



wwPDB EM Validation Summary Report ⓘ

Oct 10, 2022 – 11:12 AM EDT

PDB ID : 7TCC
EMDB ID : EMD-25808
Title : Cryo-EM structure of SARS-CoV-2 Omicron spike in complex with antibodies A19-46.1 and B1-182.1
Authors : Zhou, T.; Kwong, P.D.
Deposited on : 2021-12-23
Resolution : 3.86 Å(reported)
Based on initial model : 7MM0

This is a wwPDB EM Validation Summary 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

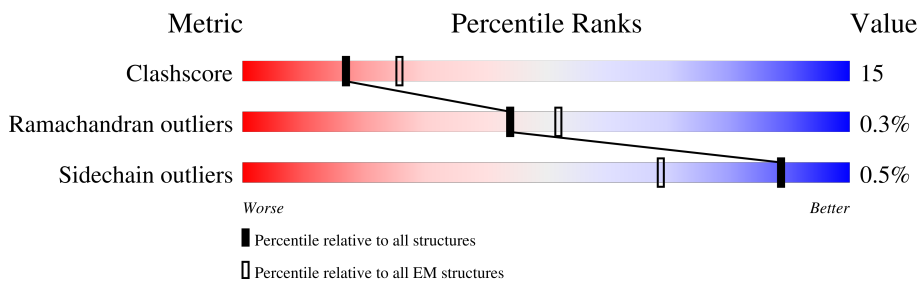
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.86 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1272	
1	B	1272	
1	C	1272	
2	D	126	
2	H	126	
2	M	126	
3	E	110	
3	L	110	

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Mol	Chain	Length	Quality of chain
3	N	110	
4	F	123	
4	J	123	
4	O	123	
5	G	108	
5	K	108	
5	P	108	
6	I	2	
6	Q	2	
6	R	2	
6	S	2	
6	T	2	
6	U	2	
6	V	2	
6	W	2	
6	X	2	
6	Y	2	
6	Z	2	
6	a	2	
6	b	2	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 37493 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
			Total	C	N	O	S		
1	A	1118	8755	5595	1464	1656	40	0	0
1	B	1116	8735	5584	1459	1652	40	0	0
1	C	1118	8755	5595	1464	1656	40	0	0

There are 384 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	conflict	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	142	ASP	TYR	conflict	UNP P0DTC2
A	212	ILE	-	insertion	UNP P0DTC2
A	213	VAL	-	insertion	UNP P0DTC2
A	214	ARG	ASN	conflict	UNP P0DTC2
A	214A	GLU	LEU	conflict	UNP P0DTC2
A	214B	PRO	VAL	conflict	UNP P0DTC2
A	214C	GLU	ARG	conflict	UNP P0DTC2
A	339	ASP	GLY	conflict	UNP P0DTC2
A	371	LEU	SER	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	conflict	UNP P0DTC2
A	496	SER	GLY	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2
A	547	LYS	THR	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	655	TYR	HIS	conflict	UNP P0DTC2
A	679	LYS	ASN	conflict	UNP P0DTC2
A	681	HIS	PRO	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	conflict	UNP P0DTC2
A	796	TYR	ASP	conflict	UNP P0DTC2
A	856	LYS	ASN	conflict	UNP P0DTC2
A	954	HIS	GLN	conflict	UNP P0DTC2
A	969	LYS	ASN	conflict	UNP P0DTC2
A	981	PHE	LEU	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1206	TYR	-	expression tag	UNP P0DTC2
A	1207	GLU	-	expression tag	UNP P0DTC2
A	1208	GLN	-	expression tag	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	conflict	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	142	ASP	TYR	conflict	UNP P0DTC2
B	212	ILE	-	insertion	UNP P0DTC2
B	213	VAL	-	insertion	UNP P0DTC2
B	213A	ARG	ASN	conflict	UNP P0DTC2
B	213B	GLU	LEU	conflict	UNP P0DTC2
B	214B	PRO	VAL	conflict	UNP P0DTC2
B	214C	GLU	ARG	conflict	UNP P0DTC2
B	339	ASP	GLY	conflict	UNP P0DTC2
B	371	LEU	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2
B	375	PHE	SER	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	478	LYS	THR	conflict	UNP P0DTC2
B	484	ALA	GLU	conflict	UNP P0DTC2
B	493	ARG	GLN	conflict	UNP P0DTC2
B	496	SER	GLY	conflict	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	505	HIS	TYR	conflict	UNP P0DTC2
B	547	LYS	THR	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	655	TYR	HIS	conflict	UNP P0DTC2
B	679	LYS	ASN	conflict	UNP P0DTC2
B	681	HIS	PRO	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	conflict	UNP P0DTC2
B	796	TYR	ASP	conflict	UNP P0DTC2
B	856	LYS	ASN	conflict	UNP P0DTC2
B	954	HIS	GLN	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	981	PHE	LEU	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1206	TYR	-	expression tag	UNP P0DTC2
B	1207	GLU	-	expression tag	UNP P0DTC2
B	1208	GLN	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	conflict	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	142	ASP	TYR	conflict	UNP P0DTC2
C	212	ILE	-	insertion	UNP P0DTC2
C	213	VAL	-	insertion	UNP P0DTC2
C	214	ARG	ASN	conflict	UNP P0DTC2
C	214A	GLU	LEU	conflict	UNP P0DTC2
C	214B	PRO	VAL	conflict	UNP P0DTC2
C	214C	GLU	ARG	conflict	UNP P0DTC2
C	339	ASP	GLY	conflict	UNP P0DTC2
C	371	LEU	SER	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	446	SER	GLY	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	484	ALA	GLU	conflict	UNP P0DTC2
C	493	ARG	GLN	conflict	UNP P0DTC2
C	496	SER	GLY	conflict	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	505	HIS	TYR	conflict	UNP P0DTC2
C	547	LYS	THR	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	HIS	PRO	conflict	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	UNP P0DTC2
C	856	LYS	ASN	conflict	UNP P0DTC2
C	954	HIS	GLN	conflict	UNP P0DTC2
C	969	LYS	ASN	conflict	UNP P0DTC2
C	981	PHE	LEU	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1206	TYR	-	expression tag	UNP P0DTC2
C	1207	GLU	-	expression tag	UNP P0DTC2
C	1208	GLN	-	expression tag	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of antibody A19-46.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	126	Total	C	N	O	S	0	0
			990	629	168	188	5		
2	H	126	Total	C	N	O	S	0	0
			990	629	168	188	5		
2	M	126	Total	C	N	O	S	0	0
			990	629	168	188	5		

- Molecule 3 is a protein called Light chain of antibody A19-46.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	110	Total	C	N	O	S	0	0
			806	507	133	163	3		
3	L	110	Total	C	N	O	S	0	0
			806	507	133	163	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	N	110	806	507	133	163	3	0	0

- Molecule 4 is a protein called heavy chain of antibody B1-182.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	122	932	584	159	181	8	1	0
4	O	122	932	584	159	181	8	1	0
4	F	122	932	584	159	181	8	1	0

- Molecule 5 is a protein called Light chain of antibody B1-182.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	108	830	522	142	164	2	1	0
5	P	108	830	522	142	164	2	1	0
5	G	108	830	522	142	164	2	1	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



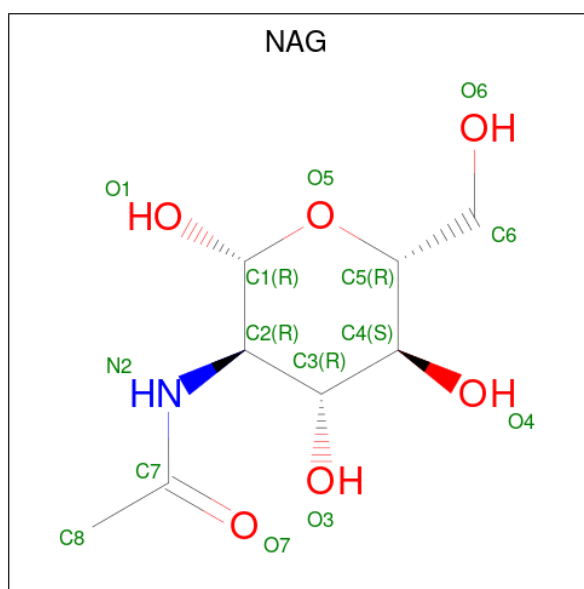
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	I	2	28	16	2	10	0	0
6	Q	2	28	16	2	10	0	0
6	R	2	28	16	2	10	0	0
6	S	2	28	16	2	10	0	0
6	T	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	U	2	Total 28	C 16	N 2	O 10	0	0
6	V	2	Total 28	C 16	N 2	O 10	0	0
6	W	2	Total 28	C 16	N 2	O 10	0	0
6	X	2	Total 28	C 16	N 2	O 10	0	0
6	Y	2	Total 28	C 16	N 2	O 10	0	0
6	Z	2	Total 28	C 16	N 2	O 10	0	0
6	a	2	Total 28	C 16	N 2	O 10	0	0
6	b	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	Total 84	C 48	N 6	O 30	0
7	A	1	Total 84	C 48	N 6	O 30	0
7	A	1	Total 84	C 48	N 6	O 30	0

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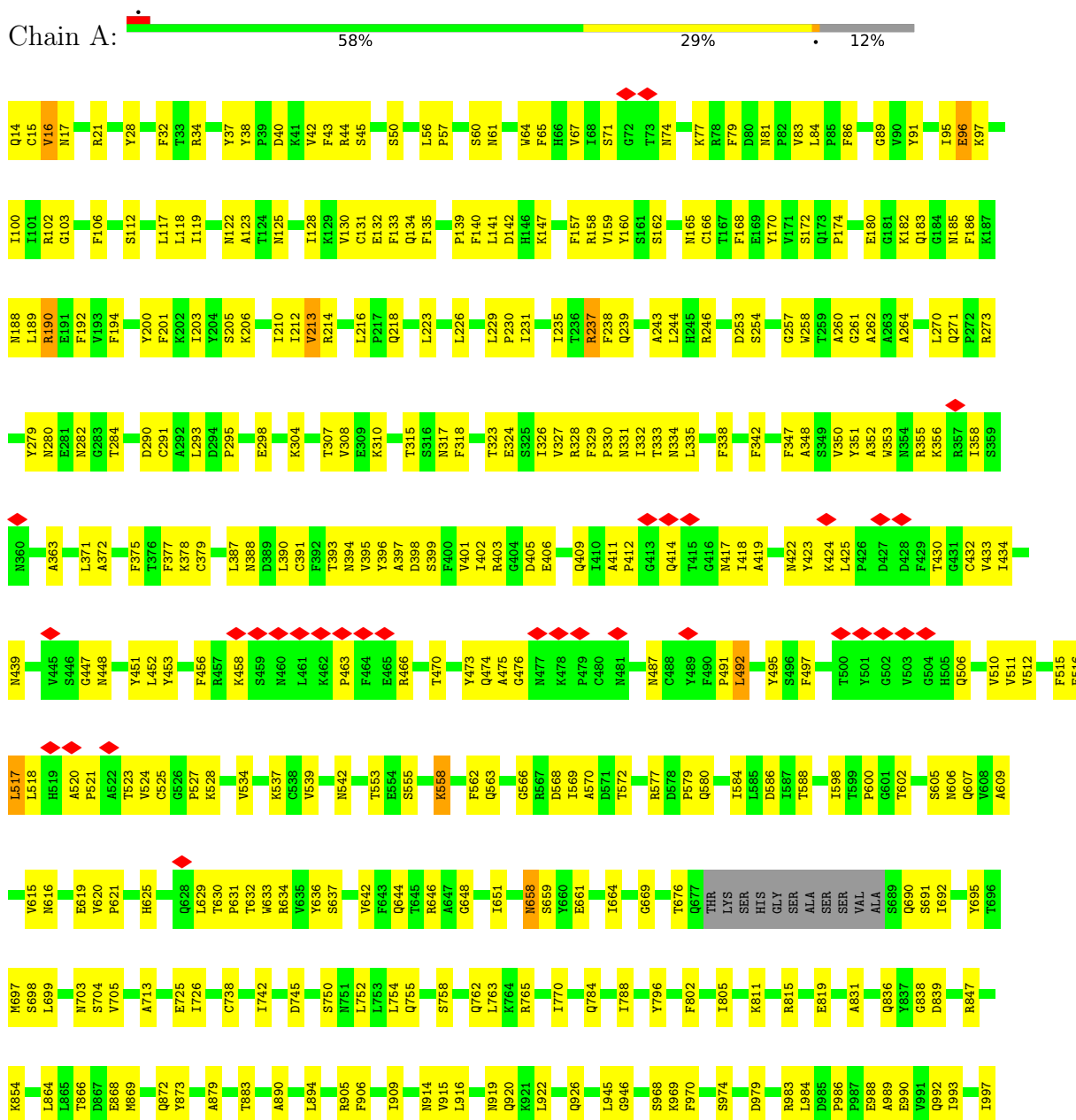
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	Total 84	C 48	N 6	O 30	0
7	A	1	Total 84	C 48	N 6	O 30	0
7	A	1	Total 84	C 48	N 6	O 30	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	C	1	Total 56	C 32	N 4	O 20	0
7	C	1	Total 56	C 32	N 4	O 20	0
7	C	1	Total 56	C 32	N 4	O 20	0
7	C	1	Total 56	C 32	N 4	O 20	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Spike glycoprotein



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

● Molecule 1: Spike glycoprotein



Q14	C15	V16	N17	R21	L24	P25	P26	A27	Y28	F32	T33	R34	R33	Y37	D40	K41	V42	F43	S46	L54	N61	R158	V62	T63	W64	V67	M165	I68	S71	G72	T73	N74	K77	R78	F79	F86	N87	D88	F92	E96	K97	S98	N99	I100	I101	T108	S112
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K113	T114	Q115	S116	L117	L118	M125	K129	E224	V130	A27	C131	L226	E132	F133	Q134	F135	F140	L141	D142	H146	K147	M148	E154	S155	L156	F157	P251	G252	V159	Y160	M164	C166	P174	M177	D178	L179	E180	G181	K182	Q183	F186	K187	M188	L189	R190	F194	I203	Y204	S205	K206	H207	T208
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F209	I210	R214	Q218	G219	L223	E224	P225	L226	W227	I231	G232	G233	R237	F238	L241	L242	A243	R246	S247	Y248	P251	G252	D253	S254	S255	S256	G257	W258	V267	Y279	L293	L296	K300	V308	K309	K310	N317	F318	R319	I326	K327	R328	F329	P330
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M331	C336	D339	V341	F342	R343	R346	F347	A348	S349	V350	Y351	A352	K356	R357	L358	V362	Y365	L371	A372	F375	F377	K378	C379	S383	K386	L387	C391	F392	T393	A397	D398	S399	F400	I402	R403	E406	F318	R493	S494	O409	I410	A411	Q414
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I418	A419	D420	N422	Y423	K424	L425	P426	D427	D428	F429	G430	C431	V433	W436	N437	S438	N439	K440	L441	D442	V445	G446	G447	Y451	L452	K458	S459	M460	L461	K462	R466	T470	I472	S471	Y473	C480	M481	F490	P491	L492	R493	S494	F497	R498	F499	V503
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G504	H505	Q506	P507	Y508	R509	V512	L513	S514	F515	E516	L517	L518	H519	A520	P521	T523	W524	C525	G526	P527	K528	L533	V534	K535	M536	K537	L546	S555	M556	K557	K558	F559	L560	Q563	G566	R567	D568	D578	P579	Q580	I584	L585	D586	G594	T602	S605	M606
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Q607	V615	T618	E619	W620	P621	V612	H625	S614	F628	L629	T630	P631	R634	S637	T638	V642	F643	R646	L650	M651	Y660	D663	I664	P665	Y674	Q675	T676	G677	THR	LYS	SER	HIS	GLY	SER	ALA	ALA	SER	SER	SER	VAL	ALA	G689	Q690	Y695	L699	E702	N703	S704
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A713	M717	S721	T724	T732	C738	I742	C743	S746	C749	S750	L754	F759	K776	M777	T778	V781	Q787	P792	I805	L806	P807	R815	S816	D820	L821	K825	W826	T827	L828	Q832	F833	R834	K835	Q836	Y837	L841	G842	D843
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Y873	L878	A879	T882	T883	Q895	R905	V915	E918	N919	I931	T934	L938	S939	K947	H954	N955	A956	Q957	V963	L966	K969	F970	G971	A972	S974	L977	I980	Q992	R995	L996	I997	R1000	L1001	N1134	N1135	T1009	Q1010	I1013
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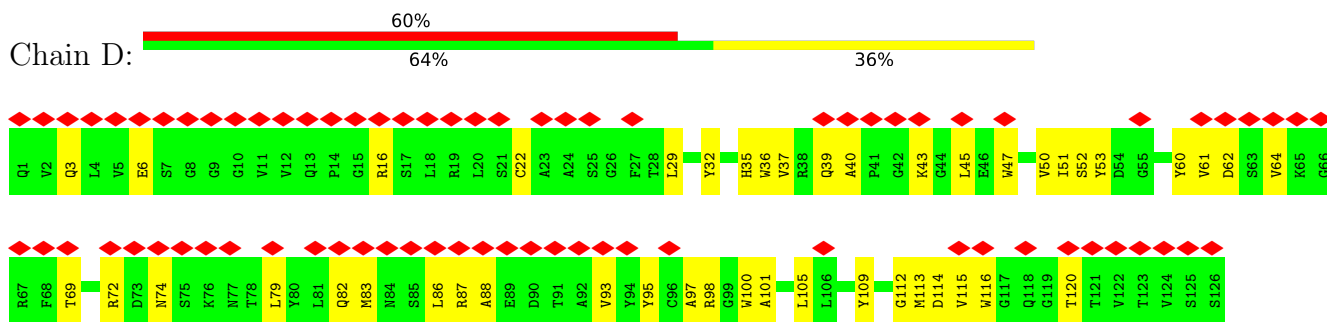
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SER	PHE	LYS	GLY	GLY	TYR	LEU	ASP	LYS	TYR	PHE	ALA	ASN	HIS	THR	SER	PRO	ALA	VAL	VAL	ASP	GLY	ILE	ASN	ILE	GLN	LEU	LEU	VAL	ILE	ASP	ARG	THR	LYS	ASN	LYS	GLY	VAL	ALA	LYS	ASN	LEU	LEU	ASN	GLY	PRO	GLY	VAL	ALA	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	LEU	ILE	ASP	ALA	TRP	LEU	GLN	GLY	LEU	GLY	LYS	TYR
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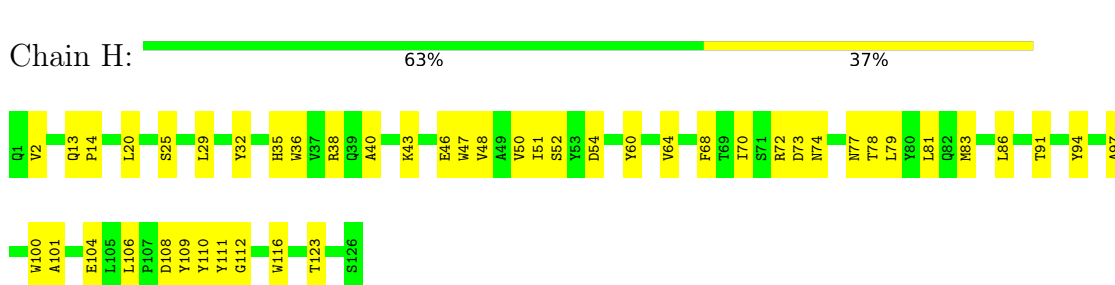
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LYS	GLY	GLY	SER	GLY	TYR	ILE	PRO	GLY	GLY	SER	SER	HIS	PRO	GLN	PHE	LYS
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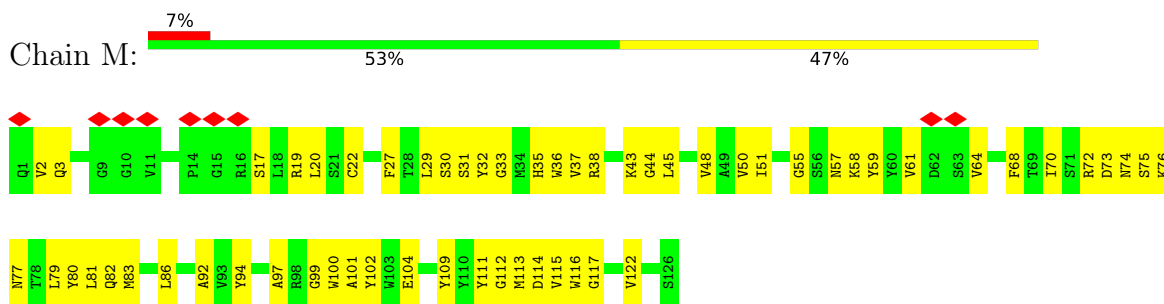
- Molecule 2: Heavy chain of antibody A19-46.1



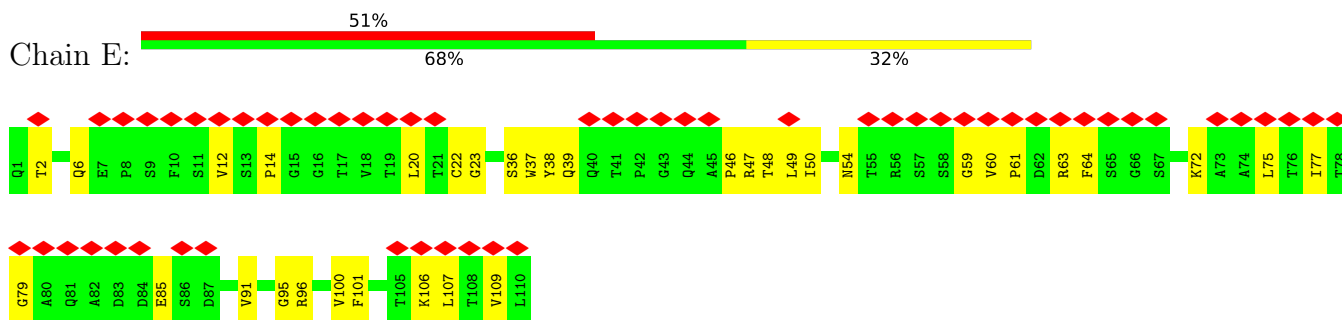
- Molecule 2: Heavy chain of antibody A19-46.1



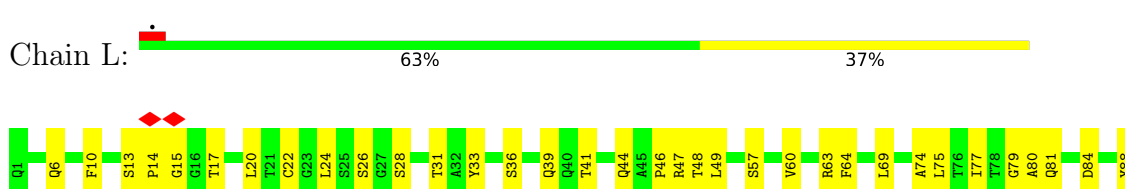
- Molecule 2: Heavy chain of antibody A19-46.1



- Molecule 3: Light chain of antibody A19-46.1

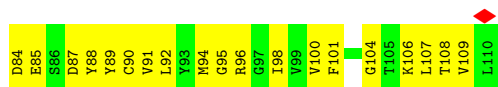
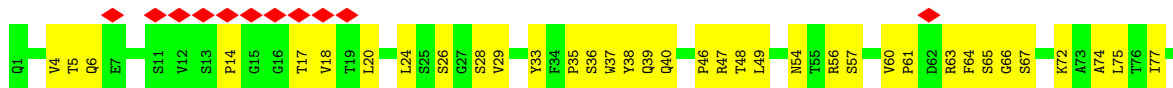


- Molecule 3: Light chain of antibody A19-46.1

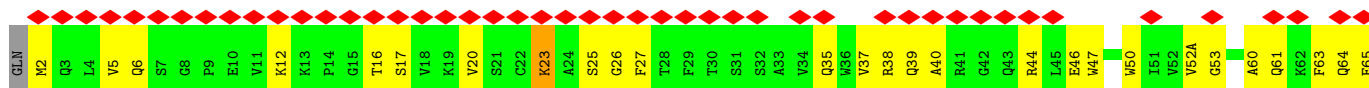




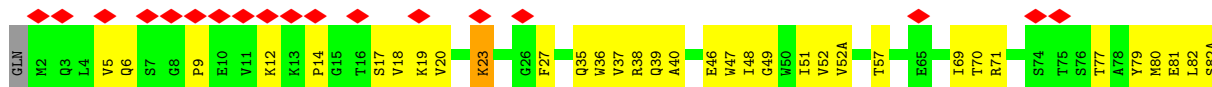
• Molecule 3: Light chain of antibody A19-46.1



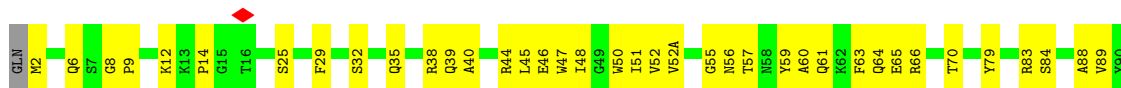
• Molecule 4: heavy chain of antibody B1-182.1



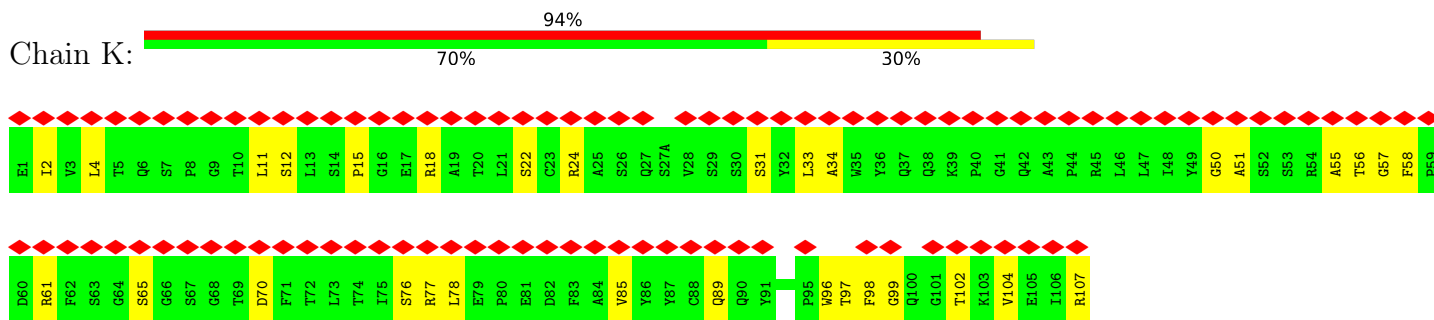
• Molecule 4: heavy chain of antibody B1-182.1



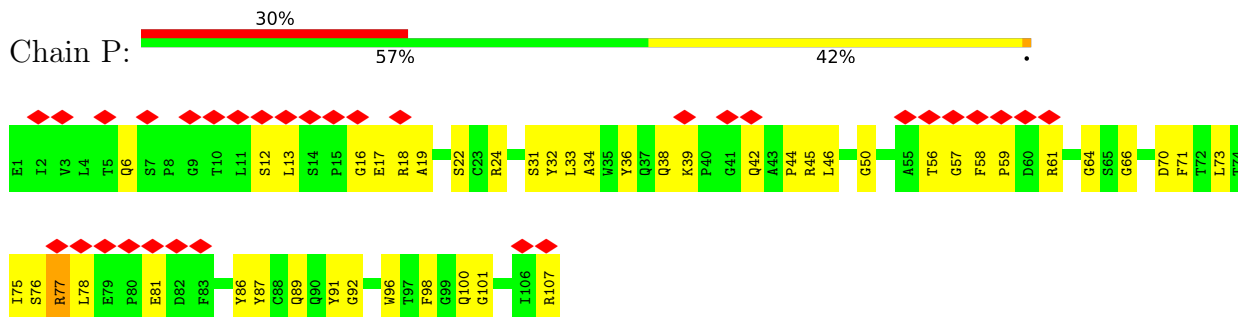
• Molecule 4: heavy chain of antibody B1-182.1



• Molecule 5: Light chain of antibody B1-182.1



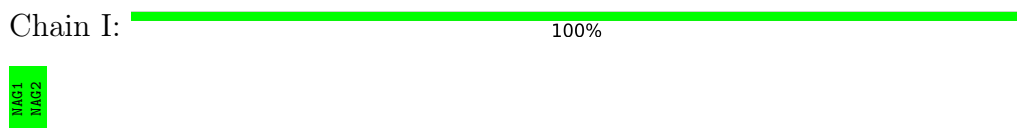
• Molecule 5: Light chain of antibody B1-182.1



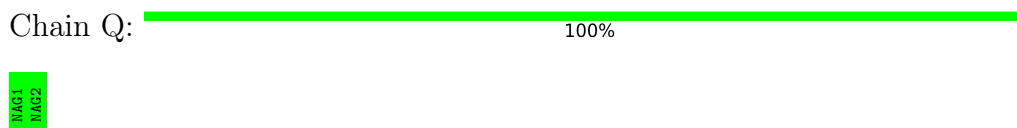
• Molecule 5: Light chain of antibody B1-182.1




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



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



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

Chain R:  100%

MAG1
MAG2

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

Chain S:  100%

MAG1
MAG2

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

Chain T:  100%

MAG1
MAG2

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

Chain U:  50% 50%

MAG1
MAG2

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

Chain V:  100%

MAG1
MAG2

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

Chain W:  100%

MAG1
MAG2

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

Chain X:  50% 50%

MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain Z:  50% 50%

MAG1
MAG2

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

Chain a:  100%

MAG1
MAG2

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

Chain b:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46244	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.797	Depositor
Minimum map value	-0.191	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.116	Depositor
Map size (Å)	513.0, 513.0, 513.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/8965	0.51	1/12202 (0.0%)
1	B	0.27	0/8944	0.51	0/12172
1	C	0.27	0/8965	0.52	2/12202 (0.0%)
2	D	0.25	0/1016	0.53	0/1381
2	H	0.26	0/1016	0.54	0/1381
2	M	0.26	0/1016	0.54	0/1381
3	E	0.26	0/823	0.51	0/1123
3	L	0.26	0/823	0.53	0/1123
3	N	0.26	0/823	0.52	0/1123
4	F	0.26	0/952	0.54	0/1289
4	J	0.24	0/952	0.54	0/1289
4	O	0.25	0/952	0.59	0/1289
5	G	0.52	1/851 (0.1%)	0.82	3/1156 (0.3%)
5	K	0.25	0/851	0.57	0/1156
5	P	0.26	0/851	0.56	0/1156
All	All	0.27	1/37800 (0.0%)	0.53	6/51423 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	8	PRO	CG-CD	-12.64	1.08	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	8	PRO	N-CD-CG	-15.40	80.11	103.20
5	G	8	PRO	CA-CB-CG	-8.38	88.08	104.00
5	G	8	PRO	CA-N-CD	-7.11	101.55	111.50
1	A	517	LEU	CA-CB-CG	5.04	126.89	115.30
1	C	452	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	GLN	Peptide

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	8755	0	8562	279	0
1	B	8735	0	8544	248	0
1	C	8755	0	8563	258	0
2	D	990	0	947	36	0
2	H	990	0	947	31	0
2	M	990	0	947	51	0
3	E	806	0	787	30	0
3	L	806	0	787	32	0
3	N	806	0	787	42	0
4	F	932	0	893	43	0
4	J	932	0	893	31	0
4	O	932	0	893	37	0
5	G	830	0	797	34	0
5	K	830	0	797	24	0
5	P	830	0	797	37	0
6	I	28	0	25	0	0
6	Q	28	0	25	0	0
6	R	28	0	25	0	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
6	U	28	0	25	1	0
6	V	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	W	28	0	25	0	0
6	X	28	0	25	0	0
6	Y	28	0	25	0	0
6	Z	28	0	25	1	0
6	a	28	0	25	0	0
6	b	28	0	25	0	0
7	A	84	0	78	1	0
7	B	70	0	65	0	0
7	C	56	0	52	1	0
All	All	37493	0	36461	1140	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 15.

The worst 5 of 1140 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)
3:N:85:GLU:HA	3:N:107:LEU:O	1.59	1.00
3:N:17:THR:HA	3:N:77:ILE:O	1.69	0.93
1:A:97:LYS:O	1:A:188:ASN:ND2	2.03	0.90
3:E:36:SER:HB2	3:E:91:VAL:HB	1.59	0.84
1:C:391:CYS:HA	1:C:525:CYS:HA	1.60	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1114/1272 (88%)	1011 (91%)	97 (9%)	6 (0%)	29 66
1	B	1110/1272 (87%)	1005 (90%)	100 (9%)	5 (0%)	29 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1114/1272 (88%)	1010 (91%)	99 (9%)	5 (0%)	34	70
2	D	124/126 (98%)	117 (94%)	7 (6%)	0	100	100
2	H	124/126 (98%)	113 (91%)	11 (9%)	0	100	100
2	M	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
3	E	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
3	L	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
3	N	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
4	F	120/123 (98%)	109 (91%)	11 (9%)	0	100	100
4	J	120/123 (98%)	108 (90%)	12 (10%)	0	100	100
4	O	120/123 (98%)	105 (88%)	15 (12%)	0	100	100
5	G	106/108 (98%)	97 (92%)	9 (8%)	0	100	100
5	K	106/108 (98%)	95 (90%)	11 (10%)	0	100	100
5	P	106/108 (98%)	98 (92%)	8 (8%)	0	100	100
All	All	4712/5217 (90%)	4289 (91%)	407 (9%)	16 (0%)	44	74

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	96	GLU
1	A	213	VAL
1	A	492	LEU
1	B	16	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	974/1100 (88%)	969 (100%)	5 (0%)	88	93
1	B	972/1100 (88%)	967 (100%)	5 (0%)	88	93
1	C	974/1100 (88%)	969 (100%)	5 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	104/104 (100%)	103 (99%)	1 (1%)	76	85
2	H	104/104 (100%)	104 (100%)	0	100	100
2	M	104/104 (100%)	104 (100%)	0	100	100
3	E	89/89 (100%)	89 (100%)	0	100	100
3	L	89/89 (100%)	89 (100%)	0	100	100
3	N	89/89 (100%)	89 (100%)	0	100	100
4	F	101/103 (98%)	99 (98%)	2 (2%)	55	74
4	J	101/103 (98%)	100 (99%)	1 (1%)	76	85
4	O	101/103 (98%)	100 (99%)	1 (1%)	76	85
5	G	90/90 (100%)	90 (100%)	0	100	100
5	K	90/90 (100%)	90 (100%)	0	100	100
5	P	90/90 (100%)	89 (99%)	1 (1%)	73	84
All	All	4072/4458 (91%)	4051 (100%)	21 (0%)	89	93

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1010	GLN
4	O	23	LYS
4	F	83	ARG
5	P	77	ARG
4	J	23	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	115	GLN
4	F	56	ASN
3	E	39	GLN
5	G	90	GLN
2	M	82	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

26 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
6	NAG	I	1	6,1	14,14,15	0.19	0	17,19,21	0.43	0
6	NAG	I	2	6	14,14,15	0.20	0	17,19,21	0.41	0
6	NAG	Q	1	6,1	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	Q	2	6	14,14,15	0.22	0	17,19,21	0.40	0
6	NAG	R	1	6,1	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	R	2	6	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	S	1	6,1	14,14,15	0.23	0	17,19,21	0.39	0
6	NAG	S	2	6	14,14,15	0.26	0	17,19,21	0.45	0
6	NAG	T	1	6,1	14,14,15	0.31	0	17,19,21	0.46	0
6	NAG	T	2	6	14,14,15	0.19	0	17,19,21	0.37	0
6	NAG	U	1	6,1	14,14,15	0.33	0	17,19,21	0.42	0
6	NAG	U	2	6	14,14,15	0.22	0	17,19,21	0.39	0
6	NAG	V	1	6,1	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	V	2	6	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	W	1	6,1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	W	2	6	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	X	1	6,1	14,14,15	0.40	0	17,19,21	0.75	1 (5%)
6	NAG	X	2	6	14,14,15	0.26	0	17,19,21	0.43	0
6	NAG	Y	1	6,1	14,14,15	0.16	0	17,19,21	0.45	0
6	NAG	Y	2	6	14,14,15	0.25	0	17,19,21	0.42	0
6	NAG	Z	1	6,1	14,14,15	0.40	0	17,19,21	0.57	0
6	NAG	Z	2	6	14,14,15	0.26	0	17,19,21	0.39	0
6	NAG	a	1	6,1	14,14,15	0.31	0	17,19,21	0.58	0
6	NAG	a	2	6	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	b	1	6,1	14,14,15	0.19	0	17,19,21	0.39	0
6	NAG	b	2	6	14,14,15	0.20	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	NAG	R	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	NAG	T	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	NAG	U	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	NAG	V	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	NAG	W	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	NAG	X	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Y	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	NAG	a	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	NAG	b	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	b	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	1	NAG	C1-O5-C5	2.51	115.59	112.19

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

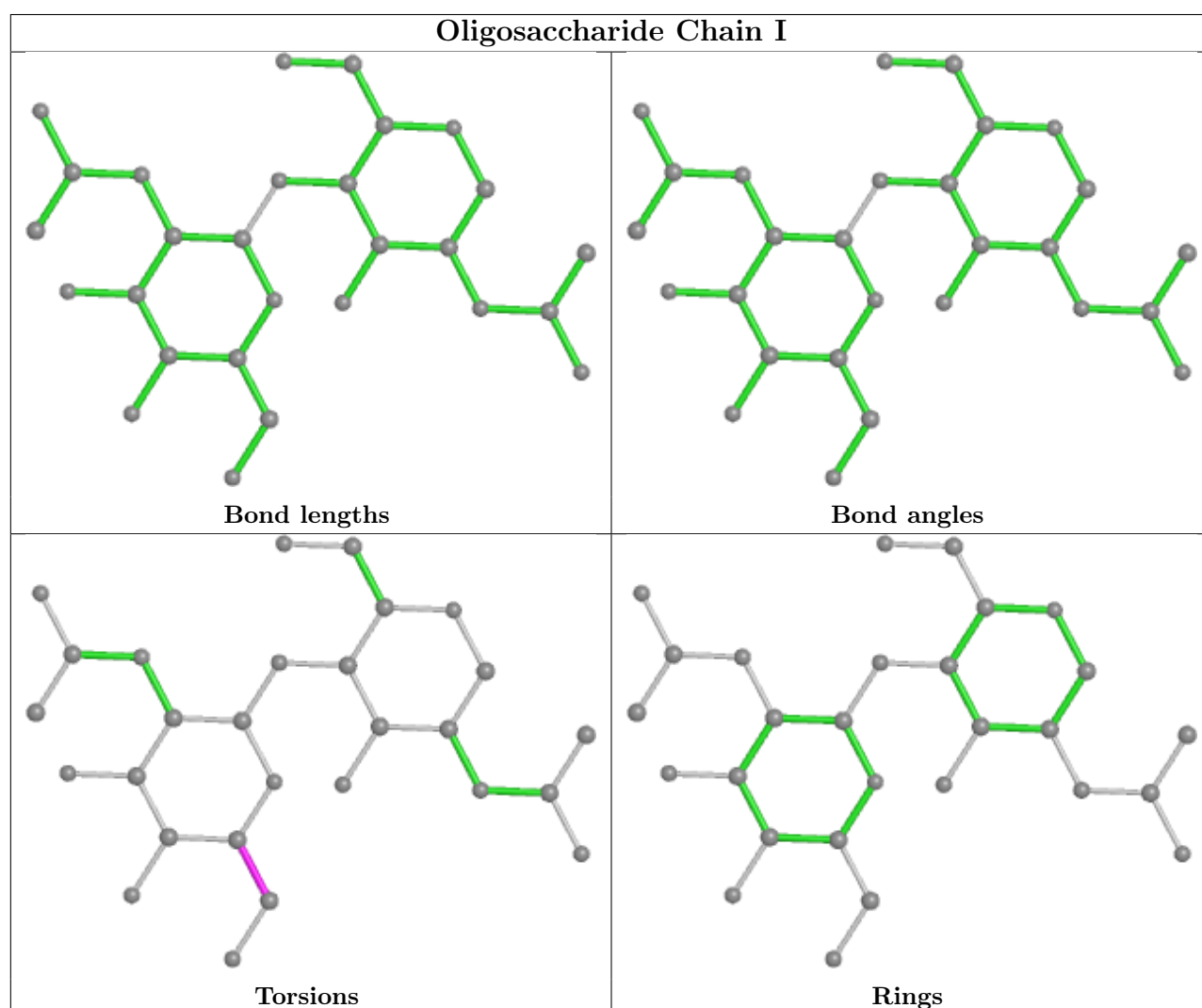
Mol	Chain	Res	Type	Atoms
6	T	1	NAG	O5-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6

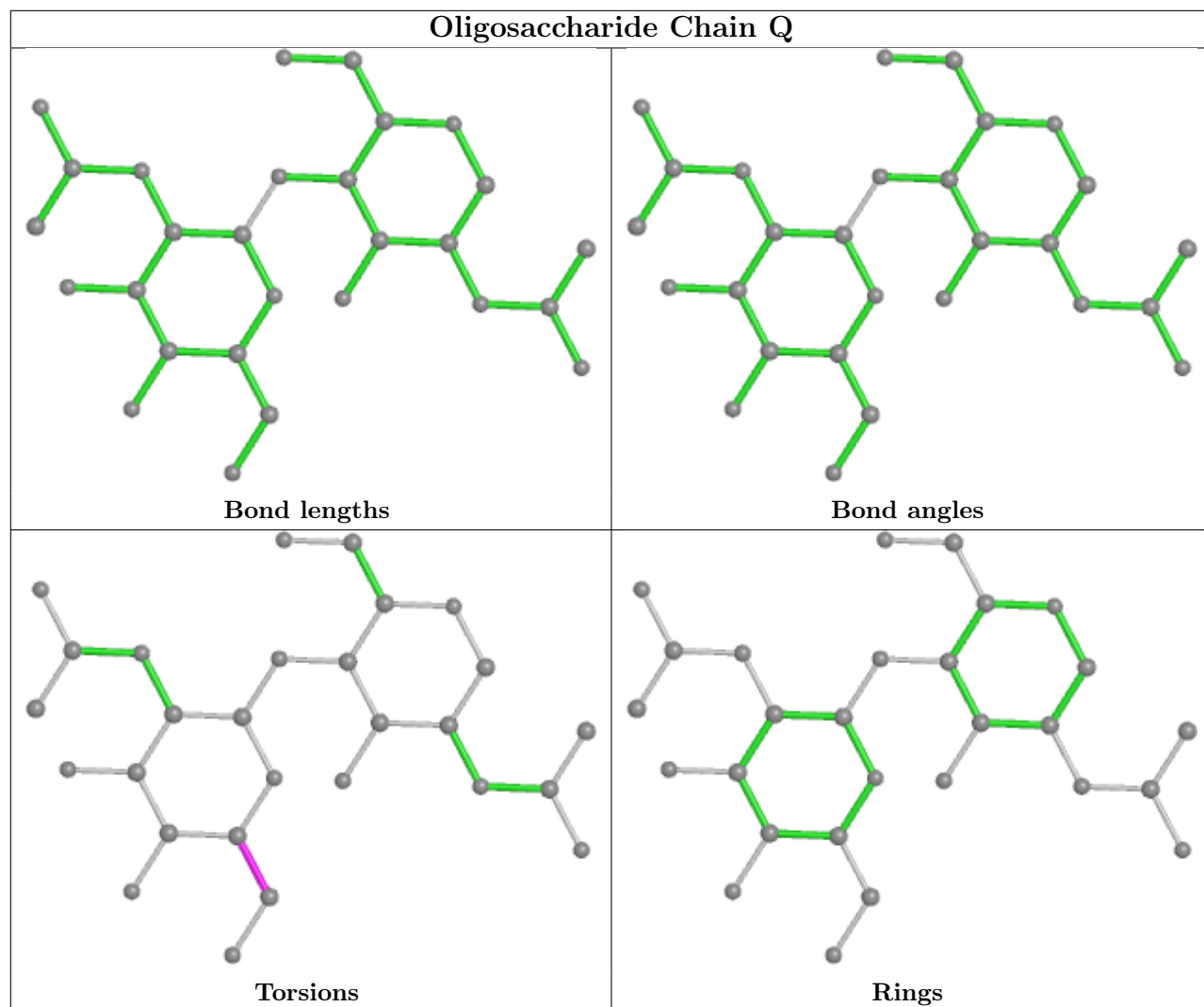
There are no ring outliers.

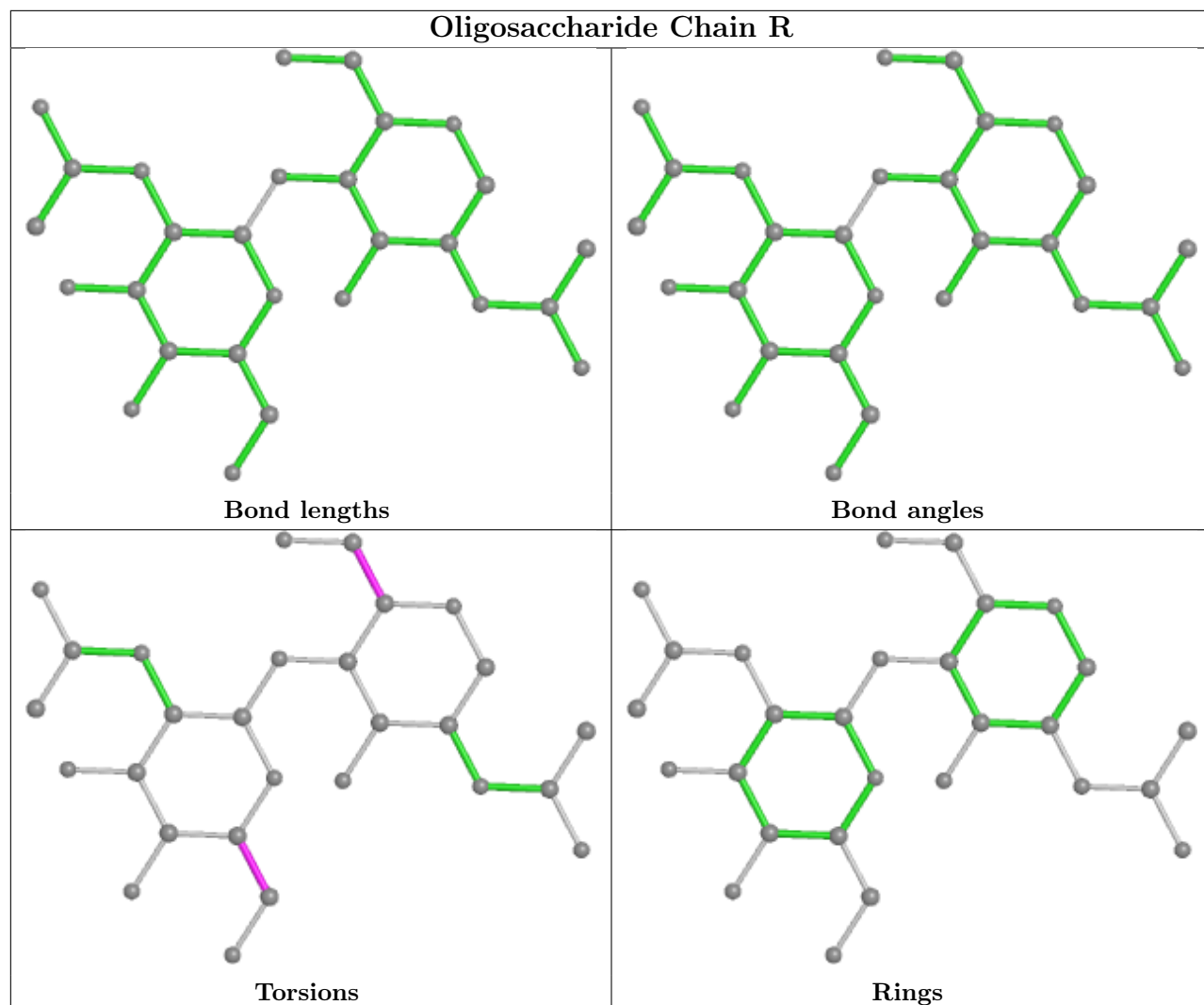
2 monomers are involved in 2 short contacts:

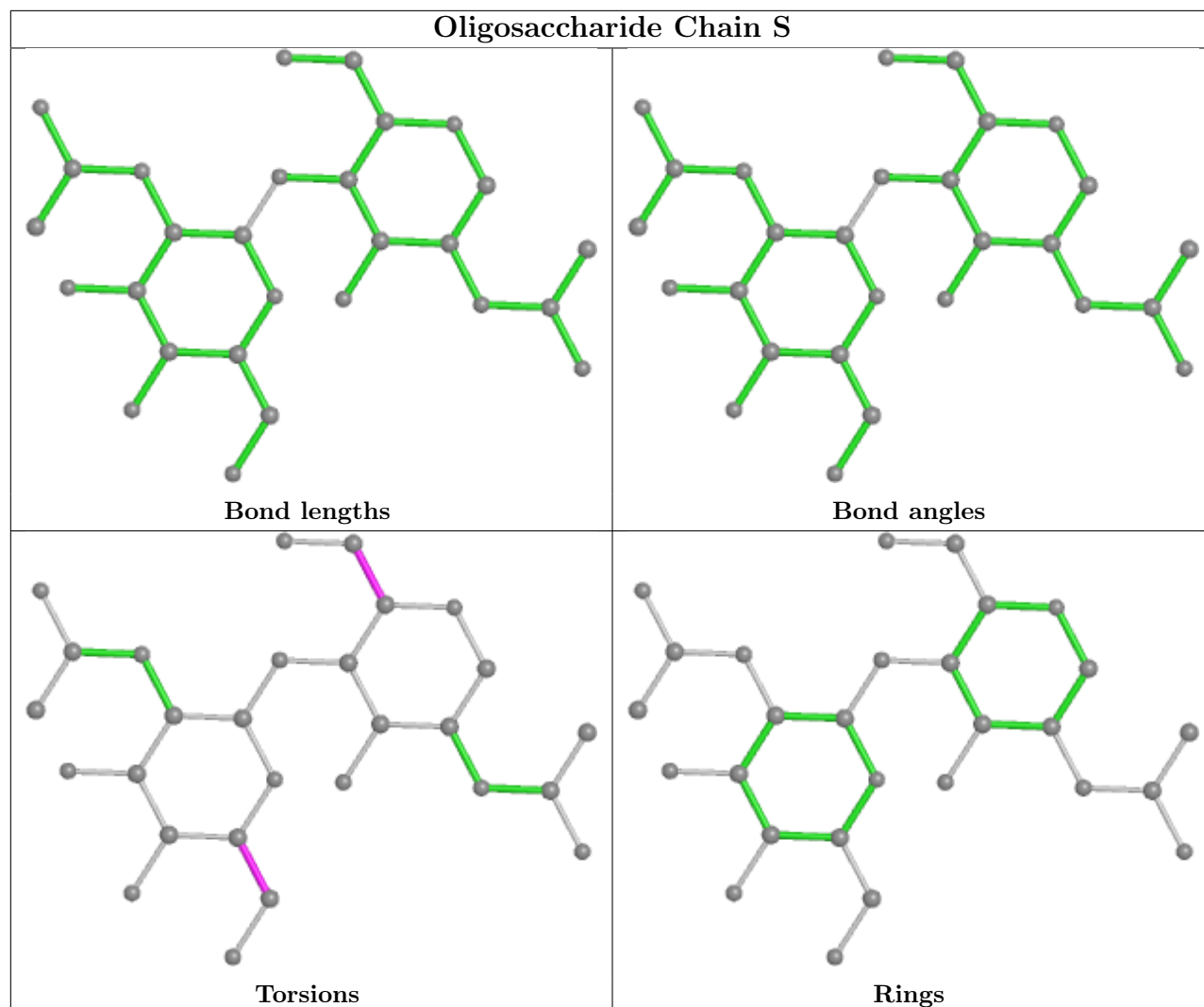
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	U	1	NAG	1	0
6	Z	1	NAG	1	0

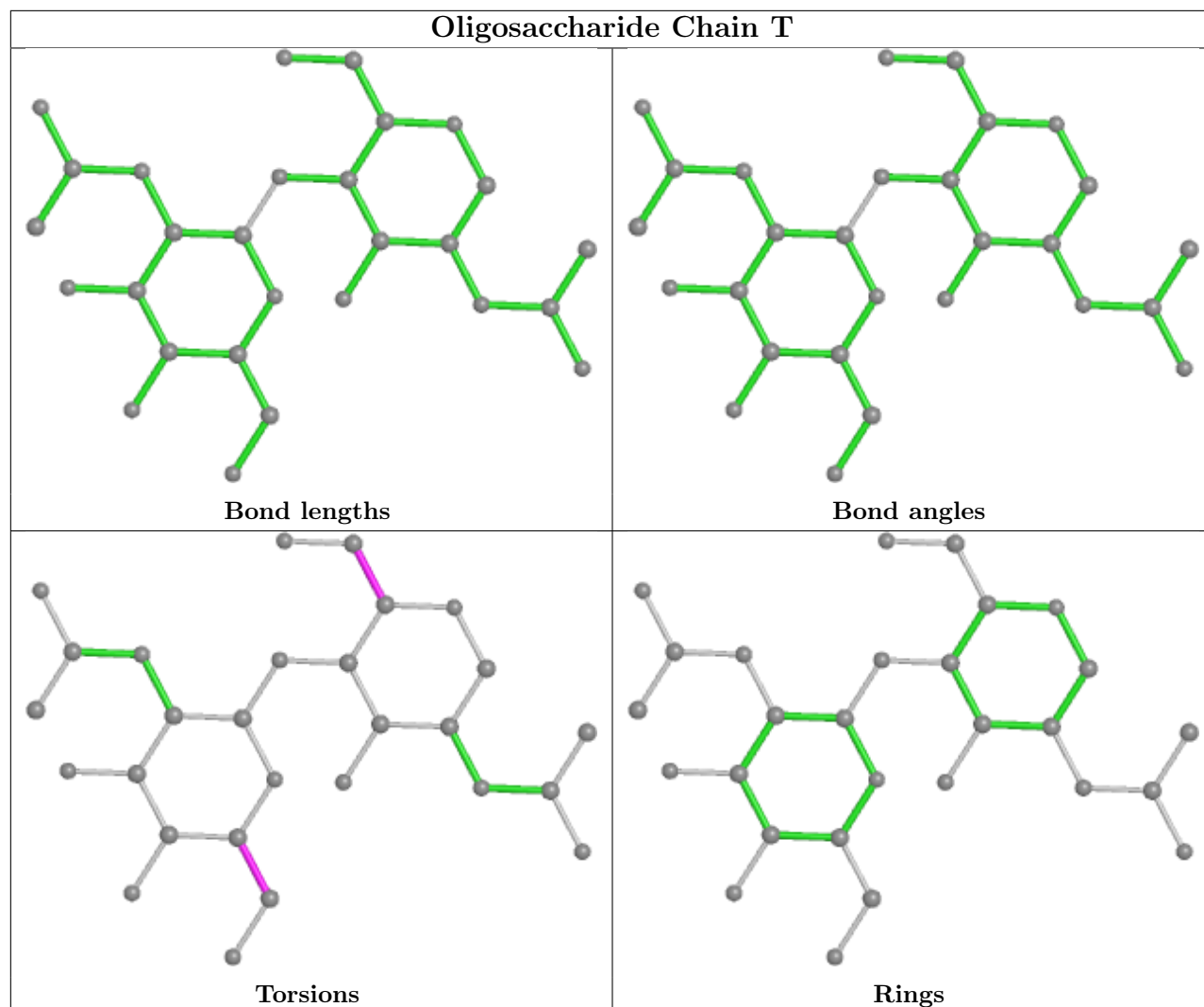
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

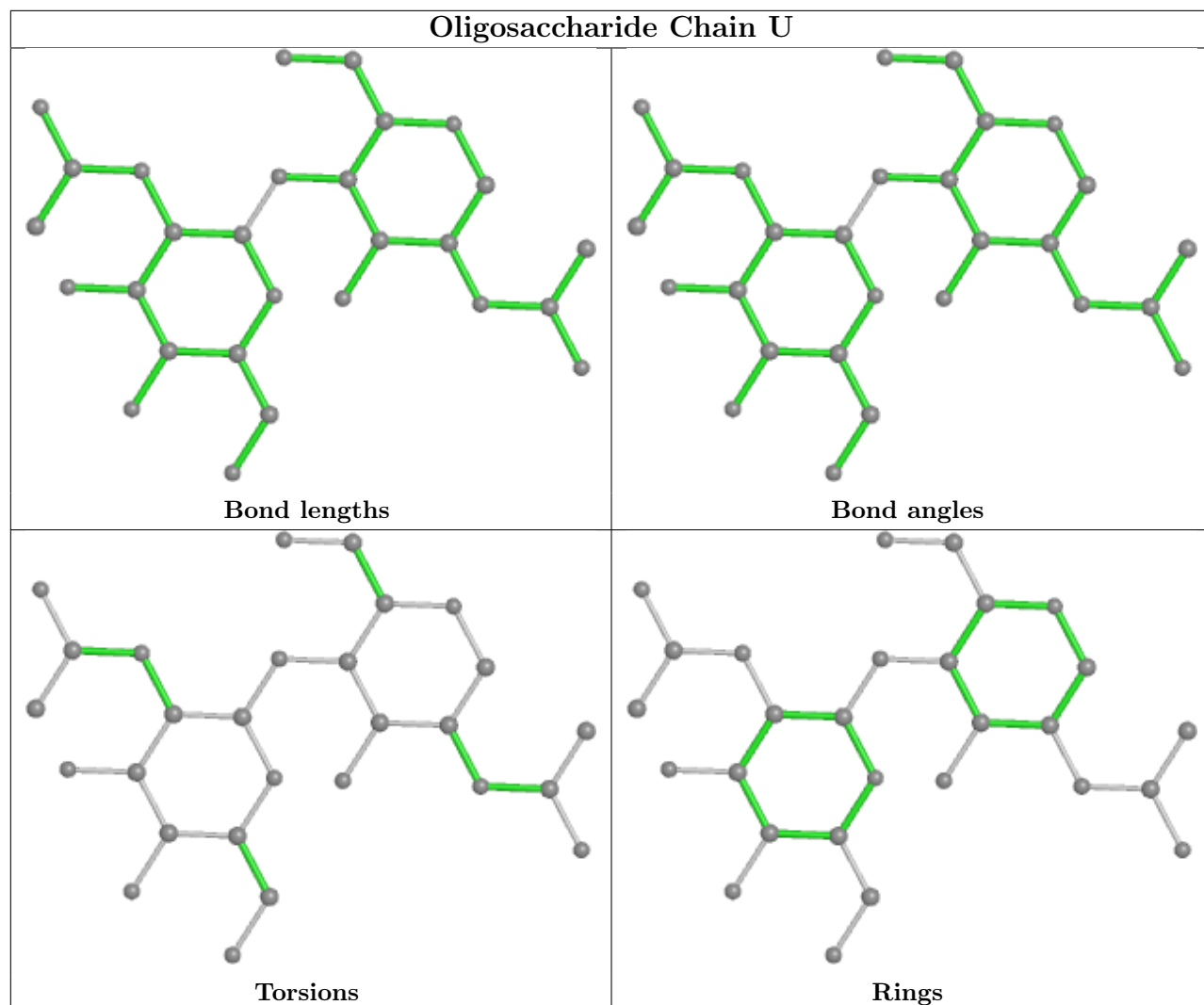


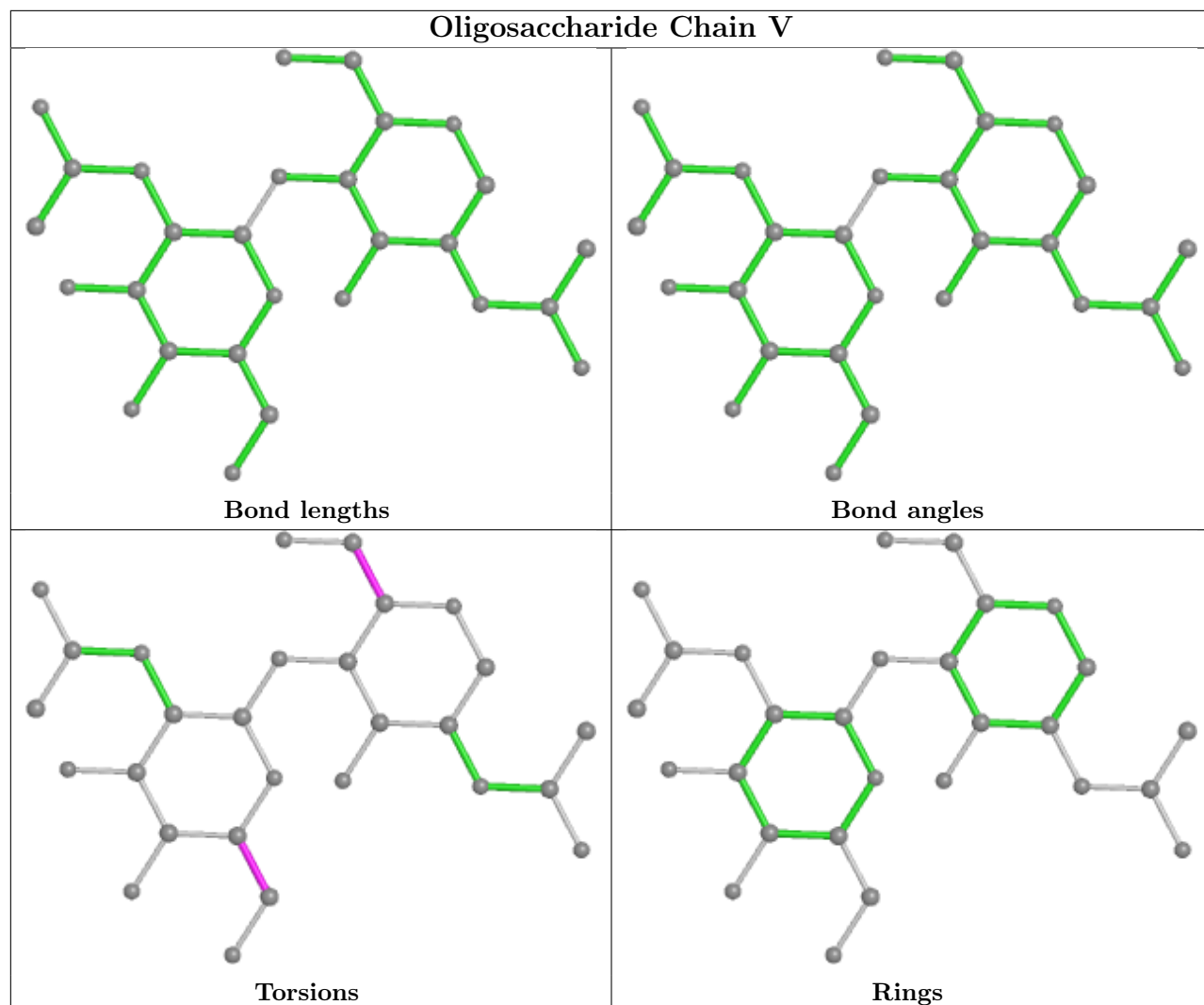


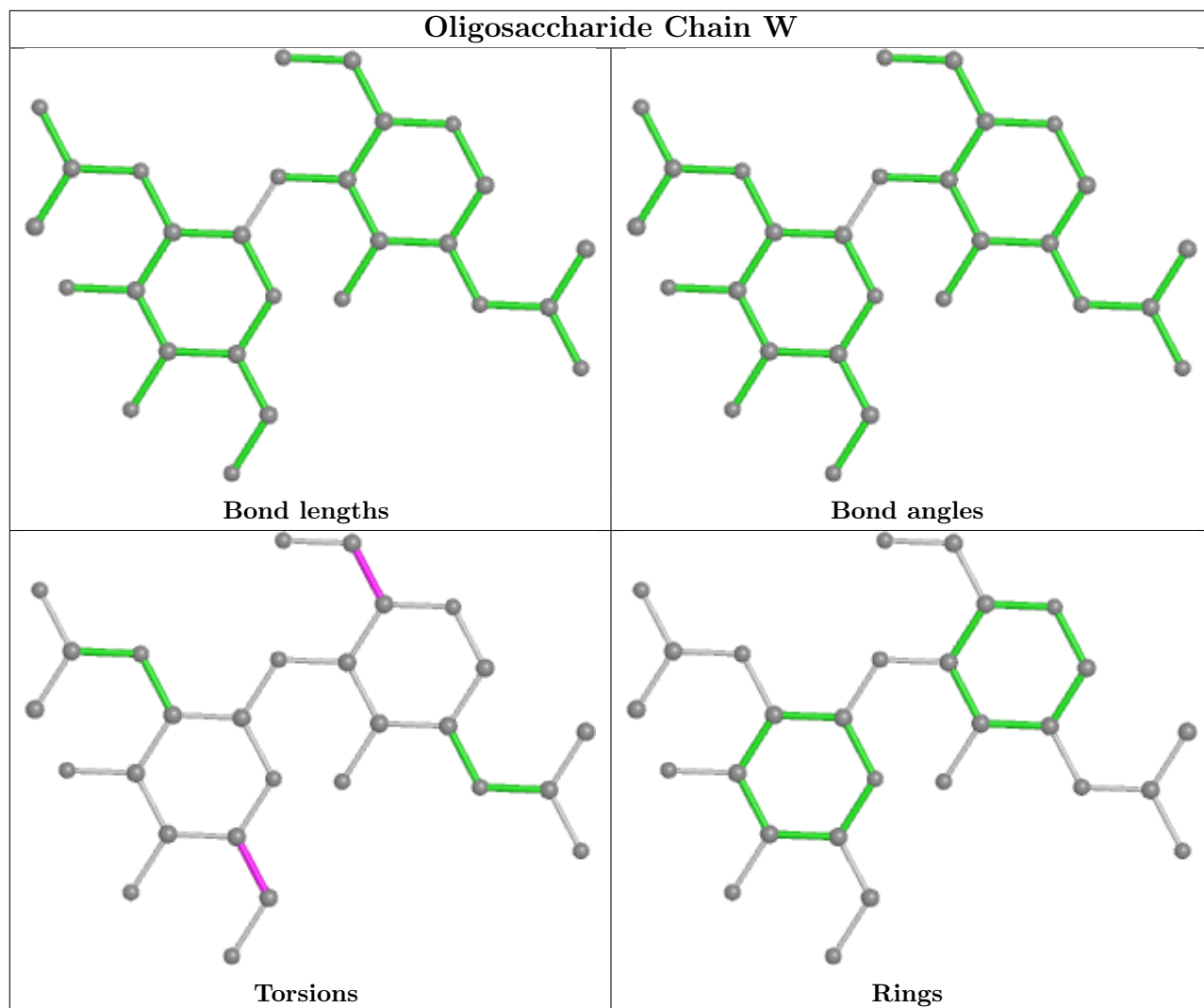


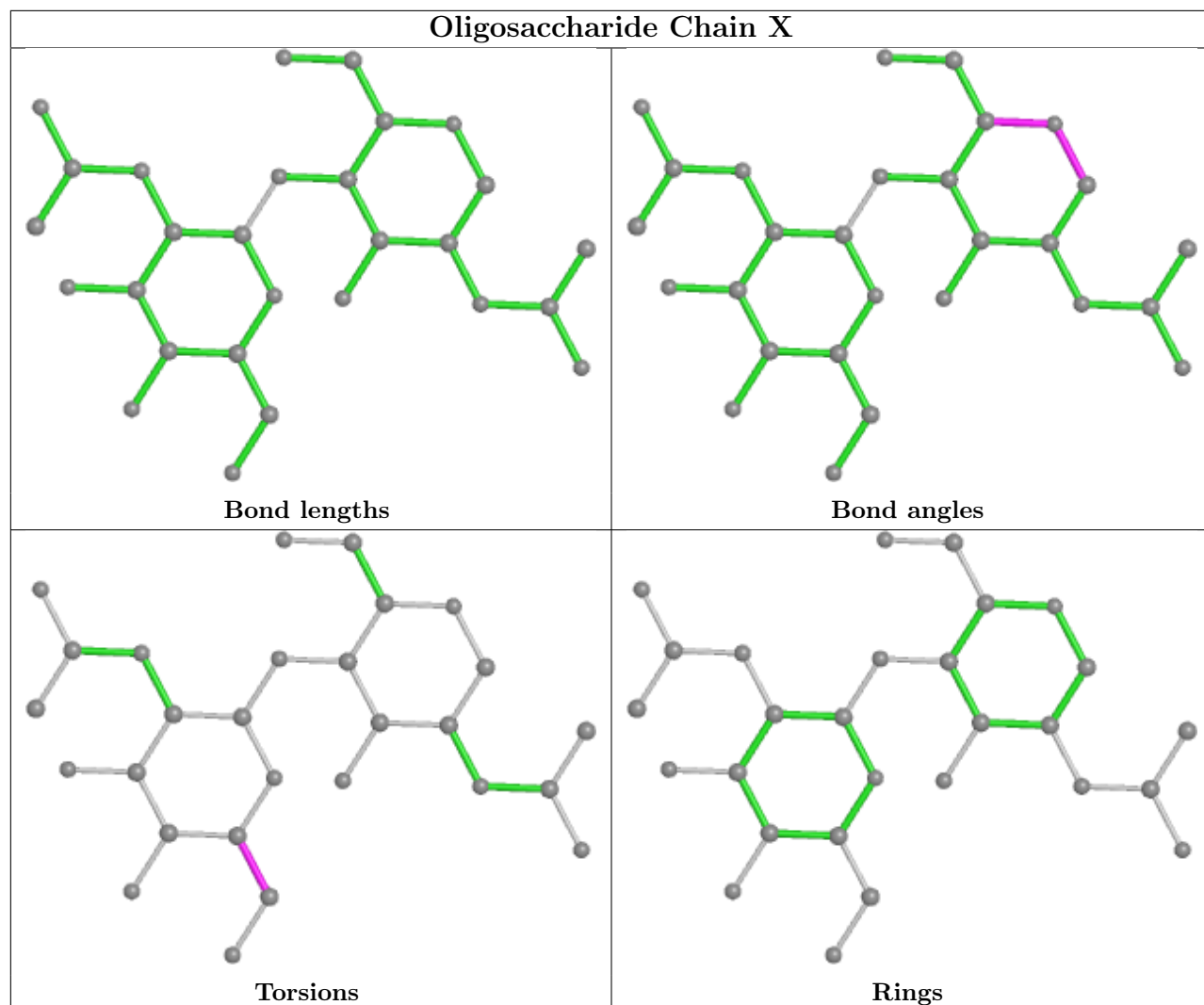


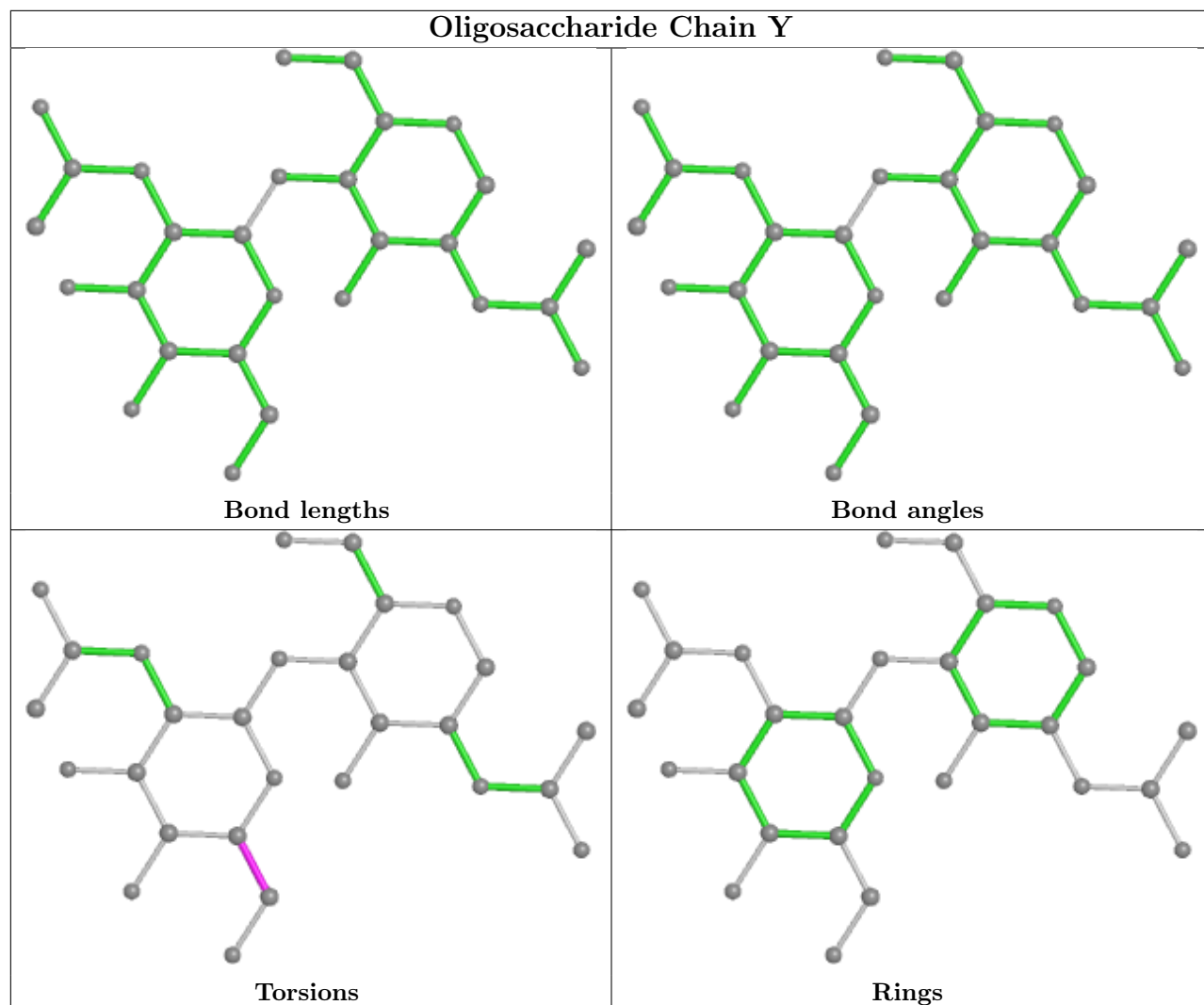


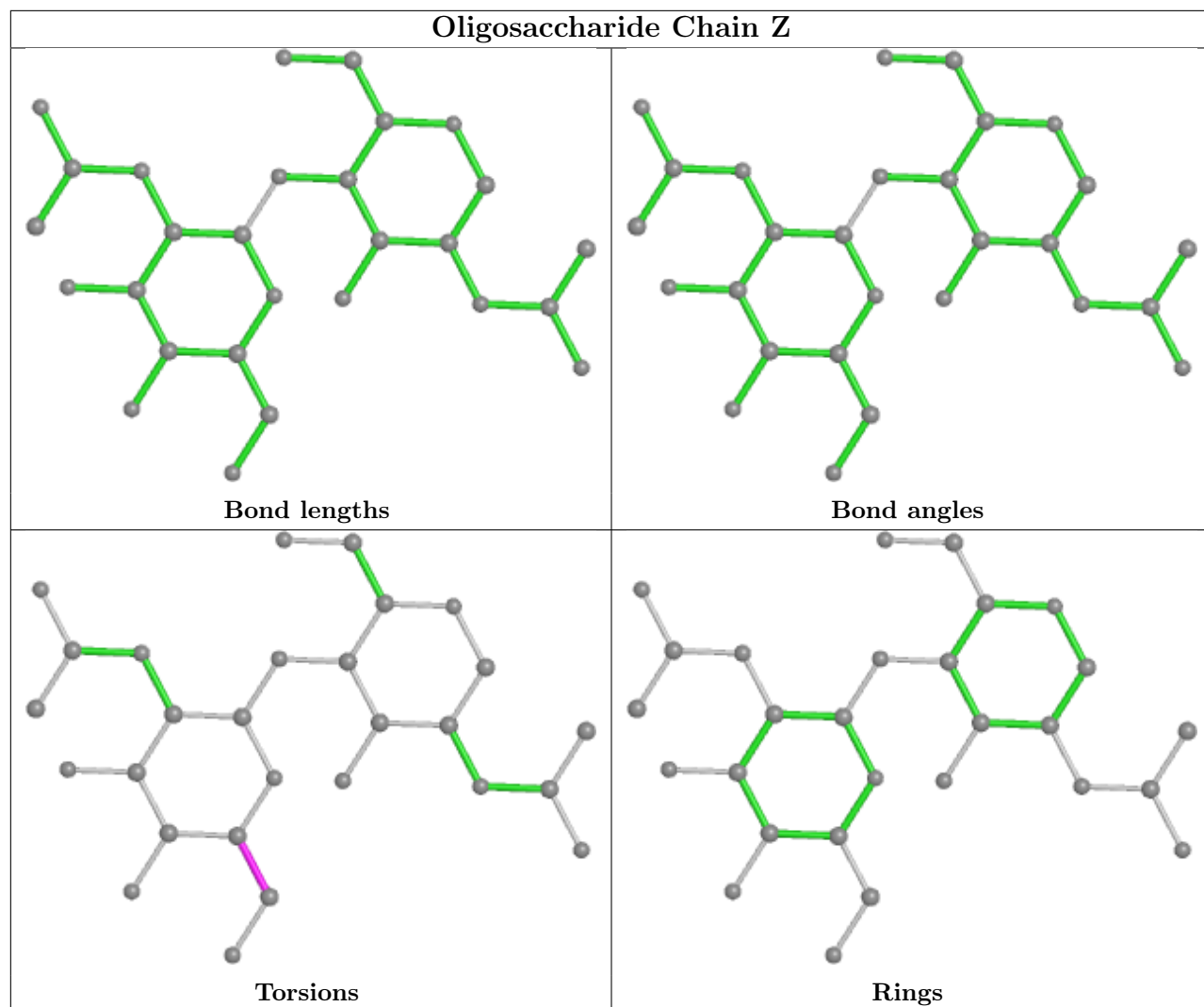


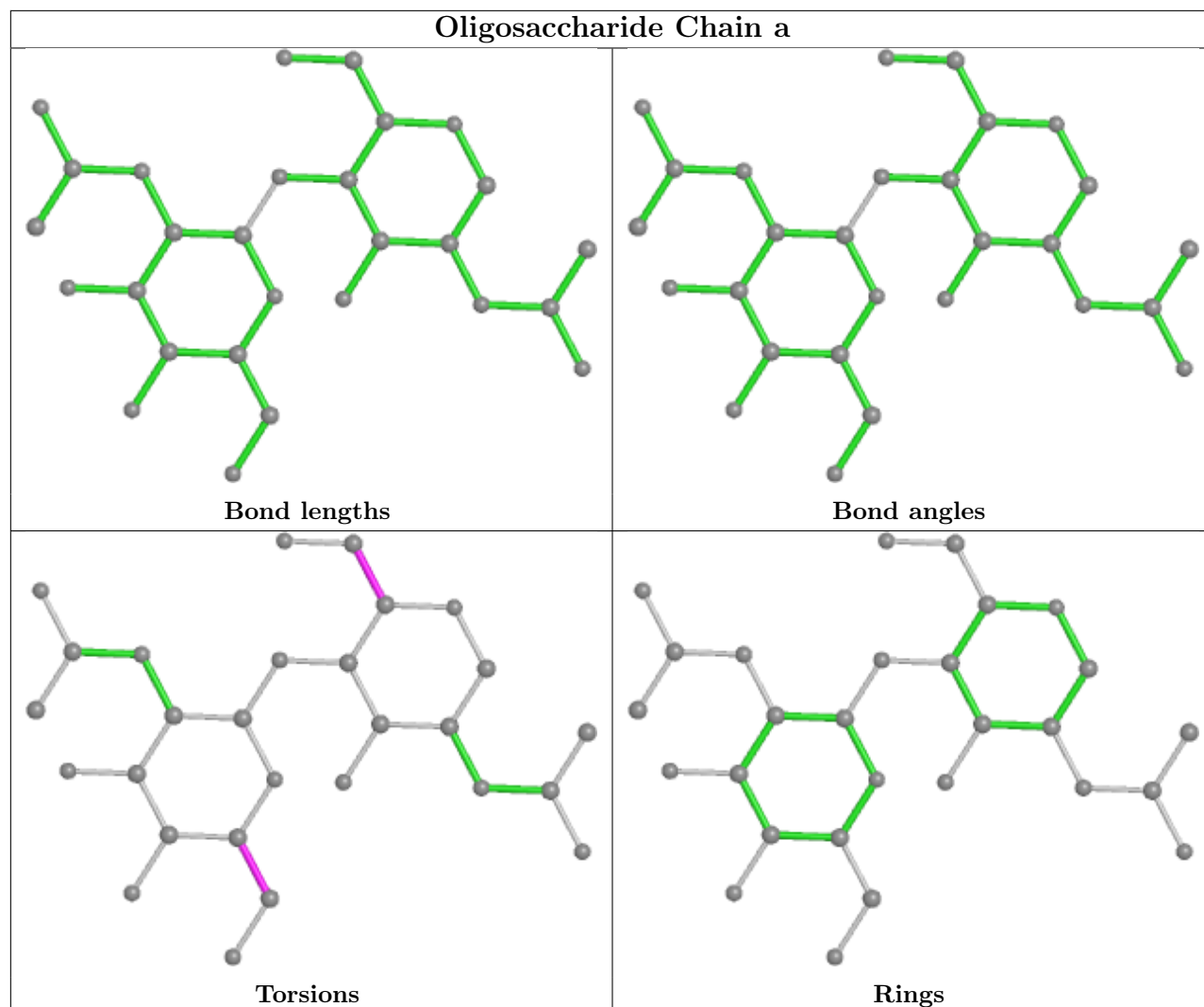


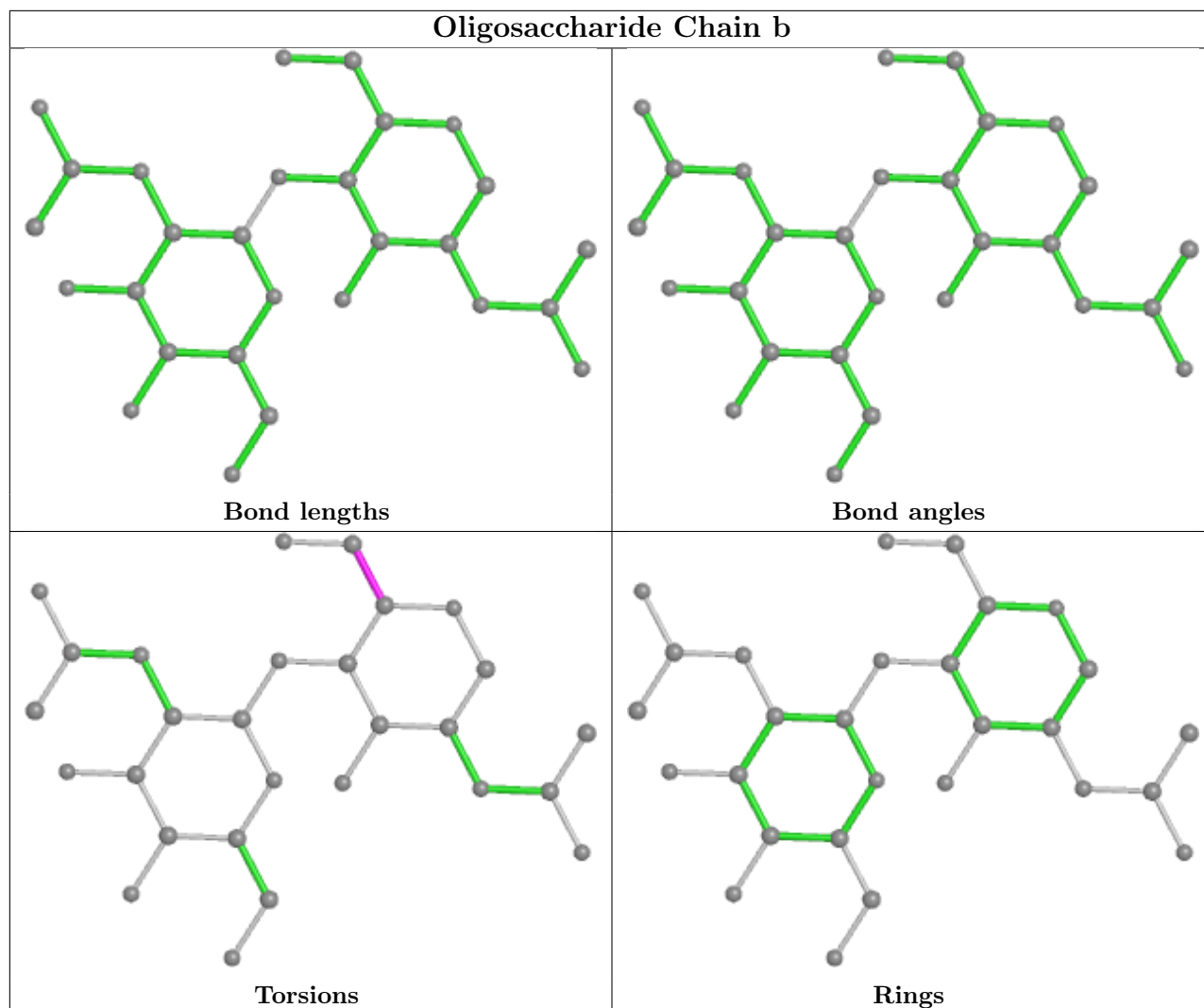












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
7	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.42	0
7	NAG	C	1302	1	14,14,15	0.26	0	17,19,21	0.40	0
7	NAG	A	1302	1	14,14,15	0.20	0	17,19,21	0.48	0
7	NAG	B	1305	1	14,14,15	0.19	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	1301	1	14,14,15	0.19	0	17,19,21	0.51	0
7	NAG	A	1301	1	14,14,15	0.20	0	17,19,21	0.47	0
7	NAG	B	1302	1	14,14,15	0.23	0	17,19,21	0.52	0
7	NAG	C	1304	1	14,14,15	0.41	0	17,19,21	0.49	0
7	NAG	B	1301	1	14,14,15	0.16	0	17,19,21	0.45	0
7	NAG	C	1303	1	14,14,15	0.27	0	17,19,21	0.46	0
7	NAG	A	1305	1	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	A	1304	1	14,14,15	0.20	0	17,19,21	0.57	0
7	NAG	B	1304	1	14,14,15	0.17	0	17,19,21	0.42	0
7	NAG	B	1303	1	14,14,15	0.23	0	17,19,21	0.53	0
7	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1301	NAG	C4-C5-C6-O6
7	B	1303	NAG	C4-C5-C6-O6
7	A	1301	NAG	O5-C5-C6-O6
7	A	1303	NAG	O5-C5-C6-O6
7	C	1304	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1301	NAG	1	0
7	A	1304	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

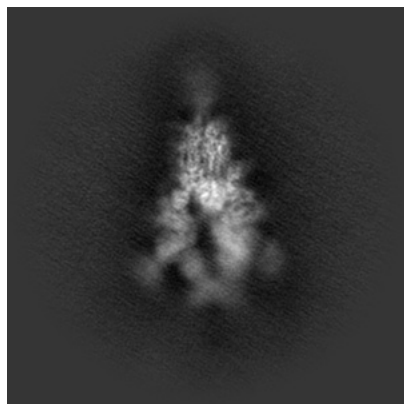
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25808. These allow visual inspection of the internal detail of the map and identification of artifacts.

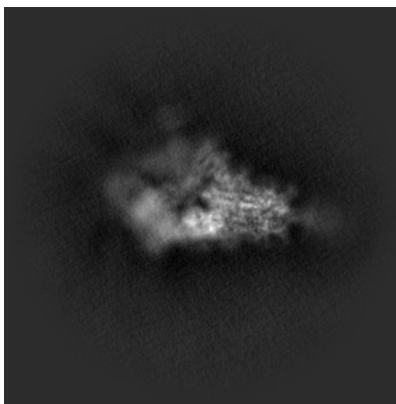
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

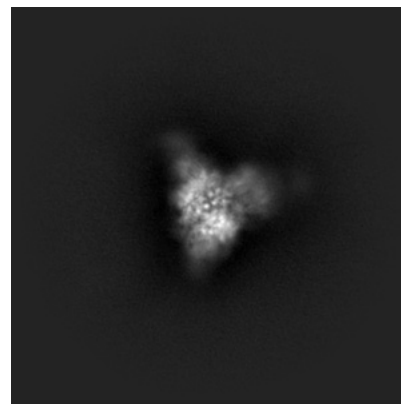
6.1.1 Primary map



X

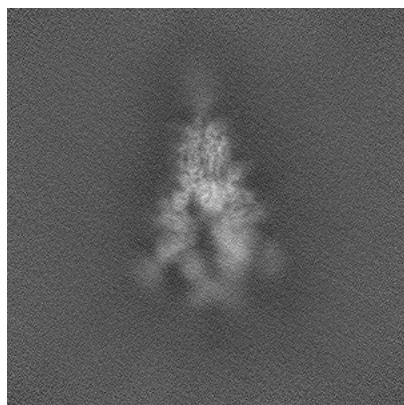


Y

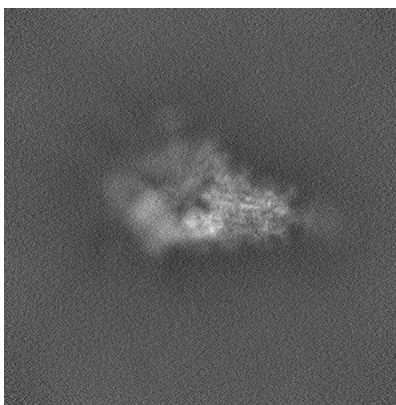


Z

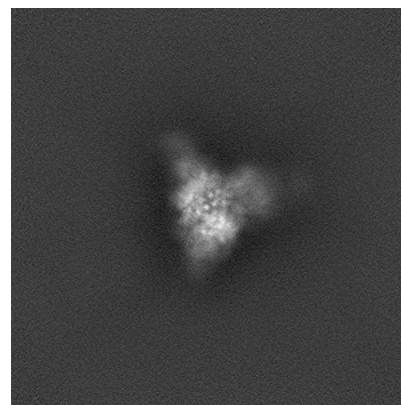
6.1.2 Raw map



X



Y

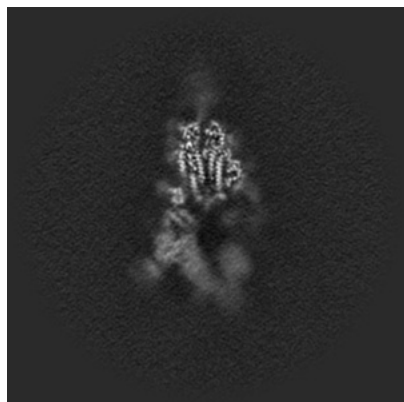


Z

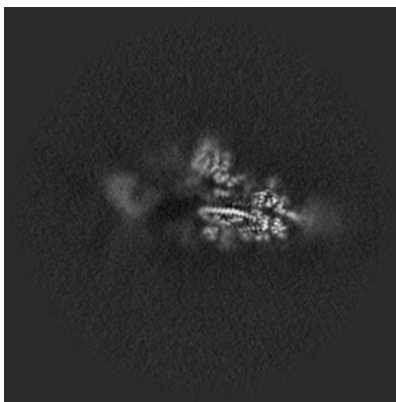
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

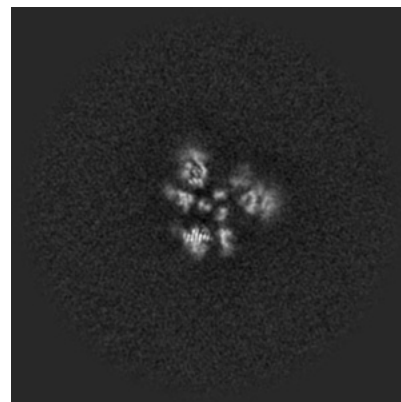
6.2.1 Primary map



X Index: 300

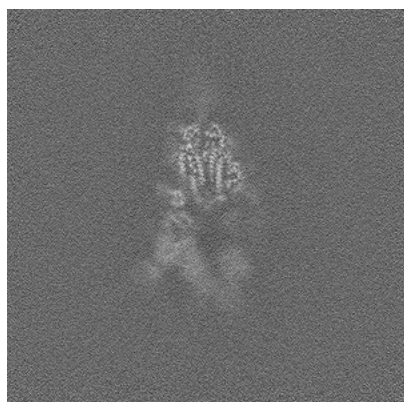


Y Index: 300



Z Index: 300

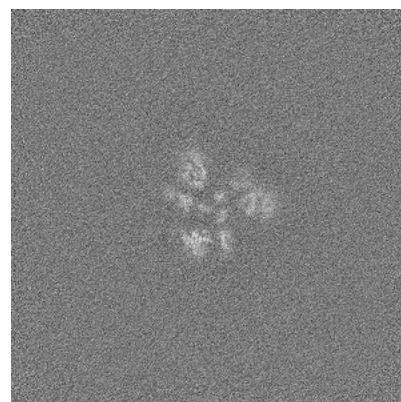
6.2.2 Raw map



X Index: 300



Y Index: 300

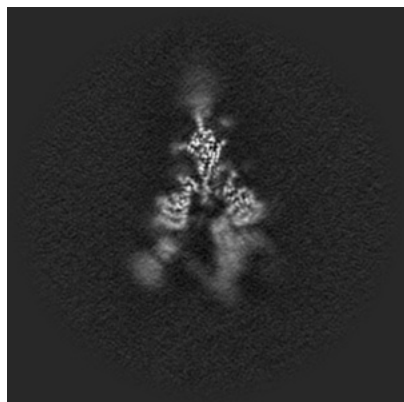


Z Index: 300

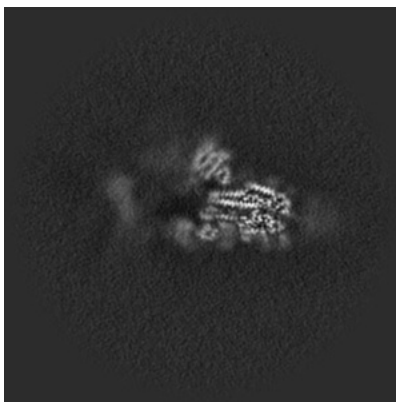
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

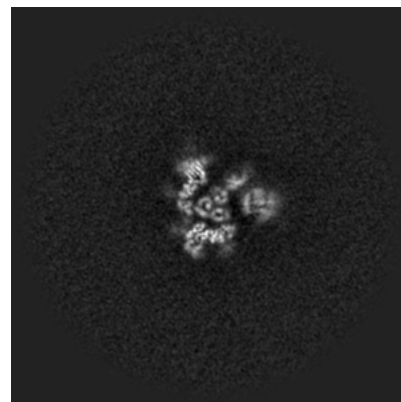
6.3.1 Primary map



X Index: 278

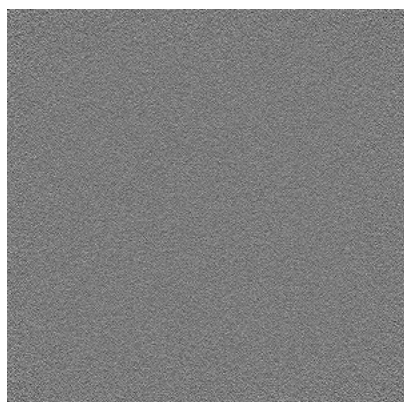


Y Index: 307

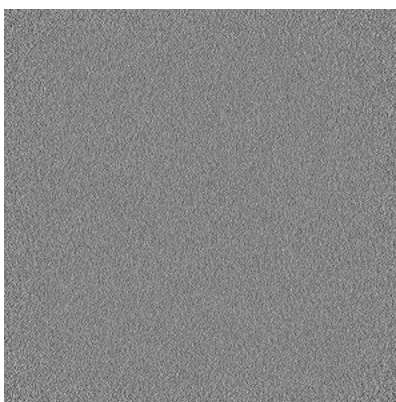


Z Index: 310

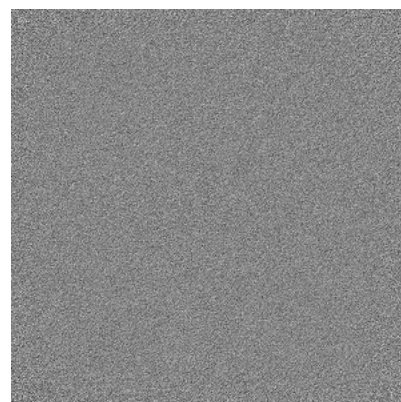
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

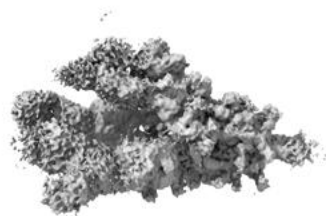
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



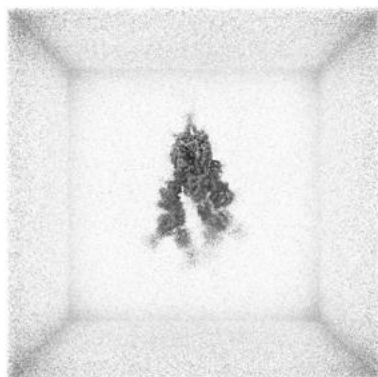
Y



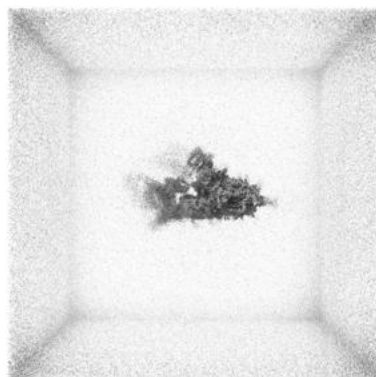
Z

The images above show the 3D surface view of the map at the recommended contour level 0.116. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

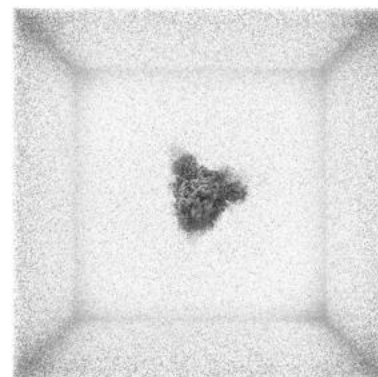
6.4.2 Raw map



X



Y



Z

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

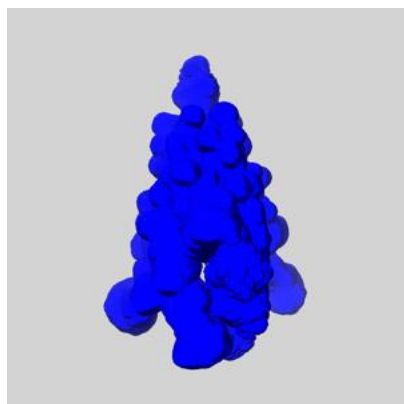
6.5 Mask visualisation [i](#)

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

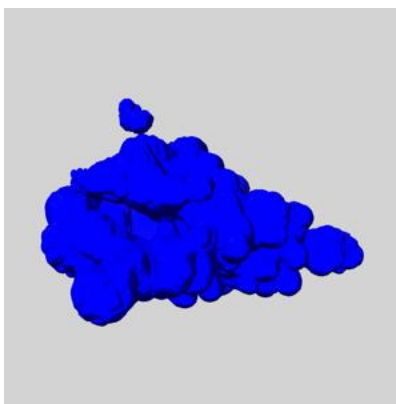
A mask typically either:

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

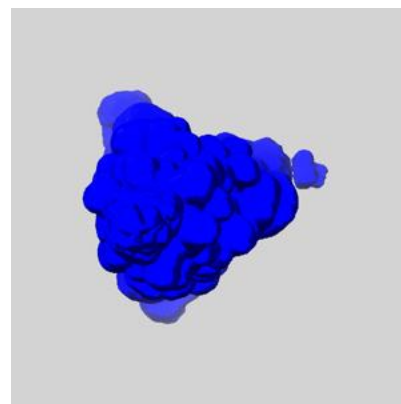
6.5.1 emd_25808_msk_1.map [i](#)



X



Y

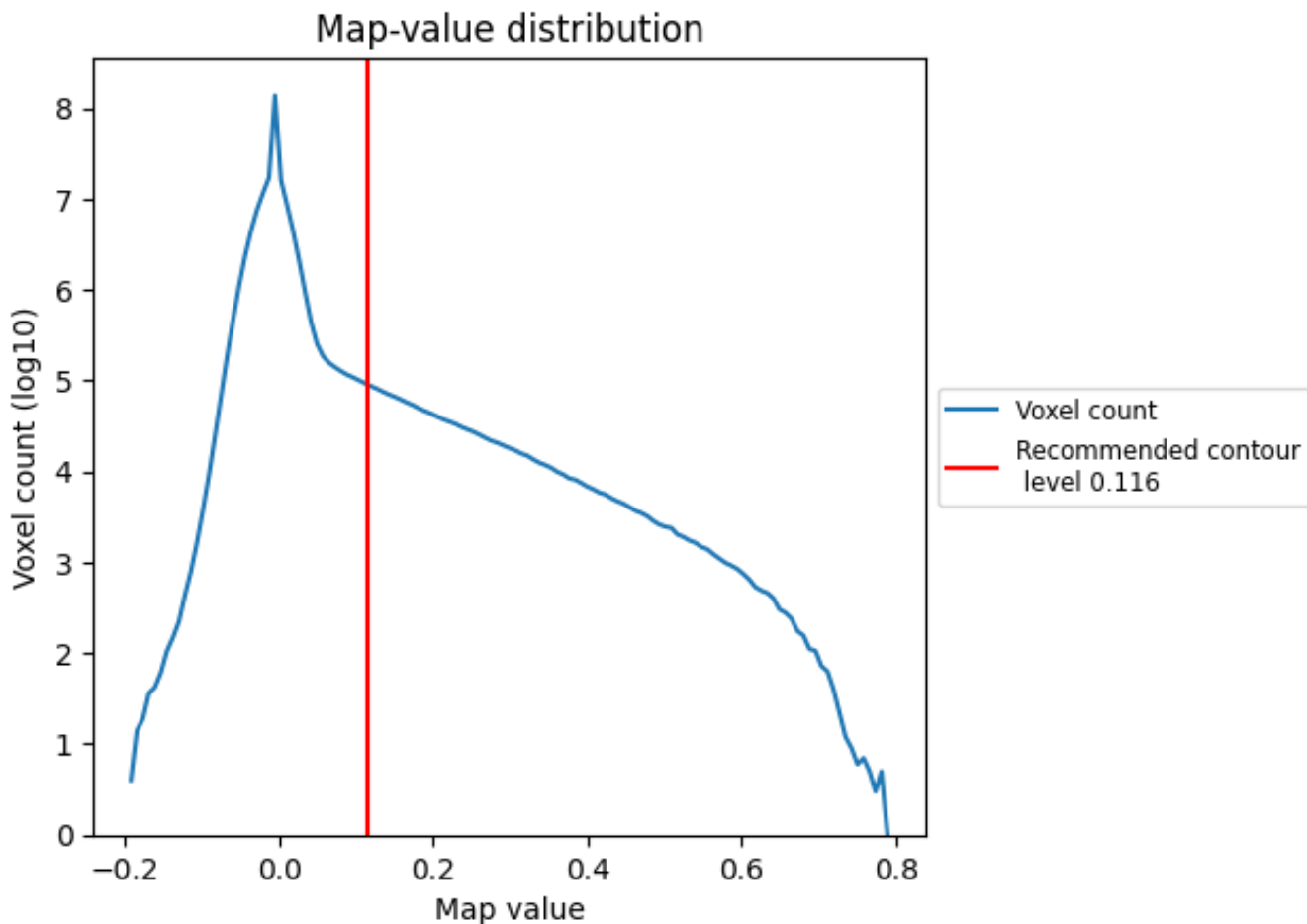


Z

7 Map analysis [i](#)

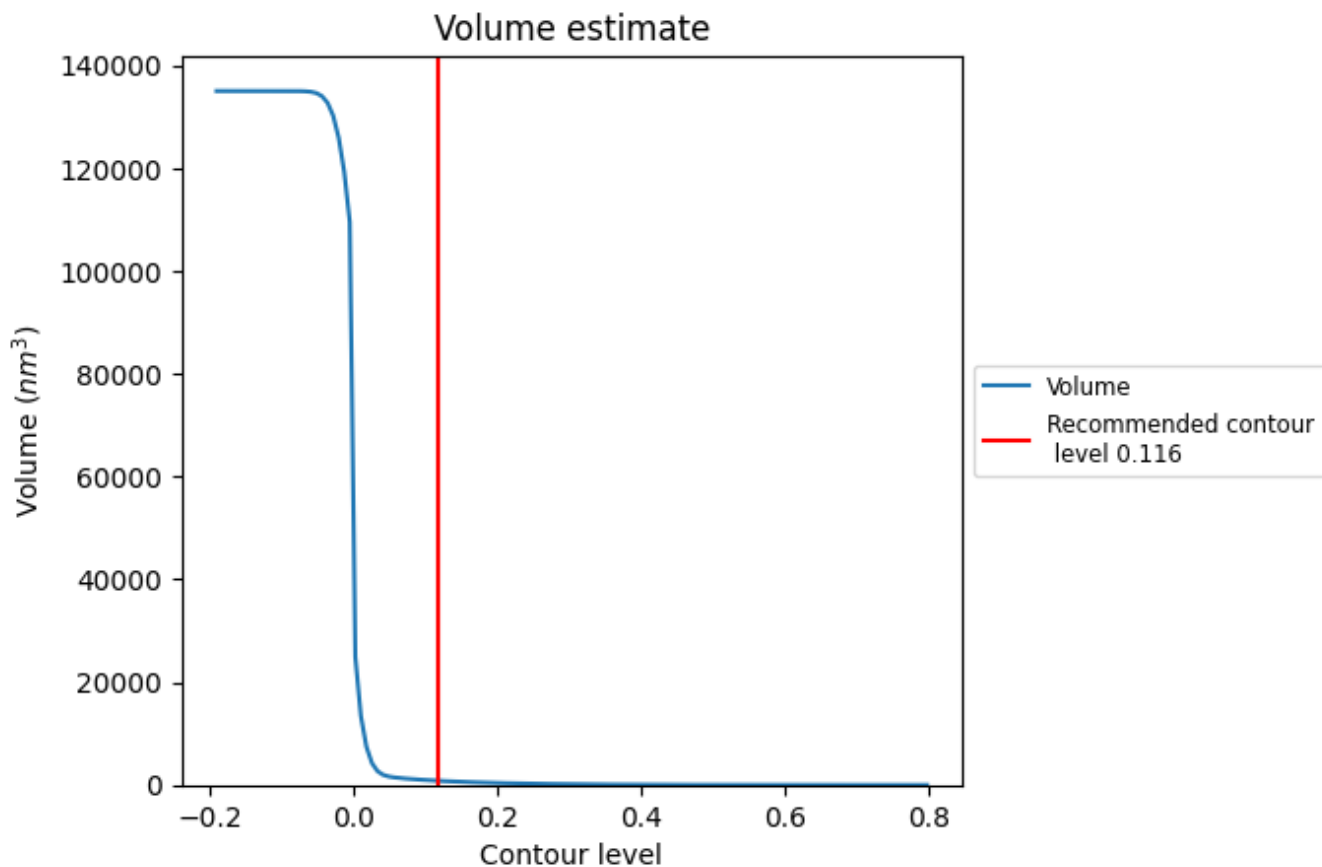
This section contains the results of statistical analysis of the map.

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.

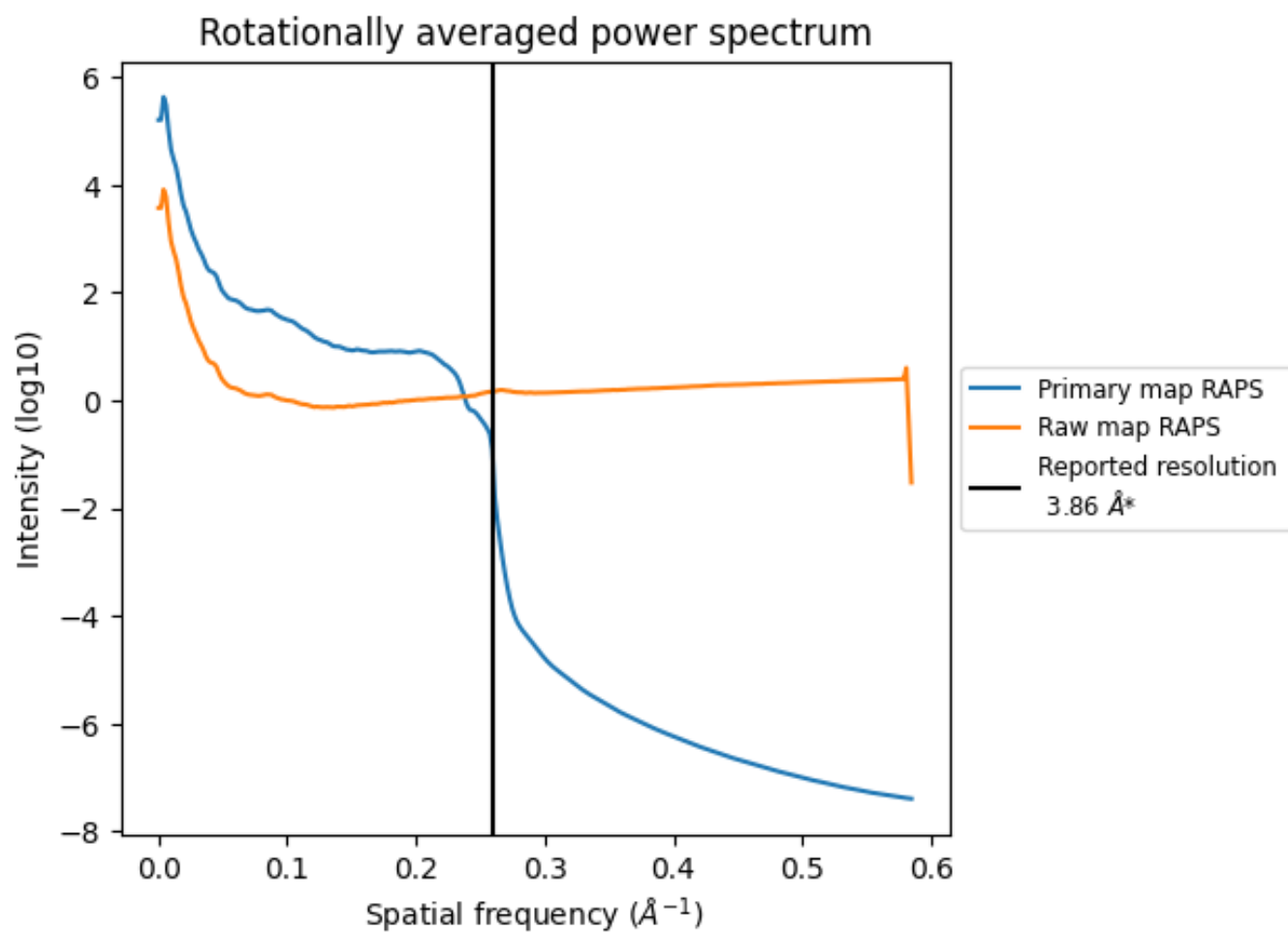
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 824 nm³; this corresponds to an approximate mass of 744 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 [i](#)

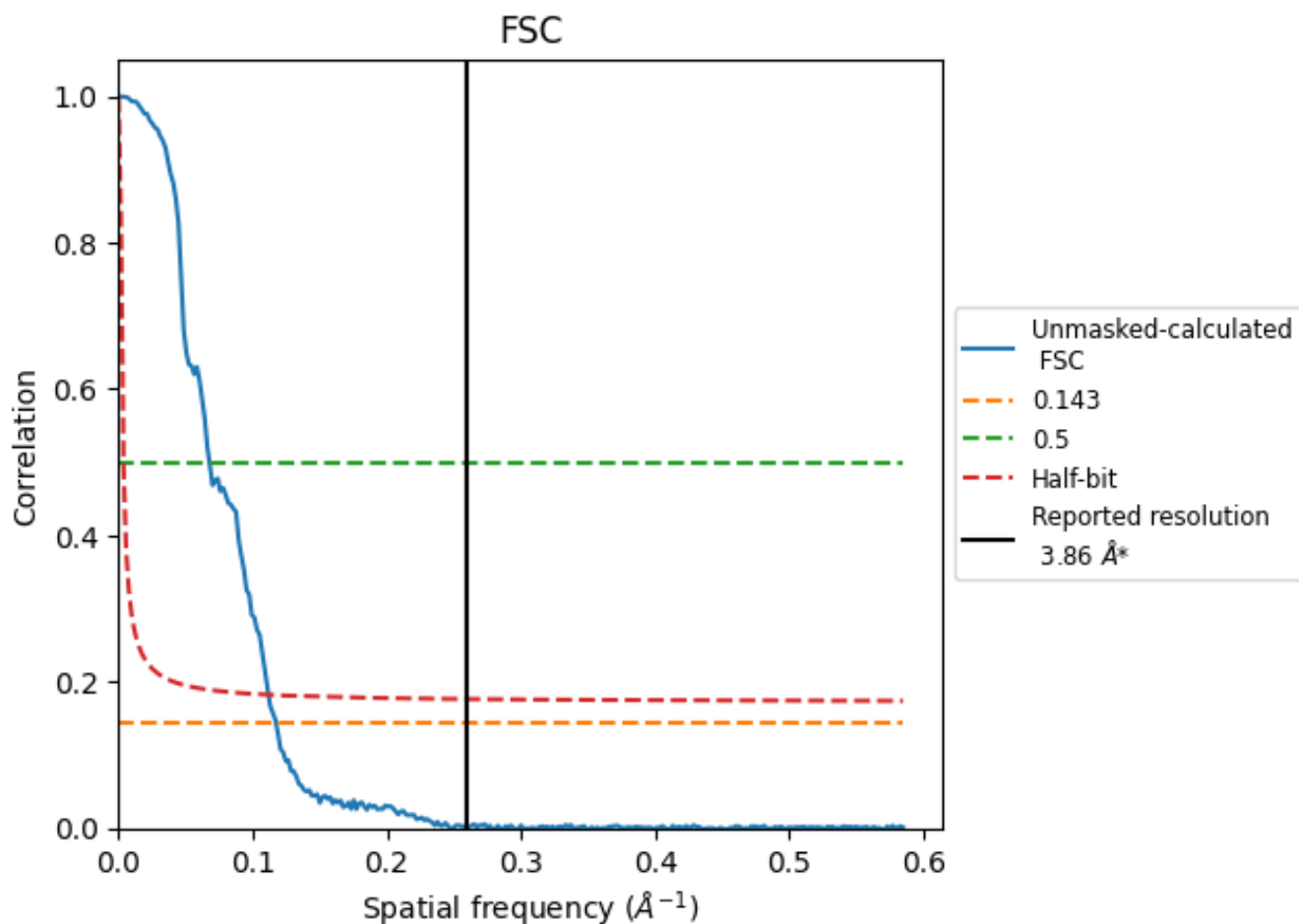


*Reported resolution corresponds to spatial frequency of 0.259 Å⁻¹

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 0.259 Å⁻¹

8.2 Resolution estimates [i](#)

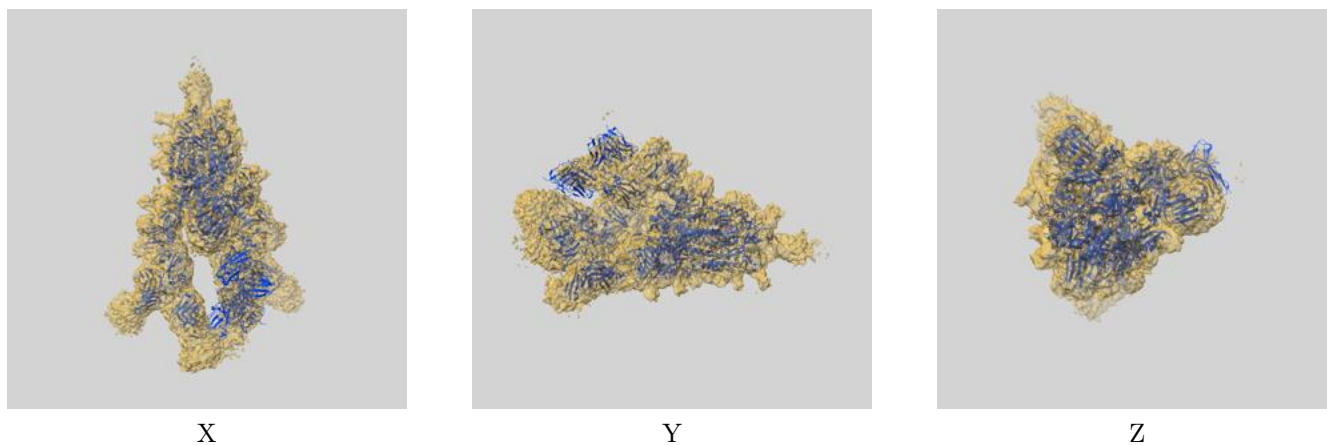
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.86	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.51	14.75	8.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 14.75 differs from the reported value 3.86 by more than 10 %

9 Map-model fit [i](#)

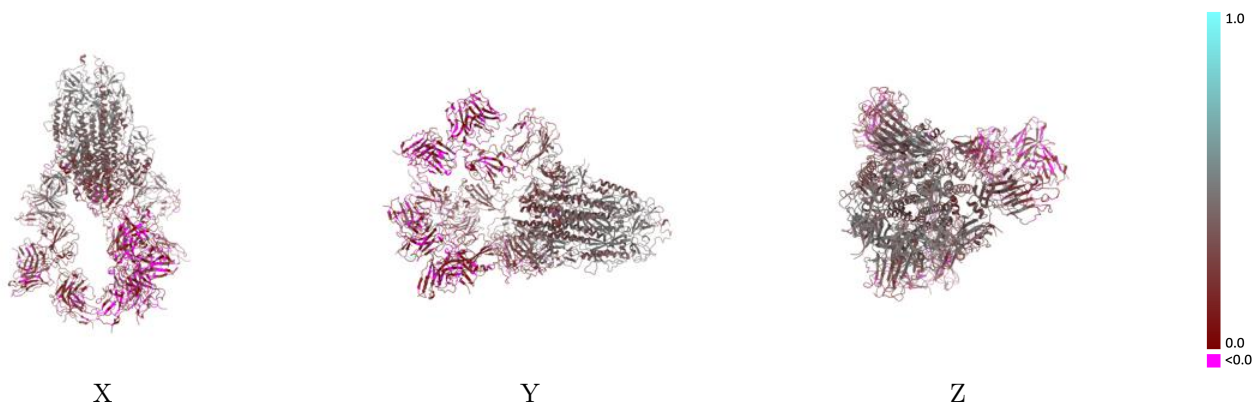
This section contains information regarding the fit between EMDB map EMD-25808 and PDB model 7TCC. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



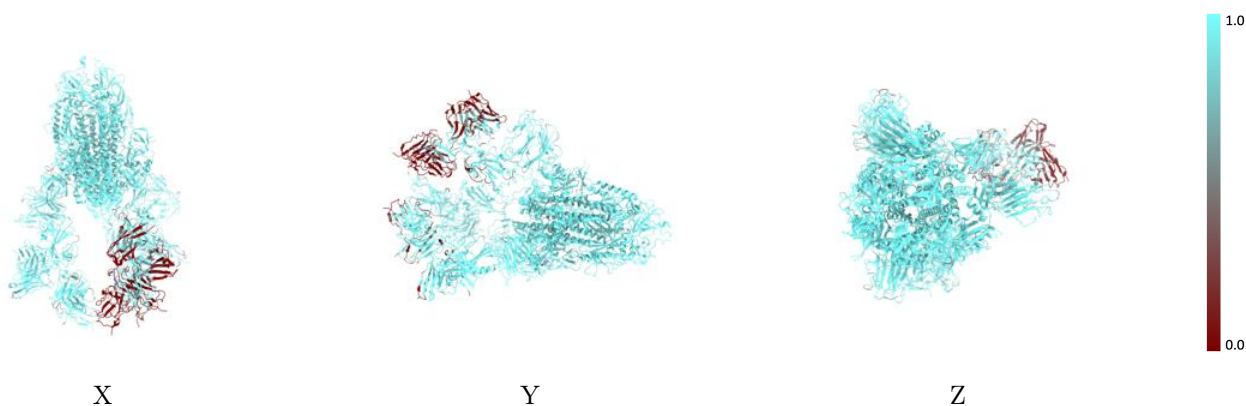
The images above show the 3D surface view of the map at the recommended contour level 0.116 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



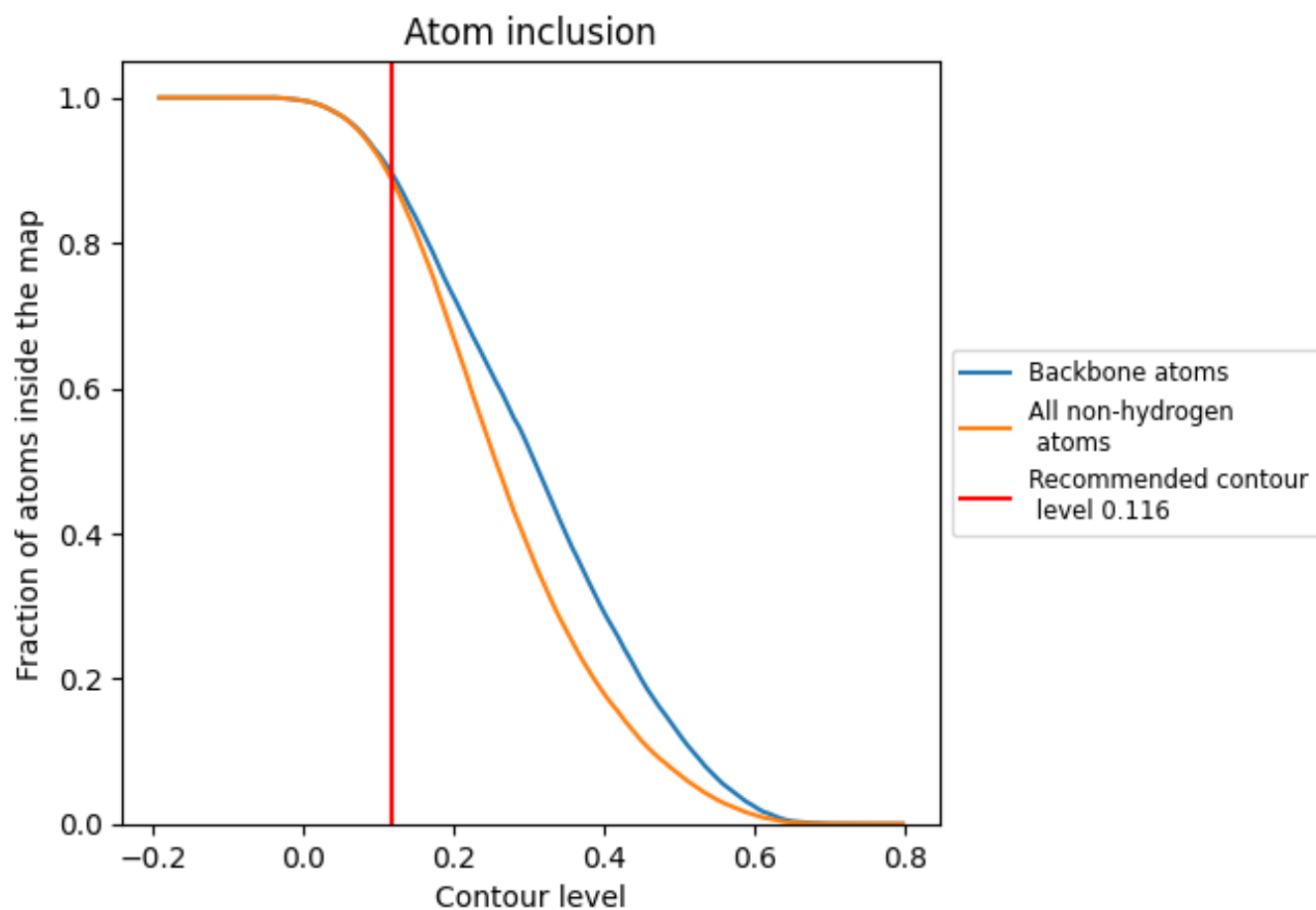
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.116).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.116) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8898	 0.2680
A	 0.9514	 0.3140
B	 0.9818	 0.3290
C	 0.9787	 0.3250
D	 0.3635	 0.1130
E	 0.4488	 0.1100
F	 0.9561	 0.1550
G	 0.9084	 0.1450
H	 0.9885	 0.1960
I	 1.0000	 0.4520
J	 0.1998	 0.0750
K	 0.0557	 0.0730
L	 0.9659	 0.1770
M	 0.9208	 0.1070
N	 0.8812	 0.1210
O	 0.7969	 0.1200
P	 0.6955	 0.1450
Q	 1.0000	 0.4020
R	 1.0000	 0.4470
S	 1.0000	 0.3940
T	 1.0000	 0.4510
U	 1.0000	 0.4190
V	 1.0000	 0.4110
W	 1.0000	 0.4180
X	 1.0000	 0.4550
Y	 1.0000	 0.3720
Z	 1.0000	 0.4320
a	 1.0000	 0.3220
b	 1.0000	 0.3600

