



# wwPDB EM Validation Summary Report ⓘ

Apr 21, 2024 – 01:53 AM EDT

PDB ID : 8EJD  
EMDB ID : EMD-28178  
Title : Structure of lineage IV Lassa virus glycoprotein complex (strain Josiah)  
Authors : Perrett, H.R.; Ward, A.B.  
Deposited on : 2022-09-16  
Resolution : 3.80 Å (reported)  
Based on initial model : 7SGD

This is a wwPDB EM Validation Summary 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>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

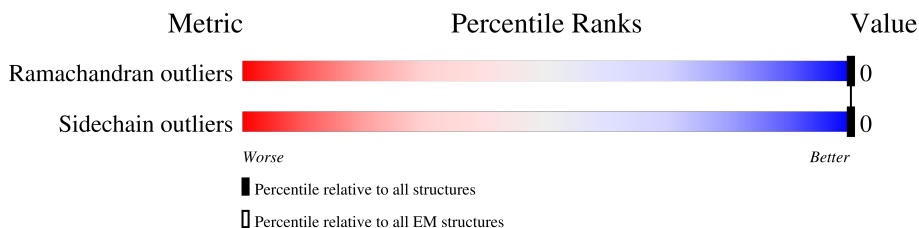
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

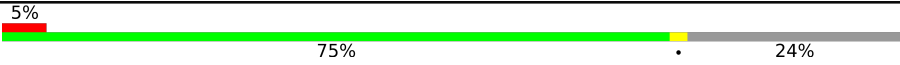




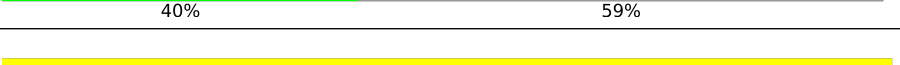
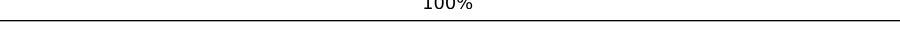
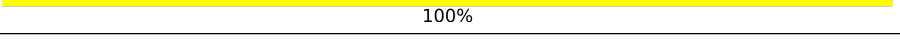
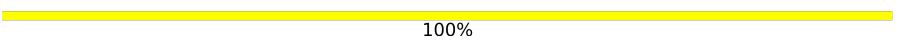
The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	259	 5% 75% 24%
1	B	259	 5% 75% 24%
1	C	259	 5% 75% 24%
2	a	406	 5% 40% 59%
2	b	406	 5% 40% 59%
2	c	406	 5% 40% 59%
3	D	3	 100%
3	E	3	 100%
3	M	3	 100%

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Mol	Chain	Length	Quality of chain
3	N	3	100%
3	V	3	100%
3	W	3	100%
4	F	2	100%
4	H	2	100%
4	I	2	100%
4	J	2	100%
4	O	2	100%
4	Q	2	100%
4	R	2	100%
4	S	2	100%
4	X	2	100%
4	Z	2	100%
4	d	2	100%
4	e	2	100%
5	G	3	100%
5	P	3	100%
5	Y	3	100%
6	K	5	60%
6	T	5	60%
6	f	5	60%
7	L	5	40%
7	U	5	40%
7	g	5	60%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9804 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 Glycoprotein G1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	197	1551	975	261	299	16	0	0
1	A	197	1551	975	261	299	16	0	0
1	B	197	1551	975	261	299	16	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	207	CYS	ARG	engineered mutation	UNP P08669
C	258	ARG	LEU	engineered mutation	UNP P08669
C	259	ARG	LEU	engineered mutation	UNP P08669
A	207	CYS	ARG	engineered mutation	UNP P08669
A	258	ARG	LEU	engineered mutation	UNP P08669
A	259	ARG	LEU	engineered mutation	UNP P08669
B	207	CYS	ARG	engineered mutation	UNP P08669
B	258	ARG	LEU	engineered mutation	UNP P08669
B	259	ARG	LEU	engineered mutation	UNP P08669

- Molecule 2 is a protein called Glycoprotein G2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	c	165	1339	842	227	255	15	0	0
2	a	165	1339	842	227	255	15	0	0
2	b	165	1339	842	227	255	15	0	0

There are 729 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	329	PRO	GLU	engineered mutation	UNP P08669
c	360	CYS	GLY	engineered mutation	UNP P08669
c	425	GLY	-	expression tag	UNP P08669
c	426	SER	-	expression tag	UNP P08669
c	427	GLY	-	expression tag	UNP P08669
c	428	GLY	-	expression tag	UNP P08669
c	429	SER	-	expression tag	UNP P08669
c	430	GLY	-	expression tag	UNP P08669
c	431	GLY	-	expression tag	UNP P08669
c	432	SER	-	expression tag	UNP P08669
c	433	GLY	-	expression tag	UNP P08669
c	434	GLY	-	expression tag	UNP P08669
c	435	SER	-	expression tag	UNP P08669
c	436	GLY	-	expression tag	UNP P08669
c	437	GLY	-	expression tag	UNP P08669
c	438	SER	-	expression tag	UNP P08669
c	439	GLU	-	expression tag	UNP P08669
c	440	LYS	-	expression tag	UNP P08669
c	441	ALA	-	expression tag	UNP P08669
c	442	ALA	-	expression tag	UNP P08669
c	443	LYS	-	expression tag	UNP P08669
c	444	ALA	-	expression tag	UNP P08669
c	445	GLU	-	expression tag	UNP P08669
c	446	GLU	-	expression tag	UNP P08669
c	447	ALA	-	expression tag	UNP P08669
c	448	ALA	-	expression tag	UNP P08669
c	449	ARG	-	expression tag	UNP P08669
c	450	LYS	-	expression tag	UNP P08669
c	451	MET	-	expression tag	UNP P08669
c	452	GLU	-	expression tag	UNP P08669
c	453	GLU	-	expression tag	UNP P08669
c	454	LEU	-	expression tag	UNP P08669
c	455	PHE	-	expression tag	UNP P08669
c	456	LYS	-	expression tag	UNP P08669
c	457	LYS	-	expression tag	UNP P08669
c	458	HIS	-	expression tag	UNP P08669
c	459	LYS	-	expression tag	UNP P08669
c	460	ILE	-	expression tag	UNP P08669
c	461	VAL	-	expression tag	UNP P08669
c	462	ALA	-	expression tag	UNP P08669
c	463	VAL	-	expression tag	UNP P08669
c	464	LEU	-	expression tag	UNP P08669
c	465	ARG	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	466	ALA	-	expression tag	UNP P08669
c	467	ASN	-	expression tag	UNP P08669
c	468	SER	-	expression tag	UNP P08669
c	469	VAL	-	expression tag	UNP P08669
c	470	GLU	-	expression tag	UNP P08669
c	471	GLU	-	expression tag	UNP P08669
c	472	ALA	-	expression tag	UNP P08669
c	473	ILE	-	expression tag	UNP P08669
c	474	GLU	-	expression tag	UNP P08669
c	475	LYS	-	expression tag	UNP P08669
c	476	ALA	-	expression tag	UNP P08669
c	477	VAL	-	expression tag	UNP P08669
c	478	ALA	-	expression tag	UNP P08669
c	479	VAL	-	expression tag	UNP P08669
c	480	PHE	-	expression tag	UNP P08669
c	481	ALA	-	expression tag	UNP P08669
c	482	GLY	-	expression tag	UNP P08669
c	483	GLY	-	expression tag	UNP P08669
c	484	VAL	-	expression tag	UNP P08669
c	485	HIS	-	expression tag	UNP P08669
c	486	LEU	-	expression tag	UNP P08669
c	487	ILE	-	expression tag	UNP P08669
c	488	GLU	-	expression tag	UNP P08669
c	489	ILE	-	expression tag	UNP P08669
c	490	THR	-	expression tag	UNP P08669
c	491	PHE	-	expression tag	UNP P08669
c	492	THR	-	expression tag	UNP P08669
c	493	VAL	-	expression tag	UNP P08669
c	494	PRO	-	expression tag	UNP P08669
c	495	ASP	-	expression tag	UNP P08669
c	496	ALA	-	expression tag	UNP P08669
c	497	ASP	-	expression tag	UNP P08669
c	498	THR	-	expression tag	UNP P08669
c	499	VAL	-	expression tag	UNP P08669
c	500	ILE	-	expression tag	UNP P08669
c	501	LYS	-	expression tag	UNP P08669
c	502	ALA	-	expression tag	UNP P08669
c	503	LEU	-	expression tag	UNP P08669
c	504	SER	-	expression tag	UNP P08669
c	505	VAL	-	expression tag	UNP P08669
c	506	LEU	-	expression tag	UNP P08669
c	507	LYS	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	508	GLU	-	expression tag	UNP P08669
c	509	LYS	-	expression tag	UNP P08669
c	510	GLY	-	expression tag	UNP P08669
c	511	ALA	-	expression tag	UNP P08669
c	512	ILE	-	expression tag	UNP P08669
c	513	ILE	-	expression tag	UNP P08669
c	514	GLY	-	expression tag	UNP P08669
c	515	ALA	-	expression tag	UNP P08669
c	516	GLY	-	expression tag	UNP P08669
c	517	THR	-	expression tag	UNP P08669
c	518	VAL	-	expression tag	UNP P08669
c	519	THR	-	expression tag	UNP P08669
c	520	SER	-	expression tag	UNP P08669
c	521	VAL	-	expression tag	UNP P08669
c	522	GLU	-	expression tag	UNP P08669
c	523	GLN	-	expression tag	UNP P08669
c	524	CYS	-	expression tag	UNP P08669
c	525	ARG	-	expression tag	UNP P08669
c	526	LYS	-	expression tag	UNP P08669
c	527	ALA	-	expression tag	UNP P08669
c	528	VAL	-	expression tag	UNP P08669
c	529	GLU	-	expression tag	UNP P08669
c	530	SER	-	expression tag	UNP P08669
c	531	GLY	-	expression tag	UNP P08669
c	532	ALA	-	expression tag	UNP P08669
c	533	GLU	-	expression tag	UNP P08669
c	534	PHE	-	expression tag	UNP P08669
c	535	ILE	-	expression tag	UNP P08669
c	536	VAL	-	expression tag	UNP P08669
c	537	SER	-	expression tag	UNP P08669
c	538	PRO	-	expression tag	UNP P08669
c	539	HIS	-	expression tag	UNP P08669
c	540	LEU	-	expression tag	UNP P08669
c	541	ASP	-	expression tag	UNP P08669
c	542	GLU	-	expression tag	UNP P08669
c	543	GLU	-	expression tag	UNP P08669
c	544	ILE	-	expression tag	UNP P08669
c	545	SER	-	expression tag	UNP P08669
c	546	GLN	-	expression tag	UNP P08669
c	547	PHE	-	expression tag	UNP P08669
c	548	CYS	-	expression tag	UNP P08669
c	549	LYS	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	550	GLU	-	expression tag	UNP P08669
c	551	LYS	-	expression tag	UNP P08669
c	552	GLY	-	expression tag	UNP P08669
c	553	VAL	-	expression tag	UNP P08669
c	554	PHE	-	expression tag	UNP P08669
c	555	TYR	-	expression tag	UNP P08669
c	556	MET	-	expression tag	UNP P08669
c	557	PRO	-	expression tag	UNP P08669
c	558	GLY	-	expression tag	UNP P08669
c	559	VAL	-	expression tag	UNP P08669
c	560	MET	-	expression tag	UNP P08669
c	561	THR	-	expression tag	UNP P08669
c	562	PRO	-	expression tag	UNP P08669
c	563	THR	-	expression tag	UNP P08669
c	564	GLU	-	expression tag	UNP P08669
c	565	LEU	-	expression tag	UNP P08669
c	566	VAL	-	expression tag	UNP P08669
c	567	LYS	-	expression tag	UNP P08669
c	568	ALA	-	expression tag	UNP P08669
c	569	MET	-	expression tag	UNP P08669
c	570	LYS	-	expression tag	UNP P08669
c	571	LEU	-	expression tag	UNP P08669
c	572	GLY	-	expression tag	UNP P08669
c	573	HIS	-	expression tag	UNP P08669
c	574	ASP	-	expression tag	UNP P08669
c	575	ILE	-	expression tag	UNP P08669
c	576	LEU	-	expression tag	UNP P08669
c	577	LYS	-	expression tag	UNP P08669
c	578	LEU	-	expression tag	UNP P08669
c	579	PHE	-	expression tag	UNP P08669
c	580	PRO	-	expression tag	UNP P08669
c	581	GLY	-	expression tag	UNP P08669
c	582	GLU	-	expression tag	UNP P08669
c	583	VAL	-	expression tag	UNP P08669
c	584	VAL	-	expression tag	UNP P08669
c	585	GLY	-	expression tag	UNP P08669
c	586	PRO	-	expression tag	UNP P08669
c	587	GLU	-	expression tag	UNP P08669
c	588	PHE	-	expression tag	UNP P08669
c	589	VAL	-	expression tag	UNP P08669
c	590	LYS	-	expression tag	UNP P08669
c	591	ALA	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	592	MET	-	expression tag	UNP P08669
c	593	LYS	-	expression tag	UNP P08669
c	594	GLY	-	expression tag	UNP P08669
c	595	PRO	-	expression tag	UNP P08669
c	596	PHE	-	expression tag	UNP P08669
c	597	PRO	-	expression tag	UNP P08669
c	598	ASN	-	expression tag	UNP P08669
c	599	VAL	-	expression tag	UNP P08669
c	600	LYS	-	expression tag	UNP P08669
c	601	PHE	-	expression tag	UNP P08669
c	602	VAL	-	expression tag	UNP P08669
c	603	PRO	-	expression tag	UNP P08669
c	604	THR	-	expression tag	UNP P08669
c	605	GLY	-	expression tag	UNP P08669
c	606	GLY	-	expression tag	UNP P08669
c	607	VAL	-	expression tag	UNP P08669
c	608	ASP	-	expression tag	UNP P08669
c	609	LEU	-	expression tag	UNP P08669
c	610	ASP	-	expression tag	UNP P08669
c	611	ASN	-	expression tag	UNP P08669
c	612	VAL	-	expression tag	UNP P08669
c	613	CYS	-	expression tag	UNP P08669
c	614	GLU	-	expression tag	UNP P08669
c	615	TRP	-	expression tag	UNP P08669
c	616	PHE	-	expression tag	UNP P08669
c	617	ASP	-	expression tag	UNP P08669
c	618	ALA	-	expression tag	UNP P08669
c	619	GLY	-	expression tag	UNP P08669
c	620	VAL	-	expression tag	UNP P08669
c	621	LEU	-	expression tag	UNP P08669
c	622	ALA	-	expression tag	UNP P08669
c	623	VAL	-	expression tag	UNP P08669
c	624	GLY	-	expression tag	UNP P08669
c	625	VAL	-	expression tag	UNP P08669
c	626	GLY	-	expression tag	UNP P08669
c	627	ASP	-	expression tag	UNP P08669
c	628	ALA	-	expression tag	UNP P08669
c	629	LEU	-	expression tag	UNP P08669
c	630	VAL	-	expression tag	UNP P08669
c	631	GLU	-	expression tag	UNP P08669
c	632	GLY	-	expression tag	UNP P08669
c	633	ASP	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	634	PRO	-	expression tag	UNP P08669
c	635	ASP	-	expression tag	UNP P08669
c	636	GLU	-	expression tag	UNP P08669
c	637	VAL	-	expression tag	UNP P08669
c	638	ARG	-	expression tag	UNP P08669
c	639	GLU	-	expression tag	UNP P08669
c	640	LYS	-	expression tag	UNP P08669
c	641	ALA	-	expression tag	UNP P08669
c	642	LYS	-	expression tag	UNP P08669
c	643	GLU	-	expression tag	UNP P08669
c	644	PHE	-	expression tag	UNP P08669
c	645	VAL	-	expression tag	UNP P08669
c	646	GLU	-	expression tag	UNP P08669
c	647	LYS	-	expression tag	UNP P08669
c	648	ILE	-	expression tag	UNP P08669
c	649	ARG	-	expression tag	UNP P08669
c	650	GLY	-	expression tag	UNP P08669
c	651	CYS	-	expression tag	UNP P08669
c	652	THR	-	expression tag	UNP P08669
c	653	GLU	-	expression tag	UNP P08669
c	654	GLY	-	expression tag	UNP P08669
c	655	SER	-	expression tag	UNP P08669
c	656	LEU	-	expression tag	UNP P08669
c	657	GLU	-	expression tag	UNP P08669
c	658	TRP	-	expression tag	UNP P08669
c	659	SER	-	expression tag	UNP P08669
c	660	HIS	-	expression tag	UNP P08669
c	661	PRO	-	expression tag	UNP P08669
c	662	GLN	-	expression tag	UNP P08669
c	663	PHE	-	expression tag	UNP P08669
c	664	GLU	-	expression tag	UNP P08669
c	665	LYS	-	expression tag	UNP P08669
a	329	PRO	GLU	engineered mutation	UNP P08669
a	360	CYS	GLY	engineered mutation	UNP P08669
a	425	GLY	-	expression tag	UNP P08669
a	426	SER	-	expression tag	UNP P08669
a	427	GLY	-	expression tag	UNP P08669
a	428	GLY	-	expression tag	UNP P08669
a	429	SER	-	expression tag	UNP P08669
a	430	GLY	-	expression tag	UNP P08669
a	431	GLY	-	expression tag	UNP P08669
a	432	SER	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
a	433	GLY	-	expression tag	UNP P08669
a	434	GLY	-	expression tag	UNP P08669
a	435	SER	-	expression tag	UNP P08669
a	436	GLY	-	expression tag	UNP P08669
a	437	GLY	-	expression tag	UNP P08669
a	438	SER	-	expression tag	UNP P08669
a	439	GLU	-	expression tag	UNP P08669
a	440	LYS	-	expression tag	UNP P08669
a	441	ALA	-	expression tag	UNP P08669
a	442	ALA	-	expression tag	UNP P08669
a	443	LYS	-	expression tag	UNP P08669
a	444	ALA	-	expression tag	UNP P08669
a	445	GLU	-	expression tag	UNP P08669
a	446	GLU	-	expression tag	UNP P08669
a	447	ALA	-	expression tag	UNP P08669
a	448	ALA	-	expression tag	UNP P08669
a	449	ARG	-	expression tag	UNP P08669
a	450	LYS	-	expression tag	UNP P08669
a	451	MET	-	expression tag	UNP P08669
a	452	GLU	-	expression tag	UNP P08669
a	453	GLU	-	expression tag	UNP P08669
a	454	LEU	-	expression tag	UNP P08669
a	455	PHE	-	expression tag	UNP P08669
a	456	LYS	-	expression tag	UNP P08669
a	457	LYS	-	expression tag	UNP P08669
a	458	HIS	-	expression tag	UNP P08669
a	459	LYS	-	expression tag	UNP P08669
a	460	ILE	-	expression tag	UNP P08669
a	461	VAL	-	expression tag	UNP P08669
a	462	ALA	-	expression tag	UNP P08669
a	463	VAL	-	expression tag	UNP P08669
a	464	LEU	-	expression tag	UNP P08669
a	465	ARG	-	expression tag	UNP P08669
a	466	ALA	-	expression tag	UNP P08669
a	467	ASN	-	expression tag	UNP P08669
a	468	SER	-	expression tag	UNP P08669
a	469	VAL	-	expression tag	UNP P08669
a	470	GLU	-	expression tag	UNP P08669
a	471	GLU	-	expression tag	UNP P08669
a	472	ALA	-	expression tag	UNP P08669
a	473	ILE	-	expression tag	UNP P08669
a	474	GLU	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
a	475	LYS	-	expression tag	UNP P08669
a	476	ALA	-	expression tag	UNP P08669
a	477	VAL	-	expression tag	UNP P08669
a	478	ALA	-	expression tag	UNP P08669
a	479	VAL	-	expression tag	UNP P08669
a	480	PHE	-	expression tag	UNP P08669
a	481	ALA	-	expression tag	UNP P08669
a	482	GLY	-	expression tag	UNP P08669
a	483	GLY	-	expression tag	UNP P08669
a	484	VAL	-	expression tag	UNP P08669
a	485	HIS	-	expression tag	UNP P08669
a	486	LEU	-	expression tag	UNP P08669
a	487	ILE	-	expression tag	UNP P08669
a	488	GLU	-	expression tag	UNP P08669
a	489	ILE	-	expression tag	UNP P08669
a	490	THR	-	expression tag	UNP P08669
a	491	PHE	-	expression tag	UNP P08669
a	492	THR	-	expression tag	UNP P08669
a	493	VAL	-	expression tag	UNP P08669
a	494	PRO	-	expression tag	UNP P08669
a	495	ASP	-	expression tag	UNP P08669
a	496	ALA	-	expression tag	UNP P08669
a	497	ASP	-	expression tag	UNP P08669
a	498	THR	-	expression tag	UNP P08669
a	499	VAL	-	expression tag	UNP P08669
a	500	ILE	-	expression tag	UNP P08669
a	501	LYS	-	expression tag	UNP P08669
a	502	ALA	-	expression tag	UNP P08669
a	503	LEU	-	expression tag	UNP P08669
a	504	SER	-	expression tag	UNP P08669
a	505	VAL	-	expression tag	UNP P08669
a	506	LEU	-	expression tag	UNP P08669
a	507	LYS	-	expression tag	UNP P08669
a	508	GLU	-	expression tag	UNP P08669
a	509	LYS	-	expression tag	UNP P08669
a	510	GLY	-	expression tag	UNP P08669
a	511	ALA	-	expression tag	UNP P08669
a	512	ILE	-	expression tag	UNP P08669
a	513	ILE	-	expression tag	UNP P08669
a	514	GLY	-	expression tag	UNP P08669
a	515	ALA	-	expression tag	UNP P08669
a	516	GLY	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
a	517	THR	-	expression tag	UNP P08669
a	518	VAL	-	expression tag	UNP P08669
a	519	THR	-	expression tag	UNP P08669
a	520	SER	-	expression tag	UNP P08669
a	521	VAL	-	expression tag	UNP P08669
a	522	GLU	-	expression tag	UNP P08669
a	523	GLN	-	expression tag	UNP P08669
a	524	CYS	-	expression tag	UNP P08669
a	525	ARG	-	expression tag	UNP P08669
a	526	LYS	-	expression tag	UNP P08669
a	527	ALA	-	expression tag	UNP P08669
a	528	VAL	-	expression tag	UNP P08669
a	529	GLU	-	expression tag	UNP P08669
a	530	SER	-	expression tag	UNP P08669
a	531	GLY	-	expression tag	UNP P08669
a	532	ALA	-	expression tag	UNP P08669
a	533	GLU	-	expression tag	UNP P08669
a	534	PHE	-	expression tag	UNP P08669
a	535	ILE	-	expression tag	UNP P08669
a	536	VAL	-	expression tag	UNP P08669
a	537	SER	-	expression tag	UNP P08669
a	538	PRO	-	expression tag	UNP P08669
a	539	HIS	-	expression tag	UNP P08669
a	540	LEU	-	expression tag	UNP P08669
a	541	ASP	-	expression tag	UNP P08669
a	542	GLU	-	expression tag	UNP P08669
a	543	GLU	-	expression tag	UNP P08669
a	544	ILE	-	expression tag	UNP P08669
a	545	SER	-	expression tag	UNP P08669
a	546	GLN	-	expression tag	UNP P08669
a	547	PHE	-	expression tag	UNP P08669
a	548	CYS	-	expression tag	UNP P08669
a	549	LYS	-	expression tag	UNP P08669
a	550	GLU	-	expression tag	UNP P08669
a	551	LYS	-	expression tag	UNP P08669
a	552	GLY	-	expression tag	UNP P08669
a	553	VAL	-	expression tag	UNP P08669
a	554	PHE	-	expression tag	UNP P08669
a	555	TYR	-	expression tag	UNP P08669
a	556	MET	-	expression tag	UNP P08669
a	557	PRO	-	expression tag	UNP P08669
a	558	GLY	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
a	559	VAL	-	expression tag	UNP P08669
a	560	MET	-	expression tag	UNP P08669
a	561	THR	-	expression tag	UNP P08669
a	562	PRO	-	expression tag	UNP P08669
a	563	THR	-	expression tag	UNP P08669
a	564	GLU	-	expression tag	UNP P08669
a	565	LEU	-	expression tag	UNP P08669
a	566	VAL	-	expression tag	UNP P08669
a	567	LYS	-	expression tag	UNP P08669
a	568	ALA	-	expression tag	UNP P08669
a	569	MET	-	expression tag	UNP P08669
a	570	LYS	-	expression tag	UNP P08669
a	571	LEU	-	expression tag	UNP P08669
a	572	GLY	-	expression tag	UNP P08669
a	573	HIS	-	expression tag	UNP P08669
a	574	ASP	-	expression tag	UNP P08669
a	575	ILE	-	expression tag	UNP P08669
a	576	LEU	-	expression tag	UNP P08669
a	577	LYS	-	expression tag	UNP P08669
a	578	LEU	-	expression tag	UNP P08669
a	579	PHE	-	expression tag	UNP P08669
a	580	PRO	-	expression tag	UNP P08669
a	581	GLY	-	expression tag	UNP P08669
a	582	GLU	-	expression tag	UNP P08669
a	583	VAL	-	expression tag	UNP P08669
a	584	VAL	-	expression tag	UNP P08669
a	585	GLY	-	expression tag	UNP P08669
a	586	PRO	-	expression tag	UNP P08669
a	587	GLU	-	expression tag	UNP P08669
a	588	PHE	-	expression tag	UNP P08669
a	589	VAL	-	expression tag	UNP P08669
a	590	LYS	-	expression tag	UNP P08669
a	591	ALA	-	expression tag	UNP P08669
a	592	MET	-	expression tag	UNP P08669
a	593	LYS	-	expression tag	UNP P08669
a	594	GLY	-	expression tag	UNP P08669
a	595	PRO	-	expression tag	UNP P08669
a	596	PHE	-	expression tag	UNP P08669
a	597	PRO	-	expression tag	UNP P08669
a	598	ASN	-	expression tag	UNP P08669
a	599	VAL	-	expression tag	UNP P08669
a	600	LYS	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
a	601	PHE	-	expression tag	UNP P08669
a	602	VAL	-	expression tag	UNP P08669
a	603	PRO	-	expression tag	UNP P08669
a	604	THR	-	expression tag	UNP P08669
a	605	GLY	-	expression tag	UNP P08669
a	606	GLY	-	expression tag	UNP P08669
a	607	VAL	-	expression tag	UNP P08669
a	608	ASP	-	expression tag	UNP P08669
a	609	LEU	-	expression tag	UNP P08669
a	610	ASP	-	expression tag	UNP P08669
a	611	ASN	-	expression tag	UNP P08669
a	612	VAL	-	expression tag	UNP P08669
a	613	CYS	-	expression tag	UNP P08669
a	614	GLU	-	expression tag	UNP P08669
a	615	TRP	-	expression tag	UNP P08669
a	616	PHE	-	expression tag	UNP P08669
a	617	ASP	-	expression tag	UNP P08669
a	618	ALA	-	expression tag	UNP P08669
a	619	GLY	-	expression tag	UNP P08669
a	620	VAL	-	expression tag	UNP P08669
a	621	LEU	-	expression tag	UNP P08669
a	622	ALA	-	expression tag	UNP P08669
a	623	VAL	-	expression tag	UNP P08669
a	624	GLY	-	expression tag	UNP P08669
a	625	VAL	-	expression tag	UNP P08669
a	626	GLY	-	expression tag	UNP P08669
a	627	ASP	-	expression tag	UNP P08669
a	628	ALA	-	expression tag	UNP P08669
a	629	LEU	-	expression tag	UNP P08669
a	630	VAL	-	expression tag	UNP P08669
a	631	GLU	-	expression tag	UNP P08669
a	632	GLY	-	expression tag	UNP P08669
a	633	ASP	-	expression tag	UNP P08669
a	634	PRO	-	expression tag	UNP P08669
a	635	ASP	-	expression tag	UNP P08669
a	636	GLU	-	expression tag	UNP P08669
a	637	VAL	-	expression tag	UNP P08669
a	638	ARG	-	expression tag	UNP P08669
a	639	GLU	-	expression tag	UNP P08669
a	640	LYS	-	expression tag	UNP P08669
a	641	ALA	-	expression tag	UNP P08669
a	642	LYS	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
a	643	GLU	-	expression tag	UNP P08669
a	644	PHE	-	expression tag	UNP P08669
a	645	VAL	-	expression tag	UNP P08669
a	646	GLU	-	expression tag	UNP P08669
a	647	LYS	-	expression tag	UNP P08669
a	648	ILE	-	expression tag	UNP P08669
a	649	ARG	-	expression tag	UNP P08669
a	650	GLY	-	expression tag	UNP P08669
a	651	CYS	-	expression tag	UNP P08669
a	652	THR	-	expression tag	UNP P08669
a	653	GLU	-	expression tag	UNP P08669
a	654	GLY	-	expression tag	UNP P08669
a	655	SER	-	expression tag	UNP P08669
a	656	LEU	-	expression tag	UNP P08669
a	657	GLU	-	expression tag	UNP P08669
a	658	TRP	-	expression tag	UNP P08669
a	659	SER	-	expression tag	UNP P08669
a	660	HIS	-	expression tag	UNP P08669
a	661	PRO	-	expression tag	UNP P08669
a	662	GLN	-	expression tag	UNP P08669
a	663	PHE	-	expression tag	UNP P08669
a	664	GLU	-	expression tag	UNP P08669
a	665	LYS	-	expression tag	UNP P08669
b	329	PRO	GLU	engineered mutation	UNP P08669
b	360	CYS	GLY	engineered mutation	UNP P08669
b	425	GLY	-	expression tag	UNP P08669
b	426	SER	-	expression tag	UNP P08669
b	427	GLY	-	expression tag	UNP P08669
b	428	GLY	-	expression tag	UNP P08669
b	429	SER	-	expression tag	UNP P08669
b	430	GLY	-	expression tag	UNP P08669
b	431	GLY	-	expression tag	UNP P08669
b	432	SER	-	expression tag	UNP P08669
b	433	GLY	-	expression tag	UNP P08669
b	434	GLY	-	expression tag	UNP P08669
b	435	SER	-	expression tag	UNP P08669
b	436	GLY	-	expression tag	UNP P08669
b	437	GLY	-	expression tag	UNP P08669
b	438	SER	-	expression tag	UNP P08669
b	439	GLU	-	expression tag	UNP P08669
b	440	LYS	-	expression tag	UNP P08669
b	441	ALA	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
b	442	ALA	-	expression tag	UNP P08669
b	443	LYS	-	expression tag	UNP P08669
b	444	ALA	-	expression tag	UNP P08669
b	445	GLU	-	expression tag	UNP P08669
b	446	GLU	-	expression tag	UNP P08669
b	447	ALA	-	expression tag	UNP P08669
b	448	ALA	-	expression tag	UNP P08669
b	449	ARG	-	expression tag	UNP P08669
b	450	LYS	-	expression tag	UNP P08669
b	451	MET	-	expression tag	UNP P08669
b	452	GLU	-	expression tag	UNP P08669
b	453	GLU	-	expression tag	UNP P08669
b	454	LEU	-	expression tag	UNP P08669
b	455	PHE	-	expression tag	UNP P08669
b	456	LYS	-	expression tag	UNP P08669
b	457	LYS	-	expression tag	UNP P08669
b	458	HIS	-	expression tag	UNP P08669
b	459	LYS	-	expression tag	UNP P08669
b	460	ILE	-	expression tag	UNP P08669
b	461	VAL	-	expression tag	UNP P08669
b	462	ALA	-	expression tag	UNP P08669
b	463	VAL	-	expression tag	UNP P08669
b	464	LEU	-	expression tag	UNP P08669
b	465	ARG	-	expression tag	UNP P08669
b	466	ALA	-	expression tag	UNP P08669
b	467	ASN	-	expression tag	UNP P08669
b	468	SER	-	expression tag	UNP P08669
b	469	VAL	-	expression tag	UNP P08669
b	470	GLU	-	expression tag	UNP P08669
b	471	GLU	-	expression tag	UNP P08669
b	472	ALA	-	expression tag	UNP P08669
b	473	ILE	-	expression tag	UNP P08669
b	474	GLU	-	expression tag	UNP P08669
b	475	LYS	-	expression tag	UNP P08669
b	476	ALA	-	expression tag	UNP P08669
b	477	VAL	-	expression tag	UNP P08669
b	478	ALA	-	expression tag	UNP P08669
b	479	VAL	-	expression tag	UNP P08669
b	480	PHE	-	expression tag	UNP P08669
b	481	ALA	-	expression tag	UNP P08669
b	482	GLY	-	expression tag	UNP P08669
b	483	GLY	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
b	484	VAL	-	expression tag	UNP P08669
b	485	HIS	-	expression tag	UNP P08669
b	486	LEU	-	expression tag	UNP P08669
b	487	ILE	-	expression tag	UNP P08669
b	488	GLU	-	expression tag	UNP P08669
b	489	ILE	-	expression tag	UNP P08669
b	490	THR	-	expression tag	UNP P08669
b	491	PHE	-	expression tag	UNP P08669
b	492	THR	-	expression tag	UNP P08669
b	493	VAL	-	expression tag	UNP P08669
b	494	PRO	-	expression tag	UNP P08669
b	495	ASP	-	expression tag	UNP P08669
b	496	ALA	-	expression tag	UNP P08669
b	497	ASP	-	expression tag	UNP P08669
b	498	THR	-	expression tag	UNP P08669
b	499	VAL	-	expression tag	UNP P08669
b	500	ILE	-	expression tag	UNP P08669
b	501	LYS	-	expression tag	UNP P08669
b	502	ALA	-	expression tag	UNP P08669
b	503	LEU	-	expression tag	UNP P08669
b	504	SER	-	expression tag	UNP P08669
b	505	VAL	-	expression tag	UNP P08669
b	506	LEU	-	expression tag	UNP P08669
b	507	LYS	-	expression tag	UNP P08669
b	508	GLU	-	expression tag	UNP P08669
b	509	LYS	-	expression tag	UNP P08669
b	510	GLY	-	expression tag	UNP P08669
b	511	ALA	-	expression tag	UNP P08669
b	512	ILE	-	expression tag	UNP P08669
b	513	ILE	-	expression tag	UNP P08669
b	514	GLY	-	expression tag	UNP P08669
b	515	ALA	-	expression tag	UNP P08669
b	516	GLY	-	expression tag	UNP P08669
b	517	THR	-	expression tag	UNP P08669
b	518	VAL	-	expression tag	UNP P08669
b	519	THR	-	expression tag	UNP P08669
b	520	SER	-	expression tag	UNP P08669
b	521	VAL	-	expression tag	UNP P08669
b	522	GLU	-	expression tag	UNP P08669
b	523	GLN	-	expression tag	UNP P08669
b	524	CYS	-	expression tag	UNP P08669
b	525	ARG	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
b	526	LYS	-	expression tag	UNP P08669
b	527	ALA	-	expression tag	UNP P08669
b	528	VAL	-	expression tag	UNP P08669
b	529	GLU	-	expression tag	UNP P08669
b	530	SER	-	expression tag	UNP P08669
b	531	GLY	-	expression tag	UNP P08669
b	532	ALA	-	expression tag	UNP P08669
b	533	GLU	-	expression tag	UNP P08669
b	534	PHE	-	expression tag	UNP P08669
b	535	ILE	-	expression tag	UNP P08669
b	536	VAL	-	expression tag	UNP P08669
b	537	SER	-	expression tag	UNP P08669
b	538	PRO	-	expression tag	UNP P08669
b	539	HIS	-	expression tag	UNP P08669
b	540	LEU	-	expression tag	UNP P08669
b	541	ASP	-	expression tag	UNP P08669
b	542	GLU	-	expression tag	UNP P08669
b	543	GLU	-	expression tag	UNP P08669
b	544	ILE	-	expression tag	UNP P08669
b	545	SER	-	expression tag	UNP P08669
b	546	GLN	-	expression tag	UNP P08669
b	547	PHE	-	expression tag	UNP P08669
b	548	CYS	-	expression tag	UNP P08669
b	549	LYS	-	expression tag	UNP P08669
b	550	GLU	-	expression tag	UNP P08669
b	551	LYS	-	expression tag	UNP P08669
b	552	GLY	-	expression tag	UNP P08669
b	553	VAL	-	expression tag	UNP P08669
b	554	PHE	-	expression tag	UNP P08669
b	555	TYR	-	expression tag	UNP P08669
b	556	MET	-	expression tag	UNP P08669
b	557	PRO	-	expression tag	UNP P08669
b	558	GLY	-	expression tag	UNP P08669
b	559	VAL	-	expression tag	UNP P08669
b	560	MET	-	expression tag	UNP P08669
b	561	THR	-	expression tag	UNP P08669
b	562	PRO	-	expression tag	UNP P08669
b	563	THR	-	expression tag	UNP P08669
b	564	GLU	-	expression tag	UNP P08669
b	565	LEU	-	expression tag	UNP P08669
b	566	VAL	-	expression tag	UNP P08669
b	567	LYS	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
b	568	ALA	-	expression tag	UNP P08669
b	569	MET	-	expression tag	UNP P08669
b	570	LYS	-	expression tag	UNP P08669
b	571	LEU	-	expression tag	UNP P08669
b	572	GLY	-	expression tag	UNP P08669
b	573	HIS	-	expression tag	UNP P08669
b	574	ASP	-	expression tag	UNP P08669
b	575	ILE	-	expression tag	UNP P08669
b	576	LEU	-	expression tag	UNP P08669
b	577	LYS	-	expression tag	UNP P08669
b	578	LEU	-	expression tag	UNP P08669
b	579	PHE	-	expression tag	UNP P08669
b	580	PRO	-	expression tag	UNP P08669
b	581	GLY	-	expression tag	UNP P08669
b	582	GLU	-	expression tag	UNP P08669
b	583	VAL	-	expression tag	UNP P08669
b	584	VAL	-	expression tag	UNP P08669
b	585	GLY	-	expression tag	UNP P08669
b	586	PRO	-	expression tag	UNP P08669
b	587	GLU	-	expression tag	UNP P08669
b	588	PHE	-	expression tag	UNP P08669
b	589	VAL	-	expression tag	UNP P08669
b	590	LYS	-	expression tag	UNP P08669
b	591	ALA	-	expression tag	UNP P08669
b	592	MET	-	expression tag	UNP P08669
b	593	LYS	-	expression tag	UNP P08669
b	594	GLY	-	expression tag	UNP P08669
b	595	PRO	-	expression tag	UNP P08669
b	596	PHE	-	expression tag	UNP P08669
b	597	PRO	-	expression tag	UNP P08669
b	598	ASN	-	expression tag	UNP P08669
b	599	VAL	-	expression tag	UNP P08669
b	600	LYS	-	expression tag	UNP P08669
b	601	PHE	-	expression tag	UNP P08669
b	602	VAL	-	expression tag	UNP P08669
b	603	PRO	-	expression tag	UNP P08669
b	604	THR	-	expression tag	UNP P08669
b	605	GLY	-	expression tag	UNP P08669
b	606	GLY	-	expression tag	UNP P08669
b	607	VAL	-	expression tag	UNP P08669
b	608	ASP	-	expression tag	UNP P08669
b	609	LEU	-	expression tag	UNP P08669

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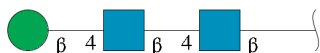
Chain	Residue	Modelled	Actual	Comment	Reference
b	610	ASP	-	expression tag	UNP P08669
b	611	ASN	-	expression tag	UNP P08669
b	612	VAL	-	expression tag	UNP P08669
b	613	CYS	-	expression tag	UNP P08669
b	614	GLU	-	expression tag	UNP P08669
b	615	TRP	-	expression tag	UNP P08669
b	616	PHE	-	expression tag	UNP P08669
b	617	ASP	-	expression tag	UNP P08669
b	618	ALA	-	expression tag	UNP P08669
b	619	GLY	-	expression tag	UNP P08669
b	620	VAL	-	expression tag	UNP P08669
b	621	LEU	-	expression tag	UNP P08669
b	622	ALA	-	expression tag	UNP P08669
b	623	VAL	-	expression tag	UNP P08669
b	624	GLY	-	expression tag	UNP P08669
b	625	VAL	-	expression tag	UNP P08669
b	626	GLY	-	expression tag	UNP P08669
b	627	ASP	-	expression tag	UNP P08669
b	628	ALA	-	expression tag	UNP P08669
b	629	LEU	-	expression tag	UNP P08669
b	630	VAL	-	expression tag	UNP P08669
b	631	GLU	-	expression tag	UNP P08669
b	632	GLY	-	expression tag	UNP P08669
b	633	ASP	-	expression tag	UNP P08669
b	634	PRO	-	expression tag	UNP P08669
b	635	ASP	-	expression tag	UNP P08669
b	636	GLU	-	expression tag	UNP P08669
b	637	VAL	-	expression tag	UNP P08669
b	638	ARG	-	expression tag	UNP P08669
b	639	GLU	-	expression tag	UNP P08669
b	640	LYS	-	expression tag	UNP P08669
b	641	ALA	-	expression tag	UNP P08669
b	642	LYS	-	expression tag	UNP P08669
b	643	GLU	-	expression tag	UNP P08669
b	644	PHE	-	expression tag	UNP P08669
b	645	VAL	-	expression tag	UNP P08669
b	646	GLU	-	expression tag	UNP P08669
b	647	LYS	-	expression tag	UNP P08669
b	648	ILE	-	expression tag	UNP P08669
b	649	ARG	-	expression tag	UNP P08669
b	650	GLY	-	expression tag	UNP P08669
b	651	CYS	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
b	652	THR	-	expression tag	UNP P08669
b	653	GLU	-	expression tag	UNP P08669
b	654	GLY	-	expression tag	UNP P08669
b	655	SER	-	expression tag	UNP P08669
b	656	LEU	-	expression tag	UNP P08669
b	657	GLU	-	expression tag	UNP P08669
b	658	TRP	-	expression tag	UNP P08669
b	659	SER	-	expression tag	UNP P08669
b	660	HIS	-	expression tag	UNP P08669
b	661	PRO	-	expression tag	UNP P08669
b	662	GLN	-	expression tag	UNP P08669
b	663	PHE	-	expression tag	UNP P08669
b	664	GLU	-	expression tag	UNP P08669
b	665	LYS	-	expression tag	UNP P08669

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



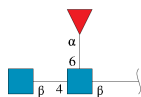
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	D	3	39	22	2	15	0	0
3	E	3	39	22	2	15	0	0
3	M	3	39	22	2	15	0	0
3	N	3	39	22	2	15	0	0
3	V	3	39	22	2	15	0	0
3	W	3	39	22	2	15	0	0

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



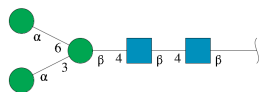
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	3	Total	C	N	O	0	0
			38	22	2	14		
5	P	3	Total	C	N	O	0	0
			38	22	2	14		
5	Y	3	Total	C	N	O	0	0
			38	22	2	14		

- 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
			Total	C	N	O		
6	K	5	61	34	2	25	0	0
6	T	5	61	34	2	25	0	0
6	f	5	61	34	2	25	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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






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

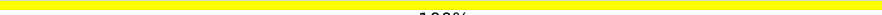




Chain D:  100%


MAG1  
MAG2  
BMA3

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

Chain E:  100%


MAG1  
MAG2  
BMA3

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

Chain M:  100%


MAG1  
MAG2  
BMA3

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

Chain N:  100%


MAG1  
MAG2  
BMA3

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

Chain V:  100%


MAG1  
MAG2  
BMA3

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

Chain W:  100%

MAG1  
MAG2  
BMA3

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

Chain F:  100%


MAG1  
MAG2

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

Chain H:  100%


MAG1  
MAG2

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

Chain I:  100%

MAG1  
MAG2

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

Chain J:  100%

MAG1  
MAG2

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

Chain O:  100%


MAG1  
MAG2

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

Chain Q:  100%

MAG1  
MAG2

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

Chain R:  100%


MAG1  
MAG2

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

Chain S:  100%

MAG1  
MAG2


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

Chain X:  100%MAG1  
MAG2

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

Chain Z:  100%MAG1  
MAG2

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

Chain d:  100%MAG1  
MAG2

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

Chain e:  100%MAG1  
MAG2

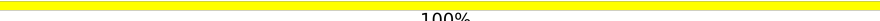
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%MAG1  
MAG2  
FUC3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%MAG1  
MAG2  
FUC3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%

MAG1  
MAG2  
FUC3

- 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

Chain K:  60% 40%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- 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

Chain T:  60% 40%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- 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

Chain f:  60% 40%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

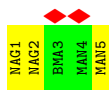
- Molecule 7: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  40% 40% 60%

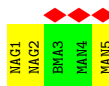
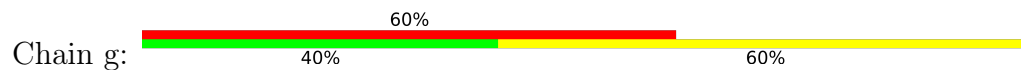
MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 7: alpha-D-mannopyranose-(1-6)-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

Chain U:  40% 40% 60%



- Molecule 7: alpha-D-mannopyranose-(1-6)-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, C3	Depositor
Number of particles used	56496	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.005	Depositor
Minimum map value	-0.541	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	294.4, 294.4, 294.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.01	2/1587 (0.1%)	0.90	2/2153 (0.1%)
1	B	1.01	2/1587 (0.1%)	0.90	2/2153 (0.1%)
1	C	1.01	2/1587 (0.1%)	0.90	2/2153 (0.1%)
2	a	1.04	0/1367	0.92	2/1845 (0.1%)
2	b	1.04	0/1367	0.92	2/1845 (0.1%)
2	c	1.04	0/1367	0.92	2/1845 (0.1%)
All	All	1.03	6/8862 (0.1%)	0.91	12/11994 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	TYR	CB-CG	-6.75	1.41	1.51
1	A	66	TYR	CB-CG	-6.75	1.41	1.51
1	B	66	TYR	CB-CG	-6.75	1.41	1.51
1	B	104	GLU	CD-OE1	-5.27	1.19	1.25
1	C	104	GLU	CD-OE1	-5.26	1.19	1.25

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	314	ARG	NE-CZ-NH2	-8.07	116.27	120.30
2	b	314	ARG	NE-CZ-NH2	-8.05	116.27	120.30
2	c	314	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	C	197	GLY	N-CA-C	-6.30	97.36	113.10
1	A	197	GLY	N-CA-C	-6.30	97.36	113.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/259 (75%)	184 (94%)	11 (6%)	0	100	100
1	B	195/259 (75%)	184 (94%)	11 (6%)	0	100	100
1	C	195/259 (75%)	184 (94%)	11 (6%)	0	100	100
2	a	163/406 (40%)	157 (96%)	6 (4%)	0	100	100
2	b	163/406 (40%)	157 (96%)	6 (4%)	0	100	100
2	c	163/406 (40%)	157 (96%)	6 (4%)	0	100	100
All	All	1074/1995 (54%)	1023 (95%)	51 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	174/228 (76%)	174 (100%)	0	100	100
1	B	174/228 (76%)	174 (100%)	0	100	100
1	C	174/228 (76%)	174 (100%)	0	100	100
2	a	148/337 (44%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	148/337 (44%)	148 (100%)	0	100	100
2	c	148/337 (44%)	148 (100%)	0	100	100
All	All	966/1695 (57%)	966 (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. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	170	HIS
1	B	232	GLN
1	A	148	ASN
1	A	170	HIS
1	A	232	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

81 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	D	1	3,1	14,14,15	2.02	5 (35%)	17,19,21	1.67	6 (35%)
3	NAG	D	2	3	14,14,15	1.91	4 (28%)	17,19,21	1.96	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	D	3	3	11,11,12	1.91	5 (45%)	15,15,17	0.69	0
3	NAG	E	1	3,1	14,14,15	1.92	4 (28%)	17,19,21	0.90	0
3	NAG	E	2	3	14,14,15	1.87	5 (35%)	17,19,21	0.88	1 (5%)
3	BMA	E	3	3	11,11,12	1.87	5 (45%)	15,15,17	0.78	0
4	NAG	F	1	1,4	14,14,15	1.99	4 (28%)	17,19,21	0.88	1 (5%)
4	NAG	F	2	4	14,14,15	1.84	4 (28%)	17,19,21	0.95	1 (5%)
5	NAG	G	1	1,5	14,14,15	1.47	2 (14%)	17,19,21	1.10	1 (5%)
5	NAG	G	2	5	14,14,15	2.17	6 (42%)	17,19,21	0.96	1 (5%)
5	FUC	G	3	5	10,10,11	1.79	4 (40%)	14,14,16	0.79	0
4	NAG	H	1	1,4	14,14,15	2.22	4 (28%)	17,19,21	1.02	0
4	NAG	H	2	4	14,14,15	1.88	5 (35%)	17,19,21	0.88	1 (5%)
4	NAG	I	1	1,4	14,14,15	1.87	4 (28%)	17,19,21	1.17	1 (5%)
4	NAG	I	2	4	14,14,15	1.94	5 (35%)	17,19,21	0.95	1 (5%)
4	NAG	J	1	1,4	14,14,15	1.86	3 (21%)	17,19,21	1.19	1 (5%)
4	NAG	J	2	4	14,14,15	1.81	5 (35%)	17,19,21	1.06	2 (11%)
6	NAG	K	1	6,2	14,14,15	0.74	0	17,19,21	1.79	3 (17%)
6	NAG	K	2	6	14,14,15	0.50	0	17,19,21	1.34	2 (11%)
6	BMA	K	3	6	11,11,12	0.40	0	15,15,17	0.76	0
6	MAN	K	4	6	11,11,12	0.38	0	15,15,17	0.75	0
6	MAN	K	5	6	11,11,12	0.27	0	15,15,17	0.60	0
7	NAG	L	1	7,2	14,14,15	1.80	3 (21%)	17,19,21	1.53	3 (17%)
7	NAG	L	2	7	14,14,15	1.90	4 (28%)	17,19,21	0.94	1 (5%)
7	BMA	L	3	7	11,11,12	0.58	0	15,15,17	0.69	0
7	MAN	L	4	7	11,11,12	0.60	0	15,15,17	0.67	0
7	MAN	L	5	7	11,11,12	1.89	5 (45%)	15,15,17	0.68	0
3	NAG	M	1	3,1	14,14,15	2.02	5 (35%)	17,19,21	1.67	6 (35%)
3	NAG	M	2	3	14,14,15	1.91	4 (28%)	17,19,21	1.96	2 (11%)
3	BMA	M	3	3	11,11,12	1.91	5 (45%)	15,15,17	0.69	0
3	NAG	N	1	3,1	14,14,15	1.92	4 (28%)	17,19,21	0.91	0
3	NAG	N	2	3	14,14,15	1.87	5 (35%)	17,19,21	0.88	1 (5%)
3	BMA	N	3	3	11,11,12	1.87	5 (45%)	15,15,17	0.78	0
4	NAG	O	1	1,4	14,14,15	1.98	4 (28%)	17,19,21	0.88	1 (5%)
4	NAG	O	2	4	14,14,15	1.84	4 (28%)	17,19,21	0.95	1 (5%)
5	NAG	P	1	1,5	14,14,15	1.48	2 (14%)	17,19,21	1.10	1 (5%)
5	NAG	P	2	5	14,14,15	2.17	6 (42%)	17,19,21	0.96	1 (5%)
5	FUC	P	3	5	10,10,11	1.79	4 (40%)	14,14,16	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	Q	1	1,4	14,14,15	2.22	4 (28%)	17,19,21	1.01	0
4	NAG	Q	2	4	14,14,15	1.88	5 (35%)	17,19,21	0.88	1 (5%)
4	NAG	R	1	1,4	14,14,15	1.87	4 (28%)	17,19,21	1.17	1 (5%)
4	NAG	R	2	4	14,14,15	1.94	5 (35%)	17,19,21	0.94	1 (5%)
4	NAG	S	1	1,4	14,14,15	1.86	3 (21%)	17,19,21	1.19	1 (5%)
4	NAG	S	2	4	14,14,15	1.81	5 (35%)	17,19,21	1.06	2 (11%)
6	NAG	T	1	6,2	14,14,15	0.74	0	17,19,21	1.79	3 (17%)
6	NAG	T	2	6	14,14,15	0.51	0	17,19,21	1.33	2 (11%)
6	BMA	T	3	6	11,11,12	0.39	0	15,15,17	0.76	0
6	MAN	T	4	6	11,11,12	0.37	0	15,15,17	0.75	0
6	MAN	T	5	6	11,11,12	0.26	0	15,15,17	0.60	0
7	NAG	U	1	7,2	14,14,15	1.80	3 (21%)	17,19,21	1.53	3 (17%)
7	NAG	U	2	7	14,14,15	1.90	3 (21%)	17,19,21	0.94	1 (5%)
7	BMA	U	3	7	11,11,12	0.58	0	15,15,17	0.69	0
7	MAN	U	4	7	11,11,12	0.59	0	15,15,17	0.68	0
7	MAN	U	5	7	11,11,12	1.89	5 (45%)	15,15,17	0.68	0
3	NAG	V	1	3,1	14,14,15	2.02	5 (35%)	17,19,21	1.67	6 (35%)
3	NAG	V	2	3	14,14,15	1.91	4 (28%)	17,19,21	1.96	2 (11%)
3	BMA	V	3	3	11,11,12	1.91	5 (45%)	15,15,17	0.69	0
3	NAG	W	1	3,1	14,14,15	1.91	4 (28%)	17,19,21	0.91	0
3	NAG	W	2	3	14,14,15	1.86	5 (35%)	17,19,21	0.89	1 (5%)
3	BMA	W	3	3	11,11,12	1.87	5 (45%)	15,15,17	0.78	0
4	NAG	X	1	1,4	14,14,15	1.98	4 (28%)	17,19,21	0.87	1 (5%)
4	NAG	X	2	4	14,14,15	1.84	4 (28%)	17,19,21	0.95	1 (5%)
5	NAG	Y	1	1,5	14,14,15	1.48	2 (14%)	17,19,21	1.10	1 (5%)
5	NAG	Y	2	5	14,14,15	2.17	6 (42%)	17,19,21	0.96	1 (5%)
5	FUC	Y	3	5	10,10,11	1.79	4 (40%)	14,14,16	0.79	0
4	NAG	Z	1	1,4	14,14,15	2.21	4 (28%)	17,19,21	1.02	1 (5%)
4	NAG	Z	2	4	14,14,15	1.88	5 (35%)	17,19,21	0.88	1 (5%)
4	NAG	d	1	1,4	14,14,15	1.87	4 (28%)	17,19,21	1.17	1 (5%)
4	NAG	d	2	4	14,14,15	1.94	5 (35%)	17,19,21	0.94	1 (5%)
4	NAG	e	1	1,4	14,14,15	1.86	3 (21%)	17,19,21	1.19	1 (5%)
4	NAG	e	2	4	14,14,15	1.81	5 (35%)	17,19,21	1.07	2 (11%)
6	NAG	f	1	6,2	14,14,15	0.73	0	17,19,21	1.79	3 (17%)
6	NAG	f	2	6	14,14,15	0.50	0	17,19,21	1.33	2 (11%)
6	BMA	f	3	6	11,11,12	0.39	0	15,15,17	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	f	4	6	11,11,12	0.38	0	15,15,17	0.75	0
6	MAN	f	5	6	11,11,12	0.26	0	15,15,17	0.60	0
7	NAG	g	1	7,2	14,14,15	1.80	3 (21%)	17,19,21	1.54	3 (17%)
7	NAG	g	2	7	14,14,15	1.89	4 (28%)	17,19,21	0.94	1 (5%)
7	BMA	g	3	7	11,11,12	0.59	0	15,15,17	0.68	0
7	MAN	g	4	7	11,11,12	0.60	0	15,15,17	0.68	0
7	MAN	g	5	7	11,11,12	1.89	5 (45%)	15,15,17	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	FUC	G	3	5	-	-	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
6	NAG	K	1	6,2	-	4/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	1/2/19/22	0/1/1/1
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
6	MAN	K	5	6	-	1/2/19/22	0/1/1/1
7	NAG	L	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
7	BMA	L	3	7	-	2/2/19/22	0/1/1/1
7	MAN	L	4	7	-	2/2/19/22	0/1/1/1
7	MAN	L	5	7	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	BMA	M	3	3	-	1/2/19/22	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	BMA	N	3	3	-	1/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	FUC	P	3	5	-	-	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
6	NAG	T	1	6,2	-	4/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	BMA	T	3	6	-	1/2/19/22	0/1/1/1
6	MAN	T	4	6	-	0/2/19/22	0/1/1/1
6	MAN	T	5	6	-	1/2/19/22	0/1/1/1
7	NAG	U	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	0/6/23/26	0/1/1/1
7	BMA	U	3	7	-	2/2/19/22	0/1/1/1
7	MAN	U	4	7	-	2/2/19/22	0/1/1/1
7	MAN	U	5	7	-	1/2/19/22	0/1/1/1
3	NAG	V	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	BMA	V	3	3	-	1/2/19/22	0/1/1/1
3	NAG	W	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	BMA	W	3	3	-	1/2/19/22	0/1/1/1
4	NAG	X	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
5	NAG	Y	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	FUC	Y	3	5	-	-	0/1/1/1
4	NAG	Z	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1
4	NAG	d	1	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1
4	NAG	e	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
6	NAG	f	1	6,2	-	4/6/23/26	0/1/1/1
6	NAG	f	2	6	-	0/6/23/26	0/1/1/1
6	BMA	f	3	6	-	1/2/19/22	0/1/1/1
6	MAN	f	4	6	-	0/2/19/22	0/1/1/1
6	MAN	f	5	6	-	1/2/19/22	0/1/1/1
7	NAG	g	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	g	2	7	-	0/6/23/26	0/1/1/1
7	BMA	g	3	7	-	2/2/19/22	0/1/1/1
7	MAN	g	4	7	-	2/2/19/22	0/1/1/1
7	MAN	g	5	7	-	1/2/19/22	0/1/1/1

The worst 5 of 257 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	C1-C2	6.11	1.61	1.52
4	Q	1	NAG	C1-C2	6.09	1.61	1.52
4	Z	1	NAG	C1-C2	6.07	1.61	1.52
5	P	2	NAG	C1-C2	5.80	1.61	1.52
5	G	2	NAG	C1-C2	5.80	1.61	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	2	NAG	C8-C7-N2	5.99	126.24	116.10
3	M	2	NAG	C8-C7-N2	5.97	126.21	116.10
3	D	2	NAG	C8-C7-N2	5.96	126.19	116.10
6	T	1	NAG	O4-C4-C5	-4.68	97.67	109.30
6	f	1	NAG	O4-C4-C5	-4.68	97.69	109.30

There are no chirality outliers.

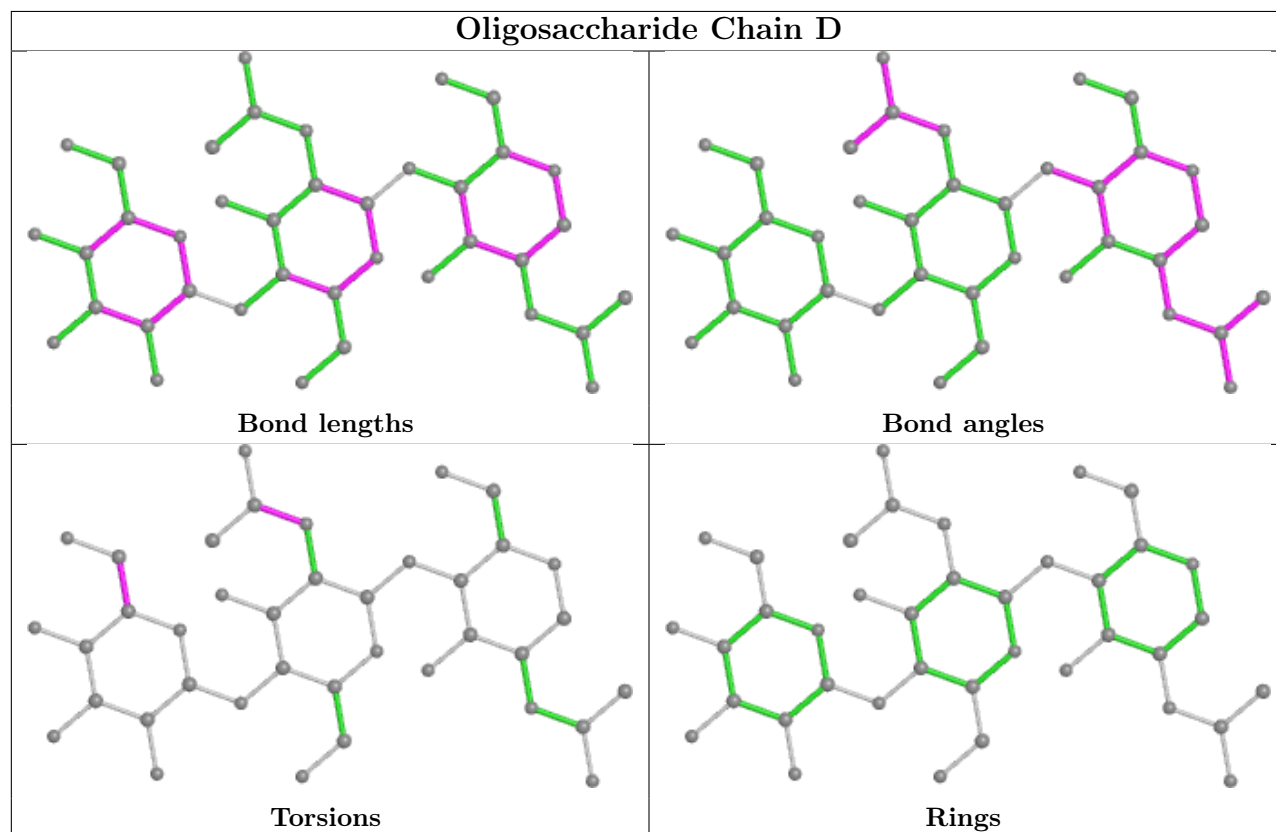
5 of 45 torsion outliers are listed below:

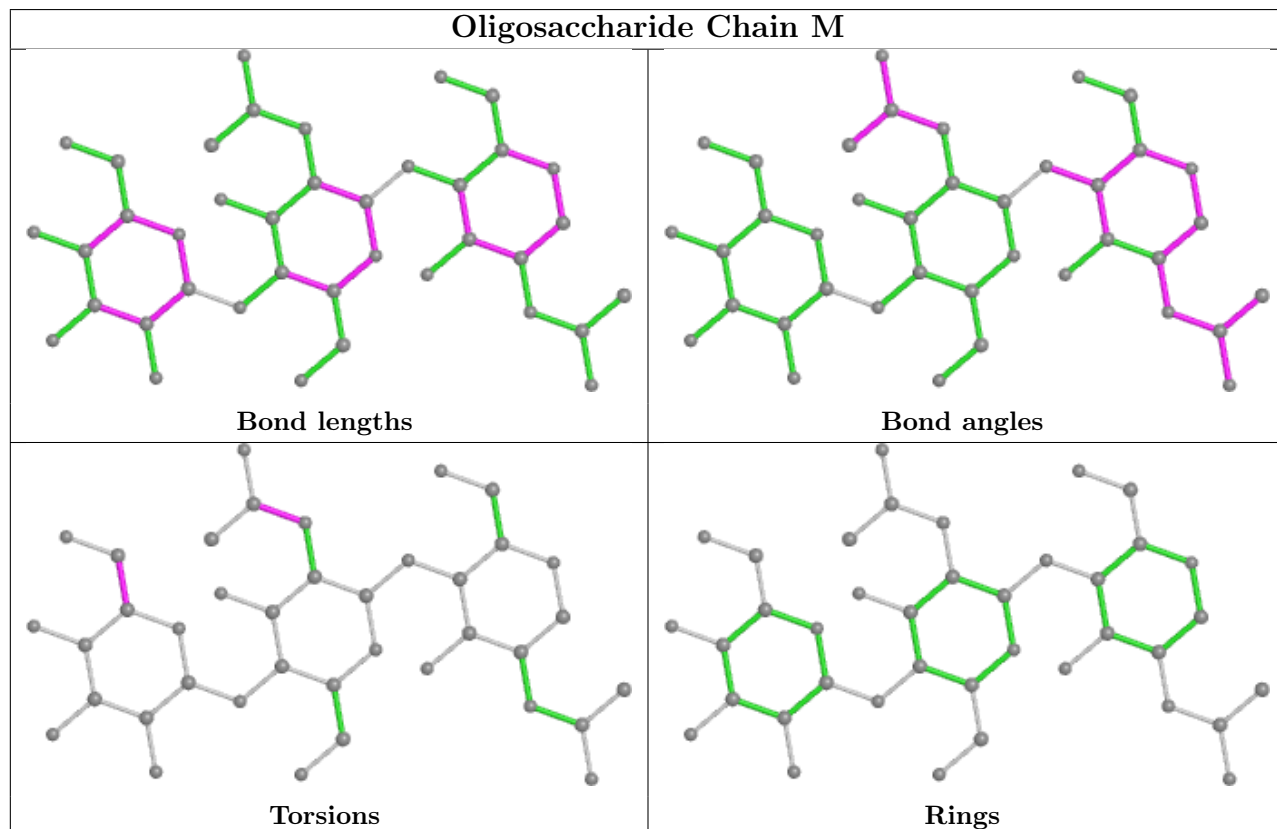
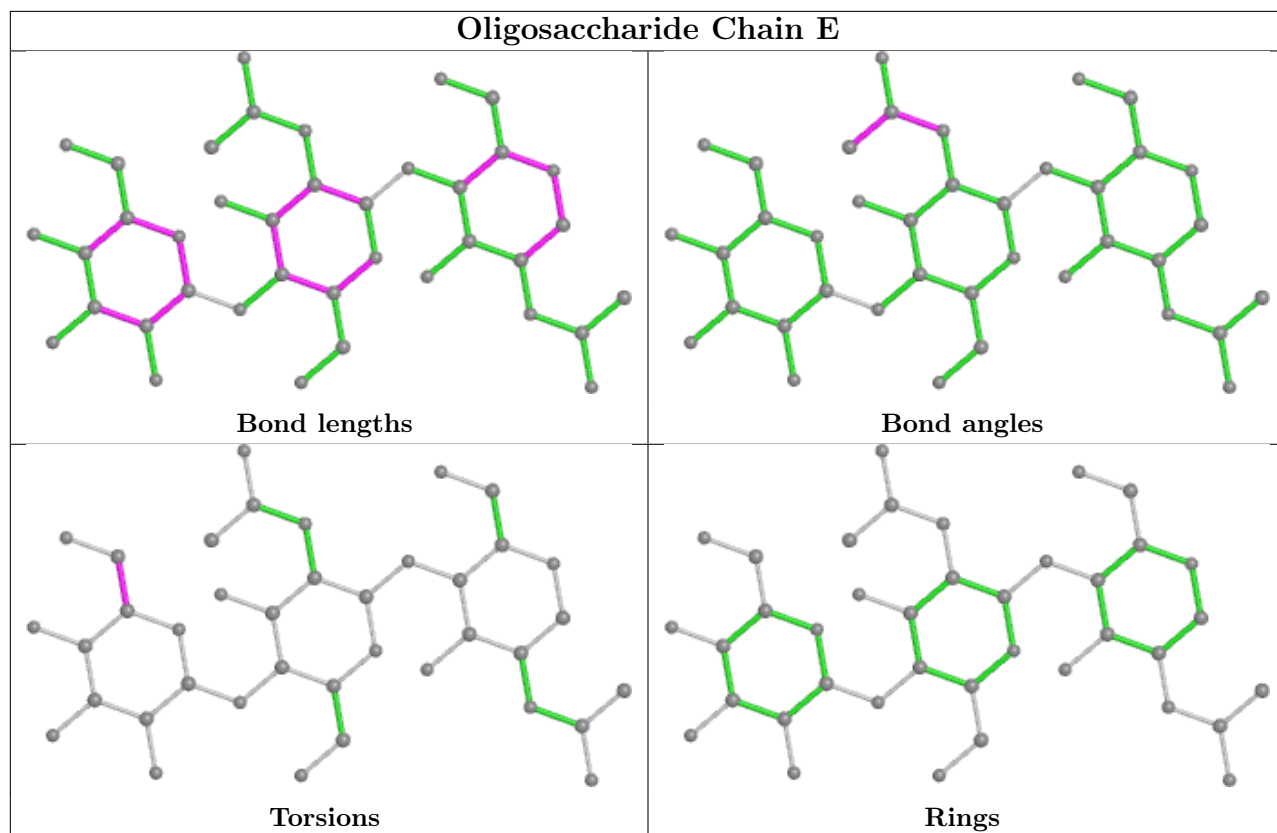
Mol	Chain	Res	Type	Atoms
6	K	1	NAG	C8-C7-N2-C2
6	K	1	NAG	O7-C7-N2-C2
6	T	1	NAG	C8-C7-N2-C2
6	T	1	NAG	O7-C7-N2-C2
6	f	1	NAG	C8-C7-N2-C2

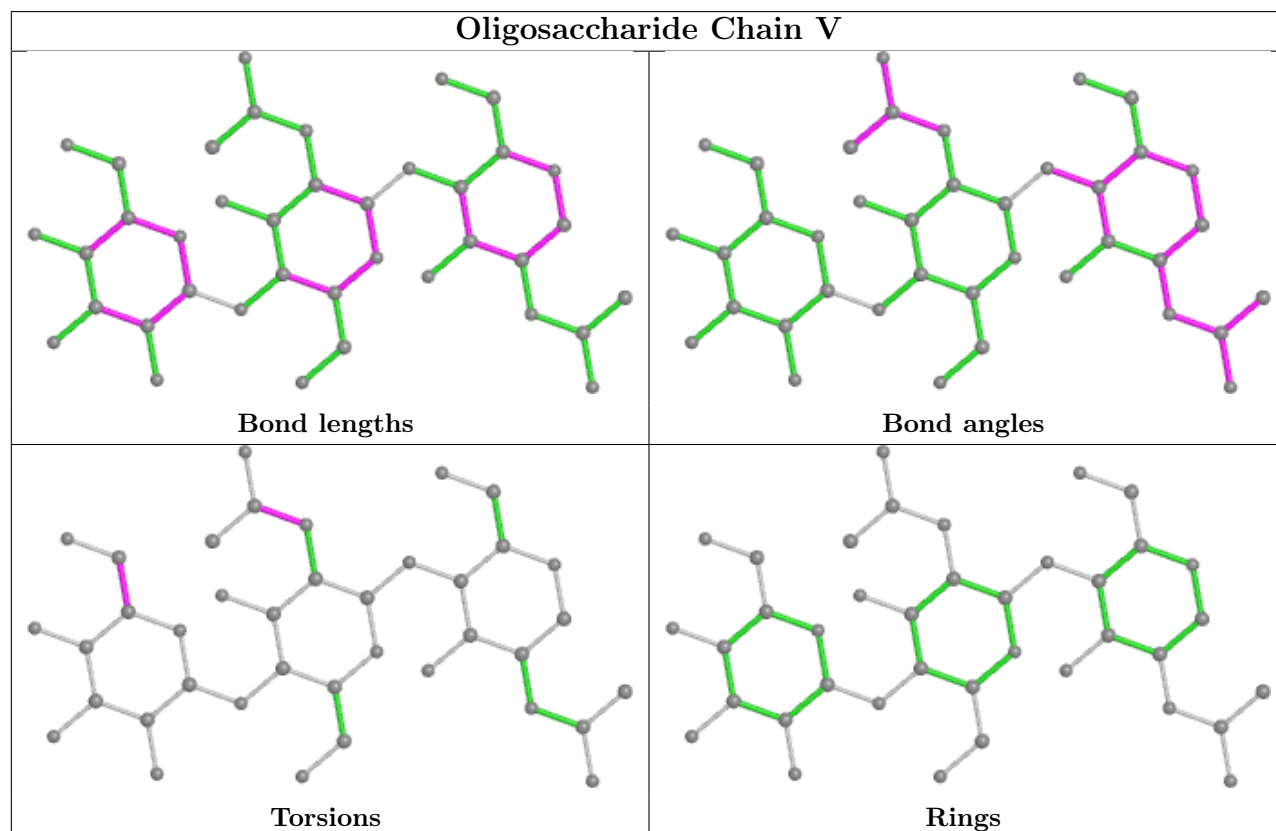
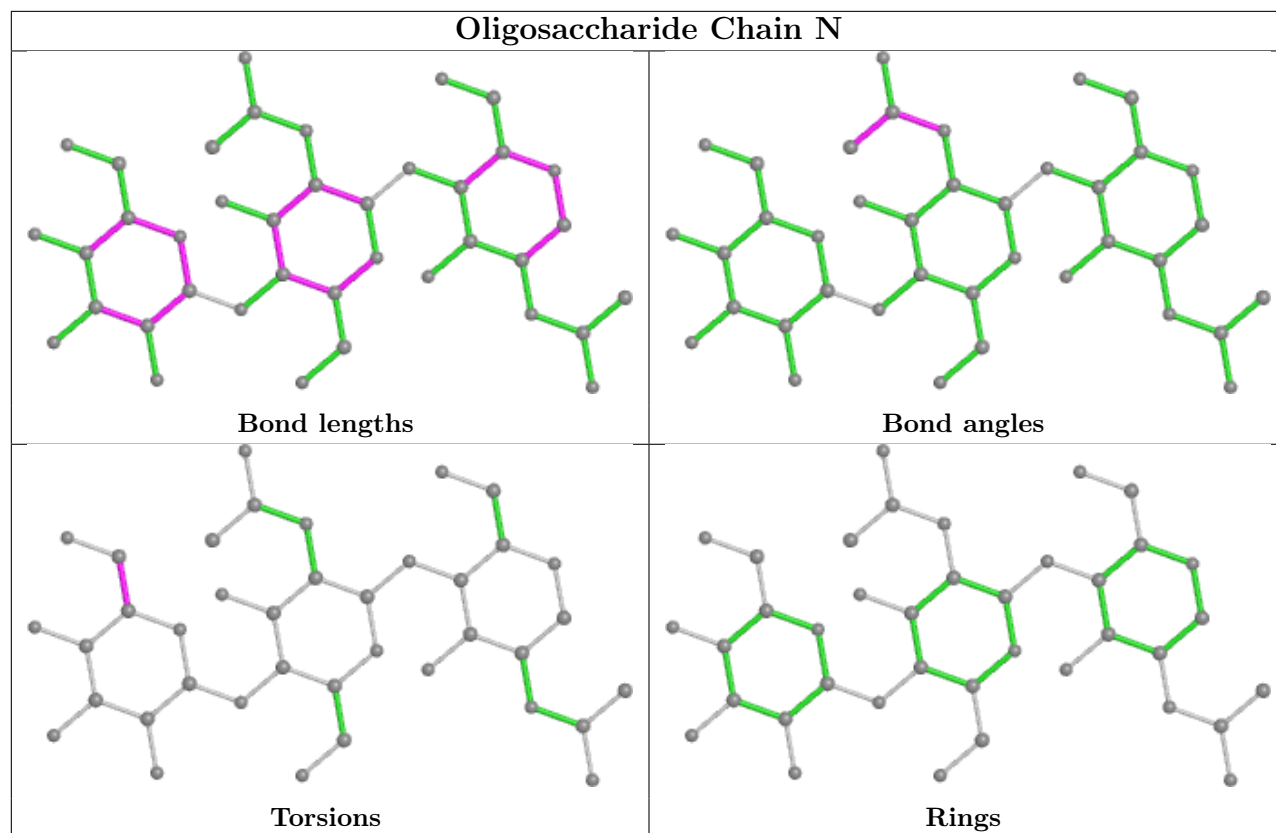
There are no ring outliers.

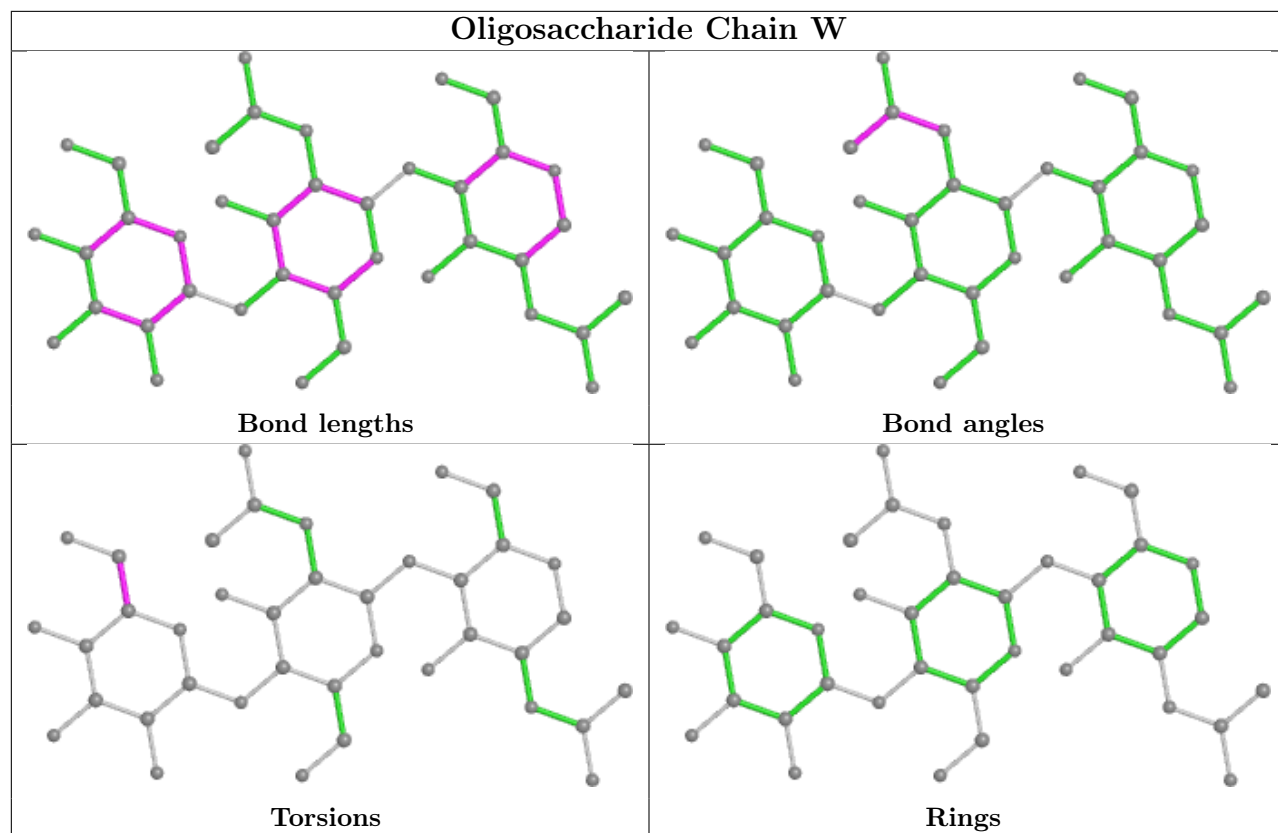
No monomer is involved in short contacts.

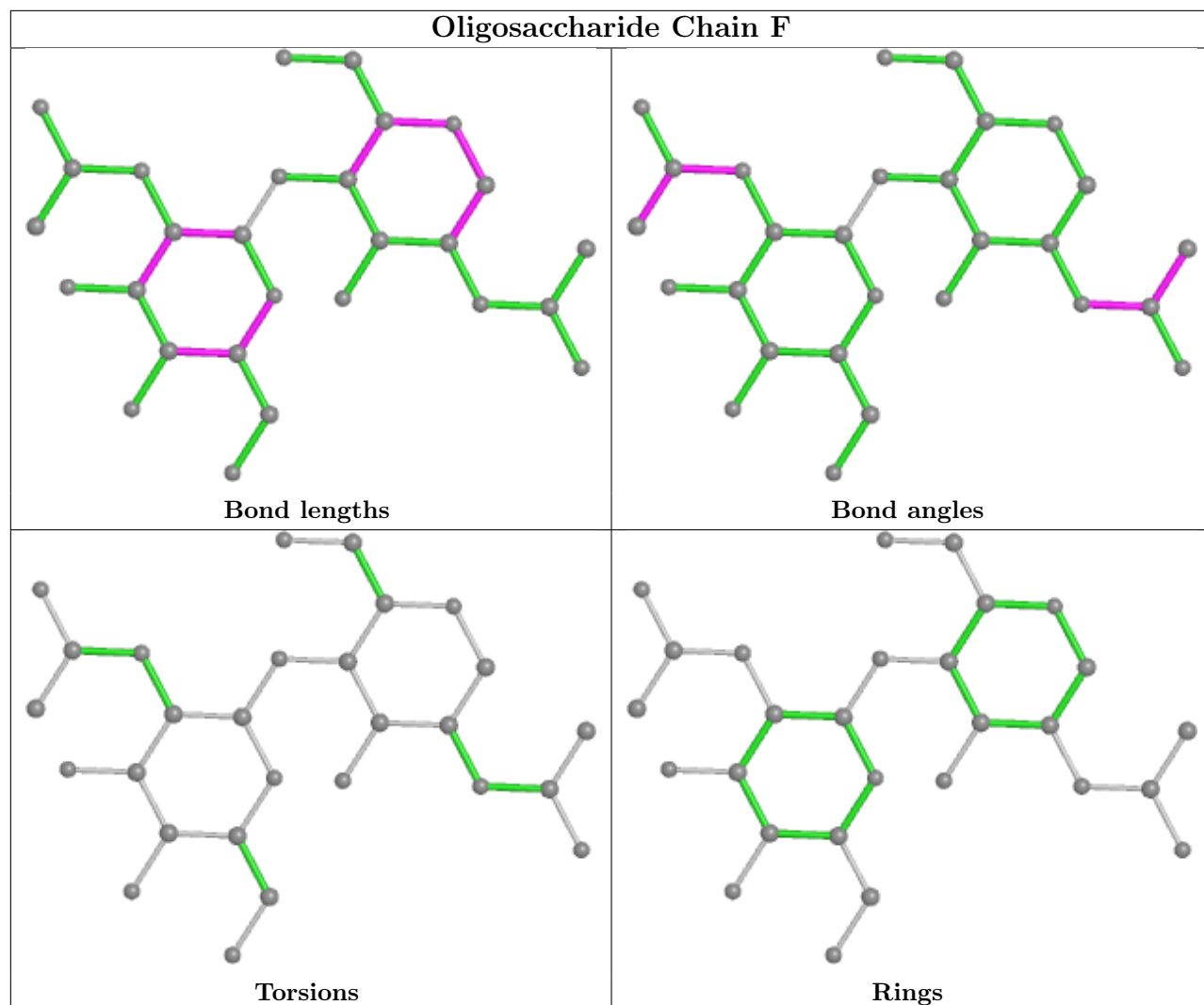
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

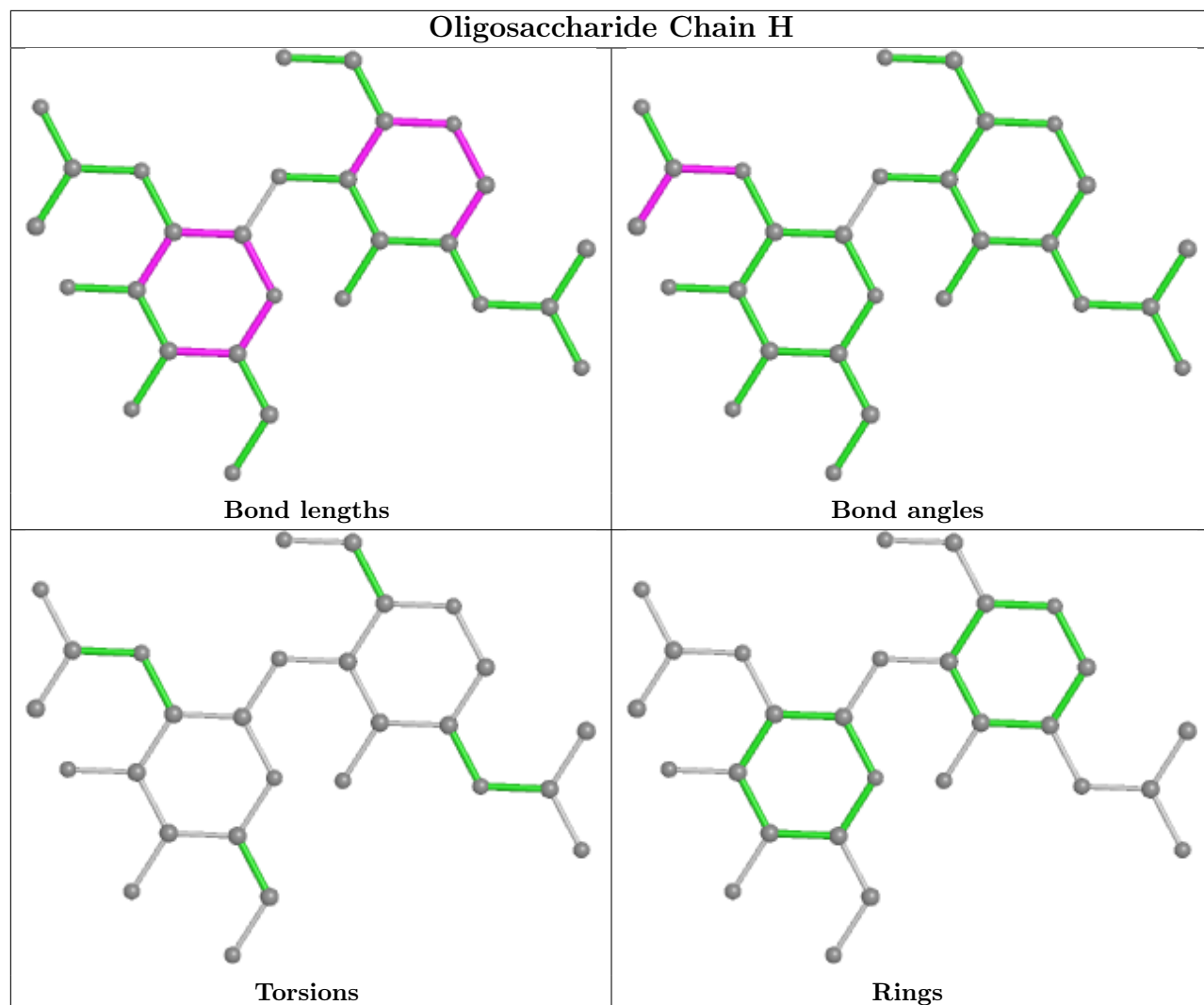


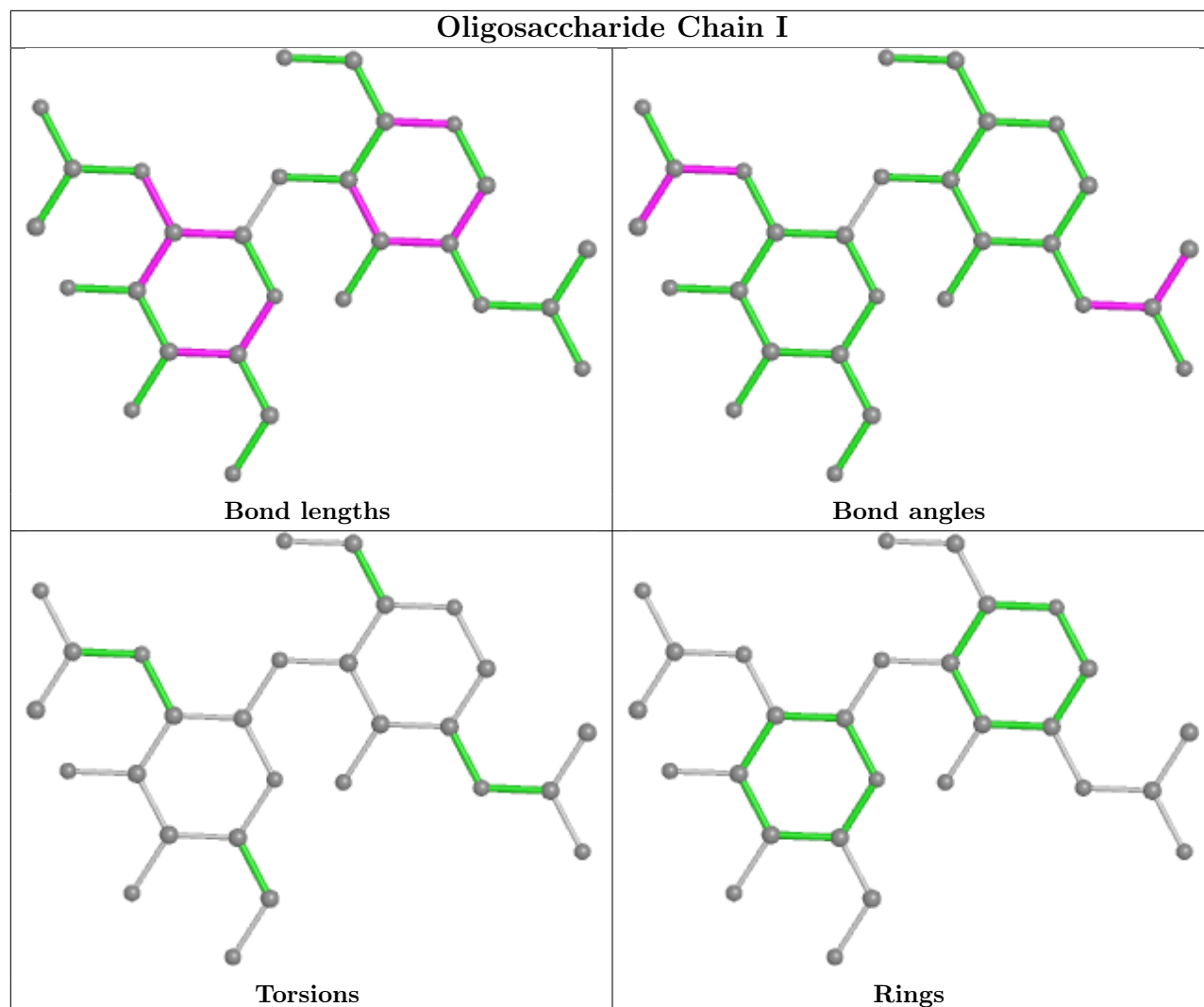




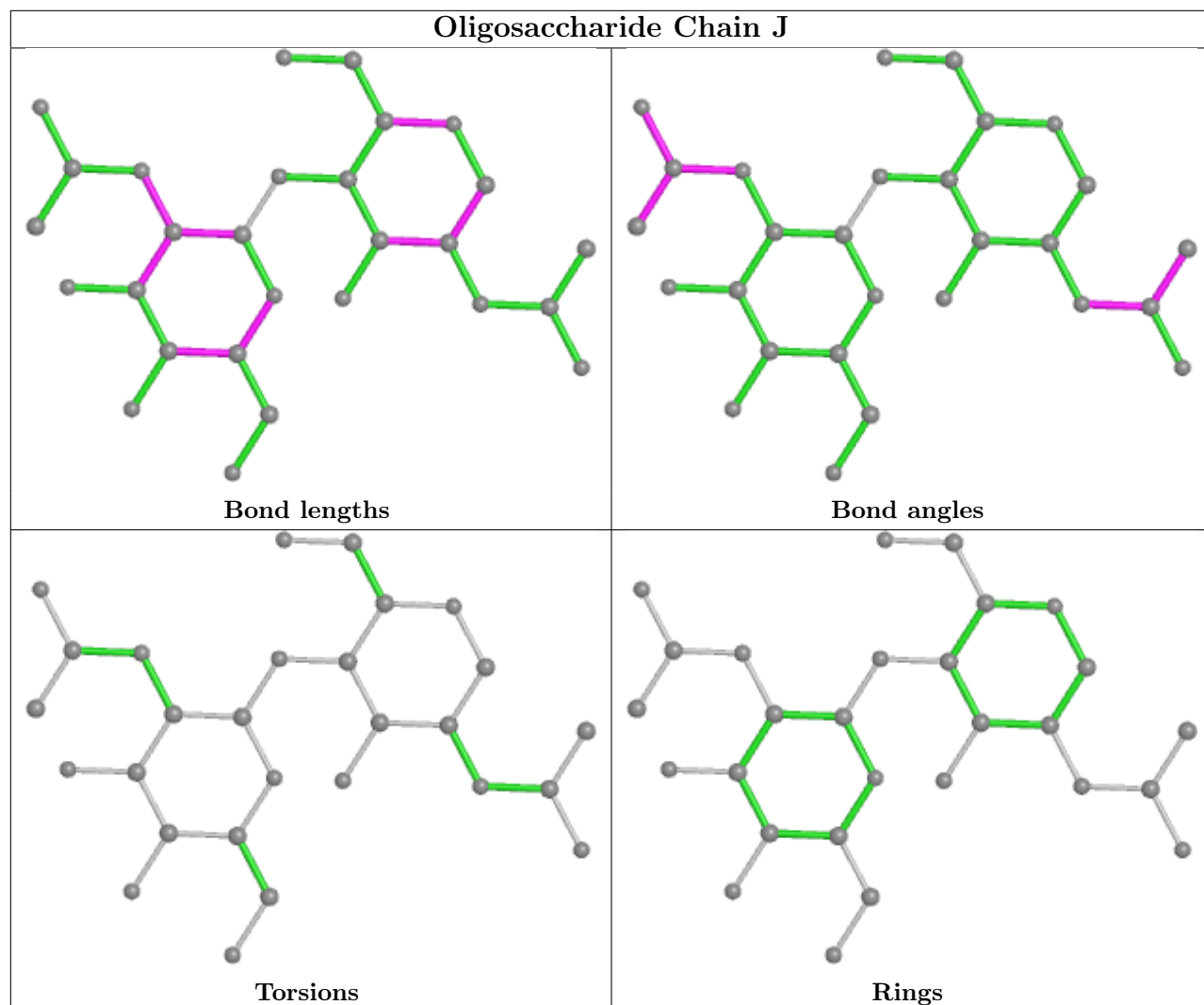


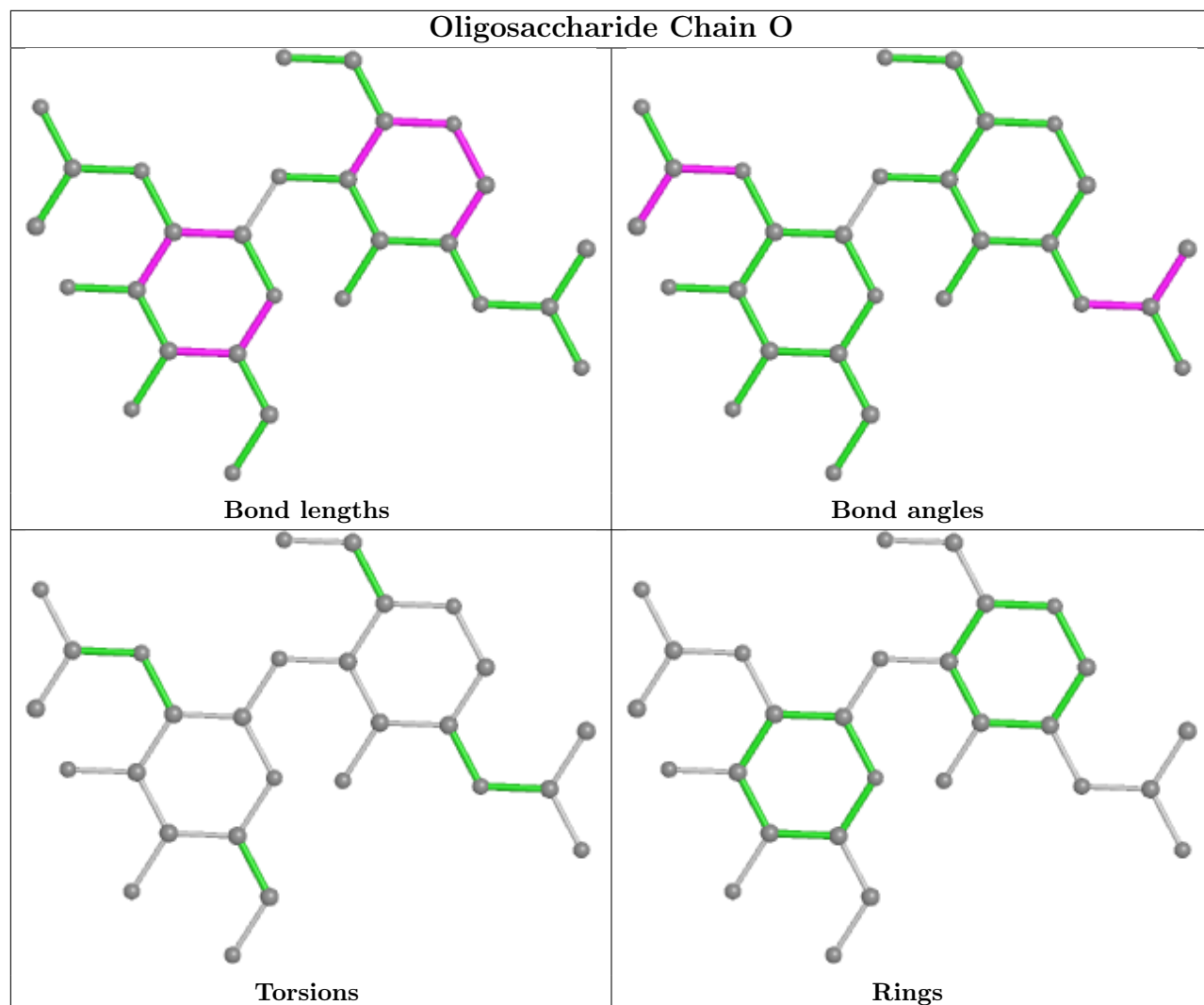


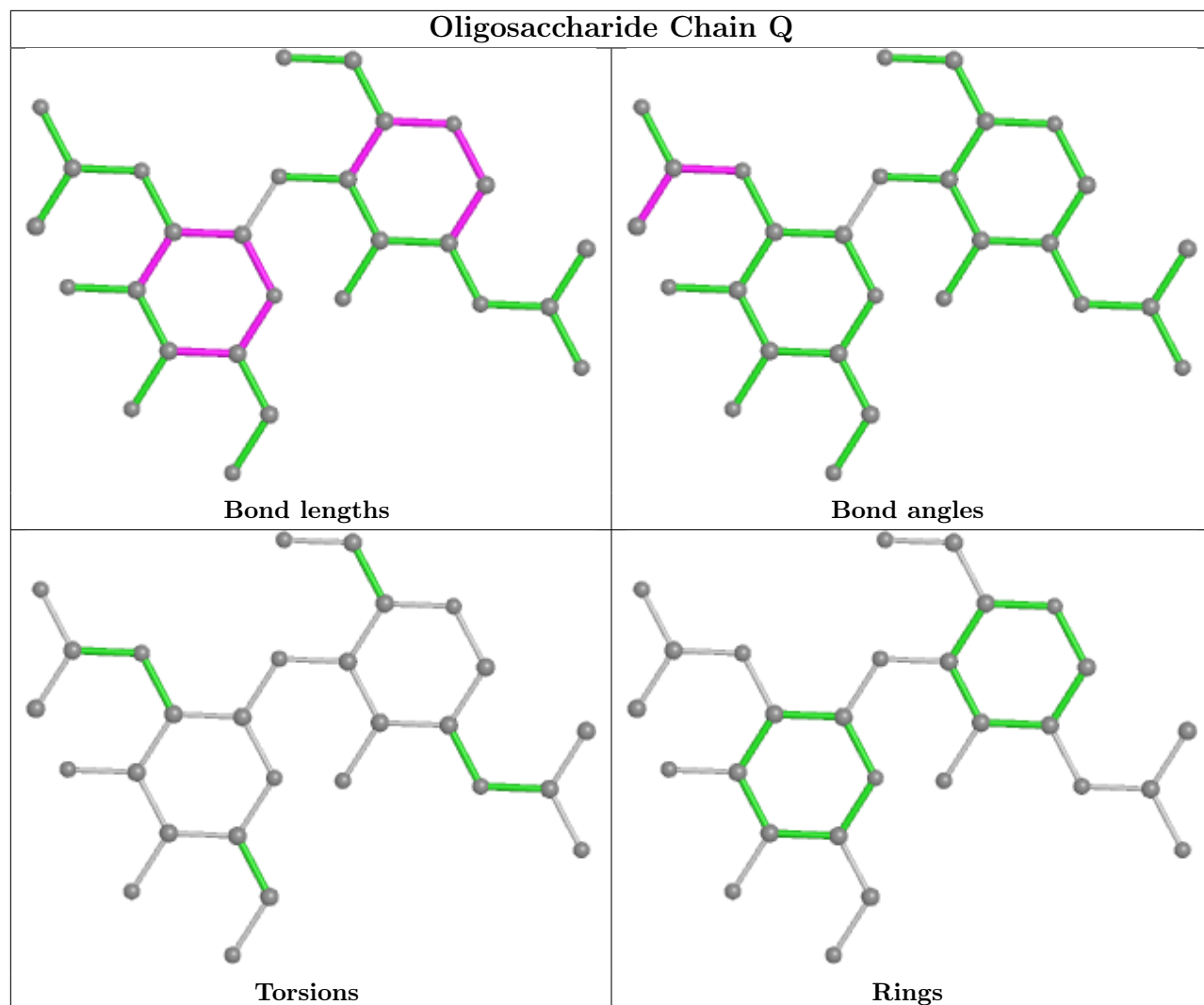


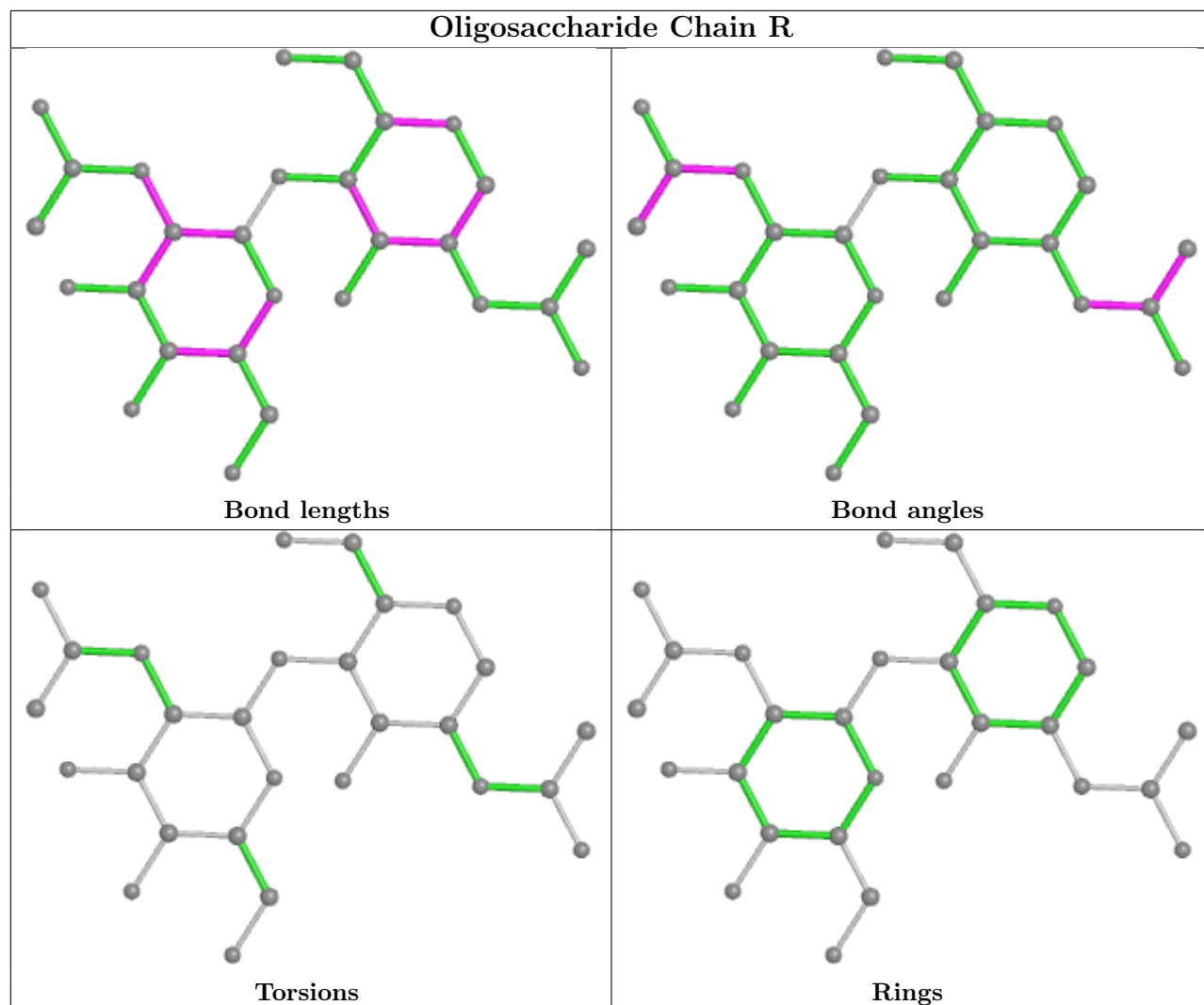


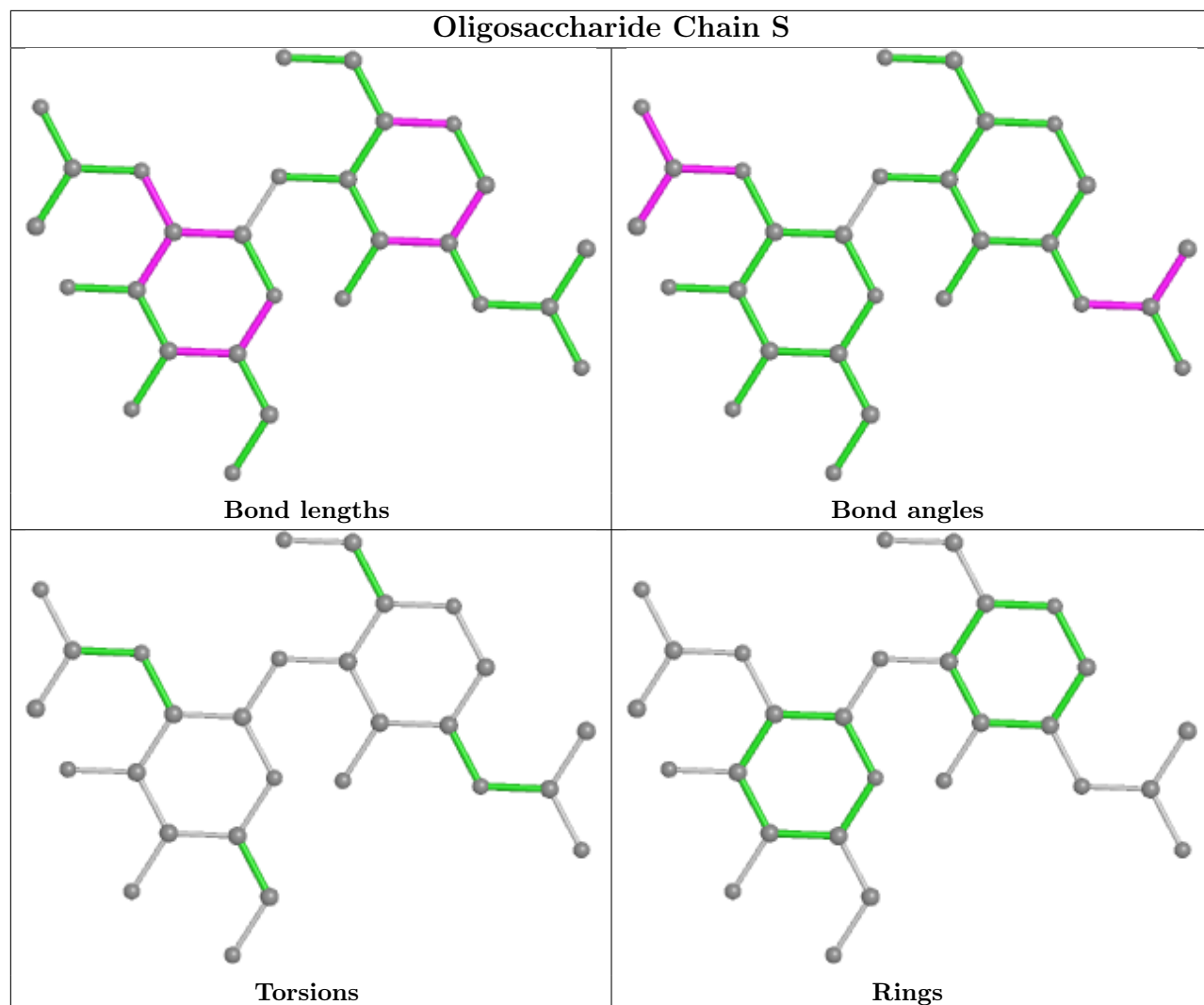


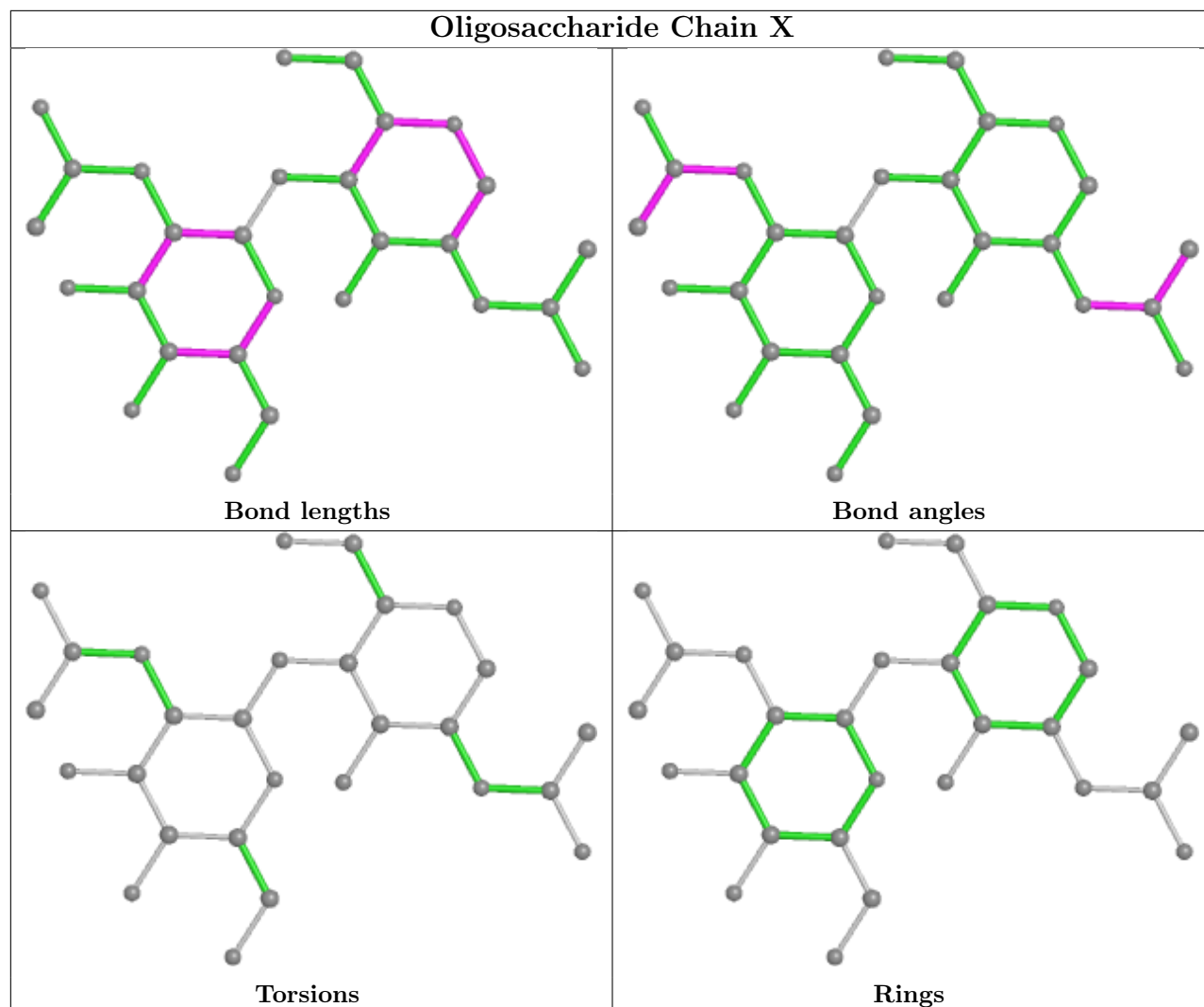


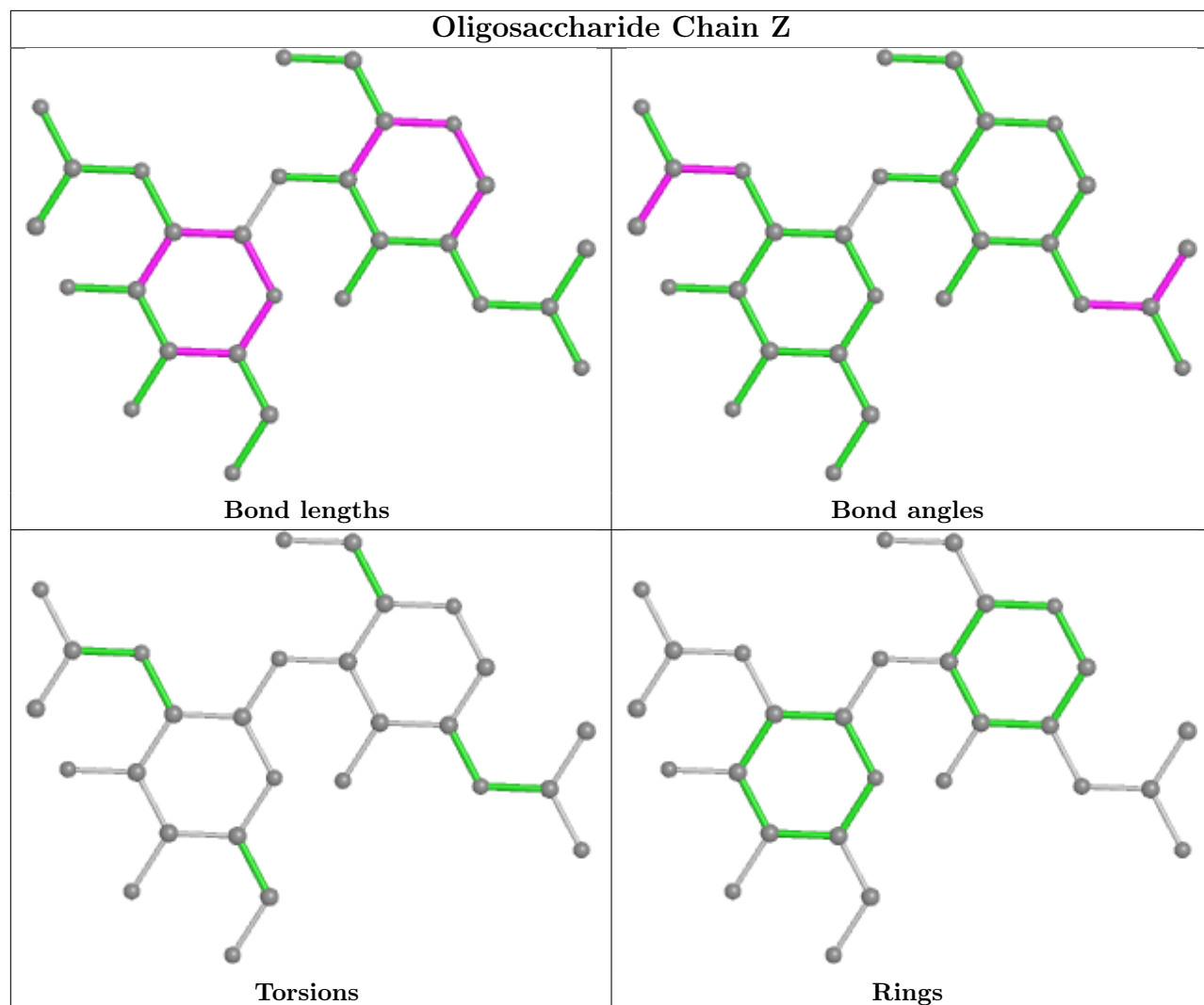


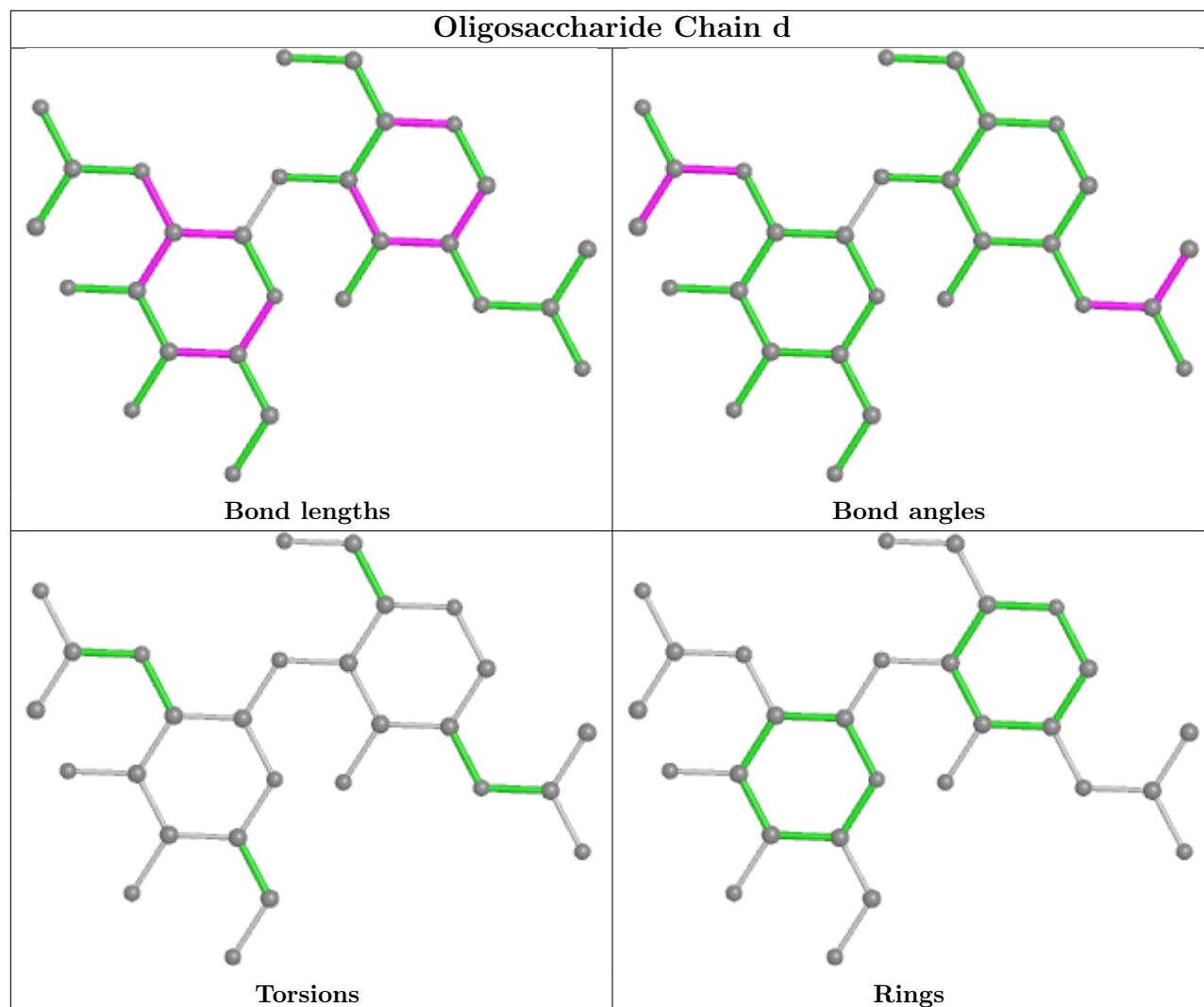




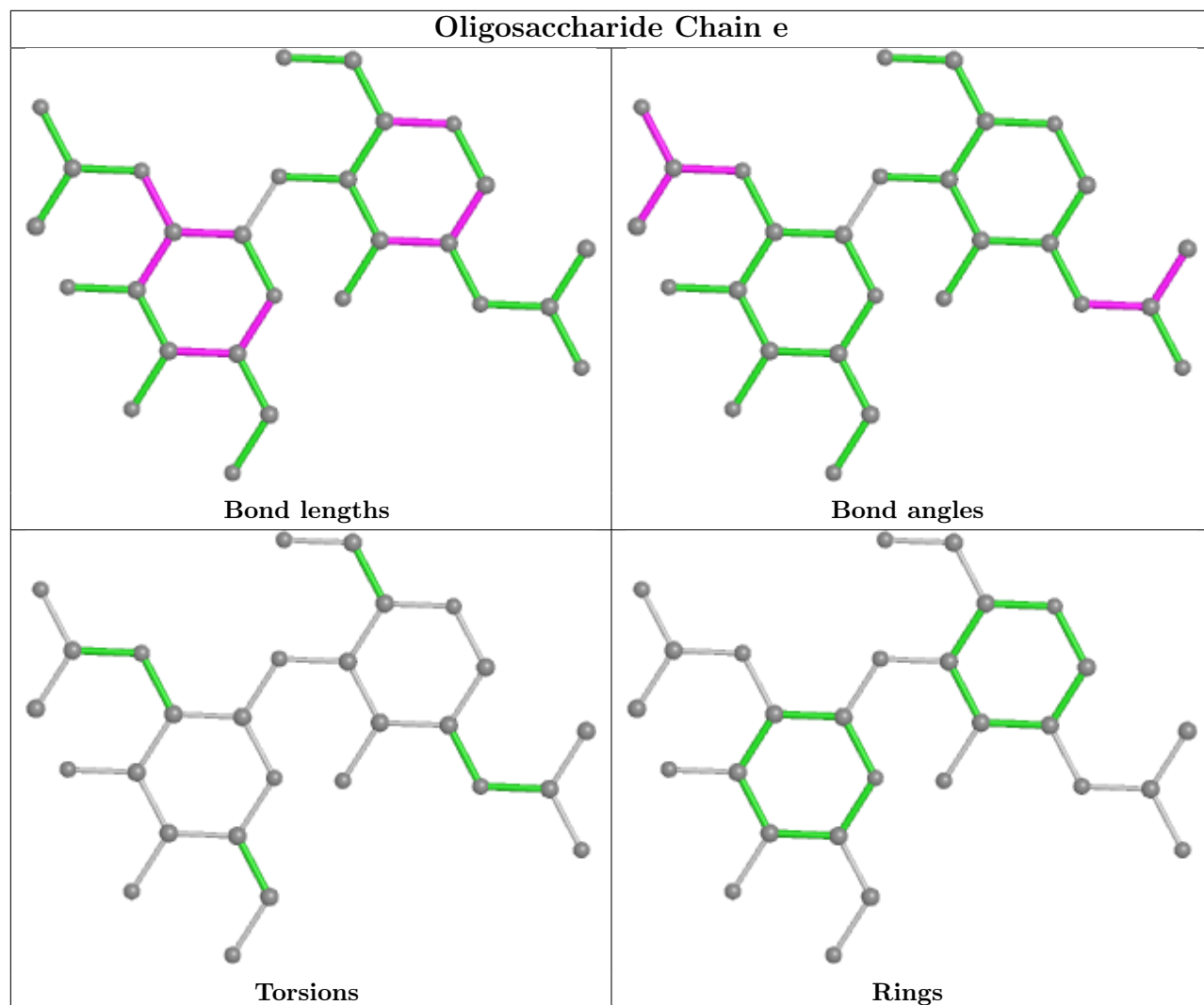


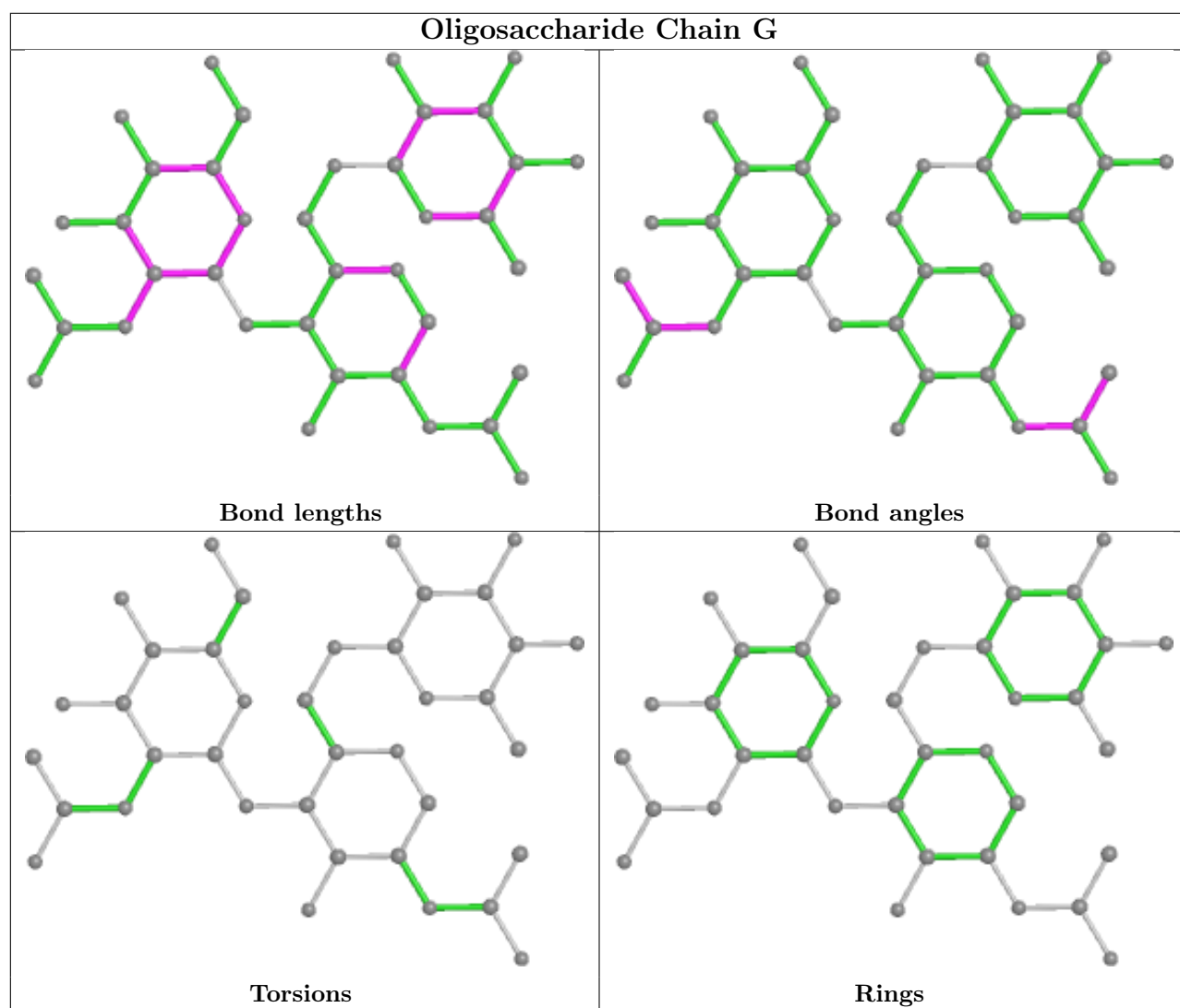


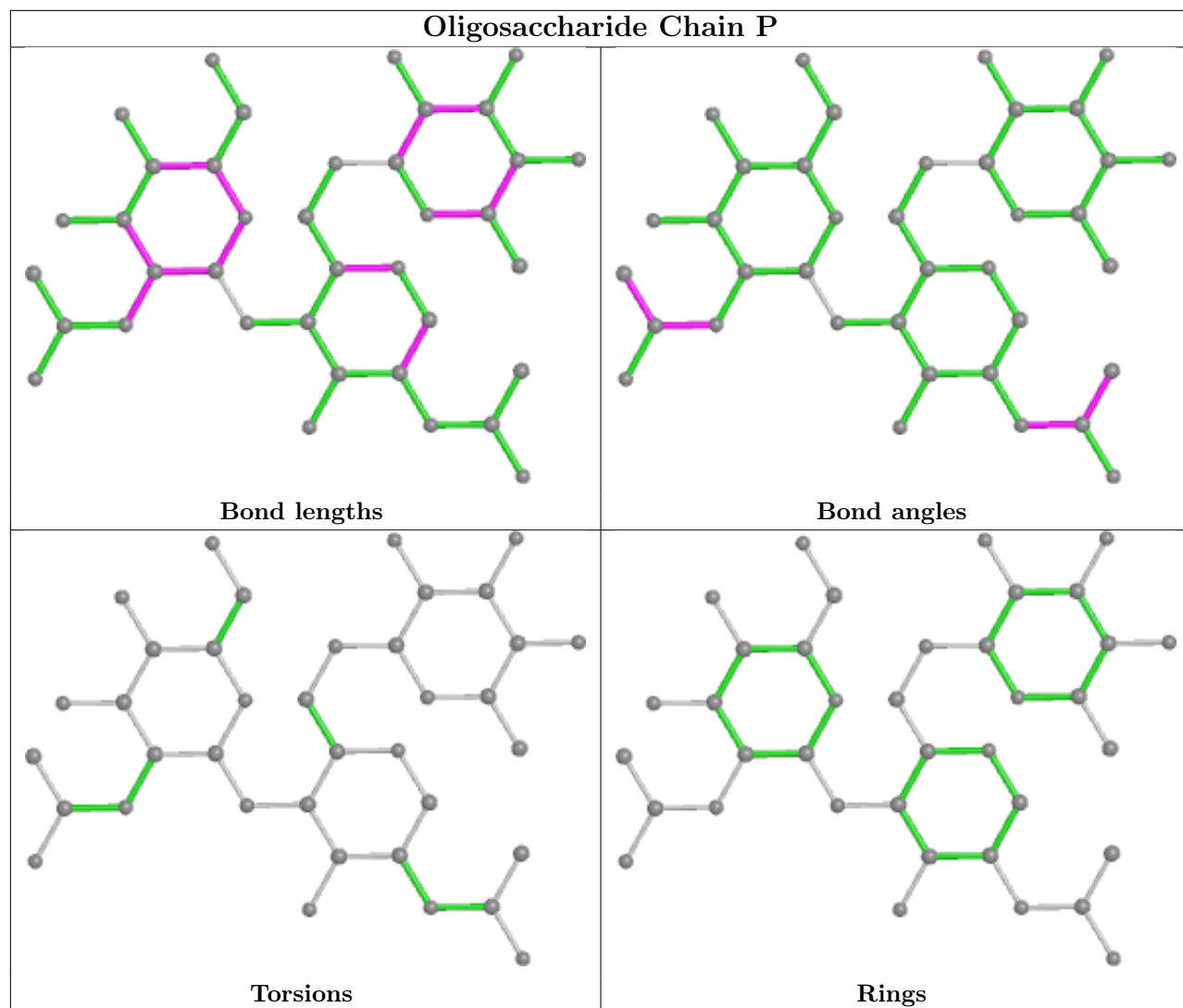


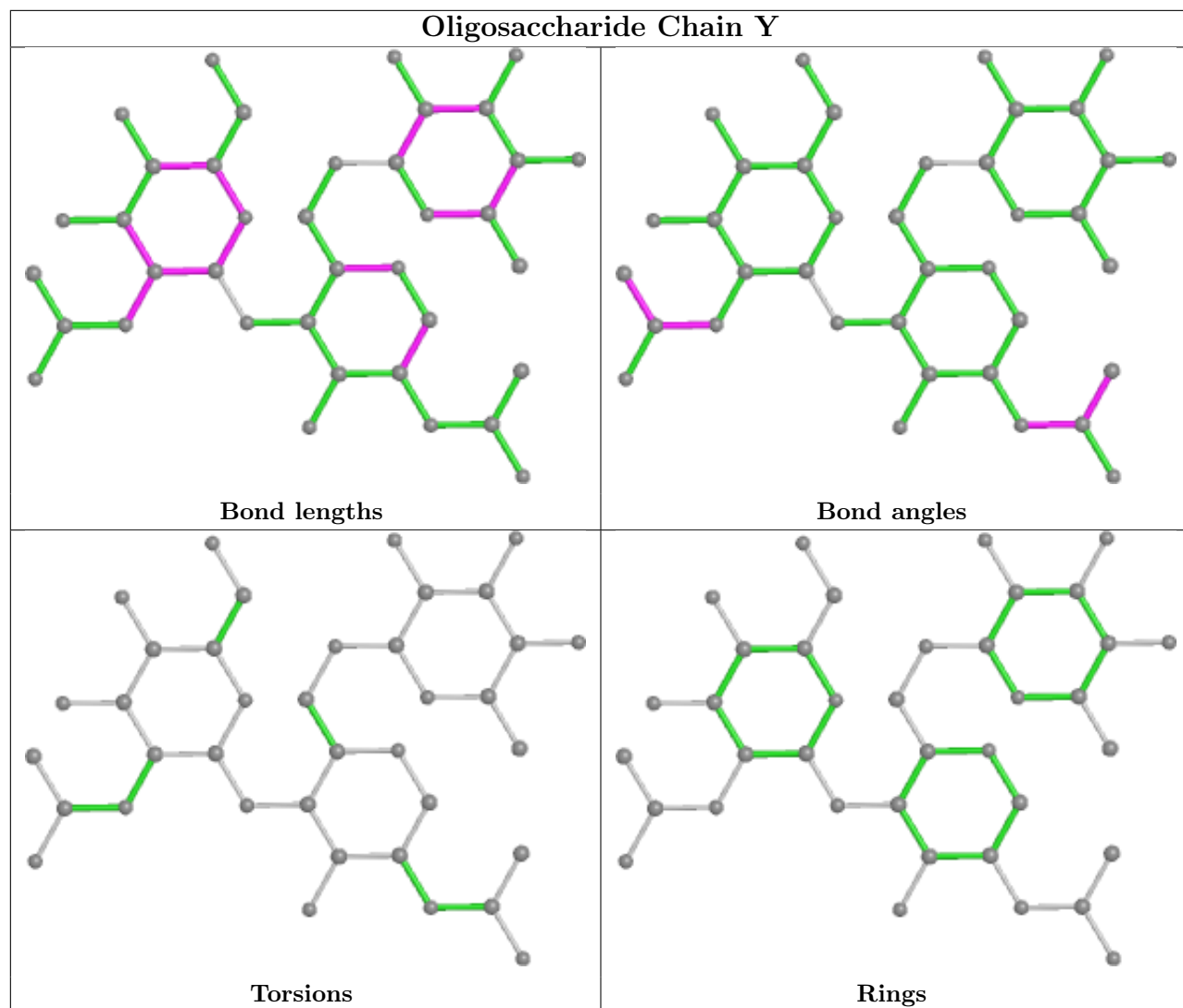


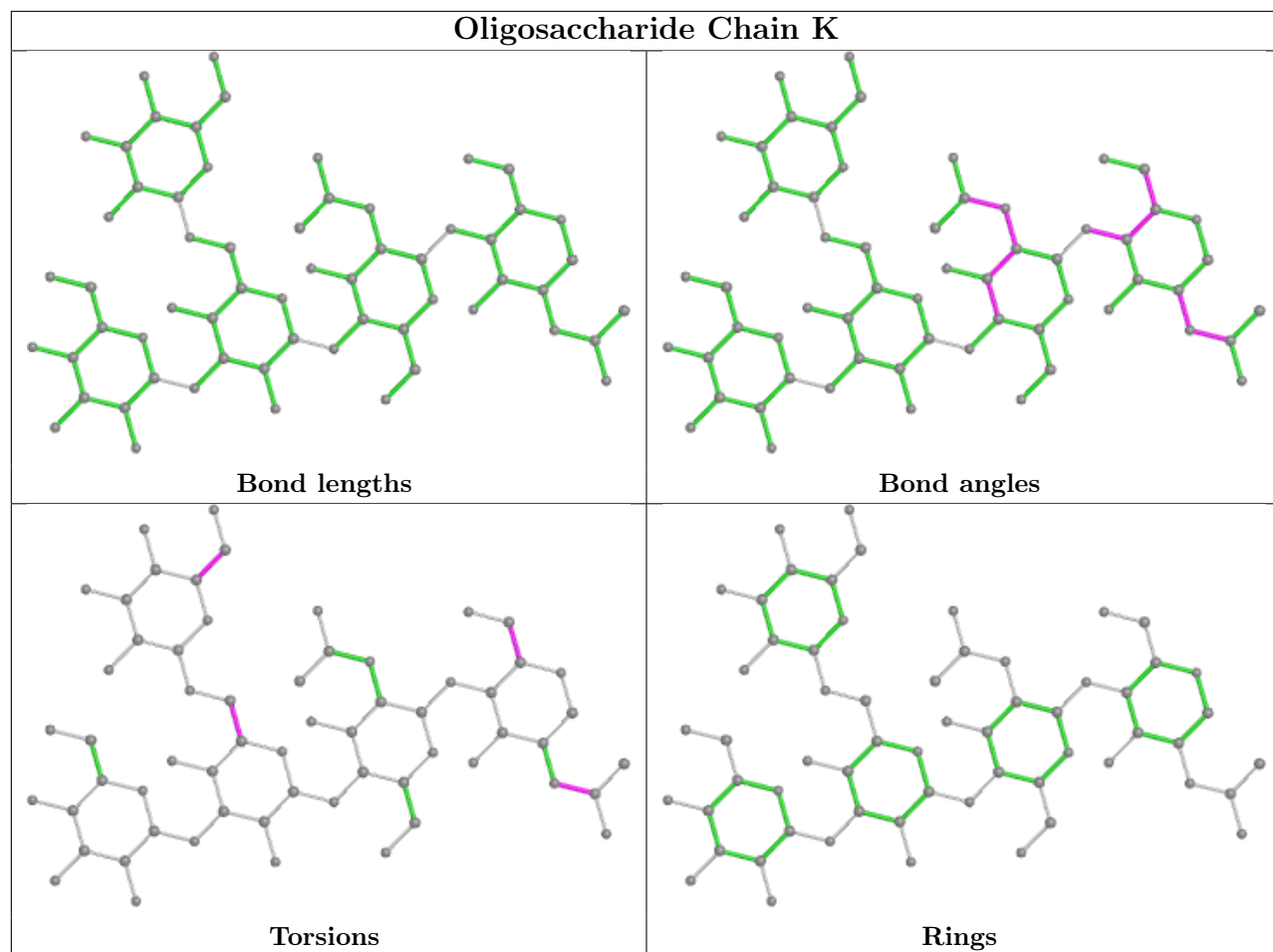


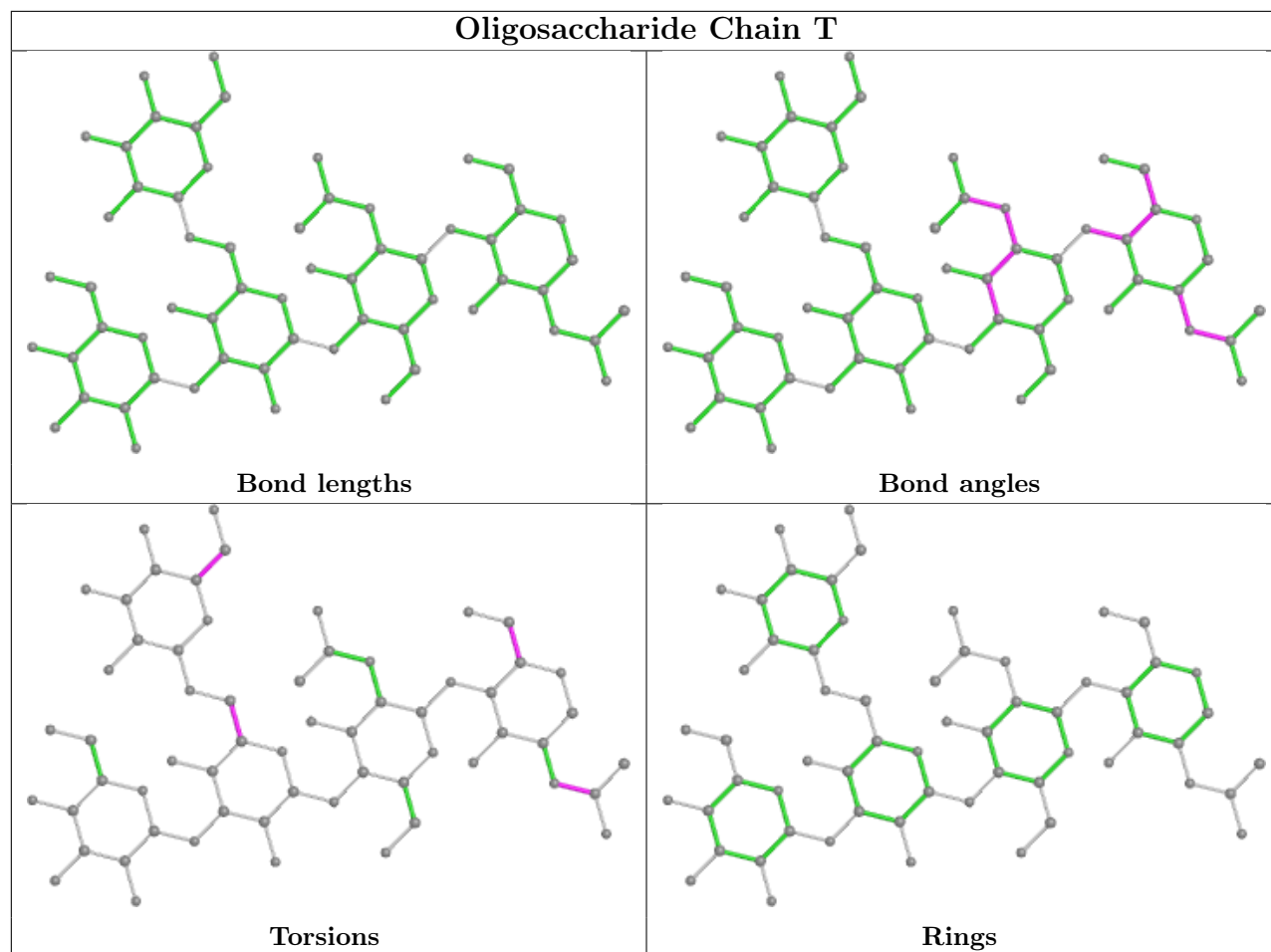


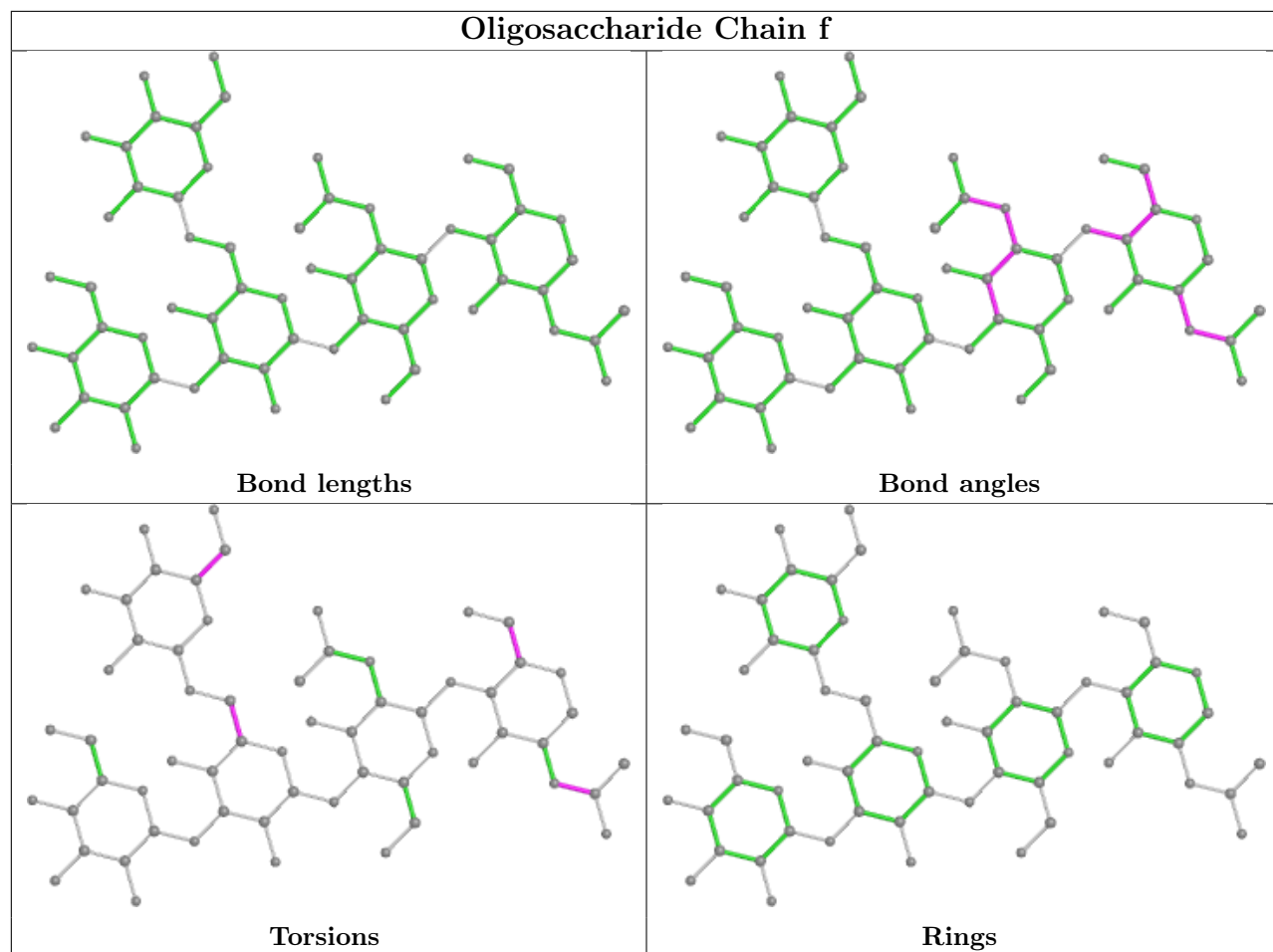


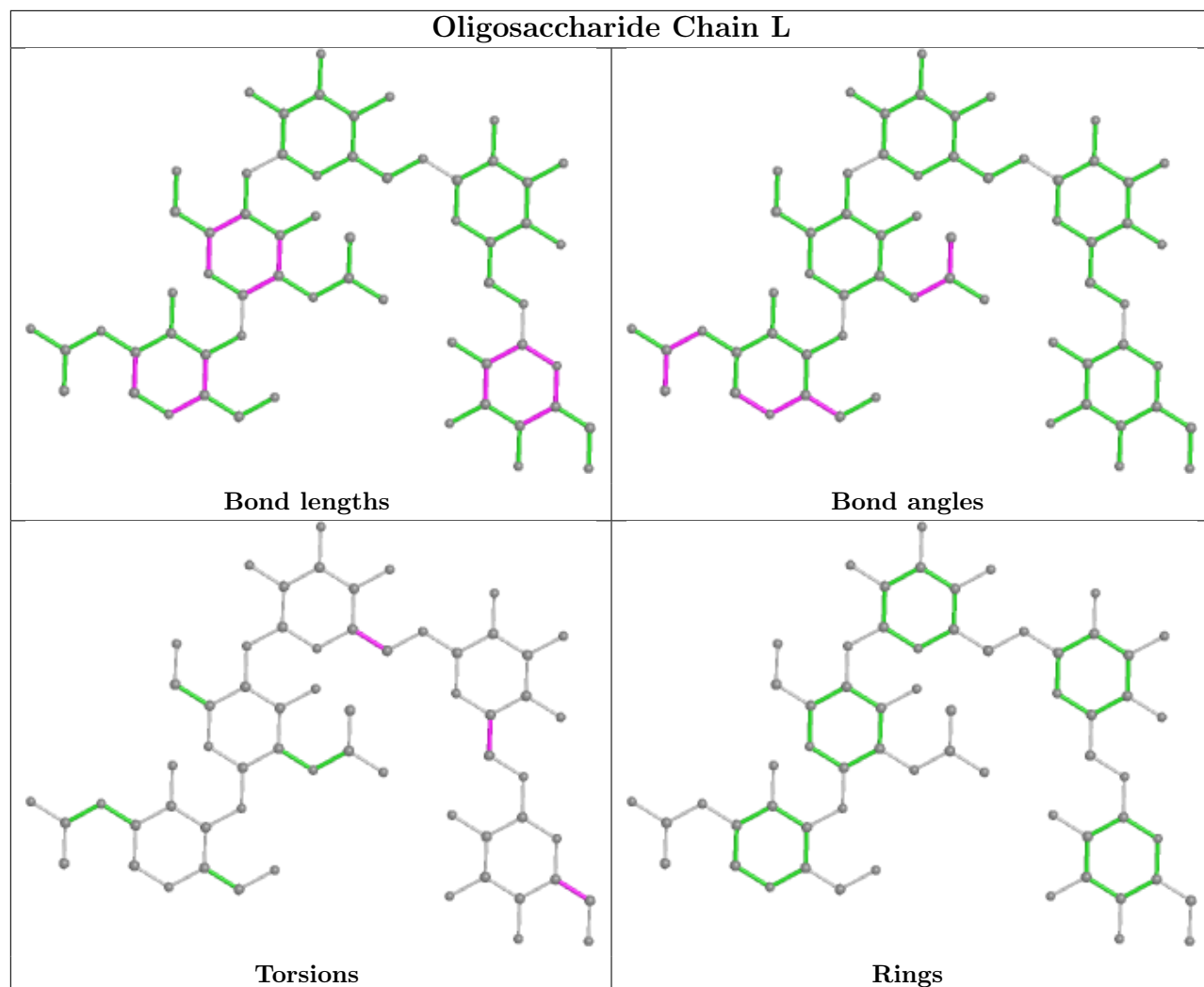




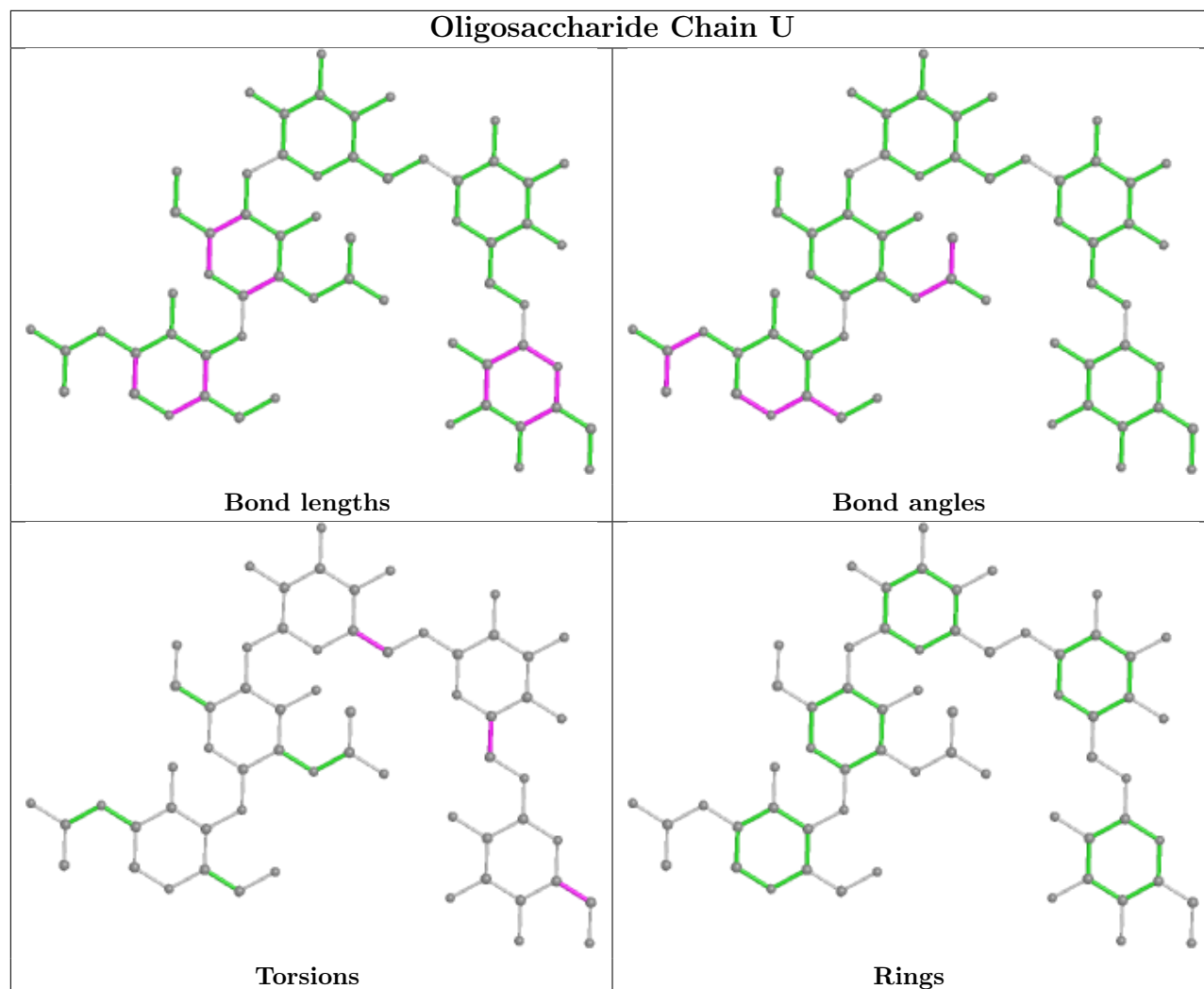


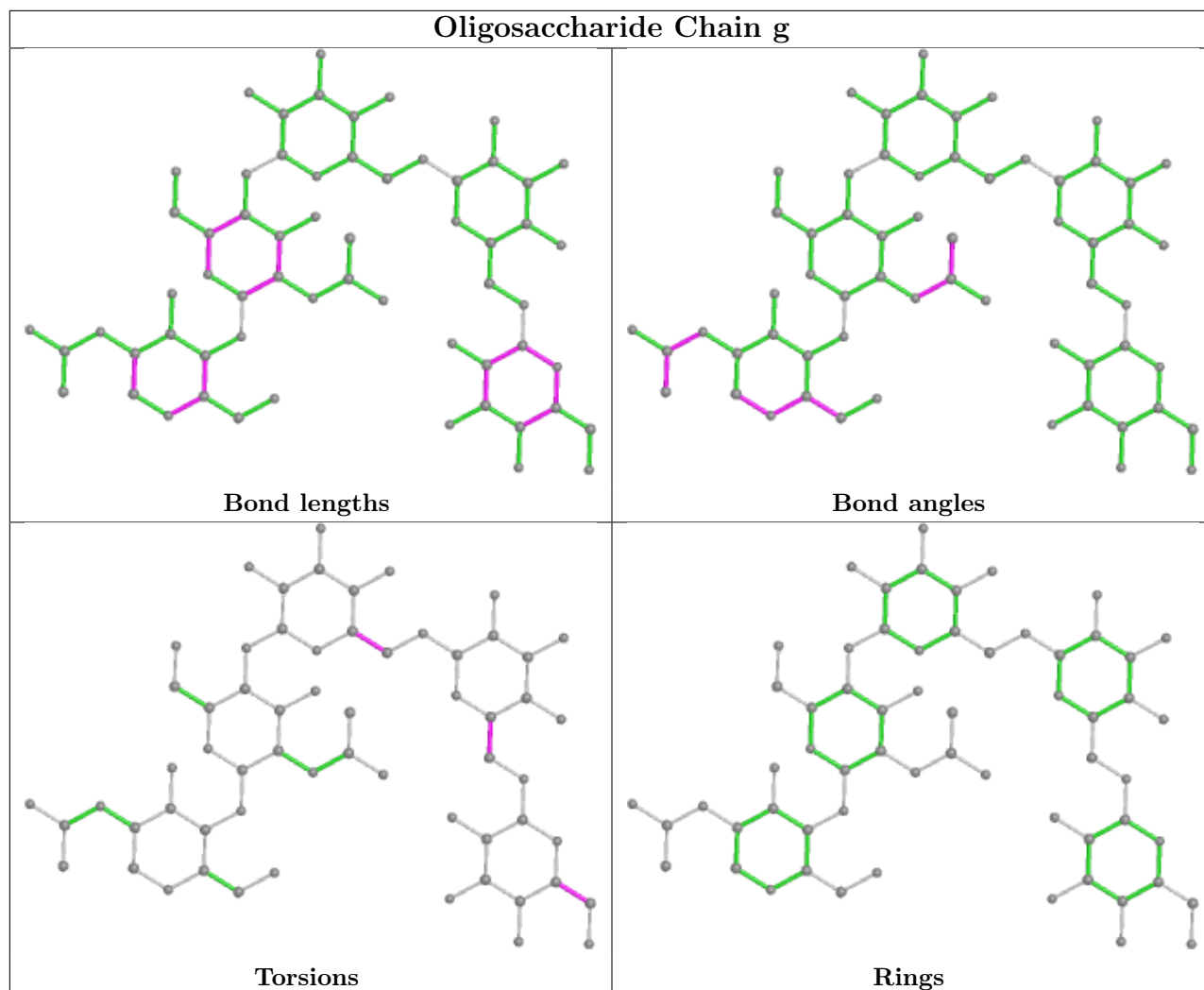












## 5.6 Ligand geometry [i](#)

6 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$
8	NAG	c	701	2	14,14,15	0.29	0	17,19,21	0.56	0
8	NAG	c	702	2	14,14,15	2.07	5 (35%)	17,19,21	0.92	1 (5%)
8	NAG	a	701	2	14,14,15	0.29	0	17,19,21	0.56	0
8	NAG	b	701	2	14,14,15	0.29	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	a	702	2	14,14,15	2.07	5 (35%)	17,19,21	0.92	1 (5%)
8	NAG	b	702	2	14,14,15	2.07	5 (35%)	17,19,21	0.91	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
8	NAG	c	701	2	-	4/6/23/26	0/1/1/1
8	NAG	c	702	2	-	1/6/23/26	0/1/1/1
8	NAG	a	701	2	-	4/6/23/26	0/1/1/1
8	NAG	b	701	2	-	4/6/23/26	0/1/1/1
8	NAG	a	702	2	-	1/6/23/26	0/1/1/1
8	NAG	b	702	2	-	1/6/23/26	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	702	NAG	C1-C2	5.05	1.59	1.52
8	c	702	NAG	C1-C2	5.04	1.59	1.52
8	b	702	NAG	C1-C2	5.03	1.59	1.52
8	c	702	NAG	O5-C5	3.22	1.50	1.43
8	a	702	NAG	O5-C5	3.20	1.49	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	c	702	NAG	C8-C7-N2	2.19	119.80	116.10
8	a	702	NAG	C8-C7-N2	2.17	119.78	116.10
8	b	702	NAG	C8-C7-N2	2.17	119.78	116.10

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	c	701	NAG	C3-C2-N2-C7
8	c	701	NAG	C8-C7-N2-C2
8	c	701	NAG	O7-C7-N2-C2
8	a	701	NAG	C3-C2-N2-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	a	701	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

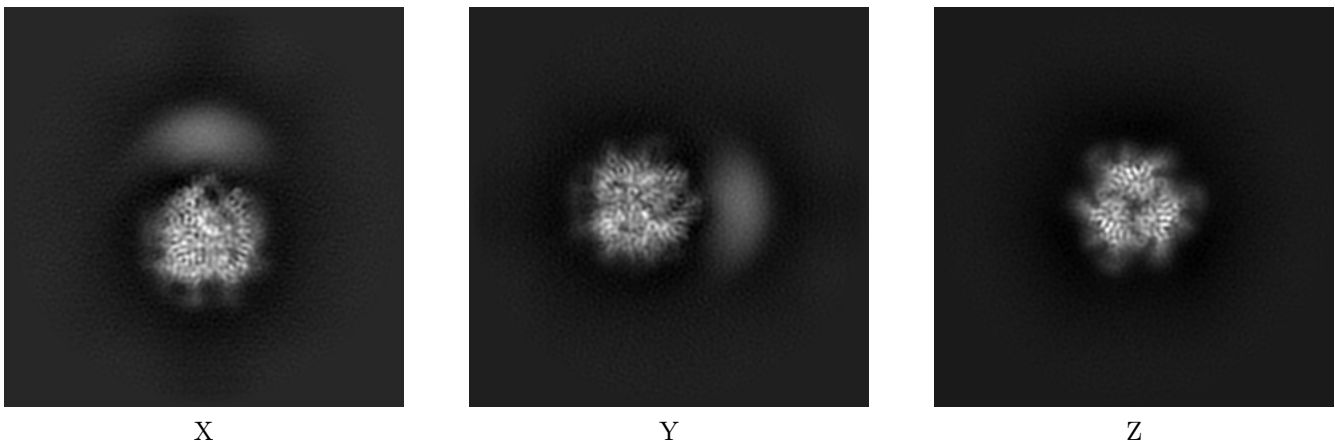
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28178. These allow visual inspection of the internal detail of the map and identification of artifacts.

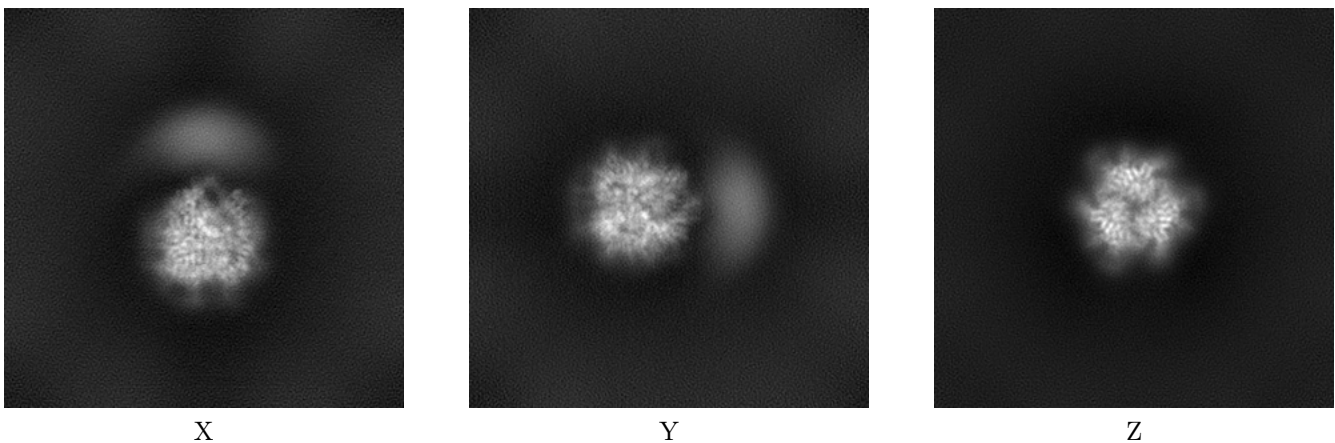
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



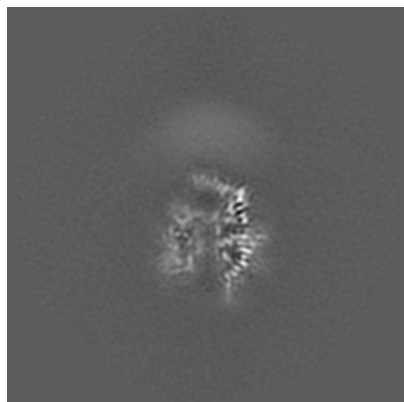
#### 6.1.2 Raw map



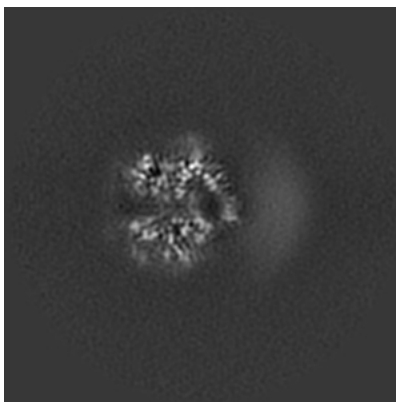
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

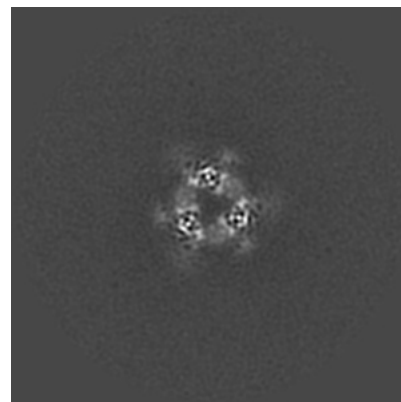
### 6.2.1 Primary map



X Index: 128

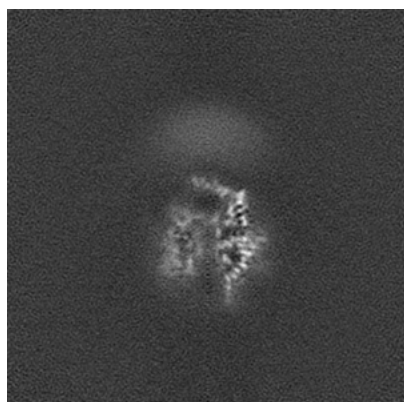


Y Index: 128

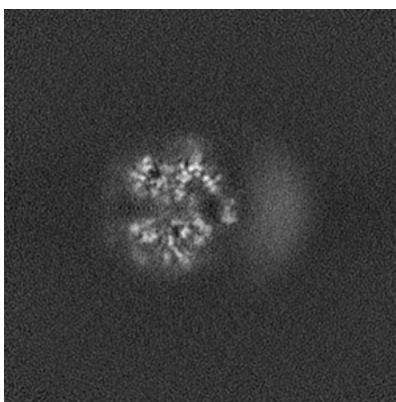


Z Index: 128

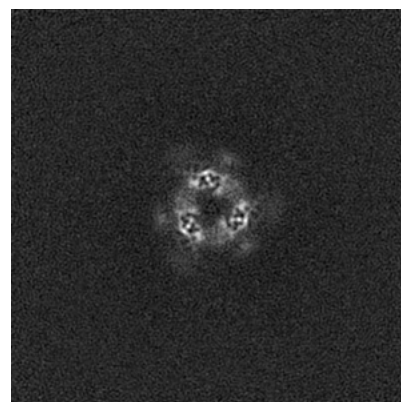
### 6.2.2 Raw map



X Index: 128



Y Index: 128

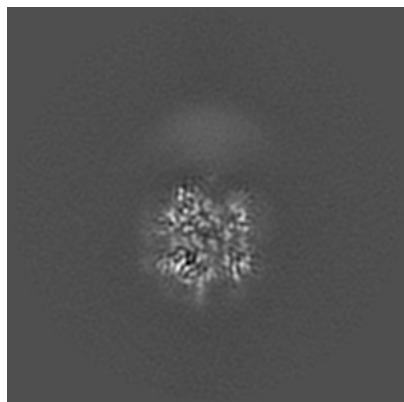


Z Index: 128

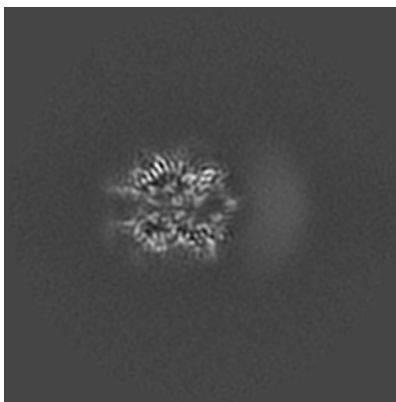
The images above show central slices of the map in three orthogonal directions.

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

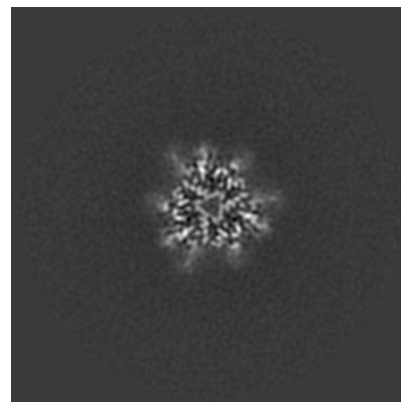
### 6.3.1 Primary map



X Index: 115

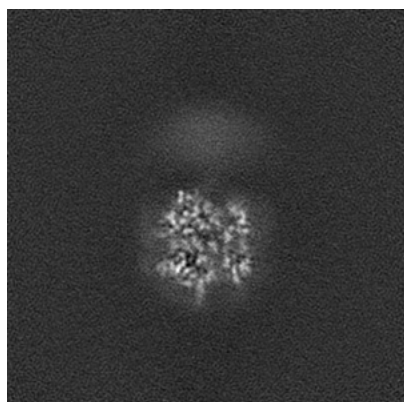


Y Index: 120

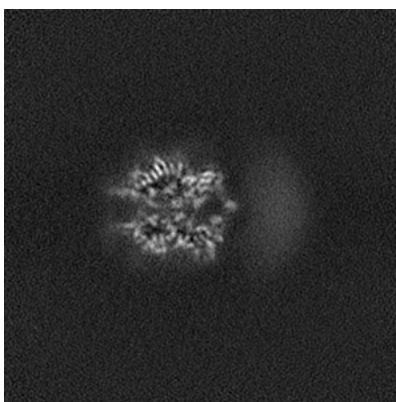


Z Index: 112

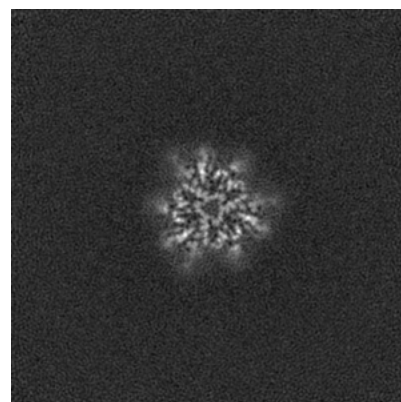
### 6.3.2 Raw map



X Index: 115



Y Index: 120

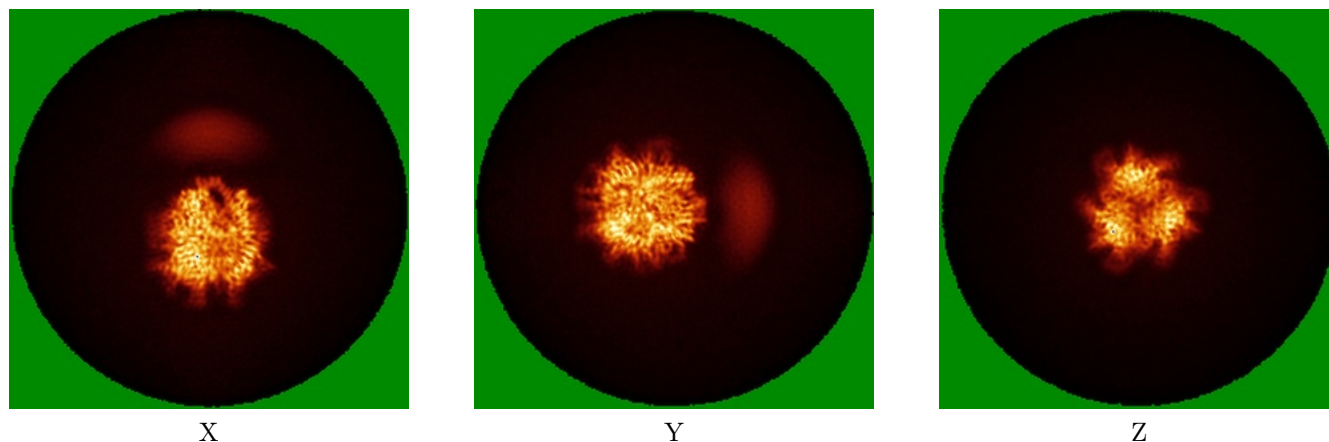


Z Index: 112

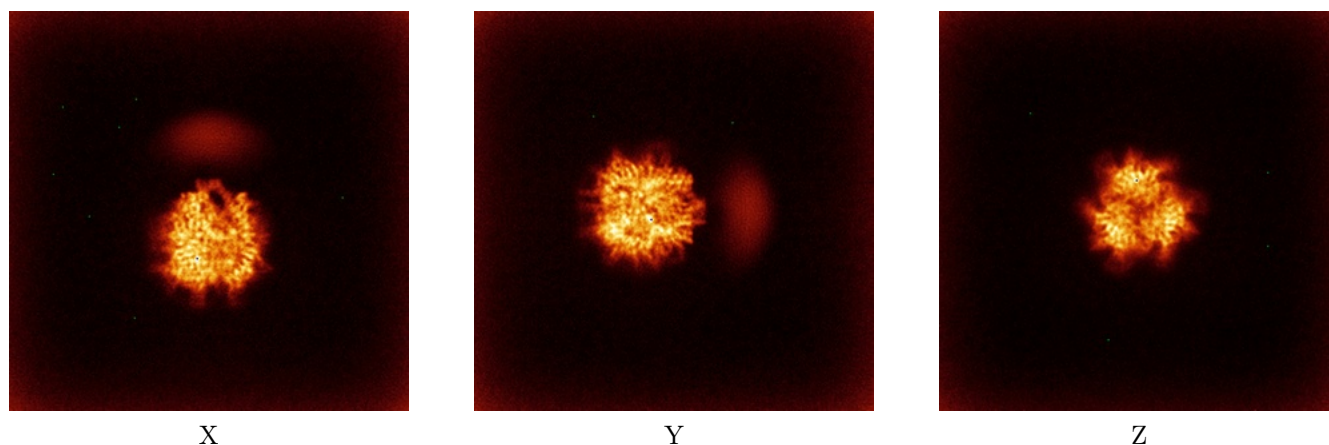
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map

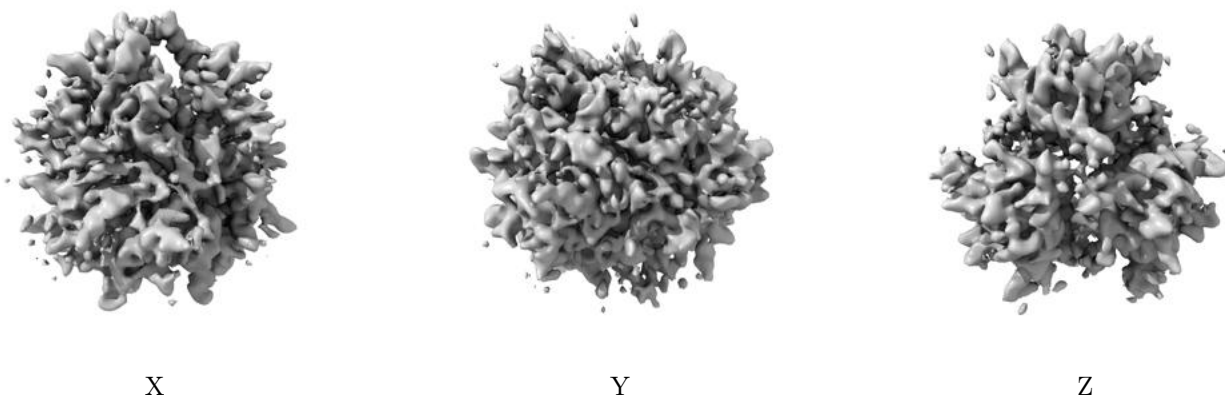


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



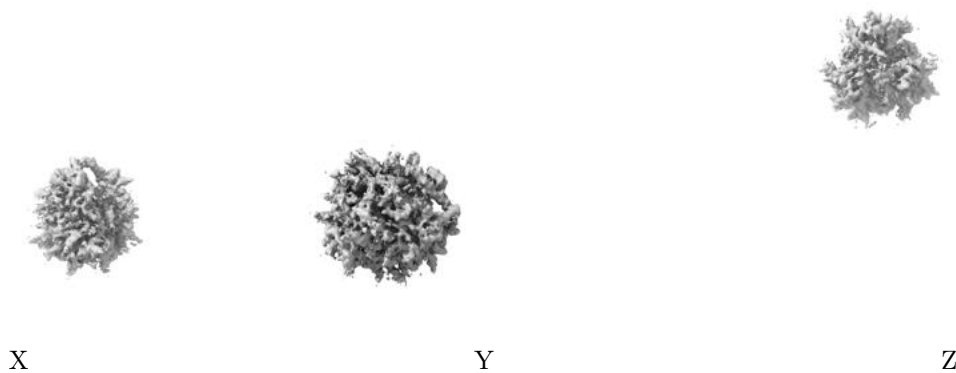
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

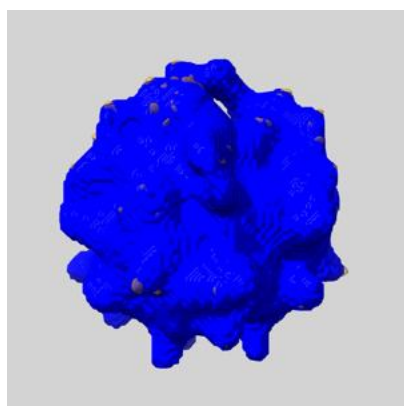
## 6.6 Mask visualisation [i](#)

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

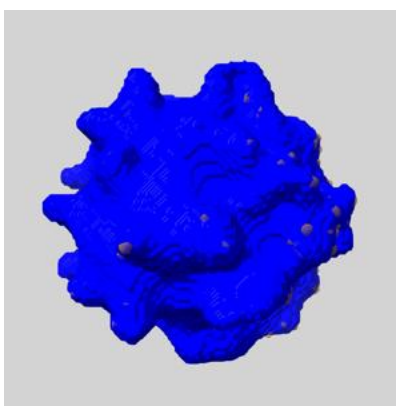
A mask typically either:

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

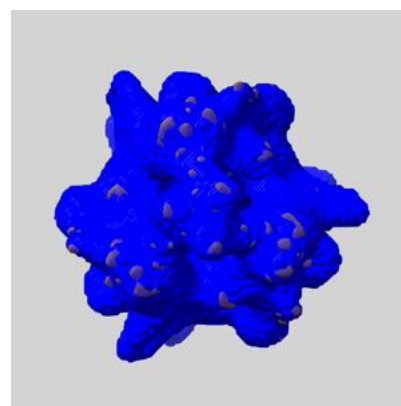
### 6.6.1 emd\_28178\_msk\_1.map [i](#)



X



Y

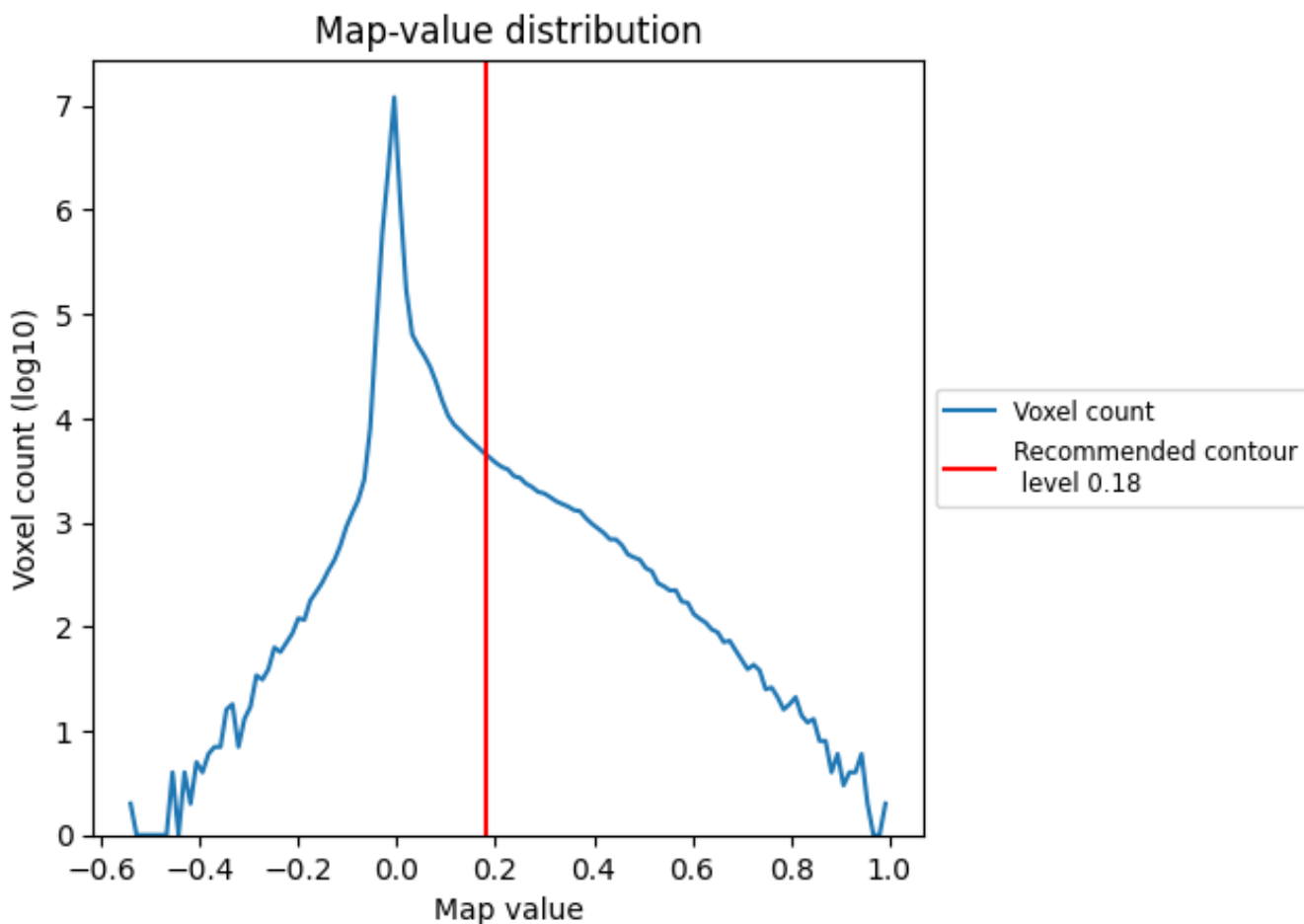


Z

## 7 Map analysis [i](#)

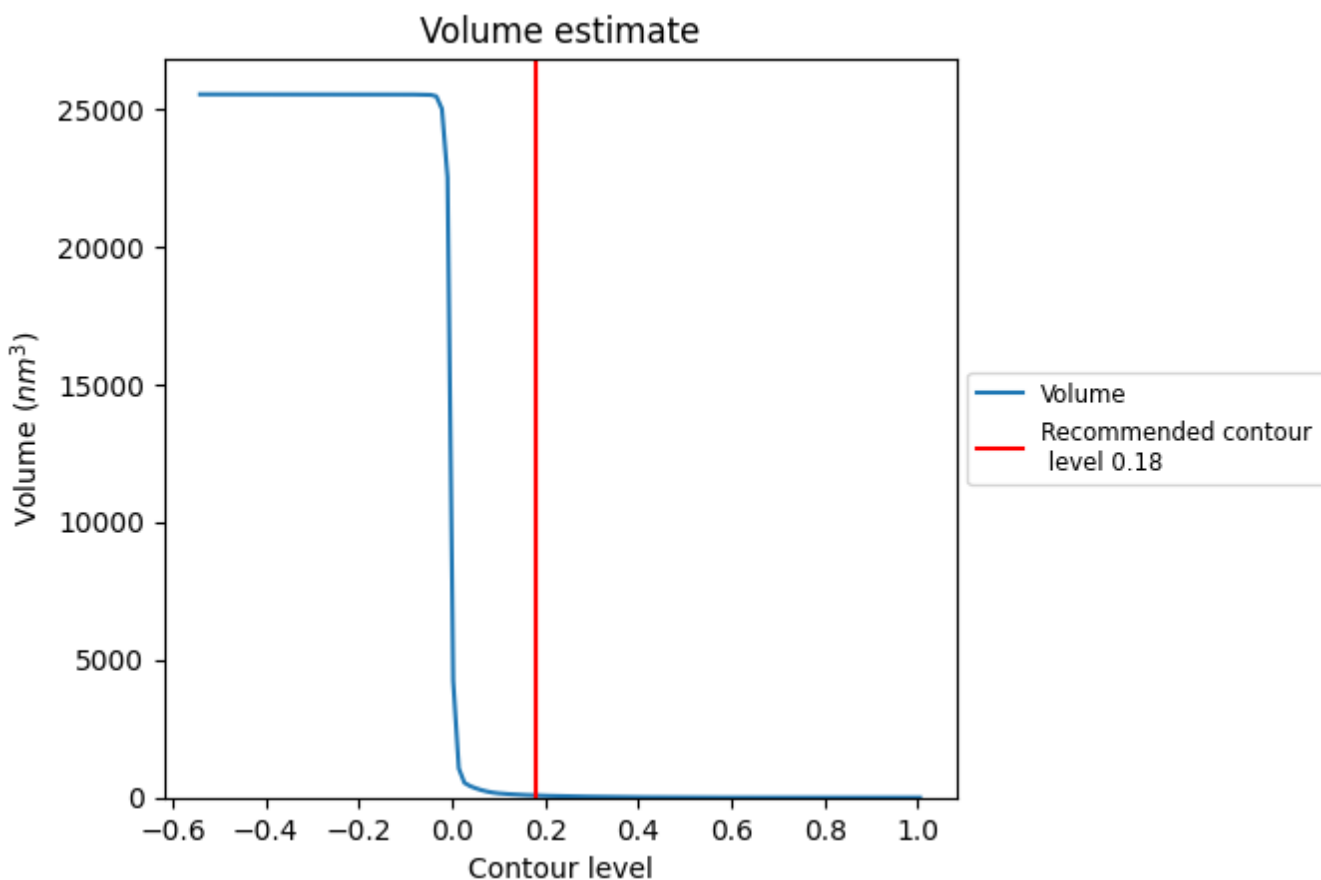
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

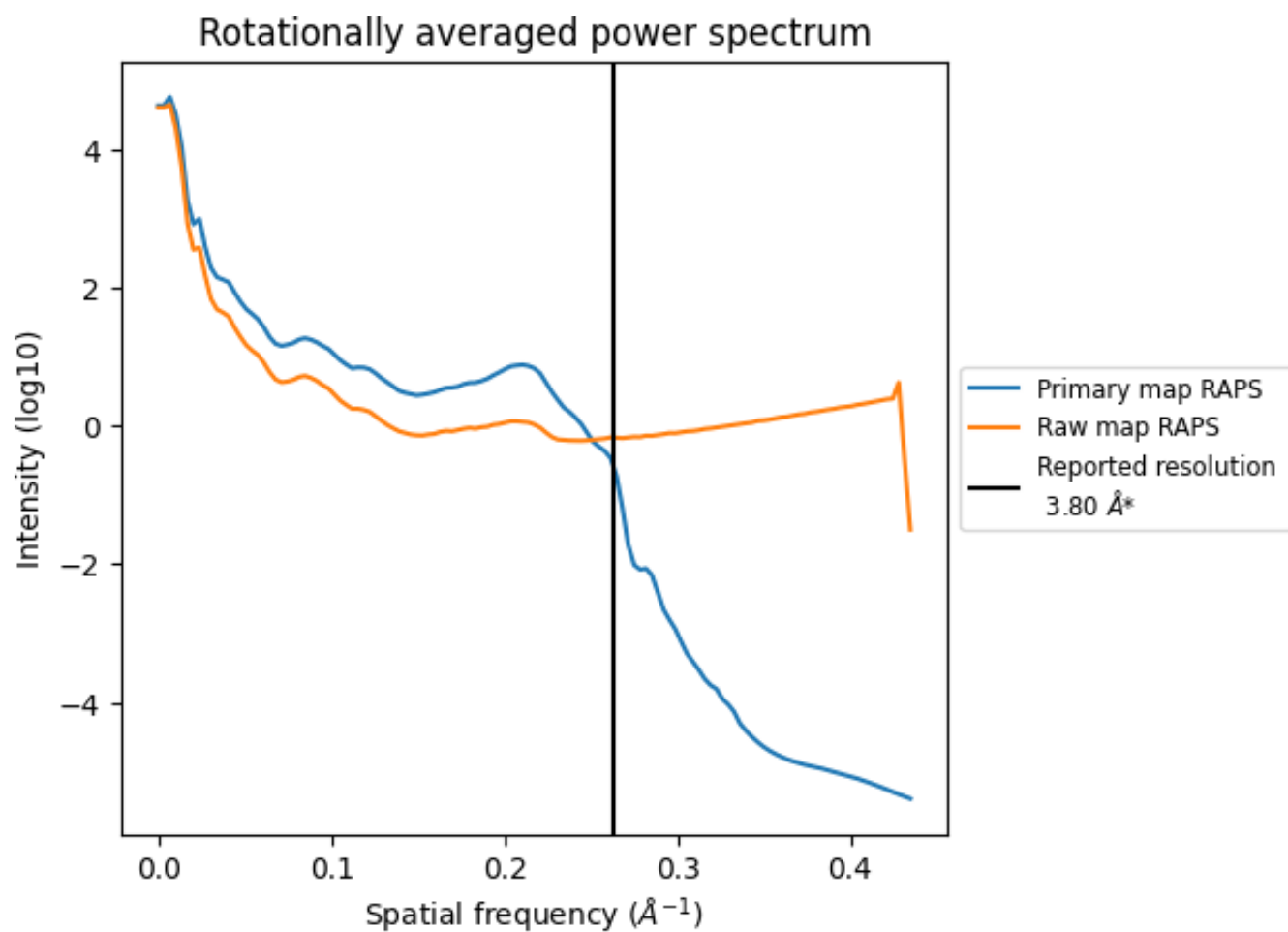
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 78 nm<sup>3</sup>; this corresponds to an approximate mass of 70 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

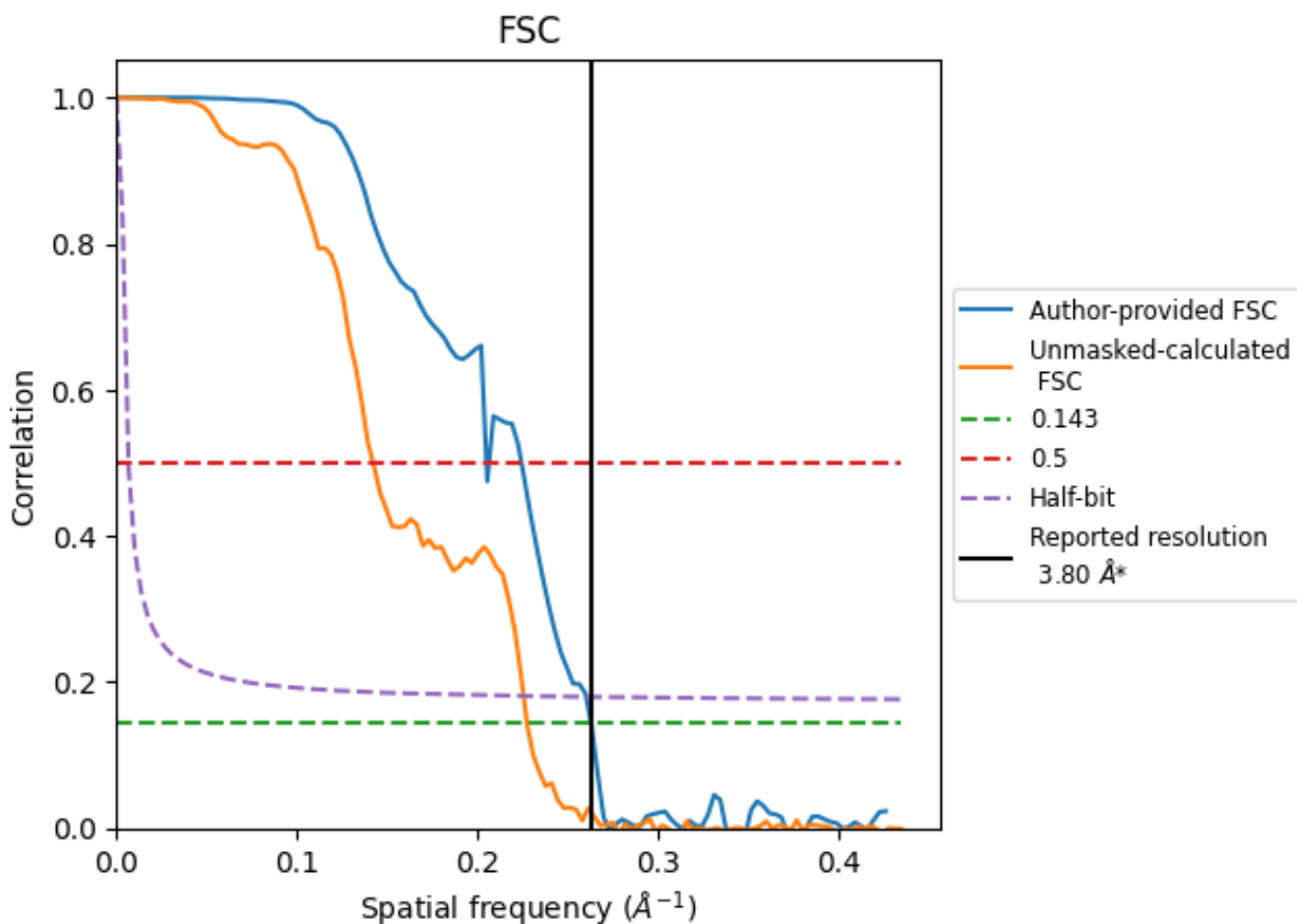


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

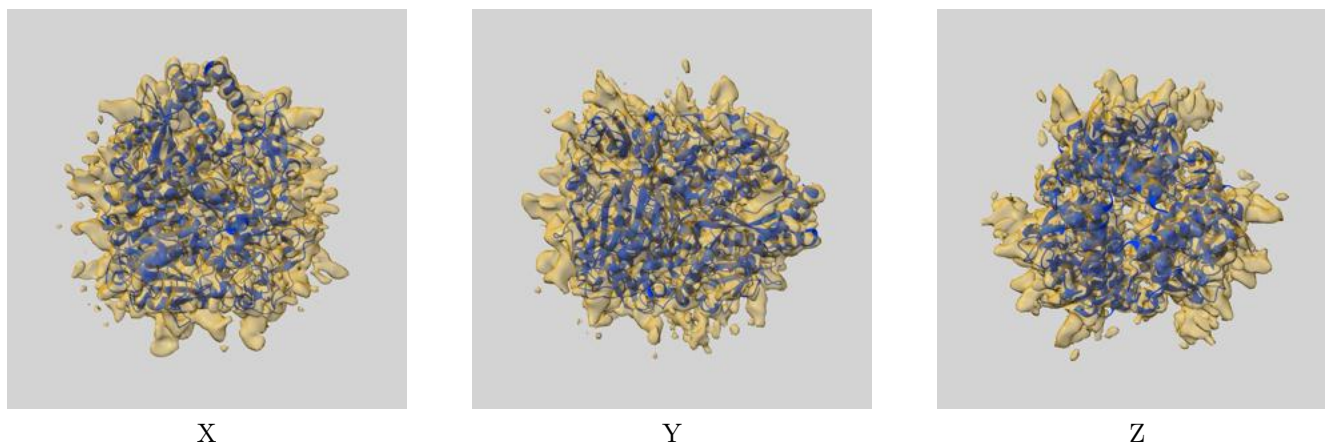
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.88	3.84
Unmasked-calculated*	4.40	7.03	4.43

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.40 differs from the reported value 3.8 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-28178 and PDB model 8EJD. Per-residue inclusion information can be found in section 3 on page 26.

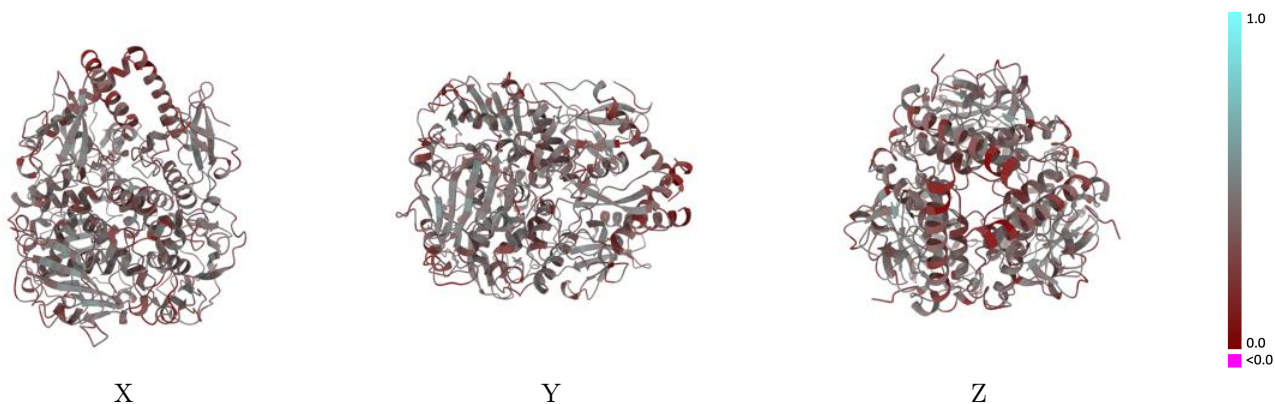
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

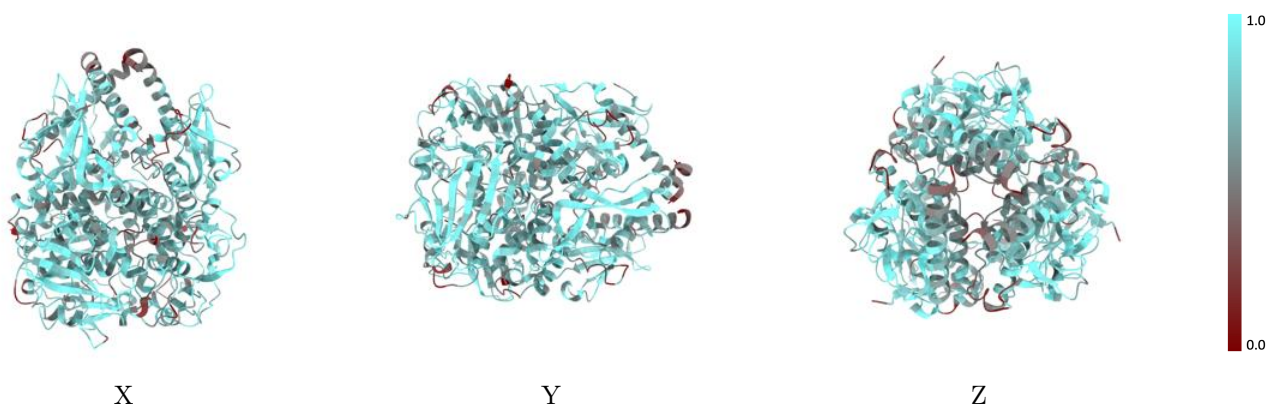


## 9.2 Q-score mapped to coordinate model [i](#)



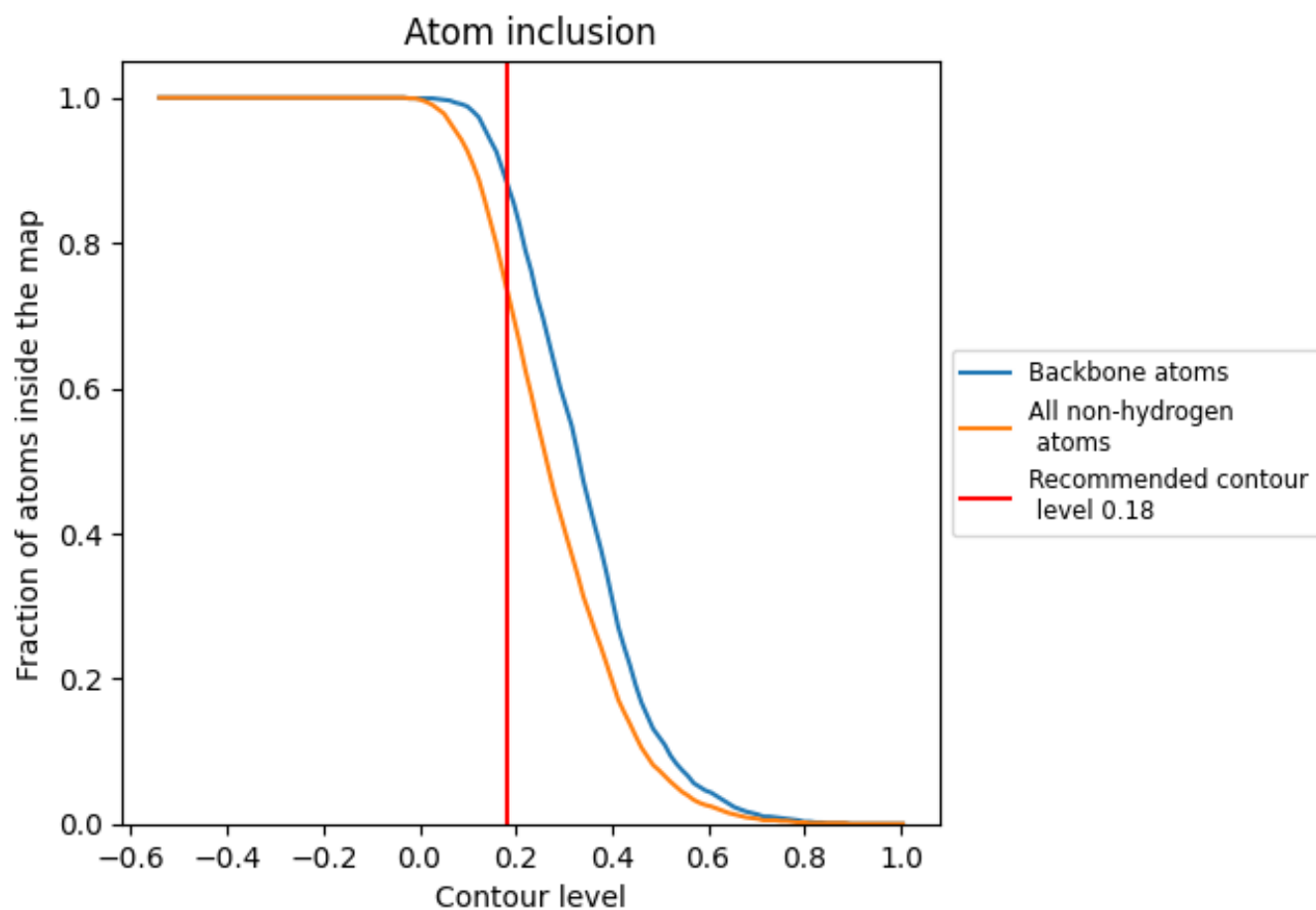
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).





































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 74% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7390	 0.3730
A	 0.7630	 0.3830
B	 0.7600	 0.3840
C	 0.7600	 0.3810
D	 0.8460	 0.3850
E	 0.7690	 0.3880
F	 0.6430	 0.3600
G	 0.7890	 0.3600
H	 0.7500	 0.3520
I	 0.7500	 0.4060
J	 0.6430	 0.3270
K	 0.9020	 0.4240
L	 0.4920	 0.3930
M	 0.8460	 0.3890
N	 0.7950	 0.3980
O	 0.6430	 0.3620
P	 0.7890	 0.3620
Q	 0.7500	 0.3560
R	 0.7500	 0.3820
S	 0.6430	 0.3310
T	 0.8850	 0.4070
U	 0.5080	 0.3930
V	 0.8460	 0.3920
W	 0.7950	 0.4040
X	 0.6430	 0.3580
Y	 0.7630	 0.3630
Z	 0.7500	 0.3660
a	 0.7160	 0.3610
b	 0.7140	 0.3600
c	 0.7150	 0.3590
d	 0.7500	 0.3960
e	 0.6430	 0.3270
f	 0.9020	 0.4150
g	 0.4920	 0.3910

