



Full wwPDB EM Validation Report ⓘ

Jul 21, 2025 – 03:09 PM EDT

PDB ID : 9P3I / pdb_00009p3i
EMDB ID : EMD-71241
Title : High-resolution in situ ANDV single tetramer structure
Authors : Luqiang, G.; McLellan, J.S.
Deposited on : 2025-06-13
Resolution : 2.35 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

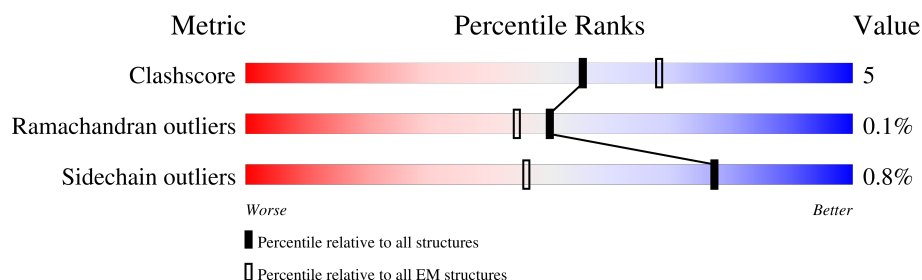
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.35 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.



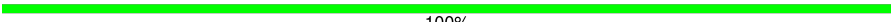
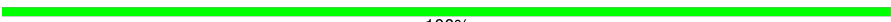








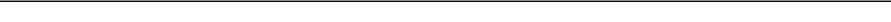

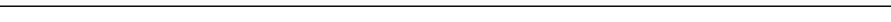


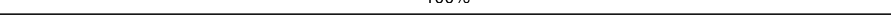
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	651	71% 8% 21%
1	C	651	71% 8% 21%
1	E	651	70% 8% 21%
1	G	651	71% 8% 21%
2	B	537	81% 8% 12%
2	D	537	80% 8% 12%
2	F	537	81% 8% 12%
2	H	537	80% 8% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	5	 100%
3	M	5	 100%
3	Q	5	 100%
3	U	5	 100%
4	J	4	 100%
4	N	4	 100%
4	R	4	 100%
4	V	4	 100%
5	K	4	 50% 50%
5	O	4	 75% 25%
5	S	4	 100%
5	W	4	 75% 25%
6	L	2	 100%
6	P	2	 100%
6	T	2	 100%
6	X	2	 100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 31608 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycoprotein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	516	Total	C	N	O	S	0	0
			3956	2522	649	749	36		
1	C	516	Total	C	N	O	S	0	0
			3956	2522	649	749	36		
1	E	516	Total	C	N	O	S	0	0
			3956	2522	649	749	36		
1	G	516	Total	C	N	O	S	0	0
			3956	2522	649	749	36		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	LYS	VAL	engineered mutation	UNP Q9E006
C	535	LYS	VAL	engineered mutation	UNP Q9E006
E	535	LYS	VAL	engineered mutation	UNP Q9E006
G	535	LYS	VAL	engineered mutation	UNP Q9E006

- Molecule 2 is a protein called Glycoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	475	Total	C	N	O	S	0	0
			3644	2307	604	696	37		
2	D	475	Total	C	N	O	S	0	0
			3644	2307	604	696	37		
2	F	475	Total	C	N	O	S	0	0
			3644	2307	604	696	37		
2	H	475	Total	C	N	O	S	0	0
			3644	2307	604	696	37		

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1096	LEU	SER	engineered mutation	UNP Q9E006

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1139	GLY	-	expression tag	UNP Q9E006
B	1140	SER	-	expression tag	UNP Q9E006
B	1141	LEU	-	expression tag	UNP Q9E006
B	1142	GLU	-	expression tag	UNP Q9E006
B	1143	VAL	-	expression tag	UNP Q9E006
B	1144	LEU	-	expression tag	UNP Q9E006
B	1145	PHE	-	expression tag	UNP Q9E006
B	1146	GLN	-	expression tag	UNP Q9E006
B	1147	GLY	-	expression tag	UNP Q9E006
B	1148	PRO	-	expression tag	UNP Q9E006
B	1149	GLY	-	expression tag	UNP Q9E006
B	1150	HIS	-	expression tag	UNP Q9E006
B	1151	HIS	-	expression tag	UNP Q9E006
B	1152	HIS	-	expression tag	UNP Q9E006
B	1153	HIS	-	expression tag	UNP Q9E006
B	1154	HIS	-	expression tag	UNP Q9E006
B	1155	HIS	-	expression tag	UNP Q9E006
B	1156	HIS	-	expression tag	UNP Q9E006
B	1157	HIS	-	expression tag	UNP Q9E006
B	1158	SER	-	expression tag	UNP Q9E006
B	1159	ALA	-	expression tag	UNP Q9E006
B	1160	TRP	-	expression tag	UNP Q9E006
B	1161	SER	-	expression tag	UNP Q9E006
B	1162	HIS	-	expression tag	UNP Q9E006
B	1163	PRO	-	expression tag	UNP Q9E006
B	1164	GLN	-	expression tag	UNP Q9E006
B	1165	PHE	-	expression tag	UNP Q9E006
B	1166	GLU	-	expression tag	UNP Q9E006
B	1167	LYS	-	expression tag	UNP Q9E006
B	1168	GLY	-	expression tag	UNP Q9E006
B	1169	GLY	-	expression tag	UNP Q9E006
B	1170	GLY	-	expression tag	UNP Q9E006
B	1171	SER	-	expression tag	UNP Q9E006
B	1172	GLY	-	expression tag	UNP Q9E006
B	1173	GLY	-	expression tag	UNP Q9E006
B	1174	GLY	-	expression tag	UNP Q9E006
B	1175	GLY	-	expression tag	UNP Q9E006
B	1176	SER	-	expression tag	UNP Q9E006
B	1177	GLY	-	expression tag	UNP Q9E006
B	1178	GLY	-	expression tag	UNP Q9E006
B	1179	SER	-	expression tag	UNP Q9E006
B	1180	ALA	-	expression tag	UNP Q9E006

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1181	TRP	-	expression tag	UNP Q9E006
B	1182	SER	-	expression tag	UNP Q9E006
B	1183	HIS	-	expression tag	UNP Q9E006
B	1184	PRO	-	expression tag	UNP Q9E006
B	1185	GLN	-	expression tag	UNP Q9E006
B	1186	PHE	-	expression tag	UNP Q9E006
B	1187	GLU	-	expression tag	UNP Q9E006
B	1188	LYS	-	expression tag	UNP Q9E006
D	1096	LEU	SER	engineered mutation	UNP Q9E006
D	1139	GLY	-	expression tag	UNP Q9E006
D	1140	SER	-	expression tag	UNP Q9E006
D	1141	LEU	-	expression tag	UNP Q9E006
D	1142	GLU	-	expression tag	UNP Q9E006
D	1143	VAL	-	expression tag	UNP Q9E006
D	1144	LEU	-	expression tag	UNP Q9E006
D	1145	PHE	-	expression tag	UNP Q9E006
D	1146	GLN	-	expression tag	UNP Q9E006
D	1147	GLY	-	expression tag	UNP Q9E006
D	1148	PRO	-	expression tag	UNP Q9E006
D	1149	GLY	-	expression tag	UNP Q9E006
D	1150	HIS	-	expression tag	UNP Q9E006
D	1151	HIS	-	expression tag	UNP Q9E006
D	1152	HIS	-	expression tag	UNP Q9E006
D	1153	HIS	-	expression tag	UNP Q9E006
D	1154	HIS	-	expression tag	UNP Q9E006
D	1155	HIS	-	expression tag	UNP Q9E006
D	1156	HIS	-	expression tag	UNP Q9E006
D	1157	HIS	-	expression tag	UNP Q9E006
D	1158	SER	-	expression tag	UNP Q9E006
D	1159	ALA	-	expression tag	UNP Q9E006
D	1160	TRP	-	expression tag	UNP Q9E006
D	1161	SER	-	expression tag	UNP Q9E006
D	1162	HIS	-	expression tag	UNP Q9E006
D	1163	PRO	-	expression tag	UNP Q9E006
D	1164	GLN	-	expression tag	UNP Q9E006
D	1165	PHE	-	expression tag	UNP Q9E006
D	1166	GLU	-	expression tag	UNP Q9E006
D	1167	LYS	-	expression tag	UNP Q9E006
D	1168	GLY	-	expression tag	UNP Q9E006
D	1169	GLY	-	expression tag	UNP Q9E006
D	1170	GLY	-	expression tag	UNP Q9E006
D	1171	SER	-	expression tag	UNP Q9E006

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1172	GLY	-	expression tag	UNP Q9E006
D	1173	GLY	-	expression tag	UNP Q9E006
D	1174	GLY	-	expression tag	UNP Q9E006
D	1175	GLY	-	expression tag	UNP Q9E006
D	1176	SER	-	expression tag	UNP Q9E006
D	1177	GLY	-	expression tag	UNP Q9E006
D	1178	GLY	-	expression tag	UNP Q9E006
D	1179	SER	-	expression tag	UNP Q9E006
D	1180	ALA	-	expression tag	UNP Q9E006
D	1181	TRP	-	expression tag	UNP Q9E006
D	1182	SER	-	expression tag	UNP Q9E006
D	1183	HIS	-	expression tag	UNP Q9E006
D	1184	PRO	-	expression tag	UNP Q9E006
D	1185	GLN	-	expression tag	UNP Q9E006
D	1186	PHE	-	expression tag	UNP Q9E006
D	1187	GLU	-	expression tag	UNP Q9E006
D	1188	LYS	-	expression tag	UNP Q9E006
F	1096	LEU	SER	engineered mutation	UNP Q9E006
F	1139	GLY	-	expression tag	UNP Q9E006
F	1140	SER	-	expression tag	UNP Q9E006
F	1141	LEU	-	expression tag	UNP Q9E006
F	1142	GLU	-	expression tag	UNP Q9E006
F	1143	VAL	-	expression tag	UNP Q9E006
F	1144	LEU	-	expression tag	UNP Q9E006
F	1145	PHE	-	expression tag	UNP Q9E006
F	1146	GLN	-	expression tag	UNP Q9E006
F	1147	GLY	-	expression tag	UNP Q9E006
F	1148	PRO	-	expression tag	UNP Q9E006
F	1149	GLY	-	expression tag	UNP Q9E006
F	1150	HIS	-	expression tag	UNP Q9E006
F	1151	HIS	-	expression tag	UNP Q9E006
F	1152	HIS	-	expression tag	UNP Q9E006
F	1153	HIS	-	expression tag	UNP Q9E006
F	1154	HIS	-	expression tag	UNP Q9E006
F	1155	HIS	-	expression tag	UNP Q9E006
F	1156	HIS	-	expression tag	UNP Q9E006
F	1157	HIS	-	expression tag	UNP Q9E006
F	1158	SER	-	expression tag	UNP Q9E006
F	1159	ALA	-	expression tag	UNP Q9E006
F	1160	TRP	-	expression tag	UNP Q9E006
F	1161	SER	-	expression tag	UNP Q9E006
F	1162	HIS	-	expression tag	UNP Q9E006

Continued on next page...

Continued from previous page...

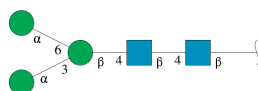
Chain	Residue	Modelled	Actual	Comment	Reference
F	1163	PRO	-	expression tag	UNP Q9E006
F	1164	GLN	-	expression tag	UNP Q9E006
F	1165	PHE	-	expression tag	UNP Q9E006
F	1166	GLU	-	expression tag	UNP Q9E006
F	1167	LYS	-	expression tag	UNP Q9E006
F	1168	GLY	-	expression tag	UNP Q9E006
F	1169	GLY	-	expression tag	UNP Q9E006
F	1170	GLY	-	expression tag	UNP Q9E006
F	1171	SER	-	expression tag	UNP Q9E006
F	1172	GLY	-	expression tag	UNP Q9E006
F	1173	GLY	-	expression tag	UNP Q9E006
F	1174	GLY	-	expression tag	UNP Q9E006
F	1175	GLY	-	expression tag	UNP Q9E006
F	1176	SER	-	expression tag	UNP Q9E006
F	1177	GLY	-	expression tag	UNP Q9E006
F	1178	GLY	-	expression tag	UNP Q9E006
F	1179	SER	-	expression tag	UNP Q9E006
F	1180	ALA	-	expression tag	UNP Q9E006
F	1181	TRP	-	expression tag	UNP Q9E006
F	1182	SER	-	expression tag	UNP Q9E006
F	1183	HIS	-	expression tag	UNP Q9E006
F	1184	PRO	-	expression tag	UNP Q9E006
F	1185	GLN	-	expression tag	UNP Q9E006
F	1186	PHE	-	expression tag	UNP Q9E006
F	1187	GLU	-	expression tag	UNP Q9E006
F	1188	LYS	-	expression tag	UNP Q9E006
H	1096	LEU	SER	engineered mutation	UNP Q9E006
H	1139	GLY	-	expression tag	UNP Q9E006
H	1140	SER	-	expression tag	UNP Q9E006
H	1141	LEU	-	expression tag	UNP Q9E006
H	1142	GLU	-	expression tag	UNP Q9E006
H	1143	VAL	-	expression tag	UNP Q9E006
H	1144	LEU	-	expression tag	UNP Q9E006
H	1145	PHE	-	expression tag	UNP Q9E006
H	1146	GLN	-	expression tag	UNP Q9E006
H	1147	GLY	-	expression tag	UNP Q9E006
H	1148	PRO	-	expression tag	UNP Q9E006
H	1149	GLY	-	expression tag	UNP Q9E006
H	1150	HIS	-	expression tag	UNP Q9E006
H	1151	HIS	-	expression tag	UNP Q9E006
H	1152	HIS	-	expression tag	UNP Q9E006
H	1153	HIS	-	expression tag	UNP Q9E006

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	1154	HIS	-	expression tag	UNP Q9E006
H	1155	HIS	-	expression tag	UNP Q9E006
H	1156	HIS	-	expression tag	UNP Q9E006
H	1157	HIS	-	expression tag	UNP Q9E006
H	1158	SER	-	expression tag	UNP Q9E006
H	1159	ALA	-	expression tag	UNP Q9E006
H	1160	TRP	-	expression tag	UNP Q9E006
H	1161	SER	-	expression tag	UNP Q9E006
H	1162	HIS	-	expression tag	UNP Q9E006
H	1163	PRO	-	expression tag	UNP Q9E006
H	1164	GLN	-	expression tag	UNP Q9E006
H	1165	PHE	-	expression tag	UNP Q9E006
H	1166	GLU	-	expression tag	UNP Q9E006
H	1167	LYS	-	expression tag	UNP Q9E006
H	1168	GLY	-	expression tag	UNP Q9E006
H	1169	GLY	-	expression tag	UNP Q9E006
H	1170	GLY	-	expression tag	UNP Q9E006
H	1171	SER	-	expression tag	UNP Q9E006
H	1172	GLY	-	expression tag	UNP Q9E006
H	1173	GLY	-	expression tag	UNP Q9E006
H	1174	GLY	-	expression tag	UNP Q9E006
H	1175	GLY	-	expression tag	UNP Q9E006
H	1176	SER	-	expression tag	UNP Q9E006
H	1177	GLY	-	expression tag	UNP Q9E006
H	1178	GLY	-	expression tag	UNP Q9E006
H	1179	SER	-	expression tag	UNP Q9E006
H	1180	ALA	-	expression tag	UNP Q9E006
H	1181	TRP	-	expression tag	UNP Q9E006
H	1182	SER	-	expression tag	UNP Q9E006
H	1183	HIS	-	expression tag	UNP Q9E006
H	1184	PRO	-	expression tag	UNP Q9E006
H	1185	GLN	-	expression tag	UNP Q9E006
H	1186	PHE	-	expression tag	UNP Q9E006
H	1187	GLU	-	expression tag	UNP Q9E006
H	1188	LYS	-	expression tag	UNP Q9E006

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	5	Total	C	N	O	0	0
			61	34	2	25		
3	M	5	Total	C	N	O	0	0
			61	34	2	25		
3	Q	5	Total	C	N	O	0	0
			61	34	2	25		
3	U	5	Total	C	N	O	0	0
			61	34	2	25		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	4	Total	C	N	O	0	0
			50	28	2	20		
4	N	4	Total	C	N	O	0	0
			50	28	2	20		
4	R	4	Total	C	N	O	0	0
			50	28	2	20		
4	V	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	4	Total	C	N	O	0	0
			50	28	2	20		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
5	O	4	Total	C	N	O	0	0
			50	28	2	20		
5	S	4	Total	C	N	O	0	0
			50	28	2	20		
5	W	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 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
6	L	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		

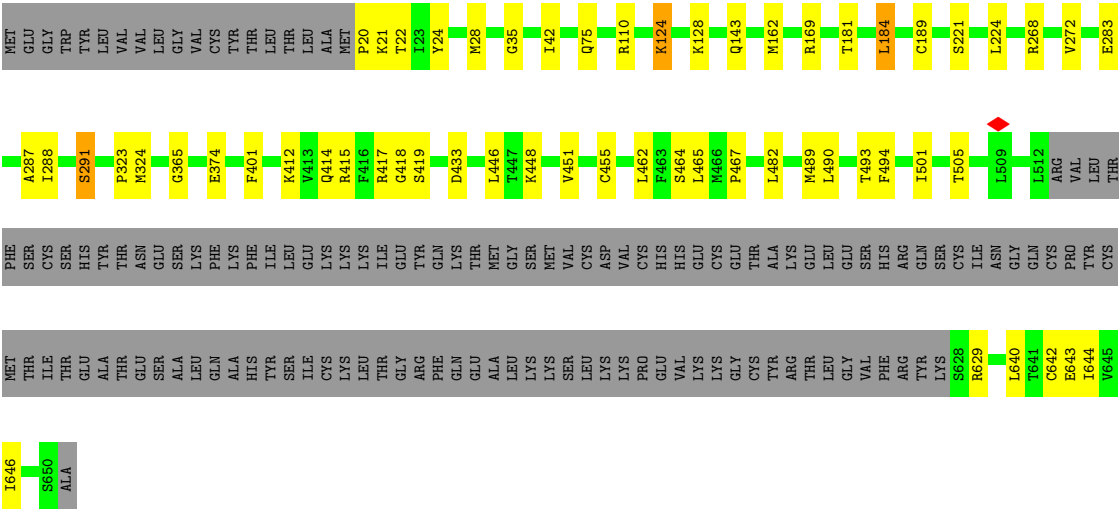
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	72	Total	O	0
			72	72	
7	B	41	Total	O	0
			41	41	
7	C	72	Total	O	0
			72	72	
7	D	41	Total	O	0
			41	41	
7	E	72	Total	O	0
			72	72	
7	F	41	Total	O	0
			41	41	
7	G	72	Total	O	0
			72	72	

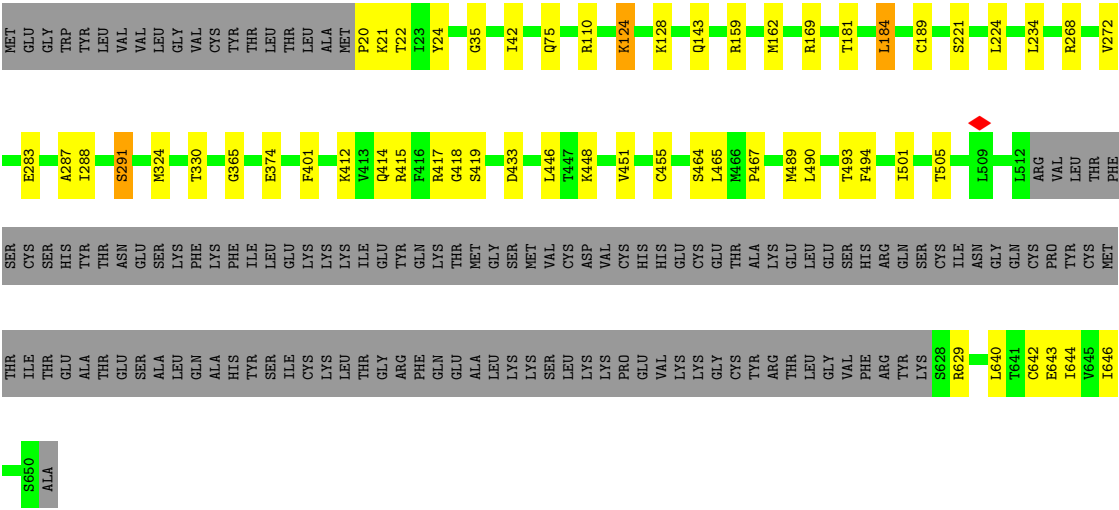
Continued on next page...

Continued from previous page...

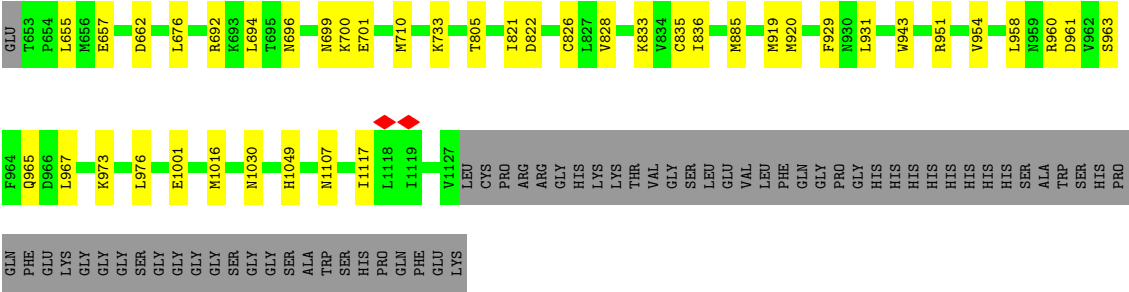
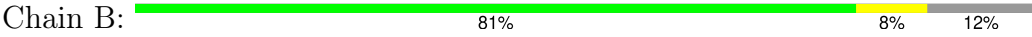
Mol	Chain	Residues	Atoms		AltConf
7	H	41	Total	O	0
			41	41	



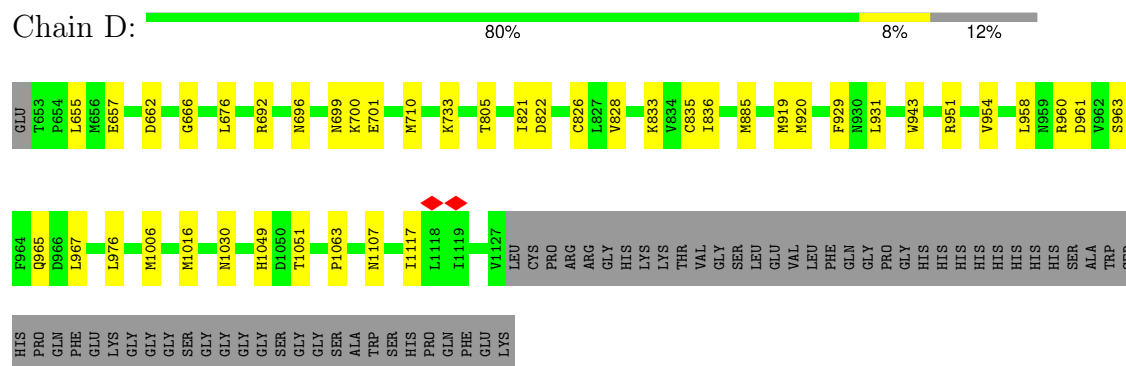
• Molecule 1: Glycoprotein N



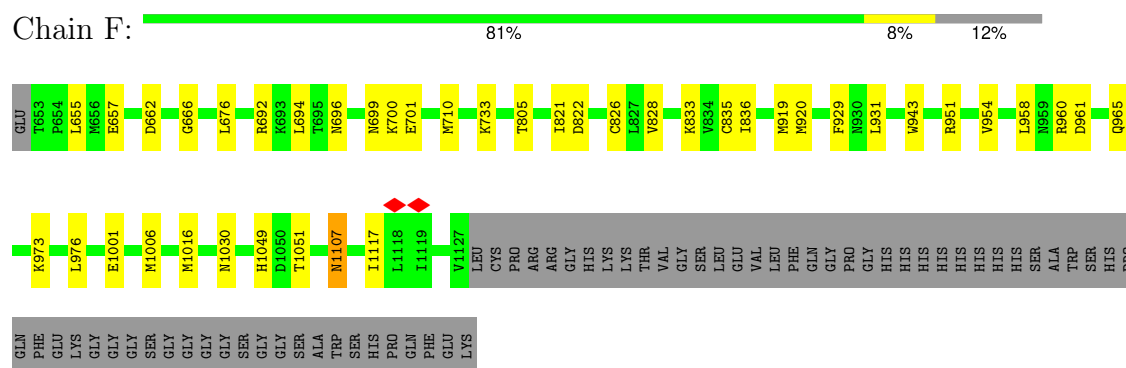
• Molecule 2: Glycoprotein C



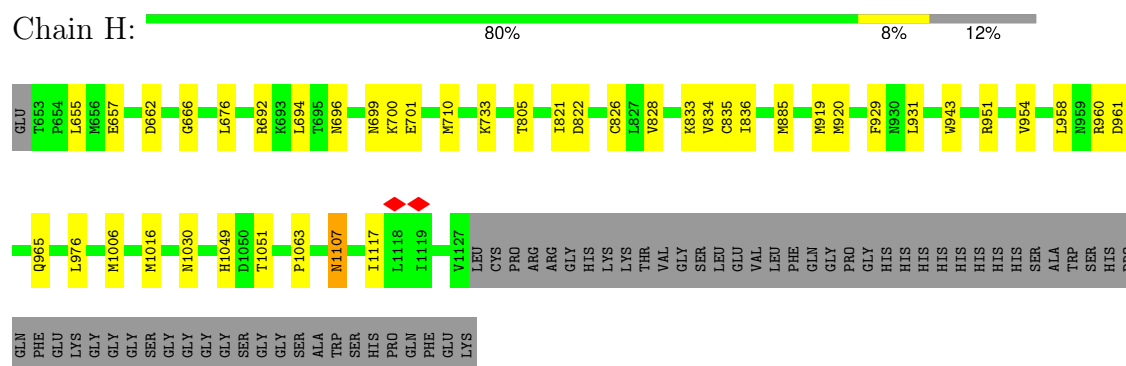
- Molecule 2: Glycoprotein C



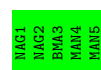
- Molecule 2: Glycoprotein C



- Molecule 2: Glycoprotein C



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



- Molecule 3: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain M:  100%



- Molecule 3: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain Q:  100%



- Molecule 3: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain U:  100%



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

Chain J:  100%



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

Chain N:  100%



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

Chain R:  100%



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

Chain V:  100%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  75% 25%




- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  75% 25%



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

Chain L:  100%



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

Chain P:  100%

MAG1
MAG2

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

Chain T:  100%MAG1
MAG2

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

Chain X:  100%MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	253514	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.190	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	372.73602, 372.73602, 372.73602	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8320001, 0.8320001, 0.8320001	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.27	0/4039	0.38	0/5499
1	C	0.27	0/4039	0.38	0/5499
1	E	0.27	0/4039	0.38	0/5499
1	G	0.27	0/4039	0.38	0/5499
2	B	0.28	0/3734	0.39	0/5070
2	D	0.28	0/3734	0.39	0/5070
2	F	0.28	0/3734	0.39	0/5070
2	H	0.28	0/3734	0.39	0/5070
All	All	0.27	0/31092	0.38	0/42276

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	G	0	1
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	629	ARG	Sidechain
2	B	692	ARG	Sidechain
1	C	629	ARG	Sidechain
2	D	692	ARG	Sidechain
1	E	629	ARG	Sidechain
2	F	692	ARG	Sidechain
1	G	629	ARG	Sidechain
2	H	692	ARG	Sidechain

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	3956	0	3976	46	0
1	C	3956	0	3976	50	0
1	E	3956	0	3976	61	0
1	G	3956	0	3976	48	0
2	B	3644	0	3529	34	0
2	D	3644	0	3529	36	0
2	F	3644	0	3529	29	0
2	H	3644	0	3529	30	0
3	I	61	0	52	0	0
3	M	61	0	52	0	0
3	Q	61	0	52	0	0
3	U	61	0	52	0	0
4	J	50	0	43	0	0
4	N	50	0	43	0	0
4	R	50	0	43	0	0
4	V	50	0	43	0	0
5	K	50	0	43	2	0
5	O	50	0	43	1	0
5	S	50	0	43	0	0
5	W	50	0	43	1	0
6	L	28	0	25	0	0
6	P	28	0	25	0	0
6	T	28	0	25	0	0
6	X	28	0	25	0	0
7	A	72	0	0	5	0
7	B	41	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	72	0	0	5	0
7	D	41	0	0	7	0
7	E	72	0	0	5	0
7	F	41	0	0	7	0
7	G	72	0	0	5	0
7	H	41	0	0	7	0
All	All	31608	0	30672	295	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 (295) 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)
2:D:1107:ASN:ND2	1:E:482:LEU:HD23	1.89	0.88
2:B:1107:ASN:ND2	1:C:482:LEU:HD23	1.92	0.85
1:C:181:THR:HG23	7:C:751:HOH:O	1.78	0.84
1:E:181:THR:HG23	7:E:751:HOH:O	1.78	0.83
1:A:181:THR:HG23	7:A:751:HOH:O	1.78	0.83
1:G:181:THR:HG23	7:G:751:HOH:O	1.78	0.82
1:E:288:ILE:HD12	1:E:323:PRO:HG2	1.62	0.80
1:E:288:ILE:HD12	1:E:323:PRO:CG	2.13	0.79
1:A:181:THR:CG2	7:A:751:HOH:O	2.31	0.78
1:G:181:THR:CG2	7:G:751:HOH:O	2.31	0.78
1:C:181:THR:CG2	7:C:751:HOH:O	2.31	0.77
2:D:1107:ASN:HD21	1:E:482:LEU:CD2	1.98	0.77
1:E:181:THR:CG2	7:E:751:HOH:O	2.31	0.76
1:C:42:ILE:HG22	7:C:737:HOH:O	1.86	0.75
2:B:1107:ASN:HD21	1:C:482:LEU:CD2	2.00	0.75
2:D:1107:ASN:HD21	1:E:482:LEU:HD23	1.52	0.75
1:A:42:ILE:HG22	7:A:737:HOH:O	1.86	0.75
2:B:836:ILE:CD1	7:B:1207:HOH:O	2.35	0.74
1:G:42:ILE:HG22	7:G:737:HOH:O	1.86	0.74
2:D:836:ILE:CD1	7:D:1207:HOH:O	2.35	0.74
1:E:42:ILE:HG22	7:E:737:HOH:O	1.86	0.74
2:D:1107:ASN:OD1	2:D:1107:ASN:O	2.06	0.74
2:H:836:ILE:CD1	7:H:1207:HOH:O	2.35	0.73
2:B:1107:ASN:OD1	2:B:1107:ASN:O	2.06	0.73
1:E:288:ILE:CD1	1:E:323:PRO:HG2	2.19	0.73
2:B:1107:ASN:HD21	1:C:482:LEU:HD23	1.54	0.72
2:F:836:ILE:CD1	7:F:1207:HOH:O	2.35	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1240:HOH:O	1:C:20:PRO:CG	2.38	0.71
1:E:288:ILE:HD12	1:E:323:PRO:HD2	1.72	0.71
2:D:1107:ASN:ND2	1:E:482:LEU:CD2	2.53	0.71
1:A:20:PRO:CG	7:H:1240:HOH:O	2.38	0.71
7:F:1240:HOH:O	1:G:20:PRO:CG	2.38	0.71
7:D:1240:HOH:O	1:E:20:PRO:CG	2.38	0.71
2:B:1107:ASN:ND2	1:C:482:LEU:CD2	2.55	0.69
1:E:288:ILE:HD12	1:E:323:PRO:CD	2.24	0.68
2:F:821:ILE:HD12	2:F:835:CYS:HA	1.76	0.68
2:D:821:ILE:HD12	2:D:835:CYS:HA	1.76	0.67
2:B:821:ILE:HD12	2:B:835:CYS:HA	1.76	0.67
2:H:821:ILE:HD12	2:H:835:CYS:HA	1.76	0.67
2:F:836:ILE:HD13	7:F:1207:HOH:O	1.95	0.65
2:H:836:ILE:HD13	7:H:1207:HOH:O	1.95	0.65
2:B:836:ILE:HD13	7:B:1207:HOH:O	1.95	0.64
2:D:836:ILE:HD13	7:D:1207:HOH:O	1.95	0.64
1:C:75:GLN:HG2	1:C:110:ARG:HB2	1.81	0.63
7:D:1231:HOH:O	1:E:20:PRO:HD2	1.99	0.63
1:A:75:GLN:HG2	1:A:110:ARG:HB2	1.81	0.63
7:F:1208:HOH:O	1:G:162:MET:HE2	2.00	0.62
1:E:75:GLN:HG2	1:E:110:ARG:HB2	1.81	0.62
7:F:1231:HOH:O	1:G:20:PRO:HD2	1.99	0.62
1:G:489:MET:O	1:G:493:THR:HG23	2.00	0.62
7:D:1208:HOH:O	1:E:162:MET:HE2	1.99	0.62
1:E:489:MET:O	1:E:493:THR:HG23	2.00	0.62
1:G:75:GLN:HG2	1:G:110:ARG:HB2	1.81	0.62
1:A:189:CYS:HB2	1:A:374:GLU:HB2	1.82	0.62
7:B:1231:HOH:O	1:C:20:PRO:HD2	1.99	0.62
1:A:35:GLY:HA2	1:A:417:ARG:HH21	1.65	0.61
1:C:489:MET:O	1:C:493:THR:HG23	2.00	0.61
1:G:189:CYS:HB2	1:G:374:GLU:HB2	1.82	0.61
1:A:20:PRO:HD2	7:H:1231:HOH:O	2.00	0.61
1:C:189:CYS:HB2	1:C:374:GLU:HB2	1.82	0.61
1:G:35:GLY:HA2	1:G:417:ARG:HH21	1.65	0.61
1:E:401:PHE:HB3	1:E:415:ARG:HG2	1.83	0.61
1:G:401:PHE:HB3	1:G:415:ARG:HG2	1.83	0.61
1:A:489:MET:O	1:A:493:THR:HG23	2.00	0.61
1:A:162:MET:HE2	7:H:1208:HOH:O	2.01	0.60
1:C:401:PHE:HB3	1:C:415:ARG:HG2	1.83	0.60
1:A:401:PHE:HB3	1:A:415:ARG:HG2	1.83	0.60
1:C:35:GLY:HA2	1:C:417:ARG:HH21	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:CYS:HB2	1:E:374:GLU:HB2	1.82	0.60
7:B:1208:HOH:O	1:C:162:MET:HE2	2.01	0.60
1:E:35:GLY:HA2	1:E:417:ARG:HH21	1.65	0.60
1:C:128:LYS:NZ	7:C:702:HOH:O	2.36	0.58
2:B:805:THR:HG22	2:B:822:ASP:HB3	1.86	0.58
2:F:805:THR:HG22	2:F:822:ASP:HB3	1.86	0.58
2:D:805:THR:HG22	2:D:822:ASP:HB3	1.86	0.58
2:H:805:THR:HG22	2:H:822:ASP:HB3	1.86	0.57
2:D:710:MET:HE1	2:D:954:VAL:HG21	1.89	0.55
1:E:128:LYS:NZ	7:E:702:HOH:O	2.36	0.55
2:H:710:MET:HE1	2:H:954:VAL:HG21	1.89	0.55
2:F:710:MET:HE1	2:F:954:VAL:HG21	1.89	0.55
1:A:128:LYS:NZ	7:A:702:HOH:O	2.36	0.54
2:B:710:MET:HE1	2:B:954:VAL:HG21	1.89	0.54
1:A:417:ARG:HD3	1:A:418:GLY:H	1.73	0.54
1:C:417:ARG:HD3	1:C:418:GLY:H	1.72	0.54
1:A:642:CYS:O	1:A:646:ILE:HD12	2.08	0.54
1:C:642:CYS:O	1:C:646:ILE:HD12	2.08	0.54
1:E:642:CYS:O	1:E:646:ILE:HD12	2.08	0.53
1:G:417:ARG:HD3	1:G:418:GLY:H	1.73	0.53
1:G:128:LYS:NZ	7:G:702:HOH:O	2.36	0.53
1:G:642:CYS:O	1:G:646:ILE:HD12	2.08	0.53
1:E:417:ARG:HD3	1:E:418:GLY:H	1.73	0.53
1:A:22:THR:HG21	1:A:24:TYR:CZ	2.45	0.52
2:D:1117:ILE:HD11	1:E:642:CYS:HB2	1.91	0.52
7:F:1231:HOH:O	1:G:20:PRO:CD	2.56	0.52
1:E:22:THR:HG21	1:E:24:TYR:CZ	2.45	0.52
2:B:676:LEU:HB3	2:B:958:LEU:HB3	1.92	0.52
7:B:1231:HOH:O	1:C:20:PRO:CD	2.56	0.52
1:G:324:MET:HE1	2:H:733:LYS:HZ3	1.75	0.52
7:B:1240:HOH:O	1:C:20:PRO:HG2	2.08	0.52
7:D:1231:HOH:O	1:E:20:PRO:CD	2.56	0.52
1:E:324:MET:HE1	2:F:733:LYS:HZ3	1.75	0.52
1:G:283:GLU:HB2	1:G:365:GLY:HA2	1.92	0.52
1:A:283:GLU:HB2	1:A:365:GLY:HA2	1.92	0.51
2:D:676:LEU:HB3	2:D:958:LEU:HB3	1.92	0.51
1:G:22:THR:HG21	1:G:24:TYR:CZ	2.45	0.51
1:A:642:CYS:HB2	2:H:1117:ILE:HD11	1.92	0.51
2:D:1117:ILE:CD1	1:E:642:CYS:HB2	2.41	0.51
1:E:283:GLU:HB2	1:E:365:GLY:HA2	1.92	0.51
2:H:676:LEU:HB3	2:H:958:LEU:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LYS:HG3	1:G:467:PRO:HB2	1.93	0.51
1:A:20:PRO:CD	7:H:1231:HOH:O	2.57	0.50
2:F:676:LEU:HB3	2:F:958:LEU:HB3	1.92	0.50
1:C:283:GLU:HB2	1:C:365:GLY:HA2	1.92	0.50
1:A:642:CYS:HB2	2:H:1117:ILE:CD1	2.41	0.50
2:F:1117:ILE:CD1	1:G:642:CYS:HB2	2.42	0.50
2:F:1117:ILE:HD11	1:G:642:CYS:HB2	1.93	0.50
1:E:467:PRO:HB2	1:G:448:LYS:HG3	1.94	0.50
2:F:828:VAL:HG22	2:F:833:LYS:HG3	1.94	0.50
1:A:20:PRO:HB3	1:A:169:ARG:HG3	1.94	0.49
1:E:143:GLN:NE2	1:E:288:ILE:HG23	2.26	0.49
1:A:467:PRO:HB2	1:C:448:LYS:HG3	1.94	0.49
1:G:124:LYS:NZ	1:G:128:LYS:HG3	2.27	0.49
2:B:655:LEU:HD13	2:B:951:ARG:HD2	1.95	0.49
1:E:124:LYS:NZ	1:E:128:LYS:HG3	2.27	0.49
1:A:124:LYS:NZ	1:A:128:LYS:HG3	2.27	0.49
2:H:655:LEU:HD13	2:H:951:ARG:HD2	1.95	0.49
1:C:124:LYS:NZ	1:C:128:LYS:HG3	2.27	0.49
1:C:324:MET:HE1	2:D:733:LYS:HZ3	1.77	0.49
2:D:655:LEU:HD13	2:D:951:ARG:HD2	1.95	0.49
2:B:1117:ILE:HD11	1:C:642:CYS:HB2	1.94	0.49
1:G:20:PRO:HB3	1:G:169:ARG:HG3	1.94	0.49
1:C:467:PRO:HB2	1:E:448:LYS:HG3	1.94	0.49
1:G:490:LEU:HD11	1:G:644:ILE:HG12	1.94	0.49
1:A:490:LEU:HD11	1:A:644:ILE:HG12	1.94	0.49
2:B:828:VAL:HG22	2:B:833:LYS:HG3	1.94	0.49
1:C:20:PRO:HB3	1:C:169:ARG:HG3	1.94	0.48
1:A:412:LYS:HB2	1:A:412:LYS:HE2	1.59	0.48
2:F:655:LEU:HD13	2:F:951:ARG:HD2	1.95	0.48
1:C:490:LEU:HD11	1:C:644:ILE:HG12	1.94	0.48
1:E:490:LEU:HD11	1:E:644:ILE:HG12	1.94	0.48
2:D:828:VAL:HG22	2:D:833:LYS:HG3	1.94	0.48
7:D:1240:HOH:O	1:E:20:PRO:HG2	2.08	0.48
1:A:414:GLN:HE22	1:A:419:SER:HA	1.78	0.48
2:H:828:VAL:HG22	2:H:833:LYS:HG3	1.94	0.48
1:A:324:MET:HE1	2:B:733:LYS:HZ3	1.78	0.48
2:B:1117:ILE:CD1	1:C:642:CYS:HB2	2.43	0.48
1:E:221:SER:HB3	1:E:224:LEU:HD12	1.96	0.48
1:C:414:GLN:HE22	1:C:419:SER:HA	1.78	0.48
2:D:826:CYS:HA	2:D:835:CYS:HB3	1.96	0.48
1:E:20:PRO:HB3	1:E:169:ARG:HG3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:GLN:HE22	1:E:419:SER:HA	1.78	0.48
1:A:20:PRO:HG2	7:H:1240:HOH:O	2.08	0.47
2:B:826:CYS:HA	2:B:835:CYS:HB3	1.96	0.47
1:C:412:LYS:HB2	1:C:412:LYS:HE2	1.59	0.47
1:G:221:SER:HB3	1:G:224:LEU:HD12	1.96	0.47
1:G:181:THR:HG22	7:G:751:HOH:O	2.08	0.47
1:E:288:ILE:HG13	1:E:323:PRO:O	2.15	0.47
7:F:1240:HOH:O	1:G:20:PRO:HG2	2.08	0.47
1:G:414:GLN:HE22	1:G:419:SER:HA	1.78	0.47
2:B:976:LEU:HD11	2:B:1049:HIS:HB3	1.97	0.47
2:D:976:LEU:HD11	2:D:1049:HIS:HB3	1.97	0.47
2:F:976:LEU:HD11	2:F:1049:HIS:HB3	1.96	0.47
1:G:412:LYS:HB2	1:G:412:LYS:HE2	1.59	0.47
2:H:826:CYS:HA	2:H:835:CYS:HB3	1.96	0.47
2:B:657:GLU:OE2	2:B:657:GLU:N	2.49	0.46
2:B:885:MET:HE2	2:B:885:MET:HB2	1.83	0.46
1:C:433:ASP:OD2	1:C:446:LEU:HD22	2.16	0.46
2:H:976:LEU:HD11	2:H:1049:HIS:HB3	1.97	0.46
2:D:657:GLU:N	2:D:657:GLU:OE2	2.49	0.46
2:F:826:CYS:HA	2:F:835:CYS:HB3	1.96	0.46
1:A:221:SER:HB3	1:A:224:LEU:HD12	1.96	0.46
1:C:221:SER:HB3	1:C:224:LEU:HD12	1.96	0.46
2:F:1107:ASN:O	2:F:1107:ASN:ND2	2.35	0.46
2:D:885:MET:HE2	2:D:885:MET:HB2	1.83	0.46
1:E:433:ASP:OD2	1:E:446:LEU:HD22	2.16	0.46
2:H:1107:ASN:O	2:H:1107:ASN:ND2	2.35	0.46
1:A:28:MET:HE3	1:A:28:MET:HB3	1.89	0.46
1:C:181:THR:HG22	7:C:751:HOH:O	2.08	0.46
2:D:1107:ASN:HD21	1:E:482:LEU:HD22	1.76	0.45
2:B:1107:ASN:HD21	1:C:482:LEU:HD22	1.77	0.45
1:A:181:THR:HG22	7:A:751:HOH:O	2.08	0.45
1:C:467:PRO:HA	1:E:451:VAL:HG11	1.98	0.45
1:G:184:LEU:HD23	1:G:184:LEU:HA	1.79	0.45
1:G:433:ASP:OD2	1:G:446:LEU:HD22	2.16	0.45
1:C:324:MET:HE1	2:D:733:LYS:NZ	2.32	0.45
1:A:433:ASP:OD2	1:A:446:LEU:HD22	2.16	0.45
2:H:657:GLU:N	2:H:657:GLU:OE2	2.49	0.45
1:E:324:MET:HE1	2:F:733:LYS:NZ	2.32	0.45
1:A:21:LYS:HD3	1:A:21:LYS:HA	1.74	0.45
1:A:324:MET:HE1	2:B:733:LYS:NZ	2.32	0.44
1:C:21:LYS:HA	1:C:21:LYS:HD3	1.74	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.79	0.44
2:H:965:GLN:CD	2:H:965:GLN:N	2.75	0.44
1:E:181:THR:HG22	7:E:751:HOH:O	2.08	0.44
2:D:965:GLN:N	2:D:965:GLN:CD	2.75	0.44
1:C:640:LEU:HD23	1:C:640:LEU:HA	1.83	0.44
2:F:965:GLN:N	2:F:965:GLN:CD	2.75	0.44
2:B:965:GLN:N	2:B:965:GLN:CD	2.75	0.44
2:D:1006:MET:HE3	2:D:1006:MET:HB3	1.81	0.44
1:G:465:LEU:HD23	1:G:465:LEU:HA	1.84	0.44
2:F:929:PHE:HE2	2:F:931:LEU:HD21	1.82	0.44
1:G:324:MET:HE1	2:H:733:LYS:NZ	2.32	0.44
1:A:464:SER:HB2	1:C:455:CYS:HB2	2.00	0.43
2:D:931:LEU:HD22	2:D:943:TRP:CG	2.53	0.43
1:G:643:GLU:HA	1:G:646:ILE:HD12	2.01	0.43
2:H:700:LYS:NZ	2:H:700:LYS:HB3	2.33	0.43
1:A:643:GLU:HA	1:A:646:ILE:HD12	2.01	0.43
2:F:657:GLU:N	2:F:657:GLU:OE2	2.49	0.43
2:F:700:LYS:NZ	2:F:700:LYS:HB3	2.33	0.43
1:A:451:VAL:HG11	1:G:467:PRO:HA	1.99	0.43
2:B:662:ASP:HB3	2:B:1016:MET:HE3	2.01	0.43
1:G:21:LYS:HA	1:G:21:LYS:HD3	1.74	0.43
2:H:662:ASP:HB3	2:H:1016:MET:HE3	2.01	0.43
2:H:885:MET:HB2	2:H:885:MET:HE2	1.84	0.43
2:B:700:LYS:NZ	2:B:700:LYS:HB3	2.33	0.43
1:C:234:LEU:HD23	1:C:234:LEU:HA	1.88	0.43
2:D:662:ASP:HB3	2:D:1016:MET:HE3	2.01	0.43
2:H:929:PHE:HE2	2:H:931:LEU:HD21	1.82	0.43
2:B:931:LEU:HD22	2:B:943:TRP:CG	2.53	0.43
1:E:21:LYS:HA	1:E:21:LYS:HD3	1.74	0.43
2:D:929:PHE:HE2	2:D:931:LEU:HD21	1.82	0.43
2:B:929:PHE:HE2	2:B:931:LEU:HD21	1.82	0.42
1:E:184:LEU:HD23	1:E:184:LEU:HA	1.79	0.42
2:F:662:ASP:HB3	2:F:1016:MET:HE3	2.01	0.42
1:E:643:GLU:HA	1:E:646:ILE:HD12	2.01	0.42
2:F:931:LEU:HD22	2:F:943:TRP:CG	2.53	0.42
2:H:931:LEU:HD22	2:H:943:TRP:CG	2.53	0.42
1:A:268:ARG:O	1:A:272:VAL:HG23	2.20	0.42
2:B:960:ARG:HH22	2:B:961:ASP:HB3	1.85	0.42
1:E:465:LEU:HD23	1:E:465:LEU:HA	1.84	0.42
1:E:467:PRO:HA	1:G:451:VAL:HG11	2.00	0.42
1:G:494:PHE:HD1	1:G:640:LEU:HD11	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1006:MET:HE3	2:H:1006:MET:HB3	1.81	0.42
1:C:643:GLU:HA	1:C:646:ILE:HD12	2.01	0.42
1:C:268:ARG:O	1:C:272:VAL:HG23	2.20	0.42
2:D:1063:PRO:HB2	1:E:446:LEU:HD11	2.01	0.42
2:F:1006:MET:HE3	2:F:1006:MET:HB3	1.81	0.42
1:G:234:LEU:HD23	1:G:234:LEU:HA	1.88	0.42
1:G:268:ARG:O	1:G:272:VAL:HG23	2.20	0.42
2:H:960:ARG:HH22	2:H:961:ASP:HB3	1.85	0.42
5:K:1:NAG:H83	5:K:1:NAG:H2	1.94	0.42
1:A:494:PHE:HD1	1:A:640:LEU:HD11	1.85	0.42
2:D:960:ARG:HH22	2:D:961:ASP:HB3	1.85	0.42
1:C:465:LEU:HD23	1:C:465:LEU:HA	1.84	0.42
1:E:22:THR:CG2	1:E:24:TYR:CZ	3.03	0.42
1:E:412:LYS:HB2	1:E:412:LYS:HE2	1.59	0.42
1:G:22:THR:CG2	1:G:24:TYR:CZ	3.03	0.42
2:D:696:ASN:HB3	2:D:699:ASN:O	2.20	0.42
1:E:501:ILE:O	1:E:505:THR:HG23	2.20	0.42
1:G:640:LEU:HD23	1:G:640:LEU:HA	1.83	0.42
2:F:696:ASN:HB3	2:F:699:ASN:O	2.20	0.42
1:A:446:LEU:HD11	2:H:1063:PRO:HB2	2.02	0.41
2:D:700:LYS:NZ	2:D:700:LYS:HB3	2.33	0.41
2:H:929:PHE:CE2	2:H:931:LEU:HD21	2.55	0.41
2:B:696:ASN:HB3	2:B:699:ASN:O	2.20	0.41
2:H:696:ASN:HB3	2:H:699:ASN:O	2.19	0.41
1:A:22:THR:CG2	1:A:24:TYR:CZ	3.03	0.41
1:A:501:ILE:O	1:A:505:THR:HG23	2.20	0.41
2:D:929:PHE:CE2	2:D:931:LEU:HD21	2.55	0.41
1:E:268:ARG:O	1:E:272:VAL:HG23	2.20	0.41
1:E:464:SER:HB2	1:G:455:CYS:HB2	2.01	0.41
1:E:640:LEU:HD23	1:E:640:LEU:HA	1.83	0.41
2:F:929:PHE:CE2	2:F:931:LEU:HD21	2.55	0.41
1:A:467:PRO:HA	1:C:451:VAL:HG11	2.02	0.41
2:B:701:GLU:OE2	2:B:701:GLU:N	2.53	0.41
2:B:919:MET:HE2	2:B:920:MET:HE2	2.03	0.41
1:E:494:PHE:HD1	1:E:640:LEU:HD11	1.85	0.41
2:F:919:MET:HE2	2:F:920:MET:HE2	2.03	0.41
1:G:501:ILE:O	1:G:505:THR:HG23	2.20	0.41
2:F:960:ARG:HH22	2:F:961:ASP:HB3	1.85	0.41
1:C:333:ARG:HA	1:C:333:ARG:HD3	1.86	0.41
1:C:501:ILE:O	1:C:505:THR:HG23	2.20	0.41
2:D:701:GLU:OE2	2:D:701:GLU:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:963:SER:O	2:D:967:LEU:HD12	2.21	0.41
1:E:28:MET:HE3	1:E:28:MET:HB3	1.89	0.41
1:G:159:ARG:NH1	5:W:2:NAG:O6	2.54	0.41
2:H:919:MET:HE2	2:H:920:MET:HE2	2.03	0.41
2:B:963:SER:O	2:B:967:LEU:HD12	2.21	0.41
2:B:973:LYS:HG3	2:B:1001:GLU:OE1	2.21	0.41
2:D:666:GLY:HA2	2:D:1051:THR:HG22	2.03	0.41
1:E:162:MET:HE3	1:E:162:MET:HB3	1.92	0.41
2:F:666:GLY:HA2	2:F:1051:THR:HG22	2.03	0.41
2:F:701:GLU:N	2:F:701:GLU:OE2	2.54	0.41
2:F:973:LYS:HG3	2:F:1001:GLU:OE1	2.21	0.41
1:G:287:ALA:HB3	1:G:291:SER:O	2.21	0.41
2:H:701:GLU:N	2:H:701:GLU:OE2	2.54	0.41
1:A:455:CYS:HB2	1:G:464:SER:HB2	2.03	0.40
1:C:159:ARG:NH1	5:O:2:NAG:O6	2.54	0.40
1:C:464:SER:HB2	1:E:455:CYS:HB2	2.03	0.40
2:H:666:GLY:HA2	2:H:1051:THR:HG22	2.03	0.40
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.89	0.40
2:B:929:PHE:CE2	2:B:931:LEU:HD21	2.55	0.40
2:D:919:MET:HE2	2:D:920:MET:HE2	2.03	0.40
1:A:159:ARG:NH1	5:K:2:NAG:O6	2.54	0.40
1:E:287:ALA:HB3	1:E:291:SER:O	2.21	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	512/651 (79%)	491 (96%)	20 (4%)	1 (0%)	44	52
1	C	512/651 (79%)	491 (96%)	20 (4%)	1 (0%)	44	52
1	E	512/651 (79%)	492 (96%)	19 (4%)	1 (0%)	44	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	512/651 (79%)	492 (96%)	19 (4%)	1 (0%)	44	52
2	B	473/537 (88%)	462 (98%)	11 (2%)	0	100	100
2	D	473/537 (88%)	462 (98%)	11 (2%)	0	100	100
2	F	473/537 (88%)	462 (98%)	11 (2%)	0	100	100
2	H	473/537 (88%)	462 (98%)	11 (2%)	0	100	100
All	All	3940/4752 (83%)	3814 (97%)	122 (3%)	4 (0%)	50	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	LYS
1	C	124	LYS
1	E	124	LYS
1	G	124	LYS

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	459/580 (79%)	454 (99%)	5 (1%)	70	81
1	C	459/580 (79%)	455 (99%)	4 (1%)	75	85
1	E	459/580 (79%)	456 (99%)	3 (1%)	81	89
1	G	459/580 (79%)	454 (99%)	5 (1%)	70	81
2	B	412/459 (90%)	410 (100%)	2 (0%)	86	93
2	D	412/459 (90%)	411 (100%)	1 (0%)	92	96
2	F	412/459 (90%)	409 (99%)	3 (1%)	81	89
2	H	412/459 (90%)	408 (99%)	4 (1%)	73	84
All	All	3484/4156 (84%)	3457 (99%)	27 (1%)	77	88

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	288	ILE
1	A	291	SER
1	A	330	THR
1	A	462	LEU
2	B	694	LEU
2	B	1030	ASN
1	C	22	THR
1	C	184	LEU
1	C	288	ILE
1	C	291	SER
2	D	1030	ASN
1	E	184	LEU
1	E	291	SER
1	E	462	LEU
2	F	694	LEU
2	F	1030	ASN
2	F	1107	ASN
1	G	143	GLN
1	G	184	LEU
1	G	288	ILE
1	G	291	SER
1	G	330	THR
2	H	694	LEU
2	H	834	VAL
2	H	1030	ASN
2	H	1107	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	38	GLN
1	A	80	GLN
1	A	108	ASN
1	A	424	ASN
2	B	816	GLN
2	B	955	ASN
2	B	959	ASN
2	B	1024	ASN
2	B	1049	HIS
2	B	1073	GLN
2	B	1107	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	32	HIS
1	C	38	GLN
1	C	80	GLN
1	C	108	ASN
1	C	143	GLN
1	C	424	ASN
2	D	716	HIS
2	D	955	ASN
2	D	1073	GLN
2	D	1107	ASN
1	E	32	HIS
1	E	38	GLN
1	E	80	GLN
1	E	108	ASN
1	E	143	GLN
1	E	411	ASN
1	E	424	ASN
2	F	716	HIS
2	F	955	ASN
2	F	1073	GLN
1	G	32	HIS
1	G	38	GLN
1	G	80	GLN
1	G	108	ASN
1	G	411	ASN
1	G	424	ASN
2	H	716	HIS
2	H	816	GLN
2	H	955	ASN
2	H	959	ASN
2	H	1024	ASN
2	H	1073	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 ⓘ

60 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	I	1	1,3	14,14,15	0.80	0	17,19,21	1.09	0
3	NAG	I	2	3	14,14,15	0.37	0	17,19,21	0.41	0
3	BMA	I	3	3	11,11,12	0.45	0	15,15,17	0.50	0
3	MAN	I	4	3	11,11,12	0.31	0	15,15,17	0.55	0
3	MAN	I	5	3	11,11,12	0.32	0	15,15,17	0.53	0
4	NAG	J	1	1,4	14,14,15	0.39	0	17,19,21	0.62	0
4	NAG	J	2	4	14,14,15	0.38	0	17,19,21	0.51	0
4	BMA	J	3	4	11,11,12	0.40	0	15,15,17	0.70	0
4	MAN	J	4	4	11,11,12	0.29	0	15,15,17	0.52	0
5	NAG	K	1	1,5	14,14,15	0.40	0	17,19,21	0.52	0
5	NAG	K	2	5	14,14,15	0.36	0	17,19,21	0.55	0
5	BMA	K	3	5	11,11,12	0.34	0	15,15,17	0.44	0
5	MAN	K	4	5	11,11,12	0.29	0	15,15,17	0.54	0
6	NAG	L	1	2,6	14,14,15	0.41	0	17,19,21	0.88	1 (5%)
6	NAG	L	2	6	14,14,15	0.69	0	17,19,21	1.19	1 (5%)
3	NAG	M	1	1,3	14,14,15	0.79	0	17,19,21	1.09	0
3	NAG	M	2	3	14,14,15	0.38	0	17,19,21	0.41	0
3	BMA	M	3	3	11,11,12	0.46	0	15,15,17	0.50	0
3	MAN	M	4	3	11,11,12	0.33	0	15,15,17	0.55	0
3	MAN	M	5	3	11,11,12	0.32	0	15,15,17	0.52	0
4	NAG	N	1	1,4	14,14,15	0.39	0	17,19,21	0.62	0
4	NAG	N	2	4	14,14,15	0.37	0	17,19,21	0.51	0
4	BMA	N	3	4	11,11,12	0.39	0	15,15,17	0.70	0
4	MAN	N	4	4	11,11,12	0.30	0	15,15,17	0.51	0
5	NAG	O	1	1,5	14,14,15	0.39	0	17,19,21	0.51	0
5	NAG	O	2	5	14,14,15	0.36	0	17,19,21	0.55	0
5	BMA	O	3	5	11,11,12	0.33	0	15,15,17	0.44	0
5	MAN	O	4	5	11,11,12	0.30	0	15,15,17	0.54	0
6	NAG	P	1	2,6	14,14,15	0.40	0	17,19,21	0.87	1 (5%)
6	NAG	P	2	6	14,14,15	0.69	0	17,19,21	1.19	1 (5%)
3	NAG	Q	1	1,3	14,14,15	0.79	0	17,19,21	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	Q	2	3	14,14,15	0.37	0	17,19,21	0.41	0
3	BMA	Q	3	3	11,11,12	0.46	0	15,15,17	0.49	0
3	MAN	Q	4	3	11,11,12	0.33	0	15,15,17	0.55	0
3	MAN	Q	5	3	11,11,12	0.32	0	15,15,17	0.53	0
4	NAG	R	1	1,4	14,14,15	0.39	0	17,19,21	0.62	0
4	NAG	R	2	4	14,14,15	0.38	0	17,19,21	0.51	0
4	BMA	R	3	4	11,11,12	0.39	0	15,15,17	0.70	0
4	MAN	R	4	4	11,11,12	0.30	0	15,15,17	0.52	0
5	NAG	S	1	1,5	14,14,15	0.39	0	17,19,21	0.51	0
5	NAG	S	2	5	14,14,15	0.36	0	17,19,21	0.54	0
5	BMA	S	3	5	11,11,12	0.33	0	15,15,17	0.44	0
5	MAN	S	4	5	11,11,12	0.30	0	15,15,17	0.54	0
6	NAG	T	1	2,6	14,14,15	0.41	0	17,19,21	0.88	1 (5%)
6	NAG	T	2	6	14,14,15	0.69	0	17,19,21	1.19	1 (5%)
3	NAG	U	1	1,3	14,14,15	0.79	0	17,19,21	1.09	0
3	NAG	U	2	3	14,14,15	0.38	0	17,19,21	0.41	0
3	BMA	U	3	3	11,11,12	0.46	0	15,15,17	0.50	0
3	MAN	U	4	3	11,11,12	0.32	0	15,15,17	0.55	0
3	MAN	U	5	3	11,11,12	0.30	0	15,15,17	0.53	0
4	NAG	V	1	1,4	14,14,15	0.40	0	17,19,21	0.61	0
4	NAG	V	2	4	14,14,15	0.38	0	17,19,21	0.51	0
4	BMA	V	3	4	11,11,12	0.38	0	15,15,17	0.69	0
4	MAN	V	4	4	11,11,12	0.29	0	15,15,17	0.52	0
5	NAG	W	1	1,5	14,14,15	0.38	0	17,19,21	0.51	0
5	NAG	W	2	5	14,14,15	0.36	0	17,19,21	0.55	0
5	BMA	W	3	5	11,11,12	0.33	0	15,15,17	0.45	0
5	MAN	W	4	5	11,11,12	0.31	0	15,15,17	0.54	0
6	NAG	X	1	2,6	14,14,15	0.40	0	17,19,21	0.88	1 (5%)
6	NAG	X	2	6	14,14,15	0.69	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
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1
3	MAN	I	5	3	-	0/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	1/2/19/22	0/1/1/1
5	MAN	K	4	5	-	1/2/19/22	0/1/1/1
6	NAG	L	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	1/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
3	MAN	M	4	3	-	0/2/19/22	0/1/1/1
3	MAN	M	5	3	-	0/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1
4	MAN	N	4	4	-	0/2/19/22	0/1/1/1
5	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
5	BMA	O	3	5	-	1/2/19/22	0/1/1/1
5	MAN	O	4	5	-	1/2/19/22	0/1/1/1
6	NAG	P	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	1/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	1/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	0/2/19/22	0/1/1/1
3	MAN	Q	5	3	-	0/2/19/22	0/1/1/1
4	NAG	R	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	BMA	R	3	4	-	0/2/19/22	0/1/1/1
4	MAN	R	4	4	-	0/2/19/22	0/1/1/1
5	NAG	S	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
5	BMA	S	3	5	-	1/2/19/22	0/1/1/1
5	MAN	S	4	5	-	1/2/19/22	0/1/1/1
6	NAG	T	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	U	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	1/6/23/26	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1
3	MAN	U	4	3	-	0/2/19/22	0/1/1/1
3	MAN	U	5	3	-	0/2/19/22	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	BMA	V	3	4	-	0/2/19/22	0/1/1/1
4	MAN	V	4	4	-	0/2/19/22	0/1/1/1
5	NAG	W	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	BMA	W	3	5	-	1/2/19/22	0/1/1/1
5	MAN	W	4	5	-	1/2/19/22	0/1/1/1
6	NAG	X	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	2	NAG	C2-N2-C7	3.17	127.15	122.90
6	P	2	NAG	C2-N2-C7	3.15	127.12	122.90
6	T	2	NAG	C2-N2-C7	3.15	127.12	122.90
6	X	2	NAG	C2-N2-C7	3.12	127.08	122.90
6	L	1	NAG	O5-C1-C2	3.01	115.95	111.29
6	T	1	NAG	O5-C1-C2	3.01	115.95	111.29
6	X	1	NAG	O5-C1-C2	3.01	115.95	111.29
6	P	1	NAG	O5-C1-C2	2.99	115.92	111.29

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
5	S	1	NAG	C8-C7-N2-C2
5	S	1	NAG	O7-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	W	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
4	V	2	NAG	C8-C7-N2-C2
4	V	2	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
6	L	1	NAG	C8-C7-N2-C2
6	P	1	NAG	C8-C7-N2-C2
6	T	1	NAG	C8-C7-N2-C2
6	X	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
6	P	1	NAG	O7-C7-N2-C2
6	T	1	NAG	O7-C7-N2-C2
6	X	1	NAG	O7-C7-N2-C2
5	K	4	MAN	O5-C5-C6-O6
5	O	4	MAN	O5-C5-C6-O6
5	S	4	MAN	O5-C5-C6-O6
5	W	4	MAN	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
6	L	2	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

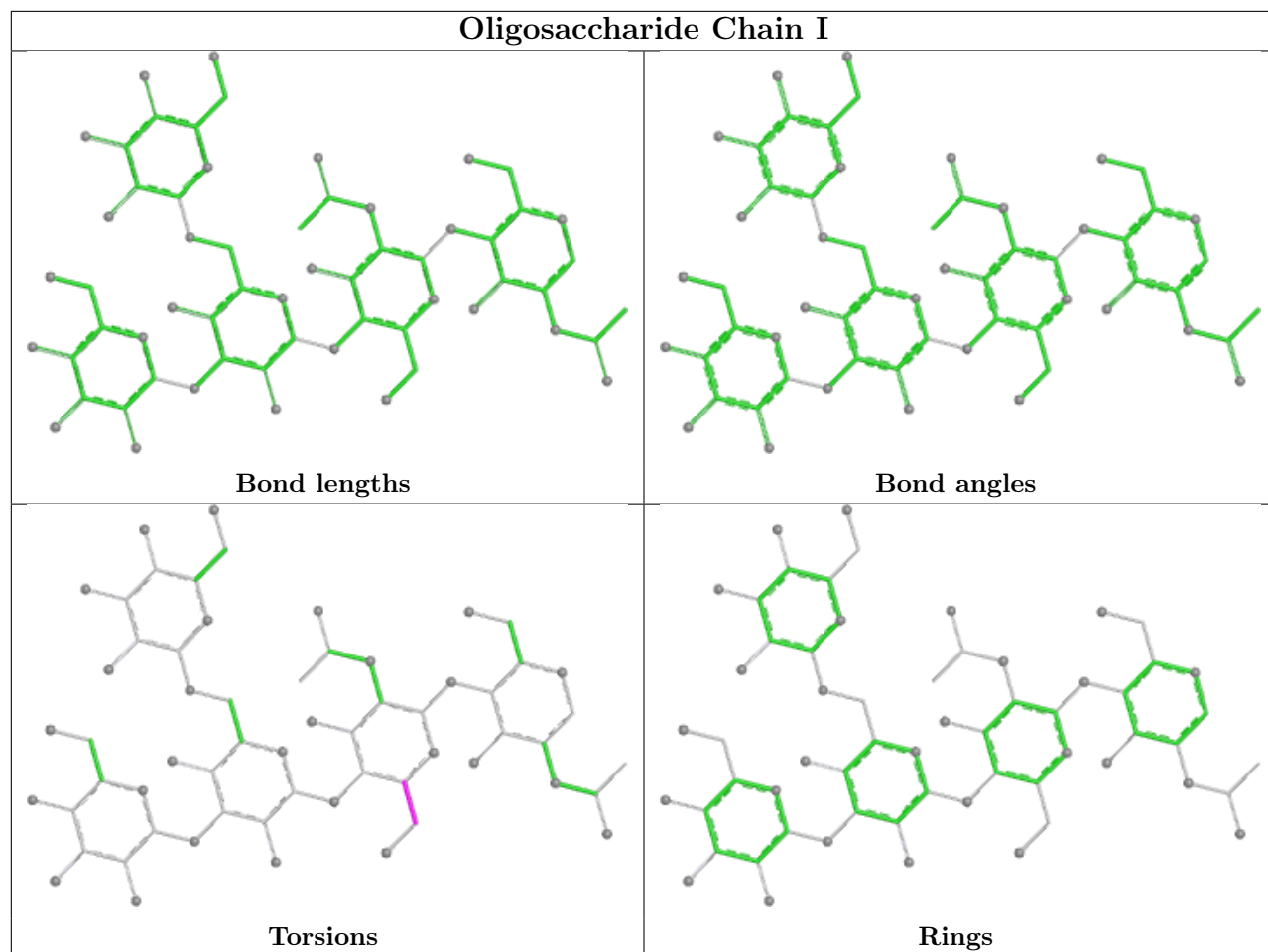
Mol	Chain	Res	Type	Atoms
6	P	2	NAG	C3-C2-N2-C7
6	T	2	NAG	C3-C2-N2-C7
6	X	2	NAG	C3-C2-N2-C7
5	O	3	BMA	O5-C5-C6-O6
5	S	3	BMA	O5-C5-C6-O6
5	W	3	BMA	O5-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6

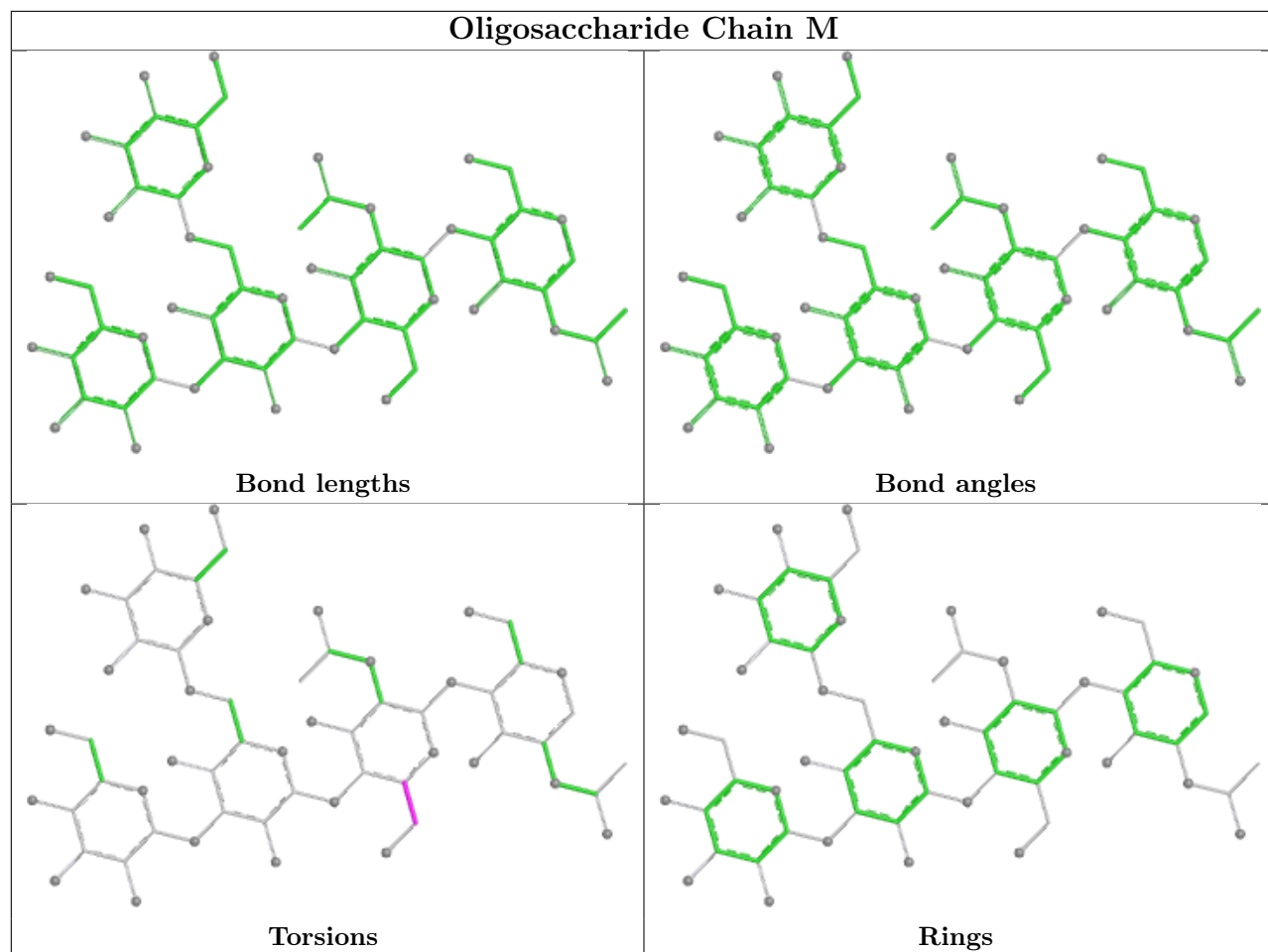
There are no ring outliers.

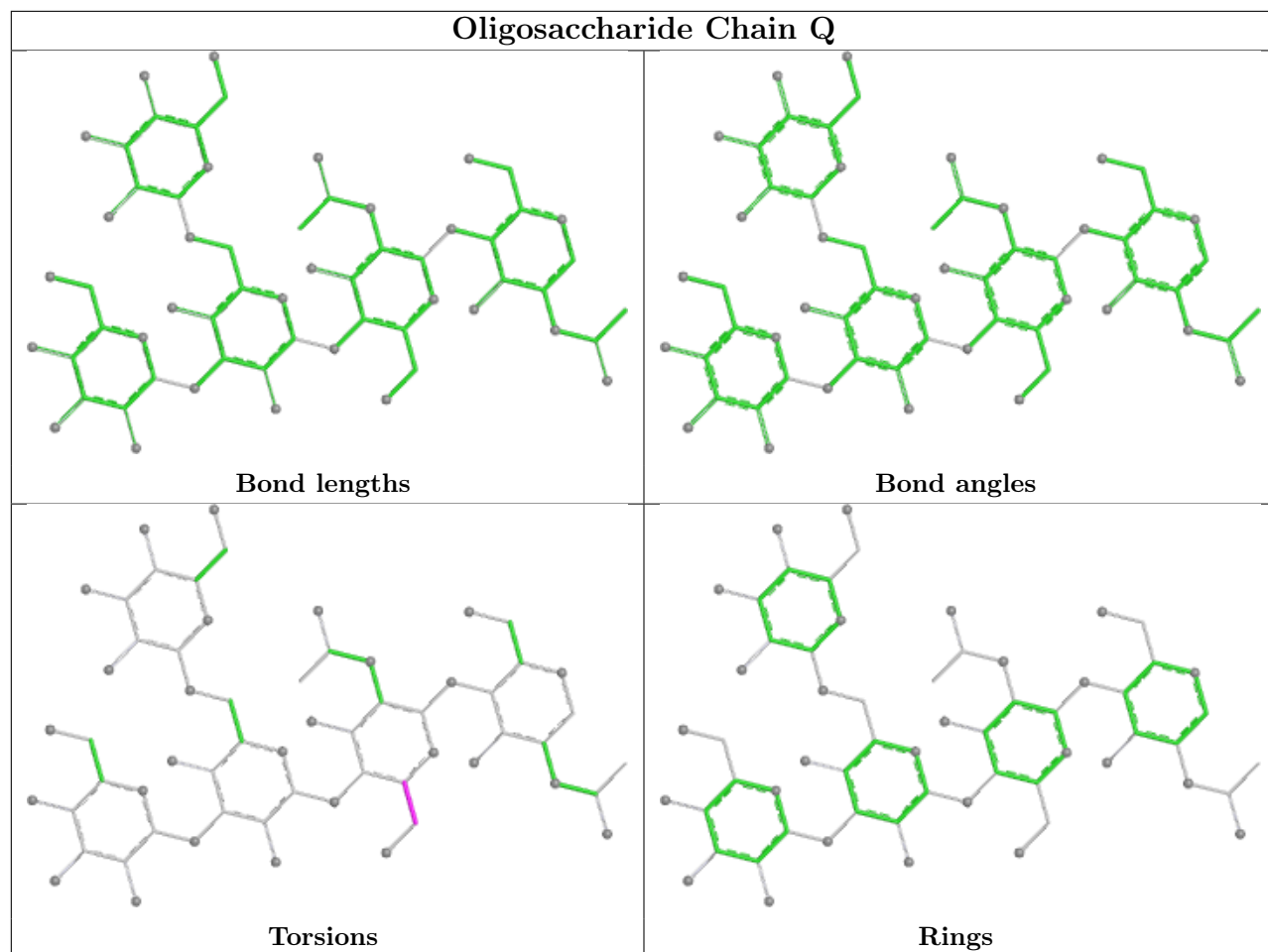
4 monomers are involved in 4 short contacts:

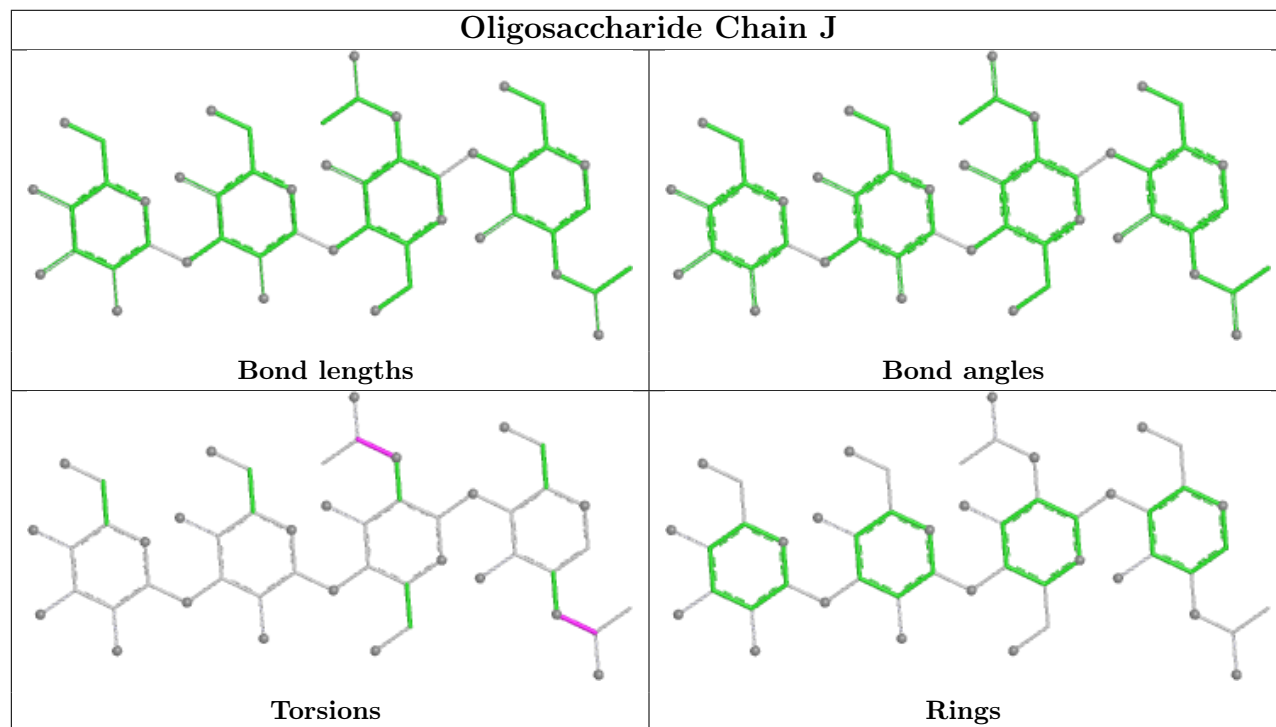
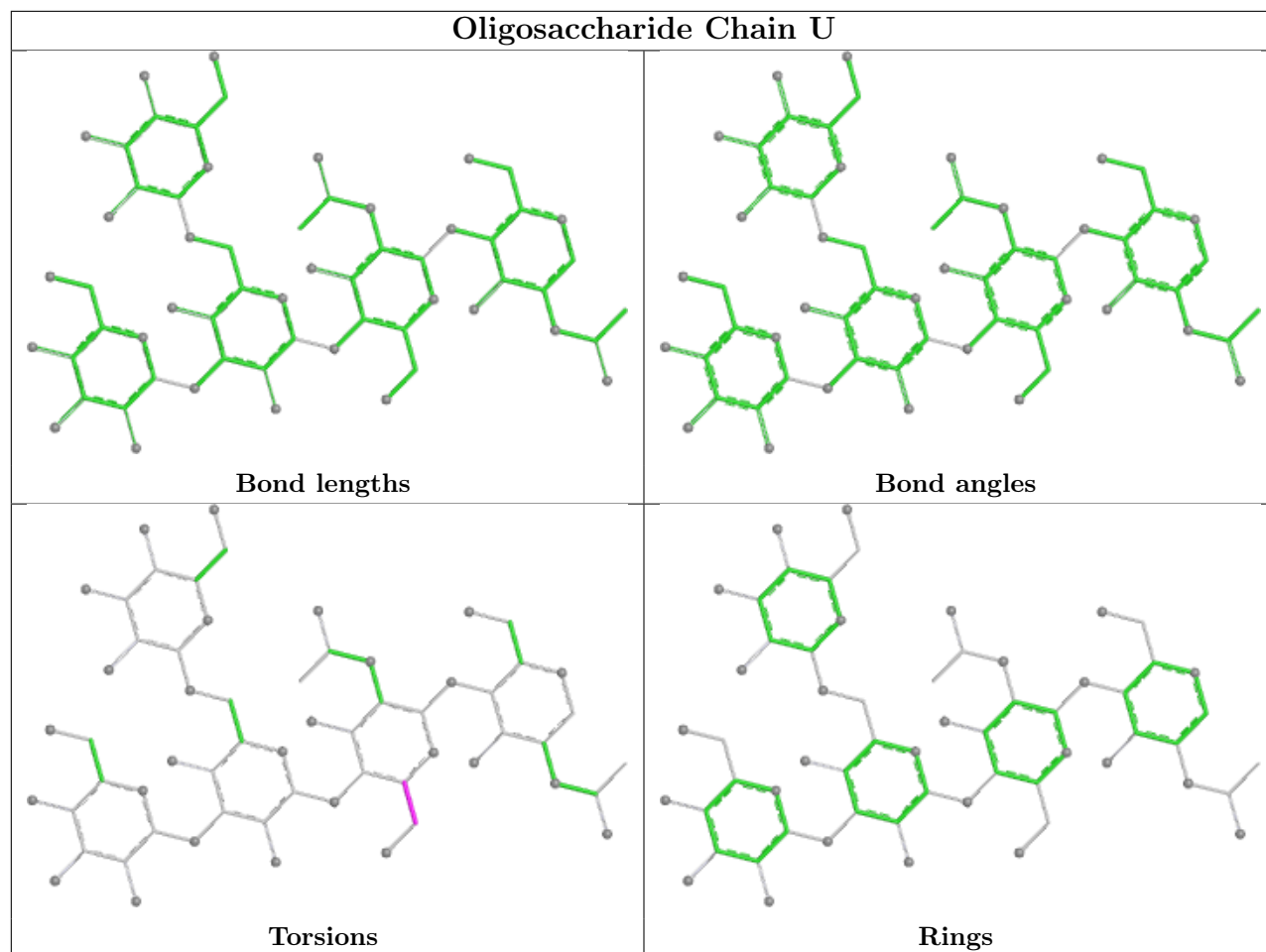
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	NAG	1	0
5	K	2	NAG	1	0
5	W	2	NAG	1	0
5	O	2	NAG	1	0

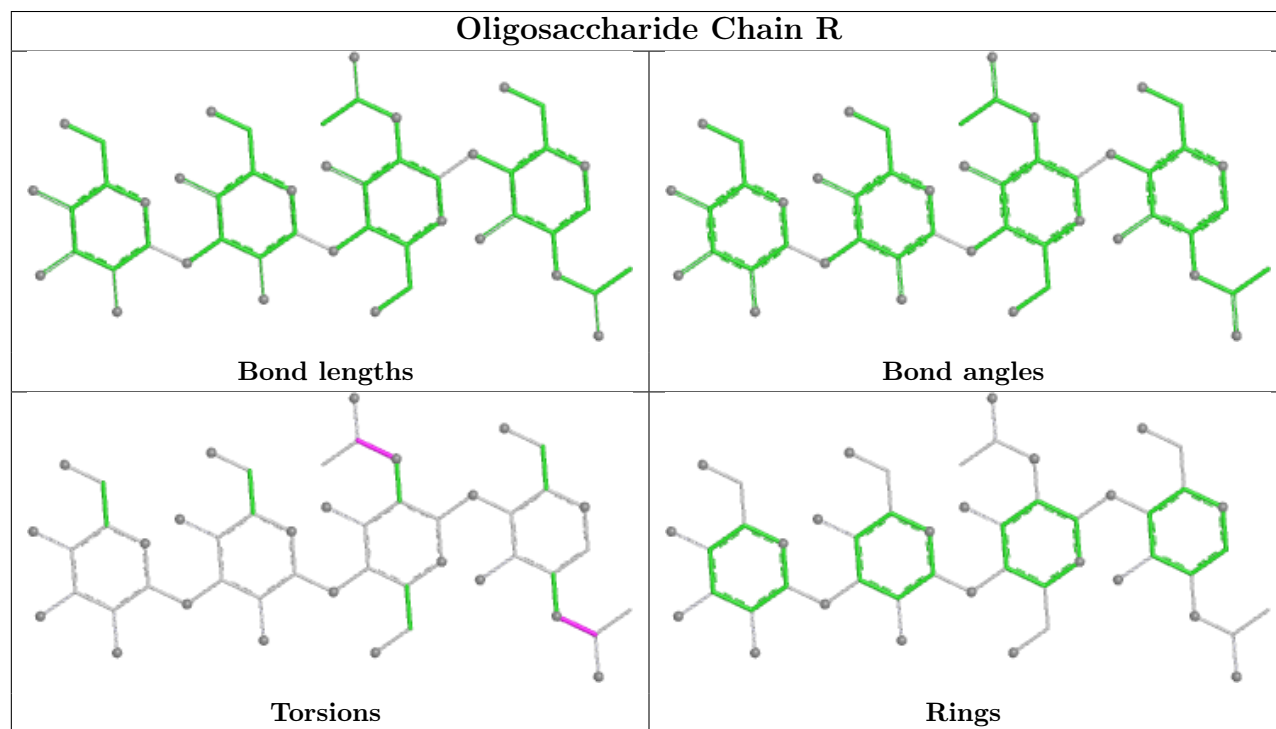
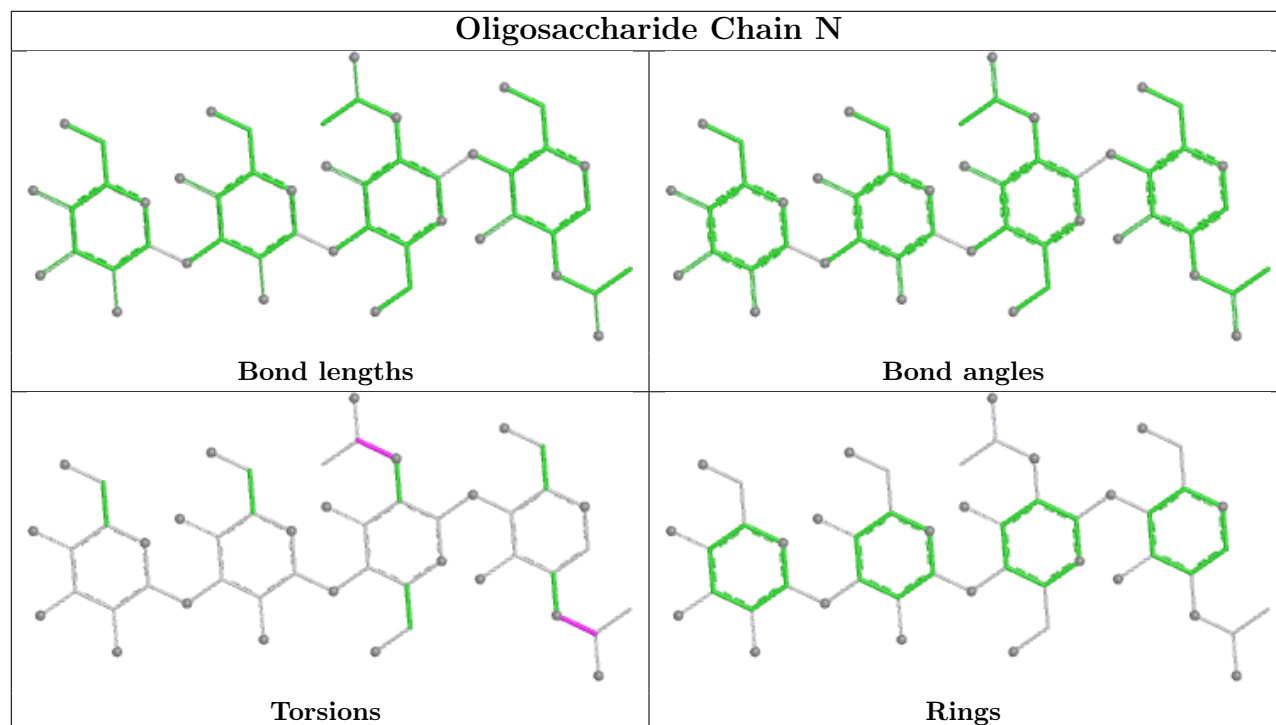
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

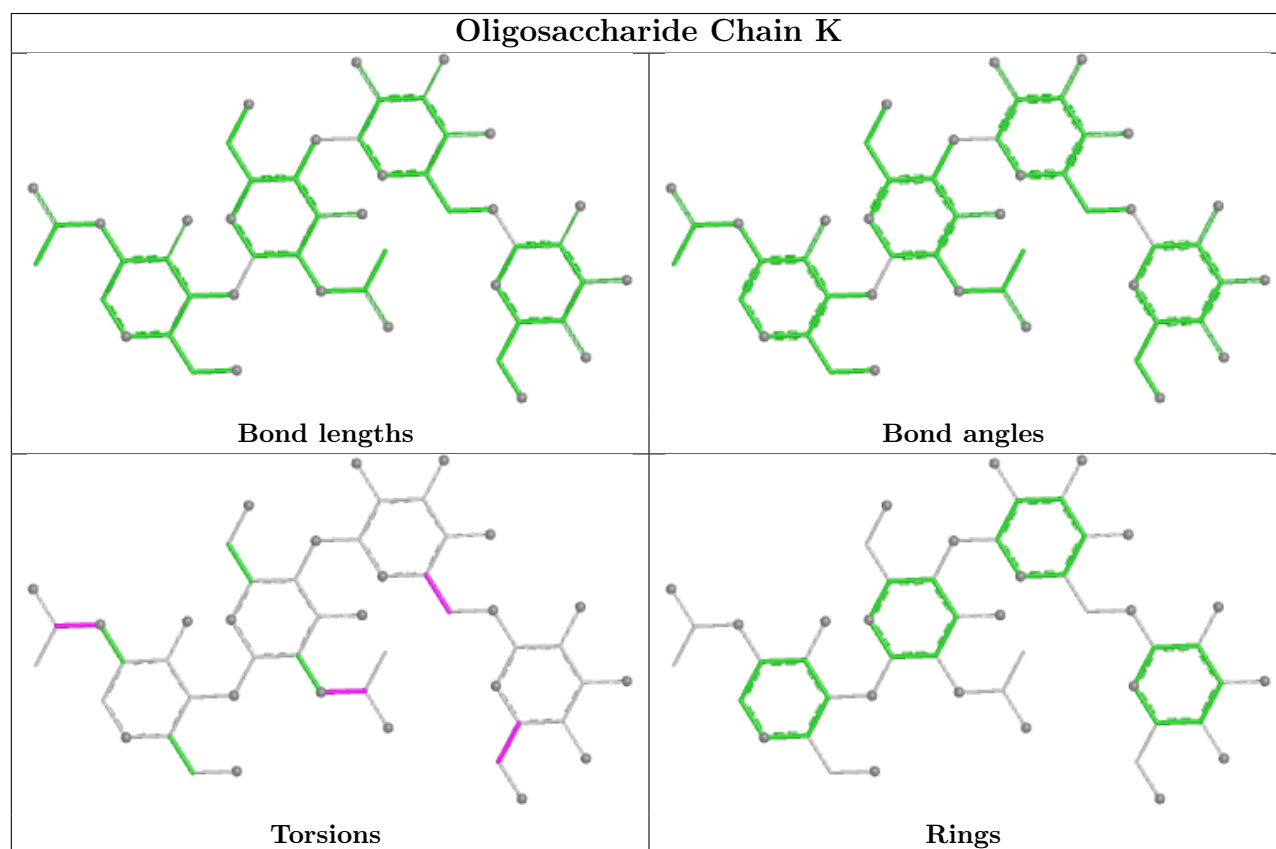
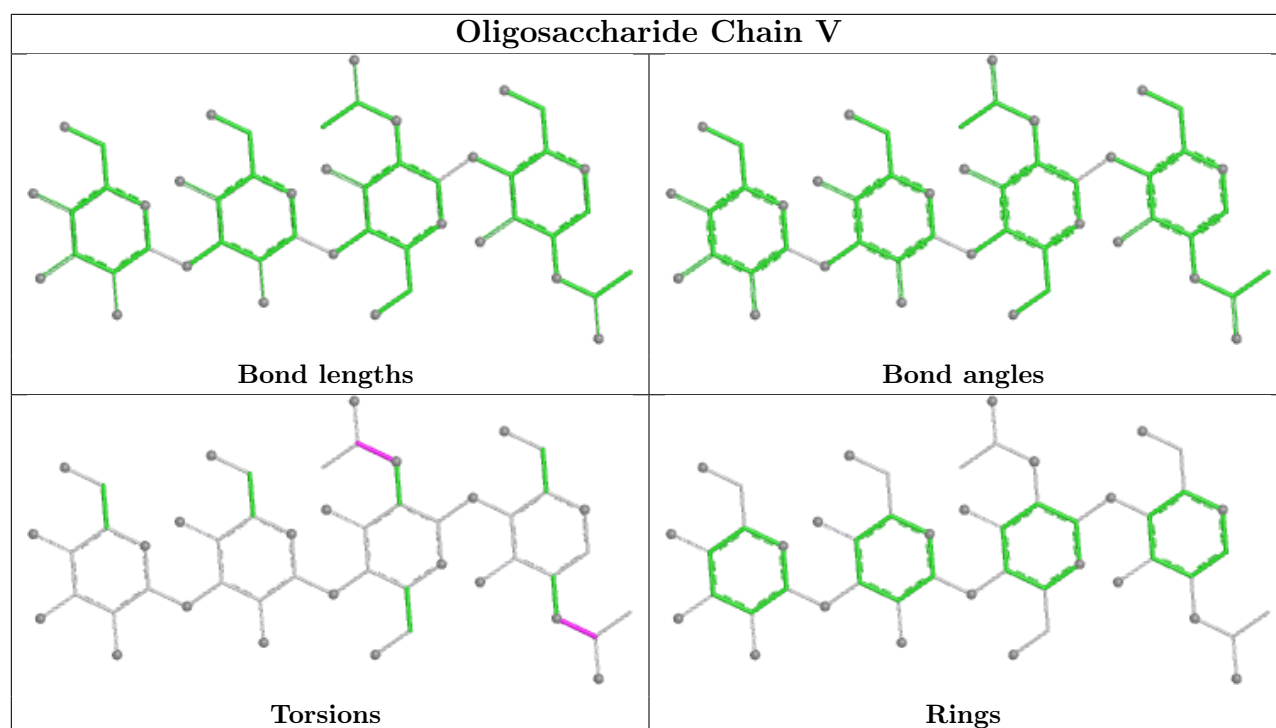


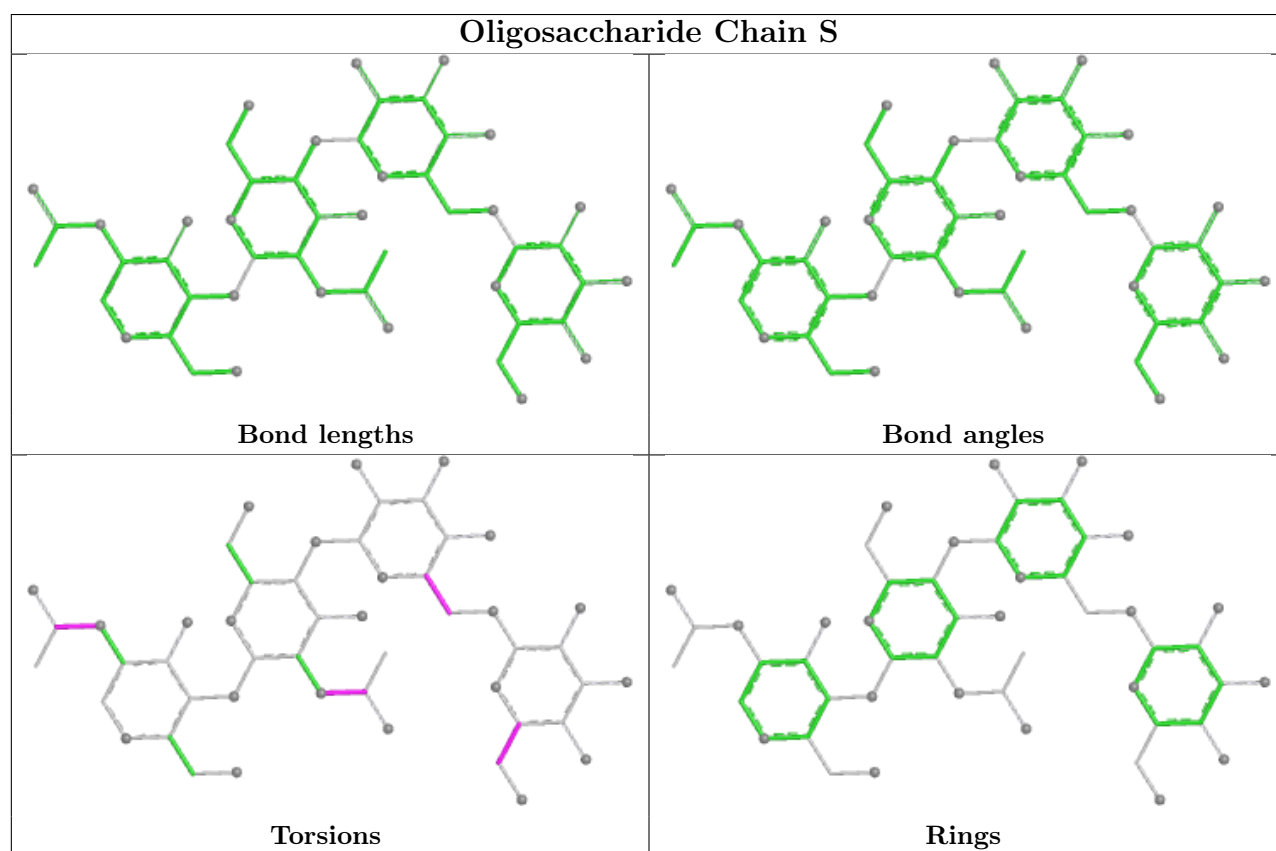
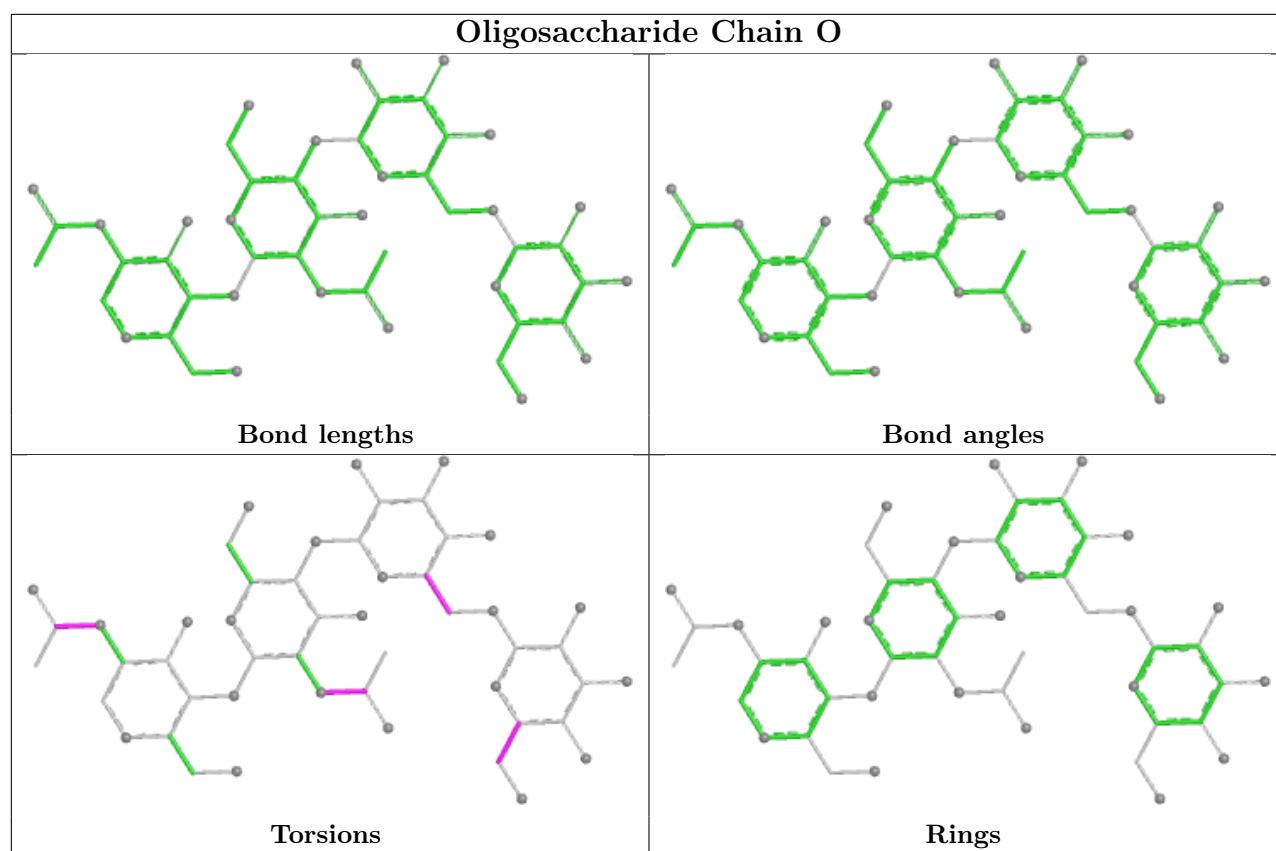


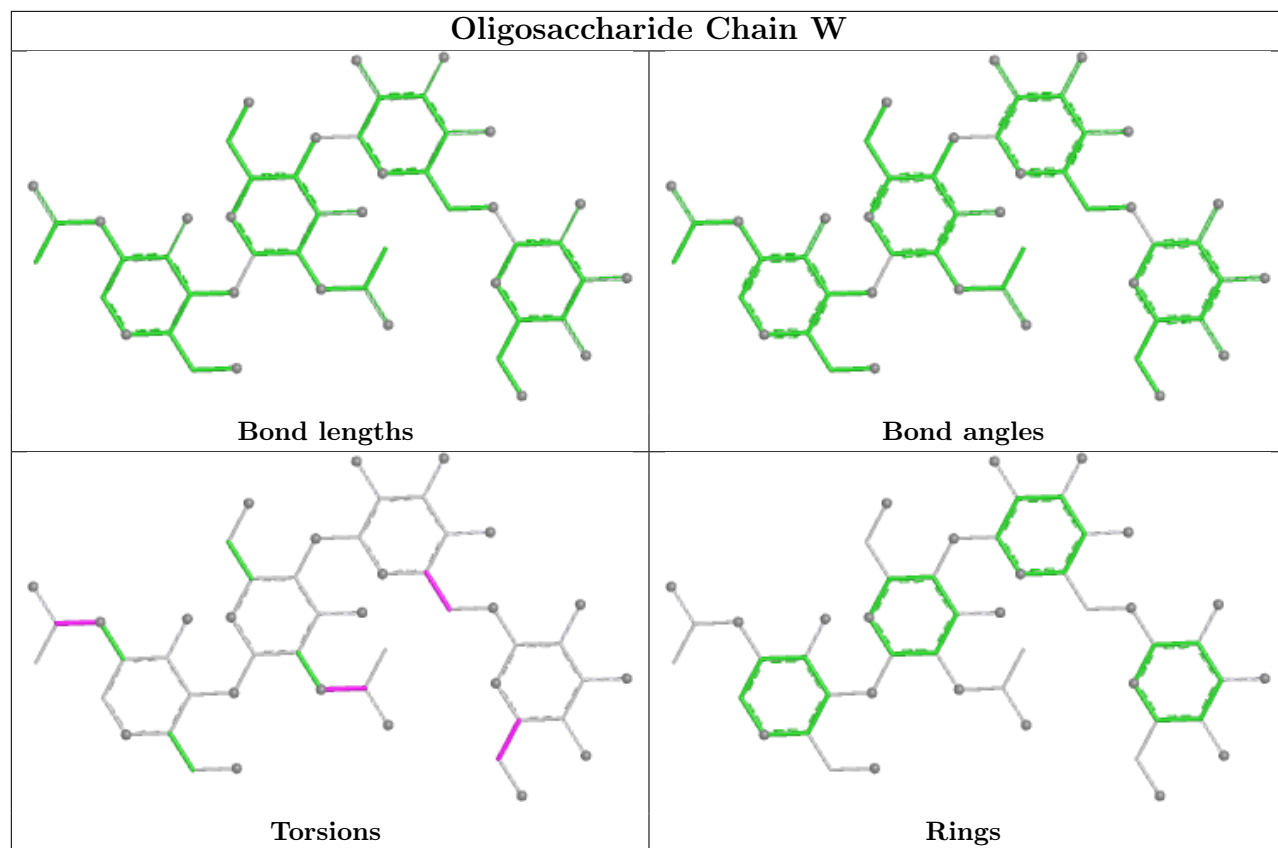


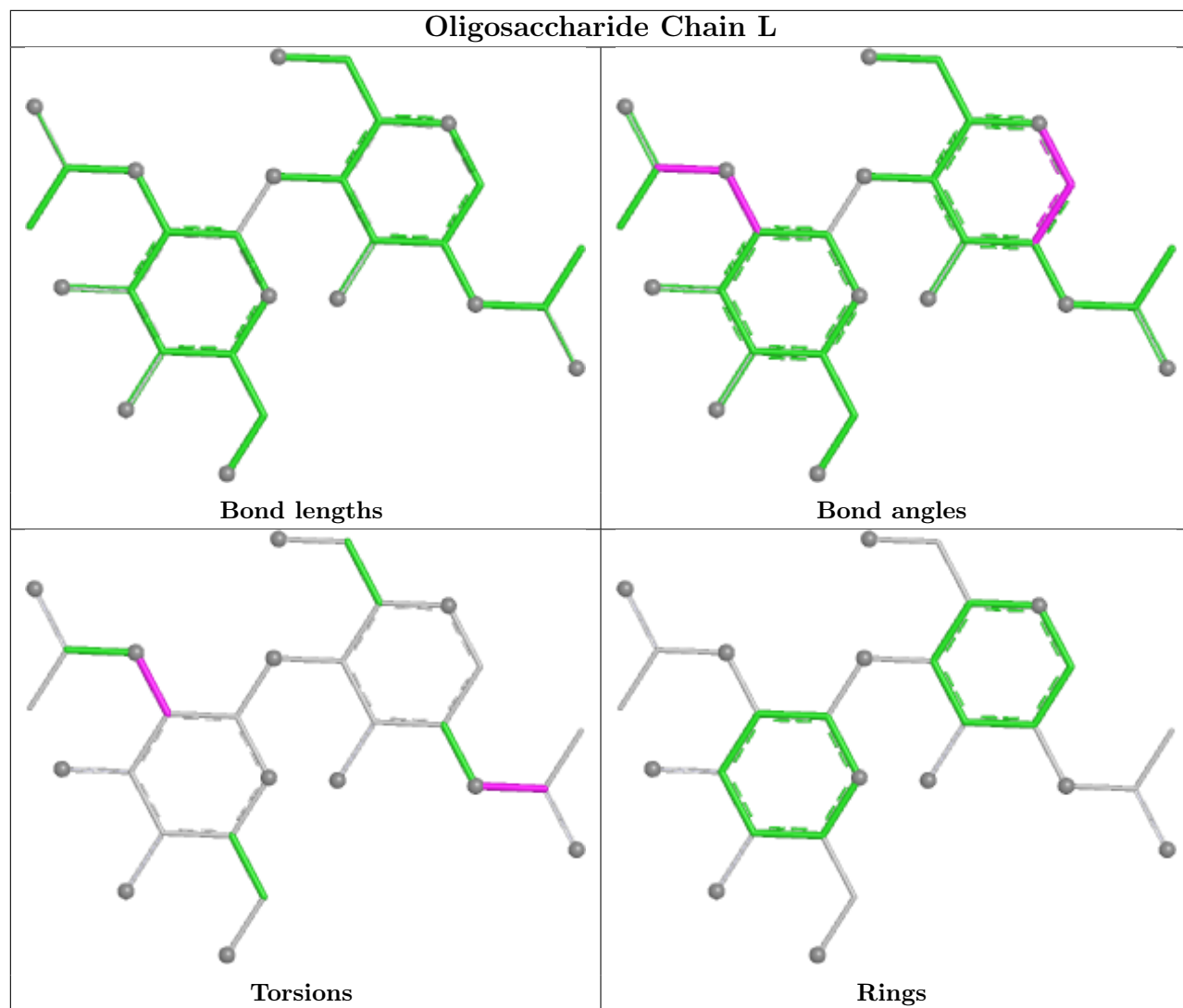


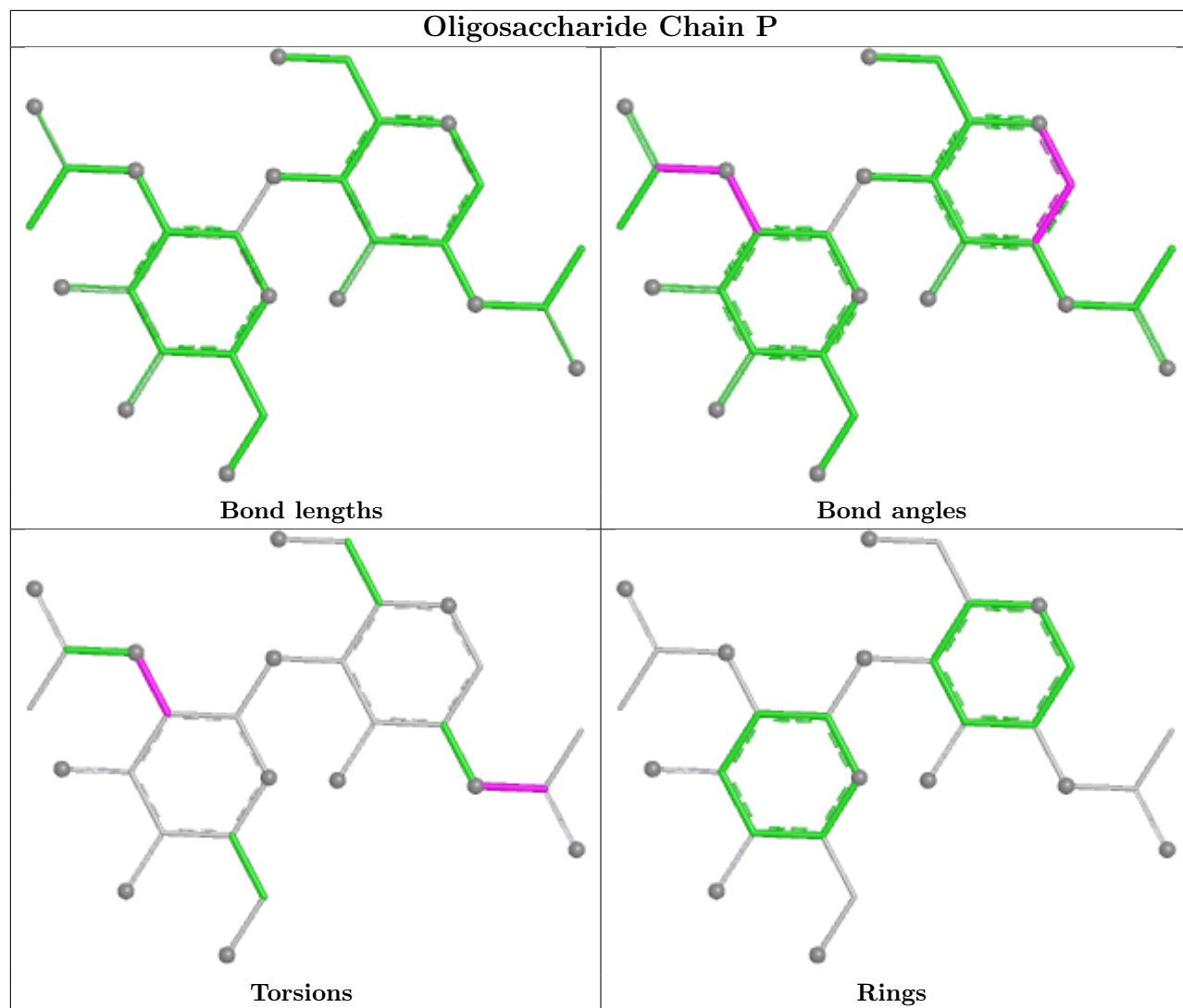


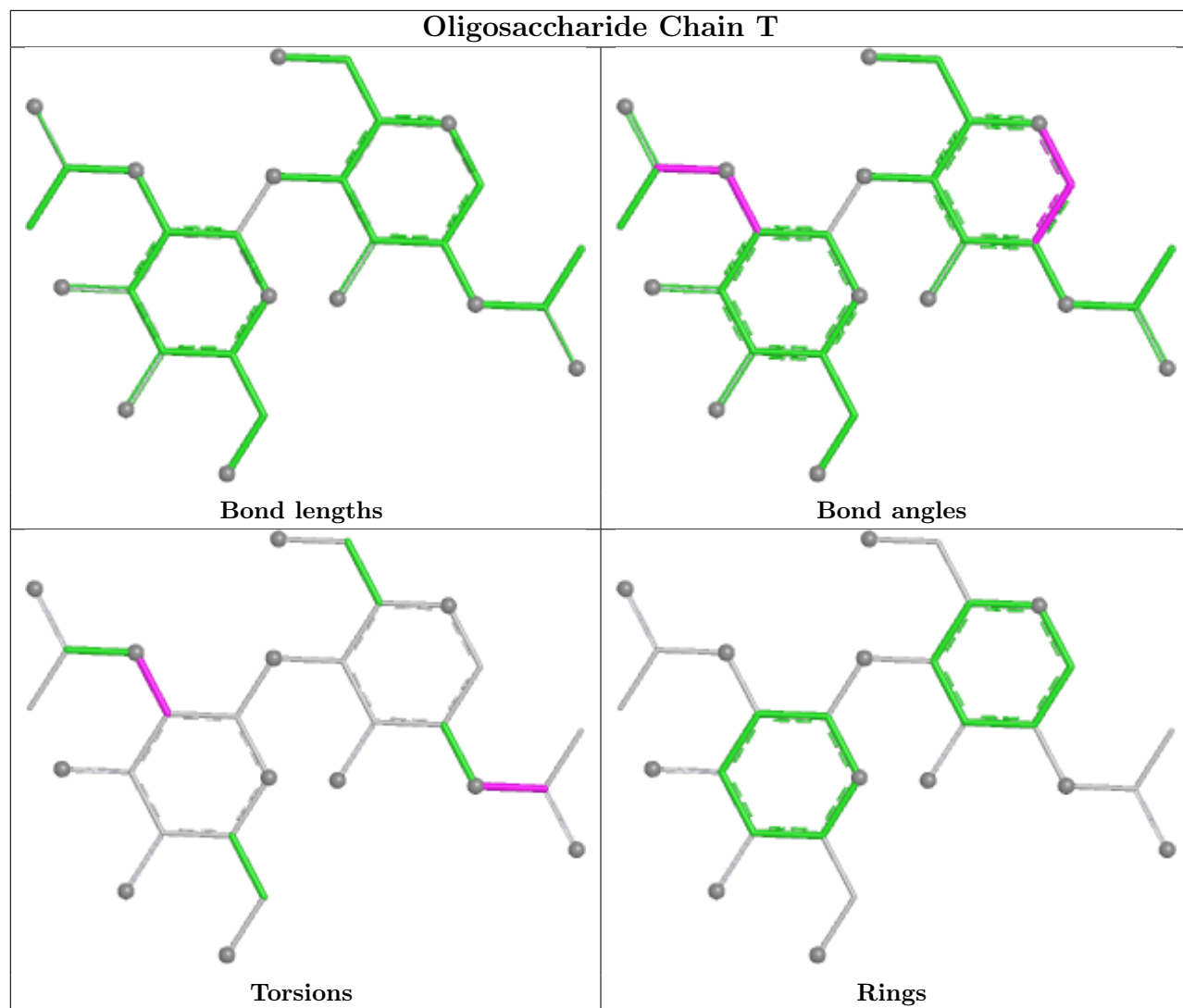


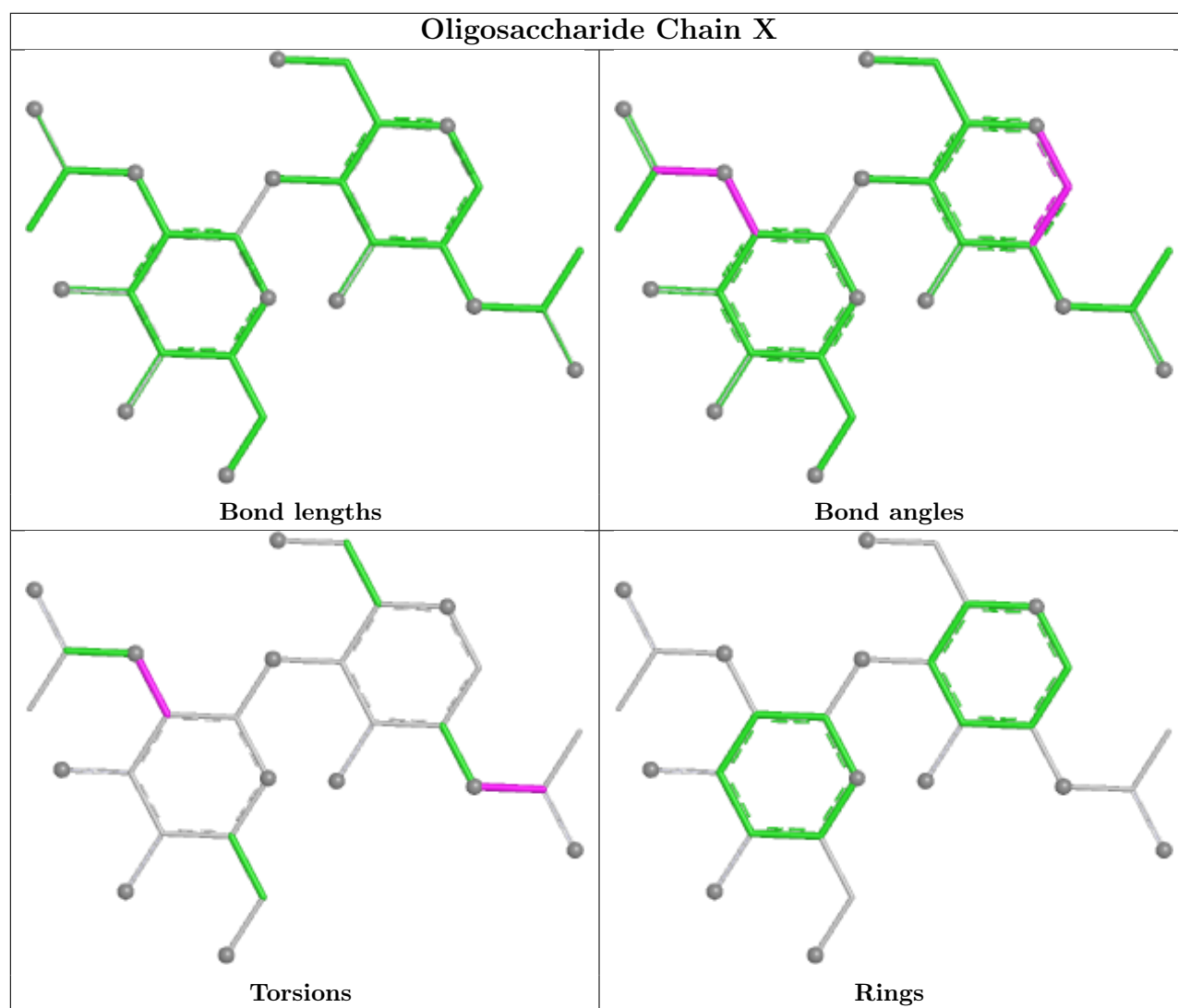












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

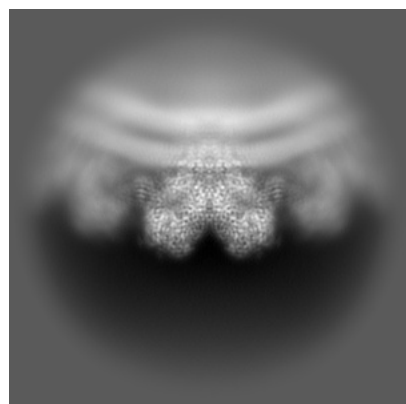
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71241. These allow visual inspection of the internal detail of the map and identification of artifacts.

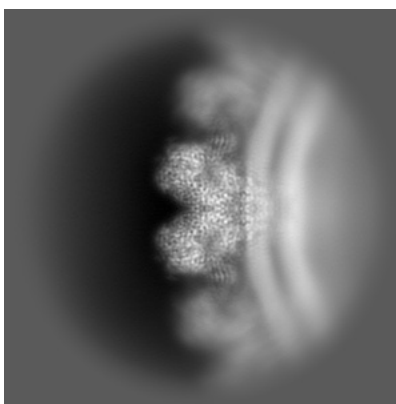
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

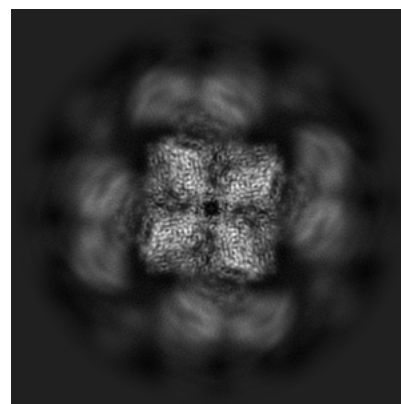
6.1.1 Primary map



X

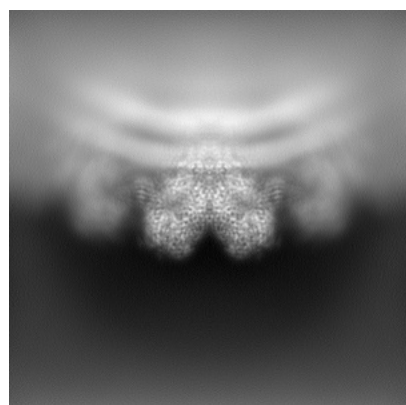


Y

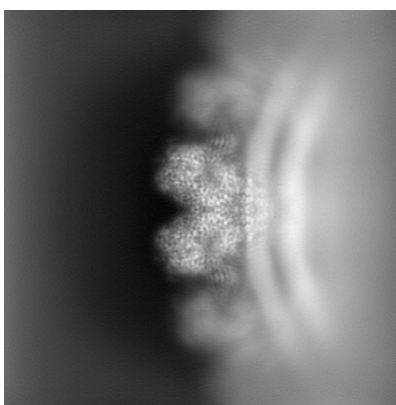


Z

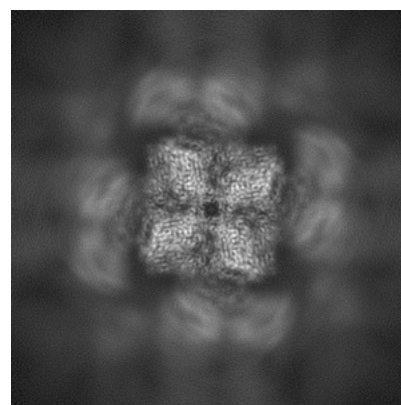
6.1.2 Raw map



X



Y

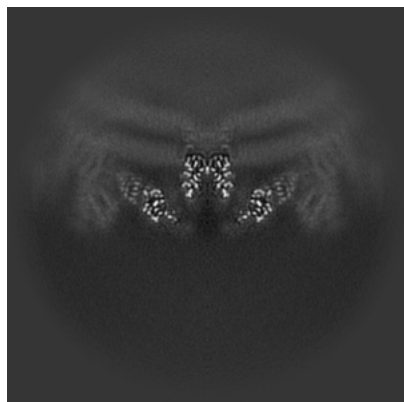


Z

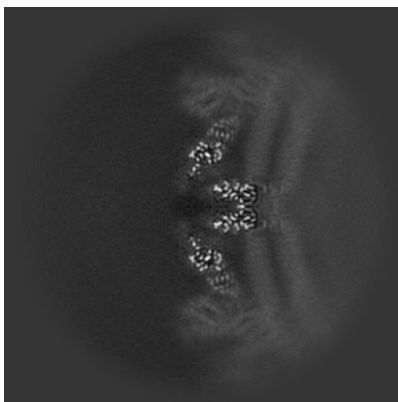
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

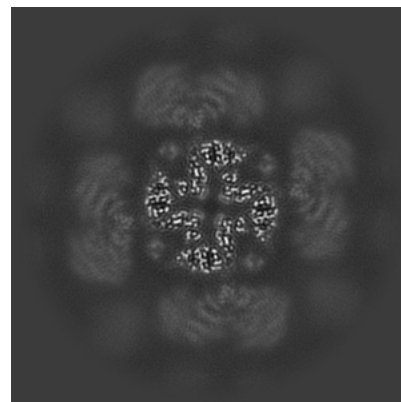
6.2.1 Primary map



X Index: 224

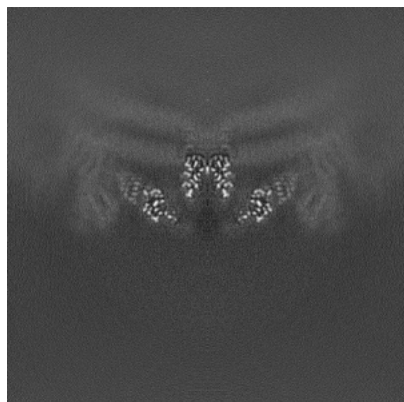


Y Index: 224

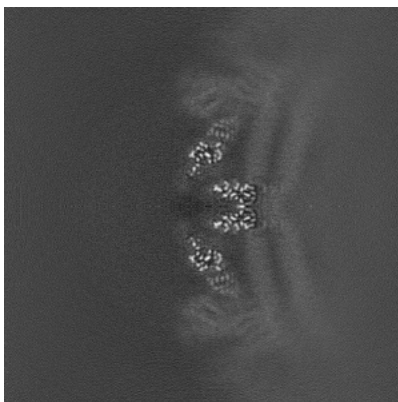


Z Index: 224

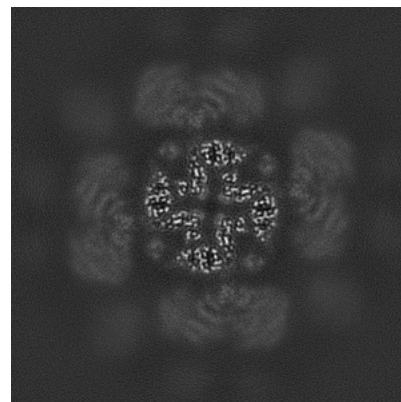
6.2.2 Raw map



X Index: 224



Y Index: 224

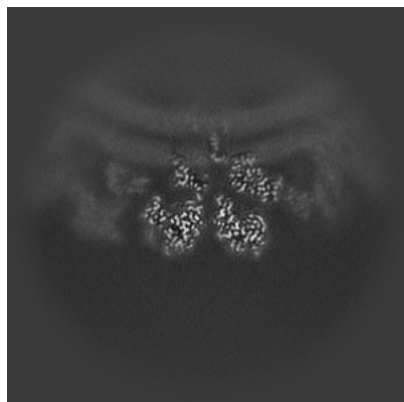


Z Index: 224

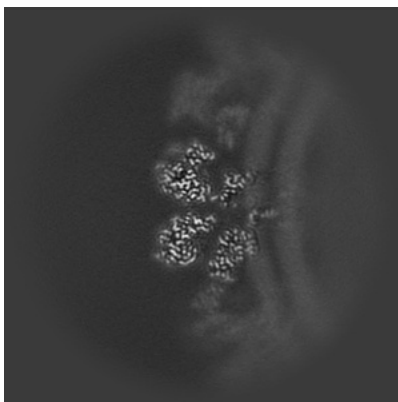
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

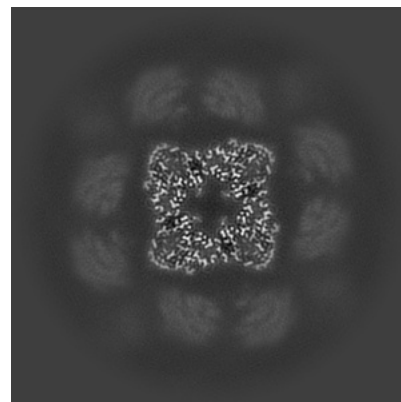
6.3.1 Primary map



X Index: 195

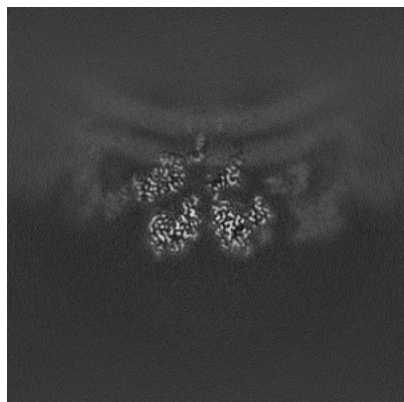


Y Index: 195

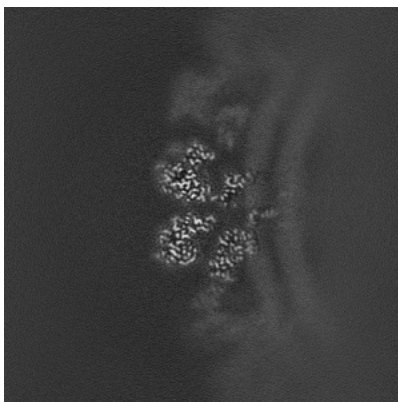


Z Index: 212

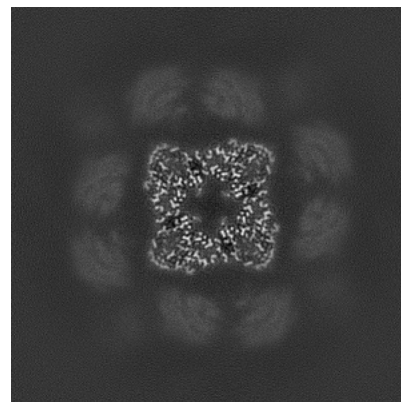
6.3.2 Raw map



X Index: 253



Y Index: 195

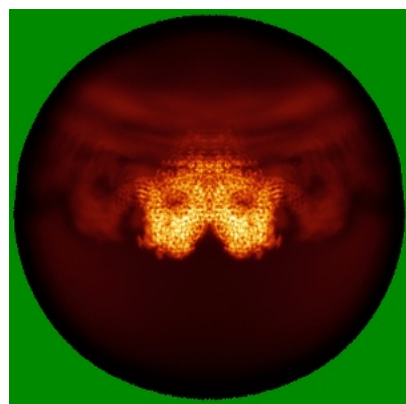


Z Index: 212

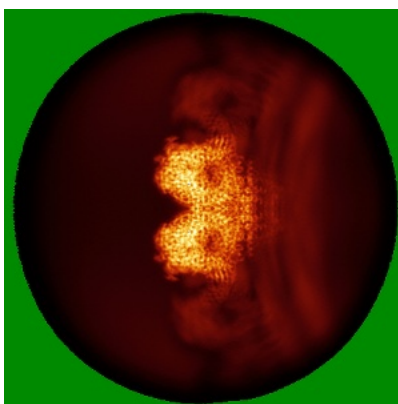
The images above show the largest variance slices of the map in three orthogonal directions.

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

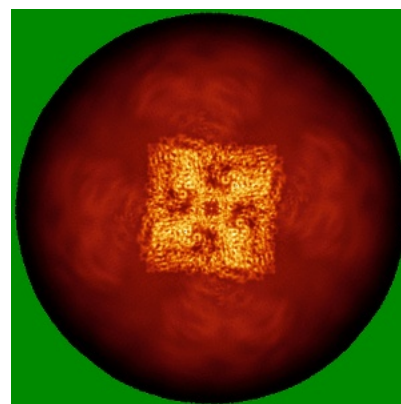
6.4.1 Primary map



X

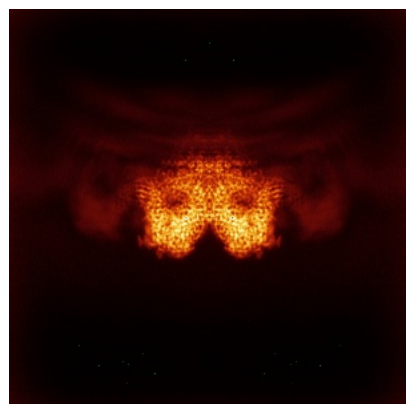


Y

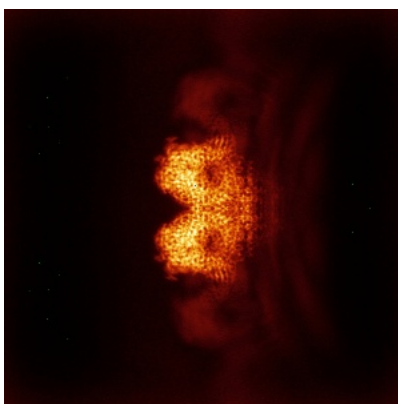


Z

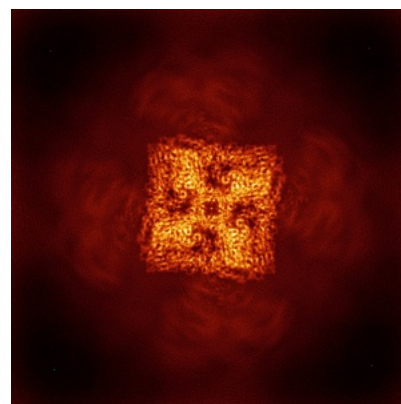
6.4.2 Raw map



X



Y

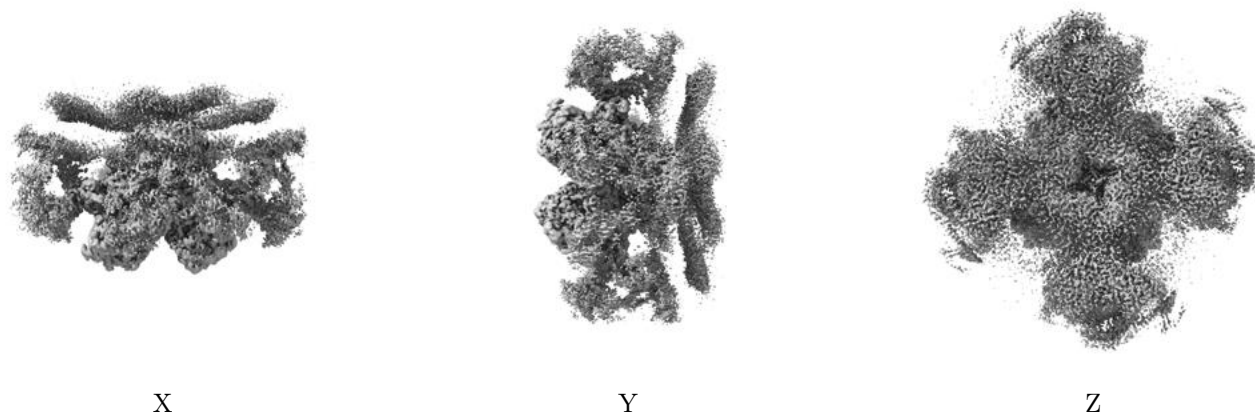


Z

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.

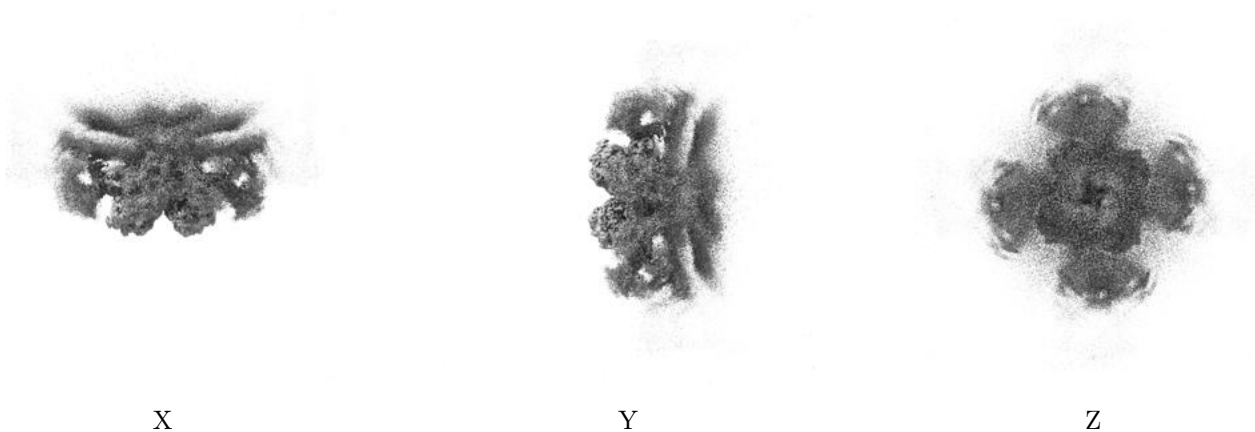
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

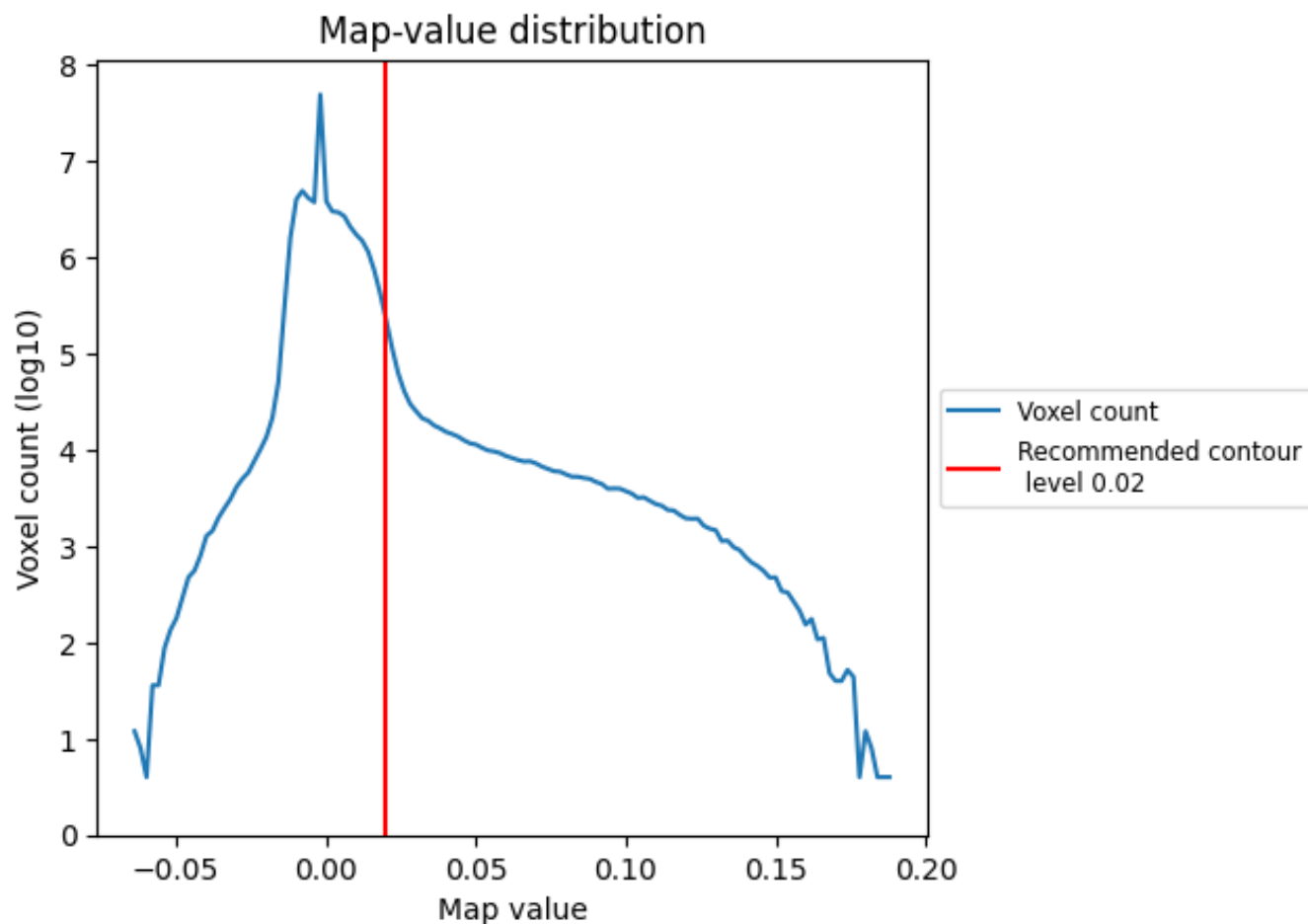
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

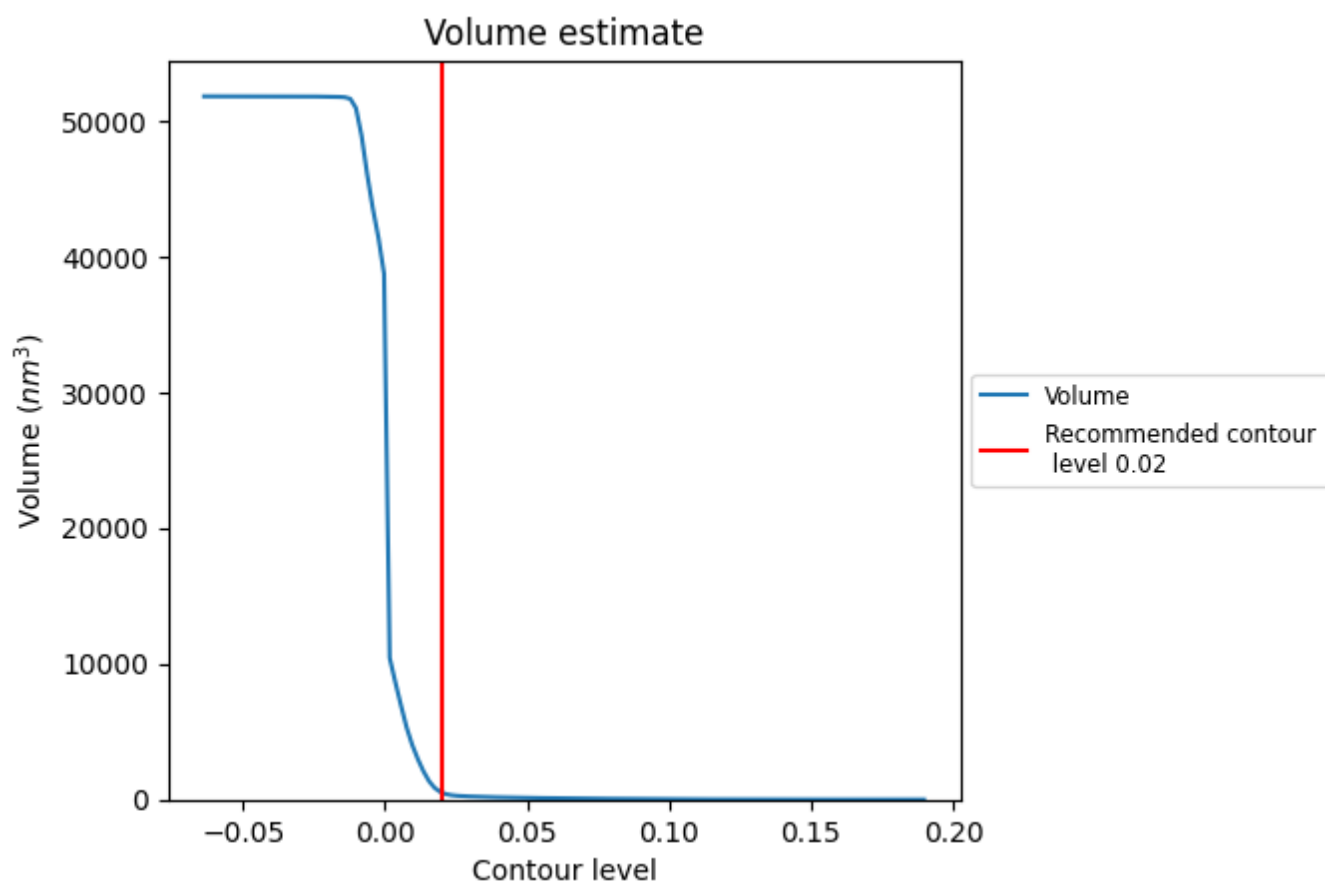
This section contains the results of statistical analysis of the map.

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.

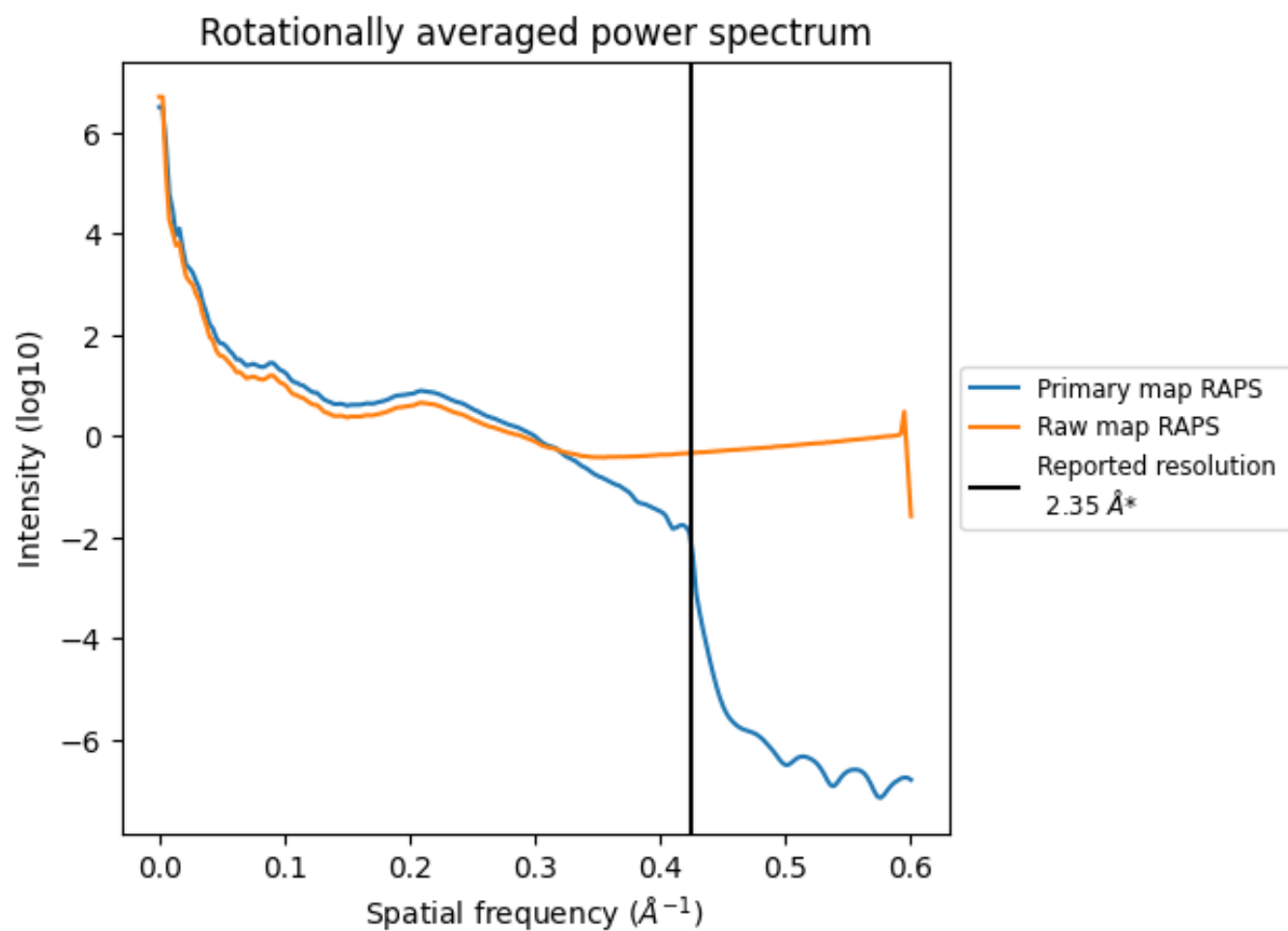
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 522 nm^3 ; this corresponds to an approximate mass of 471 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 ⓘ

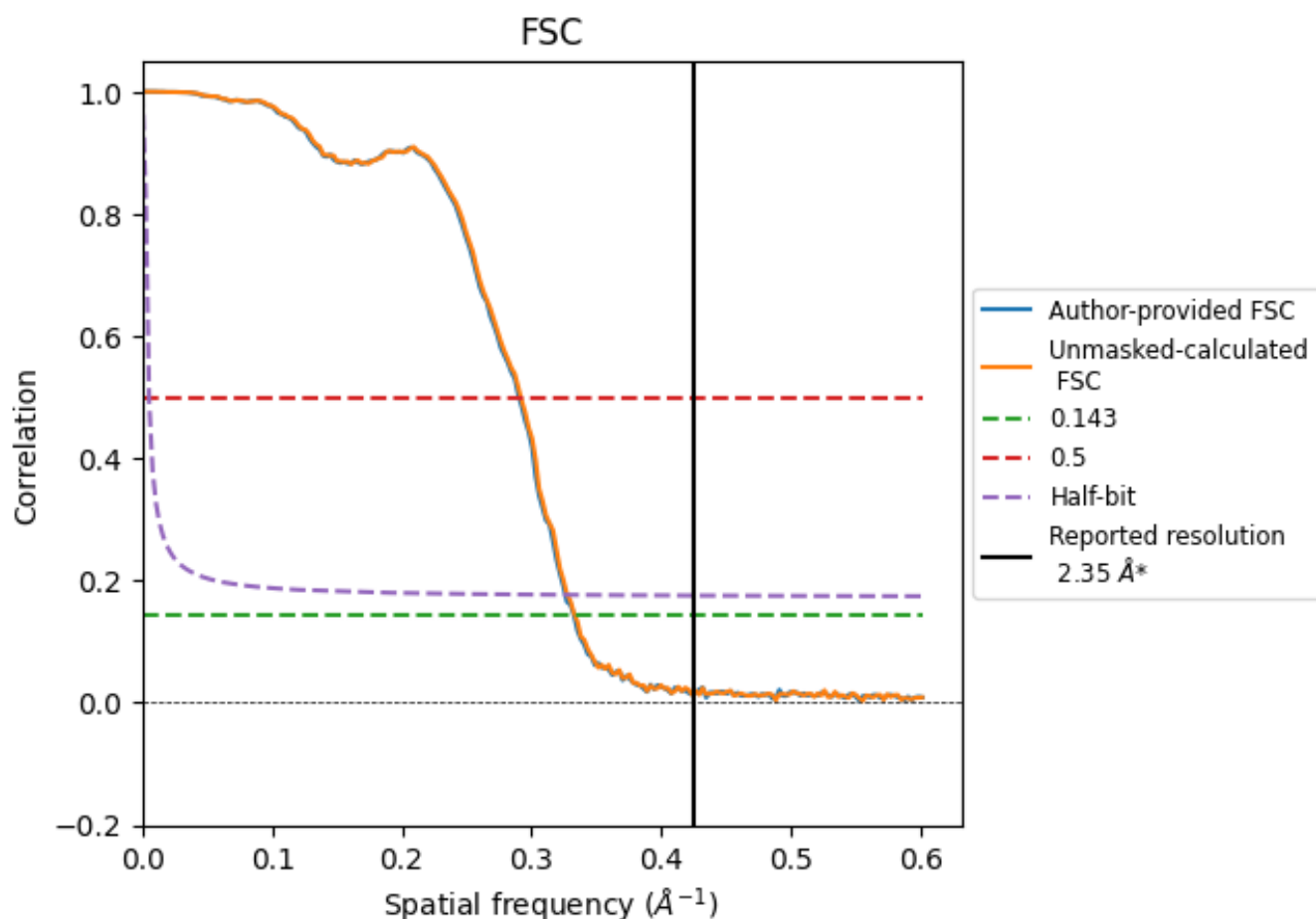


*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

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 0.426 \AA^{-1}

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	3.01	3.44	3.07
Unmasked-calculated*	3.00	3.43	3.05

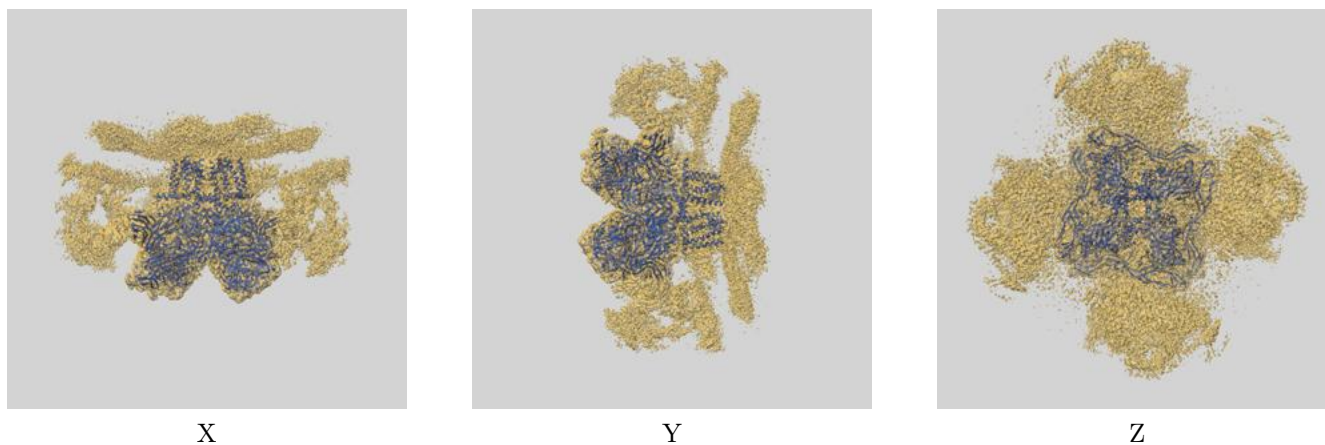
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.01 differs from the reported value 2.35 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.00 differs from the reported value 2.35 by more than 10 %

9 Map-model fit [i](#)

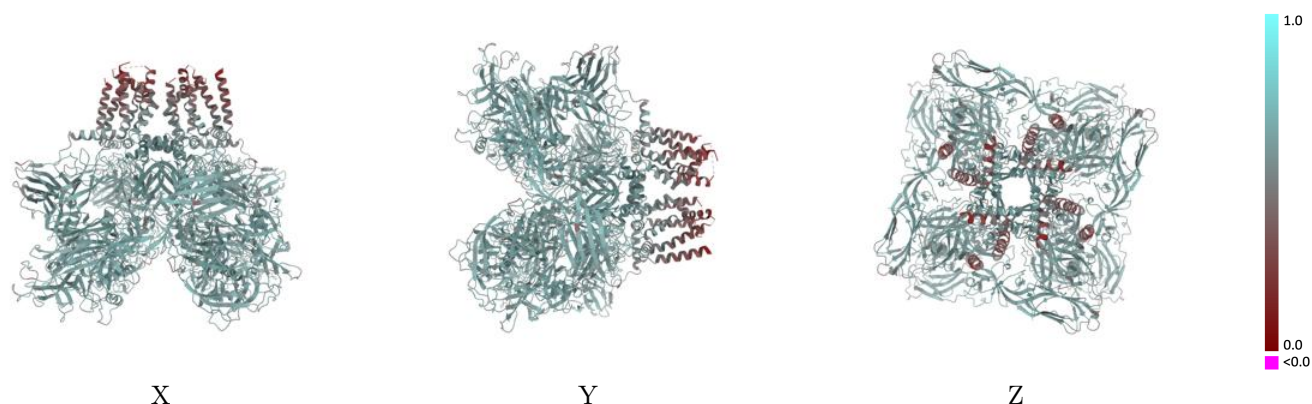
This section contains information regarding the fit between EMDB map EMD-71241 and PDB model 9P3I. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



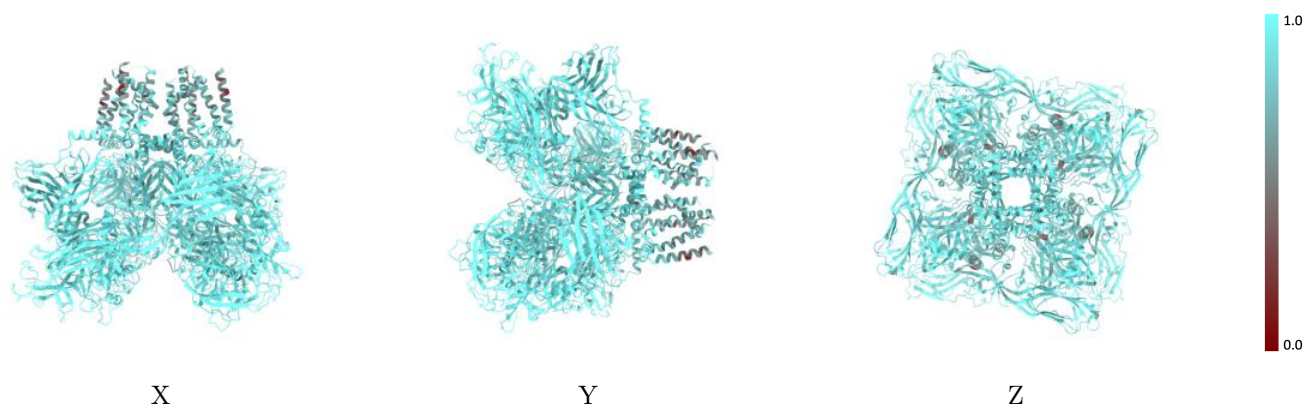
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



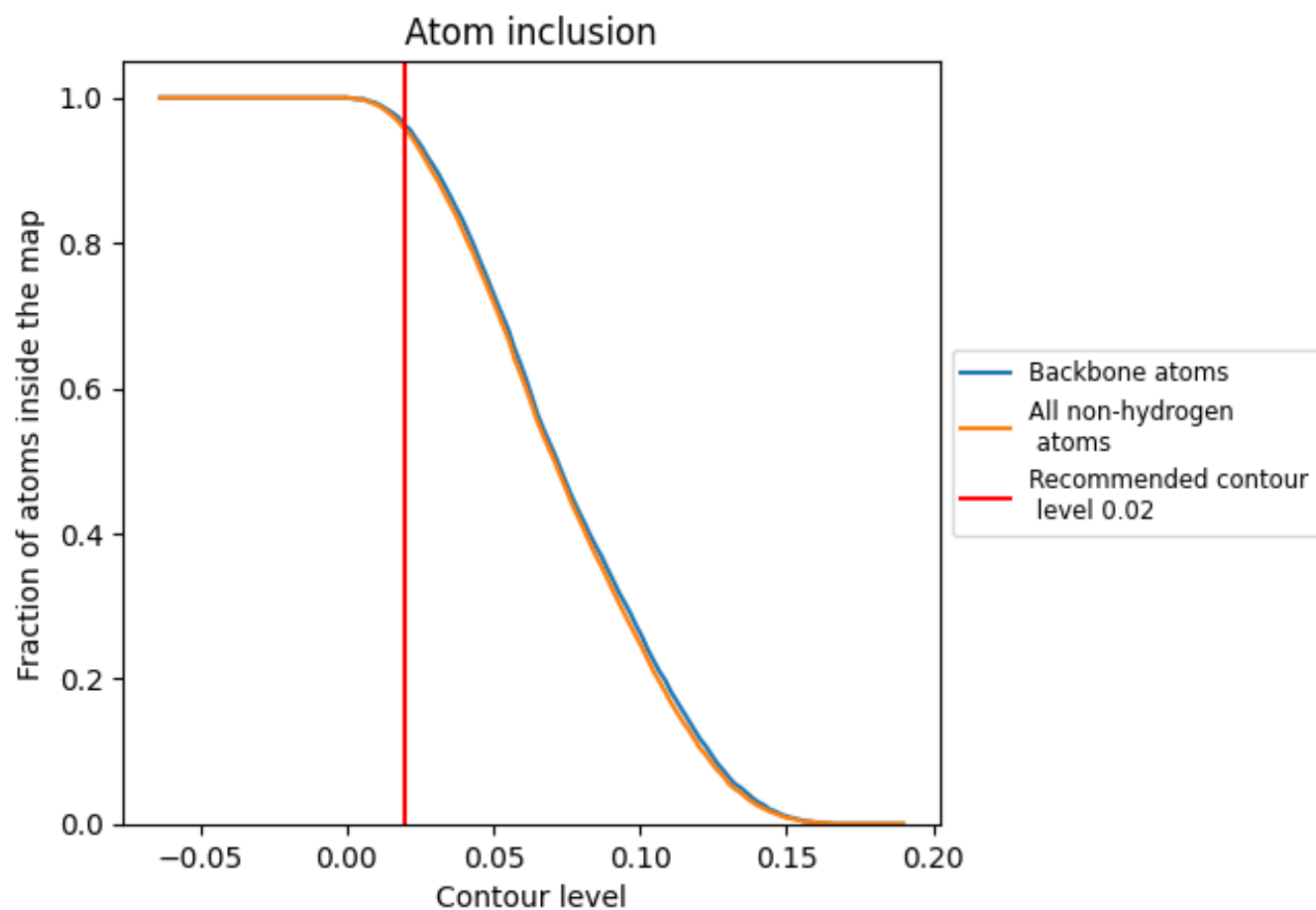
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9550	 0.5850
A	 0.9570	 0.5880
B	 0.9540	 0.5850
C	 0.9580	 0.5890
D	 0.9540	 0.5860
E	 0.9570	 0.5860
F	 0.9540	 0.5850
G	 0.9580	 0.5860
H	 0.9540	 0.5840
I	 0.9840	 0.5540
J	 0.9600	 0.5130
K	 0.9800	 0.5370
L	 0.7500	 0.4930
M	 0.9840	 0.5480
N	 0.9600	 0.5160
O	 0.9800	 0.5300
P	 0.7500	 0.5100
Q	 0.9840	 0.5470
R	 0.9600	 0.5080
S	 0.9800	 0.5280
T	 0.7500	 0.4760
U	 0.9840	 0.5450
V	 0.9600	 0.5120
W	 0.9800	 0.5410
X	 0.7500	 0.4860

