



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2025 – 04:29 PM EDT

PDB ID : 8VPF  
EMDB ID : EMD-43407  
Title : Structure of SARS-CoV spike in complex with CoV1-65 Fab (NTD-bound)  
Authors : Bangaru, S.; Ward, A.B.  
Deposited on : 2024-01-16  
Resolution : 3.20 Å(reported)  
Based on initial model : 6crx

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

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

A user guide is available at

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

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 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) : 2.41.4

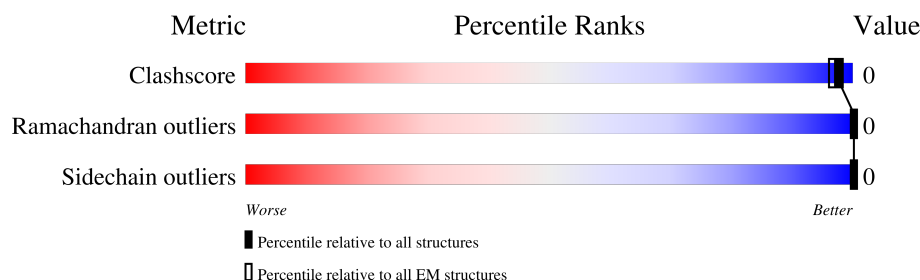
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1249	
1	B	1249	
1	C	1249	
2	D	231	
2	E	231	
2	M	231	
3	F	217	
3	G	217	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	N	217	 47% 51%
4	H	2	 50% 100%
4	I	2	 50% 100%
4	K	2	 100%
4	L	2	 50% 100%
4	O	2	 50% 100%
4	Q	2	 100%
4	R	2	 50% 100%
4	S	2	 50% 100%
4	U	2	 100%
5	J	3	 33% 100%
5	P	3	 33% 100%
5	T	3	 33% 100%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 23832 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	776	Total	C	N	O	S	0	0
			6011	3836	997	1148	30		
1	B	776	Total	C	N	O	S	0	0
			6011	3836	997	1148	30		
1	C	776	Total	C	N	O	S	0	0
			6011	3836	997	1148	30		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	577	ALA	SER	variant	UNP P59594
A	968	PRO	LYS	conflict	UNP P59594
A	969	PRO	VAL	conflict	UNP P59594
A	1191	GLY	-	expression tag	UNP P59594
A	1192	SER	-	expression tag	UNP P59594
A	1193	GLY	-	expression tag	UNP P59594
A	1194	TYR	-	expression tag	UNP P59594
A	1195	ILE	-	expression tag	UNP P59594
A	1196	PRO	-	expression tag	UNP P59594
A	1197	GLU	-	expression tag	UNP P59594
A	1198	ALA	-	expression tag	UNP P59594
A	1199	PRO	-	expression tag	UNP P59594
A	1200	ARG	-	expression tag	UNP P59594
A	1201	ASP	-	expression tag	UNP P59594
A	1202	GLY	-	expression tag	UNP P59594
A	1203	GLN	-	expression tag	UNP P59594
A	1204	ALA	-	expression tag	UNP P59594
A	1205	TYR	-	expression tag	UNP P59594
A	1206	VAL	-	expression tag	UNP P59594
A	1207	ARG	-	expression tag	UNP P59594
A	1208	LYS	-	expression tag	UNP P59594
A	1209	ASP	-	expression tag	UNP P59594
A	1210	GLY	-	expression tag	UNP P59594
A	1211	GLU	-	expression tag	UNP P59594

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	1212	TRP	-	expression tag	UNP P59594
A	1213	VAL	-	expression tag	UNP P59594
A	1214	LEU	-	expression tag	UNP P59594
A	1215	LEU	-	expression tag	UNP P59594
A	1216	SER	-	expression tag	UNP P59594
A	1217	THR	-	expression tag	UNP P59594
A	1218	PHE	-	expression tag	UNP P59594
A	1219	LEU	-	expression tag	UNP P59594
A	1220	GLY	-	expression tag	UNP P59594
A	1221	ARG	-	expression tag	UNP P59594
A	1222	SER	-	expression tag	UNP P59594
A	1223	LEU	-	expression tag	UNP P59594
A	1224	GLU	-	expression tag	UNP P59594
A	1225	VAL	-	expression tag	UNP P59594
A	1226	LEU	-	expression tag	UNP P59594
A	1227	PHE	-	expression tag	UNP P59594
A	1228	GLN	-	expression tag	UNP P59594
A	1229	GLY	-	expression tag	UNP P59594
A	1230	PRO	-	expression tag	UNP P59594
A	1231	GLY	-	expression tag	UNP P59594
A	1232	HIS	-	expression tag	UNP P59594
A	1233	HIS	-	expression tag	UNP P59594
A	1234	HIS	-	expression tag	UNP P59594
A	1235	HIS	-	expression tag	UNP P59594
A	1236	HIS	-	expression tag	UNP P59594
A	1237	HIS	-	expression tag	UNP P59594
A	1238	HIS	-	expression tag	UNP P59594
A	1239	HIS	-	expression tag	UNP P59594
A	1240	SER	-	expression tag	UNP P59594
A	1241	ALA	-	expression tag	UNP P59594
A	1242	TRP	-	expression tag	UNP P59594
A	1243	SER	-	expression tag	UNP P59594
A	1244	HIS	-	expression tag	UNP P59594
A	1245	PRO	-	expression tag	UNP P59594
A	1246	GLN	-	expression tag	UNP P59594
A	1247	PHE	-	expression tag	UNP P59594
A	1248	GLU	-	expression tag	UNP P59594
A	1249	LYS	-	expression tag	UNP P59594
B	577	ALA	SER	variant	UNP P59594
B	968	PRO	LYS	conflict	UNP P59594
B	969	PRO	VAL	conflict	UNP P59594
B	1191	GLY	-	expression tag	UNP P59594

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	1192	SER	-	expression tag	UNP P59594
B	1193	GLY	-	expression tag	UNP P59594
B	1194	TYR	-	expression tag	UNP P59594
B	1195	ILE	-	expression tag	UNP P59594
B	1196	PRO	-	expression tag	UNP P59594
B	1197	GLU	-	expression tag	UNP P59594
B	1198	ALA	-	expression tag	UNP P59594
B	1199	PRO	-	expression tag	UNP P59594
B	1200	ARG	-	expression tag	UNP P59594
B	1201	ASP	-	expression tag	UNP P59594
B	1202	GLY	-	expression tag	UNP P59594
B	1203	GLN	-	expression tag	UNP P59594
B	1204	ALA	-	expression tag	UNP P59594
B	1205	TYR	-	expression tag	UNP P59594
B	1206	VAL	-	expression tag	UNP P59594
B	1207	ARG	-	expression tag	UNP P59594
B	1208	LYS	-	expression tag	UNP P59594
B	1209	ASP	-	expression tag	UNP P59594
B	1210	GLY	-	expression tag	UNP P59594
B	1211	GLU	-	expression tag	UNP P59594
B	1212	TRP	-	expression tag	UNP P59594
B	1213	VAL	-	expression tag	UNP P59594
B	1214	LEU	-	expression tag	UNP P59594
B	1215	LEU	-	expression tag	UNP P59594
B	1216	SER	-	expression tag	UNP P59594
B	1217	THR	-	expression tag	UNP P59594
B	1218	PHE	-	expression tag	UNP P59594
B	1219	LEU	-	expression tag	UNP P59594
B	1220	GLY	-	expression tag	UNP P59594
B	1221	ARG	-	expression tag	UNP P59594
B	1222	SER	-	expression tag	UNP P59594
B	1223	LEU	-	expression tag	UNP P59594
B	1224	GLU	-	expression tag	UNP P59594
B	1225	VAL	-	expression tag	UNP P59594
B	1226	LEU	-	expression tag	UNP P59594
B	1227	PHE	-	expression tag	UNP P59594
B	1228	GLN	-	expression tag	UNP P59594
B	1229	GLY	-	expression tag	UNP P59594
B	1230	PRO	-	expression tag	UNP P59594
B	1231	GLY	-	expression tag	UNP P59594
B	1232	HIS	-	expression tag	UNP P59594
B	1233	HIS	-	expression tag	UNP P59594

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	1234	HIS	-	expression tag	UNP P59594
B	1235	HIS	-	expression tag	UNP P59594
B	1236	HIS	-	expression tag	UNP P59594
B	1237	HIS	-	expression tag	UNP P59594
B	1238	HIS	-	expression tag	UNP P59594
B	1239	HIS	-	expression tag	UNP P59594
B	1240	SER	-	expression tag	UNP P59594
B	1241	ALA	-	expression tag	UNP P59594
B	1242	TRP	-	expression tag	UNP P59594
B	1243	SER	-	expression tag	UNP P59594
B	1244	HIS	-	expression tag	UNP P59594
B	1245	PRO	-	expression tag	UNP P59594
B	1246	GLN	-	expression tag	UNP P59594
B	1247	PHE	-	expression tag	UNP P59594
B	1248	GLU	-	expression tag	UNP P59594
B	1249	LYS	-	expression tag	UNP P59594
C	577	ALA	SER	variant	UNP P59594
C	968	PRO	LYS	conflict	UNP P59594
C	969	PRO	VAL	conflict	UNP P59594
C	1191	GLY	-	expression tag	UNP P59594
C	1192	SER	-	expression tag	UNP P59594
C	1193	GLY	-	expression tag	UNP P59594
C	1194	TYR	-	expression tag	UNP P59594
C	1195	ILE	-	expression tag	UNP P59594
C	1196	PRO	-	expression tag	UNP P59594
C	1197	GLU	-	expression tag	UNP P59594
C	1198	ALA	-	expression tag	UNP P59594
C	1199	PRO	-	expression tag	UNP P59594
C	1200	ARG	-	expression tag	UNP P59594
C	1201	ASP	-	expression tag	UNP P59594
C	1202	GLY	-	expression tag	UNP P59594
C	1203	GLN	-	expression tag	UNP P59594
C	1204	ALA	-	expression tag	UNP P59594
C	1205	TYR	-	expression tag	UNP P59594
C	1206	VAL	-	expression tag	UNP P59594
C	1207	ARG	-	expression tag	UNP P59594
C	1208	LYS	-	expression tag	UNP P59594
C	1209	ASP	-	expression tag	UNP P59594
C	1210	GLY	-	expression tag	UNP P59594
C	1211	GLU	-	expression tag	UNP P59594
C	1212	TRP	-	expression tag	UNP P59594
C	1213	VAL	-	expression tag	UNP P59594

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	1214	LEU	-	expression tag	UNP P59594
C	1215	LEU	-	expression tag	UNP P59594
C	1216	SER	-	expression tag	UNP P59594
C	1217	THR	-	expression tag	UNP P59594
C	1218	PHE	-	expression tag	UNP P59594
C	1219	LEU	-	expression tag	UNP P59594
C	1220	GLY	-	expression tag	UNP P59594
C	1221	ARG	-	expression tag	UNP P59594
C	1222	SER	-	expression tag	UNP P59594
C	1223	LEU	-	expression tag	UNP P59594
C	1224	GLU	-	expression tag	UNP P59594
C	1225	VAL	-	expression tag	UNP P59594
C	1226	LEU	-	expression tag	UNP P59594
C	1227	PHE	-	expression tag	UNP P59594
C	1228	GLN	-	expression tag	UNP P59594
C	1229	GLY	-	expression tag	UNP P59594
C	1230	PRO	-	expression tag	UNP P59594
C	1231	GLY	-	expression tag	UNP P59594
C	1232	HIS	-	expression tag	UNP P59594
C	1233	HIS	-	expression tag	UNP P59594
C	1234	HIS	-	expression tag	UNP P59594
C	1235	HIS	-	expression tag	UNP P59594
C	1236	HIS	-	expression tag	UNP P59594
C	1237	HIS	-	expression tag	UNP P59594
C	1238	HIS	-	expression tag	UNP P59594
C	1239	HIS	-	expression tag	UNP P59594
C	1240	SER	-	expression tag	UNP P59594
C	1241	ALA	-	expression tag	UNP P59594
C	1242	TRP	-	expression tag	UNP P59594
C	1243	SER	-	expression tag	UNP P59594
C	1244	HIS	-	expression tag	UNP P59594
C	1245	PRO	-	expression tag	UNP P59594
C	1246	GLN	-	expression tag	UNP P59594
C	1247	PHE	-	expression tag	UNP P59594
C	1248	GLU	-	expression tag	UNP P59594
C	1249	LYS	-	expression tag	UNP P59594

- Molecule 2 is a protein called CoV1-65 antibody heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	126	Total	C	N	O	S	
			953	600	167	182	4	
								0
								0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	126	Total	C	N	O	S	0	0
			953	600	167	182	4		
2	E	126	Total	C	N	O	S	0	0
			953	600	167	182	4		

- Molecule 3 is a protein called CoV1-65 antibody light chain.

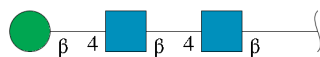
Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	107	Total	C	N	O	S	0	0
			787	494	130	160	3		
3	F	107	Total	C	N	O	S	0	0
			787	494	130	160	3		
3	G	107	Total	C	N	O	S	0	0
			787	494	130	160	3		

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



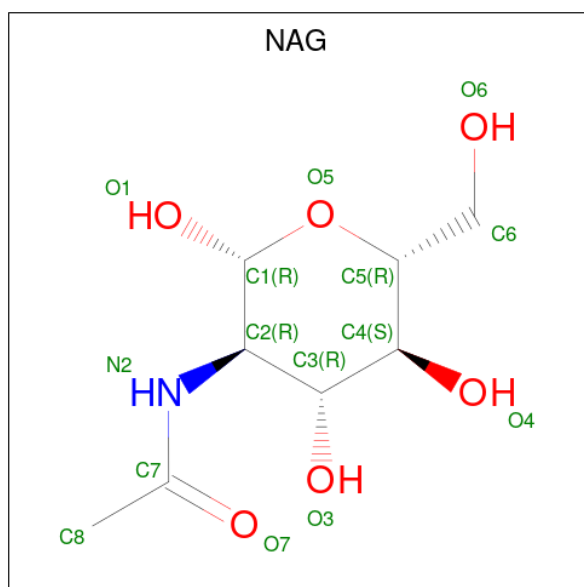
Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	3	Total	C	N	O	0	0
			39	22	2	15		
5	P	3	Total	C	N	O	0	0
			39	22	2	15		
5	T	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

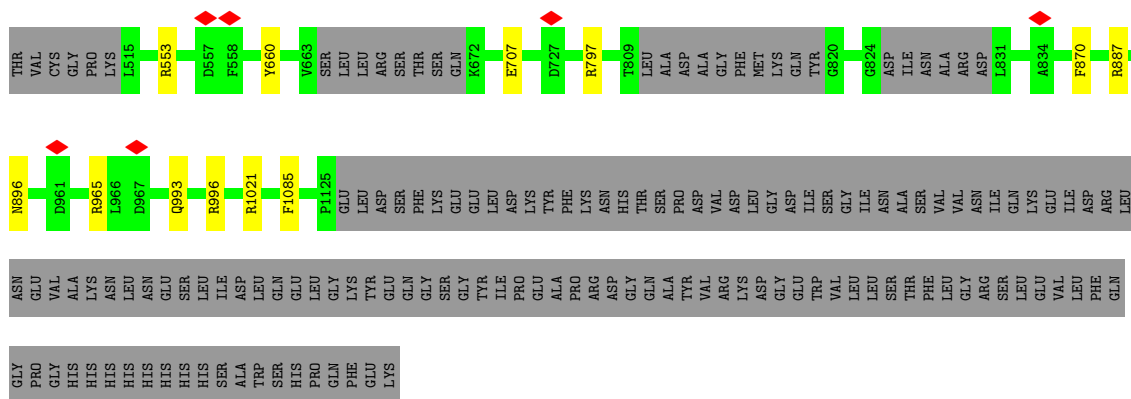
Continued on next page...

*Continued from previous page...*

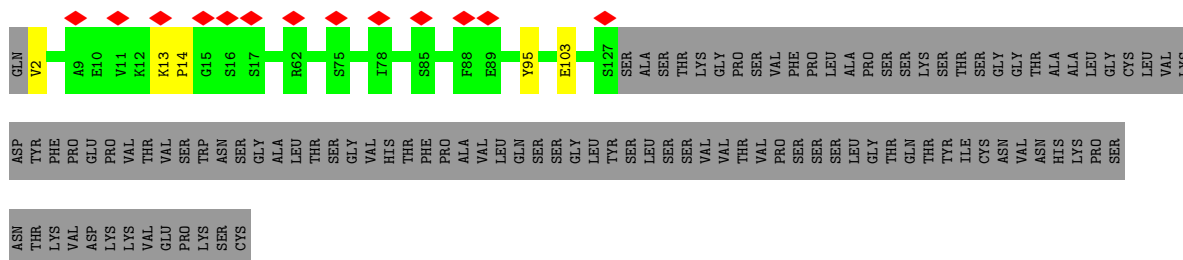
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6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



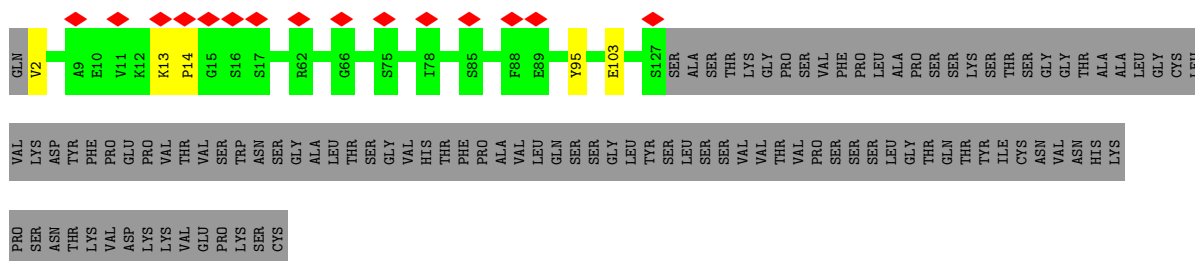




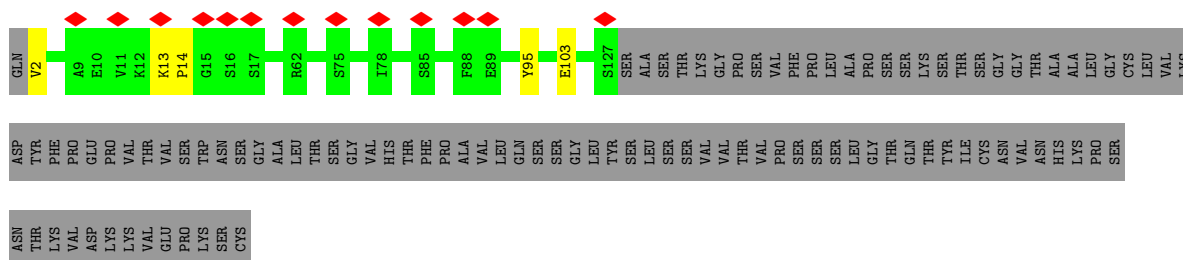
- Molecule 2: CoV1-65 antibody heavy chain



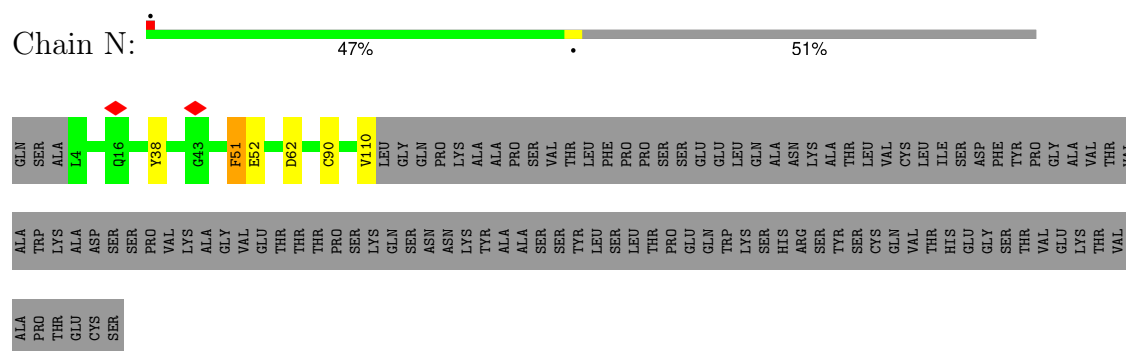
- Molecule 2: CoV1-65 antibody heavy chain



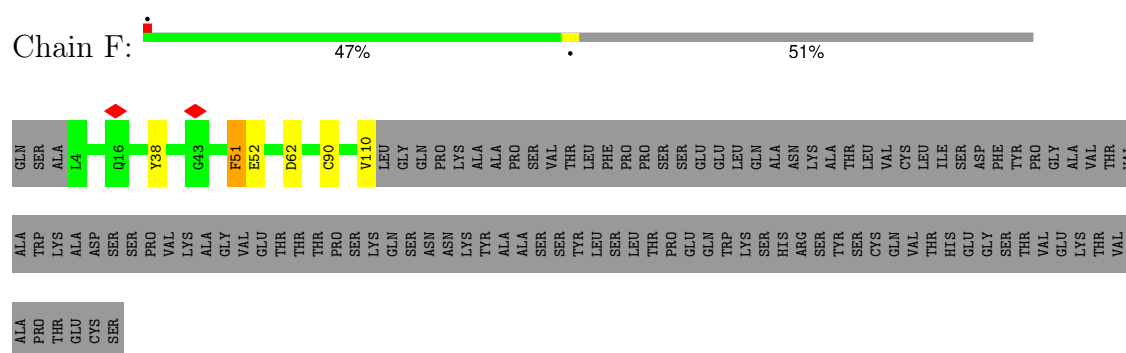
- Molecule 2: CoV1-65 antibody heavy chain



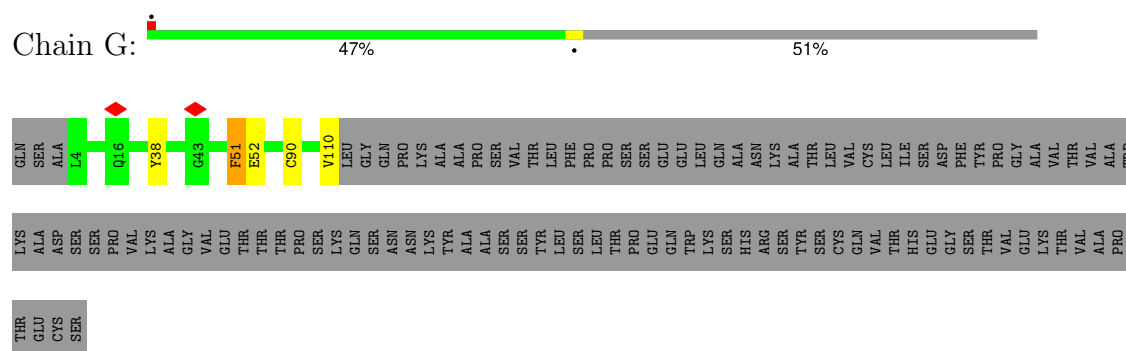
- Molecule 3: CoV1-65 antibody light chain



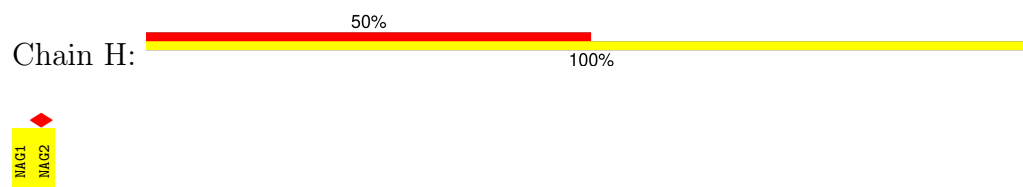
- Molecule 3: CoV1-65 antibody light chain



- Molecule 3: CoV1-65 antibody light chain



- 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 K:  100%



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

Chain L:  50%  
 100%



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

Chain O:  50%  
 100%



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

Chain Q:  100%



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

Chain R:  50%  
 100%



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

Chain S:  50%  
 100%





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

Chain U:  100%



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

Chain J:  33% 100%



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

Chain P:  33% 100%



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

Chain T:  33% 100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	190300	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.011	Depositor
Minimum map value	-1.240	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	417.99997, 417.99997, 417.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.10	16/6137 (0.3%)	0.93	18/8342 (0.2%)
1	B	1.10	16/6137 (0.3%)	0.93	18/8342 (0.2%)
1	C	1.10	16/6137 (0.3%)	0.93	18/8342 (0.2%)
2	D	1.01	2/972 (0.2%)	0.89	1/1318 (0.1%)
2	E	1.01	2/972 (0.2%)	0.89	1/1318 (0.1%)
2	M	1.02	2/972 (0.2%)	0.89	1/1318 (0.1%)
3	F	1.10	5/806 (0.6%)	1.02	1/1094 (0.1%)
3	G	1.10	5/806 (0.6%)	1.02	1/1094 (0.1%)
3	N	1.10	5/806 (0.6%)	1.02	1/1094 (0.1%)
All	All	1.09	69/23745 (0.3%)	0.94	60/32262 (0.2%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	TYR	CG-CD2	8.09	1.49	1.39
1	B	30	TYR	CG-CD2	8.07	1.49	1.39
1	C	30	TYR	CG-CD2	8.07	1.49	1.39
1	B	30	TYR	CE1-CZ	7.51	1.48	1.38
1	C	30	TYR	CE1-CZ	7.51	1.48	1.38
1	C	30	TYR	CG-CD1	7.49	1.48	1.39
1	A	30	TYR	CG-CD1	7.48	1.48	1.39
1	B	30	TYR	CG-CD1	7.47	1.48	1.39
1	A	30	TYR	CE1-CZ	7.46	1.48	1.38
1	B	896	ASN	CB-CG	-6.99	1.34	1.51
1	A	896	ASN	CB-CG	-6.98	1.34	1.51
1	C	896	ASN	CB-CG	-6.97	1.35	1.51
3	F	38	TYR	CB-CG	-6.84	1.41	1.51
3	G	38	TYR	CB-CG	-6.81	1.41	1.51
3	N	38	TYR	CB-CG	-6.78	1.41	1.51
1	A	30	TYR	CE2-CZ	6.43	1.47	1.38
1	A	184	GLU	CD-OE2	-6.43	1.18	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	TYR	CE2-CZ	6.42	1.46	1.38
1	C	30	TYR	CE2-CZ	6.41	1.46	1.38
1	B	184	GLU	CD-OE2	-6.41	1.18	1.25
1	C	184	GLU	CD-OE2	-6.40	1.18	1.25
1	B	870	PHE	CB-CG	-5.88	1.41	1.51
1	A	870	PHE	CB-CG	-5.87	1.41	1.51
1	C	870	PHE	CB-CG	-5.86	1.41	1.51
3	N	38	TYR	CD2-CE2	-5.70	1.30	1.39
3	F	38	TYR	CD2-CE2	-5.69	1.30	1.39
3	G	38	TYR	CD2-CE2	-5.67	1.30	1.39
3	G	51	PHE	CB-CG	-5.66	1.41	1.51
1	B	184	GLU	CD-OE1	-5.64	1.19	1.25
3	N	51	PHE	CB-CG	-5.64	1.41	1.51
3	F	51	PHE	CB-CG	-5.63	1.41	1.51
1	C	184	GLU	CD-OE1	-5.60	1.19	1.25
1	A	1085	PHE	CB-CG	-5.59	1.41	1.51
1	A	184	GLU	CD-OE1	-5.58	1.19	1.25
1	B	1085	PHE	CB-CG	-5.56	1.41	1.51
1	C	1085	PHE	CB-CG	-5.56	1.41	1.51
2	M	2	VAL	CB-CG1	5.53	1.64	1.52
2	E	2	VAL	CB-CG1	5.52	1.64	1.52
2	D	2	VAL	CB-CG1	5.51	1.64	1.52
1	C	285	GLU	CG-CD	-5.50	1.43	1.51
1	A	30	TYR	CB-CG	5.50	1.59	1.51
1	B	30	TYR	CB-CG	5.49	1.59	1.51
1	A	285	GLU	CG-CD	-5.48	1.43	1.51
1	C	30	TYR	CB-CG	5.48	1.59	1.51
1	B	285	GLU	CG-CD	-5.47	1.43	1.51
1	A	707	GLU	CD-OE2	-5.40	1.19	1.25
1	A	30	TYR	CD1-CE1	5.38	1.47	1.39
1	C	30	TYR	CD1-CE1	5.37	1.47	1.39
1	C	707	GLU	CD-OE2	-5.35	1.19	1.25
1	B	707	GLU	CD-OE2	-5.35	1.19	1.25
1	B	30	TYR	CD1-CE1	5.34	1.47	1.39
1	C	707	GLU	CD-OE1	-5.22	1.20	1.25
1	B	63	TYR	CD2-CE2	-5.21	1.31	1.39
1	B	93	GLU	CG-CD	-5.21	1.44	1.51
1	A	93	GLU	CG-CD	-5.20	1.44	1.51
1	B	707	GLU	CD-OE1	-5.20	1.20	1.25
1	C	63	TYR	CD2-CE2	-5.20	1.31	1.39
3	N	90	CYS	CB-SG	-5.19	1.73	1.81
3	N	110	VAL	CB-CG1	5.19	1.63	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	90	CYS	CB-SG	-5.19	1.73	1.81
1	C	93	GLU	CG-CD	-5.18	1.44	1.51
3	G	110	VAL	CB-CG1	5.18	1.63	1.52
1	A	707	GLU	CD-OE1	-5.18	1.20	1.25
1	A	63	TYR	CD2-CE2	-5.18	1.31	1.39
3	F	110	VAL	CB-CG1	5.17	1.63	1.52
3	G	90	CYS	CB-SG	-5.16	1.73	1.81
2	M	103	GLU	CD-OE1	-5.11	1.20	1.25
2	E	103	GLU	CD-OE1	-5.09	1.20	1.25
2	D	103	GLU	CD-OE1	-5.05	1.20	1.25

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	797	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	A	797	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	C	797	ARG	NE-CZ-NH2	-9.43	115.58	120.30
3	G	38	TYR	CB-CG-CD2	-8.07	116.16	121.00
1	A	887	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	B	887	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	C	887	ARG	NE-CZ-NH2	-8.03	116.28	120.30
3	N	38	TYR	CB-CG-CD2	-8.01	116.19	121.00
3	F	38	TYR	CB-CG-CD2	-8.00	116.20	121.00
1	C	262	PHE	CB-CG-CD2	-7.10	115.83	120.80
1	B	262	PHE	CB-CG-CD2	-7.10	115.83	120.80
1	A	262	PHE	CB-CG-CD2	-7.09	115.83	120.80
1	A	197	TYR	CB-CG-CD2	-7.03	116.78	121.00
1	C	197	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	B	197	TYR	CB-CG-CD2	-6.95	116.83	121.00
1	A	797	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	B	797	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	797	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	870	PHE	CB-CG-CD2	-6.70	116.11	120.80
1	C	870	PHE	CB-CG-CD2	-6.67	116.13	120.80
1	A	870	PHE	CB-CG-CD2	-6.65	116.15	120.80
1	C	1021	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	266	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	A	63	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	A	1021	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	266	TYR	CB-CG-CD2	-6.47	117.11	121.00
1	C	63	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	B	63	TYR	CB-CG-CD2	-6.45	117.13	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1021	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	965	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	965	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	C	965	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	C	266	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	A	315	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	C	315	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	315	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	262	PHE	CB-CG-CD1	6.22	125.16	120.80
1	B	262	PHE	CB-CG-CD1	6.22	125.16	120.80
1	C	262	PHE	CB-CG-CD1	6.19	125.13	120.80
1	C	88	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	B	88	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	A	88	TYR	CB-CG-CD2	-6.11	117.34	121.00
1	A	660	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	B	660	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	C	660	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	B	48	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	C	48	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	48	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	887	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	887	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	887	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	553	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	553	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	553	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	315	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	315	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	C	315	ARG	NE-CZ-NH2	-5.23	117.68	120.30
2	M	95	TYR	CB-CG-CD1	-5.08	117.95	121.00
2	D	95	TYR	CB-CG-CD1	-5.04	117.97	121.00
2	E	95	TYR	CB-CG-CD1	-5.04	117.98	121.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6011	0	5893	3	0
1	B	6011	0	5893	4	0
1	C	6011	0	5893	3	0
2	D	953	0	941	1	0
2	E	953	0	941	1	0
2	M	953	0	941	1	0
3	F	787	0	747	2	0
3	G	787	0	747	1	0
3	N	787	0	747	2	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	K	28	0	24	0	0
4	L	28	0	25	0	0
4	O	28	0	25	0	0
4	Q	28	0	24	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	U	28	0	24	0	0
5	J	39	0	34	0	0
5	P	39	0	34	0	0
5	T	39	0	34	0	0
6	A	70	0	65	0	0
6	B	70	0	65	0	0
6	C	70	0	65	0	0
All	All	23832	0	23262	18	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 0.

All (18) 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:B:183:ARG:HG2	1:B:200:TYR:CD1	2.46	0.51
1:C:183:ARG:HG2	1:C:200:TYR:CD1	2.46	0.51
1:A:183:ARG:HG2	1:A:200:TYR:CD1	2.46	0.51
3:N:51:PHE:CZ	3:N:52:GLU:OE2	2.69	0.46
3:F:51:PHE:CZ	3:F:52:GLU:OE2	2.69	0.46
3:G:51:PHE:CZ	3:G:52:GLU:OE2	2.69	0.45
1:B:281:ASN:HB2	1:B:282:PRO:HD2	2.00	0.43
1:A:281:ASN:HB2	1:A:282:PRO:HD2	2.00	0.43
1:C:281:ASN:HB2	1:C:282:PRO:HD2	2.00	0.42
3:F:62:ASP:OD1	3:F:62:ASP:N	2.53	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:993:GLN:OE1	1:B:996:ARG:NH1	2.54	0.41
2:M:13:LYS:HB3	2:M:14:PRO:HD2	2.03	0.41
1:A:993:GLN:OE1	1:A:996:ARG:NH1	2.54	0.41
1:C:993:GLN:OE1	1:C:996:ARG:NH1	2.54	0.41
1:B:727:ASP:OD1	1:B:727:ASP:N	2.52	0.40
2:E:13:LYS:HB3	2:E:14:PRO:HD2	2.03	0.40
3:N:62:ASP:N	3:N:62:ASP:OD1	2.53	0.40
2:D:13:LYS:HB3	2:D:14:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	758/1249 (61%)	749 (99%)	9 (1%)	0	100	100
1	B	758/1249 (61%)	749 (99%)	9 (1%)	0	100	100
1	C	758/1249 (61%)	749 (99%)	9 (1%)	0	100	100
2	D	124/231 (54%)	121 (98%)	3 (2%)	0	100	100
2	E	124/231 (54%)	121 (98%)	3 (2%)	0	100	100
2	M	124/231 (54%)	121 (98%)	3 (2%)	0	100	100
3	F	105/217 (48%)	101 (96%)	4 (4%)	0	100	100
3	G	105/217 (48%)	101 (96%)	4 (4%)	0	100	100
3	N	105/217 (48%)	101 (96%)	4 (4%)	0	100	100
All	All	2961/5091 (58%)	2913 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	667/1083 (62%)	667 (100%)	0	100	100
1	B	667/1083 (62%)	667 (100%)	0	100	100
1	C	667/1083 (62%)	667 (100%)	0	100	100
2	D	101/192 (53%)	101 (100%)	0	100	100
2	E	101/192 (53%)	101 (100%)	0	100	100
2	M	101/192 (53%)	101 (100%)	0	100	100
3	F	87/181 (48%)	87 (100%)	0	100	100
3	G	87/181 (48%)	87 (100%)	0	100	100
3	N	87/181 (48%)	87 (100%)	0	100	100
All	All	2565/4368 (59%)	2565 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	B	78	ASN
1	C	78	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 ⓘ

27 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	H	1	1,4	14,14,15	2.19	5 (35%)	17,19,21	1.03	1 (5%)
4	NAG	H	2	4	14,14,15	2.03	6 (42%)	17,19,21	0.88	0
4	NAG	I	1	1,4	14,14,15	2.26	6 (42%)	17,19,21	1.03	0
4	NAG	I	2	4	14,14,15	2.12	6 (42%)	17,19,21	0.82	0
5	NAG	J	1	5,1	14,14,15	2.04	5 (35%)	17,19,21	1.07	1 (5%)
5	NAG	J	2	5	14,14,15	2.03	5 (35%)	17,19,21	0.98	2 (11%)
5	BMA	J	3	5	11,11,12	1.96	6 (54%)	15,15,17	0.74	0
4	NAG	K	1	1,4	14,14,15	2.21	7 (50%)	17,19,21	1.11	2 (11%)
4	NAG	K	2	4	14,14,15	2.01	5 (35%)	17,19,21	6.80	4 (23%)
4	NAG	L	1	1,4	14,14,15	2.18	5 (35%)	17,19,21	1.03	1 (5%)
4	NAG	L	2	4	14,14,15	2.03	6 (42%)	17,19,21	0.88	0
4	NAG	O	1	1,4	14,14,15	2.25	6 (42%)	17,19,21	1.03	0
4	NAG	O	2	4	14,14,15	2.12	6 (42%)	17,19,21	0.83	0
5	NAG	P	1	5,1	14,14,15	2.04	5 (35%)	17,19,21	1.07	1 (5%)
5	NAG	P	2	5	14,14,15	2.03	5 (35%)	17,19,21	0.98	2 (11%)
5	BMA	P	3	5	11,11,12	1.96	6 (54%)	15,15,17	0.74	0
4	NAG	Q	1	1,4	14,14,15	2.21	7 (50%)	17,19,21	1.11	2 (11%)
4	NAG	Q	2	4	14,14,15	2.00	5 (35%)	17,19,21	6.80	4 (23%)
4	NAG	R	1	1,4	14,14,15	2.19	5 (35%)	17,19,21	1.03	1 (5%)
4	NAG	R	2	4	14,14,15	2.03	6 (42%)	17,19,21	0.89	0
4	NAG	S	1	1,4	14,14,15	2.26	6 (42%)	17,19,21	1.03	0
4	NAG	S	2	4	14,14,15	2.12	6 (42%)	17,19,21	0.83	0
5	NAG	T	1	5,1	14,14,15	2.04	5 (35%)	17,19,21	1.07	1 (5%)
5	NAG	T	2	5	14,14,15	2.02	5 (35%)	17,19,21	0.97	2 (11%)
5	BMA	T	3	5	11,11,12	1.96	6 (54%)	15,15,17	0.74	0
4	NAG	U	1	1,4	14,14,15	2.21	7 (50%)	17,19,21	1.11	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	U	2	4	14,14,15	2.01	5 (35%)	17,19,21	6.81	4 (23%)

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	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	BMA	J	3	5	-	1/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	1/2/19/22	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
5	NAG	T	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
5	BMA	T	3	5	-	1/2/19/22	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	1	NAG	C1-C2	6.01	1.60	1.52
4	I	1	NAG	C1-C2	6.01	1.60	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	1	NAG	C1-C2	5.98	1.60	1.52
4	K	1	NAG	C1-C2	5.66	1.60	1.52
4	Q	1	NAG	C1-C2	5.64	1.60	1.52
4	U	1	NAG	C1-C2	5.63	1.60	1.52
5	T	1	NAG	C1-C2	5.41	1.59	1.52
5	J	1	NAG	C1-C2	5.41	1.59	1.52
5	P	1	NAG	C1-C2	5.39	1.59	1.52
4	H	1	NAG	C1-C2	5.38	1.59	1.52
4	L	1	NAG	C1-C2	5.38	1.59	1.52
4	R	1	NAG	C1-C2	5.35	1.59	1.52
4	I	2	NAG	C1-C2	5.04	1.59	1.52
4	S	2	NAG	C1-C2	5.04	1.59	1.52
4	O	2	NAG	C1-C2	5.02	1.59	1.52
4	K	2	NAG	C1-C2	4.80	1.58	1.52
4	U	2	NAG	C1-C2	4.78	1.58	1.52
4	H	2	NAG	C1-C2	4.75	1.58	1.52
4	Q	2	NAG	C1-C2	4.74	1.58	1.52
4	L	2	NAG	C1-C2	4.74	1.58	1.52
4	R	2	NAG	C1-C2	4.74	1.58	1.52
5	P	2	NAG	C1-C2	4.71	1.58	1.52
5	J	2	NAG	C1-C2	4.71	1.58	1.52
5	T	2	NAG	C1-C2	4.69	1.58	1.52
4	O	2	NAG	O5-C5	3.36	1.50	1.43
4	I	2	NAG	O5-C5	3.34	1.49	1.43
4	S	2	NAG	O5-C5	3.33	1.49	1.43
4	R	1	NAG	O5-C5	3.29	1.49	1.43
4	L	1	NAG	O5-C5	3.28	1.49	1.43
4	H	1	NAG	O5-C5	3.28	1.49	1.43
4	R	2	NAG	O5-C5	3.23	1.49	1.43
4	H	2	NAG	O5-C5	3.23	1.49	1.43
4	L	2	NAG	O5-C5	3.22	1.49	1.43
5	T	3	BMA	C2-C3	3.19	1.57	1.52
5	J	3	BMA	C2-C3	3.18	1.57	1.52
5	P	3	BMA	C2-C3	3.16	1.57	1.52
5	J	3	BMA	O5-C5	3.10	1.49	1.43
5	P	3	BMA	O5-C5	3.08	1.49	1.43
4	Q	1	NAG	O5-C5	3.07	1.49	1.43
5	T	3	BMA	O5-C5	3.07	1.49	1.43
4	K	1	NAG	O5-C5	3.07	1.49	1.43
4	U	1	NAG	O5-C5	3.06	1.49	1.43
4	Q	2	NAG	O5-C5	3.03	1.49	1.43
5	J	2	NAG	O5-C5	3.03	1.49	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	2	NAG	O5-C5	3.03	1.49	1.43
4	U	2	NAG	O5-C5	3.02	1.49	1.43
5	P	2	NAG	O5-C5	3.01	1.49	1.43
5	T	2	NAG	O5-C5	2.99	1.49	1.43
4	S	1	NAG	O5-C5	2.83	1.49	1.43
4	I	1	NAG	O5-C5	2.83	1.48	1.43
4	O	1	NAG	O5-C5	2.81	1.48	1.43
5	J	3	BMA	C1-C2	2.71	1.58	1.52
5	T	3	BMA	C1-C2	2.70	1.58	1.52
5	P	3	BMA	C1-C2	2.69	1.58	1.52
4	O	2	NAG	C3-C2	2.63	1.58	1.52
4	I	2	NAG	C3-C2	2.61	1.58	1.52
4	S	2	NAG	C3-C2	2.61	1.58	1.52
4	H	1	NAG	O5-C1	2.58	1.48	1.43
4	Q	1	NAG	C4-C5	2.57	1.58	1.53
4	K	1	NAG	C4-C5	2.57	1.58	1.53
4	U	1	NAG	C4-C5	2.57	1.58	1.53
4	R	1	NAG	O5-C1	2.57	1.48	1.43
4	L	1	NAG	O5-C1	2.54	1.48	1.43
4	L	2	NAG	C3-C2	2.51	1.57	1.52
4	H	2	NAG	C3-C2	2.51	1.57	1.52
5	T	2	NAG	C4-C5	2.50	1.58	1.53
5	P	2	NAG	C4-C5	2.50	1.58	1.53
5	T	3	BMA	C4-C5	2.49	1.58	1.53
4	R	2	NAG	C3-C2	2.48	1.57	1.52
5	J	2	NAG	C4-C5	2.48	1.58	1.53
5	J	3	BMA	C4-C5	2.48	1.58	1.53
5	P	3	BMA	C4-C5	2.47	1.58	1.53
4	O	1	NAG	C4-C5	2.46	1.58	1.53
4	I	1	NAG	C4-C5	2.46	1.58	1.53
4	S	1	NAG	C4-C5	2.43	1.58	1.53
4	L	1	NAG	C3-C2	2.43	1.57	1.52
4	H	1	NAG	C3-C2	2.42	1.57	1.52
4	R	1	NAG	C3-C2	2.42	1.57	1.52
5	P	2	NAG	C3-C2	2.40	1.57	1.52
5	J	2	NAG	C3-C2	2.40	1.57	1.52
4	K	2	NAG	C3-C2	2.39	1.57	1.52
5	T	2	NAG	C3-C2	2.39	1.57	1.52
4	L	2	NAG	C4-C5	2.37	1.58	1.53
4	U	2	NAG	C3-C2	2.37	1.57	1.52
4	H	2	NAG	C4-C5	2.37	1.58	1.53
4	R	2	NAG	C4-C5	2.37	1.58	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	2	NAG	C3-C2	2.37	1.57	1.52
5	J	1	NAG	O5-C5	2.35	1.48	1.43
5	P	1	NAG	O5-C5	2.35	1.48	1.43
4	U	2	NAG	C4-C5	2.35	1.58	1.53
5	T	1	NAG	O5-C5	2.34	1.48	1.43
5	J	1	NAG	C3-C2	2.33	1.57	1.52
5	P	1	NAG	C3-C2	2.33	1.57	1.52
4	Q	2	NAG	C4-C5	2.33	1.58	1.53
5	T	1	NAG	C3-C2	2.32	1.57	1.52
4	I	2	NAG	C4-C5	2.31	1.58	1.53
4	K	2	NAG	C4-C5	2.31	1.57	1.53
4	O	2	NAG	C4-C5	2.31	1.57	1.53
4	S	2	NAG	C4-C5	2.30	1.57	1.53
4	S	1	NAG	C3-C2	2.27	1.57	1.52
4	I	1	NAG	C3-C2	2.26	1.57	1.52
4	O	1	NAG	C3-C2	2.24	1.57	1.52
4	U	1	NAG	C3-C2	2.22	1.57	1.52
4	K	1	NAG	C3-C2	2.21	1.57	1.52
4	K	2	NAG	C4-C3	2.20	1.58	1.52
4	Q	2	NAG	C4-C3	2.20	1.58	1.52
4	U	2	NAG	C4-C3	2.20	1.58	1.52
4	Q	1	NAG	C3-C2	2.20	1.57	1.52
4	I	2	NAG	C2-N2	2.18	1.49	1.46
4	O	2	NAG	C2-N2	2.17	1.49	1.46
4	S	2	NAG	C2-N2	2.16	1.49	1.46
4	S	1	NAG	O5-C1	2.15	1.47	1.43
5	T	2	NAG	C4-C3	2.15	1.57	1.52
4	O	1	NAG	O5-C1	2.15	1.47	1.43
4	I	1	NAG	O5-C1	2.15	1.47	1.43
5	J	2	NAG	C4-C3	2.14	1.57	1.52
4	O	1	NAG	C4-C3	2.14	1.57	1.52
4	I	1	NAG	C4-C3	2.13	1.57	1.52
4	S	1	NAG	C4-C3	2.13	1.57	1.52
5	P	2	NAG	C4-C3	2.12	1.57	1.52
4	Q	1	NAG	C2-N2	2.10	1.49	1.46
4	U	1	NAG	C2-N2	2.09	1.49	1.46
4	H	2	NAG	C4-C3	2.08	1.57	1.52
4	H	2	NAG	C2-N2	2.08	1.49	1.46
4	R	2	NAG	C4-C3	2.08	1.57	1.52
4	K	1	NAG	C2-N2	2.07	1.49	1.46
4	L	2	NAG	C4-C3	2.07	1.57	1.52
5	P	1	NAG	C4-C3	2.07	1.57	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	1	NAG	C4-C3	2.07	1.57	1.52
4	R	1	NAG	C4-C5	2.06	1.57	1.53
4	U	1	NAG	C4-C3	2.06	1.57	1.52
4	Q	1	NAG	O5-C1	2.06	1.47	1.43
4	K	1	NAG	O5-C1	2.06	1.47	1.43
4	U	1	NAG	O5-C1	2.06	1.47	1.43
4	Q	1	NAG	C4-C3	2.06	1.57	1.52
4	S	2	NAG	C4-C3	2.06	1.57	1.52
4	L	2	NAG	C2-N2	2.06	1.49	1.46
4	I	2	NAG	C4-C3	2.06	1.57	1.52
5	T	3	BMA	O5-C1	2.06	1.47	1.43
5	J	1	NAG	C4-C3	2.05	1.57	1.52
5	J	3	BMA	C4-C3	2.05	1.57	1.52
4	O	2	NAG	C4-C3	2.05	1.57	1.52
5	P	3	BMA	C4-C3	2.05	1.57	1.52
4	R	2	NAG	C2-N2	2.05	1.49	1.46
5	P	3	BMA	O5-C1	2.05	1.47	1.43
5	T	3	BMA	C4-C3	2.05	1.57	1.52
5	P	1	NAG	C4-C5	2.04	1.57	1.53
4	H	1	NAG	C4-C5	2.04	1.57	1.53
4	L	1	NAG	C4-C5	2.04	1.57	1.53
4	K	1	NAG	C4-C3	2.04	1.57	1.52
5	J	3	BMA	O5-C1	2.04	1.47	1.43
5	J	1	NAG	C4-C5	2.03	1.57	1.53
5	T	1	NAG	C4-C5	2.02	1.57	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	2	NAG	C2-N2-C7	27.34	159.53	122.90
4	Q	2	NAG	C2-N2-C7	27.32	159.52	122.90
4	K	2	NAG	C2-N2-C7	27.32	159.51	122.90
4	Q	2	NAG	C8-C7-N2	4.91	124.27	116.12
4	U	2	NAG	C8-C7-N2	4.91	124.26	116.12
4	K	2	NAG	C8-C7-N2	4.91	124.26	116.12
4	U	1	NAG	O4-C4-C3	-2.53	104.42	110.38
4	Q	1	NAG	O4-C4-C3	-2.51	104.46	110.38
4	K	1	NAG	O4-C4-C3	-2.51	104.46	110.38
4	U	2	NAG	O7-C7-N2	-2.48	117.60	121.98
4	K	2	NAG	O7-C7-N2	-2.46	117.64	121.98
4	Q	2	NAG	O7-C7-N2	-2.46	117.64	121.98
4	L	1	NAG	C8-C7-N2	2.43	120.15	116.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C8-C7-N2	2.42	120.14	116.12
4	R	1	NAG	C8-C7-N2	2.42	120.13	116.12
5	J	2	NAG	C8-C7-N2	2.40	120.09	116.12
5	P	2	NAG	C8-C7-N2	2.39	120.09	116.12
5	T	2	NAG	C8-C7-N2	2.38	120.07	116.12
5	T	1	NAG	C1-O5-C5	2.25	115.21	112.19
5	P	1	NAG	C1-O5-C5	2.25	115.20	112.19
5	J	1	NAG	C1-O5-C5	2.25	115.19	112.19
4	Q	2	NAG	O7-C7-C8	-2.22	118.10	122.05
4	K	2	NAG	O7-C7-C8	-2.22	118.11	122.05
4	U	2	NAG	O7-C7-C8	-2.20	118.14	122.05
5	J	2	NAG	O7-C7-C8	-2.10	118.32	122.05
4	K	1	NAG	C8-C7-N2	2.09	119.59	116.12
5	P	2	NAG	O7-C7-C8	-2.09	118.34	122.05
4	U	1	NAG	C8-C7-N2	2.08	119.56	116.12
5	T	2	NAG	O7-C7-C8	-2.08	118.36	122.05
4	Q	1	NAG	C8-C7-N2	2.07	119.56	116.12

There are no chirality outliers.

All (9) torsion outliers are listed below:

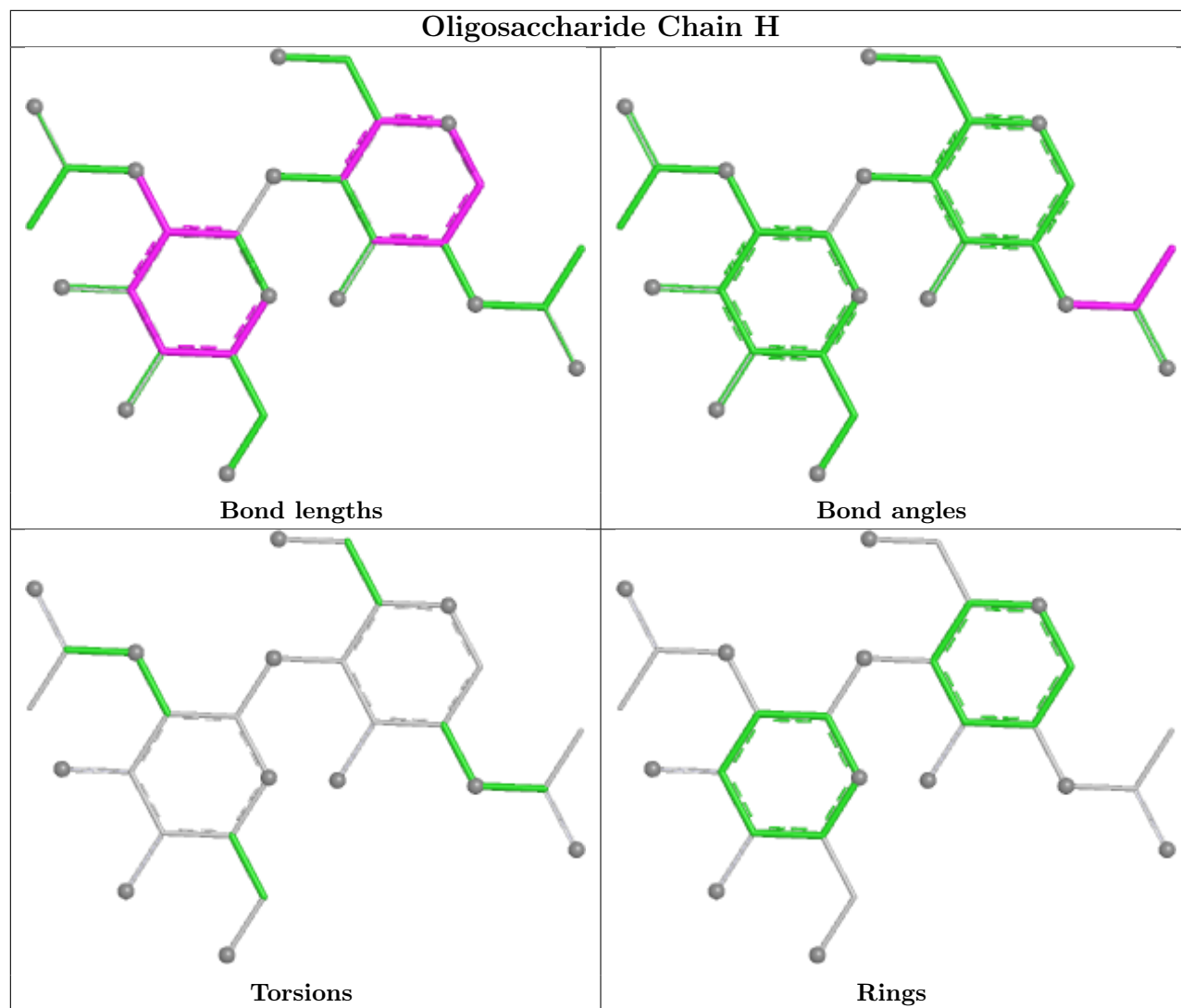
Mol	Chain	Res	Type	Atoms
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
5	J	3	BMA	O5-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6

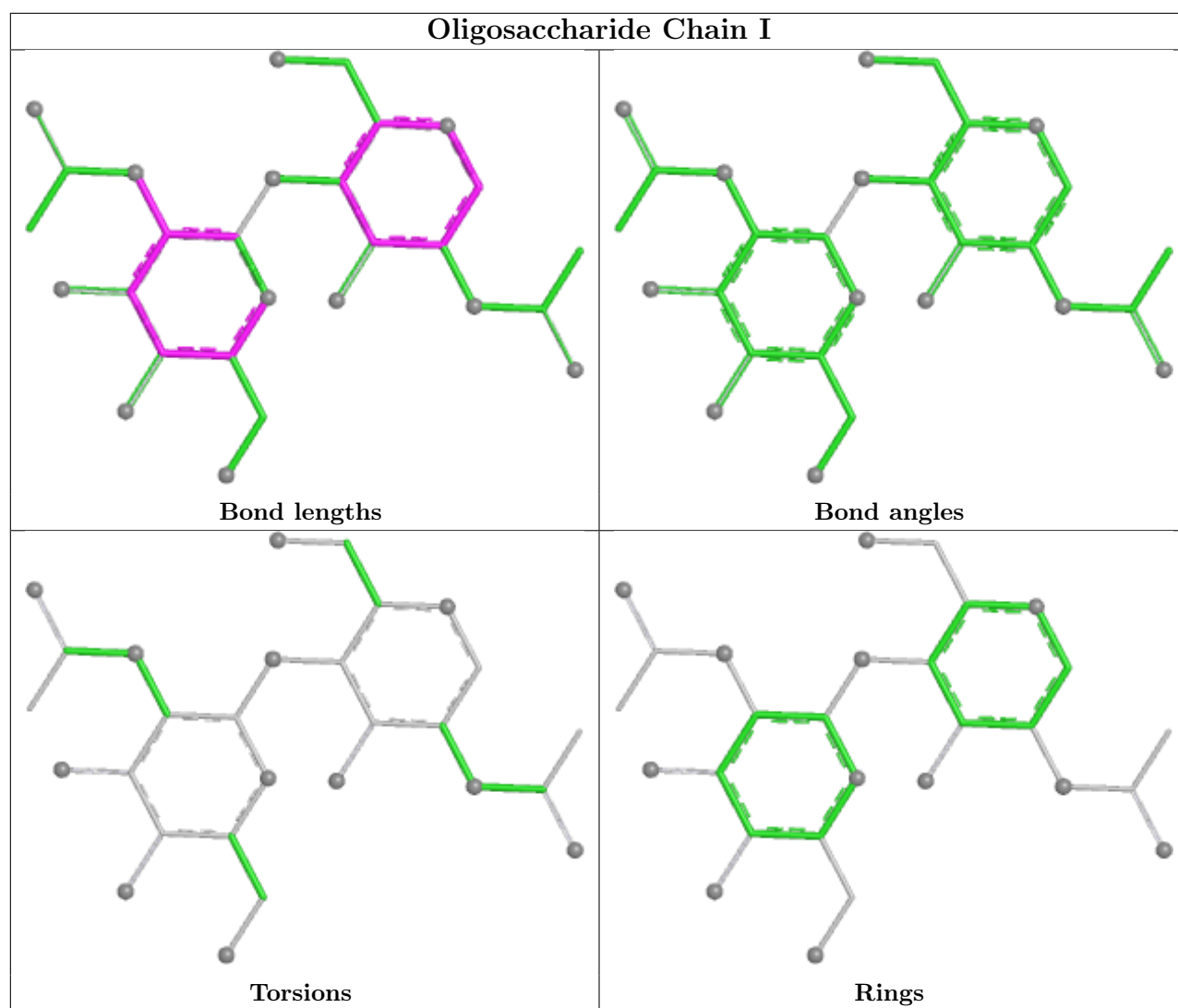
There are no ring outliers.

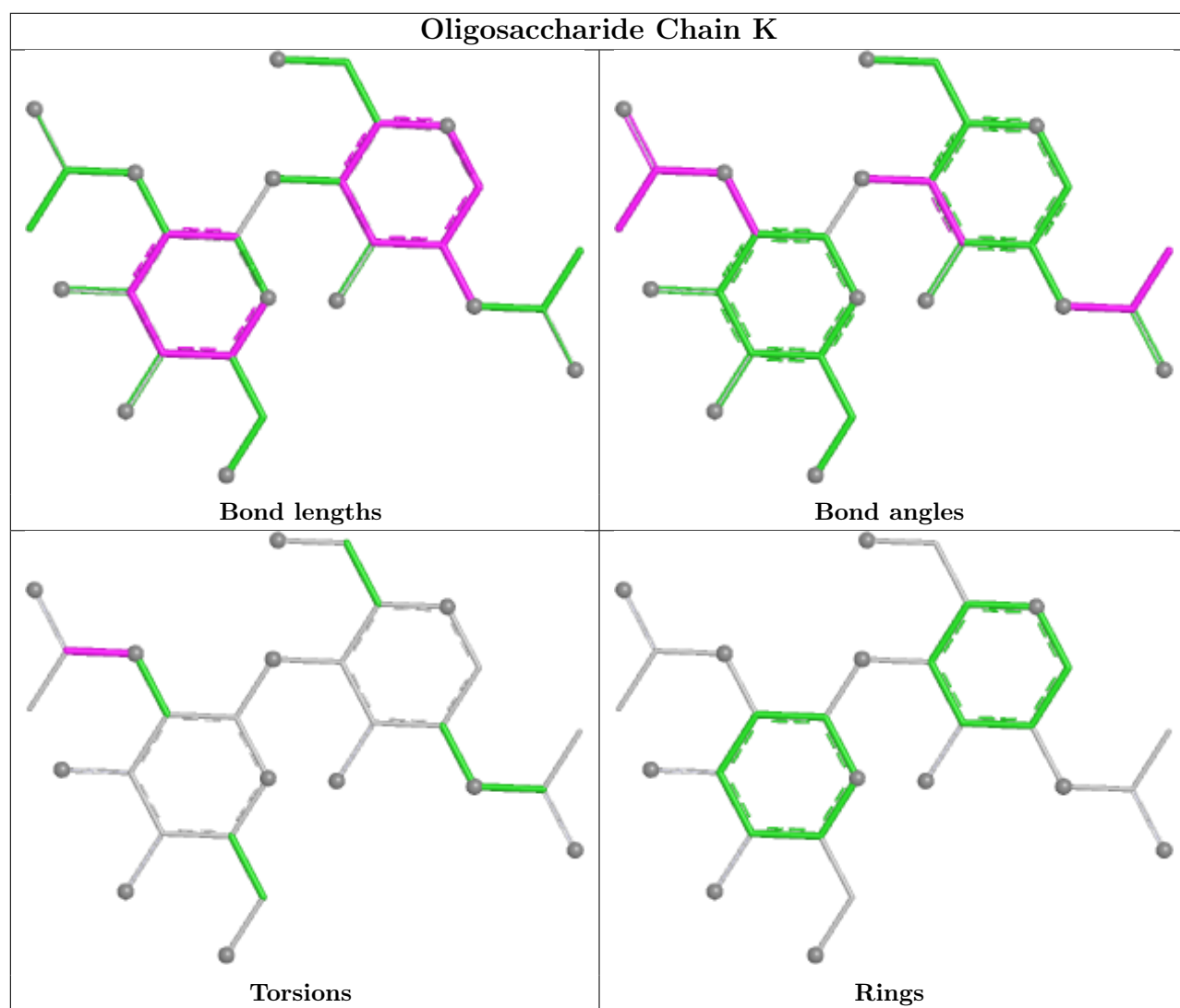
No monomer is involved in short contacts.

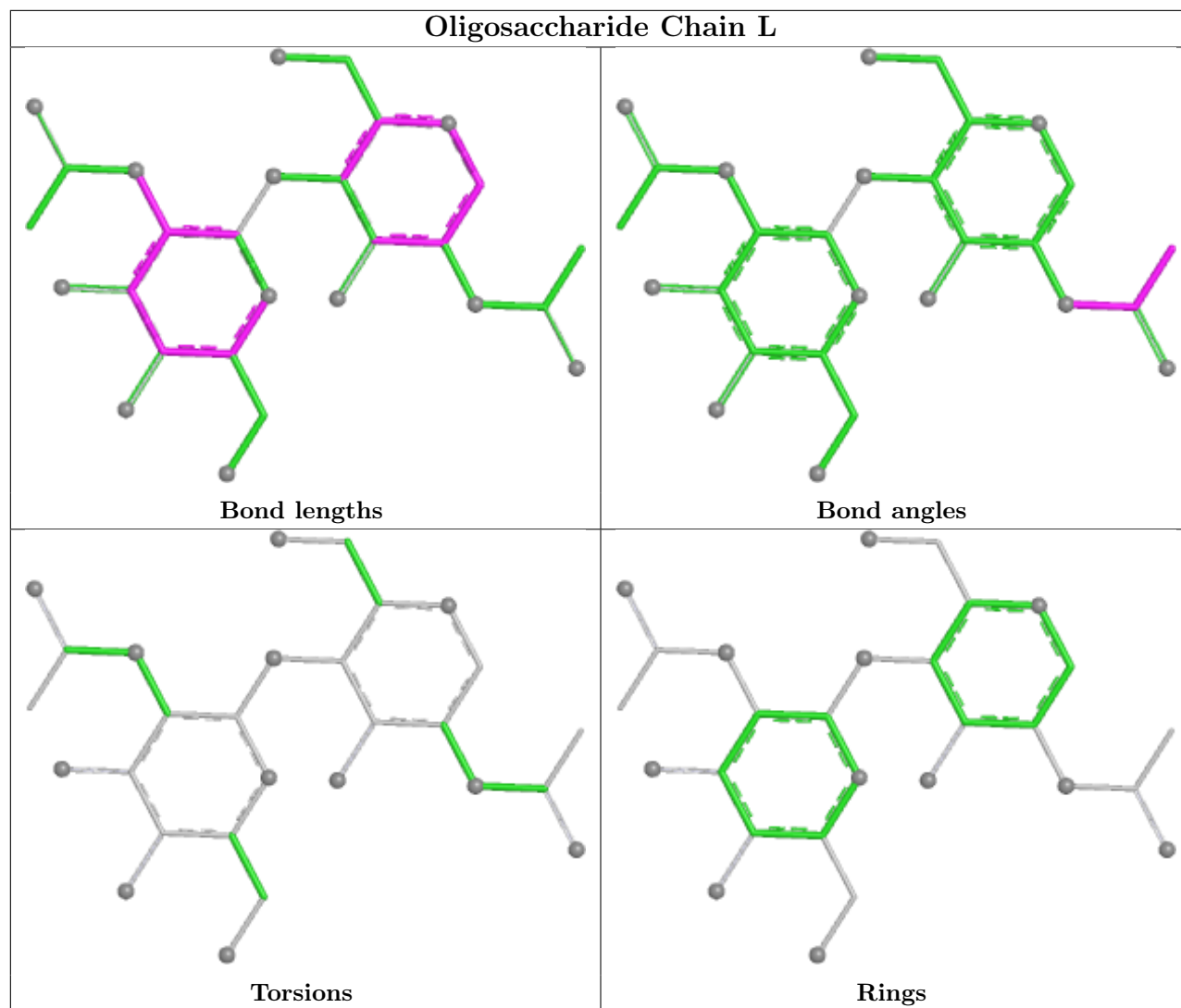
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

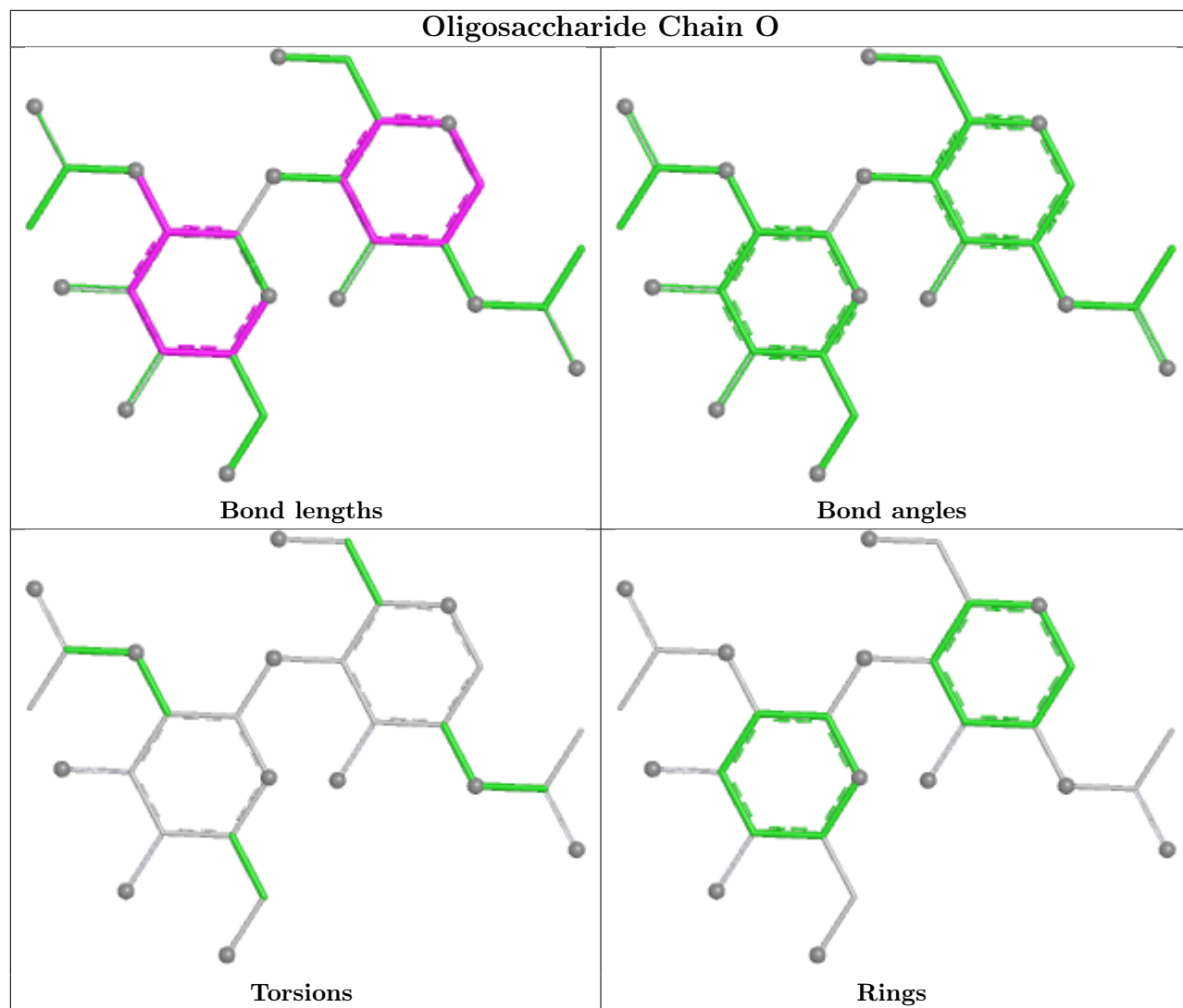


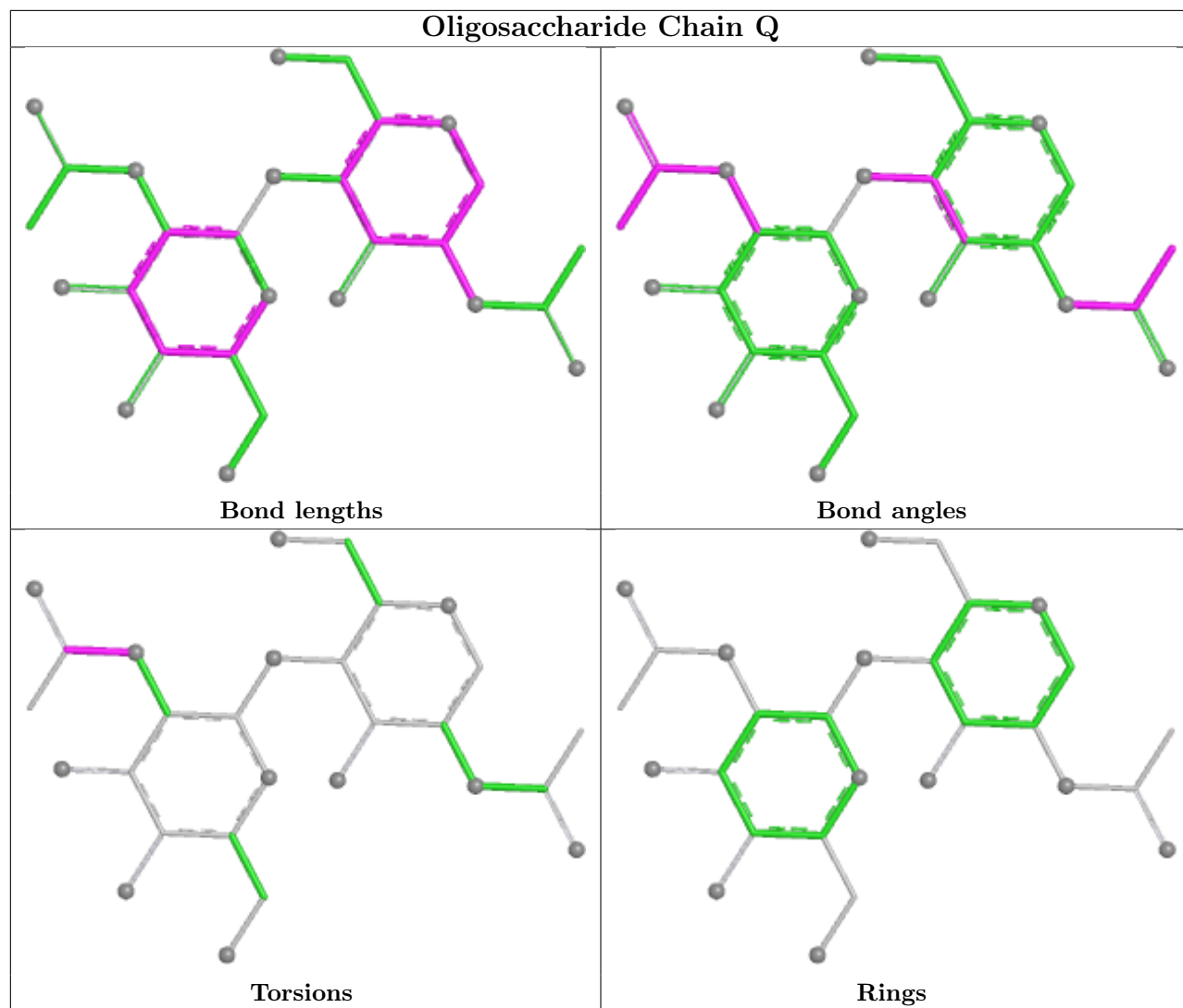


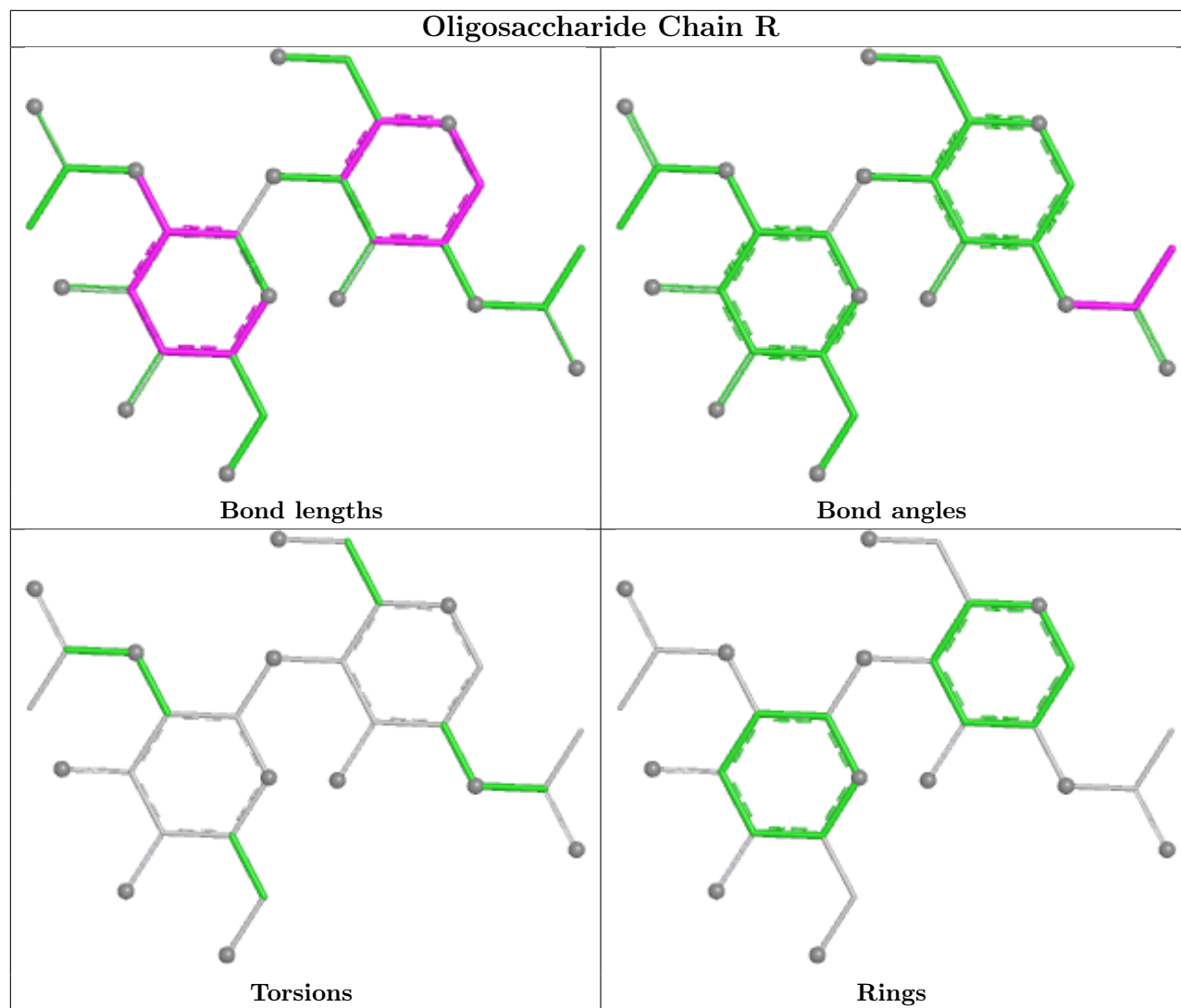


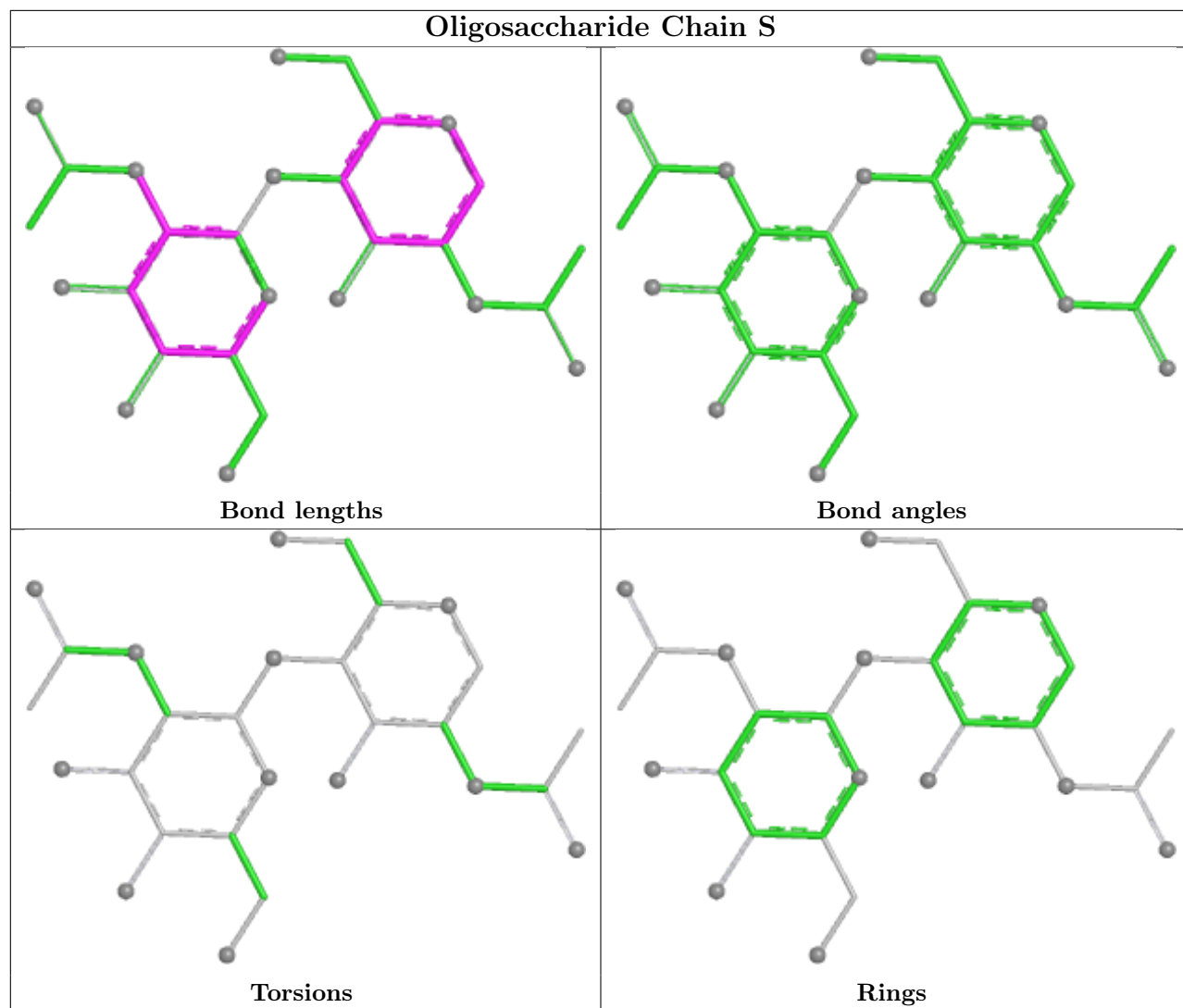




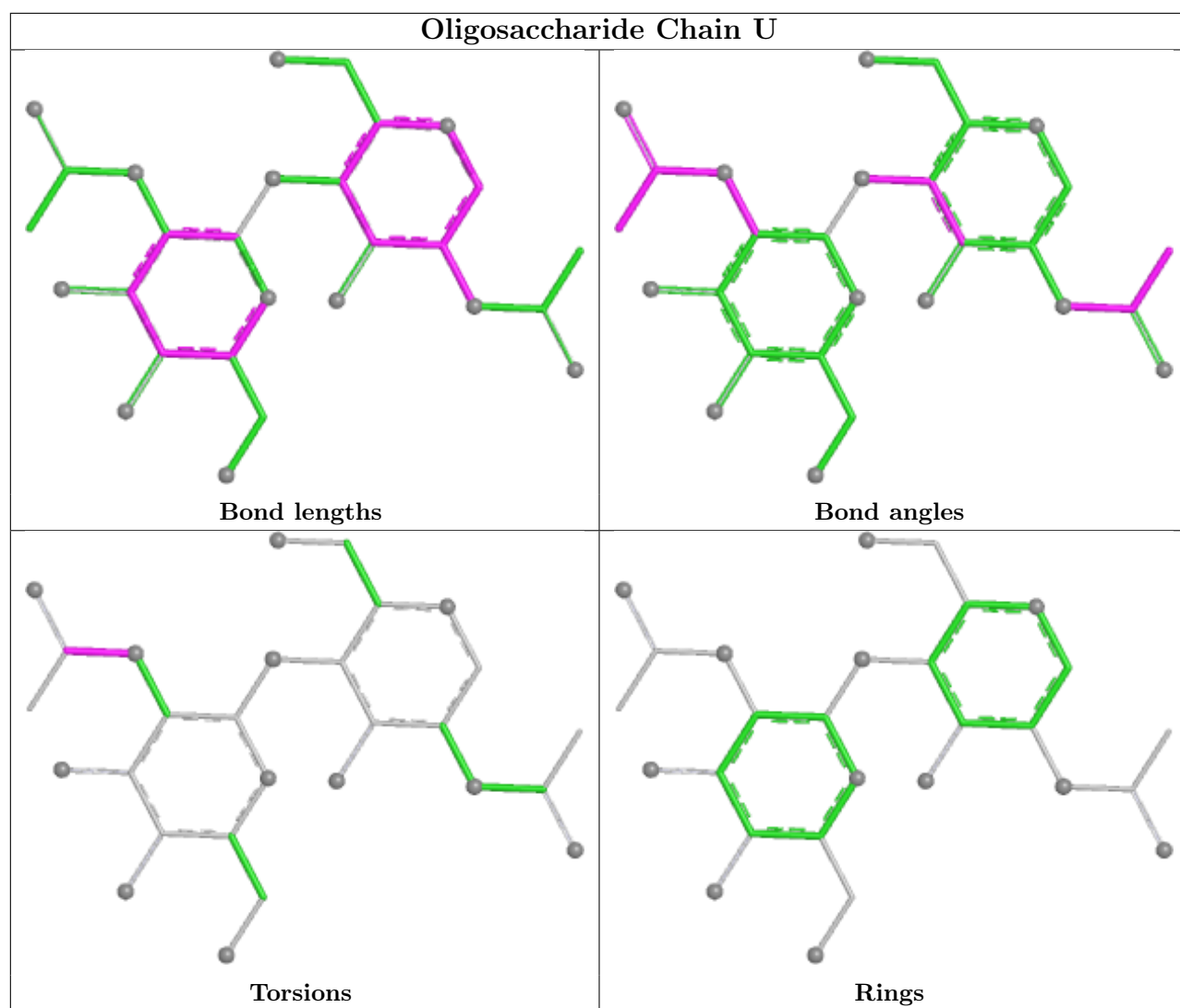


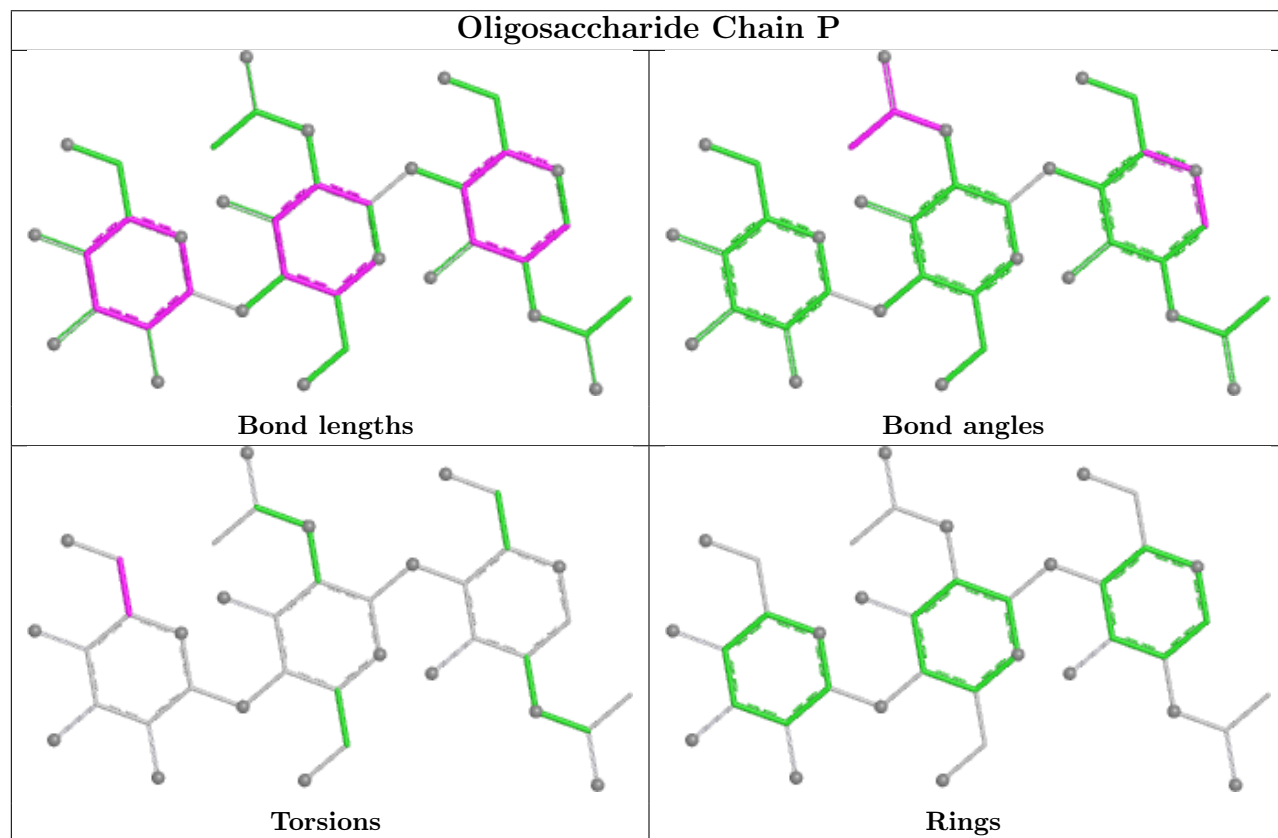
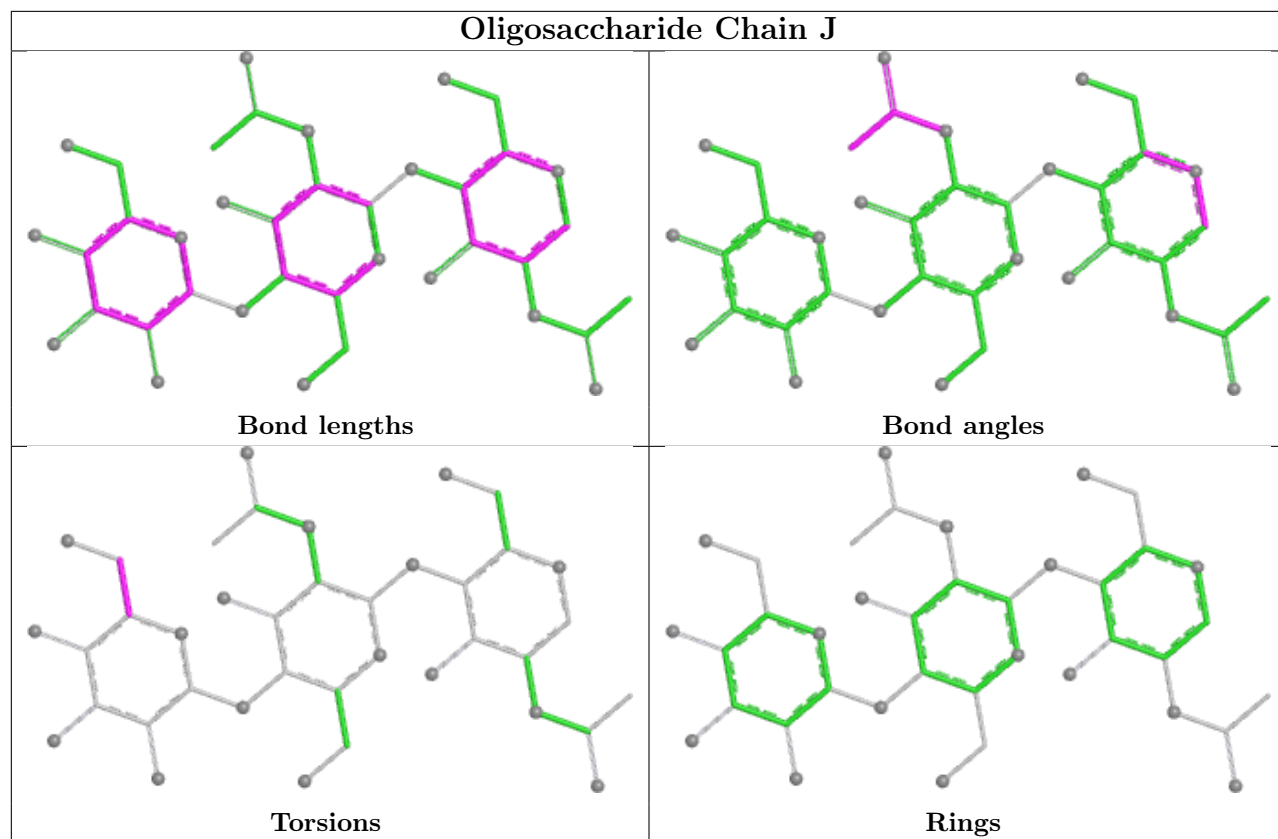


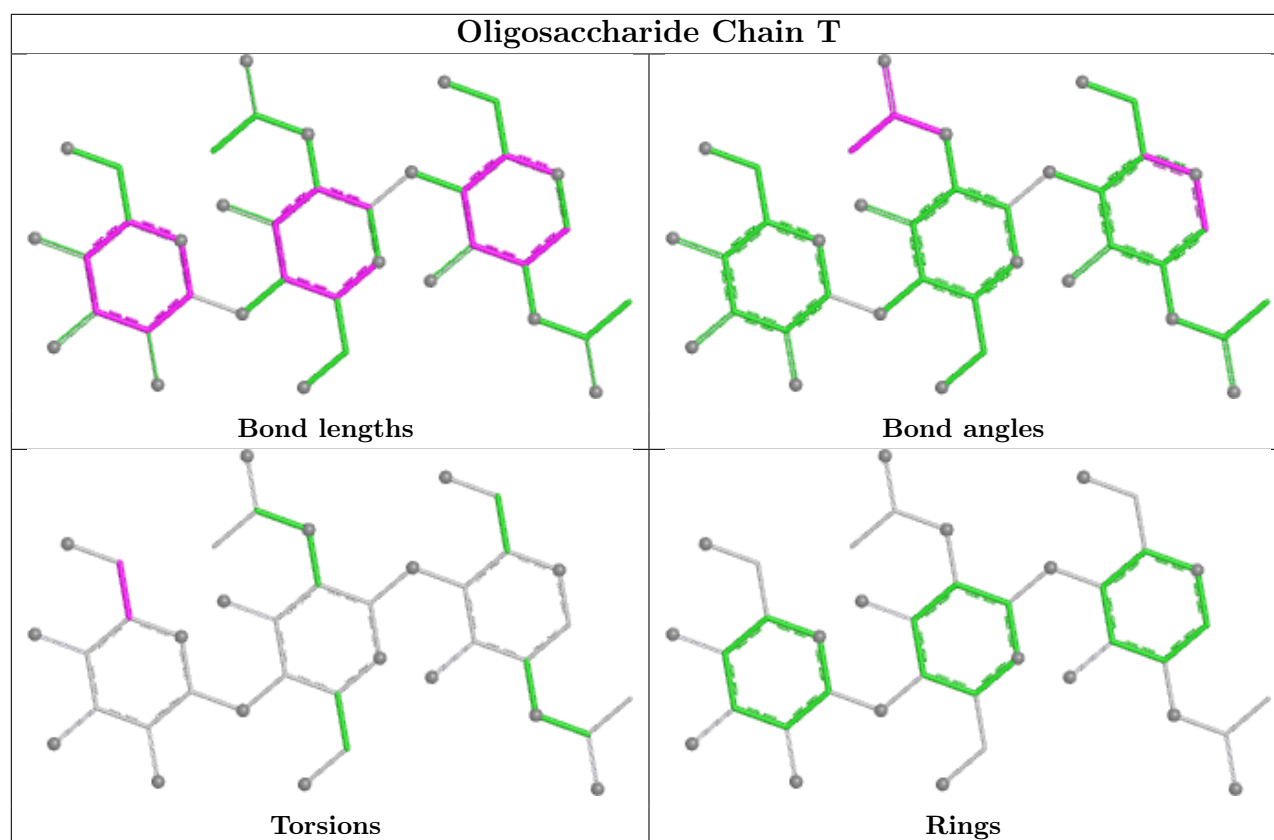












## 5.6 Ligand geometry [i](#)

15 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	$\# Z  > 2$
6	NAG	C	1305	1	14,14,15	2.25	5 (35%)	17,19,21	1.07	2 (11%)
6	NAG	A	1301	1	14,14,15	2.26	6 (42%)	17,19,21	2.25	4 (23%)
6	NAG	A	1305	1	14,14,15	2.25	5 (35%)	17,19,21	1.08	2 (11%)
6	NAG	C	1301	1	14,14,15	2.26	6 (42%)	17,19,21	2.25	4 (23%)
6	NAG	B	1303	1	14,14,15	2.26	7 (50%)	17,19,21	0.98	1 (5%)
6	NAG	B	1305	1	14,14,15	2.24	5 (35%)	17,19,21	1.07	2 (11%)
6	NAG	B	1302	1	14,14,15	2.20	7 (50%)	17,19,21	1.06	2 (11%)
6	NAG	C	1302	1	14,14,15	2.21	7 (50%)	17,19,21	1.06	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	C	1303	1	14,14,15	2.26	7 (50%)	17,19,21	0.98	1 (5%)
6	NAG	A	1304	1	14,14,15	2.24	6 (42%)	17,19,21	1.07	1 (5%)
6	NAG	A	1303	1	14,14,15	2.26	7 (50%)	17,19,21	0.98	1 (5%)
6	NAG	B	1301	1	14,14,15	2.25	6 (42%)	17,19,21	2.25	4 (23%)
6	NAG	B	1304	1	14,14,15	2.25	7 (50%)	17,19,21	1.07	1 (5%)
6	NAG	A	1302	1	14,14,15	2.20	7 (50%)	17,19,21	1.06	2 (11%)
6	NAG	C	1304	1	14,14,15	2.25	6 (42%)	17,19,21	1.06	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
6	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	2/6/23/26	0/1/1/1

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1301	NAG	C1-C2	5.91	1.60	1.52
6	C	1301	NAG	C1-C2	5.90	1.60	1.52
6	B	1301	NAG	C1-C2	5.89	1.60	1.52
6	B	1303	NAG	C1-C2	5.79	1.60	1.52
6	A	1303	NAG	C1-C2	5.77	1.60	1.52
6	C	1303	NAG	C1-C2	5.76	1.60	1.52

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1305	NAG	C1-C2	5.69	1.60	1.52
6	C	1305	NAG	C1-C2	5.66	1.60	1.52
6	B	1305	NAG	C1-C2	5.66	1.60	1.52
6	C	1302	NAG	C1-C2	5.51	1.59	1.52
6	B	1302	NAG	C1-C2	5.48	1.59	1.52
6	C	1304	NAG	C1-C2	5.46	1.59	1.52
6	B	1304	NAG	C1-C2	5.46	1.59	1.52
6	A	1302	NAG	C1-C2	5.45	1.59	1.52
6	A	1304	NAG	C1-C2	5.45	1.59	1.52
6	B	1304	NAG	O5-C5	3.63	1.50	1.43
6	C	1304	NAG	O5-C5	3.59	1.50	1.43
6	A	1304	NAG	O5-C5	3.59	1.50	1.43
6	A	1305	NAG	O5-C5	3.48	1.50	1.43
6	B	1305	NAG	O5-C5	3.47	1.50	1.43
6	C	1305	NAG	O5-C5	3.47	1.50	1.43
6	A	1302	NAG	O5-C5	3.25	1.49	1.43
6	C	1302	NAG	O5-C5	3.25	1.49	1.43
6	A	1303	NAG	O5-C5	3.23	1.49	1.43
6	B	1302	NAG	O5-C5	3.23	1.49	1.43
6	B	1303	NAG	O5-C5	3.22	1.49	1.43
6	C	1303	NAG	O5-C5	3.21	1.49	1.43
6	A	1301	NAG	O5-C5	2.91	1.49	1.43
6	C	1301	NAG	O5-C5	2.90	1.49	1.43
6	B	1301	NAG	O5-C5	2.89	1.49	1.43
6	C	1305	NAG	O5-C1	2.73	1.48	1.43
6	B	1305	NAG	O5-C1	2.71	1.48	1.43
6	C	1304	NAG	O5-C1	2.69	1.48	1.43
6	A	1305	NAG	O5-C1	2.69	1.48	1.43
6	A	1304	NAG	O5-C1	2.69	1.48	1.43
6	B	1304	NAG	O5-C1	2.68	1.48	1.43
6	A	1302	NAG	O5-C1	2.66	1.48	1.43
6	B	1302	NAG	O5-C1	2.64	1.48	1.43
6	C	1302	NAG	O5-C1	2.63	1.48	1.43
6	B	1303	NAG	O5-C1	2.60	1.48	1.43
6	C	1301	NAG	O5-C1	2.58	1.48	1.43
6	C	1303	NAG	O5-C1	2.58	1.48	1.43
6	C	1301	NAG	C3-C2	2.58	1.57	1.52
6	A	1303	NAG	O5-C1	2.58	1.48	1.43
6	B	1301	NAG	O5-C1	2.57	1.48	1.43
6	A	1301	NAG	O5-C1	2.56	1.48	1.43
6	A	1301	NAG	C3-C2	2.55	1.57	1.52
6	B	1301	NAG	C3-C2	2.55	1.57	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1304	NAG	C3-C2	2.50	1.57	1.52
6	B	1304	NAG	C3-C2	2.47	1.57	1.52
6	A	1304	NAG	C3-C2	2.47	1.57	1.52
6	C	1303	NAG	C3-C2	2.40	1.57	1.52
6	B	1303	NAG	C3-C2	2.39	1.57	1.52
6	A	1303	NAG	C3-C2	2.38	1.57	1.52
6	C	1303	NAG	C4-C5	2.36	1.58	1.53
6	A	1303	NAG	C4-C5	2.35	1.58	1.53
6	B	1303	NAG	C4-C5	2.35	1.58	1.53
6	C	1302	NAG	C4-C5	2.32	1.58	1.53
6	C	1305	NAG	C3-C2	2.32	1.57	1.52
6	B	1305	NAG	C3-C2	2.32	1.57	1.52
6	A	1302	NAG	C4-C5	2.32	1.58	1.53
6	B	1301	NAG	C2-N2	2.30	1.50	1.46
6	A	1305	NAG	C3-C2	2.30	1.57	1.52
6	B	1302	NAG	C4-C5	2.29	1.57	1.53
6	C	1304	NAG	C4-C5	2.28	1.57	1.53
6	A	1304	NAG	C4-C5	2.28	1.57	1.53
6	A	1301	NAG	C2-N2	2.27	1.50	1.46
6	C	1301	NAG	C2-N2	2.27	1.50	1.46
6	B	1304	NAG	C4-C5	2.26	1.57	1.53
6	A	1305	NAG	C4-C5	2.21	1.57	1.53
6	C	1305	NAG	C4-C5	2.21	1.57	1.53
6	B	1305	NAG	C4-C5	2.21	1.57	1.53
6	A	1302	NAG	C3-C2	2.18	1.57	1.52
6	B	1302	NAG	C3-C2	2.18	1.57	1.52
6	C	1302	NAG	C3-C2	2.18	1.57	1.52
6	B	1302	NAG	C2-N2	2.17	1.49	1.46
6	A	1302	NAG	C2-N2	2.14	1.49	1.46
6	C	1302	NAG	C2-N2	2.12	1.49	1.46
6	B	1301	NAG	C4-C5	2.09	1.57	1.53
6	C	1301	NAG	C4-C5	2.09	1.57	1.53
6	A	1304	NAG	C2-N2	2.07	1.49	1.46
6	C	1304	NAG	C2-N2	2.07	1.49	1.46
6	A	1301	NAG	C4-C5	2.07	1.57	1.53
6	B	1304	NAG	C2-N2	2.06	1.49	1.46
6	C	1302	NAG	C4-C3	2.06	1.57	1.52
6	C	1303	NAG	C4-C3	2.05	1.57	1.52
6	B	1303	NAG	C4-C3	2.05	1.57	1.52
6	A	1302	NAG	C4-C3	2.04	1.57	1.52
6	C	1303	NAG	C2-N2	2.04	1.49	1.46
6	B	1302	NAG	C4-C3	2.04	1.57	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1303	NAG	C4-C3	2.04	1.57	1.52
6	A	1303	NAG	C2-N2	2.02	1.49	1.46
6	B	1303	NAG	C2-N2	2.02	1.49	1.46
6	B	1304	NAG	C4-C3	2.01	1.57	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1301	NAG	C8-C7-N2	6.94	127.63	116.12
6	C	1301	NAG	C8-C7-N2	6.94	127.63	116.12
6	B	1301	NAG	C8-C7-N2	6.93	127.61	116.12
6	C	1301	NAG	O7-C7-N2	-4.49	114.04	121.98
6	B	1301	NAG	O7-C7-N2	-4.49	114.05	121.98
6	A	1301	NAG	O7-C7-N2	-4.49	114.06	121.98
6	A	1305	NAG	C8-C7-N2	2.63	120.48	116.12
6	B	1305	NAG	C8-C7-N2	2.62	120.46	116.12
6	A	1302	NAG	C8-C7-N2	2.61	120.44	116.12
6	C	1305	NAG	C8-C7-N2	2.61	120.44	116.12
6	B	1302	NAG	C8-C7-N2	2.59	120.42	116.12
6	C	1302	NAG	C8-C7-N2	2.59	120.42	116.12
6	B	1301	NAG	C2-N2-C7	2.28	125.96	122.90
6	A	1301	NAG	C2-N2-C7	2.28	125.95	122.90
6	C	1301	NAG	C2-N2-C7	2.27	125.95	122.90
6	B	1305	NAG	O7-C7-C8	-2.15	118.22	122.05
6	A	1305	NAG	O7-C7-C8	-2.14	118.24	122.05
6	A	1304	NAG	C2-N2-C7	2.13	125.75	122.90
6	C	1305	NAG	O7-C7-C8	-2.12	118.28	122.05
6	B	1304	NAG	C2-N2-C7	2.12	125.74	122.90
6	A	1301	NAG	O7-C7-C8	-2.10	118.31	122.05
6	C	1304	NAG	C2-N2-C7	2.09	125.70	122.90
6	B	1302	NAG	O7-C7-C8	-2.09	118.33	122.05
6	C	1301	NAG	O7-C7-C8	-2.09	118.33	122.05
6	C	1302	NAG	O7-C7-C8	-2.09	118.34	122.05
6	B	1301	NAG	O7-C7-C8	-2.08	118.34	122.05
6	A	1302	NAG	O7-C7-C8	-2.08	118.35	122.05
6	A	1303	NAG	C8-C7-N2	2.04	119.50	116.12
6	B	1303	NAG	C8-C7-N2	2.04	119.50	116.12
6	C	1303	NAG	C8-C7-N2	2.02	119.47	116.12

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1301	NAG	C8-C7-N2-C2
6	A	1301	NAG	O7-C7-N2-C2
6	B	1301	NAG	C8-C7-N2-C2
6	B	1301	NAG	O7-C7-N2-C2
6	C	1301	NAG	C8-C7-N2-C2
6	C	1301	NAG	O7-C7-N2-C2
6	A	1304	NAG	C1-C2-N2-C7
6	B	1304	NAG	C1-C2-N2-C7
6	C	1304	NAG	C1-C2-N2-C7
6	B	1303	NAG	C4-C5-C6-O6
6	C	1303	NAG	C4-C5-C6-O6
6	A	1303	NAG	C4-C5-C6-O6
6	A	1304	NAG	C3-C2-N2-C7
6	B	1304	NAG	C3-C2-N2-C7
6	C	1304	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



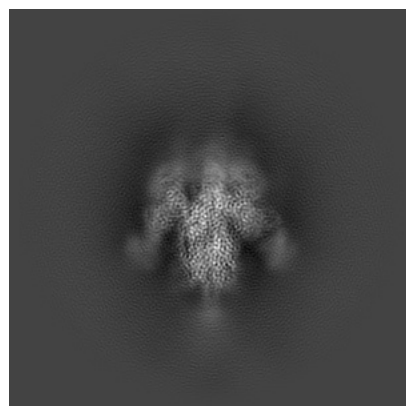
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43407. These allow visual inspection of the internal detail of the map and identification of artifacts.

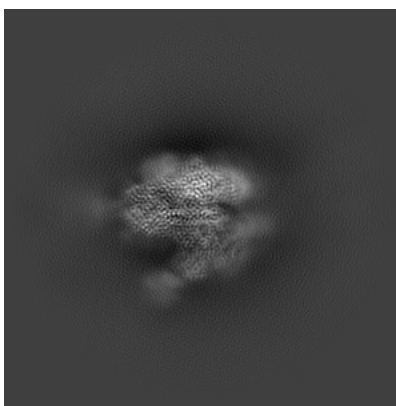
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

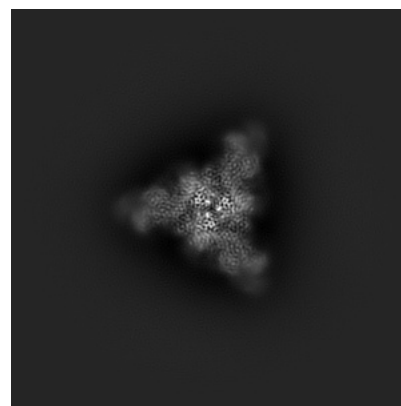
#### 6.1.1 Primary map



X

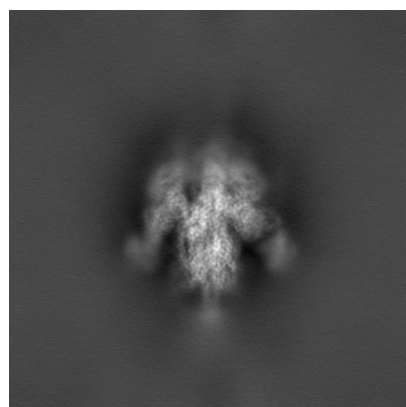


Y

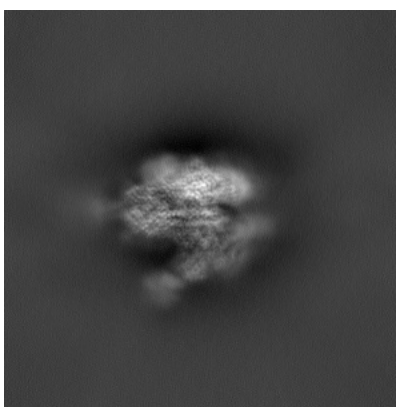


Z

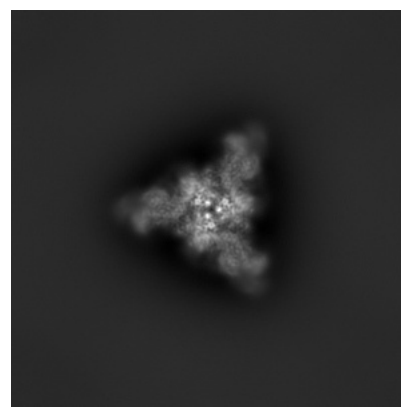
#### 6.1.2 Raw map



X



Y

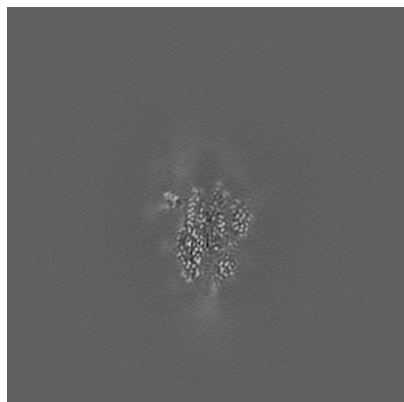


Z

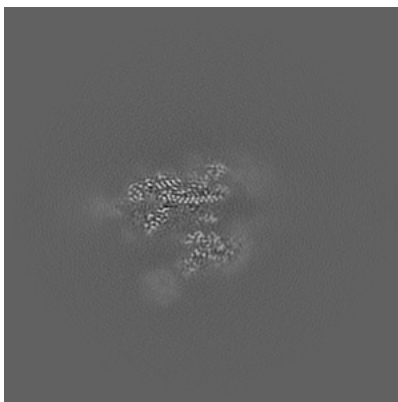
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

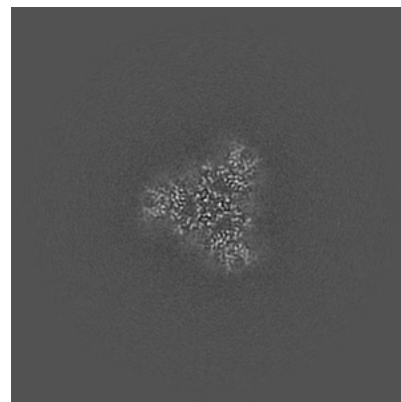
### 6.2.1 Primary map



X Index: 200

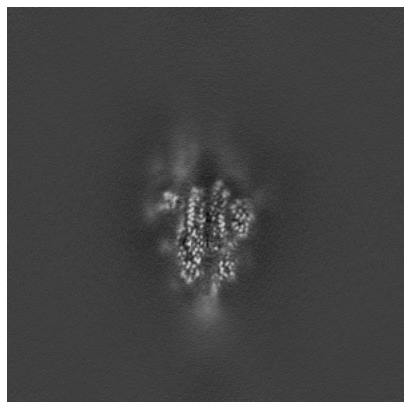


Y Index: 200

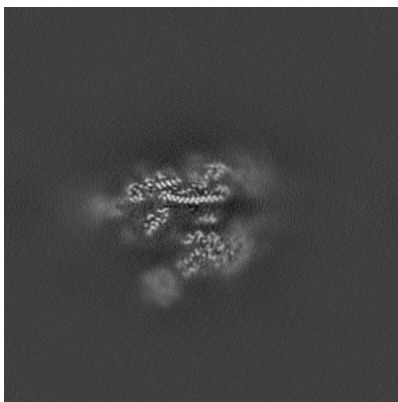


Z Index: 200

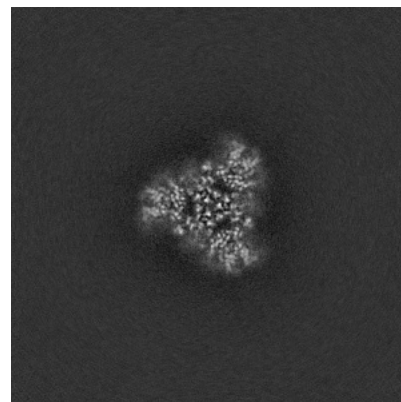
### 6.2.2 Raw map



X Index: 200



Y Index: 200

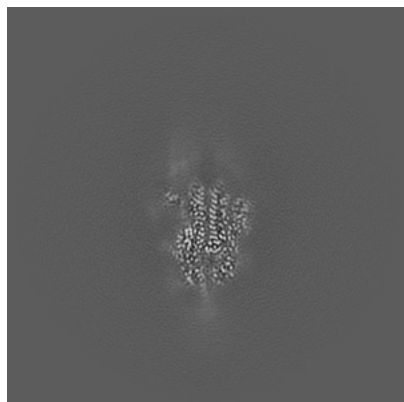


Z Index: 200

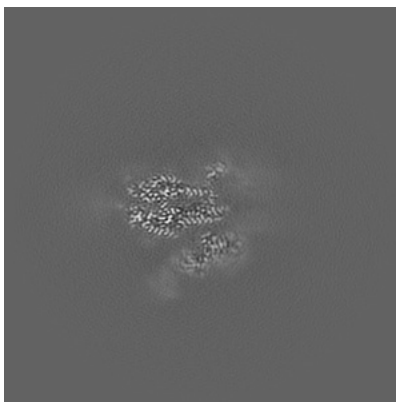
The images above show central slices of the map in three orthogonal directions.

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

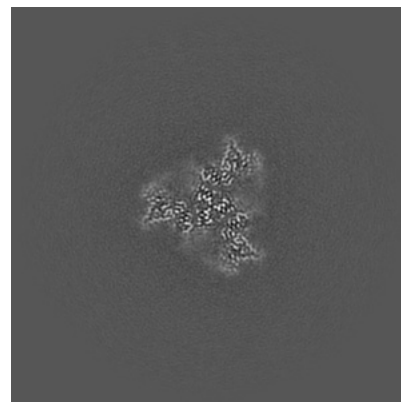
### 6.3.1 Primary map



X Index: 195

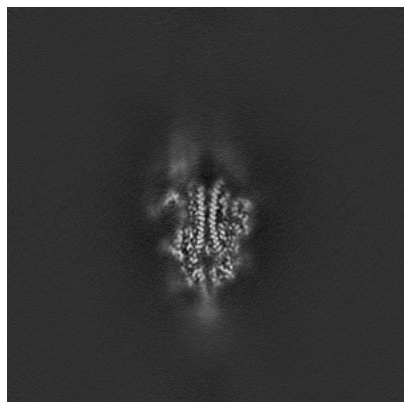


Y Index: 209

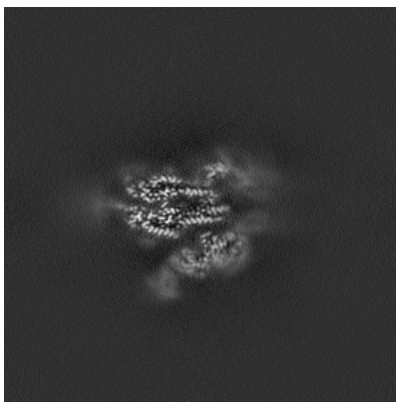


Z Index: 193

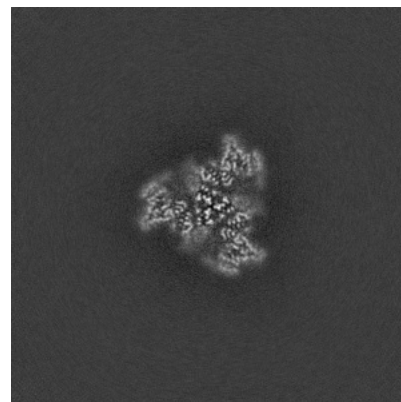
### 6.3.2 Raw map



X Index: 196



Y Index: 209

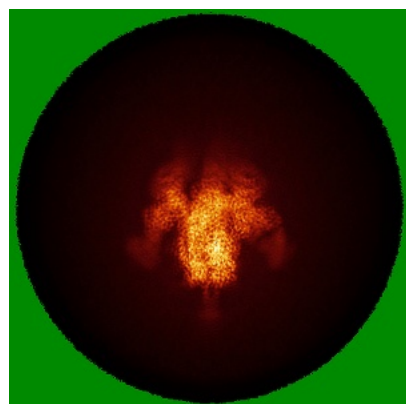


Z Index: 193

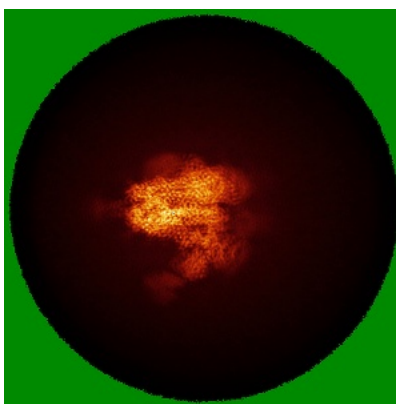
The images above show the largest variance slices of the map in three orthogonal directions.

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

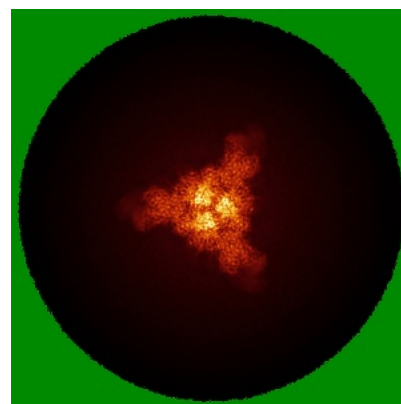
### 6.4.1 Primary map



X

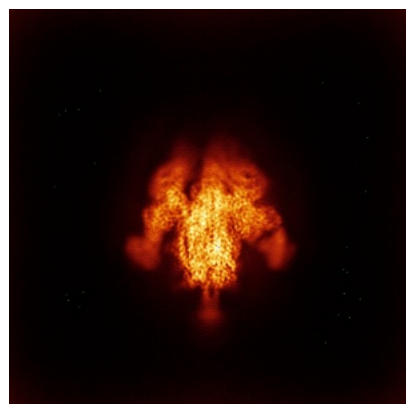


Y

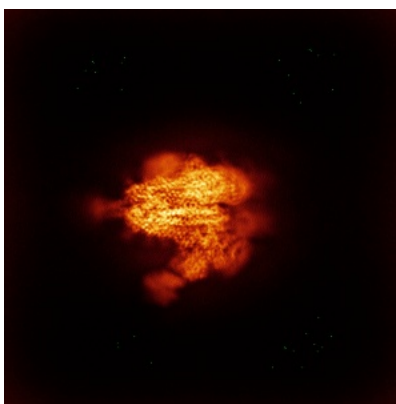


Z

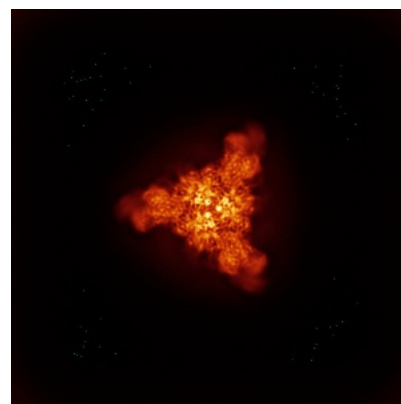
### 6.4.2 Raw map



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.

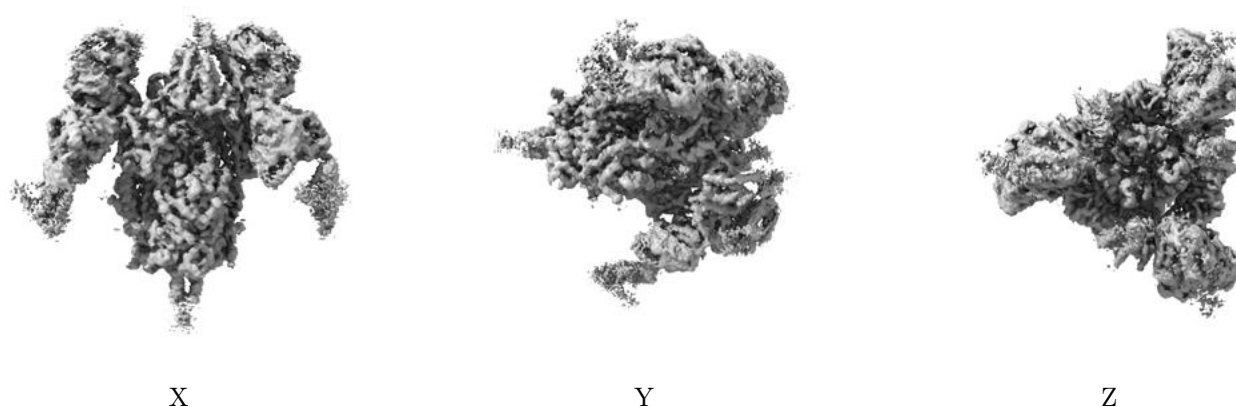
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

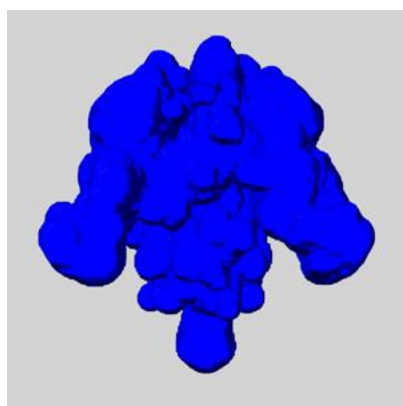
## 6.6 Mask visualisation [i](#)

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

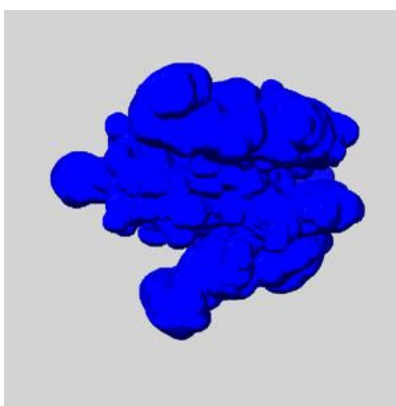
A mask typically either:

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

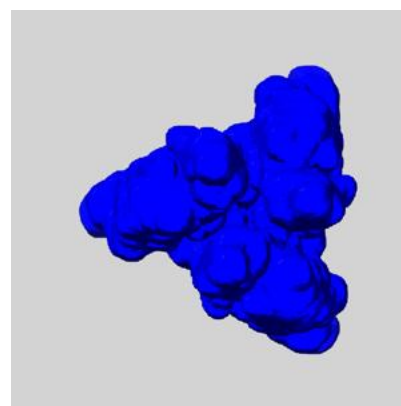
### 6.6.1 emd\_43407\_msk\_1.map [i](#)



X



Y



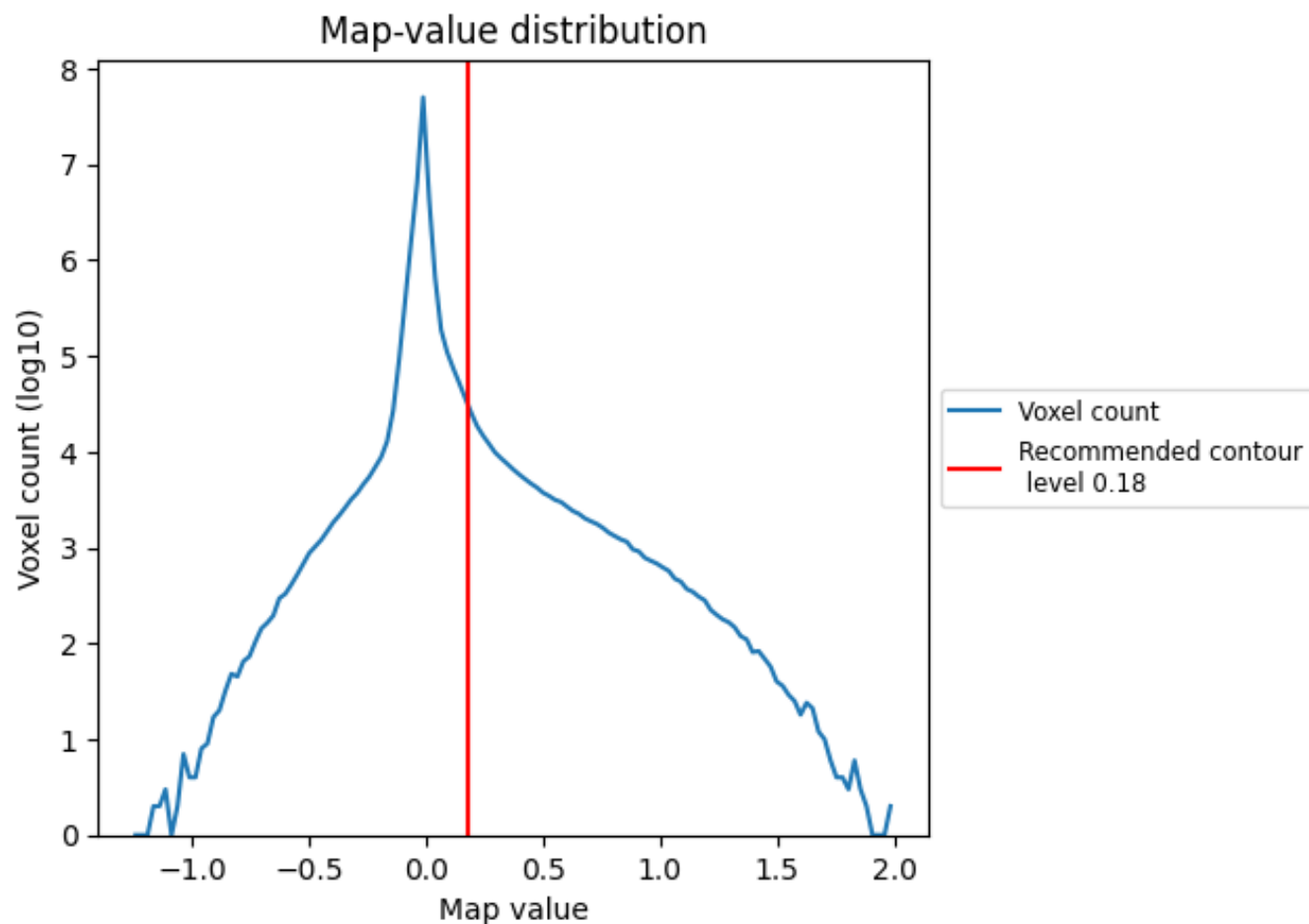
Z



## 7 Map analysis [i](#)

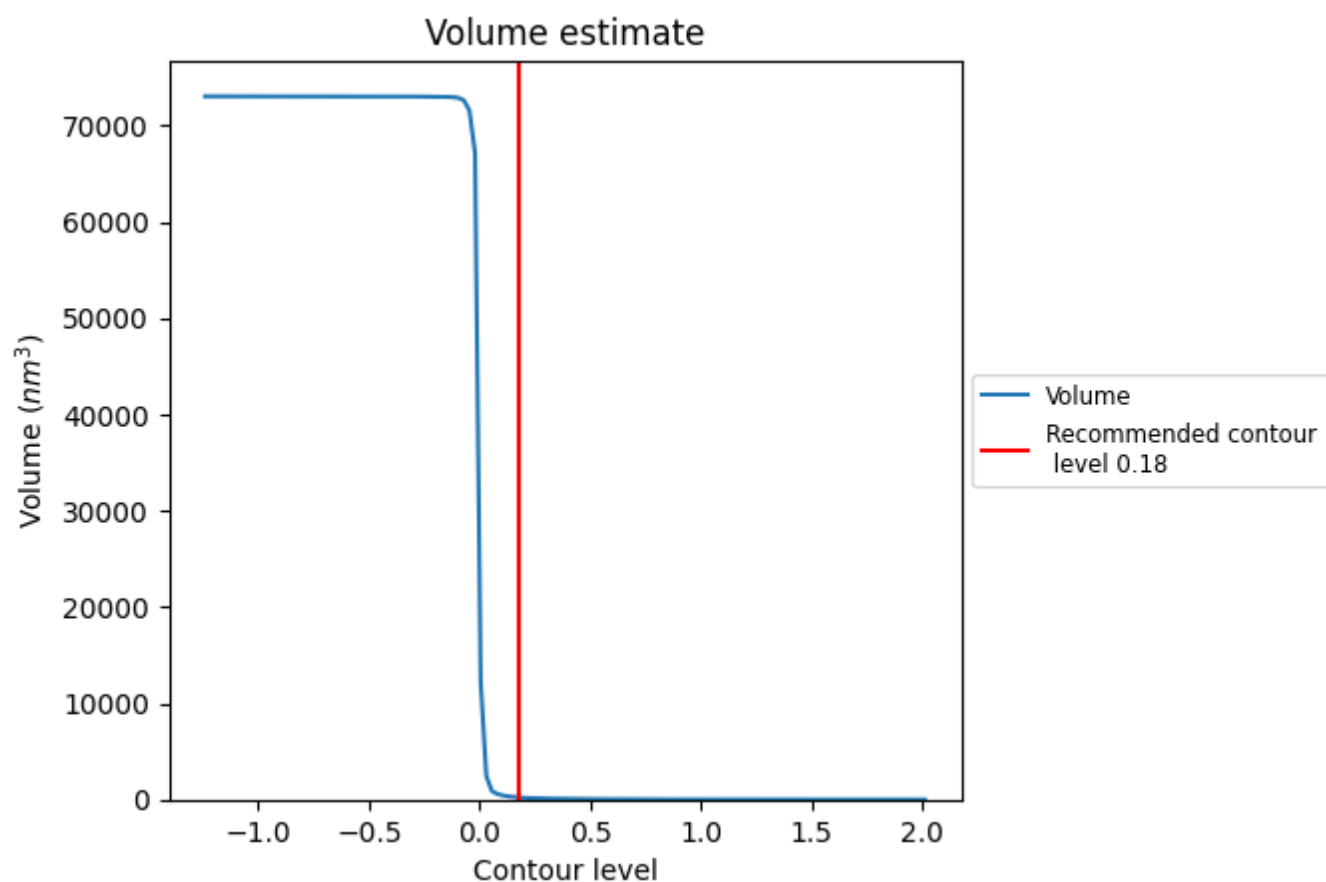
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

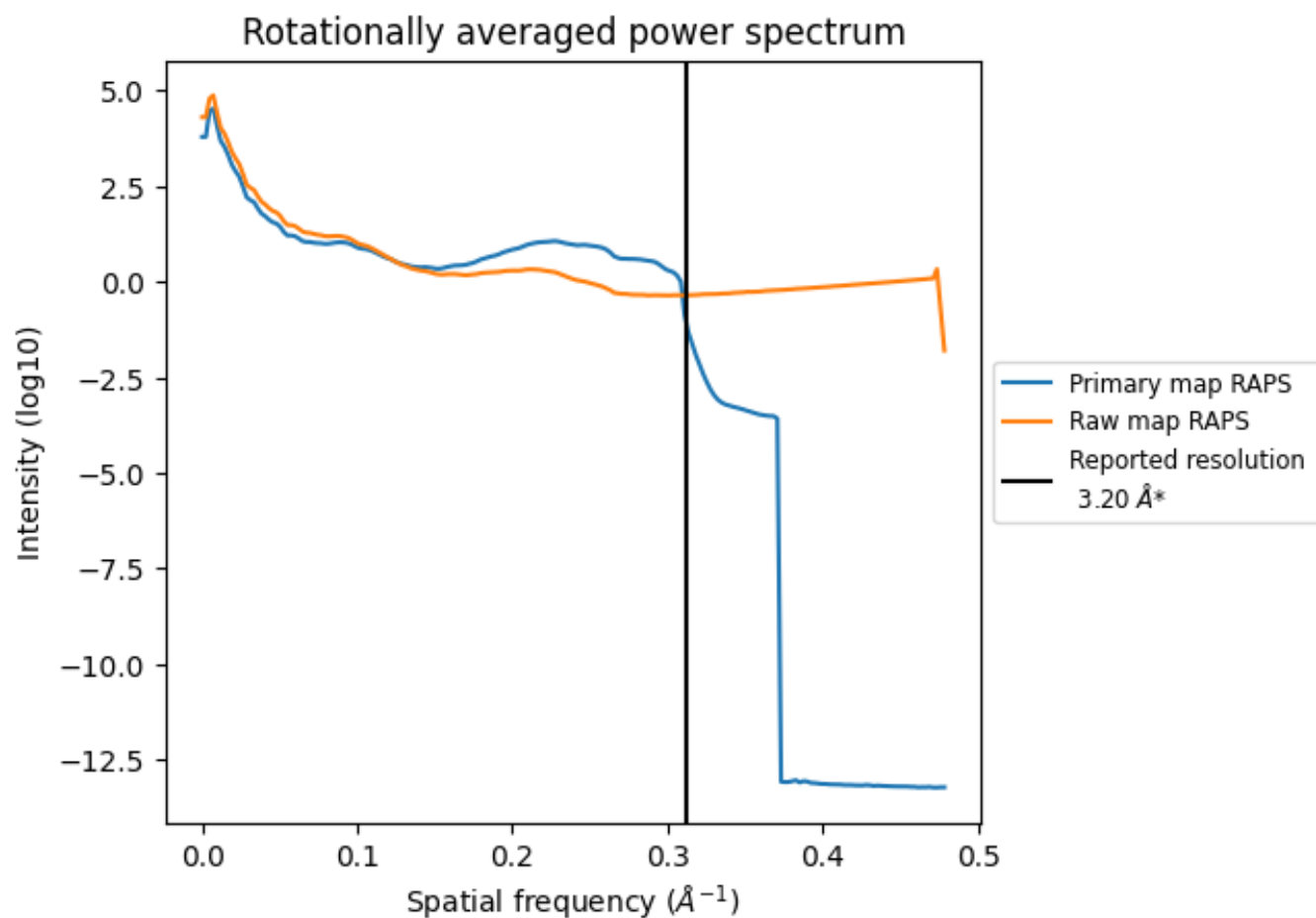


The volume at the recommended contour level is 209 nm<sup>3</sup>; this corresponds to an approximate mass of 189 kDa.

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 ⓘ

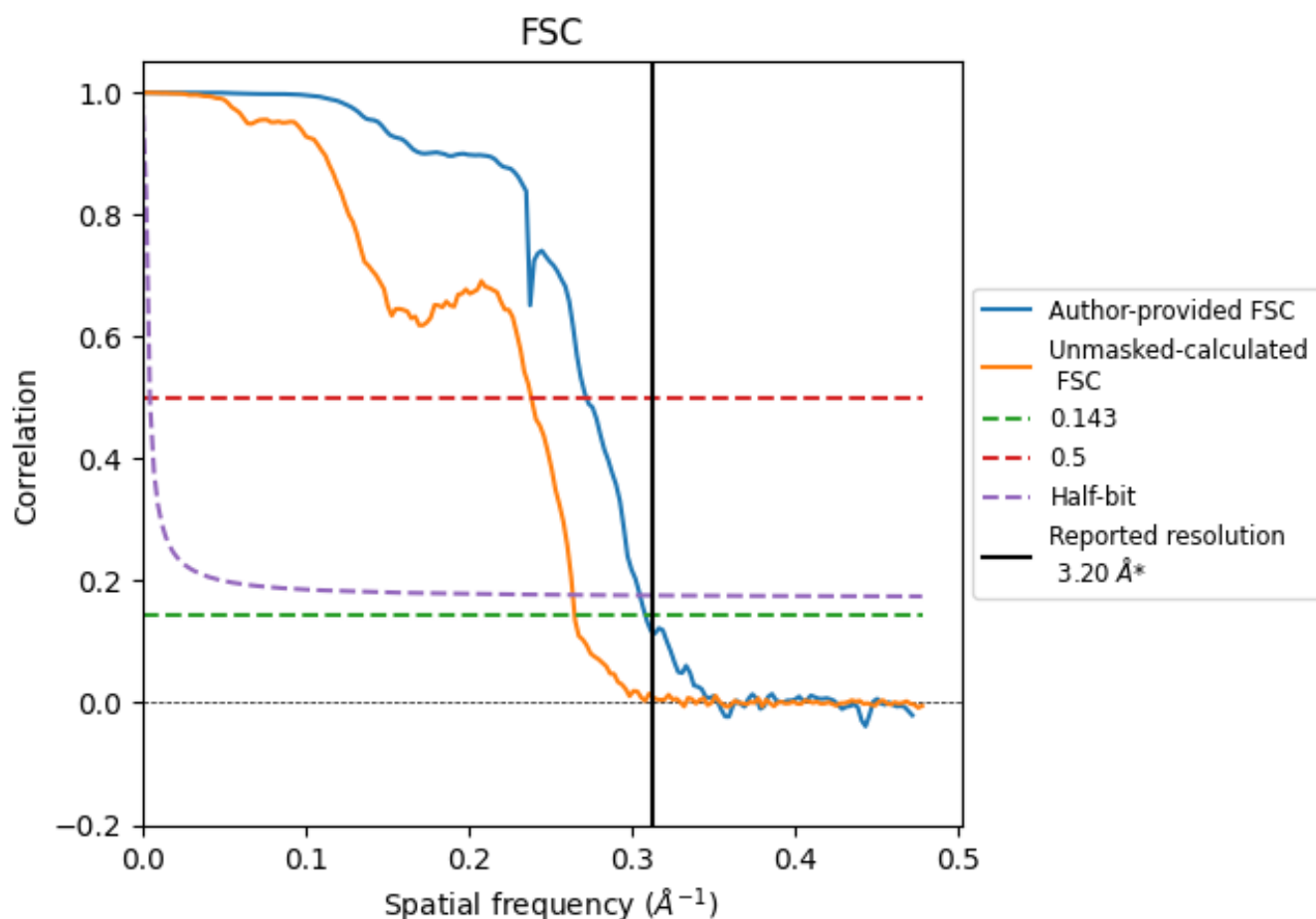


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.312 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

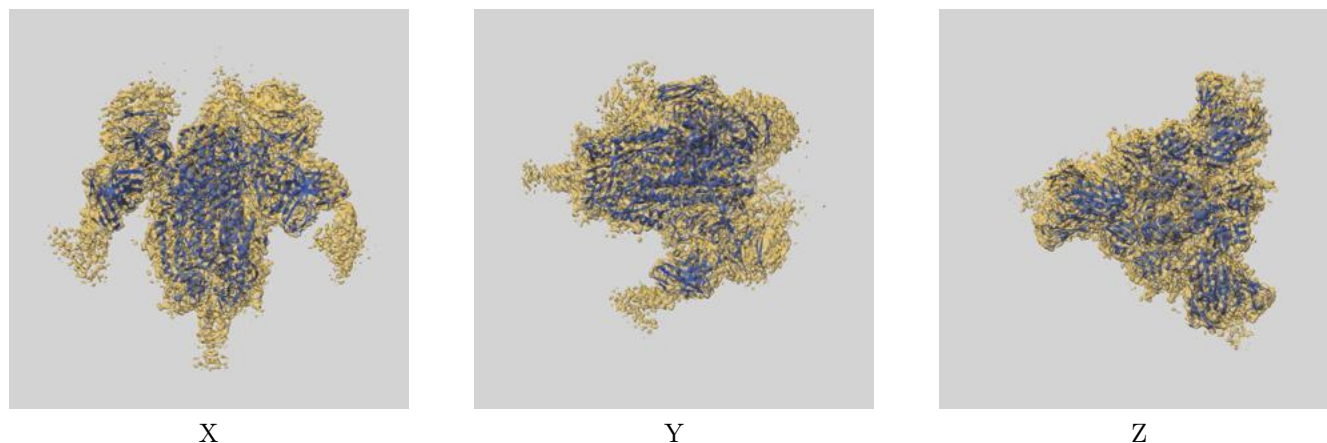
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.24	3.67	3.27
Unmasked-calculated*	3.77	4.19	3.79

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.77 differs from the reported value 3.2 by more than 10 %

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

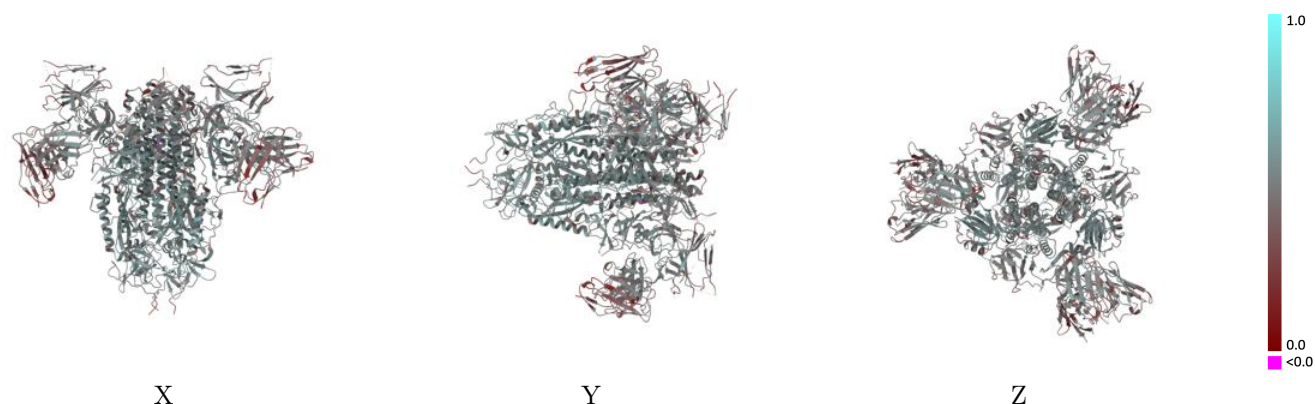
This section contains information regarding the fit between EMDB map EMD-43407 and PDB model 8VPF. Per-residue inclusion information can be found in section 3 on page 12.

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



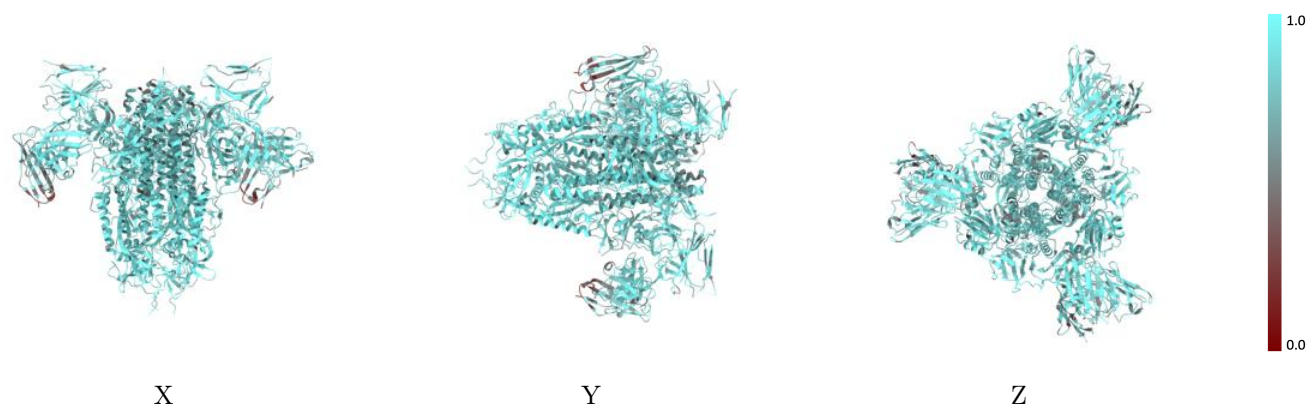
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



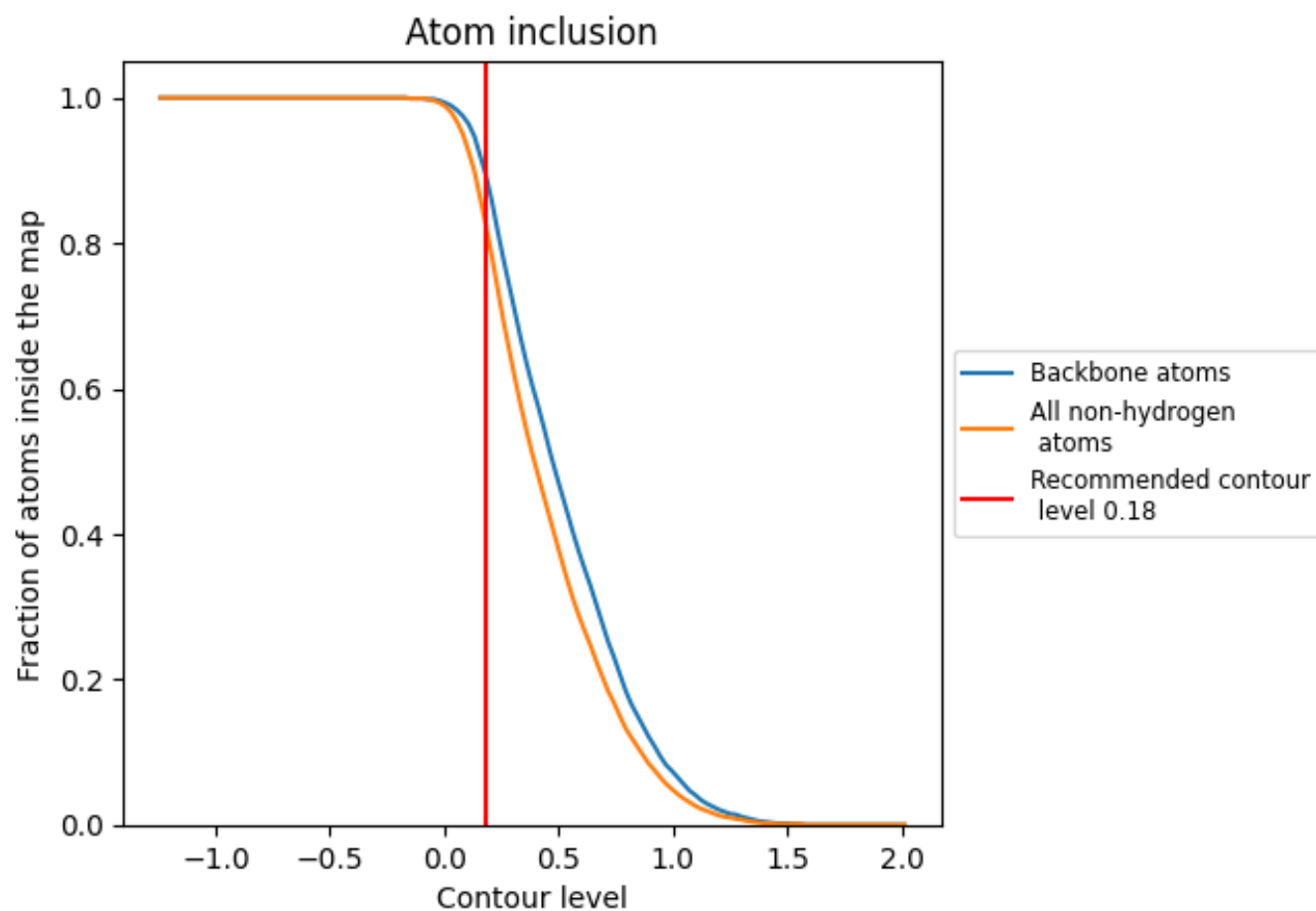
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.4760
A	 0.8520	 0.4930
B	 0.8510	 0.4930
C	 0.8500	 0.4930
D	 0.7160	 0.3990
E	 0.7120	 0.3970
F	 0.8210	 0.4560
G	 0.8210	 0.4540
H	 0.5710	 0.4070
I	 0.5000	 0.2640
J	 0.5900	 0.3980
K	 0.7140	 0.3890
L	 0.5710	 0.4120
M	 0.7190	 0.4000
N	 0.8220	 0.4620
O	 0.4640	 0.2710
P	 0.5640	 0.4090
Q	 0.7140	 0.3840
R	 0.5710	 0.3980
S	 0.5000	 0.2490
T	 0.5640	 0.3920
U	 0.7140	 0.3890

