



## Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 02:15 PM EDT

PDB ID : 9NVV / pdb\_00009nvv  
EMDB ID : EMD-49865  
Title : Cryo-EM structure of V2 apex germline-targeting HIV Env trimer Q23-APEX-GT2  
Authors : Roark, R.S.; Shapiro, L.S.; Kwong, P.D.  
Deposited on : 2025-03-21  
Resolution : 2.90 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](mailto: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

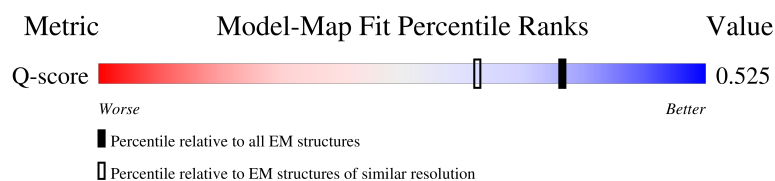
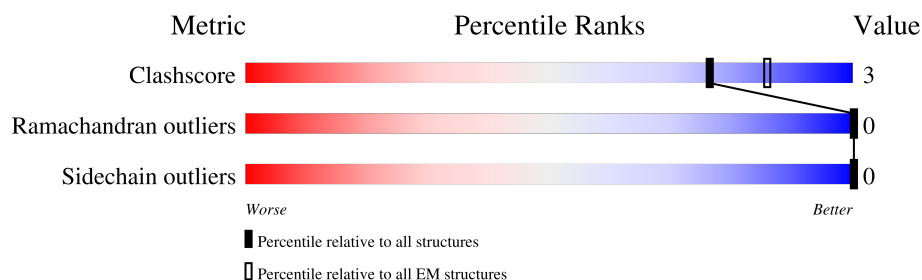
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




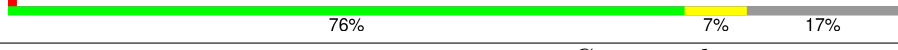
The reported resolution of this entry is 2.90 Å.

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.





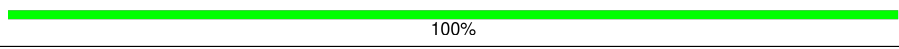

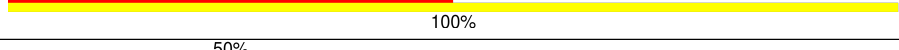
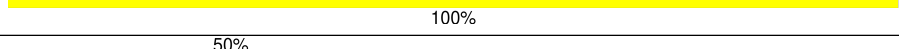
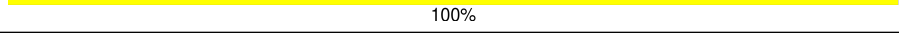
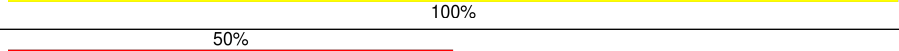


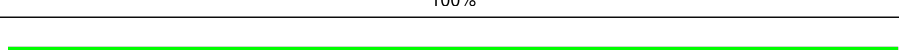


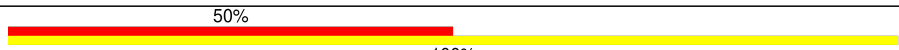
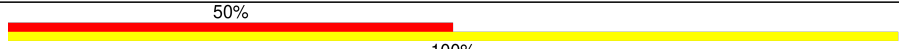
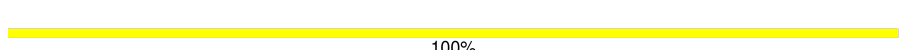




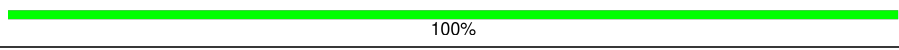
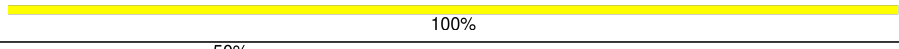
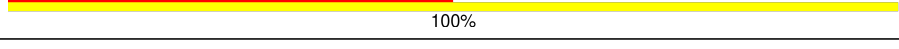
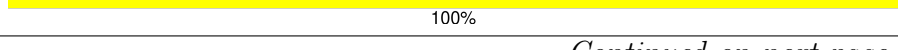

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 ( 2.40 - 3.40 )

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  $\geq 3$ , 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	b	763	
1	d	763	
1	f	763	
2	c	153	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	e	153	
2	g	153	
3	A	2	
3	D	2	
3	E	2	
3	F	2	
3	G	2	
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	U	2	
3	V	2	
3	W	2	
3	X	2	
3	Y	2	
3	Z	2	
3	i	2	
3	j	2	
3	k	2	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	l	2	
3	n	2	
3	o	2	
3	p	2	
3	q	2	
4	B	3	
4	H	3	
4	N	3	
4	T	3	
4	a	3	
4	h	3	
4	m	3	
5	C	4	
6	O	5	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15284 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 HIV envelope gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	b	445	Total	C	N	O	S	0	0
			3530	2221	624	656	29		
1	d	445	Total	C	N	O	S	0	0
			3530	2221	624	656	29		
1	f	445	Total	C	N	O	S	0	0
			3530	2221	624	656	29		

There are 867 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	31	ALA	VAL	conflict	UNP O55774
b	49	GLU	ASP	conflict	UNP O55774
b	132	ARG	THR	conflict	UNP O55774
b	153	GLU	GLY	conflict	UNP O55774
b	158	THR	SER	conflict	UNP O55774
b	201	CYS	ILE	conflict	UNP O55774
b	219	ALA	THR	conflict	UNP O55774
b	302	TYR	ASN	conflict	UNP O55774
b	320	MET	THR	conflict	UNP O55774
b	334	SER	THR	conflict	UNP O55774
b	433	CYS	ALA	conflict	UNP O55774
b	501	CYS	ALA	conflict	UNP O55774
b	508	GLY	ARG	conflict	UNP O55774
b	509	GLY	GLU	conflict	UNP O55774
b	510	GLY	LYS	conflict	UNP O55774
b	511	GLY	ARG	conflict	UNP O55774
b	512	SER	ALA	conflict	UNP O55774
b	513	GLY	VAL	conflict	UNP O55774
b	515	GLY	ILE	conflict	UNP O55774
b	517	SER	ALA	conflict	UNP O55774
b	518	PHE	-	insertion	UNP O55774
b	519	GLU	-	insertion	UNP O55774
b	520	PRO	-	insertion	UNP O55774
b	521	ILE	VAL	conflict	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
b	522	PRO	PHE	conflict	UNP O55774
b	523	ILE	LEU	conflict	UNP O55774
b	524	HIS	GLY	conflict	UNP O55774
b	525	TYR	PHE	conflict	UNP O55774
b	526	CYS	LEU	conflict	UNP O55774
b	527	ALA	GLY	conflict	UNP O55774
b	528	PRO	ALA	conflict	UNP O55774
b	531	PHE	-	insertion	UNP O55774
b	532	ALA	-	insertion	UNP O55774
b	533	ILE	-	insertion	UNP O55774
b	534	LEU	-	insertion	UNP O55774
b	535	LYS	-	insertion	UNP O55774
b	536	CYS	-	insertion	UNP O55774
b	537	LYS	-	insertion	UNP O55774
b	538	ASP	-	insertion	UNP O55774
b	539	GLU	-	insertion	UNP O55774
b	540	GLY	-	insertion	UNP O55774
b	541	PHE	-	insertion	UNP O55774
b	542	ASN	-	insertion	UNP O55774
b	543	GLY	-	insertion	UNP O55774
b	544	THR	-	insertion	UNP O55774
b	545	GLY	-	insertion	UNP O55774
b	546	LEU	-	insertion	UNP O55774
b	547	CYS	-	insertion	UNP O55774
b	548	LYS	-	insertion	UNP O55774
b	549	ASN	-	insertion	UNP O55774
b	550	VAL	-	insertion	UNP O55774
b	553	VAL	MET	conflict	UNP O55774
b	554	GLN	GLY	conflict	UNP O55774
b	555	CYS	ALA	conflict	UNP O55774
b	557	HIS	-	insertion	UNP O55774
b	558	GLY	SER	conflict	UNP O55774
b	560	LYS	THR	conflict	UNP O55774
b	561	PRO	LEU	conflict	UNP O55774
b	562	VAL	THR	conflict	UNP O55774
b	564	SER	GLN	conflict	UNP O55774
b	565	THR	ALA	conflict	UNP O55774
b	566	GLN	ARG	conflict	UNP O55774
b	567	LEU	GLN	conflict	UNP O55774
b	570	ASN	SER	conflict	UNP O55774
b	572	SER	ILE	conflict	UNP O55774
b	573	LEU	VAL	conflict	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
b	574	ALA	GLN	conflict	UNP O55774
b	575	GLU	GLN	conflict	UNP O55774
b	576	LYS	GLN	conflict	UNP O55774
b	578	ILE	ASN	conflict	UNP O55774
b	579	THR	LEU	conflict	UNP O55774
b	580	ILE	LEU	conflict	UNP O55774
b	582	SER	ALA	conflict	UNP O55774
b	583	GLU	ILE	conflict	UNP O55774
b	584	ASN	GLU	conflict	UNP O55774
b	585	ILE	ALA	conflict	UNP O55774
b	586	THR	GLN	conflict	UNP O55774
b	587	ASN	GLN	conflict	UNP O55774
b	588	ASN	HIS	conflict	UNP O55774
b	589	ALA	LEU	conflict	UNP O55774
b	590	LYS	LEU	conflict	UNP O55774
b	591	ILE	LYS	conflict	UNP O55774
b	592	ILE	LEU	conflict	UNP O55774
b	593	ILE	THR	conflict	UNP O55774
b	595	GLN	TRP	conflict	UNP O55774
b	596	LEU	GLY	conflict	UNP O55774
b	597	VAL	ILE	conflict	UNP O55774
b	598	GLN	LYS	conflict	UNP O55774
b	599	PRO	GLN	conflict	UNP O55774
b	600	VAL	LEU	conflict	UNP O55774
b	601	THR	GLN	conflict	UNP O55774
b	602	ILE	ALA	conflict	UNP O55774
b	603	LYS	ARG	conflict	UNP O55774
b	604	CYS	VAL	conflict	UNP O55774
b	605	ILE	LEU	conflict	UNP O55774
b	606	ARG	ALA	conflict	UNP O55774
b	607	PRO	VAL	conflict	UNP O55774
b	608	ASN	GLU	conflict	UNP O55774
b	609	ASN	ARG	conflict	UNP O55774
b	611	THR	LEU	conflict	UNP O55774
b	613	LYS	ASP	conflict	UNP O55774
b	614	SER	GLN	conflict	UNP O55774
b	615	ILE	GLN	conflict	UNP O55774
b	616	ARG	LEU	conflict	UNP O55774
b	617	ILE	LEU	conflict	UNP O55774
b	619	PRO	-	expression tag	UNP O55774
b	620	GLY	-	expression tag	UNP O55774
b	621	GLN	-	expression tag	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
b	622	ALA	-	expression tag	UNP O55774
b	623	PHE	-	expression tag	UNP O55774
b	624	TYR	-	expression tag	UNP O55774
b	625	ALA	-	expression tag	UNP O55774
b	626	MET	-	expression tag	UNP O55774
b	627	GLY	-	expression tag	UNP O55774
b	628	ASP	-	expression tag	UNP O55774
b	629	ILE	-	expression tag	UNP O55774
b	630	ILE	-	expression tag	UNP O55774
b	631	GLY	-	expression tag	UNP O55774
b	632	ASP	-	expression tag	UNP O55774
b	633	ILE	-	expression tag	UNP O55774
b	634	ARG	-	expression tag	UNP O55774
b	635	GLN	-	expression tag	UNP O55774
b	636	ALA	-	expression tag	UNP O55774
b	637	HIS	-	expression tag	UNP O55774
b	638	CYS	-	expression tag	UNP O55774
b	639	ASN	-	expression tag	UNP O55774
b	640	VAL	-	expression tag	UNP O55774
b	641	SER	-	expression tag	UNP O55774
b	642	ARG	-	expression tag	UNP O55774
b	643	SER	-	expression tag	UNP O55774
b	644	ARG	-	expression tag	UNP O55774
b	645	TRP	-	expression tag	UNP O55774
b	646	ASN	-	expression tag	UNP O55774
b	647	LYS	-	expression tag	UNP O55774
b	648	THR	-	expression tag	UNP O55774
b	649	LEU	-	expression tag	UNP O55774
b	650	GLN	-	expression tag	UNP O55774
b	651	GLU	-	expression tag	UNP O55774
b	652	VAL	-	expression tag	UNP O55774
b	653	ALA	-	expression tag	UNP O55774
b	654	GLU	-	expression tag	UNP O55774
b	655	LYS	-	expression tag	UNP O55774
b	656	LEU	-	expression tag	UNP O55774
b	657	ARG	-	expression tag	UNP O55774
b	658	THR	-	expression tag	UNP O55774
b	659	TYR	-	expression tag	UNP O55774
b	660	PHE	-	expression tag	UNP O55774
b	661	GLY	-	expression tag	UNP O55774
b	662	ASN	-	expression tag	UNP O55774
b	663	LYS	-	expression tag	UNP O55774

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
b	664	THR	-	expression tag	UNP O55774
b	665	ILE	-	expression tag	UNP O55774
b	666	ILE	-	expression tag	UNP O55774
b	667	PHE	-	expression tag	UNP O55774
b	668	ALA	-	expression tag	UNP O55774
b	669	ASN	-	expression tag	UNP O55774
b	670	SER	-	expression tag	UNP O55774
b	671	SER	-	expression tag	UNP O55774
b	672	GLY	-	expression tag	UNP O55774
b	673	GLY	-	expression tag	UNP O55774
b	674	ASP	-	expression tag	UNP O55774
b	675	LEU	-	expression tag	UNP O55774
b	676	GLU	-	expression tag	UNP O55774
b	677	ILE	-	expression tag	UNP O55774
b	678	THR	-	expression tag	UNP O55774
b	679	THR	-	expression tag	UNP O55774
b	680	HIS	-	expression tag	UNP O55774
b	681	SER	-	expression tag	UNP O55774
b	682	PHE	-	expression tag	UNP O55774
b	683	ASN	-	expression tag	UNP O55774
b	684	CYS	-	expression tag	UNP O55774
b	685	GLY	-	expression tag	UNP O55774
b	686	GLY	-	expression tag	UNP O55774
b	687	GLU	-	expression tag	UNP O55774
b	688	PHE	-	expression tag	UNP O55774
b	689	PHE	-	expression tag	UNP O55774
b	690	TYR	-	expression tag	UNP O55774
b	691	CYS	-	expression tag	UNP O55774
b	692	ASN	-	expression tag	UNP O55774
b	693	THR	-	expression tag	UNP O55774
b	694	SER	-	expression tag	UNP O55774
b	695	GLY	-	expression tag	UNP O55774
b	696	LEU	-	expression tag	UNP O55774
b	697	PHE	-	expression tag	UNP O55774
b	698	ASN	-	expression tag	UNP O55774
b	699	SER	-	expression tag	UNP O55774
b	700	THR	-	expression tag	UNP O55774
b	701	TRP	-	expression tag	UNP O55774
b	702	TYR	-	expression tag	UNP O55774
b	703	VAL	-	expression tag	UNP O55774
b	704	ASN	-	expression tag	UNP O55774
b	705	SER	-	expression tag	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
b	706	THR	-	expression tag	UNP O55774
b	707	TRP	-	expression tag	UNP O55774
b	708	ASN	-	expression tag	UNP O55774
b	709	SER	-	expression tag	UNP O55774
b	710	ASN	-	expression tag	UNP O55774
b	711	ASP	-	expression tag	UNP O55774
b	712	THR	-	expression tag	UNP O55774
b	713	ILE	-	expression tag	UNP O55774
b	714	THR	-	expression tag	UNP O55774
b	715	LEU	-	expression tag	UNP O55774
b	716	PRO	-	expression tag	UNP O55774
b	717	CYS	-	expression tag	UNP O55774
b	718	ARG	-	expression tag	UNP O55774
b	719	ILE	-	expression tag	UNP O55774
b	720	LYS	-	expression tag	UNP O55774
b	721	GLN	-	expression tag	UNP O55774
b	722	ILE	-	expression tag	UNP O55774
b	723	ILE	-	expression tag	UNP O55774
b	724	ASN	-	expression tag	UNP O55774
b	725	MET	-	expression tag	UNP O55774
b	726	TRP	-	expression tag	UNP O55774
b	727	GLN	-	expression tag	UNP O55774
b	728	ARG	-	expression tag	UNP O55774
b	729	ALA	-	expression tag	UNP O55774
b	730	GLY	-	expression tag	UNP O55774
b	731	GLN	-	expression tag	UNP O55774
b	732	CYS	-	expression tag	UNP O55774
b	733	MET	-	expression tag	UNP O55774
b	734	TYR	-	expression tag	UNP O55774
b	735	ALA	-	expression tag	UNP O55774
b	736	PRO	-	expression tag	UNP O55774
b	737	PRO	-	expression tag	UNP O55774
b	738	ILE	-	expression tag	UNP O55774
b	739	PRO	-	expression tag	UNP O55774
b	740	GLY	-	expression tag	UNP O55774
b	741	VAL	-	expression tag	UNP O55774
b	742	ILE	-	expression tag	UNP O55774
b	743	LYS	-	expression tag	UNP O55774
b	744	CYS	-	expression tag	UNP O55774
b	745	GLU	-	expression tag	UNP O55774
b	746	SER	-	expression tag	UNP O55774
b	747	ASN	-	expression tag	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
b	748	ILE	-	expression tag	UNP O55774
b	749	THR	-	expression tag	UNP O55774
b	750	GLY	-	expression tag	UNP O55774
b	751	LEU	-	expression tag	UNP O55774
b	752	LEU	-	expression tag	UNP O55774
b	753	LEU	-	expression tag	UNP O55774
b	754	THR	-	expression tag	UNP O55774
b	755	ARG	-	expression tag	UNP O55774
b	756	ASP	-	expression tag	UNP O55774
b	757	GLY	-	expression tag	UNP O55774
b	758	GLY	-	expression tag	UNP O55774
b	759	LYS	-	expression tag	UNP O55774
b	760	ASP	-	expression tag	UNP O55774
b	761	ASN	-	expression tag	UNP O55774
b	762	ASN	-	expression tag	UNP O55774
b	763	VAL	-	expression tag	UNP O55774
b	764	ASN	-	expression tag	UNP O55774
b	765	GLU	-	expression tag	UNP O55774
b	766	THR	-	expression tag	UNP O55774
b	767	PHE	-	expression tag	UNP O55774
b	768	ARG	-	expression tag	UNP O55774
b	769	PRO	-	expression tag	UNP O55774
b	770	GLY	-	expression tag	UNP O55774
b	771	GLY	-	expression tag	UNP O55774
b	772	GLY	-	expression tag	UNP O55774
b	773	ASP	-	expression tag	UNP O55774
b	774	MET	-	expression tag	UNP O55774
b	775	ARG	-	expression tag	UNP O55774
b	776	ASP	-	expression tag	UNP O55774
b	777	ASN	-	expression tag	UNP O55774
b	778	TRP	-	expression tag	UNP O55774
b	779	ARG	-	expression tag	UNP O55774
b	780	SER	-	expression tag	UNP O55774
b	781	GLU	-	expression tag	UNP O55774
b	782	LEU	-	expression tag	UNP O55774
b	783	TYR	-	expression tag	UNP O55774
b	784	LYS	-	expression tag	UNP O55774
b	785	TYR	-	expression tag	UNP O55774
b	786	LYS	-	expression tag	UNP O55774
b	787	VAL	-	expression tag	UNP O55774
b	788	VAL	-	expression tag	UNP O55774
b	789	GLU	-	expression tag	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
b	790	ILE	-	expression tag	UNP O55774
b	791	GLU	-	expression tag	UNP O55774
b	792	PRO	-	expression tag	UNP O55774
b	793	LEU	-	expression tag	UNP O55774
b	794	GLY	-	expression tag	UNP O55774
b	795	VAL	-	expression tag	UNP O55774
b	796	ALA	-	expression tag	UNP O55774
b	797	PRO	-	expression tag	UNP O55774
b	798	THR	-	expression tag	UNP O55774
b	799	ARG	-	expression tag	UNP O55774
b	800	CYS	-	expression tag	UNP O55774
b	801	LYS	-	expression tag	UNP O55774
b	802	ARG	-	expression tag	UNP O55774
d	31	ALA	VAL	conflict	UNP O55774
d	49	GLU	ASP	conflict	UNP O55774
d	132	ARG	THR	conflict	UNP O55774
d	153	GLU	GLY	conflict	UNP O55774
d	158	THR	SER	conflict	UNP O55774
d	201	CYS	ILE	conflict	UNP O55774
d	219	ALA	THR	conflict	UNP O55774
d	302	TYR	ASN	conflict	UNP O55774
d	320	MET	THR	conflict	UNP O55774
d	334	SER	THR	conflict	UNP O55774
d	433	CYS	ALA	conflict	UNP O55774
d	501	CYS	ALA	conflict	UNP O55774
d	508	GLY	ARG	conflict	UNP O55774
d	509	GLY	GLU	conflict	UNP O55774
d	510	GLY	LYS	conflict	UNP O55774
d	511	GLY	ARG	conflict	UNP O55774
d	512	SER	ALA	conflict	UNP O55774
d	513	GLY	VAL	conflict	UNP O55774
d	515	GLY	ILE	conflict	UNP O55774
d	517	SER	ALA	conflict	UNP O55774
d	518	PHE	-	insertion	UNP O55774
d	519	GLU	-	insertion	UNP O55774
d	520	PRO	-	insertion	UNP O55774
d	521	ILE	VAL	conflict	UNP O55774
d	522	PRO	PHE	conflict	UNP O55774
d	523	ILE	LEU	conflict	UNP O55774
d	524	HIS	GLY	conflict	UNP O55774
d	525	TYR	PHE	conflict	UNP O55774
d	526	CYS	LEU	conflict	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
d	527	ALA	GLY	conflict	UNP O55774
d	528	PRO	ALA	conflict	UNP O55774
d	531	PHE	-	insertion	UNP O55774
d	532	ALA	-	insertion	UNP O55774
d	533	ILE	-	insertion	UNP O55774
d	534	LEU	-	insertion	UNP O55774
d	535	LYS	-	insertion	UNP O55774
d	536	CYS	-	insertion	UNP O55774
d	537	LYS	-	insertion	UNP O55774
d	538	ASP	-	insertion	UNP O55774
d	539	GLU	-	insertion	UNP O55774
d	540	GLY	-	insertion	UNP O55774
d	541	PHE	-	insertion	UNP O55774
d	542	ASN	-	insertion	UNP O55774
d	543	GLY	-	insertion	UNP O55774
d	544	THR	-	insertion	UNP O55774
d	545	GLY	-	insertion	UNP O55774
d	546	LEU	-	insertion	UNP O55774
d	547	CYS	-	insertion	UNP O55774
d	548	LYS	-	insertion	UNP O55774
d	549	ASN	-	insertion	UNP O55774
d	550	VAL	-	insertion	UNP O55774
d	553	VAL	MET	conflict	UNP O55774
d	554	GLN	GLY	conflict	UNP O55774
d	555	CYS	ALA	conflict	UNP O55774
d	557	HIS	-	insertion	UNP O55774
d	558	GLY	SER	conflict	UNP O55774
d	560	LYS	THR	conflict	UNP O55774
d	561	PRO	LEU	conflict	UNP O55774
d	562	VAL	THR	conflict	UNP O55774
d	564	SER	GLN	conflict	UNP O55774
d	565	THR	ALA	conflict	UNP O55774
d	566	GLN	ARG	conflict	UNP O55774
d	567	LEU	GLN	conflict	UNP O55774
d	570	ASN	SER	conflict	UNP O55774
d	572	SER	ILE	conflict	UNP O55774
d	573	LEU	VAL	conflict	UNP O55774
d	574	ALA	GLN	conflict	UNP O55774
d	575	GLU	GLN	conflict	UNP O55774
d	576	LYS	GLN	conflict	UNP O55774
d	578	ILE	ASN	conflict	UNP O55774
d	579	THR	LEU	conflict	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
d	580	ILE	LEU	conflict	UNP O55774
d	582	SER	ALA	conflict	UNP O55774
d	583	GLU	ILE	conflict	UNP O55774
d	584	ASN	GLU	conflict	UNP O55774
d	585	ILE	ALA	conflict	UNP O55774
d	586	THR	GLN	conflict	UNP O55774
d	587	ASN	GLN	conflict	UNP O55774
d	588	ASN	HIS	conflict	UNP O55774
d	589	ALA	LEU	conflict	UNP O55774
d	590	LYS	LEU	conflict	UNP O55774
d	591	ILE	LYS	conflict	UNP O55774
d	592	ILE	LEU	conflict	UNP O55774
d	593	ILE	THR	conflict	UNP O55774
d	595	GLN	TRP	conflict	UNP O55774
d	596	LEU	GLY	conflict	UNP O55774
d	597	VAL	ILE	conflict	UNP O55774
d	598	GLN	LYS	conflict	UNP O55774
d	599	PRO	GLN	conflict	UNP O55774
d	600	VAL	LEU	conflict	UNP O55774
d	601	THR	GLN	conflict	UNP O55774
d	602	ILE	ALA	conflict	UNP O55774
d	603	LYS	ARG	conflict	UNP O55774
d	604	CYS	VAL	conflict	UNP O55774
d	605	ILE	LEU	conflict	UNP O55774
d	606	ARG	ALA	conflict	UNP O55774
d	607	PRO	VAL	conflict	UNP O55774
d	608	ASN	GLU	conflict	UNP O55774
d	609	ASN	ARG	conflict	UNP O55774
d	611	THR	LEU	conflict	UNP O55774
d	613	LYS	ASP	conflict	UNP O55774
d	614	SER	GLN	conflict	UNP O55774
d	615	ILE	GLN	conflict	UNP O55774
d	616	ARG	LEU	conflict	UNP O55774
d	617	ILE	LEU	conflict	UNP O55774
d	619	PRO	-	expression tag	UNP O55774
d	620	GLY	-	expression tag	UNP O55774
d	621	GLN	-	expression tag	UNP O55774
d	622	ALA	-	expression tag	UNP O55774
d	623	PHE	-	expression tag	UNP O55774
d	624	TYR	-	expression tag	UNP O55774
d	625	ALA	-	expression tag	UNP O55774
d	626	MET	-	expression tag	UNP O55774

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
d	627	GLY	-	expression tag	UNP O55774
d	628	ASP	-	expression tag	UNP O55774
d	629	ILE	-	expression tag	UNP O55774
d	630	ILE	-	expression tag	UNP O55774
d	631	GLY	-	expression tag	UNP O55774
d	632	ASP	-	expression tag	UNP O55774
d	633	ILE	-	expression tag	UNP O55774
d	634	ARG	-	expression tag	UNP O55774
d	635	GLN	-	expression tag	UNP O55774
d	636	ALA	-	expression tag	UNP O55774
d	637	HIS	-	expression tag	UNP O55774
d	638	CYS	-	expression tag	UNP O55774
d	639	ASN	-	expression tag	UNP O55774
d	640	VAL	-	expression tag	UNP O55774
d	641	SER	-	expression tag	UNP O55774
d	642	ARG	-	expression tag	UNP O55774
d	643	SER	-	expression tag	UNP O55774
d	644	ARG	-	expression tag	UNP O55774
d	645	TRP	-	expression tag	UNP O55774
d	646	ASN	-	expression tag	UNP O55774
d	647	LYS	-	expression tag	UNP O55774
d	648	THR	-	expression tag	UNP O55774
d	649	LEU	-	expression tag	UNP O55774
d	650	GLN	-	expression tag	UNP O55774
d	651	GLU	-	expression tag	UNP O55774
d	652	VAL	-	expression tag	UNP O55774
d	653	ALA	-	expression tag	UNP O55774
d	654	GLU	-	expression tag	UNP O55774
d	655	LYS	-	expression tag	UNP O55774
d	656	LEU	-	expression tag	UNP O55774
d	657	ARG	-	expression tag	UNP O55774
d	658	THR	-	expression tag	UNP O55774
d	659	TYR	-	expression tag	UNP O55774
d	660	PHE	-	expression tag	UNP O55774
d	661	GLY	-	expression tag	UNP O55774
d	662	ASN	-	expression tag	UNP O55774
d	663	LYS	-	expression tag	UNP O55774
d	664	THR	-	expression tag	UNP O55774
d	665	ILE	-	expression tag	UNP O55774
d	666	ILE	-	expression tag	UNP O55774
d	667	PHE	-	expression tag	UNP O55774
d	668	ALA	-	expression tag	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
d	669	ASN	-	expression tag	UNP O55774
d	670	SER	-	expression tag	UNP O55774
d	671	SER	-	expression tag	UNP O55774
d	672	GLY	-	expression tag	UNP O55774
d	673	GLY	-	expression tag	UNP O55774
d	674	ASP	-	expression tag	UNP O55774
d	675	LEU	-	expression tag	UNP O55774
d	676	GLU	-	expression tag	UNP O55774
d	677	ILE	-	expression tag	UNP O55774
d	678	THR	-	expression tag	UNP O55774
d	679	THR	-	expression tag	UNP O55774
d	680	HIS	-	expression tag	UNP O55774
d	681	SER	-	expression tag	UNP O55774
d	682	PHE	-	expression tag	UNP O55774
d	683	ASN	-	expression tag	UNP O55774
d	684	CYS	-	expression tag	UNP O55774
d	685	GLY	-	expression tag	UNP O55774
d	686	GLY	-	expression tag	UNP O55774
d	687	GLU	-	expression tag	UNP O55774
d	688	PHE	-	expression tag	UNP O55774
d	689	PHE	-	expression tag	UNP O55774
d	690	TYR	-	expression tag	UNP O55774
d	691	CYS	-	expression tag	UNP O55774
d	692	ASN	-	expression tag	UNP O55774
d	693	THR	-	expression tag	UNP O55774
d	694	SER	-	expression tag	UNP O55774
d	695	GLY	-	expression tag	UNP O55774
d	696	LEU	-	expression tag	UNP O55774
d	697	PHE	-	expression tag	UNP O55774
d	698	ASN	-	expression tag	UNP O55774
d	699	SER	-	expression tag	UNP O55774
d	700	THR	-	expression tag	UNP O55774
d	701	TRP	-	expression tag	UNP O55774
d	702	TYR	-	expression tag	UNP O55774
d	703	VAL	-	expression tag	UNP O55774
d	704	ASN	-	expression tag	UNP O55774
d	705	SER	-	expression tag	UNP O55774
d	706	THR	-	expression tag	UNP O55774
d	707	TRP	-	expression tag	UNP O55774
d	708	ASN	-	expression tag	UNP O55774
d	709	SER	-	expression tag	UNP O55774
d	710	ASN	-	expression tag	UNP O55774

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
d	711	ASP	-	expression tag	UNP O55774
d	712	THR	-	expression tag	UNP O55774
d	713	ILE	-	expression tag	UNP O55774
d	714	THR	-	expression tag	UNP O55774
d	715	LEU	-	expression tag	UNP O55774
d	716	PRO	-	expression tag	UNP O55774
d	717	CYS	-	expression tag	UNP O55774
d	718	ARG	-	expression tag	UNP O55774
d	719	ILE	-	expression tag	UNP O55774
d	720	LYS	-	expression tag	UNP O55774
d	721	GLN	-	expression tag	UNP O55774
d	722	ILE	-	expression tag	UNP O55774
d	723	ILE	-	expression tag	UNP O55774
d	724	ASN	-	expression tag	UNP O55774
d	725	MET	-	expression tag	UNP O55774
d	726	TRP	-	expression tag	UNP O55774
d	727	GLN	-	expression tag	UNP O55774
d	728	ARG	-	expression tag	UNP O55774
d	729	ALA	-	expression tag	UNP O55774
d	730	GLY	-	expression tag	UNP O55774
d	731	GLN	-	expression tag	UNP O55774
d	732	CYS	-	expression tag	UNP O55774
d	733	MET	-	expression tag	UNP O55774
d	734	TYR	-	expression tag	UNP O55774
d	735	ALA	-	expression tag	UNP O55774
d	736	PRO	-	expression tag	UNP O55774
d	737	PRO	-	expression tag	UNP O55774
d	738	ILE	-	expression tag	UNP O55774
d	739	PRO	-	expression tag	UNP O55774
d	740	GLY	-	expression tag	UNP O55774
d	741	VAL	-	expression tag	UNP O55774
d	742	ILE	-	expression tag	UNP O55774
d	743	LYS	-	expression tag	UNP O55774
d	744	CYS	-	expression tag	UNP O55774
d	745	GLU	-	expression tag	UNP O55774
d	746	SER	-	expression tag	UNP O55774
d	747	ASN	-	expression tag	UNP O55774
d	748	ILE	-	expression tag	UNP O55774
d	749	THR	-	expression tag	UNP O55774
d	750	GLY	-	expression tag	UNP O55774
d	751	LEU	-	expression tag	UNP O55774
d	752	LEU	-	expression tag	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
d	753	LEU	-	expression tag	UNP O55774
d	754	THR	-	expression tag	UNP O55774
d	755	ARG	-	expression tag	UNP O55774
d	756	ASP	-	expression tag	UNP O55774
d	757	GLY	-	expression tag	UNP O55774
d	758	GLY	-	expression tag	UNP O55774
d	759	LYS	-	expression tag	UNP O55774
d	760	ASP	-	expression tag	UNP O55774
d	761	ASN	-	expression tag	UNP O55774
d	762	ASN	-	expression tag	UNP O55774
d	763	VAL	-	expression tag	UNP O55774
d	764	ASN	-	expression tag	UNP O55774
d	765	GLU	-	expression tag	UNP O55774
d	766	THR	-	expression tag	UNP O55774
d	767	PHE	-	expression tag	UNP O55774
d	768	ARG	-	expression tag	UNP O55774
d	769	PRO	-	expression tag	UNP O55774
d	770	GLY	-	expression tag	UNP O55774
d	771	GLY	-	expression tag	UNP O55774
d	772	GLY	-	expression tag	UNP O55774
d	773	ASP	-	expression tag	UNP O55774
d	774	MET	-	expression tag	UNP O55774
d	775	ARG	-	expression tag	UNP O55774
d	776	ASP	-	expression tag	UNP O55774
d	777	ASN	-	expression tag	UNP O55774
d	778	TRP	-	expression tag	UNP O55774
d	779	ARG	-	expression tag	UNP O55774
d	780	SER	-	expression tag	UNP O55774
d	781	GLU	-	expression tag	UNP O55774
d	782	LEU	-	expression tag	UNP O55774
d	783	TYR	-	expression tag	UNP O55774
d	784	LYS	-	expression tag	UNP O55774
d	785	TYR	-	expression tag	UNP O55774
d	786	LYS	-	expression tag	UNP O55774
d	787	VAL	-	expression tag	UNP O55774
d	788	VAL	-	expression tag	UNP O55774
d	789	GLU	-	expression tag	UNP O55774
d	790	ILE	-	expression tag	UNP O55774
d	791	GLU	-	expression tag	UNP O55774
d	792	PRO	-	expression tag	UNP O55774
d	793	LEU	-	expression tag	UNP O55774
d	794	GLY	-	expression tag	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
d	795	VAL	-	expression tag	UNP O55774
d	796	ALA	-	expression tag	UNP O55774
d	797	PRO	-	expression tag	UNP O55774
d	798	THR	-	expression tag	UNP O55774
d	799	ARG	-	expression tag	UNP O55774
d	800	CYS	-	expression tag	UNP O55774
d	801	LYS	-	expression tag	UNP O55774
d	802	ARG	-	expression tag	UNP O55774
f	31	ALA	VAL	conflict	UNP O55774
f	49	GLU	ASP	conflict	UNP O55774
f	132	ARG	THR	conflict	UNP O55774
f	153	GLU	GLY	conflict	UNP O55774
f	158	THR	SER	conflict	UNP O55774
f	201	CYS	ILE	conflict	UNP O55774
f	219	ALA	THR	conflict	UNP O55774
f	302	TYR	ASN	conflict	UNP O55774
f	320	MET	THR	conflict	UNP O55774
f	334	SER	THR	conflict	UNP O55774
f	433	CYS	ALA	conflict	UNP O55774
f	501	CYS	ALA	conflict	UNP O55774
f	508	GLY	ARG	conflict	UNP O55774
f	509	GLY	GLU	conflict	UNP O55774
f	510	GLY	LYS	conflict	UNP O55774
f	511	GLY	ARG	conflict	UNP O55774
f	512	SER	ALA	conflict	UNP O55774
f	513	GLY	VAL	conflict	UNP O55774
f	515	GLY	ILE	conflict	UNP O55774
f	517	SER	ALA	conflict	UNP O55774
f	518	PHE	-	insertion	UNP O55774
f	519	GLU	-	insertion	UNP O55774
f	520	PRO	-	insertion	UNP O55774
f	521	ILE	VAL	conflict	UNP O55774
f	522	PRO	PHE	conflict	UNP O55774
f	523	ILE	LEU	conflict	UNP O55774
f	524	HIS	GLY	conflict	UNP O55774
f	525	TYR	PHE	conflict	UNP O55774
f	526	CYS	LEU	conflict	UNP O55774
f	527	ALA	GLY	conflict	UNP O55774
f	528	PRO	ALA	conflict	UNP O55774
f	531	PHE	-	insertion	UNP O55774
f	532	ALA	-	insertion	UNP O55774
f	533	ILE	-	insertion	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
f	534	LEU	-	insertion	UNP O55774
f	535	LYS	-	insertion	UNP O55774
f	536	CYS	-	insertion	UNP O55774
f	537	LYS	-	insertion	UNP O55774
f	538	ASP	-	insertion	UNP O55774
f	539	GLU	-	insertion	UNP O55774
f	540	GLY	-	insertion	UNP O55774
f	541	PHE	-	insertion	UNP O55774
f	542	ASN	-	insertion	UNP O55774
f	543	GLY	-	insertion	UNP O55774
f	544	THR	-	insertion	UNP O55774
f	545	GLY	-	insertion	UNP O55774
f	546	LEU	-	insertion	UNP O55774
f	547	CYS	-	insertion	UNP O55774
f	548	LYS	-	insertion	UNP O55774
f	549	ASN	-	insertion	UNP O55774
f	550	VAL	-	insertion	UNP O55774
f	553	VAL	MET	conflict	UNP O55774
f	554	GLN	GLY	conflict	UNP O55774
f	555	CYS	ALA	conflict	UNP O55774
f	557	HIS	-	insertion	UNP O55774
f	558	GLY	SER	conflict	UNP O55774
f	560	LYS	THR	conflict	UNP O55774
f	561	PRO	LEU	conflict	UNP O55774
f	562	VAL	THR	conflict	UNP O55774
f	564	SER	GLN	conflict	UNP O55774
f	565	THR	ALA	conflict	UNP O55774
f	566	GLN	ARG	conflict	UNP O55774
f	567	LEU	GLN	conflict	UNP O55774
f	570	ASN	SER	conflict	UNP O55774
f	572	SER	ILE	conflict	UNP O55774
f	573	LEU	VAL	conflict	UNP O55774
f	574	ALA	GLN	conflict	UNP O55774
f	575	GLU	GLN	conflict	UNP O55774
f	576	LYS	GLN	conflict	UNP O55774
f	578	ILE	ASN	conflict	UNP O55774
f	579	THR	LEU	conflict	UNP O55774
f	580	ILE	LEU	conflict	UNP O55774
f	582	SER	ALA	conflict	UNP O55774
f	583	GLU	ILE	conflict	UNP O55774
f	584	ASN	GLU	conflict	UNP O55774
f	585	ILE	ALA	conflict	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
f	586	THR	GLN	conflict	UNP O55774
f	587	ASN	GLN	conflict	UNP O55774
f	588	ASN	HIS	conflict	UNP O55774
f	589	ALA	LEU	conflict	UNP O55774
f	590	LYS	LEU	conflict	UNP O55774
f	591	ILE	LYS	conflict	UNP O55774
f	592	ILE	LEU	conflict	UNP O55774
f	593	ILE	THR	conflict	UNP O55774
f	595	GLN	TRP	conflict	UNP O55774
f	596	LEU	GLY	conflict	UNP O55774
f	597	VAL	ILE	conflict	UNP O55774
f	598	GLN	LYS	conflict	UNP O55774
f	599	PRO	GLN	conflict	UNP O55774
f	600	VAL	LEU	conflict	UNP O55774
f	601	THR	GLN	conflict	UNP O55774
f	602	ILE	ALA	conflict	UNP O55774
f	603	LYS	ARG	conflict	UNP O55774
f	604	CYS	VAL	conflict	UNP O55774
f	605	ILE	LEU	conflict	UNP O55774
f	606	ARG	ALA	conflict	UNP O55774
f	607	PRO	VAL	conflict	UNP O55774
f	608	ASN	GLU	conflict	UNP O55774
f	609	ASN	ARG	conflict	UNP O55774
f	611	THR	LEU	conflict	UNP O55774
f	613	LYS	ASP	conflict	UNP O55774
f	614	SER	GLN	conflict	UNP O55774
f	615	ILE	GLN	conflict	UNP O55774
f	616	ARG	LEU	conflict	UNP O55774
f	617	ILE	LEU	conflict	UNP O55774
f	619	PRO	-	expression tag	UNP O55774
f	620	GLY	-	expression tag	UNP O55774
f	621	GLN	-	expression tag	UNP O55774
f	622	ALA	-	expression tag	UNP O55774
f	623	PHE	-	expression tag	UNP O55774
f	624	TYR	-	expression tag	UNP O55774
f	625	ALA	-	expression tag	UNP O55774
f	626	MET	-	expression tag	UNP O55774
f	627	GLY	-	expression tag	UNP O55774
f	628	ASP	-	expression tag	UNP O55774
f	629	ILE	-	expression tag	UNP O55774
f	630	ILE	-	expression tag	UNP O55774
f	631	GLY	-	expression tag	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
f	632	ASP	-	expression tag	UNP O55774
f	633	ILE	-	expression tag	UNP O55774
f	634	ARG	-	expression tag	UNP O55774
f	635	GLN	-	expression tag	UNP O55774
f	636	ALA	-	expression tag	UNP O55774
f	637	HIS	-	expression tag	UNP O55774
f	638	CYS	-	expression tag	UNP O55774
f	639	ASN	-	expression tag	UNP O55774
f	640	VAL	-	expression tag	UNP O55774
f	641	SER	-	expression tag	UNP O55774
f	642	ARG	-	expression tag	UNP O55774
f	643	SER	-	expression tag	UNP O55774
f	644	ARG	-	expression tag	UNP O55774
f	645	TRP	-	expression tag	UNP O55774
f	646	ASN	-	expression tag	UNP O55774
f	647	LYS	-	expression tag	UNP O55774
f	648	THR	-	expression tag	UNP O55774
f	649	LEU	-	expression tag	UNP O55774
f	650	GLN	-	expression tag	UNP O55774
f	651	GLU	-	expression tag	UNP O55774
f	652	VAL	-	expression tag	UNP O55774
f	653	ALA	-	expression tag	UNP O55774
f	654	GLU	-	expression tag	UNP O55774
f	655	LYS	-	expression tag	UNP O55774
f	656	LEU	-	expression tag	UNP O55774
f	657	ARG	-	expression tag	UNP O55774
f	658	THR	-	expression tag	UNP O55774
f	659	TYR	-	expression tag	UNP O55774
f	660	PHE	-	expression tag	UNP O55774
f	661	GLY	-	expression tag	UNP O55774
f	662	ASN	-	expression tag	UNP O55774
f	663	LYS	-	expression tag	UNP O55774
f	664	THR	-	expression tag	UNP O55774
f	665	ILE	-	expression tag	UNP O55774
f	666	ILE	-	expression tag	UNP O55774
f	667	PHE	-	expression tag	UNP O55774
f	668	ALA	-	expression tag	UNP O55774
f	669	ASN	-	expression tag	UNP O55774
f	670	SER	-	expression tag	UNP O55774
f	671	SER	-	expression tag	UNP O55774
f	672	GLY	-	expression tag	UNP O55774
f	673	GLY	-	expression tag	UNP O55774

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
f	674	ASP	-	expression tag	UNP O55774
f	675	LEU	-	expression tag	UNP O55774
f	676	GLU	-	expression tag	UNP O55774
f	677	ILE	-	expression tag	UNP O55774
f	678	THR	-	expression tag	UNP O55774
f	679	THR	-	expression tag	UNP O55774
f	680	HIS	-	expression tag	UNP O55774
f	681	SER	-	expression tag	UNP O55774
f	682	PHE	-	expression tag	UNP O55774
f	683	ASN	-	expression tag	UNP O55774
f	684	CYS	-	expression tag	UNP O55774
f	685	GLY	-	expression tag	UNP O55774
f	686	GLY	-	expression tag	UNP O55774
f	687	GLU	-	expression tag	UNP O55774
f	688	PHE	-	expression tag	UNP O55774
f	689	PHE	-	expression tag	UNP O55774
f	690	TYR	-	expression tag	UNP O55774
f	691	CYS	-	expression tag	UNP O55774
f	692	ASN	-	expression tag	UNP O55774
f	693	THR	-	expression tag	UNP O55774
f	694	SER	-	expression tag	UNP O55774
f	695	GLY	-	expression tag	UNP O55774
f	696	LEU	-	expression tag	UNP O55774
f	697	PHE	-	expression tag	UNP O55774
f	698	ASN	-	expression tag	UNP O55774
f	699	SER	-	expression tag	UNP O55774
f	700	THR	-	expression tag	UNP O55774
f	701	TRP	-	expression tag	UNP O55774
f	702	TYR	-	expression tag	UNP O55774
f	703	VAL	-	expression tag	UNP O55774
f	704	ASN	-	expression tag	UNP O55774
f	705	SER	-	expression tag	UNP O55774
f	706	THR	-	expression tag	UNP O55774
f	707	TRP	-	expression tag	UNP O55774
f	708	ASN	-	expression tag	UNP O55774
f	709	SER	-	expression tag	UNP O55774
f	710	ASN	-	expression tag	UNP O55774
f	711	ASP	-	expression tag	UNP O55774
f	712	THR	-	expression tag	UNP O55774
f	713	ILE	-	expression tag	UNP O55774
f	714	THR	-	expression tag	UNP O55774
f	715	LEU	-	expression tag	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
f	716	PRO	-	expression tag	UNP O55774
f	717	CYS	-	expression tag	UNP O55774
f	718	ARG	-	expression tag	UNP O55774
f	719	ILE	-	expression tag	UNP O55774
f	720	LYS	-	expression tag	UNP O55774
f	721	GLN	-	expression tag	UNP O55774
f	722	ILE	-	expression tag	UNP O55774
f	723	ILE	-	expression tag	UNP O55774
f	724	ASN	-	expression tag	UNP O55774
f	725	MET	-	expression tag	UNP O55774
f	726	TRP	-	expression tag	UNP O55774
f	727	GLN	-	expression tag	UNP O55774
f	728	ARG	-	expression tag	UNP O55774
f	729	ALA	-	expression tag	UNP O55774
f	730	GLY	-	expression tag	UNP O55774
f	731	GLN	-	expression tag	UNP O55774
f	732	CYS	-	expression tag	UNP O55774
f	733	MET	-	expression tag	UNP O55774
f	734	TYR	-	expression tag	UNP O55774
f	735	ALA	-	expression tag	UNP O55774
f	736	PRO	-	expression tag	UNP O55774
f	737	PRO	-	expression tag	UNP O55774
f	738	ILE	-	expression tag	UNP O55774
f	739	PRO	-	expression tag	UNP O55774
f	740	GLY	-	expression tag	UNP O55774
f	741	VAL	-	expression tag	UNP O55774
f	742	ILE	-	expression tag	UNP O55774
f	743	LYS	-	expression tag	UNP O55774
f	744	CYS	-	expression tag	UNP O55774
f	745	GLU	-	expression tag	UNP O55774
f	746	SER	-	expression tag	UNP O55774
f	747	ASN	-	expression tag	UNP O55774
f	748	ILE	-	expression tag	UNP O55774
f	749	THR	-	expression tag	UNP O55774
f	750	GLY	-	expression tag	UNP O55774
f	751	LEU	-	expression tag	UNP O55774
f	752	LEU	-	expression tag	UNP O55774
f	753	LEU	-	expression tag	UNP O55774
f	754	THR	-	expression tag	UNP O55774
f	755	ARG	-	expression tag	UNP O55774
f	756	ASP	-	expression tag	UNP O55774
f	757	GLY	-	expression tag	UNP O55774

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
f	758	GLY	-	expression tag	UNP O55774
f	759	LYS	-	expression tag	UNP O55774
f	760	ASP	-	expression tag	UNP O55774
f	761	ASN	-	expression tag	UNP O55774
f	762	ASN	-	expression tag	UNP O55774
f	763	VAL	-	expression tag	UNP O55774
f	764	ASN	-	expression tag	UNP O55774
f	765	GLU	-	expression tag	UNP O55774
f	766	THR	-	expression tag	UNP O55774
f	767	PHE	-	expression tag	UNP O55774
f	768	ARG	-	expression tag	UNP O55774
f	769	PRO	-	expression tag	UNP O55774
f	770	GLY	-	expression tag	UNP O55774
f	771	GLY	-	expression tag	UNP O55774
f	772	GLY	-	expression tag	UNP O55774
f	773	ASP	-	expression tag	UNP O55774
f	774	MET	-	expression tag	UNP O55774
f	775	ARG	-	expression tag	UNP O55774
f	776	ASP	-	expression tag	UNP O55774
f	777	ASN	-	expression tag	UNP O55774
f	778	TRP	-	expression tag	UNP O55774
f	779	ARG	-	expression tag	UNP O55774
f	780	SER	-	expression tag	UNP O55774
f	781	GLU	-	expression tag	UNP O55774
f	782	LEU	-	expression tag	UNP O55774
f	783	TYR	-	expression tag	UNP O55774
f	784	LYS	-	expression tag	UNP O55774
f	785	TYR	-	expression tag	UNP O55774
f	786	LYS	-	expression tag	UNP O55774
f	787	VAL	-	expression tag	UNP O55774
f	788	VAL	-	expression tag	UNP O55774
f	789	GLU	-	expression tag	UNP O55774
f	790	ILE	-	expression tag	UNP O55774
f	791	GLU	-	expression tag	UNP O55774
f	792	PRO	-	expression tag	UNP O55774
f	793	LEU	-	expression tag	UNP O55774
f	794	GLY	-	expression tag	UNP O55774
f	795	VAL	-	expression tag	UNP O55774
f	796	ALA	-	expression tag	UNP O55774
f	797	PRO	-	expression tag	UNP O55774
f	798	THR	-	expression tag	UNP O55774
f	799	ARG	-	expression tag	UNP O55774

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
f	800	CYS	-	expression tag	UNP O55774
f	801	LYS	-	expression tag	UNP O55774
f	802	ARG	-	expression tag	UNP O55774

- Molecule 2 is a protein called HIV envelope gp41 ectodomain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	127	Total	C	N	O	S	0	0
			1026	650	184	187	5		
2	e	127	Total	C	N	O	S	0	0
			1026	650	184	187	5		
2	g	127	Total	C	N	O	S	0	0
			1026	650	184	187	5		

There are 27 discrepancies between the modelled and reference sequences:

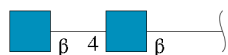
Chain	Residue	Modelled	Actual	Comment	Reference
c	519	ARG	PHE	conflict	UNP O55774
c	520	ARG	LEU	conflict	UNP O55774
c	533	ALA	THR	conflict	UNP O55774
c	551	PRO	GLN	conflict	UNP O55774
c	559	PRO	ILE	conflict	UNP O55774
c	569	GLY	THR	conflict	UNP O55774
c	605	CYS	THR	conflict	UNP O55774
c	636	GLY	ASN	conflict	UNP O55774
c	662	ALA	GLU	conflict	UNP O55774
e	519	ARG	PHE	conflict	UNP O55774
e	520	ARG	LEU	conflict	UNP O55774
e	533	ALA	THR	conflict	UNP O55774
e	551	PRO	GLN	conflict	UNP O55774
e	559	PRO	ILE	conflict	UNP O55774
e	569	GLY	THR	conflict	UNP O55774
e	605	CYS	THR	conflict	UNP O55774
e	636	GLY	ASN	conflict	UNP O55774
e	662	ALA	GLU	conflict	UNP O55774
g	519	ARG	PHE	conflict	UNP O55774
g	520	ARG	LEU	conflict	UNP O55774
g	533	ALA	THR	conflict	UNP O55774
g	551	PRO	GLN	conflict	UNP O55774
g	559	PRO	ILE	conflict	UNP O55774
g	569	GLY	THR	conflict	UNP O55774
g	605	CYS	THR	conflict	UNP O55774

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
g	636	GLY	ASN	conflict	UNP O55774
g	662	ALA	GLU	conflict	UNP O55774

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



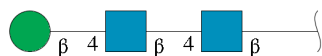
Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		
3	j	2	Total	C	N	O	0	0
			28	16	2	10		
3	k	2	Total	C	N	O	0	0
			28	16	2	10		
3	l	2	Total	C	N	O	0	0
			28	16	2	10		
3	n	2	Total	C	N	O	0	0
			28	16	2	10		
3	o	2	Total	C	N	O	0	0
			28	16	2	10		
3	p	2	Total	C	N	O	0	0
			28	16	2	10		
3	q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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.



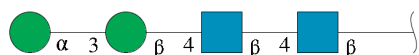
Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	H	3	Total	C	N	O	0	0
			39	22	2	15		
4	N	3	Total	C	N	O	0	0
			39	22	2	15		
4	T	3	Total	C	N	O	0	0
			39	22	2	15		
4	a	3	Total	C	N	O	0	0
			39	22	2	15		

Continued on next page...

Continued from previous page...

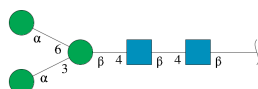
Mol	Chain	Residues	Atoms				AltConf	Trace
4	h	3	Total	C	N	O	0	0
			39	22	2	15		
4	m	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
5	C	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 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
6	O	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
7	b	1	Total	C	N	O	0
			14	8	1	5	
7	b	1	Total	C	N	O	0
			14	8	1	5	
7	b	1	Total	C	N	O	0
			14	8	1	5	
7	b	1	Total	C	N	O	0
			14	8	1	5	
7	b	1	Total	C	N	O	0
			14	8	1	5	
7	b	1	Total	C	N	O	0
			14	8	1	5	
7	b	1	Total	C	N	O	0
			14	8	1	5	
7	c	1	Total	C	N	O	0
			14	8	1	5	
7	c	1	Total	C	N	O	0
			14	8	1	5	
7	c	1	Total	C	N	O	0
			14	8	1	5	
7	d	1	Total	C	N	O	0
			14	8	1	5	
7	d	1	Total	C	N	O	0
			14	8	1	5	
7	d	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

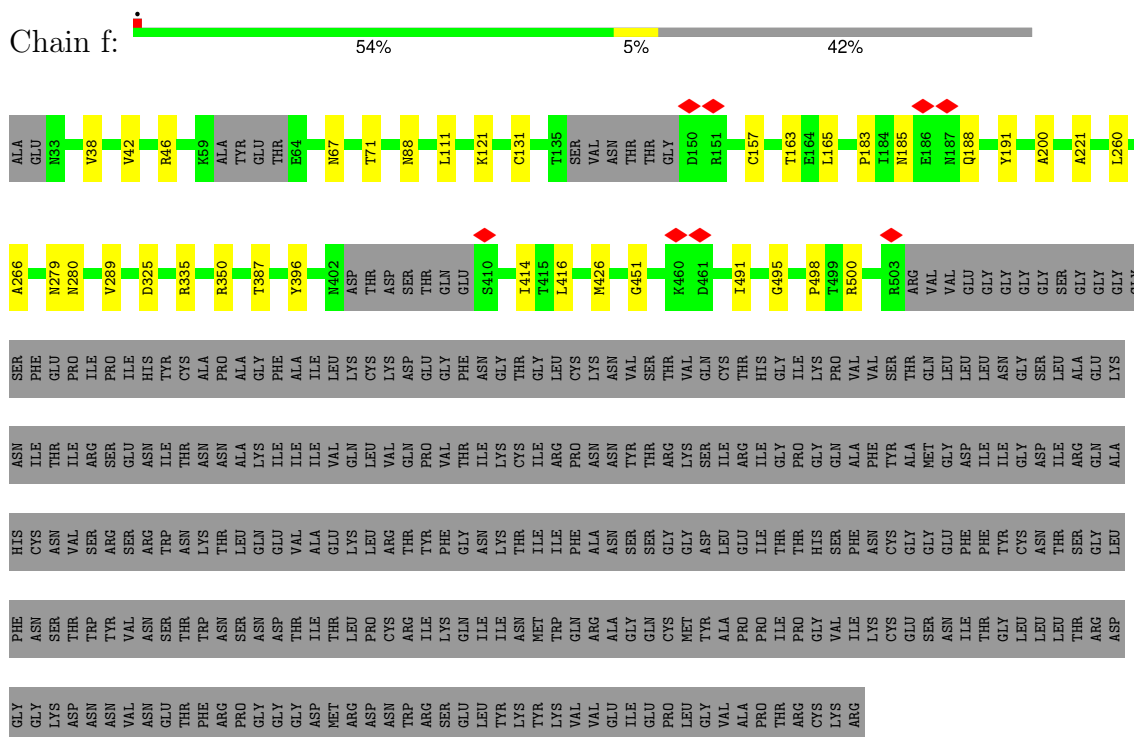
*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
7	d	1	Total	C	N	O	0
			14	8	1	5	
7	d	1	Total	C	N	O	0
			14	8	1	5	
7	d	1	Total	C	N	O	0
			14	8	1	5	
7	d	1	Total	C	N	O	0
			14	8	1	5	
7	e	1	Total	C	N	O	0
			14	8	1	5	
7	e	1	Total	C	N	O	0
			14	8	1	5	
7	e	1	Total	C	N	O	0
			14	8	1	5	
7	f	1	Total	C	N	O	0
			14	8	1	5	
7	f	1	Total	C	N	O	0
			14	8	1	5	
7	f	1	Total	C	N	O	0
			14	8	1	5	
7	f	1	Total	C	N	O	0
			14	8	1	5	
7	f	1	Total	C	N	O	0
			14	8	1	5	
7	f	1	Total	C	N	O	0
			14	8	1	5	
7	f	1	Total	C	N	O	0
			14	8	1	5	
7	f	1	Total	C	N	O	0
			14	8	1	5	
7	g	1	Total	C	N	O	0
			14	8	1	5	
7	g	1	Total	C	N	O	0
			14	8	1	5	
7	g	1	Total	C	N	O	0
			14	8	1	5	

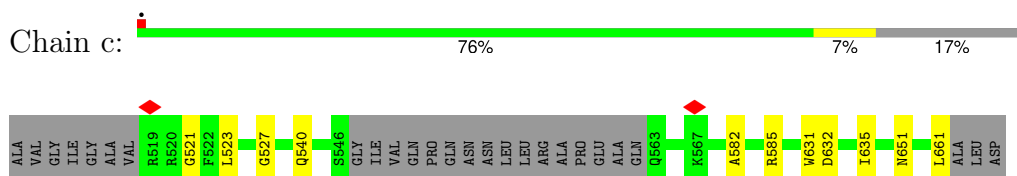




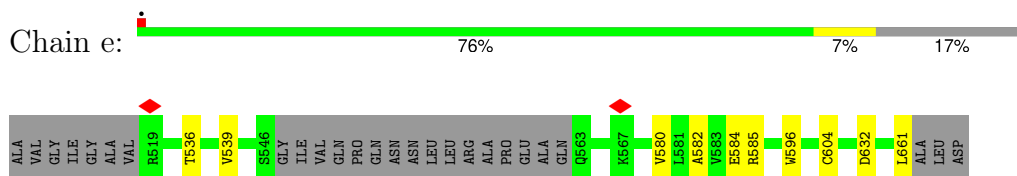
- Molecule 1: HIV envelope gp120



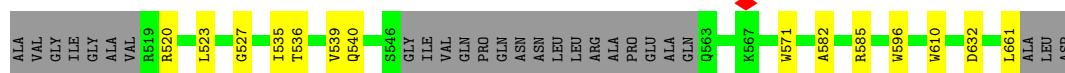
- Molecule 2: HIV envelope gp41 ectodomain



- Molecule 2: HIV envelope gp41 ectodomain



- Molecule 2: HIV envelope gp41 ectodomain



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



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



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



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



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



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

Chain I:  100%

MAG1  
MAG2

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

Chain J:  50%  
 100%

MAG1  
MAG2

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

Chain K:  50%  
 100%

MAG1  
MAG2

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

Chain L:  50%  
 100%


MAG1  
MAG2

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

Chain M:  100%

MAG1  
MAG2

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

Chain P:  50%  
 50%

MAG1  
MAG2

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

Chain Q:  50%  
 100%



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



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



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



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



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



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





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



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



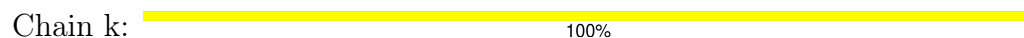
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

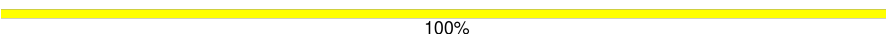


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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

Chain n:  100%



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

Chain o:  50% 100%



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

Chain p:  50% 100%



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

Chain q:  50% 50% 50%



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

Chain B:  33% 100%



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

Chain H:  67% 100%



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



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



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



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



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



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: 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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101320	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.546	Depositor
Minimum map value	-0.200	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.12	Depositor
Map size ( $\text{\AA}$ )	318.72, 318.72, 318.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	b	0.15	0/3606	0.47	0/4894
1	d	0.16	0/3606	0.48	0/4894
1	f	0.15	0/3606	0.47	0/4894
2	c	0.15	0/1044	0.43	0/1410
2	e	0.18	0/1044	0.42	0/1410
2	g	0.18	0/1044	0.47	1/1410 (0.1%)
All	All	0.16	0/13950	0.47	1/18912 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	g	520	ARG	CB-CA-C	-5.63	110.07	116.54

There are no chirality outliers.

There are no planarity outliers.

### 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	b	3530	0	3451	27	0
1	d	3530	0	3451	34	0
1	f	3530	0	3452	23	0
2	c	1026	0	1025	9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	e	1026	0	1025	8	0
2	g	1026	0	1025	11	0
3	A	28	0	25	0	0
3	D	28	0	25	1	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	P	28	0	25	1	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	i	28	0	25	0	0
3	j	28	0	25	0	0
3	k	28	0	25	0	0
3	l	28	0	25	0	0
3	n	28	0	25	0	0
3	o	28	0	25	0	0
3	p	28	0	25	0	0
3	q	28	0	25	0	0
4	B	39	0	34	0	0
4	H	39	0	34	0	0
4	N	39	0	34	0	0
4	T	39	0	34	0	0
4	a	39	0	34	0	0
4	h	39	0	34	0	0
4	m	39	0	34	0	0
5	C	50	0	43	1	0
6	O	61	0	52	0	0
7	b	112	0	104	0	0
7	c	42	0	39	0	0
7	d	98	0	91	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	e	42	0	39	0	0
7	f	112	0	104	0	0
7	g	42	0	39	0	0
All	All	15284	0	14878	91	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 3.

All (91) 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:d:185:ASN:HD22	1:d:188:GLN:CB	1.97	0.77
1:d:185:ASN:HD22	1:d:188:GLN:HB2	1.57	0.69
1:d:184:ILE:HG13	1:d:185:ASN:N	2.07	0.68
2:c:651:ASN:ND2	2:g:535:ILE:O	2.29	0.66
1:d:55:ALA:HB3	1:d:216:HIS:HB2	1.79	0.64
1:d:500:ARG:HD2	2:g:661:LEU:HD12	1.80	0.64
1:b:55:ALA:HB3	1:b:216:HIS:HB2	1.80	0.64
1:d:54:CYS:SG	1:d:55:ALA:N	2.72	0.63
1:b:54:CYS:SG	1:b:55:ALA:N	2.72	0.63
1:b:500:ARG:HD2	2:e:661:LEU:HD12	1.81	0.62
2:c:661:LEU:HD12	1:f:500:ARG:HD2	1.82	0.62
1:d:185:ASN:ND2	1:d:188:GLN:HB2	2.16	0.60
1:f:491:ILE:O	2:g:585:ARG:NH2	2.34	0.60
1:d:184:ILE:HD11	1:d:190:GLU:OE1	2.03	0.59
1:b:46:ARG:NH1	2:c:632:ASP:OD2	2.38	0.57
1:d:184:ILE:HG13	1:d:185:ASN:H	1.69	0.57
1:b:491:ILE:O	2:c:585:ARG:NH2	2.38	0.57
1:b:163:THR:HG23	1:b:165:LEU:H	1.70	0.56
1:d:46:ARG:NH1	2:e:632:ASP:OD2	2.38	0.56
1:f:46:ARG:NH1	2:g:632:ASP:OD2	2.39	0.55
1:b:65:LYS:HZ2	5:C:4:MAN:H4	1.72	0.55
1:d:491:ILE:O	2:e:585:ARG:NH2	2.40	0.55
1:d:37:THR:OG1	2:e:604:CYS:O	2.20	0.54
1:d:185:ASN:ND2	1:d:188:GLN:H	2.05	0.54
1:b:277:ILE:O	1:b:456:ARG:NH1	2.40	0.53
1:f:38:VAL:HG21	2:g:596:TRP:HZ3	1.74	0.52
1:b:368:ASP:N	1:b:368:ASP:OD1	2.42	0.52
1:f:131:CYS:HA	1:f:157:CYS:HA	1.91	0.52
1:d:121:LYS:HE2	1:d:200:ALA:HB3	1.93	0.51
1:d:185:ASN:HD22	1:d:188:GLN:H	1.59	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:580:VAL:O	2:e:584:GLU:HG3	2.12	0.50
1:b:121:LYS:HE2	1:b:200:ALA:HB3	1.92	0.50
1:d:132:ARG:NH2	3:P:1:NAG:O6	2.45	0.50
1:d:131:CYS:HA	1:d:157:CYS:HA	1.94	0.49
1:f:221:ALA:HB3	2:g:582:ALA:HB1	1.95	0.49
1:b:131:CYS:HA	1:b:157:CYS:HA	1.95	0.48
1:f:279:ASN:OD1	1:f:280:ASN:N	2.46	0.48
1:d:184:ILE:HG22	1:d:192:ARG:HE	1.78	0.48
1:b:221:ALA:HB3	2:c:582:ALA:HB1	1.96	0.48
1:d:38:VAL:HG21	2:e:596:TRP:HZ3	1.78	0.48
1:b:280:ASN:OD1	1:b:456:ARG:NH2	2.47	0.47
1:d:163:THR:HG23	1:d:165:LEU:H	1.79	0.47
1:d:337:ARG:O	1:d:341:THR:HG23	2.15	0.47
1:b:84:ILE:HG12	2:c:521:GLY:HA3	1.95	0.47
1:f:325:ASP:OD1	1:f:325:ASP:N	2.48	0.46
1:b:369:LEU:O	1:b:373:THR:OG1	2.27	0.46
1:f:67:ASN:ND2	1:f:71:THR:OG1	2.42	0.45
1:f:88:ASN:HB2	2:g:527:GLY:HA3	1.98	0.45
1:f:260:LEU:HD12	1:f:451:GLY:HA3	1.99	0.45
1:d:260:LEU:HD12	1:d:451:GLY:HA3	1.99	0.45
1:f:111:LEU:HD11	2:g:571:TRP:CZ2	2.52	0.45
1:f:42:VAL:HG21	1:f:495:GLY:HA3	1.99	0.44
1:b:132:ARG:NH2	3:D:1:NAG:O6	2.50	0.44
1:d:184:ILE:CD1	1:d:190:GLU:OE1	2.66	0.44
1:d:221:ALA:HB3	2:e:582:ALA:HB1	1.98	0.44
1:b:260:LEU:HD12	1:b:451:GLY:HA3	1.99	0.44
1:b:279:ASN:OD1	1:b:280:ASN:N	2.50	0.44
1:b:88:ASN:HB2	2:c:527:GLY:HA3	2.00	0.43
1:f:335:ARG:HG3	1:f:414:ILE:HD11	2.00	0.43
1:f:387:THR:HG22	1:f:416:LEU:HD23	2.00	0.43
1:f:163:THR:HG23	1:f:165:LEU:H	1.82	0.43
1:b:42:VAL:HG21	1:b:495:GLY:HA3	2.01	0.42
1:f:350:ARG:NH2	1:f:396:TYR:O	2.51	0.42
1:d:339:ASN:HA	1:d:342:LEU:HB2	2.01	0.42
1:f:183:PRO:HA	1:f:191:TYR:HA	2.02	0.42
1:f:266:ALA:HB3	1:f:289:VAL:HG12	2.02	0.42
1:d:54:CYS:HB3	1:d:74:CYS:HB2	1.96	0.41
1:b:38:VAL:HG12	1:b:496:VAL:HG22	2.02	0.41
1:b:501:CYS:SG	1:b:502:LYS:N	2.93	0.41
2:c:631:TRP:CE2	2:c:635:ILE:HD13	2.55	0.41
1:d:42:VAL:HG21	1:d:495:GLY:HA3	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:185:ASN:HD22	1:d:188:GLN:HB3	1.82	0.41
1:d:350:ARG:NH2	1:d:396:TYR:O	2.54	0.41
1:f:498:PRO:HG3	2:g:610:TRP:CE2	2.56	0.41
1:b:258:GLN:NE2	1:b:371:ILE:O	2.51	0.41
1:f:121:LYS:HE2	1:f:200:ALA:HB3	2.02	0.41
1:f:185:ASN:HB2	1:f:188:GLN:HB3	2.03	0.41
1:b:54:CYS:HB3	1:b:74:CYS:HB2	1.95	0.41
1:b:356:LYS:HE2	1:b:463:ASN:HA	2.02	0.41
1:d:280:ASN:OD1	1:d:456:ARG:NH2	2.53	0.41
2:g:523:LEU:HD12	2:g:540:GLN:HG2	2.03	0.41
2:g:536:THR:O	2:g:539:VAL:HG22	2.21	0.41
1:d:41:GLY:N	1:d:493:PRO:O	2.53	0.41
1:d:98:ASN:OD1	1:d:100:MET:HG3	2.20	0.41
1:b:161:MET:HE2	1:b:161:MET:HA	2.03	0.40
1:b:266:ALA:HB3	1:b:289:VAL:HG12	2.03	0.40
1:d:325:ASP:N	1:d:325:ASP:OD1	2.53	0.40
2:e:536:THR:O	2:e:539:VAL:HG22	2.22	0.40
2:c:523:LEU:HD12	2:c:540:GLN:HG2	2.03	0.40
1:d:163:THR:OG1	1:d:164:GLU:N	2.54	0.40
1:f:426:MET:HE2	1:f:426:MET:HB3	1.80	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	437/763 (57%)	427 (98%)	10 (2%)	0	100	100
1	d	437/763 (57%)	425 (97%)	12 (3%)	0	100	100
1	f	437/763 (57%)	430 (98%)	7 (2%)	0	100	100
2	c	123/153 (80%)	121 (98%)	2 (2%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	e	123/153 (80%)	122 (99%)	1 (1%)	0	100	100
2	g	123/153 (80%)	122 (99%)	1 (1%)	0	100	100
All	All	1680/2748 (61%)	1647 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	b	398/667 (60%)	398 (100%)	0	100	100
1	d	398/667 (60%)	398 (100%)	0	100	100
1	f	398/667 (60%)	398 (100%)	0	100	100
2	c	110/128 (86%)	110 (100%)	0	100	100
2	e	110/128 (86%)	110 (100%)	0	100	100
2	g	110/128 (86%)	110 (100%)	0	100	100
All	All	1524/2385 (64%)	1524 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	66	HIS
1	b	72	HIS
1	b	85	HIS
1	b	99	ASN
1	b	462	ASN
2	c	543	GLN
1	d	66	HIS
1	d	72	HIS
1	d	82	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	d	99	ASN
1	d	185	ASN
1	d	188	GLN
2	e	543	GLN
1	f	82	GLN
1	f	85	HIS
1	f	130	HIS
1	f	462	ASN
2	g	543	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

86 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	$\# Z  > 2$
3	NAG	A	1	3,1	14,14,15	0.71	0	17,19,21	0.86	0
3	NAG	A	2	3	14,14,15	0.70	0	17,19,21	0.77	0
4	NAG	B	1	4,1	14,14,15	0.69	0	17,19,21	0.89	1 (5%)
4	NAG	B	2	4	14,14,15	0.67	0	17,19,21	1.41	2 (11%)
4	BMA	B	3	4	11,11,12	0.86	0	15,15,17	2.21	4 (26%)
5	NAG	C	1	5,1	14,14,15	0.74	0	17,19,21	1.00	1 (5%)
5	NAG	C	2	5	14,14,15	0.72	0	17,19,21	0.89	0
5	BMA	C	3	5	11,11,12	0.81	0	15,15,17	2.49	6 (40%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	C	4	5	11,11,12	0.62	0	15,15,17	1.46	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.73	0	17,19,21	1.03	1 (5%)
3	NAG	D	2	3	14,14,15	0.70	0	17,19,21	1.39	1 (5%)
3	NAG	E	1	3,1	14,14,15	0.75	0	17,19,21	1.11	1 (5%)
3	NAG	E	2	3	14,14,15	0.69	0	17,19,21	0.83	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.71	0	17,19,21	1.44	1 (5%)
3	NAG	F	2	3	14,14,15	0.71	0	17,19,21	1.40	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.69	0	17,19,21	1.25	3 (17%)
3	NAG	G	2	3	14,14,15	0.79	0	17,19,21	1.12	1 (5%)
4	NAG	H	1	4,1	14,14,15	0.76	0	17,19,21	1.18	2 (11%)
4	NAG	H	2	4	14,14,15	0.83	1 (7%)	17,19,21	1.34	1 (5%)
4	BMA	H	3	4	11,11,12	0.85	0	15,15,17	2.23	3 (20%)
3	NAG	I	1	3,1	14,14,15	0.73	0	17,19,21	1.70	4 (23%)
3	NAG	I	2	3	14,14,15	0.81	0	17,19,21	1.00	1 (5%)
3	NAG	J	1	3,1	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
3	NAG	J	2	3	14,14,15	0.79	1 (7%)	17,19,21	1.63	3 (17%)
3	NAG	K	1	3,1	14,14,15	0.73	0	17,19,21	0.97	1 (5%)
3	NAG	K	2	3	14,14,15	0.78	0	17,19,21	1.14	1 (5%)
3	NAG	L	1	3,1	14,14,15	0.67	0	17,19,21	1.06	1 (5%)
3	NAG	L	2	3	14,14,15	0.72	0	17,19,21	1.44	2 (11%)
3	NAG	M	1	3,1	14,14,15	0.73	0	17,19,21	0.91	0
3	NAG	M	2	3	14,14,15	0.69	0	17,19,21	0.78	0
4	NAG	N	1	4,1	14,14,15	0.69	0	17,19,21	0.90	1 (5%)
4	NAG	N	2	4	14,14,15	0.69	0	17,19,21	1.40	1 (5%)
4	BMA	N	3	4	11,11,12	0.86	0	15,15,17	2.21	3 (20%)
6	NAG	O	1	6,1	14,14,15	0.74	0	17,19,21	1.04	1 (5%)
6	NAG	O	2	6	14,14,15	0.71	0	17,19,21	1.02	1 (5%)
6	BMA	O	3	6	11,11,12	0.83	0	15,15,17	2.28	4 (26%)
6	MAN	O	4	6	11,11,12	0.63	0	15,15,17	1.46	1 (6%)
6	MAN	O	5	6	11,11,12	0.68	0	15,15,17	1.35	1 (6%)
3	NAG	P	1	3,1	14,14,15	0.74	0	17,19,21	1.04	1 (5%)
3	NAG	P	2	3	14,14,15	0.71	0	17,19,21	1.40	1 (5%)
3	NAG	Q	1	3,1	14,14,15	0.75	0	17,19,21	1.06	1 (5%)
3	NAG	Q	2	3	14,14,15	0.68	0	17,19,21	0.84	1 (5%)
3	NAG	R	1	3,1	14,14,15	0.70	0	17,19,21	1.43	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	R	2	3	14,14,15	0.71	0	17,19,21	1.40	1 (5%)
3	NAG	S	1	3,1	14,14,15	0.69	0	17,19,21	1.25	3 (17%)
3	NAG	S	2	3	14,14,15	0.77	0	17,19,21	1.11	1 (5%)
4	NAG	T	1	4,1	14,14,15	0.74	0	17,19,21	1.20	2 (11%)
4	NAG	T	2	4	14,14,15	0.82	0	17,19,21	1.33	1 (5%)
4	BMA	T	3	4	11,11,12	0.85	0	15,15,17	2.22	3 (20%)
3	NAG	U	1	3,1	14,14,15	0.73	0	17,19,21	1.68	4 (23%)
3	NAG	U	2	3	14,14,15	0.78	0	17,19,21	0.97	1 (5%)
3	NAG	V	1	3,1	14,14,15	0.71	0	17,19,21	0.85	1 (5%)
3	NAG	V	2	3	14,14,15	0.80	1 (7%)	17,19,21	1.65	3 (17%)
3	NAG	W	1	3,1	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
3	NAG	W	2	3	14,14,15	0.73	0	17,19,21	1.05	1 (5%)
3	NAG	X	1	3,1	14,14,15	0.75	0	17,19,21	1.07	1 (5%)
3	NAG	X	2	3	14,14,15	0.79	0	17,19,21	1.26	1 (5%)
3	NAG	Y	1	3,1	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
3	NAG	Y	2	3	14,14,15	0.70	0	17,19,21	1.41	1 (5%)
3	NAG	Z	1	3,1	14,14,15	0.72	0	17,19,21	0.89	0
3	NAG	Z	2	3	14,14,15	0.68	0	17,19,21	0.78	0
4	NAG	a	1	4,1	14,14,15	0.72	0	17,19,21	0.90	0
4	NAG	a	2	4	14,14,15	0.69	0	17,19,21	1.42	1 (5%)
4	BMA	a	3	4	11,11,12	0.87	0	15,15,17	2.27	4 (26%)
4	NAG	h	1	4,1	14,14,15	0.71	0	17,19,21	0.99	1 (5%)
4	NAG	h	2	4	14,14,15	0.71	0	17,19,21	0.95	1 (5%)
4	BMA	h	3	4	11,11,12	0.87	0	15,15,17	2.24	4 (26%)
3	NAG	i	1	3,1	14,14,15	0.77	0	17,19,21	1.19	3 (17%)
3	NAG	i	2	3	14,14,15	0.71	0	17,19,21	1.40	1 (5%)
3	NAG	j	1	3,1	14,14,15	0.74	0	17,19,21	1.05	1 (5%)
3	NAG	j	2	3	14,14,15	0.69	0	17,19,21	0.84	1 (5%)
3	NAG	k	1	3,1	14,14,15	0.70	0	17,19,21	1.43	1 (5%)
3	NAG	k	2	3	14,14,15	0.70	0	17,19,21	1.40	1 (5%)
3	NAG	l	1	3,1	14,14,15	0.68	0	17,19,21	1.25	3 (17%)
3	NAG	l	2	3	14,14,15	0.79	0	17,19,21	1.15	1 (5%)
4	NAG	m	1	4,1	14,14,15	0.76	0	17,19,21	1.19	2 (11%)
4	NAG	m	2	4	14,14,15	0.81	0	17,19,21	1.34	1 (5%)
4	BMA	m	3	4	11,11,12	0.86	0	15,15,17	2.23	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	n	1	3,1	14,14,15	0.75	0	17,19,21	1.76	4 (23%)
3	NAG	n	2	3	14,14,15	0.81	0	17,19,21	1.03	1 (5%)
3	NAG	o	1	3,1	14,14,15	0.71	0	17,19,21	0.93	1 (5%)
3	NAG	o	2	3	14,14,15	0.79	1 (7%)	17,19,21	1.62	2 (11%)
3	NAG	p	1	3,1	14,14,15	0.74	0	17,19,21	0.92	1 (5%)
3	NAG	p	2	3	14,14,15	0.79	0	17,19,21	1.13	1 (5%)
3	NAG	q	1	3,1	14,14,15	0.74	0	17,19,21	0.81	0
3	NAG	q	2	3	14,14,15	0.83	1 (7%)	17,19,21	1.70	3 (17%)

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
3	NAG	A	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
4	NAG	B	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
5	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
5	MAN	C	4	5	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	1/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	3/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1
6	NAG	O	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	2/2/19/22	0/1/1/1
6	MAN	O	4	6	-	0/2/19/22	0/1/1/1
6	MAN	O	5	6	-	2/2/19/22	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	1/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	1/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	BMA	T	3	4	-	1/2/19/22	0/1/1/1
3	NAG	U	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	3/6/23/26	0/1/1/1
3	NAG	W	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	NAG	X	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	1/6/23/26	0/1/1/1
3	NAG	Y	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	3/6/23/26	0/1/1/1
3	NAG	Z	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
4	NAG	a	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	BMA	a	3	4	-	0/2/19/22	0/1/1/1
4	NAG	h	1	4,1	-	0/6/23/26	0/1/1/1

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	h	2	4	-	0/6/23/26	0/1/1/1
4	BMA	h	3	4	-	0/2/19/22	0/1/1/1
3	NAG	i	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	i	2	3	-	2/6/23/26	0/1/1/1
3	NAG	j	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	j	2	3	-	1/6/23/26	0/1/1/1
3	NAG	k	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	k	2	3	-	3/6/23/26	0/1/1/1
3	NAG	l	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	l	2	3	-	1/6/23/26	0/1/1/1
4	NAG	m	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	m	2	4	-	0/6/23/26	0/1/1/1
4	BMA	m	3	4	-	1/2/19/22	0/1/1/1
3	NAG	n	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	n	2	3	-	0/6/23/26	0/1/1/1
3	NAG	o	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	o	2	3	-	3/6/23/26	0/1/1/1
3	NAG	p	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	p	2	3	-	1/6/23/26	0/1/1/1
3	NAG	q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	q	2	3	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	q	2	NAG	C1-C2	2.26	1.55	1.52
3	V	2	NAG	C1-C2	2.05	1.55	1.52
3	J	2	NAG	C1-C2	2.02	1.55	1.52
4	H	2	NAG	C1-C2	2.02	1.55	1.52
3	o	2	NAG	C1-C2	2.01	1.55	1.52

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3	BMA	C1-O5-C5	7.39	122.09	112.19
4	B	3	BMA	C1-O5-C5	6.80	121.30	112.19
4	N	3	BMA	C1-O5-C5	6.79	121.29	112.19
4	H	3	BMA	C1-O5-C5	6.75	121.23	112.19
4	m	3	BMA	C1-O5-C5	6.74	121.21	112.19
4	a	3	BMA	C1-O5-C5	6.67	121.13	112.19
4	T	3	BMA	C1-O5-C5	6.66	121.11	112.19

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	h	3	BMA	C1-O5-C5	6.52	120.93	112.19
6	O	3	BMA	C1-O5-C5	6.39	120.74	112.19
5	C	4	MAN	C1-O5-C5	4.78	118.59	112.19
6	O	4	MAN	C1-O5-C5	4.76	118.56	112.19
3	Y	2	NAG	C2-N2-C7	4.25	128.60	122.90
3	P	2	NAG	C2-N2-C7	4.24	128.59	122.90
3	n	1	NAG	C2-N2-C7	4.23	128.57	122.90
3	U	1	NAG	C2-N2-C7	4.20	128.52	122.90
3	I	1	NAG	C2-N2-C7	4.18	128.51	122.90
4	N	2	NAG	C2-N2-C7	4.18	128.50	122.90
4	B	2	NAG	C2-N2-C7	4.18	128.50	122.90
3	D	2	NAG	C2-N2-C7	4.17	128.49	122.90
3	R	2	NAG	C2-N2-C7	4.17	128.49	122.90
4	a	2	NAG	C2-N2-C7	4.15	128.46	122.90
3	F	1	NAG	C2-N2-C7	4.15	128.46	122.90
3	i	2	NAG	C2-N2-C7	4.14	128.45	122.90
3	F	2	NAG	C2-N2-C7	4.14	128.44	122.90
3	k	2	NAG	C2-N2-C7	4.11	128.41	122.90
3	k	1	NAG	C2-N2-C7	4.08	128.37	122.90
3	R	1	NAG	C2-N2-C7	4.07	128.35	122.90
3	L	2	NAG	C2-N2-C7	4.02	128.29	122.90
3	q	2	NAG	C2-N2-C7	3.94	128.18	122.90
6	O	5	MAN	C1-O5-C5	3.94	117.47	112.19
3	V	2	NAG	C2-N2-C7	3.92	128.15	122.90
3	J	2	NAG	C2-N2-C7	3.91	128.14	122.90
3	o	2	NAG	C2-N2-C7	3.87	128.08	122.90
3	X	2	NAG	C1-O5-C5	3.85	117.35	112.19
3	q	2	NAG	C1-O5-C5	3.67	117.11	112.19
4	m	2	NAG	C1-O5-C5	3.59	117.00	112.19
3	V	2	NAG	C1-O5-C5	3.57	116.97	112.19
4	H	2	NAG	C1-O5-C5	3.55	116.94	112.19
3	J	2	NAG	C1-O5-C5	3.52	116.90	112.19
3	o	2	NAG	C1-O5-C5	3.51	116.89	112.19
4	T	2	NAG	C1-O5-C5	3.45	116.81	112.19
5	C	3	BMA	C3-C4-C5	3.29	116.19	110.23
3	p	2	NAG	C1-O5-C5	3.19	116.46	112.19
3	K	2	NAG	C1-O5-C5	3.18	116.45	112.19
3	X	1	NAG	O5-C1-C2	-3.09	106.51	111.29
3	l	1	NAG	O5-C1-C2	-3.08	106.52	111.29
4	H	1	NAG	O5-C1-C2	-3.03	106.60	111.29
6	O	3	BMA	C3-C4-C5	3.03	115.73	110.23
3	S	1	NAG	O5-C1-C2	-3.02	106.62	111.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	l	2	NAG	C1-O5-C5	2.97	116.17	112.19
4	T	1	NAG	O5-C1-C2	-2.97	106.70	111.29
4	m	1	NAG	O5-C1-C2	-2.95	106.72	111.29
4	a	3	BMA	C3-C4-C5	2.91	115.51	110.23
3	G	1	NAG	O5-C1-C2	-2.91	106.79	111.29
4	h	3	BMA	C3-C4-C5	2.89	115.47	110.23
3	n	1	NAG	O5-C1-C2	-2.86	106.87	111.29
3	G	2	NAG	C1-O5-C5	2.81	115.96	112.19
3	S	2	NAG	C1-O5-C5	2.76	115.88	112.19
4	a	3	BMA	C2-C3-C4	2.74	115.69	110.86
4	h	3	BMA	C2-C3-C4	2.72	115.65	110.86
4	m	3	BMA	C2-C3-C4	2.67	115.56	110.86
3	L	1	NAG	O5-C1-C2	-2.65	107.18	111.29
4	H	3	BMA	C2-C3-C4	2.64	115.51	110.86
4	T	3	BMA	C2-C3-C4	2.64	115.51	110.86
3	U	1	NAG	O5-C1-C2	-2.61	107.26	111.29
3	n	1	NAG	O4-C4-C3	-2.60	104.25	110.38
3	o	1	NAG	O5-C1-C2	-2.58	107.30	111.29
3	U	2	NAG	O5-C1-C2	-2.58	107.30	111.29
6	O	3	BMA	C2-C3-C4	2.57	115.37	110.86
5	C	3	BMA	O4-C4-C3	-2.55	104.38	110.38
3	I	1	NAG	O4-C4-C3	-2.53	104.41	110.38
3	J	1	NAG	O5-C1-C2	-2.53	107.38	111.29
3	I	1	NAG	O5-C1-C2	-2.51	107.40	111.29
3	U	1	NAG	O4-C4-C3	-2.51	104.45	110.38
5	C	1	NAG	C1-O5-C5	2.50	115.54	112.19
3	K	1	NAG	O5-C1-C2	-2.50	107.43	111.29
6	O	1	NAG	C1-O5-C5	2.49	115.52	112.19
3	I	2	NAG	O5-C1-C2	-2.48	107.46	111.29
4	T	3	BMA	C3-C4-C5	2.43	114.64	110.23
3	W	2	NAG	C1-O5-C5	2.43	115.44	112.19
3	E	1	NAG	C1-O5-C5	2.42	115.44	112.19
5	C	3	BMA	C2-C3-C4	2.42	115.12	110.86
4	H	3	BMA	C3-C4-C5	2.41	114.60	110.23
4	m	3	BMA	C3-C4-C5	2.40	114.59	110.23
3	V	1	NAG	O5-C1-C2	-2.37	107.63	111.29
4	h	1	NAG	C1-O5-C5	2.36	115.34	112.19
4	h	2	NAG	O5-C1-C2	-2.35	107.66	111.29
3	L	2	NAG	C1-O5-C5	2.34	115.32	112.19
6	O	3	BMA	O4-C4-C3	-2.33	104.88	110.38
3	i	1	NAG	O4-C4-C3	-2.32	104.92	110.38
3	W	1	NAG	O5-C1-C2	-2.31	107.72	111.29

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	n	1	NAG	C4-C3-C2	2.30	114.39	111.02
3	S	1	NAG	O3-C3-C4	2.28	115.76	110.38
3	n	2	NAG	O5-C1-C2	-2.26	107.79	111.29
3	G	1	NAG	O3-C3-C4	2.26	115.70	110.38
4	B	3	BMA	O3-C3-C2	-2.26	105.45	110.05
3	Q	2	NAG	O5-C1-C2	-2.25	107.81	111.29
4	T	1	NAG	O3-C3-C2	-2.25	104.73	109.40
6	O	2	NAG	O4-C4-C3	-2.25	105.07	110.38
3	j	1	NAG	C1-O5-C5	2.25	115.20	112.19
3	G	1	NAG	C4-C3-C2	-2.25	107.73	111.02
3	l	1	NAG	O3-C3-C4	2.24	115.66	110.38
4	N	3	BMA	O3-C3-C2	-2.24	105.48	110.05
3	Q	1	NAG	C1-O5-C5	2.24	115.19	112.19
3	I	1	NAG	C4-C3-C2	2.22	114.28	111.02
3	U	1	NAG	C4-C3-C2	2.22	114.28	111.02
3	q	2	NAG	C1-C2-N2	2.22	113.93	110.43
4	m	1	NAG	O3-C3-C2	-2.20	104.82	109.40
3	D	1	NAG	O4-C4-C3	-2.19	105.21	110.38
3	S	1	NAG	C4-C3-C2	-2.19	107.81	111.02
3	j	2	NAG	O5-C1-C2	-2.18	107.92	111.29
4	B	3	BMA	C2-C3-C4	2.18	114.69	110.86
4	H	1	NAG	O3-C3-C2	-2.17	104.89	109.40
4	N	3	BMA	C2-C3-C4	2.17	114.67	110.86
3	P	1	NAG	O4-C4-C3	-2.15	105.32	110.38
3	E	2	NAG	O5-C1-C2	-2.15	107.97	111.29
3	p	1	NAG	O5-C1-C2	-2.15	107.97	111.29
3	i	1	NAG	C4-C3-C2	2.15	114.16	111.02
4	h	3	BMA	O4-C4-C3	-2.13	105.36	110.38
3	l	1	NAG	C4-C3-C2	-2.12	107.91	111.02
4	B	1	NAG	O5-C1-C2	-2.11	108.02	111.29
4	N	1	NAG	O5-C1-C2	-2.11	108.03	111.29
4	a	3	BMA	O4-C4-C3	-2.11	105.41	110.38
3	Y	1	NAG	O5-C1-C2	-2.10	108.04	111.29
4	B	2	NAG	O5-C1-C2	-2.09	108.05	111.29
3	J	2	NAG	C1-C2-N2	2.07	113.69	110.43
3	V	2	NAG	C1-C2-N2	2.05	113.66	110.43
5	C	3	BMA	O3-C3-C4	2.03	115.15	110.38
3	i	1	NAG	O5-C1-C2	-2.01	108.18	111.29
5	C	3	BMA	O5-C5-C4	2.01	115.71	110.83
4	B	3	BMA	O4-C4-C3	-2.01	105.64	110.38

There are no chirality outliers.



All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	n	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	n	1	NAG	C4-C5-C6-O6
6	O	3	BMA	O5-C5-C6-O6
6	O	5	MAN	O5-C5-C6-O6
6	O	5	MAN	C4-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
4	T	3	BMA	O5-C5-C6-O6
4	m	3	BMA	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	l	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	p	2	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	o	2	NAG	O5-C5-C6-O6
3	q	2	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	j	2	NAG	O5-C5-C6-O6
3	k	2	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	m	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C1-C2-N2-C7
3	F	2	NAG	C1-C2-N2-C7
3	I	1	NAG	C1-C2-N2-C7
3	J	2	NAG	C1-C2-N2-C7
3	L	2	NAG	C1-C2-N2-C7
3	P	2	NAG	C1-C2-N2-C7
3	R	2	NAG	C1-C2-N2-C7
3	U	1	NAG	C1-C2-N2-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	V	2	NAG	C1-C2-N2-C7
3	Y	2	NAG	C1-C2-N2-C7
3	i	2	NAG	C1-C2-N2-C7
3	n	1	NAG	C1-C2-N2-C7
3	o	2	NAG	C1-C2-N2-C7
3	q	2	NAG	C1-C2-N2-C7
4	B	2	NAG	C1-C2-N2-C7
4	N	2	NAG	C1-C2-N2-C7
4	a	2	NAG	C1-C2-N2-C7
6	O	3	BMA	C4-C5-C6-O6
3	F	1	NAG	C3-C2-N2-C7
3	I	1	NAG	C3-C2-N2-C7
3	J	2	NAG	C3-C2-N2-C7
3	R	1	NAG	C3-C2-N2-C7
3	R	2	NAG	C3-C2-N2-C7
3	V	2	NAG	C3-C2-N2-C7
3	k	1	NAG	C3-C2-N2-C7
3	k	2	NAG	C3-C2-N2-C7
3	n	1	NAG	C3-C2-N2-C7
3	o	2	NAG	C3-C2-N2-C7
3	F	1	NAG	C1-C2-N2-C7
3	R	1	NAG	C1-C2-N2-C7
3	k	1	NAG	C1-C2-N2-C7
3	k	2	NAG	C1-C2-N2-C7
3	D	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
3	L	2	NAG	C3-C2-N2-C7
3	P	2	NAG	C3-C2-N2-C7
3	U	1	NAG	C3-C2-N2-C7
3	Y	2	NAG	C3-C2-N2-C7
3	i	2	NAG	C3-C2-N2-C7
3	q	2	NAG	C3-C2-N2-C7
4	B	2	NAG	C3-C2-N2-C7
4	N	2	NAG	C3-C2-N2-C7
4	a	2	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

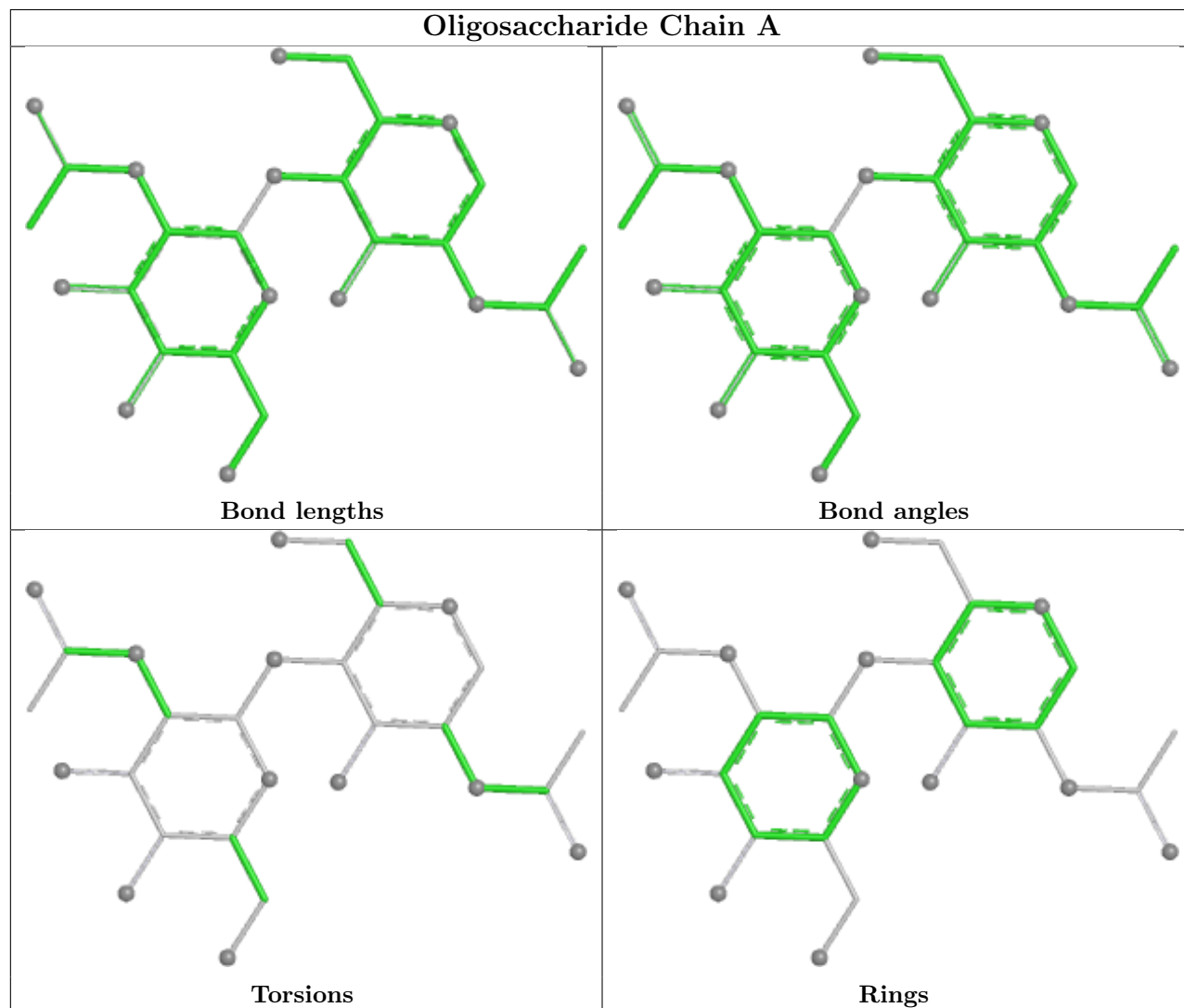
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	4	MAN	1	0
3	D	1	NAG	1	0

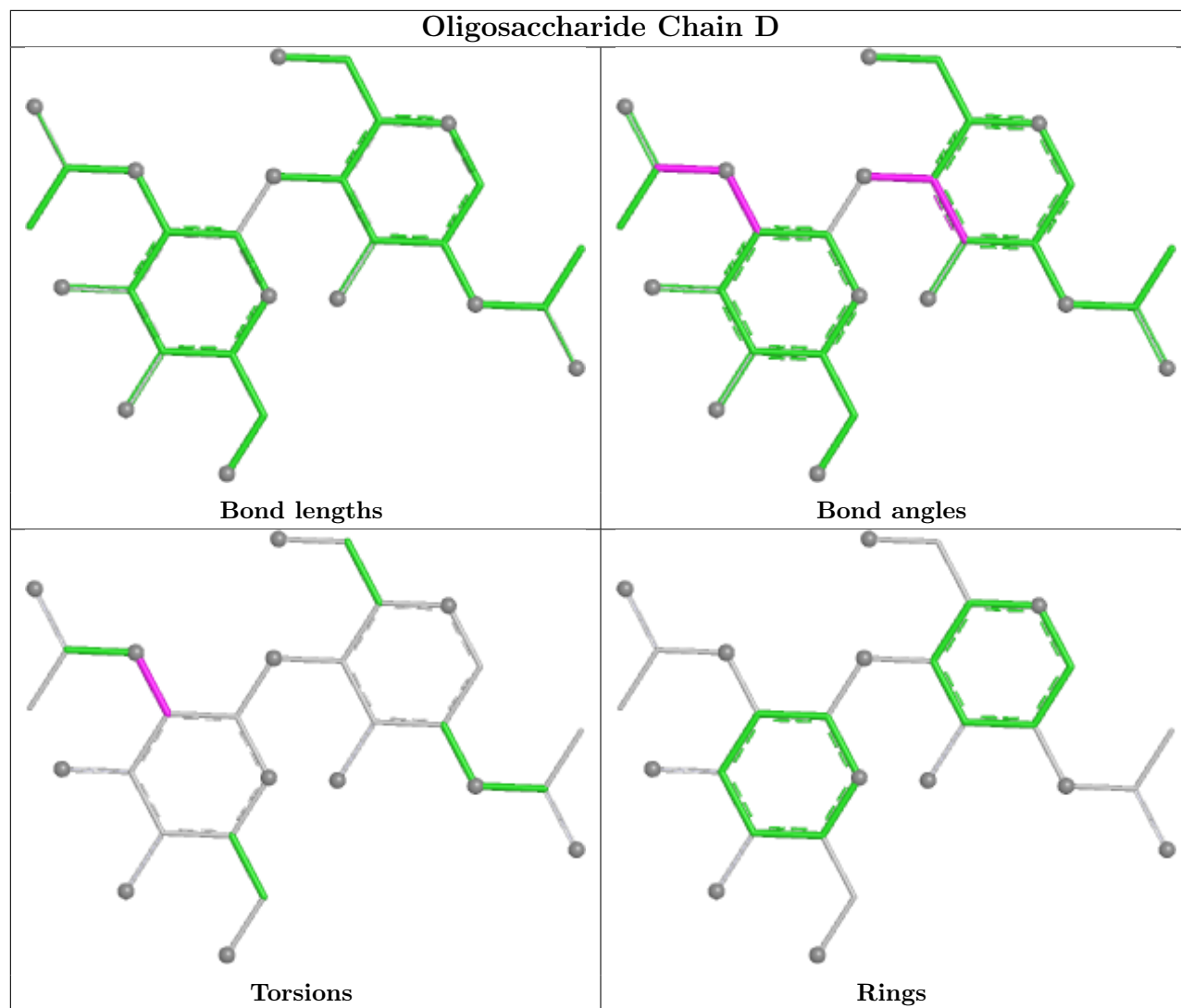
*Continued on next page...*

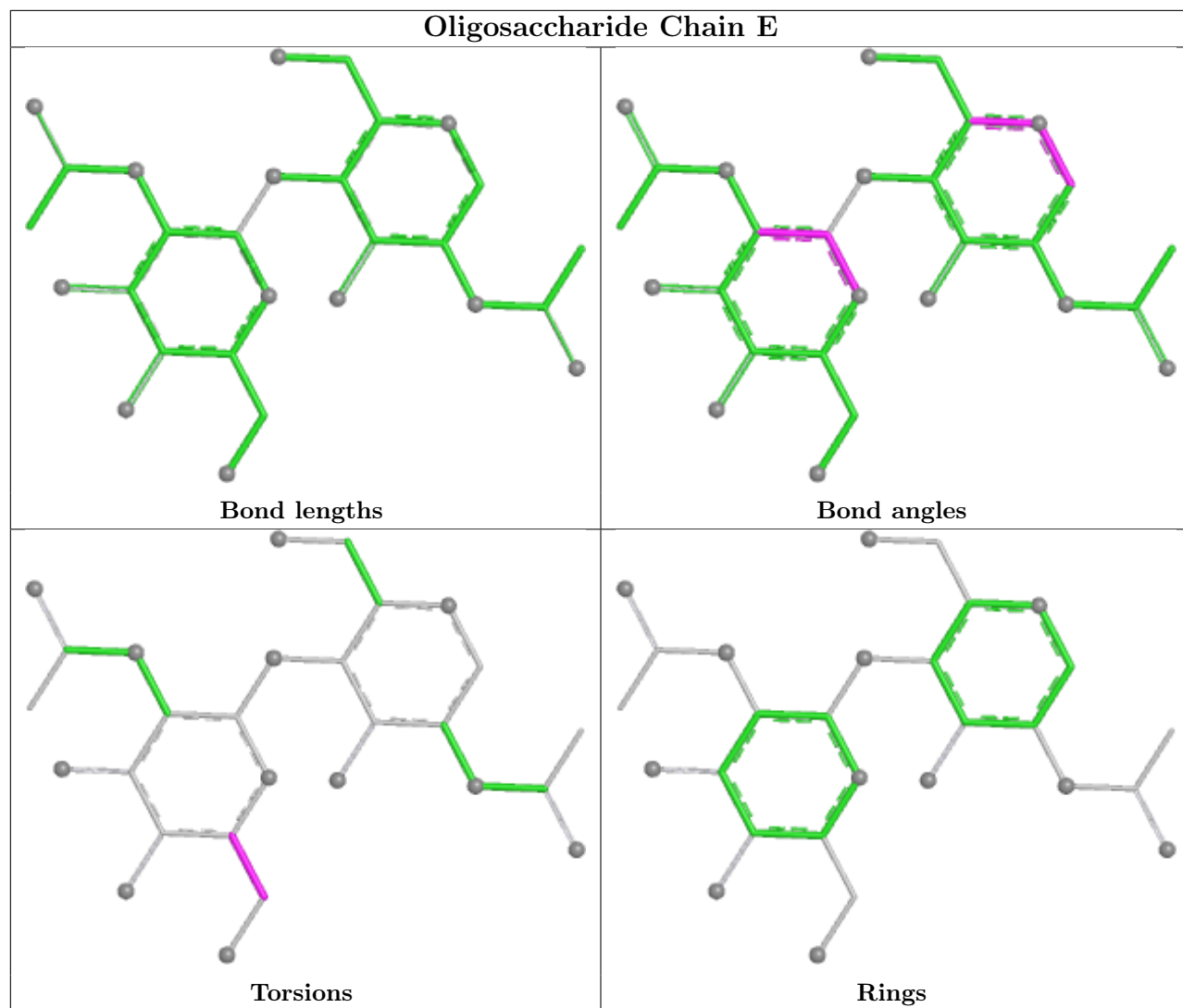
*Continued from previous page...*

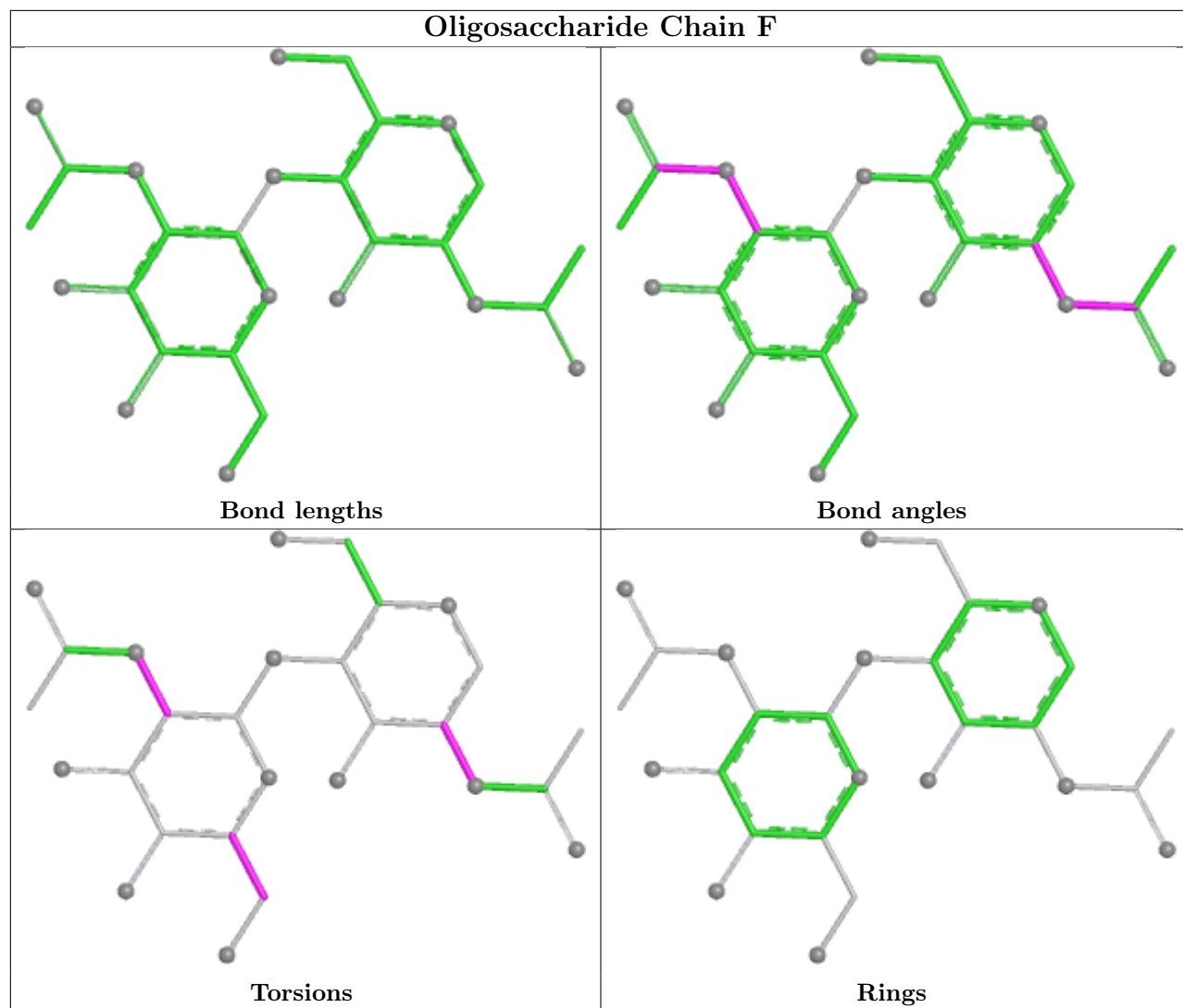
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	1	NAG	1	0

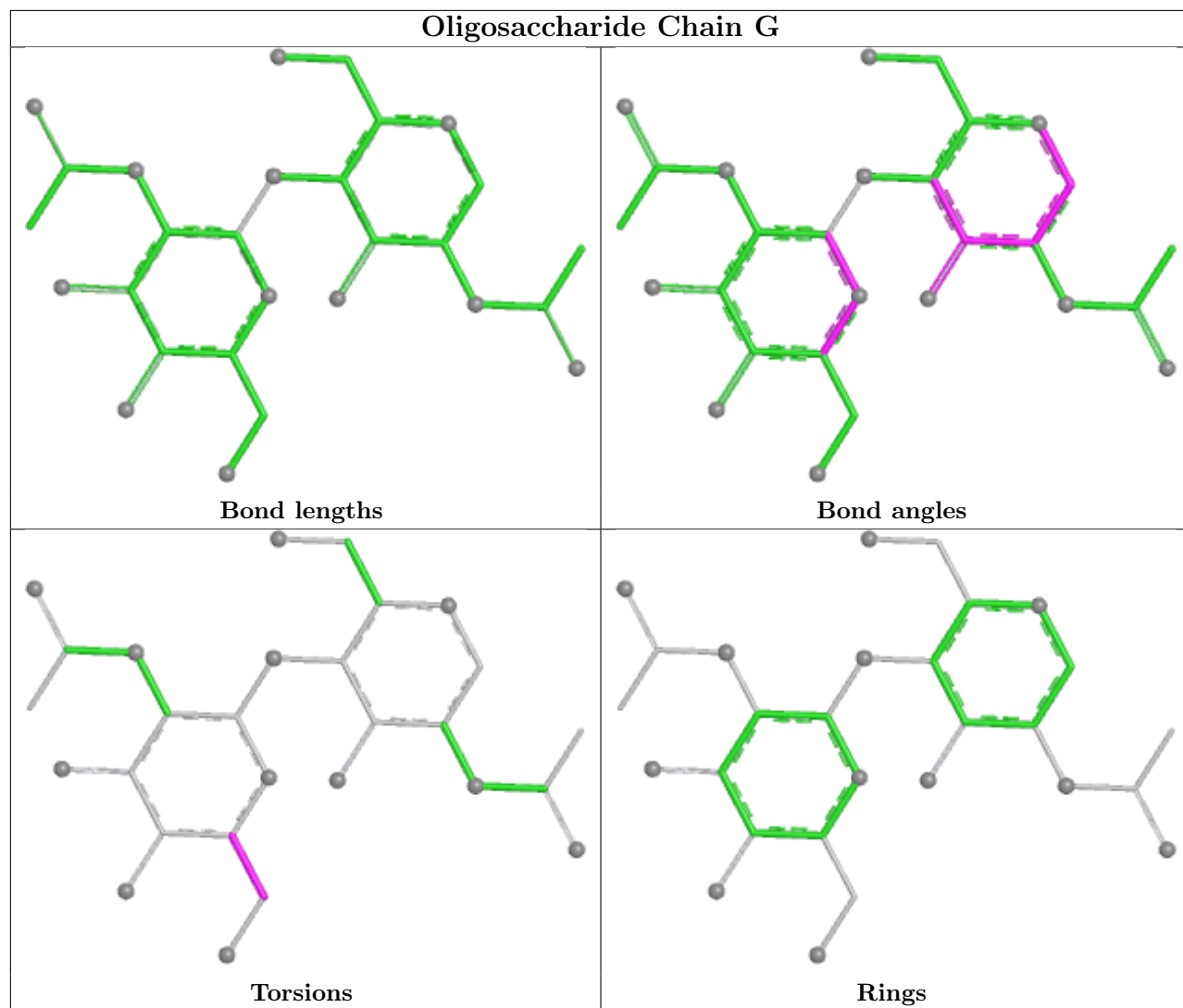
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

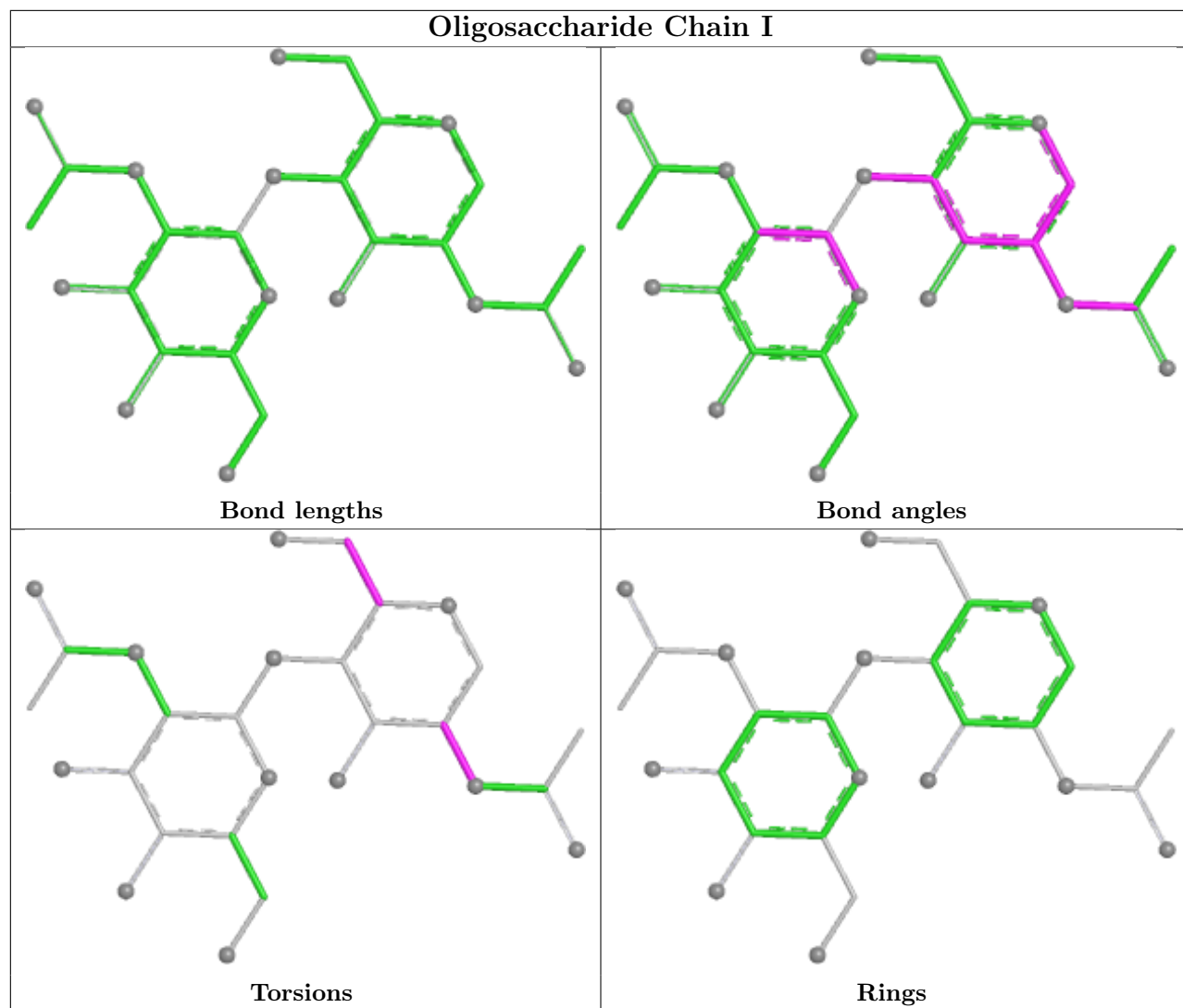




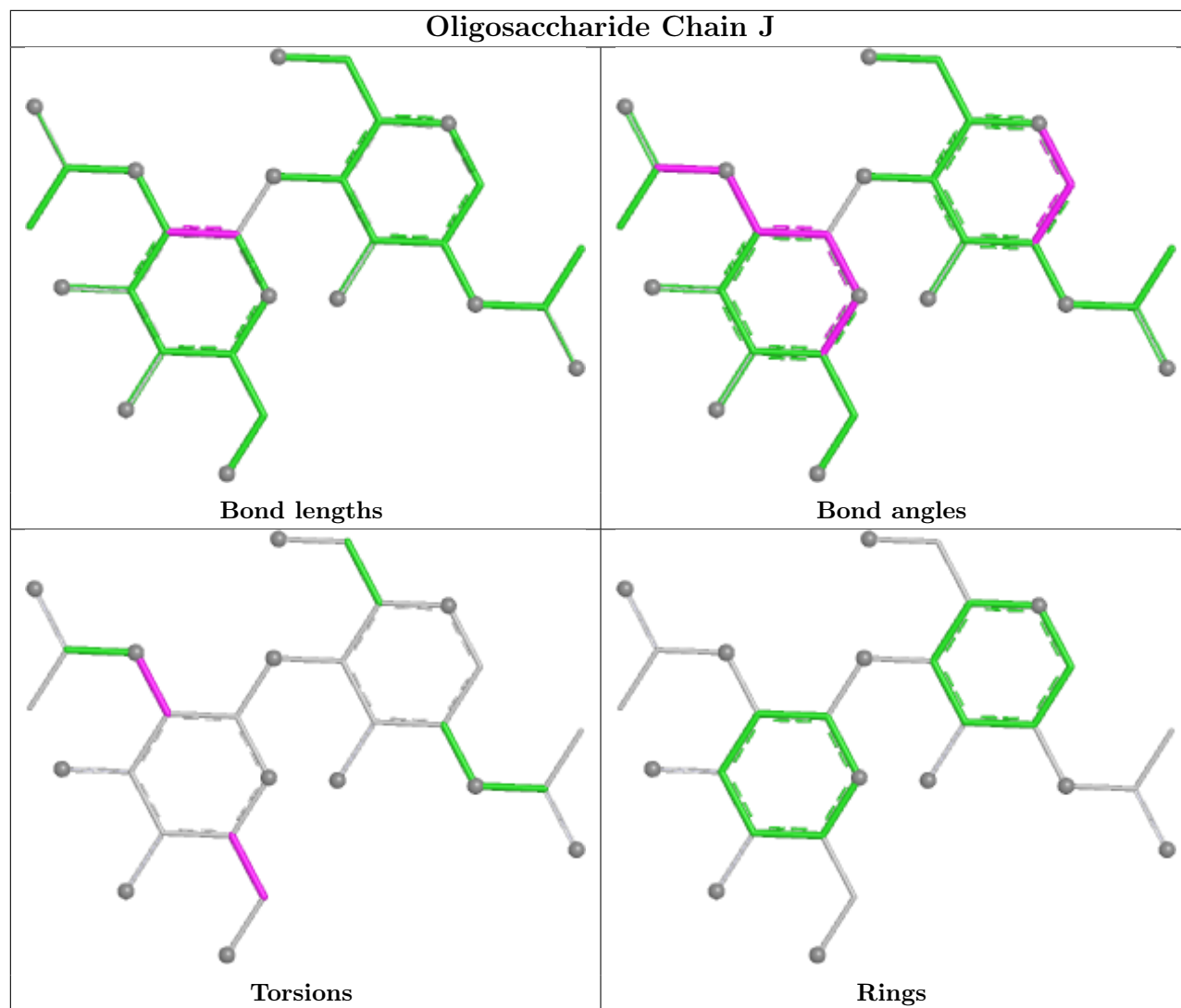


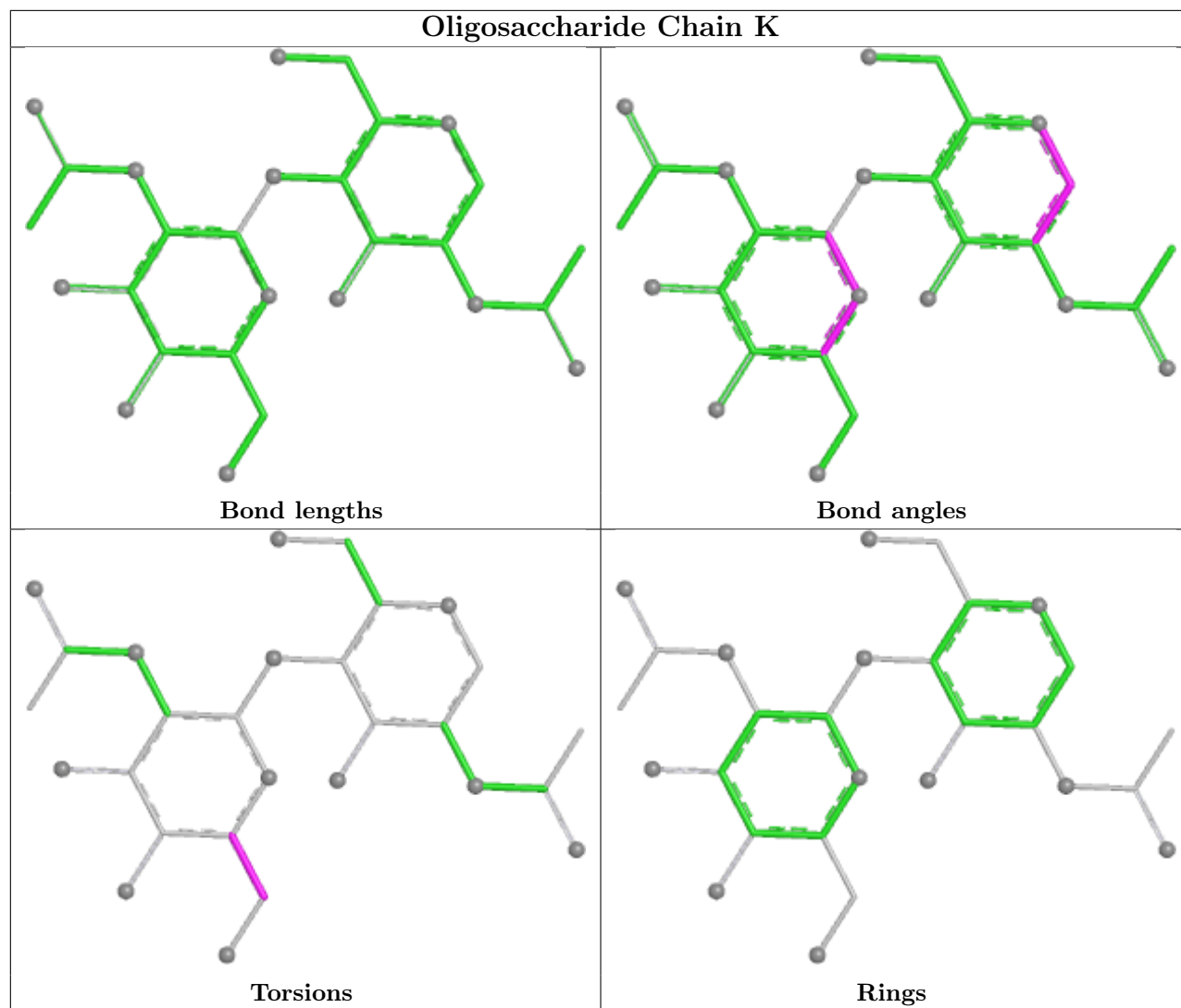


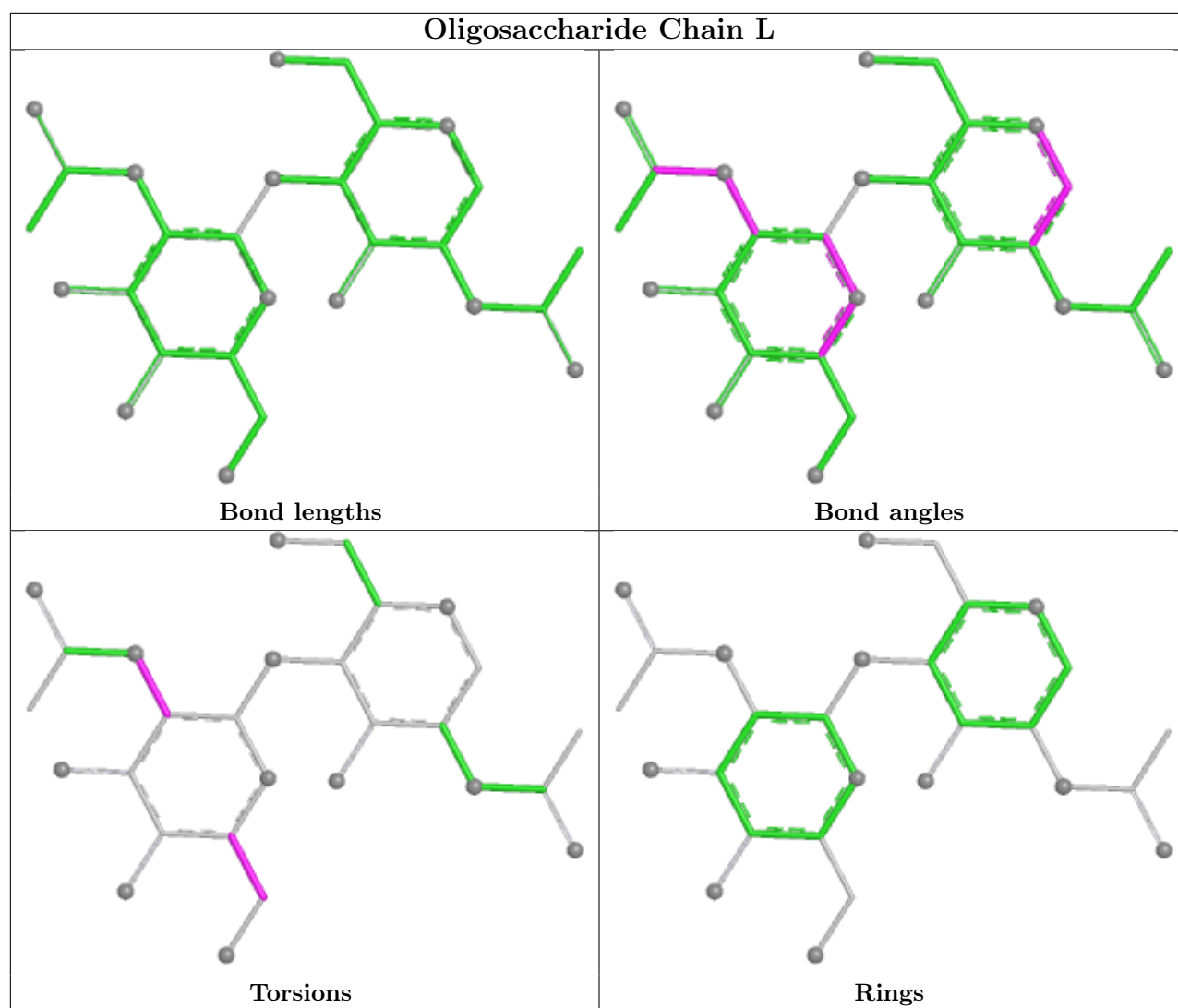


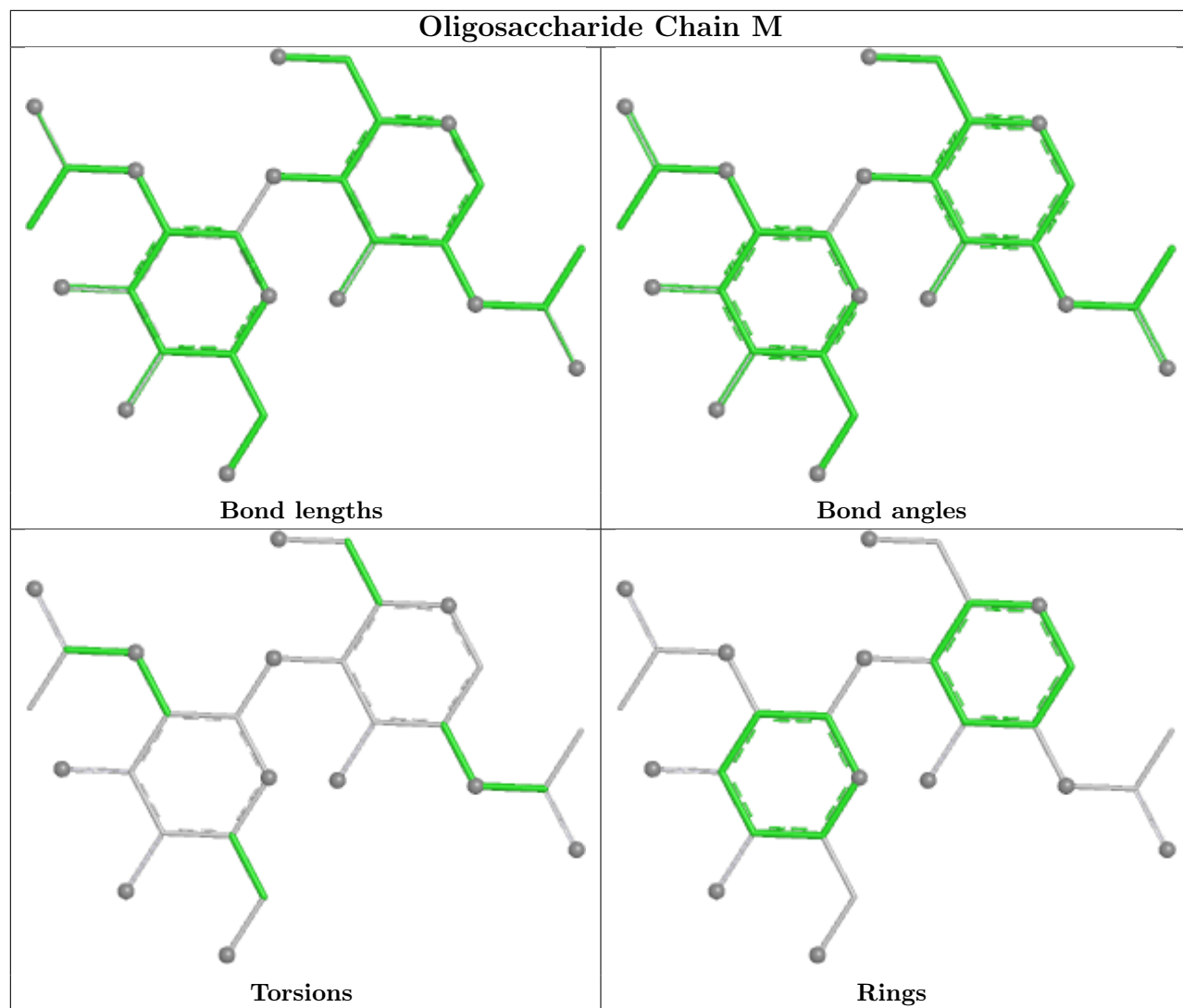


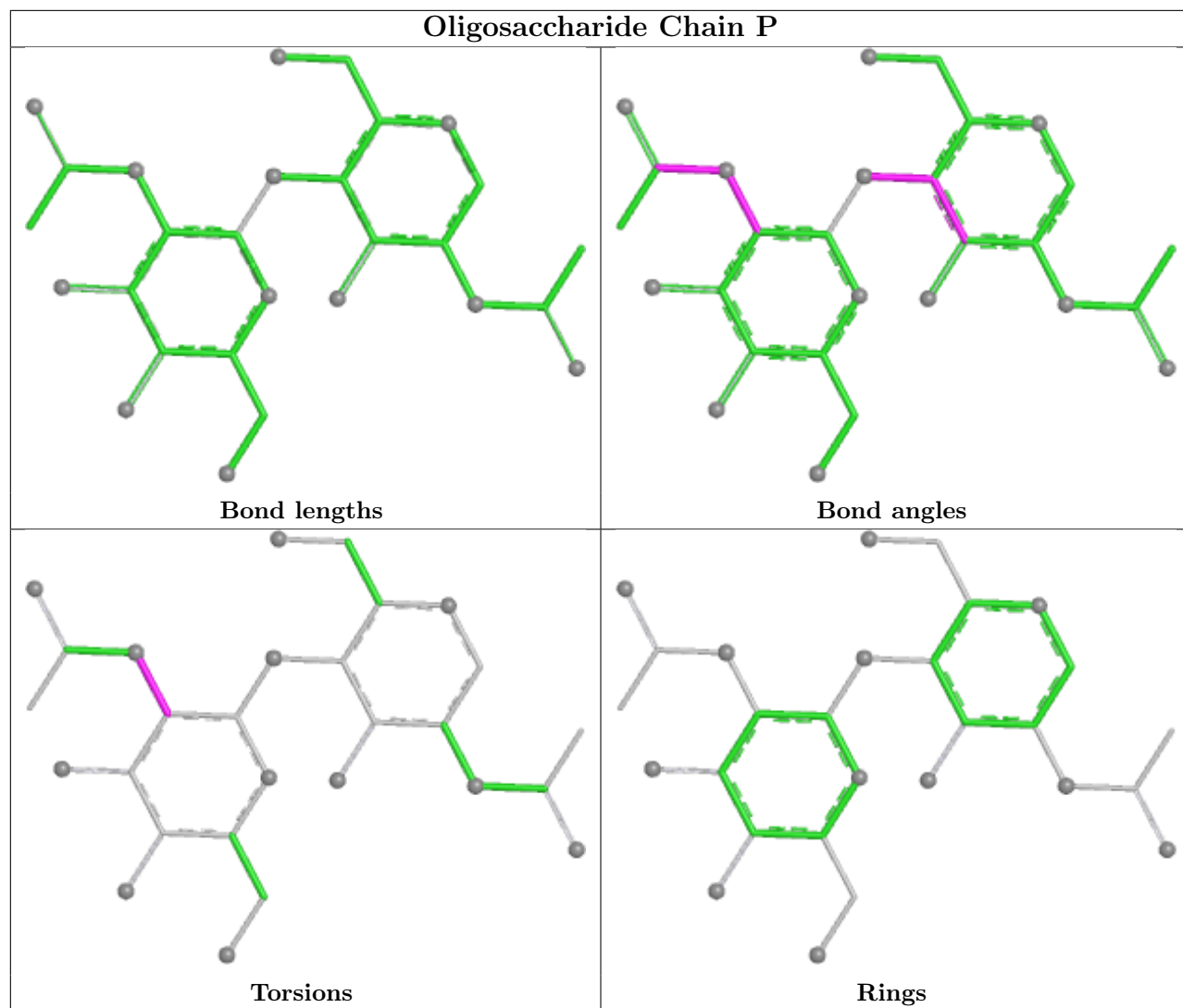


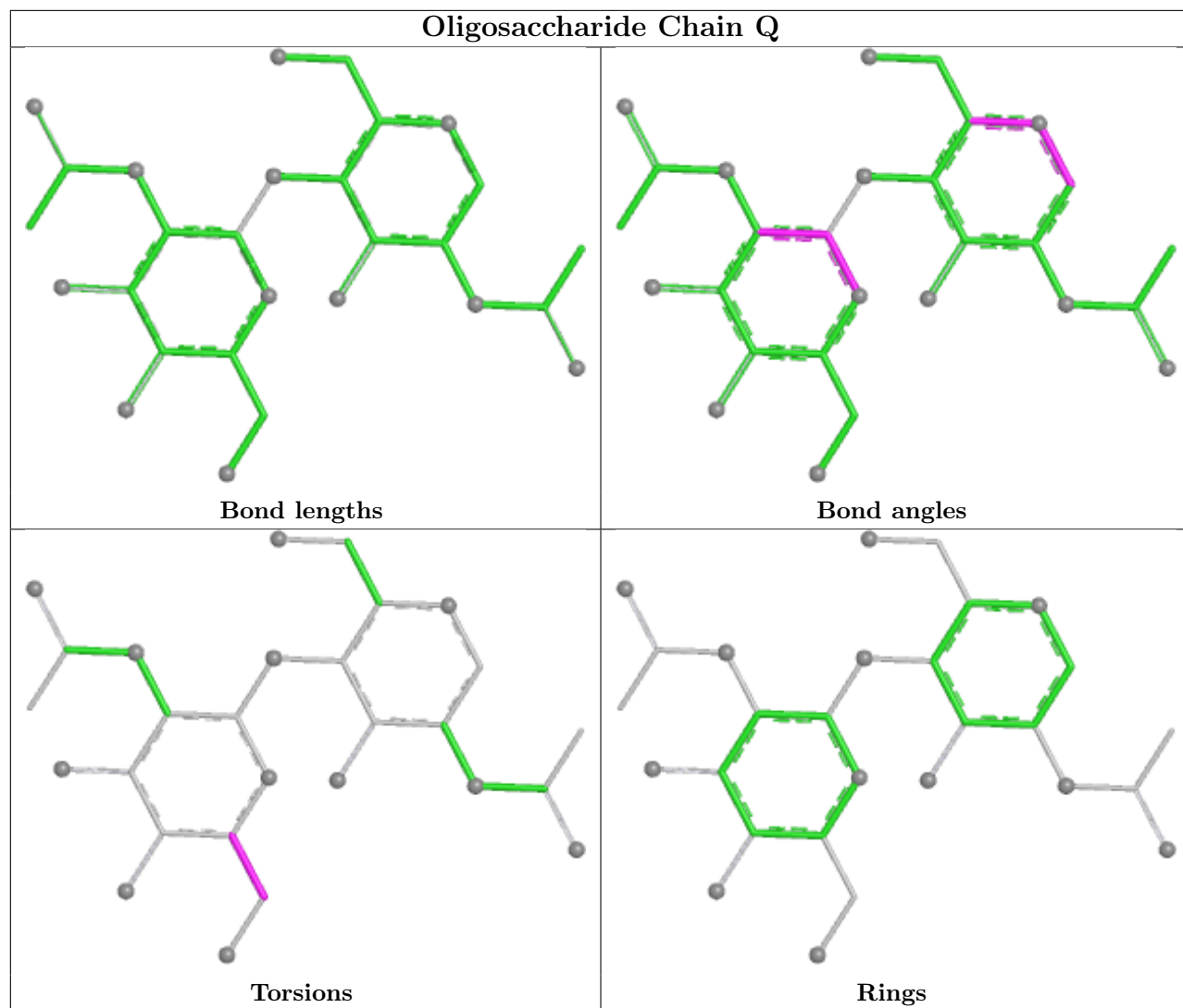


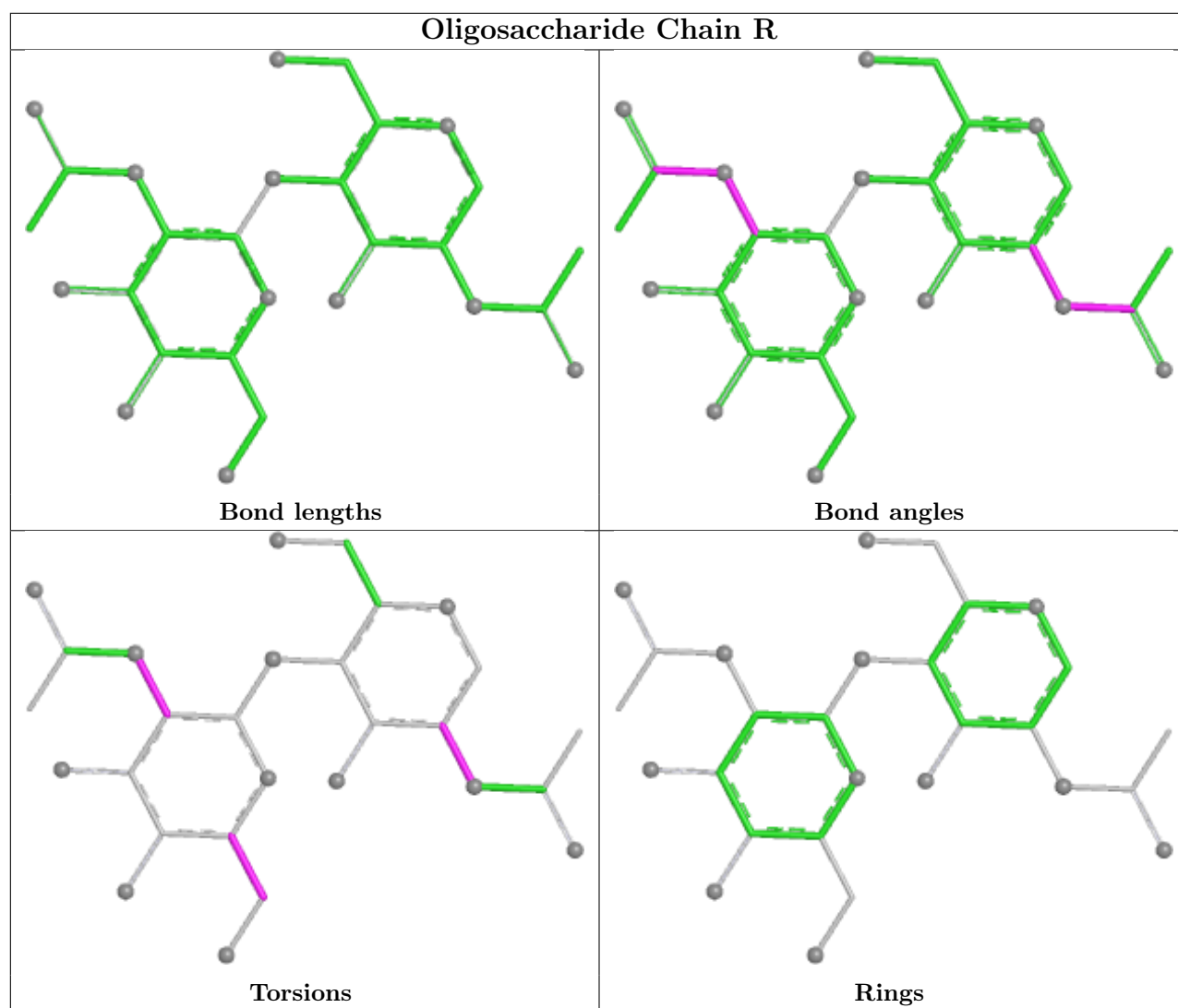


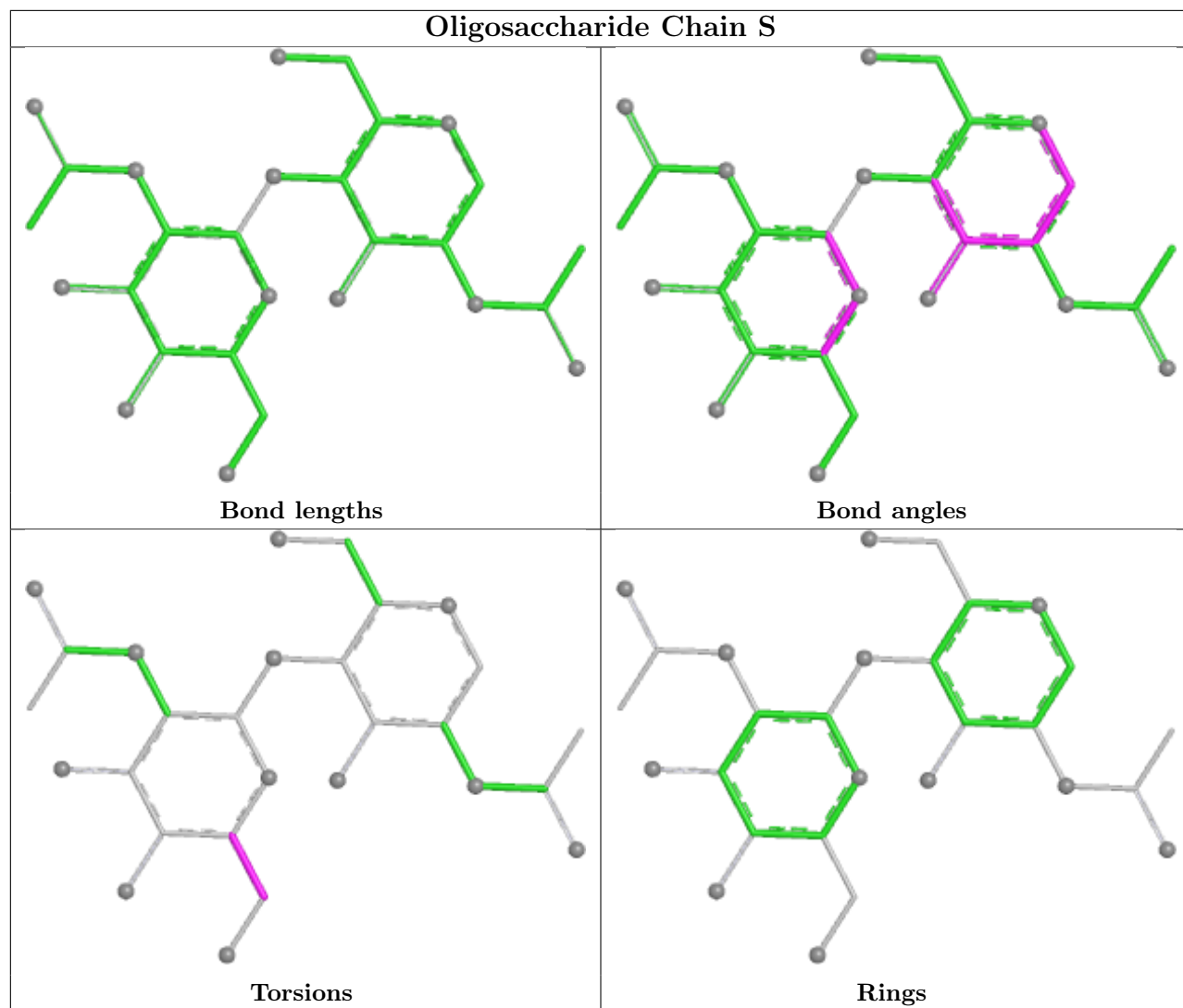




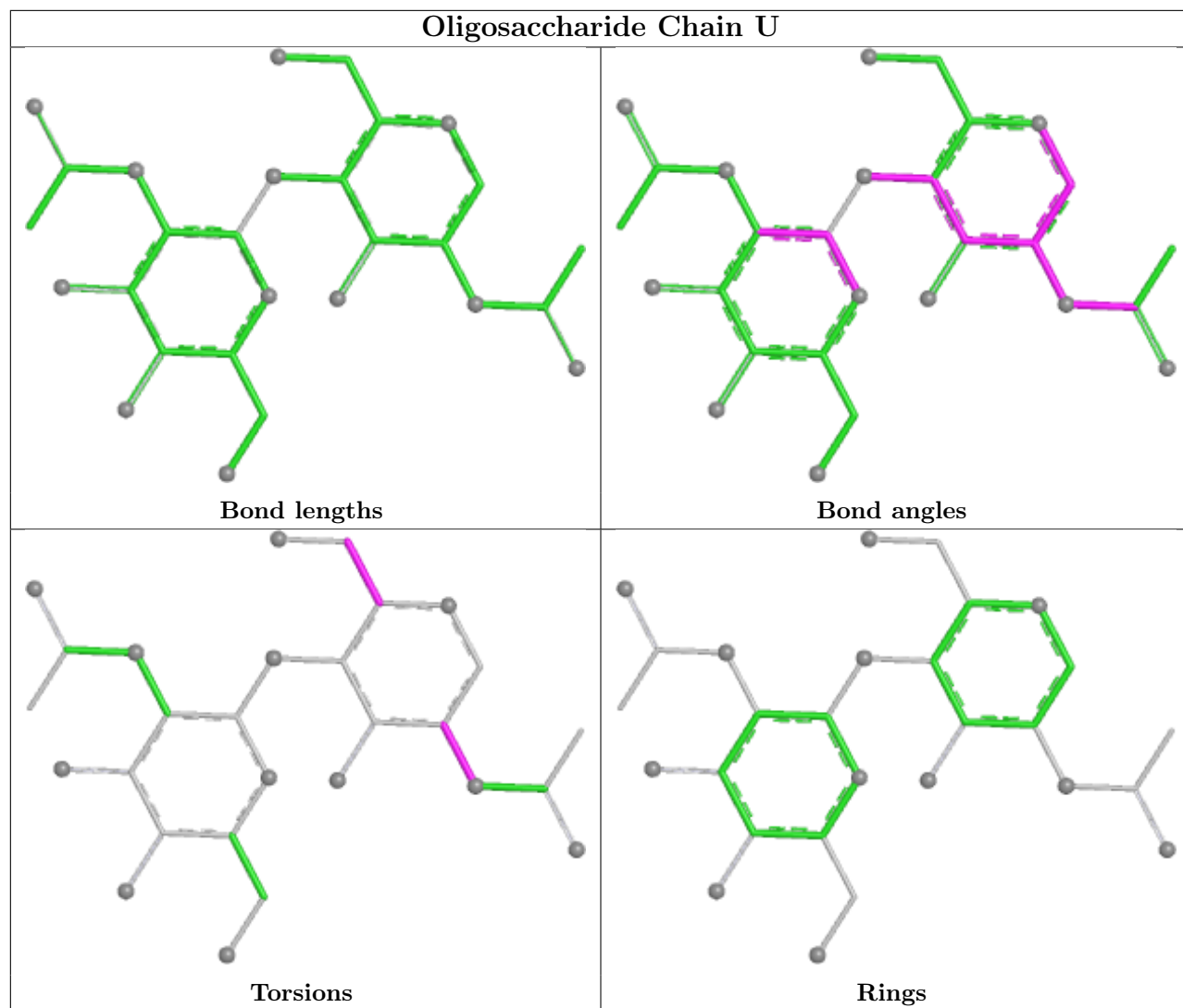


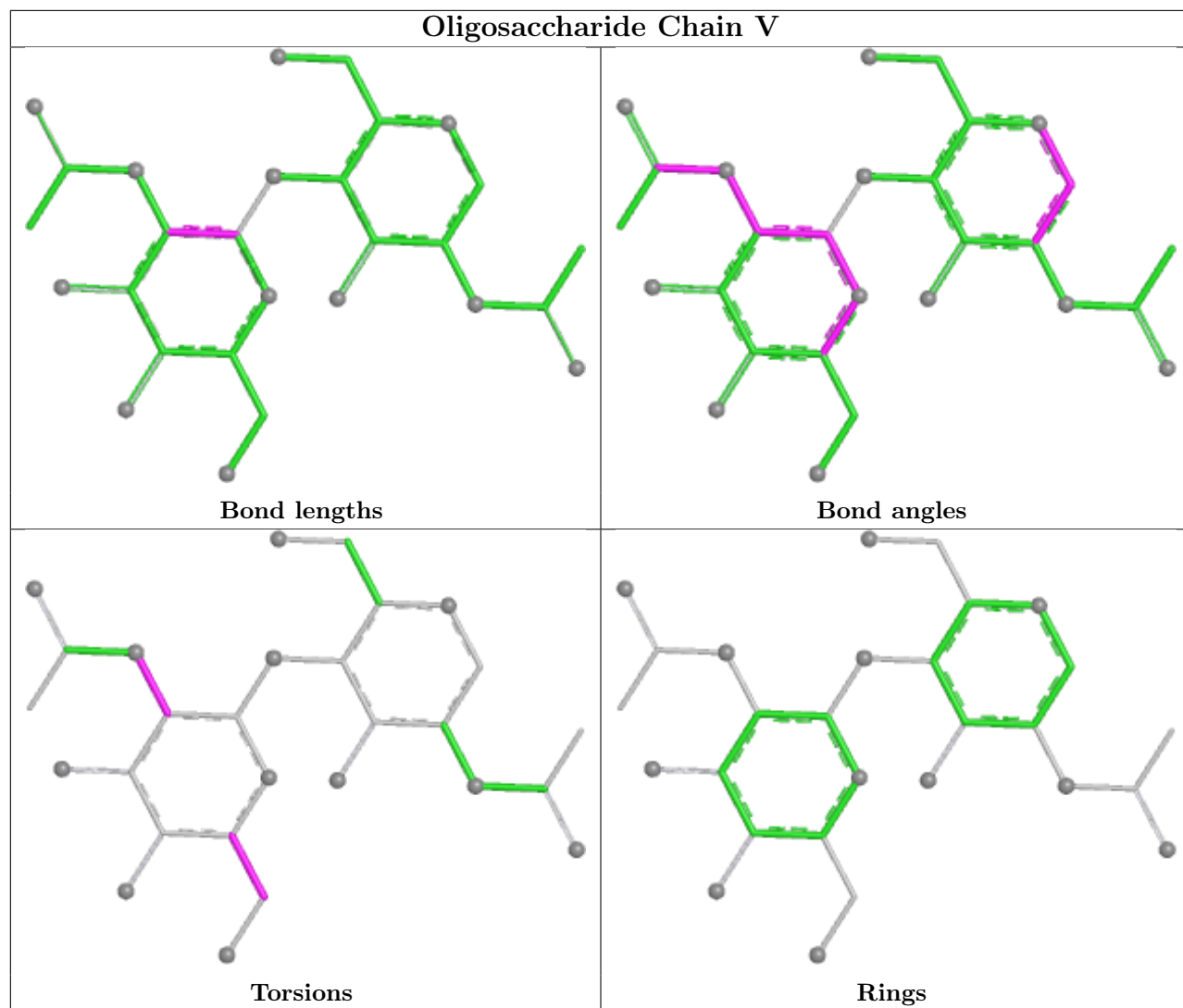


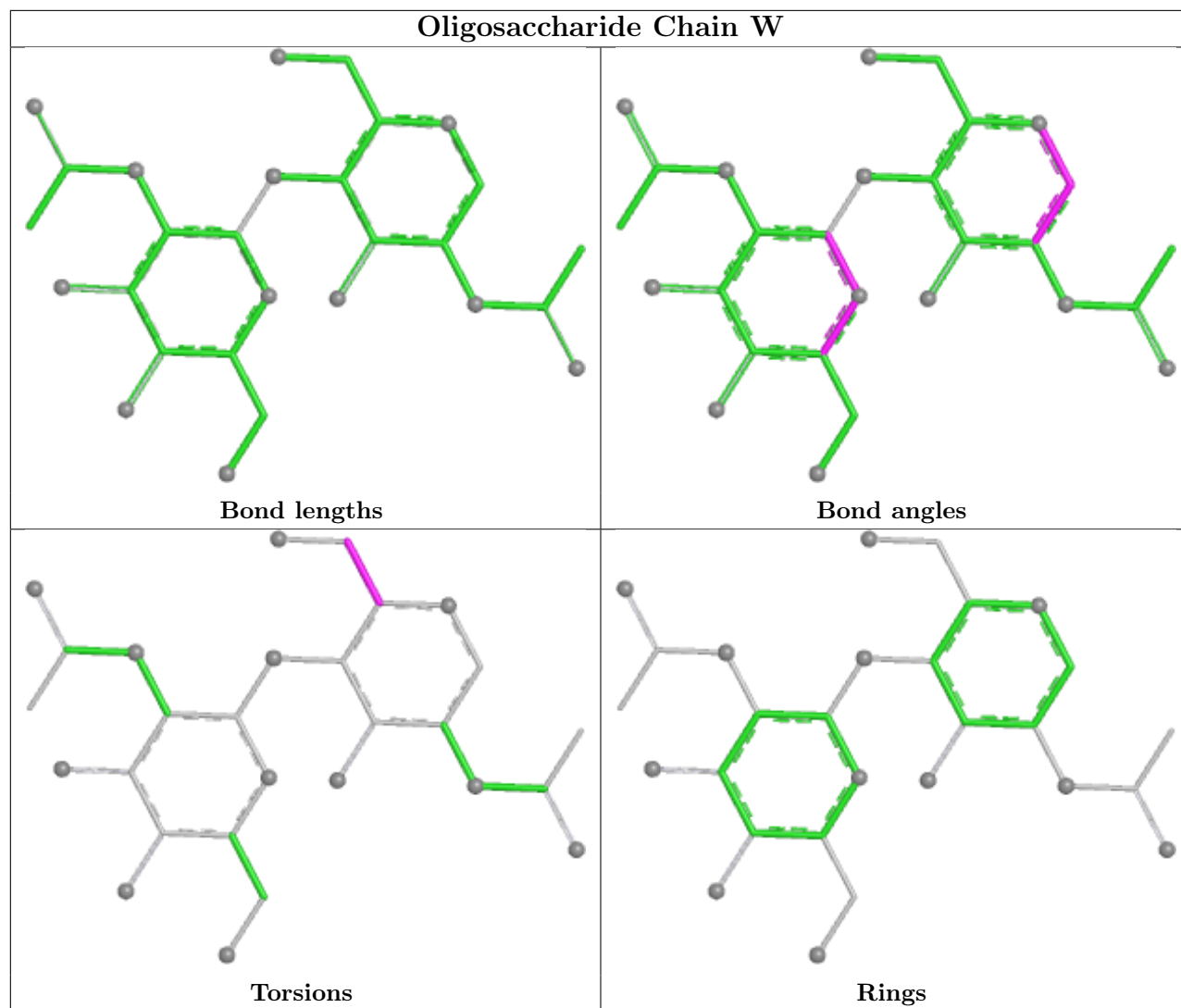


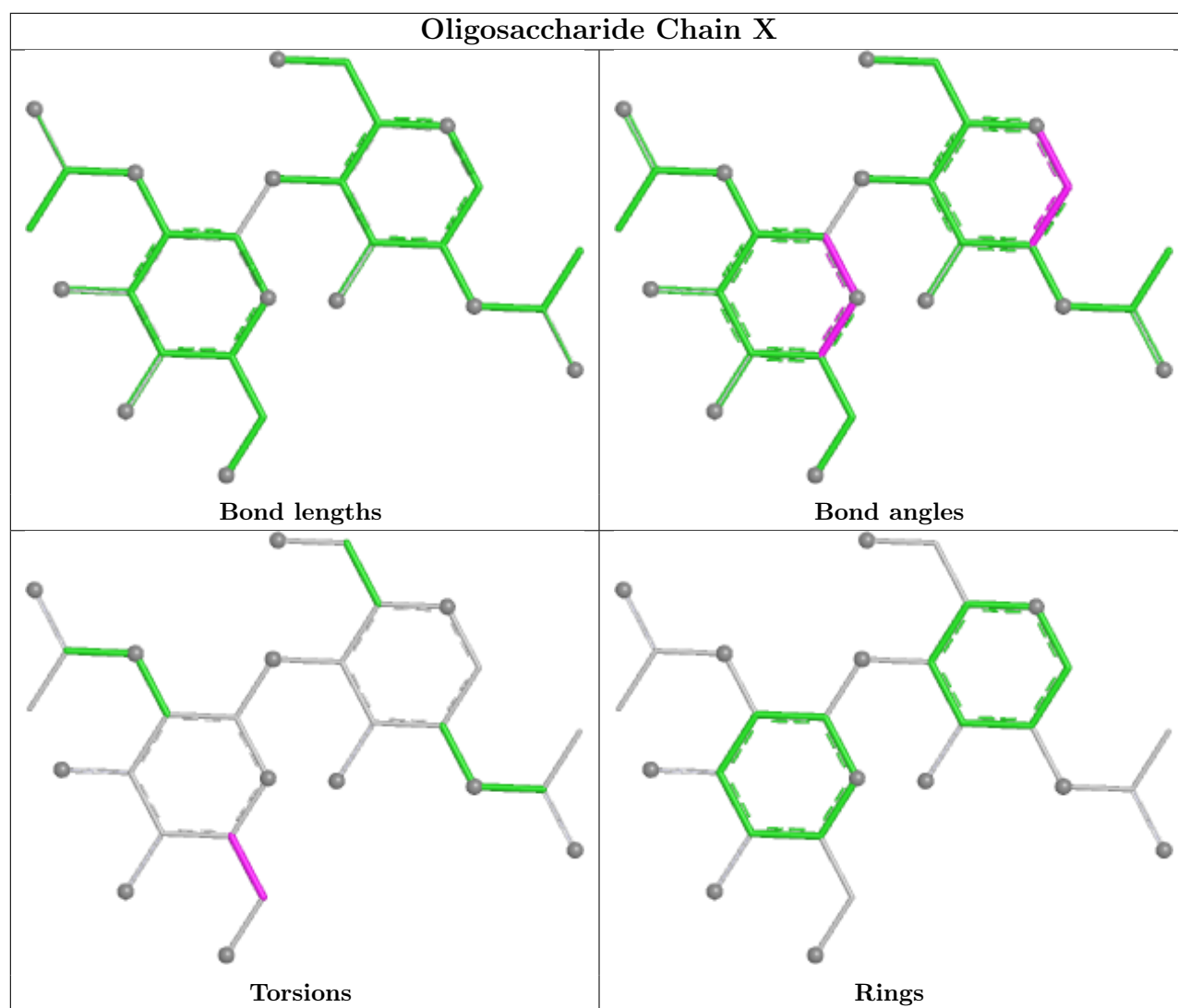


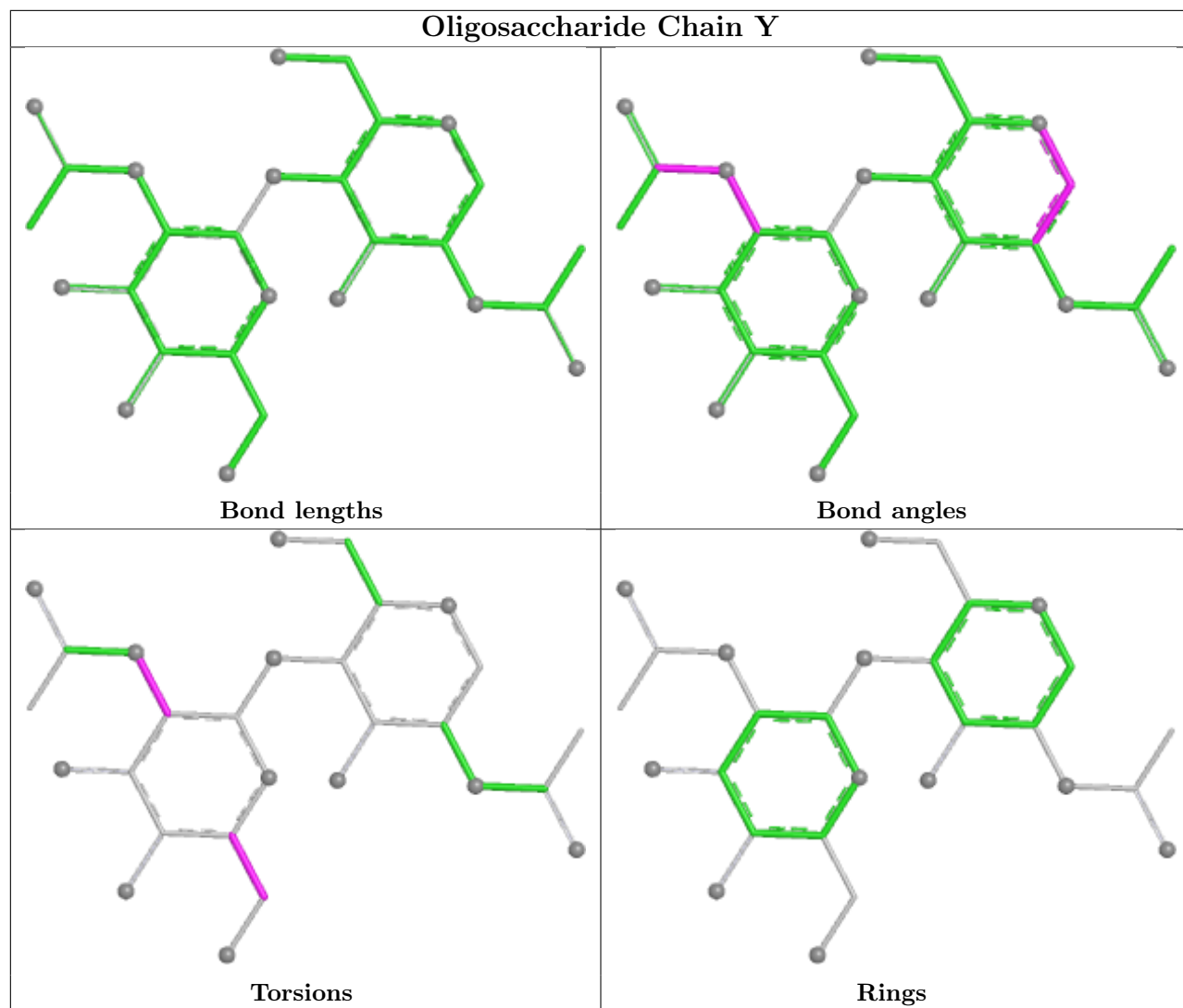


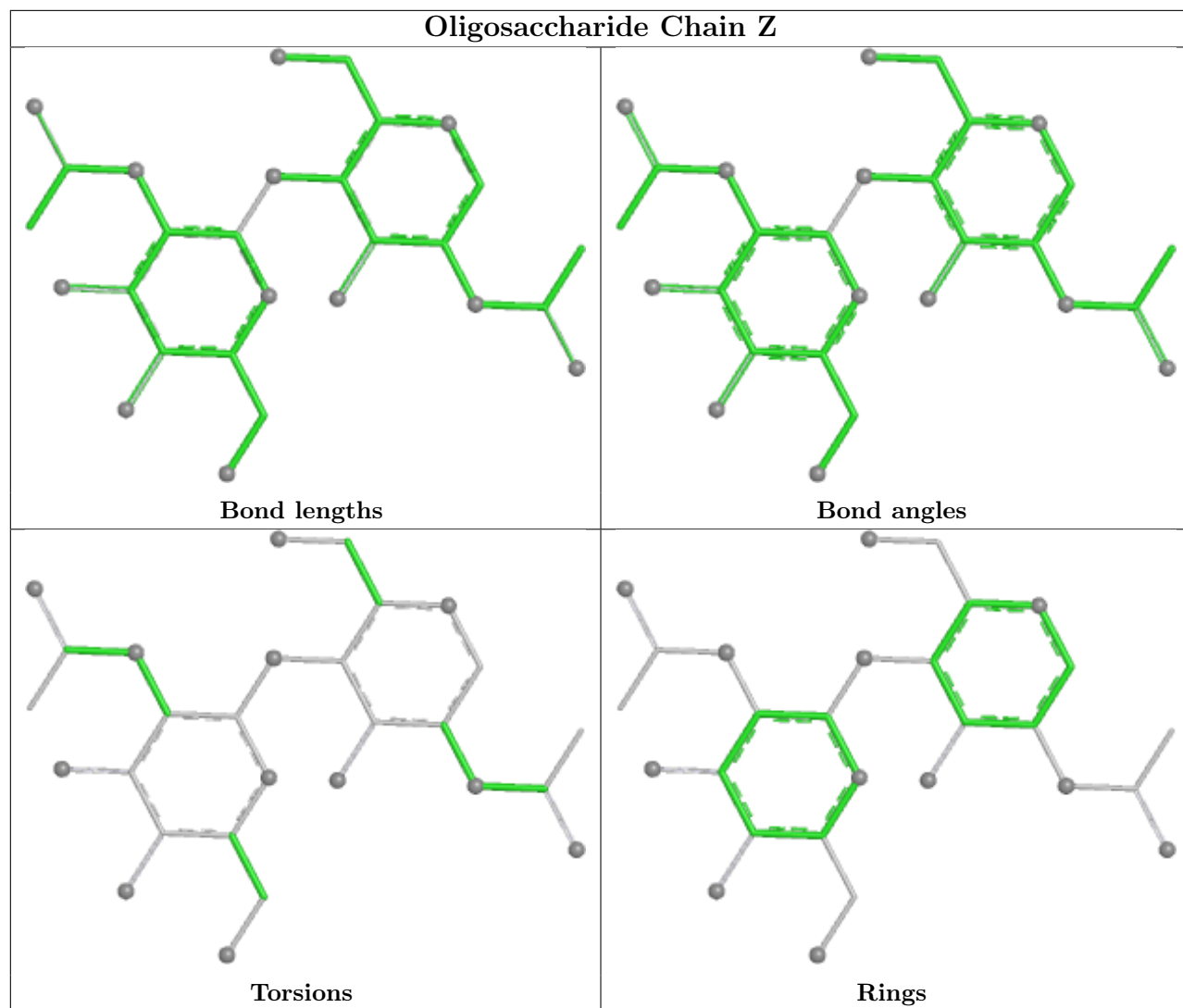


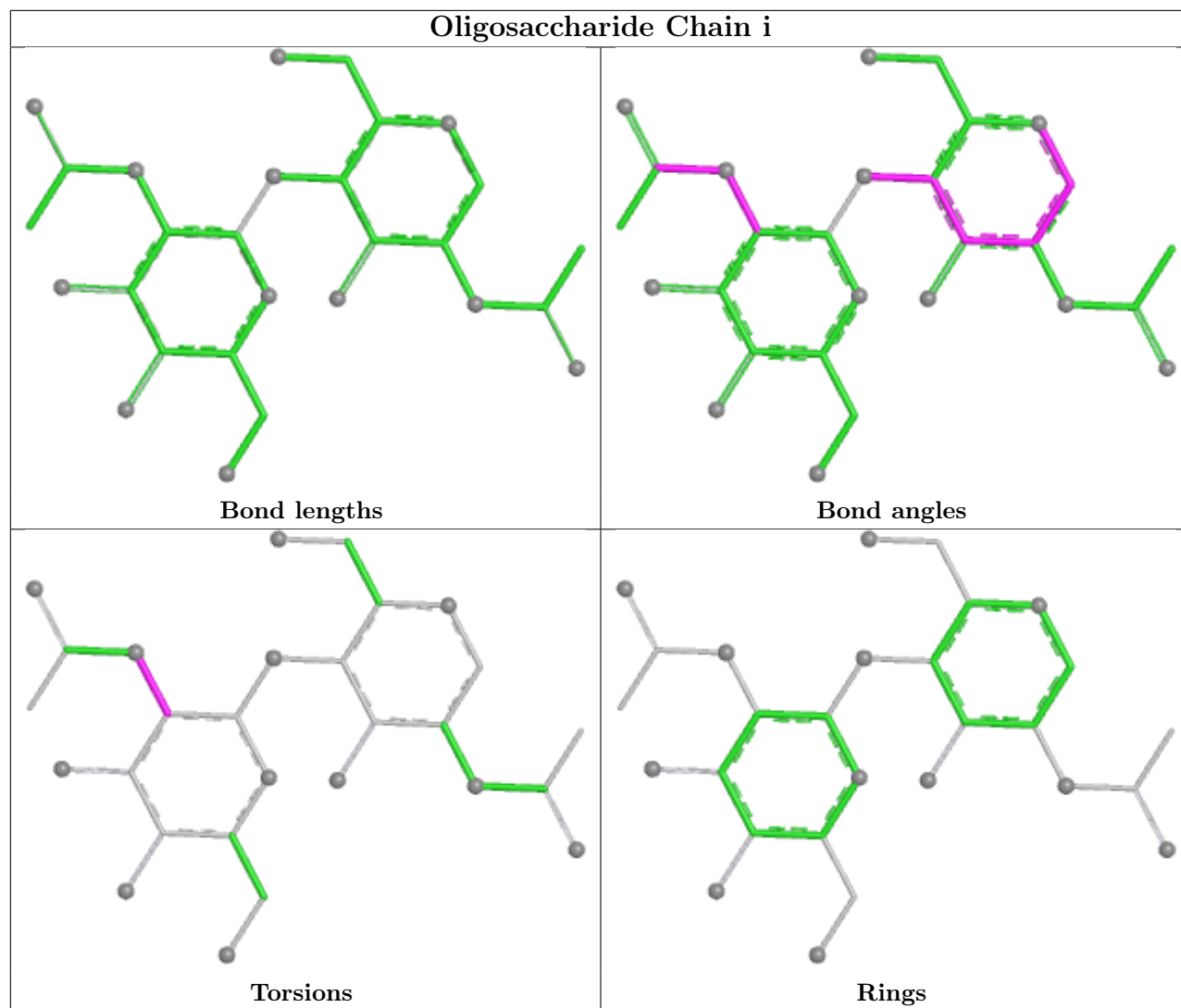


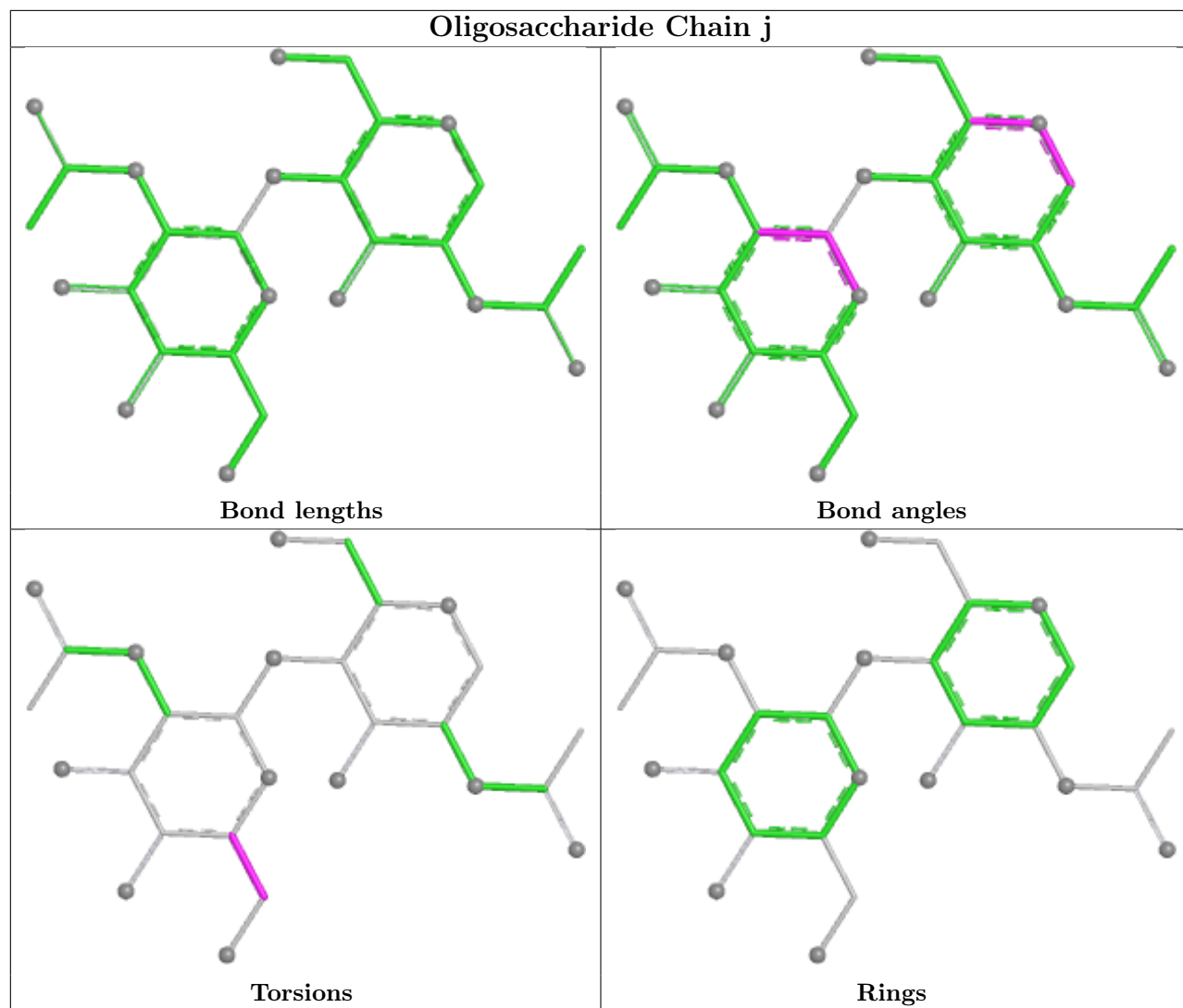




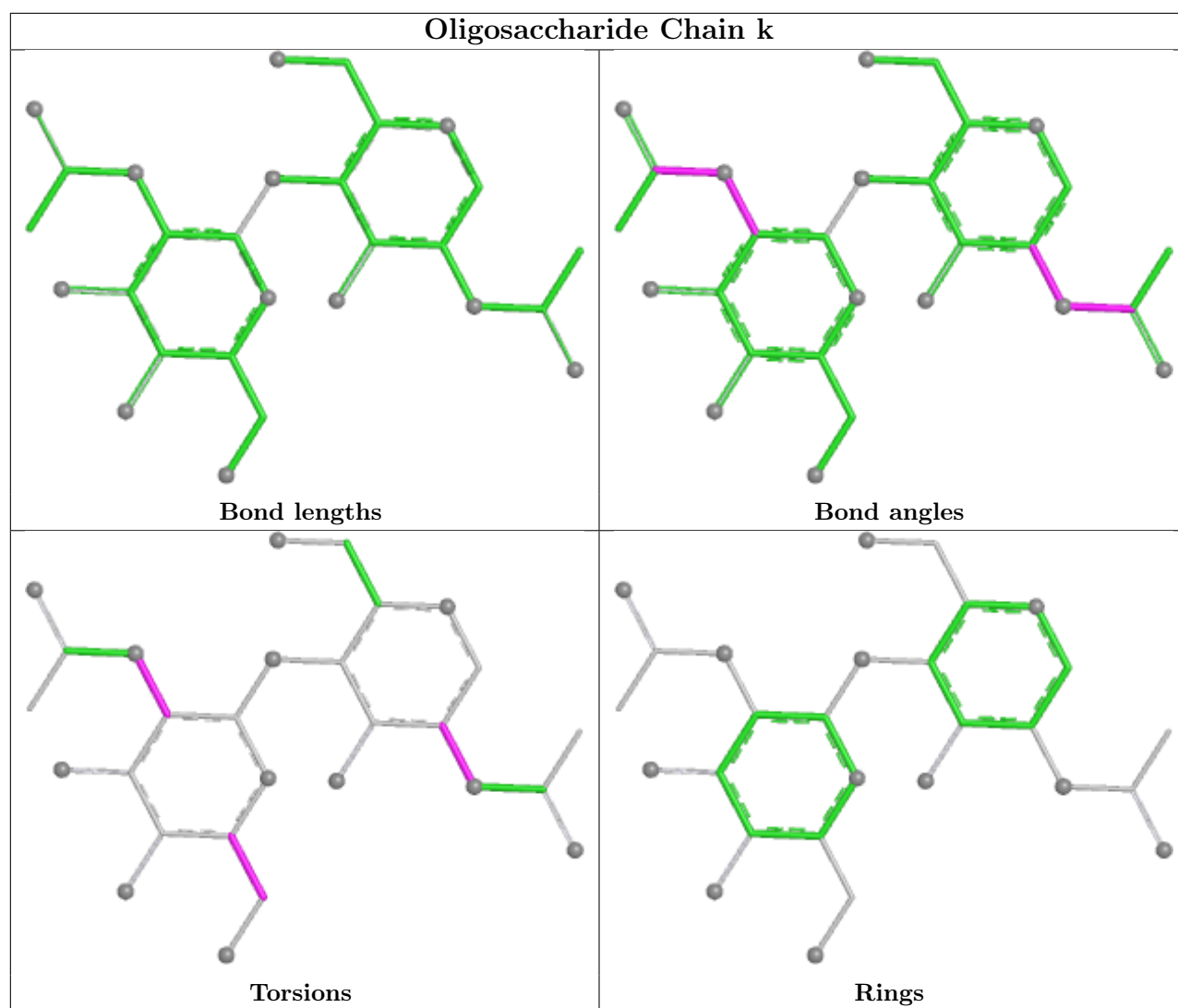


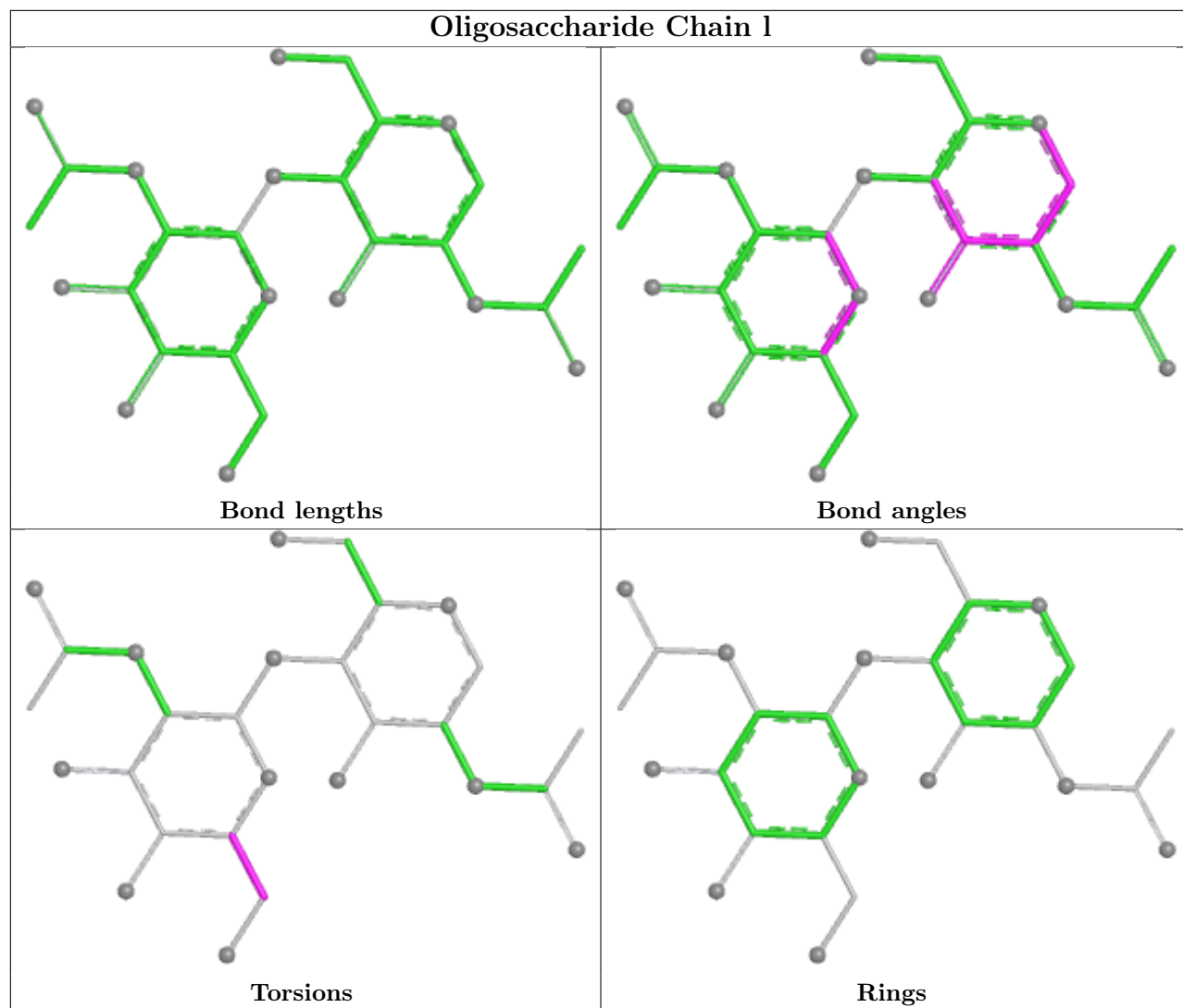


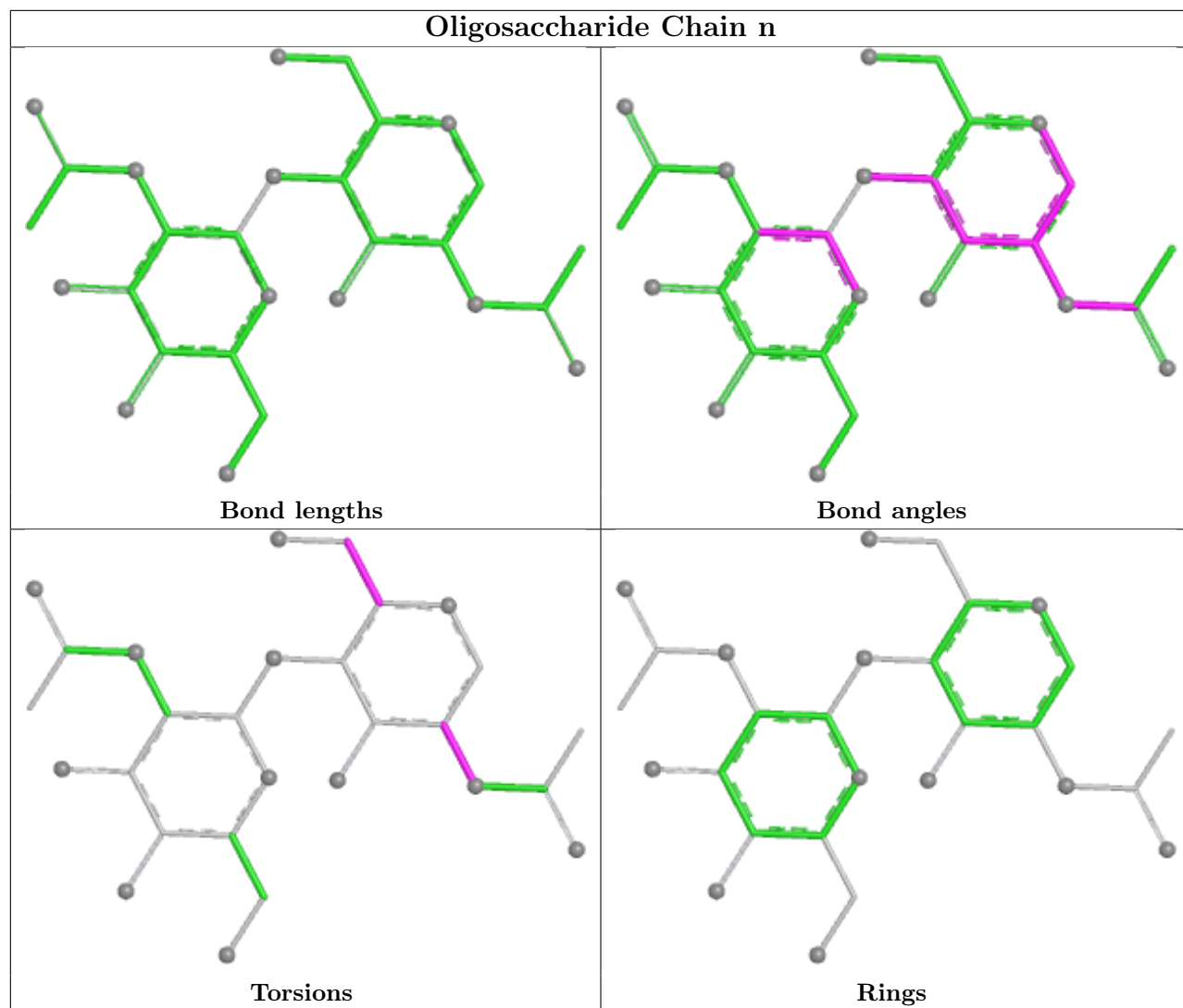


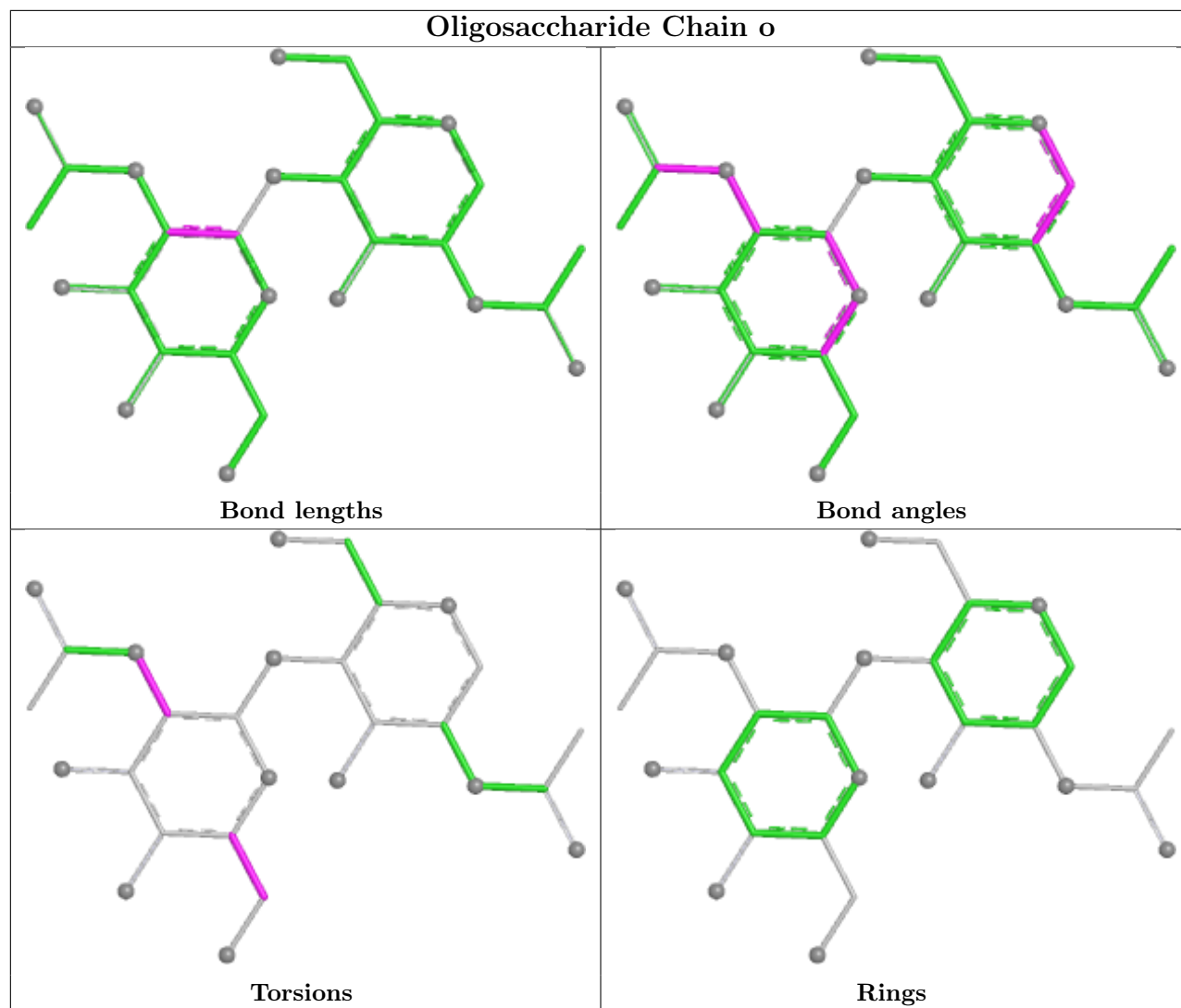


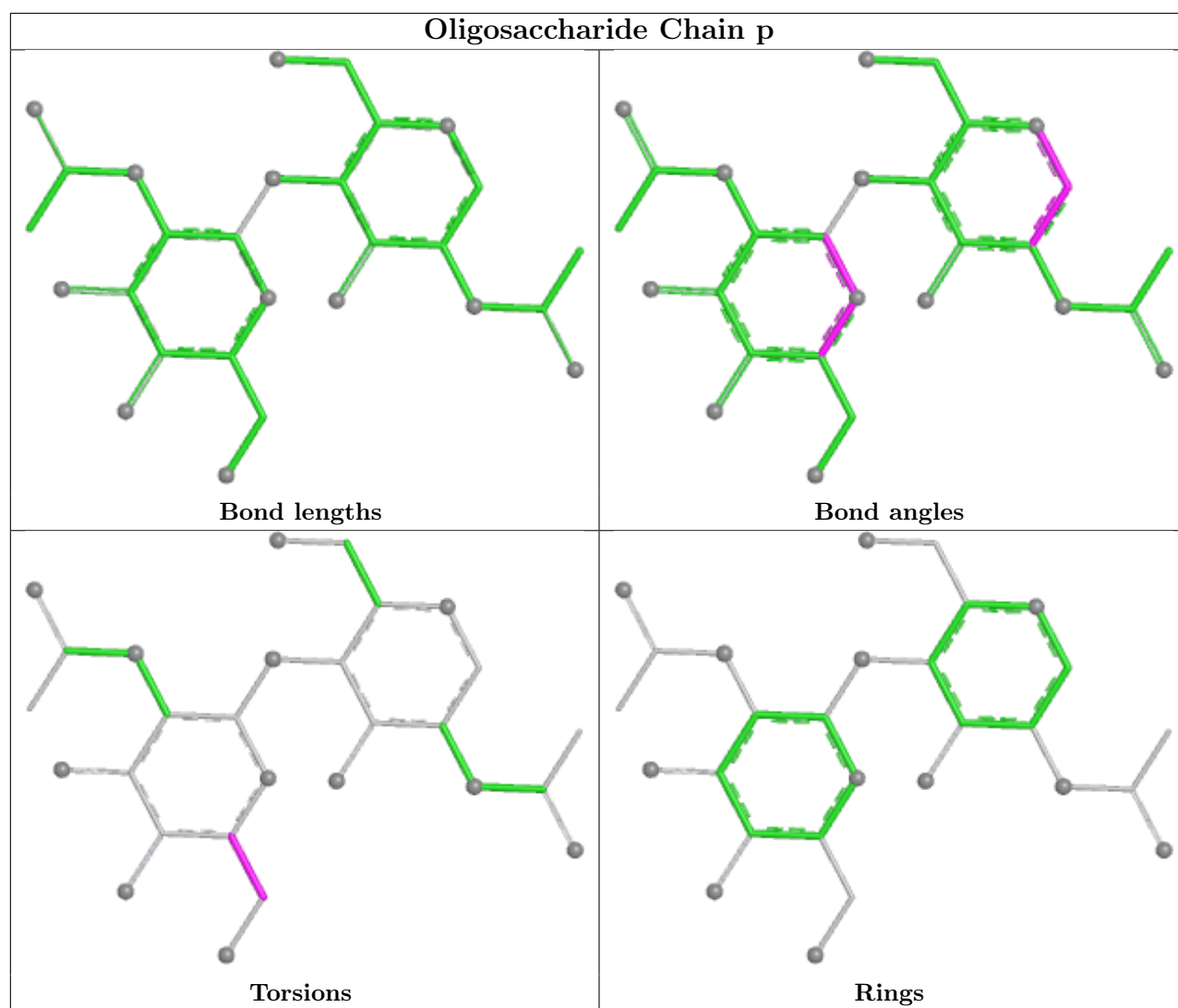


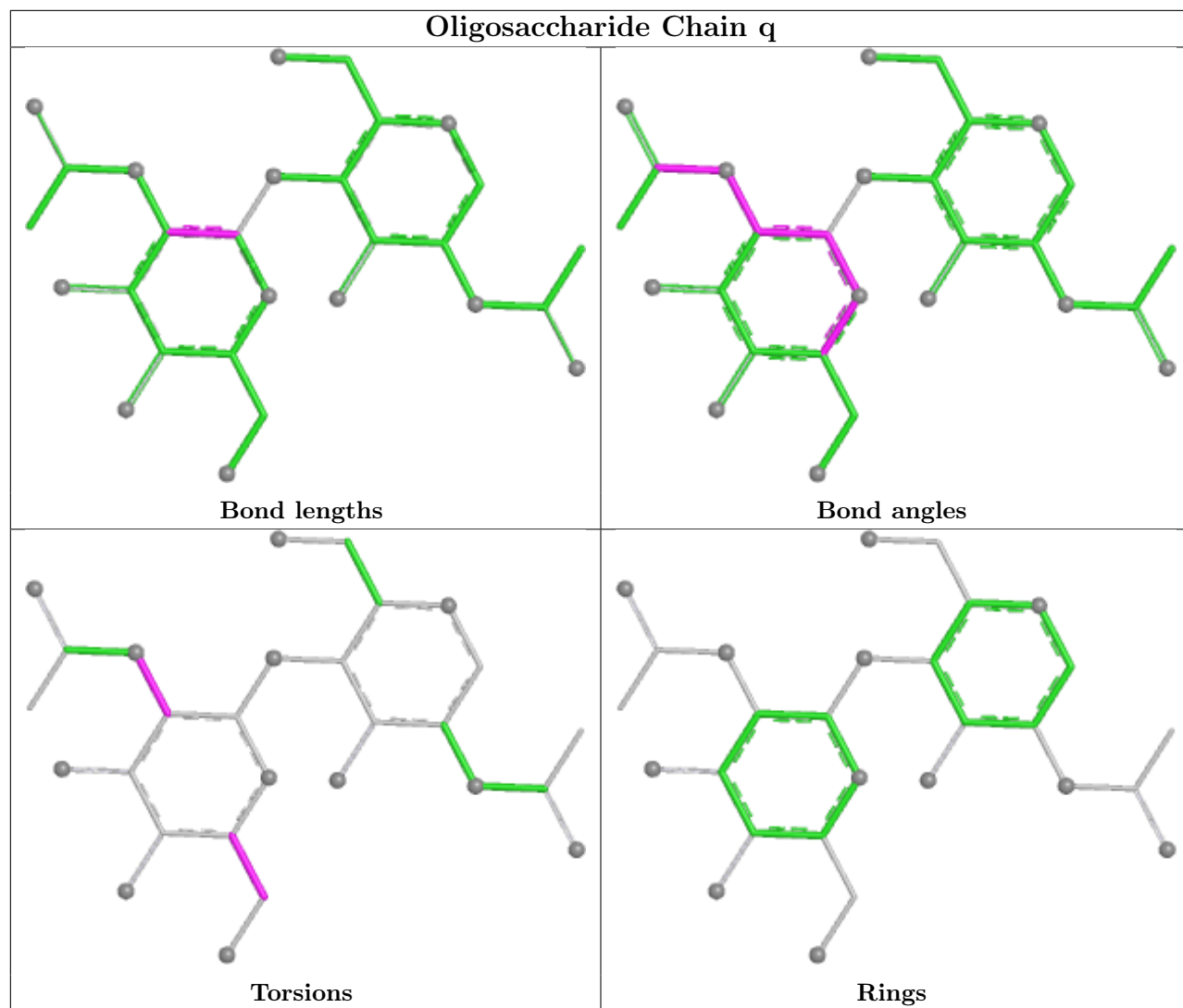


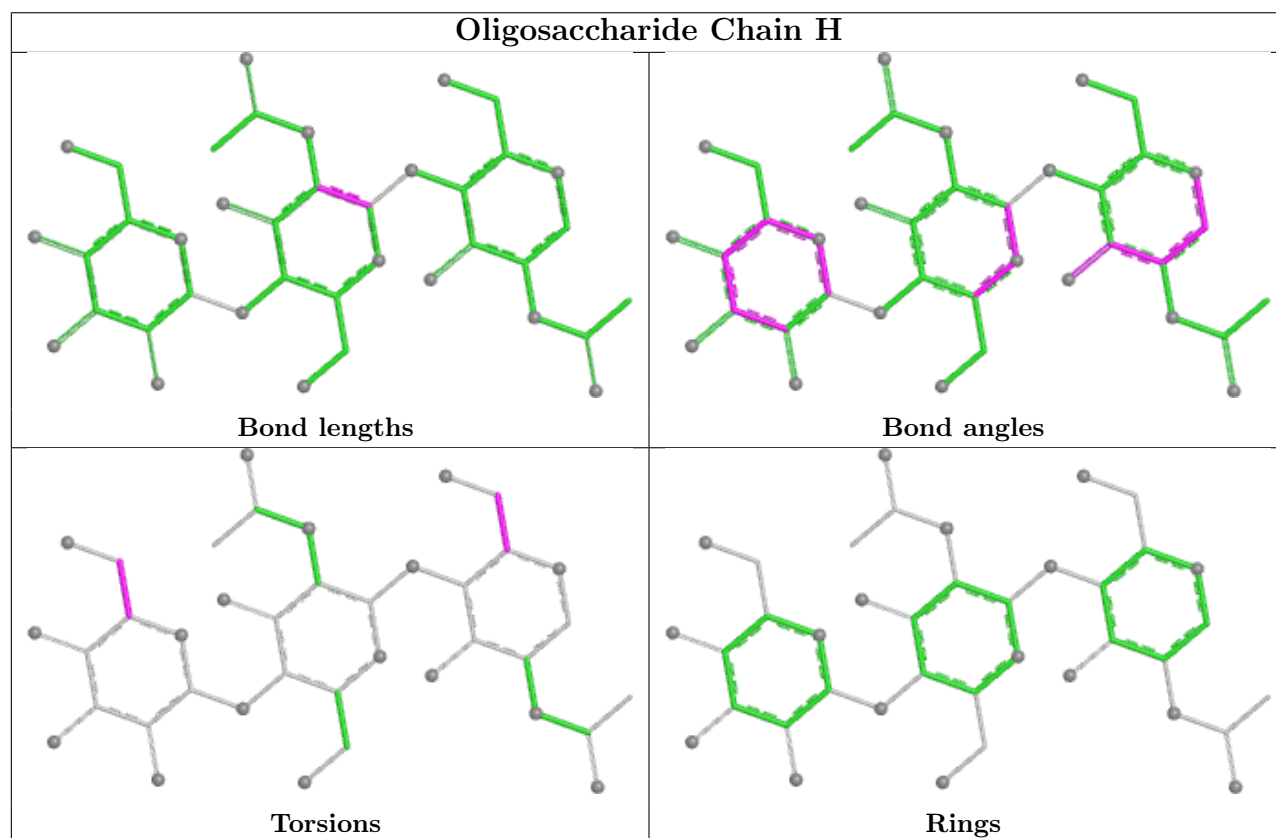
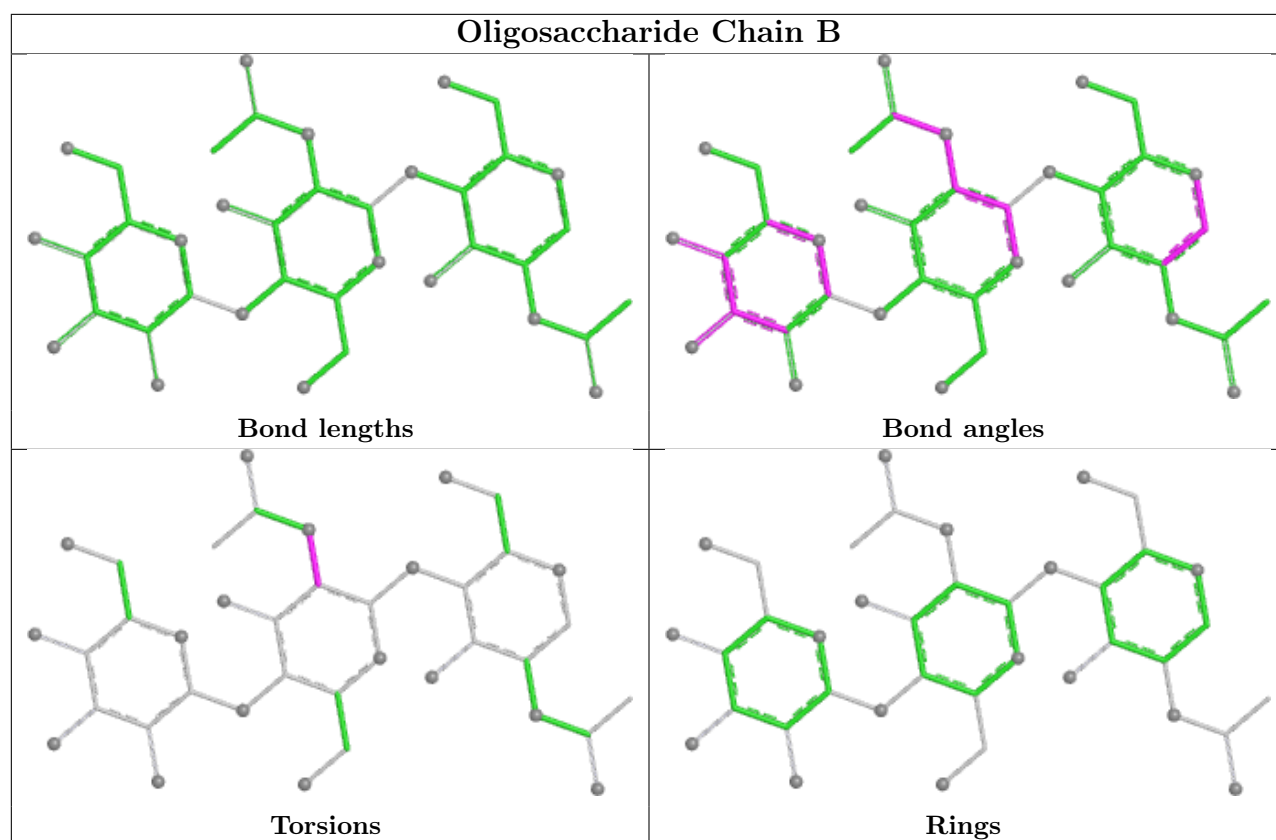


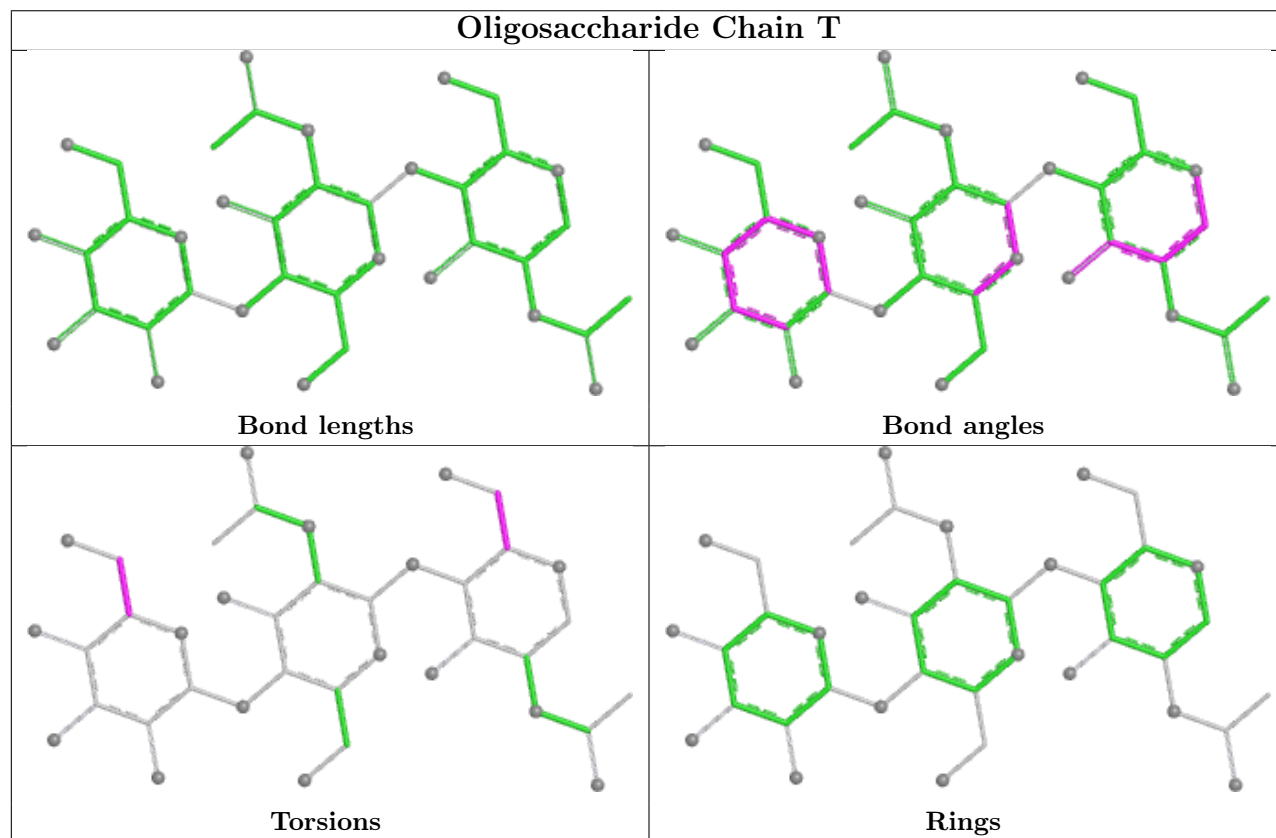
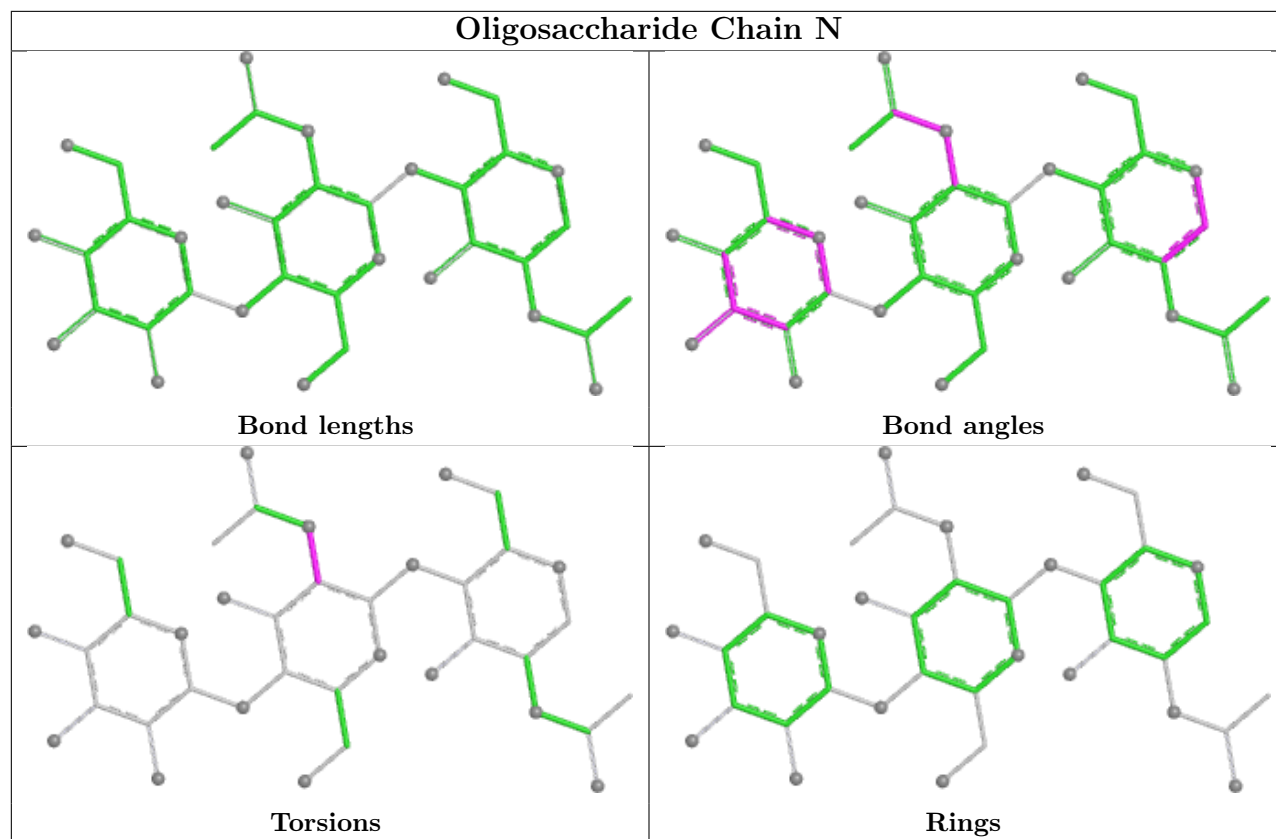




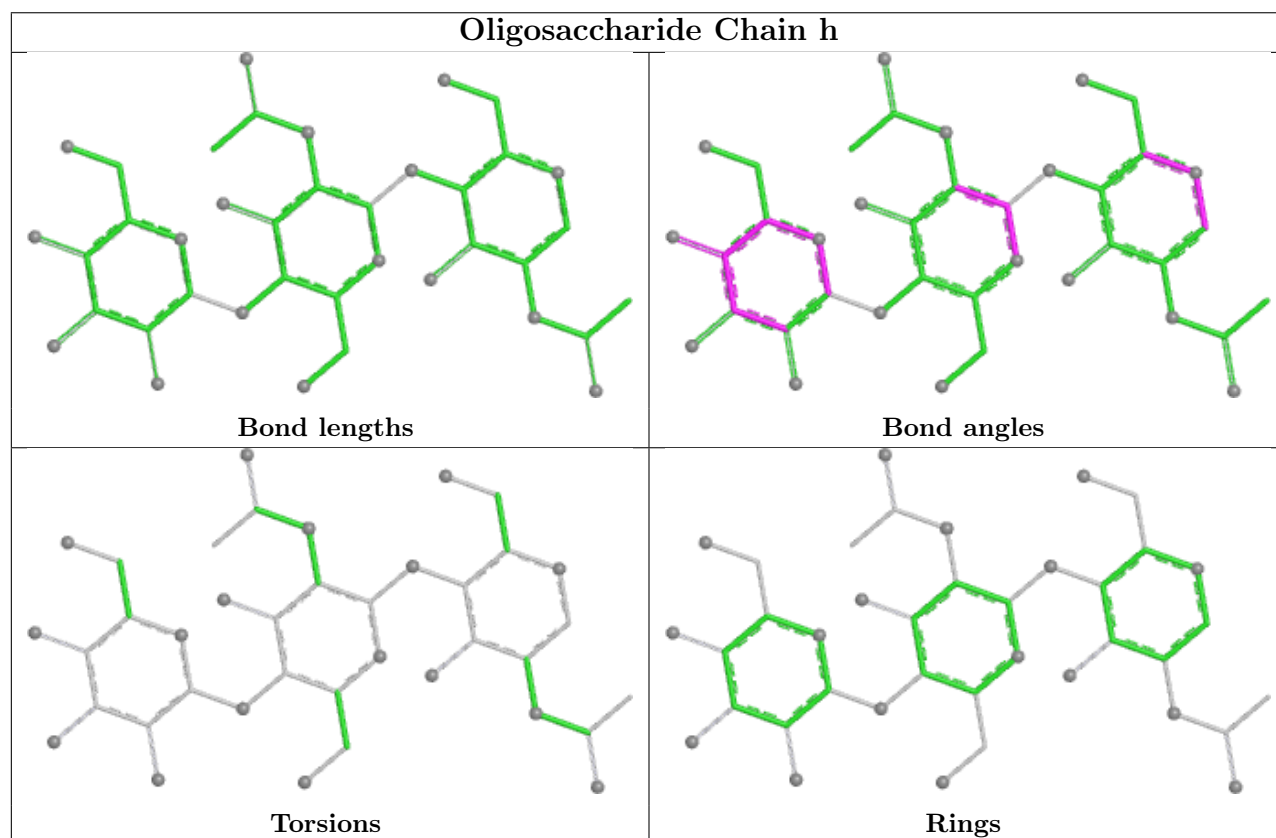
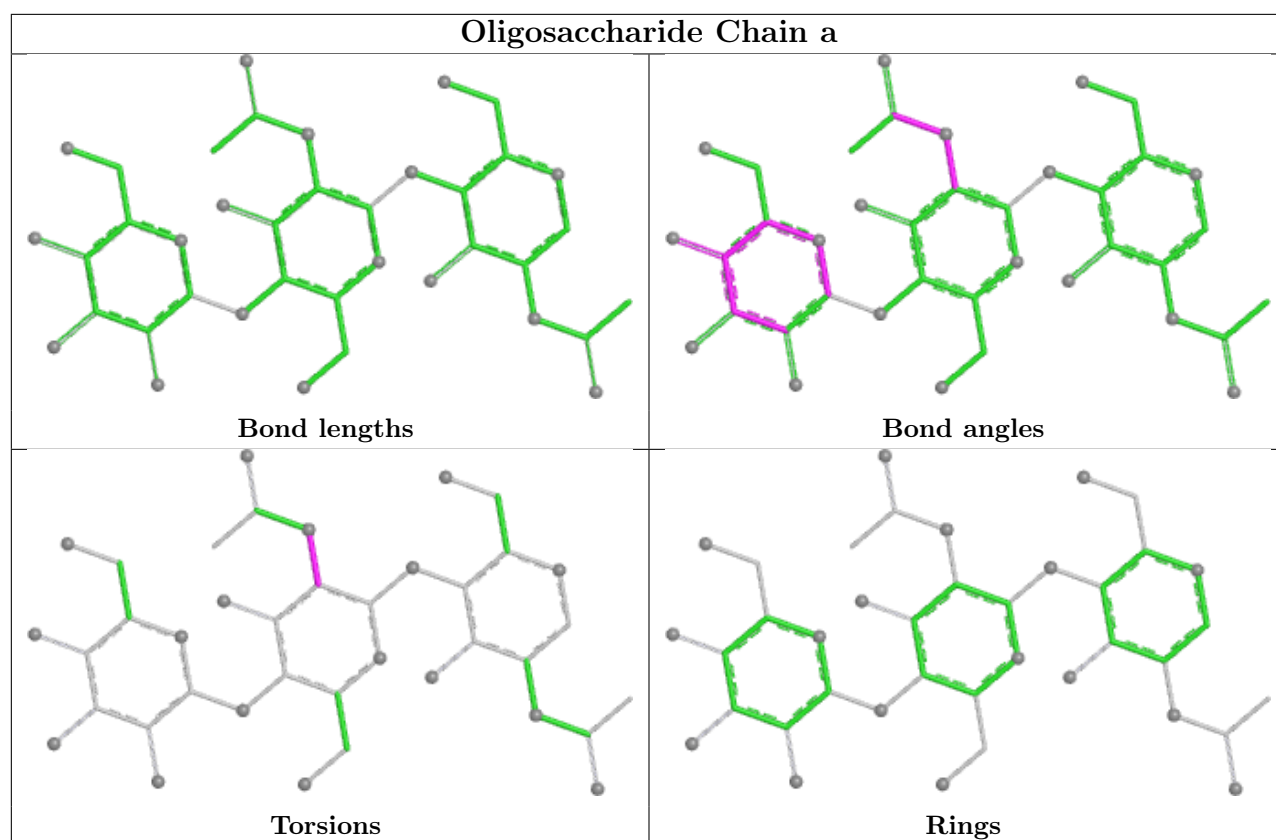


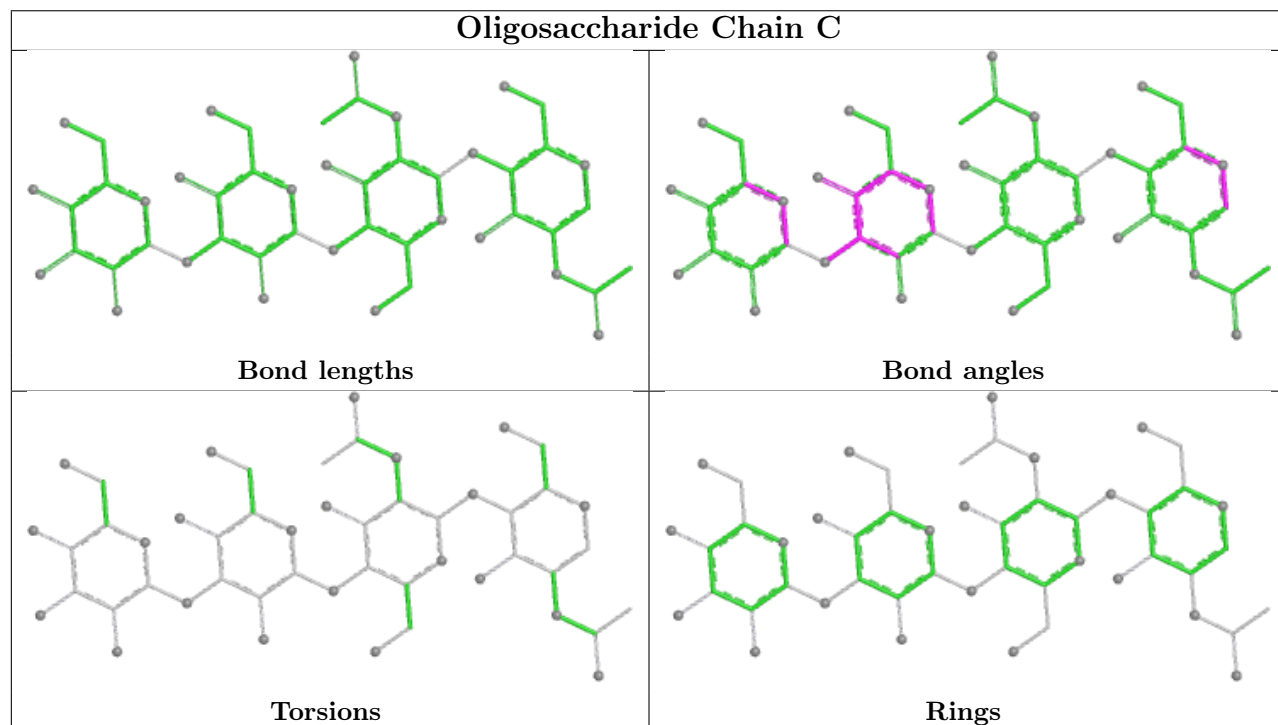
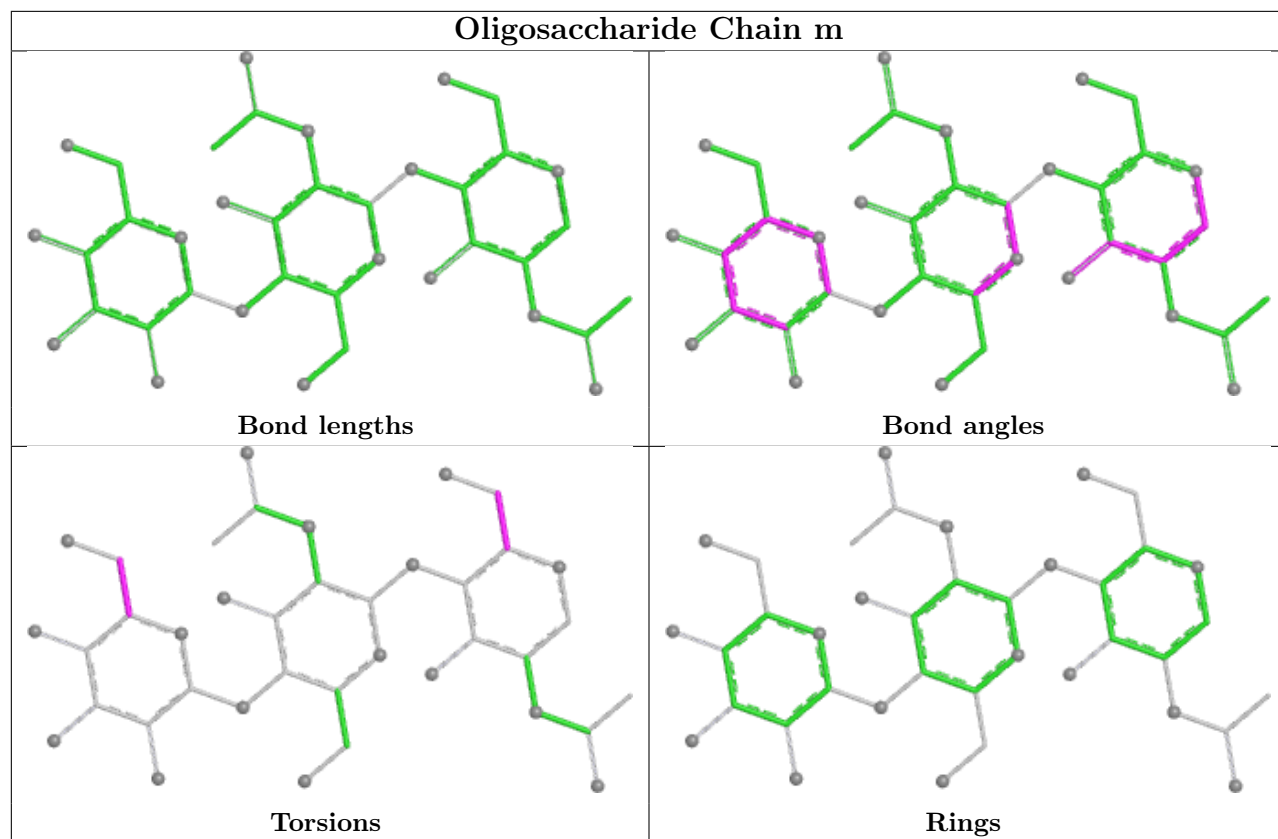


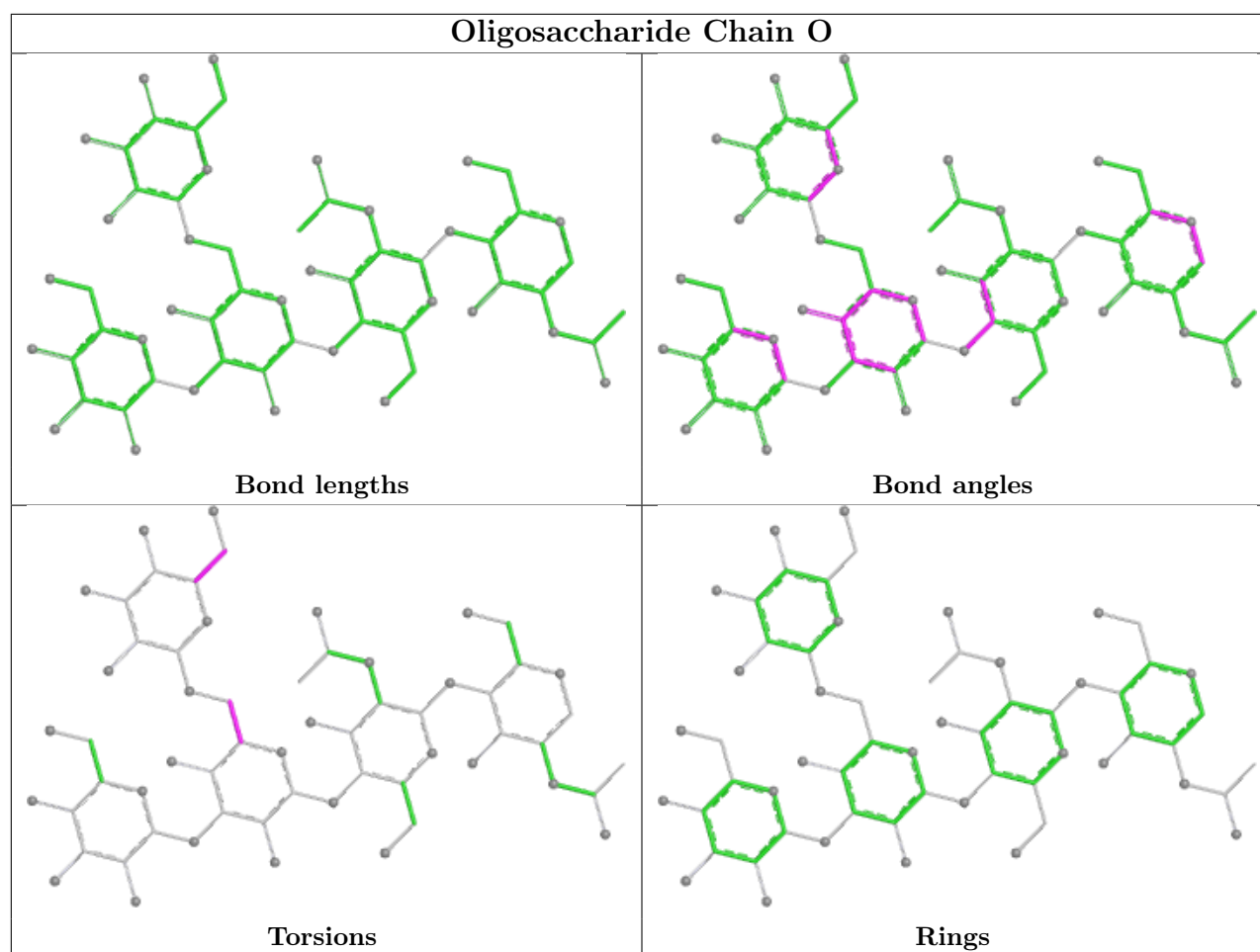












## 5.6 Ligand geometry [i](#)

32 ligands 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	$\# Z  > 2$
7	NAG	b	906	1	14,14,15	0.71	0	17,19,21	1.41	1 (5%)
7	NAG	d	907	1	14,14,15	0.71	0	17,19,21	0.84	0
7	NAG	b	904	1	14,14,15	0.71	0	17,19,21	0.96	1 (5%)
7	NAG	c	703	2	14,14,15	0.72	0	17,19,21	0.86	0
7	NAG	g	702	2	14,14,15	0.71	0	17,19,21	0.94	1 (5%)
7	NAG	f	903	1	14,14,15	0.77	0	17,19,21	1.63	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	b	903	1	14,14,15	0.75	0	17,19,21	1.84	3 (17%)
7	NAG	d	904	1	14,14,15	0.72	0	17,19,21	0.88	1 (5%)
7	NAG	e	702	2	14,14,15	0.70	0	17,19,21	0.93	1 (5%)
7	NAG	b	907	1	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
7	NAG	d	905	1	14,14,15	0.71	0	17,19,21	0.87	1 (5%)
7	NAG	e	701	2	14,14,15	0.70	0	17,19,21	0.86	0
7	NAG	c	702	2	14,14,15	0.71	0	17,19,21	0.90	1 (5%)
7	NAG	e	703	2	14,14,15	0.71	0	17,19,21	0.82	0
7	NAG	g	701	2	14,14,15	0.69	0	17,19,21	0.87	0
7	NAG	b	902	1	14,14,15	0.69	0	17,19,21	0.79	0
7	NAG	b	908	1	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
7	NAG	c	701	2	14,14,15	0.70	0	17,19,21	0.87	0
7	NAG	d	901	1	14,14,15	0.71	0	17,19,21	0.90	1 (5%)
7	NAG	d	903	1	14,14,15	0.78	0	17,19,21	1.75	4 (23%)
7	NAG	f	904	1	14,14,15	0.73	0	17,19,21	0.84	0
7	NAG	f	901	1	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
7	NAG	g	703	2	14,14,15	0.72	0	17,19,21	0.85	0
7	NAG	b	901	1	14,14,15	0.70	0	17,19,21	0.90	1 (5%)
7	NAG	d	906	1	14,14,15	0.74	0	17,19,21	1.24	1 (5%)
7	NAG	f	905	1	14,14,15	0.72	0	17,19,21	0.91	1 (5%)
7	NAG	d	902	1	14,14,15	0.70	0	17,19,21	0.80	0
7	NAG	f	907	1	14,14,15	0.72	0	17,19,21	0.88	0
7	NAG	f	908	1	14,14,15	0.75	0	17,19,21	0.92	0
7	NAG	b	905	1	14,14,15	0.71	0	17,19,21	0.87	1 (5%)
7	NAG	f	902	1	14,14,15	0.68	0	17,19,21	0.79	0
7	NAG	f	906	1	14,14,15	0.73	0	17,19,21	1.48	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
7	NAG	b	906	1	-	3/6/23/26	0/1/1/1
7	NAG	d	907	1	-	0/6/23/26	0/1/1/1
7	NAG	b	904	1	-	0/6/23/26	0/1/1/1
7	NAG	c	703	2	-	0/6/23/26	0/1/1/1
7	NAG	g	702	2	-	0/6/23/26	0/1/1/1
7	NAG	f	903	1	-	2/6/23/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	b	903	1	-	2/6/23/26	0/1/1/1
7	NAG	d	904	1	-	0/6/23/26	0/1/1/1
7	NAG	e	702	2	-	0/6/23/26	0/1/1/1
7	NAG	b	907	1	-	0/6/23/26	0/1/1/1
7	NAG	d	905	1	-	0/6/23/26	0/1/1/1
7	NAG	e	701	2	-	0/6/23/26	0/1/1/1
7	NAG	c	702	2	-	0/6/23/26	0/1/1/1
7	NAG	e	703	2	-	0/6/23/26	0/1/1/1
7	NAG	g	701	2	-	0/6/23/26	0/1/1/1
7	NAG	b	902	1	-	0/6/23/26	0/1/1/1
7	NAG	b	908	1	-	0/6/23/26	0/1/1/1
7	NAG	c	701	2	-	0/6/23/26	0/1/1/1
7	NAG	d	901	1	-	0/6/23/26	0/1/1/1
7	NAG	d	903	1	-	1/6/23/26	0/1/1/1
7	NAG	f	904	1	-	0/6/23/26	0/1/1/1
7	NAG	f	901	1	-	0/6/23/26	0/1/1/1
7	NAG	g	703	2	-	0/6/23/26	0/1/1/1
7	NAG	b	901	1	-	0/6/23/26	0/1/1/1
7	NAG	d	906	1	-	0/6/23/26	0/1/1/1
7	NAG	f	905	1	-	0/6/23/26	0/1/1/1
7	NAG	d	902	1	-	0/6/23/26	0/1/1/1
7	NAG	f	907	1	-	0/6/23/26	0/1/1/1
7	NAG	f	908	1	-	0/6/23/26	0/1/1/1
7	NAG	b	905	1	-	0/6/23/26	0/1/1/1
7	NAG	f	902	1	-	0/6/23/26	0/1/1/1
7	NAG	f	906	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	f	906	NAG	C2-N2-C7	4.56	129.01	122.90
7	b	906	NAG	C2-N2-C7	4.32	128.69	122.90
7	d	903	NAG	C2-N2-C7	4.29	128.65	122.90
7	b	903	NAG	C1-O5-C5	4.09	117.66	112.19
7	b	903	NAG	C2-N2-C7	3.95	128.19	122.90
7	f	903	NAG	C2-N2-C7	3.89	128.11	122.90
7	d	906	NAG	C1-O5-C5	3.49	116.86	112.19
7	f	903	NAG	C1-O5-C5	2.64	115.73	112.19
7	f	901	NAG	O5-C1-C2	-2.50	107.43	111.29
7	d	903	NAG	O7-C7-N2	2.44	126.30	121.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	702	NAG	C1-O5-C5	2.43	115.44	112.19
7	d	901	NAG	O5-C1-C2	-2.38	107.60	111.29
7	b	901	NAG	O5-C1-C2	-2.37	107.62	111.29
7	e	702	NAG	C1-O5-C5	2.37	115.36	112.19
7	b	903	NAG	O7-C7-N2	2.30	126.04	121.98
7	f	905	NAG	C1-O5-C5	2.27	115.23	112.19
7	f	903	NAG	O7-C7-N2	2.22	125.90	121.98
7	b	908	NAG	C1-O5-C5	2.18	115.11	112.19
7	c	702	NAG	C1-O5-C5	2.16	115.08	112.19
7	b	905	NAG	C1-O5-C5	2.16	115.08	112.19
7	d	903	NAG	C1-O5-C5	2.15	115.07	112.19
7	b	904	NAG	C1-O5-C5	2.14	115.05	112.19
7	d	903	NAG	C1-C2-N2	2.11	113.75	110.43
7	b	907	NAG	C1-O5-C5	2.09	114.99	112.19
7	d	904	NAG	C1-O5-C5	2.05	114.94	112.19
7	d	905	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	f	906	NAG	O5-C5-C6-O6
7	b	906	NAG	O5-C5-C6-O6
7	b	903	NAG	C3-C2-N2-C7
7	b	906	NAG	C3-C2-N2-C7
7	d	903	NAG	C3-C2-N2-C7
7	f	903	NAG	C3-C2-N2-C7
7	f	906	NAG	C3-C2-N2-C7
7	b	903	NAG	C1-C2-N2-C7
7	b	906	NAG	C1-C2-N2-C7
7	f	903	NAG	C1-C2-N2-C7
7	f	906	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

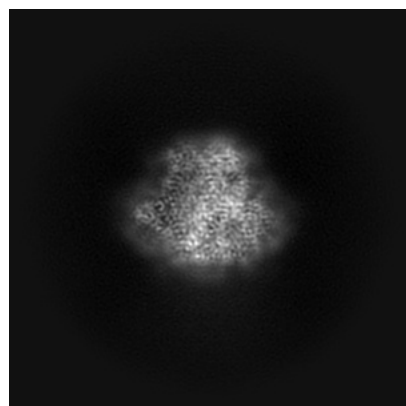
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49865. These allow visual inspection of the internal detail of the map and identification of artifacts.

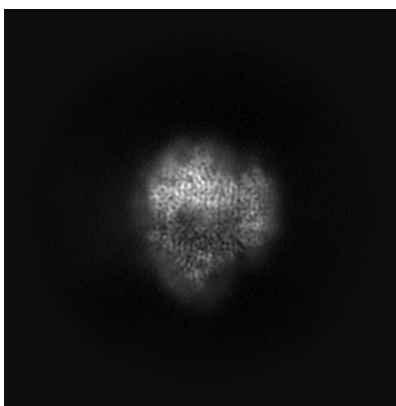
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

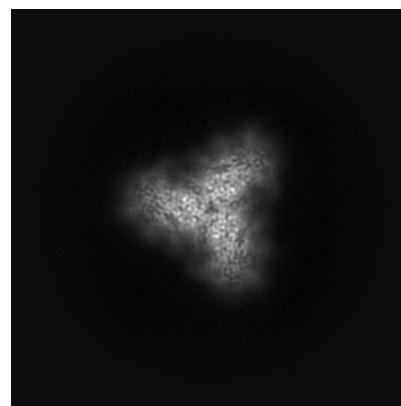
#### 6.1.1 Primary map



X

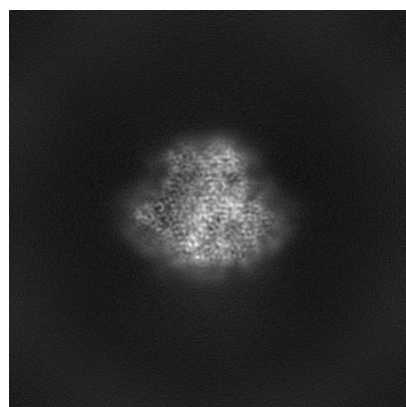


Y

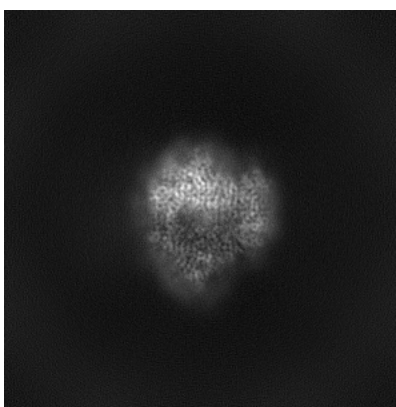


Z

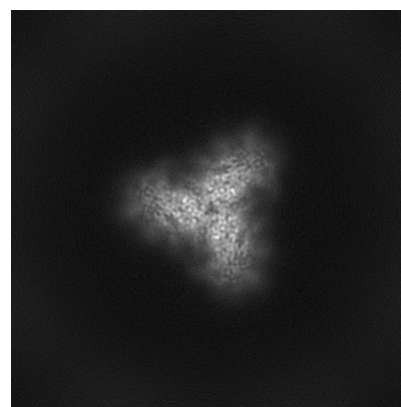
#### 6.1.2 Raw map



X



Y



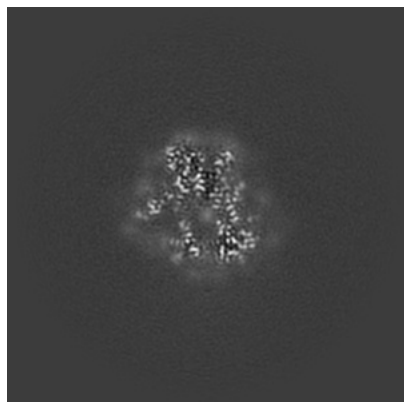
Z

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

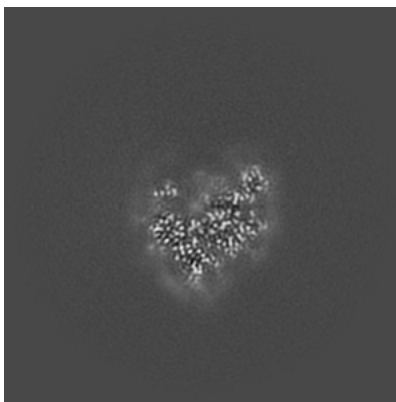


## 6.2 Central slices [i](#)

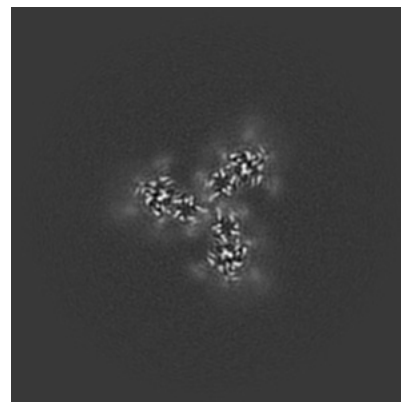
### 6.2.1 Primary map



X Index: 192

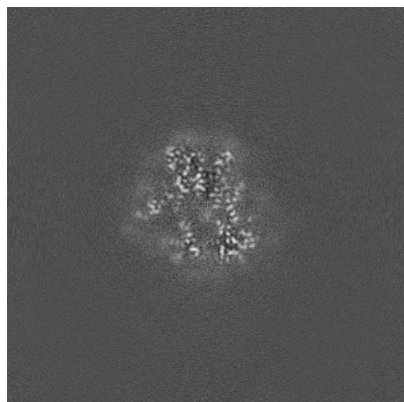


Y Index: 192

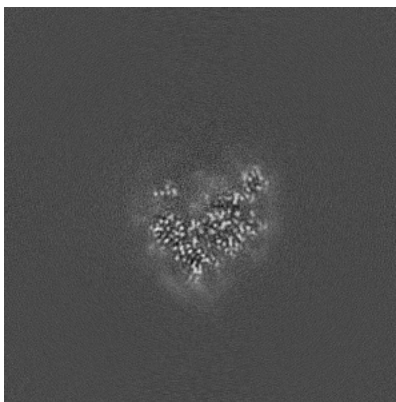


Z Index: 192

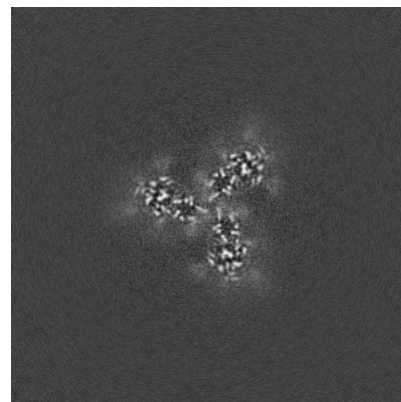
### 6.2.2 Raw map



X Index: 192



Y Index: 192

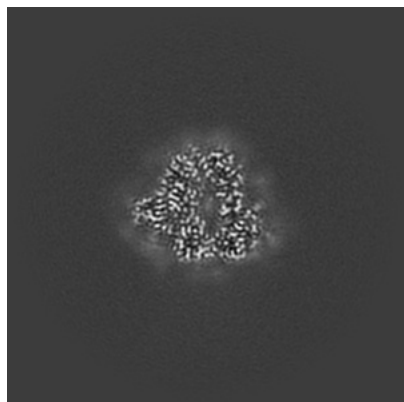


Z Index: 192

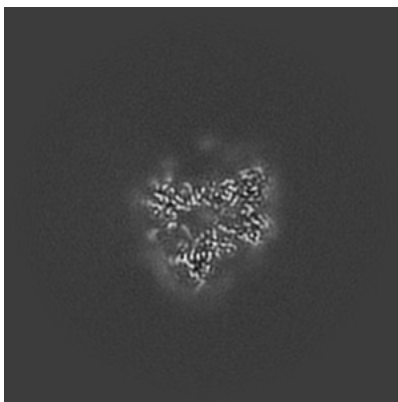
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

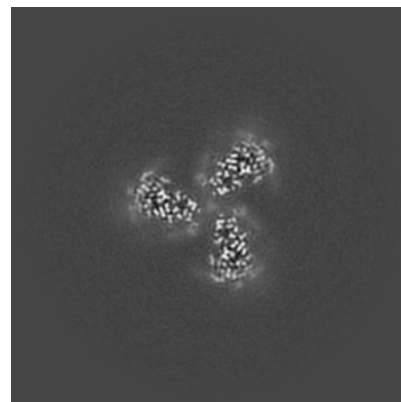
### 6.3.1 Primary map



X Index: 204

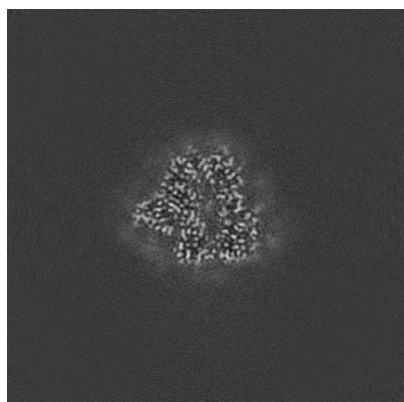


Y Index: 205

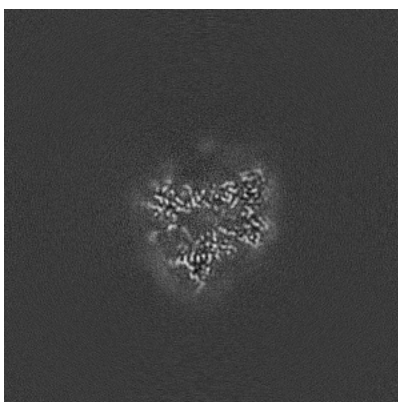


Z Index: 186

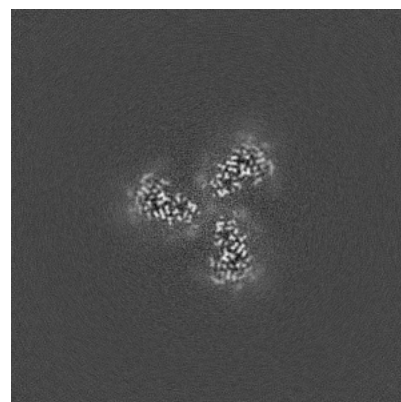
### 6.3.2 Raw map



X Index: 203



Y Index: 205

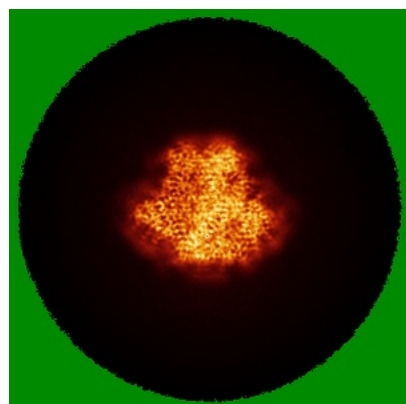


Z Index: 186

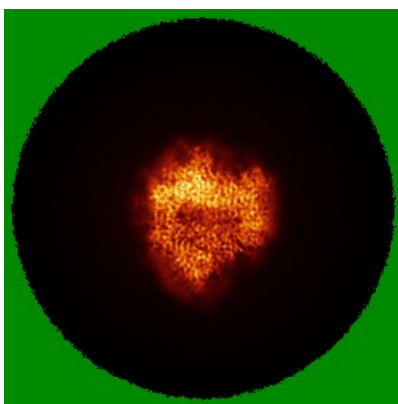
The images above show the largest variance slices of the map in three orthogonal directions.

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

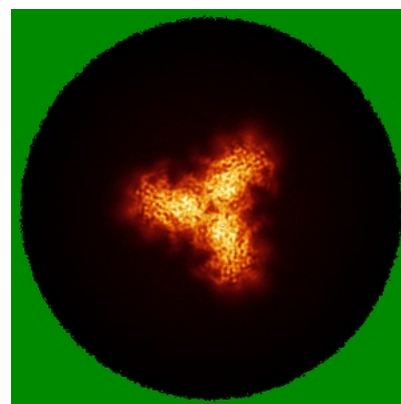
### 6.4.1 Primary map



X

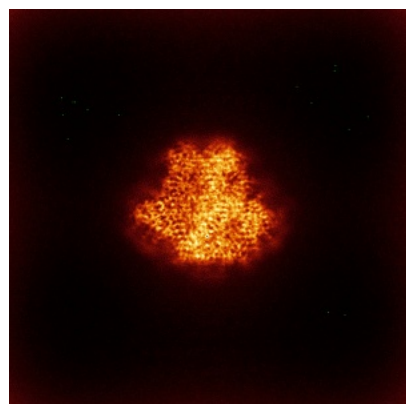


Y

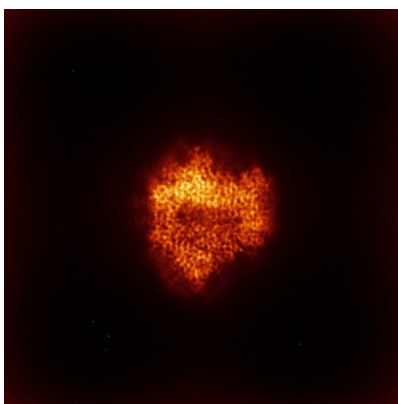


Z

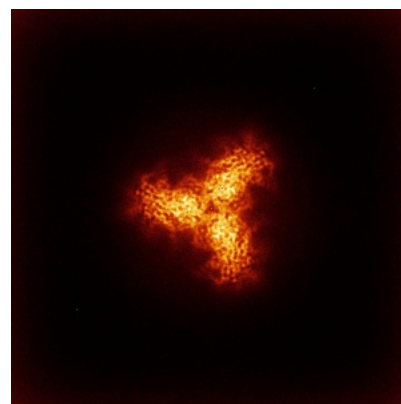
### 6.4.2 Raw map



X



Y

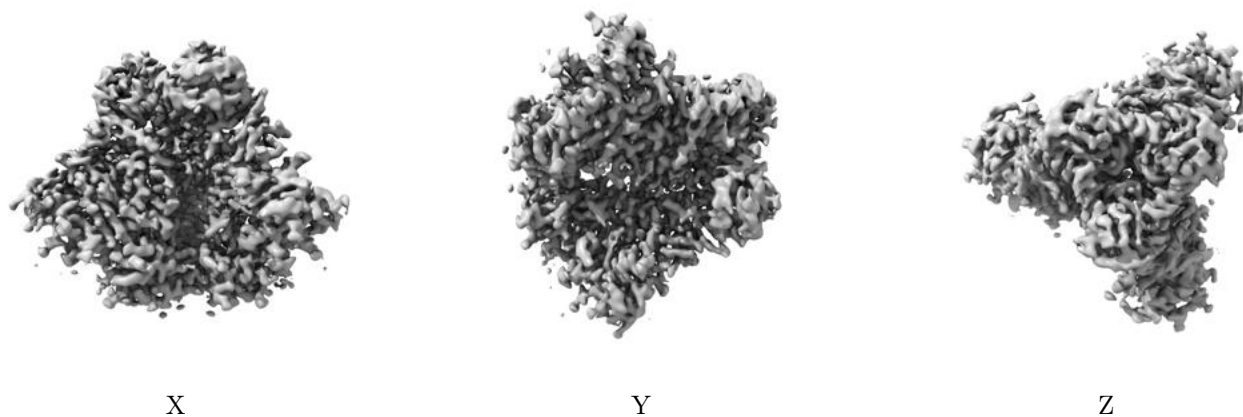


Z

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

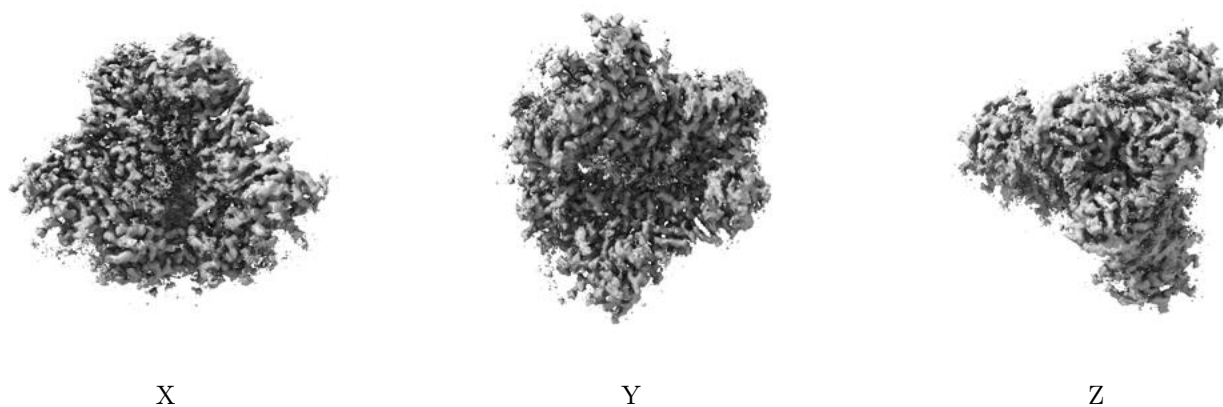
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

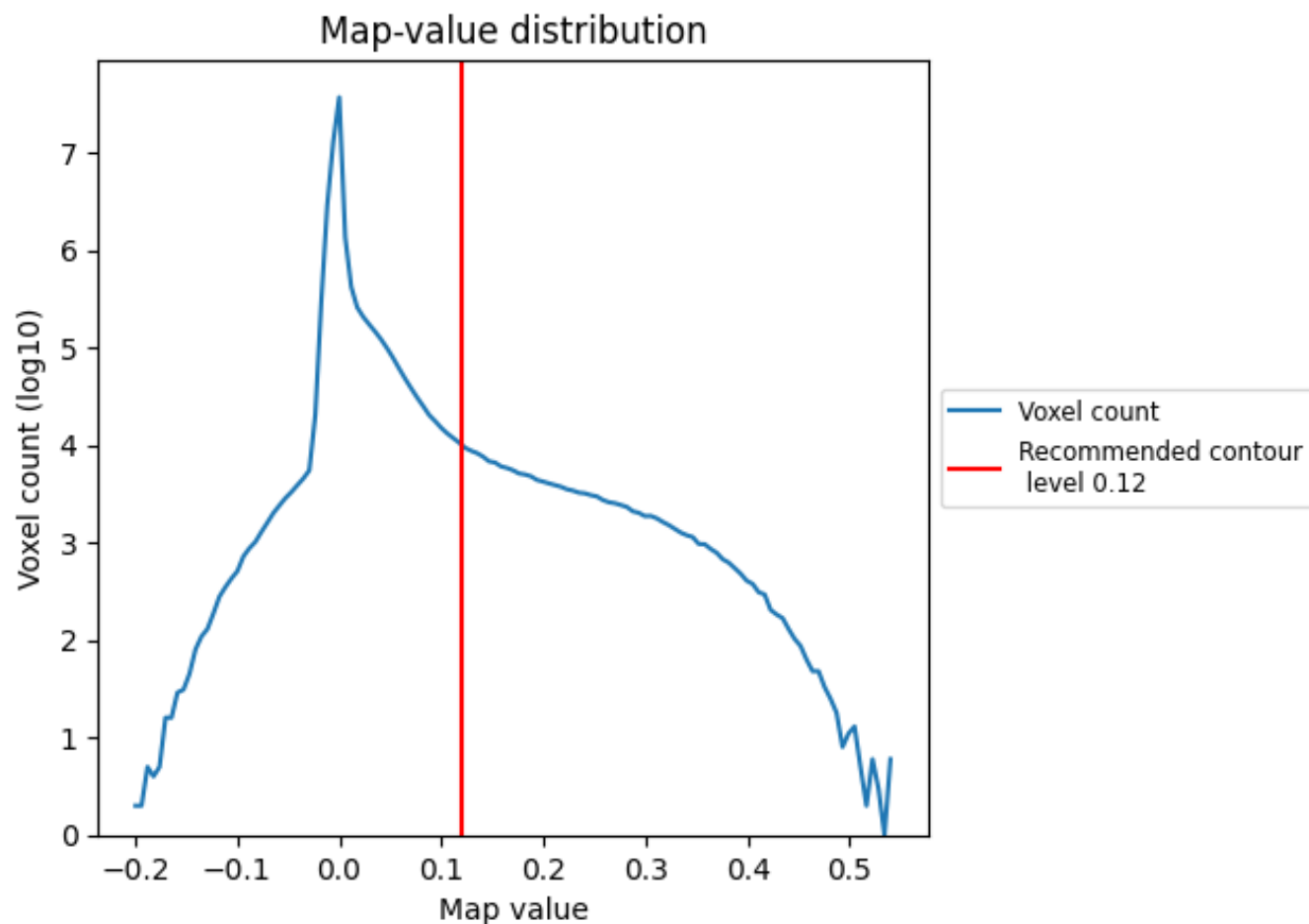
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

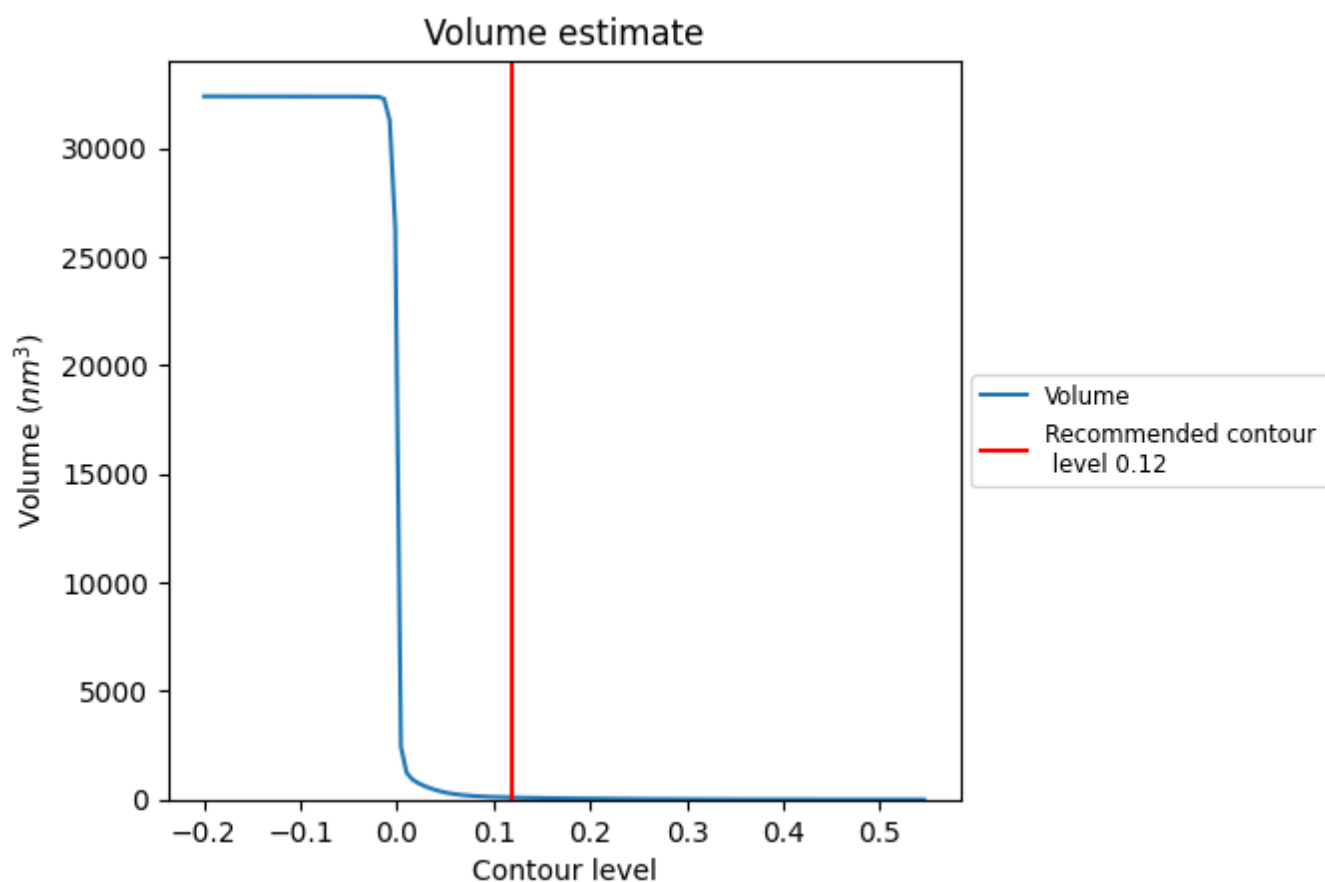
This section contains the results of statistical analysis of the map.

### 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.

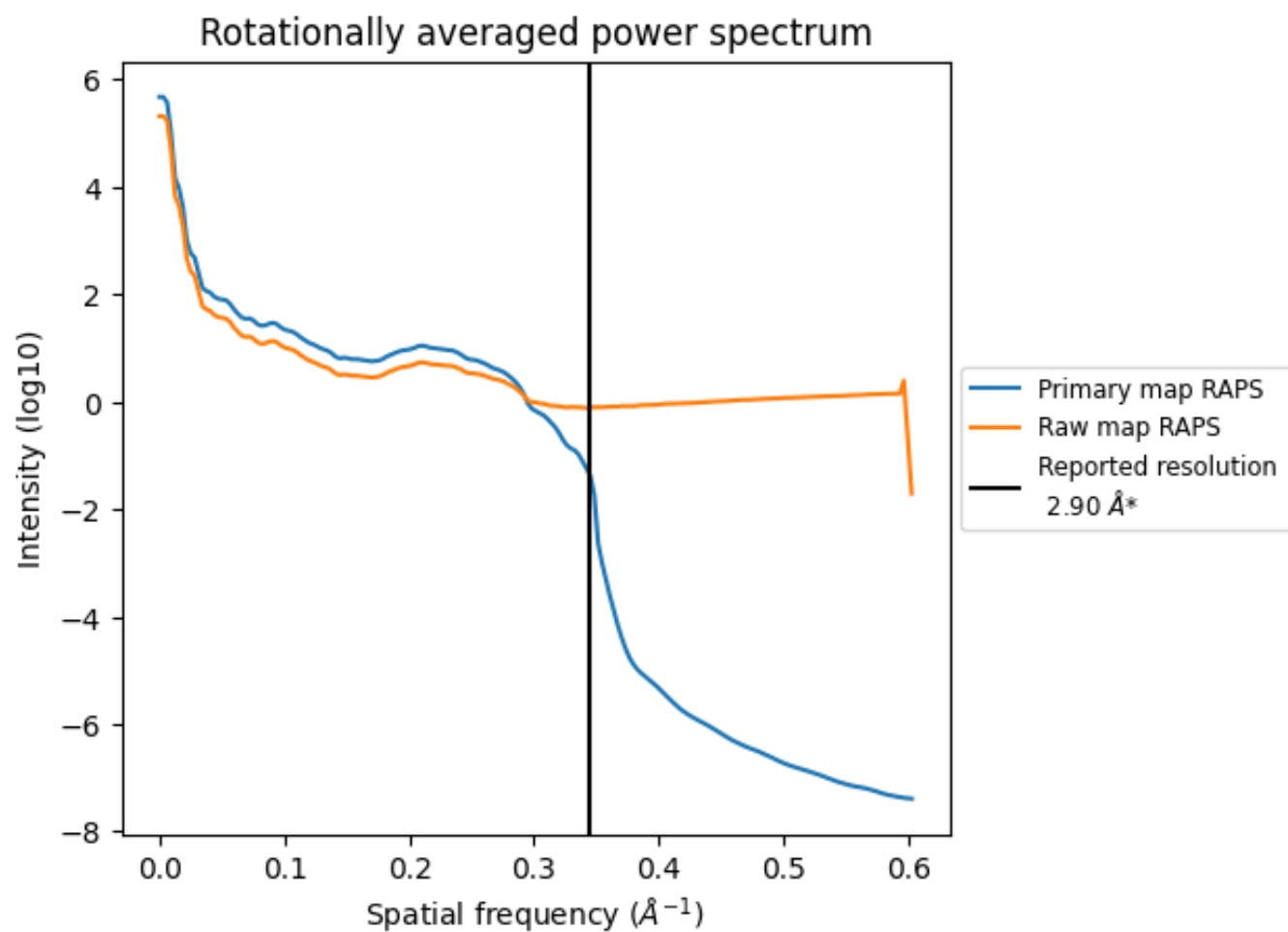
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 94 nm<sup>3</sup>; this corresponds to an approximate mass of 85 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

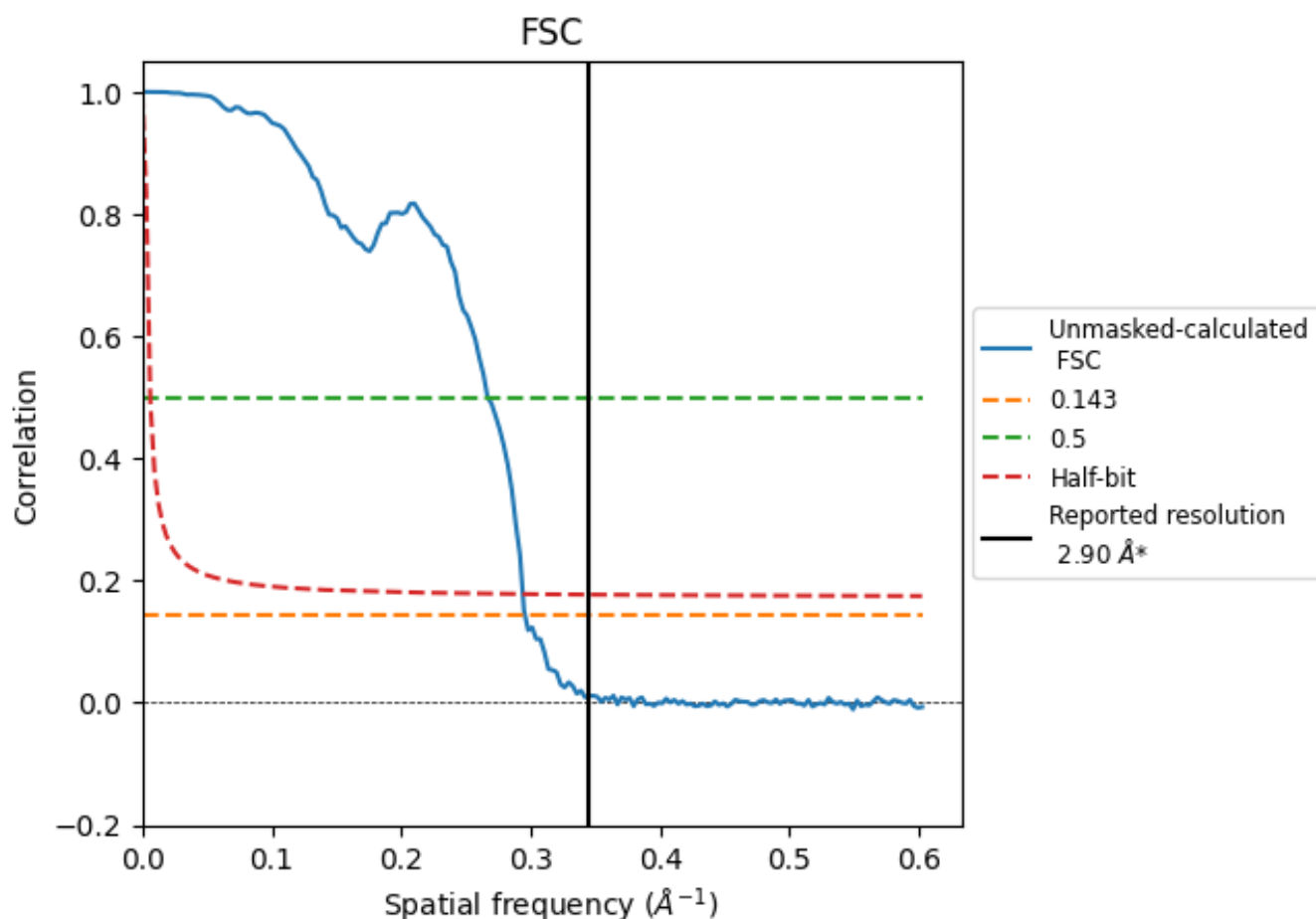


\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

## 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  $0.345 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

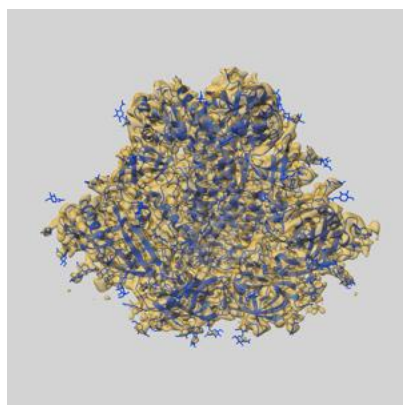
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	3.75	3.40

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.38 differs from the reported value 2.9 by more than 10 %

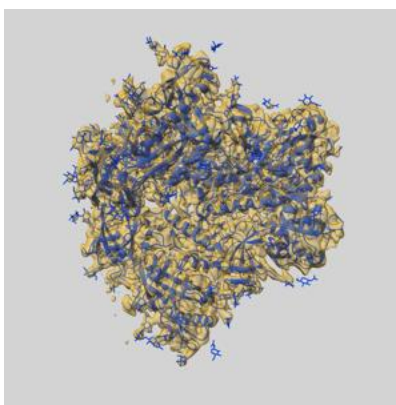
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49865 and PDB model 9NVV. Per-residue inclusion information can be found in section [3](#) on page [32](#).

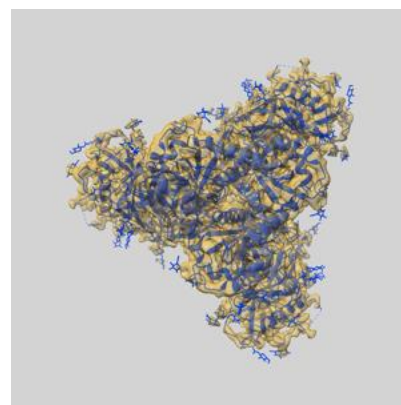
### 9.1 Map-model overlay [i](#)



X



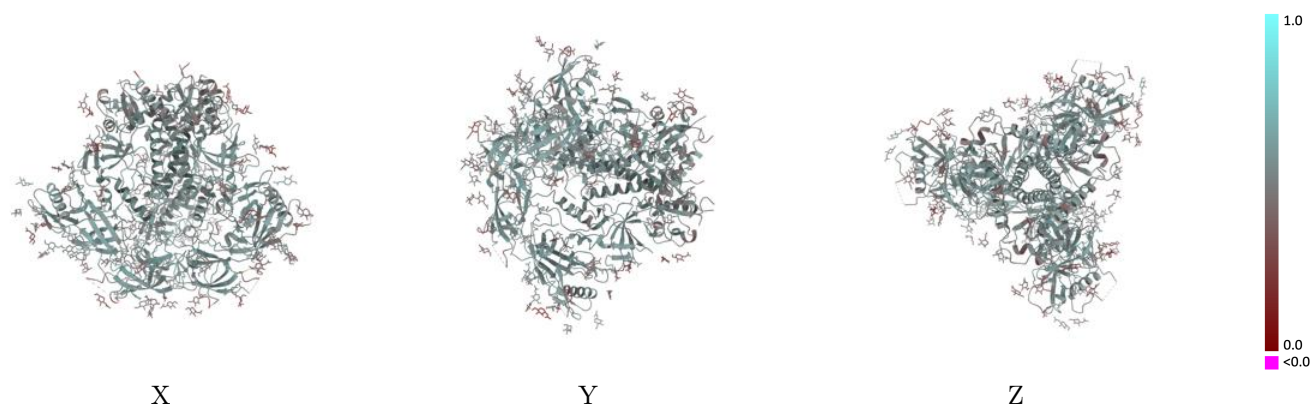
Y



Z

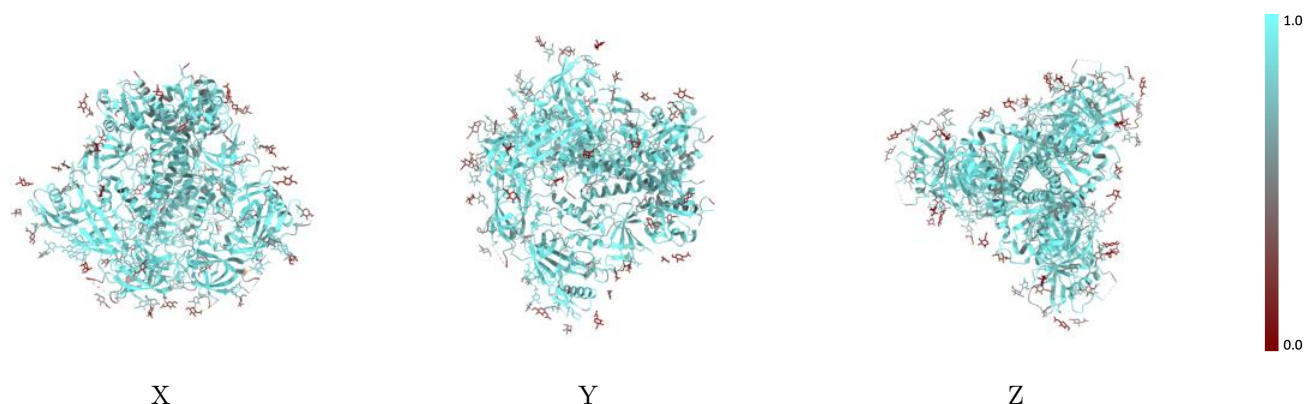
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



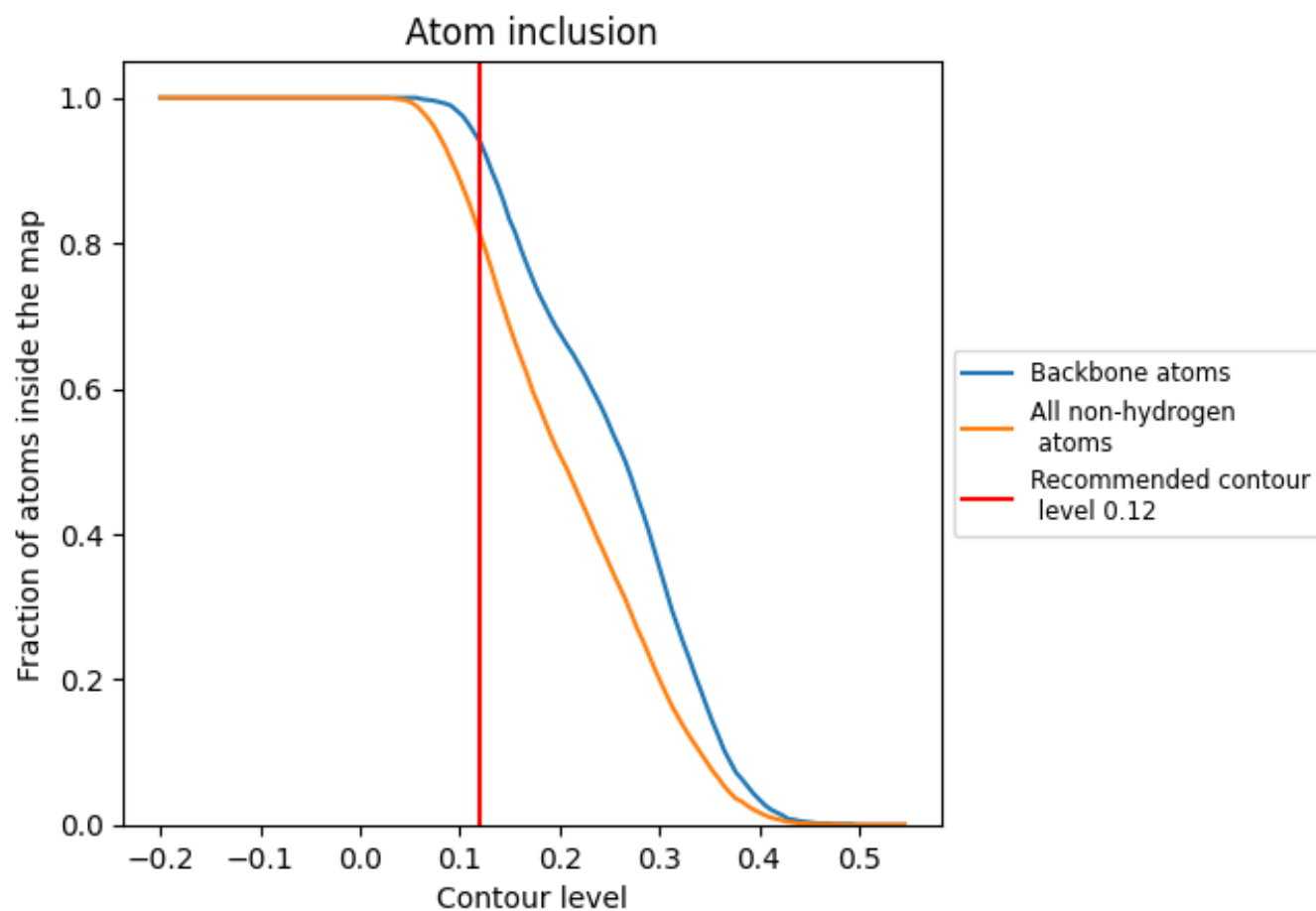
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 81% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8140	 0.5250
A	 0.6430	 0.4630
B	 0.5640	 0.4690
C	 0.8200	 0.5090
D	 0.7140	 0.4950
E	 0.3570	 0.3940
F	 0.6070	 0.4620
G	 0.5360	 0.4240
H	 0.3850	 0.3490
I	 0.5360	 0.3840
J	 0.3570	 0.3870
K	 0.3210	 0.3840
L	 0.4290	 0.3390
M	 0.6430	 0.4710
N	 0.5900	 0.4850
O	 0.6720	 0.4710
P	 0.7140	 0.4970
Q	 0.3570	 0.3960
R	 0.6070	 0.4620
S	 0.5360	 0.3970
T	 0.3850	 0.3500
U	 0.5360	 0.3930
V	 0.3570	 0.3860
W	 0.8570	 0.4230
X	 0.3210	 0.3640
Y	 0.4640	 0.3930
Z	 0.6430	 0.4650
a	 0.5640	 0.4600
b	 0.8540	 0.5410
c	 0.7830	 0.5130
d	 0.8490	 0.5380
e	 0.7840	 0.5130
f	 0.8560	 0.5380
g	 0.7850	 0.5160
h	 0.8720	 0.5260



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.6790	 0.4640
j	 0.3570	 0.3880
k	 0.6430	 0.4720
l	 0.5000	 0.4070
m	 0.3850	 0.3520
n	 0.5360	 0.3940
o	 0.3570	 0.3830
p	 0.3210	 0.3950
q	 0.3930	 0.3010