



Full wwPDB EM Validation Report ⓘ

Dec 16, 2024 – 06:09 PM EST

PDB ID : 5W9I
EMDB ID : EMD-8784
Title : MERS S ectodomain trimer in complex with variable domain of neutralizing antibody G4
Authors : Pallesen, J.; Ward, A.B.
Deposited on : 2017-06-23
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.40

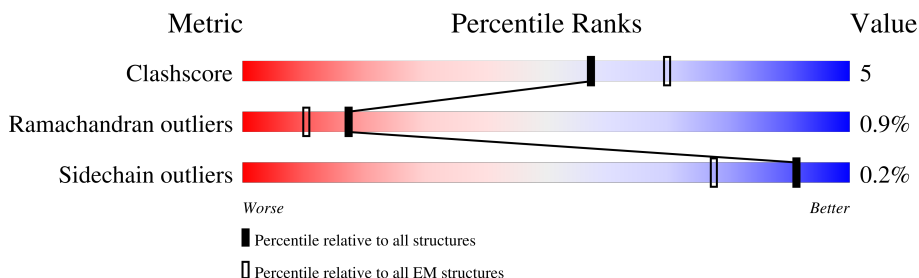
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.











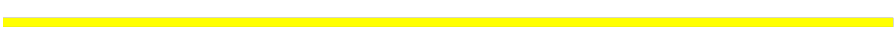








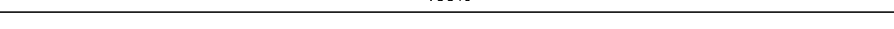
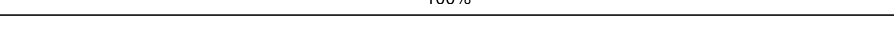
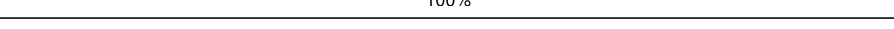
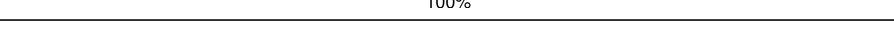
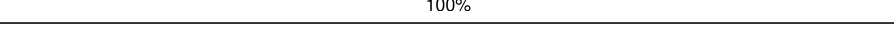

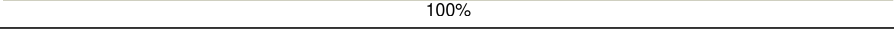
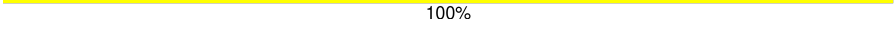
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	1329	
1	B	1329	
1	E	1329	
1	F	1329	
1	I	1329	
1	J	1329	
2	C	233	
2	G	233	

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Mol	Chain	Length	Quality of chain
2	K	233	
3	D	218	
3	H	218	
3	L	218	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	V	2	
4	W	2	
4	X	2	
4	Y	2	
4	Z	2	
4	a	2	
4	b	2	
4	c	2	
4	d	2	
4	e	2	
4	f	2	
4	g	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28896 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	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	B	513	Total	C	N	O	S	0	0
			4010	2549	664	774	23		
1	E	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	F	513	Total	C	N	O	S	0	0
			4010	2549	664	774	23		
1	I	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	J	513	Total	C	N	O	S	0	0
			4010	2549	664	774	23		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	506	PHE	LEU	conflict	UNP W5ZZF5
A	748	ALA	ARG	conflict	UNP W5ZZF5
A	751	GLY	ARG	conflict	UNP W5ZZF5
A	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
A	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
A	1292	GLY	-	expression tag	UNP W5ZZF5
A	1293	SER	-	expression tag	UNP W5ZZF5
A	1294	GLY	-	expression tag	UNP W5ZZF5
A	1295	TYR	-	expression tag	UNP W5ZZF5
A	1296	ILE	-	expression tag	UNP W5ZZF5
A	1297	PRO	-	expression tag	UNP W5ZZF5
A	1298	GLU	-	expression tag	UNP W5ZZF5
A	1299	ALA	-	expression tag	UNP W5ZZF5
A	1300	PRO	-	expression tag	UNP W5ZZF5
A	1301	ARG	-	expression tag	UNP W5ZZF5
A	1302	ASP	-	expression tag	UNP W5ZZF5
A	1303	GLY	-	expression tag	UNP W5ZZF5
A	1304	GLN	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1305	ALA	-	expression tag	UNP W5ZZF5
A	1306	TYR	-	expression tag	UNP W5ZZF5
A	1307	VAL	-	expression tag	UNP W5ZZF5
A	1308	ARG	-	expression tag	UNP W5ZZF5
A	1309	LYS	-	expression tag	UNP W5ZZF5
A	1310	ASP	-	expression tag	UNP W5ZZF5
A	1311	GLY	-	expression tag	UNP W5ZZF5
A	1312	GLU	-	expression tag	UNP W5ZZF5
A	1313	TRP	-	expression tag	UNP W5ZZF5
A	1314	VAL	-	expression tag	UNP W5ZZF5
A	1315	LEU	-	expression tag	UNP W5ZZF5
A	1316	LEU	-	expression tag	UNP W5ZZF5
A	1317	SER	-	expression tag	UNP W5ZZF5
A	1318	THR	-	expression tag	UNP W5ZZF5
A	1319	PHE	-	expression tag	UNP W5ZZF5
A	1320	LEU	-	expression tag	UNP W5ZZF5
A	1321	GLY	-	expression tag	UNP W5ZZF5
A	1322	ARG	-	expression tag	UNP W5ZZF5
A	1323	SER	-	expression tag	UNP W5ZZF5
A	1324	LEU	-	expression tag	UNP W5ZZF5
A	1325	GLU	-	expression tag	UNP W5ZZF5
A	1326	VAL	-	expression tag	UNP W5ZZF5
A	1327	LEU	-	expression tag	UNP W5ZZF5
A	1328	PHE	-	expression tag	UNP W5ZZF5
A	1329	GLN	-	expression tag	UNP W5ZZF5
B	506	PHE	LEU	conflict	UNP W5ZZF5
B	748	ALA	ARG	conflict	UNP W5ZZF5
B	751	GLY	ARG	conflict	UNP W5ZZF5
B	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
B	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
B	1292	GLY	-	expression tag	UNP W5ZZF5
B	1293	SER	-	expression tag	UNP W5ZZF5
B	1294	GLY	-	expression tag	UNP W5ZZF5
B	1295	TYR	-	expression tag	UNP W5ZZF5
B	1296	ILE	-	expression tag	UNP W5ZZF5
B	1297	PRO	-	expression tag	UNP W5ZZF5
B	1298	GLU	-	expression tag	UNP W5ZZF5
B	1299	ALA	-	expression tag	UNP W5ZZF5
B	1300	PRO	-	expression tag	UNP W5ZZF5
B	1301	ARG	-	expression tag	UNP W5ZZF5
B	1302	ASP	-	expression tag	UNP W5ZZF5
B	1303	GLY	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1304	GLN	-	expression tag	UNP W5ZZF5
B	1305	ALA	-	expression tag	UNP W5ZZF5
B	1306	TYR	-	expression tag	UNP W5ZZF5
B	1307	VAL	-	expression tag	UNP W5ZZF5
B	1308	ARG	-	expression tag	UNP W5ZZF5
B	1309	LYS	-	expression tag	UNP W5ZZF5
B	1310	ASP	-	expression tag	UNP W5ZZF5
B	1311	GLY	-	expression tag	UNP W5ZZF5
B	1312	GLU	-	expression tag	UNP W5ZZF5
B	1313	TRP	-	expression tag	UNP W5ZZF5
B	1314	VAL	-	expression tag	UNP W5ZZF5
B	1315	LEU	-	expression tag	UNP W5ZZF5
B	1316	LEU	-	expression tag	UNP W5ZZF5
B	1317	SER	-	expression tag	UNP W5ZZF5
B	1318	THR	-	expression tag	UNP W5ZZF5
B	1319	PHE	-	expression tag	UNP W5ZZF5
B	1320	LEU	-	expression tag	UNP W5ZZF5
B	1321	GLY	-	expression tag	UNP W5ZZF5
B	1322	ARG	-	expression tag	UNP W5ZZF5
B	1323	SER	-	expression tag	UNP W5ZZF5
B	1324	LEU	-	expression tag	UNP W5ZZF5
B	1325	GLU	-	expression tag	UNP W5ZZF5
B	1326	VAL	-	expression tag	UNP W5ZZF5
B	1327	LEU	-	expression tag	UNP W5ZZF5
B	1328	PHE	-	expression tag	UNP W5ZZF5
B	1329	GLN	-	expression tag	UNP W5ZZF5
E	506	PHE	LEU	conflict	UNP W5ZZF5
E	748	ALA	ARG	conflict	UNP W5ZZF5
E	751	GLY	ARG	conflict	UNP W5ZZF5
E	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
E	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
E	1292	GLY	-	expression tag	UNP W5ZZF5
E	1293	SER	-	expression tag	UNP W5ZZF5
E	1294	GLY	-	expression tag	UNP W5ZZF5
E	1295	TYR	-	expression tag	UNP W5ZZF5
E	1296	ILE	-	expression tag	UNP W5ZZF5
E	1297	PRO	-	expression tag	UNP W5ZZF5
E	1298	GLU	-	expression tag	UNP W5ZZF5
E	1299	ALA	-	expression tag	UNP W5ZZF5
E	1300	PRO	-	expression tag	UNP W5ZZF5
E	1301	ARG	-	expression tag	UNP W5ZZF5
E	1302	ASP	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1303	GLY	-	expression tag	UNP W5ZZF5
E	1304	GLN	-	expression tag	UNP W5ZZF5
E	1305	ALA	-	expression tag	UNP W5ZZF5
E	1306	TYR	-	expression tag	UNP W5ZZF5
E	1307	VAL	-	expression tag	UNP W5ZZF5
E	1308	ARG	-	expression tag	UNP W5ZZF5
E	1309	LYS	-	expression tag	UNP W5ZZF5
E	1310	ASP	-	expression tag	UNP W5ZZF5
E	1311	GLY	-	expression tag	UNP W5ZZF5
E	1312	GLU	-	expression tag	UNP W5ZZF5
E	1313	TRP	-	expression tag	UNP W5ZZF5
E	1314	VAL	-	expression tag	UNP W5ZZF5
E	1315	LEU	-	expression tag	UNP W5ZZF5
E	1316	LEU	-	expression tag	UNP W5ZZF5
E	1317	SER	-	expression tag	UNP W5ZZF5
E	1318	THR	-	expression tag	UNP W5ZZF5
E	1319	PHE	-	expression tag	UNP W5ZZF5
E	1320	LEU	-	expression tag	UNP W5ZZF5
E	1321	GLY	-	expression tag	UNP W5ZZF5
E	1322	ARG	-	expression tag	UNP W5ZZF5
E	1323	SER	-	expression tag	UNP W5ZZF5
E	1324	LEU	-	expression tag	UNP W5ZZF5
E	1325	GLU	-	expression tag	UNP W5ZZF5
E	1326	VAL	-	expression tag	UNP W5ZZF5
E	1327	LEU	-	expression tag	UNP W5ZZF5
E	1328	PHE	-	expression tag	UNP W5ZZF5
E	1329	GLN	-	expression tag	UNP W5ZZF5
F	506	PHE	LEU	conflict	UNP W5ZZF5
F	748	ALA	ARG	conflict	UNP W5ZZF5
F	751	GLY	ARG	conflict	UNP W5ZZF5
F	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
F	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
F	1292	GLY	-	expression tag	UNP W5ZZF5
F	1293	SER	-	expression tag	UNP W5ZZF5
F	1294	GLY	-	expression tag	UNP W5ZZF5
F	1295	TYR	-	expression tag	UNP W5ZZF5
F	1296	ILE	-	expression tag	UNP W5ZZF5
F	1297	PRO	-	expression tag	UNP W5ZZF5
F	1298	GLU	-	expression tag	UNP W5ZZF5
F	1299	ALA	-	expression tag	UNP W5ZZF5
F	1300	PRO	-	expression tag	UNP W5ZZF5
F	1301	ARG	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1302	ASP	-	expression tag	UNP W5ZZF5
F	1303	GLY	-	expression tag	UNP W5ZZF5
F	1304	GLN	-	expression tag	UNP W5ZZF5
F	1305	ALA	-	expression tag	UNP W5ZZF5
F	1306	TYR	-	expression tag	UNP W5ZZF5
F	1307	VAL	-	expression tag	UNP W5ZZF5
F	1308	ARG	-	expression tag	UNP W5ZZF5
F	1309	LYS	-	expression tag	UNP W5ZZF5
F	1310	ASP	-	expression tag	UNP W5ZZF5
F	1311	GLY	-	expression tag	UNP W5ZZF5
F	1312	GLU	-	expression tag	UNP W5ZZF5
F	1313	TRP	-	expression tag	UNP W5ZZF5
F	1314	VAL	-	expression tag	UNP W5ZZF5
F	1315	LEU	-	expression tag	UNP W5ZZF5
F	1316	LEU	-	expression tag	UNP W5ZZF5
F	1317	SER	-	expression tag	UNP W5ZZF5
F	1318	THR	-	expression tag	UNP W5ZZF5
F	1319	PHE	-	expression tag	UNP W5ZZF5
F	1320	LEU	-	expression tag	UNP W5ZZF5
F	1321	GLY	-	expression tag	UNP W5ZZF5
F	1322	ARG	-	expression tag	UNP W5ZZF5
F	1323	SER	-	expression tag	UNP W5ZZF5
F	1324	LEU	-	expression tag	UNP W5ZZF5
F	1325	GLU	-	expression tag	UNP W5ZZF5
F	1326	VAL	-	expression tag	UNP W5ZZF5
F	1327	LEU	-	expression tag	UNP W5ZZF5
F	1328	PHE	-	expression tag	UNP W5ZZF5
F	1329	GLN	-	expression tag	UNP W5ZZF5
I	506	PHE	LEU	conflict	UNP W5ZZF5
I	748	ALA	ARG	conflict	UNP W5ZZF5
I	751	GLY	ARG	conflict	UNP W5ZZF5
I	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
I	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
I	1292	GLY	-	expression tag	UNP W5ZZF5
I	1293	SER	-	expression tag	UNP W5ZZF5
I	1294	GLY	-	expression tag	UNP W5ZZF5
I	1295	TYR	-	expression tag	UNP W5ZZF5
I	1296	ILE	-	expression tag	UNP W5ZZF5
I	1297	PRO	-	expression tag	UNP W5ZZF5
I	1298	GLU	-	expression tag	UNP W5ZZF5
I	1299	ALA	-	expression tag	UNP W5ZZF5
I	1300	PRO	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1301	ARG	-	expression tag	UNP W5ZZF5
I	1302	ASP	-	expression tag	UNP W5ZZF5
I	1303	GLY	-	expression tag	UNP W5ZZF5
I	1304	GLN	-	expression tag	UNP W5ZZF5
I	1305	ALA	-	expression tag	UNP W5ZZF5
I	1306	TYR	-	expression tag	UNP W5ZZF5
I	1307	VAL	-	expression tag	UNP W5ZZF5
I	1308	ARG	-	expression tag	UNP W5ZZF5
I	1309	LYS	-	expression tag	UNP W5ZZF5
I	1310	ASP	-	expression tag	UNP W5ZZF5
I	1311	GLY	-	expression tag	UNP W5ZZF5
I	1312	GLU	-	expression tag	UNP W5ZZF5
I	1313	TRP	-	expression tag	UNP W5ZZF5
I	1314	VAL	-	expression tag	UNP W5ZZF5
I	1315	LEU	-	expression tag	UNP W5ZZF5
I	1316	LEU	-	expression tag	UNP W5ZZF5
I	1317	SER	-	expression tag	UNP W5ZZF5
I	1318	THR	-	expression tag	UNP W5ZZF5
I	1319	PHE	-	expression tag	UNP W5ZZF5
I	1320	LEU	-	expression tag	UNP W5ZZF5
I	1321	GLY	-	expression tag	UNP W5ZZF5
I	1322	ARG	-	expression tag	UNP W5ZZF5
I	1323	SER	-	expression tag	UNP W5ZZF5
I	1324	LEU	-	expression tag	UNP W5ZZF5
I	1325	GLU	-	expression tag	UNP W5ZZF5
I	1326	VAL	-	expression tag	UNP W5ZZF5
I	1327	LEU	-	expression tag	UNP W5ZZF5
I	1328	PHE	-	expression tag	UNP W5ZZF5
I	1329	GLN	-	expression tag	UNP W5ZZF5
J	506	PHE	LEU	conflict	UNP W5ZZF5
J	748	ALA	ARG	conflict	UNP W5ZZF5
J	751	GLY	ARG	conflict	UNP W5ZZF5
J	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
J	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
J	1292	GLY	-	expression tag	UNP W5ZZF5
J	1293	SER	-	expression tag	UNP W5ZZF5
J	1294	GLY	-	expression tag	UNP W5ZZF5
J	1295	TYR	-	expression tag	UNP W5ZZF5
J	1296	ILE	-	expression tag	UNP W5ZZF5
J	1297	PRO	-	expression tag	UNP W5ZZF5
J	1298	GLU	-	expression tag	UNP W5ZZF5
J	1299	ALA	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1300	PRO	-	expression tag	UNP W5ZZF5
J	1301	ARG	-	expression tag	UNP W5ZZF5
J	1302	ASP	-	expression tag	UNP W5ZZF5
J	1303	GLY	-	expression tag	UNP W5ZZF5
J	1304	GLN	-	expression tag	UNP W5ZZF5
J	1305	ALA	-	expression tag	UNP W5ZZF5
J	1306	TYR	-	expression tag	UNP W5ZZF5
J	1307	VAL	-	expression tag	UNP W5ZZF5
J	1308	ARG	-	expression tag	UNP W5ZZF5
J	1309	LYS	-	expression tag	UNP W5ZZF5
J	1310	ASP	-	expression tag	UNP W5ZZF5
J	1311	GLY	-	expression tag	UNP W5ZZF5
J	1312	GLU	-	expression tag	UNP W5ZZF5
J	1313	TRP	-	expression tag	UNP W5ZZF5
J	1314	VAL	-	expression tag	UNP W5ZZF5
J	1315	LEU	-	expression tag	UNP W5ZZF5
J	1316	LEU	-	expression tag	UNP W5ZZF5
J	1317	SER	-	expression tag	UNP W5ZZF5
J	1318	THR	-	expression tag	UNP W5ZZF5
J	1319	PHE	-	expression tag	UNP W5ZZF5
J	1320	LEU	-	expression tag	UNP W5ZZF5
J	1321	GLY	-	expression tag	UNP W5ZZF5
J	1322	ARG	-	expression tag	UNP W5ZZF5
J	1323	SER	-	expression tag	UNP W5ZZF5
J	1324	LEU	-	expression tag	UNP W5ZZF5
J	1325	GLU	-	expression tag	UNP W5ZZF5
J	1326	VAL	-	expression tag	UNP W5ZZF5
J	1327	LEU	-	expression tag	UNP W5ZZF5
J	1328	PHE	-	expression tag	UNP W5ZZF5
J	1329	GLN	-	expression tag	UNP W5ZZF5

- Molecule 2 is a protein called G4 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	G	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	K	119	Total	C	N	O	S	0	0
			948	602	156	185	5		

- Molecule 3 is a protein called G4 VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	111	Total	C	N	O	S	0	0
			835	522	143	166	4		
3	H	111	Total	C	N	O	S	0	0
			835	522	143	166	4		
3	L	111	Total	C	N	O	S	0	0
			835	522	143	166	4		

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



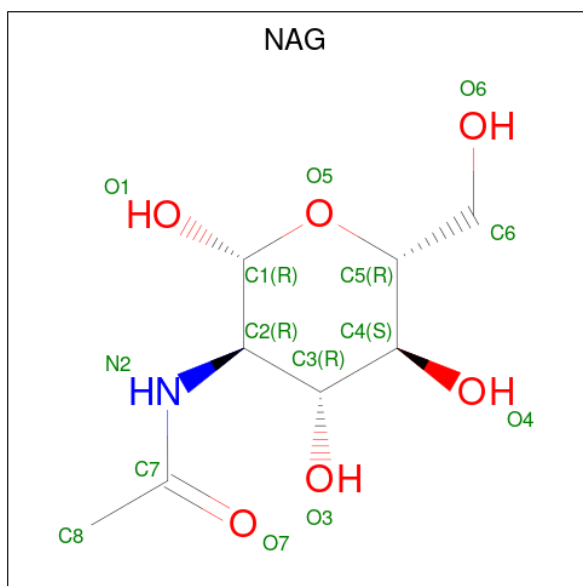
Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	

[illegible]

- Molecule 1: Spike glycoprotein



MET	ILE	HIS	SER	PHE	LEU	LEU	THR	PRO	THR	GLU	SER	TYR	VAL	ASP	VAL	GLY	PRO	ASP	SER	VAL	LYS	SER	ALA	CYS	ILE	GLU	VAL	ASP	ILE	GLN	GLN	THR	PHE	PHE	ASP	ASP	LYS	THR	TRP	PRO	PRO	ARG	ARG	PRO	PRO	ILE	ASP	VAL	SER	LYS	ALA	LYS	ASP	GLY	ILE	ILE	TYR	TYR	PRO	GLN
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GLY	ARG	THR	TYR	SER	ASN	ILE	THR	THR	THR	GLN	GLY	LEU	PHE	PRO	PRO	GLN	TYR	GLY	ASP	HIS	GLY	ASP	MET	VAL	VAL	TYR	TYR	SER	SER	ALA	ALA	GLY	HIS	ALA	THR	THR	GLY	THR	THR	THR	PRO	PRO	GLN	GLN	LYS	GLN	PHE	PHE	VAL	VAL	VAL	VAL	ARG	ILE
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GLY	ALA	ALA	ALA	ASN	SER	THR	GLY	THR	VAL	ILE	ILE	SER	PRO	SER	THR	SER	ALA	THR	ILE	ARG	LYS	ILE	TYR	PRO	ALA	PHE	MET	LEU	GLY	SER	SER	VAL	GLY	ASN	PHE	SER	ASP	GLY	LYS	MET	GLY	ARG	PHE	ASN	ASN	HIS	THR	LEU	VAL	LEU	PRO	ASP	GLY	CYS	THR	GLY	LEU
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ARG	ALA	ALA	PHE	TYR	CYS	ILE	LEU	GLU	PRO	ARG	SER	GLY	ASN	ASN	HIS	CYS	PRO	ALA	ALA	GLY	ASN	SER	TYR	THR	SER	PHE	ALA	ALA	THR	TYR	HIS	THR	THR	PRO	ALA	ALA	THR	ASP	CYS	SER	SER	ASP	GLY	ASN	TYR	TYR	ARG	ASN	ASN	SER	PHE	LYS	GLU	TYR	PHE	ASN	LEU	ARG	ASN	CYS	THR	PHE	ASP
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Tyr	Ser	Ser	Ser	Phe	Glu	Ala	Lys	Gly	Ser	Val	Glu	Gln	Ala	Glu	Gly	Glu	Cys	Asp	Phe	Ser	Pro	Pro	Gln	Val	Tyr	Thr	Thr	Arg	Leu	Val	Phe	Thr	Asn	Cys	Asn	Tyr	Ser	Ser	Leu	Phe	Ser	Val
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ASN	ASP	PHE	THR	CYS	SER	GLN	ILE	ALA	ALA	ALA	ILE	ILE	ALA	ASN	CYS	TYR	SER	SER	LEU	LEU	ASP	TYR	PHE	SER	PRO	TYR	LEU	LEU	SER	LYS	MET	ASN	SER	SER	ASP	LEU	LEU	SER	VAL	PRO	ILE	PRO	SER	SER	GLN	PHE	ASN	TYR	TYR	GLN	LYS	GLN	PHE	SER	SER	ASN	PRO	PRO	THR	CYS	TYR	LEU	ILE	TYR
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LEU	ALA	THR	VAL	PRO	HIS	ASN	LEU	THR	THR	ILE	THR	LYS	PRO	LEU	LEU	LYS	TYR	SER	TYR	ILE	ASN	CYS	SER	ARG	PHE	LEU	LEU	SER	ASP	ASP	ASP	ARG	THR	GLU	VAL	VAL	PRO	GLN	LEU	VAL	ASN	ASN	ALA	ALA	GLN	TYR	SER	PRO	CYS	CYS	VAL	SER	ILE	VAL	PRO	GLU	GLY	ASP	TYR
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TYR	ARG	LYS	GLN	LEU	SER	PRO	LEU	GLY	GLY	GLY	TRP	LEU	VAL	ALA	SER	ALA	GLY	SER	THR	THR	ALA	ALA	MET	GLU	GLN	LEU	GLN	MET	GLY	PHE	GLY	ILE	THR	THR	VAL	GLN	TYR	GLY	THR	THR	ASP	ASN	THR	THR	ASN	SER	VAL	CYS	PRO	PRO	LYS	LEU	GLU	GLY	PHE	ALA	ALA	ALA	THR	LYS	ILE	ILE	ALA	ALA	SER	SER	GLN	LEU
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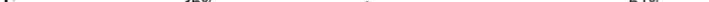
VAL	ILE	TYR	ASP	LYS	GLU	THR	LYS	THR	HIS	HIS	ALA	ALA	LEU	PHE	GLY	SER	VAL	VAL	ALA	CYS	GLU	HIS	ILE	SER	SER	THR	MET	GLN	TYR	SER	ARG	SER	THR	THR	ARG	ASP	SER	THR	TYR	GLY	PRO	PRO	VAL	VAL	GLY	CYS	VAL	LEU	LEU	GLY	VAL	ASN	SER
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SER	LEU	PHE	VAL	GLN	ASP	CYS	LYS	LEU	PRO	LEU	GLY	GLN	SER	SER	CYS	ALA	PRO	ASP	THR	PRO	SER	THR	LEU	PRO	ALA	VAL	GLY	SER	V753	R758	C806	Q808	D869	V877	SER	ILE	SER	THR	GLY	SER	ARG	SER	A886	A901	P903	G904	Y905	N906	O907
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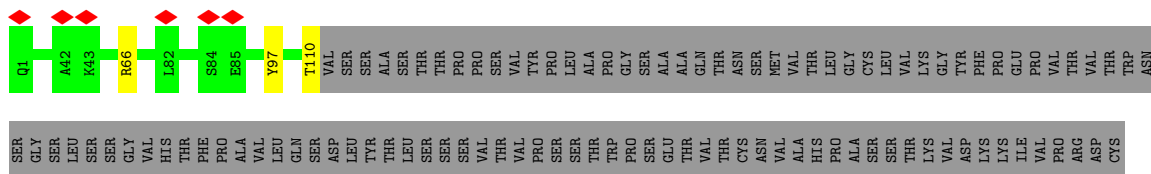
Q914	Q915	Q916	S919	A920	R921	D922	L923	R924	Y932	P936	R955	A956	G957	V958	F972	S975	Q988	K1108	A1109	R1113	F1116	V1124	N1160	T1175	E1195	P1219	P1220	L1233	GLY	ASN	SER	THR	GLY	ILE	ASP	PHE	GLN	ASP	GLU	LEU	ASP	THR
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PHE PHE LYS LYS VAL SER THR SER SER PRO ILE ASN ASN PHE GLY SER LEU LEU THR THR GLN ILE ASN THR THR THR LEU LEU ASP LEU TYR MET MET GLU LEU LEU SER SER GLN GLN VAL VAL LYS ALA LEU LEU LEU LEU LYS ASN SER TYR TYR ILE ASP LEU LEU TYR THR TYR TYR GLY SER GLY TYR ILE PHE

GLU
ALA
PRO
ARG
ASP
GLY
GLN
ALA
TYR
VAL
ARG
LYS
ASP
GLY
GLU
TRP
VAL
LEU
LEU
SER
THR
PHE
LEU
GLY
ARG
SER
SER
LEU
GLU
VAL
LEU
PHE
GLN

Chain F:  36% 61%






THR
CYS
GLU
ALA
THR
HIS
LYS
THR
THR
SER
SER
PRO
ILE
VAL
LYS
SER
PHE
ASN
ARG
ASN
GLU
CYS

• Molecule 3: G4 VL

Chain L: 

 ARG
THR
ASP
ASP
ALA
ALA
PRO
THR
VAL
SER
ILE
PHE
PRO
PRO
SER
SER
GLN
LEU
THR
SER
GLY
GLY
ALA
SER
VAL
VAL
CYS
PHE
LEU
ASN
ASN

PHE
THR
PRO
LYS
ASP
ILE
ASN
VAL
LYS
LYS
TRP
LYS
ILE
ASP
GLY
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TYR

LYS
THR
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THR
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ILE
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LYS
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ASN
ARG
ASN
GLU
CYS

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

Chain M: 

MAG1
MAG2

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

Chain N: 

MAG1
MAG2

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

Chain O: 

MAG1
MAG2

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

Chain P: 

MAG1
MAG2

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

Chain Q: 



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



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



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



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



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



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

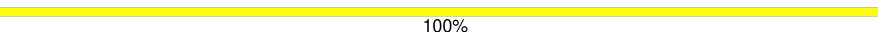


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  50% 50%

MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain Z:  100%

MAG1
MAG2

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

Chain a:  100%

MAG1
MAG2

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

Chain b:  100%

MAG1
MAG2

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

Chain c:  100%

MAG1
MAG2

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

Chain d:  50% 50%



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	37180	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 ($e^-/\text{\AA}^2$)	1.89	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	310.08, 310.08, 310.08	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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: 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	0.75	0/3618	0.84	6/4921 (0.1%)
1	B	0.72	0/4112	0.90	9/5590 (0.2%)
1	E	0.75	0/3618	0.81	2/4921 (0.0%)
1	F	0.71	0/4112	0.90	10/5590 (0.2%)
1	I	0.76	0/3618	0.84	6/4921 (0.1%)
1	J	0.72	0/4112	0.89	8/5590 (0.1%)
2	C	0.72	0/972	0.88	2/1317 (0.2%)
2	G	0.71	0/972	0.87	2/1317 (0.2%)
2	K	0.71	0/972	0.87	2/1317 (0.2%)
3	D	0.73	0/852	0.88	1/1153 (0.1%)
3	H	0.74	0/852	0.87	0/1153
3	L	0.74	0/852	0.86	0/1153
All	All	0.73	0/28662	0.87	48/38943 (0.1%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	642	TYR	CB-CG-CD1	-8.74	115.75	121.00
1	B	642	TYR	CB-CG-CD1	-8.61	115.83	121.00
1	J	334	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	F	334	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	B	334	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	I	940	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	E	932	TYR	CB-CG-CD2	-7.88	116.27	121.00
1	I	932	TYR	CB-CG-CD2	-7.86	116.28	121.00
1	A	932	TYR	CB-CG-CD2	-7.83	116.30	121.00
1	J	642	TYR	CB-CG-CD1	-7.70	116.38	121.00
1	I	940	ASP	CB-CG-OD1	7.56	125.11	118.30
1	J	58	TYR	CB-CG-CD2	-7.20	116.68	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	TYR	CB-CG-CD2	-7.09	116.75	121.00
1	F	58	TYR	CB-CG-CD2	-7.06	116.76	121.00
1	A	940	ASP	CB-CG-OD2	-6.93	112.07	118.30
1	J	184	TYR	CB-CG-CD1	-6.39	117.16	121.00
1	I	1117	CYS	N-CA-CB	6.26	121.88	110.60
1	A	1117	CYS	N-CA-CB	6.26	121.87	110.60
1	A	940	ASP	CB-CG-OD1	6.22	123.90	118.30
1	I	909	TYR	CB-CG-CD1	-6.12	117.33	121.00
2	C	66	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	323	PHE	CB-CG-CD1	6.09	125.06	120.80
1	J	323	PHE	CB-CG-CD1	6.07	125.05	120.80
1	F	323	PHE	CB-CG-CD1	6.06	125.04	120.80
2	G	66	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	909	TYR	CB-CG-CD1	-5.96	117.42	121.00
2	K	66	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	G	97	TYR	CB-CG-CD1	-5.76	117.55	121.00
2	K	97	TYR	CB-CG-CD1	-5.74	117.56	121.00
2	C	97	TYR	CB-CG-CD1	-5.65	117.61	121.00
1	B	323	PHE	CB-CG-CD2	-5.63	116.86	120.80
1	J	323	PHE	CB-CG-CD2	-5.58	116.90	120.80
1	F	323	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	F	184	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	B	184	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	F	652	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	307	ARG	NE-CZ-NH2	5.28	122.94	120.30
3	D	96	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	A	868	ASP	CB-CG-OD2	5.21	122.99	118.30
1	F	593	ASP	CB-CG-OD2	5.19	122.97	118.30
1	J	593	ASP	CB-CG-OD2	5.19	122.97	118.30
1	I	868	ASP	CB-CG-OD2	5.19	122.97	118.30
1	F	307	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	B	593	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	868	ASP	CB-CG-OD2	5.16	122.94	118.30
1	F	163	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	J	369	LYS	C-N-CD	5.04	138.99	128.40
1	B	663	TYR	CB-CG-CD1	-5.00	118.00	121.00

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	3545	0	3467	38	0
1	B	4010	0	3808	38	0
1	E	3545	0	3467	39	0
1	F	4010	0	3808	42	0
1	I	3545	0	3467	45	0
1	J	4010	0	3810	67	0
2	C	948	0	904	1	0
2	G	948	0	904	2	0
2	K	948	0	904	2	0
3	D	835	0	816	1	0
3	H	835	0	816	1	0
3	L	835	0	816	0	0
4	M	28	0	25	1	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	1	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	24	0	0
4	Z	28	0	25	0	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	c	28	0	25	0	0
4	d	28	0	25	0	0
4	e	28	0	25	0	0
4	f	28	0	25	0	0
4	g	28	0	25	0	0
5	A	14	0	13	0	0
5	B	84	0	78	1	0
5	E	14	0	13	0	0
5	F	84	0	78	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	14	0	13	0	0
5	J	84	0	75	0	0
All	All	28896	0	27781	259	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.

All (259) 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:905:TYR:OH	1:A:936:PRO:CA	1.68	1.41
1:E:905:TYR:OH	1:E:936:PRO:CA	1.70	1.39
1:I:905:TYR:OH	1:I:936:PRO:HA	1.26	1.34
1:I:905:TYR:OH	1:I:936:PRO:CA	1.75	1.32
1:A:905:TYR:OH	1:A:936:PRO:HA	1.13	1.24
1:J:688:GLN:HB2	1:J:689:TYR:HA	1.18	1.13
1:F:688:GLN:HB2	1:F:689:TYR:HA	1.19	1.11
1:E:958:VAL:HG11	1:E:1108:LYS:O	1.50	1.11
1:J:602:ASN:O	1:J:616:VAL:HB	1.48	1.11
1:B:688:GLN:HB2	1:B:689:TYR:HA	1.19	1.11
1:I:958:VAL:HG11	1:I:1108:LYS:O	1.51	1.10
1:E:905:TYR:OH	1:E:936:PRO:HA	0.93	1.09
1:I:958:VAL:HG21	1:I:1109:ALA:HA	1.11	1.08
1:F:621:THR:O	1:F:648:TYR:HD2	1.35	1.08
1:J:602:ASN:O	1:J:616:VAL:CB	2.02	1.07
1:E:905:TYR:CZ	1:E:936:PRO:HA	1.88	1.07
1:E:958:VAL:HG21	1:E:1109:ALA:HA	1.09	1.05
1:F:689:TYR:HD1	1:F:690:SER:N	1.55	1.04
1:I:905:TYR:OH	1:I:936:PRO:N	1.89	1.02
1:I:1116:PHE:O	1:I:1117:CYS:SG	2.18	1.02
1:A:905:TYR:OH	1:A:936:PRO:N	1.93	1.01
1:A:905:TYR:CZ	1:A:936:PRO:HA	1.93	1.01
1:J:689:TYR:HD1	1:J:690:SER:N	1.63	0.97
1:I:905:TYR:CZ	1:I:936:PRO:HA	2.00	0.96
1:E:806:CYS:O	1:E:808:GLN:N	1.99	0.94
1:A:905:TYR:CZ	1:A:936:PRO:CA	2.50	0.93
1:E:807:LYS:HD2	1:J:691:ARG:NH2	1.85	0.92
1:F:689:TYR:CD1	1:F:690:SER:N	2.36	0.92
1:A:1121:THR:HG22	1:I:964:LEU:HD12	1.52	0.92
1:I:905:TYR:CZ	1:I:936:PRO:CA	2.55	0.90
1:F:371:SER:HB3	1:F:604:VAL:HG12	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:621:THR:O	1:F:648:TYR:CD2	2.25	0.88
1:J:688:GLN:CB	1:J:689:TYR:HA	2.04	0.88
1:F:688:GLN:CB	1:F:689:TYR:HA	2.04	0.87
1:E:905:TYR:CZ	1:E:936:PRO:CA	2.52	0.87
1:J:689:TYR:CD1	1:J:690:SER:N	2.44	0.84
1:B:688:GLN:HB2	1:B:689:TYR:CA	2.09	0.82
1:J:602:ASN:O	1:J:616:VAL:CA	2.28	0.81
1:E:807:LYS:HD2	1:J:691:ARG:HH22	1.42	0.81
1:B:688:GLN:CB	1:B:689:TYR:HA	2.05	0.81
1:A:905:TYR:CZ	1:A:936:PRO:HB3	2.16	0.80
1:J:371:SER:HB2	1:J:604:VAL:HG12	1.62	0.80
1:J:621:THR:O	1:J:648:TYR:HD2	1.64	0.79
1:I:958:VAL:CG1	1:I:1108:LYS:O	2.31	0.79
1:E:905:TYR:CZ	1:E:936:PRO:HB3	2.19	0.78
1:J:369:LYS:HD2	1:J:370:PRO:HD2	1.66	0.78
1:F:371:SER:CB	1:F:604:VAL:HG12	2.14	0.77
1:E:958:VAL:CG1	1:E:1108:LYS:O	2.32	0.76
1:E:905:TYR:CE1	1:E:936:PRO:HB3	2.20	0.76
1:F:688:GLN:HB2	1:F:689:TYR:CA	2.10	0.76
1:I:905:TYR:CZ	1:I:936:PRO:HB3	2.21	0.75
1:B:689:TYR:HD1	1:B:690:SER:N	1.84	0.74
1:A:985:ILE:HG13	1:A:1190:SER:OG	1.88	0.74
1:A:905:TYR:CZ	1:A:936:PRO:CB	2.72	0.73
1:E:905:TYR:OH	1:E:936:PRO:N	2.22	0.73
1:A:905:TYR:CE1	1:A:936:PRO:HB3	2.24	0.73
1:J:621:THR:O	1:J:648:TYR:CD2	2.43	0.72
1:J:688:GLN:HB2	1:J:689:TYR:CA	2.10	0.72
1:B:371:SER:HB3	1:B:604:VAL:HG12	1.72	0.72
1:F:330:ASP:O	1:J:624:GLY:HA3	1.89	0.71
1:J:371:SER:CB	1:J:604:VAL:HG12	2.21	0.71
1:E:905:TYR:CZ	1:E:936:PRO:CB	2.75	0.70
1:F:621:THR:HG22	1:F:622:ALA:N	2.07	0.69
1:F:330:ASP:C	1:J:624:GLY:HA3	2.13	0.69
1:B:372:GLY:O	1:B:604:VAL:HB	1.93	0.68
1:I:905:TYR:OH	1:I:935:LEU:C	2.32	0.68
1:I:958:VAL:HG11	1:I:1108:LYS:C	2.13	0.68
1:I:904:GLY:O	1:I:905:TYR:HB2	1.94	0.67
1:I:905:TYR:CZ	1:I:936:PRO:CB	2.77	0.67
1:A:904:GLY:O	1:A:905:TYR:HB2	1.93	0.67
1:B:689:TYR:CD1	1:B:690:SER:N	2.63	0.67
1:A:1113:ARG:O	1:A:1114:SER:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:GLY:HA3	1:J:330:ASP:O	1.95	0.67
1:F:689:TYR:HD1	1:F:690:SER:H	1.39	0.66
1:J:602:ASN:HA	1:J:616:VAL:HG23	1.78	0.66
1:B:172:LEU:HD12	1:B:172:LEU:O	1.96	0.66
1:J:172:LEU:HD12	1:J:172:LEU:O	1.96	0.65
1:B:371:SER:CB	1:B:604:VAL:HG12	2.27	0.65
1:E:958:VAL:HG11	1:E:1108:LYS:C	2.18	0.64
1:A:985:ILE:CG1	1:A:1190:SER:OG	2.46	0.64
1:E:958:VAL:HG21	1:E:1109:ALA:CA	2.05	0.64
1:F:594:THR:HB	1:F:595:LYS:HA	1.81	0.63
1:I:960:TRP:O	1:I:961:THR:HB	1.97	0.63
1:F:621:THR:HG22	1:F:622:ALA:H	1.63	0.63
1:B:330:ASP:O	1:F:624:GLY:HA3	1.97	0.62
1:B:624:GLY:HA3	1:J:330:ASP:C	2.20	0.62
1:B:594:THR:HB	1:B:595:LYS:HA	1.82	0.62
1:J:594:THR:HB	1:J:595:LYS:HA	1.82	0.62
1:A:1106:CYS:SG	1:A:1138:HIS:CE1	2.93	0.61
1:A:905:TYR:OH	1:A:935:LEU:C	2.38	0.61
1:I:905:TYR:CE1	1:I:936:PRO:HB3	2.35	0.60
1:J:616:VAL:HG13	1:J:616:VAL:O	1.99	0.60
1:I:960:TRP:O	1:I:961:THR:CB	2.48	0.60
1:A:907:GLN:N	1:A:907:GLN:OE1	2.35	0.60
1:A:1116:PHE:O	1:A:1117:CYS:SG	2.61	0.59
1:F:371:SER:HB3	1:F:604:VAL:CG1	2.31	0.59
1:A:1169:ASN:HA	1:I:961:THR:OG1	2.02	0.59
1:J:602:ASN:O	1:J:616:VAL:HA	2.02	0.58
1:A:1121:THR:HG22	1:I:964:LEU:CD1	2.31	0.58
1:I:907:GLN:N	1:I:907:GLN:OE1	2.36	0.58
1:J:369:LYS:CD	1:J:370:PRO:HD2	2.33	0.57
1:E:904:GLY:O	1:E:906:MET:N	2.37	0.57
1:I:956:ALA:HB2	1:I:972:PHE:HA	1.86	0.57
1:F:622:ALA:HB1	1:F:642:TYR:OH	2.05	0.57
1:I:958:VAL:HG21	1:I:1109:ALA:CA	2.07	0.57
1:J:367:GLU:O	1:J:368:ALA:HB2	2.05	0.57
2:C:110:THR:HG22	2:C:110:THR:O	2.06	0.56
1:B:714:VAL:HB	1:B:717:LEU:HD23	1.88	0.56
2:G:85:GLU:OE1	2:G:85:GLU:N	2.37	0.56
1:F:368:ALA:O	1:F:369:LYS:CB	2.54	0.56
1:F:367:GLU:O	1:F:368:ALA:HB2	2.05	0.56
2:K:110:THR:O	2:K:110:THR:HG22	2.05	0.56
2:G:110:THR:HG22	2:G:110:THR:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:626:ARG:O	1:J:627:GLN:HB2	2.07	0.55
1:F:368:ALA:O	1:F:369:LYS:HB3	2.07	0.55
1:A:907:GLN:CD	1:A:907:GLN:H	2.09	0.55
2:K:85:GLU:OE1	2:K:85:GLU:N	2.38	0.55
1:J:377:GLN:OE1	1:J:377:GLN:O	2.25	0.54
1:A:955:ILE:O	1:A:956:ALA:HB3	2.07	0.54
1:J:602:ASN:CA	1:J:616:VAL:HG23	2.38	0.54
1:B:377:GLN:O	1:B:377:GLN:OE1	2.25	0.54
1:E:955:ILE:O	1:E:956:ALA:HB3	2.08	0.54
1:I:907:GLN:H	1:I:907:GLN:CD	2.10	0.54
1:E:956:ALA:N	1:E:957:GLY:HA2	2.22	0.54
1:J:621:THR:HG22	1:J:622:ALA:N	2.23	0.54
1:F:377:GLN:OE1	1:F:377:GLN:O	2.26	0.53
1:F:626:ARG:O	1:F:627:GLN:HB2	2.08	0.53
1:B:620:CYS:CB	1:B:650:CYS:SG	2.96	0.53
1:E:907:GLN:OE1	1:E:907:GLN:N	2.38	0.53
1:I:1115:GLY:O	1:I:1116:PHE:HB2	2.08	0.53
1:J:602:ASN:O	1:J:616:VAL:CG2	2.56	0.53
1:J:334:ARG:HA	1:J:334:ARG:NE	2.24	0.53
1:J:689:TYR:HD1	1:J:690:SER:H	1.52	0.53
1:F:334:ARG:HA	1:F:334:ARG:NE	2.24	0.52
1:J:67:ILE:HG13	1:J:67:ILE:O	2.08	0.52
1:E:905:TYR:O	1:E:906:MET:HE2	2.08	0.52
1:F:689:TYR:HD1	1:F:690:SER:CA	2.21	0.52
1:A:1175:THR:HG23	1:A:1175:THR:O	2.09	0.52
1:B:334:ARG:NE	1:B:334:ARG:HA	2.24	0.52
1:J:369:LYS:CD	1:J:370:PRO:CD	2.87	0.52
1:B:616:VAL:O	1:B:616:VAL:HG13	2.10	0.52
1:E:988:GLN:HB3	1:E:1195:GLU:OE2	2.11	0.51
1:F:616:VAL:HG13	1:F:616:VAL:O	2.10	0.51
1:B:67:ILE:HG13	1:B:67:ILE:O	2.09	0.51
1:E:807:LYS:CD	1:J:691:ARG:NH2	2.67	0.51
1:E:956:ALA:HA	1:E:975:SER:CB	2.40	0.51
1:E:956:ALA:HA	1:E:975:SER:HB3	1.93	0.51
1:A:1114:SER:HB2	1:I:964:LEU:HD21	1.92	0.51
1:I:983:VAL:O	1:I:1190:SER:OG	2.16	0.51
1:E:758:ARG:HA	1:F:717:LEU:O	2.11	0.51
1:I:988:GLN:HB3	1:I:1195:GLU:OE2	2.11	0.51
1:I:1102:LYS:HE2	1:I:1116:PHE:CE2	2.46	0.51
1:F:621:THR:CG2	1:F:622:ALA:N	2.74	0.50
1:B:374:VAL:CG2	1:B:604:VAL:HG21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:ILE:HG13	1:F:67:ILE:O	2.10	0.50
1:F:372:GLY:O	1:F:604:VAL:HB	2.11	0.50
1:B:334:ARG:HA	1:B:334:ARG:HE	1.77	0.50
1:J:372:GLY:O	1:J:604:VAL:HB	2.11	0.50
1:J:334:ARG:HA	1:J:334:ARG:HE	1.77	0.49
1:B:604:VAL:HG23	1:B:604:VAL:O	2.13	0.49
1:F:334:ARG:HA	1:F:334:ARG:HE	1.77	0.49
1:E:1175:THR:O	1:E:1175:THR:HG23	2.12	0.49
1:E:905:TYR:CE1	1:E:936:PRO:CB	2.93	0.49
1:B:330:ASP:C	1:F:624:GLY:HA3	2.33	0.49
1:I:758:ARG:HA	1:J:717:LEU:O	2.12	0.49
1:I:1175:THR:HG23	1:I:1175:THR:O	2.12	0.49
1:J:689:TYR:CD1	1:J:689:TYR:C	2.87	0.49
1:A:988:GLN:HB3	1:A:1195:GLU:OE2	2.12	0.48
1:B:714:VAL:HG21	1:B:717:LEU:HG	1.95	0.48
1:J:369:LYS:HB2	1:J:688:GLN:HA	1.95	0.48
1:E:1113:ARG:O	1:E:1113:ARG:HG2	2.12	0.48
1:F:367:GLU:HB2	1:F:689:TYR:O	2.13	0.48
1:B:689:TYR:CD1	1:B:689:TYR:C	2.86	0.48
1:F:689:TYR:CD1	1:F:689:TYR:C	2.87	0.47
1:A:1121:THR:HA	1:I:964:LEU:HD13	1.96	0.47
1:B:154:GLY:HA2	5:B:1402:NAG:H82	1.96	0.47
1:E:807:LYS:CD	1:J:691:ARG:HH22	2.19	0.47
1:F:689:TYR:HD1	1:F:690:SER:C	2.18	0.47
1:J:714:VAL:HG21	1:J:717:LEU:HG	1.95	0.47
1:F:621:THR:CG2	1:F:622:ALA:H	2.26	0.47
1:J:689:TYR:HD1	1:J:690:SER:CA	2.28	0.47
1:A:904:GLY:O	1:A:905:TYR:CB	2.60	0.47
1:F:104:ASN:O	1:F:104:ASN:CG	2.53	0.47
1:I:956:ALA:N	1:I:957:GLY:HA2	2.30	0.46
1:A:1116:PHE:O	1:A:1117:CYS:CB	2.63	0.46
1:I:1102:LYS:HG2	1:I:1116:PHE:CE2	2.51	0.46
1:J:374:VAL:CG2	1:J:604:VAL:HG21	2.45	0.46
1:J:594:THR:CB	1:J:595:LYS:HA	2.43	0.46
1:A:956:ALA:N	1:A:957:GLY:HA2	2.30	0.46
3:D:1:ASP:OD1	3:D:1:ASP:C	2.53	0.46
1:I:1219:PRO:HB2	1:I:1220:PRO:HD3	1.98	0.46
1:E:956:ALA:HB2	1:E:972:PHE:HA	1.98	0.46
1:F:714:VAL:HG21	1:F:717:LEU:HG	1.97	0.46
1:J:616:VAL:O	1:J:616:VAL:CG1	2.64	0.46
1:E:1116:PHE:N	1:E:1116:PHE:CD1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:371:SER:OG	1:F:604:VAL:HG12	2.16	0.46
1:J:104:ASN:O	1:J:104:ASN:CG	2.53	0.46
1:E:1219:PRO:HB2	1:E:1220:PRO:HD3	1.98	0.45
1:F:689:TYR:CD1	1:F:690:SER:C	2.90	0.45
1:J:104:ASN:OD1	1:J:104:ASN:C	2.55	0.45
1:B:621:THR:O	1:B:648:TYR:HB3	2.16	0.45
1:B:221:ARG:NH2	4:R:1:NAG:O6	2.38	0.45
1:B:374:VAL:HG23	1:B:604:VAL:HG21	1.97	0.45
1:E:907:GLN:H	1:E:907:GLN:CD	2.18	0.45
1:A:1003:GLN:HE22	4:M:2:NAG:H81	1.81	0.45
1:J:622:ALA:HB1	1:J:642:TYR:OH	2.17	0.45
1:A:1219:PRO:HB2	1:A:1220:PRO:HD3	1.98	0.44
1:B:672:THR:HG22	1:B:715:LEU:HB2	1.98	0.44
1:B:371:SER:OG	1:B:604:VAL:HG12	2.16	0.44
1:J:369:LYS:HD2	1:J:370:PRO:CD	2.42	0.44
1:J:371:SER:HB2	1:J:604:VAL:CG1	2.41	0.44
1:J:689:TYR:HD1	1:J:690:SER:C	2.21	0.44
1:B:371:SER:HB3	1:B:604:VAL:CG1	2.44	0.44
1:A:905:TYR:CE1	1:A:936:PRO:CB	2.97	0.44
1:E:1116:PHE:N	1:E:1116:PHE:HD1	2.16	0.43
1:J:624:GLY:HA2	1:J:625:VAL:HA	1.71	0.43
1:J:626:ARG:O	1:J:627:GLN:CB	2.66	0.43
1:E:806:CYS:C	1:E:808:GLN:N	2.65	0.43
1:I:956:ALA:HA	1:I:975:SER:HB3	2.00	0.43
1:E:1160:ASN:OD1	1:E:1160:ASN:C	2.57	0.43
1:J:374:VAL:HG23	1:J:604:VAL:HG21	2.01	0.42
1:B:594:THR:HB	1:B:595:LYS:CA	2.49	0.42
1:B:600:LEU:HA	1:B:601:GLY:HA3	1.74	0.42
1:E:906:MET:HA	1:E:907:GLN:HA	1.81	0.42
1:I:786:PHE:CD1	1:I:786:PHE:C	2.92	0.42
1:I:961:THR:O	1:I:963:GLY:N	2.52	0.42
1:B:104:ASN:OD1	1:B:104:ASN:C	2.57	0.42
1:I:904:GLY:O	1:I:905:TYR:CB	2.61	0.42
1:J:172:LEU:HD12	1:J:172:LEU:C	2.39	0.42
1:A:1106:CYS:SG	1:A:1138:HIS:ND1	2.93	0.42
1:B:689:TYR:HD1	1:B:690:SER:C	2.23	0.42
1:J:600:LEU:HA	1:J:601:GLY:HA3	1.62	0.42
1:B:602:ASN:O	1:B:616:VAL:HB	2.20	0.42
1:J:330:ASP:C	1:J:330:ASP:OD1	2.58	0.42
1:J:625:VAL:HG12	1:J:626:ARG:N	2.35	0.42
1:J:368:ALA:O	1:J:369:LYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:594:THR:HB	1:J:595:LYS:CA	2.49	0.41
1:A:1120:GLY:O	1:A:1121:THR:OG1	2.29	0.41
1:F:330:ASP:C	1:F:330:ASP:OD1	2.58	0.41
1:I:965:SER:OG	1:I:966:SER:N	2.53	0.41
1:I:1160:ASN:C	1:I:1160:ASN:OD1	2.58	0.41
1:J:714:VAL:HB	1:J:717:LEU:HD23	2.03	0.41
3:H:43:PRO:HA	3:H:44:PRO:HD3	1.94	0.41
1:I:956:ALA:HA	1:I:975:SER:CB	2.50	0.41
1:I:906:MET:HA	1:I:907:GLN:HA	1.80	0.41
1:A:936:PRO:HA	1:A:937:PRO:HD3	1.92	0.41
1:J:209:THR:O	1:J:209:THR:HG22	2.21	0.41
1:I:1124:VAL:O	1:I:1124:VAL:HG13	2.20	0.41
1:E:1124:VAL:O	1:E:1124:VAL:HG13	2.21	0.41
1:A:965:SER:OG	1:A:966:SER:N	2.54	0.41
1:I:1102:LYS:HG2	1:I:1116:PHE:HE2	1.86	0.41
1:J:130:VAL:O	1:J:130:VAL:HG12	2.21	0.41
1:J:689:TYR:CD1	1:J:690:SER:C	2.95	0.41
1:J:664:ASP:OD1	1:J:664:ASP:C	2.57	0.40
1:A:786:PHE:CD1	1:A:786:PHE:C	2.93	0.40
1:B:172:LEU:HD12	1:B:172:LEU:C	2.41	0.40
1:A:826:GLN:OE1	1:A:826:GLN:N	2.35	0.40
1:A:1124:VAL:O	1:A:1124:VAL:HG13	2.21	0.40
1:F:104:ASN:OD1	1:F:104:ASN:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	459/1329 (34%)	441 (96%)	14 (3%)	4 (1%)	14 48
1	B	509/1329 (38%)	478 (94%)	27 (5%)	4 (1%)	16 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	459/1329 (34%)	435 (95%)	20 (4%)	4 (1%)	14	48
1	F	509/1329 (38%)	475 (93%)	29 (6%)	5 (1%)	13	46
1	I	459/1329 (34%)	438 (95%)	14 (3%)	7 (2%)	8	39
1	J	509/1329 (38%)	475 (93%)	30 (6%)	4 (1%)	16	51
2	C	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
2	G	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
2	K	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
3	D	109/218 (50%)	105 (96%)	3 (3%)	1 (1%)	14	48
3	H	109/218 (50%)	105 (96%)	3 (3%)	1 (1%)	14	48
3	L	109/218 (50%)	105 (96%)	3 (3%)	1 (1%)	14	48
All	All	3582/9327 (38%)	3402 (95%)	149 (4%)	31 (1%)	17	48

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1114	SER
1	A	1117	CYS
1	E	806	CYS
1	E	807	LYS
1	F	367	GLU
1	F	368	ALA
1	I	1116	PHE
1	I	1117	CYS
1	J	368	ALA
1	A	1220	PRO
1	B	718	VAL
1	E	1220	PRO
1	F	369	LYS
1	F	603	CYS
1	I	1115	GLY
1	J	367	GLU
1	I	961	THR
1	I	962	ALA
1	I	1220	PRO
1	E	905	TYR
1	F	718	VAL
1	A	940	ASP
1	B	368	ALA

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Mol	Chain	Res	Type
1	B	369	LYS
1	B	621	THR
1	I	940	ASP
1	J	718	VAL
3	D	77	PRO
3	H	77	PRO
3	L	77	PRO
1	J	369	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/1148 (34%)	387 (100%)	1 (0%)	91	96
1	B	442/1148 (38%)	441 (100%)	1 (0%)	92	96
1	E	388/1148 (34%)	388 (100%)	0	100	100
1	F	442/1148 (38%)	440 (100%)	2 (0%)	86	93
1	I	388/1148 (34%)	387 (100%)	1 (0%)	91	96
1	J	442/1148 (38%)	441 (100%)	1 (0%)	92	96
2	C	102/202 (50%)	102 (100%)	0	100	100
2	G	102/202 (50%)	102 (100%)	0	100	100
2	K	102/202 (50%)	102 (100%)	0	100	100
3	D	93/192 (48%)	93 (100%)	0	100	100
3	H	93/192 (48%)	93 (100%)	0	100	100
3	L	93/192 (48%)	93 (100%)	0	100	100
All	All	3075/8070 (38%)	3069 (100%)	6 (0%)	91	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1116	PHE
1	B	621	THR

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Mol	Chain	Res	Type
1	F	104	ASN
1	F	367	GLU
1	I	1116	PHE
1	J	104	ASN

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

Mol	Chain	Res	Type
1	A	1003	GLN
1	I	1169	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 ⓘ

42 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	$\# Z > 2$
4	NAG	M	1	4,1	14,14,15	0.46	0	17,19,21	0.87	1 (5%)
4	NAG	M	2	4	14,14,15	0.63	0	17,19,21	0.94	1 (5%)
4	NAG	N	1	4,1	14,14,15	0.78	1 (7%)	17,19,21	0.51	0
4	NAG	N	2	4	14,14,15	0.25	0	17,19,21	0.58	0
4	NAG	O	1	4,1	14,14,15	0.33	0	17,19,21	0.47	0
4	NAG	O	2	4	14,14,15	0.34	0	17,19,21	0.64	1 (5%)
4	NAG	P	1	4,1	14,14,15	0.39	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	P	2	4	14,14,15	0.30	0	17,19,21	0.44	0
4	NAG	Q	1	4,1	14,14,15	0.92	1 (7%)	17,19,21	0.71	0
4	NAG	Q	2	4	14,14,15	0.19	0	17,19,21	0.70	1 (5%)
4	NAG	R	1	4,1	14,14,15	1.30	1 (7%)	17,19,21	1.27	2 (11%)
4	NAG	R	2	4	14,14,15	0.65	1 (7%)	17,19,21	0.50	0
4	NAG	S	1	4,1	14,14,15	1.44	3 (21%)	17,19,21	1.48	2 (11%)
4	NAG	S	2	4	14,14,15	0.60	0	17,19,21	0.72	0
4	NAG	T	1	4,1	14,14,15	0.60	0	17,19,21	0.83	0
4	NAG	T	2	4	14,14,15	0.84	1 (7%)	17,19,21	2.38	3 (17%)
4	NAG	U	1	4,1	14,14,15	0.51	0	17,19,21	1.12	1 (5%)
4	NAG	U	2	4	14,14,15	0.21	0	17,19,21	0.51	0
4	NAG	V	1	4,1	14,14,15	0.44	0	17,19,21	0.69	0
4	NAG	V	2	4	14,14,15	0.28	0	17,19,21	0.53	0
4	NAG	W	1	4,1	14,14,15	0.33	0	17,19,21	0.90	0
4	NAG	W	2	4	14,14,15	0.66	1 (7%)	17,19,21	0.65	1 (5%)
4	NAG	X	1	4,1	14,14,15	0.46	0	17,19,21	1.46	3 (17%)
4	NAG	X	2	4	14,14,15	0.27	0	17,19,21	0.61	0
4	NAG	Y	1	4,1	14,14,15	0.70	1 (7%)	17,19,21	1.09	1 (5%)
4	NAG	Y	2	4	14,14,15	0.64	0	17,19,21	1.00	1 (5%)
4	NAG	Z	1	4,1	14,14,15	0.32	0	17,19,21	0.60	0
4	NAG	Z	2	4	14,14,15	0.36	0	17,19,21	0.55	0
4	NAG	a	1	4,1	14,14,15	0.30	0	17,19,21	0.68	0
4	NAG	a	2	4	14,14,15	0.50	0	17,19,21	0.57	0
4	NAG	b	1	4,1	14,14,15	1.09	1 (7%)	17,19,21	0.69	1 (5%)
4	NAG	b	2	4	14,14,15	0.42	0	17,19,21	0.75	1 (5%)
4	NAG	c	1	4,1	14,14,15	0.21	0	17,19,21	1.17	2 (11%)
4	NAG	c	2	4	14,14,15	0.42	0	17,19,21	1.09	1 (5%)
4	NAG	d	1	4,1	14,14,15	0.54	0	17,19,21	0.74	1 (5%)
4	NAG	d	2	4	14,14,15	0.26	0	17,19,21	0.57	0
4	NAG	e	1	4,1	14,14,15	0.80	1 (7%)	17,19,21	1.24	2 (11%)
4	NAG	e	2	4	14,14,15	0.73	0	17,19,21	0.98	1 (5%)
4	NAG	f	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	1.20	2 (11%)
4	NAG	f	2	4	14,14,15	1.76	2 (14%)	17,19,21	1.38	1 (5%)
4	NAG	g	1	4,1	14,14,15	0.19	0	17,19,21	0.61	0
4	NAG	g	2	4	14,14,15	0.29	0	17,19,21	0.44	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	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	3/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	4/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	1/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	5/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	X	2	4	-	3/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	3/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	NAG	a	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	NAG	b	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	2/6/23/26	0/1/1/1
4	NAG	c	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	c	2	4	-	4/6/23/26	0/1/1/1

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	f	2	NAG	O5-C1	5.26	1.52	1.43
4	R	1	NAG	O5-C1	-4.63	1.35	1.43
4	b	1	NAG	O5-C1	-3.70	1.37	1.43
4	f	2	NAG	C1-C2	3.69	1.57	1.52
4	S	1	NAG	O5-C1	-3.63	1.37	1.43
4	Q	1	NAG	O5-C1	-3.12	1.38	1.43
4	S	1	NAG	C1-C2	3.09	1.56	1.52
4	T	2	NAG	C1-C2	2.53	1.55	1.52
4	N	1	NAG	O5-C1	-2.48	1.39	1.43
4	f	1	NAG	C1-C2	2.45	1.55	1.52
4	Y	1	NAG	O5-C1	-2.39	1.39	1.43
4	W	2	NAG	C1-C2	2.39	1.55	1.52
4	S	1	NAG	C3-C2	2.37	1.57	1.52
4	e	1	NAG	O5-C1	-2.22	1.40	1.43
4	R	2	NAG	O5-C1	2.20	1.47	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	2	NAG	C2-N2-C7	8.34	134.07	122.90
4	f	2	NAG	C1-O5-C5	5.09	119.01	112.19
4	S	1	NAG	C4-C3-C2	4.36	117.41	111.02
4	T	2	NAG	C1-C2-N2	3.90	116.58	110.43
4	X	1	NAG	C1-O5-C5	3.86	117.35	112.19
4	R	1	NAG	C2-N2-C7	3.47	127.55	122.90
4	Y	1	NAG	C2-N2-C7	3.36	127.40	122.90
4	e	1	NAG	C2-N2-C7	3.31	127.33	122.90
4	e	2	NAG	C2-N2-C7	3.25	127.26	122.90
4	c	1	NAG	C2-N2-C7	3.23	127.23	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	2	NAG	C2-N2-C7	3.21	127.20	122.90
4	M	2	NAG	C2-N2-C7	3.19	127.18	122.90
4	c	2	NAG	C2-N2-C7	3.18	127.16	122.90
4	X	1	NAG	C2-N2-C7	3.11	127.07	122.90
4	U	1	NAG	C2-N2-C7	3.00	126.92	122.90
4	f	1	NAG	C2-N2-C7	2.99	126.91	122.90
4	S	1	NAG	C2-N2-C7	2.75	126.59	122.90
4	M	1	NAG	C1-O5-C5	2.72	115.83	112.19
4	X	1	NAG	C1-C2-N2	2.66	114.62	110.43
4	c	1	NAG	C1-O5-C5	2.35	115.34	112.19
4	e	1	NAG	C1-O5-C5	-2.32	109.08	112.19
4	f	1	NAG	C1-C2-N2	2.31	114.07	110.43
4	d	1	NAG	C1-O5-C5	2.25	115.20	112.19
4	Q	2	NAG	C1-O5-C5	2.22	115.16	112.19
4	T	2	NAG	C8-C7-N2	2.18	119.73	116.12
4	b	2	NAG	C1-O5-C5	2.09	114.99	112.19
4	O	2	NAG	C1-O5-C5	2.09	114.99	112.19
4	W	2	NAG	C1-O5-C5	2.07	114.97	112.19
4	R	1	NAG	O4-C4-C3	-2.06	105.52	110.38
4	b	1	NAG	C1-O5-C5	-2.02	109.47	112.19

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	1	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
4	e	1	NAG	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	Q	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	f	2	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	e	1	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
4	S	2	NAG	C8-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
4	T	1	NAG	C8-C7-N2-C2
4	T	1	NAG	O7-C7-N2-C2
4	T	2	NAG	C8-C7-N2-C2
4	T	2	NAG	O7-C7-N2-C2
4	X	2	NAG	C8-C7-N2-C2
4	X	2	NAG	O7-C7-N2-C2
4	b	2	NAG	C8-C7-N2-C2
4	b	2	NAG	O7-C7-N2-C2
4	d	1	NAG	C8-C7-N2-C2
4	d	1	NAG	O7-C7-N2-C2
4	f	2	NAG	C8-C7-N2-C2
4	f	2	NAG	O7-C7-N2-C2
4	a	2	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
4	f	1	NAG	O5-C5-C6-O6
4	g	1	NAG	O5-C5-C6-O6

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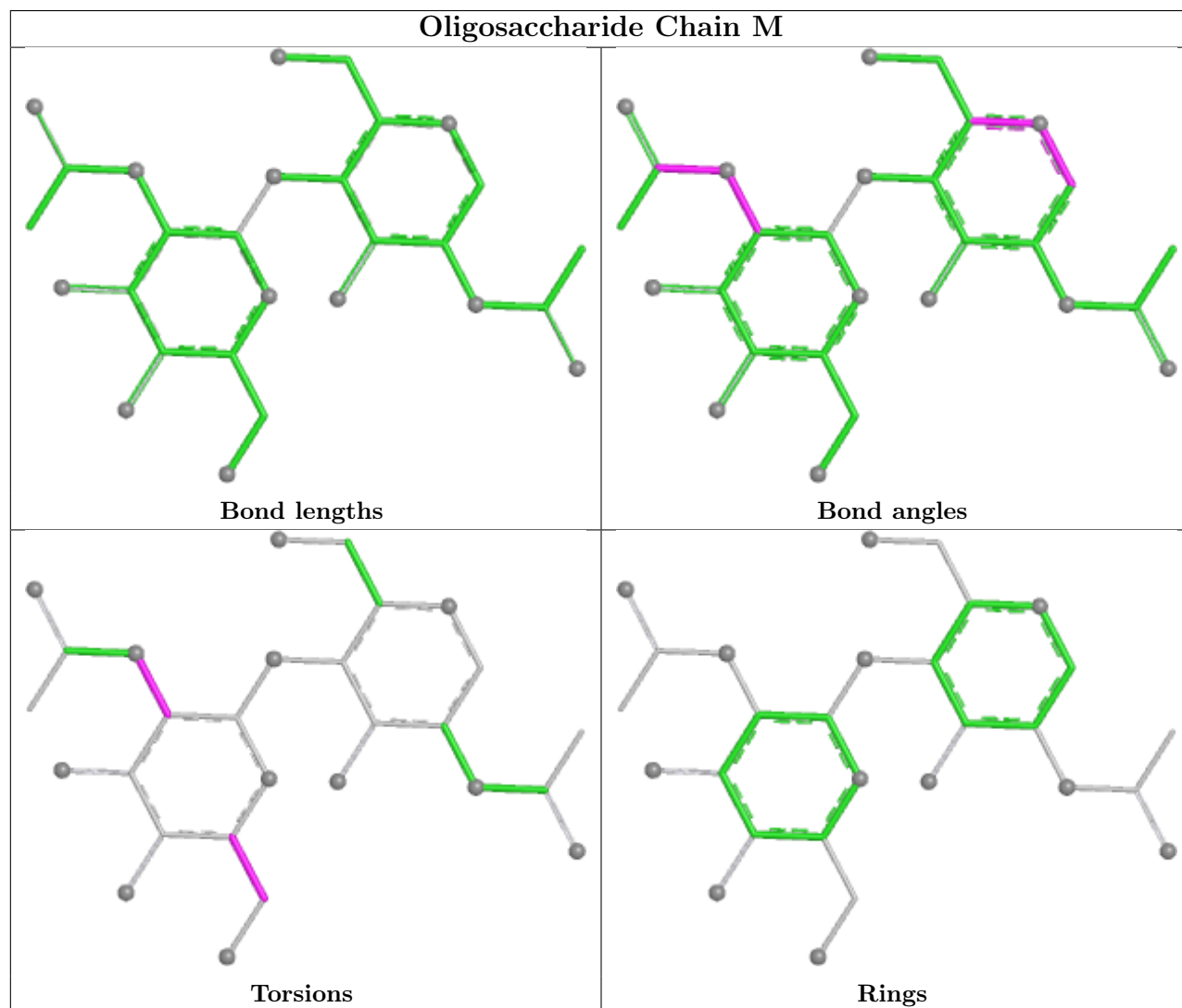
Mol	Chain	Res	Type	Atoms
4	T	2	NAG	O5-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C1-C2-N2-C7
4	R	1	NAG	C1-C2-N2-C7
4	Y	1	NAG	C1-C2-N2-C7
4	Y	2	NAG	C1-C2-N2-C7
4	c	1	NAG	C1-C2-N2-C7
4	c	2	NAG	C1-C2-N2-C7
4	e	1	NAG	C1-C2-N2-C7
4	e	2	NAG	C1-C2-N2-C7
4	a	1	NAG	C4-C5-C6-O6
4	S	1	NAG	C3-C2-N2-C7
4	T	2	NAG	C3-C2-N2-C7
4	U	1	NAG	C3-C2-N2-C7
4	e	1	NAG	C3-C2-N2-C7
4	N	1	NAG	C1-C2-N2-C7
4	S	1	NAG	C1-C2-N2-C7
4	T	2	NAG	C1-C2-N2-C7
4	U	1	NAG	C1-C2-N2-C7
4	X	1	NAG	C1-C2-N2-C7
4	f	1	NAG	C1-C2-N2-C7
4	M	2	NAG	C3-C2-N2-C7
4	R	1	NAG	C3-C2-N2-C7
4	X	1	NAG	C3-C2-N2-C7
4	Y	1	NAG	C3-C2-N2-C7
4	Y	2	NAG	C3-C2-N2-C7
4	c	1	NAG	C3-C2-N2-C7
4	c	2	NAG	C3-C2-N2-C7
4	e	2	NAG	C3-C2-N2-C7
4	f	1	NAG	C3-C2-N2-C7
4	W	1	NAG	C4-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6

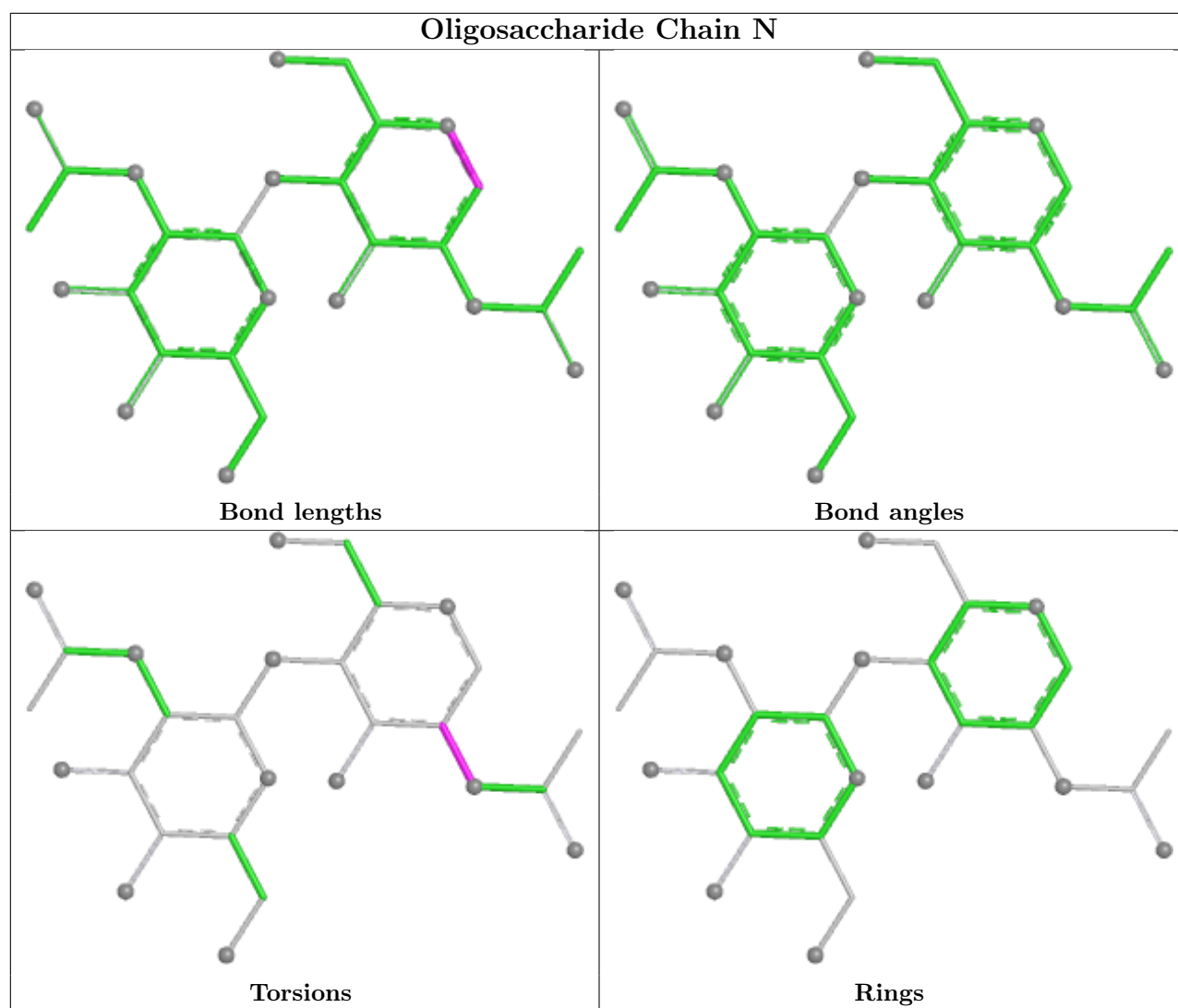
There are no ring outliers.

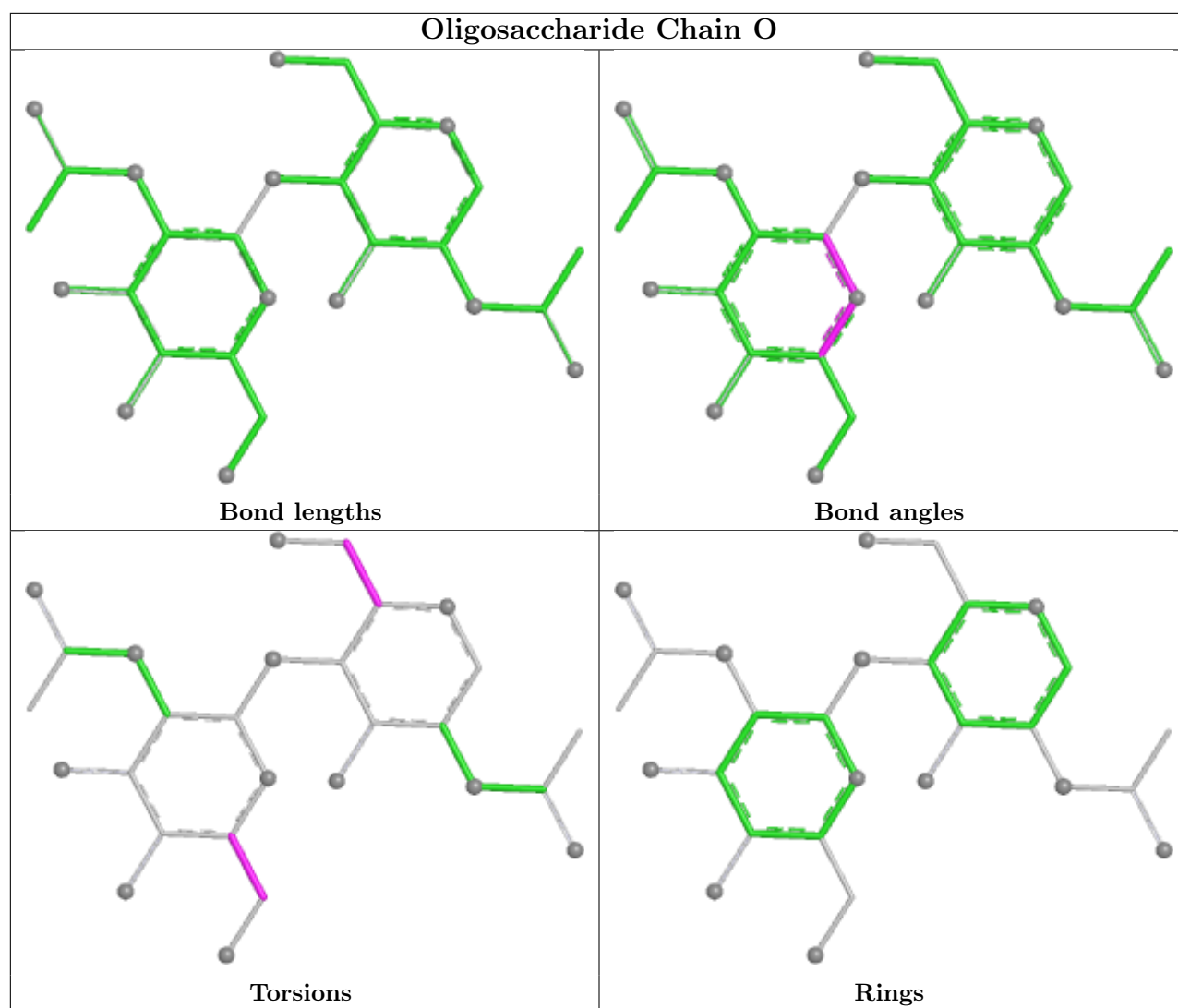
2 monomers are involved in 2 short contacts:

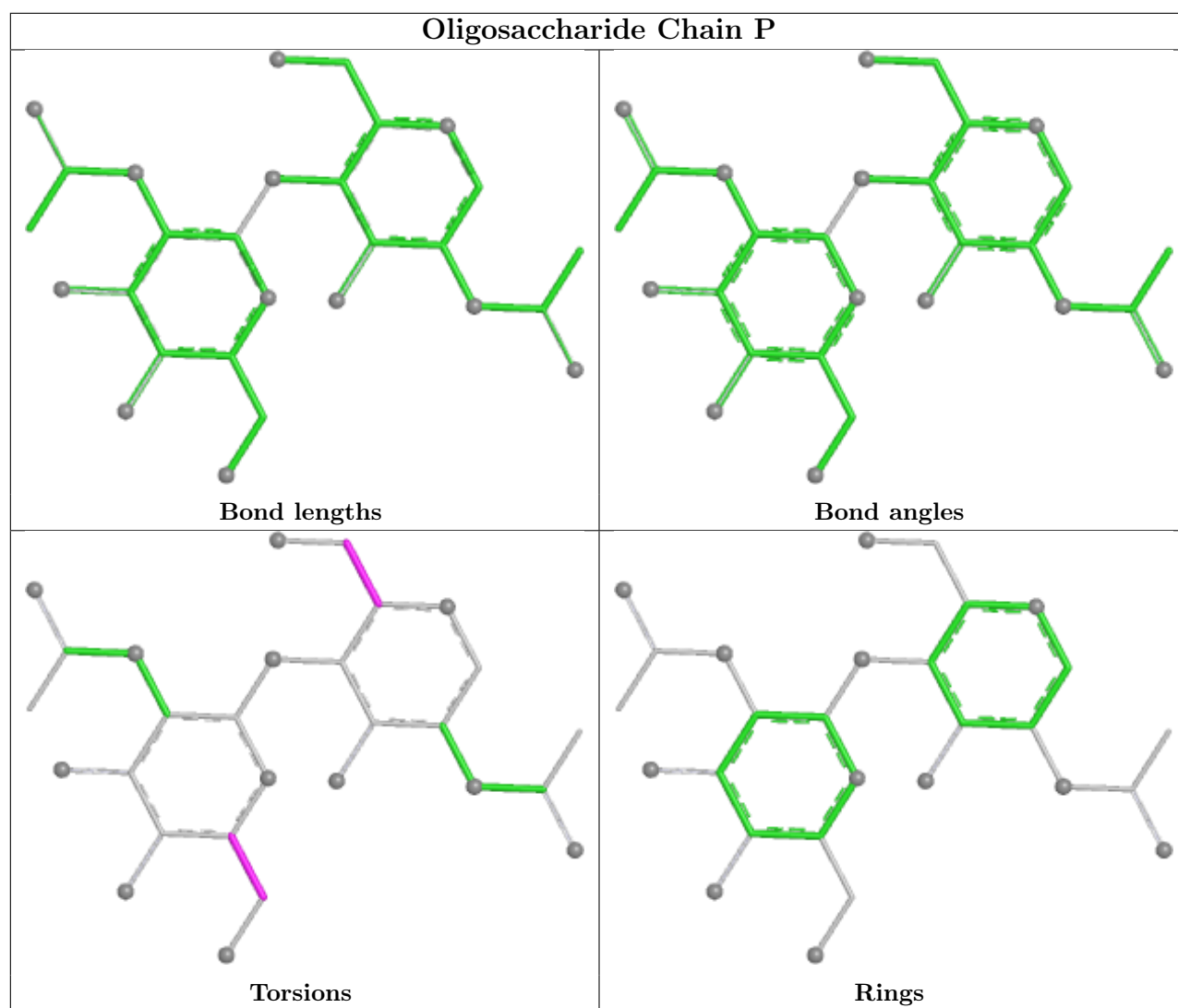
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	1	NAG	1	0
4	M	2	NAG	1	0

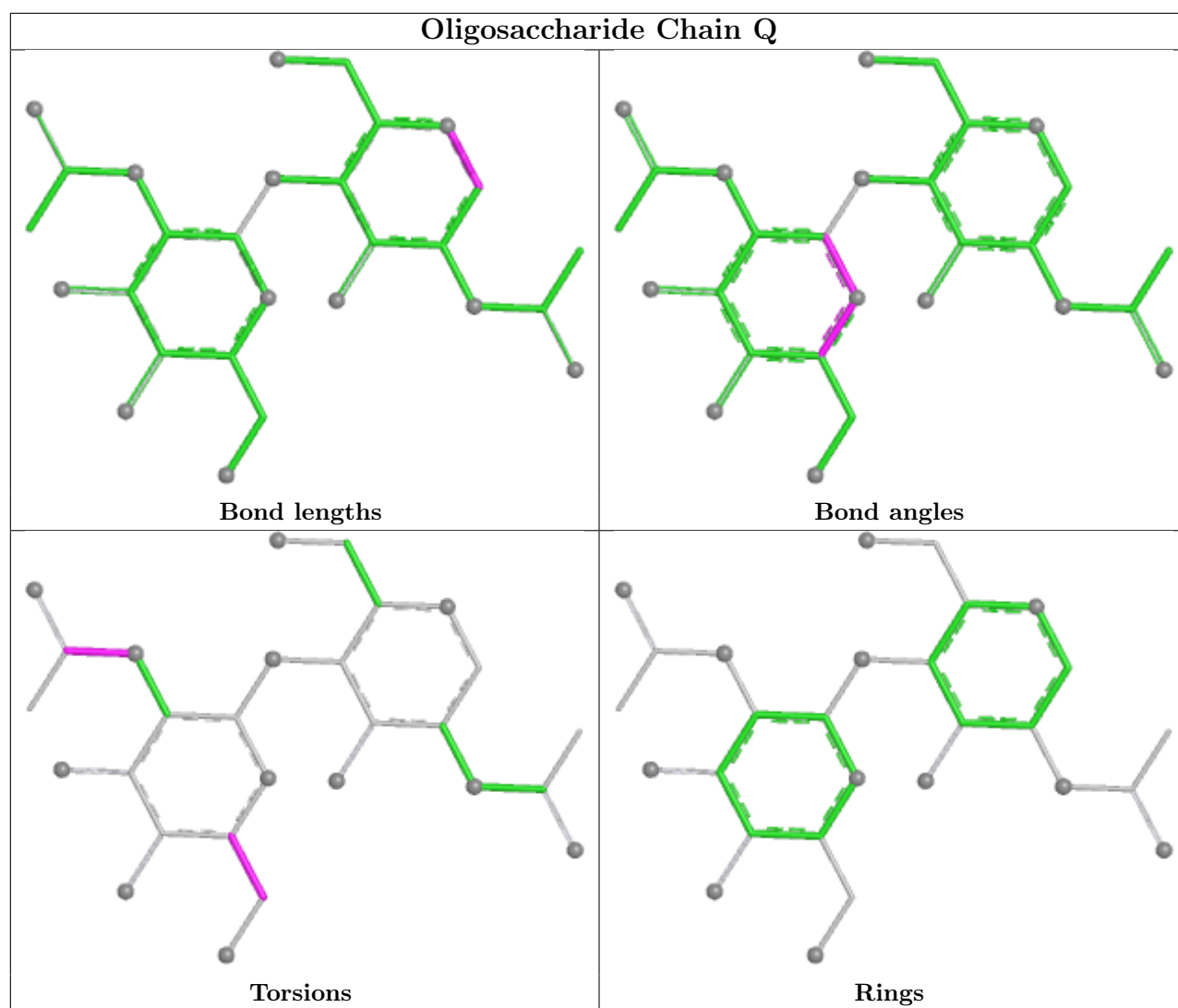
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

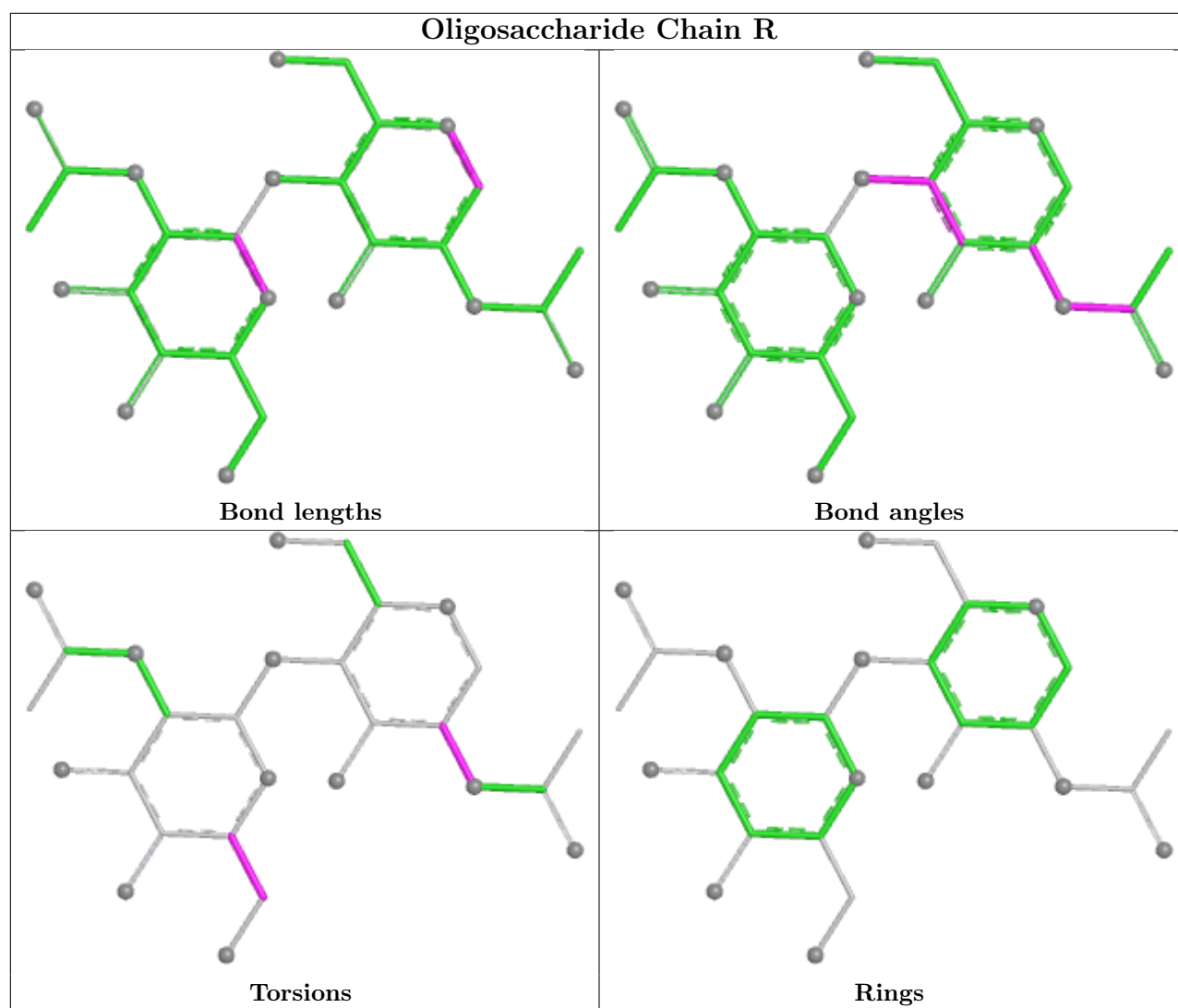


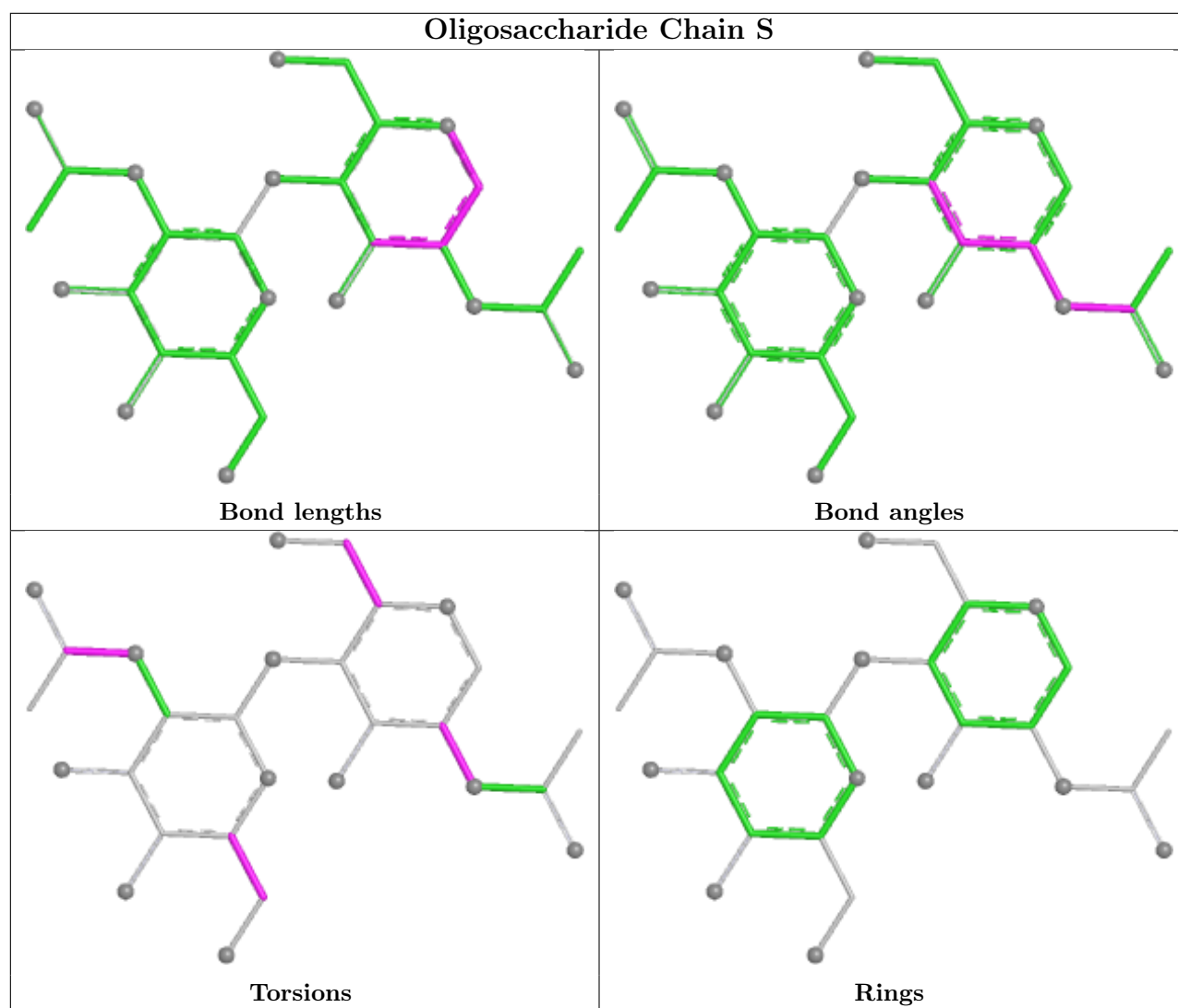


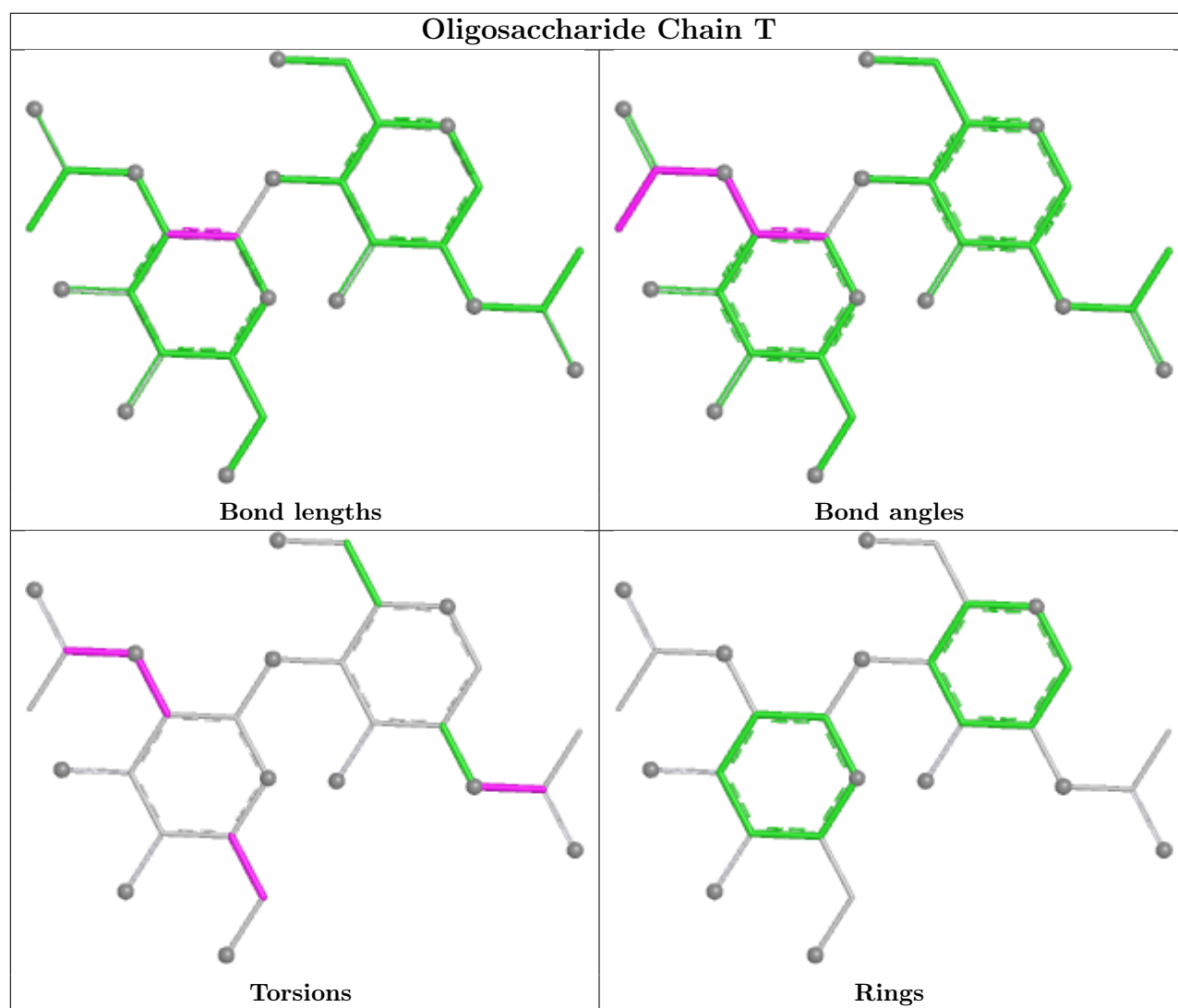


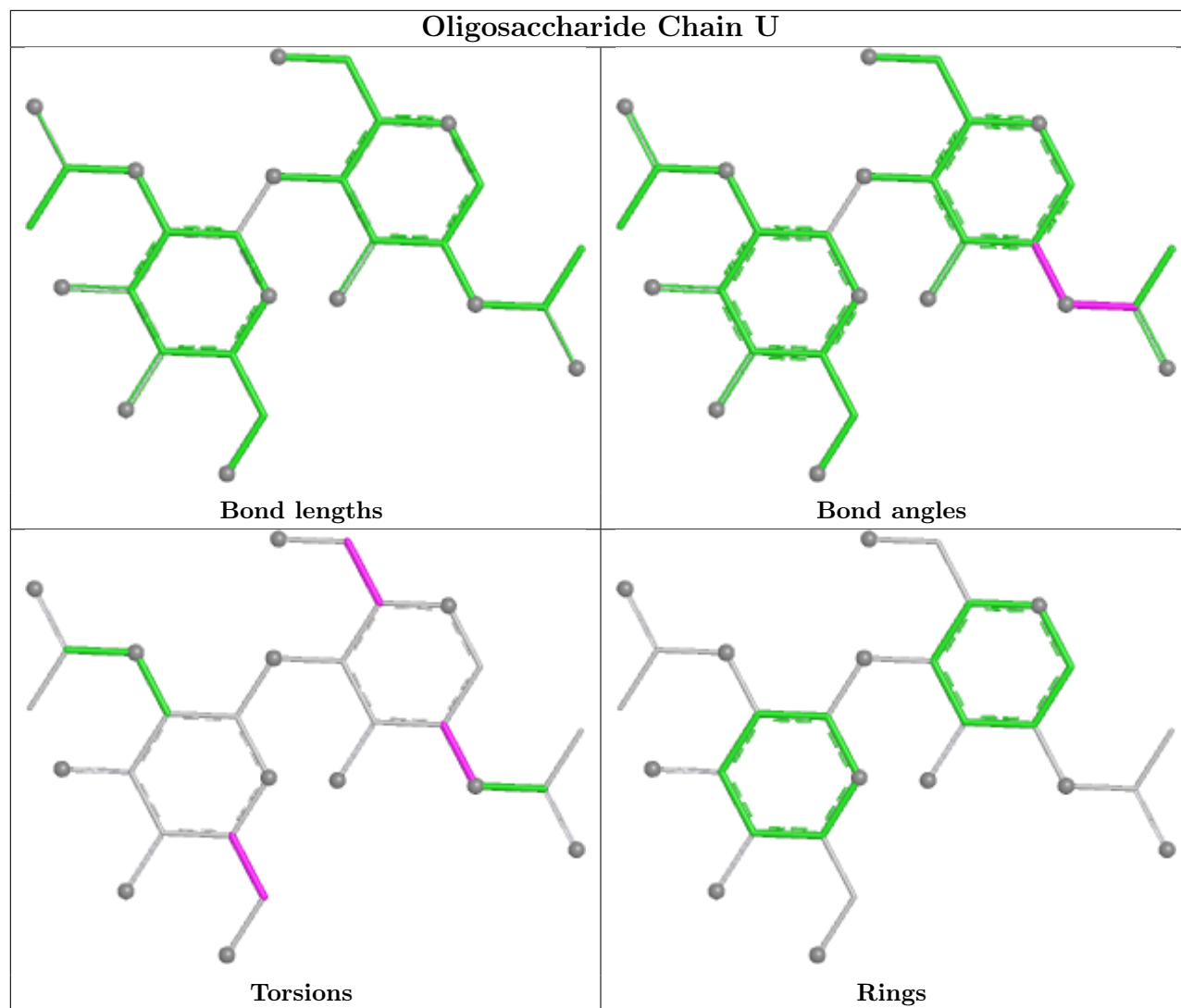


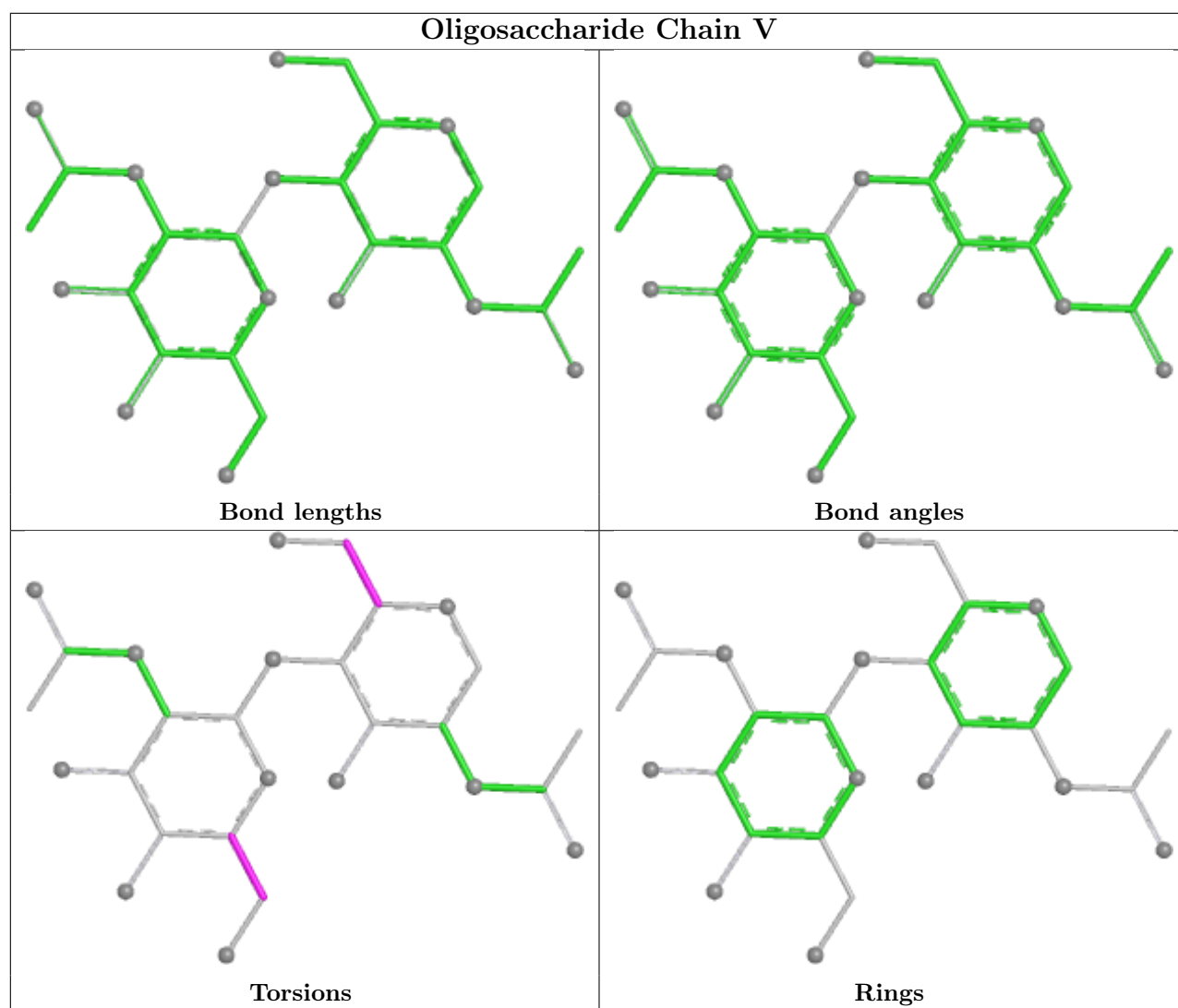


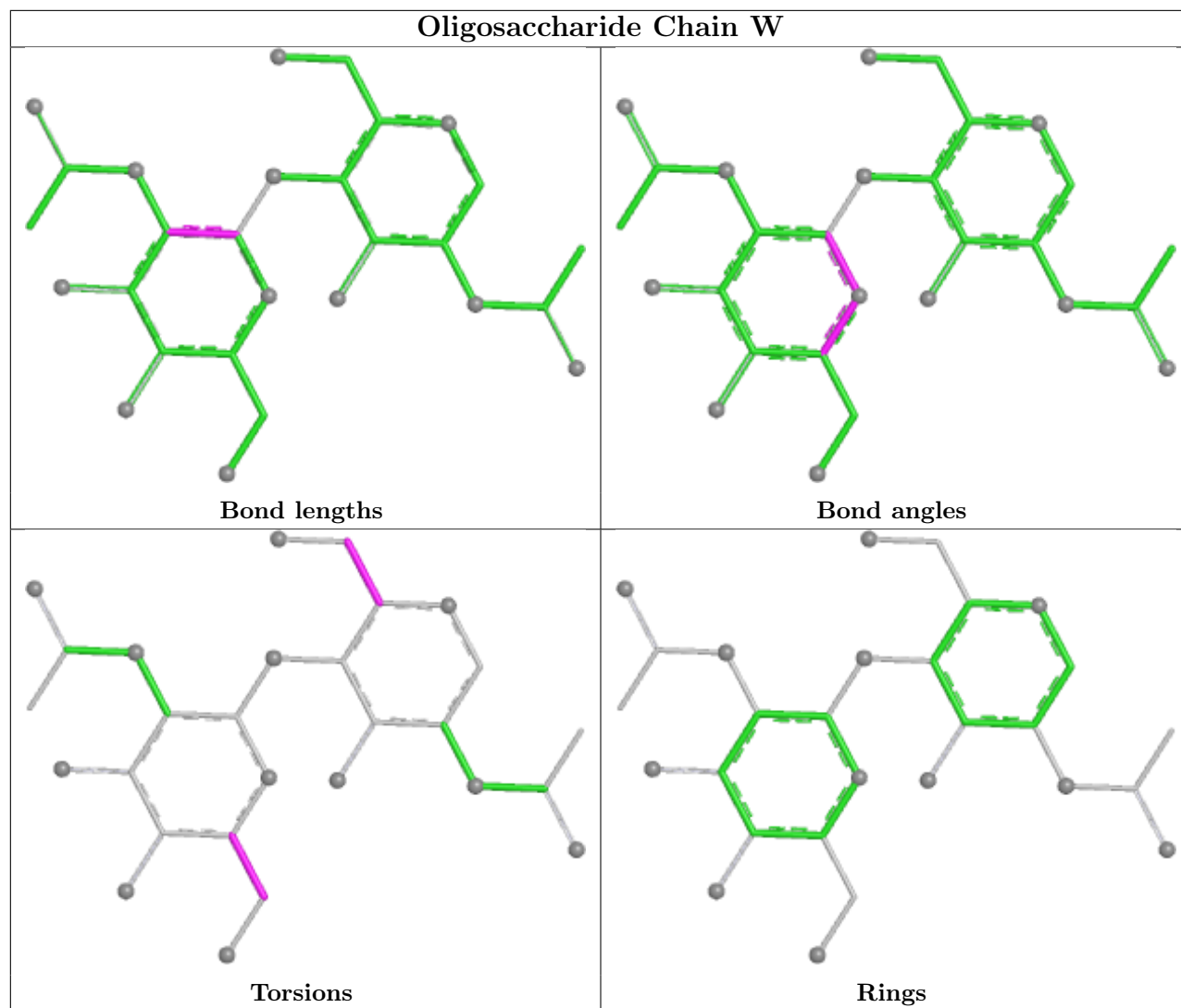


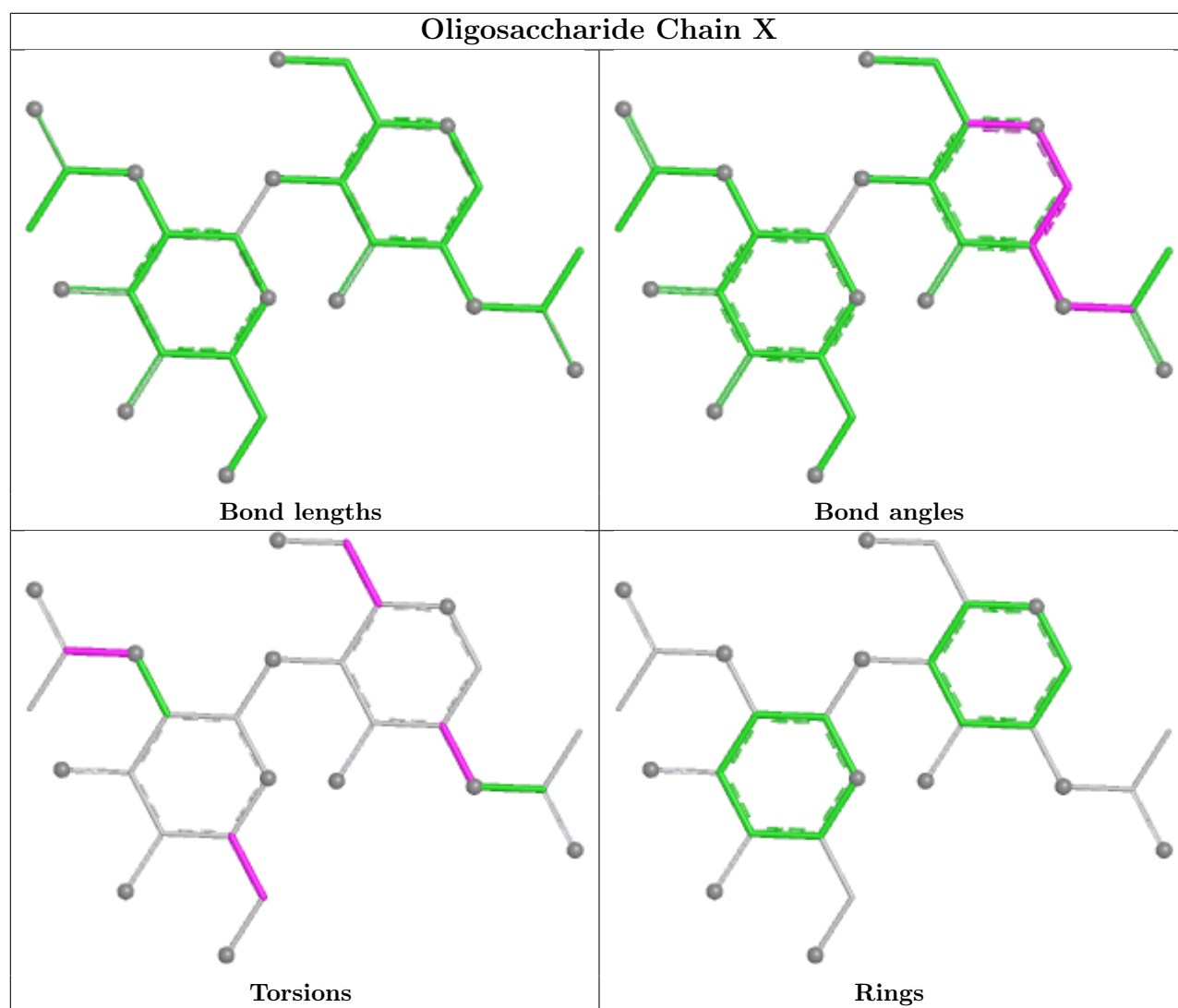


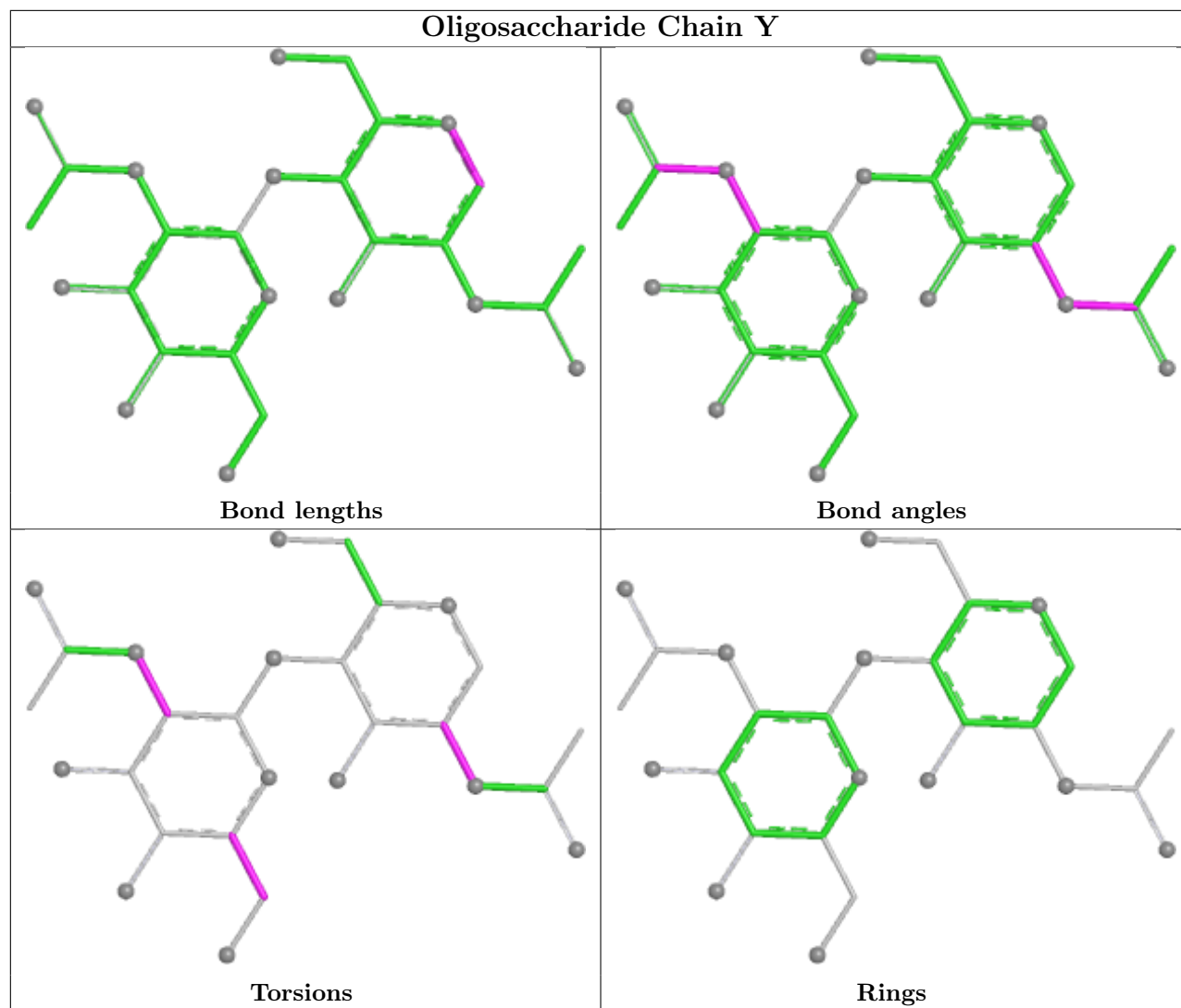


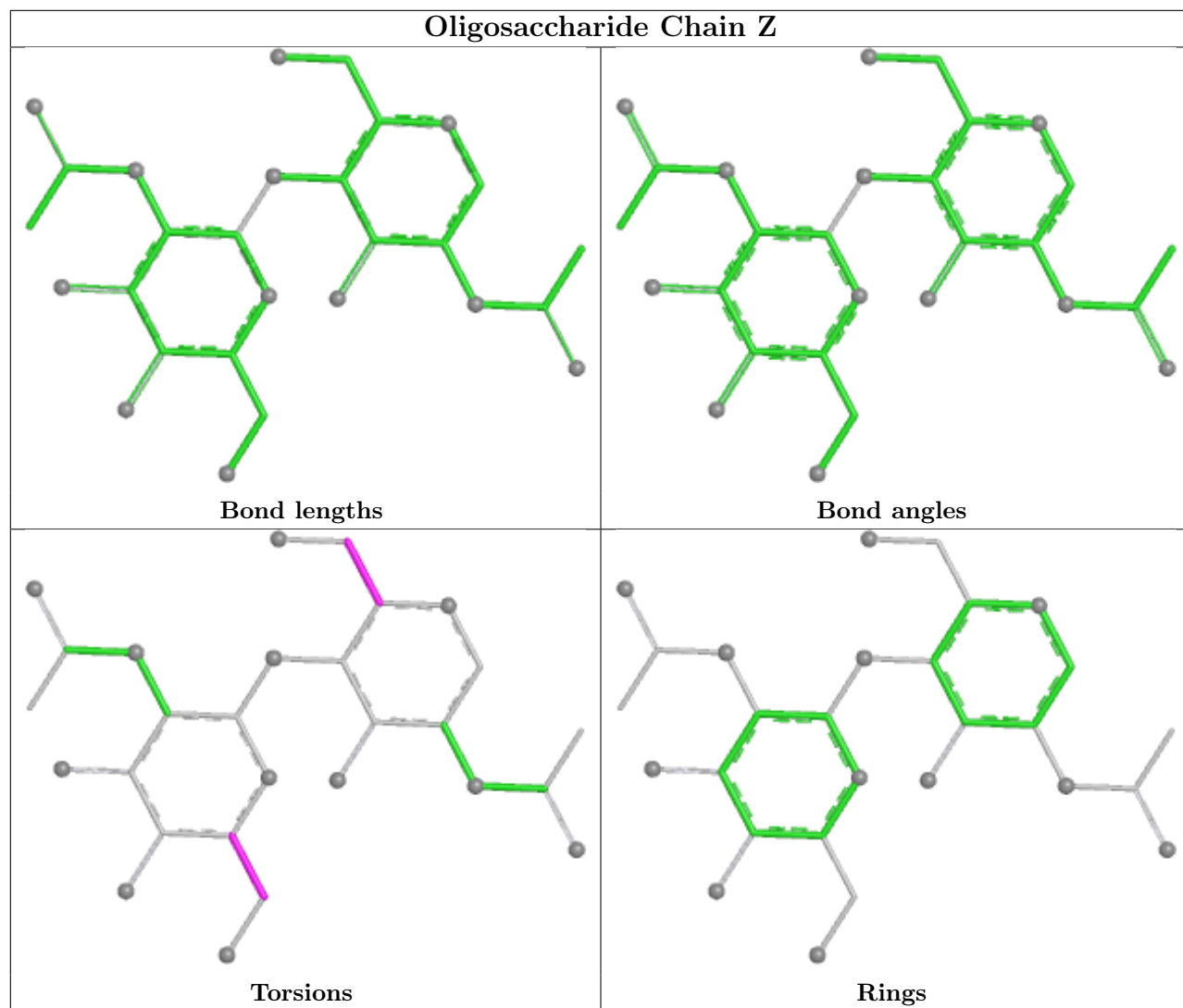


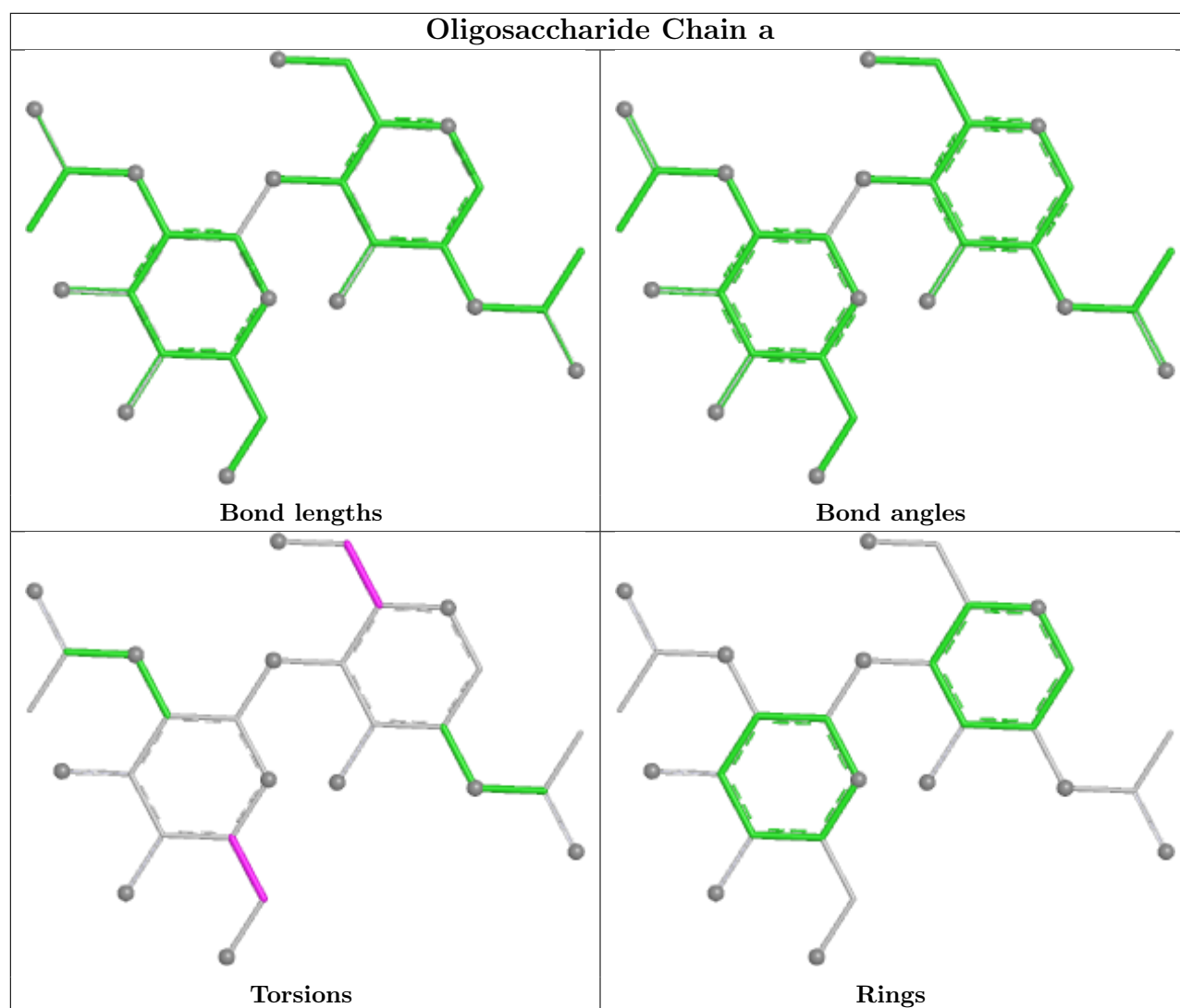


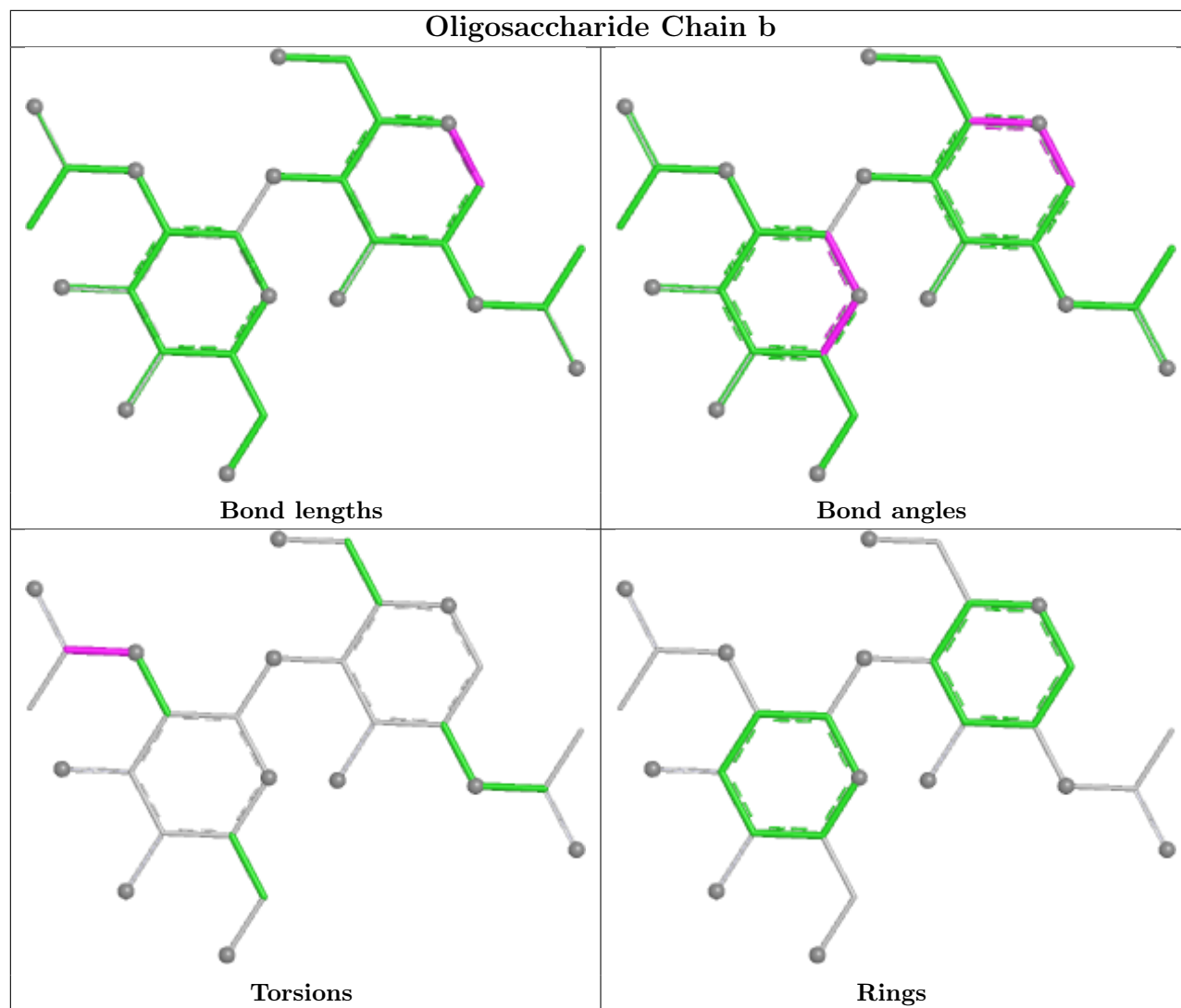


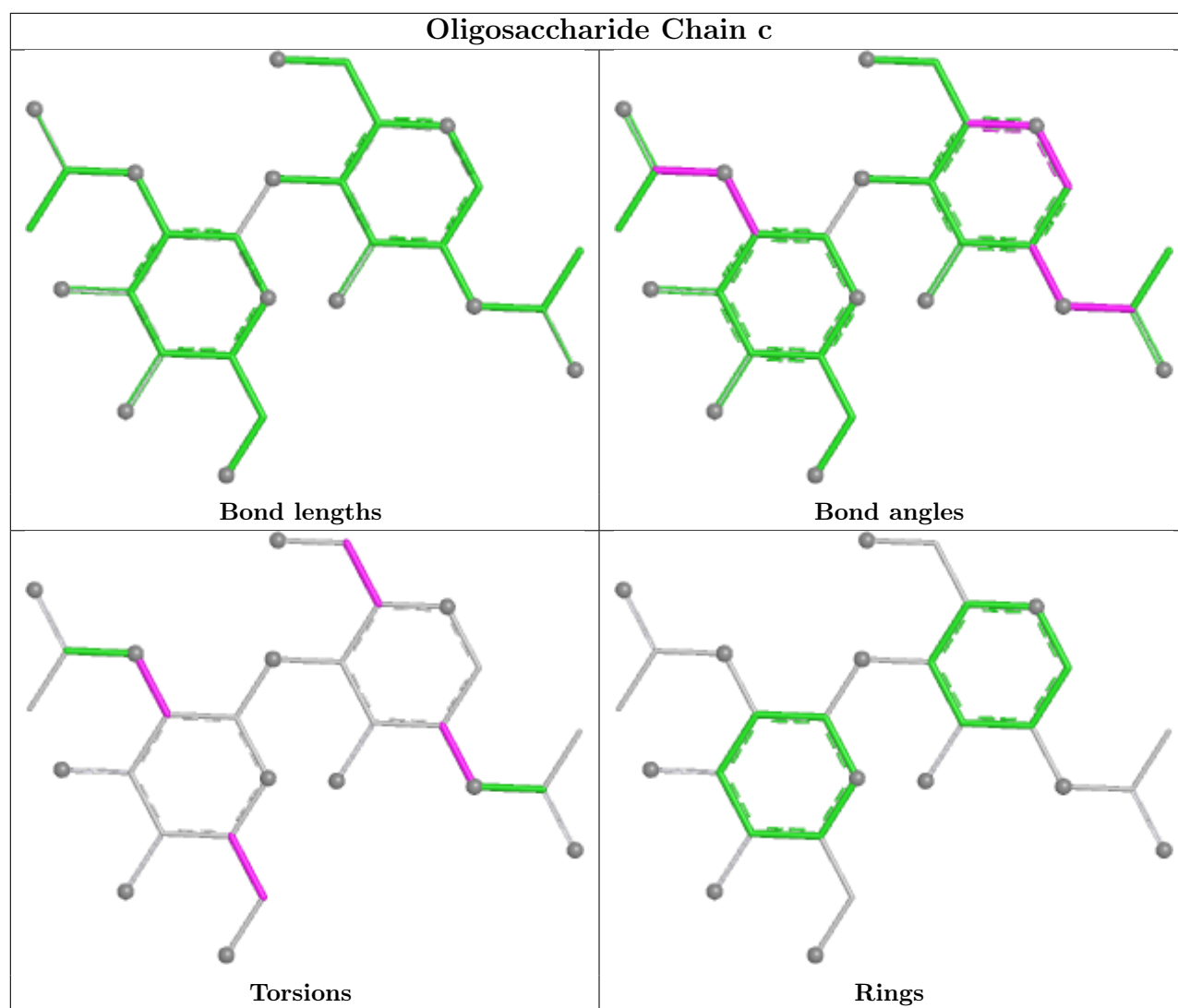


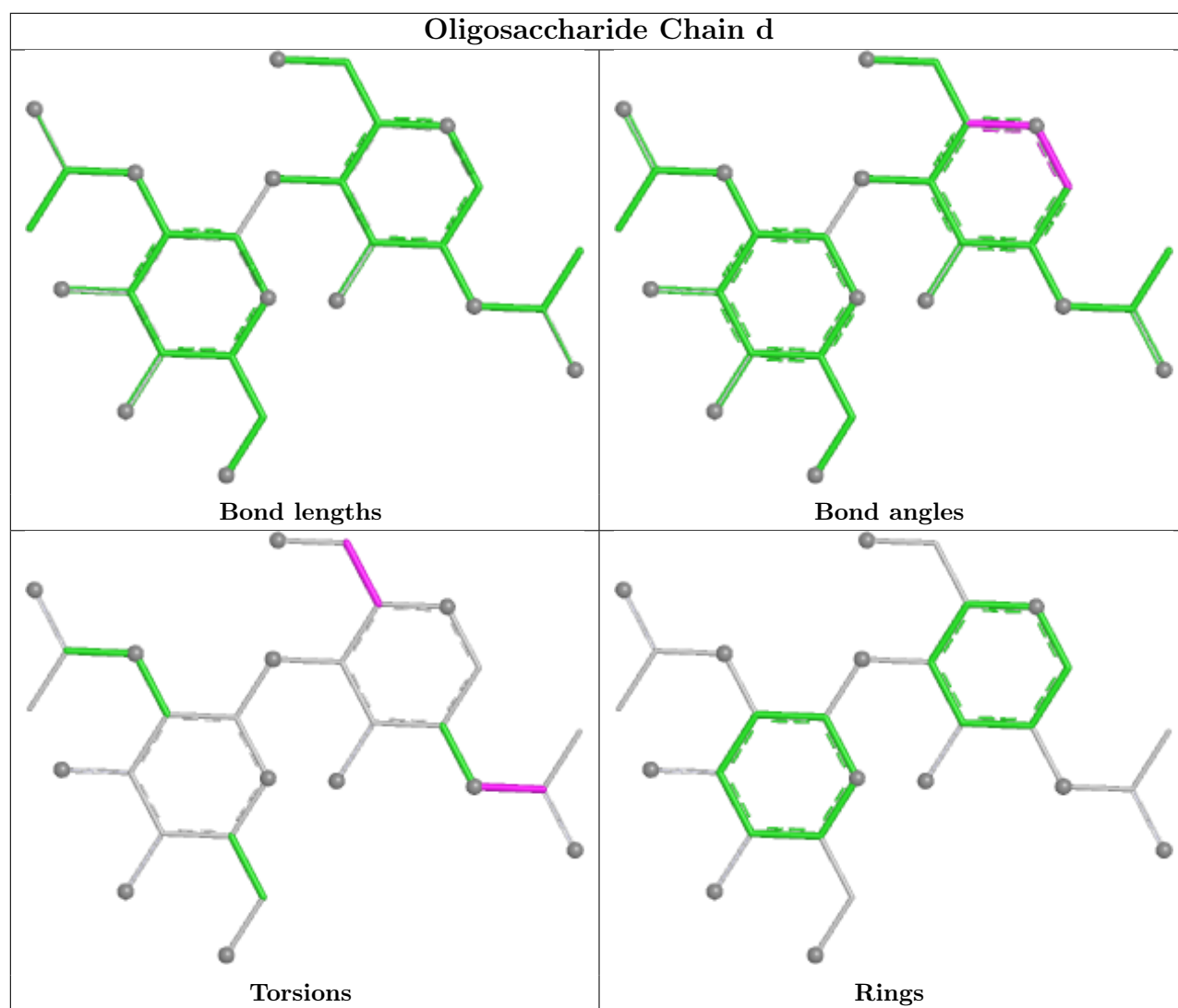


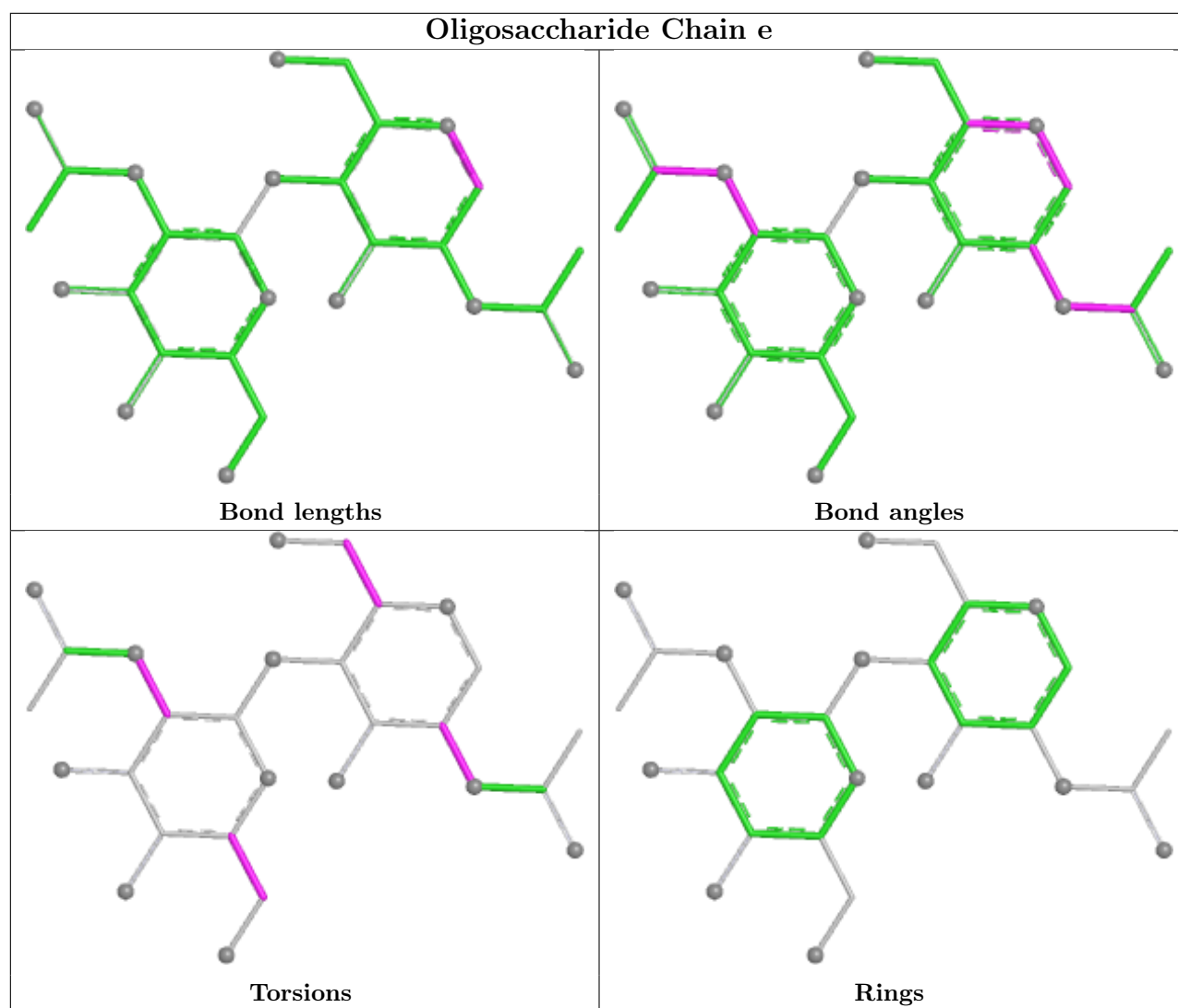


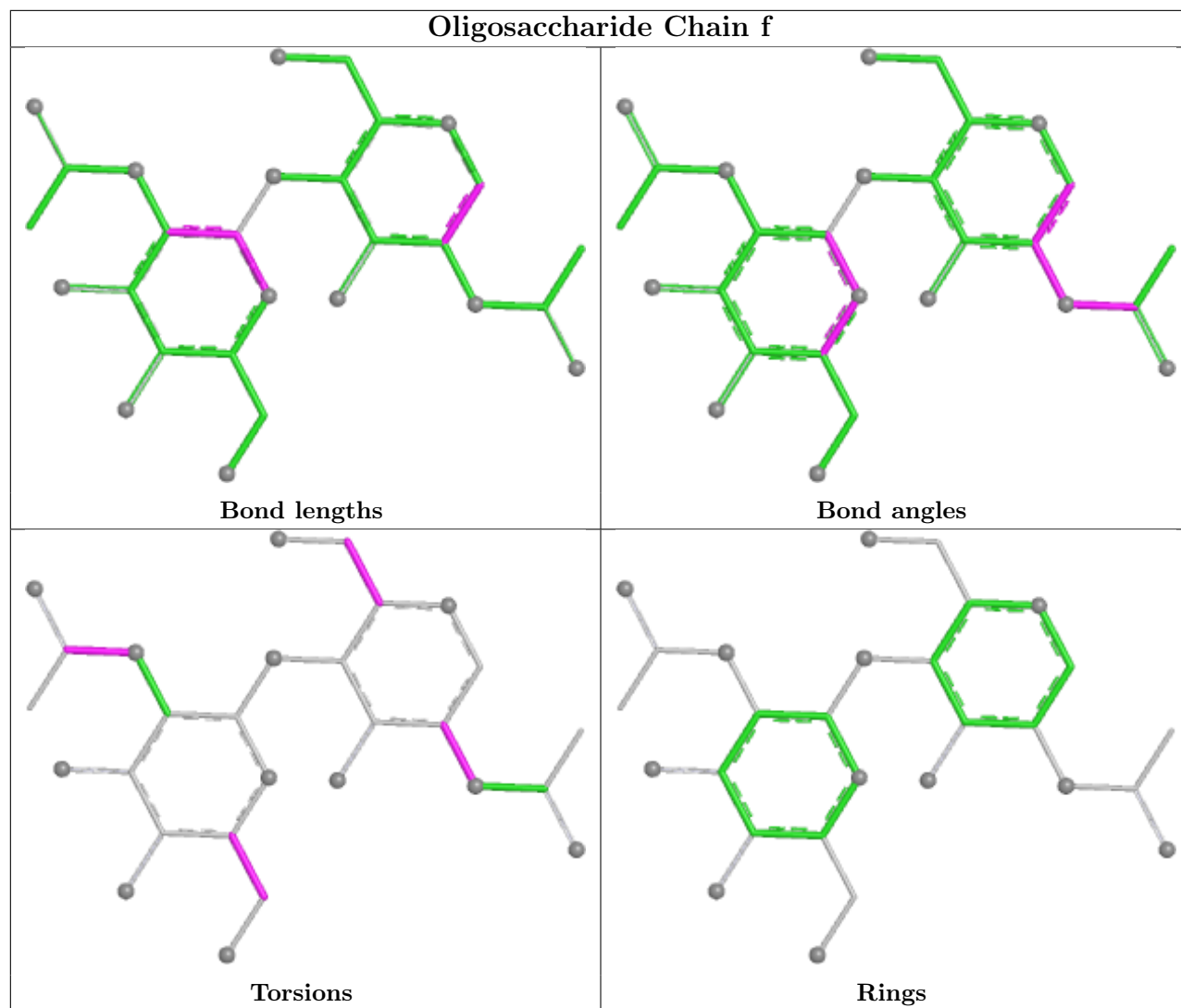


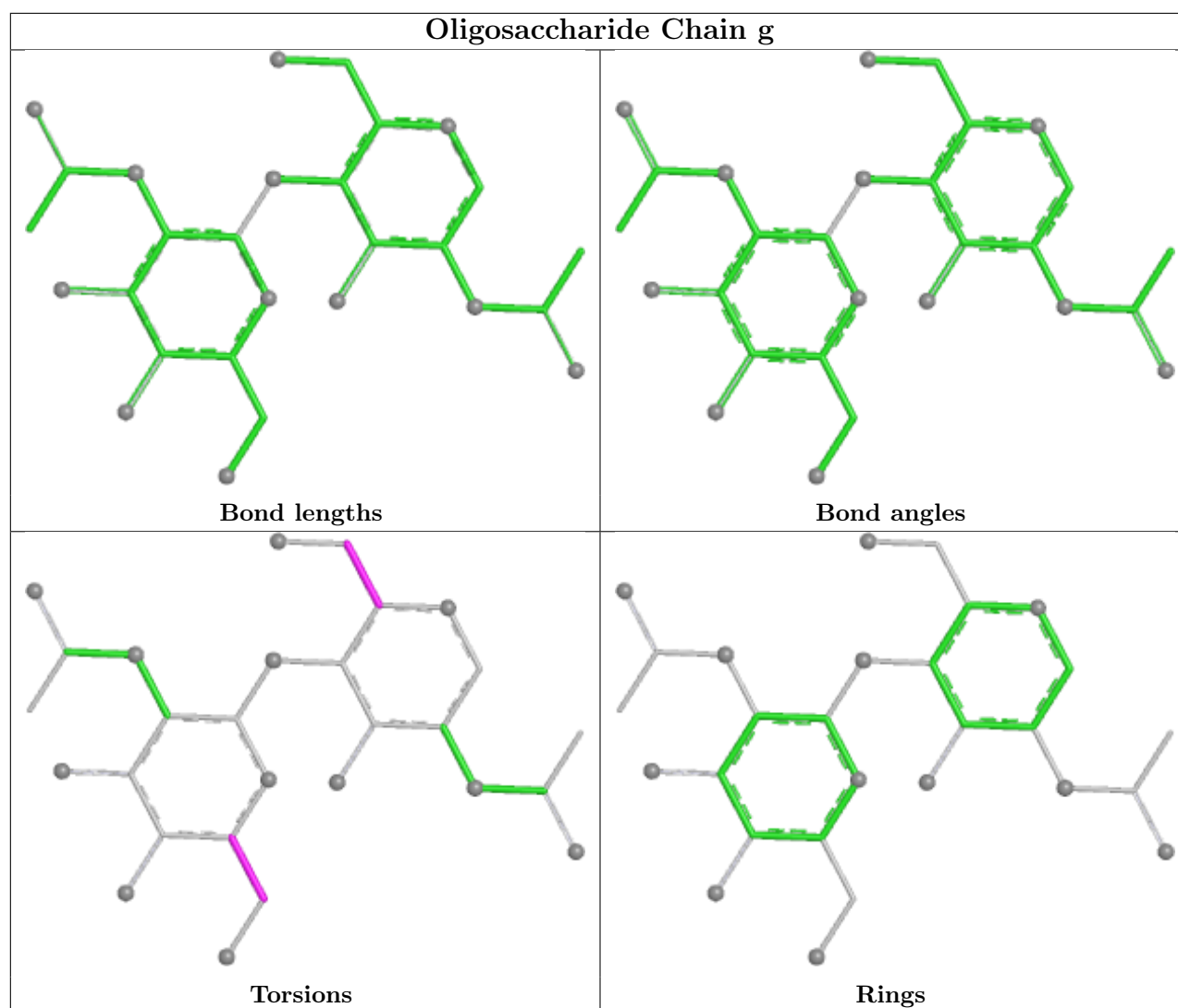












5.6 Ligand geometry [i](#)

21 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	$\# Z > 2$
5	NAG	J	1404	1	14,14,15	0.47	0	17,19,21	0.44	0
5	NAG	F	1402	1	14,14,15	0.28	0	17,19,21	0.67	1 (5%)
5	NAG	F	1403	1	14,14,15	1.28	1 (7%)	17,19,21	2.31	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1405	1	14,14,15	0.69	0	17,19,21	0.65	0
5	NAG	J	1402	1	14,14,15	0.34	0	17,19,21	0.81	1 (5%)
5	NAG	J	1403	1	14,14,15	0.43	0	17,19,21	0.57	0
5	NAG	F	1404	1	14,14,15	0.55	0	17,19,21	0.76	1 (5%)
5	NAG	J	1406	1	14,14,15	0.60	0	17,19,21	0.64	0
5	NAG	B	1401	1	14,14,15	1.99	1 (7%)	17,19,21	1.99	3 (17%)
5	NAG	B	1402	1	14,14,15	0.47	0	17,19,21	0.66	1 (5%)
5	NAG	J	1401	1	14,14,15	0.70	0	17,19,21	0.79	1 (5%)
5	NAG	A	1401	1	14,14,15	0.61	0	17,19,21	1.10	1 (5%)
5	NAG	F	1405	1	14,14,15	0.71	0	17,19,21	0.65	0
5	NAG	J	1405	1	14,14,15	0.22	0	17,19,21	0.57	0
5	NAG	B	1403	1	14,14,15	0.77	1 (7%)	17,19,21	1.02	1 (5%)
5	NAG	I	1401	1	14,14,15	0.32	0	17,19,21	0.80	1 (5%)
5	NAG	B	1406	1	14,14,15	0.50	0	17,19,21	0.70	0
5	NAG	F	1406	1	14,14,15	0.64	0	17,19,21	0.76	1 (5%)
5	NAG	B	1404	1	14,14,15	0.75	1 (7%)	17,19,21	1.18	3 (17%)
5	NAG	E	1401	1	14,14,15	0.37	0	17,19,21	0.92	1 (5%)
5	NAG	F	1401	1	14,14,15	0.51	0	17,19,21	1.04	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
5	NAG	J	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	F	1402	1	-	3/6/23/26	0/1/1/1
5	NAG	F	1403	1	-	6/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	J	1402	1	-	4/6/23/26	0/1/1/1
5	NAG	J	1403	1	-	1/6/23/26	0/1/1/1
5	NAG	F	1404	1	-	4/6/23/26	0/1/1/1
5	NAG	J	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	J	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	F	1405	1	-	3/6/23/26	0/1/1/1
5	NAG	J	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	4/6/23/26	0/1/1/1
5	NAG	I	1401	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	3/6/23/26	0/1/1/1
5	NAG	F	1406	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	3/6/23/26	0/1/1/1
5	NAG	E	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	F	1401	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1401	NAG	C1-C2	7.16	1.62	1.52
5	F	1403	NAG	C1-C2	4.12	1.58	1.52
5	B	1403	NAG	C1-C2	2.42	1.55	1.52
5	B	1404	NAG	O5-C1	2.26	1.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1403	NAG	C2-N2-C7	8.19	133.88	122.90
5	B	1401	NAG	C2-N2-C7	6.26	131.29	122.90
5	E	1401	NAG	C1-O5-C5	3.42	116.78	112.19
5	A	1401	NAG	C2-N2-C7	3.30	127.32	122.90
5	F	1401	NAG	C2-N2-C7	3.26	127.28	122.90
5	B	1404	NAG	C2-N2-C7	3.21	127.20	122.90
5	F	1403	NAG	C1-C2-N2	3.10	115.31	110.43
5	B	1403	NAG	C2-N2-C7	3.08	127.03	122.90
5	B	1401	NAG	C1-C2-N2	3.02	115.19	110.43
5	B	1401	NAG	C1-O5-C5	2.89	116.06	112.19
5	I	1401	NAG	C1-O5-C5	2.65	115.73	112.19
5	J	1401	NAG	C1-O5-C5	2.53	115.58	112.19
5	B	1404	NAG	C1-C2-N2	2.47	114.33	110.43
5	F	1406	NAG	C1-O5-C5	2.36	115.35	112.19
5	F	1403	NAG	C8-C7-N2	2.26	119.87	116.12
5	J	1402	NAG	C2-N2-C7	2.16	125.79	122.90
5	F	1404	NAG	C2-N2-C7	2.11	125.73	122.90
5	B	1404	NAG	C1-O5-C5	2.06	114.95	112.19
5	B	1402	NAG	C1-O5-C5	2.06	114.94	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1402	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1402	NAG	O5-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	J	1401	NAG	O5-C5-C6-O6
5	J	1404	NAG	O5-C5-C6-O6
5	J	1404	NAG	C4-C5-C6-O6
5	E	1401	NAG	O5-C5-C6-O6
5	F	1403	NAG	O5-C5-C6-O6
5	I	1401	NAG	O5-C5-C6-O6
5	J	1402	NAG	C4-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	E	1401	NAG	C4-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	B	1405	NAG	C8-C7-N2-C2
5	B	1405	NAG	O7-C7-N2-C2
5	B	1406	NAG	C8-C7-N2-C2
5	B	1406	NAG	O7-C7-N2-C2
5	F	1402	NAG	C8-C7-N2-C2
5	F	1402	NAG	O7-C7-N2-C2
5	F	1403	NAG	C8-C7-N2-C2
5	F	1403	NAG	O7-C7-N2-C2
5	F	1404	NAG	C8-C7-N2-C2
5	F	1404	NAG	O7-C7-N2-C2
5	F	1405	NAG	C8-C7-N2-C2
5	F	1405	NAG	O7-C7-N2-C2
5	I	1401	NAG	C8-C7-N2-C2
5	I	1401	NAG	O7-C7-N2-C2
5	J	1402	NAG	C8-C7-N2-C2
5	J	1402	NAG	O7-C7-N2-C2
5	B	1403	NAG	C4-C5-C6-O6
5	J	1401	NAG	C4-C5-C6-O6
5	J	1406	NAG	O5-C5-C6-O6
5	I	1401	NAG	C4-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	J	1403	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1406	NAG	O5-C5-C6-O6
5	F	1402	NAG	O5-C5-C6-O6
5	F	1406	NAG	O5-C5-C6-O6
5	A	1401	NAG	C1-C2-N2-C7
5	F	1401	NAG	C1-C2-N2-C7
5	F	1404	NAG	C4-C5-C6-O6
5	J	1406	NAG	C4-C5-C6-O6
5	F	1405	NAG	O5-C5-C6-O6
5	F	1403	NAG	C4-C5-C6-O6
5	B	1403	NAG	C3-C2-N2-C7
5	F	1401	NAG	C3-C2-N2-C7
5	F	1403	NAG	C3-C2-N2-C7
5	B	1403	NAG	C1-C2-N2-C7
5	B	1404	NAG	C1-C2-N2-C7
5	F	1403	NAG	C1-C2-N2-C7
5	B	1401	NAG	O7-C7-N2-C2
5	A	1401	NAG	C3-C2-N2-C7
5	B	1404	NAG	C3-C2-N2-C7
5	F	1404	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	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.

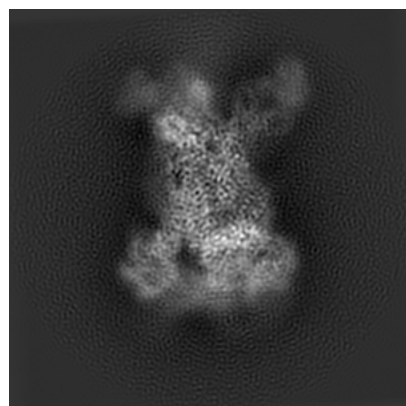
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8784. These allow visual inspection of the internal detail of the map and identification of artifacts.

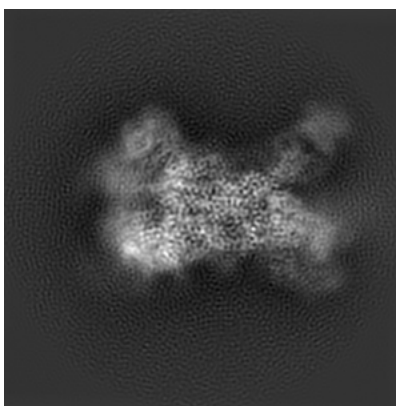
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

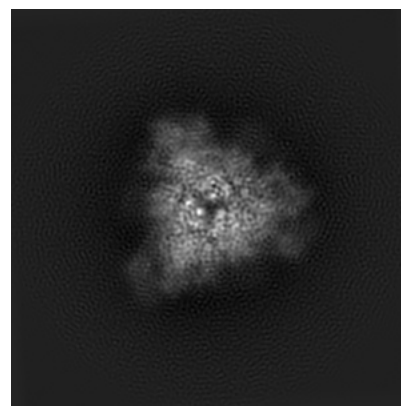
6.1.1 Primary map



X

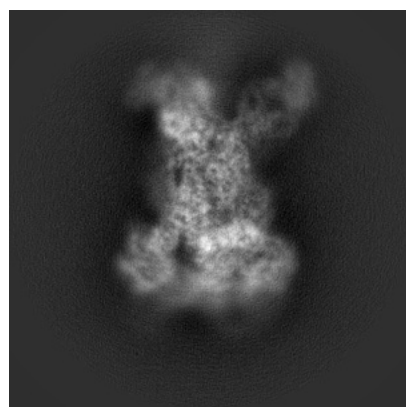


Y

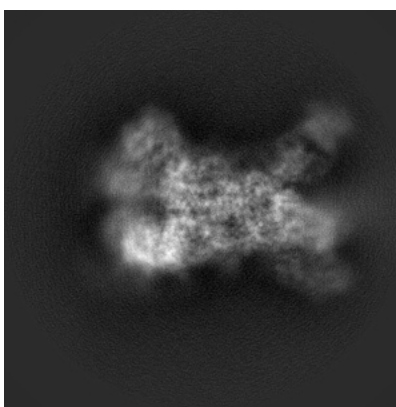


Z

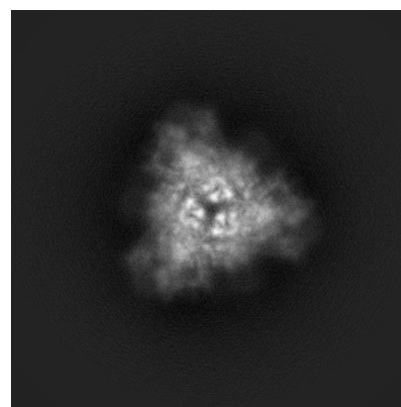
6.1.2 Raw map



X



Y

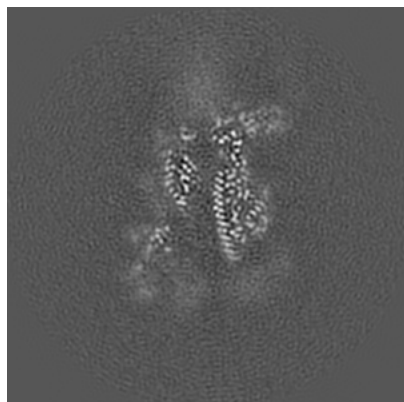


Z

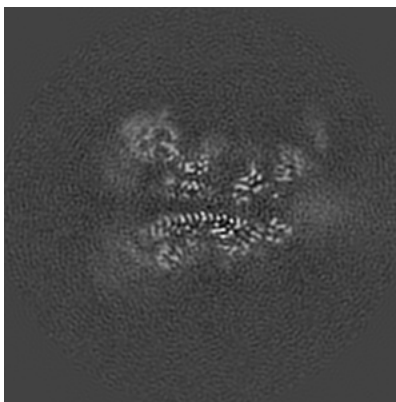
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

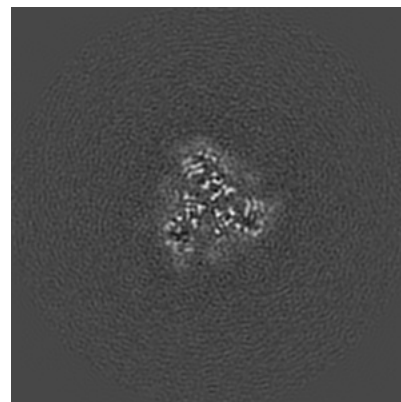
6.2.1 Primary map



X Index: 152

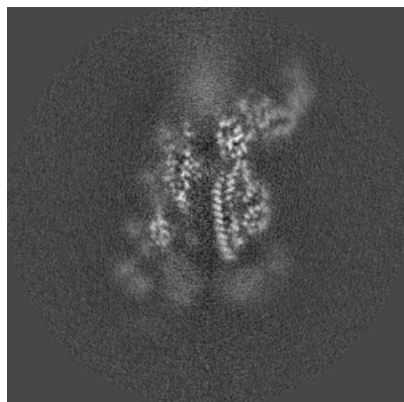


Y Index: 152

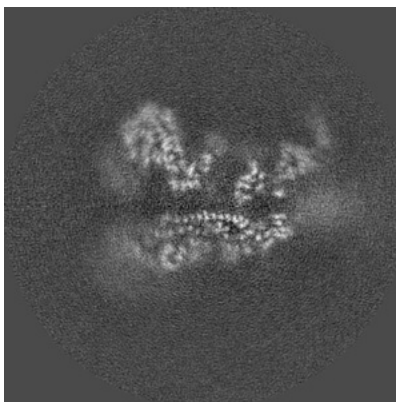


Z Index: 152

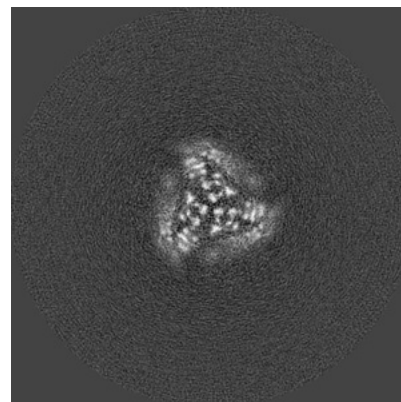
6.2.2 Raw map



X Index: 152



Y Index: 152

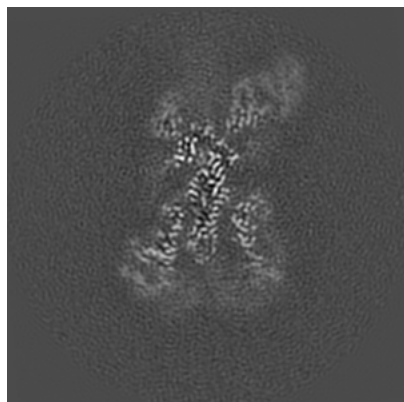


Z Index: 152

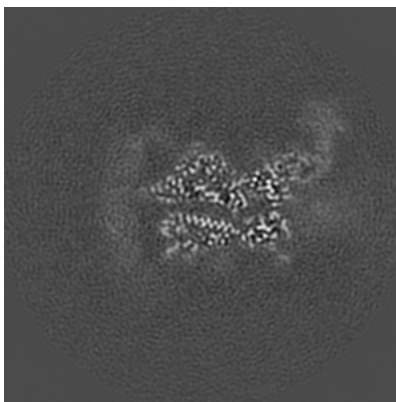
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

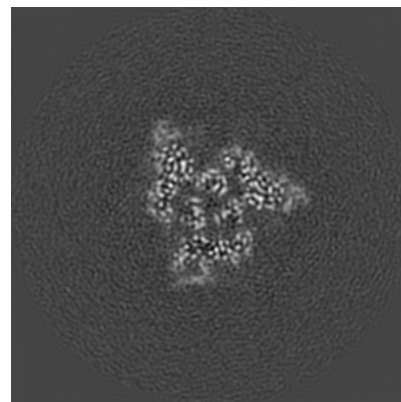
6.3.1 Primary map



X Index: 136

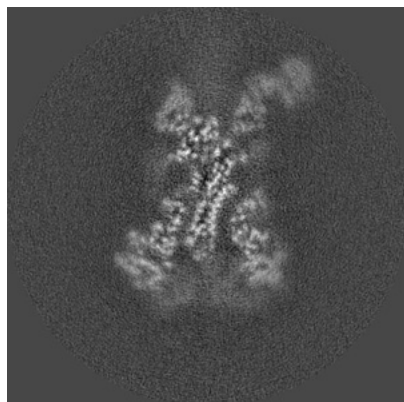


Y Index: 141

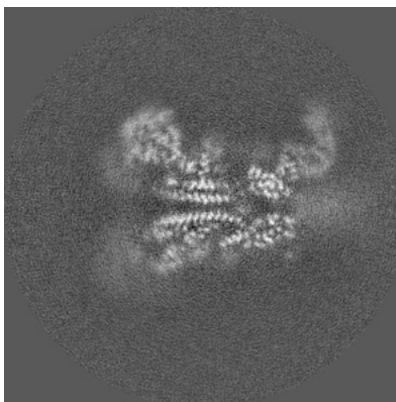


Z Index: 126

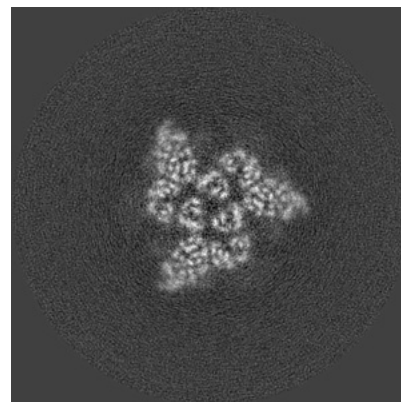
6.3.2 Raw map



X Index: 135



Y Index: 148

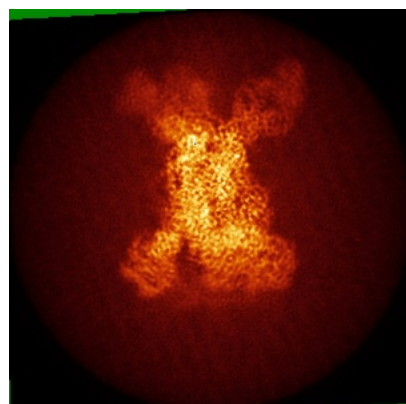


Z Index: 127

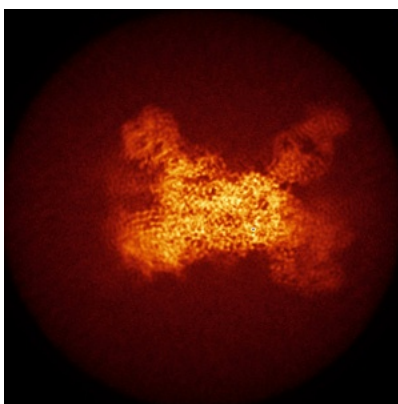
The images above show the largest variance slices of the map in three orthogonal directions.

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

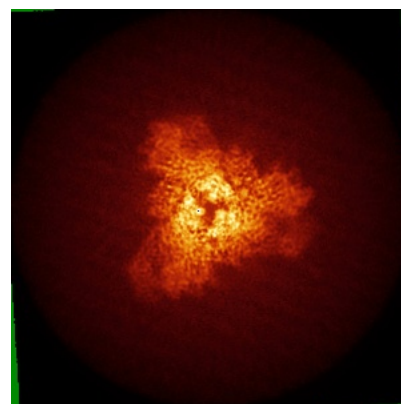
6.4.1 Primary map



X

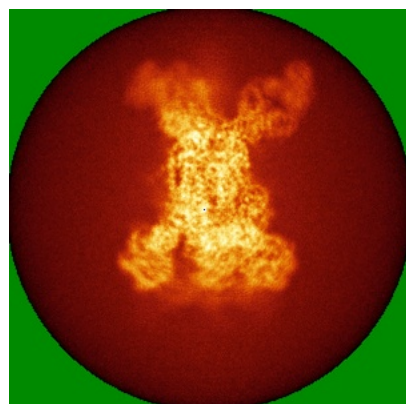


Y

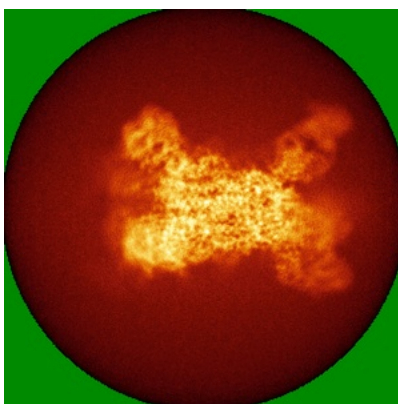


Z

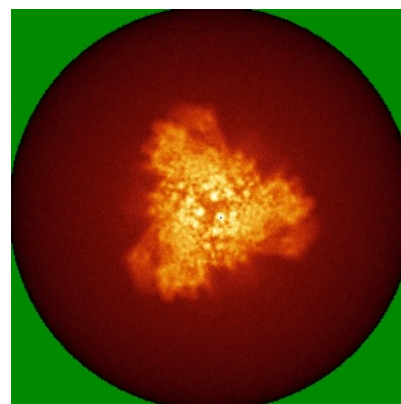
6.4.2 Raw map



X



Y

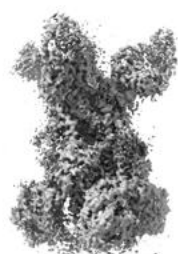


Z

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



X



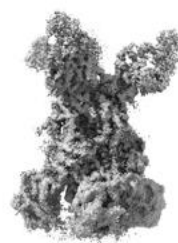
Y



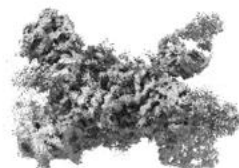
Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

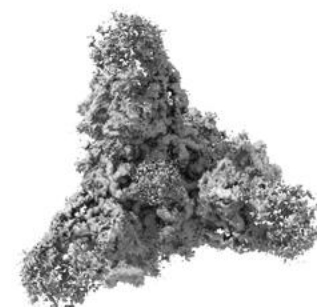
6.5.2 Raw map



X



Y



Z

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.

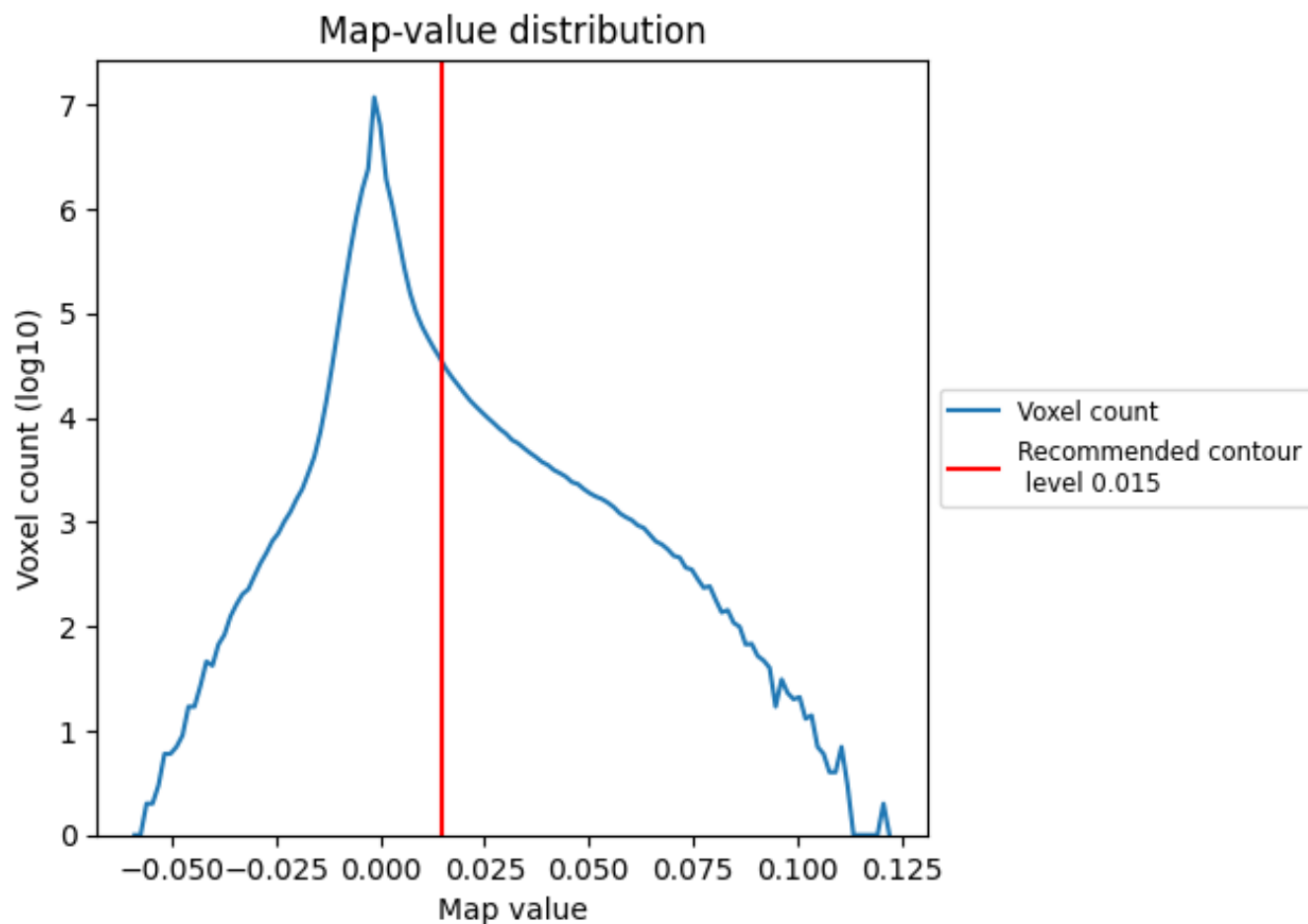
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

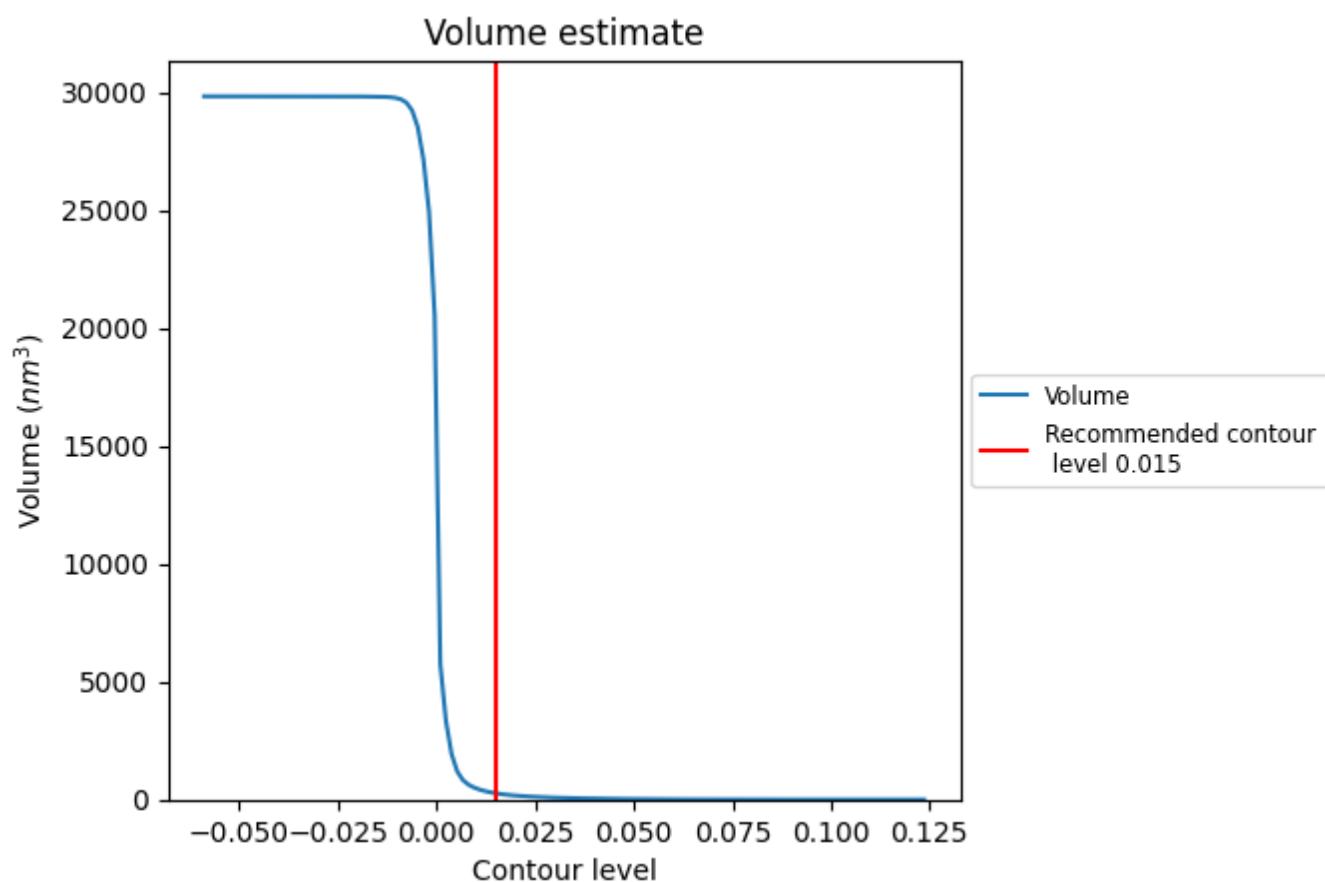
This section contains the results of statistical analysis of the map.

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.

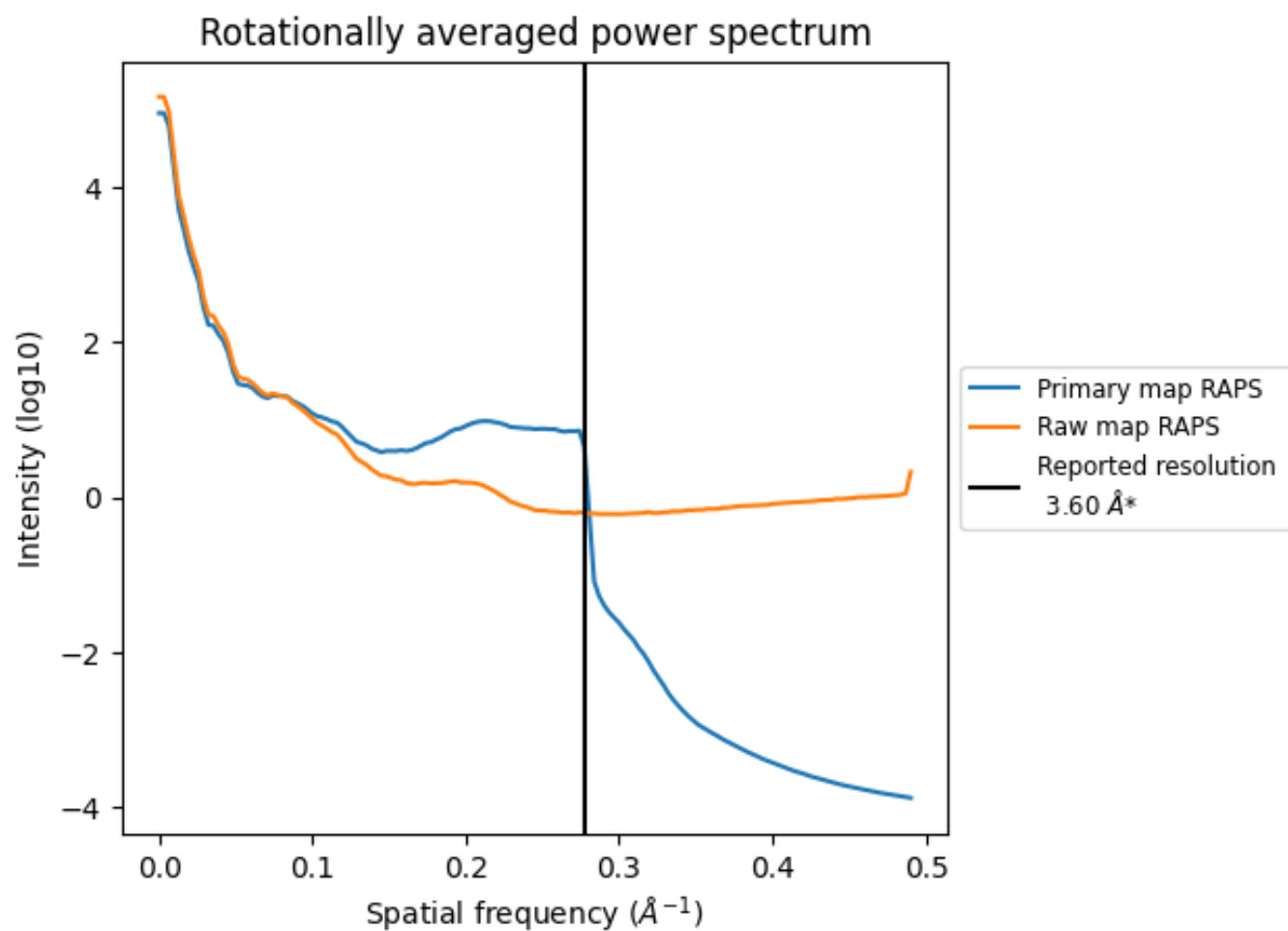
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 266 nm³; this corresponds to an approximate mass of 241 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 ⓘ

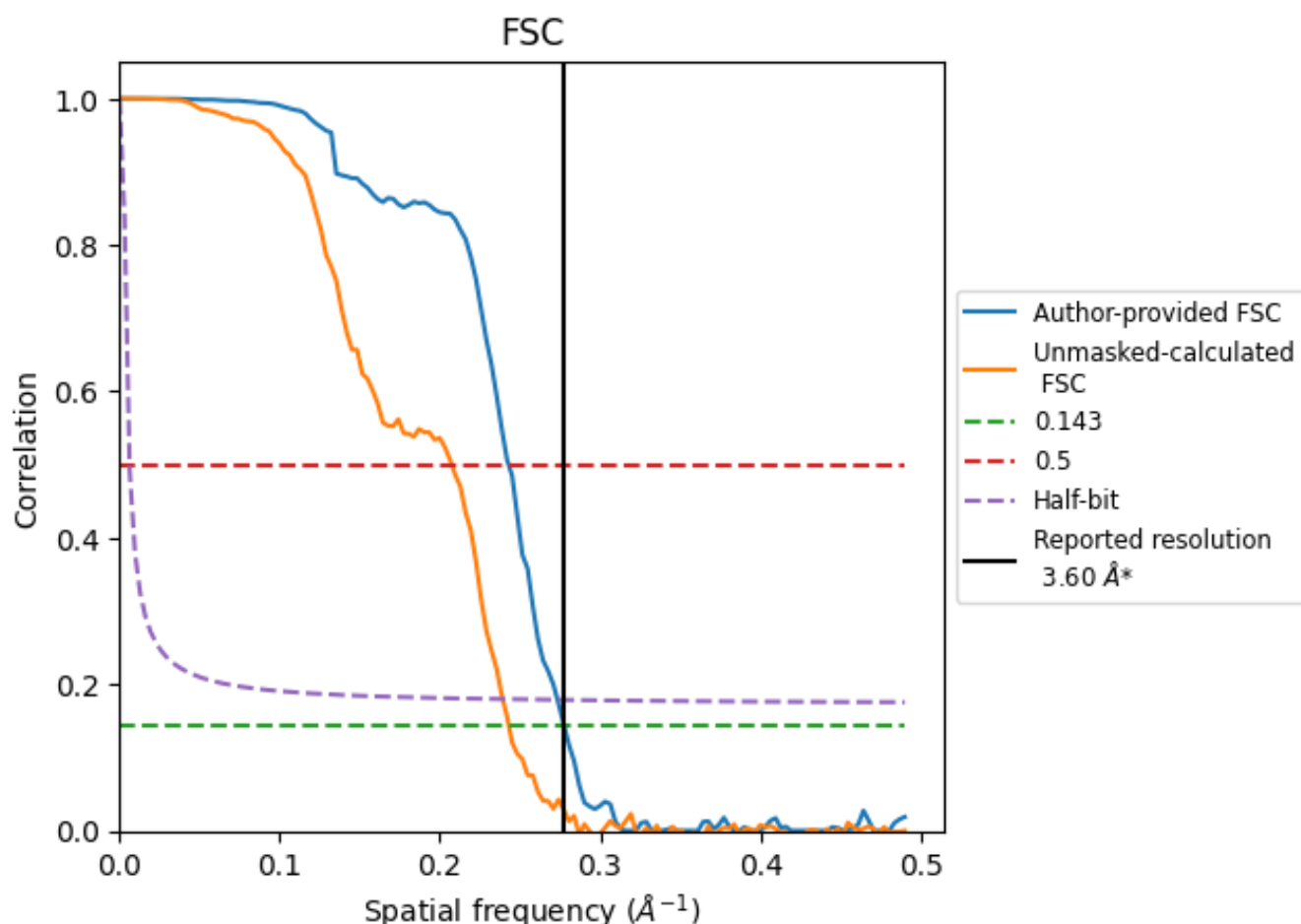


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

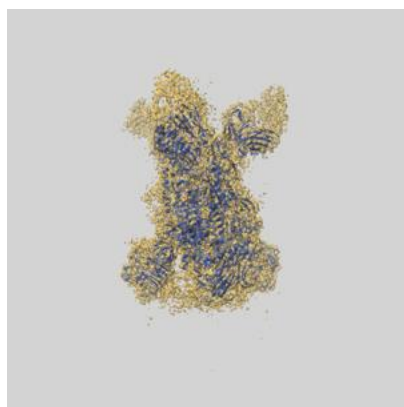
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.12	3.66
Unmasked-calculated*	4.11	4.82	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.11 differs from the reported value 3.6 by more than 10 %

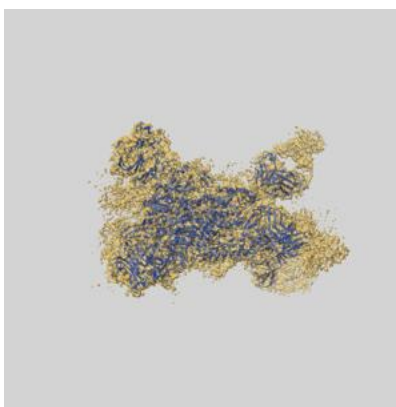
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8784 and PDB model 5W9I. Per-residue inclusion information can be found in section [3](#) on page [14](#).

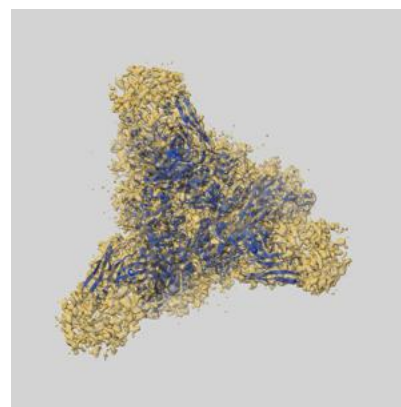
9.1 Map-model overlay [i](#)



X



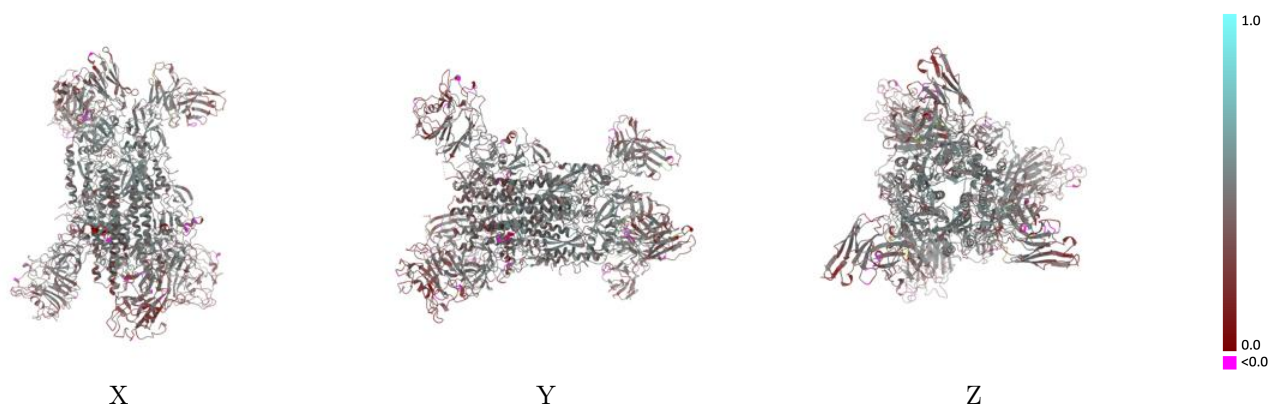
Y



Z

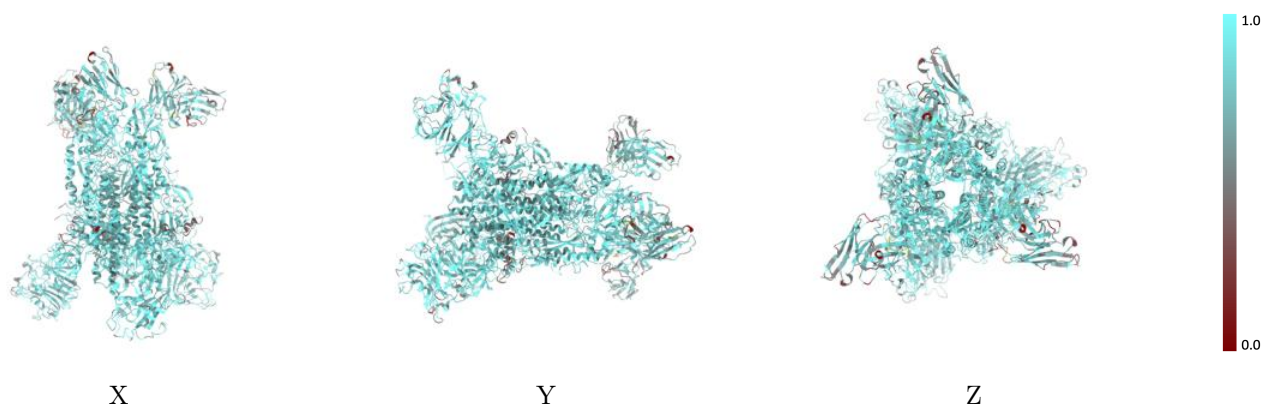
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



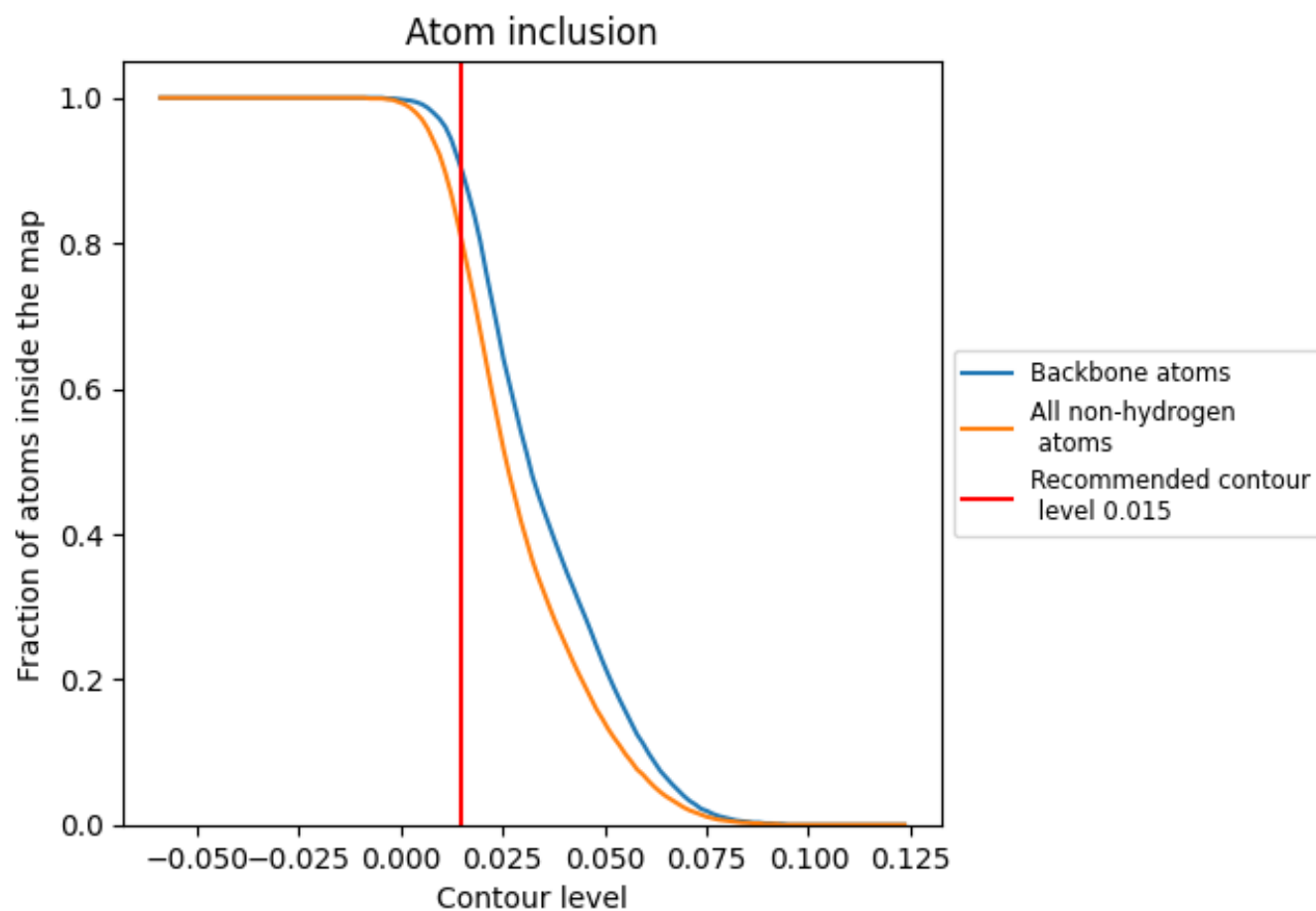
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 80% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8030	 0.4140
A	 0.8450	 0.4580
B	 0.8230	 0.3930
C	 0.7450	 0.4070
D	 0.6300	 0.3480
E	 0.8440	 0.4600
F	 0.8240	 0.3950
G	 0.7400	 0.4010
H	 0.6260	 0.3460
I	 0.8440	 0.4620
J	 0.8230	 0.3930
K	 0.7380	 0.4090
L	 0.6320	 0.3490
M	 0.6430	 0.3210
N	 0.6070	 0.3020
O	 0.7860	 0.4420
P	 0.7860	 0.4600
Q	 0.6070	 0.3100
R	 0.6430	 0.3240
S	 0.8570	 0.3380
T	 0.5710	 0.2840
U	 0.7860	 0.3840
V	 0.6430	 0.3240
W	 0.6790	 0.3760
X	 0.5710	 0.3490
Y	 0.5360	 0.2730
Z	 0.7140	 0.3030
a	 0.7140	 0.4280
b	 0.6070	 0.2610
c	 0.6070	 0.3170
d	 0.7860	 0.4620
e	 0.3210	 0.2230
f	 0.5710	 0.3510
g	 0.8210	 0.3460

