



## Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 06:54 PM UTC

PDB ID : 9D8J / pdb\_00009d8j  
EMDB ID : EMD-46639  
Title : KP.2 SARS-COV-2 Spike 3-down conformation  
Authors : Windsor, I.W.; Wu, H.  
Deposited on : 2024-08-19  
Resolution : 2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

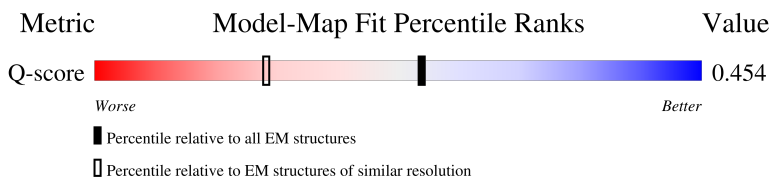
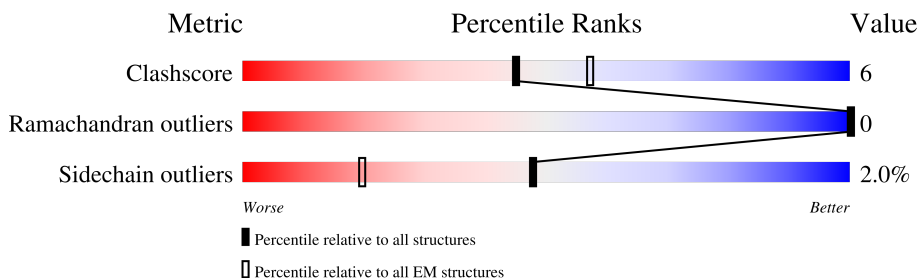
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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

















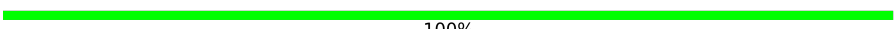
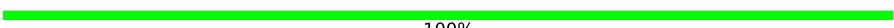
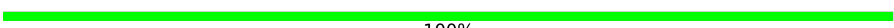
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 ( 2.40 - 3.40 )

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

Mol	Chain	Length	Quality of chain
1	A	1305	<div> <div>10%</div> <div>71%</div> <div>14%</div> <div>15%</div> </div>
1	B	1305	<div> <div>9%</div> <div>71%</div> <div>14%</div> <div>15%</div> </div>
1	C	1305	<div> <div>10%</div> <div>70%</div> <div>14%</div> <div>15%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	2	 50% 50%
2	F	2	 50% 50%
2	G	2	 50% 50%
2	I	2	 50% 50%
2	J	2	 50% 50%
2	K	2	 50% 50%
2	L	2	 50% 50%
2	M	2	 50% 50%
2	O	2	 50% 50%
2	P	2	 50% 50%
2	Q	2	 50% 50%
2	R	2	 50% 50%
2	S	2	 50% 50%
2	U	2	 50% 50%
3	H	3	 100%
3	N	3	 100%
3	T	3	 100%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27666 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1112	Total	C	N	O	S	23	0
			8918	5708	1475	1695	40		
1	B	1112	Total	C	N	O	S	23	0
			8918	5708	1475	1695	40		
1	C	1112	Total	C	N	O	S	23	0
			8918	5708	1475	1695	40		

There are 363 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A6N0C4S6
A	2	PHE	-	expression tag	UNP A0A6N0C4S6
A	3	VAL	-	expression tag	UNP A0A6N0C4S6
A	4	PHE	-	expression tag	UNP A0A6N0C4S6
A	5	LEU	-	expression tag	UNP A0A6N0C4S6
A	6	VAL	-	expression tag	UNP A0A6N0C4S6
A	7	LEU	-	expression tag	UNP A0A6N0C4S6
A	8	LEU	-	expression tag	UNP A0A6N0C4S6
A	9	PRO	-	expression tag	UNP A0A6N0C4S6
A	10	LEU	-	expression tag	UNP A0A6N0C4S6
A	11	VAL	-	expression tag	UNP A0A6N0C4S6
A	12	SER	-	expression tag	UNP A0A6N0C4S6
A	13	SER	-	expression tag	UNP A0A6N0C4S6
A	14	GLN	-	expression tag	UNP A0A6N0C4S6
A	15	CYS	-	expression tag	UNP A0A6N0C4S6
A	16	VAL	-	expression tag	UNP A0A6N0C4S6
A	17	MET	-	expression tag	UNP A0A6N0C4S6
A	18	PRO	-	expression tag	UNP A0A6N0C4S6
A	19	LEU	-	expression tag	UNP A0A6N0C4S6
A	20	PHE	-	expression tag	UNP A0A6N0C4S6
A	21	ASN	-	expression tag	UNP A0A6N0C4S6
A	22	LEU	-	expression tag	UNP A0A6N0C4S6
A	23	ILE	-	expression tag	UNP A0A6N0C4S6
A	24	THR	-	expression tag	UNP A0A6N0C4S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	THR	-	expression tag	UNP A0A6N0C4S6
A	26	THR	-	expression tag	UNP A0A6N0C4S6
A	27	GLN	-	expression tag	UNP A0A6N0C4S6
A	28	SER	-	expression tag	UNP A0A6N0C4S6
A	51	LEU	SER	conflict	UNP A0A6N0C4S6
A	?	-	HIS	deletion	UNP A0A6N0C4S6
A	?	-	VAL	deletion	UNP A0A6N0C4S6
A	126	PHE	VAL	conflict	UNP A0A6N0C4S6
A	141	ASP	GLY	conflict	UNP A0A6N0C4S6
A	?	-	TYR	deletion	UNP A0A6N0C4S6
A	155	SER	PHE	conflict	UNP A0A6N0C4S6
A	156	GLY	ARG	conflict	UNP A0A6N0C4S6
A	?	-	ASN	deletion	UNP A0A6N0C4S6
A	209	ILE	LEU	conflict	UNP A0A6N0C4S6
A	210	GLY	VAL	conflict	UNP A0A6N0C4S6
A	213	PHE	LEU	conflict	UNP A0A6N0C4S6
A	242	ASN	HIS	conflict	UNP A0A6N0C4S6
A	261	ASP	ALA	conflict	UNP A0A6N0C4S6
A	329	VAL	ILE	conflict	UNP A0A6N0C4S6
A	336	HIS	GLY	conflict	UNP A0A6N0C4S6
A	343	THR	ARG	conflict	UNP A0A6N0C4S6
A	353	THR	LYS	conflict	UNP A0A6N0C4S6
A	368	PHE	SER	conflict	UNP A0A6N0C4S6
A	370	PRO	SER	conflict	UNP A0A6N0C4S6
A	372	PHE	SER	conflict	UNP A0A6N0C4S6
A	373	ALA	THR	conflict	UNP A0A6N0C4S6
A	400	LYS	ARG	conflict	UNP A0A6N0C4S6
A	402	ASN	ASP	conflict	UNP A0A6N0C4S6
A	405	SER	ARG	conflict	UNP A0A6N0C4S6
A	414	ASN	LYS	conflict	UNP A0A6N0C4S6
A	437	LYS	ASN	conflict	UNP A0A6N0C4S6
A	442	HIS	VAL	conflict	UNP A0A6N0C4S6
A	443	SER	GLY	conflict	UNP A0A6N0C4S6
A	447	ASP	ASN	conflict	UNP A0A6N0C4S6
A	449	TRP	LEU	conflict	UNP A0A6N0C4S6
A	452	SER	LEU	conflict	UNP A0A6N0C4S6
A	453	LEU	PHE	conflict	UNP A0A6N0C4S6
A	457	LYS	ASN	conflict	UNP A0A6N0C4S6
A	474	ASN	SER	conflict	UNP A0A6N0C4S6
A	475	LYS	THR	conflict	UNP A0A6N0C4S6
A	478	LYS	ASN	conflict	UNP A0A6N0C4S6
A	?	-	VAL	deletion	UNP A0A6N0C4S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	480	LYS	GLU	conflict	UNP A0A6N0C4S6
A	482	PRO	PHE	conflict	UNP A0A6N0C4S6
A	494	ARG	GLN	conflict	UNP A0A6N0C4S6
A	497	TYR	ASN	conflict	UNP A0A6N0C4S6
A	501	HIS	TYR	conflict	UNP A0A6N0C4S6
A	550	LYS	GLU	conflict	UNP A0A6N0C4S6
A	566	VAL	ALA	conflict	UNP A0A6N0C4S6
A	617	SER	PRO	conflict	UNP A0A6N0C4S6
A	651	TYR	HIS	conflict	UNP A0A6N0C4S6
A	675	LYS	ASN	conflict	UNP A0A6N0C4S6
A	677	ARG	PRO	conflict	UNP A0A6N0C4S6
A	760	LYS	ASN	conflict	UNP A0A6N0C4S6
A	792	TYR	ASP	conflict	UNP A0A6N0C4S6
A	935	PHE	SER	conflict	UNP A0A6N0C4S6
A	950	HIS	GLN	conflict	UNP A0A6N0C4S6
A	965	LYS	ASN	conflict	UNP A0A6N0C4S6
A	982	PRO	LYS	conflict	UNP A0A6N0C4S6
A	983	PRO	VAL	conflict	UNP A0A6N0C4S6
A	1139	LEU	PRO	conflict	UNP A0A6N0C4S6
A	1270	GLY	-	expression tag	UNP A0A6N0C4S6
A	1271	GLY	-	expression tag	UNP A0A6N0C4S6
A	1272	GLY	-	expression tag	UNP A0A6N0C4S6
A	1273	GLY	-	expression tag	UNP A0A6N0C4S6
A	1274	SER	-	expression tag	UNP A0A6N0C4S6
A	1275	GLY	-	expression tag	UNP A0A6N0C4S6
A	1276	GLY	-	expression tag	UNP A0A6N0C4S6
A	1277	GLY	-	expression tag	UNP A0A6N0C4S6
A	1278	GLY	-	expression tag	UNP A0A6N0C4S6
A	1279	SER	-	expression tag	UNP A0A6N0C4S6
A	1280	TRP	-	expression tag	UNP A0A6N0C4S6
A	1281	SER	-	expression tag	UNP A0A6N0C4S6
A	1282	HIS	-	expression tag	UNP A0A6N0C4S6
A	1283	PRO	-	expression tag	UNP A0A6N0C4S6
A	1284	GLN	-	expression tag	UNP A0A6N0C4S6
A	1285	PHE	-	expression tag	UNP A0A6N0C4S6
A	1286	GLU	-	expression tag	UNP A0A6N0C4S6
A	1287	LYS	-	expression tag	UNP A0A6N0C4S6
A	1288	GLY	-	expression tag	UNP A0A6N0C4S6
A	1289	GLY	-	expression tag	UNP A0A6N0C4S6
A	1290	GLY	-	expression tag	UNP A0A6N0C4S6
A	1291	GLY	-	expression tag	UNP A0A6N0C4S6
A	1292	SER	-	expression tag	UNP A0A6N0C4S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1293	GLY	-	expression tag	UNP A0A6N0C4S6
A	1294	GLY	-	expression tag	UNP A0A6N0C4S6
A	1295	GLY	-	expression tag	UNP A0A6N0C4S6
A	1296	GLY	-	expression tag	UNP A0A6N0C4S6
A	1297	SER	-	expression tag	UNP A0A6N0C4S6
A	1298	TRP	-	expression tag	UNP A0A6N0C4S6
A	1299	SER	-	expression tag	UNP A0A6N0C4S6
A	1300	HIS	-	expression tag	UNP A0A6N0C4S6
A	1301	PRO	-	expression tag	UNP A0A6N0C4S6
A	1302	GLN	-	expression tag	UNP A0A6N0C4S6
A	1303	PHE	-	expression tag	UNP A0A6N0C4S6
A	1304	GLU	-	expression tag	UNP A0A6N0C4S6
A	1305	LYS	-	expression tag	UNP A0A6N0C4S6
B	1	MET	-	initiating methionine	UNP A0A6N0C4S6
B	2	PHE	-	expression tag	UNP A0A6N0C4S6
B	3	VAL	-	expression tag	UNP A0A6N0C4S6
B	4	PHE	-	expression tag	UNP A0A6N0C4S6
B	5	LEU	-	expression tag	UNP A0A6N0C4S6
B	6	VAL	-	expression tag	UNP A0A6N0C4S6
B	7	LEU	-	expression tag	UNP A0A6N0C4S6
B	8	LEU	-	expression tag	UNP A0A6N0C4S6
B	9	PRO	-	expression tag	UNP A0A6N0C4S6
B	10	LEU	-	expression tag	UNP A0A6N0C4S6
B	11	VAL	-	expression tag	UNP A0A6N0C4S6
B	12	SER	-	expression tag	UNP A0A6N0C4S6
B	13	SER	-	expression tag	UNP A0A6N0C4S6
B	14	GLN	-	expression tag	UNP A0A6N0C4S6
B	15	CYS	-	expression tag	UNP A0A6N0C4S6
B	16	VAL	-	expression tag	UNP A0A6N0C4S6
B	17	MET	-	expression tag	UNP A0A6N0C4S6
B	18	PRO	-	expression tag	UNP A0A6N0C4S6
B	19	LEU	-	expression tag	UNP A0A6N0C4S6
B	20	PHE	-	expression tag	UNP A0A6N0C4S6
B	21	ASN	-	expression tag	UNP A0A6N0C4S6
B	22	LEU	-	expression tag	UNP A0A6N0C4S6
B	23	ILE	-	expression tag	UNP A0A6N0C4S6
B	24	THR	-	expression tag	UNP A0A6N0C4S6
B	25	THR	-	expression tag	UNP A0A6N0C4S6
B	26	THR	-	expression tag	UNP A0A6N0C4S6
B	27	GLN	-	expression tag	UNP A0A6N0C4S6
B	28	SER	-	expression tag	UNP A0A6N0C4S6
B	51	LEU	SER	conflict	UNP A0A6N0C4S6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	HIS	deletion	UNP A0A6N0C4S6
B	?	-	VAL	deletion	UNP A0A6N0C4S6
B	126	PHE	VAL	conflict	UNP A0A6N0C4S6
B	141	ASP	GLY	conflict	UNP A0A6N0C4S6
B	?	-	TYR	deletion	UNP A0A6N0C4S6
B	155	SER	PHE	conflict	UNP A0A6N0C4S6
B	156	GLY	ARG	conflict	UNP A0A6N0C4S6
B	?	-	ASN	deletion	UNP A0A6N0C4S6
B	209	ILE	LEU	conflict	UNP A0A6N0C4S6
B	210	GLY	VAL	conflict	UNP A0A6N0C4S6
B	213	PHE	LEU	conflict	UNP A0A6N0C4S6
B	242	ASN	HIS	conflict	UNP A0A6N0C4S6
B	261	ASP	ALA	conflict	UNP A0A6N0C4S6
B	329	VAL	ILE	conflict	UNP A0A6N0C4S6
B	336	HIS	GLY	conflict	UNP A0A6N0C4S6
B	343	THR	ARG	conflict	UNP A0A6N0C4S6
B	353	THR	LYS	conflict	UNP A0A6N0C4S6
B	368	PHE	SER	conflict	UNP A0A6N0C4S6
B	370	PRO	SER	conflict	UNP A0A6N0C4S6
B	372	PHE	SER	conflict	UNP A0A6N0C4S6
B	373	ALA	THR	conflict	UNP A0A6N0C4S6
B	400	LYS	ARG	conflict	UNP A0A6N0C4S6
B	402	ASN	ASP	conflict	UNP A0A6N0C4S6
B	405	SER	ARG	conflict	UNP A0A6N0C4S6
B	414	ASN	LYS	conflict	UNP A0A6N0C4S6
B	437	LYS	ASN	conflict	UNP A0A6N0C4S6
B	442	HIS	VAL	conflict	UNP A0A6N0C4S6
B	443	SER	GLY	conflict	UNP A0A6N0C4S6
B	447	ASP	ASN	conflict	UNP A0A6N0C4S6
B	449	TRP	LEU	conflict	UNP A0A6N0C4S6
B	452	SER	LEU	conflict	UNP A0A6N0C4S6
B	453	LEU	PHE	conflict	UNP A0A6N0C4S6
B	457	LYS	ASN	conflict	UNP A0A6N0C4S6
B	474	ASN	SER	conflict	UNP A0A6N0C4S6
B	475	LYS	THR	conflict	UNP A0A6N0C4S6
B	478	LYS	ASN	conflict	UNP A0A6N0C4S6
B	?	-	VAL	deletion	UNP A0A6N0C4S6
B	480	LYS	GLU	conflict	UNP A0A6N0C4S6
B	482	PRO	PHE	conflict	UNP A0A6N0C4S6
B	494	ARG	GLN	conflict	UNP A0A6N0C4S6
B	497	TYR	ASN	conflict	UNP A0A6N0C4S6
B	501	HIS	TYR	conflict	UNP A0A6N0C4S6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	550	LYS	GLU	conflict	UNP A0A6N0C4S6
B	566	VAL	ALA	conflict	UNP A0A6N0C4S6
B	617	SER	PRO	conflict	UNP A0A6N0C4S6
B	651	TYR	HIS	conflict	UNP A0A6N0C4S6
B	675	LYS	ASN	conflict	UNP A0A6N0C4S6
B	677	ARG	PRO	conflict	UNP A0A6N0C4S6
B	760	LYS	ASN	conflict	UNP A0A6N0C4S6
B	792	TYR	ASP	conflict	UNP A0A6N0C4S6
B	935	PHE	SER	conflict	UNP A0A6N0C4S6
B	950	HIS	GLN	conflict	UNP A0A6N0C4S6
B	965	LYS	ASN	conflict	UNP A0A6N0C4S6
B	982	PRO	LYS	conflict	UNP A0A6N0C4S6
B	983	PRO	VAL	conflict	UNP A0A6N0C4S6
B	1139	LEU	PRO	conflict	UNP A0A6N0C4S6
B	1270	GLY	-	expression tag	UNP A0A6N0C4S6
B	1271	GLY	-	expression tag	UNP A0A6N0C4S6
B	1272	GLY	-	expression tag	UNP A0A6N0C4S6
B	1273	GLY	-	expression tag	UNP A0A6N0C4S6
B	1274	SER	-	expression tag	UNP A0A6N0C4S6
B	1275	GLY	-	expression tag	UNP A0A6N0C4S6
B	1276	GLY	-	expression tag	UNP A0A6N0C4S6
B	1277	GLY	-	expression tag	UNP A0A6N0C4S6
B	1278	GLY	-	expression tag	UNP A0A6N0C4S6
B	1279	SER	-	expression tag	UNP A0A6N0C4S6
B	1280	TRP	-	expression tag	UNP A0A6N0C4S6
B	1281	SER	-	expression tag	UNP A0A6N0C4S6
B	1282	HIS	-	expression tag	UNP A0A6N0C4S6
B	1283	PRO	-	expression tag	UNP A0A6N0C4S6
B	1284	GLN	-	expression tag	UNP A0A6N0C4S6
B	1285	PHE	-	expression tag	UNP A0A6N0C4S6
B	1286	GLU	-	expression tag	UNP A0A6N0C4S6
B	1287	LYS	-	expression tag	UNP A0A6N0C4S6
B	1288	GLY	-	expression tag	UNP A0A6N0C4S6
B	1289	GLY	-	expression tag	UNP A0A6N0C4S6
B	1290	GLY	-	expression tag	UNP A0A6N0C4S6
B	1291	GLY	-	expression tag	UNP A0A6N0C4S6
B	1292	SER	-	expression tag	UNP A0A6N0C4S6
B	1293	GLY	-	expression tag	UNP A0A6N0C4S6
B	1294	GLY	-	expression tag	UNP A0A6N0C4S6
B	1295	GLY	-	expression tag	UNP A0A6N0C4S6
B	1296	GLY	-	expression tag	UNP A0A6N0C4S6
B	1297	SER	-	expression tag	UNP A0A6N0C4S6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1298	TRP	-	expression tag	UNP A0A6N0C4S6
B	1299	SER	-	expression tag	UNP A0A6N0C4S6
B	1300	HIS	-	expression tag	UNP A0A6N0C4S6
B	1301	PRO	-	expression tag	UNP A0A6N0C4S6
B	1302	GLN	-	expression tag	UNP A0A6N0C4S6
B	1303	PHE	-	expression tag	UNP A0A6N0C4S6
B	1304	GLU	-	expression tag	UNP A0A6N0C4S6
B	1305	LYS	-	expression tag	UNP A0A6N0C4S6
C	1	MET	-	initiating methionine	UNP A0A6N0C4S6
C	2	PHE	-	expression tag	UNP A0A6N0C4S6
C	3	VAL	-	expression tag	UNP A0A6N0C4S6
C	4	PHE	-	expression tag	UNP A0A6N0C4S6
C	5	LEU	-	expression tag	UNP A0A6N0C4S6
C	6	VAL	-	expression tag	UNP A0A6N0C4S6
C	7	LEU	-	expression tag	UNP A0A6N0C4S6
C	8	LEU	-	expression tag	UNP A0A6N0C4S6
C	9	PRO	-	expression tag	UNP A0A6N0C4S6
C	10	LEU	-	expression tag	UNP A0A6N0C4S6
C	11	VAL	-	expression tag	UNP A0A6N0C4S6
C	12	SER	-	expression tag	UNP A0A6N0C4S6
C	13	SER	-	expression tag	UNP A0A6N0C4S6
C	14	GLN	-	expression tag	UNP A0A6N0C4S6
C	15	CYS	-	expression tag	UNP A0A6N0C4S6
C	16	VAL	-	expression tag	UNP A0A6N0C4S6
C	17	MET	-	expression tag	UNP A0A6N0C4S6
C	18	PRO	-	expression tag	UNP A0A6N0C4S6
C	19	LEU	-	expression tag	UNP A0A6N0C4S6
C	20	PHE	-	expression tag	UNP A0A6N0C4S6
C	21	ASN	-	expression tag	UNP A0A6N0C4S6
C	22	LEU	-	expression tag	UNP A0A6N0C4S6
C	23	ILE	-	expression tag	UNP A0A6N0C4S6
C	24	THR	-	expression tag	UNP A0A6N0C4S6
C	25	THR	-	expression tag	UNP A0A6N0C4S6
C	26	THR	-	expression tag	UNP A0A6N0C4S6
C	27	GLN	-	expression tag	UNP A0A6N0C4S6
C	28	SER	-	expression tag	UNP A0A6N0C4S6
C	51	LEU	SER	conflict	UNP A0A6N0C4S6
C	?	-	HIS	deletion	UNP A0A6N0C4S6
C	?	-	VAL	deletion	UNP A0A6N0C4S6
C	126	PHE	VAL	conflict	UNP A0A6N0C4S6
C	141	ASP	GLY	conflict	UNP A0A6N0C4S6
C	?	-	TYR	deletion	UNP A0A6N0C4S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	155	SER	PHE	conflict	UNP A0A6N0C4S6
C	156	GLY	ARG	conflict	UNP A0A6N0C4S6
C	?	-	ASN	deletion	UNP A0A6N0C4S6
C	209	ILE	LEU	conflict	UNP A0A6N0C4S6
C	210	GLY	VAL	conflict	UNP A0A6N0C4S6
C	213	PHE	LEU	conflict	UNP A0A6N0C4S6
C	242	ASN	HIS	conflict	UNP A0A6N0C4S6
C	261	ASP	ALA	conflict	UNP A0A6N0C4S6
C	329	VAL	ILE	conflict	UNP A0A6N0C4S6
C	336	HIS	GLY	conflict	UNP A0A6N0C4S6
C	343	THR	ARG	conflict	UNP A0A6N0C4S6
C	353	THR	LYS	conflict	UNP A0A6N0C4S6
C	368	PHE	SER	conflict	UNP A0A6N0C4S6
C	370	PRO	SER	conflict	UNP A0A6N0C4S6
C	372	PHE	SER	conflict	UNP A0A6N0C4S6
C	373	ALA	THR	conflict	UNP A0A6N0C4S6
C	400	LYS	ARG	conflict	UNP A0A6N0C4S6
C	402	ASN	ASP	conflict	UNP A0A6N0C4S6
C	405	SER	ARG	conflict	UNP A0A6N0C4S6
C	414	ASN	LYS	conflict	UNP A0A6N0C4S6
C	437	LYS	ASN	conflict	UNP A0A6N0C4S6
C	442	HIS	VAL	conflict	UNP A0A6N0C4S6
C	443	SER	GLY	conflict	UNP A0A6N0C4S6
C	447	ASP	ASN	conflict	UNP A0A6N0C4S6
C	449	TRP	LEU	conflict	UNP A0A6N0C4S6
C	452	SER	LEU	conflict	UNP A0A6N0C4S6
C	453	LEU	PHE	conflict	UNP A0A6N0C4S6
C	457	LYS	ASN	conflict	UNP A0A6N0C4S6
C	474	ASN	SER	conflict	UNP A0A6N0C4S6
C	475	LYS	THR	conflict	UNP A0A6N0C4S6
C	478	LYS	ASN	conflict	UNP A0A6N0C4S6
C	?	-	VAL	deletion	UNP A0A6N0C4S6
C	480	LYS	GLU	conflict	UNP A0A6N0C4S6
C	482	PRO	PHE	conflict	UNP A0A6N0C4S6
C	494	ARG	GLN	conflict	UNP A0A6N0C4S6
C	497	TYR	ASN	conflict	UNP A0A6N0C4S6
C	501	HIS	TYR	conflict	UNP A0A6N0C4S6
C	550	LYS	GLU	conflict	UNP A0A6N0C4S6
C	566	VAL	ALA	conflict	UNP A0A6N0C4S6
C	617	SER	PRO	conflict	UNP A0A6N0C4S6
C	651	TYR	HIS	conflict	UNP A0A6N0C4S6
C	675	LYS	ASN	conflict	UNP A0A6N0C4S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	677	ARG	PRO	conflict	UNP A0A6N0C4S6
C	760	LYS	ASN	conflict	UNP A0A6N0C4S6
C	792	TYR	ASP	conflict	UNP A0A6N0C4S6
C	935	PHE	SER	conflict	UNP A0A6N0C4S6
C	950	HIS	GLN	conflict	UNP A0A6N0C4S6
C	965	LYS	ASN	conflict	UNP A0A6N0C4S6
C	982	PRO	LYS	conflict	UNP A0A6N0C4S6
C	983	PRO	VAL	conflict	UNP A0A6N0C4S6
C	1139	LEU	PRO	conflict	UNP A0A6N0C4S6
C	1270	GLY	-	expression tag	UNP A0A6N0C4S6
C	1271	GLY	-	expression tag	UNP A0A6N0C4S6
C	1272	GLY	-	expression tag	UNP A0A6N0C4S6
C	1273	GLY	-	expression tag	UNP A0A6N0C4S6
C	1274	SER	-	expression tag	UNP A0A6N0C4S6
C	1275	GLY	-	expression tag	UNP A0A6N0C4S6
C	1276	GLY	-	expression tag	UNP A0A6N0C4S6
C	1277	GLY	-	expression tag	UNP A0A6N0C4S6
C	1278	GLY	-	expression tag	UNP A0A6N0C4S6
C	1279	SER	-	expression tag	UNP A0A6N0C4S6
C	1280	TRP	-	expression tag	UNP A0A6N0C4S6
C	1281	SER	-	expression tag	UNP A0A6N0C4S6
C	1282	HIS	-	expression tag	UNP A0A6N0C4S6
C	1283	PRO	-	expression tag	UNP A0A6N0C4S6
C	1284	GLN	-	expression tag	UNP A0A6N0C4S6
C	1285	PHE	-	expression tag	UNP A0A6N0C4S6
C	1286	GLU	-	expression tag	UNP A0A6N0C4S6
C	1287	LYS	-	expression tag	UNP A0A6N0C4S6
C	1288	GLY	-	expression tag	UNP A0A6N0C4S6
C	1289	GLY	-	expression tag	UNP A0A6N0C4S6
C	1290	GLY	-	expression tag	UNP A0A6N0C4S6
C	1291	GLY	-	expression tag	UNP A0A6N0C4S6
C	1292	SER	-	expression tag	UNP A0A6N0C4S6
C	1293	GLY	-	expression tag	UNP A0A6N0C4S6
C	1294	GLY	-	expression tag	UNP A0A6N0C4S6
C	1295	GLY	-	expression tag	UNP A0A6N0C4S6
C	1296	GLY	-	expression tag	UNP A0A6N0C4S6
C	1297	SER	-	expression tag	UNP A0A6N0C4S6
C	1298	TRP	-	expression tag	UNP A0A6N0C4S6
C	1299	SER	-	expression tag	UNP A0A6N0C4S6
C	1300	HIS	-	expression tag	UNP A0A6N0C4S6
C	1301	PRO	-	expression tag	UNP A0A6N0C4S6
C	1302	GLN	-	expression tag	UNP A0A6N0C4S6

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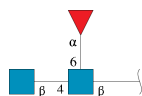
Chain	Residue	Modelled	Actual	Comment	Reference
C	1303	PHE	-	expression tag	UNP A0A6N0C4S6
C	1304	GLU	-	expression tag	UNP A0A6N0C4S6
C	1305	LYS	-	expression tag	UNP A0A6N0C4S6

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



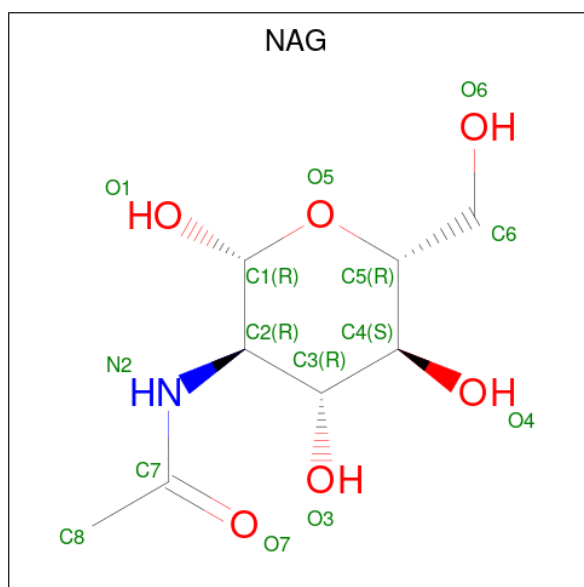
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16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

- Molecule 3 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
3	H	3	Total	C	N	O	0	0
			38	22	2	14		
3	N	3	Total	C	N	O	0	0
			38	22	2	14		
3	T	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

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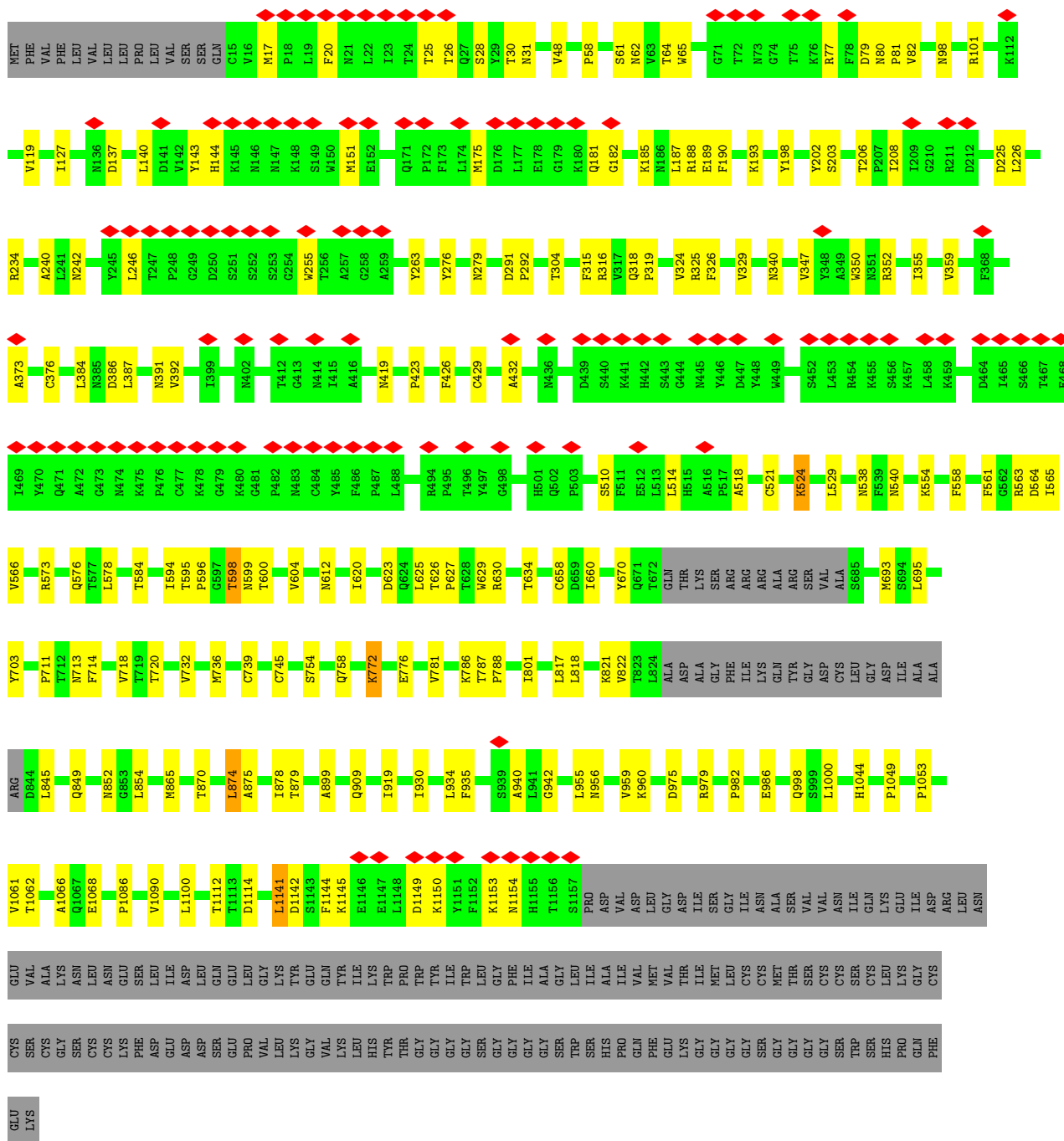
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	C	1	14	8	1	5	0

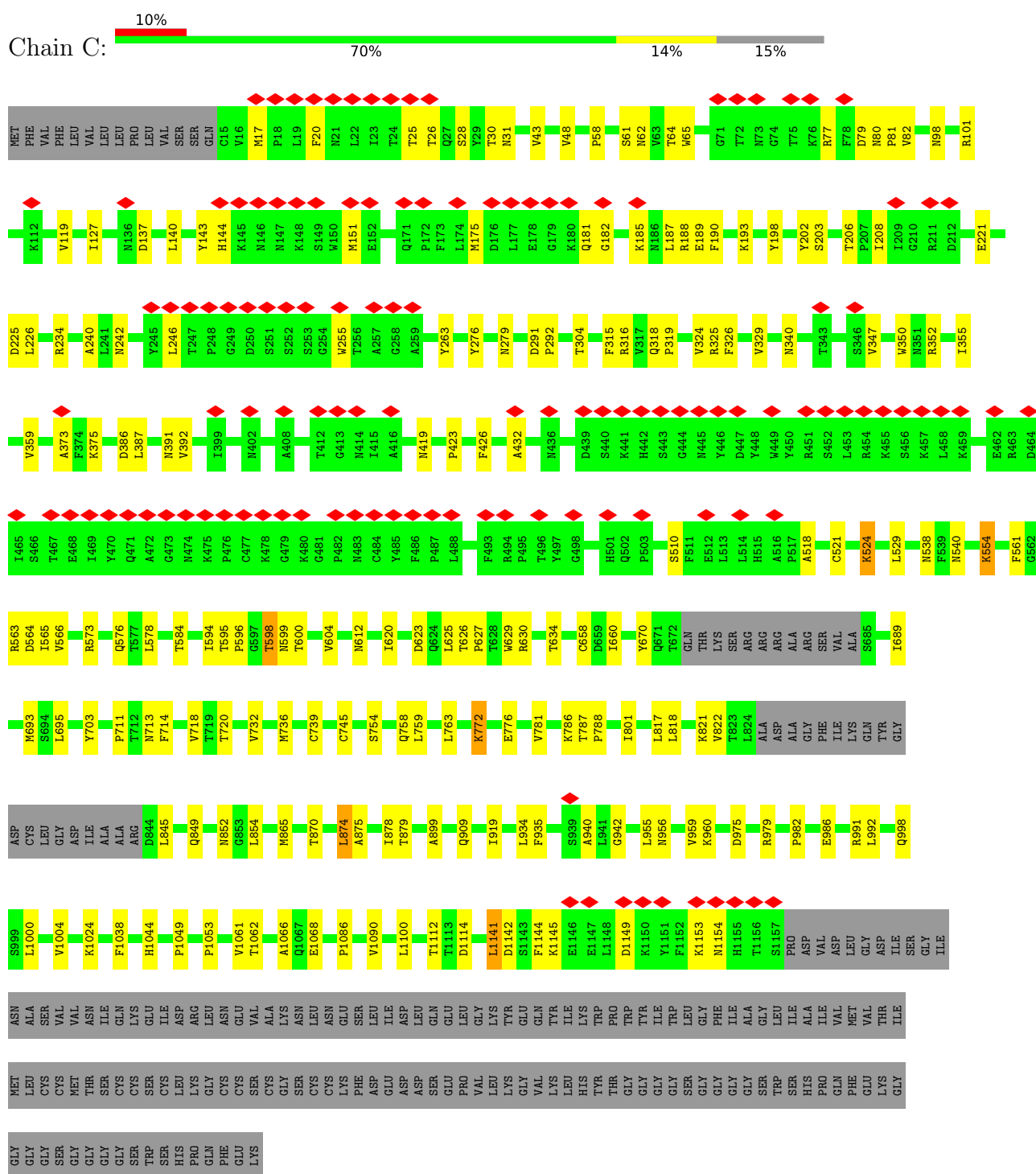




- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein



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

Chain D: 



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

Chain E:  50% 50%



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

Chain F:  50% 50%



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

Chain G:  50% 50%



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

Chain I:  50% 50%



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

Chain J:  50% 50%



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

Chain K:  50% 50%



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

Chain L:  50% 50%



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



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



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



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



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



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



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

Chain U:  50% 50%

MAG1  
MAG2

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

Chain H:  100%

MAG1  
MAG2  
FUC3

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

Chain N:  100%

MAG1  
MAG2  
FUC3

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

Chain T:  100%

MAG1  
MAG2  
FUC3

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66711	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 ( $e^-/\text{\AA}^2$ )	40.0	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.151	Depositor
Minimum map value	-0.822	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.06	Depositor
Map size ( $\text{\AA}$ )	263.88, 263.88, 263.88	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.73300004, 0.73300004, 0.73300004	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.19	0/9135	0.34	0/12425
1	B	0.20	0/9135	0.34	0/12425
1	C	0.20	0/9135	0.34	0/12425
All	All	0.20	0/27405	0.34	0/37275

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

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	8918	0	8685	115	0
1	B	8918	0	8685	122	0
1	C	8918	0	8685	127	0
2	D	28	0	25	1	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0
2	K	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	1	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	U	28	0	25	0	0
3	H	38	0	34	0	0
3	N	38	0	34	0	0
3	T	38	0	34	0	0
4	A	126	0	117	3	0
4	B	126	0	117	3	0
4	C	126	0	117	3	0
All	All	27666	0	26883	341	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 6.

All (341) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:MET:SD	1:C:316:ARG:NH2	2.46	0.88
1:B:316:ARG:NH2	1:C:736:MET:SD	2.47	0.87
1:B:355:ILE:HB	1:B:392:VAL:HB	1.66	0.78
1:C:187:LEU:HB3	1:C:206:THR:O	1.85	0.77
1:A:187:LEU:HB3	1:A:206:THR:O	1.85	0.77
1:B:187:LEU:HB3	1:B:206:THR:O	1.85	0.77
1:C:355:ILE:HB	1:C:392:VAL:HB	1.66	0.76
1:A:355:ILE:HB	1:A:392:VAL:HB	1.66	0.76
1:A:732:VAL:HG11	1:A:1000:LEU:HD21	1.67	0.75
1:C:732:VAL:HG11	1:C:1000:LEU:HD21	1.66	0.75
1:B:732:VAL:HG11	1:B:1000:LEU:HD21	1.67	0.75
1:A:316:ARG:NH2	1:B:736:MET:SD	2.59	0.74
1:A:620:ILE:HG13	1:A:630:ARG:HD2	1.72	0.72
1:A:82:VAL:HB	1:A:234:ARG:HH12	1.54	0.72
1:B:620:ILE:HG13	1:B:630:ARG:HD2	1.72	0.71
1:C:82:VAL:HB	1:C:234:ARG:HH12	1.54	0.71
1:C:1112:THR:HG22	1:C:1114:ASP:H	1.55	0.71
1:A:1112:THR:HG22	1:A:1114:ASP:H	1.55	0.71
1:B:82:VAL:HB	1:B:234:ARG:HH12	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1112:THR:HG22	1:B:1114:ASP:H	1.55	0.70
1:C:620:ILE:HG13	1:C:630:ARG:HD2	1.72	0.70
1:A:899:ALA:HB1	1:A:909:GLN:HB2	1.76	0.68
1:C:899:ALA:HB1	1:C:909:GLN:HB2	1.76	0.68
1:C:318:GLN:OE1	1:C:626:THR:OG1	2.12	0.67
1:B:318:GLN:OE1	1:B:626:THR:OG1	2.12	0.67
1:B:324:VAL:HG12	1:B:538:ASN:HB3	1.77	0.67
1:C:324:VAL:HG12	1:C:538:ASN:HB3	1.77	0.67
1:B:899:ALA:HB1	1:B:909:GLN:HB2	1.76	0.66
1:A:318:GLN:OE1	1:A:626:THR:OG1	2.12	0.66
1:A:324:VAL:HG12	1:A:538:ASN:HB3	1.77	0.66
1:A:182:GLY:H	1:A:185:LYS:HE3	1.61	0.65
1:C:350:TRP:HZ3	1:C:352:ARG:HE	1.45	0.65
1:A:713:ASN:HB3	1:A:1066:ALA:HB3	1.79	0.64
1:B:182:GLY:H	1:B:185:LYS:HE3	1.61	0.64
1:A:350:TRP:HZ3	1:A:352:ARG:HE	1.45	0.64
1:A:788:PRO:HG3	1:C:703:TYR:HB3	1.80	0.63
1:B:350:TRP:HZ3	1:B:352:ARG:HE	1.44	0.63
1:C:182:GLY:H	1:C:185:LYS:HE3	1.61	0.63
1:C:713:ASN:HB3	1:C:1066:ALA:HB3	1.79	0.63
1:C:62:ASN:HD22	4:C:1407:NAG:C7	2.11	0.63
1:B:713:ASN:HB3	1:B:1066:ALA:HB3	1.79	0.62
1:A:62:ASN:HD22	4:A:1407:NAG:C7	2.11	0.62
1:B:62:ASN:HD22	4:B:1407:NAG:C7	2.11	0.61
1:A:960:LYS:HD3	1:C:566:VAL:HG12	1.83	0.61
1:B:875:ALA:O	1:B:879:THR:OG1	2.17	0.60
1:A:875:ALA:O	1:A:879:THR:OG1	2.17	0.60
1:B:347:VAL:HG22	1:B:419:ASN:HB3	1.85	0.59
1:C:347:VAL:HG22	1:C:419:ASN:HB3	1.85	0.59
1:B:518:ALA:HB1	1:B:540:ASN:HD22	1.68	0.59
1:B:772:LYS:O	1:B:776:GLU:HG2	2.04	0.58
1:A:518:ALA:HB1	1:A:540:ASN:HD22	1.68	0.58
1:C:518:ALA:HB1	1:C:540:ASN:HD22	1.68	0.58
1:B:20:PHE:HZ	1:B:255:TRP:HB2	1.69	0.57
1:C:875:ALA:O	1:C:879:THR:OG1	2.17	0.57
1:A:347:VAL:HG22	1:A:419:ASN:HB3	1.85	0.57
1:A:187:LEU:CB	1:A:206:THR:O	2.53	0.57
1:A:772:LYS:O	1:A:776:GLU:HG2	2.04	0.57
1:C:187:LEU:CB	1:C:206:THR:O	2.53	0.57
1:C:772:LYS:O	1:C:776:GLU:HG2	2.04	0.57
1:A:20:PHE:HZ	1:A:255:TRP:HB2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:GLN:NE2	1:A:956:ASN:OD1	2.38	0.56
1:B:187:LEU:CB	1:B:206:THR:O	2.53	0.56
1:C:119:VAL:HG13	1:C:140:LEU:HD11	1.88	0.56
1:B:119:VAL:HG13	1:B:140:LEU:HD11	1.88	0.56
1:C:718:VAL:HG22	1:C:1061:VAL:HG22	1.88	0.56
1:A:119:VAL:HG13	1:A:140:LEU:HD11	1.88	0.55
1:A:623:ASP:HA	1:A:630:ARG:HH12	1.72	0.55
1:A:718:VAL:HG22	1:A:1061:VAL:HG22	1.88	0.55
1:B:101:ARG:HG3	1:B:240:ALA:HB2	1.89	0.55
1:C:20:PHE:HZ	1:C:255:TRP:HB2	1.69	0.55
1:C:849:GLN:NE2	1:C:956:ASN:OD1	2.38	0.55
1:B:573:ARG:HD3	1:B:578:LEU:HD13	1.89	0.55
1:B:718:VAL:HG22	1:B:1061:VAL:HG22	1.88	0.55
1:C:720:THR:HG21	1:C:934:LEU:HD13	1.89	0.55
1:A:703:TYR:HB3	1:B:788:PRO:HG3	1.88	0.55
1:A:101:ARG:HG3	1:A:240:ALA:HB2	1.89	0.55
1:B:849:GLN:NE2	1:B:956:ASN:OD1	2.38	0.55
1:A:595:THR:HG22	1:A:604:VAL:HG12	1.88	0.55
1:C:623:ASP:HA	1:C:630:ARG:HH12	1.71	0.55
1:A:325:ARG:HH11	1:A:529:LEU:HB2	1.72	0.55
1:B:720:THR:HG21	1:B:934:LEU:HD13	1.89	0.55
1:C:101:ARG:HG3	1:C:240:ALA:HB2	1.89	0.55
1:B:595:THR:HG22	1:B:604:VAL:HG12	1.88	0.55
1:C:325:ARG:HH11	1:C:529:LEU:HB2	1.72	0.55
1:B:325:ARG:HH11	1:B:529:LEU:HB2	1.72	0.54
1:A:720:THR:HG21	1:A:934:LEU:HD13	1.89	0.54
1:B:623:ASP:HA	1:B:630:ARG:HH12	1.72	0.54
1:C:181:GLN:HB2	1:C:185:LYS:HD2	1.90	0.54
1:A:817:LEU:HB3	1:A:935:PHE:CZ	2.43	0.54
1:C:573:ARG:HD3	1:C:578:LEU:HD13	1.89	0.54
1:C:595:THR:HG22	1:C:604:VAL:HG12	1.88	0.54
1:B:982:PRO:O	1:B:986:GLU:HG2	2.09	0.53
1:C:817:LEU:HB3	1:C:935:PHE:CZ	2.43	0.53
1:C:982:PRO:O	1:C:986:GLU:HG2	2.08	0.53
1:C:318:GLN:HE21	1:C:319:PRO:HD2	1.73	0.53
1:A:573:ARG:HD3	1:A:578:LEU:HD13	1.89	0.53
1:B:25:THR:HG21	1:B:81:PRO:HG3	1.91	0.53
1:B:817:LEU:HB3	1:B:935:PHE:CZ	2.43	0.53
1:A:181:GLN:HB2	1:A:185:LYS:HD2	1.90	0.53
1:A:318:GLN:HE21	1:A:319:PRO:HD2	1.73	0.53
1:A:982:PRO:O	1:A:986:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:GLN:HB2	1:B:185:LYS:HD2	1.90	0.53
1:C:25:THR:HG21	1:C:81:PRO:HG3	1.91	0.53
1:A:28:SER:HB2	1:A:65:TRP:HB3	1.91	0.53
1:A:564:ASP:OD1	1:A:565:ILE:N	2.38	0.53
1:B:423:PRO:HG2	1:B:426:PHE:HB2	1.91	0.52
1:C:28:SER:HB2	1:C:65:TRP:HB3	1.91	0.52
1:C:612:ASN:OD1	4:C:1405:NAG:N2	2.42	0.52
1:B:318:GLN:HE21	1:B:319:PRO:HD2	1.73	0.52
1:B:612:ASN:OD1	4:B:1405:NAG:N2	2.42	0.52
1:C:315:PHE:HA	1:C:627:PRO:HD3	1.92	0.52
1:A:423:PRO:HG2	1:A:426:PHE:HB2	1.91	0.52
1:B:315:PHE:HA	1:B:627:PRO:HD3	1.92	0.52
1:A:25:THR:HG21	1:A:81:PRO:HG3	1.91	0.52
1:C:423:PRO:HG2	1:C:426:PHE:HB2	1.91	0.51
1:A:612:ASN:OD1	4:A:1405:NAG:N2	2.42	0.51
1:B:28:SER:HB2	1:B:65:TRP:HB3	1.91	0.51
1:B:703:TYR:HB3	1:C:788:PRO:HG3	1.91	0.51
1:A:315:PHE:HA	1:A:627:PRO:HD3	1.92	0.51
1:B:566:VAL:HG12	1:C:960:LYS:HD3	1.93	0.51
1:A:340:ASN:O	4:A:1402:NAG:N2	2.44	0.50
1:A:979:ARG:HG2	1:C:387:LEU:HD21	1.93	0.50
1:B:143:TYR:CZ	1:B:151:MET:HE1	2.47	0.50
1:B:304:THR:HA	1:B:598:THR:HG21	1.94	0.50
1:B:1044:HIS:HA	1:B:1062:THR:HG22	1.94	0.50
1:B:340:ASN:O	4:B:1402:NAG:N2	2.44	0.50
1:B:58:PRO:O	1:B:61:SER:HB2	2.12	0.49
1:C:58:PRO:O	1:C:61:SER:HB2	2.12	0.49
1:C:143:TYR:CZ	1:C:151:MET:HE1	2.47	0.49
1:C:1044:HIS:HA	1:C:1062:THR:HG22	1.94	0.49
1:A:143:TYR:CZ	1:A:151:MET:HE1	2.47	0.49
1:A:304:THR:HA	1:A:598:THR:HG21	1.94	0.49
1:C:198:TYR:HD2	1:C:225:ASP:OD2	1.96	0.49
1:C:564:ASP:OD1	1:C:565:ILE:N	2.38	0.49
1:C:564:ASP:OD1	1:C:565:ILE:HG22	2.13	0.49
1:A:198:TYR:HD2	1:A:225:ASP:OD2	1.96	0.49
1:A:1044:HIS:HA	1:A:1062:THR:HG22	1.94	0.49
1:B:198:TYR:HD2	1:B:225:ASP:OD2	1.96	0.49
1:B:564:ASP:OD1	1:B:565:ILE:HG22	2.13	0.49
1:B:563:ARG:HG3	1:C:43:VAL:CG1	2.43	0.48
1:A:58:PRO:O	1:A:61:SER:HB2	2.12	0.48
1:C:304:THR:HA	1:C:598:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ASP:OD1	1:B:565:ILE:N	2.38	0.48
1:A:564:ASP:OD1	1:A:565:ILE:HG22	2.13	0.48
1:B:386:ASP:OD2	1:B:524:LYS:NZ	2.47	0.47
1:C:386:ASP:OD2	1:C:524:LYS:NZ	2.47	0.47
1:C:821:LYS:HG2	1:C:935:PHE:CD1	2.49	0.47
1:C:1153[A]:LYS:HB3	1:C:1153[A]:LYS:HE3	1.63	0.47
1:A:386:ASP:OD2	1:A:524:LYS:NZ	2.47	0.47
1:A:739:CYS:HB3	1:A:745:CYS:HB3	1.68	0.47
1:C:1142[A]:ASP:HA	1:C:1145[A]:LYS:HB3	1.97	0.47
1:A:127:ILE:HG21	1:A:226:LEU:HD13	1.96	0.47
1:C:340:ASN:O	4:C:1402:NAG:N2	2.44	0.47
1:A:865:MET:HB3	1:C:695:LEU:HD11	1.95	0.47
1:B:127:ILE:HG21	1:B:226:LEU:HD13	1.95	0.47
1:B:1141[A]:LEU:HA	1:B:1144[A]:PHE:CE2	2.50	0.47
1:A:975:ASP:O	1:A:979:ARG:HG3	2.14	0.47
1:B:821:LYS:HG2	1:B:935:PHE:CD1	2.49	0.47
1:C:1141[A]:LEU:HA	1:C:1144[A]:PHE:CE2	2.50	0.47
1:B:561:PHE:CE2	1:C:43:VAL:HG22	2.49	0.47
1:B:975:ASP:O	1:B:979:ARG:HG3	2.14	0.47
1:A:821:LYS:HG2	1:A:935:PHE:CD1	2.49	0.47
1:A:1142[A]:ASP:HA	1:A:1145[A]:LYS:HB3	1.97	0.47
1:B:563:ARG:HG3	1:C:43:VAL:HG11	1.96	0.47
1:B:1142[A]:ASP:HA	1:B:1145[A]:LYS:HB3	1.97	0.47
1:C:127:ILE:HG21	1:C:226:LEU:HD13	1.96	0.47
1:A:596:PRO:HB3	1:A:670:TYR:HB2	1.97	0.47
1:A:1141[A]:LEU:HA	1:A:1144[A]:PHE:CE2	2.50	0.47
1:C:711:PRO:HA	1:C:1068:GLU:HA	1.97	0.47
1:A:711:PRO:HA	1:A:1068:GLU:HA	1.97	0.46
1:A:329:VAL:HG12	1:A:359:VAL:HG13	1.97	0.46
1:C:594:ILE:HG23	1:C:660:ILE:HG21	1.97	0.46
1:A:594:ILE:HG23	1:A:660:ILE:HG21	1.97	0.46
1:C:193:LYS:HD3	1:C:202:TYR:HE1	1.81	0.46
1:B:711:PRO:HA	1:B:1068:GLU:HA	1.98	0.46
1:C:329:VAL:HG12	1:C:359:VAL:HG13	1.97	0.46
1:A:391:ASN:N	1:A:391:ASN:OD1	2.48	0.46
1:B:594:ILE:HG23	1:B:660:ILE:HG21	1.96	0.46
1:C:98:ASN:O	1:C:101:ARG:NE	2.49	0.46
1:C:326:PHE:O	1:C:576:GLN:NE2	2.49	0.46
1:C:975:ASP:O	1:C:979:ARG:HG3	2.15	0.46
1:B:20:PHE:CZ	1:B:255:TRP:HB2	2.50	0.46
1:C:596:PRO:HB3	1:C:670:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:845:LEU:HD13	1:C:956:ASN:HD21	1.81	0.46
1:A:326:PHE:O	1:A:576:GLN:NE2	2.49	0.46
1:B:845:LEU:HD13	1:B:956:ASN:HD21	1.81	0.46
1:A:98:ASN:O	1:A:101:ARG:NE	2.49	0.46
1:C:373:ALA:HB3	1:C:432:ALA:HB3	1.98	0.46
1:C:391:ASN:OD1	1:C:391:ASN:N	2.48	0.46
1:A:193:LYS:HD3	1:A:202:TYR:HE1	1.81	0.46
1:B:391:ASN:OD1	1:B:391:ASN:N	2.48	0.46
1:B:596:PRO:HB3	1:B:670:TYR:HB2	1.97	0.46
1:B:326:PHE:O	1:B:576:GLN:NE2	2.49	0.45
1:B:329:VAL:HG12	1:B:359:VAL:HG13	1.97	0.45
1:C:1086:PRO:HB3	1:C:1100:LEU:HD11	1.99	0.45
1:A:43:VAL:HG22	1:C:561:PHE:CE2	2.52	0.45
1:A:175:MET:HG3	1:A:188:ARG:HH21	1.80	0.45
1:A:1000:LEU:HD23	1:A:1000:LEU:HA	1.79	0.45
1:A:1086:PRO:HB3	1:A:1100:LEU:HD11	1.98	0.45
1:B:695:LEU:HD11	1:C:865:MET:HB3	1.97	0.45
1:C:739:CYS:HB3	1:C:745:CYS:HB3	1.68	0.45
1:A:373:ALA:HB3	1:A:432:ALA:HB3	1.98	0.45
1:A:852:ASN:O	1:A:854:LEU:HG	2.17	0.45
1:B:1000:LEU:HD23	1:B:1000:LEU:HA	1.79	0.45
1:C:175:MET:HG3	1:C:188:ARG:HH21	1.81	0.45
1:C:852:ASN:O	1:C:854:LEU:HG	2.17	0.45
1:A:845:LEU:HD13	1:A:956:ASN:HD21	1.81	0.45
1:B:98:ASN:O	1:B:101:ARG:NE	2.49	0.45
1:B:175:MET:HG3	1:B:188:ARG:HH21	1.80	0.45
1:B:1153[B]:LYS:HA	1:B:1153[B]:LYS:HD3	1.67	0.45
1:A:20:PHE:CZ	1:A:255:TRP:HB2	2.50	0.45
1:B:1153[A]:LYS:HB3	1:B:1153[A]:LYS:HE3	1.63	0.45
1:C:786:LYS:HE2	1:C:786:LYS:HB2	1.64	0.45
1:A:26:THR:OG1	1:A:77:ARG:NH2	2.50	0.45
1:B:26:THR:OG1	1:B:77:ARG:NH2	2.50	0.45
1:C:787:THR:HG21	1:C:878:ILE:HD11	1.99	0.45
1:A:786:LYS:HB2	1:A:786:LYS:HE2	1.64	0.45
1:A:1153[B]:LYS:HA	1:A:1153[B]:LYS:HD3	1.68	0.45
1:B:786:LYS:HE2	1:B:786:LYS:HB2	1.64	0.45
1:B:1086:PRO:HB3	1:B:1100:LEU:HD11	1.99	0.44
1:A:292:PRO:HB2	1:A:604:VAL:HG21	2.00	0.44
1:A:772:LYS:HB2	1:A:772:LYS:HE2	1.69	0.44
1:B:373:ALA:HB3	1:B:432:ALA:HB3	1.98	0.44
1:B:193:LYS:HD3	1:B:202:TYR:HE1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:772:LYS:HB2	1:C:772:LYS:HE2	1.69	0.44
1:B:291:ASP:HA	1:B:629:TRP:HB2	1.99	0.44
1:A:714:PHE:HE1	1:A:919:ILE:HG12	1.83	0.44
1:C:26:THR:OG1	1:C:77:ARG:NH2	2.50	0.44
1:A:955:LEU:HD23	1:A:955:LEU:HA	1.80	0.44
1:C:188:ARG:HB3	1:C:190:PHE:HE1	1.83	0.44
1:C:874:LEU:HD12	1:C:1049:PRO:HD2	2.00	0.44
1:A:291:ASP:HA	1:A:629:TRP:HB2	1.99	0.44
1:B:188:ARG:HB3	1:B:190:PHE:HE1	1.83	0.44
1:B:852:ASN:O	1:B:854:LEU:HG	2.17	0.44
1:A:188:ARG:HB3	1:A:190:PHE:HE1	1.83	0.43
1:A:1141[A]:LEU:HD22	1:A:1144[A]:PHE:HE2	1.83	0.43
1:B:1141[A]:LEU:HD22	1:B:1144[A]:PHE:HE2	1.83	0.43
1:C:291:ASP:HA	1:C:629:TRP:HB2	1.99	0.43
1:C:1141[A]:LEU:HD22	1:C:1144[A]:PHE:HE2	1.83	0.43
1:B:48:VAL:HG12	1:B:276:TYR:HB2	2.01	0.43
1:B:787:THR:HG21	1:B:878:ILE:HD11	1.99	0.43
1:C:1153[B]:LYS:HA	1:C:1153[B]:LYS:HD3	1.67	0.43
1:A:787:THR:HG21	1:A:878:ILE:HD11	1.99	0.43
1:B:384:LEU:HD23	1:B:384:LEU:HA	1.84	0.43
1:C:17:MET:HE2	1:C:17:MET:HA	2.00	0.43
1:C:48:VAL:HG12	1:C:276:TYR:HB2	2.01	0.43
1:A:1150[A]:LYS:HE3	1:A:1150[A]:LYS:HB3	1.84	0.43
1:B:292:PRO:HB2	1:B:604:VAL:HG21	2.00	0.43
1:C:1024:LYS:NZ	1:C:1038:PHE:O	2.48	0.43
1:A:17:MET:HA	1:A:17:MET:HE2	2.00	0.43
1:B:1150[A]:LYS:HB3	1:B:1150[A]:LYS:HE3	1.84	0.43
1:B:558:PHE:HE1	1:C:221:GLU:HG2	1.84	0.43
1:B:739:CYS:HB3	1:B:745:CYS:HB3	1.68	0.43
1:C:1000:LEU:HA	1:C:1000:LEU:HD23	1.79	0.43
1:A:48:VAL:HG12	1:A:276:TYR:HB2	2.01	0.43
1:A:566:VAL:HG12	1:B:960:LYS:HD3	2.01	0.43
1:A:991:ARG:HE	1:A:991:ARG:HB3	1.73	0.43
1:C:714:PHE:HE1	1:C:919:ILE:HG12	1.83	0.43
1:A:1153[A]:LYS:HB3	1:A:1153[A]:LYS:HE3	1.64	0.43
1:C:991:ARG:HE	1:C:991:ARG:HB3	1.74	0.43
1:A:874:LEU:HD12	1:A:1049:PRO:HD2	2.00	0.42
1:B:17:MET:HE2	1:B:17:MET:HA	2.00	0.42
1:B:30:THR:OG1	1:B:31:ASN:N	2.52	0.42
1:C:30:THR:OG1	1:C:31:ASN:N	2.52	0.42
1:B:874:LEU:HD12	1:B:1049:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:PHE:CZ	1:C:255:TRP:HB2	2.50	0.42
1:C:80:ASN:OD1	1:C:80:ASN:N	2.52	0.42
1:A:80:ASN:HD21	1:A:137:ASP:HB3	1.84	0.42
1:A:187:LEU:HB2	1:A:208:ILE:HG13	2.00	0.42
1:B:187:LEU:HB2	1:B:208:ILE:HG13	2.00	0.42
1:C:80:ASN:HD21	1:C:137:ASP:HB3	1.84	0.42
1:A:30:THR:OG1	1:A:31:ASN:N	2.52	0.42
1:C:187:LEU:HB2	1:C:208:ILE:HG13	2.00	0.42
1:C:292:PRO:HB2	1:C:604:VAL:HG21	2.00	0.42
1:C:940:ALA:C	1:C:942:GLY:H	2.28	0.42
1:A:43:VAL:HG11	1:C:563:ARG:HG3	2.02	0.42
1:A:695:LEU:HD11	1:B:865:MET:HB3	2.00	0.42
1:A:818:LEU:HD21	1:A:934:LEU:HD21	2.01	0.42
1:B:80:ASN:OD1	1:B:80:ASN:N	2.52	0.42
1:C:625:LEU:HD23	1:C:625:LEU:HA	1.84	0.42
1:C:955:LEU:HD23	1:C:955:LEU:HA	1.80	0.42
1:A:754:SER:O	1:A:758:GLN:HG3	2.20	0.42
1:B:324:VAL:O	1:B:325:ARG:HD2	2.20	0.42
1:B:930:ILE:HD13	1:B:930:ILE:HA	1.90	0.42
1:C:242:ASN:HB2	1:C:246:LEU:HD21	2.02	0.42
1:B:242:ASN:HB2	1:B:246:LEU:HD21	2.02	0.42
1:B:714:PHE:HE1	1:B:919:ILE:HG12	1.83	0.42
1:C:754:SER:O	1:C:758:GLN:HG3	2.20	0.42
1:A:518:ALA:CB	1:A:540:ASN:HD22	2.31	0.42
1:A:801:ILE:HD12	1:A:874:LEU:HD11	2.02	0.42
1:B:80:ASN:HD21	1:B:137:ASP:HB3	1.84	0.42
1:B:561:PHE:CZ	1:C:43:VAL:HG22	2.55	0.42
1:B:818:LEU:HD21	1:B:934:LEU:HD21	2.01	0.42
1:A:324:VAL:O	1:A:325:ARG:HD2	2.20	0.41
1:A:763:LEU:HD23	1:A:763:LEU:HA	1.88	0.41
1:B:518:ALA:CB	1:B:540:ASN:HD22	2.31	0.41
1:B:658:CYS:HB2	1:B:693:MET:HG2	2.02	0.41
1:B:754:SER:O	1:B:758:GLN:HG3	2.20	0.41
1:A:127:ILE:HD13	1:A:226:LEU:HD11	2.02	0.41
1:C:822:VAL:HB	1:C:1053:PRO:HG2	2.02	0.41
1:A:940:ALA:C	1:A:942:GLY:H	2.28	0.41
1:B:77:ARG:NE	1:B:79:ASP:OD2	2.32	0.41
1:B:772:LYS:HB2	1:B:772:LYS:HE2	1.69	0.41
1:B:822:VAL:HB	1:B:1053:PRO:HG2	2.02	0.41
1:C:189:GLU:O	1:C:203:SER:HA	2.21	0.41
1:C:763:LEU:HD23	1:C:763:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:818:LEU:HD21	1:C:934:LEU:HD21	2.01	0.41
1:A:80:ASN:OD1	1:A:80:ASN:N	2.52	0.41
1:A:279:ASN:OD1	2:D:1:NAG:N2	2.54	0.41
1:B:279:ASN:OD1	2:J:1:NAG:N2	2.54	0.41
1:B:940:ALA:C	1:B:942:GLY:H	2.28	0.41
1:C:554:LYS:H	1:C:554:LYS:HG2	1.73	0.41
1:A:375:LYS:H	1:A:375:LYS:HG2	1.62	0.41
1:A:822:VAL:HB	1:A:1053:PRO:HG2	2.02	0.41
1:B:514:LEU:HD23	1:B:514:LEU:HA	1.81	0.41
1:C:375:LYS:H	1:C:375:LYS:HG2	1.62	0.41
1:C:518:ALA:CB	1:C:540:ASN:HD22	2.31	0.41
1:A:658:CYS:HB2	1:A:693:MET:HG2	2.02	0.41
1:B:625:LEU:HD23	1:B:625:LEU:HA	1.84	0.41
1:C:992:LEU:HD23	1:C:992:LEU:HA	1.88	0.41
1:A:376:CYS:HA	1:A:429:CYS:HA	2.03	0.41
1:A:242:ASN:HB2	1:A:246:LEU:HD21	2.02	0.41
1:A:1102:GLN:HG3	1:A:1105:PHE:O	2.21	0.41
1:B:189:GLU:O	1:B:203:SER:HA	2.21	0.41
1:B:998:GLN:NE2	1:C:998:GLN:HE22	2.19	0.41
1:C:279:ASN:OD1	2:P:1:NAG:N2	2.54	0.41
1:C:324:VAL:O	1:C:325:ARG:HD2	2.20	0.41
1:C:599:ASN:OD1	1:C:600:THR:N	2.54	0.41
1:C:658:CYS:HB2	1:C:693:MET:HG2	2.02	0.41
1:B:376:CYS:HA	1:B:429:CYS:HA	2.03	0.41
1:B:801:ILE:HD12	1:B:874:LEU:HD11	2.02	0.41
1:A:759:LEU:HD22	1:A:1004:VAL:HG21	2.03	0.40
1:B:127:ILE:HD13	1:B:226:LEU:HD11	2.02	0.40
1:B:387:LEU:HD21	1:C:979:ARG:HG2	2.02	0.40
1:B:599:ASN:OD1	1:B:600:THR:N	2.54	0.40
1:C:77:ARG:NE	1:C:79:ASP:OD2	2.32	0.40
1:C:759:LEU:HD22	1:C:1004:VAL:HG21	2.03	0.40
1:B:955:LEU:HD23	1:B:955:LEU:HA	1.80	0.40
1:C:127:ILE:HD13	1:C:226:LEU:HD11	2.02	0.40
1:C:801:ILE:HD12	1:C:874:LEU:HD11	2.02	0.40
1:B:558:PHE:CE1	1:C:221:GLU:HG2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1128/1305 (86%)	1080 (96%)	48 (4%)	0	100	100
1	B	1128/1305 (86%)	1081 (96%)	47 (4%)	0	100	100
1	C	1128/1305 (86%)	1080 (96%)	48 (4%)	0	100	100
All	All	3384/3915 (86%)	3241 (96%)	143 (4%)	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	997/1130 (88%)	975 (98%)	22 (2%)	45	77
1	B	997/1130 (88%)	975 (98%)	22 (2%)	45	77
1	C	997/1130 (88%)	974 (98%)	23 (2%)	44	76
All	All	2991/3390 (88%)	2924 (98%)	67 (2%)	48	77

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	144	HIS
1	A	263	TYR
1	A	510	SER
1	A	521	CYS

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Mol	Chain	Res	Type
1	A	524	LYS
1	A	554	LYS
1	A	584	THR
1	A	598	THR
1	A	634	THR
1	A	772	LYS
1	A	781	VAL
1	A	870	THR
1	A	874	LEU
1	A	959	VAL
1	A	1090	VAL
1	A	1141[A]	LEU
1	A	1141[B]	LEU
1	A	1149[A]	ASP
1	A	1149[B]	ASP
1	A	1154[A]	ASN
1	A	1154[B]	ASN
1	B	64	THR
1	B	144	HIS
1	B	263	TYR
1	B	510	SER
1	B	521	CYS
1	B	524	LYS
1	B	554	LYS
1	B	584	THR
1	B	598	THR
1	B	634	THR
1	B	772	LYS
1	B	781	VAL
1	B	870	THR
1	B	874	LEU
1	B	959	VAL
1	B	1090	VAL
1	B	1141[A]	LEU
1	B	1141[B]	LEU
1	B	1149[A]	ASP
1	B	1149[B]	ASP
1	B	1154[A]	ASN
1	B	1154[B]	ASN
1	C	64	THR
1	C	144	HIS
1	C	263	TYR

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Mol	Chain	Res	Type
1	C	510	SER
1	C	521	CYS
1	C	524	LYS
1	C	554	LYS
1	C	584	THR
1	C	598	THR
1	C	634	THR
1	C	689	ILE
1	C	772	LYS
1	C	781	VAL
1	C	870	THR
1	C	874	LEU
1	C	959	VAL
1	C	1090	VAL
1	C	1141[A]	LEU
1	C	1141[B]	LEU
1	C	1149[A]	ASP
1	C	1149[B]	ASP
1	C	1154[A]	ASN
1	C	1154[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	162	ASN
1	A	194	ASN
1	A	242	ASN
1	A	501	HIS
1	A	536	ASN
1	A	540	ASN
1	A	560	GLN
1	A	770	GLN
1	A	903	ASN
1	A	931	GLN
1	A	945	GLN
1	A	988	GLN
1	A	1102	GLN
1	A	1109	GLN
1	B	114	GLN
1	B	144	HIS
1	B	162	ASN

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Mol	Chain	Res	Type
1	B	194	ASN
1	B	242	ASN
1	B	536	ASN
1	B	540	ASN
1	B	560	GLN
1	B	621	HIS
1	B	783	GLN
1	B	903	ASN
1	B	909	GLN
1	B	931	GLN
1	B	945	GLN
1	B	988	GLN
1	B	998	GLN
1	B	1102	GLN
1	B	1109	GLN
1	C	31	ASN
1	C	114	GLN
1	C	162	ASN
1	C	194	ASN
1	C	242	ASN
1	C	318	GLN
1	C	536	ASN
1	C	540	ASN
1	C	560	GLN
1	C	609	GLN
1	C	621	HIS
1	C	751	GLN
1	C	783	GLN
1	C	903	ASN
1	C	931	GLN
1	C	945	GLN
1	C	988	GLN
1	C	998	GLN
1	C	1102	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

39 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	$\# Z  > 2$
2	NAG	D	1	1,2	14,14,15	0.76	0	17,19,21	1.06	2 (11%)
2	NAG	D	2	2	14,14,15	0.67	0	17,19,21	0.93	0
2	NAG	E	1	1,2	14,14,15	0.65	0	17,19,21	1.45	2 (11%)
2	NAG	E	2	2	14,14,15	0.71	0	17,19,21	0.82	0
2	NAG	F	1	1,2	14,14,15	0.82	0	17,19,21	1.25	2 (11%)
2	NAG	F	2	2	14,14,15	0.74	0	17,19,21	0.88	0
2	NAG	G	1	1,2	14,14,15	0.75	0	17,19,21	1.32	2 (11%)
2	NAG	G	2	2	14,14,15	0.73	0	17,19,21	0.91	0
3	NAG	H	1	1,3	14,14,15	0.76	0	17,19,21	0.89	0
3	NAG	H	2	3	14,14,15	0.71	0	17,19,21	0.79	0
3	FUC	H	3	3	10,10,11	0.79	0	14,14,16	0.88	0
2	NAG	I	1	1,2	14,14,15	0.73	0	17,19,21	0.78	0
2	NAG	I	2	2	14,14,15	0.71	0	17,19,21	1.18	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.77	0	17,19,21	1.06	2 (11%)
2	NAG	J	2	2	14,14,15	0.69	0	17,19,21	0.92	0
2	NAG	K	1	1,2	14,14,15	0.66	0	17,19,21	1.45	2 (11%)
2	NAG	K	2	2	14,14,15	0.71	0	17,19,21	0.81	0
2	NAG	L	1	1,2	14,14,15	0.81	0	17,19,21	1.25	2 (11%)
2	NAG	L	2	2	14,14,15	0.74	0	17,19,21	0.88	0
2	NAG	M	1	1,2	14,14,15	0.77	0	17,19,21	1.32	2 (11%)
2	NAG	M	2	2	14,14,15	0.73	0	17,19,21	0.91	0
3	NAG	N	1	1,3	14,14,15	0.77	0	17,19,21	0.90	0
3	NAG	N	2	3	14,14,15	0.71	0	17,19,21	0.78	0
3	FUC	N	3	3	10,10,11	0.79	0	14,14,16	0.87	0
2	NAG	O	1	1,2	14,14,15	0.75	0	17,19,21	0.79	0
2	NAG	O	2	2	14,14,15	0.71	0	17,19,21	1.17	1 (5%)
2	NAG	P	1	1,2	14,14,15	0.76	0	17,19,21	1.06	2 (11%)
2	NAG	P	2	2	14,14,15	0.67	0	17,19,21	0.92	0
2	NAG	Q	1	1,2	14,14,15	0.65	0	17,19,21	1.45	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	Q	2	2	14,14,15	0.72	0	17,19,21	0.82	0
2	NAG	R	1	1,2	14,14,15	0.82	0	17,19,21	1.25	2 (11%)
2	NAG	R	2	2	14,14,15	0.74	0	17,19,21	0.88	0
2	NAG	S	1	1,2	14,14,15	0.76	0	17,19,21	1.31	2 (11%)
2	NAG	S	2	2	14,14,15	0.73	0	17,19,21	0.91	0
3	NAG	T	1	1,3	14,14,15	0.76	0	17,19,21	0.89	0
3	NAG	T	2	3	14,14,15	0.71	0	17,19,21	0.79	0
3	FUC	T	3	3	10,10,11	0.80	0	14,14,16	0.87	0
2	NAG	U	1	1,2	14,14,15	0.73	0	17,19,21	0.78	0
2	NAG	U	2	2	14,14,15	0.71	0	17,19,21	1.18	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
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	FUC	H	3	3	-	-	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	3/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	K	2	2	-	1/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	N	3	3	-	-	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	3/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	1/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	FUC	T	3	3	-	-	0/1/1/1
2	NAG	U	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	1	NAG	C2-N2-C7	4.03	128.30	122.90
2	K	1	NAG	C2-N2-C7	4.02	128.29	122.90
2	E	1	NAG	C2-N2-C7	4.01	128.27	122.90
2	G	1	NAG	C1-O5-C5	3.97	117.50	112.19
2	M	1	NAG	C1-O5-C5	3.97	117.50	112.19
2	S	1	NAG	C1-O5-C5	3.95	117.48	112.19
2	R	1	NAG	O5-C1-C2	-3.56	105.78	111.29
2	F	1	NAG	O5-C1-C2	-3.55	105.79	111.29
2	L	1	NAG	O5-C1-C2	-3.54	105.82	111.29
2	I	2	NAG	C2-N2-C7	3.20	127.19	122.90
2	O	2	NAG	C2-N2-C7	3.18	127.17	122.90
2	U	2	NAG	C2-N2-C7	3.17	127.15	122.90
2	F	1	NAG	C1-O5-C5	2.63	115.71	112.19
2	R	1	NAG	C1-O5-C5	2.59	115.66	112.19
2	L	1	NAG	C1-O5-C5	2.59	115.65	112.19
2	Q	1	NAG	O5-C1-C2	-2.48	107.45	111.29
2	K	1	NAG	O5-C1-C2	-2.48	107.46	111.29
2	E	1	NAG	O5-C1-C2	-2.47	107.46	111.29
2	M	1	NAG	O5-C1-C2	-2.32	107.70	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	O5-C1-C2	-2.31	107.71	111.29
2	S	1	NAG	O5-C1-C2	-2.29	107.75	111.29
2	J	1	NAG	O5-C1-C2	-2.27	107.78	111.29
2	D	1	NAG	O5-C1-C2	-2.25	107.80	111.29
2	P	1	NAG	O5-C1-C2	-2.25	107.81	111.29
2	P	1	NAG	C2-N2-C7	2.12	125.74	122.90
2	D	1	NAG	C2-N2-C7	2.10	125.71	122.90
2	J	1	NAG	C2-N2-C7	2.10	125.71	122.90

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C1-C2-N2-C7
2	K	1	NAG	C1-C2-N2-C7
2	Q	1	NAG	C1-C2-N2-C7
2	G	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	P	1	NAG	C8-C7-N2-C2
2	P	1	NAG	O7-C7-N2-C2
2	P	2	NAG	C8-C7-N2-C2
2	P	2	NAG	O7-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6

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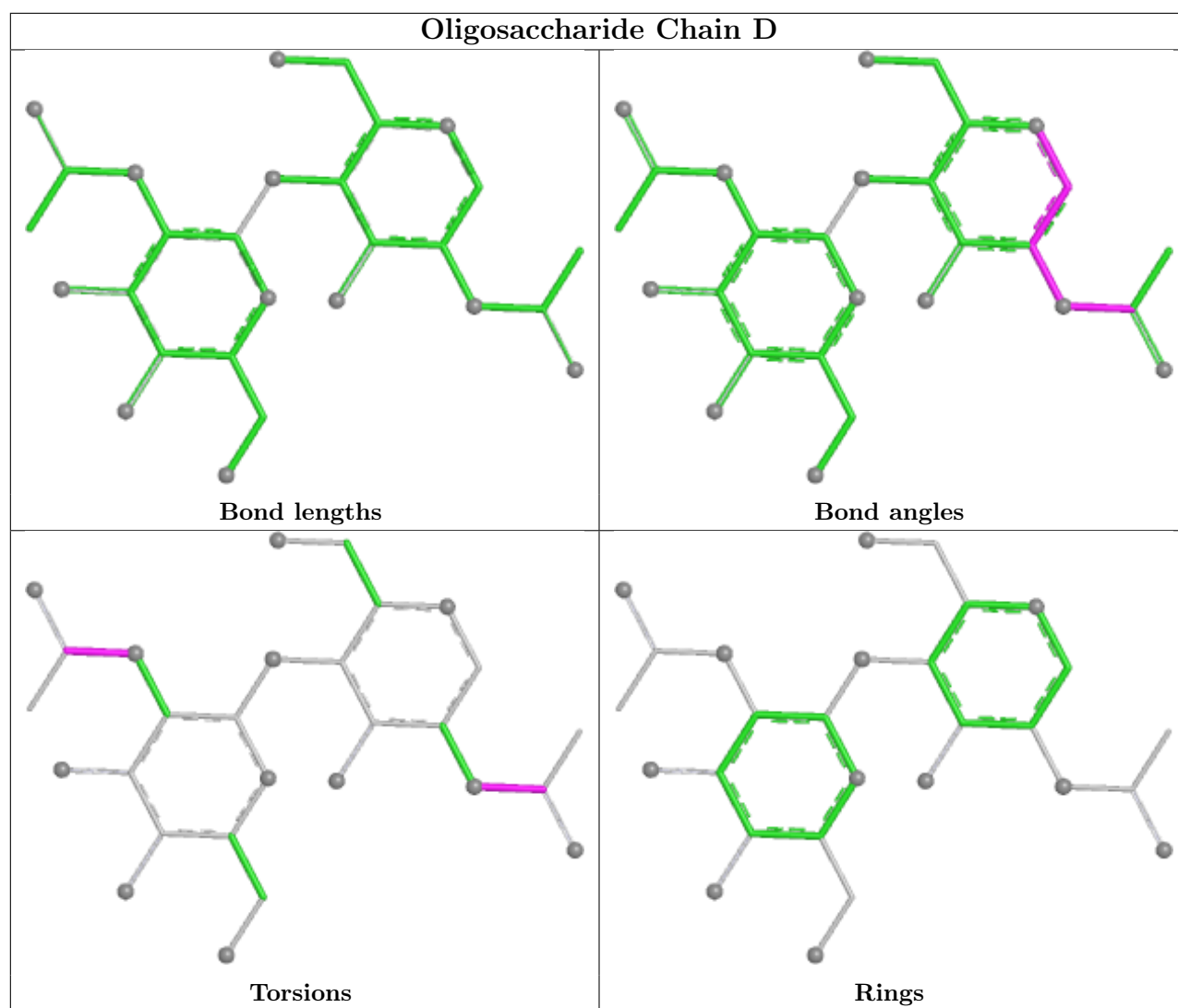
Mol	Chain	Res	Type	Atoms
2	Q	1	NAG	O5-C5-C6-O6
2	I	2	NAG	C1-C2-N2-C7
2	O	2	NAG	C1-C2-N2-C7
2	U	2	NAG	C1-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
2	K	1	NAG	C3-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
2	Q	1	NAG	C3-C2-N2-C7
2	U	2	NAG	C3-C2-N2-C7

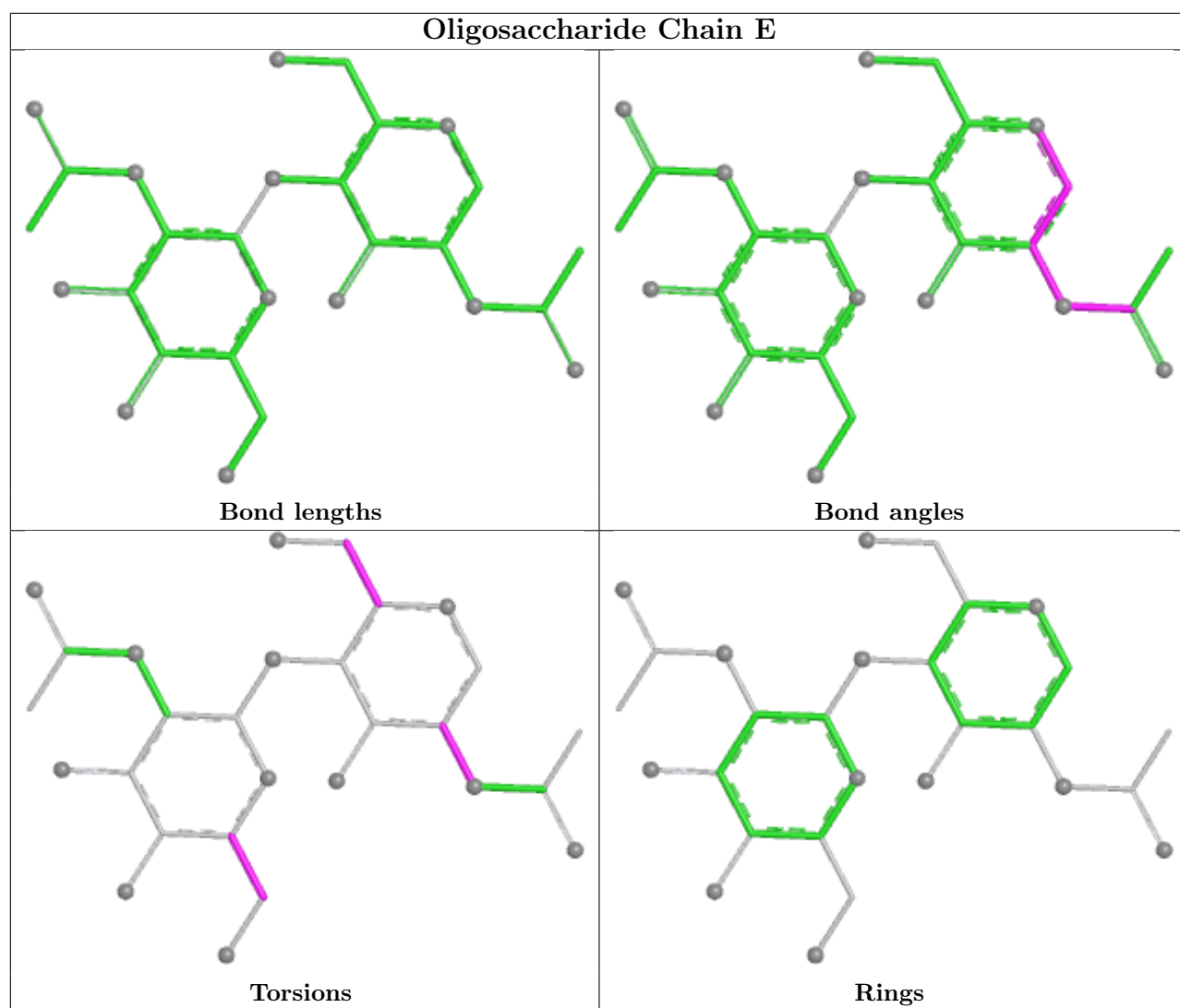
There are no ring outliers.

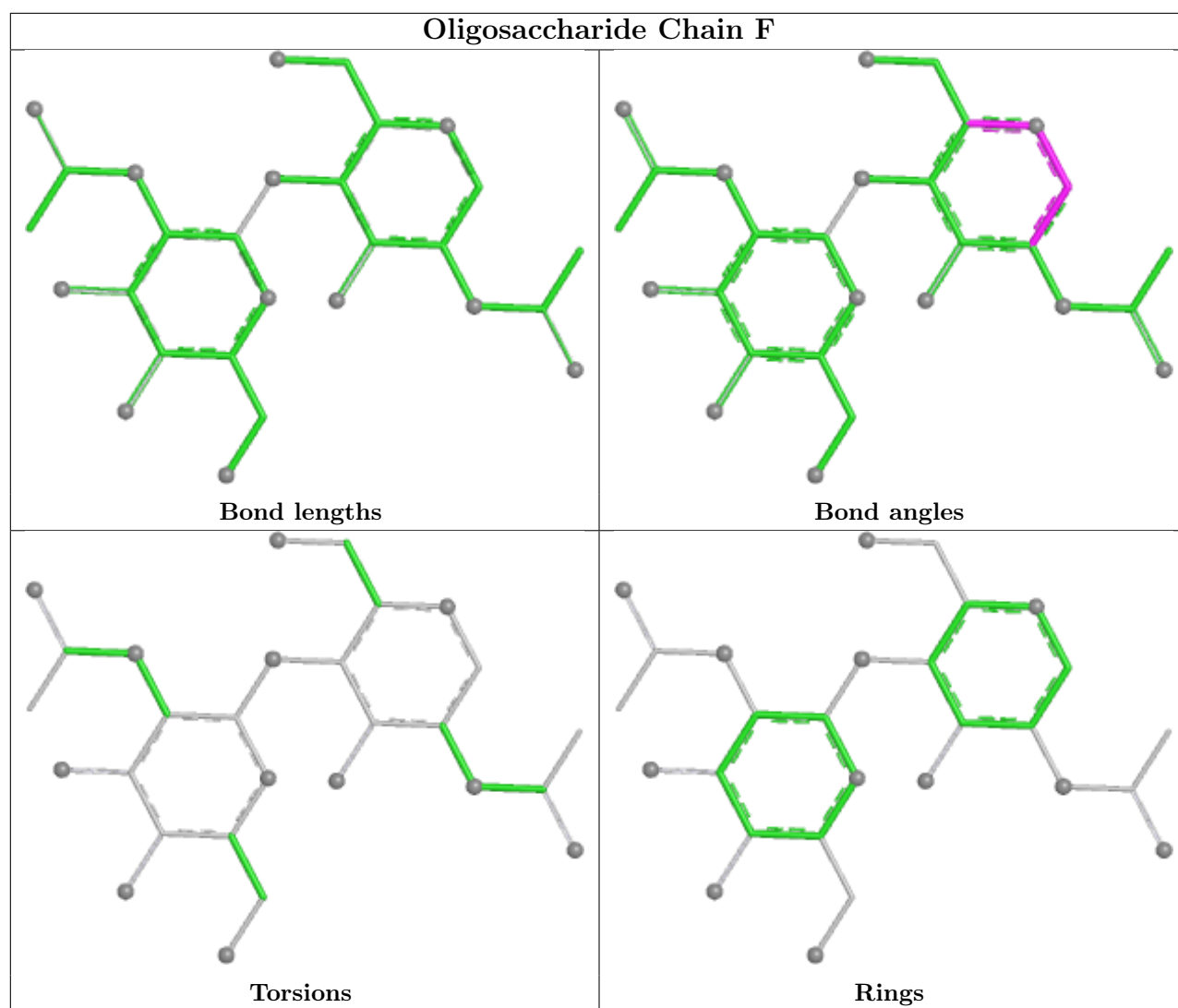
3 monomers are involved in 3 short contacts:

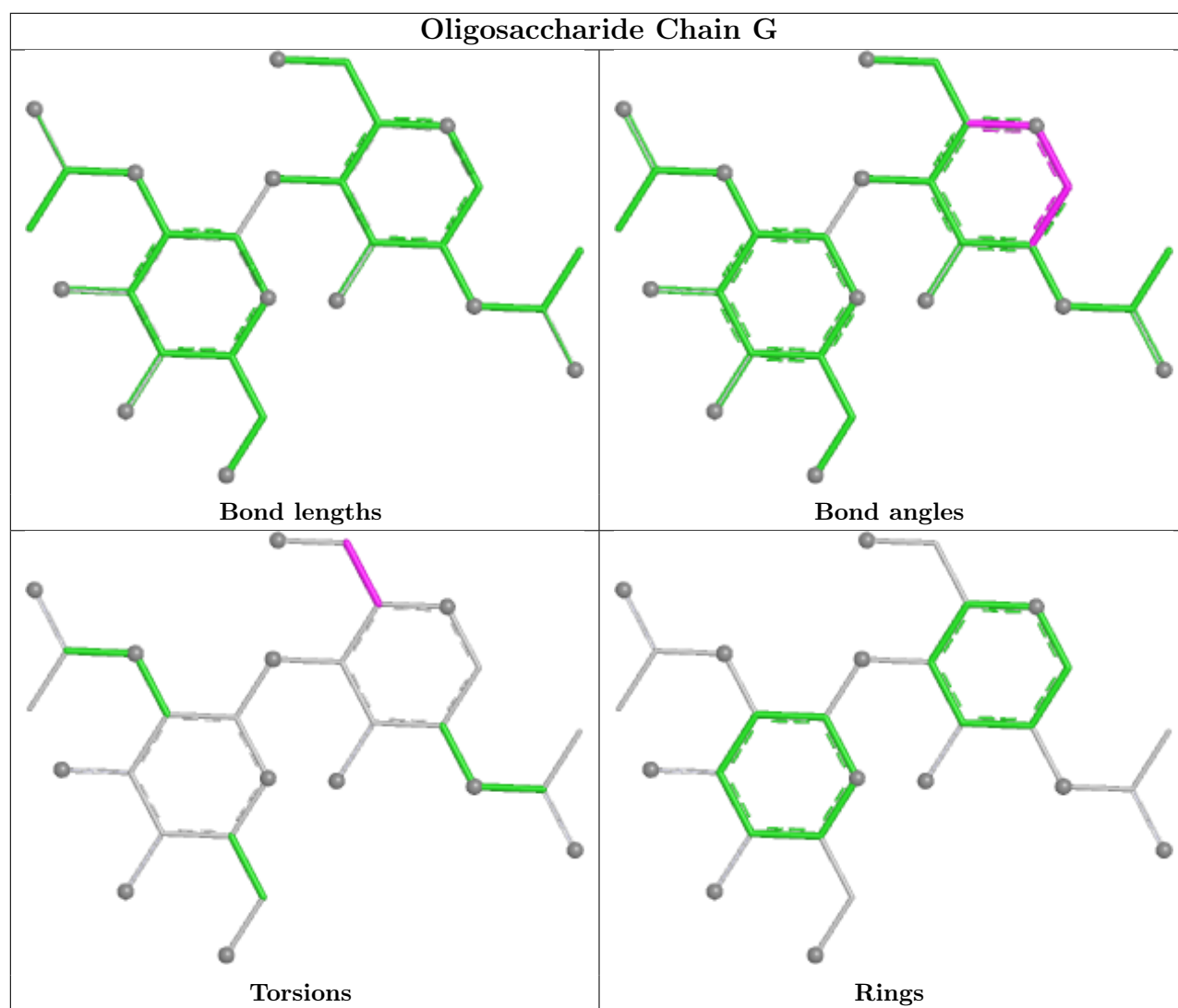
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	J	1	NAG	1	0
2	P	1	NAG	1	0

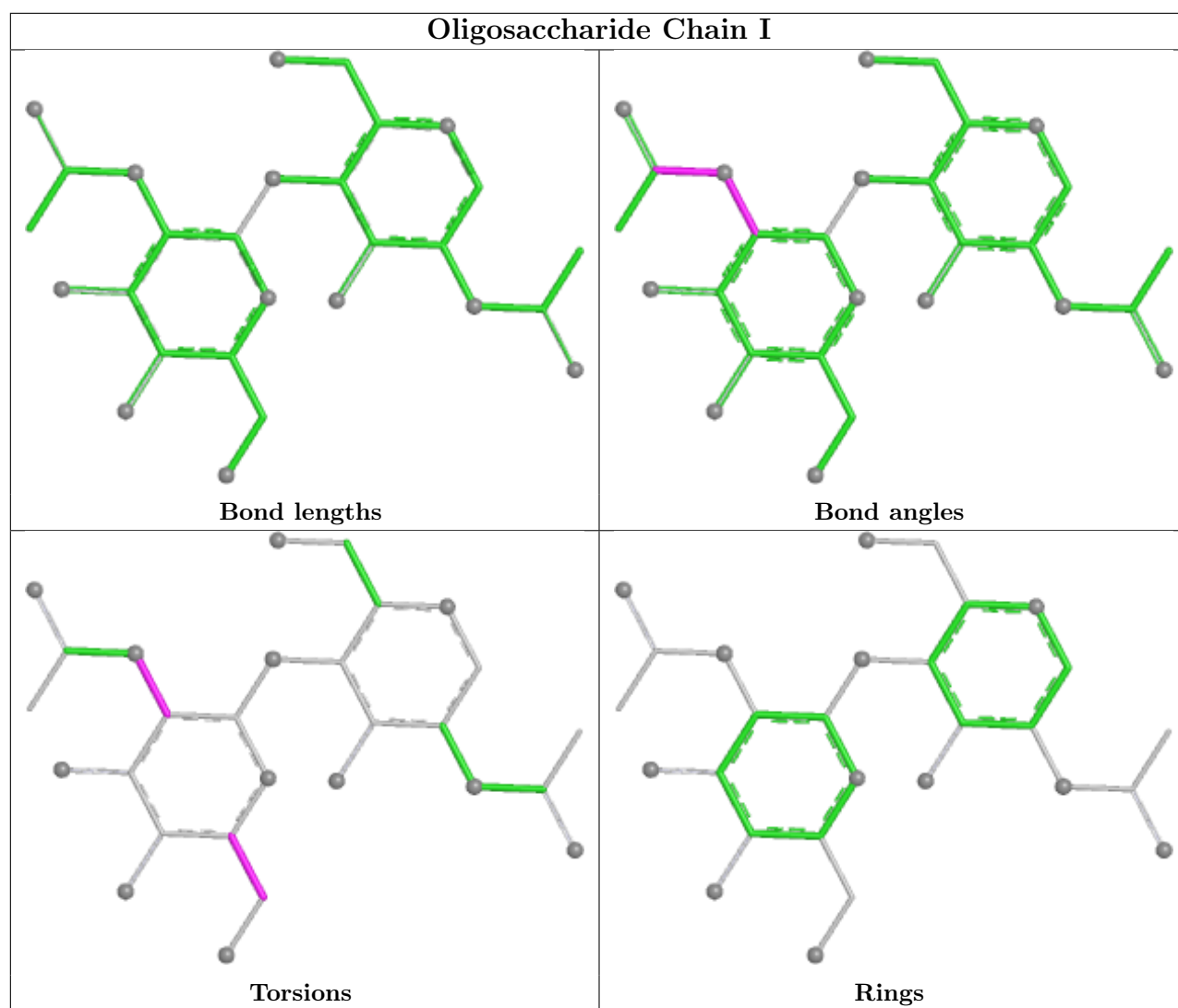
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

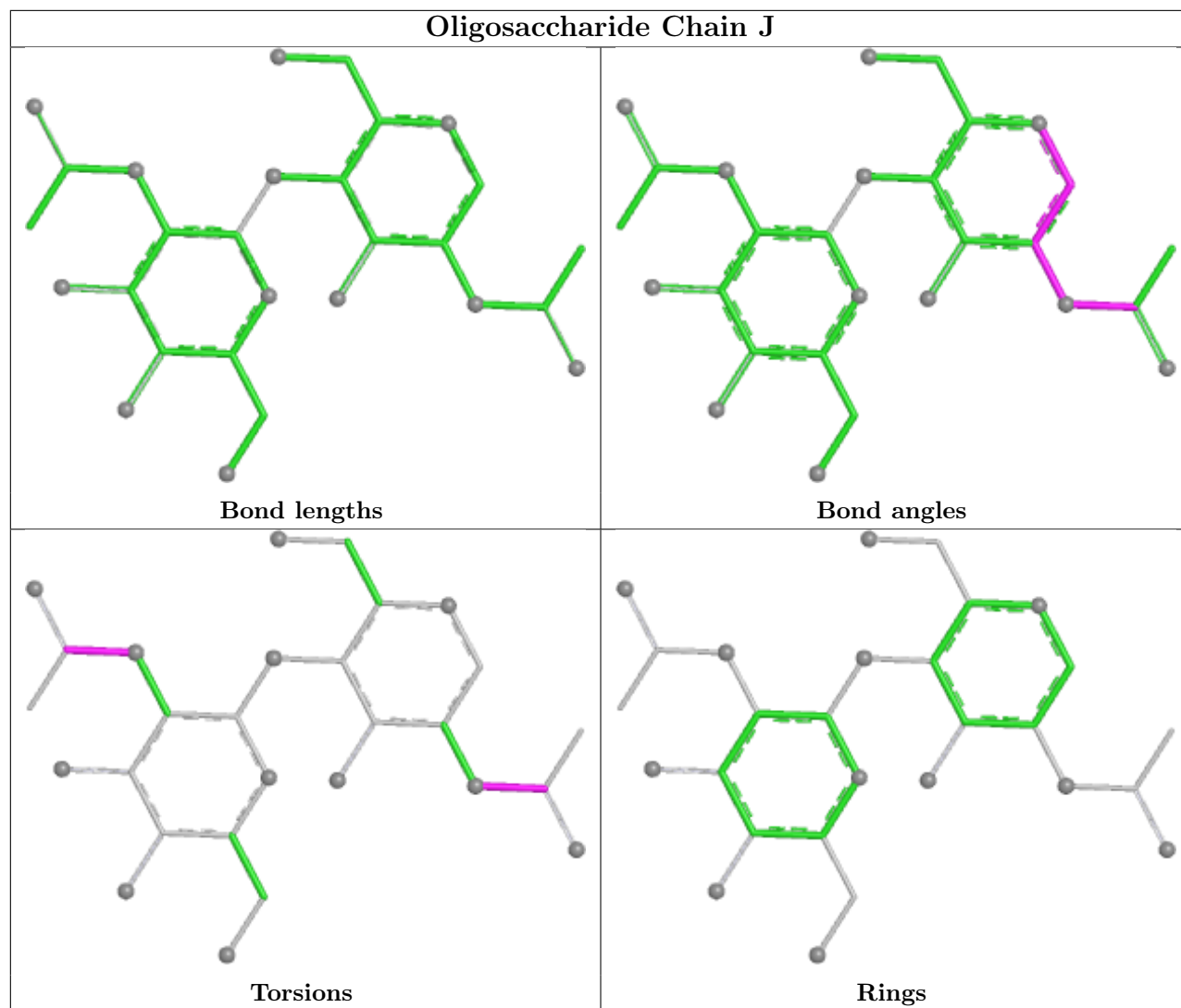




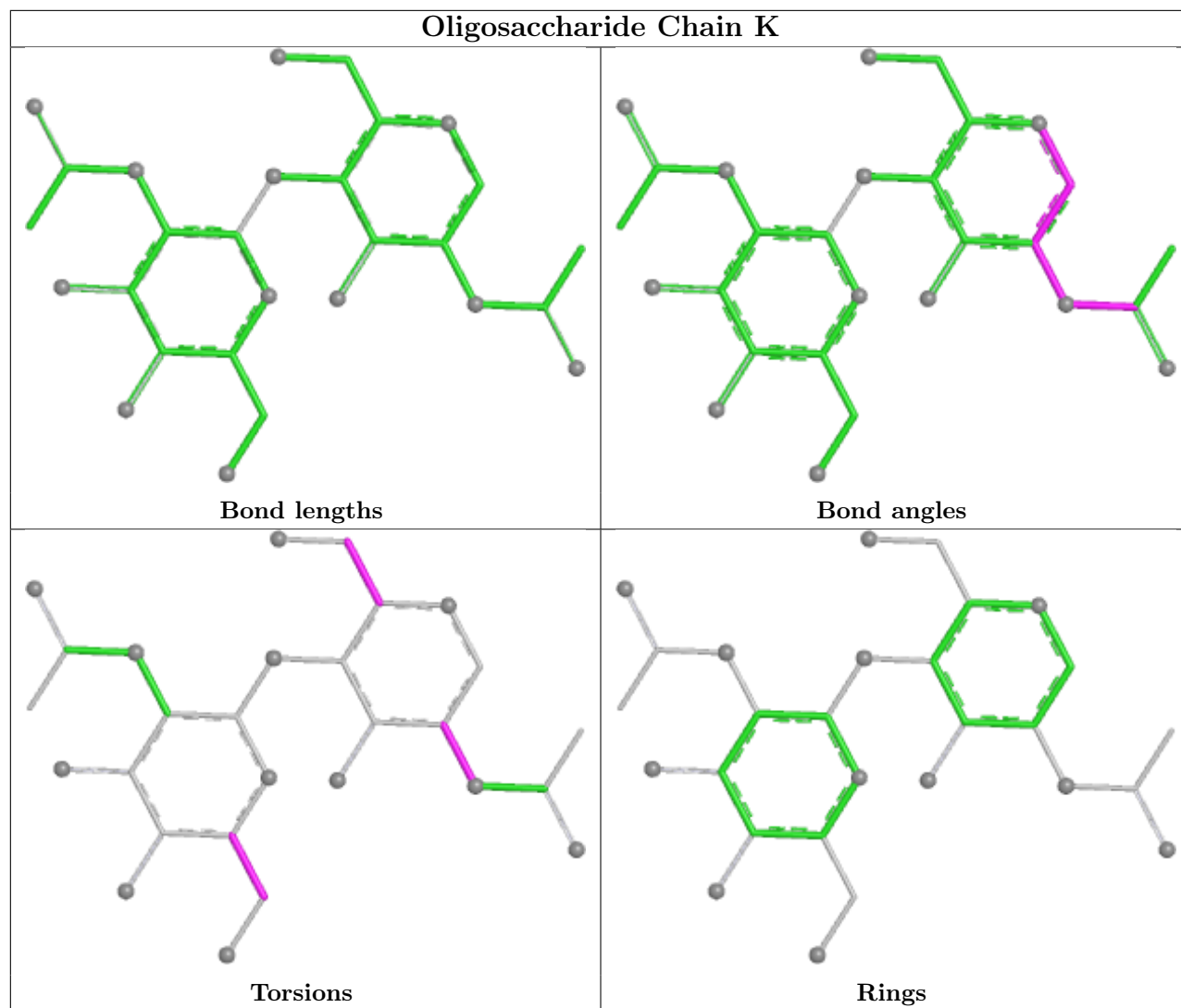


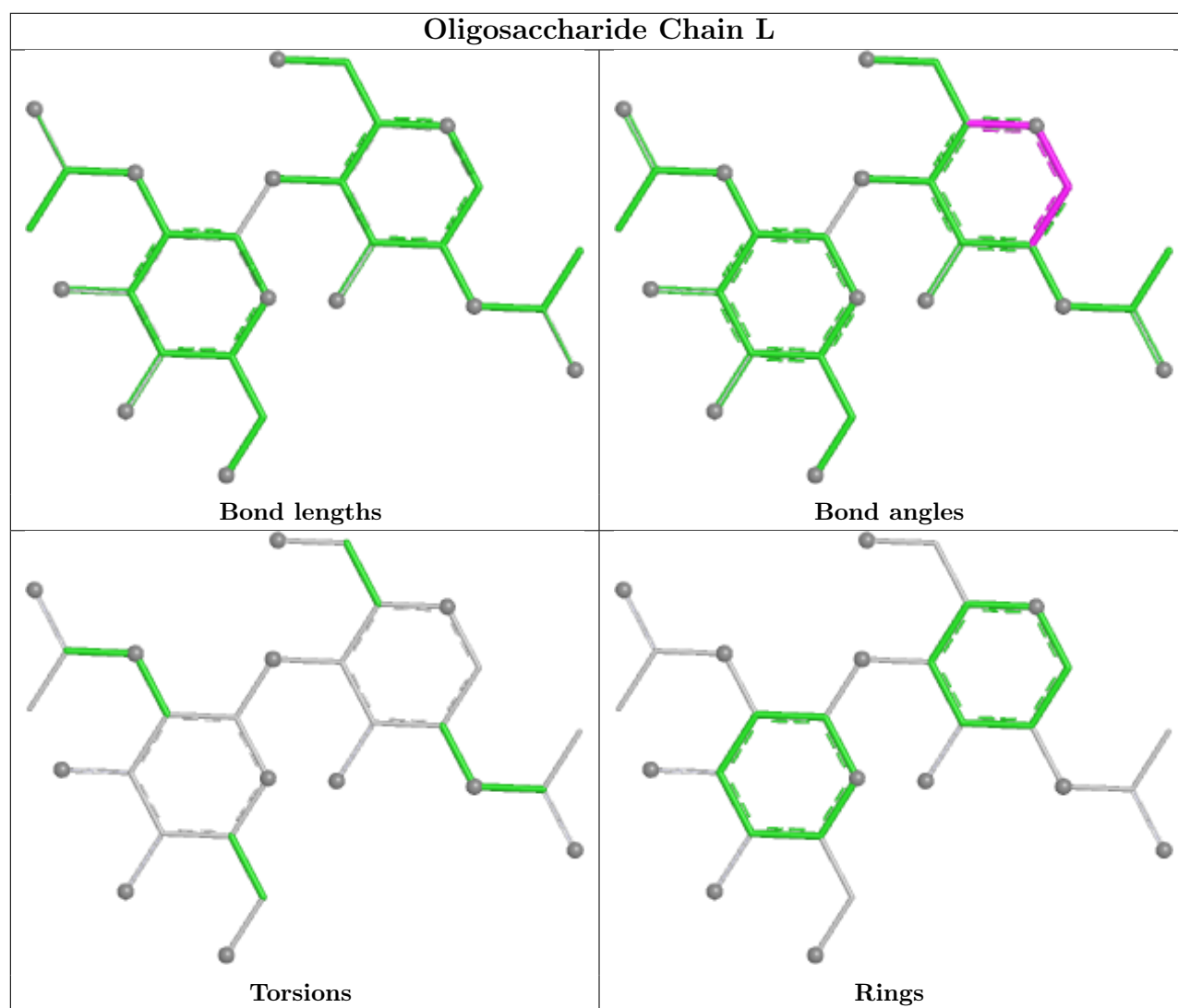


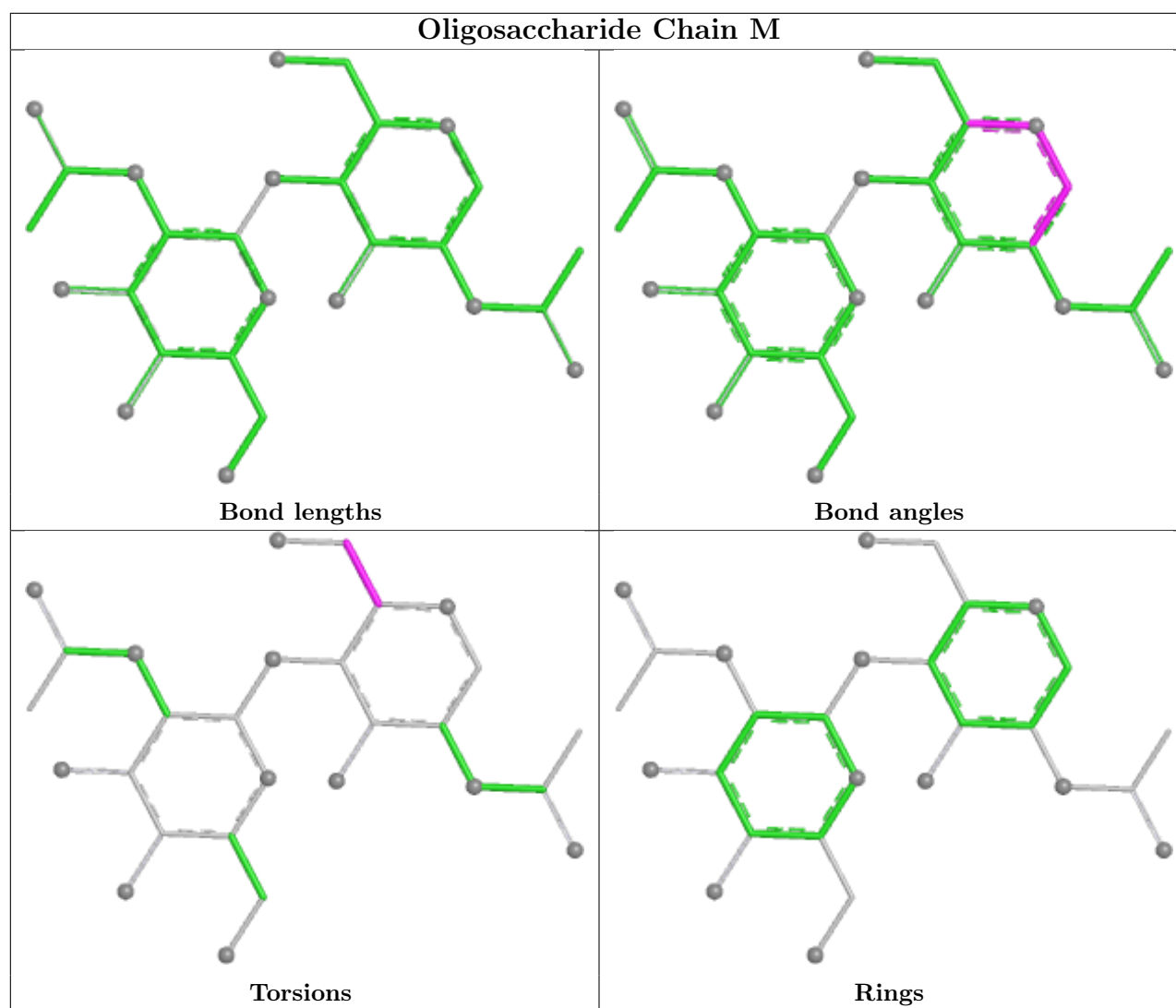


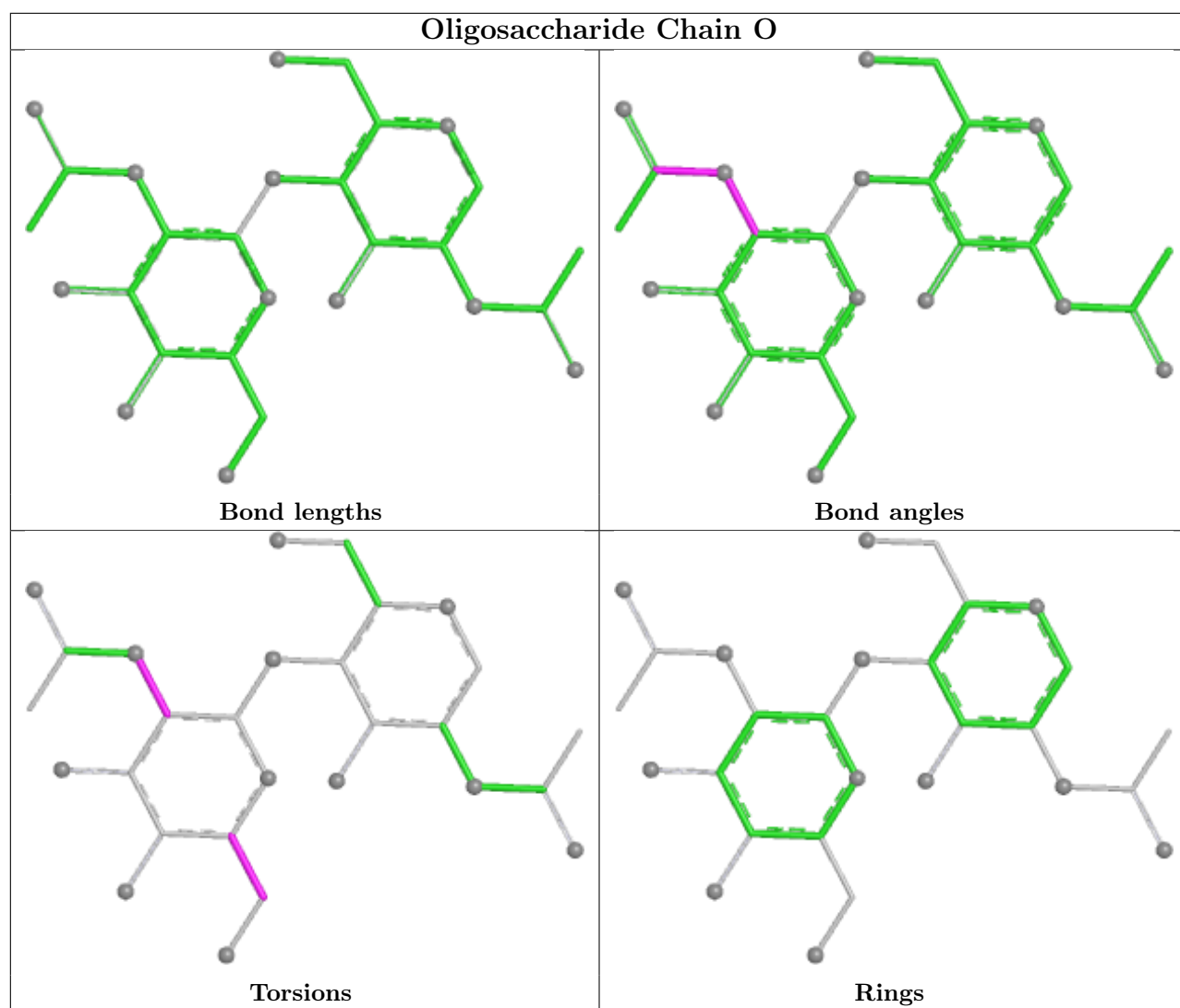


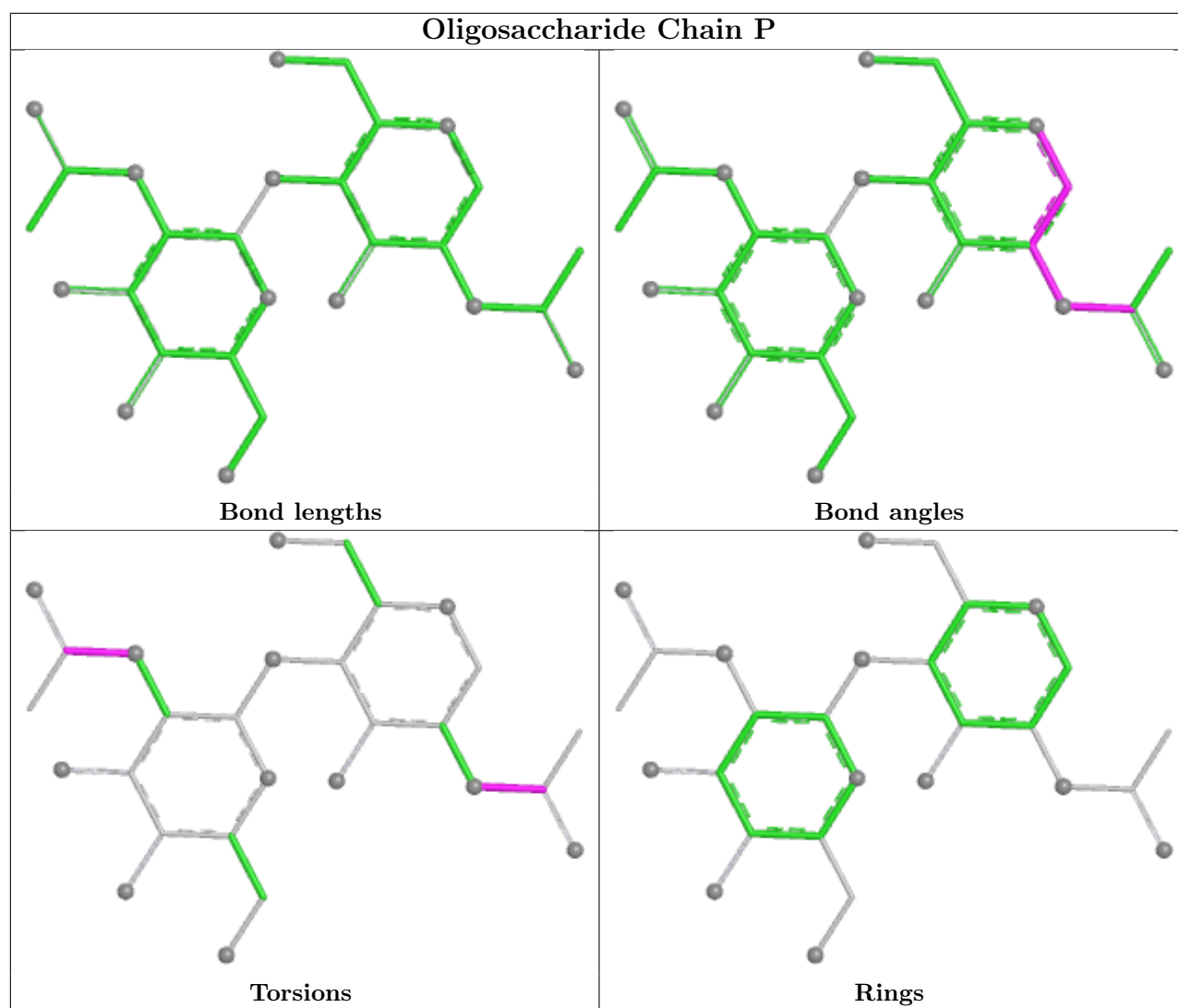


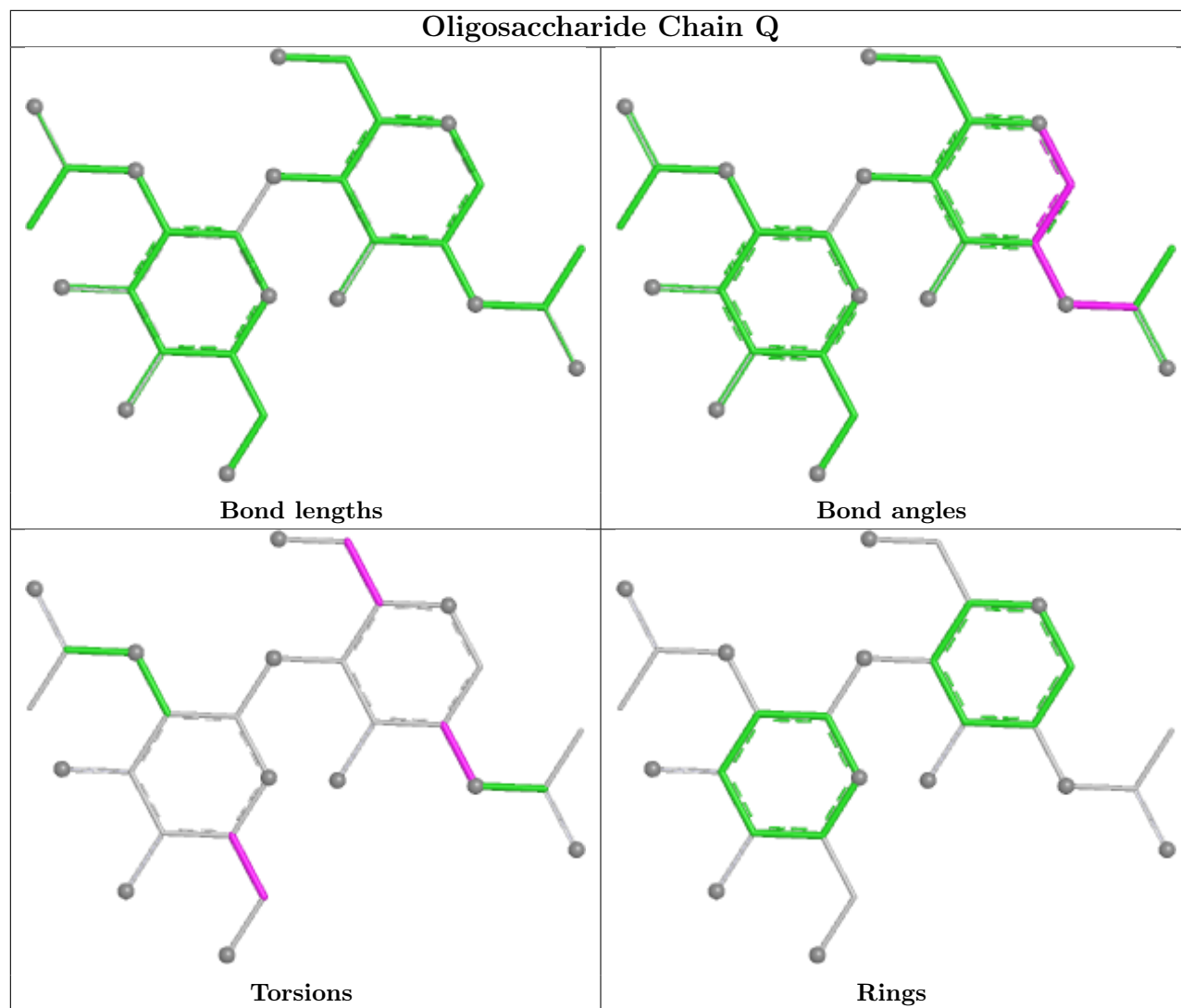


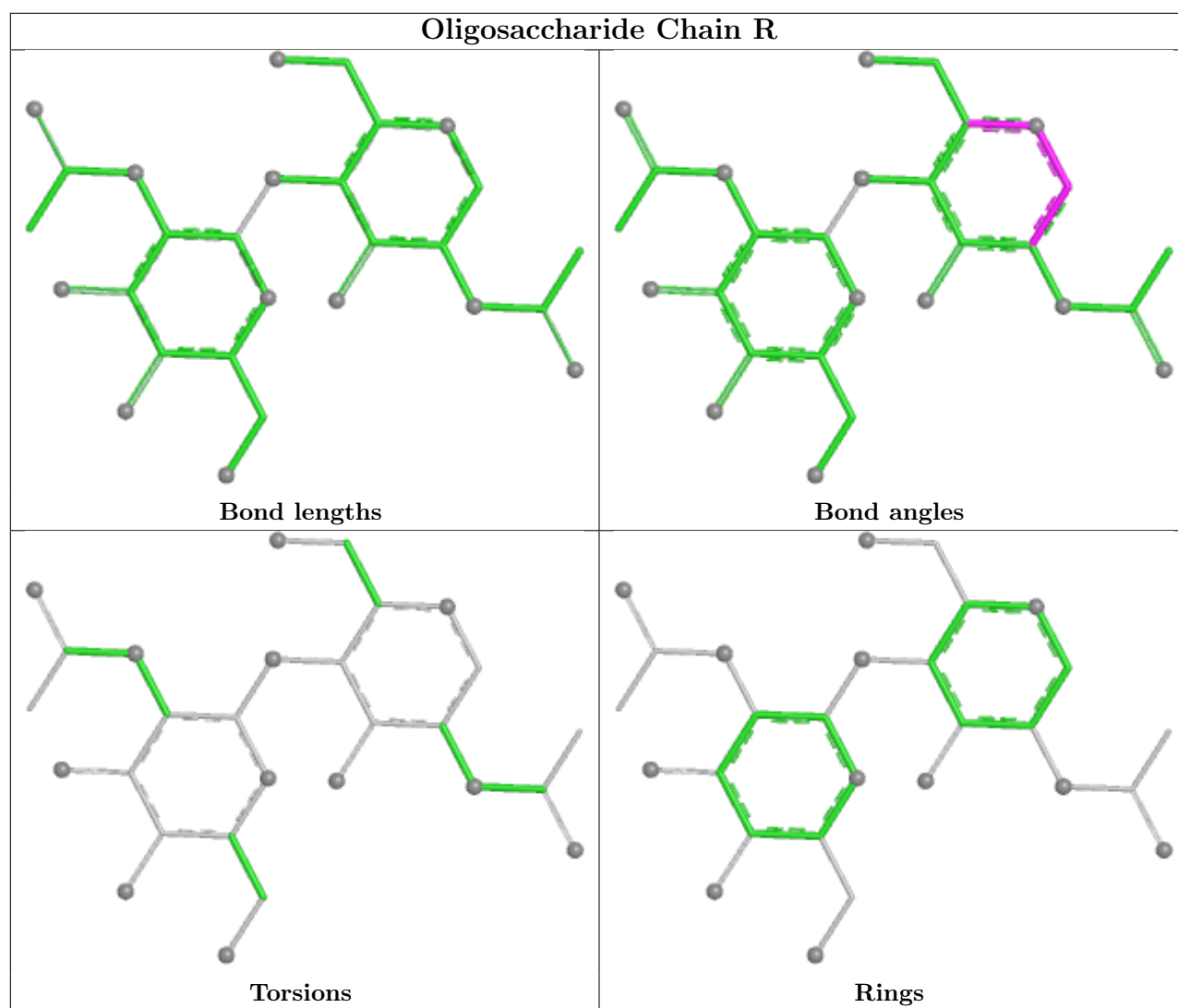


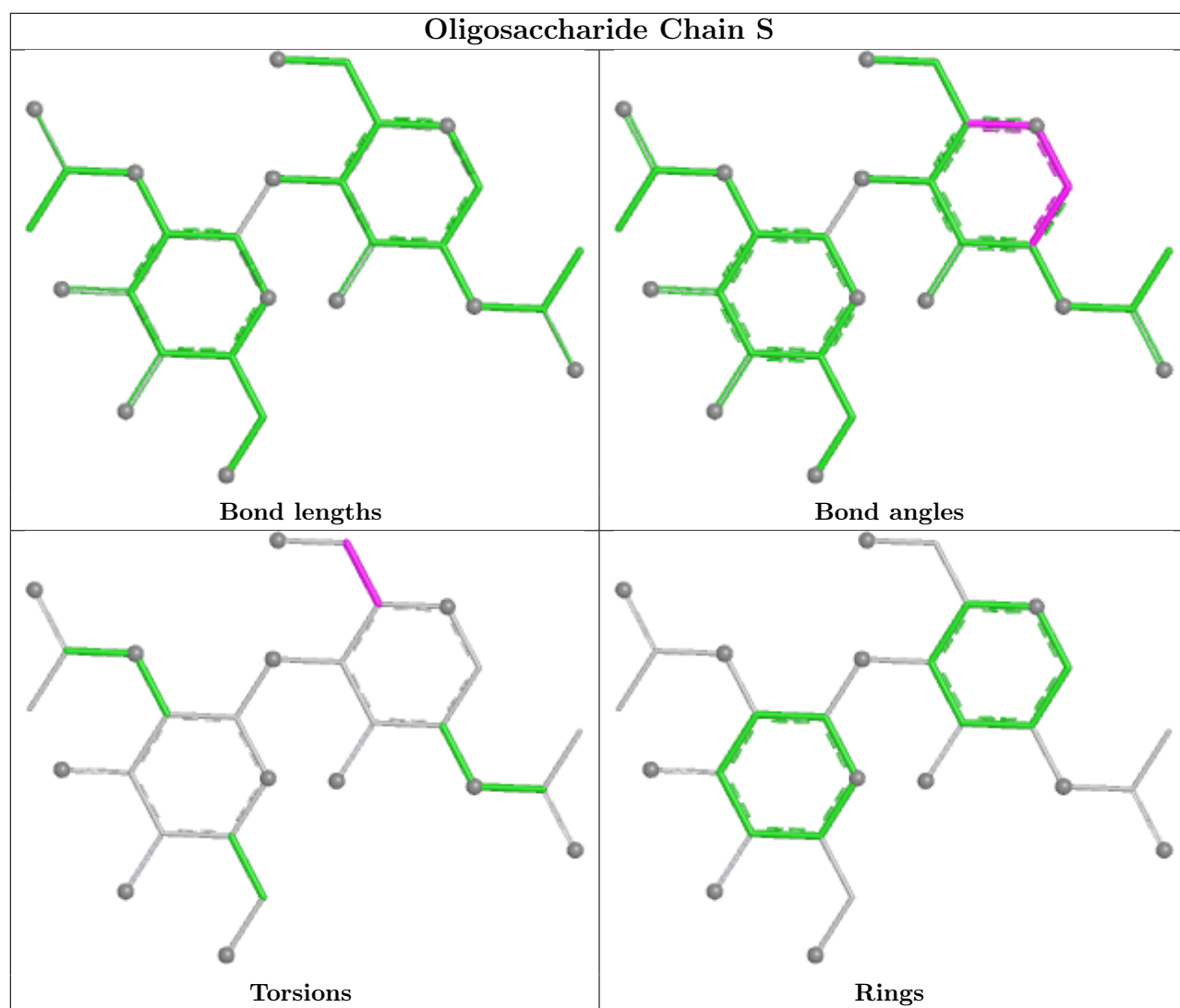




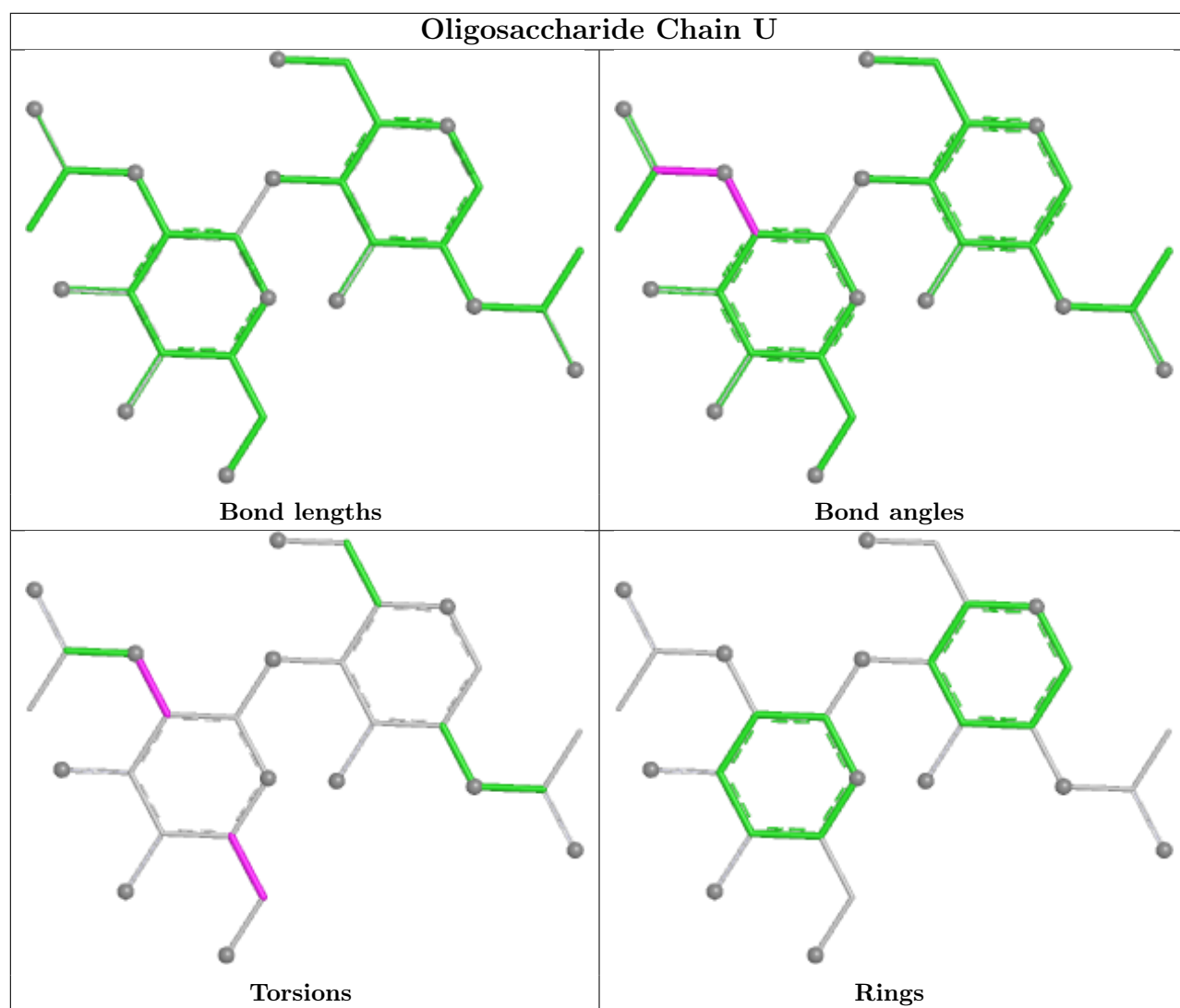


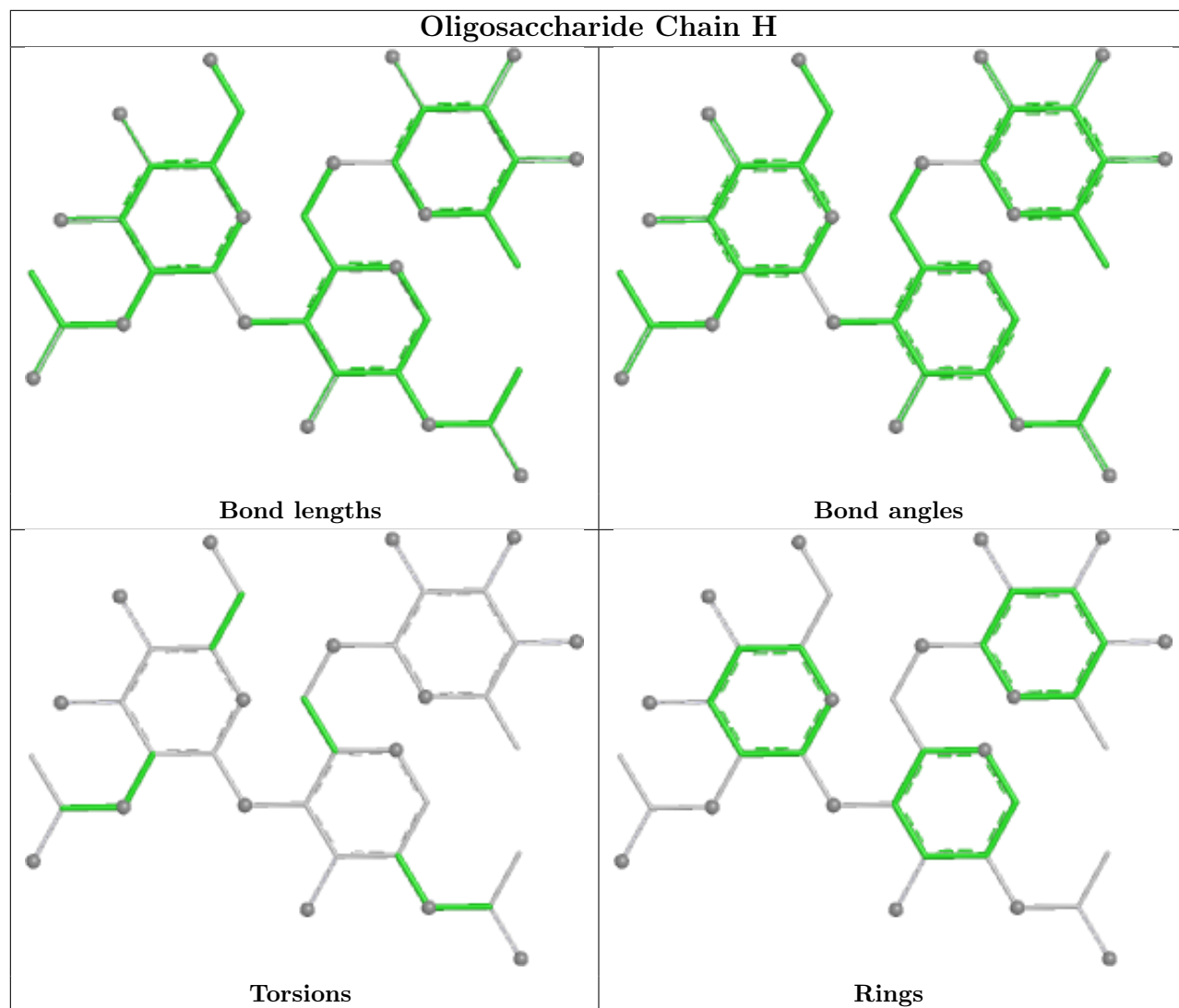


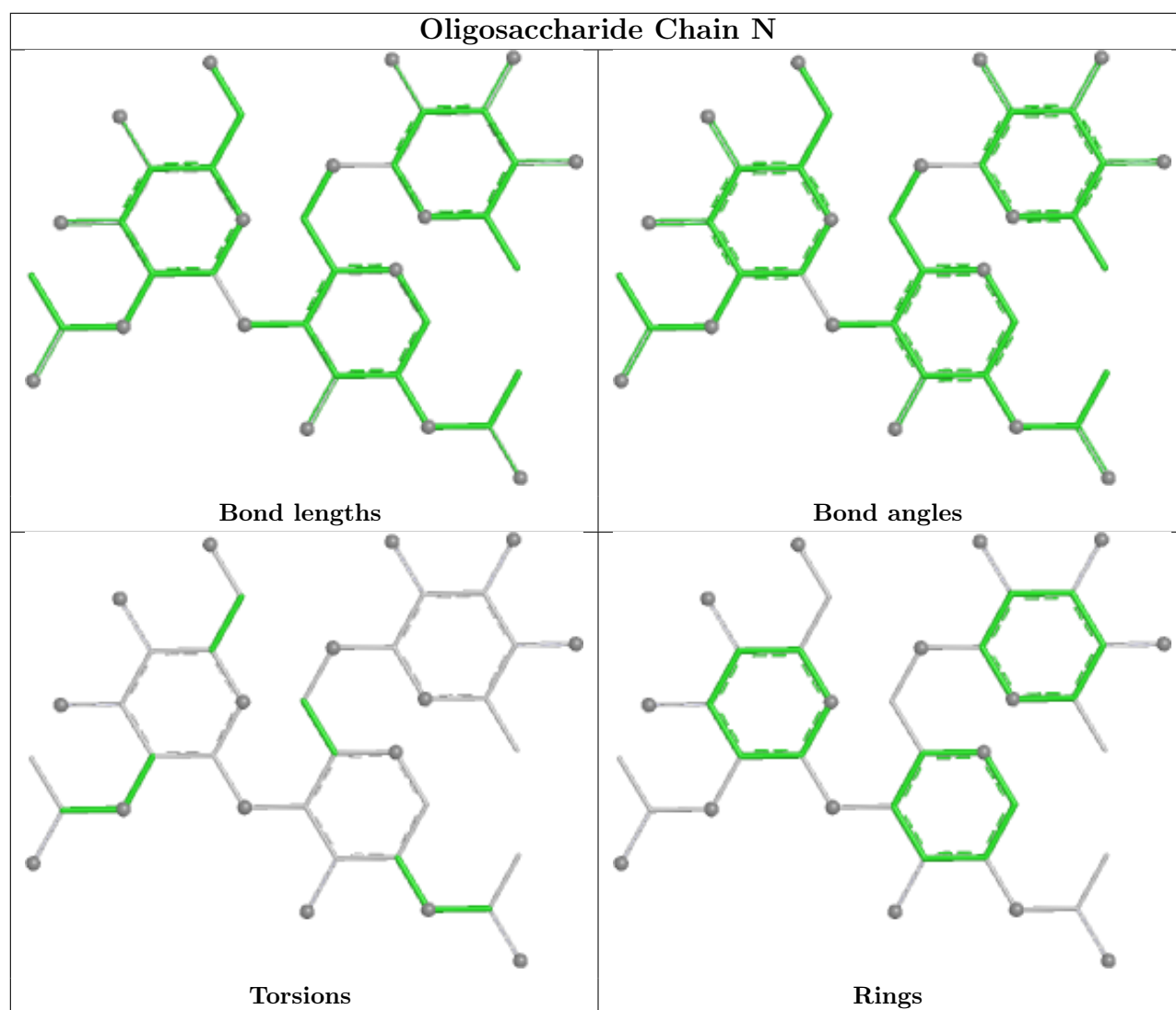


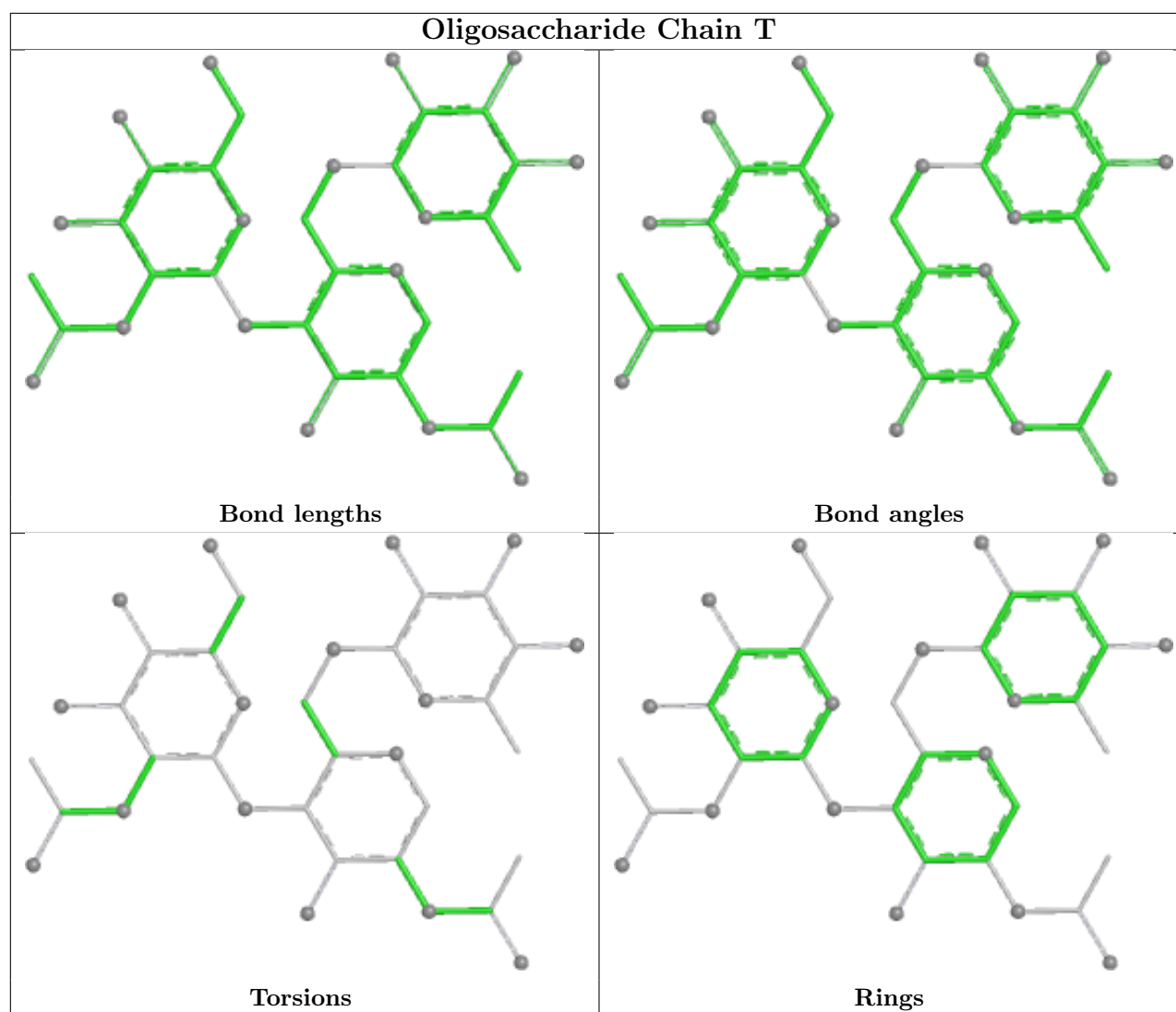












## 5.6 Ligand geometry [i](#)

27 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	$\# Z  > 2$
4	NAG	C	1403	1	14,14,15	0.75	0	17,19,21	1.38	2 (11%)
4	NAG	C	1409	1	14,14,15	0.71	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
4	NAG	A	1408	1	14,14,15	0.80	0	17,19,21	2.38	4 (23%)
4	NAG	A	1407	1	14,14,15	0.69	0	17,19,21	1.93	3 (17%)
4	NAG	B	1404	1	14,14,15	0.70	0	17,19,21	1.36	3 (17%)
4	NAG	C	1405	1	14,14,15	0.80	0	17,19,21	0.95	1 (5%)
4	NAG	B	1407	1	14,14,15	0.68	0	17,19,21	1.93	3 (17%)
4	NAG	C	1408	1	14,14,15	0.80	0	17,19,21	2.38	4 (23%)
4	NAG	C	1406	1	14,14,15	0.72	0	17,19,21	0.85	0
4	NAG	A	1402	1	14,14,15	0.70	0	17,19,21	0.83	0
4	NAG	A	1401	1	14,14,15	0.82	1 (7%)	17,19,21	1.17	1 (5%)
4	NAG	A	1409	1	14,14,15	0.71	0	17,19,21	1.17	1 (5%)
4	NAG	B	1409	1	14,14,15	0.71	0	17,19,21	1.17	1 (5%)
4	NAG	C	1404	1	14,14,15	0.71	0	17,19,21	1.36	3 (17%)
4	NAG	A	1403	1	14,14,15	0.74	0	17,19,21	1.38	2 (11%)
4	NAG	C	1407	1	14,14,15	0.68	0	17,19,21	1.93	3 (17%)
4	NAG	B	1405	1	14,14,15	0.80	0	17,19,21	0.96	1 (5%)
4	NAG	A	1405	1	14,14,15	0.81	0	17,19,21	0.95	1 (5%)
4	NAG	C	1402	1	14,14,15	0.71	0	17,19,21	0.84	0
4	NAG	C	1401	1	14,14,15	0.82	1 (7%)	17,19,21	1.17	1 (5%)
4	NAG	B	1403	1	14,14,15	0.75	0	17,19,21	1.39	2 (11%)
4	NAG	A	1404	1	14,14,15	0.70	0	17,19,21	1.35	3 (17%)
4	NAG	A	1406	1	14,14,15	0.73	0	17,19,21	0.85	0
4	NAG	B	1402	1	14,14,15	0.70	0	17,19,21	0.83	0
4	NAG	B	1401	1	14,14,15	0.83	1 (7%)	17,19,21	1.17	2 (11%)
4	NAG	B	1408	1	14,14,15	0.80	0	17,19,21	2.38	4 (23%)
4	NAG	B	1406	1	14,14,15	0.73	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
4	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1406	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1401	NAG	C1-C2	2.06	1.55	1.52
4	A	1401	NAG	C1-C2	2.05	1.55	1.52
4	B	1401	NAG	C1-C2	2.01	1.55	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1408	NAG	C2-N2-C7	8.21	133.90	122.90
4	A	1408	NAG	C2-N2-C7	8.21	133.90	122.90
4	C	1408	NAG	C2-N2-C7	8.21	133.90	122.90
4	B	1407	NAG	C1-O5-C5	-5.93	104.24	112.19
4	A	1407	NAG	C1-O5-C5	-5.88	104.30	112.19
4	C	1407	NAG	C1-O5-C5	-5.88	104.31	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1403	NAG	C1-O5-C5	4.15	117.75	112.19
4	C	1403	NAG	C1-O5-C5	4.14	117.73	112.19
4	A	1403	NAG	C1-O5-C5	4.13	117.73	112.19
4	B	1409	NAG	C2-N2-C7	3.24	127.24	122.90
4	B	1404	NAG	O5-C1-C2	-3.24	106.28	111.29
4	C	1409	NAG	C2-N2-C7	3.24	127.24	122.90
4	A	1404	NAG	O5-C1-C2	-3.23	106.30	111.29
4	A	1409	NAG	C2-N2-C7	3.22	127.22	122.90
4	C	1404	NAG	O5-C1-C2	-3.22	106.31	111.29
4	B	1401	NAG	C2-N2-C7	3.05	126.99	122.90
4	A	1401	NAG	C2-N2-C7	3.02	126.95	122.90
4	C	1401	NAG	C2-N2-C7	3.02	126.94	122.90
4	A	1407	NAG	O5-C5-C6	2.84	113.20	107.66
4	C	1407	NAG	O5-C5-C6	2.82	113.16	107.66
4	B	1407	NAG	O5-C5-C6	2.82	113.15	107.66
4	B	1408	NAG	C8-C7-N2	2.68	120.56	116.12
4	A	1408	NAG	C8-C7-N2	2.66	120.53	116.12
4	C	1408	NAG	C8-C7-N2	2.65	120.51	116.12
4	C	1407	NAG	O4-C4-C3	-2.48	104.52	110.38
4	B	1407	NAG	O4-C4-C3	-2.48	104.53	110.38
4	A	1407	NAG	O4-C4-C3	-2.48	104.54	110.38
4	B	1403	NAG	O5-C1-C2	-2.46	107.49	111.29
4	C	1404	NAG	C1-O5-C5	2.46	115.48	112.19
4	B	1404	NAG	C1-O5-C5	2.45	115.46	112.19
4	A	1403	NAG	O5-C1-C2	-2.43	107.53	111.29
4	A	1404	NAG	C1-O5-C5	2.42	115.43	112.19
4	C	1403	NAG	O5-C1-C2	-2.42	107.55	111.29
4	B	1408	NAG	C1-O5-C5	2.39	115.39	112.19
4	A	1408	NAG	C1-O5-C5	2.37	115.36	112.19
4	C	1408	NAG	C1-O5-C5	2.36	115.35	112.19
4	B	1408	NAG	C1-C2-N2	2.34	114.12	110.43
4	C	1408	NAG	C1-C2-N2	2.34	114.12	110.43
4	A	1408	NAG	C1-C2-N2	2.33	114.10	110.43
4	A	1404	NAG	C1-C2-N2	2.29	114.04	110.43
4	C	1404	NAG	C1-C2-N2	2.28	114.02	110.43
4	B	1404	NAG	C1-C2-N2	2.27	114.02	110.43
4	B	1405	NAG	C1-O5-C5	2.27	115.23	112.19
4	A	1405	NAG	C1-O5-C5	2.24	115.19	112.19
4	C	1405	NAG	C1-O5-C5	2.24	115.19	112.19
4	B	1401	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1401	NAG	C8-C7-N2-C2
4	A	1401	NAG	O7-C7-N2-C2
4	A	1402	NAG	C8-C7-N2-C2
4	A	1402	NAG	O7-C7-N2-C2
4	A	1408	NAG	C8-C7-N2-C2
4	A	1408	NAG	O7-C7-N2-C2
4	B	1401	NAG	C8-C7-N2-C2
4	B	1401	NAG	O7-C7-N2-C2
4	B	1402	NAG	C8-C7-N2-C2
4	B	1402	NAG	O7-C7-N2-C2
4	B	1408	NAG	C8-C7-N2-C2
4	B	1408	NAG	O7-C7-N2-C2
4	C	1401	NAG	C8-C7-N2-C2
4	C	1401	NAG	O7-C7-N2-C2
4	C	1402	NAG	C8-C7-N2-C2
4	C	1402	NAG	O7-C7-N2-C2
4	C	1408	NAG	C8-C7-N2-C2
4	C	1408	NAG	O7-C7-N2-C2
4	A	1407	NAG	O5-C5-C6-O6
4	C	1407	NAG	O5-C5-C6-O6
4	B	1407	NAG	O5-C5-C6-O6
4	A	1409	NAG	C1-C2-N2-C7
4	B	1409	NAG	C1-C2-N2-C7
4	C	1409	NAG	C1-C2-N2-C7
4	A	1404	NAG	O5-C5-C6-O6
4	C	1404	NAG	O5-C5-C6-O6
4	B	1404	NAG	O5-C5-C6-O6
4	A	1408	NAG	C1-C2-N2-C7
4	B	1408	NAG	C1-C2-N2-C7
4	C	1408	NAG	C1-C2-N2-C7
4	A	1404	NAG	C4-C5-C6-O6
4	B	1404	NAG	C4-C5-C6-O6
4	C	1404	NAG	C4-C5-C6-O6
4	A	1408	NAG	C3-C2-N2-C7
4	A	1409	NAG	C3-C2-N2-C7
4	B	1408	NAG	C3-C2-N2-C7
4	B	1409	NAG	C3-C2-N2-C7
4	C	1408	NAG	C3-C2-N2-C7
4	C	1409	NAG	C3-C2-N2-C7

There are no ring outliers.

9 monomers are involved in 9 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1407	NAG	1	0
4	C	1405	NAG	1	0
4	B	1407	NAG	1	0
4	A	1402	NAG	1	0
4	C	1407	NAG	1	0
4	B	1405	NAG	1	0
4	A	1405	NAG	1	0
4	C	1402	NAG	1	0
4	B	1402	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.

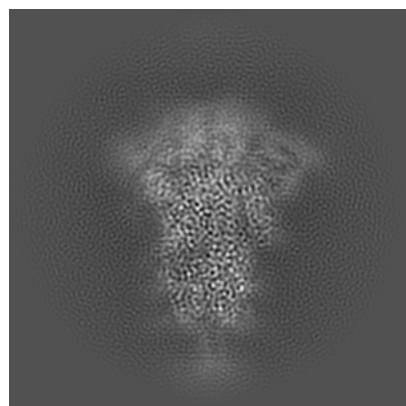
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46639. These allow visual inspection of the internal detail of the map and identification of artifacts.

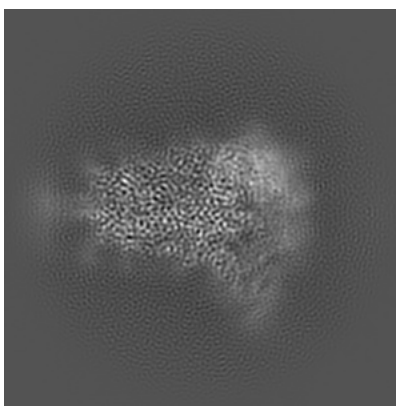
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

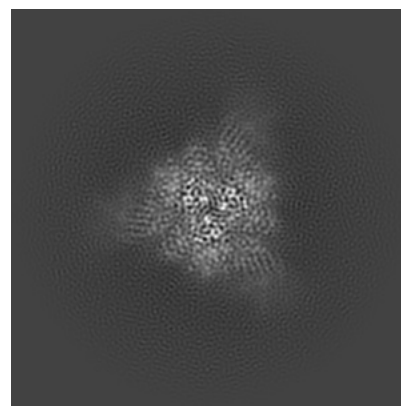
#### 6.1.1 Primary map



X

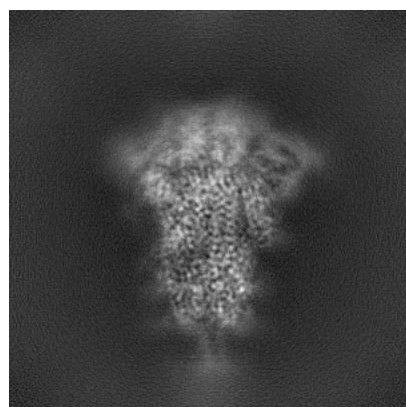


Y

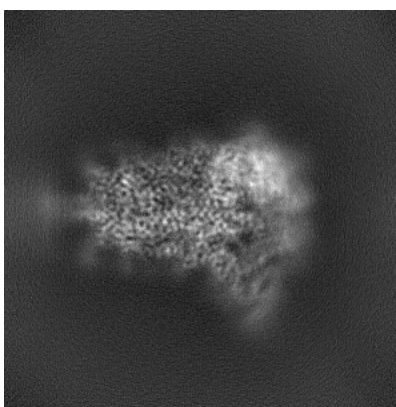


Z

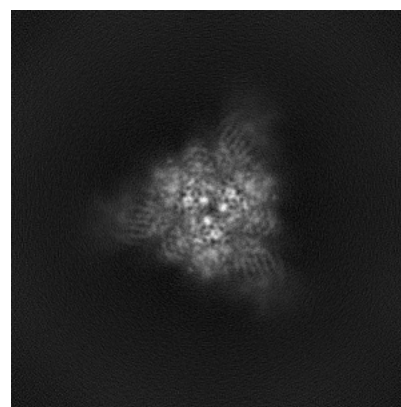
#### 6.1.2 Raw map



X



Y

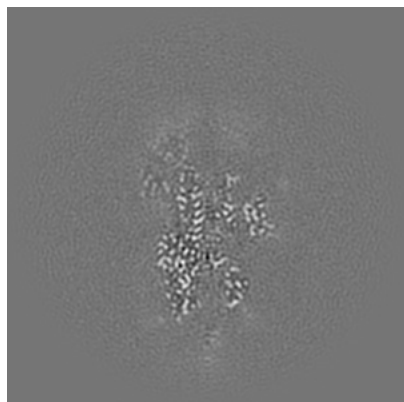


Z

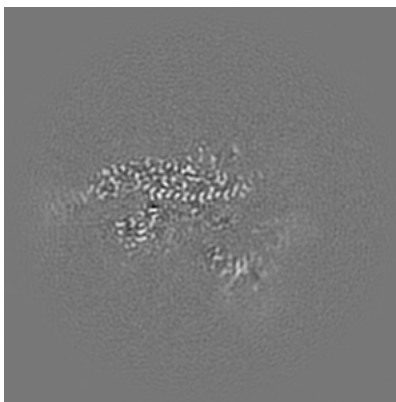
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

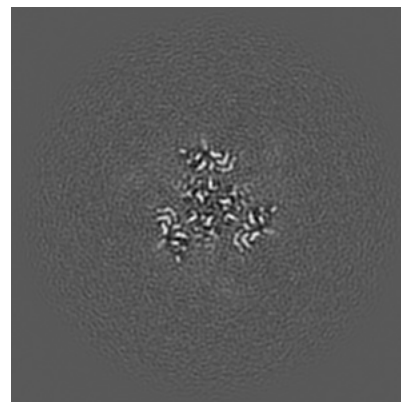
### 6.2.1 Primary map



X Index: 180

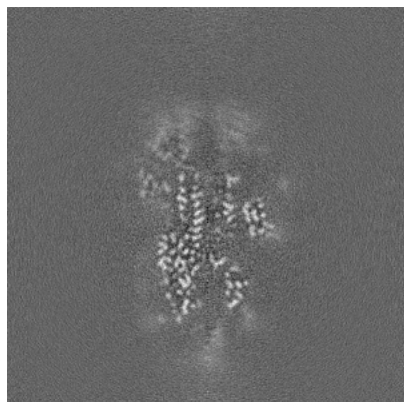


Y Index: 180

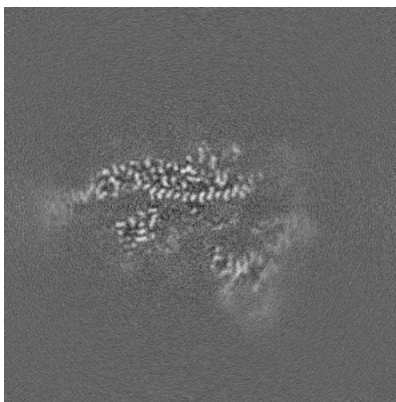


Z Index: 180

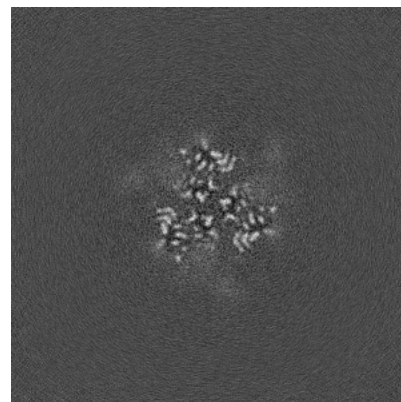
### 6.2.2 Raw map



X Index: 180



Y Index: 180

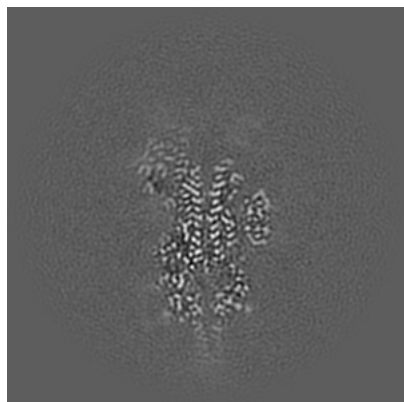


Z Index: 180

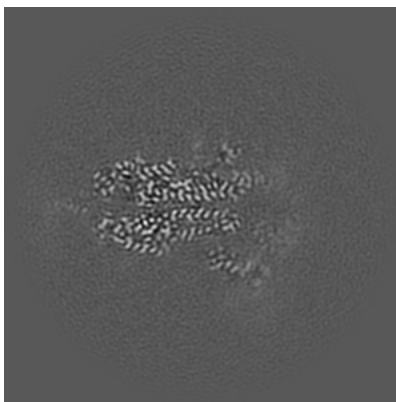
The images above show central slices of the map in three orthogonal directions.

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

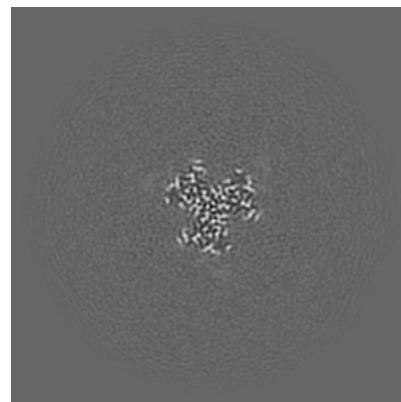
### 6.3.1 Primary map



X Index: 175

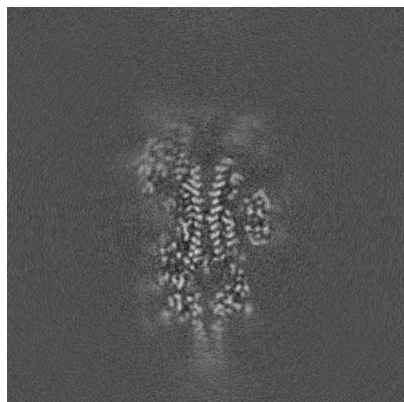


Y Index: 185

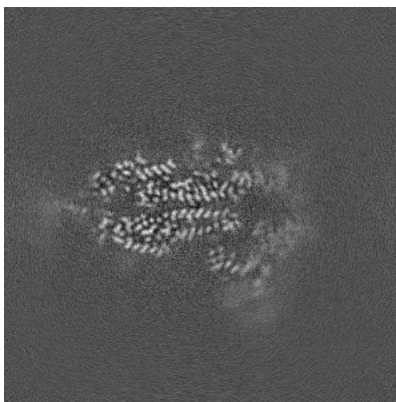


Z Index: 133

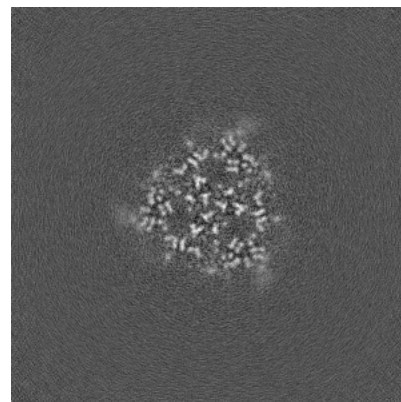
### 6.3.2 Raw map



X Index: 175



Y Index: 185



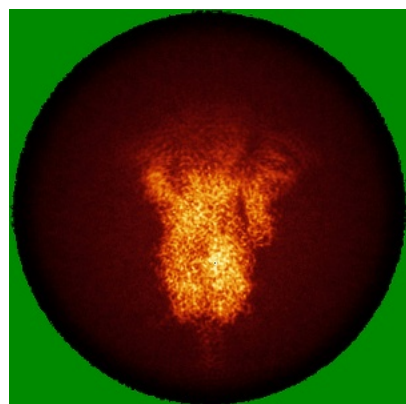
Z Index: 192

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

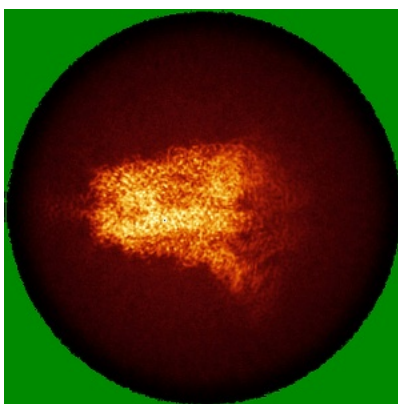


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

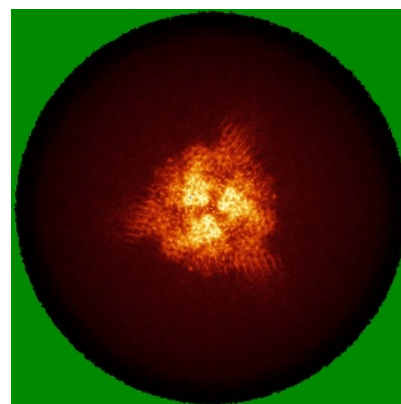
### 6.4.1 Primary map



X

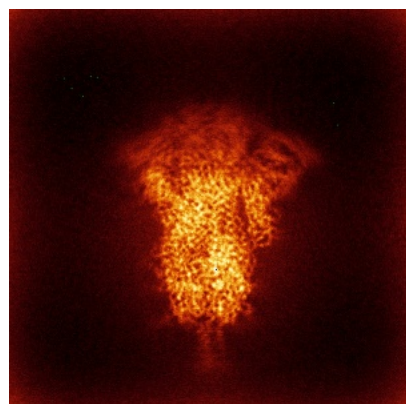


Y

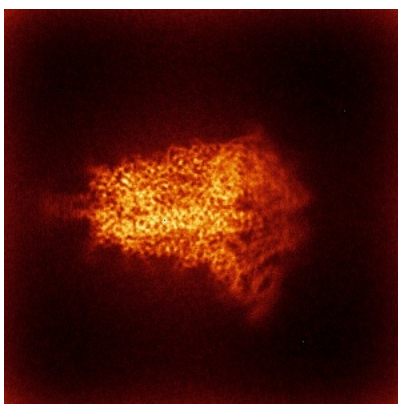


Z

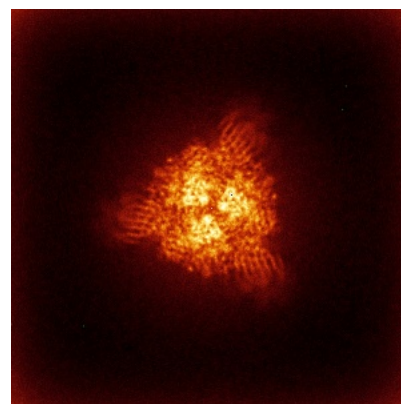
### 6.4.2 Raw map



X



Y

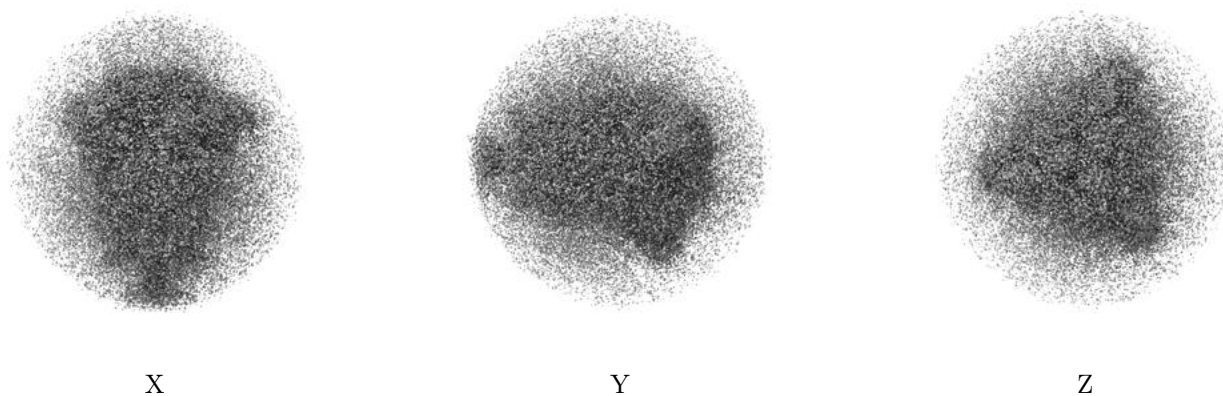


Z

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.

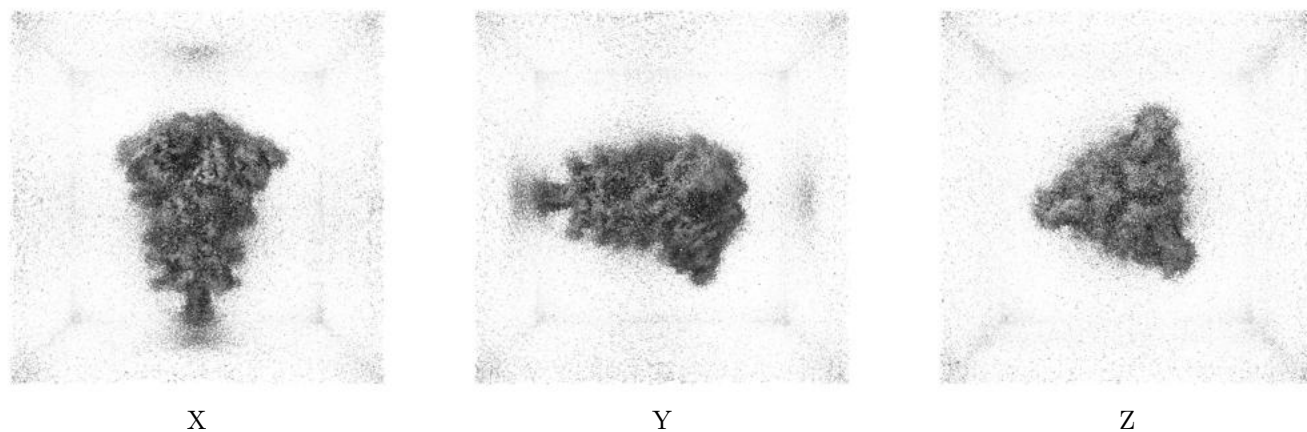
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

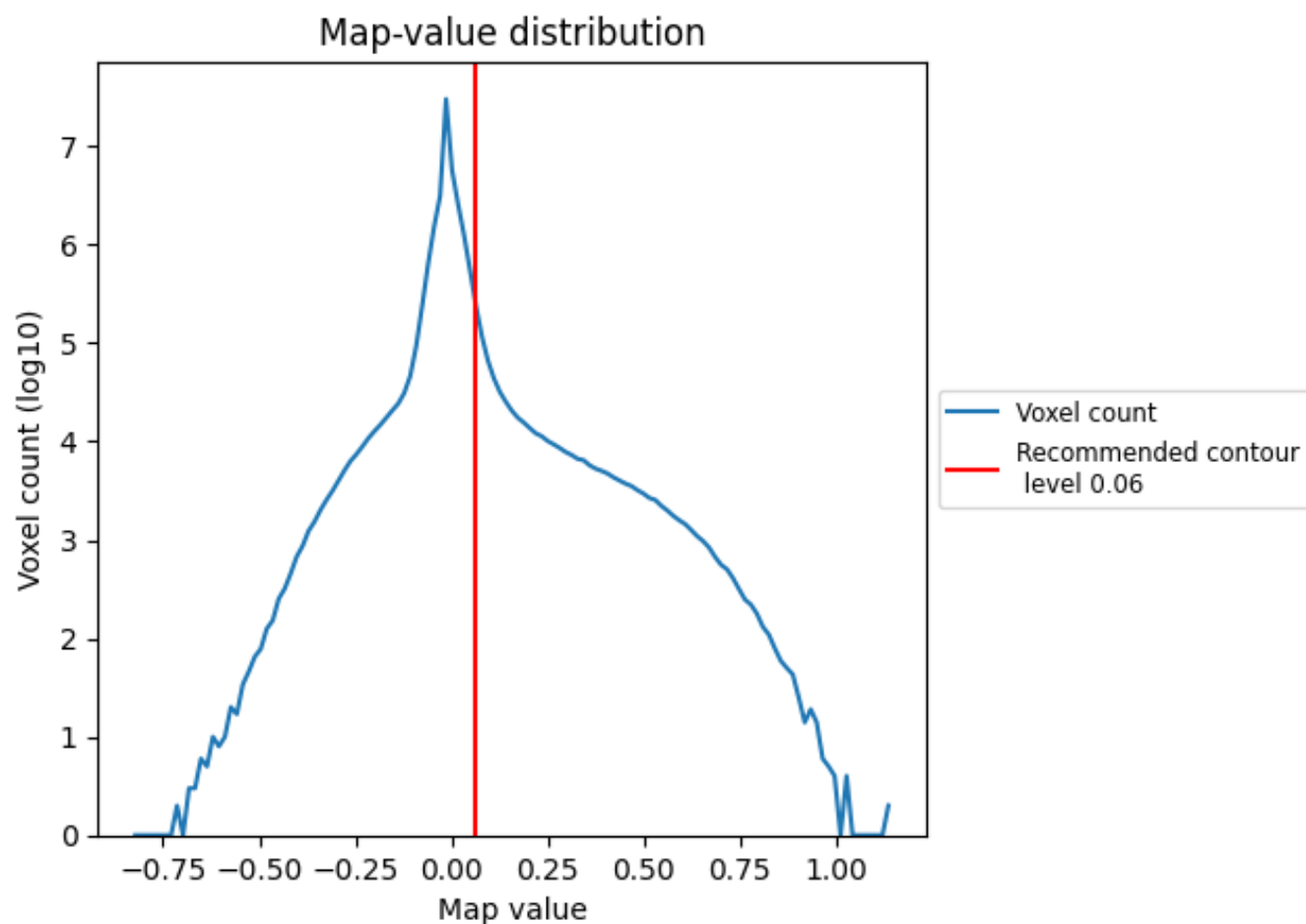
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

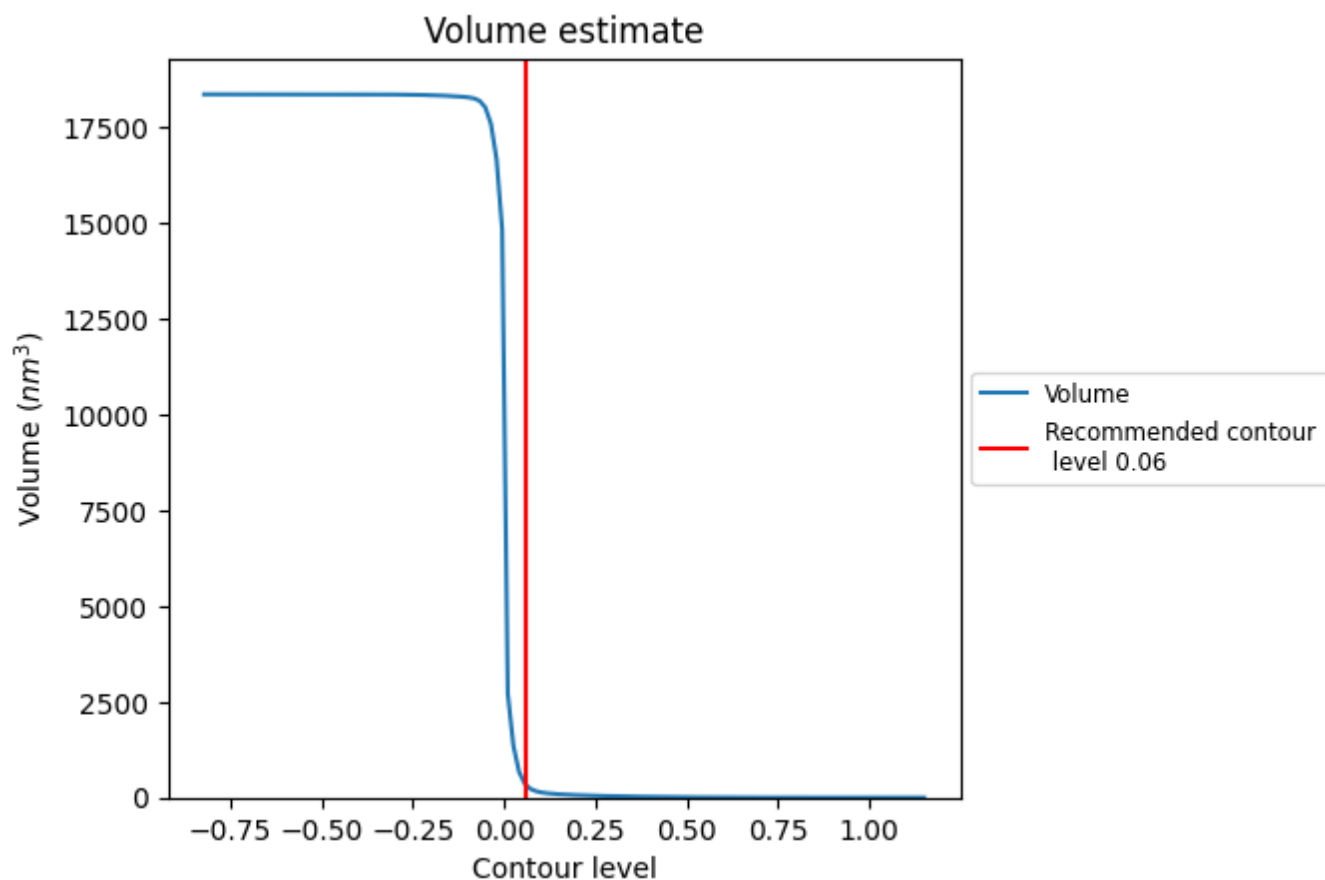
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

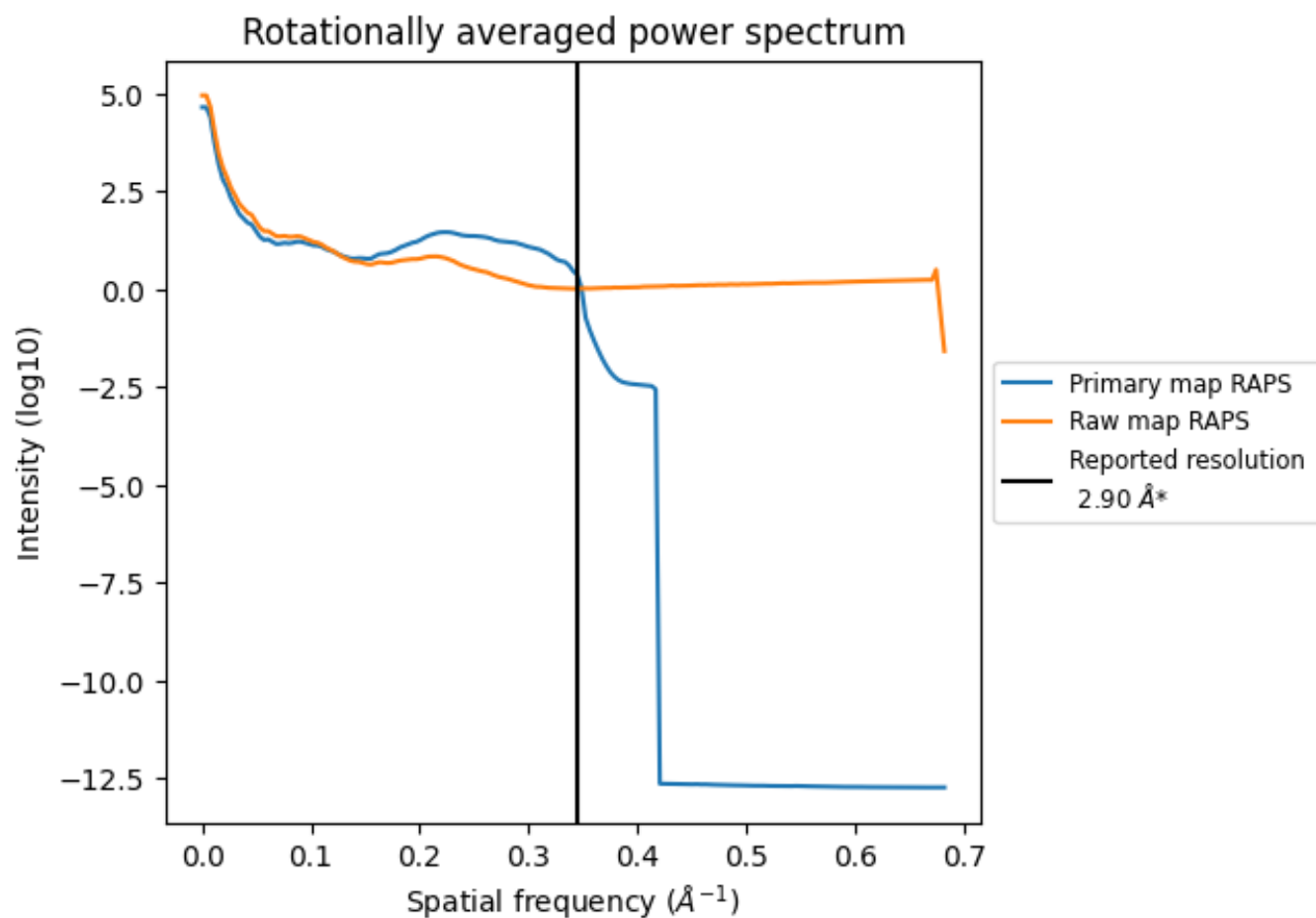


The volume at the recommended contour level is 334  $\text{nm}^3$ ; this corresponds to an approximate mass of 302 kDa.

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 ⓘ

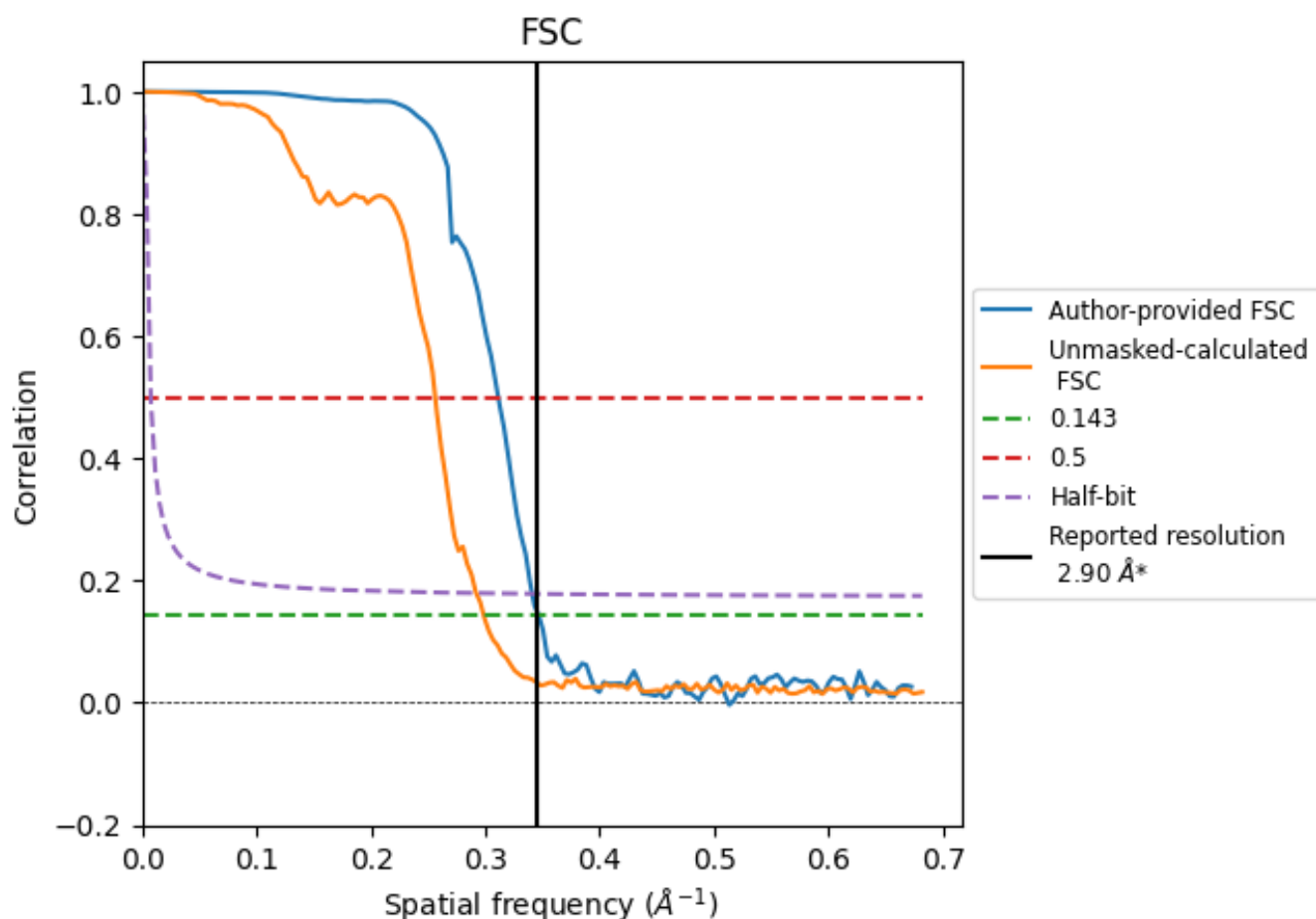


\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



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

## 8.2 Resolution estimates [i](#)

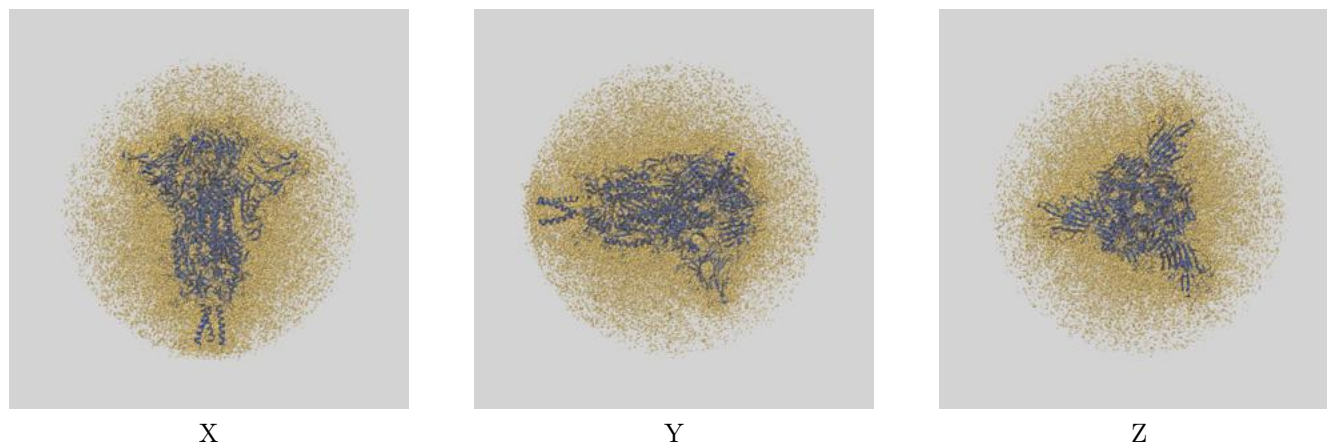
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.21	2.93
Unmasked-calculated*	3.35	3.90	3.42

\*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 3.35 differs from the reported value 2.9 by more than 10 %

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

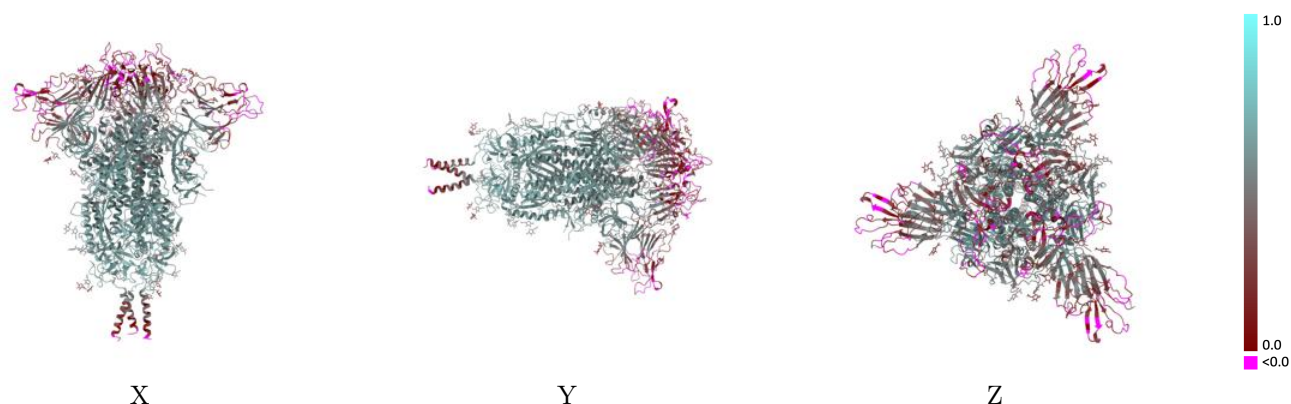
This section contains information regarding the fit between EMDB map EMD-46639 and PDB model 9D8J. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



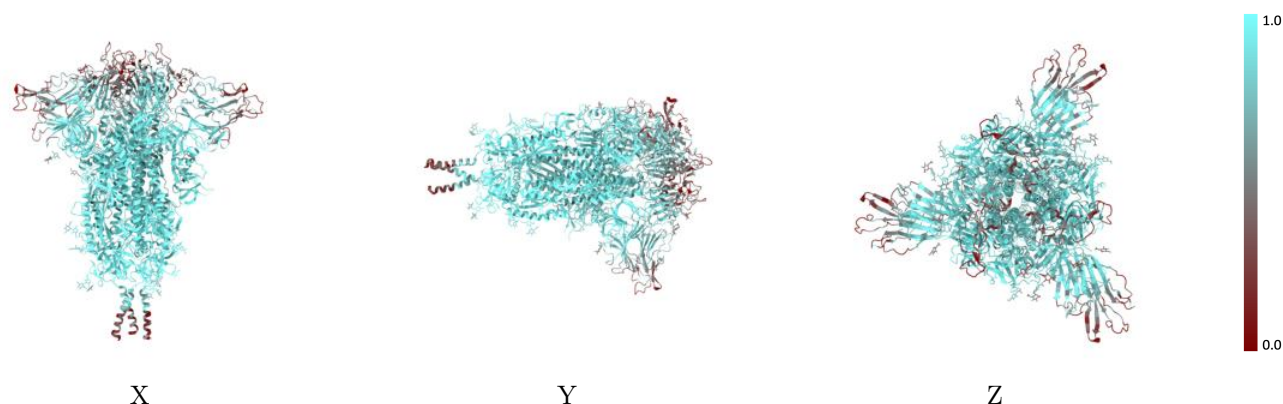
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



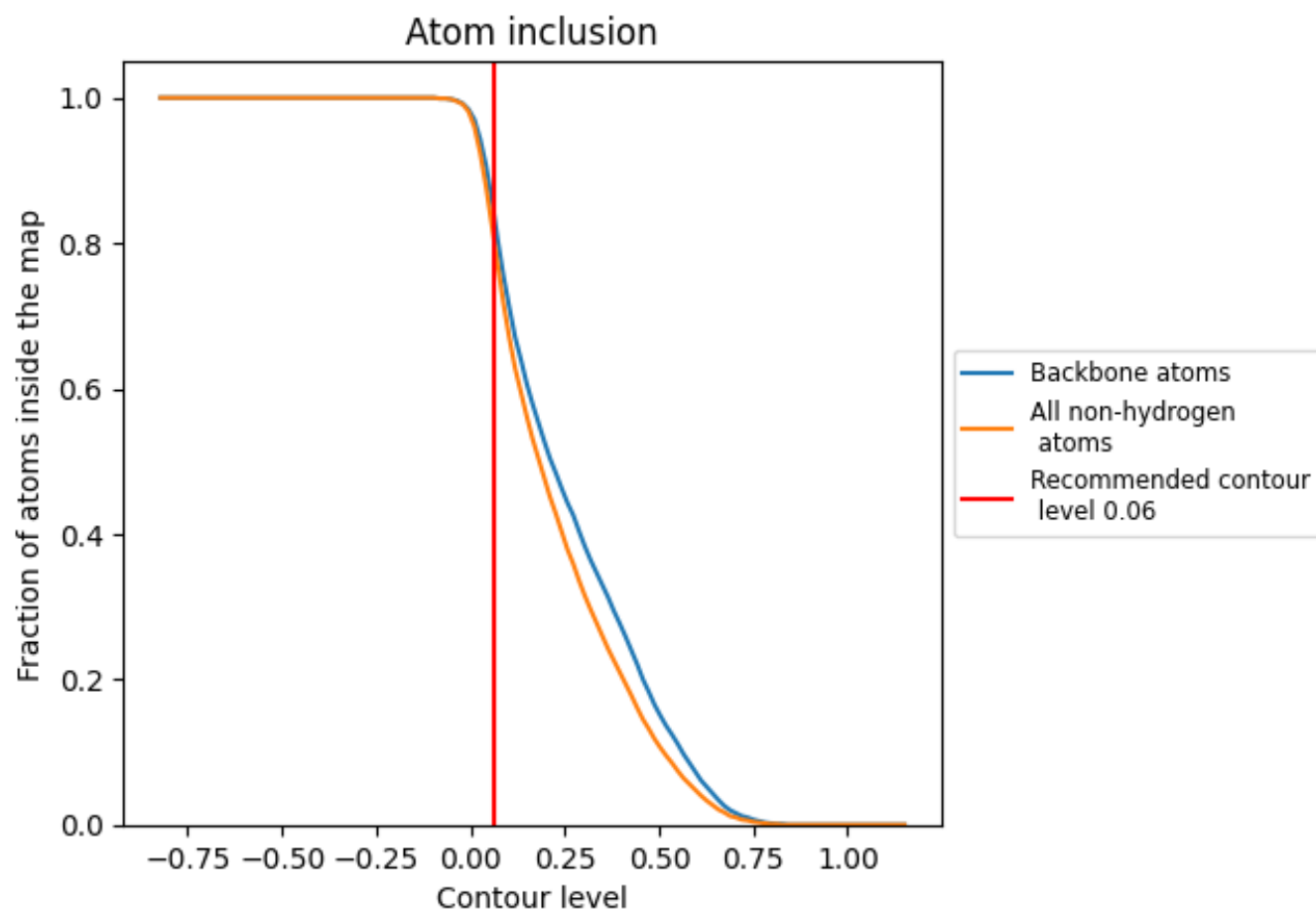
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8120	 0.4540
A	 0.8140	 0.4570
B	 0.8140	 0.4550
C	 0.8130	 0.4550
D	 0.5710	 0.2220
E	 0.8210	 0.4680
F	 0.9290	 0.5100
G	 0.8210	 0.4800
H	 0.7370	 0.3320
I	 0.6070	 0.2840
J	 0.5710	 0.2570
K	 0.8210	 0.4660
L	 0.9290	 0.5010
M	 0.8210	 0.4880
N	 0.7630	 0.3400
O	 0.5000	 0.2600
P	 0.5710	 0.2520
Q	 0.8210	 0.4530
R	 0.9290	 0.5120
S	 0.8210	 0.4820
T	 0.7370	 0.3290
U	 0.5710	 0.3020

