



# wwPDB EM Validation Summary Report ⓘ

Apr 15, 2025 – 10:37 am BST

PDB ID : 9F02 / pdb\_00009f02  
EMDB ID : EMD-50092  
Title : HIV-1 envelope glycoprotein (BG505 gp140 SOSIP.664) trimer in complex with three copies of ELC07 broadly neutralizing antibody.  
Authors : Hope, J.; Alguel, Y.; Nans, A.; Cherepanov, P.  
Deposited on : 2024-04-15  
Resolution : 3.02 Å (reported)  
Based on initial models : ., 8FR6

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.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

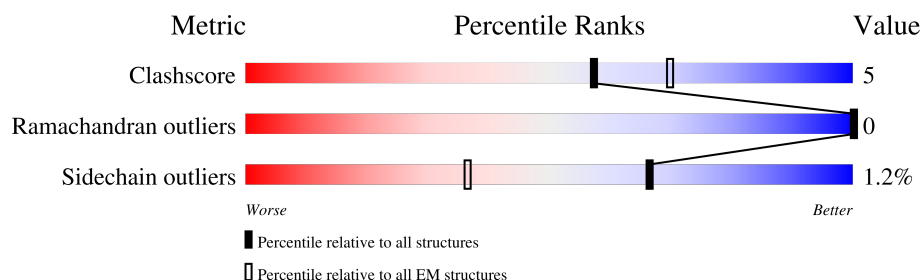
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.02 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	170	
1	E	170	
1	F	170	
2	C	516	
2	G	516	
2	N	516	
3	H	268	
3	I	268	

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Mol	Chain	Length	Quality of chain
3	K	268	
4	J	235	
4	L	235	
4	M	235	
5	d	4	
5	e	4	
5	g	4	
6	f	3	
6	h	3	
6	q	3	
7	B	2	
7	D	2	
7	O	2	
7	P	2	
7	Q	2	
7	R	2	
7	S	2	
7	T	2	
7	U	2	
7	V	2	
7	W	2	
7	X	2	
7	Y	2	
7	Z	2	
7	a	2	

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Mol	Chain	Length	Quality of chain
7	b	2	<div><div></div><div>50%</div><div></div><div></div><div>100%</div></div>
7	c	2	<div><div></div><div>50%</div><div></div><div></div><div>100%</div></div>
7	u	2	<div><div></div><div>50%</div><div></div><div></div><div>100%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24183 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 Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	112	Total	C	N	O	S	0	0
			882	557	154	165	6		
1	F	112	Total	C	N	O	S	0	0
			882	557	154	165	6		
1	E	112	Total	C	N	O	S	0	0
			882	557	154	165	6		

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	PRO	ILE	conflict	UNP Q2N0S8
A	605	CYS	THR	conflict	UNP Q2N0S8
A	665	GLY	-	expression tag	UNP Q2N0S8
A	666	SER	-	expression tag	UNP Q2N0S8
A	667	GLY	-	expression tag	UNP Q2N0S8
A	668	LEU	-	expression tag	UNP Q2N0S8
A	669	ASN	-	expression tag	UNP Q2N0S8
A	670	ASP	-	expression tag	UNP Q2N0S8
A	671	ILE	-	expression tag	UNP Q2N0S8
A	672	PHE	-	expression tag	UNP Q2N0S8
A	673	GLU	-	expression tag	UNP Q2N0S8
A	674	ALA	-	expression tag	UNP Q2N0S8
A	675	GLN	-	expression tag	UNP Q2N0S8
A	676	LYS	-	expression tag	UNP Q2N0S8
A	677	ILE	-	expression tag	UNP Q2N0S8
A	678	GLU	-	expression tag	UNP Q2N0S8
A	679	TRP	-	expression tag	UNP Q2N0S8
A	680	HIS	-	expression tag	UNP Q2N0S8
A	681	GLU	-	expression tag	UNP Q2N0S8
F	559	PRO	ILE	conflict	UNP Q2N0S8
F	605	CYS	THR	conflict	UNP Q2N0S8
F	665	GLY	-	expression tag	UNP Q2N0S8
F	666	SER	-	expression tag	UNP Q2N0S8
F	667	GLY	-	expression tag	UNP Q2N0S8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	668	LEU	-	expression tag	UNP Q2N0S8
F	669	ASN	-	expression tag	UNP Q2N0S8
F	670	ASP	-	expression tag	UNP Q2N0S8
F	671	ILE	-	expression tag	UNP Q2N0S8
F	672	PHE	-	expression tag	UNP Q2N0S8
F	673	GLU	-	expression tag	UNP Q2N0S8
F	674	ALA	-	expression tag	UNP Q2N0S8
F	675	GLN	-	expression tag	UNP Q2N0S8
F	676	LYS	-	expression tag	UNP Q2N0S8
F	677	ILE	-	expression tag	UNP Q2N0S8
F	678	GLU	-	expression tag	UNP Q2N0S8
F	679	TRP	-	expression tag	UNP Q2N0S8
F	680	HIS	-	expression tag	UNP Q2N0S8
F	681	GLU	-	expression tag	UNP Q2N0S8
E	559	PRO	ILE	conflict	UNP Q2N0S8
E	605	CYS	THR	conflict	UNP Q2N0S8
E	665	GLY	-	expression tag	UNP Q2N0S8
E	666	SER	-	expression tag	UNP Q2N0S8
E	667	GLY	-	expression tag	UNP Q2N0S8
E	668	LEU	-	expression tag	UNP Q2N0S8
E	669	ASN	-	expression tag	UNP Q2N0S8
E	670	ASP	-	expression tag	UNP Q2N0S8
E	671	ILE	-	expression tag	UNP Q2N0S8
E	672	PHE	-	expression tag	UNP Q2N0S8
E	673	GLU	-	expression tag	UNP Q2N0S8
E	674	ALA	-	expression tag	UNP Q2N0S8
E	675	GLN	-	expression tag	UNP Q2N0S8
E	676	LYS	-	expression tag	UNP Q2N0S8
E	677	ILE	-	expression tag	UNP Q2N0S8
E	678	GLU	-	expression tag	UNP Q2N0S8
E	679	TRP	-	expression tag	UNP Q2N0S8
E	680	HIS	-	expression tag	UNP Q2N0S8
E	681	GLU	-	expression tag	UNP Q2N0S8

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	442	Total	C	N	O	S	0	0
			3470	2180	613	649	28		
2	G	442	Total	C	N	O	S	0	0
			3470	2180	613	649	28		
2	N	442	Total	C	N	O	S	0	0
			3470	2180	613	649	28		

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	MET	-	initiating methionine	UNP Q2N0S8
C	-3	ASP	-	expression tag	UNP Q2N0S8
C	-2	ALA	-	expression tag	UNP Q2N0S8
C	-1	MET	-	expression tag	UNP Q2N0S8
C	0	LYS	-	expression tag	UNP Q2N0S8
C	1	ARG	-	expression tag	UNP Q2N0S8
C	2	GLY	-	expression tag	UNP Q2N0S8
C	3	LEU	-	expression tag	UNP Q2N0S8
C	4	CYS	-	expression tag	UNP Q2N0S8
C	5	CYS	-	expression tag	UNP Q2N0S8
C	6	VAL	-	expression tag	UNP Q2N0S8
C	7	LEU	-	expression tag	UNP Q2N0S8
C	8	LEU	-	expression tag	UNP Q2N0S8
C	9	LEU	-	expression tag	UNP Q2N0S8
C	10	CYS	-	expression tag	UNP Q2N0S8
C	11	GLY	-	expression tag	UNP Q2N0S8
C	12	ALA	-	expression tag	UNP Q2N0S8
C	13	VAL	-	expression tag	UNP Q2N0S8
C	14	PHE	-	expression tag	UNP Q2N0S8
C	15	VAL	-	expression tag	UNP Q2N0S8
C	16	SER	-	expression tag	UNP Q2N0S8
C	17	PRO	-	expression tag	UNP Q2N0S8
C	18	SER	-	expression tag	UNP Q2N0S8
C	19	GLN	-	expression tag	UNP Q2N0S8
C	20	GLU	-	expression tag	UNP Q2N0S8
C	21	ILE	-	expression tag	UNP Q2N0S8
C	22	HIS	-	expression tag	UNP Q2N0S8
C	23	ALA	-	expression tag	UNP Q2N0S8
C	24	ARG	-	expression tag	UNP Q2N0S8
C	25	PHE	-	expression tag	UNP Q2N0S8
C	26	ARG	-	expression tag	UNP Q2N0S8
C	27	ARG	-	expression tag	UNP Q2N0S8
C	28	GLY	-	expression tag	UNP Q2N0S8
C	29	ALA	-	expression tag	UNP Q2N0S8
C	30	ARG	-	expression tag	UNP Q2N0S8
C	62	GLU	LYS	variant	UNP Q2N0S8
C	99	ASN	SER	variant	UNP Q2N0S8
C	117	LYS	GLU	variant	UNP Q2N0S8
C	?	-	ASN	deletion	UNP Q2N0S8
C	?	-	VAL	deletion	UNP Q2N0S8
C	134	VAL	THR	variant	UNP Q2N0S8
C	135	THR	ASN	variant	UNP Q2N0S8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	136	ASN	ALA	variant	UNP Q2N0S8
C	185F	ARG	SER	variant	UNP Q2N0S8
C	185H	ASN	LYS	variant	UNP Q2N0S8
C	185I	ASN	SER	variant	UNP Q2N0S8
C	234	ASN	THR	variant	UNP Q2N0S8
C	240	PRO	SER	variant	UNP Q2N0S8
C	241	SER	ASN	variant	UNP Q2N0S8
C	308	ARG	HIS	variant	UNP Q2N0S8
C	325	ASP	ASN	variant	UNP Q2N0S8
C	330	HIS	GLN	variant	UNP Q2N0S8
C	332	ASN	THR	variant	UNP Q2N0S8
C	343	GLY	GLU	variant	UNP Q2N0S8
C	351	LYS	GLU	variant	UNP Q2N0S8
C	358	ILE	THR	variant	UNP Q2N0S8
C	360	ARG	ILE	variant	UNP Q2N0S8
C	363	ASN	SER	variant	UNP Q2N0S8
C	409	GLY	GLU	variant	UNP Q2N0S8
C	411	ASN	SER	variant	UNP Q2N0S8
C	413	SER	THR	variant	UNP Q2N0S8
C	461	THR	ASN	variant	UNP Q2N0S8
C	465	THR	ASN	variant	UNP Q2N0S8
C	501	CYS	ALA	conflict	UNP Q2N0S8
C	509	ARG	GLU	conflict	UNP Q2N0S8
C	510	ARG	LYS	conflict	UNP Q2N0S8
C	512	ARG	ALA	conflict	UNP Q2N0S8
C	513	ARG	VAL	conflict	UNP Q2N0S8
G	-4	MET	-	initiating methionine	UNP Q2N0S8
G	-3	ASP	-	expression tag	UNP Q2N0S8
G	-2	ALA	-	expression tag	UNP Q2N0S8
G	-1	MET	-	expression tag	UNP Q2N0S8
G	0	LYS	-	expression tag	UNP Q2N0S8
G	1	ARG	-	expression tag	UNP Q2N0S8
G	2	GLY	-	expression tag	UNP Q2N0S8
G	3	LEU	-	expression tag	UNP Q2N0S8
G	4	CYS	-	expression tag	UNP Q2N0S8
G	5	CYS	-	expression tag	UNP Q2N0S8
G	6	VAL	-	expression tag	UNP Q2N0S8
G	7	LEU	-	expression tag	UNP Q2N0S8
G	8	LEU	-	expression tag	UNP Q2N0S8
G	9	LEU	-	expression tag	UNP Q2N0S8
G	10	CYS	-	expression tag	UNP Q2N0S8
G	11	GLY	-	expression tag	UNP Q2N0S8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	12	ALA	-	expression tag	UNP Q2N0S8
G	13	VAL	-	expression tag	UNP Q2N0S8
G	14	PHE	-	expression tag	UNP Q2N0S8
G	15	VAL	-	expression tag	UNP Q2N0S8
G	16	SER	-	expression tag	UNP Q2N0S8
G	17	PRO	-	expression tag	UNP Q2N0S8
G	18	SER	-	expression tag	UNP Q2N0S8
G	19	GLN	-	expression tag	UNP Q2N0S8
G	20	GLU	-	expression tag	UNP Q2N0S8
G	21	ILE	-	expression tag	UNP Q2N0S8
G	22	HIS	-	expression tag	UNP Q2N0S8
G	23	ALA	-	expression tag	UNP Q2N0S8
G	24	ARG	-	expression tag	UNP Q2N0S8
G	25	PHE	-	expression tag	UNP Q2N0S8
G	26	ARG	-	expression tag	UNP Q2N0S8
G	27	ARG	-	expression tag	UNP Q2N0S8
G	28	GLY	-	expression tag	UNP Q2N0S8
G	29	ALA	-	expression tag	UNP Q2N0S8
G	30	ARG	-	expression tag	UNP Q2N0S8
G	62	GLU	LYS	variant	UNP Q2N0S8
G	99	ASN	SER	variant	UNP Q2N0S8
G	117	LYS	GLU	variant	UNP Q2N0S8
G	?	-	ASN	deletion	UNP Q2N0S8
G	?	-	VAL	deletion	UNP Q2N0S8
G	134	VAL	THR	variant	UNP Q2N0S8
G	135	THR	ASN	variant	UNP Q2N0S8
G	136	ASN	ALA	variant	UNP Q2N0S8
G	185F	ARG	SER	variant	UNP Q2N0S8
G	185H	ASN	LYS	variant	UNP Q2N0S8
G	185I	ASN	SER	variant	UNP Q2N0S8
G	234	ASN	THR	variant	UNP Q2N0S8
G	240	PRO	SER	variant	UNP Q2N0S8
G	241	SER	ASN	variant	UNP Q2N0S8
G	308	ARG	HIS	variant	UNP Q2N0S8
G	325	ASP	ASN	variant	UNP Q2N0S8
G	330	HIS	GLN	variant	UNP Q2N0S8
G	332	ASN	THR	variant	UNP Q2N0S8
G	343	GLY	GLU	variant	UNP Q2N0S8
G	351	LYS	GLU	variant	UNP Q2N0S8
G	358	ILE	THR	variant	UNP Q2N0S8
G	360	ARG	ILE	variant	UNP Q2N0S8
G	363	ASN	SER	variant	UNP Q2N0S8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	409	GLY	GLU	variant	UNP Q2N0S8
G	411	ASN	SER	variant	UNP Q2N0S8
G	413	SER	THR	variant	UNP Q2N0S8
G	461	THR	ASN	variant	UNP Q2N0S8
G	465	THR	ASN	variant	UNP Q2N0S8
G	501	CYS	ALA	conflict	UNP Q2N0S8
G	509	ARG	GLU	conflict	UNP Q2N0S8
G	510	ARG	LYS	conflict	UNP Q2N0S8
G	512	ARG	ALA	conflict	UNP Q2N0S8
G	513	ARG	VAL	conflict	UNP Q2N0S8
N	-4	MET	-	initiating methionine	UNP Q2N0S8
N	-3	ASP	-	expression tag	UNP Q2N0S8
N	-2	ALA	-	expression tag	UNP Q2N0S8
N	-1	MET	-	expression tag	UNP Q2N0S8
N	0	LYS	-	expression tag	UNP Q2N0S8
N	1	ARG	-	expression tag	UNP Q2N0S8
N	2	GLY	-	expression tag	UNP Q2N0S8
N	3	LEU	-	expression tag	UNP Q2N0S8
N	4	CYS	-	expression tag	UNP Q2N0S8
N	5	CYS	-	expression tag	UNP Q2N0S8
N	6	VAL	-	expression tag	UNP Q2N0S8
N	7	LEU	-	expression tag	UNP Q2N0S8
N	8	LEU	-	expression tag	UNP Q2N0S8
N	9	LEU	-	expression tag	UNP Q2N0S8
N	10	CYS	-	expression tag	UNP Q2N0S8
N	11	GLY	-	expression tag	UNP Q2N0S8
N	12	ALA	-	expression tag	UNP Q2N0S8
N	13	VAL	-	expression tag	UNP Q2N0S8
N	14	PHE	-	expression tag	UNP Q2N0S8
N	15	VAL	-	expression tag	UNP Q2N0S8
N	16	SER	-	expression tag	UNP Q2N0S8
N	17	PRO	-	expression tag	UNP Q2N0S8
N	18	SER	-	expression tag	UNP Q2N0S8
N	19	GLN	-	expression tag	UNP Q2N0S8
N	20	GLU	-	expression tag	UNP Q2N0S8
N	21	ILE	-	expression tag	UNP Q2N0S8
N	22	HIS	-	expression tag	UNP Q2N0S8
N	23	ALA	-	expression tag	UNP Q2N0S8
N	24	ARG	-	expression tag	UNP Q2N0S8
N	25	PHE	-	expression tag	UNP Q2N0S8
N	26	ARG	-	expression tag	UNP Q2N0S8
N	27	ARG	-	expression tag	UNP Q2N0S8

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Chain	Residue	Modelled	Actual	Comment	Reference
N	28	GLY	-	expression tag	UNP Q2N0S8
N	29	ALA	-	expression tag	UNP Q2N0S8
N	30	ARG	-	expression tag	UNP Q2N0S8
N	62	GLU	LYS	variant	UNP Q2N0S8
N	99	ASN	SER	variant	UNP Q2N0S8
N	117	LYS	GLU	variant	UNP Q2N0S8
N	?	-	ASN	deletion	UNP Q2N0S8
N	?	-	VAL	deletion	UNP Q2N0S8
N	134	VAL	THR	variant	UNP Q2N0S8
N	135	THR	ASN	variant	UNP Q2N0S8
N	136	ASN	ALA	variant	UNP Q2N0S8
N	185F	ARG	SER	variant	UNP Q2N0S8
N	185H	ASN	LYS	variant	UNP Q2N0S8
N	185I	ASN	SER	variant	UNP Q2N0S8
N	234	ASN	THR	variant	UNP Q2N0S8
N	240	PRO	SER	variant	UNP Q2N0S8
N	241	SER	ASN	variant	UNP Q2N0S8
N	308	ARG	HIS	variant	UNP Q2N0S8
N	325	ASP	ASN	variant	UNP Q2N0S8
N	330	HIS	GLN	variant	UNP Q2N0S8
N	332	ASN	THR	variant	UNP Q2N0S8
N	343	GLY	GLU	variant	UNP Q2N0S8
N	351	LYS	GLU	variant	UNP Q2N0S8
N	358	ILE	THR	variant	UNP Q2N0S8
N	360	ARG	ILE	variant	UNP Q2N0S8
N	363	ASN	SER	variant	UNP Q2N0S8
N	409	GLY	GLU	variant	UNP Q2N0S8
N	411	ASN	SER	variant	UNP Q2N0S8
N	413	SER	THR	variant	UNP Q2N0S8
N	461	THR	ASN	variant	UNP Q2N0S8
N	465	THR	ASN	variant	UNP Q2N0S8
N	501	CYS	ALA	conflict	UNP Q2N0S8
N	509	ARG	GLU	conflict	UNP Q2N0S8
N	510	ARG	LYS	conflict	UNP Q2N0S8
N	512	ARG	ALA	conflict	UNP Q2N0S8
N	513	ARG	VAL	conflict	UNP Q2N0S8

- Molecule 3 is a protein called ELC07 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	230	Total	C	N	O	S	0	0
			1711	1081	292	331	7		

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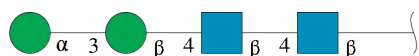
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	230	Total	C	N	O	S	0	0
			1711	1081	292	331	7		
3	K	230	Total	C	N	O	S	0	0
			1711	1081	292	331	7		

- Molecule 4 is a protein called ELC07 light chain.

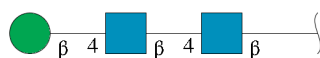
Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	213	Total	C	N	O	S	0	0
			1629	1019	278	326	6		
4	J	213	Total	C	N	O	S	0	0
			1629	1019	278	326	6		
4	M	213	Total	C	N	O	S	0	0
			1629	1019	278	326	6		

- 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	e	4	Total	C	N	O	0	0
			50	28	2	20		
5	d	4	Total	C	N	O	0	0
			50	28	2	20		
5	g	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 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
6	q	3	Total	C	N	O	0	0
			39	22	2	15		

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

- Molecule 7 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
7	u	2	Total	C	N	O	0	0
			28	16	2	10		
7	B	2	Total	C	N	O	0	0
			28	16	2	10		
7	D	2	Total	C	N	O	0	0
			28	16	2	10		
7	O	2	Total	C	N	O	0	0
			28	16	2	10		
7	P	2	Total	C	N	O	0	0
			28	16	2	10		
7	Q	2	Total	C	N	O	0	0
			28	16	2	10		
7	R	2	Total	C	N	O	0	0
			28	16	2	10		
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		
7	Y	2	Total	C	N	O	0	0
			28	16	2	10		
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	a	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		
7	c	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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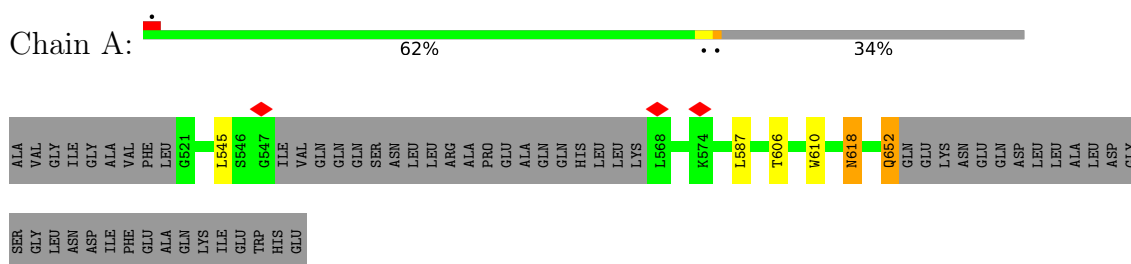
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Mol	Chain	Residues	Atoms				AltConf
8	G	1	Total 14	C 8	N 1	O 5	0
8	G	1	Total 14	C 8	N 1	O 5	0
8	G	1	Total 14	C 8	N 1	O 5	0
8	G	1	Total 14	C 8	N 1	O 5	0
8	G	1	Total 14	C 8	N 1	O 5	0
8	G	1	Total 14	C 8	N 1	O 5	0
8	G	1	Total 14	C 8	N 1	O 5	0
8	G	1	Total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

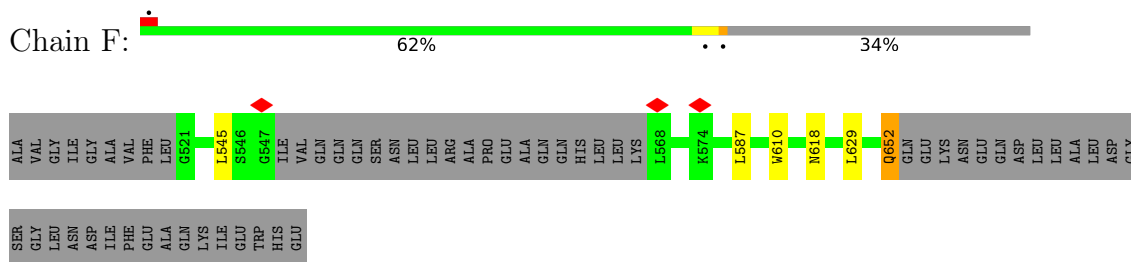
### 3 Residue-property plots [i](#)

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

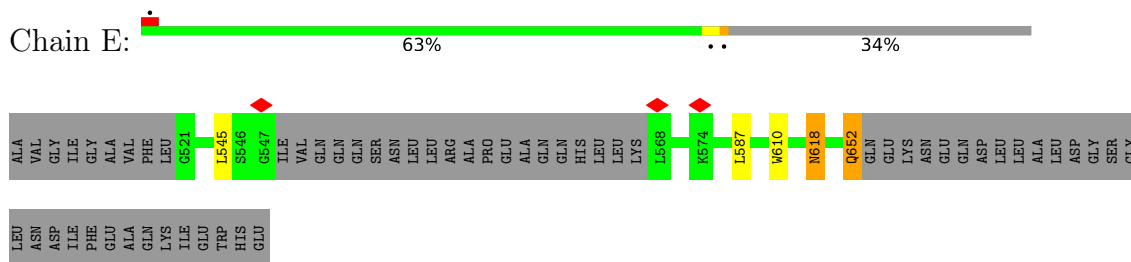
- Molecule 1: Transmembrane protein gp41



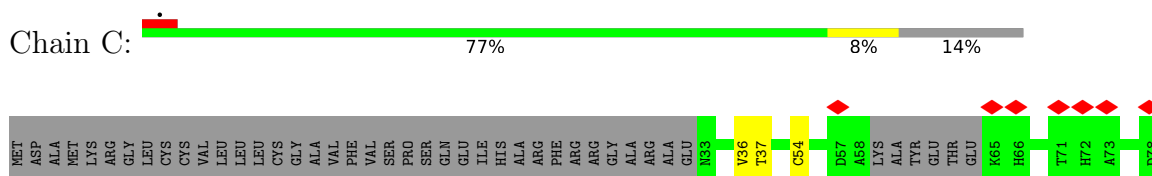
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41

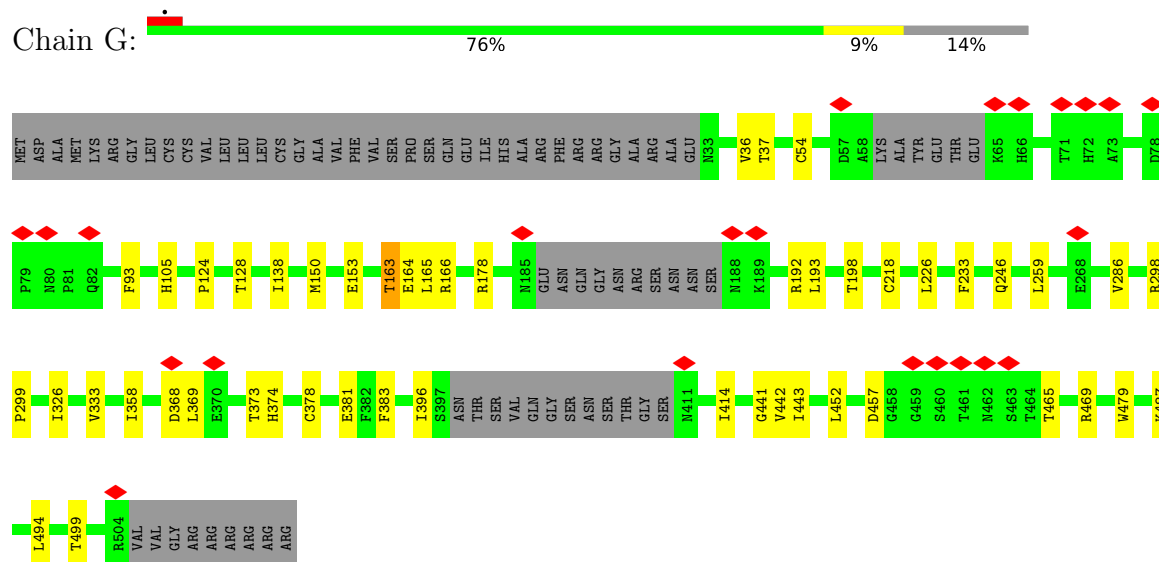


- Molecule 2: Envelope glycoprotein gp160

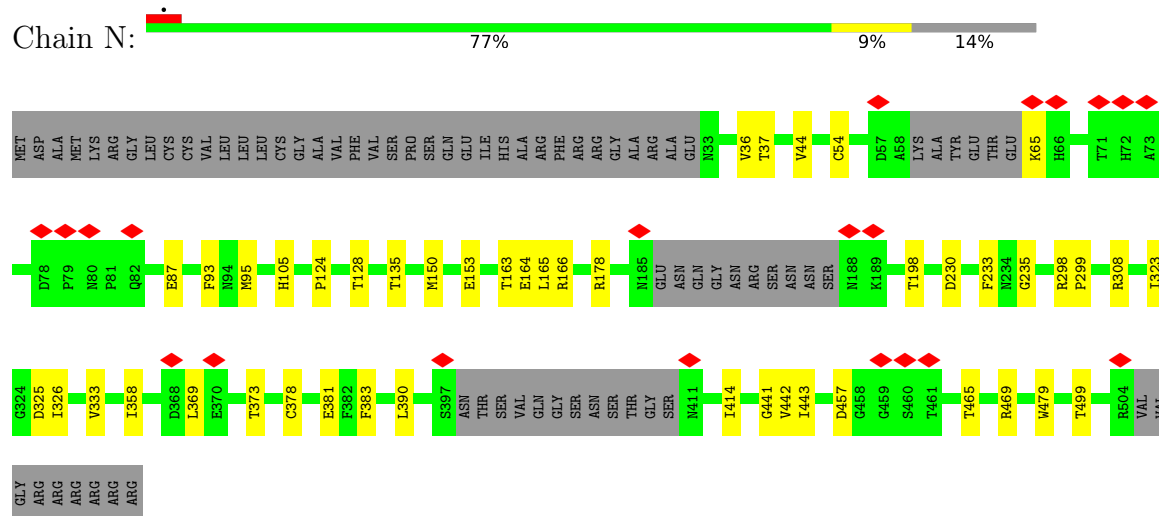




- Molecule 2: Envelope glycoprotein gp160

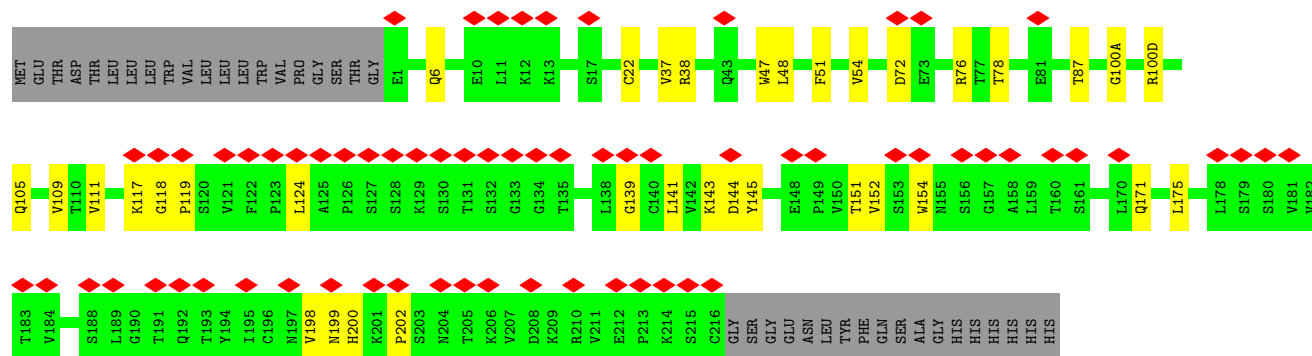


- Molecule 2: Envelope glycoprotein gp160

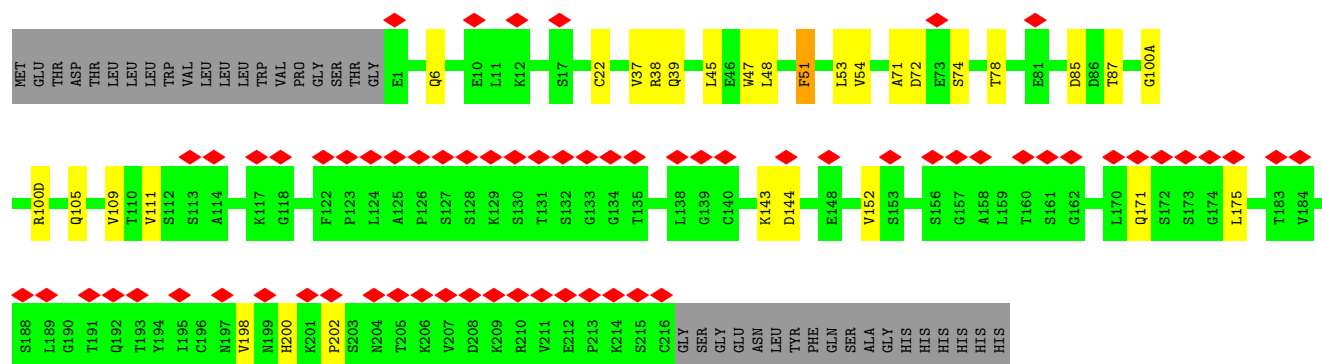
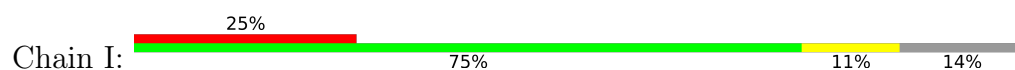


- Molecule 3: ELC07 heavy chain

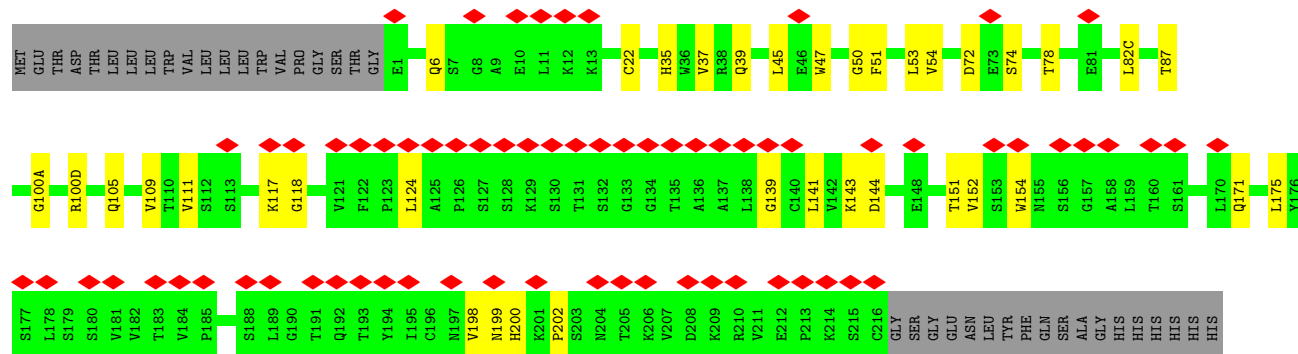
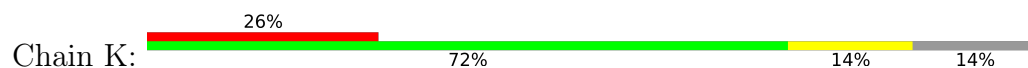




• Molecule 3: ELC07 heavy chain

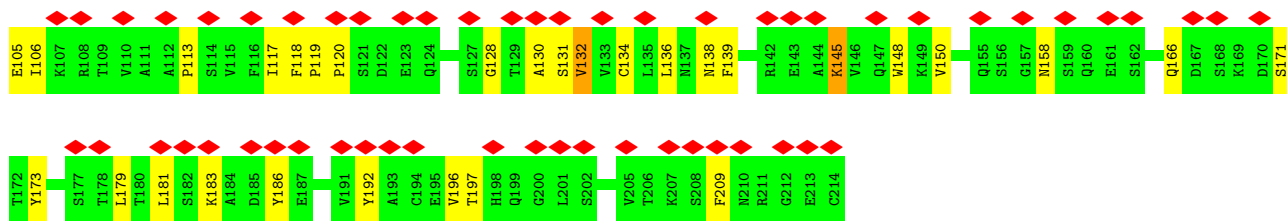


• Molecule 3: ELC07 heavy chain

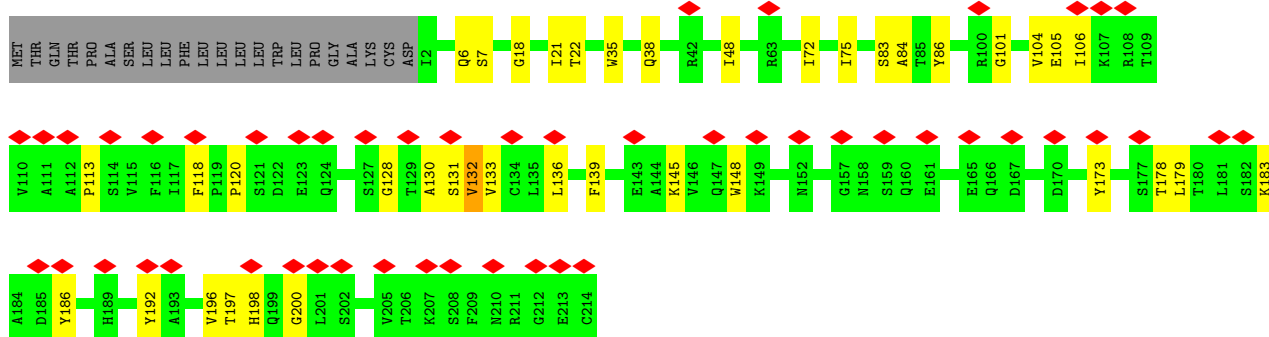
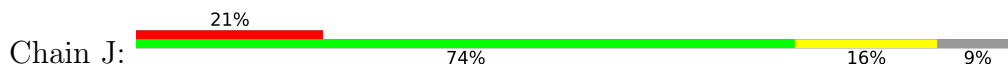


• Molecule 4: ELC07 light chain

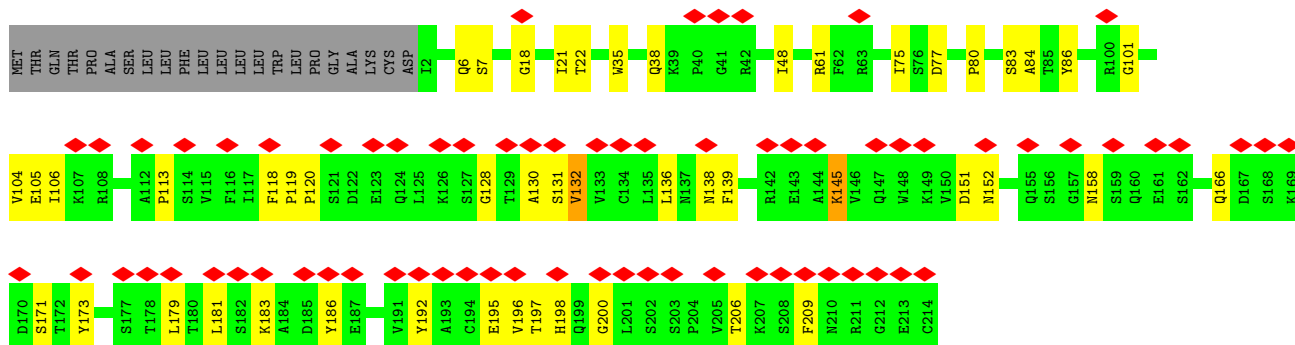




• Molecule 4: ELC07 light chain



• Molecule 4: ELC07 light chain



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



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



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



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



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





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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



- Molecule 7: 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	35337	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	33	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.610	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.139	Depositor
Map size (Å)	342.0, 342.0, 342.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.23	0/899	0.44	0/1220
1	E	0.23	0/899	0.43	0/1220
1	F	0.23	0/899	0.43	0/1220
2	C	0.25	0/3542	0.49	0/4809
2	G	0.25	0/3542	0.49	0/4809
2	N	0.25	0/3542	0.49	0/4809
3	H	0.25	0/1754	0.48	0/2384
3	I	0.25	0/1754	0.49	0/2384
3	K	0.25	0/1754	0.48	0/2384
4	J	0.25	0/1665	0.47	0/2261
4	L	0.25	0/1665	0.47	0/2261
4	M	0.25	0/1665	0.47	0/2261
All	All	0.25	0/23580	0.48	0/32022

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	882	0	858	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	882	0	858	6	0
1	F	882	0	858	5	0
2	C	3470	0	3406	27	0
2	G	3470	0	3406	30	0
2	N	3470	0	3406	28	0
3	H	1711	0	1675	18	0
3	I	1711	0	1675	16	0
3	K	1711	0	1675	18	0
4	J	1629	0	1586	24	0
4	L	1629	0	1586	30	0
4	M	1629	0	1586	28	0
5	d	50	0	43	0	0
5	e	50	0	43	0	0
5	g	50	0	43	0	0
6	f	39	0	34	0	0
6	h	39	0	34	0	0
6	q	39	0	34	0	0
7	B	28	0	25	0	0
7	D	28	0	25	0	0
7	O	28	0	25	0	0
7	P	28	0	25	0	0
7	Q	28	0	25	0	0
7	R	28	0	25	1	0
7	S	28	0	25	0	0
7	T	28	0	25	0	0
7	U	28	0	25	0	0
7	V	28	0	25	0	0
7	W	28	0	25	0	0
7	X	28	0	25	0	0
7	Y	28	0	25	0	0
7	Z	28	0	25	0	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
7	u	28	0	25	0	0
8	C	112	0	104	1	0
8	G	112	0	104	1	0
8	N	112	0	104	1	0
All	All	24183	0	23568	217	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 5.

The worst 5 of 217 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)
4:M:136:LEU:HD11	4:M:196:VAL:HG21	1.73	0.68
3:I:6:GLN:H	3:I:105:GLN:HE22	1.41	0.67
4:J:136:LEU:HD11	4:J:196:VAL:HG21	1.77	0.67
4:J:113:PRO:HB3	4:J:139:PHE:HB3	1.77	0.65
4:L:136:LEU:HD11	4:L:196:VAL:HG21	1.77	0.65

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	108/170 (64%)	107 (99%)	1 (1%)	0	100	100
1	E	108/170 (64%)	107 (99%)	1 (1%)	0	100	100
1	F	108/170 (64%)	105 (97%)	3 (3%)	0	100	100
2	C	434/516 (84%)	413 (95%)	21 (5%)	0	100	100
2	G	434/516 (84%)	411 (95%)	23 (5%)	0	100	100
2	N	434/516 (84%)	412 (95%)	22 (5%)	0	100	100
3	H	228/268 (85%)	224 (98%)	4 (2%)	0	100	100
3	I	228/268 (85%)	227 (100%)	1 (0%)	0	100	100
3	K	228/268 (85%)	224 (98%)	4 (2%)	0	100	100
4	J	211/235 (90%)	208 (99%)	3 (1%)	0	100	100
4	L	211/235 (90%)	207 (98%)	4 (2%)	0	100	100
4	M	211/235 (90%)	207 (98%)	4 (2%)	0	100	100
All	All	2943/3567 (82%)	2852 (97%)	91 (3%)	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	A	94/143 (66%)	92 (98%)	2 (2%)	48	76
1	E	94/143 (66%)	92 (98%)	2 (2%)	48	76
1	F	94/143 (66%)	92 (98%)	2 (2%)	48	76
2	C	393/456 (86%)	391 (100%)	2 (0%)	86	94
2	G	393/456 (86%)	390 (99%)	3 (1%)	79	90
2	N	393/456 (86%)	388 (99%)	5 (1%)	65	84
3	H	187/219 (85%)	185 (99%)	2 (1%)	70	87
3	I	187/219 (85%)	185 (99%)	2 (1%)	70	87
3	K	187/219 (85%)	183 (98%)	4 (2%)	48	76
4	J	185/204 (91%)	183 (99%)	2 (1%)	70	87
4	L	185/204 (91%)	183 (99%)	2 (1%)	70	87
4	M	185/204 (91%)	182 (98%)	3 (2%)	58	81
All	All	2577/3066 (84%)	2546 (99%)	31 (1%)	66	85

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	145	LYS
2	N	87	GLU
4	J	132	VAL
2	N	163	THR
4	M	145	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	J	198	HIS
4	M	152	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

57 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	$\# Z  > 2$
7	NAG	B	1	2,7	14,14,15	0.74	0	17,19,21	0.99	1 (5%)
7	NAG	B	2	7	14,14,15	0.71	0	17,19,21	0.83	0
7	NAG	D	1	2,7	14,14,15	0.72	0	17,19,21	0.90	0
7	NAG	D	2	7	14,14,15	0.71	0	17,19,21	0.88	0
7	NAG	O	1	2,7	14,14,15	0.77	0	17,19,21	1.20	2 (11%)
7	NAG	O	2	7	14,14,15	0.78	0	17,19,21	0.89	0
7	NAG	P	1	2,7	14,14,15	0.75	0	17,19,21	0.94	1 (5%)
7	NAG	P	2	7	14,14,15	0.70	0	17,19,21	1.16	1 (5%)
7	NAG	Q	1	2,7	14,14,15	0.74	0	17,19,21	0.83	0
7	NAG	Q	2	7	14,14,15	0.73	0	17,19,21	0.81	0
7	NAG	R	1	2,7	14,14,15	0.74	0	17,19,21	0.94	1 (5%)
7	NAG	R	2	7	14,14,15	0.73	0	17,19,21	0.85	0
7	NAG	S	1	2,7	14,14,15	0.73	0	17,19,21	1.16	1 (5%)
7	NAG	S	2	7	14,14,15	0.73	0	17,19,21	0.83	0
7	NAG	T	1	2,7	14,14,15	0.73	0	17,19,21	0.88	0
7	NAG	T	2	7	14,14,15	0.71	0	17,19,21	0.85	0
7	NAG	U	1	2,7	14,14,15	0.78	0	17,19,21	1.21	2 (11%)
7	NAG	U	2	7	14,14,15	0.77	0	17,19,21	0.89	0
7	NAG	V	1	2,7	14,14,15	0.74	0	17,19,21	0.96	1 (5%)
7	NAG	V	2	7	14,14,15	0.70	0	17,19,21	1.17	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	W	1	2,7	14,14,15	0.74	0	17,19,21	0.84	0
7	NAG	W	2	7	14,14,15	0.72	0	17,19,21	0.81	0
7	NAG	X	1	2,7	14,14,15	0.73	0	17,19,21	0.93	1 (5%)
7	NAG	X	2	7	14,14,15	0.74	0	17,19,21	0.84	0
7	NAG	Y	1	2,7	14,14,15	0.75	0	17,19,21	1.12	1 (5%)
7	NAG	Y	2	7	14,14,15	0.72	0	17,19,21	0.83	0
7	NAG	Z	1	2,7	14,14,15	0.73	0	17,19,21	0.90	0
7	NAG	Z	2	7	14,14,15	0.69	0	17,19,21	0.86	0
7	NAG	a	1	2,7	14,14,15	0.79	0	17,19,21	1.20	2 (11%)
7	NAG	a	2	7	14,14,15	0.76	0	17,19,21	0.90	0
7	NAG	b	1	2,7	14,14,15	0.76	0	17,19,21	0.94	1 (5%)
7	NAG	b	2	7	14,14,15	0.71	0	17,19,21	1.16	1 (5%)
7	NAG	c	1	2,7	14,14,15	0.73	0	17,19,21	0.83	0
7	NAG	c	2	7	14,14,15	0.71	0	17,19,21	0.82	0
5	NAG	d	1	2,5	14,14,15	0.76	0	17,19,21	1.03	1 (5%)
5	NAG	d	2	5	14,14,15	0.72	0	17,19,21	0.96	1 (5%)
5	BMA	d	3	5	11,11,12	0.85	0	15,15,17	2.14	4 (26%)
5	MAN	d	4	5	11,11,12	0.71	0	15,15,17	1.18	1 (6%)
5	NAG	e	1	2,5	14,14,15	0.74	0	17,19,21	1.04	1 (5%)
5	NAG	e	2	5	14,14,15	0.73	0	17,19,21	0.95	1 (5%)
5	BMA	e	3	5	11,11,12	0.84	0	15,15,17	2.14	4 (26%)
5	MAN	e	4	5	11,11,12	0.72	0	15,15,17	1.15	1 (6%)
6	NAG	f	1	2,6	14,14,15	0.76	0	17,19,21	0.94	1 (5%)
6	NAG	f	2	6	14,14,15	0.74	0	17,19,21	0.89	0
6	BMA	f	3	6	11,11,12	0.86	0	15,15,17	2.20	4 (26%)
5	NAG	g	1	2,5	14,14,15	0.77	0	17,19,21	1.04	0
5	NAG	g	2	5	14,14,15	0.72	0	17,19,21	0.91	1 (5%)
5	BMA	g	3	5	11,11,12	0.85	0	15,15,17	2.17	4 (26%)
5	MAN	g	4	5	11,11,12	0.71	0	15,15,17	1.18	1 (6%)
6	NAG	h	1	2,6	14,14,15	0.77	0	17,19,21	0.93	0
6	NAG	h	2	6	14,14,15	0.73	0	17,19,21	0.88	0
6	BMA	h	3	6	11,11,12	0.87	0	15,15,17	2.21	4 (26%)
6	NAG	q	1	2,6	14,14,15	0.74	0	17,19,21	0.96	1 (5%)
6	NAG	q	2	6	14,14,15	0.73	0	17,19,21	0.87	0
6	BMA	q	3	6	11,11,12	0.86	0	15,15,17	2.21	4 (26%)
7	NAG	u	1	2,7	14,14,15	0.75	0	17,19,21	0.90	0
7	NAG	u	2	7	14,14,15	0.72	0	17,19,21	0.85	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
7	NAG	B	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	B	2	7	-	0/6/23/26	0/1/1/1
7	NAG	D	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	D	2	7	-	0/6/23/26	0/1/1/1
7	NAG	O	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	1/6/23/26	0/1/1/1
7	NAG	P	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	P	2	7	-	1/6/23/26	0/1/1/1
7	NAG	Q	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	NAG	R	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	R	2	7	-	0/6/23/26	0/1/1/1
7	NAG	S	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1
7	NAG	T	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	NAG	U	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	0/6/23/26	0/1/1/1
7	NAG	V	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	V	2	7	-	2/6/23/26	0/1/1/1
7	NAG	W	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
7	NAG	X	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	X	2	7	-	0/6/23/26	0/1/1/1
7	NAG	Y	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	0/6/23/26	0/1/1/1
7	NAG	Z	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	0/6/23/26	0/1/1/1
7	NAG	a	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	a	2	7	-	1/6/23/26	0/1/1/1
7	NAG	b	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	b	2	7	-	2/6/23/26	0/1/1/1
7	NAG	c	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
5	NAG	d	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	0/6/23/26	0/1/1/1
5	BMA	d	3	5	-	0/2/19/22	0/1/1/1

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

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	h	3	BMA	C1-O5-C5	6.54	121.05	112.19
6	f	3	BMA	C1-O5-C5	6.50	120.99	112.19
6	q	3	BMA	C1-O5-C5	6.45	120.93	112.19
5	g	3	BMA	C1-O5-C5	6.37	120.83	112.19
5	d	3	BMA	C1-O5-C5	6.23	120.64	112.19

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	e	4	MAN	C4-C5-C6-O6
5	d	4	MAN	C4-C5-C6-O6
5	g	4	MAN	C4-C5-C6-O6
5	e	4	MAN	O5-C5-C6-O6
5	g	4	MAN	O5-C5-C6-O6

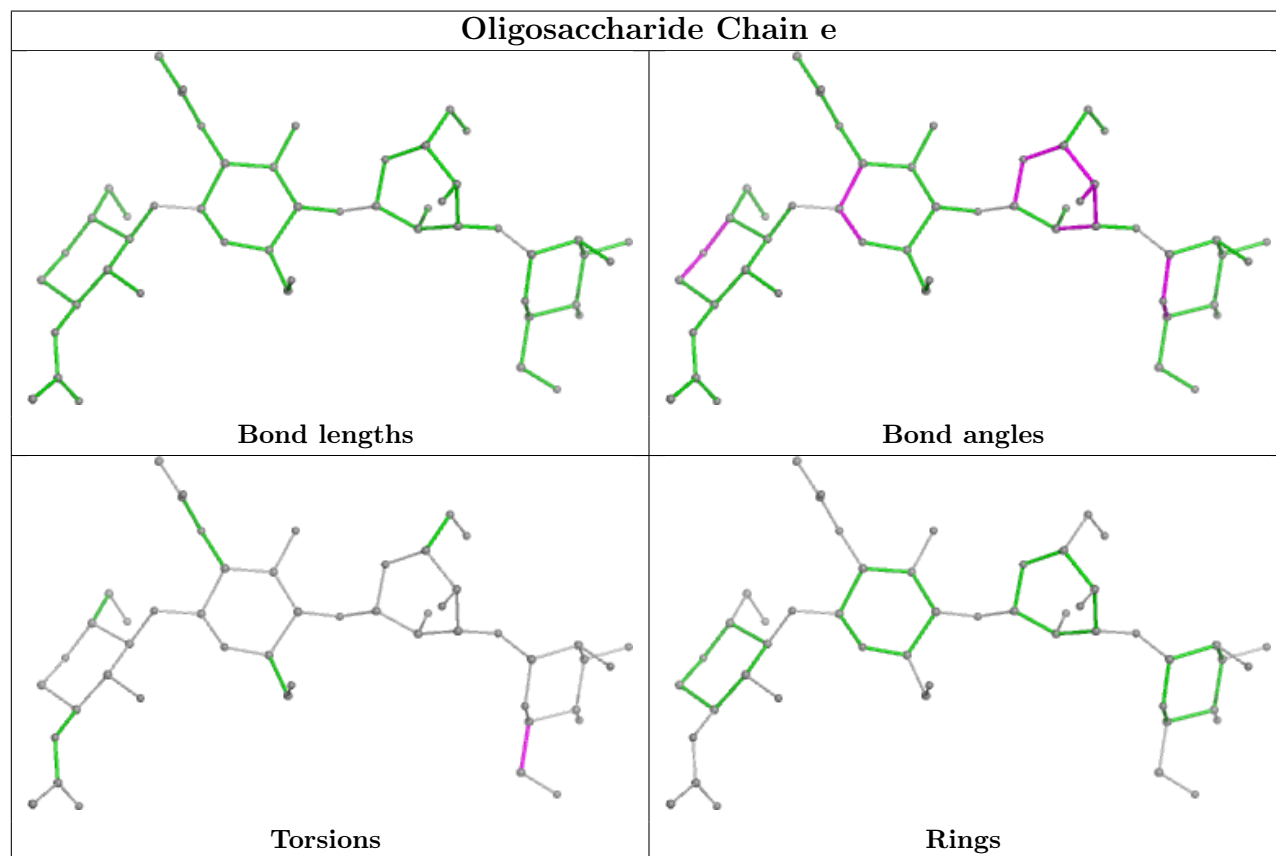


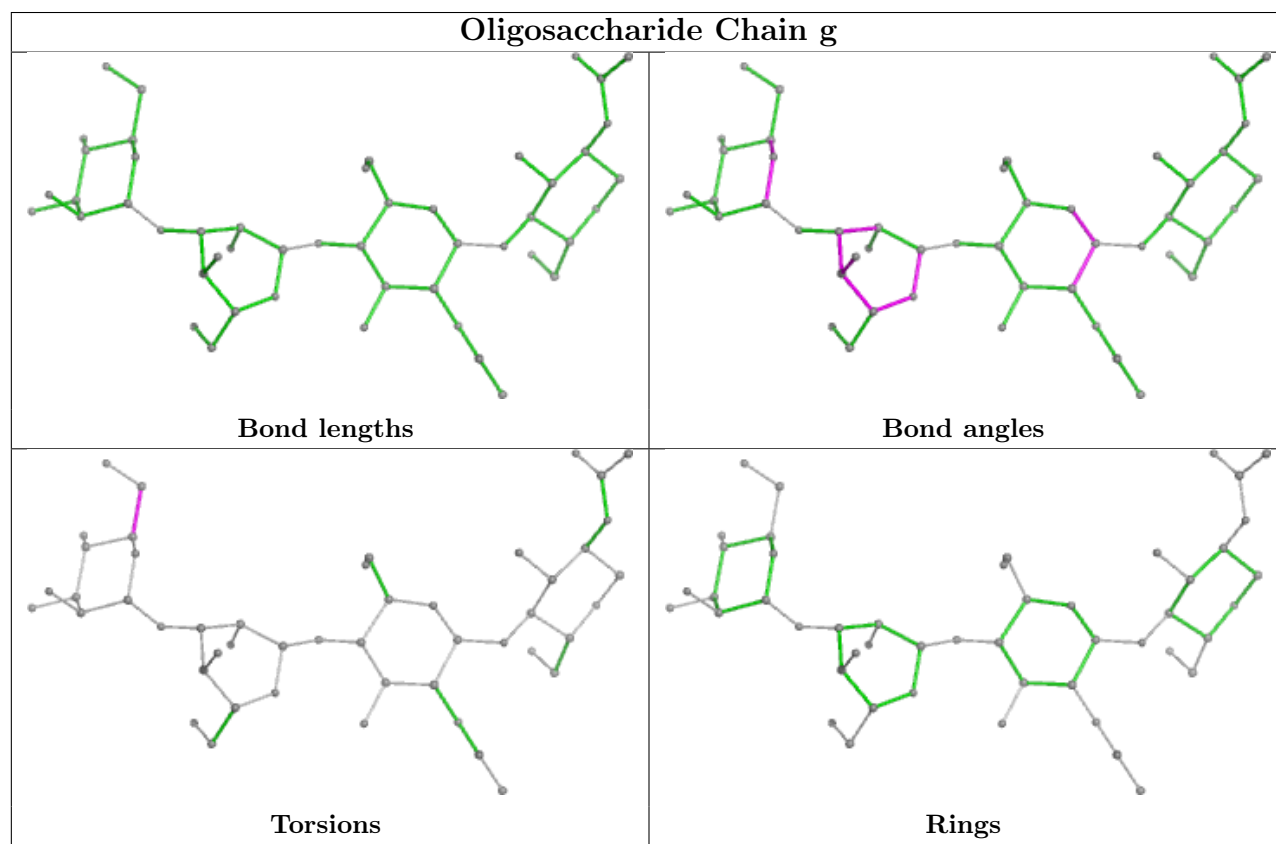
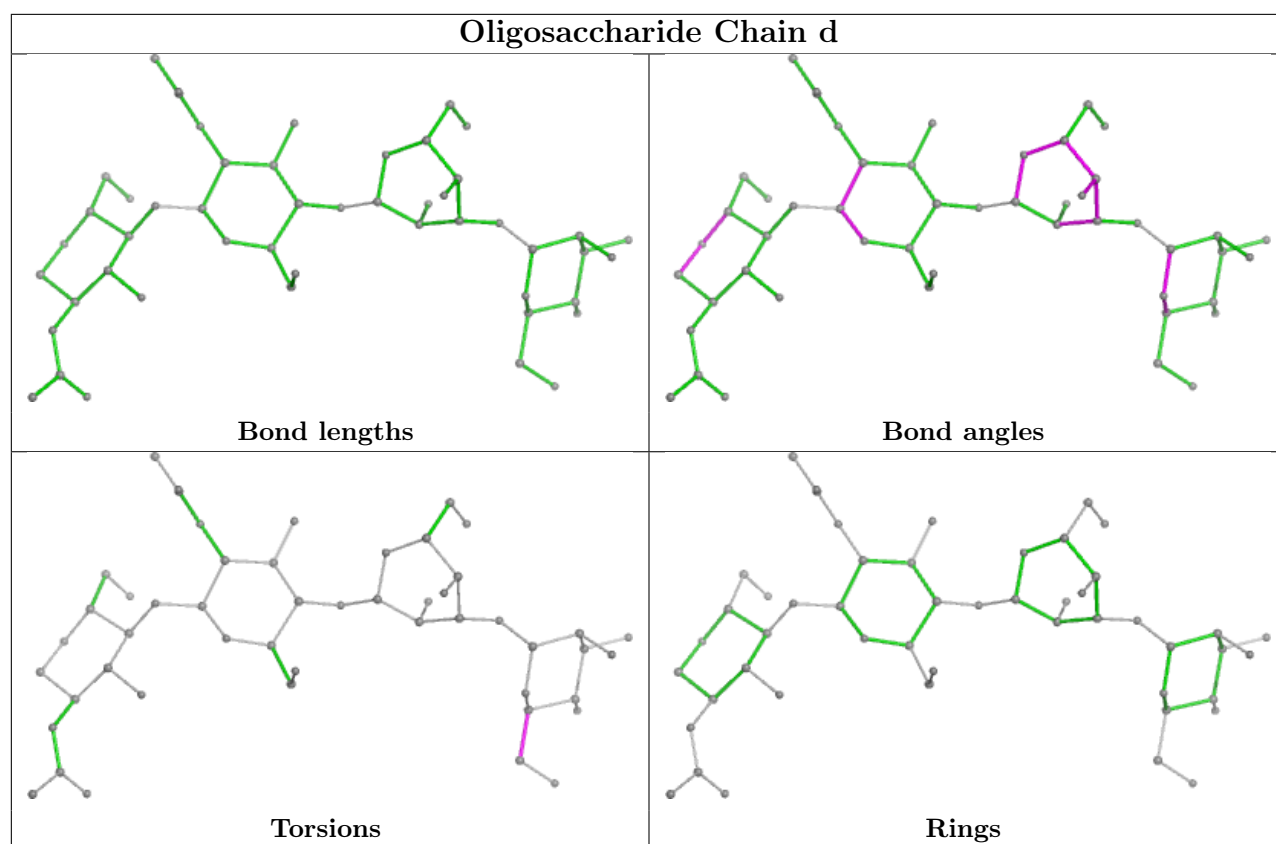
There are no ring outliers.

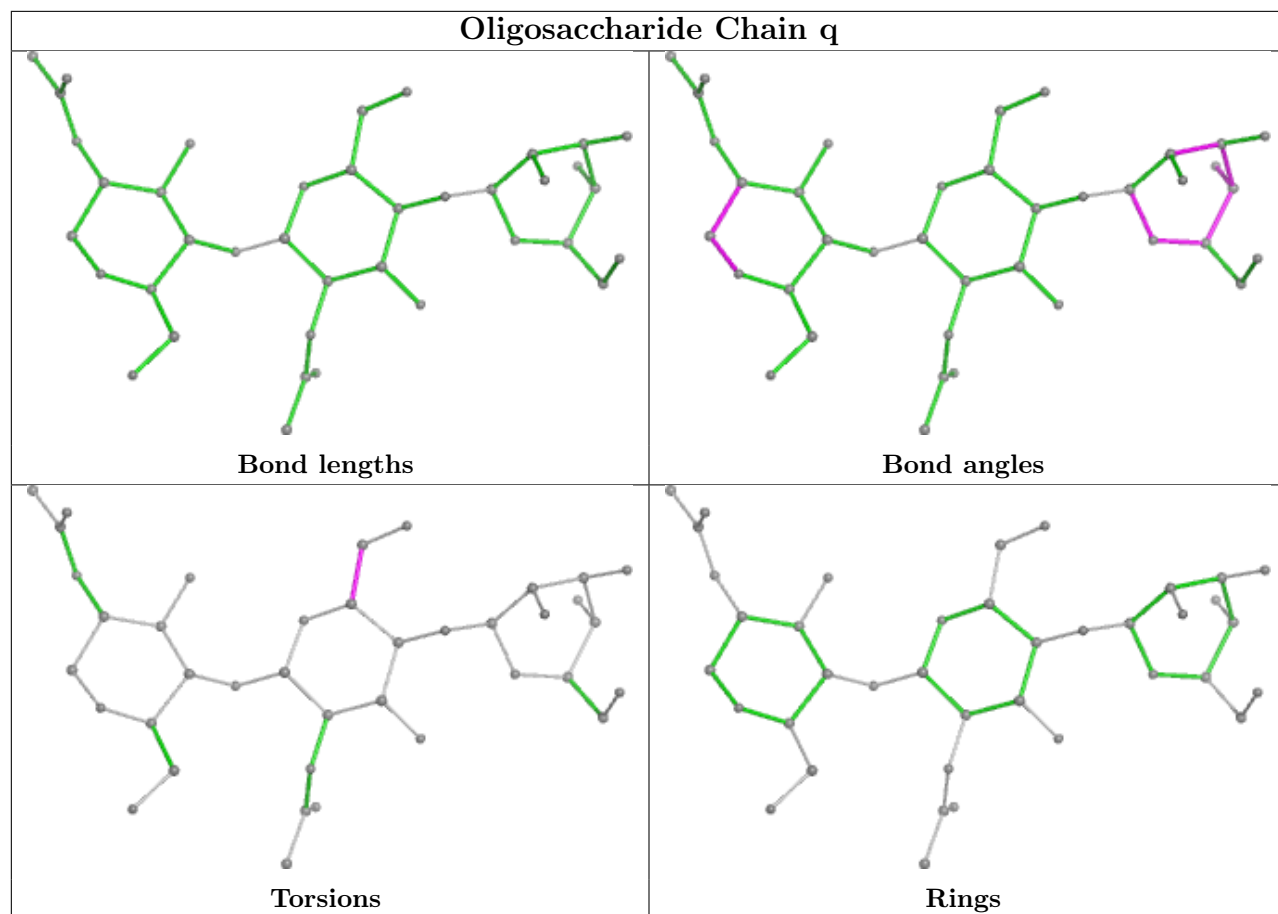
2 monomers are involved in 1 short contact:

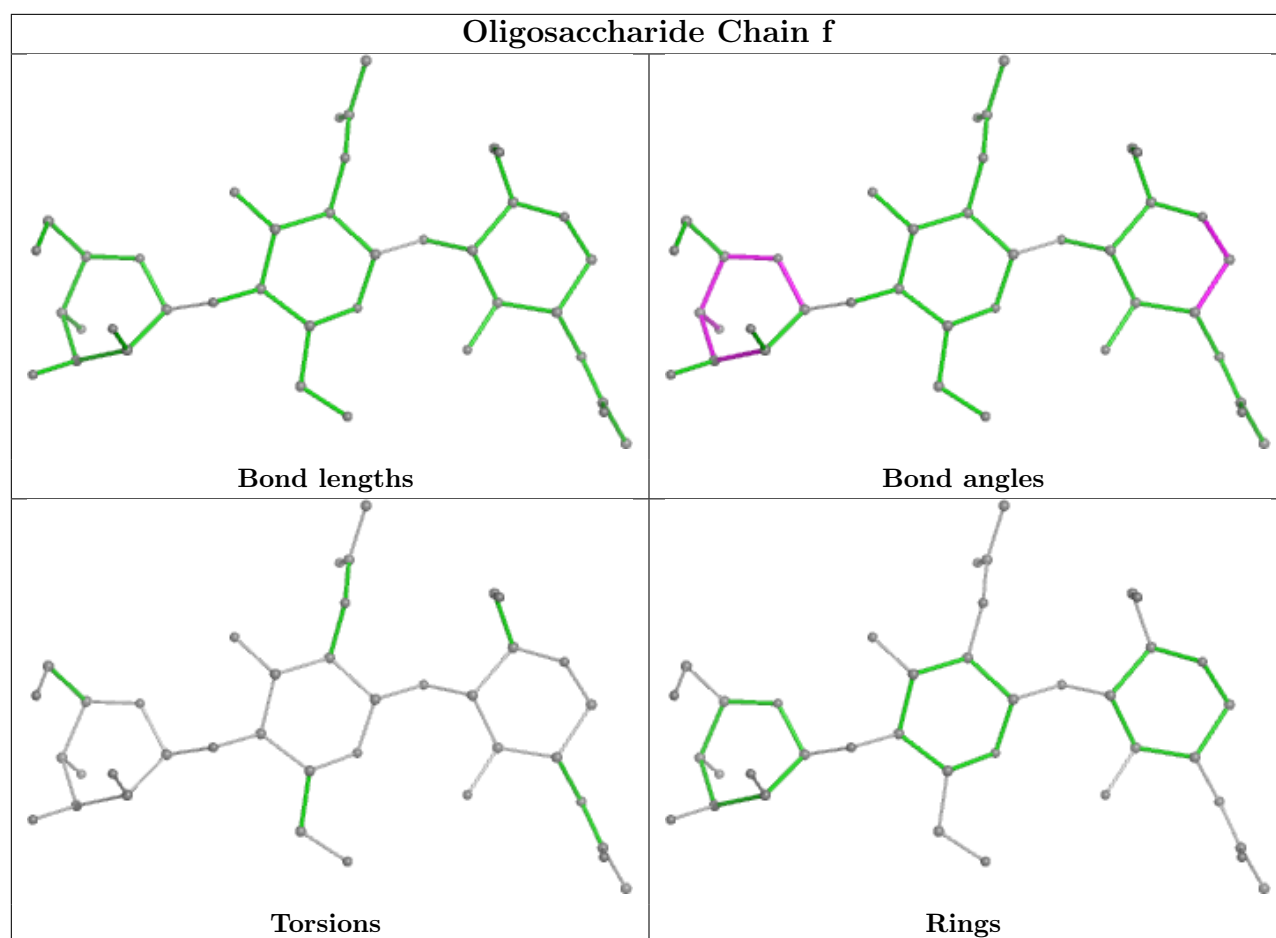
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	1	NAG	1	0
7	R	2	NAG	1	0

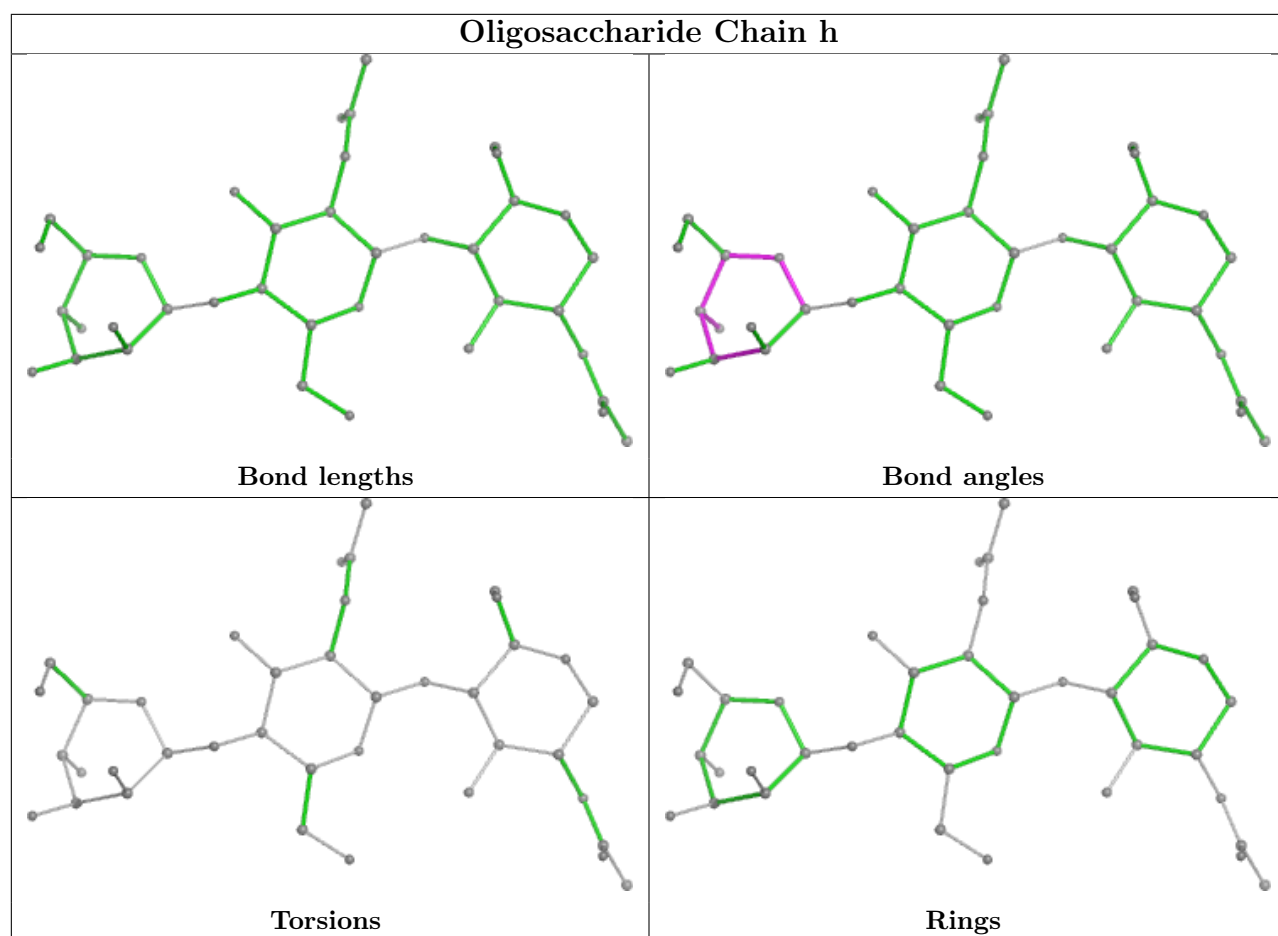
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

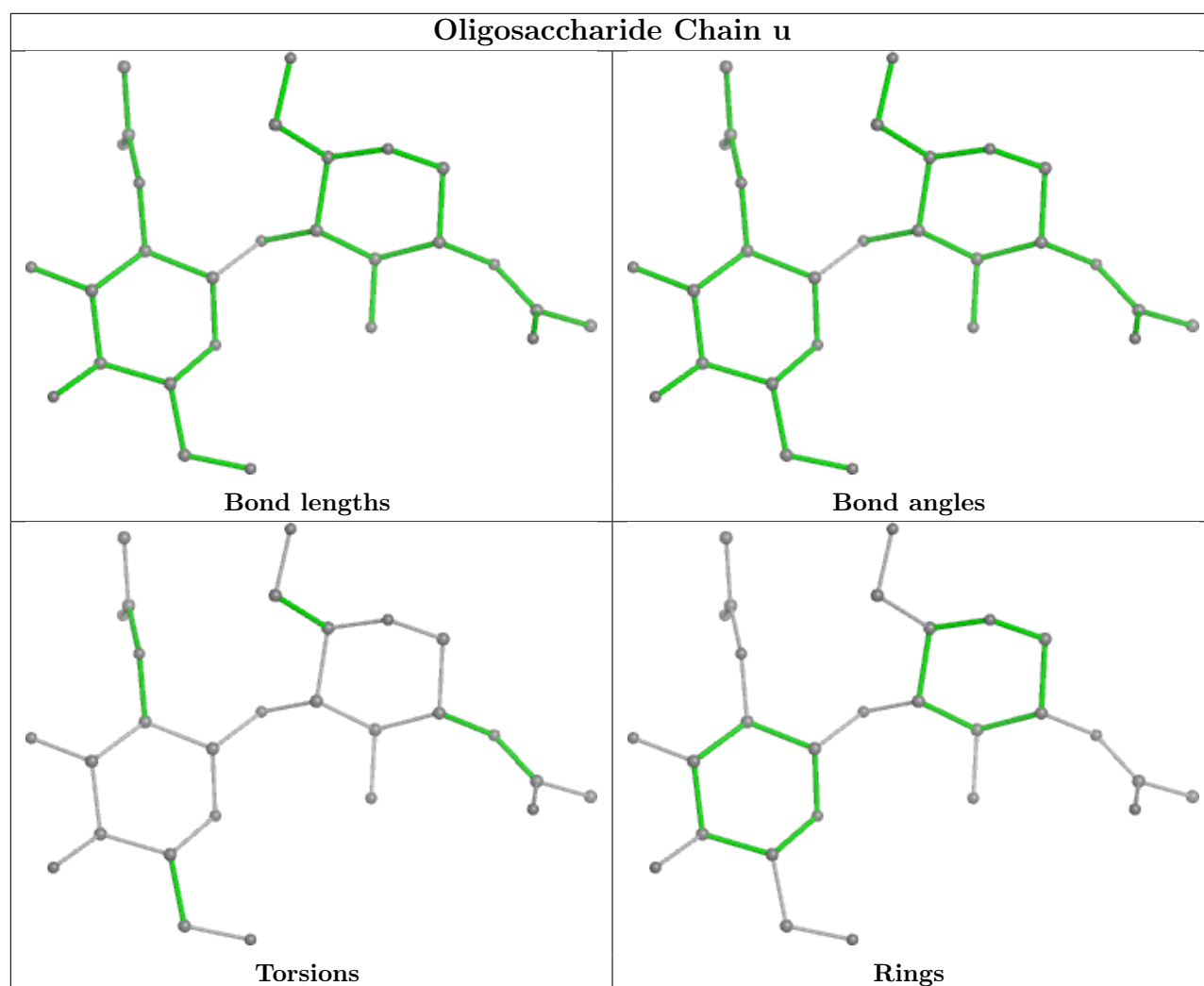


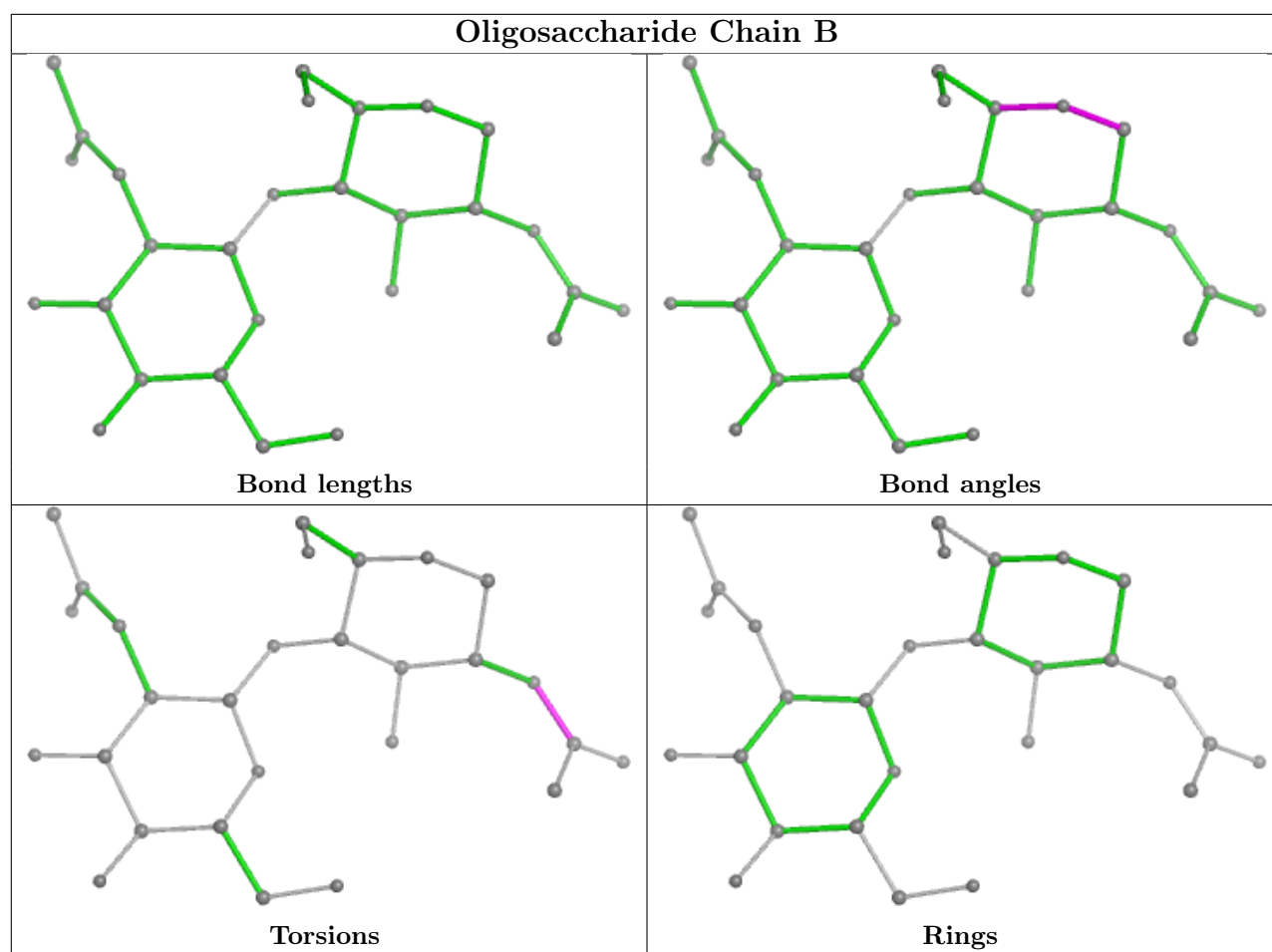


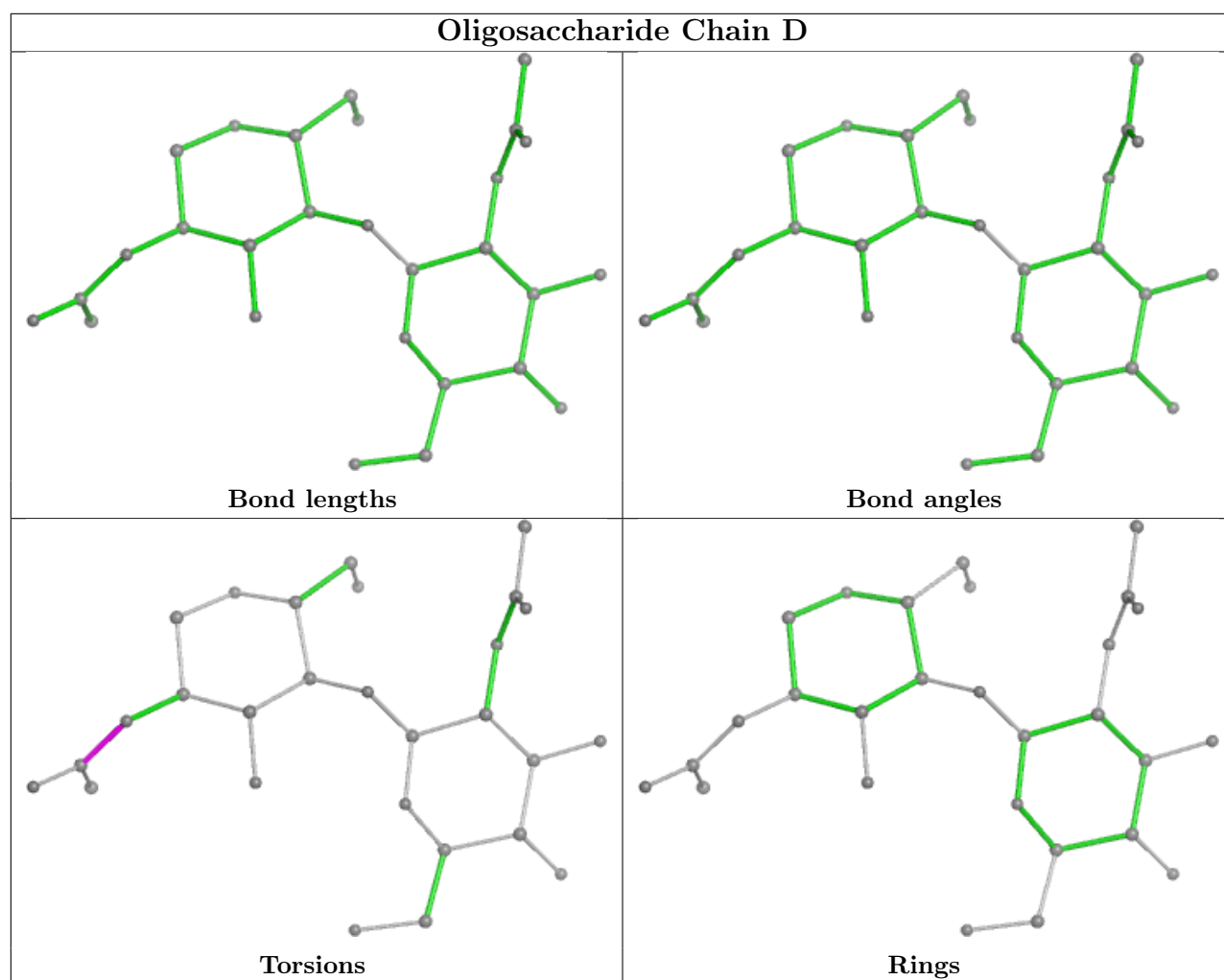




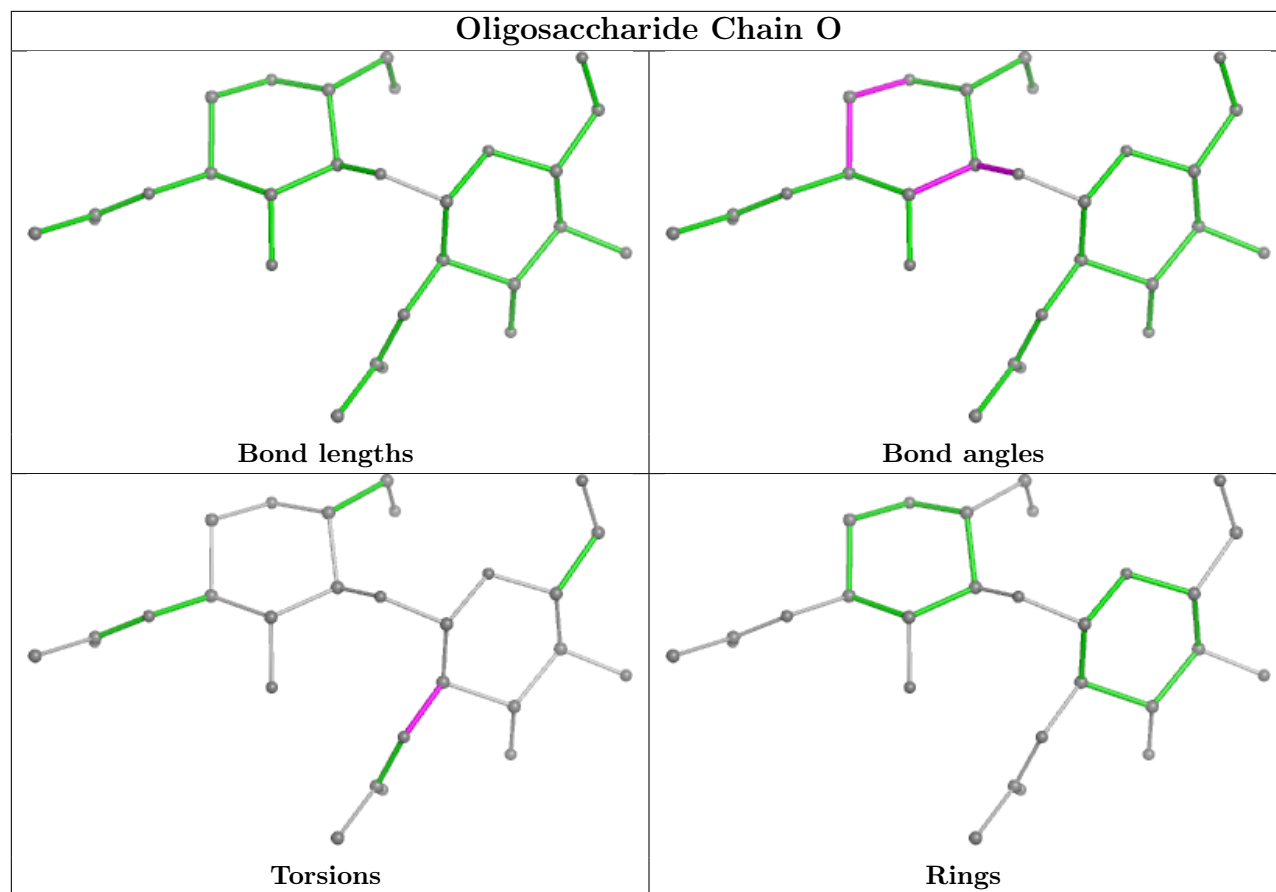


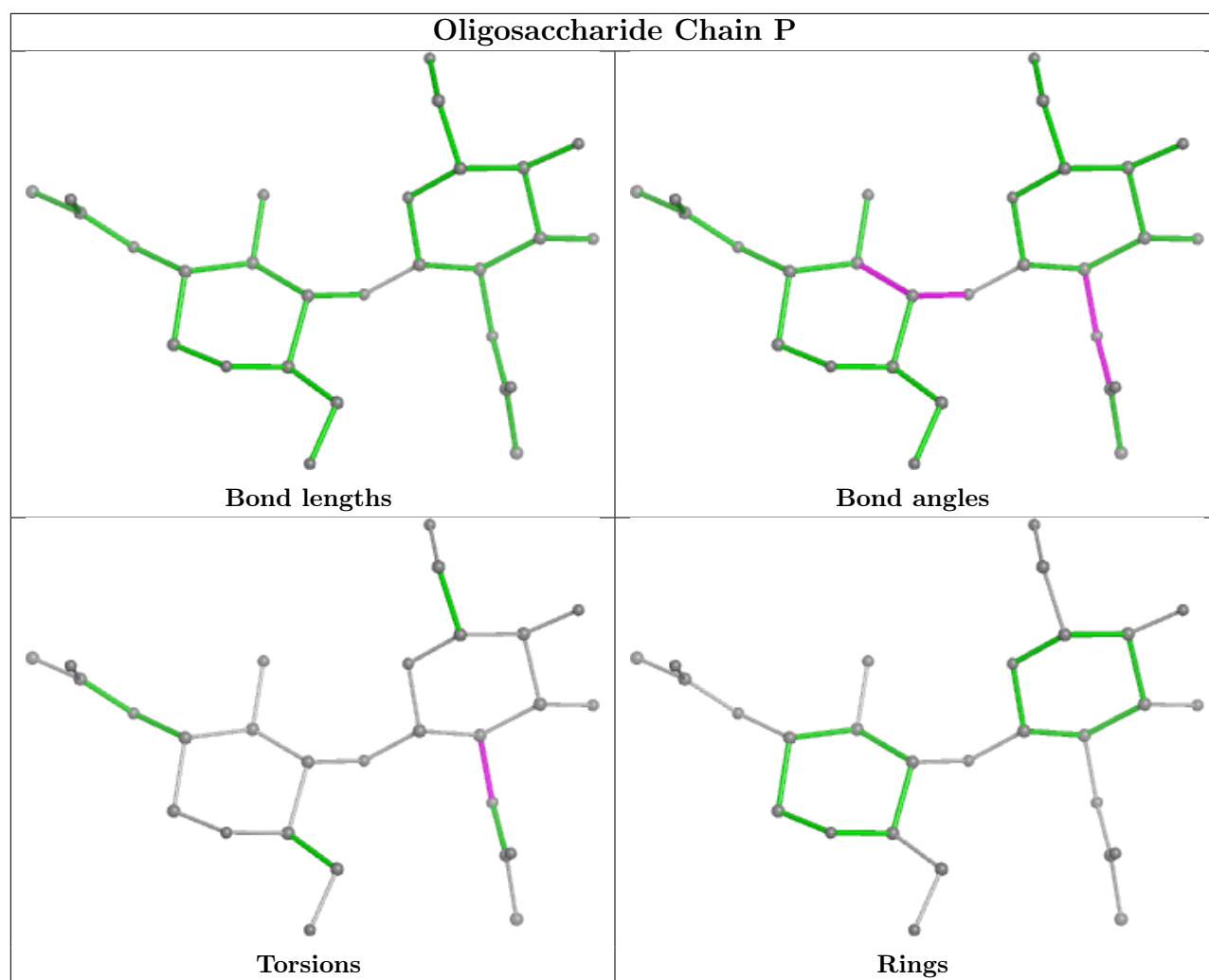


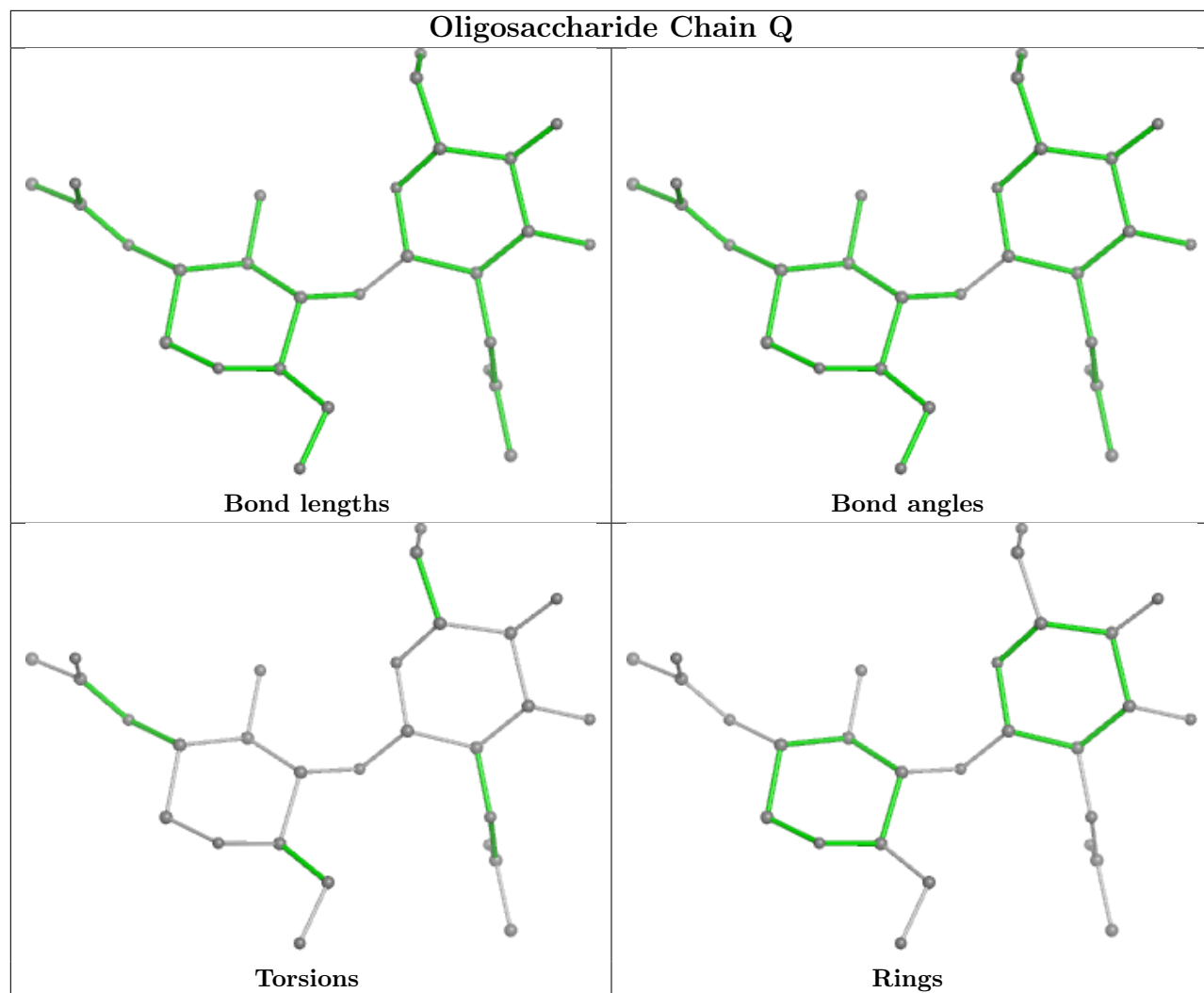


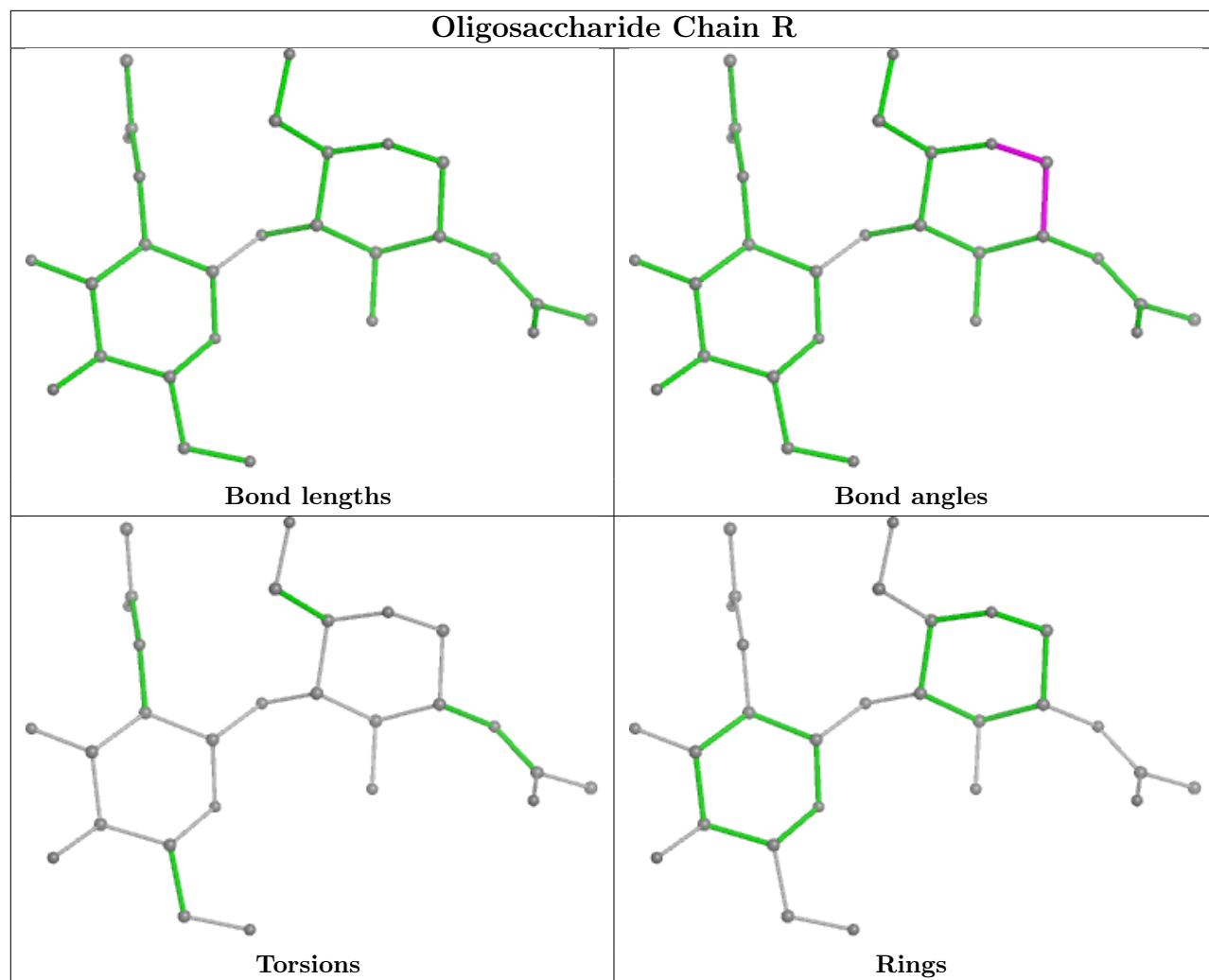


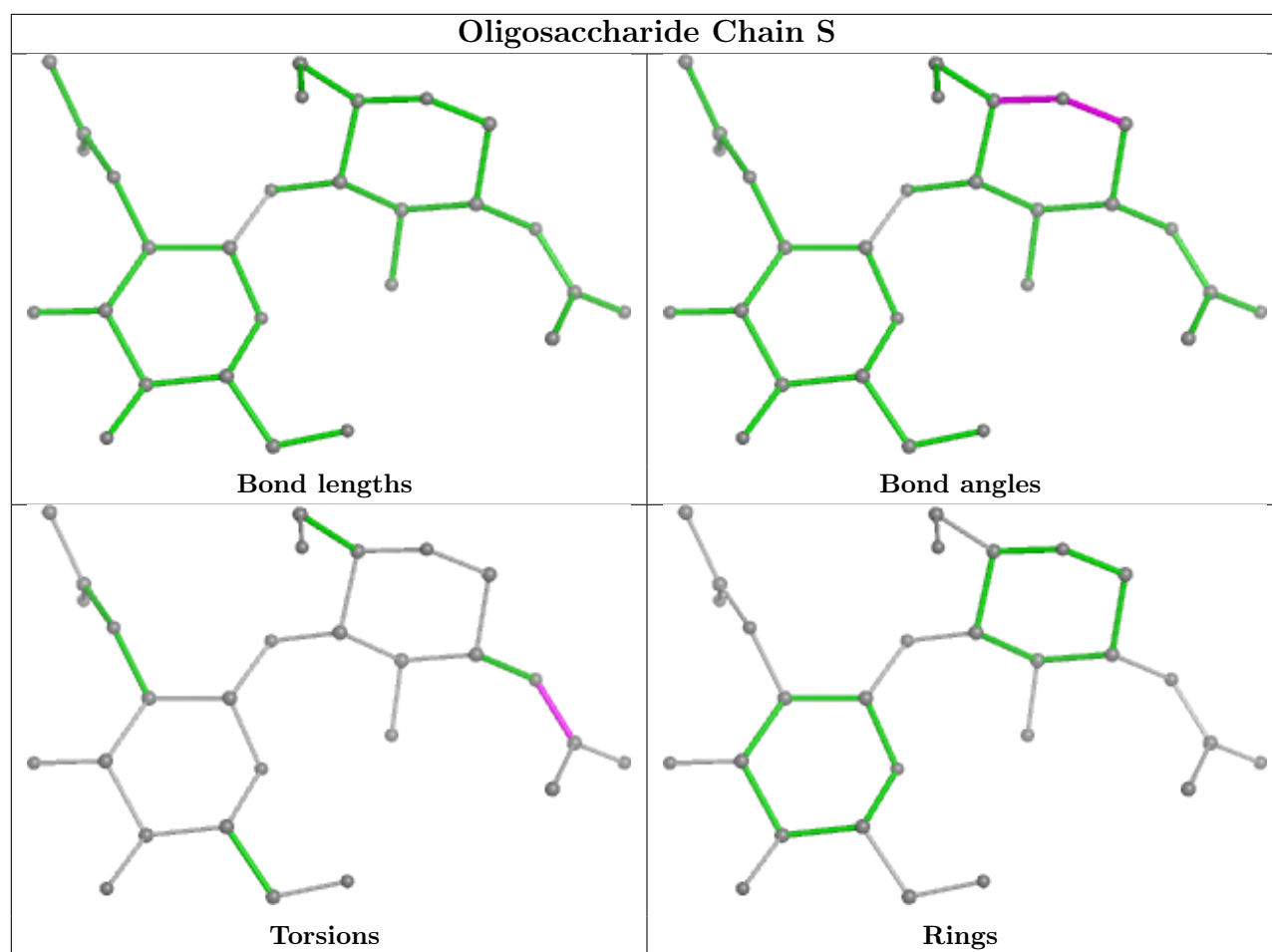


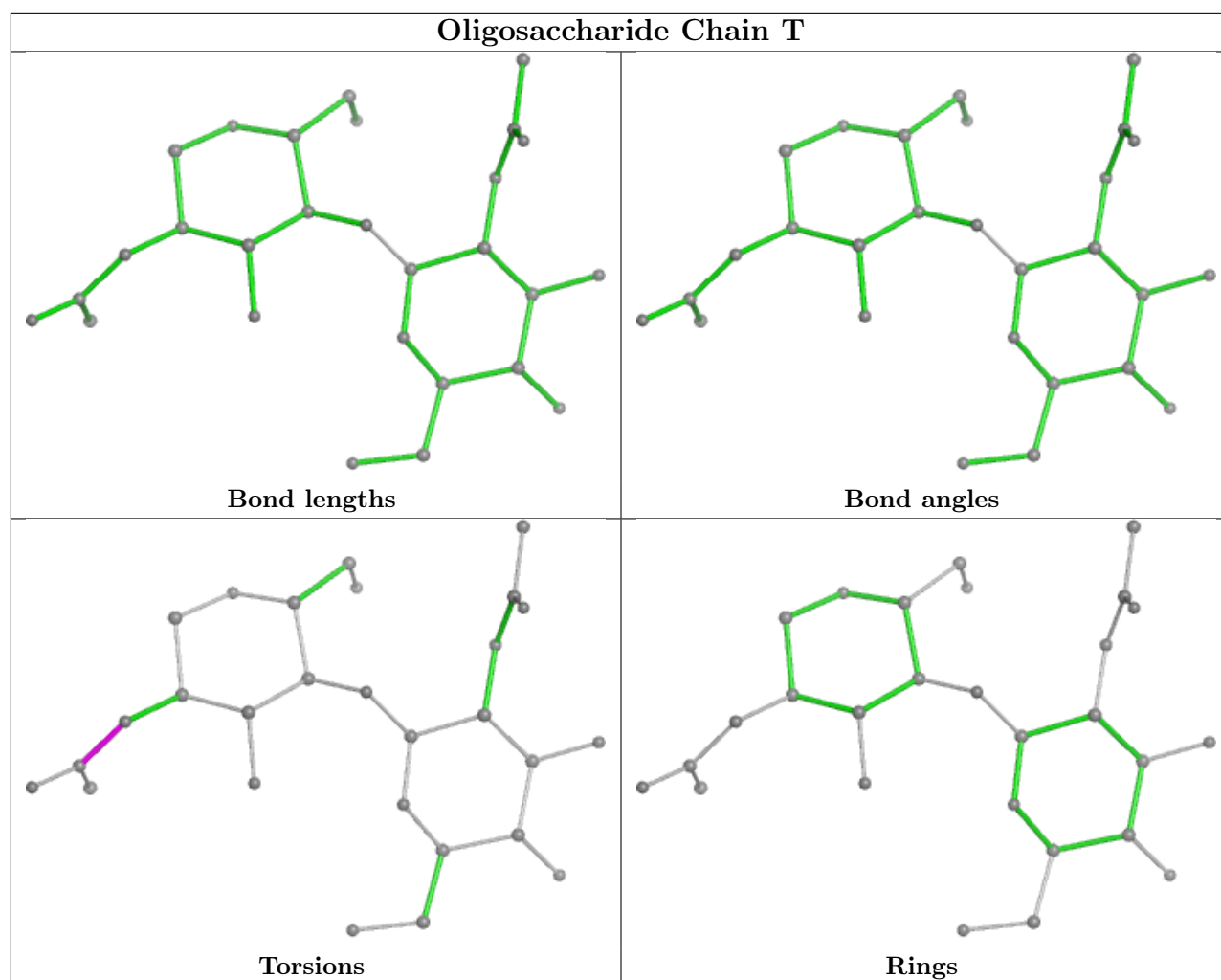


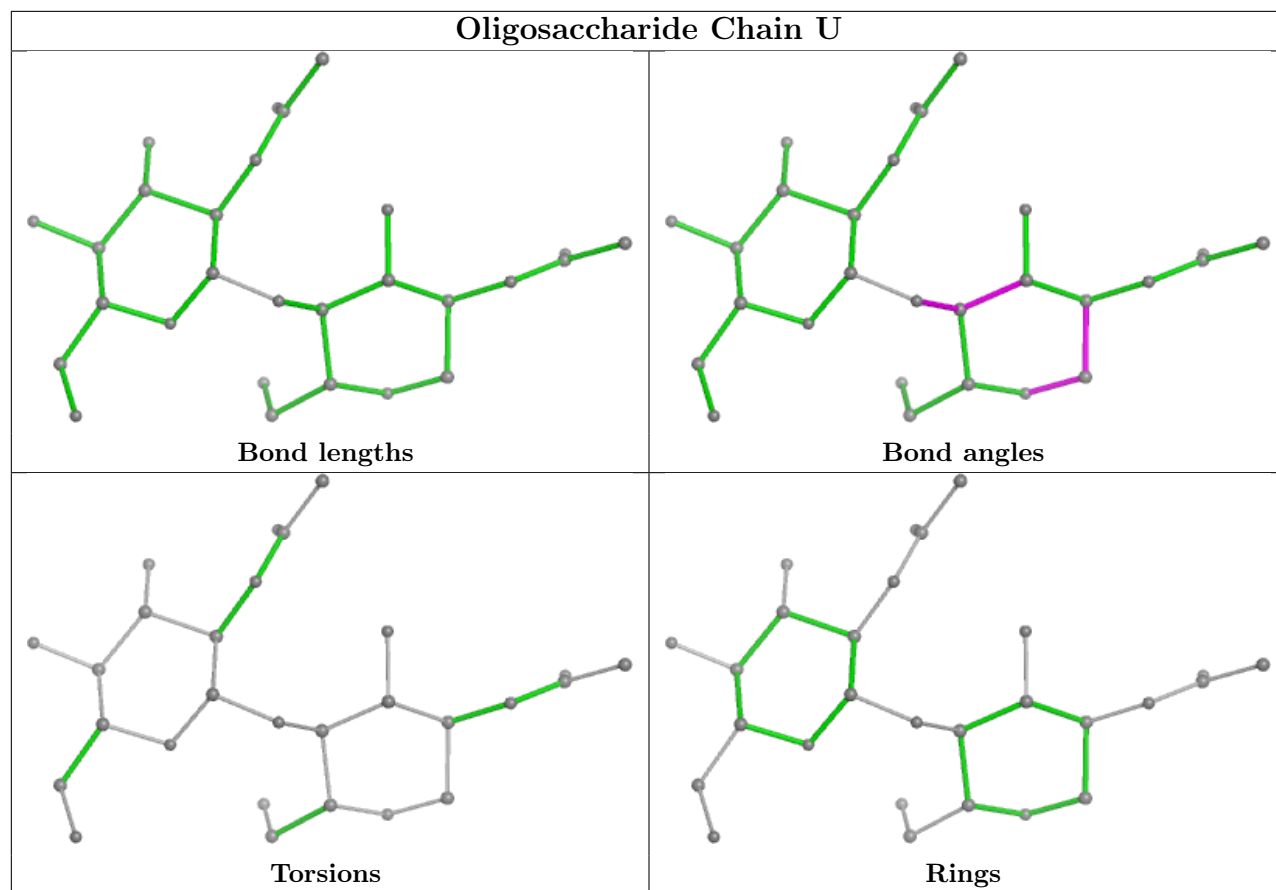


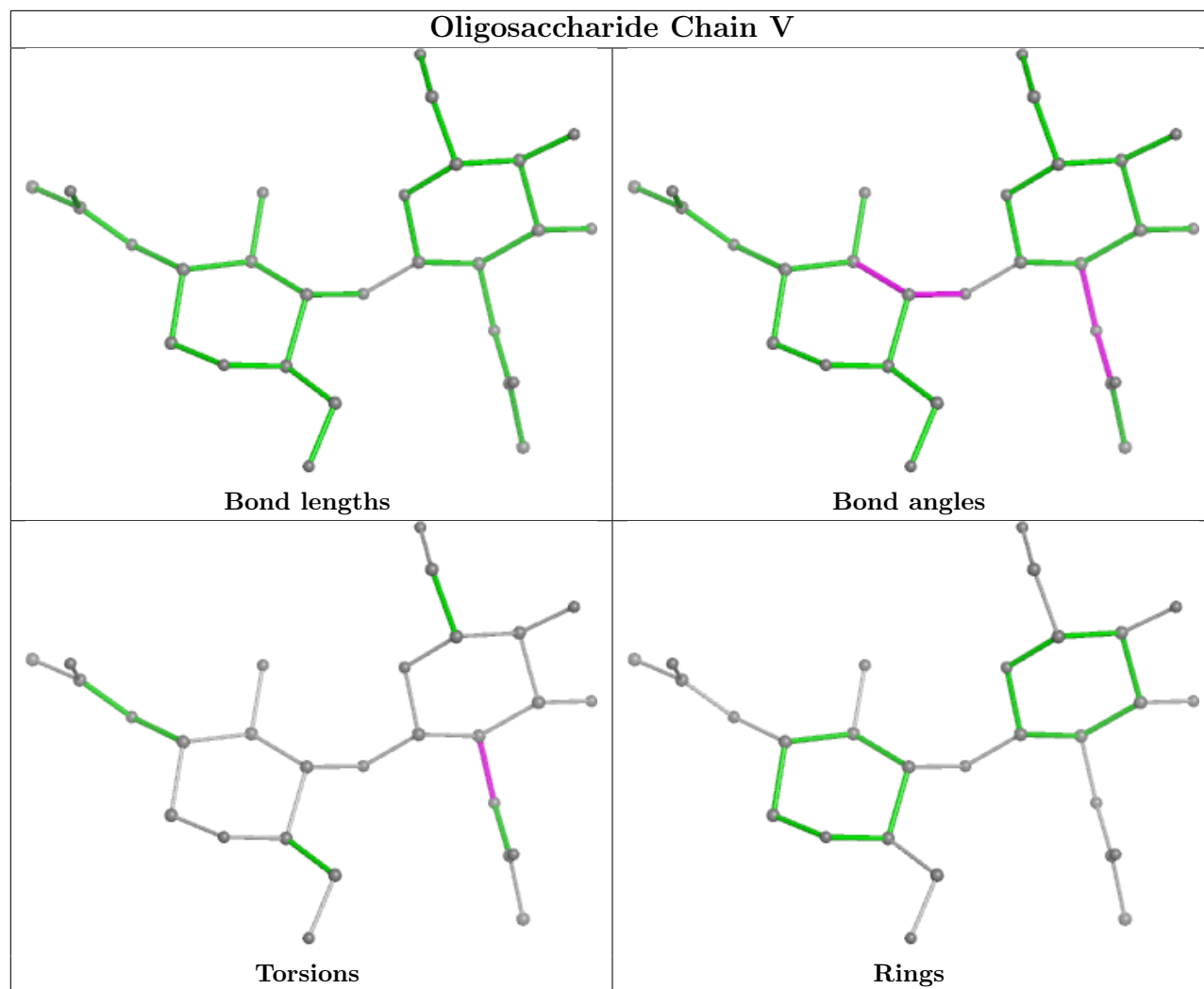






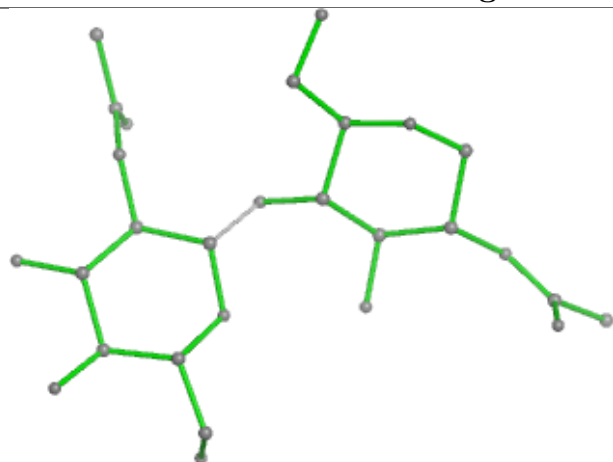




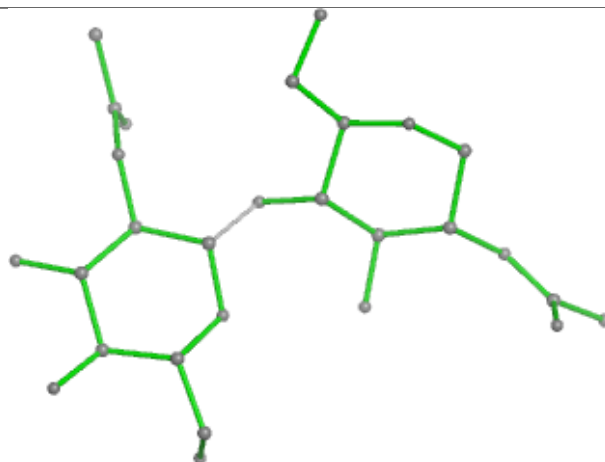




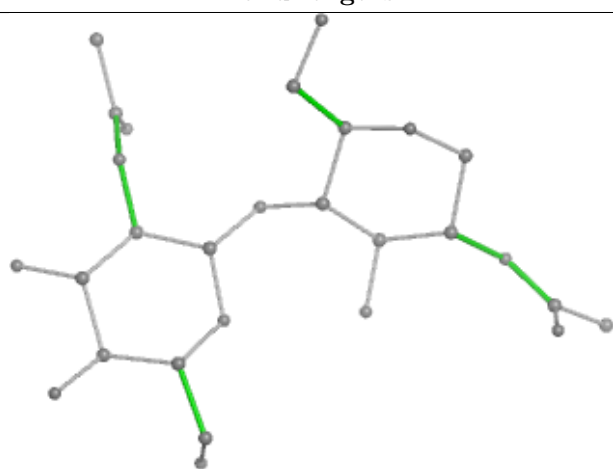
## Oligosaccharide Chain W



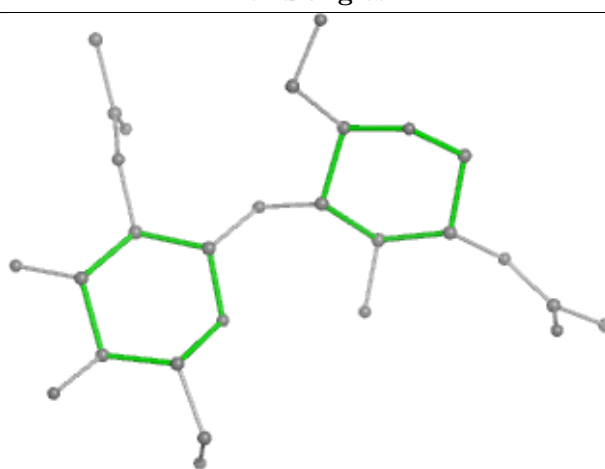
Bond lengths



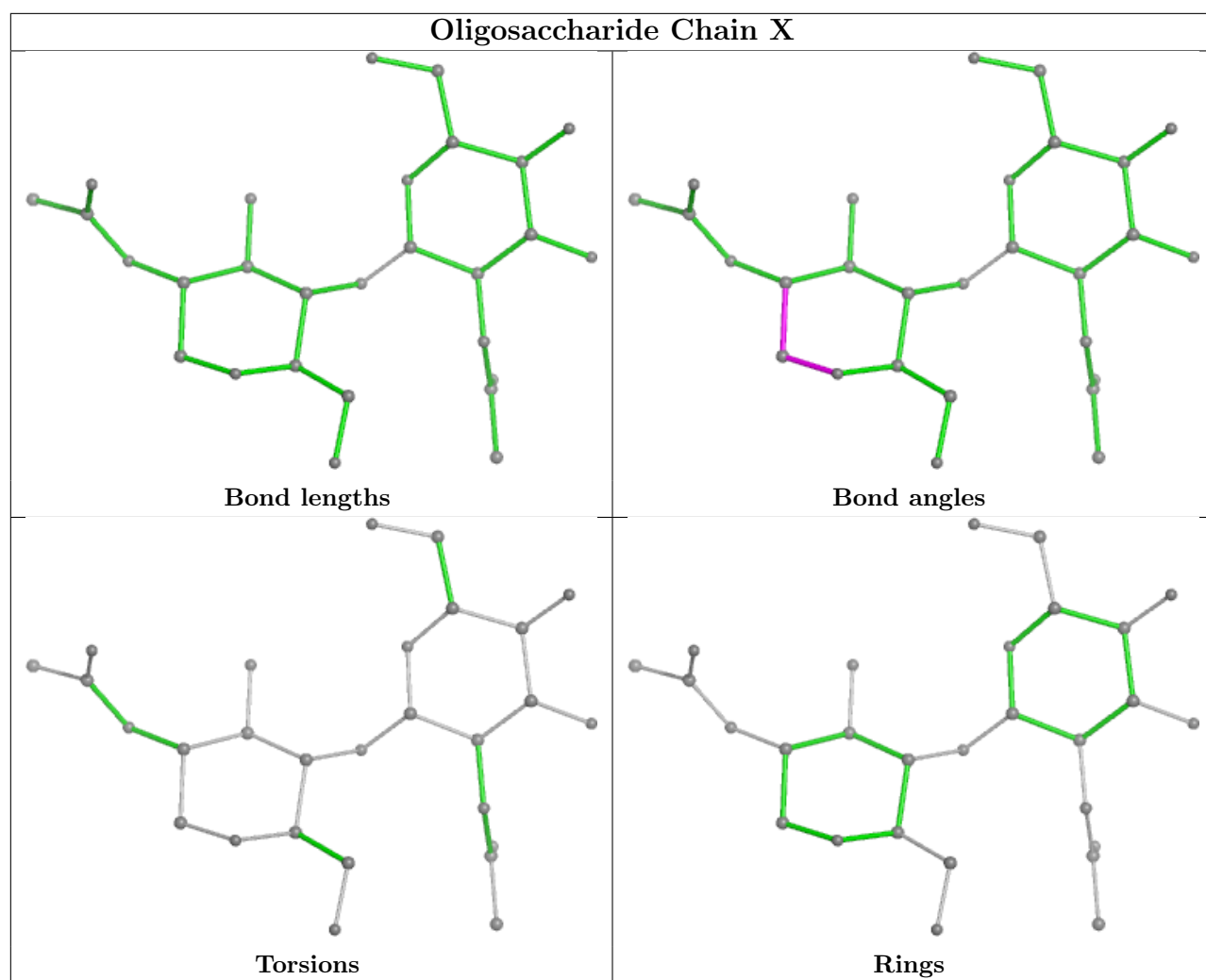
Bond angles

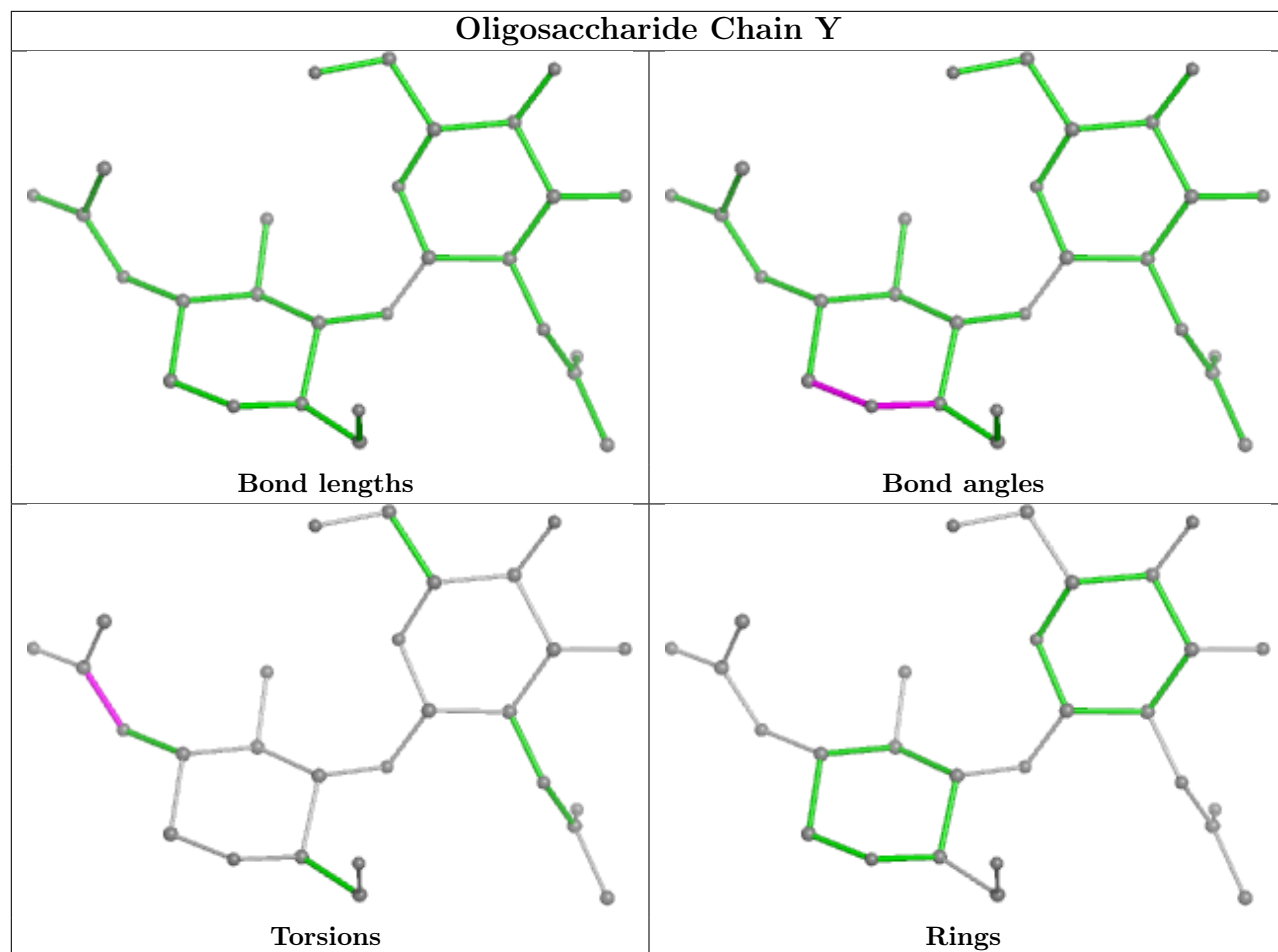


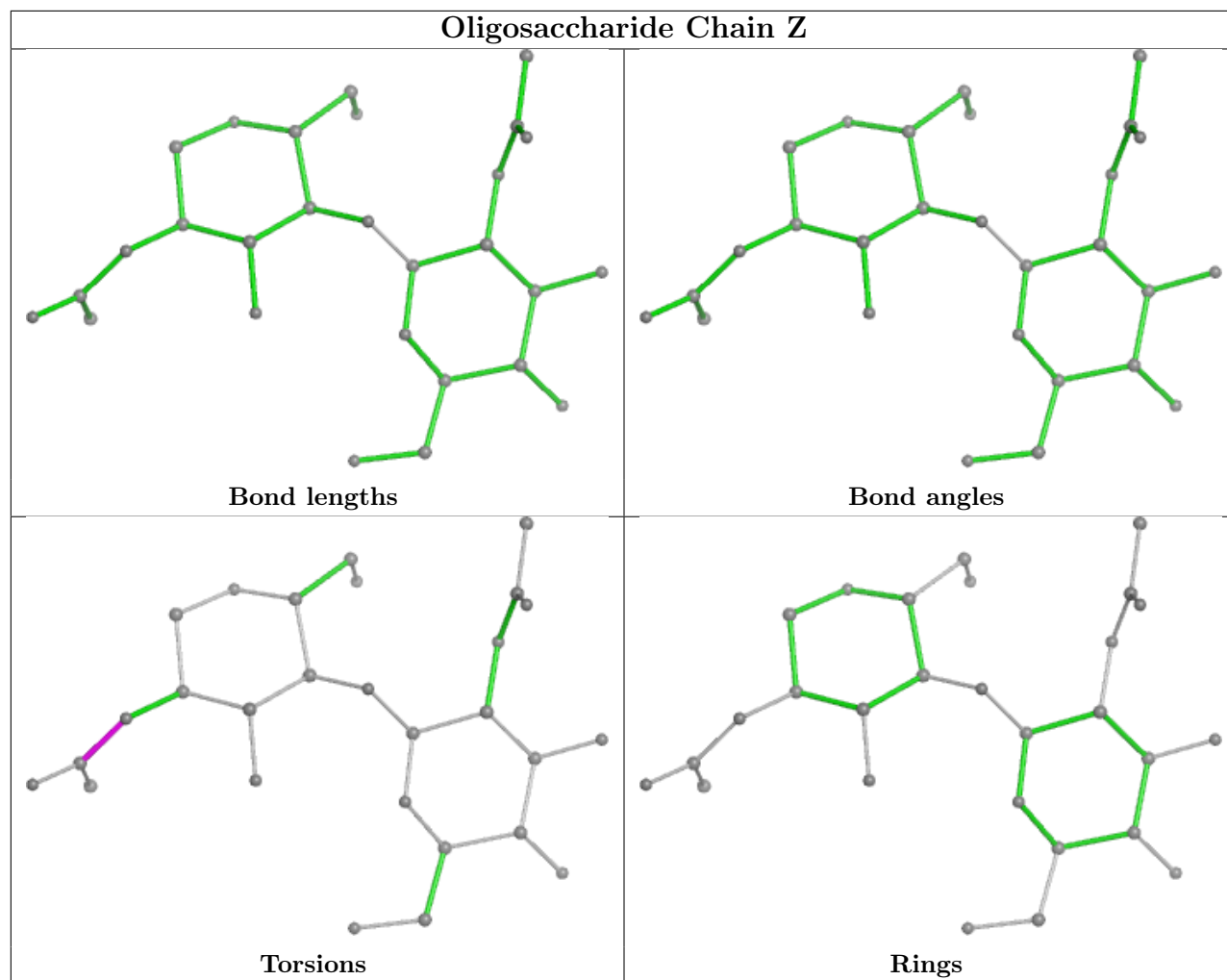
Torsions

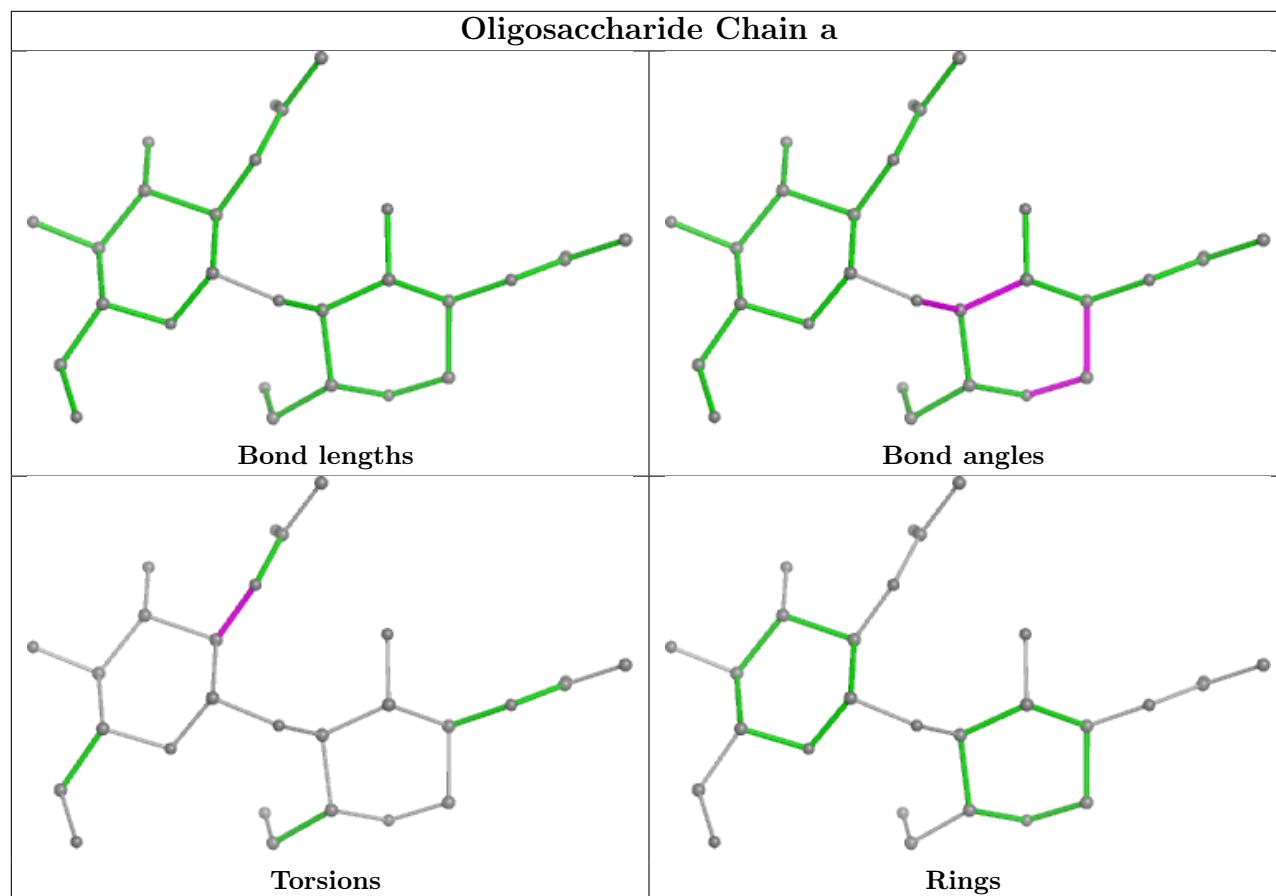


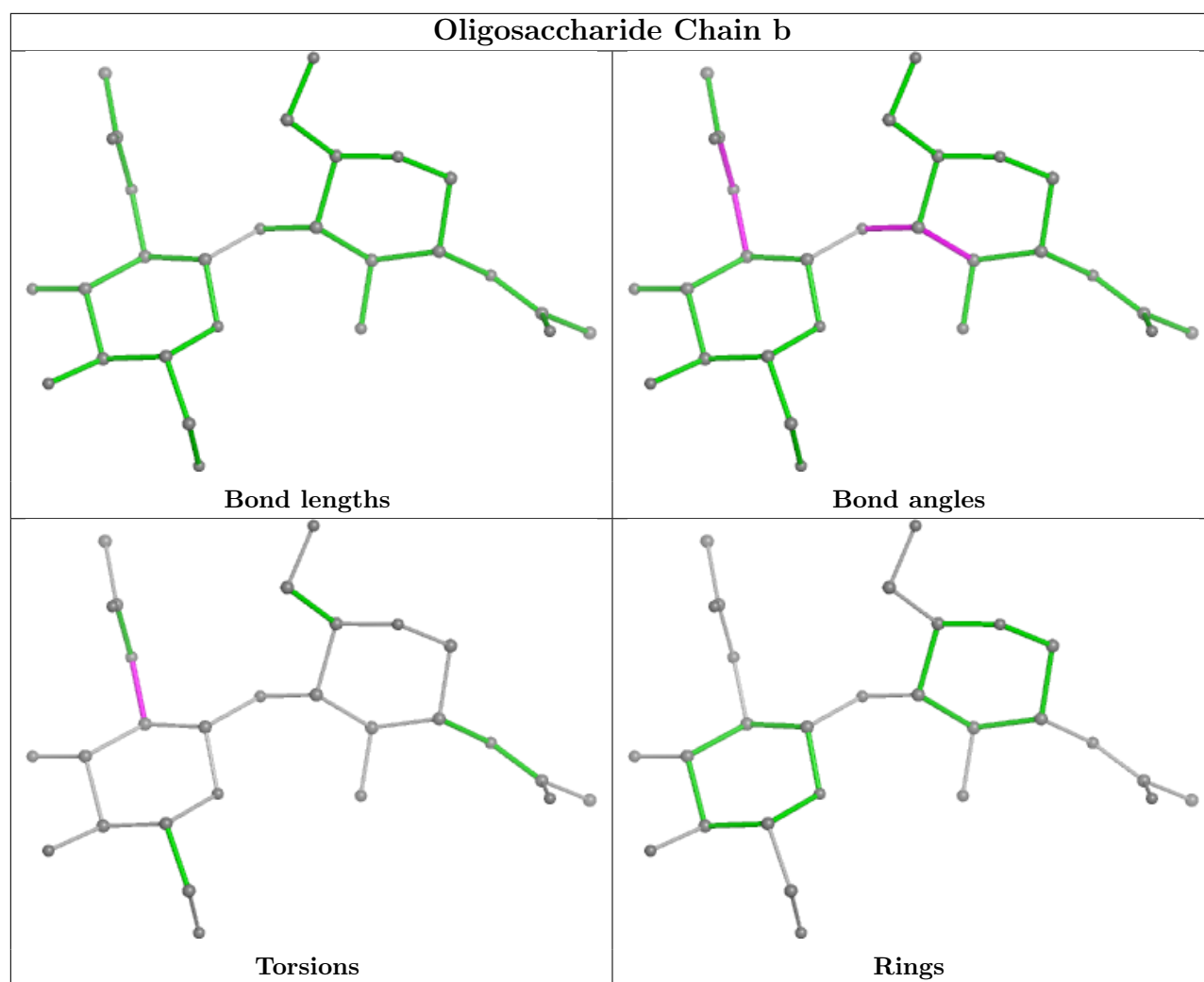
Rings

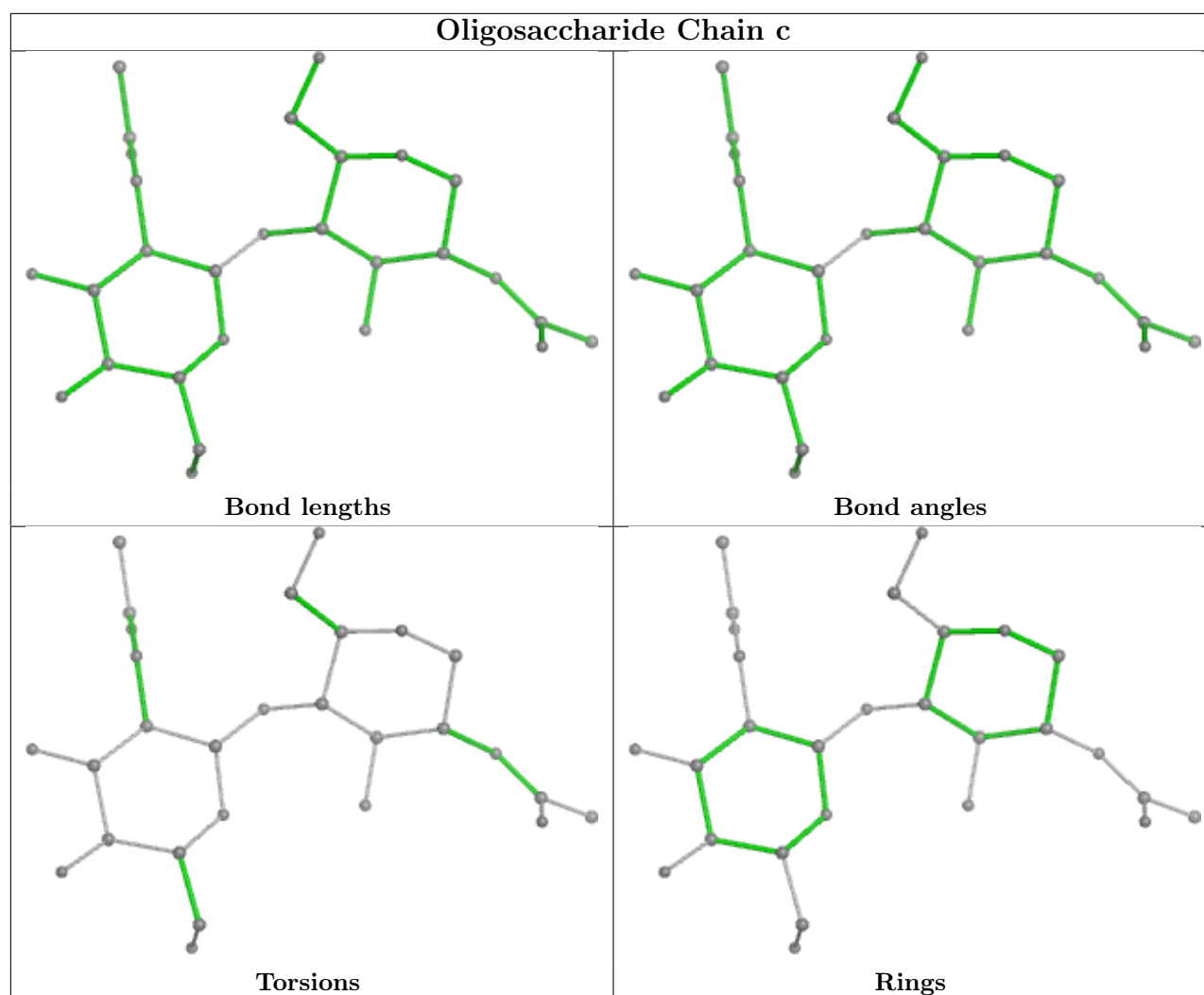












## 5.6 Ligand geometry [i](#)

24 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	N	604	2	14,14,15	0.72	0	17,19,21	0.88	0
8	NAG	N	608	2	14,14,15	0.74	0	17,19,21	1.00	1 (5%)
8	NAG	G	605	2	14,14,15	0.70	0	17,19,21	0.85	0
8	NAG	G	604	2	14,14,15	0.70	0	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	C	605	2	14,14,15	0.70	0	17,19,21	0.88	0
8	NAG	G	602	2	14,14,15	0.70	0	17,19,21	0.88	0
8	NAG	G	603	2	14,14,15	0.74	0	17,19,21	0.90	0
8	NAG	C	602	2	14,14,15	0.71	0	17,19,21	0.89	0
8	NAG	C	601	2	14,14,15	0.70	0	17,19,21	0.86	0
8	NAG	C	604	2	14,14,15	0.71	0	17,19,21	0.85	0
8	NAG	N	601	2	14,14,15	0.71	0	17,19,21	0.85	0
8	NAG	G	607	2	14,14,15	0.77	0	17,19,21	2.28	3 (17%)
8	NAG	C	603	2	14,14,15	0.73	0	17,19,21	0.91	0
8	NAG	C	608	2	14,14,15	0.73	0	17,19,21	1.13	2 (11%)
8	NAG	G	601	2	14,14,15	0.70	0	17,19,21	0.87	0
8	NAG	N	605	2	14,14,15	0.71	0	17,19,21	0.87	0
8	NAG	N	603	2	14,14,15	0.71	0	17,19,21	1.06	2 (11%)
8	NAG	C	606	2	14,14,15	0.74	0	17,19,21	0.94	1 (5%)
8	NAG	G	606	2	14,14,15	0.74	0	17,19,21	0.97	1 (5%)
8	NAG	G	608	2	14,14,15	0.69	0	17,19,21	1.55	2 (11%)
8	NAG	N	607	2	14,14,15	0.77	0	17,19,21	2.26	2 (11%)
8	NAG	C	607	2	14,14,15	0.76	0	17,19,21	2.26	2 (11%)
8	NAG	N	602	2	14,14,15	0.70	0	17,19,21	0.87	0
8	NAG	N	606	2	14,14,15	0.76	0	17,19,21	0.97	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	N	604	2	-	3/6/23/26	0/1/1/1
8	NAG	N	608	2	-	2/6/23/26	0/1/1/1
8	NAG	G	605	2	-	2/6/23/26	0/1/1/1
8	NAG	G	604	2	-	3/6/23/26	0/1/1/1
8	NAG	C	605	2	-	2/6/23/26	0/1/1/1
8	NAG	G	602	2	-	2/6/23/26	0/1/1/1
8	NAG	G	603	2	-	2/6/23/26	0/1/1/1
8	NAG	C	602	2	-	2/6/23/26	0/1/1/1
8	NAG	C	601	2	-	0/6/23/26	0/1/1/1
8	NAG	C	604	2	-	3/6/23/26	0/1/1/1
8	NAG	N	601	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	G	607	2	-	3/6/23/26	0/1/1/1
8	NAG	C	603	2	-	2/6/23/26	0/1/1/1
8	NAG	C	608	2	-	0/6/23/26	0/1/1/1
8	NAG	G	601	2	-	0/6/23/26	0/1/1/1
8	NAG	N	605	2	-	2/6/23/26	0/1/1/1
8	NAG	N	603	2	-	2/6/23/26	0/1/1/1
8	NAG	C	606	2	-	0/6/23/26	0/1/1/1
8	NAG	G	606	2	-	0/6/23/26	0/1/1/1
8	NAG	G	608	2	-	1/6/23/26	0/1/1/1
8	NAG	N	607	2	-	3/6/23/26	0/1/1/1
8	NAG	C	607	2	-	3/6/23/26	0/1/1/1
8	NAG	N	602	2	-	2/6/23/26	0/1/1/1
8	NAG	N	606	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	607	NAG	C2-N2-C7	7.83	134.06	122.90
8	C	607	NAG	C2-N2-C7	7.78	133.99	122.90
8	N	607	NAG	C2-N2-C7	7.78	133.98	122.90
8	G	608	NAG	C2-N2-C7	4.10	128.74	122.90
8	C	607	NAG	C8-C7-N2	2.67	120.63	116.10

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	602	NAG	C8-C7-N2-C2
8	C	602	NAG	O7-C7-N2-C2
8	C	603	NAG	C8-C7-N2-C2
8	C	603	NAG	O7-C7-N2-C2
8	C	604	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	606	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	606	NAG	1	0
8	N	606	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

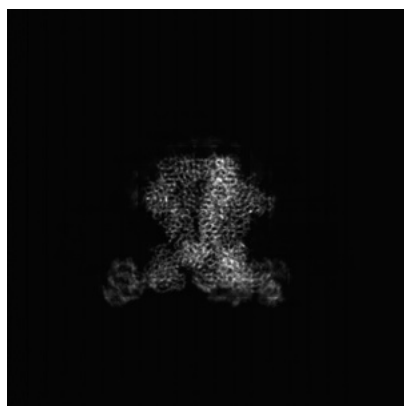
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50092. These allow visual inspection of the internal detail of the map and identification of artifacts.

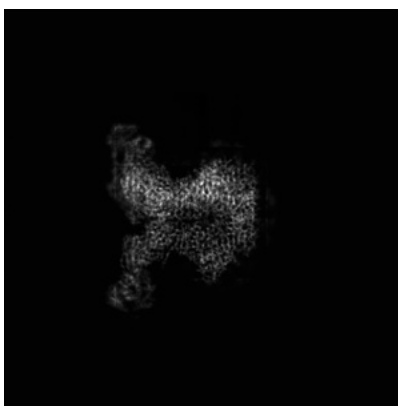
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

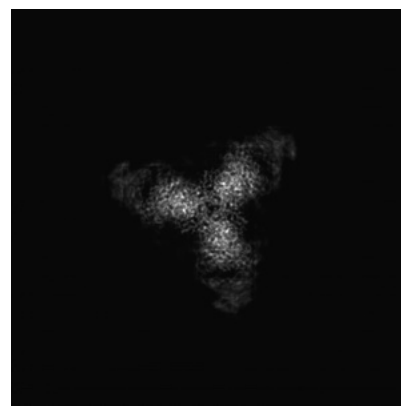
#### 6.1.1 Primary map



X

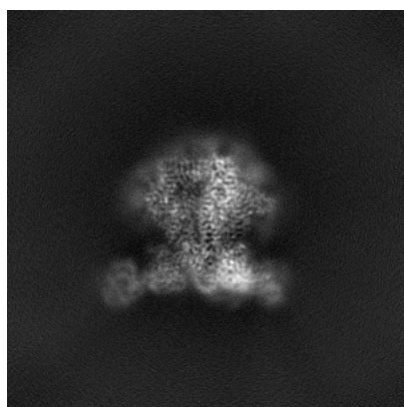


Y

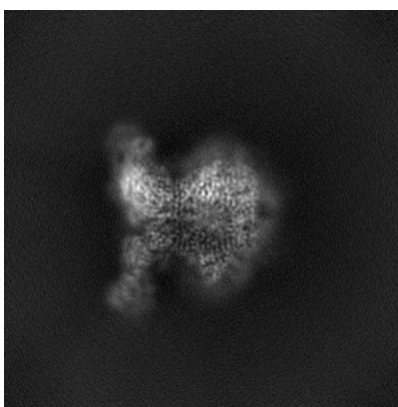


Z

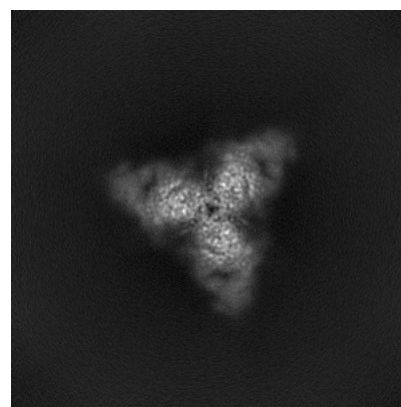
#### 6.1.2 Raw map



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: 180

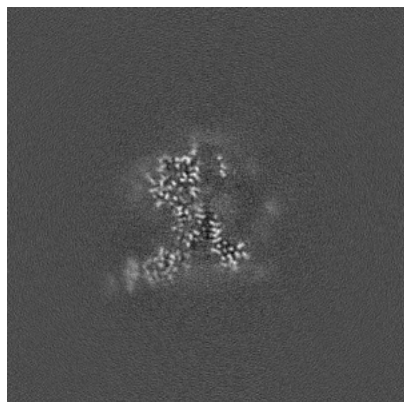


Y Index: 180

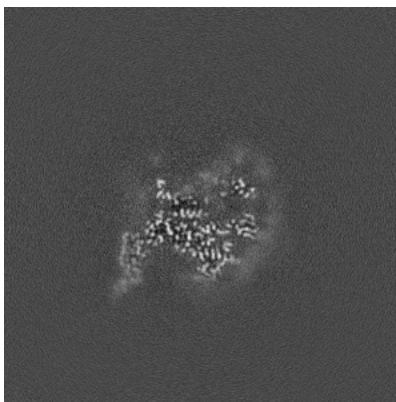


Z Index: 180

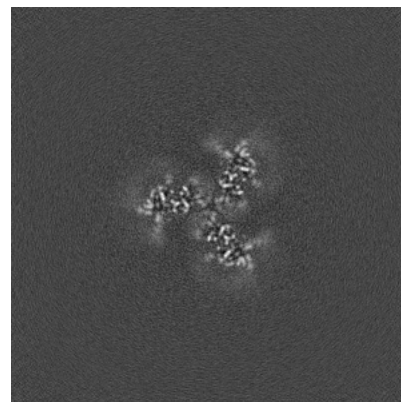
### 6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

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: 191

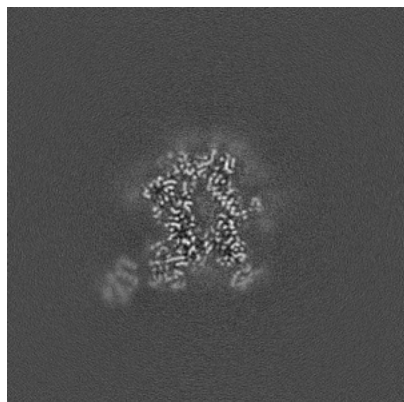


Y Index: 197

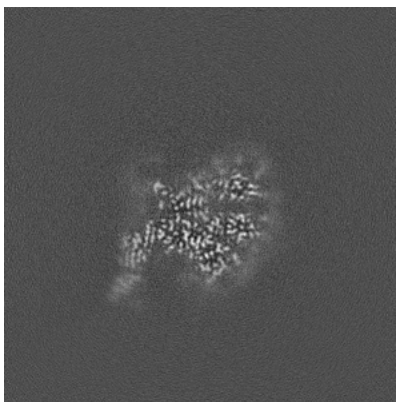


Z Index: 188

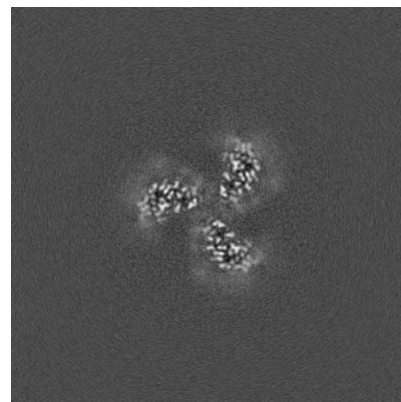
### 6.3.2 Raw map



X Index: 191



Y Index: 184

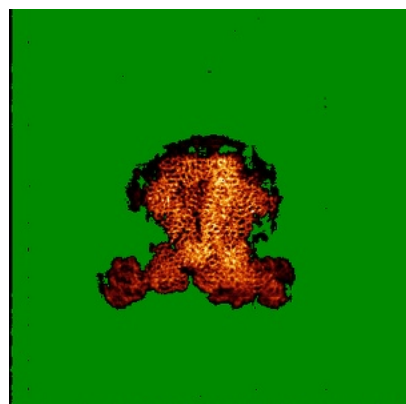


Z Index: 188

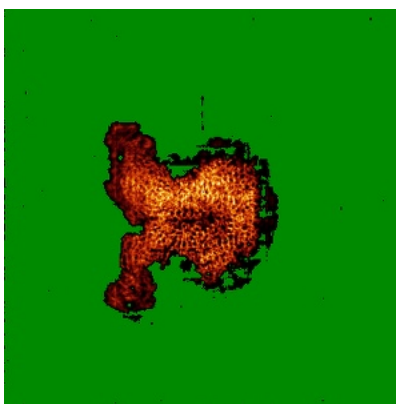
The images above show the largest variance slices of the map in three orthogonal directions.

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

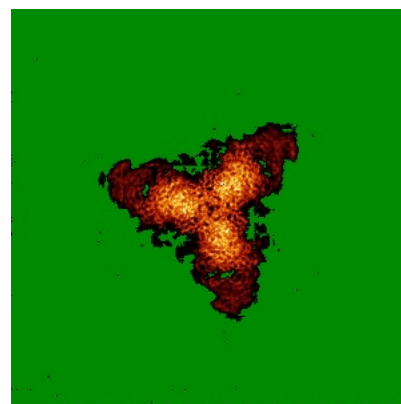
### 6.4.1 Primary map



X

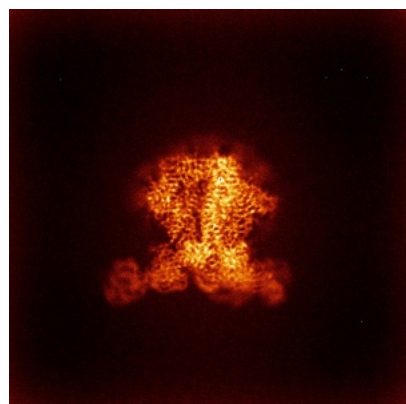


Y

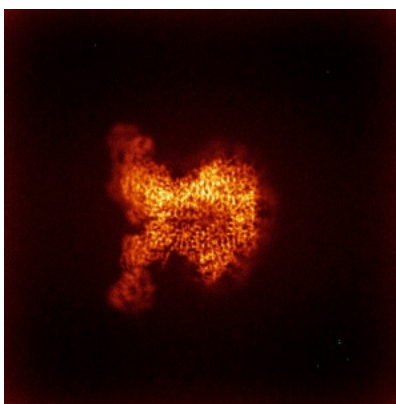


Z

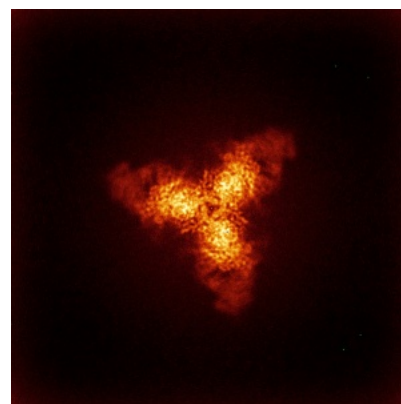
### 6.4.2 Raw map



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.



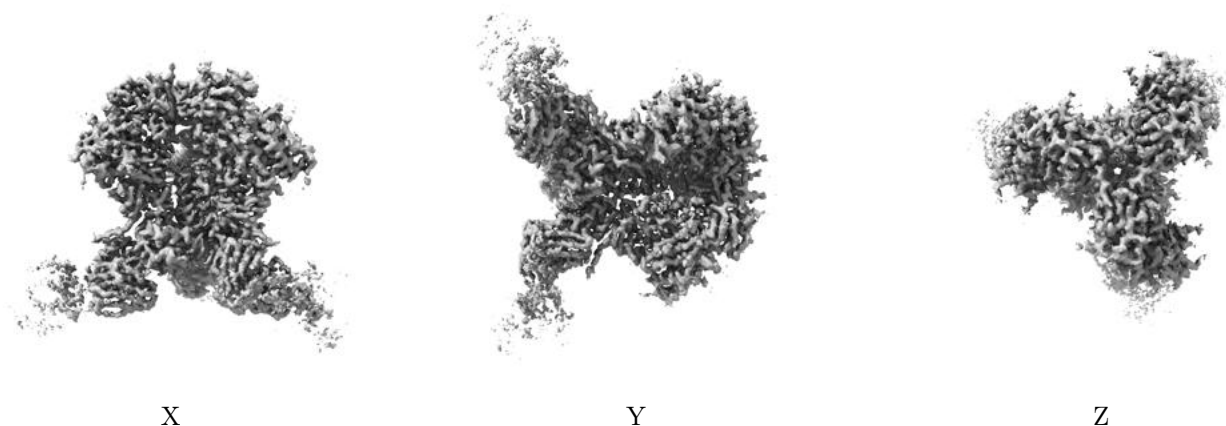
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.139. 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.

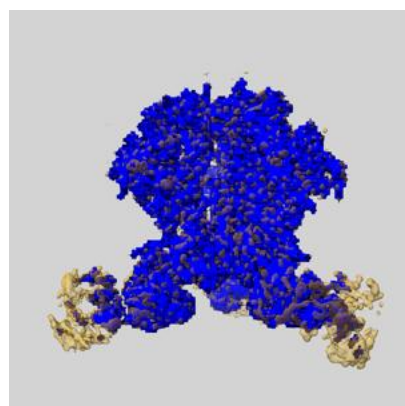
## 6.6 Mask visualisation [i](#)

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

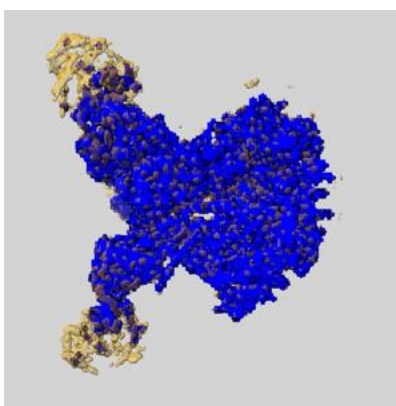
A mask typically either:

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

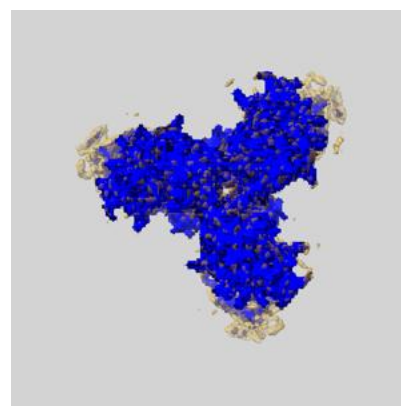
### 6.6.1 emd\_50092\_msk\_1.map [i](#)



X



Y



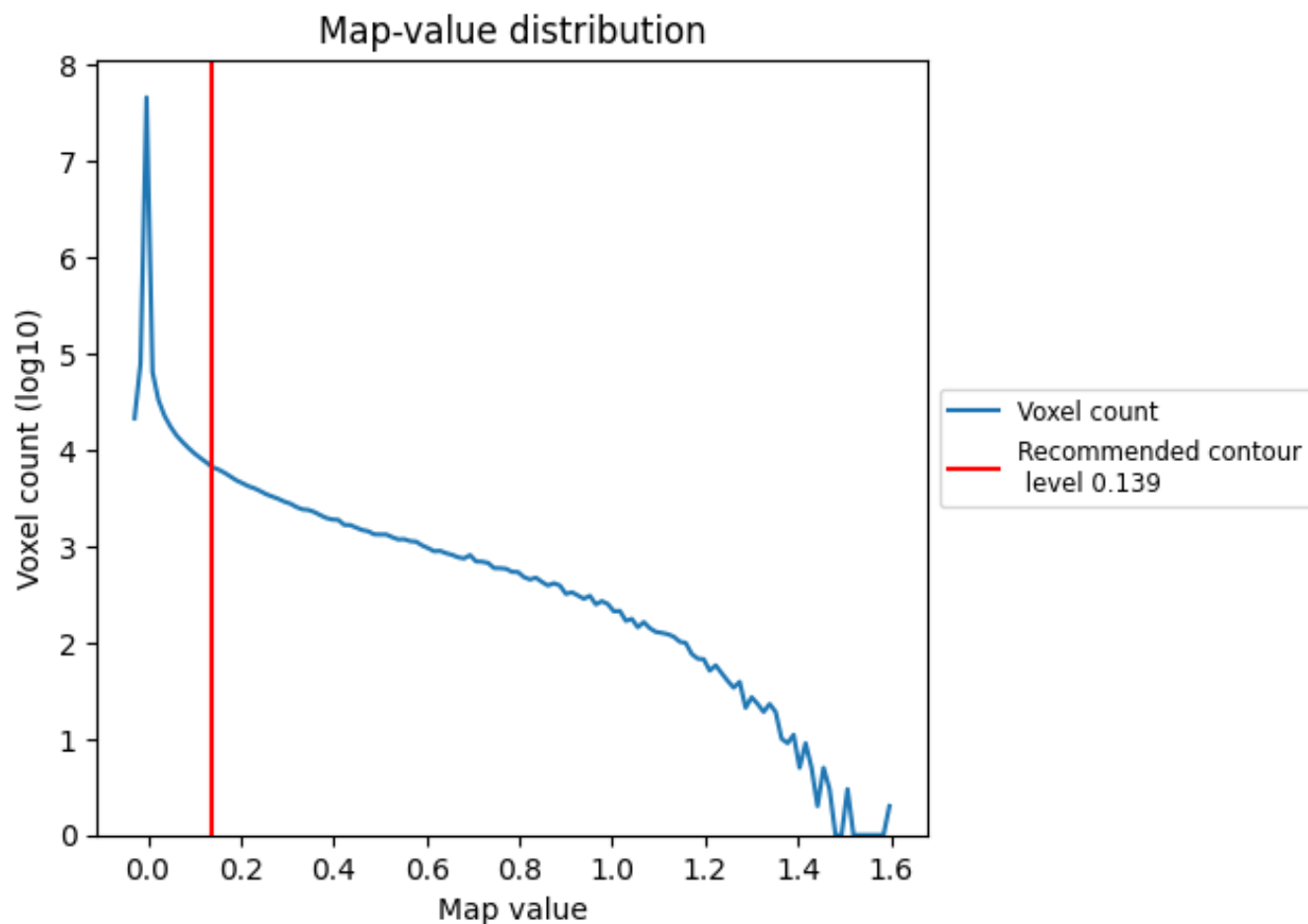
Z



## 7 Map analysis [i](#)

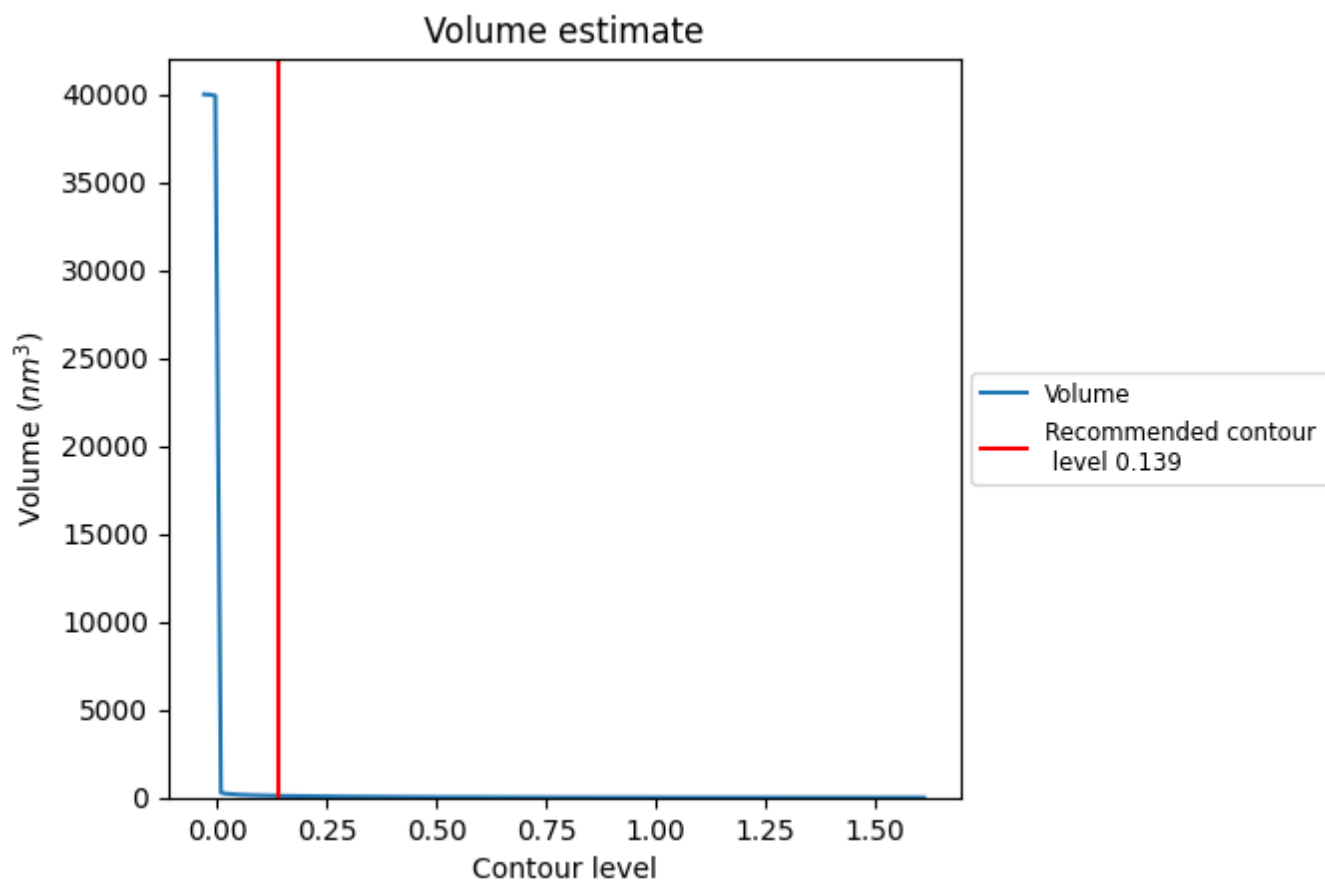
This section contains the results of statistical analysis of the map.

### 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.

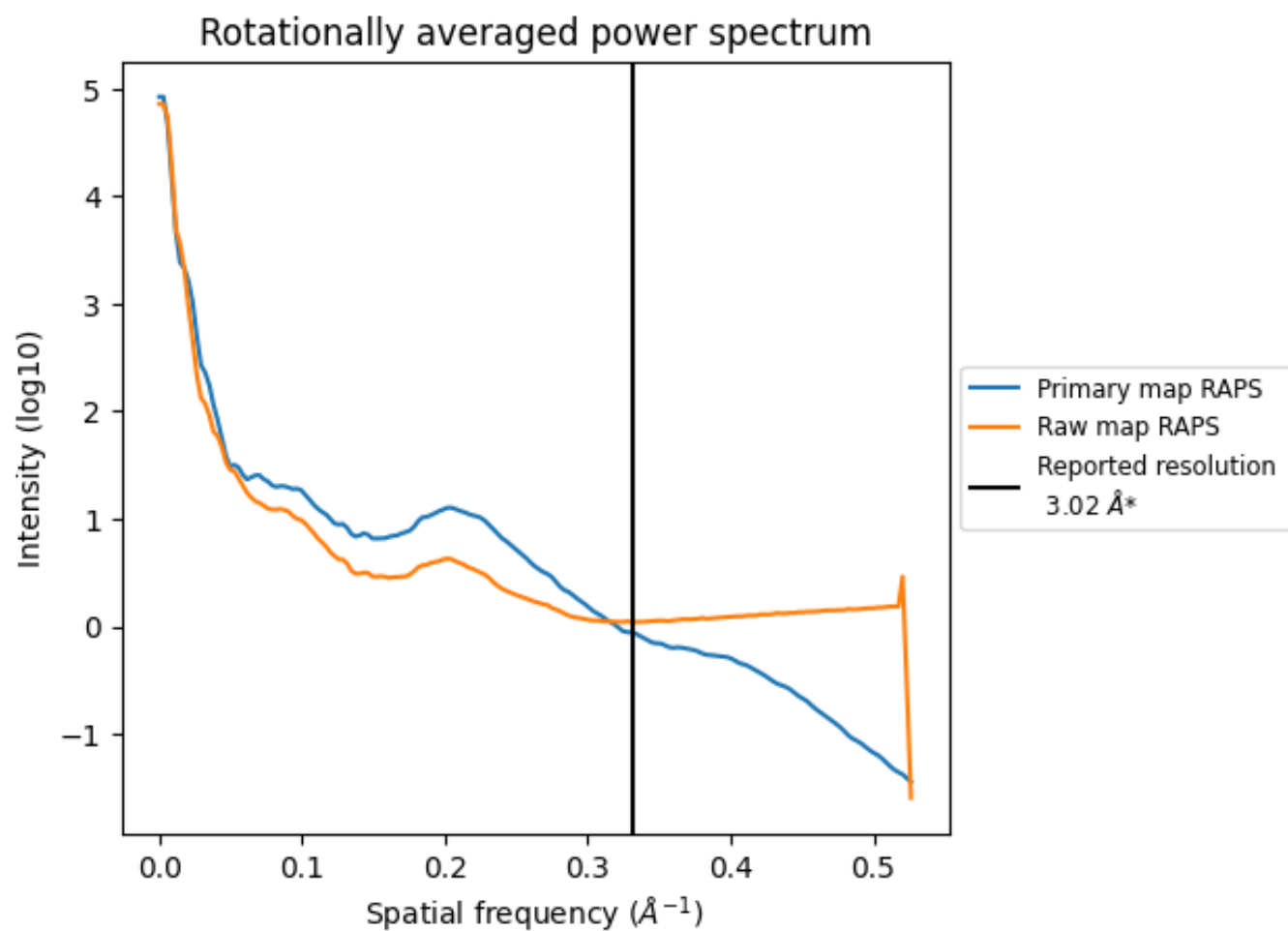
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100  $\text{nm}^3$ ; this corresponds to an approximate mass of 90 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

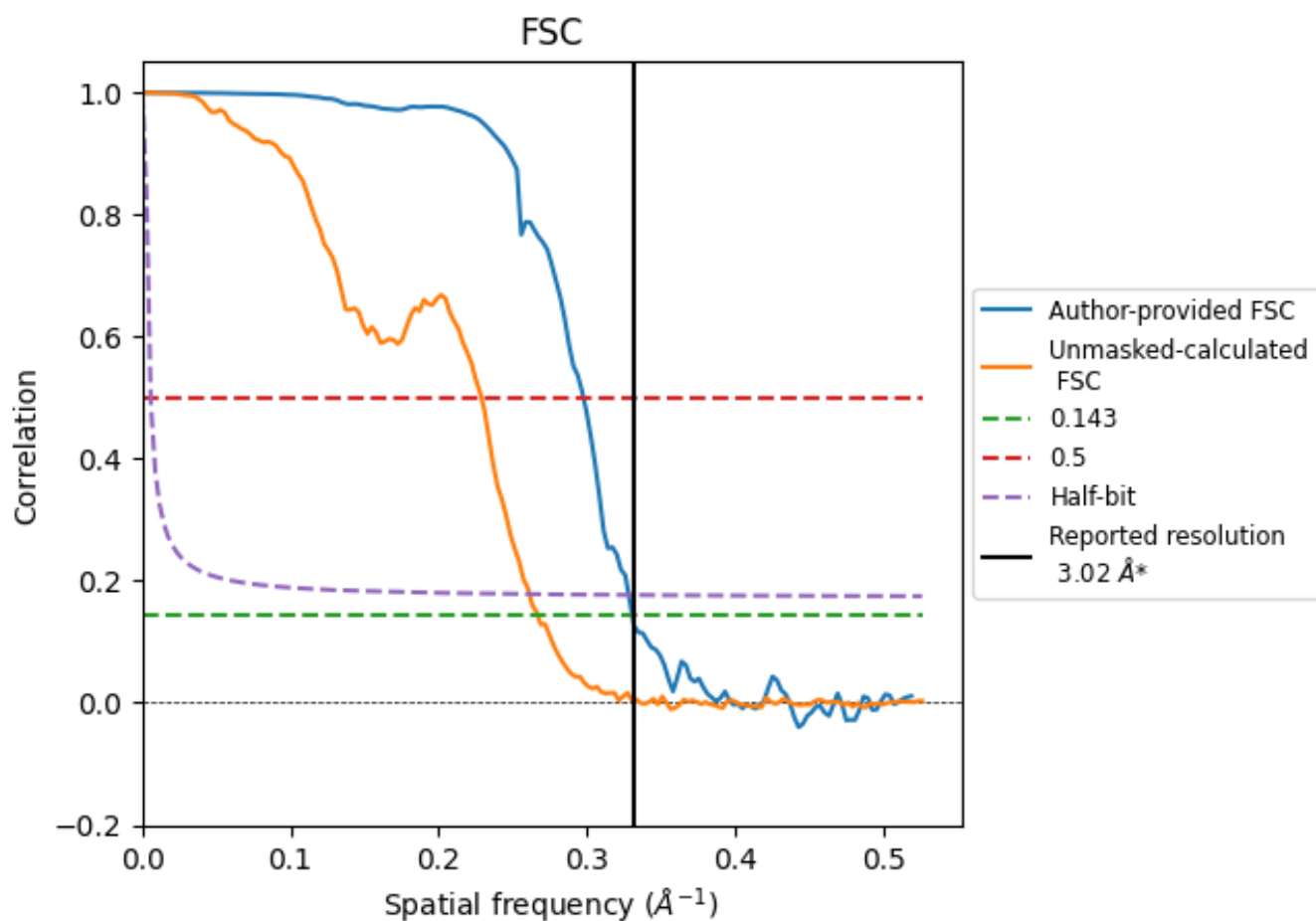


\*Reported resolution corresponds to spatial frequency of  $0.331 \text{ \AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

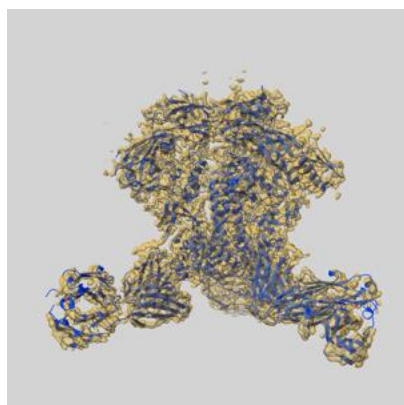
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.36	3.05
Unmasked-calculated*	3.75	4.37	3.83

\*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 3.75 differs from the reported value 3.02 by more than 10 %

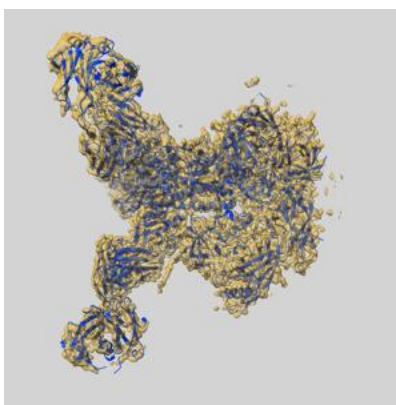
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50092 and PDB model 9F02. Per-residue inclusion information can be found in section 3 on page 16.

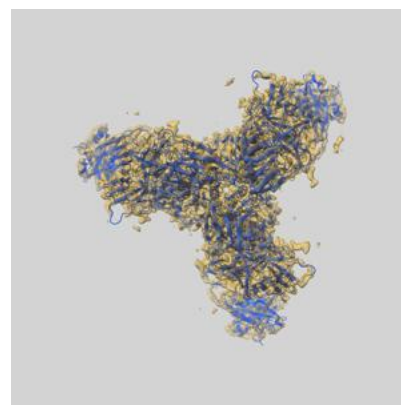
### 9.1 Map-model overlay [i](#)



X



Y



Z

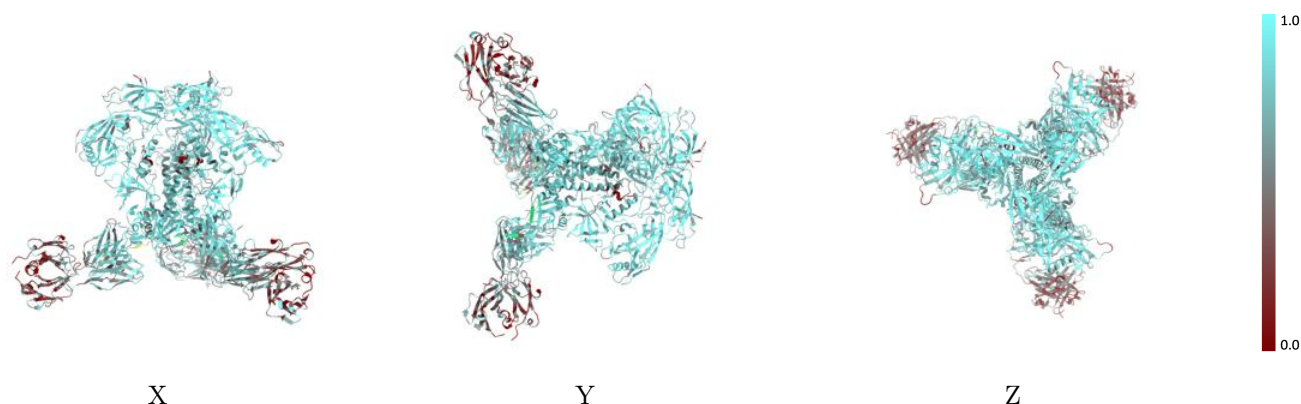
The images above show the 3D surface view of the map at the recommended contour level 0.139 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



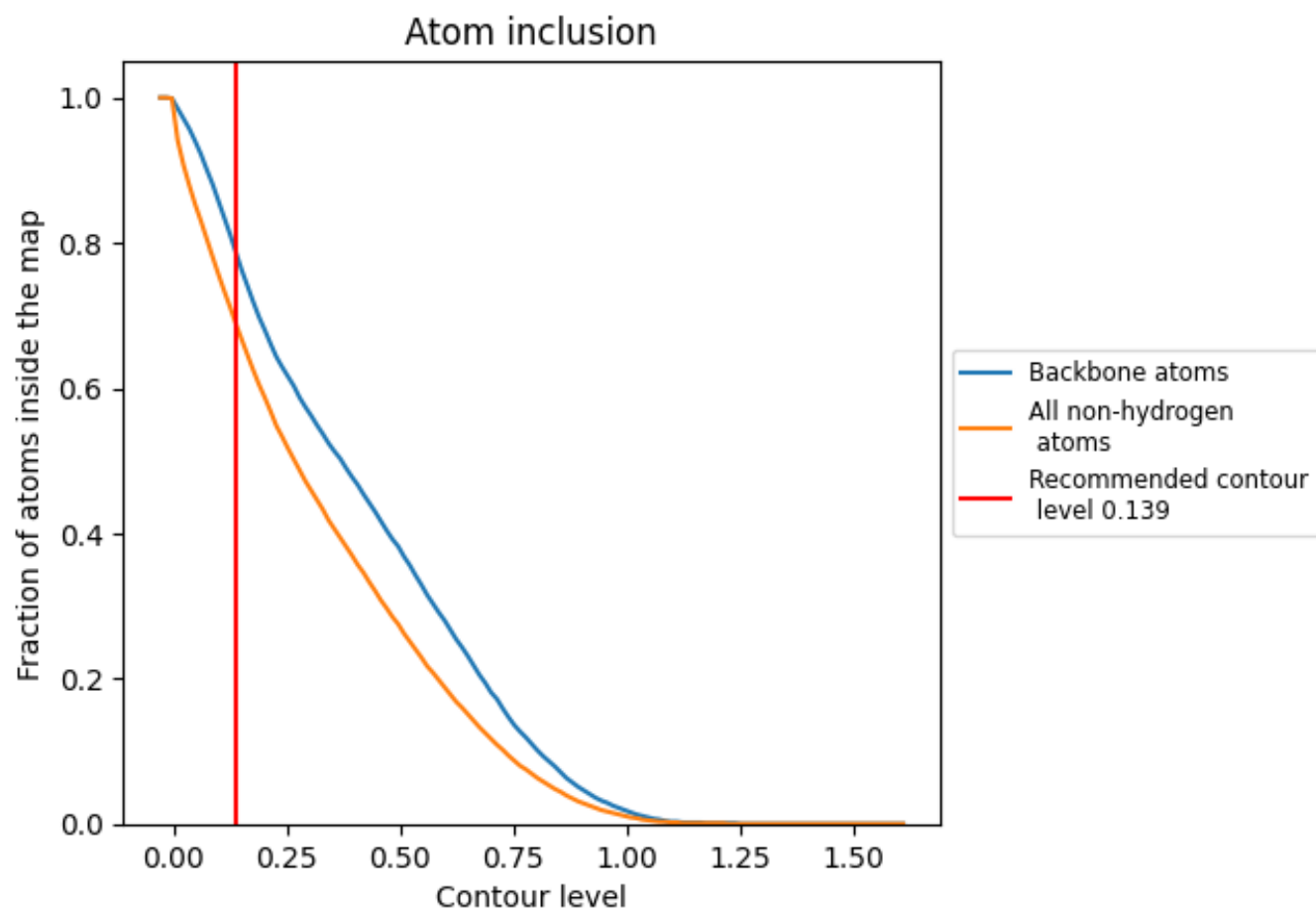
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.139).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 78% of all backbone atoms, 69% 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 (0.139) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6870	 0.4600
A	 0.8250	 0.5690
B	 0.4640	 0.3430
C	 0.7990	 0.5490
D	 0.3930	 0.2880
E	 0.8180	 0.5730
F	 0.8210	 0.5720
G	 0.7890	 0.5450
H	 0.5690	 0.3630
I	 0.5750	 0.3680
J	 0.5660	 0.3250
K	 0.5680	 0.3680
L	 0.5280	 0.3090
M	 0.5290	 0.3110
N	 0.7890	 0.5480
O	 0.5360	 0.3830
P	 0.4640	 0.4670
Q	 0.3210	 0.3890
R	 0.3570	 0.4060
S	 0.4290	 0.3300
T	 0.3210	 0.3490
U	 0.5000	 0.3720
V	 0.3210	 0.4330
W	 0.2860	 0.4370
X	 0.6070	 0.4000
Y	 0.4290	 0.3410
Z	 0.3570	 0.2810
a	 0.3930	 0.3680
b	 0.2500	 0.4380
c	 0.2860	 0.4150
d	 0.5600	 0.4690
e	 0.3800	 0.4420
f	 0.7440	 0.5370
g	 0.4400	 0.4450
h	 0.6670	 0.5340



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Chain	Atom inclusion	Q-score
q	 0.7440	 0.5100
u	 0.2860	 0.3500