



Full wwPDB EM Validation Report ⓘ

May 26, 2025 – 12:33 PM EDT

PDB ID : 8VPF / pdb_00008vpf
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

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) : 2.43.1

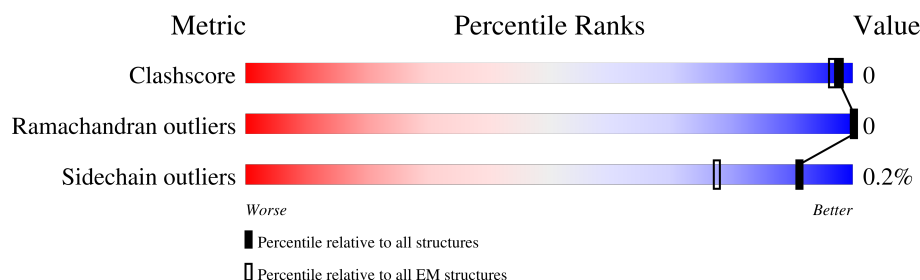
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY






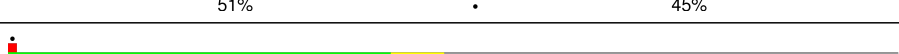
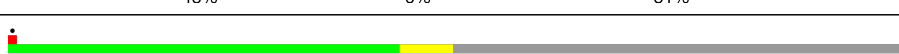

The reported resolution of this entry is 3.20 Å.

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 ≥ 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	

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Mol	Chain	Length	Quality of chain
3	N	217	 43% 6% 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

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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

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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

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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

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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

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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.

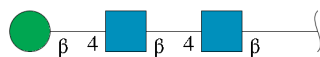
Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	107	Total	C	N	O	S	0	0
			787	494	130	160	3		
3	F	107	Total	C	N	O	S	0	0
			787	494	130	160	3		
3	G	107	Total	C	N	O	S	0	0
			787	494	130	160	3		

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



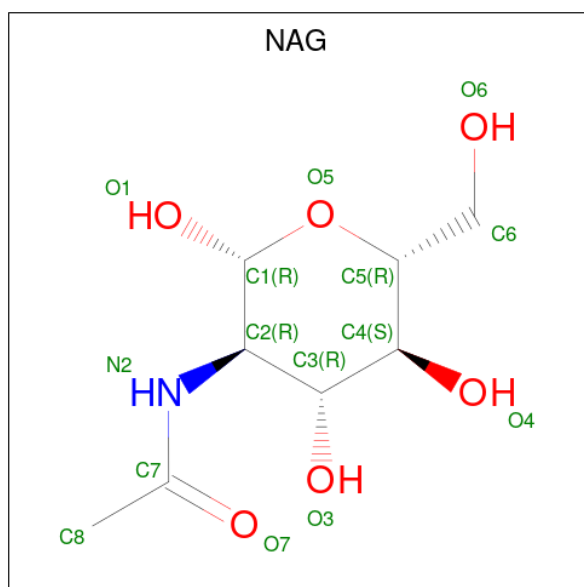
Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

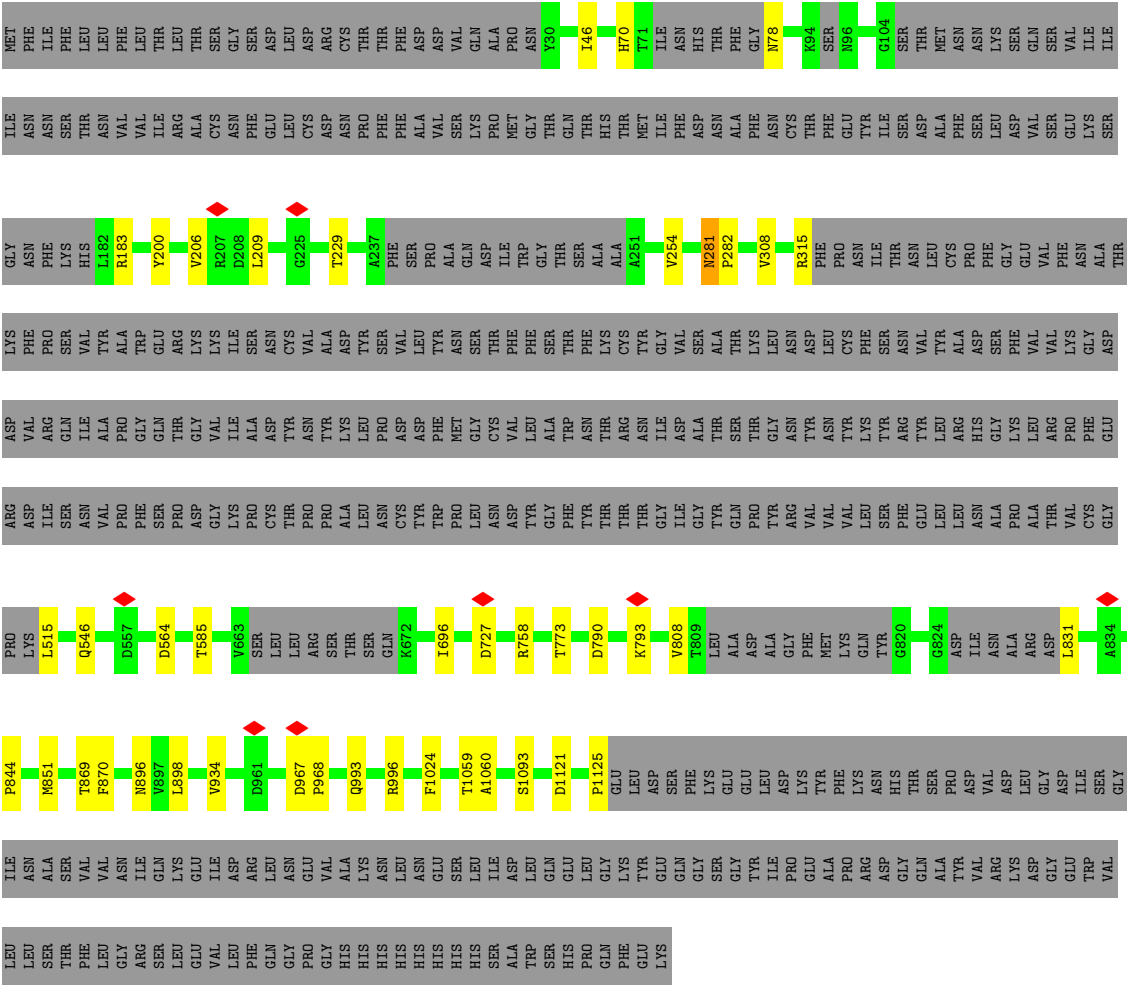


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	

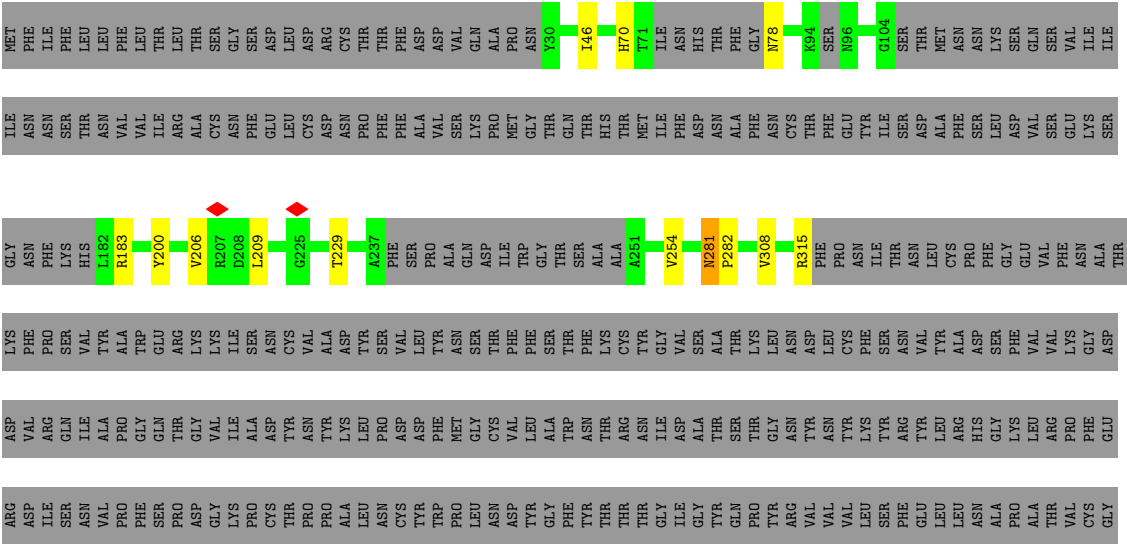
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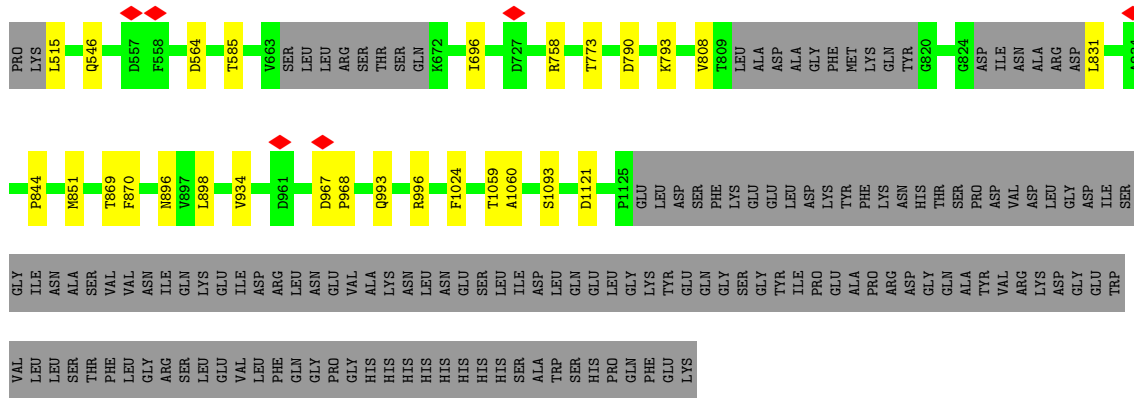
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Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C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

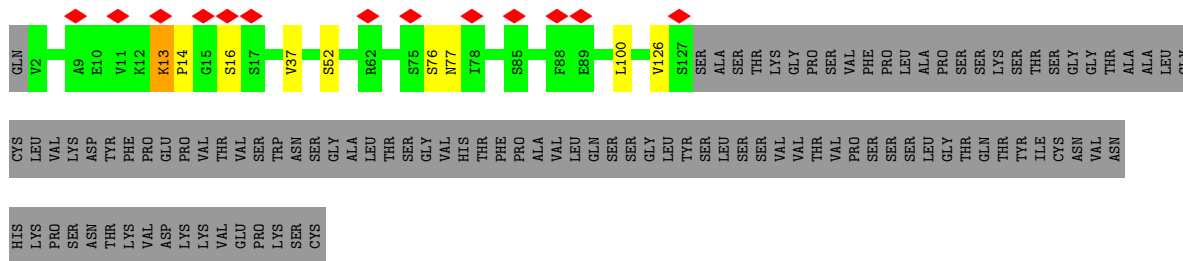


● Molecule 1: Spike glycoprotein

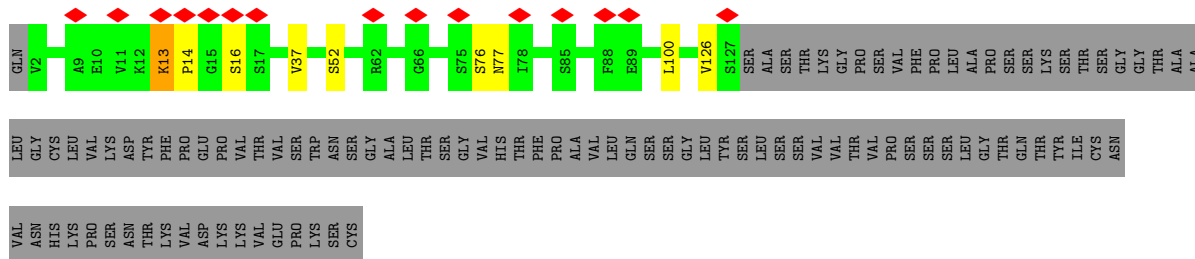




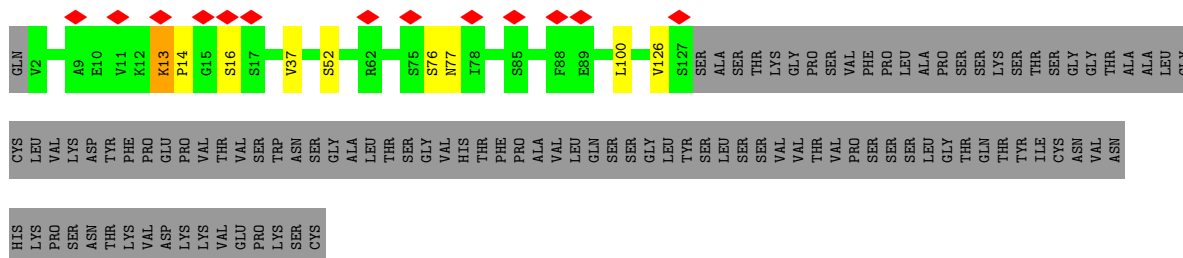
- Molecule 2: CoV1-65 antibody heavy chain



- Molecule 2: CoV1-65 antibody heavy chain



- Molecule 2: CoV1-65 antibody heavy chain





- 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	6/6137 (0.1%)	1.26	46/8342 (0.6%)
1	B	1.10	7/6137 (0.1%)	1.26	48/8342 (0.6%)
1	C	1.10	6/6137 (0.1%)	1.26	48/8342 (0.6%)
2	D	0.96	0/972	1.29	8/1318 (0.6%)
2	E	0.96	0/972	1.29	8/1318 (0.6%)
2	M	0.96	0/972	1.29	8/1318 (0.6%)
3	F	1.04	0/806	1.48	16/1094 (1.5%)
3	G	1.04	0/806	1.48	16/1094 (1.5%)
3	N	1.04	0/806	1.48	16/1094 (1.5%)
All	All	1.08	19/23745 (0.1%)	1.29	214/32262 (0.7%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	896	ASN	CB-CG	-6.83	1.34	1.52
1	A	896	ASN	CB-CG	-6.82	1.34	1.52
1	C	896	ASN	CB-CG	-6.81	1.35	1.52
1	A	831	LEU	CB-CG	5.79	1.65	1.53
1	B	831	LEU	CB-CG	5.78	1.65	1.53
1	C	831	LEU	CB-CG	5.77	1.65	1.53
1	B	515	LEU	CB-CG	5.33	1.64	1.53
1	C	515	LEU	CB-CG	5.33	1.64	1.53
1	A	515	LEU	CB-CG	5.32	1.64	1.53
1	A	78	ASN	C-N	5.27	1.39	1.33
1	B	78	ASN	C-N	5.25	1.39	1.33
1	C	78	ASN	C-N	5.25	1.39	1.33
1	B	315	ARG	NE-CZ	5.18	1.38	1.33
1	A	315	ARG	NE-CZ	5.16	1.38	1.33
1	C	315	ARG	NE-CZ	5.11	1.38	1.33
1	C	898	LEU	CG-CD2	-5.05	1.35	1.52
1	A	898	LEU	CG-CD2	-5.03	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	898	LEU	CG-CD2	-5.02	1.35	1.52
1	B	1125	PRO	N-CD	5.02	1.54	1.47

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	95	GLY	N-CA-C	-9.86	102.58	111.95
3	F	95	GLY	N-CA-C	-9.86	102.59	111.95
3	G	95	GLY	N-CA-C	-9.82	102.62	111.95
2	D	13	LYS	CA-C-N	8.78	128.42	119.82
2	D	13	LYS	C-N-CA	8.78	128.42	119.82
2	E	13	LYS	CA-C-N	8.77	128.41	119.82
2	E	13	LYS	C-N-CA	8.77	128.41	119.82
2	M	13	LYS	CA-C-N	8.75	128.39	119.82
2	M	13	LYS	C-N-CA	8.75	128.39	119.82
1	A	1121	ASP	CA-C-N	8.10	127.75	119.82
1	A	1121	ASP	C-N-CA	8.10	127.75	119.82
1	C	1121	ASP	CA-C-N	8.07	127.73	119.82
1	C	1121	ASP	C-N-CA	8.07	127.73	119.82
1	B	1121	ASP	CA-C-N	8.07	127.73	119.82
1	B	1121	ASP	C-N-CA	8.07	127.73	119.82
1	A	229	THR	N-CA-C	-7.36	105.21	114.56
1	C	229	THR	N-CA-C	-7.35	105.23	114.56
2	E	76	SER	N-CA-C	-7.34	103.92	114.12
2	M	76	SER	N-CA-C	-7.34	103.92	114.12
1	B	229	THR	N-CA-C	-7.33	105.25	114.56
2	D	76	SER	N-CA-C	-7.32	103.94	114.12
1	B	844	PRO	CA-C-N	7.32	127.27	120.03
1	B	844	PRO	C-N-CA	7.32	127.27	120.03
1	A	844	PRO	CA-C-N	7.28	127.24	120.03
1	A	844	PRO	C-N-CA	7.28	127.24	120.03
1	B	308	VAL	CA-C-N	7.28	127.26	119.76
1	B	308	VAL	C-N-CA	7.28	127.26	119.76
1	A	308	VAL	CA-C-N	7.28	127.25	119.76
1	A	308	VAL	C-N-CA	7.28	127.25	119.76
1	C	308	VAL	CA-C-N	7.27	127.25	119.76
1	C	308	VAL	C-N-CA	7.27	127.25	119.76
1	C	844	PRO	CA-C-N	7.27	127.23	120.03
1	C	844	PRO	C-N-CA	7.27	127.23	120.03
1	A	870	PHE	CA-CB-CG	7.22	121.02	113.80
1	B	870	PHE	CA-CB-CG	7.22	121.02	113.80
1	C	870	PHE	CA-CB-CG	7.21	121.01	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	30	GLY	N-CA-C	-6.98	102.82	112.18
3	G	30	GLY	N-CA-C	-6.98	102.82	112.18
3	N	30	GLY	N-CA-C	-6.97	102.84	112.18
1	A	206	VAL	N-CA-C	6.95	117.91	111.45
1	B	206	VAL	N-CA-C	6.94	117.90	111.45
1	C	206	VAL	N-CA-C	6.93	117.89	111.45
3	G	6	GLN	CA-C-N	6.79	124.55	119.66
3	G	6	GLN	C-N-CA	6.79	124.55	119.66
3	N	6	GLN	CA-C-N	6.79	124.55	119.66
3	N	6	GLN	C-N-CA	6.79	124.55	119.66
3	F	6	GLN	CA-C-N	6.78	124.54	119.66
3	F	6	GLN	C-N-CA	6.78	124.54	119.66
3	N	26	TYR	CA-C-N	6.78	133.44	122.53
3	N	26	TYR	C-N-CA	6.78	133.44	122.53
3	F	26	TYR	CA-C-N	6.76	133.41	122.53
3	F	26	TYR	C-N-CA	6.76	133.41	122.53
3	G	26	TYR	CA-C-N	6.75	133.41	122.53
3	G	26	TYR	C-N-CA	6.75	133.41	122.53
1	A	564	ASP	CA-C-N	6.67	126.37	119.56
1	A	564	ASP	C-N-CA	6.67	126.37	119.56
1	C	564	ASP	CA-C-N	6.66	126.36	119.56
1	C	564	ASP	C-N-CA	6.66	126.36	119.56
1	B	564	ASP	CA-C-N	6.65	126.34	119.56
1	B	564	ASP	C-N-CA	6.65	126.34	119.56
1	A	70	HIS	CA-C-N	6.60	133.57	121.70
1	A	70	HIS	C-N-CA	6.60	133.57	121.70
1	B	70	HIS	CA-C-N	6.60	133.58	121.70
1	B	70	HIS	C-N-CA	6.60	133.58	121.70
1	C	70	HIS	CA-C-N	6.59	133.56	121.70
1	C	70	HIS	C-N-CA	6.59	133.56	121.70
1	B	793	LYS	CA-C-N	6.57	126.27	119.56
1	B	793	LYS	C-N-CA	6.57	126.27	119.56
1	A	793	LYS	CA-C-N	6.56	126.25	119.56
1	A	793	LYS	C-N-CA	6.56	126.25	119.56
1	A	696	ILE	CA-C-N	6.55	126.51	119.76
1	A	696	ILE	C-N-CA	6.55	126.51	119.76
1	C	793	LYS	CA-C-N	6.54	126.23	119.56
1	C	793	LYS	C-N-CA	6.54	126.23	119.56
1	C	696	ILE	CA-C-N	6.53	126.49	119.76
1	C	696	ILE	C-N-CA	6.53	126.49	119.76
1	B	696	ILE	CA-C-N	6.53	126.49	119.76
1	B	696	ILE	C-N-CA	6.53	126.49	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	87	ASP	CA-CB-CG	6.45	119.05	112.60
3	N	87	ASP	CA-CB-CG	6.44	119.04	112.60
3	G	87	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	934	VAL	N-CA-C	-6.39	104.62	110.82
1	B	934	VAL	N-CA-C	-6.37	104.64	110.82
1	C	934	VAL	N-CA-C	-6.37	104.64	110.82
1	A	78	ASN	CA-C-N	6.30	126.49	120.31
1	A	78	ASN	C-N-CA	6.30	126.49	120.31
1	B	78	ASN	CA-C-N	6.30	126.48	120.31
1	B	78	ASN	C-N-CA	6.30	126.48	120.31
1	C	78	ASN	CA-C-N	6.30	126.48	120.31
1	C	78	ASN	C-N-CA	6.30	126.48	120.31
1	C	585	THR	CA-C-N	6.25	126.37	119.87
1	C	585	THR	C-N-CA	6.25	126.37	119.87
3	G	27	ASN	N-CA-C	-6.23	100.08	108.86
3	N	27	ASN	N-CA-C	-6.22	100.08	108.86
1	B	585	THR	CA-C-N	6.22	126.34	119.87
1	B	585	THR	C-N-CA	6.22	126.34	119.87
3	F	27	ASN	N-CA-C	-6.22	100.09	108.86
1	A	585	THR	CA-C-N	6.21	126.32	119.87
1	A	585	THR	C-N-CA	6.21	126.32	119.87
1	B	851	MET	N-CA-C	-6.09	103.99	112.45
1	A	851	MET	N-CA-C	-6.09	103.99	112.45
2	M	52	SER	CA-C-N	6.08	126.52	119.47
2	M	52	SER	C-N-CA	6.08	126.52	119.47
1	C	851	MET	N-CA-C	-6.08	104.00	112.45
2	E	52	SER	CA-C-N	6.07	126.51	119.47
2	E	52	SER	C-N-CA	6.07	126.51	119.47
2	D	52	SER	CA-C-N	6.04	126.48	119.47
2	D	52	SER	C-N-CA	6.04	126.48	119.47
1	A	808	VAL	CA-C-N	6.03	132.56	121.70
1	A	808	VAL	C-N-CA	6.03	132.56	121.70
1	C	808	VAL	CA-C-N	6.03	132.56	121.70
1	C	808	VAL	C-N-CA	6.03	132.56	121.70
1	B	808	VAL	CA-C-N	6.02	132.53	121.70
1	B	808	VAL	C-N-CA	6.02	132.53	121.70
3	F	56	ARG	CA-C-N	6.02	126.48	120.52
3	F	56	ARG	C-N-CA	6.02	126.48	120.52
2	M	77	ASN	CA-CB-CG	6.02	118.62	112.60
3	N	56	ARG	CA-C-N	6.01	126.47	120.52
3	N	56	ARG	C-N-CA	6.01	126.47	120.52
2	D	77	ASN	CA-CB-CG	6.01	118.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	56	ARG	CA-C-N	6.01	126.47	120.52
3	G	56	ARG	C-N-CA	6.01	126.47	120.52
2	E	77	ASN	CA-CB-CG	5.99	118.59	112.60
1	C	46	ILE	N-CA-C	5.95	116.50	108.17
1	A	46	ILE	N-CA-C	5.95	116.50	108.17
1	B	968	PRO	N-CA-C	5.95	117.95	110.70
1	C	968	PRO	N-CA-C	5.95	117.95	110.70
1	A	968	PRO	N-CA-C	5.94	117.95	110.70
1	B	46	ILE	N-CA-C	5.94	116.49	108.17
1	C	967	ASP	CA-C-N	5.91	126.47	120.38
1	C	967	ASP	C-N-CA	5.91	126.47	120.38
1	B	967	ASP	CA-C-N	5.90	126.46	120.38
1	B	967	ASP	C-N-CA	5.90	126.46	120.38
1	A	967	ASP	CA-C-N	5.88	126.44	120.38
1	A	967	ASP	C-N-CA	5.88	126.44	120.38
1	B	790	ASP	CA-C-N	5.81	125.43	119.56
1	B	790	ASP	C-N-CA	5.81	125.43	119.56
1	A	790	ASP	CA-C-N	5.81	125.42	119.56
1	A	790	ASP	C-N-CA	5.81	125.42	119.56
1	C	790	ASP	CA-C-N	5.81	125.43	119.56
1	C	790	ASP	C-N-CA	5.81	125.43	119.56
1	B	1024	PHE	N-CA-C	-5.66	100.01	109.24
1	C	1024	PHE	N-CA-C	-5.65	100.03	109.24
1	C	209	LEU	N-CA-C	-5.65	102.53	109.65
1	A	209	LEU	N-CA-C	-5.65	102.53	109.65
1	B	209	LEU	N-CA-C	-5.64	102.54	109.65
1	A	1024	PHE	N-CA-C	-5.64	100.05	109.24
2	E	16	SER	N-CA-C	5.56	116.70	108.86
2	M	16	SER	N-CA-C	5.56	116.70	108.86
3	N	28	ASP	CB-CA-C	-5.55	109.68	117.23
2	D	16	SER	N-CA-C	5.55	116.68	108.86
3	G	28	ASP	CB-CA-C	-5.54	109.70	117.23
3	F	28	ASP	CB-CA-C	-5.54	109.70	117.23
1	A	758	ARG	N-CA-C	-5.51	104.78	112.45
1	B	758	ARG	N-CA-C	-5.51	104.80	112.45
1	C	758	ARG	N-CA-C	-5.50	104.81	112.45
1	B	1059	THR	N-CA-C	5.46	118.17	109.81
1	C	1059	THR	N-CA-C	5.46	118.16	109.81
1	A	1059	THR	N-CA-C	5.45	118.15	109.81
1	A	1093	SER	CA-C-N	5.36	125.12	119.76
1	A	1093	SER	C-N-CA	5.36	125.12	119.76
1	B	1093	SER	CA-C-N	5.35	125.11	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1093	SER	C-N-CA	5.35	125.11	119.76
1	C	1093	SER	CA-C-N	5.34	125.10	119.76
1	C	1093	SER	C-N-CA	5.34	125.10	119.76
1	A	1060	ALA	CA-C-N	5.32	124.93	119.56
1	A	1060	ALA	C-N-CA	5.32	124.93	119.56
3	N	5	THR	N-CA-C	5.32	117.63	109.07
3	G	5	THR	N-CA-C	5.30	117.61	109.07
3	F	5	THR	N-CA-C	5.30	117.60	109.07
1	B	1060	ALA	CA-C-N	5.29	124.91	119.56
1	B	1060	ALA	C-N-CA	5.29	124.91	119.56
1	C	1060	ALA	CA-C-N	5.29	124.90	119.56
1	C	1060	ALA	C-N-CA	5.29	124.90	119.56
1	B	869	THR	CA-C-N	5.27	127.34	120.28
1	B	869	THR	C-N-CA	5.27	127.34	120.28
1	A	869	THR	CA-C-N	5.26	127.33	120.28
1	A	869	THR	C-N-CA	5.26	127.33	120.28
1	C	869	THR	CA-C-N	5.25	127.31	120.28
1	C	869	THR	C-N-CA	5.25	127.31	120.28
1	A	546	GLN	CA-C-N	5.25	126.40	119.84
1	A	546	GLN	C-N-CA	5.25	126.40	119.84
1	B	546	GLN	CA-C-N	5.25	126.40	119.84
1	B	546	GLN	C-N-CA	5.25	126.40	119.84
1	C	546	GLN	CA-C-N	5.24	126.39	119.84
1	C	546	GLN	C-N-CA	5.24	126.39	119.84
1	B	773	THR	CA-C-N	5.24	125.17	119.78
1	B	773	THR	C-N-CA	5.24	125.17	119.78
1	C	773	THR	CA-C-N	5.24	125.17	119.78
1	C	773	THR	C-N-CA	5.24	125.17	119.78
1	A	773	THR	CA-C-N	5.21	125.15	119.78
1	A	773	THR	C-N-CA	5.21	125.15	119.78
2	D	37	VAL	N-CA-C	5.19	115.45	107.77
3	N	60	VAL	CA-C-N	5.18	125.16	120.03
3	N	60	VAL	C-N-CA	5.18	125.16	120.03
3	G	60	VAL	CA-C-N	5.18	125.16	120.03
3	G	60	VAL	C-N-CA	5.18	125.16	120.03
3	F	60	VAL	CA-C-N	5.18	125.16	120.03
3	F	60	VAL	C-N-CA	5.18	125.16	120.03
2	E	37	VAL	N-CA-C	5.18	115.43	107.77
2	M	37	VAL	N-CA-C	5.17	115.42	107.77
3	G	95	GLY	CA-C-O	-5.14	118.88	122.22
3	F	95	GLY	CA-C-O	-5.14	118.88	122.22
3	F	27	ASN	CA-CB-CG	5.12	117.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	95	GLY	CA-C-O	-5.11	118.90	122.22
3	N	27	ASN	CA-CB-CG	5.11	117.71	112.60
3	G	27	ASN	CA-CB-CG	5.09	117.69	112.60
1	C	254	VAL	N-CA-C	5.08	115.44	108.12
1	B	254	VAL	N-CA-C	5.07	115.42	108.12
1	A	254	VAL	N-CA-C	5.07	115.41	108.12
1	B	281	ASN	CA-C-N	5.01	124.67	119.56
1	B	281	ASN	C-N-CA	5.01	124.67	119.56
1	C	281	ASN	CA-C-N	5.00	124.66	119.56
1	C	281	ASN	C-N-CA	5.00	124.66	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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	3	0
3	G	787	0	747	1	0
3	N	787	0	747	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	20	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 (20) 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
3:N:52:GLU:O	3:N:53:VAL:C	2.60	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
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
3:F:52:GLU:O	3:F:53:VAL:C	2.60	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%)	99 (98%)	2 (2%)	50	75
2	E	101/192 (53%)	99 (98%)	2 (2%)	50	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	101/192 (53%)	99 (98%)	2 (2%)	50	75
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%)	2559 (100%)	6 (0%)	91	97

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

Mol	Chain	Res	Type
2	M	100	LEU
2	M	126	VAL
2	D	100	LEU
2	D	126	VAL
2	E	100	LEU
2	E	126	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	895	GLN
1	A	947	GLN
1	A	951	ASN
2	M	65	GLN
3	N	27	ASN
1	B	304	ASN
1	B	737	GLN
1	B	947	GLN
1	B	951	ASN
2	D	65	GLN
3	F	27	ASN
1	C	304	ASN
1	C	737	GLN
1	C	895	GLN
1	C	947	GLN
2	E	65	GLN
3	G	27	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	4,1	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	4,1	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	4,1	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	4,1	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	4,1	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	4,1	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	R	1	4,1	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	4,1	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	4,1	14,14,15	2.21	7 (50%)	17,19,21	1.11	2 (11%)
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	4,1	-	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	4,1	-	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	4,1	-	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	4,1	-	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	4,1	-	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	4,1	-	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	4,1	-	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	4,1	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	T	3	5	-	1/2/19/22	0/1/1/1
4	NAG	U	1	4,1	-	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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.

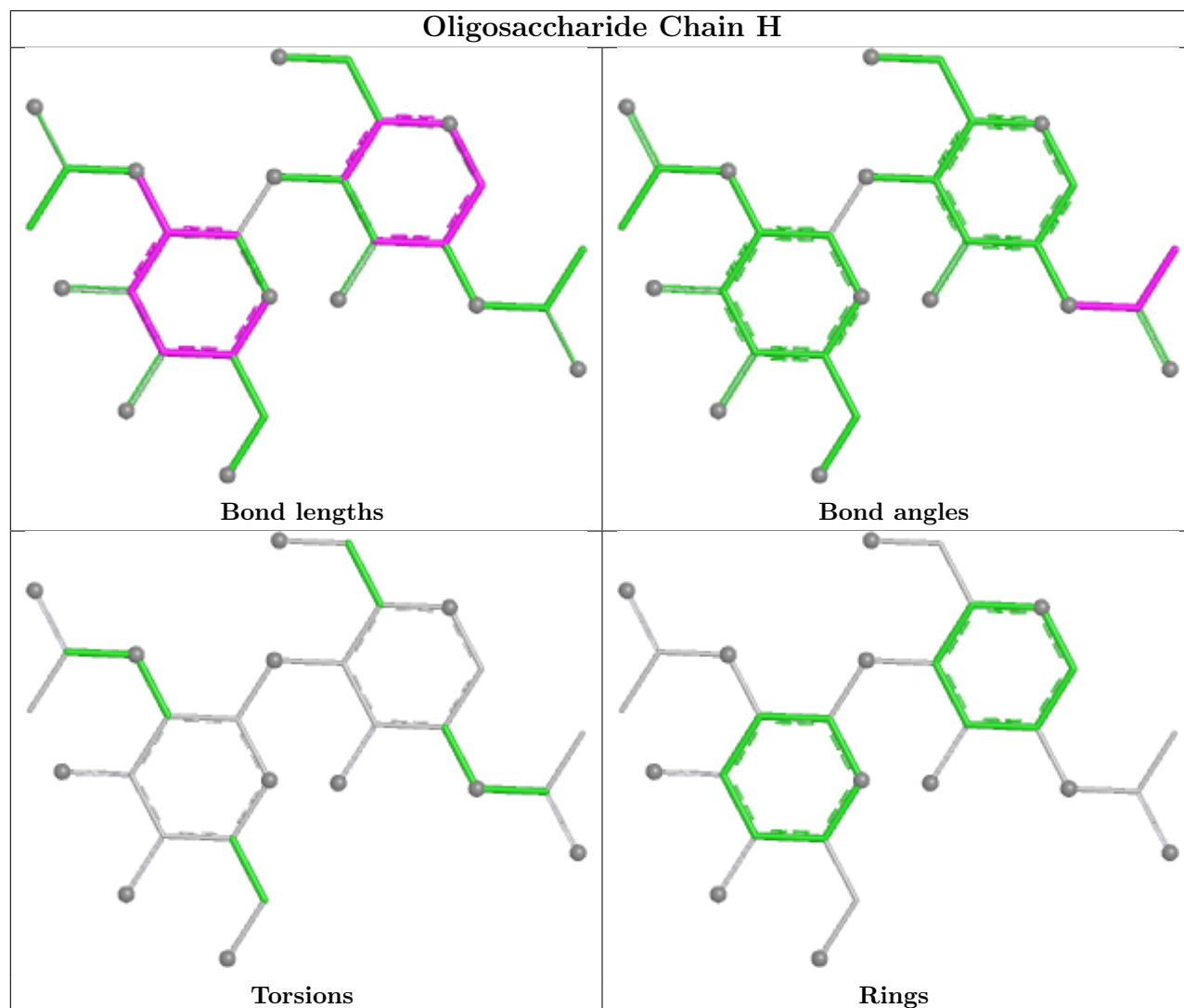
All (9) torsion outliers are listed below:

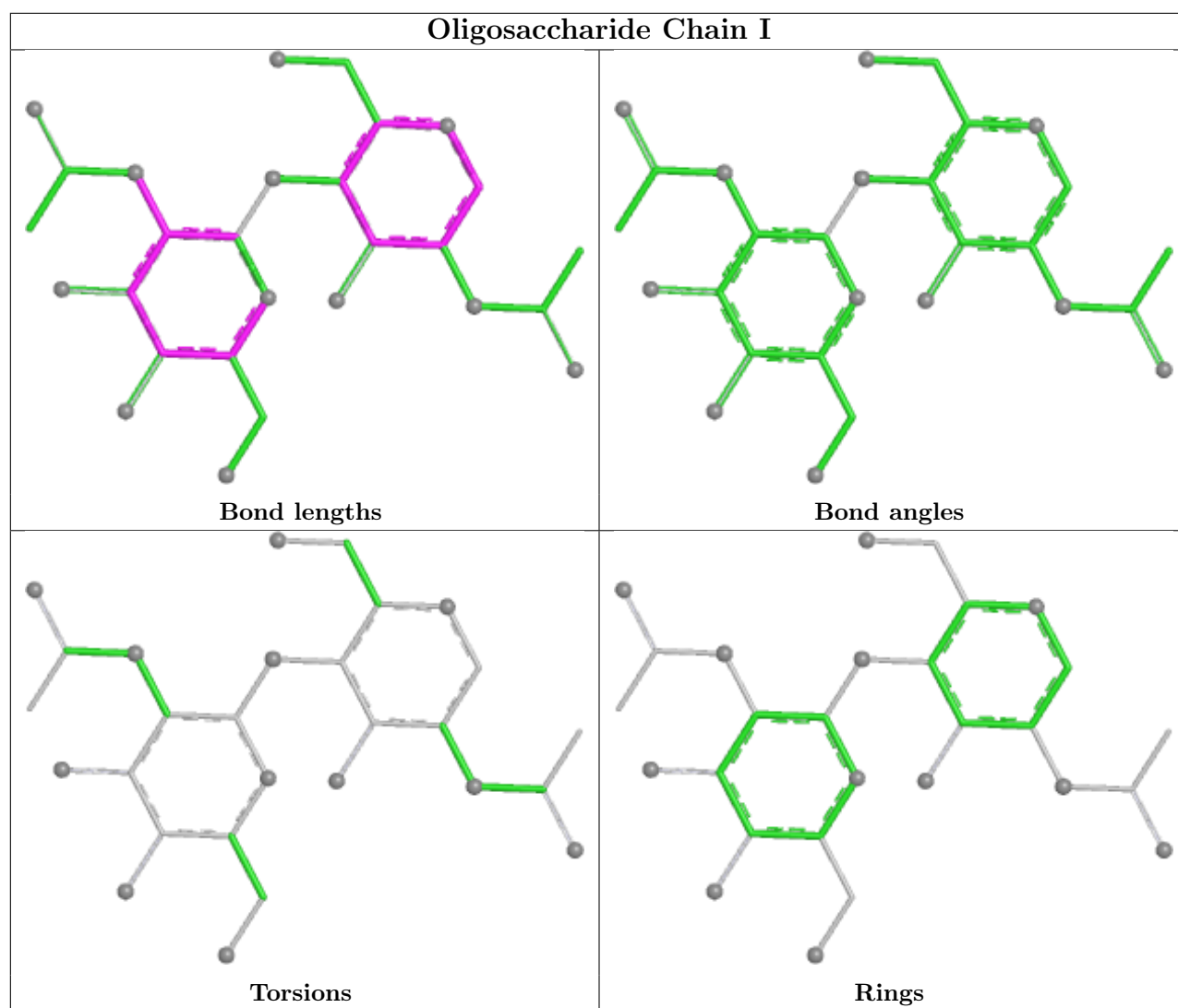
Mol	Chain	Res	Type	Atoms
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
5	J	3	BMA	O5-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6

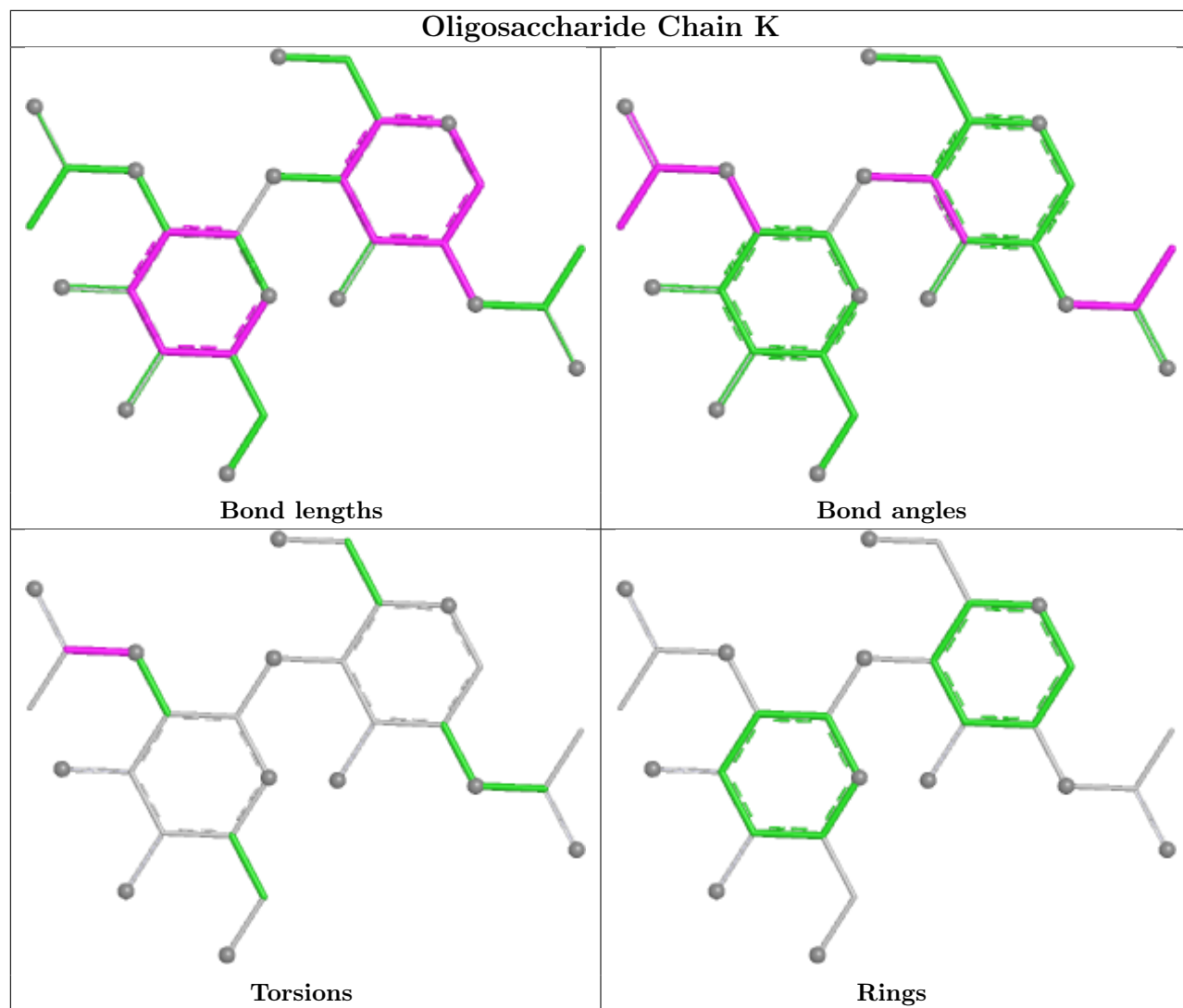
There are no ring outliers.

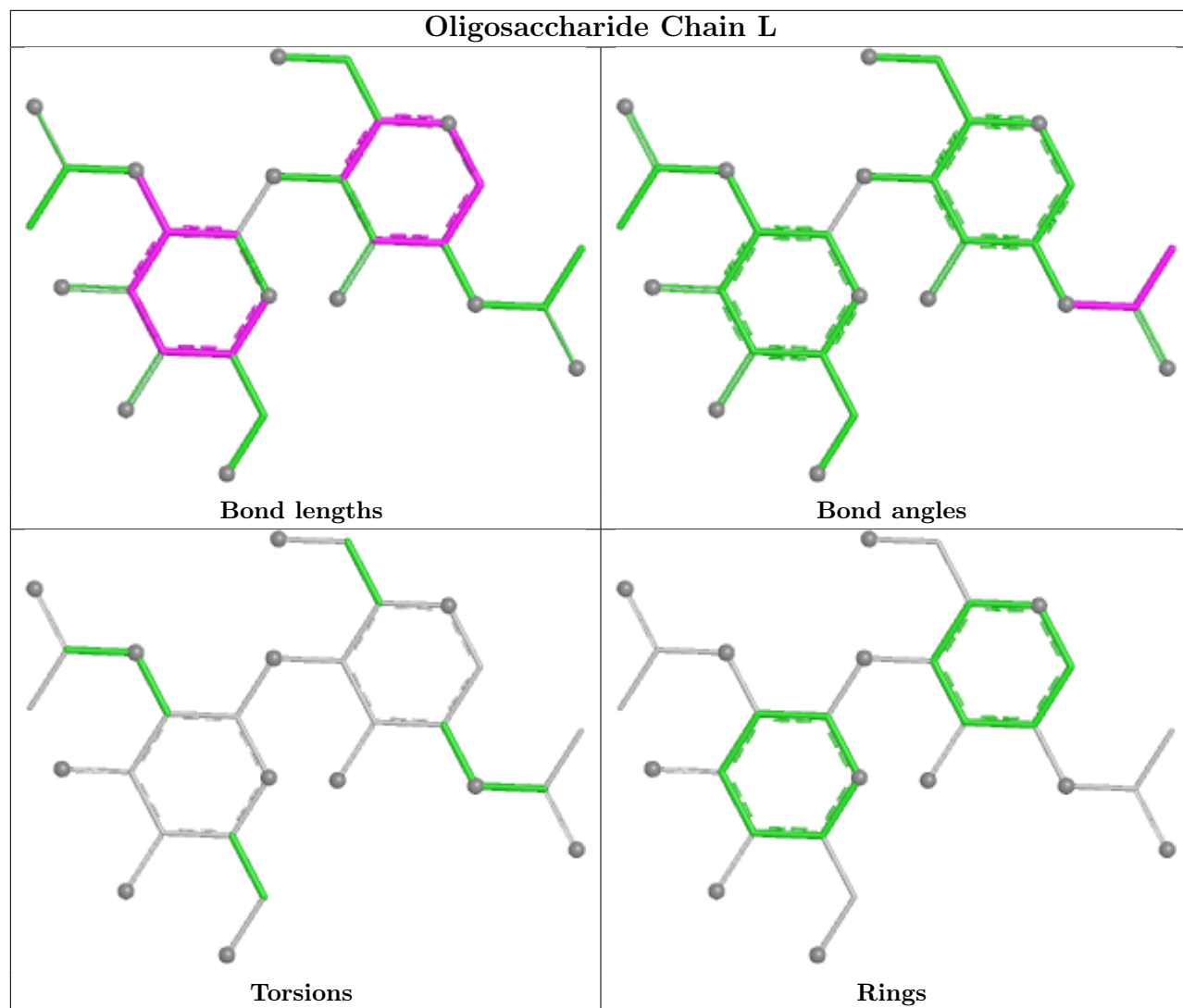
No monomer is involved in short contacts.

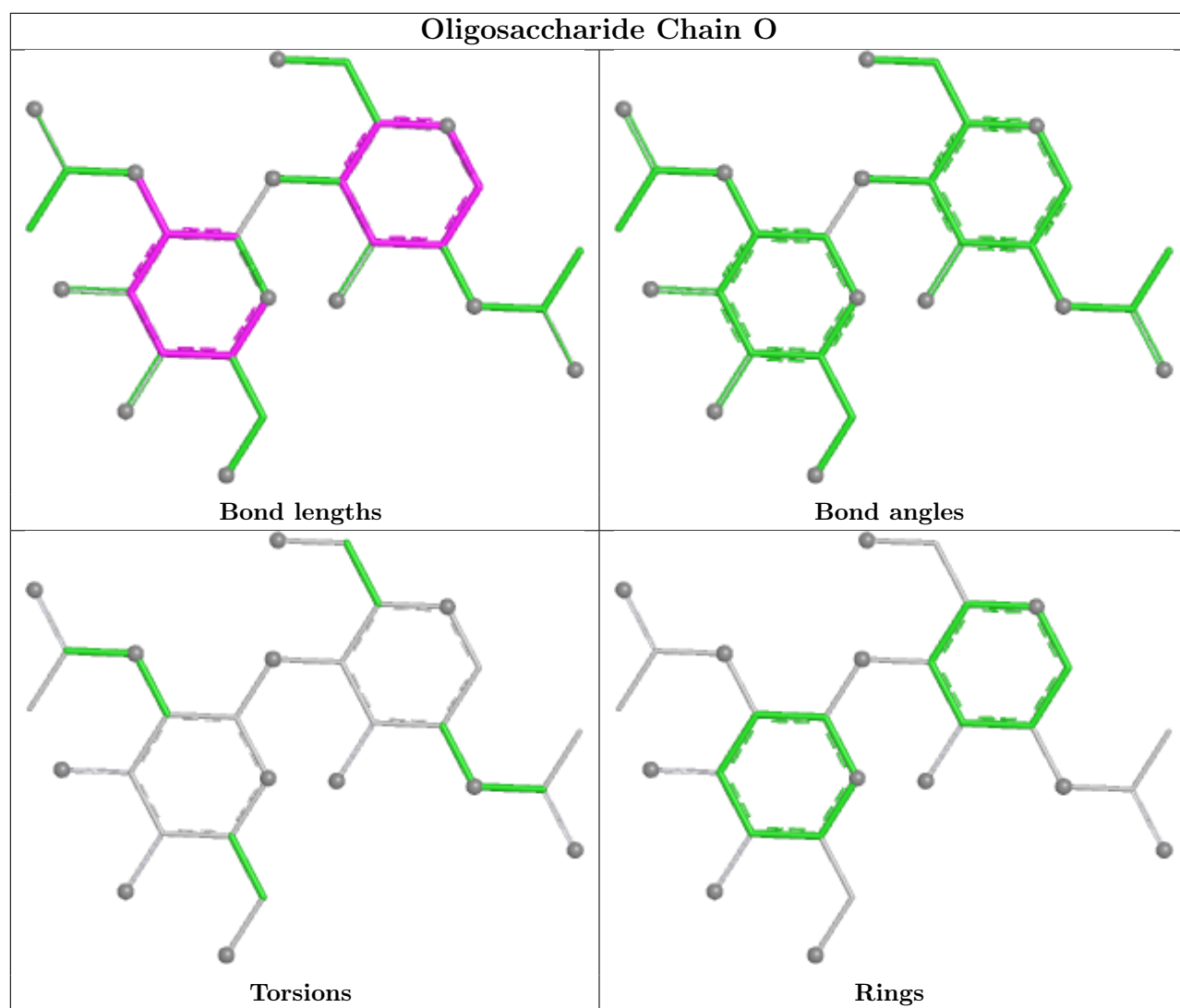
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

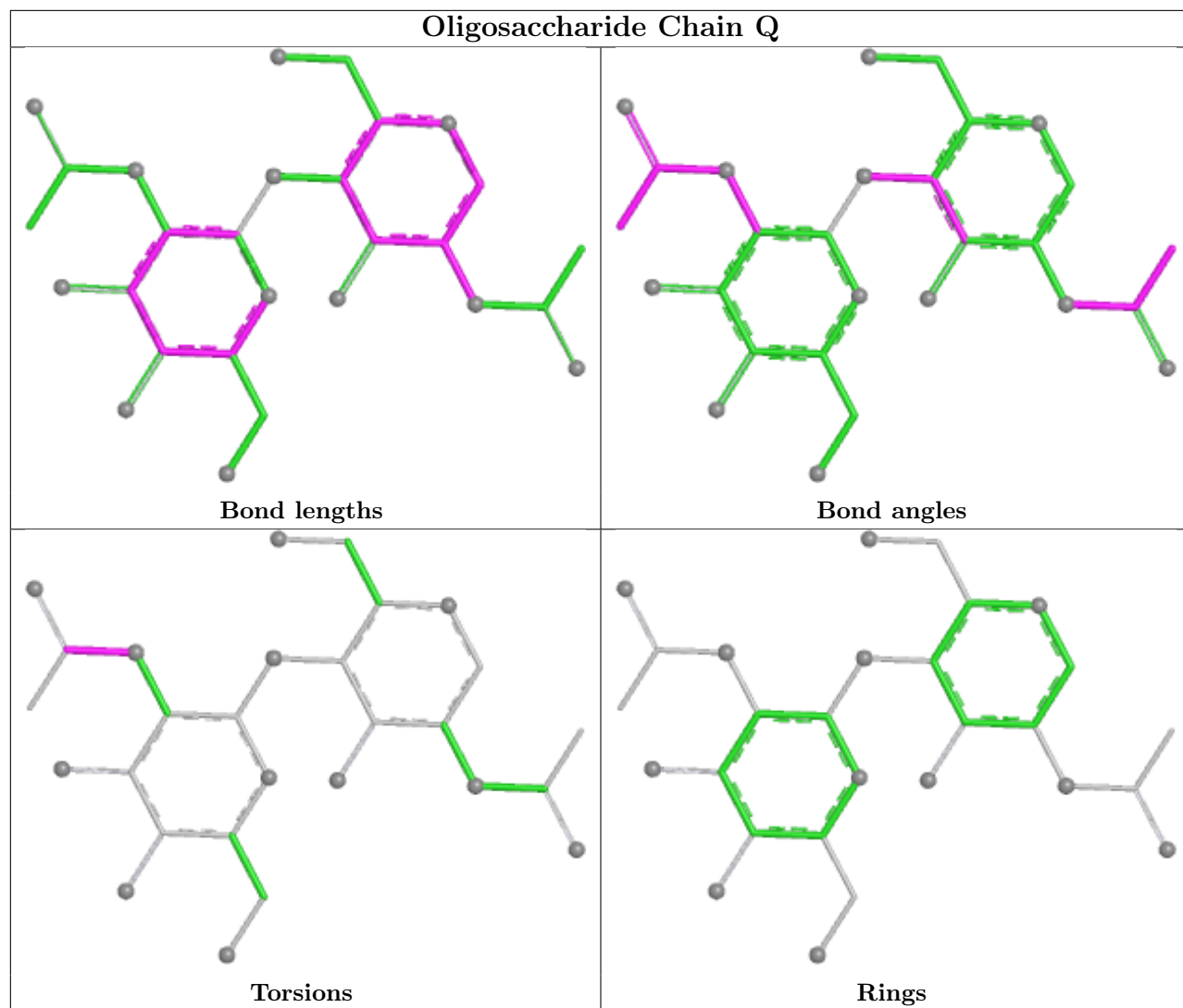


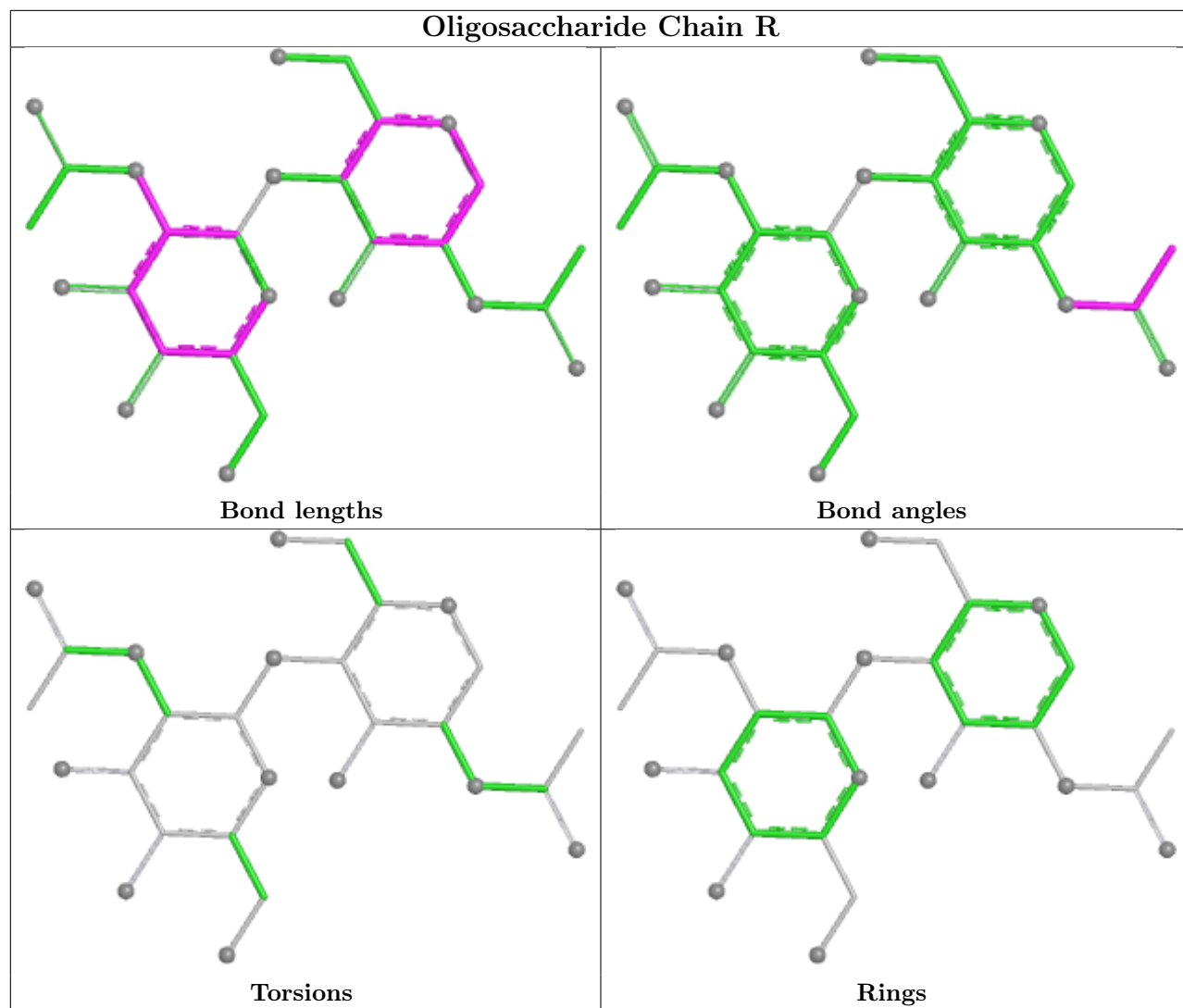


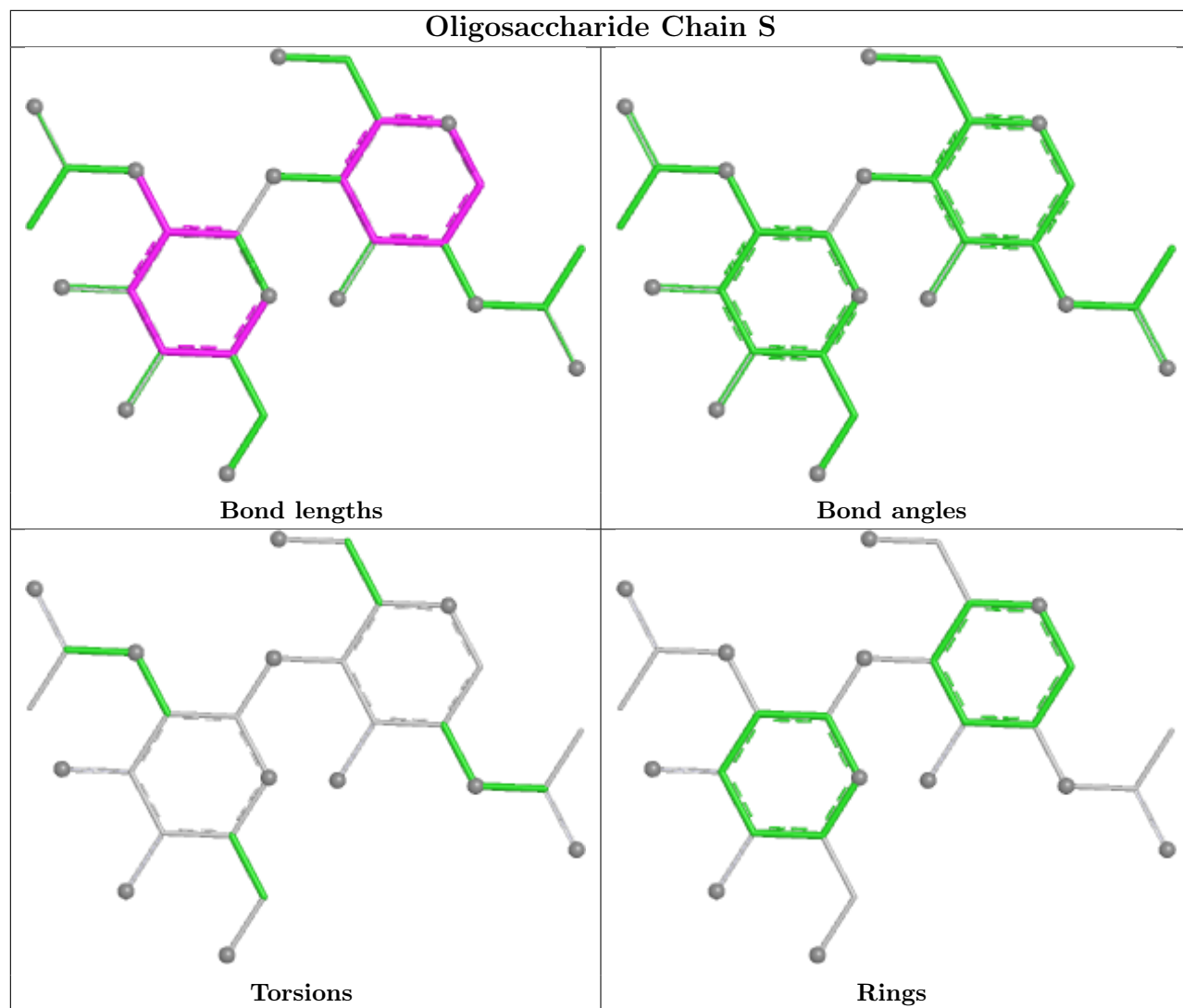


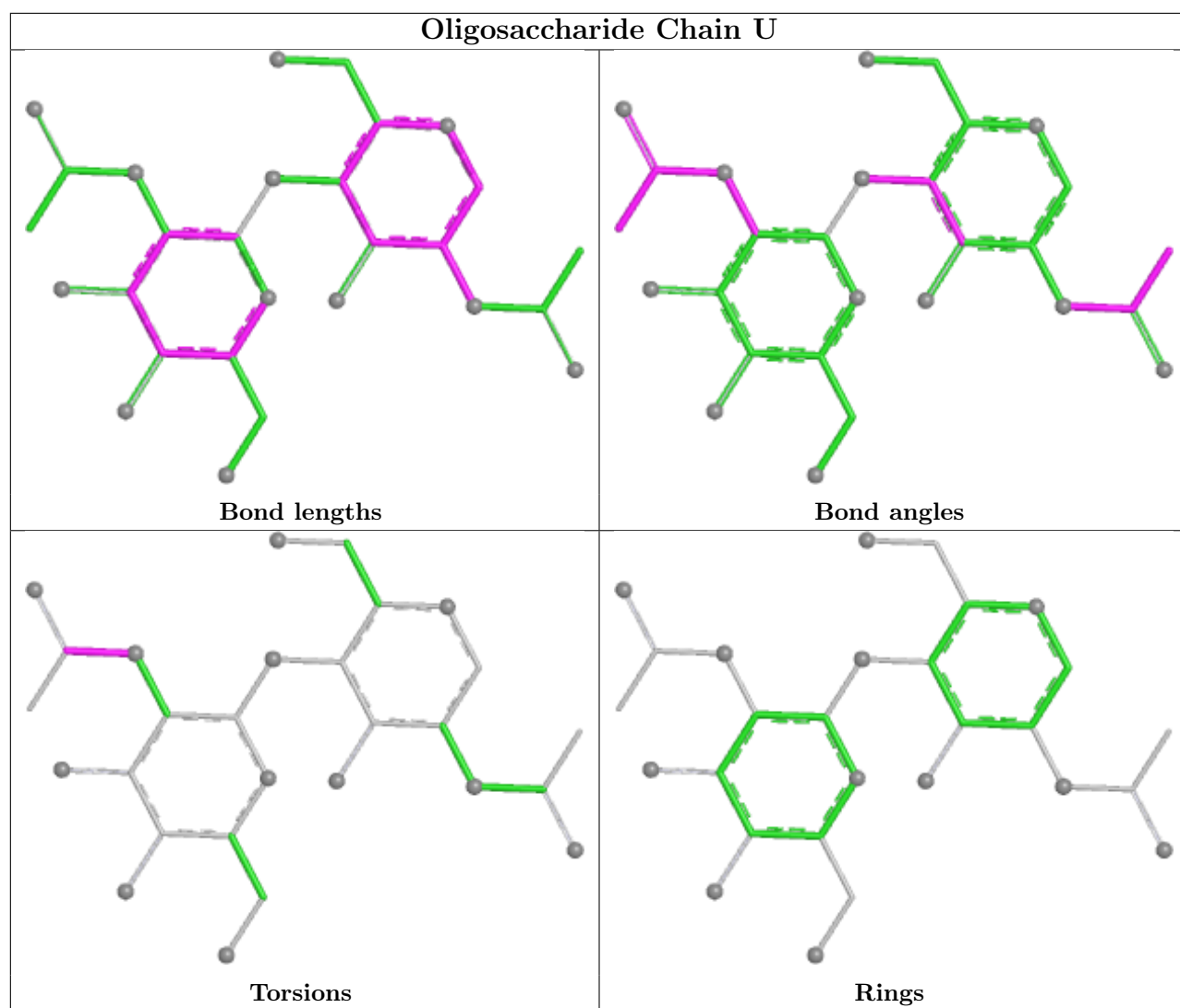


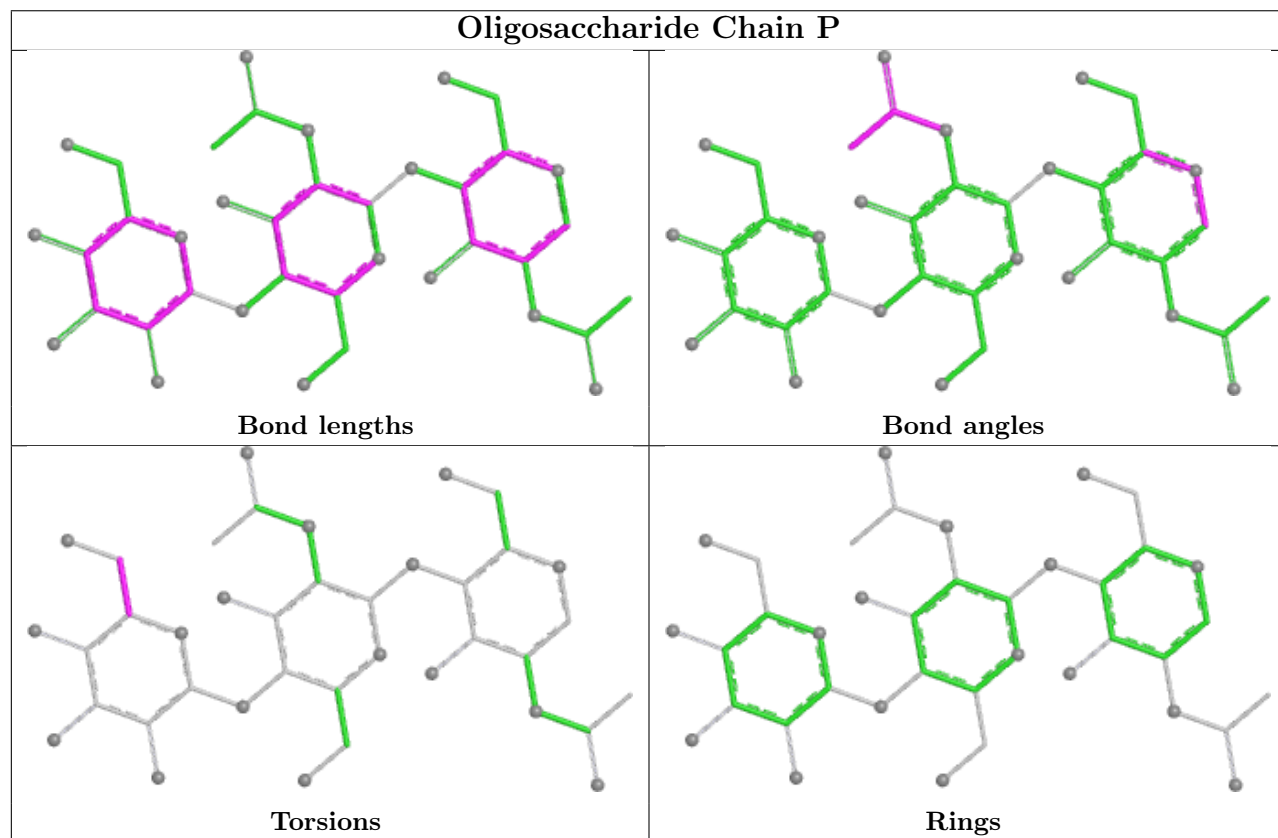
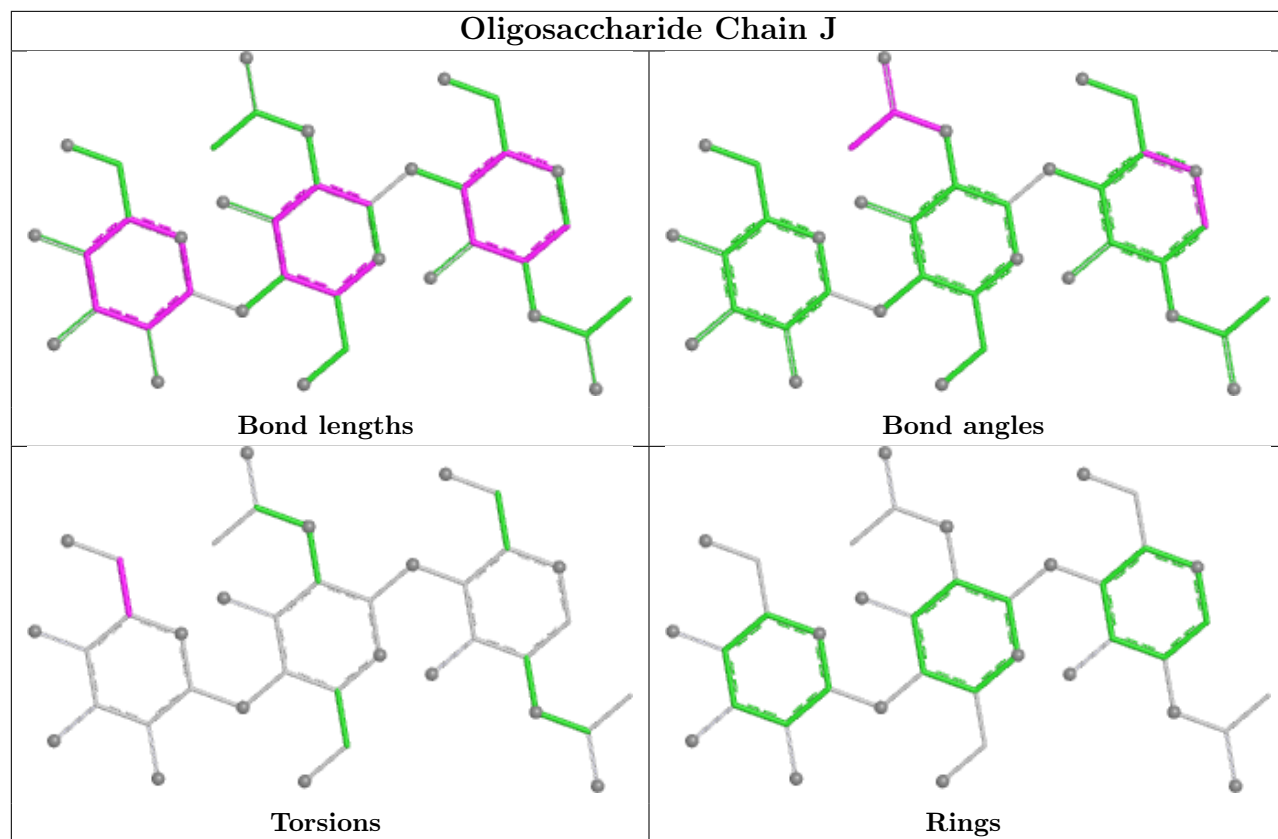


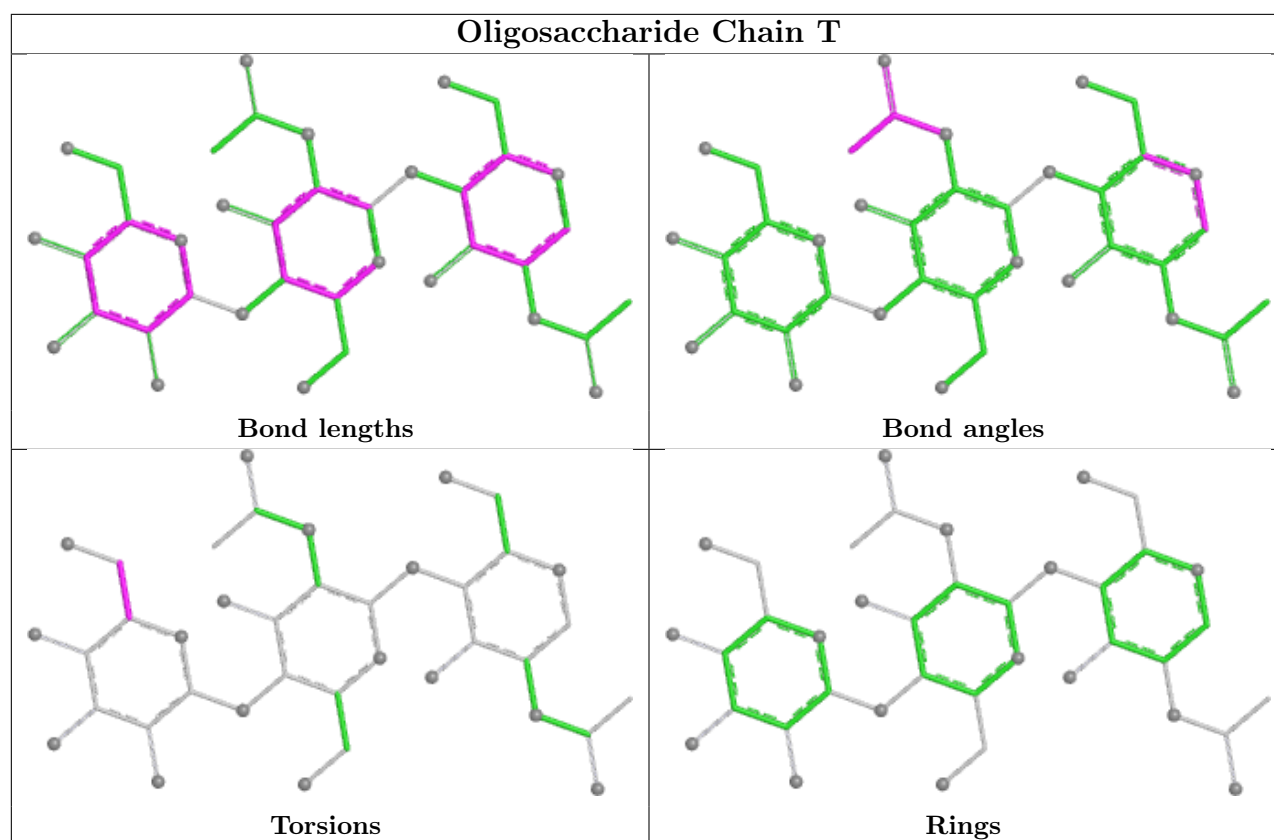












5.6 Ligand geometry [i](#)

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	1304	1	14,14,15	2.25	6 (42%)	17,19,21	1.06	1 (5%)
6	NAG	A	1304	1	14,14,15	2.24	6 (42%)	17,19,21	1.07	1 (5%)
6	NAG	B	1304	1	14,14,15	2.25	7 (50%)	17,19,21	1.07	1 (5%)
6	NAG	C	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	C	1305	1	14,14,15	2.25	5 (35%)	17,19,21	1.07	2 (11%)
6	NAG	B	1303	1	14,14,15	2.26	7 (50%)	17,19,21	0.98	1 (5%)
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	1301	1	14,14,15	2.26	6 (42%)	17,19,21	2.25	4 (23%)
6	NAG	B	1302	1	14,14,15	2.20	7 (50%)	17,19,21	1.06	2 (11%)
6	NAG	B	1305	1	14,14,15	2.24	5 (35%)	17,19,21	1.07	2 (11%)
6	NAG	A	1303	1	14,14,15	2.26	7 (50%)	17,19,21	0.98	1 (5%)
6	NAG	A	1305	1	14,14,15	2.25	5 (35%)	17,19,21	1.08	2 (11%)
6	NAG	A	1301	1	14,14,15	2.26	6 (42%)	17,19,21	2.25	4 (23%)
6	NAG	A	1302	1	14,14,15	2.20	7 (50%)	17,19,21	1.06	2 (11%)

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	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	C	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	C	1305	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1302	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	1302	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
6	NAG	A	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	1302	1	-	0/6/23/26	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

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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

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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

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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.

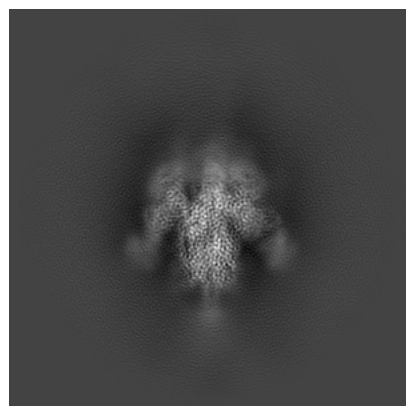
6 Map visualisation [i](#)

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.

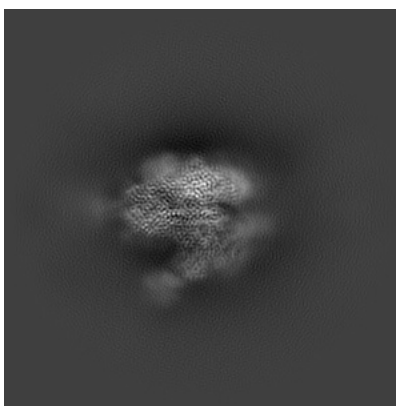
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

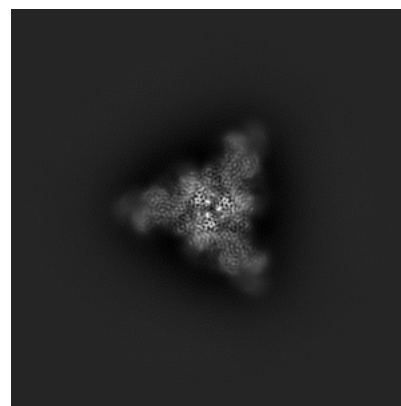
6.1.1 Primary map



X

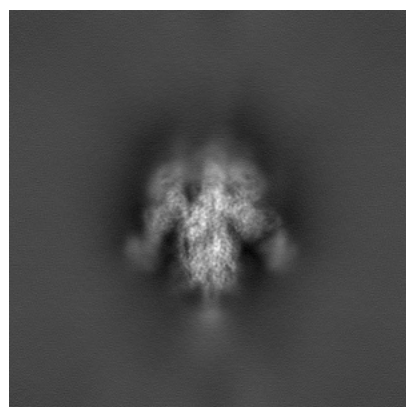


Y

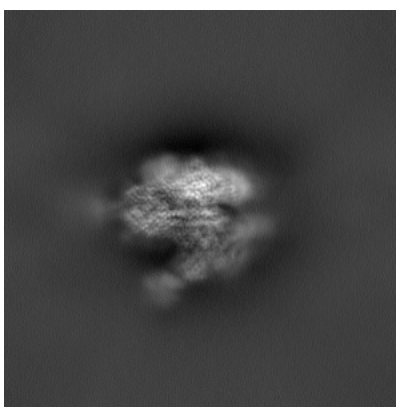


Z

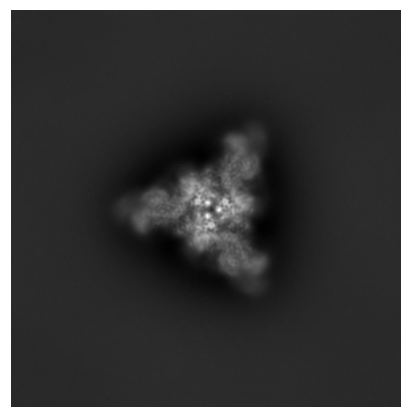
6.1.2 Raw map



X



Y

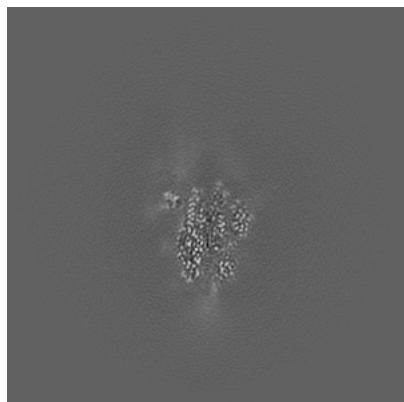


Z

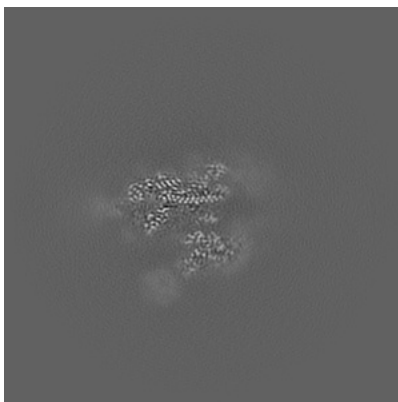
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

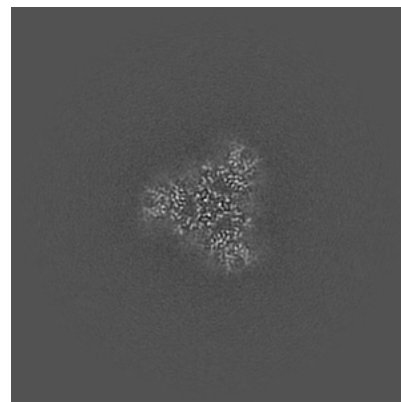
6.2.1 Primary map



X Index: 200

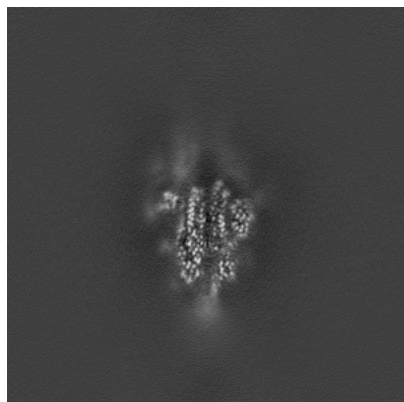


Y Index: 200

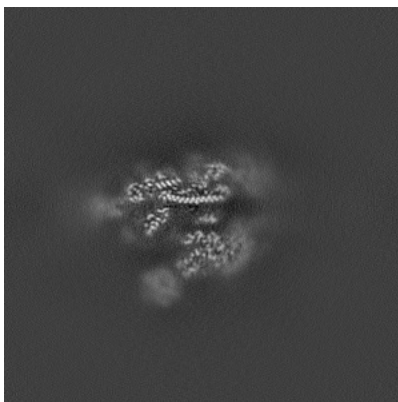


Z Index: 200

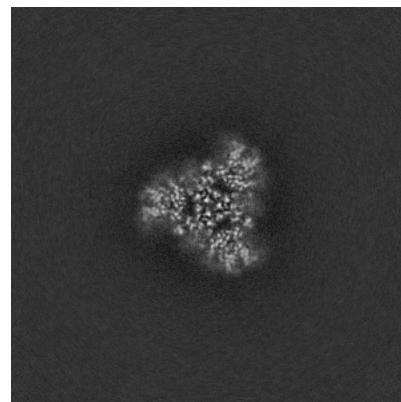
6.2.2 Raw map



X Index: 200



Y Index: 200

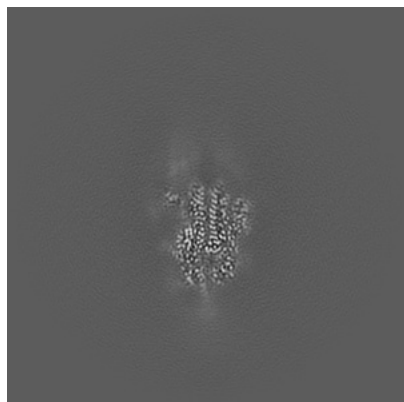


Z Index: 200

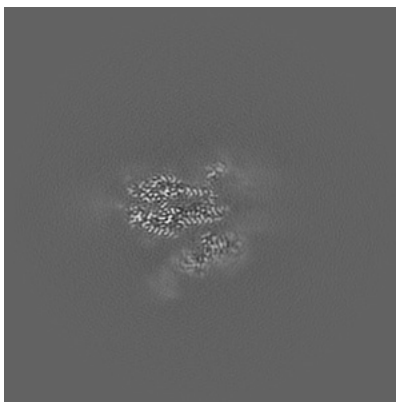
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

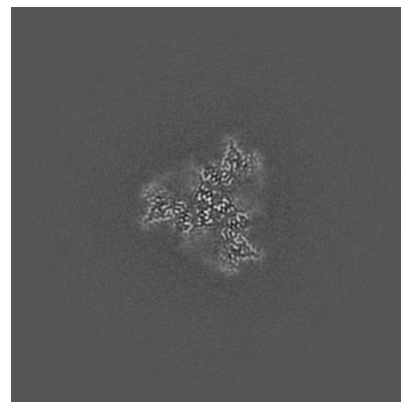
6.3.1 Primary map



X Index: 195

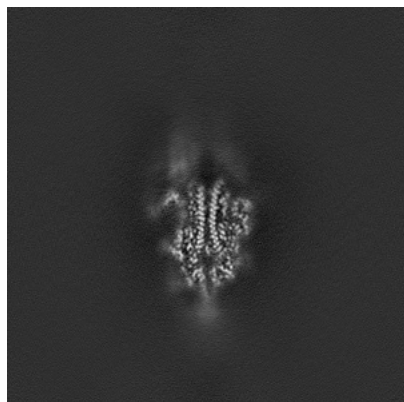


Y Index: 209

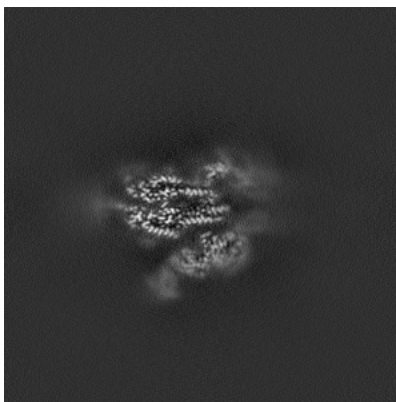


Z Index: 193

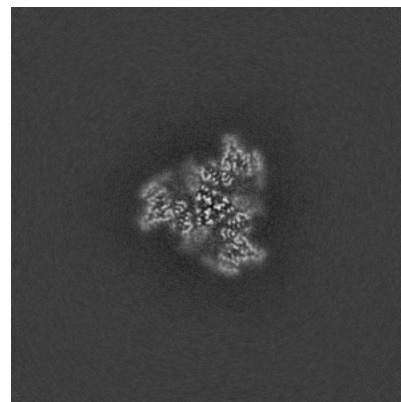
6.3.2 Raw map



X Index: 196



Y Index: 209

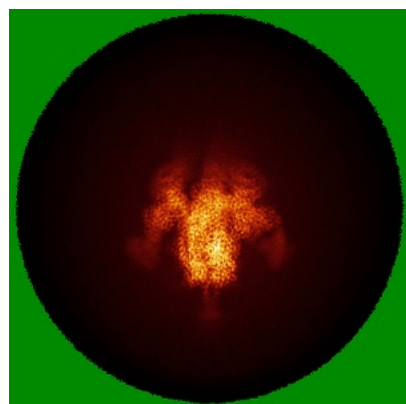


Z Index: 193

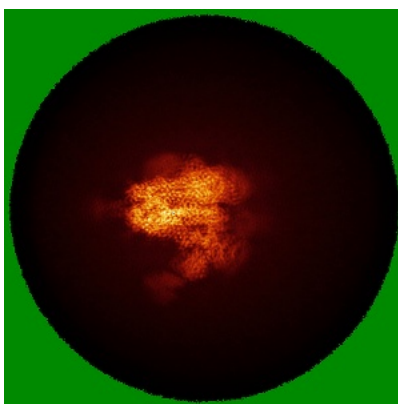
The images above show the largest variance slices of the map in three orthogonal directions.

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

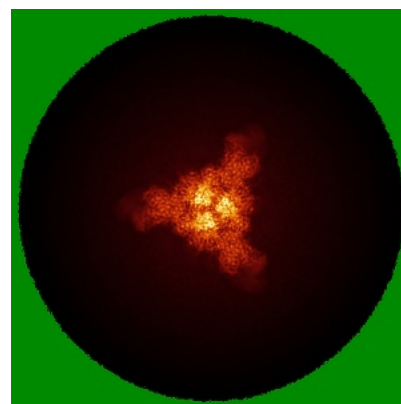
6.4.1 Primary map



X

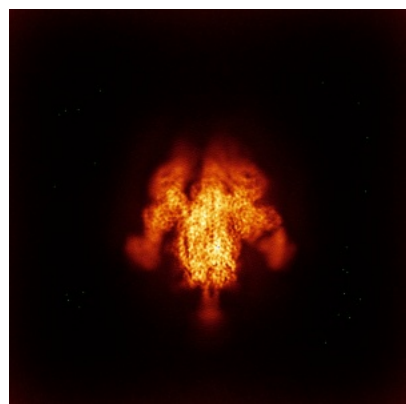


Y

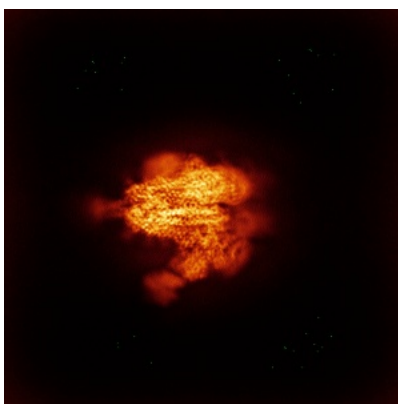


Z

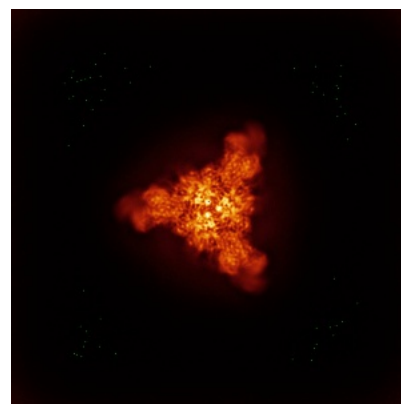
6.4.2 Raw map



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.

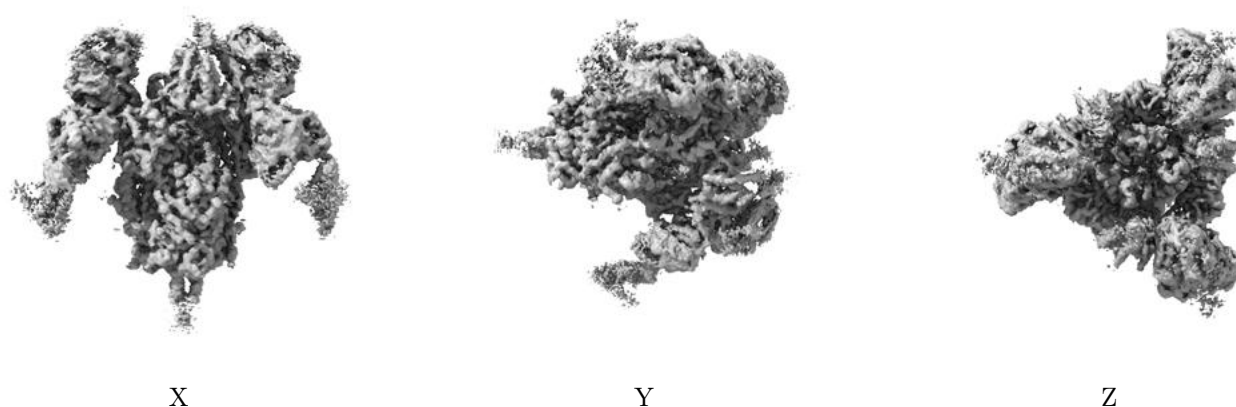
6.5 Orthogonal surface views [i](#)

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.

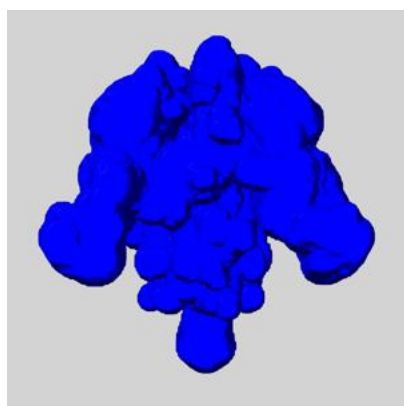
6.6 Mask visualisation [i](#)

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

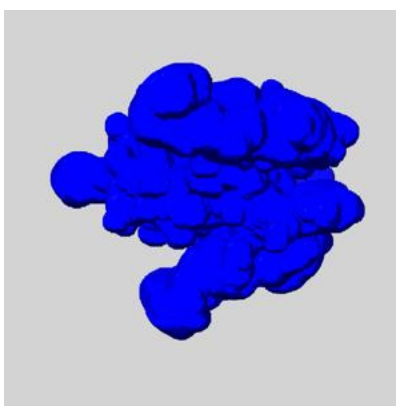
A mask typically either:

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

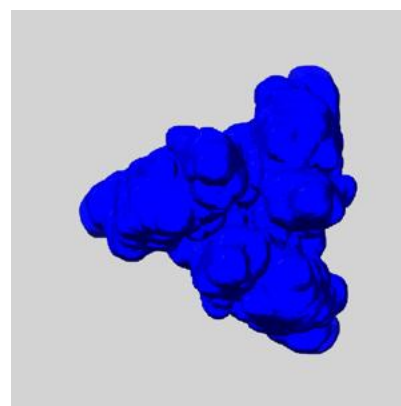
6.6.1 emd_43407_msk_1.map [i](#)



X



Y

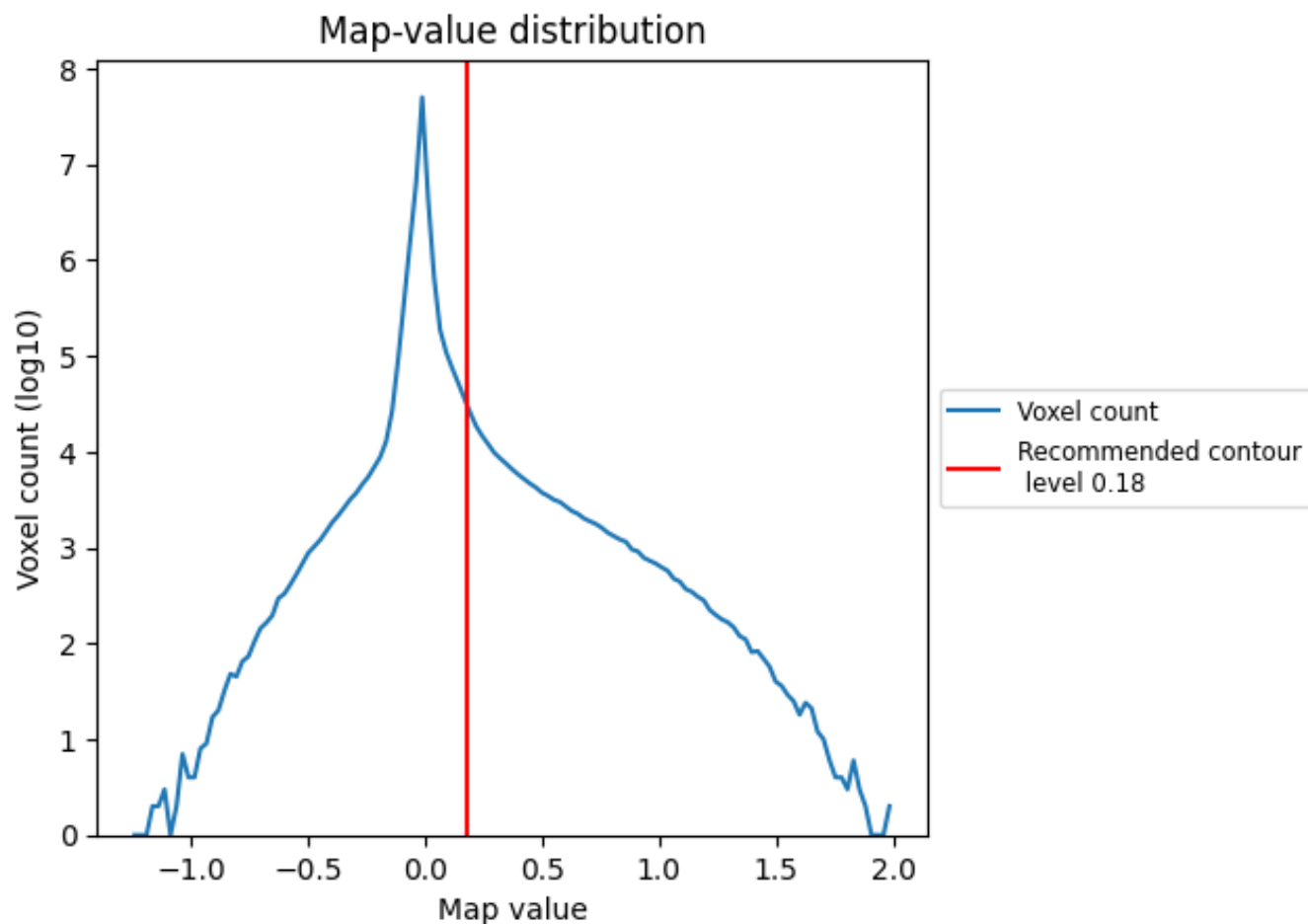


Z

7 Map analysis [i](#)

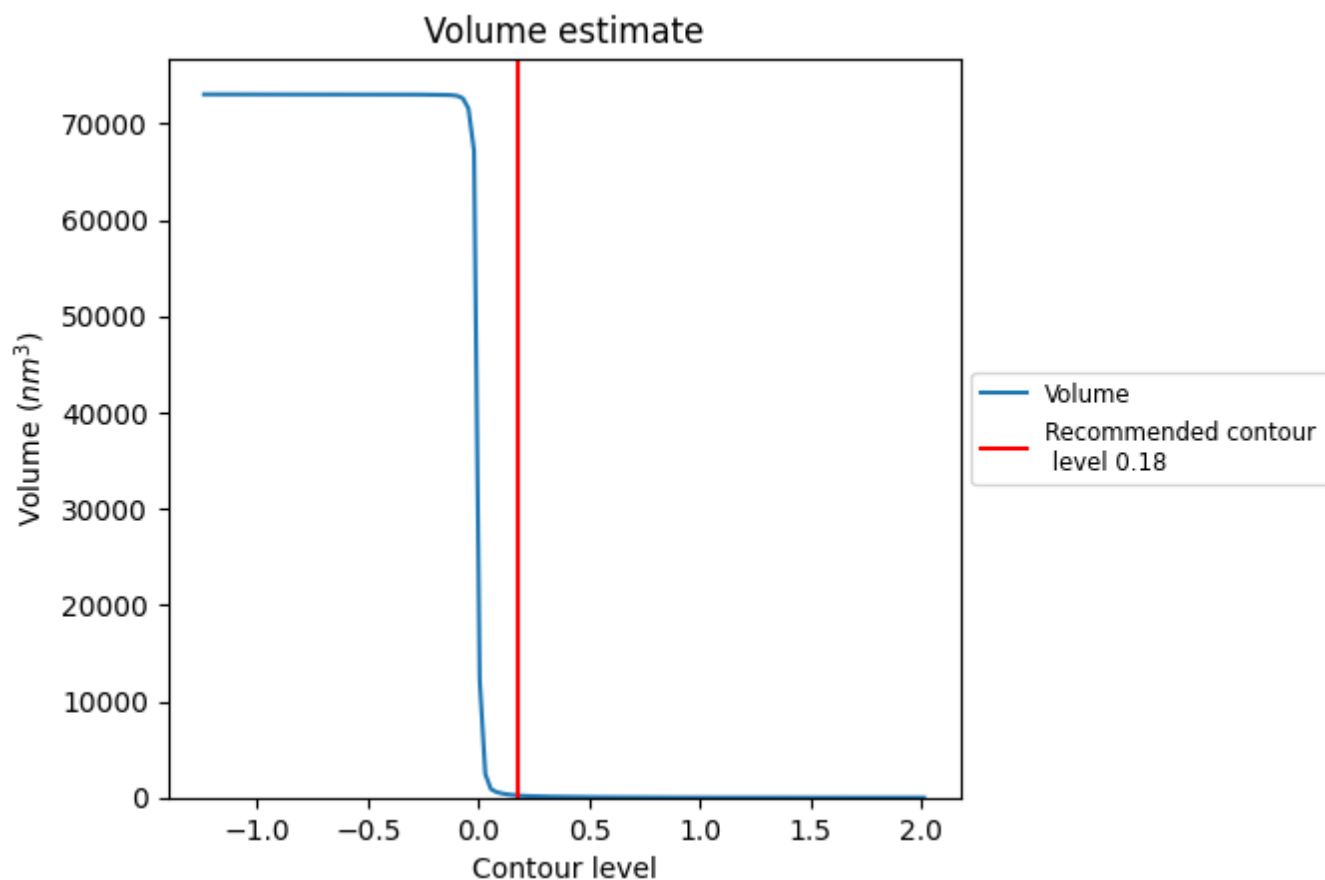
This section contains the results of statistical analysis of the map.

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.

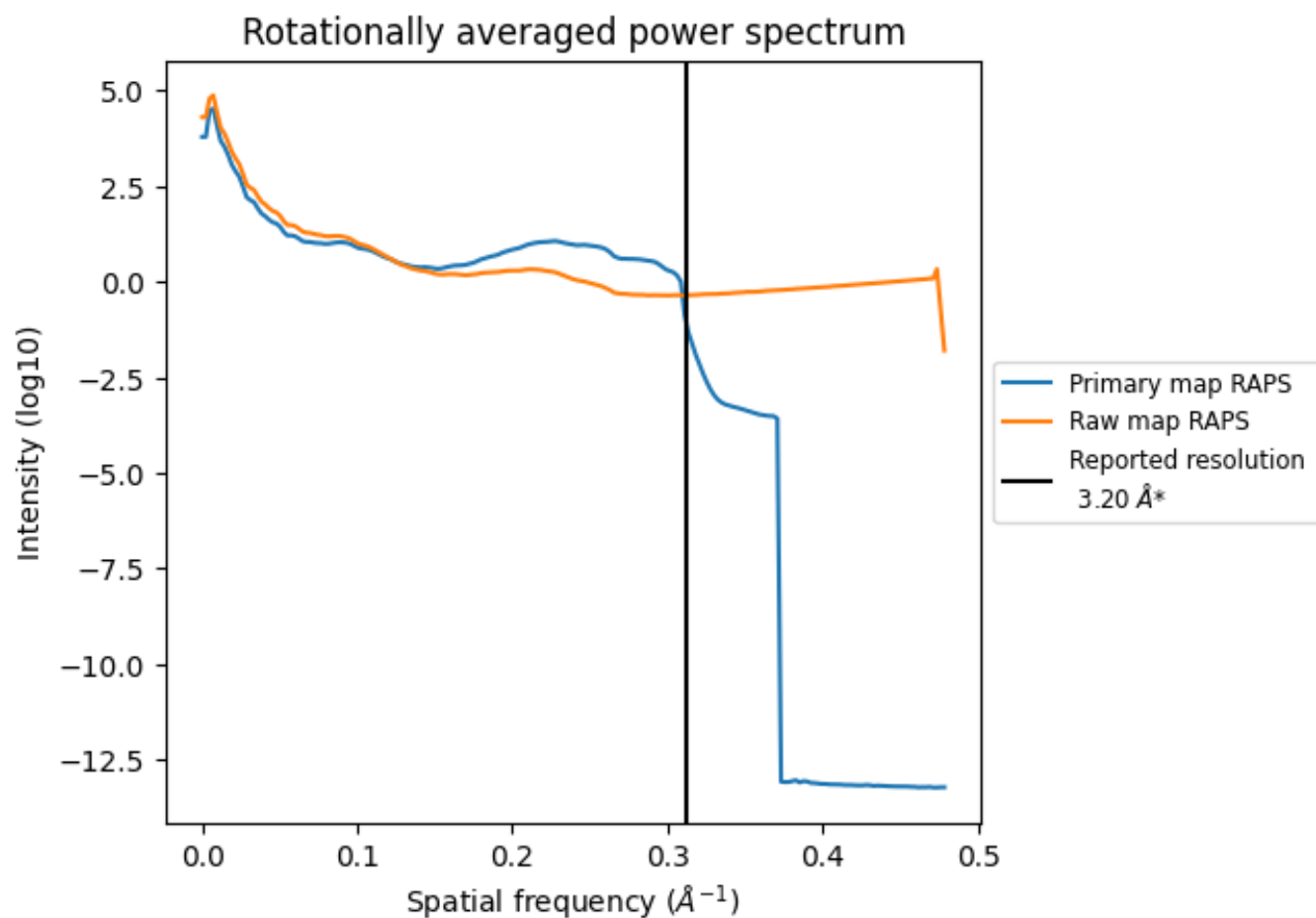
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 209 nm³; 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 ⓘ

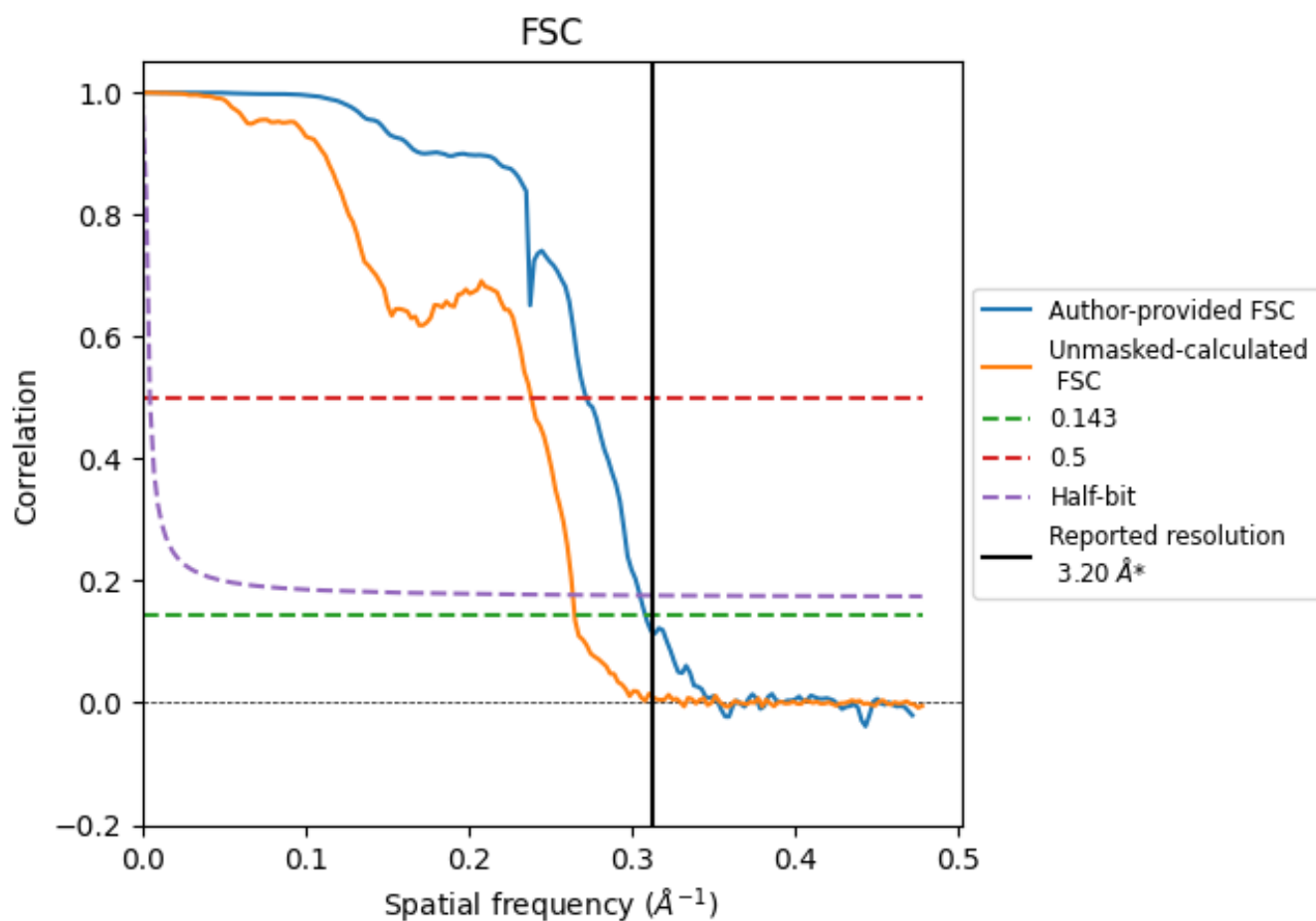


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

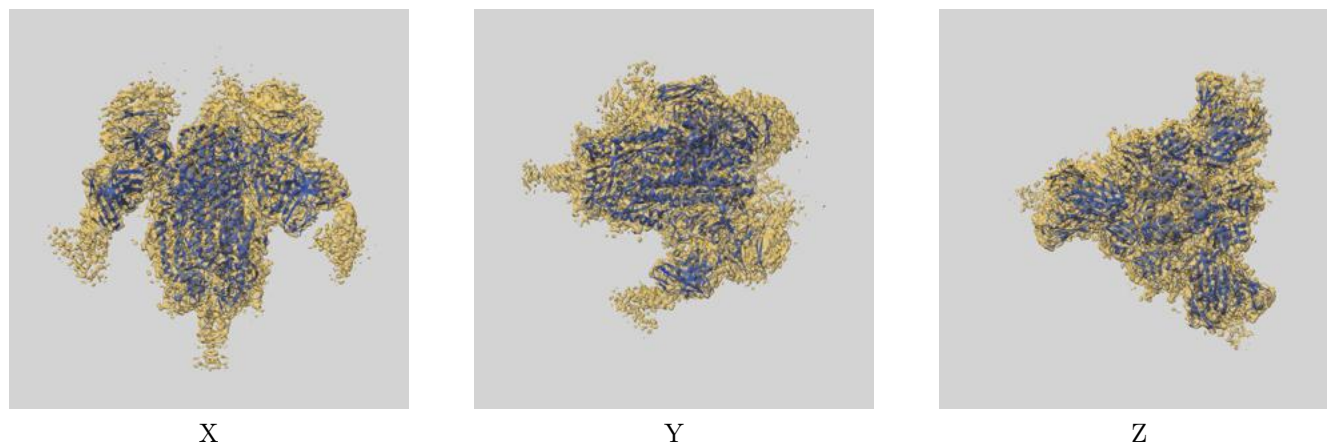
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.24	3.67	3.27
Unmasked-calculated*	3.77	4.19	3.79

*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](#)



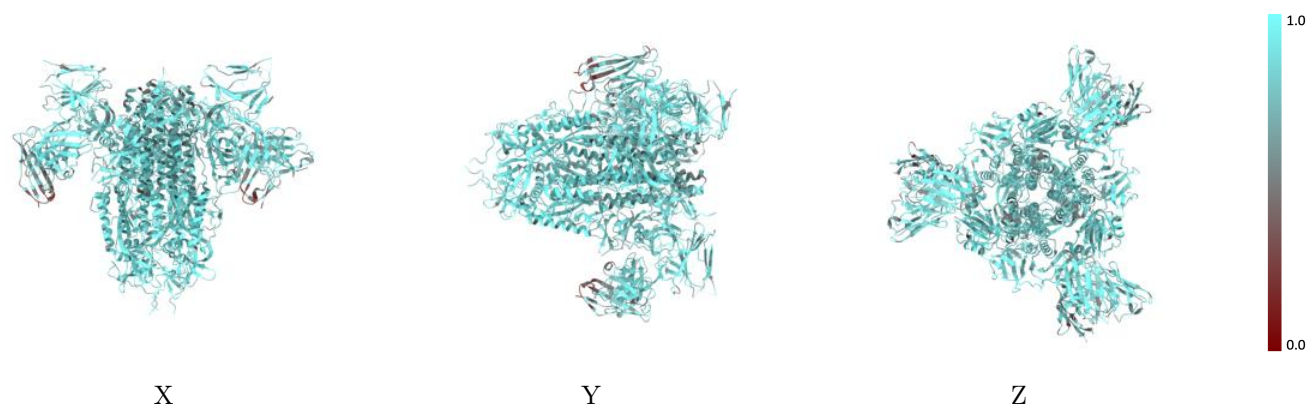
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



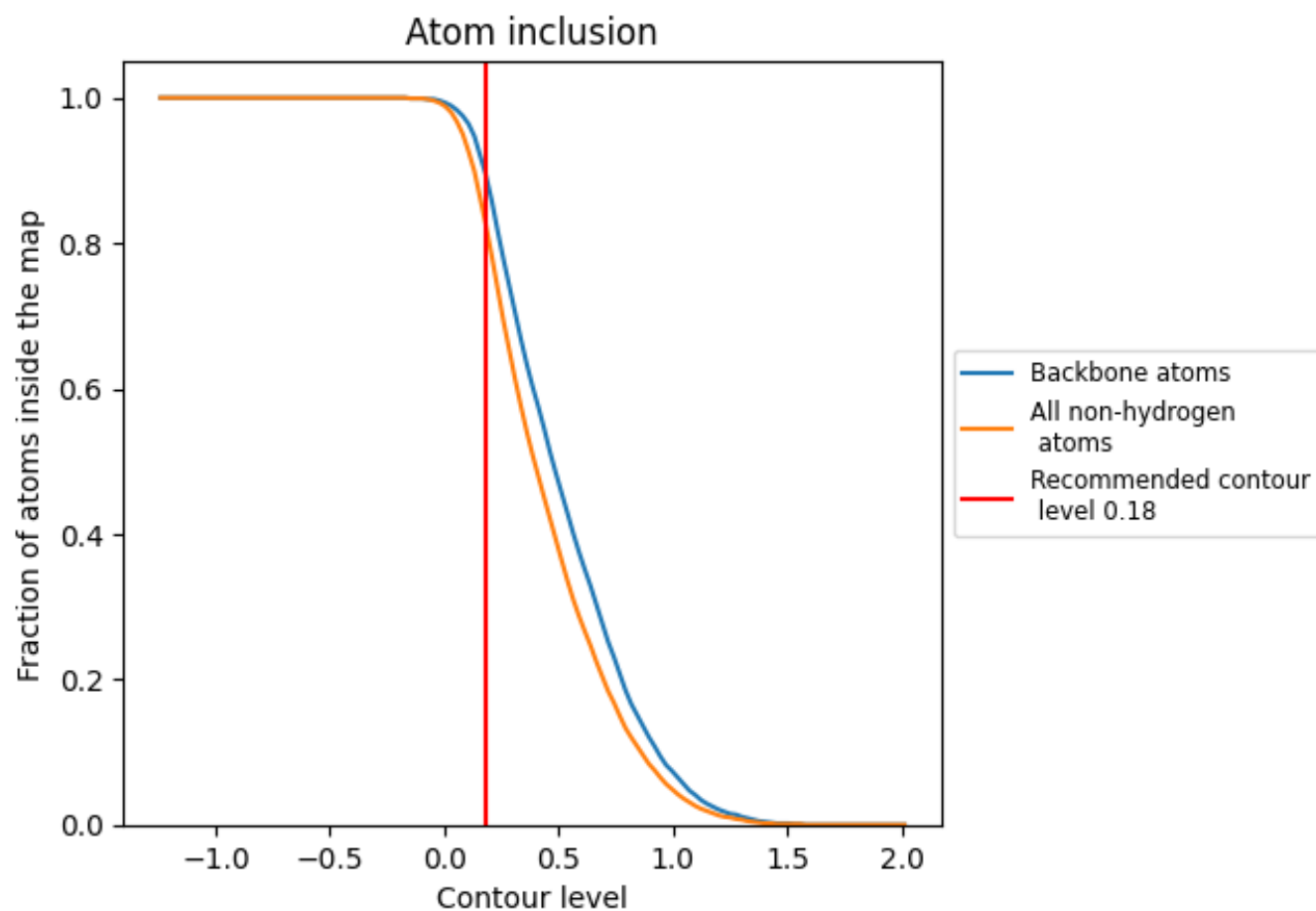
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

