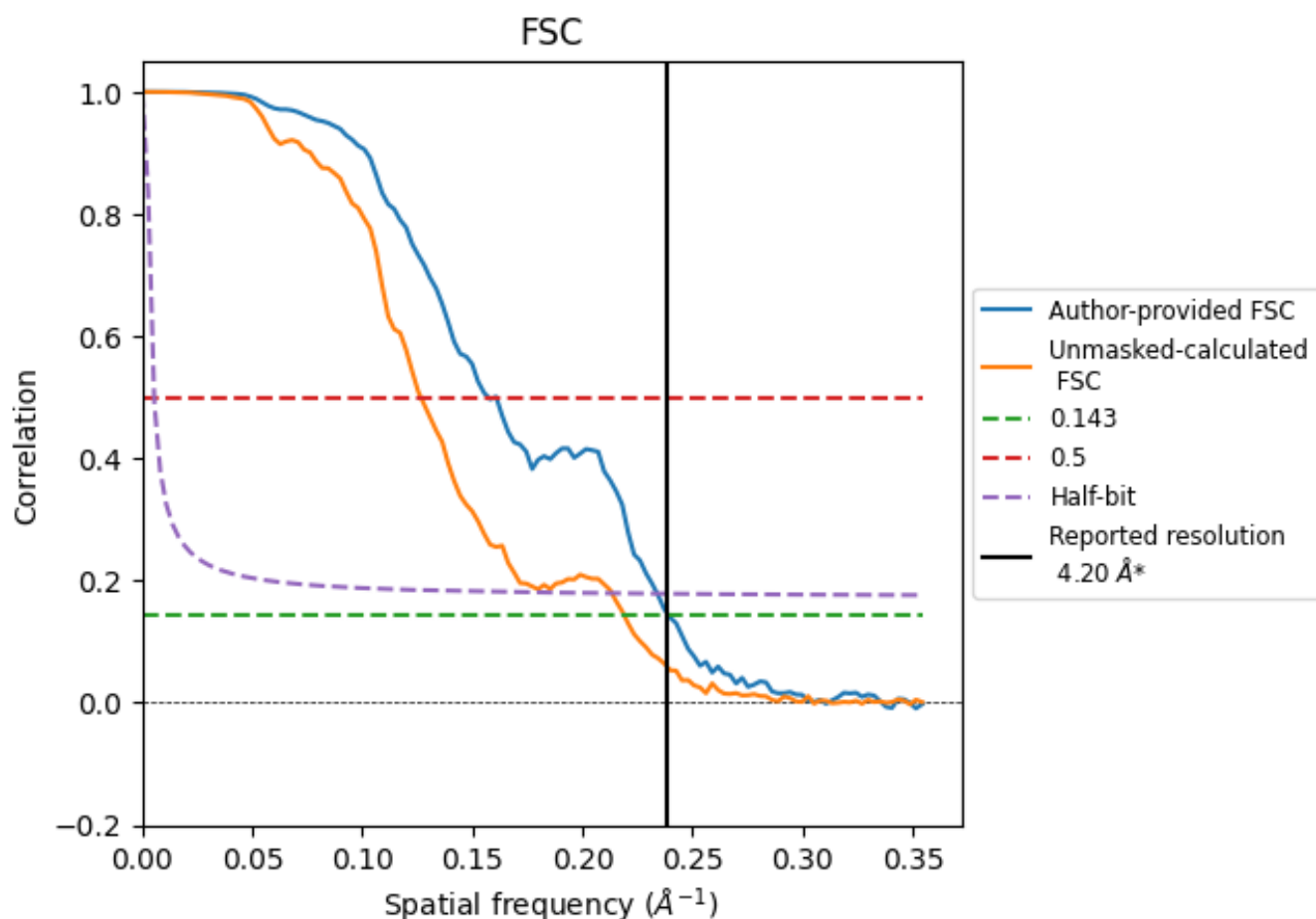


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

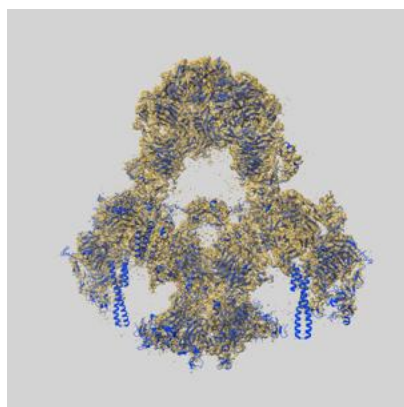
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	6.36	4.27
Unmasked-calculated*	4.57	7.90	4.69

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

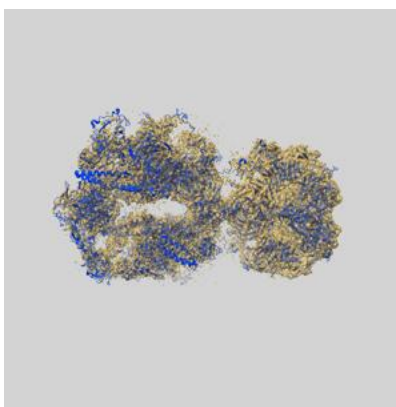
9 Map-model fit [i](#)

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

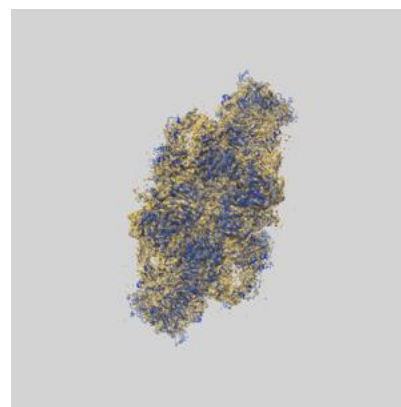
9.1 Map-model overlay [i](#)



X



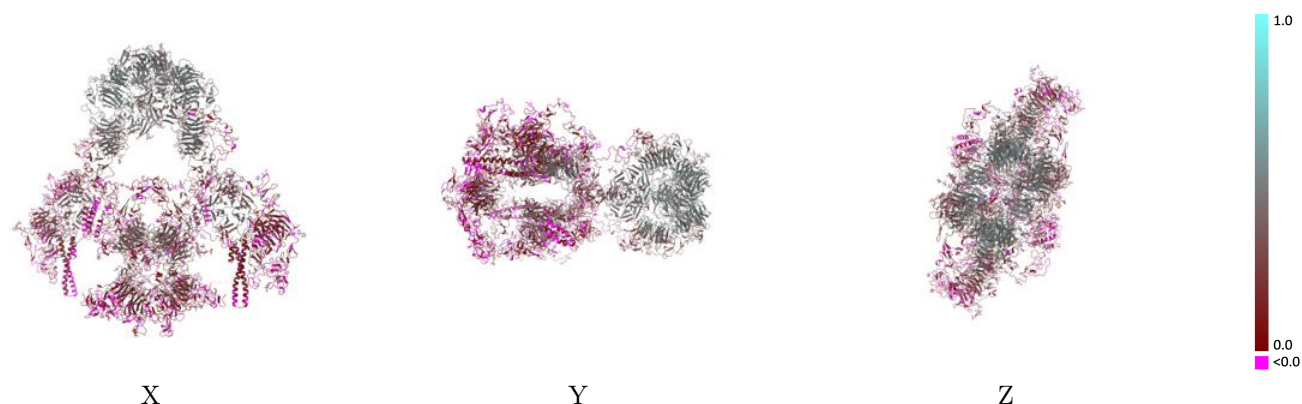
Y



Z

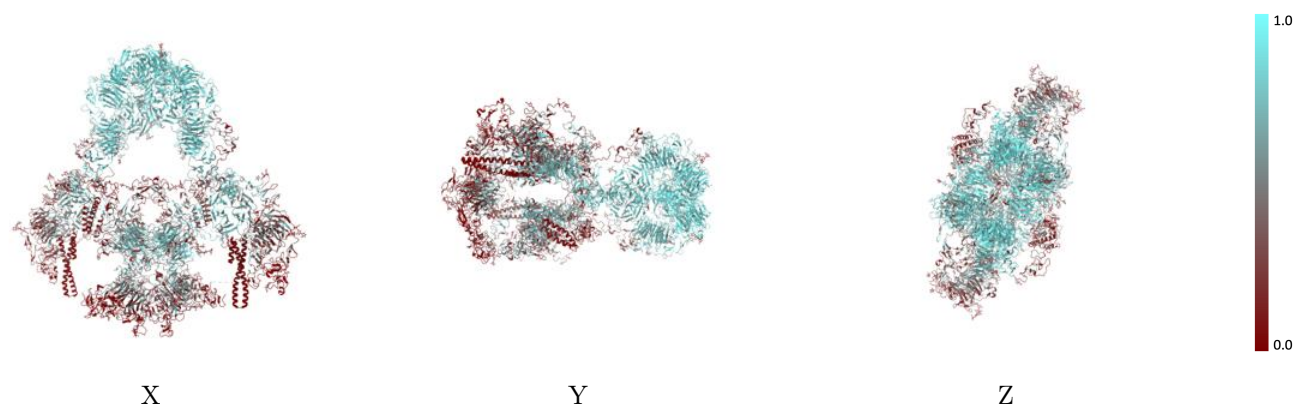
The images above show the 3D surface view of the map at the recommended contour level 0.0242 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



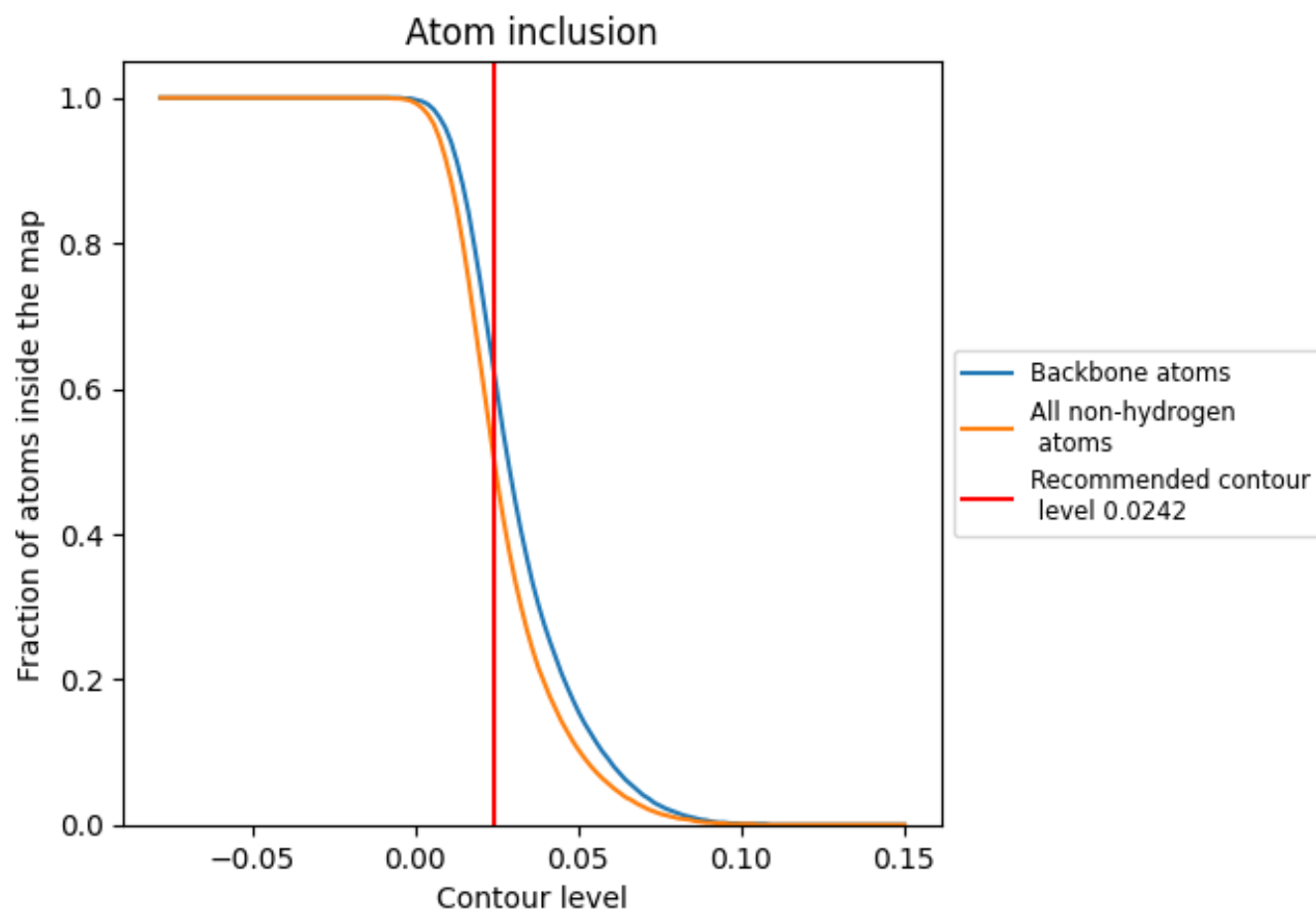
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0242).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0242) and Q-score for the entire model and for each chain.

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



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