



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:53 PM UTC

PDB ID : 7T9K / pdb_00007t9k
EMDB ID : EMD-25760
Title : Cryo-EM structure of SARS-CoV-2 Omicron spike protein in complex with human ACE2
Authors : Zhu, X.; Mannar, D.; Saville, J.W.; Srivastava, S.S.; Berezuk, A.M.; Tuttle, K.S.; Subramaniam, S.
Deposited on : 2021-12-19
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

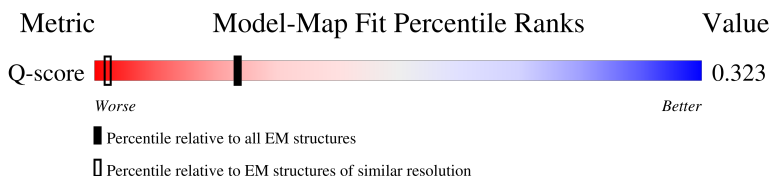
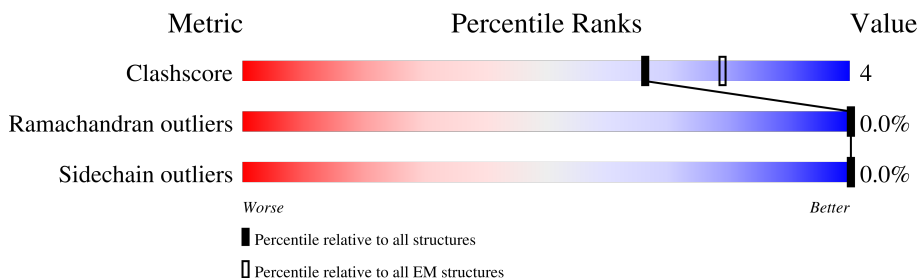
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.45 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5931 (1.96 - 2.95)

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	1285	20% 72% 8% 20%
1	B	1285	18% 71% 9% 20%
1	C	1285	• 57% 7% 35%
2	D	606	97% 88% 10% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	606	98% 87% 11%
3	F	2	100% 50% 50%
3	G	2	50% 50%
3	H	2	50% 50%
3	I	2	50% 100%
3	J	2	50% 100%
3	K	2	50% 100%
3	L	2	100% 100%
3	M	2	50% 50%
3	N	2	50% 50%
3	O	2	50% 100%
3	P	2	50% 100%
3	Q	2	50% 50%
3	R	2	100% 100%
3	S	2	50% 50%
3	T	2	50% 50%
3	U	2	50% 100%
3	V	2	50% 100%
3	W	2	50% 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33398 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	1032	Total	C	N	O	S	0	0
			8101	5189	1349	1526	37		
1	B	1032	Total	C	N	O	S	0	0
			8101	5189	1349	1526	37		
1	C	833	Total	C	N	O	S	0	0
			6502	4158	1078	1237	29		

There are 387 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	210A	ILE	-	insertion	UNP P0DTC2
A	210B	VAL	-	insertion	UNP P0DTC2
A	210C	ARG	ASN	conflict	UNP P0DTC2
A	210D	GLU	LEU	conflict	UNP P0DTC2
A	210E	PRO	VAL	conflict	UNP P0DTC2
A	210F	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

Continued on next page...

Continued from previous page...

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	817	PRO	PHE	conflict	UNP P0DTC2
A	856	LYS	ASN	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	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	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1226	LYS	-	expression tag	UNP P0DTC2
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1268	GLY	-	expression tag	UNP P0DTC2
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	210A	ILE	-	insertion	UNP P0DTC2
B	210B	VAL	-	insertion	UNP P0DTC2
B	210C	ARG	ASN	conflict	UNP P0DTC2
B	210D	GLU	LEU	conflict	UNP P0DTC2
B	210E	PRO	VAL	conflict	UNP P0DTC2
B	210F	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	477	ASN	SER	conflict	UNP P0DTC2
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	817	PRO	PHE	conflict	UNP P0DTC2
B	856	LYS	ASN	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	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	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
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	210A	ILE	-	insertion	UNP P0DTC2
C	210B	VAL	-	insertion	UNP P0DTC2
C	210C	ARG	ASN	conflict	UNP P0DTC2
C	210D	GLU	LEU	conflict	UNP P0DTC2
C	210E	PRO	VAL	conflict	UNP P0DTC2
C	210F	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
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	817	PRO	PHE	conflict	UNP P0DTC2
C	856	LYS	ASN	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	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	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		
2	E	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1
D	622	HIS	-	expression tag	UNP Q9BYF1
D	623	HIS	-	expression tag	UNP Q9BYF1
E	616	HIS	-	expression tag	UNP Q9BYF1
E	617	HIS	-	expression tag	UNP Q9BYF1
E	618	HIS	-	expression tag	UNP Q9BYF1
E	619	HIS	-	expression tag	UNP Q9BYF1
E	620	HIS	-	expression tag	UNP Q9BYF1
E	621	HIS	-	expression tag	UNP Q9BYF1
E	622	HIS	-	expression tag	UNP Q9BYF1
E	623	HIS	-	expression tag	UNP Q9BYF1

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



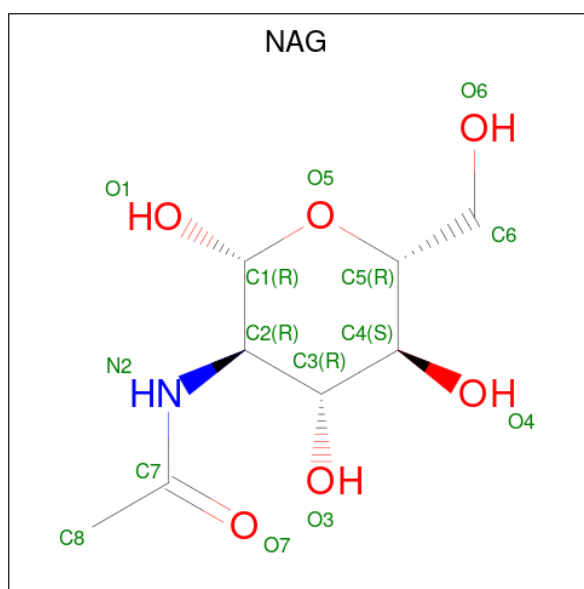
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

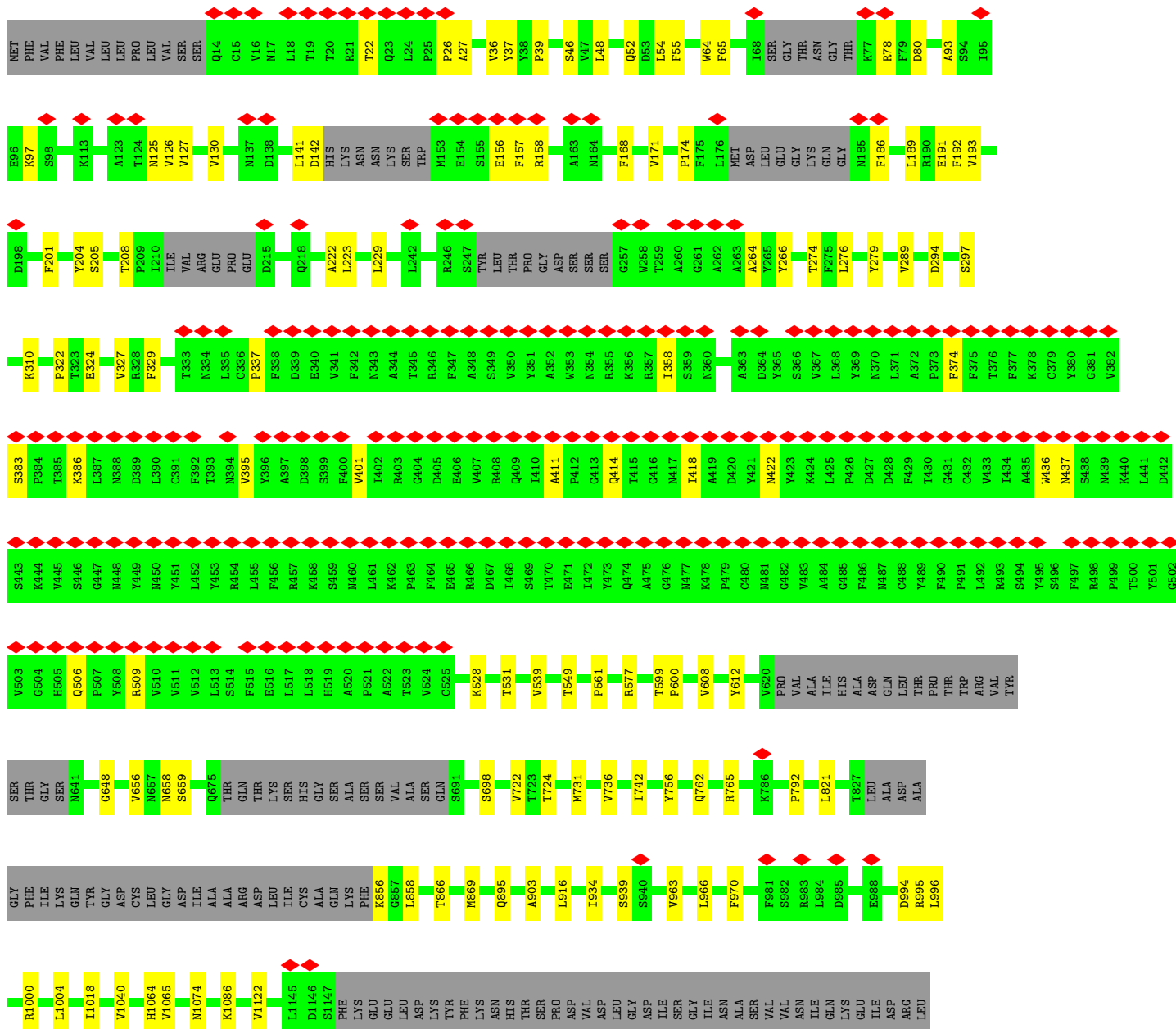
Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	



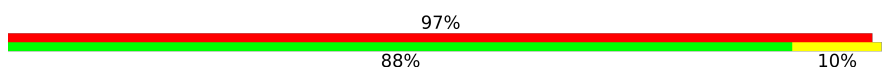
ASN	GLU	VAL	ALA	LYS	ASN	LEU	ASN	GLU	LEU	ASN	SER	ILE	ASP	LEU	GLN	GLU	LEU	GLY	LYS	TYR	GLY	GLY	SER	GLY	TYR	ILE	GLY	PRO	GLY	GLU	ALA	PRO	ARG	ASP	GLY	GLY	GLN	ALA	TRP	TRP	VAL	ARG	LYS	LYS	ASP	GLY	GLY	GLU	TRP	TRP	VAL	LEU	LEU	SER	THR	PHE	LEU	GLY	ARG	SER	SER	LEU	VAL	VAL	LEU	PHE	GLN
GLY	PRO	GLY	HIS	HIS	HIS	HIS	HIS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

• Molecule 1: Spike glycoprotein

Chain C:  57% 7% 35%

SER	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLY	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

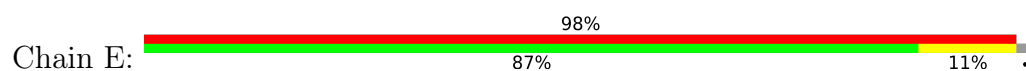
• Molecule 2: Processed angiotensin-converting enzyme 2

Chain D:  97% 88% 10%

HIS	L558	C498	F438	H378	V318	P258	D198	P138	T78
	H559	D499	L439	I379	G319	T259	Y199	Q139	L79
	L560	P500	L440	Q380	L320	G260	G200	E140	A80
	G561	A501	K441	Y381	P321	C261	D201	C141	Q81
HIS	K562	S502	Q442	D382	N322	L282	Y202	L142	M82
	S563	L503	A443	H383	H323	P283	W203	L143	Y83
	E564	F504	L444	A384	T324	A284	R204	L144	P84
	P565	H505	T445	Y385	Q325	H285	G205	E145	L85
HIS	W566	V506	I446	A386	G326	L286	D206	P146	K26
	T567	S507	V447	A387	F327	L287	Y207	G147	E87
	L568	N508	Q448	Q388	W328	G288	E208	L148	F28
	A569	D509	T449	P389	E329	D289	V209	M149	Q89
HIS	L570	Y510	L450	F390	N330	M270	N210	E150	N90
	E571	S511	P451	L391	S331	W271	G211	T151	L91
	N572	F512	F452	L392	N332	G272	V212	M152	T92
	V573	I513	T453	R393	L333	R273	D213	A153	Y93
HIS	V574	R514	Y454	N394	T334	F274	G214	N154	K94
	G575	Y515	M455	G395	D335	W275	Y215	S155	L95
	A576	V516	L456	A396	P336	T276	D216	L156	A36
	K577	T517	E457	N397	G337	W277	Y217	D157	Q96
HIS	N578	R518	K458	E398	N338	L278	S218	Y158	L97
	M579	T519	W459	F400	V339	Y279	R219	N159	Q98
	N580	L520	R460	F401	Q340	S280	G220	E160	L39
	V581	Y521	W461	E402	K341	L281	Q221	R161	A99
HIS	R582	Q522	M462	A403	A342	T282	L222	L162	L100
	P583	F523	V463	Y404	V343	V283	T223	W163	Q101
	L584	Q524	F464	G405	C344	P284	E224	A164	G42
	L585	F525	K465	E406	H345	F285	D225	W165	S43
HIS	N586	Q526	G466	I407	P346	G286	V226	E166	S106
	V587	E527	E467	M408	T347	Q287	E227	S167	S47
	F588	A528	I468	S409	A348	K288	H228	W168	W48
	E589	L529	P469	L410	W349	P289	T229	R169	N49
HIS	P590	C530	K470	L411	D350	N290	F230	S170	Y50
	L591	Q531	D471	A412	L351	T291	E231	E171	E10
	F592	A532	Q472	A413	G352	D292	E232	W172	D11
	T593	A533	W473	T414	K353	V293	T233	G173	K112
HIS	W594	K534	M474	P415	G354	T294	K234	K174	S113
	L595	H535	K475	P416	D355	D295	P235	Q175	R114
	K596	E536	K476	H417	F356	A296	L236	L176	R115
	D597	Q537	W477	L418	R357	W297	Y237	R177	L116
HIS	Q598	P538	W478	K419	L358	V298	E238	P178	M58
	N599	L539	E479	L419	L359	D299	H239	L179	T118
	K600	H540	M480	S420	N360	Q300	L240	Y180	I119
	N601	K541	K481	I421	C361	A301	H241	E181	L120
HIS	S602	C542	R482	G422	T362	W302	A242	E182	N121
	F603	D543	E483	L423	K363	D303	Y243	M123	M62
	V604	I544	L484	S425	V364	A304	V244	S124	M64
	G605	S545	V485	P426	T365	Q305	R245	V185	A65
HIS	W606	N546	G486	D427	N366	R306	A246	L186	G66
	S607	S547	W487	F428	D367	I307	K247	K187	D67
	T608	T548	V488	Q429	D368	F308	L248	N188	K68
	D609	E549	E489	Q429	F369	K309	M249	E189	W69
HIS	W610	A550	P490	E430	L370	E310	N250	M190	S70
	S611	G551	V491	D431	T371	A311	A251	A191	A71
	P612	Q552	P492	N432	A372	E312	Y252	R192	F72
	V613	K553	H493	E433	H373	K313	P253	A193	L73
HIS	ALA	L554	D494	T434	H374	F314	S254	N194	K74
	ASP	F555	E495	E435	E375	F315	Y255	H195	E75
	HIS	N556	T496	I436	E376	V316	T256	P195	Q76
	HIS	N557	W557	Y497	N437	G377	S317	E257	S77

HIS
HIS
HIS
HIS
HIS

● Molecule 2: Processed angiotensin-converting enzyme 2



GLN	S19	T20	T21	E22	E23	Q24	A25	K26	T27	F28	L29	D30	K31	F32	N33	H34	E35	A36	E37	D38	L39	F40	Y41	Q42	S43	S44	L45	A46	S47	W48	N49	Y50	N51	T52	N53	T54	T55	E56	E57	N58	V59	Q60	N61	H62	N63	N64	A65	G66	D67	K68	W69	S70	A71	F72	L73	K74	E75	Q76	S77
T78	L79	A80	Q81	H82	Y83	P84	L85	Q86	E87	I88	Q89	N90	L91	T92	V93	K94	L95	Q96	L97	Q98	A99	L100	Q101	Q102	N103	G104	S105	S106	S107	L108	S109	E110	D111	K112	S113	K114	R115	L116	N117	T118	V119	L120	N121	E122	M123	S124	T125	I126	K127	S128	T129	G130	K131	V132	C133	N134	P135	D136	N137

Chain H:  50% 50%



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

Chain I:  50% 100%



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

Chain J:  50% 100%

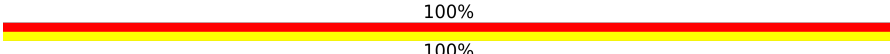


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 100%



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

Chain L:  100% 100%



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

Chain M:  50% 50%



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

Chain N:  50% 50%



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

Chain O:  50% 100%



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

Chain P:  50% 100%



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

Chain Q:  50% 50% 50%



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

Chain R:  100% 100%



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

Chain S:  50% 50%



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

Chain T:  50% 50%



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

Chain U:  50% 100%



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

Chain V:  50% 100%



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

Chain W:  50% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	272266	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.148	Depositor
Minimum map value	-0.416	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.152	Depositor
Map size (Å)	400.0, 400.0, 400.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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	0.20	0/8292	0.50	0/11281
1	B	0.22	0/8292	0.51	0/11281
1	C	0.22	0/6644	0.52	0/9036
2	D	0.21	0/4994	0.49	0/6785
2	E	0.21	0/4994	0.48	0/6785
All	All	0.21	0/33216	0.50	0/45168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8101	0	7925	65	0
1	B	8101	0	7925	71	0
1	C	6502	0	6386	60	0
2	D	4857	0	4630	37	0
2	E	4857	0	4630	36	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
4	A	112	0	104	0	0
4	B	112	0	104	1	0
4	C	84	0	78	1	0
4	D	84	0	78	0	0
4	E	84	0	78	0	0
All	All	33398	0	32388	256	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 4.

All (256) 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:C:142:ASP:HB2	1:C:156:GLU:HB3	1.74	0.69
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.77	0.65
1:B:856:LYS:HD3	1:B:966:LEU:HD12	1.78	0.65
1:B:46:SER:HA	1:B:279:TYR:O	1.97	0.65
1:B:156:GLU:OE2	1:B:158:ARG:NH1	2.32	0.63
1:C:156:GLU:OE2	1:C:158:ARG:NH1	2.32	0.62
2:E:170:SER:OG	2:E:174:LYS:NZ	2.34	0.60
1:A:572:THR:HG22	1:B:856:LYS:HE3	1.84	0.60
1:B:327:VAL:H	1:B:531:THR:HB	1.66	0.59
1:C:51:THR:O	1:C:274:THR:HA	2.02	0.59
1:A:156:GLU:OE2	1:A:158:ARG:NH1	2.34	0.59
2:E:85:LEU:HD12	2:E:94:LYS:HG3	1.84	0.59
1:B:26:PRO:HB3	1:B:65:PHE:HE1	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:LEU:HD12	2:D:94:LYS:HG3	1.85	0.59
2:E:169:ARG:HH22	2:E:271:TRP:HA	1.68	0.59
2:D:170:SER:OG	2:D:174:LYS:NZ	2.36	0.58
1:A:105:ILE:HB	1:A:239:GLN:HB2	1.84	0.58
1:C:22:THR:O	1:C:78:ARG:NH1	2.35	0.58
1:C:821:LEU:HD11	1:C:939:SER:HB3	1.86	0.58
2:E:475:LYS:NZ	2:E:495:GLU:OE1	2.37	0.57
1:B:142:ASP:HB2	1:B:156:GLU:HB3	1.86	0.57
1:C:278:LYS:HE3	1:C:287:ASP:HB2	1.87	0.57
1:A:978:ASN:ND2	1:C:547:LYS:O	2.36	0.57
1:B:659:SER:HB3	1:B:698:SER:HB3	1.88	0.56
1:B:762:GLN:OE1	1:B:765:ARG:NH1	2.39	0.56
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.70	0.56
1:B:970:PHE:O	1:B:995:ARG:NH2	2.38	0.55
1:B:78:ARG:NH2	1:B:80:ASP:OD1	2.40	0.55
1:B:126:VAL:HG13	1:B:174:PRO:HA	1.88	0.55
1:C:985:ASP:OD1	1:C:985:ASP:N	2.38	0.54
1:B:821:LEU:HD11	1:B:939:SER:HB2	1.87	0.54
1:B:22:THR:O	1:B:78:ARG:NH1	2.39	0.54
1:C:294:ASP:OD1	1:C:294:ASP:N	2.40	0.54
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.26	0.54
1:A:821:LEU:HD11	1:A:939:SER:HB3	1.90	0.54
2:E:44:SER:HB3	2:E:351:LEU:HD22	1.89	0.54
1:A:294:ASP:OD1	1:A:294:ASP:N	2.40	0.53
1:A:22:THR:O	1:A:78:ARG:NH1	2.41	0.53
1:A:383:SER:HB3	1:A:386:LYS:HG2	1.90	0.53
2:D:288:LYS:HE3	2:D:289:PRO:HD2	1.90	0.53
2:D:261:CYS:HB2	2:D:488:VAL:HB	1.91	0.53
2:D:482:ARG:NH1	2:D:608:THR:O	2.42	0.53
1:C:40:ASP:N	1:C:40:ASP:OD1	2.43	0.52
1:A:856:LYS:HZ2	1:C:570:ALA:HB3	1.73	0.52
1:C:226:LEU:HG	1:C:227:VAL:HG23	1.92	0.52
1:B:1074:ASN:OD1	1:C:895:GLN:NE2	2.42	0.52
1:C:93:ALA:HB3	1:C:266:TYR:HB2	1.92	0.52
2:D:44:SER:HB3	2:D:351:LEU:HD22	1.91	0.52
1:B:383:SER:HB3	1:B:386:LYS:HG2	1.91	0.52
2:D:475:LYS:NZ	2:D:495:GLU:OE1	2.35	0.52
1:A:78:ARG:NH2	1:A:80:ASP:OD1	2.43	0.52
1:A:1086:LYS:HD2	1:A:1122:VAL:HG11	1.92	0.52
1:C:289:VAL:HG13	1:C:297:SER:HB3	1.91	0.52
1:B:599:THR:HB	1:B:608:VAL:HG12	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:THR:OG1	1:C:324:GLU:OE1	2.28	0.51
2:E:288:LYS:HE3	2:E:289:PRO:HD2	1.92	0.51
1:B:294:ASP:N	1:B:294:ASP:OD1	2.42	0.51
1:B:437:ASN:ND2	1:B:506:GLN:OE1	2.44	0.51
1:A:599:THR:HB	1:A:608:VAL:HG12	1.93	0.51
2:D:80:ALA:O	2:D:101:GLN:NE2	2.44	0.51
2:E:80:ALA:O	2:E:101:GLN:NE2	2.43	0.50
1:A:189:LEU:HB3	1:A:208:THR:HB	1.94	0.50
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.94	0.50
2:D:462:MET:HE3	2:D:468:ILE:HD11	1.93	0.50
1:C:858:LEU:HD21	1:C:962:LEU:HD23	1.94	0.50
1:C:656:VAL:HG12	1:C:658:ASN:H	1.77	0.50
2:E:462:MET:HE3	2:E:468:ILE:HD11	1.94	0.49
1:C:127:VAL:HG21	4:C:1302:NAG:H62	1.94	0.49
2:D:152:MET:O	2:D:161:ARG:NH1	2.46	0.49
1:A:97:LYS:HG2	1:A:186:PHE:HD1	1.77	0.49
1:B:193:VAL:HG23	1:B:223:LEU:HD22	1.95	0.49
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	1.94	0.49
1:B:324:GLU:H	1:B:539:VAL:HG12	1.77	0.49
1:B:93:ALA:HB3	1:B:266:TYR:HB2	1.94	0.48
2:D:169:ARG:HH22	2:D:271:TRP:HA	1.77	0.48
1:A:393:THR:HG21	1:A:518:LEU:HB2	1.95	0.48
1:A:125:ASN:HD22	1:A:171:VAL:HG13	1.78	0.48
1:C:78:ARG:NH2	1:C:80:ASP:OD1	2.46	0.48
1:A:289:VAL:HG13	1:A:297:SER:HB3	1.95	0.48
1:A:128:ILE:HD13	1:A:170:TYR:HD2	1.79	0.48
1:A:474:GLN:NE2	1:A:478:LYS:O	2.39	0.48
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.96	0.48
1:A:46:SER:HA	1:A:279:TYR:O	2.13	0.48
1:B:561:PRO:HA	1:B:577:ARG:HH12	1.77	0.48
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.95	0.48
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.78	0.48
1:A:570:ALA:HB1	1:B:963:VAL:HG11	1.96	0.48
2:D:148:LEU:HA	2:D:151:ILE:HG22	1.96	0.48
1:A:142:ASP:HB2	1:A:156:GLU:HB3	1.96	0.48
2:E:261:CYS:HB2	2:E:488:VAL:HB	1.96	0.48
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.96	0.47
1:A:126:VAL:HG23	1:A:174:PRO:HA	1.96	0.47
1:A:139:PRO:HB3	1:A:159:VAL:HG13	1.97	0.47
1:A:1029:MET:HE2	1:A:1029:MET:HB2	1.82	0.47
1:C:659:SER:HB3	1:C:698:SER:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:527:GLU:OE2	2:D:586:ASN:ND2	2.47	0.47
2:E:21:ILE:HD13	2:E:87:GLU:HG3	1.96	0.47
1:B:656:VAL:HG12	1:B:658:ASN:H	1.79	0.47
1:B:36:VAL:HG23	1:B:222:ALA:HA	1.97	0.47
1:C:48:LEU:HB3	1:C:276:LEU:HD11	1.97	0.47
1:C:320:VAL:HG13	1:C:590:CYS:HB3	1.97	0.47
2:E:527:GLU:OE2	2:E:586:ASN:ND2	2.42	0.47
1:A:914:ASN:ND2	1:A:1111:GLU:OE2	2.42	0.46
2:D:457:GLU:HG2	2:D:512:PHE:HB3	1.97	0.46
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.97	0.46
1:A:193:VAL:HB	1:A:204:TYR:HB2	1.97	0.46
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.97	0.46
1:B:189:LEU:HB3	1:B:208:THR:HB	1.98	0.46
1:C:858:LEU:HD23	1:C:959:LEU:HD22	1.98	0.46
2:E:148:LEU:HA	2:E:151:ILE:HG22	1.98	0.46
1:A:978:ASN:HB3	1:C:547:LYS:HB2	1.98	0.46
1:B:97:LYS:HG2	1:B:186:PHE:HD1	1.81	0.46
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.98	0.46
1:C:129:LYS:NZ	1:C:160:TYR:OH	2.49	0.46
1:C:724:THR:HG23	1:C:934:ILE:HD12	1.98	0.46
1:B:1040:VAL:HG21	1:C:1035:GLY:HA3	1.98	0.46
2:E:260:GLY:HA3	2:E:612:PRO:HD3	1.97	0.46
2:E:332:MET:HE2	2:E:332:MET:HB3	1.85	0.46
1:C:38:TYR:HB2	1:C:225:PRO:HD3	1.97	0.46
1:A:1074:ASN:OD1	1:B:895:GLN:NE2	2.43	0.45
1:B:289:VAL:HG13	1:B:297:SER:HB3	1.97	0.45
1:B:1086:LYS:HD2	1:B:1122:VAL:HG11	1.98	0.45
1:C:14:GLN:HB3	1:C:158:ARG:HE	1.81	0.45
1:B:127:VAL:HG22	1:B:171:VAL:HG22	1.97	0.45
1:A:731:MET:HG3	1:A:1018:ILE:HG13	1.96	0.45
1:A:736:VAL:HG11	1:A:1004:LEU:HD11	1.99	0.45
1:A:37:TYR:OH	1:A:54:LEU:O	2.26	0.45
1:A:96:GLU:O	1:A:188:ASN:HB2	2.17	0.45
1:B:52:GLN:OE1	1:B:274:THR:OG1	2.31	0.45
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.99	0.45
1:B:193:VAL:HB	1:B:204:TYR:HB2	1.98	0.45
2:E:381:TYR:HD1	2:E:558:LEU:HG	1.82	0.45
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.98	0.45
1:B:736:VAL:HG11	1:B:1004:LEU:HD11	1.98	0.45
1:C:192:PHE:HA	1:C:204:TYR:O	2.17	0.45
2:E:152:MET:O	2:E:161:ARG:NH1	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:CD2	1:B:528:LYS:HB3	2.52	0.45
1:C:21:ARG:NH2	1:C:138:ASP:OD2	2.43	0.45
2:D:479:GLU:HA	2:D:482:ARG:HD2	1.99	0.45
1:A:358:ILE:HB	1:A:395:VAL:HB	1.99	0.44
1:B:756:TYR:OH	1:B:994:ASP:OD1	2.27	0.44
1:C:128:ILE:HD13	1:C:170:TYR:HD2	1.82	0.44
2:E:535:HIS:NE2	2:E:538:PRO:O	2.49	0.44
1:C:599:THR:HB	1:C:608:VAL:HG12	1.98	0.44
1:A:659:SER:HB3	1:A:698:SER:HB3	1.99	0.44
1:A:934:ILE:HD13	1:A:934:ILE:HA	1.84	0.44
1:B:191:GLU:O	1:B:205:SER:HA	2.17	0.44
2:D:168:TRP:HE1	2:D:502:SER:HB2	1.83	0.44
1:A:656:VAL:HG12	1:A:658:ASN:H	1.83	0.44
1:B:127:VAL:HG21	4:B:1302:NAG:H62	2.00	0.44
2:D:332:MET:HE2	2:D:332:MET:HB3	1.87	0.44
1:B:358:ILE:HB	1:B:395:VAL:HB	2.00	0.44
1:C:89:GLY:HA3	1:C:270:LEU:HD12	2.00	0.44
1:C:916:LEU:HD22	1:C:923:ILE:HD13	2.00	0.44
2:D:524:GLN:HB3	2:D:574:VAL:HG11	2.00	0.44
1:B:192:PHE:HA	1:B:204:TYR:O	2.18	0.44
1:C:229:LEU:HG	1:C:231:ILE:HG23	2.00	0.44
1:B:125:ASN:HD22	1:B:171:VAL:HG13	1.82	0.44
1:B:736:VAL:HG22	1:B:858:LEU:HD23	2.00	0.44
1:A:40:ASP:OD1	1:A:40:ASP:N	2.51	0.43
1:B:310:LYS:HG3	1:B:600:PRO:HA	2.00	0.43
1:C:756:TYR:OH	1:C:994:ASP:OD1	2.34	0.43
2:D:230:PHE:HA	2:D:233:ILE:HB	2.00	0.43
2:E:574:VAL:HG23	2:E:576:ALA:H	1.82	0.43
1:B:39:PRO:HG3	1:B:55:PHE:HZ	1.83	0.43
1:C:612:TYR:O	1:C:648:GLY:HA3	2.18	0.43
1:A:128:ILE:HG21	1:A:229:LEU:HD13	2.01	0.43
1:B:731:MET:HG3	1:B:1018:ILE:HG13	2.00	0.43
2:E:307:ILE:HG23	2:E:369:PHE:HD1	1.83	0.43
1:A:278:LYS:HE3	1:A:278:LYS:HB2	1.85	0.43
1:A:374:PHE:HA	1:A:436:TRP:HB3	2.01	0.43
1:A:412:PRO:HB3	1:A:427:ASP:HA	2.01	0.43
1:A:790:LYS:HB3	1:A:790:LYS:HE2	1.75	0.43
1:A:48:LEU:HB3	1:A:276:LEU:HD11	1.99	0.43
1:B:996:LEU:HD23	1:B:996:LEU:HA	1.93	0.43
1:C:34:ARG:NH2	1:C:221:SER:OG	2.51	0.43
1:C:532:ASN:OD1	1:C:533:LEU:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:168:TRP:CD1	2:E:270:MET:HE2	2.54	0.43
2:E:326:GLY:O	2:E:330:ASN:ND2	2.51	0.43
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.83	0.42
2:D:97:LEU:HD23	2:D:97:LEU:HA	1.89	0.42
2:E:582:ARG:HH12	2:E:585:LEU:HB2	1.84	0.42
1:A:707:TYR:HB3	1:B:792:PRO:HG3	2.00	0.42
2:D:260:GLY:HA3	2:D:612:PRO:HD3	2.01	0.42
2:E:460:ARG:HA	2:E:463:VAL:HG12	2.02	0.42
1:B:612:TYR:O	1:B:648:GLY:HA3	2.19	0.42
1:C:1048:HIS:HA	1:C:1066:THR:HG22	2.01	0.42
2:E:458:LYS:HD2	2:E:462:MET:HE2	2.01	0.42
1:A:354:ASN:O	1:A:398:ASP:HA	2.19	0.42
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.85	0.42
1:C:97:LYS:HG2	1:C:186:PHE:HD1	1.84	0.42
1:B:724:THR:HG23	1:B:934:ILE:HD12	2.01	0.42
2:D:574:VAL:HG23	2:D:576:ALA:H	1.85	0.42
1:A:903:ALA:HB2	1:A:916:LEU:HD12	2.01	0.42
1:B:201:PHE:HB3	1:B:229:LEU:HB2	2.02	0.42
2:D:458:LYS:HD2	2:D:462:MET:HE2	2.02	0.42
2:D:460:ARG:HD3	2:D:506:VAL:HG23	2.02	0.42
1:B:934:ILE:HD13	1:B:934:ILE:HA	1.83	0.42
2:D:381:TYR:HD1	2:D:558:LEU:HG	1.84	0.42
2:E:457:GLU:HG2	2:E:512:PHE:HB3	2.02	0.42
1:A:487:ASN:OD1	2:D:83:TYR:OH	2.37	0.42
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.02	0.42
1:C:68:ILE:HG22	1:C:78:ARG:HB2	2.02	0.42
2:E:460:ARG:HD3	2:E:506:VAL:HG23	2.02	0.42
2:D:557:MET:HE3	2:D:557:MET:HB3	1.89	0.42
2:E:482:ARG:NH1	2:E:608:THR:O	2.53	0.42
1:A:80:ASP:O	1:A:265:TYR:OH	2.33	0.41
1:A:93:ALA:HB3	1:A:266:TYR:HB2	2.02	0.41
1:B:46:SER:CA	1:B:279:TYR:O	2.65	0.41
2:D:178:PRO:HA	2:D:181:GLU:HB2	2.02	0.41
2:D:528:ALA:HB2	2:D:574:VAL:HG12	2.01	0.41
1:B:322:PRO:HG3	1:B:549:THR:HG21	2.02	0.41
1:C:27:ALA:HB3	1:C:64:TRP:HB3	2.02	0.41
2:D:524:GLN:HE21	2:D:574:VAL:HG21	1.86	0.41
2:D:535:HIS:NE2	2:D:538:PRO:O	2.52	0.41
1:A:907:ASN:HD22	1:C:1107:ARG:HH22	1.68	0.41
2:D:326:GLY:O	2:D:330:ASN:ND2	2.53	0.41
2:E:528:ALA:HB2	2:E:574:VAL:HG12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:VAL:HA	1:A:1064:HIS:O	2.20	0.41
1:C:996:LEU:HD23	1:C:996:LEU:HA	1.91	0.41
2:E:162:LEU:HD13	2:E:265:HIS:CE1	2.55	0.41
2:E:217:TYR:OH	2:E:225:ASP:OD2	2.31	0.41
1:C:48:LEU:HD21	1:C:306:PHE:HD1	1.86	0.41
1:C:717:ASN:ND2	1:C:1071:GLN:OE1	2.54	0.41
1:B:411:ALA:HB3	1:B:414:GLN:HG3	2.01	0.41
2:D:460:ARG:HA	2:D:463:VAL:HG12	2.02	0.41
2:E:230:PHE:HA	2:E:233:ILE:HB	2.01	0.41
1:B:903:ALA:HB2	1:B:916:LEU:HD12	2.02	0.41
2:E:144:LEU:HA	2:E:148:LEU:HB2	2.02	0.41
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.48	0.41
1:A:1035:GLY:HA3	1:C:1040:VAL:HG21	2.02	0.41
1:B:37:TYR:OH	1:B:54:LEU:O	2.29	0.41
1:B:48:LEU:HB3	1:B:276:LEU:HD11	2.01	0.41
1:C:736:VAL:HG11	1:C:1004:LEU:HD11	2.03	0.41
1:C:913:GLN:H	1:C:913:GLN:HG2	1.64	0.41
1:C:1086:LYS:HB2	1:C:1086:LYS:HE2	1.90	0.41
2:D:529:LEU:HD11	2:D:554:LEU:HD22	2.03	0.41
2:E:156:LEU:HD11	2:E:281:LEU:HD21	2.02	0.41
1:B:1086:LYS:HB2	1:B:1086:LYS:HE2	1.87	0.41
1:C:52:GLN:HB2	1:C:274:THR:HG22	2.03	0.41
1:A:192:PHE:HA	1:A:204:TYR:O	2.21	0.40
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.96	0.40
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.42	0.40
1:A:895:GLN:NE2	1:C:1074:ASN:OD1	2.46	0.40
1:B:722:VAL:HA	1:B:1064:HIS:O	2.21	0.40
1:B:866:THR:H	1:B:869:MET:HE3	1.86	0.40
2:D:156:LEU:HD11	2:D:281:LEU:HD21	2.03	0.40
2:D:252:TYR:HA	2:D:253:PRO:HD3	1.96	0.40
2:E:183:TYR:OH	2:E:509:ASP:OD1	2.34	0.40
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.85	0.40
1:C:776:LYS:NZ	1:C:780:GLU:OE2	2.54	0.40
2:D:168:TRP:CD1	2:D:270:MET:HE2	2.56	0.40
2:E:524:GLN:HE21	2:E:574:VAL:HG21	1.85	0.40
1:A:724:THR:HG23	1:A:934:ILE:HD12	2.02	0.40
1:B:141:LEU:HD22	1:B:157:PHE:CD1	2.56	0.40
2:E:178:PRO:HA	2:E:181:GLU:HB2	2.04	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	1014/1285 (79%)	993 (98%)	21 (2%)	0	100	100
1	B	1014/1285 (79%)	992 (98%)	21 (2%)	1 (0%)	48	61
1	C	813/1285 (63%)	801 (98%)	12 (2%)	0	100	100
2	D	593/606 (98%)	577 (97%)	16 (3%)	0	100	100
2	E	593/606 (98%)	577 (97%)	16 (3%)	0	100	100
All	All	4027/5067 (80%)	3940 (98%)	86 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	337	PRO

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	907/1116 (81%)	907 (100%)	0	100	100
1	B	907/1116 (81%)	907 (100%)	0	100	100
1	C	733/1116 (66%)	732 (100%)	1 (0%)	88	93
2	D	526/536 (98%)	526 (100%)	0	100	100
2	E	526/536 (98%)	526 (100%)	0	100	100
All	All	3599/4420 (81%)	3598 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	913	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	ASN
1	A	536	ASN
1	A	542	ASN
1	A	607	GLN
1	A	779	GLN
1	A	824	ASN
1	A	872	GLN
1	A	907	ASN
1	A	992	GLN
1	B	14	GLN
1	B	245	HIS
1	B	317	ASN
1	B	544	ASN
1	B	607	GLN
1	B	824	ASN
1	B	955	ASN
1	B	992	GLN
1	B	1011	GLN
1	C	121	ASN
1	C	239	GLN
1	C	314	GLN
1	C	824	ASN
1	C	907	ASN
1	C	913	GLN
1	C	1011	GLN
2	D	89	GLN
2	D	154	ASN
2	D	175	GLN
2	D	239	HIS
2	D	250	ASN
2	D	325	GLN
2	D	417	HIS
2	D	472	GLN
2	D	599	ASN
2	E	24	GLN
2	E	89	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	154	ASN
2	E	325	GLN
2	E	330	ASN
2	E	417	HIS
2	E	472	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	F	1	1,3	14,14,15	0.74	0	17,19,21	0.67	1 (5%)
3	NAG	F	2	3	14,14,15	0.34	0	17,19,21	0.41	0
3	NAG	G	1	1,3	14,14,15	0.32	0	17,19,21	0.62	1 (5%)
3	NAG	G	2	3	14,14,15	0.34	0	17,19,21	0.50	0
3	NAG	H	1	1,3	14,14,15	0.51	0	17,19,21	1.16	2 (11%)
3	NAG	H	2	3	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	I	1	1,3	14,14,15	0.22	0	17,19,21	0.52	0
3	NAG	I	2	3	14,14,15	0.28	0	17,19,21	0.48	0
3	NAG	J	1	1,3	14,14,15	0.27	0	17,19,21	0.57	0
3	NAG	J	2	3	14,14,15	0.36	0	17,19,21	0.41	0
3	NAG	K	1	1,3	14,14,15	0.29	0	17,19,21	0.59	0
3	NAG	K	2	3	14,14,15	0.37	0	17,19,21	0.54	0
3	NAG	L	1	1,3	14,14,15	0.59	0	17,19,21	0.62	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	L	2	3	14,14,15	0.43	0	17,19,21	0.76	1 (5%)
3	NAG	M	1	1,3	14,14,15	0.33	0	17,19,21	0.66	1 (5%)
3	NAG	M	2	3	14,14,15	0.28	0	17,19,21	0.45	0
3	NAG	N	1	1,3	14,14,15	0.47	0	17,19,21	1.09	2 (11%)
3	NAG	N	2	3	14,14,15	0.36	0	17,19,21	0.50	0
3	NAG	O	1	1,3	14,14,15	0.21	0	17,19,21	0.56	0
3	NAG	O	2	3	14,14,15	0.31	0	17,19,21	0.44	0
3	NAG	P	1	1,3	14,14,15	0.33	0	17,19,21	0.53	0
3	NAG	P	2	3	14,14,15	0.34	0	17,19,21	0.40	0
3	NAG	Q	1	1,3	14,14,15	0.41	0	17,19,21	0.67	1 (5%)
3	NAG	Q	2	3	14,14,15	0.45	0	17,19,21	0.47	0
3	NAG	R	1	1,3	14,14,15	0.55	0	17,19,21	0.60	0
3	NAG	R	2	3	14,14,15	0.40	0	17,19,21	0.52	0
3	NAG	S	1	1,3	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
3	NAG	S	2	3	14,14,15	0.38	0	17,19,21	0.47	0
3	NAG	T	1	1,3	14,14,15	0.42	0	17,19,21	1.11	2 (11%)
3	NAG	T	2	3	14,14,15	0.39	0	17,19,21	0.60	0
3	NAG	U	1	1,3	14,14,15	0.24	0	17,19,21	0.55	0
3	NAG	U	2	3	14,14,15	0.34	0	17,19,21	0.46	0
3	NAG	V	1	1,3	14,14,15	0.28	0	17,19,21	0.58	0
3	NAG	V	2	3	14,14,15	0.35	0	17,19,21	0.44	0
3	NAG	W	1	1,3	14,14,15	0.24	0	17,19,21	0.53	0
3	NAG	W	2	3	14,14,15	0.42	0	17,19,21	0.47	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
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	1/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1	NAG	C2-N2-C7	3.23	127.22	122.90
3	N	1	NAG	C2-N2-C7	3.19	127.18	122.90
3	H	1	NAG	C2-N2-C7	3.19	127.17	122.90
3	L	2	NAG	C1-O5-C5	2.90	116.07	112.19
3	H	1	NAG	C1-O5-C5	2.60	115.66	112.19
3	F	1	NAG	C1-O5-C5	2.32	115.30	112.19
3	Q	1	NAG	C1-O5-C5	2.29	115.25	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1	NAG	C1-O5-C5	2.28	115.24	112.19
3	T	1	NAG	C1-O5-C5	2.21	115.15	112.19
3	S	1	NAG	C1-O5-C5	2.12	115.02	112.19
3	G	1	NAG	C1-O5-C5	2.10	115.00	112.19
3	N	1	NAG	C1-O5-C5	2.09	114.99	112.19
3	L	1	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6

Continued on next page...

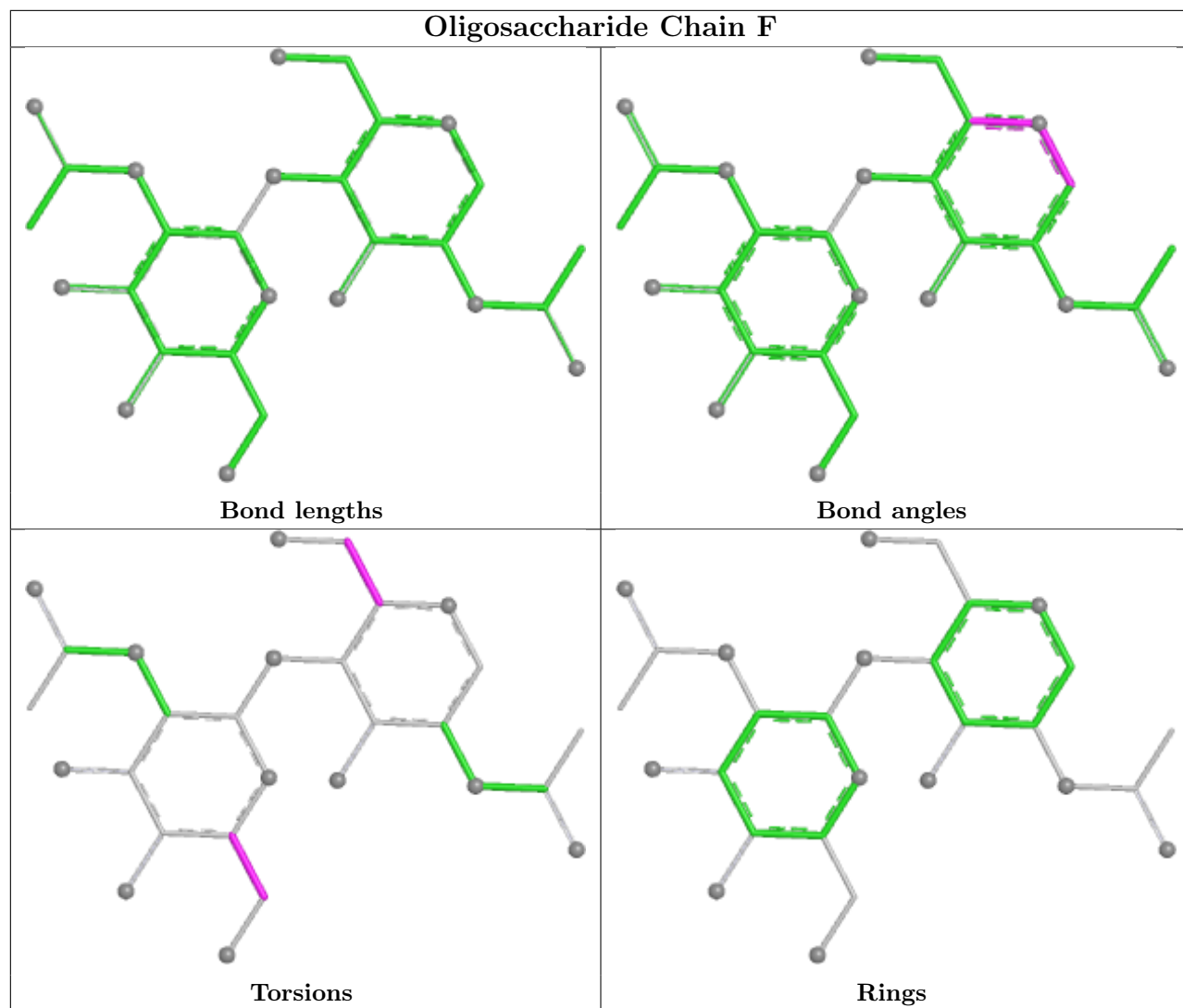
Continued from previous page...

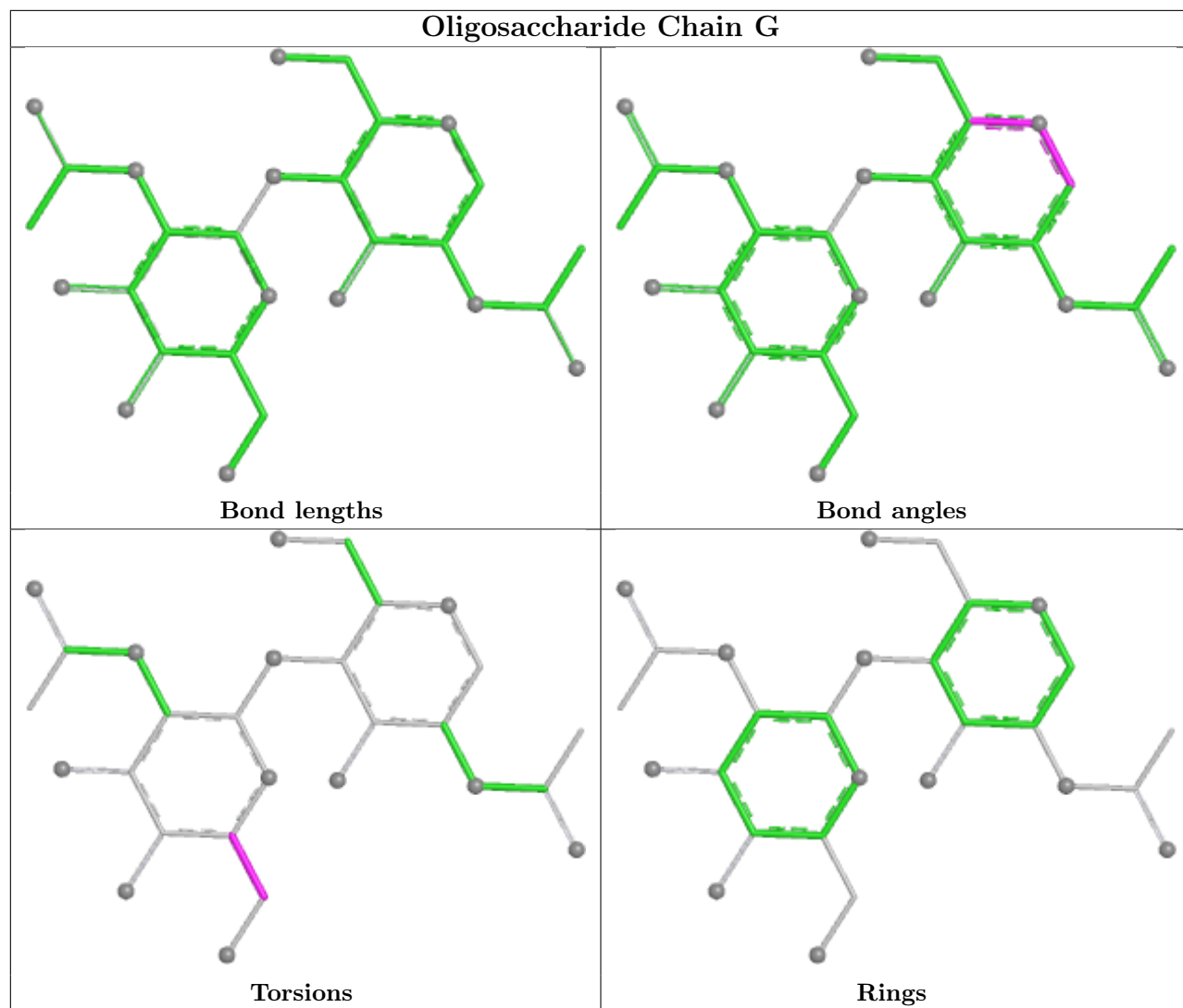
Mol	Chain	Res	Type	Atoms
3	S	1	NAG	C4-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C1-C2-N2-C7
3	N	1	NAG	C1-C2-N2-C7
3	T	1	NAG	C1-C2-N2-C7
3	H	1	NAG	C3-C2-N2-C7
3	N	1	NAG	C3-C2-N2-C7
3	T	1	NAG	C3-C2-N2-C7
3	V	2	NAG	O5-C5-C6-O6

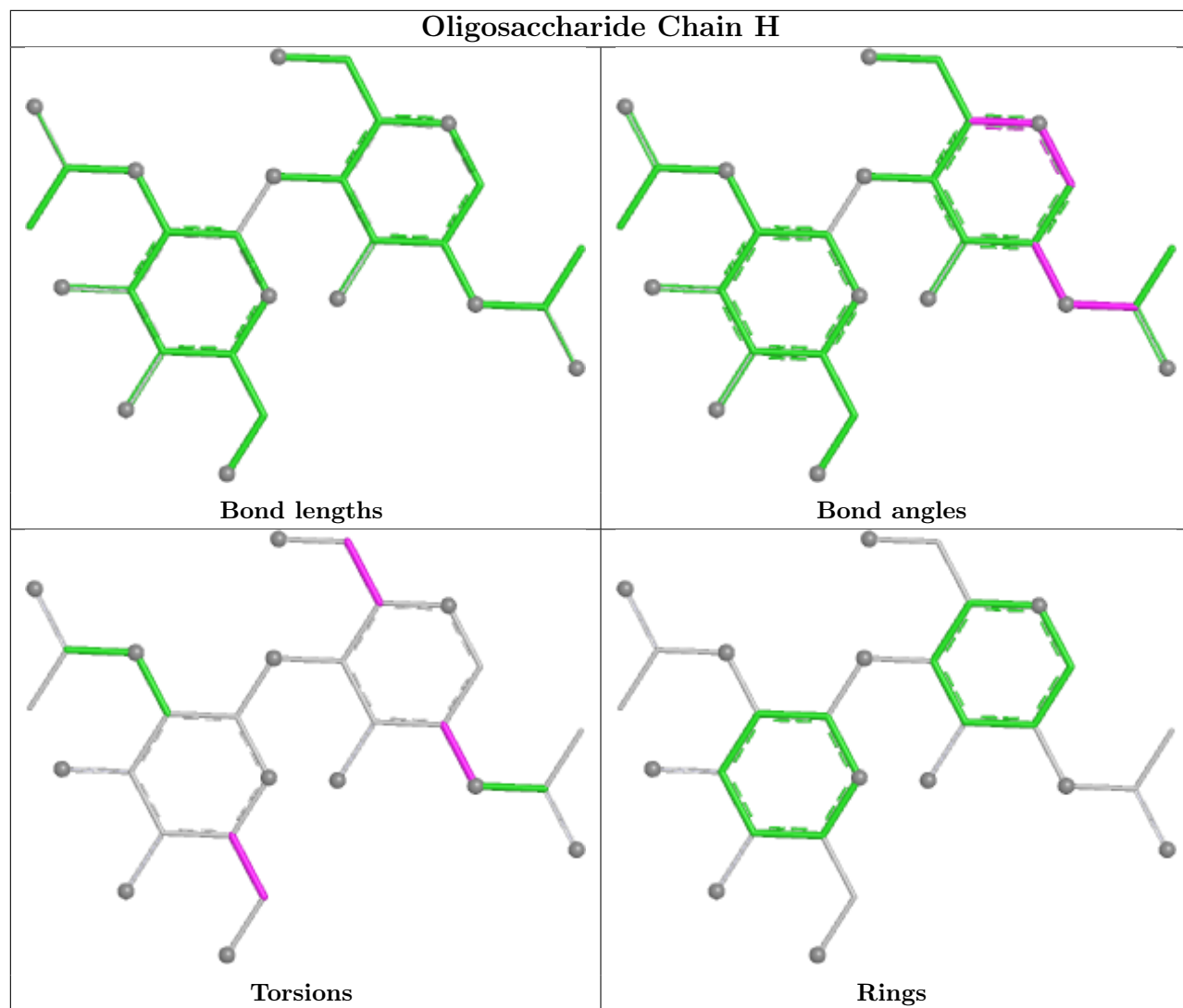
There are no ring outliers.

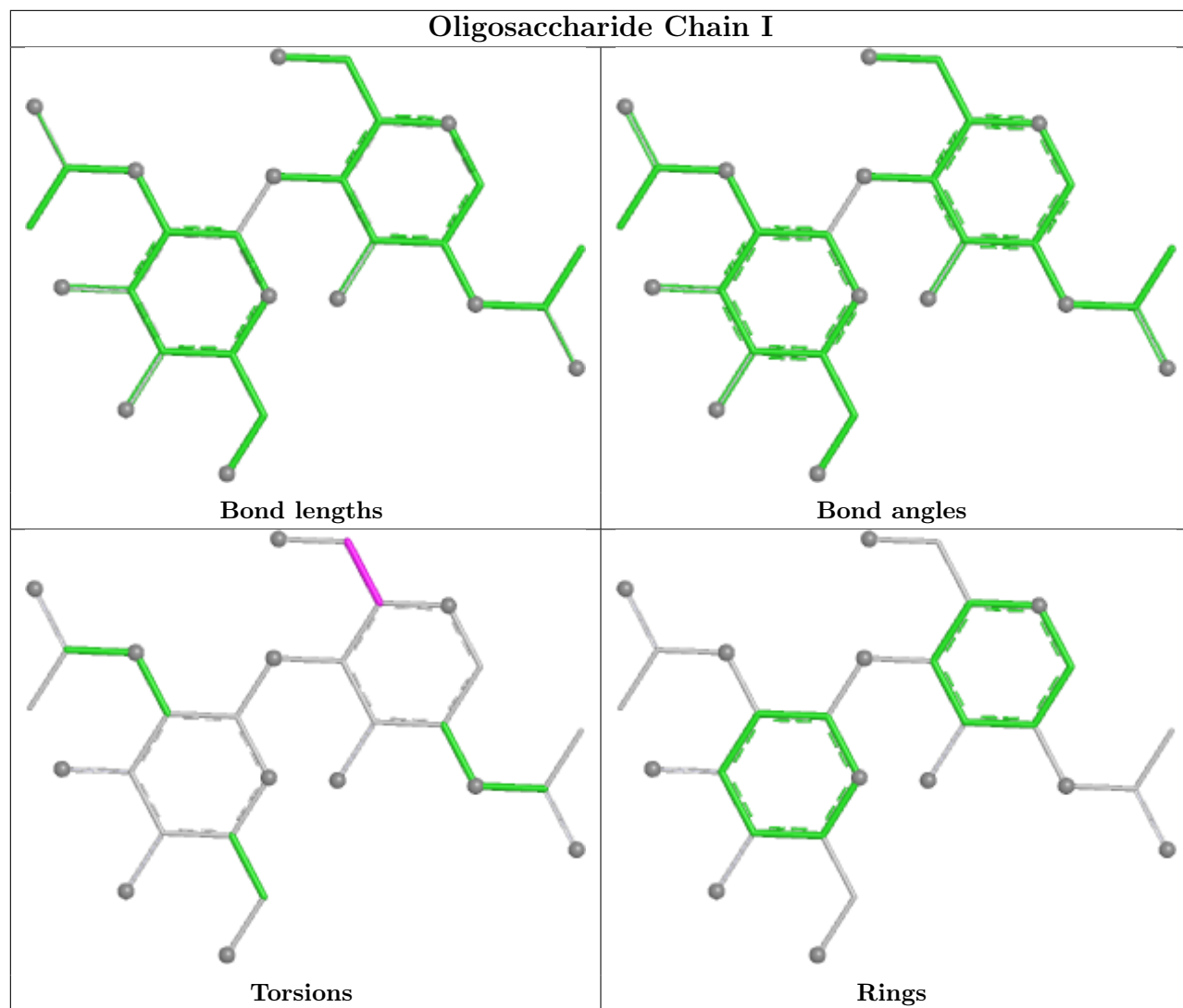
No monomer is involved in short contacts.

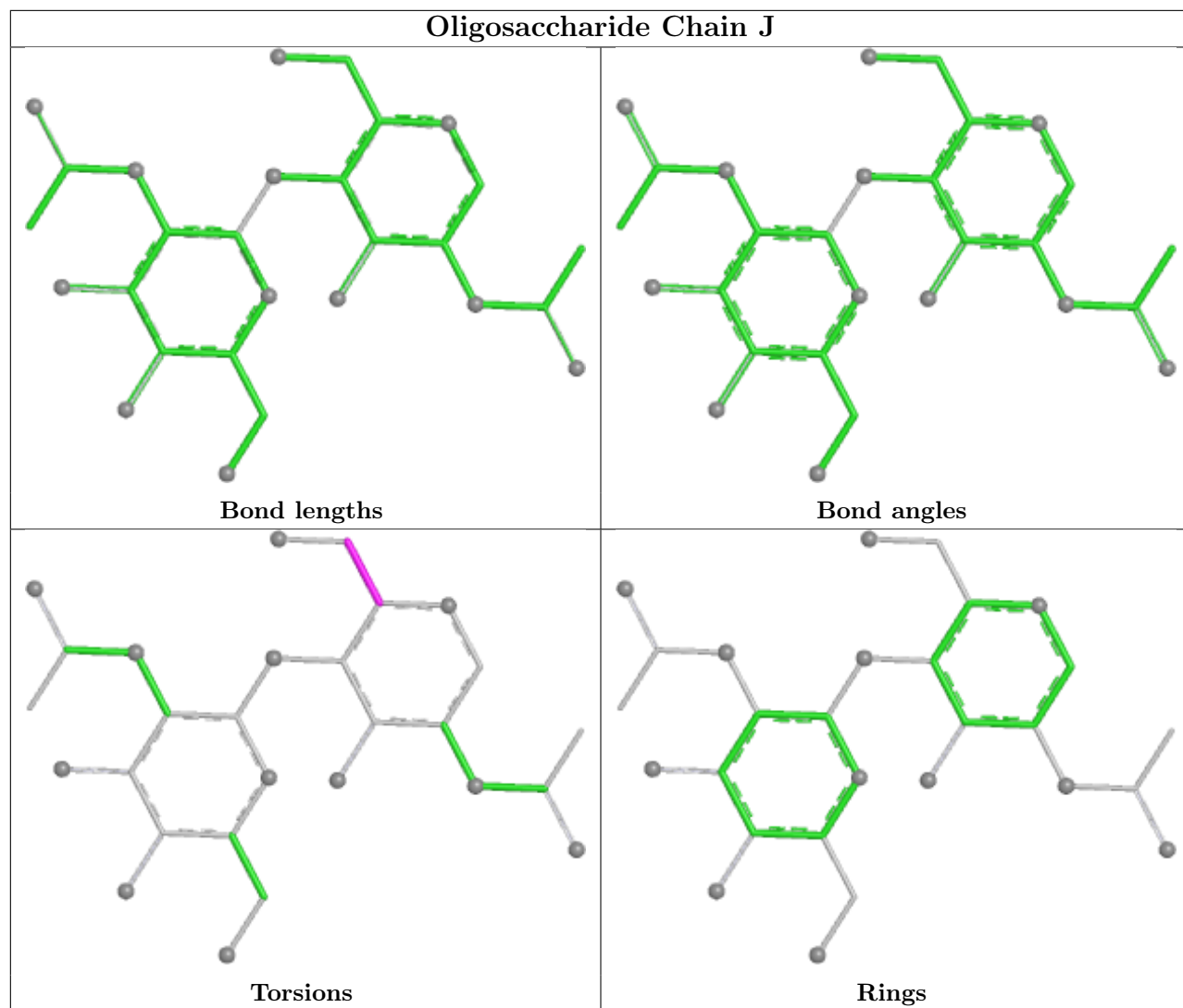
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

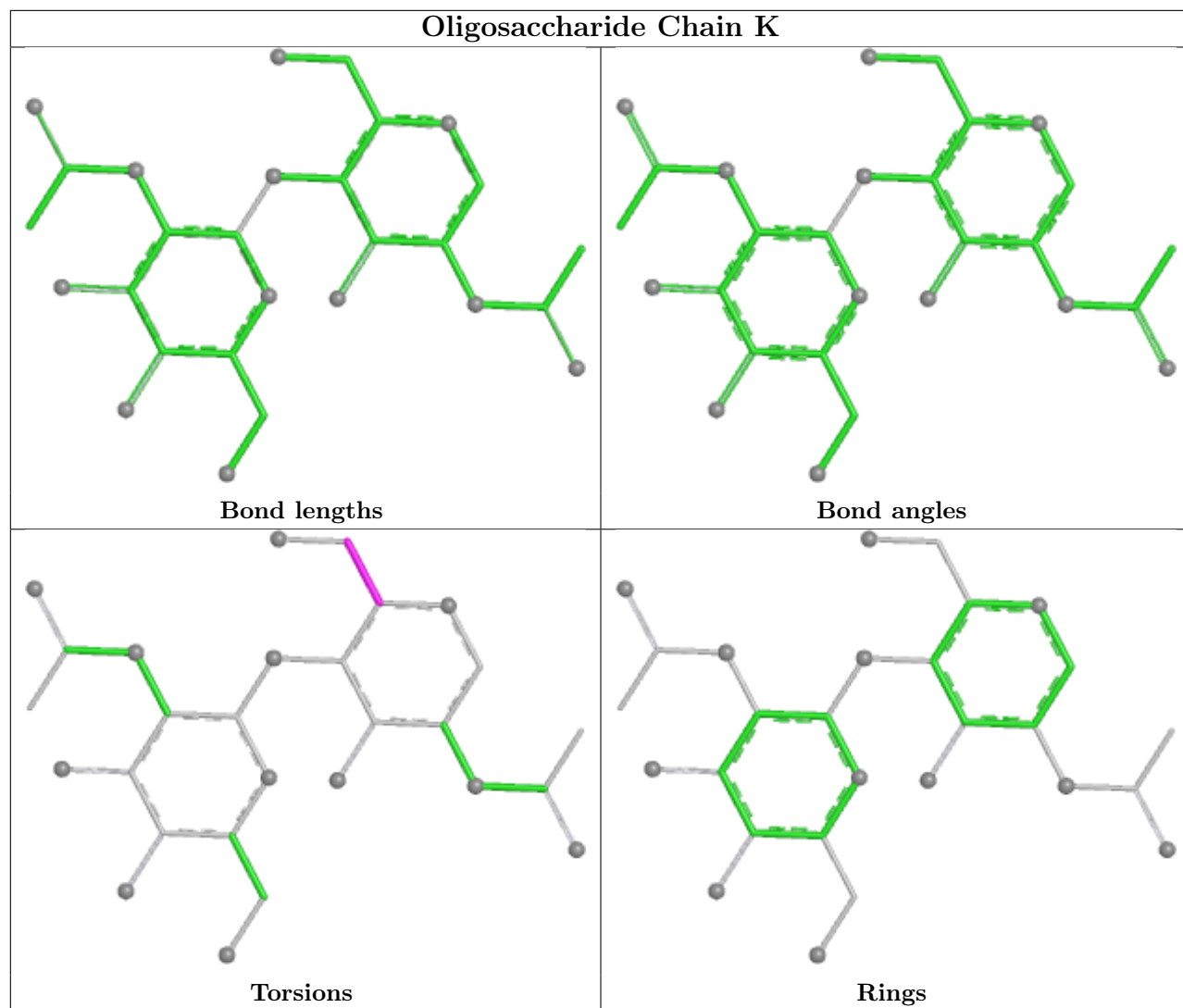


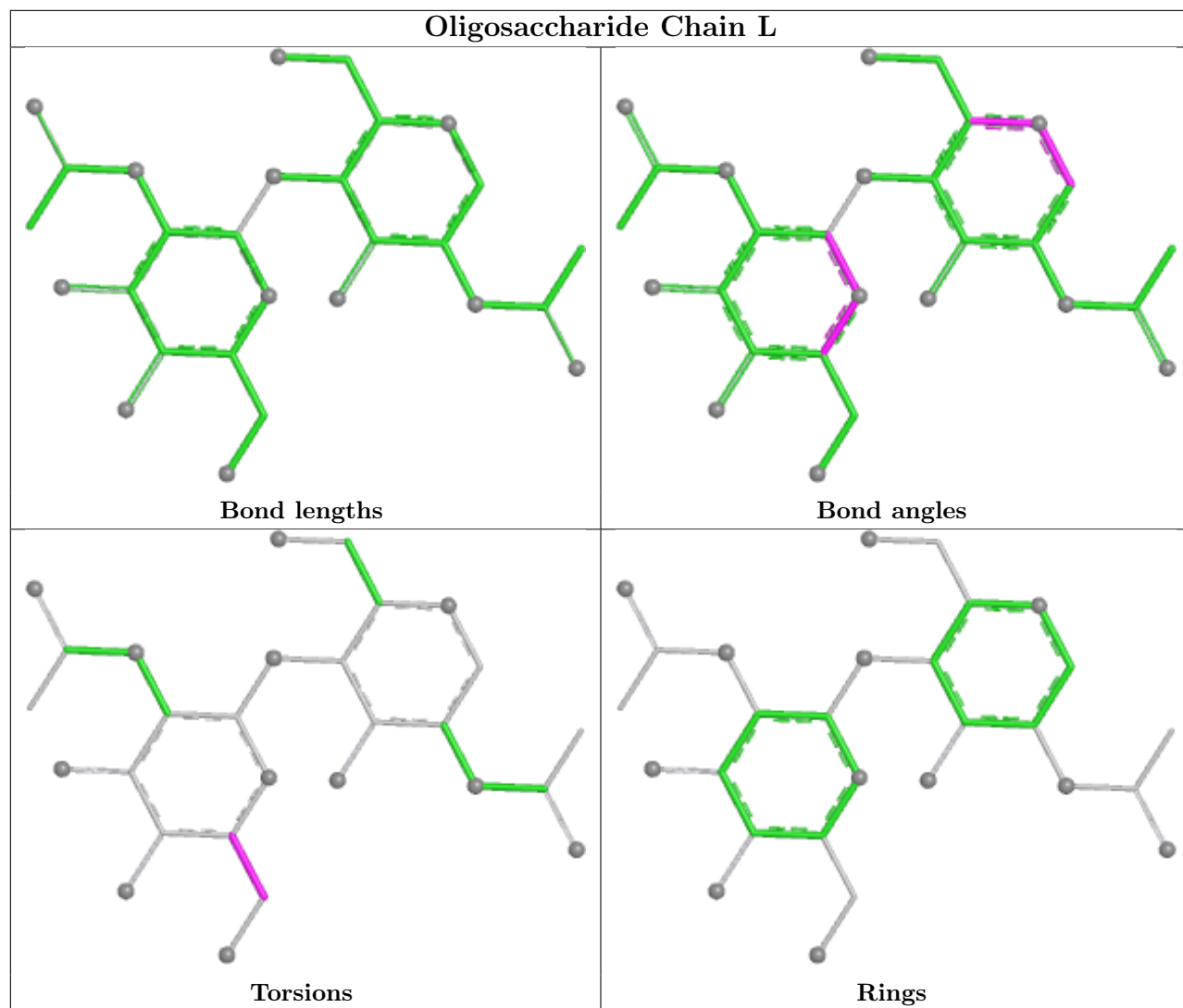


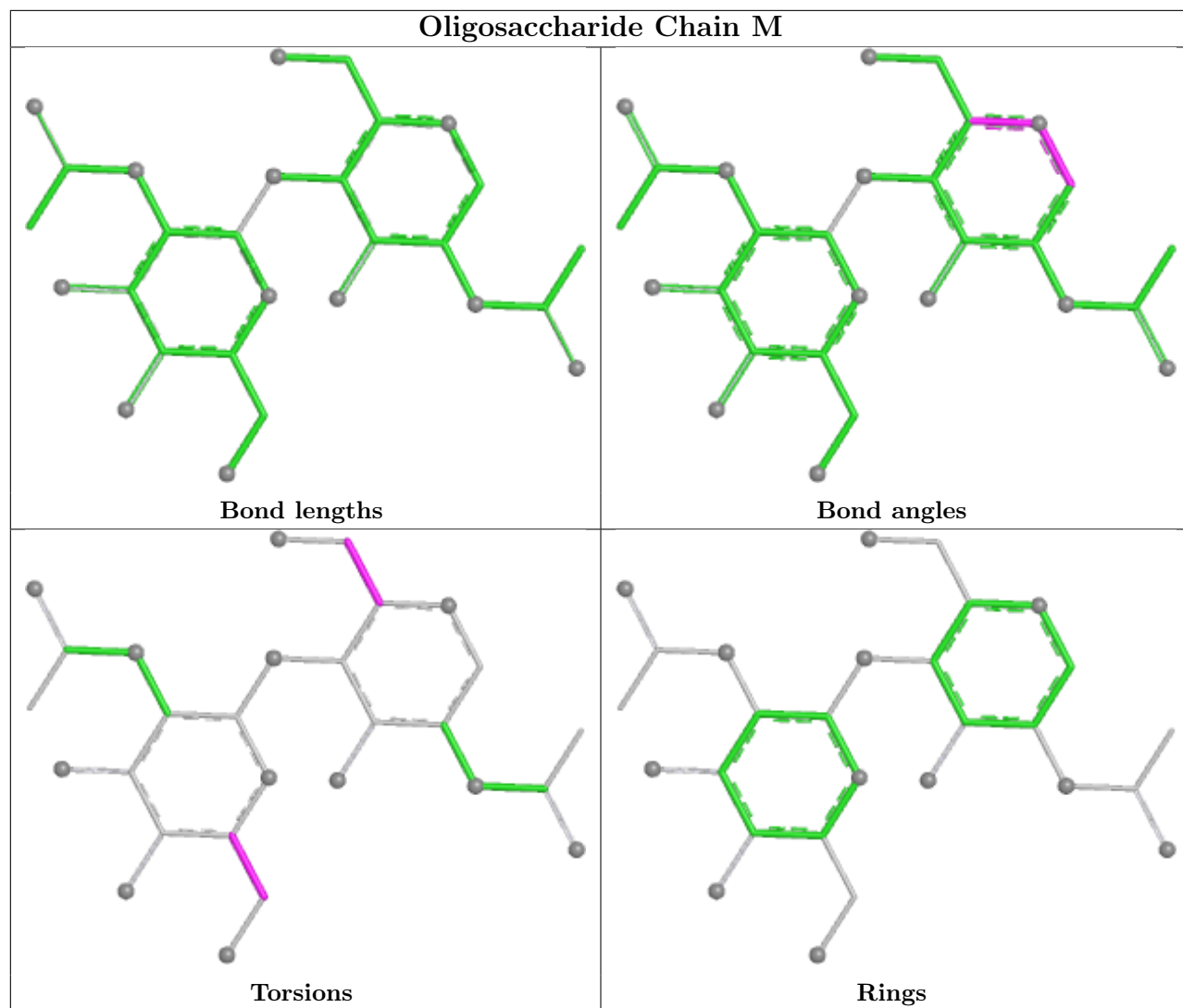


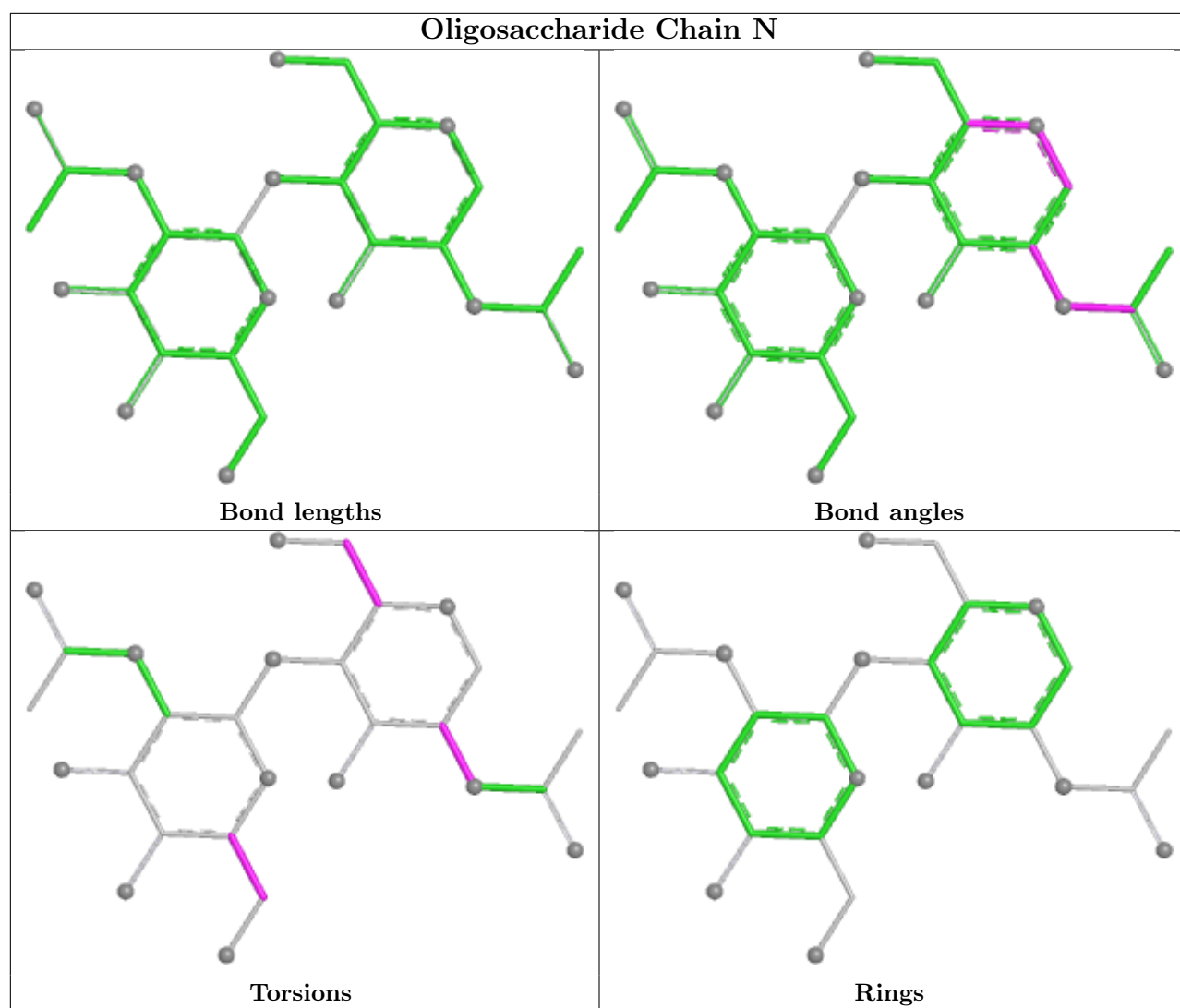


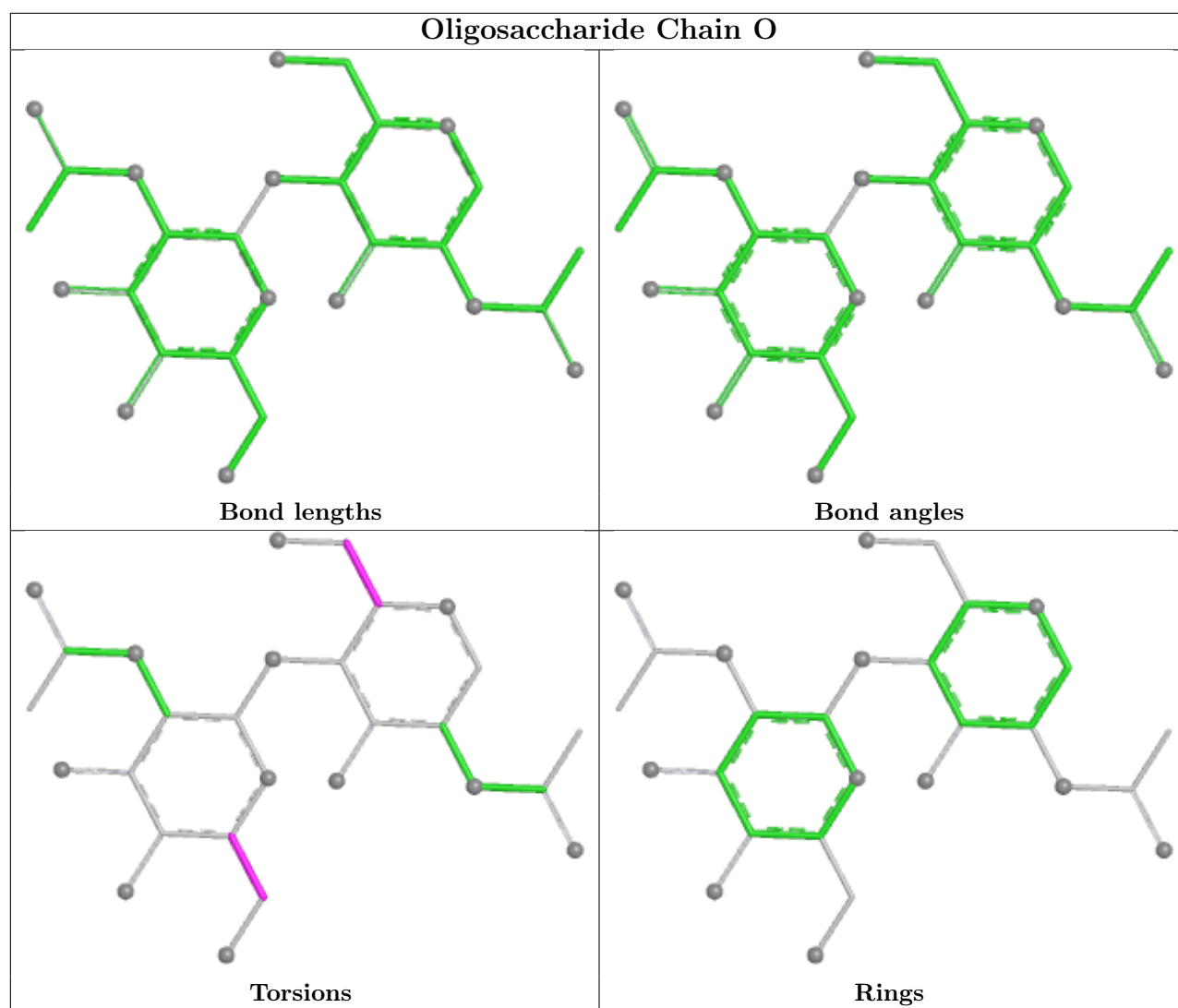


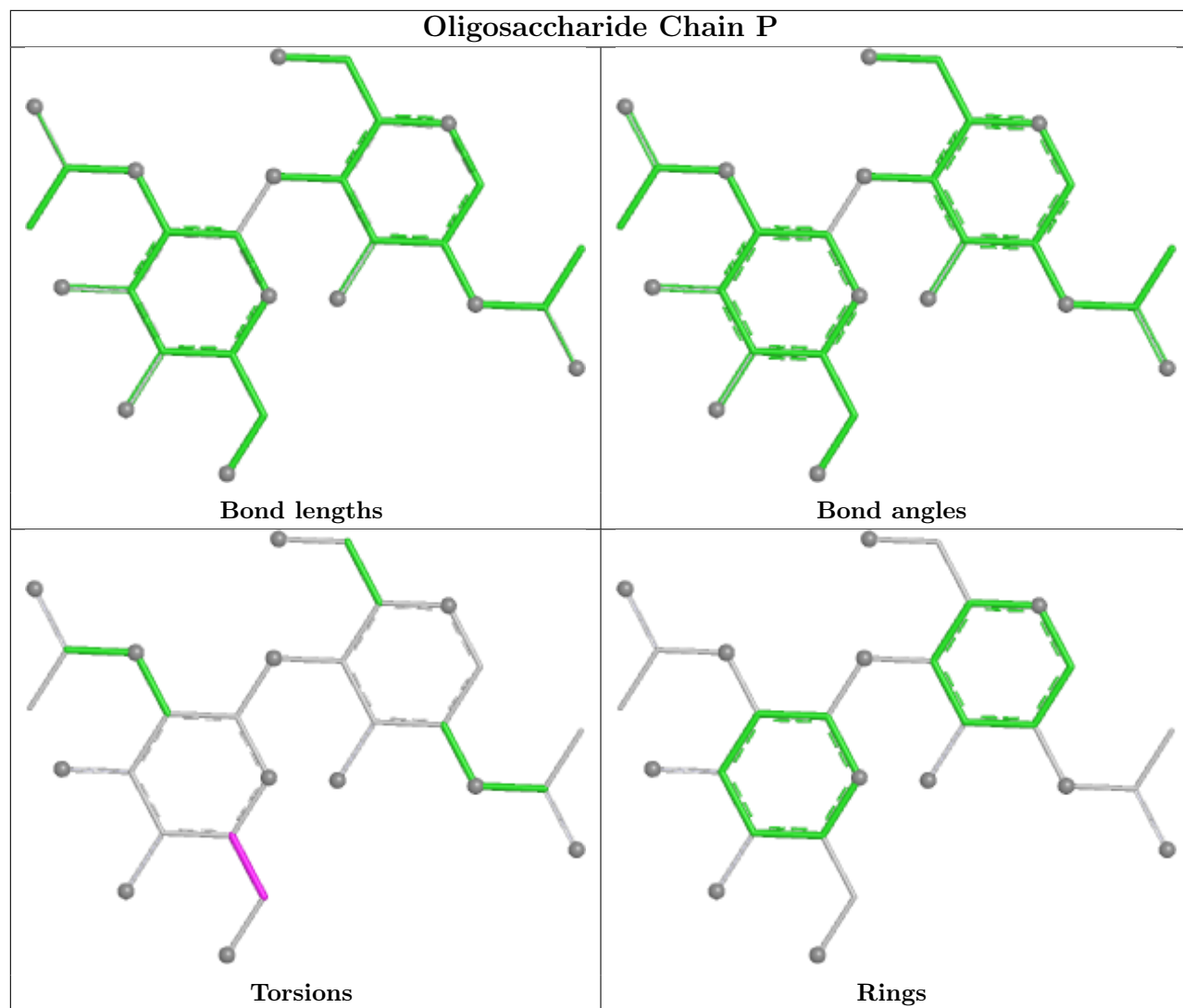


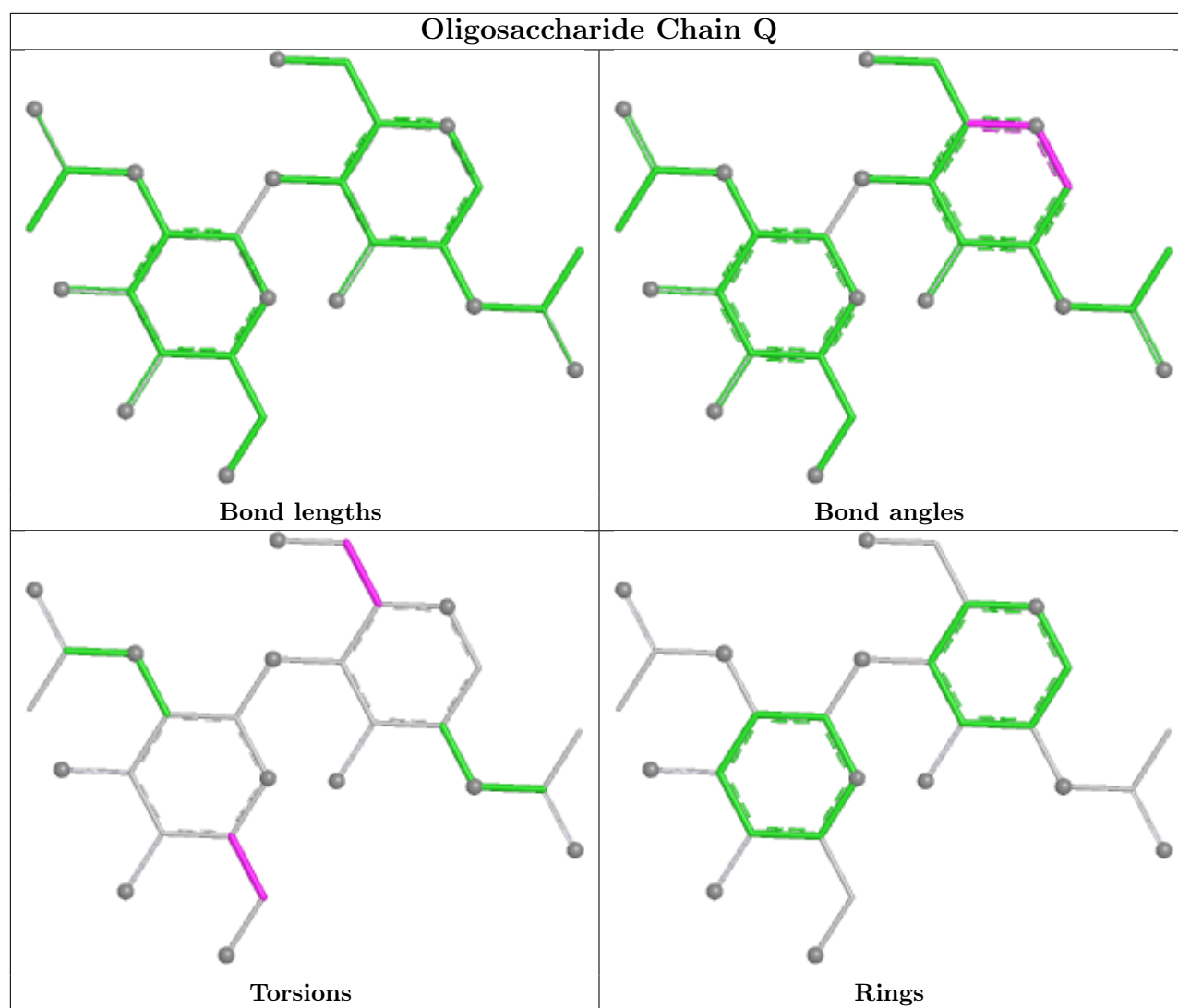


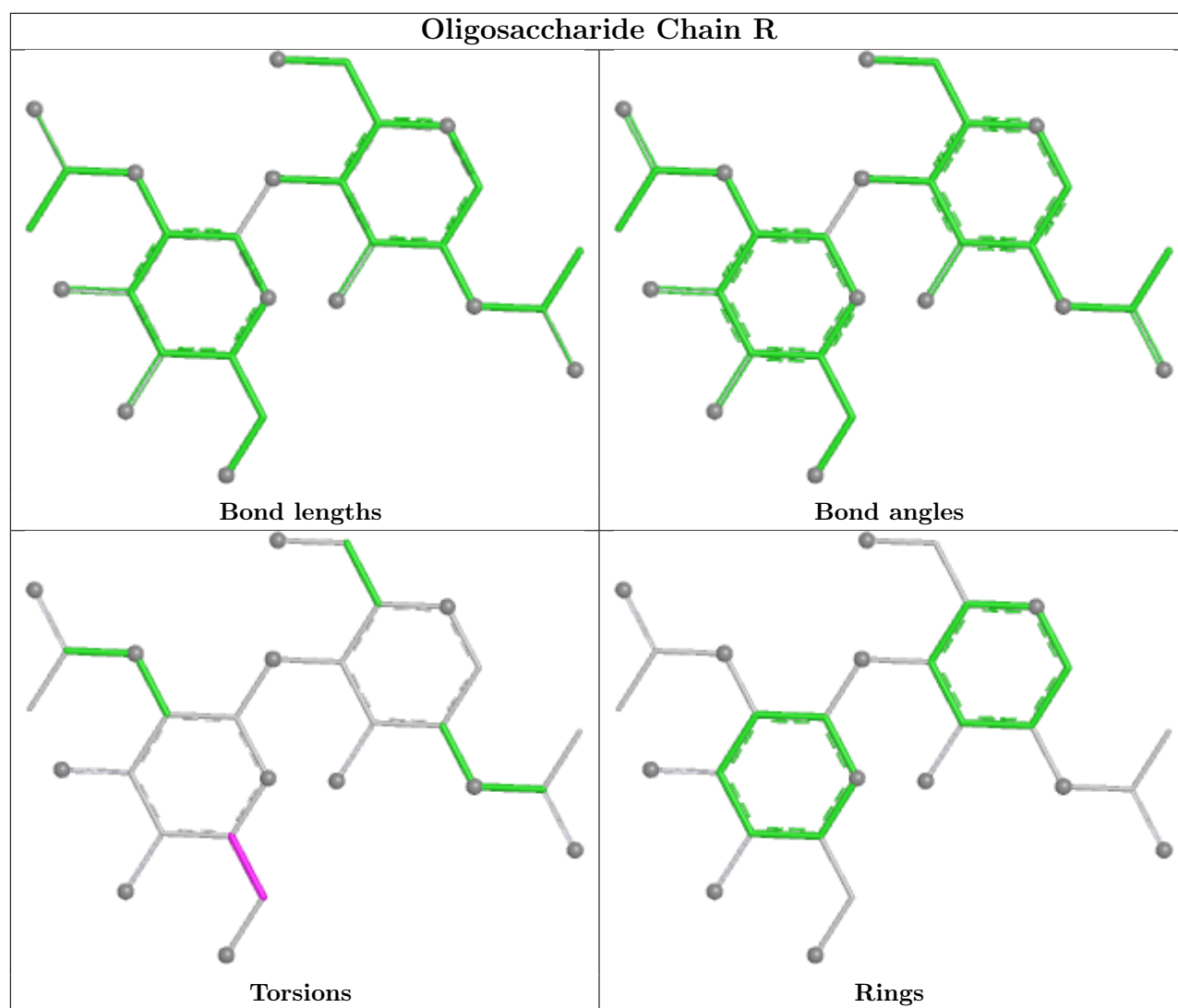


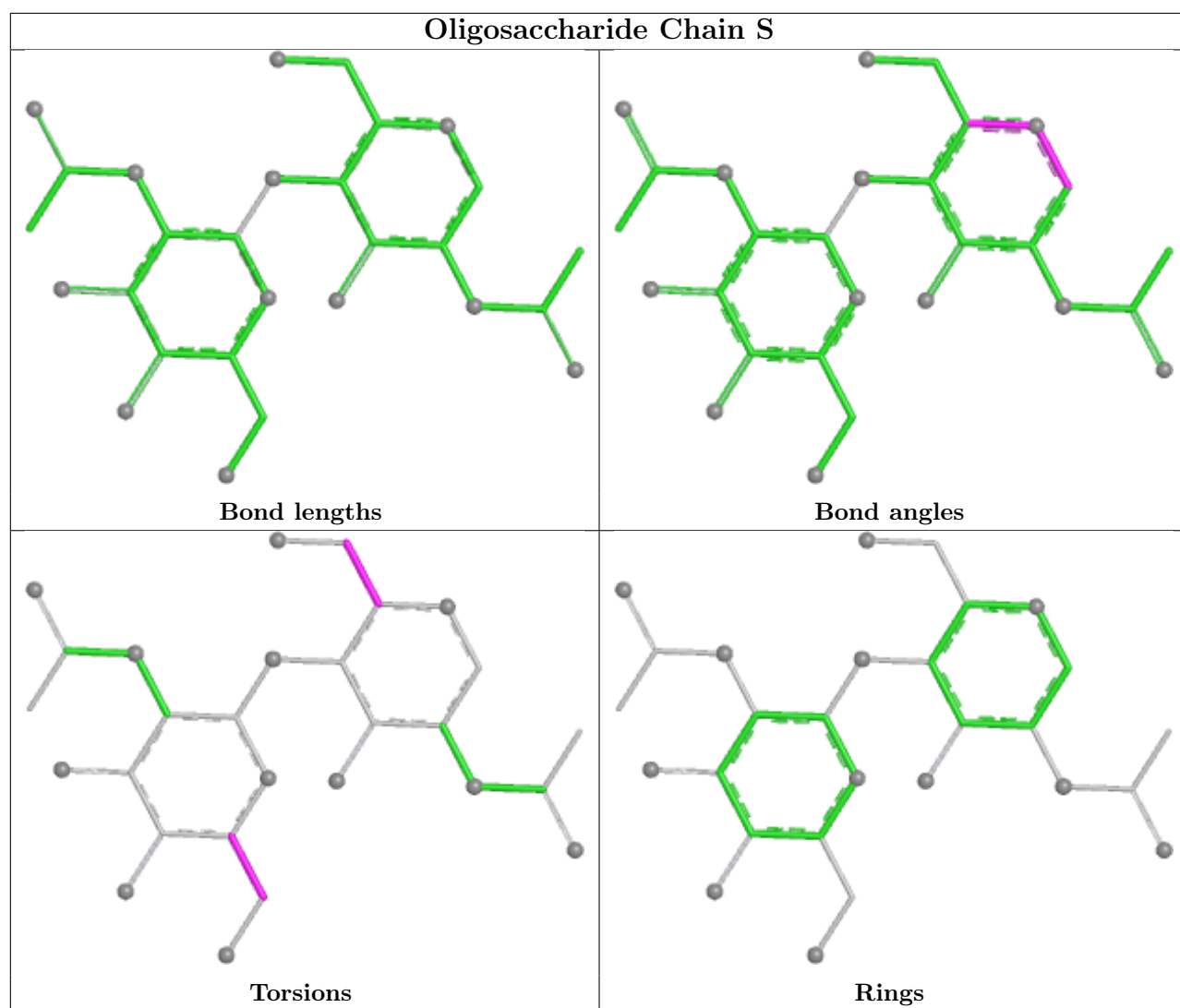


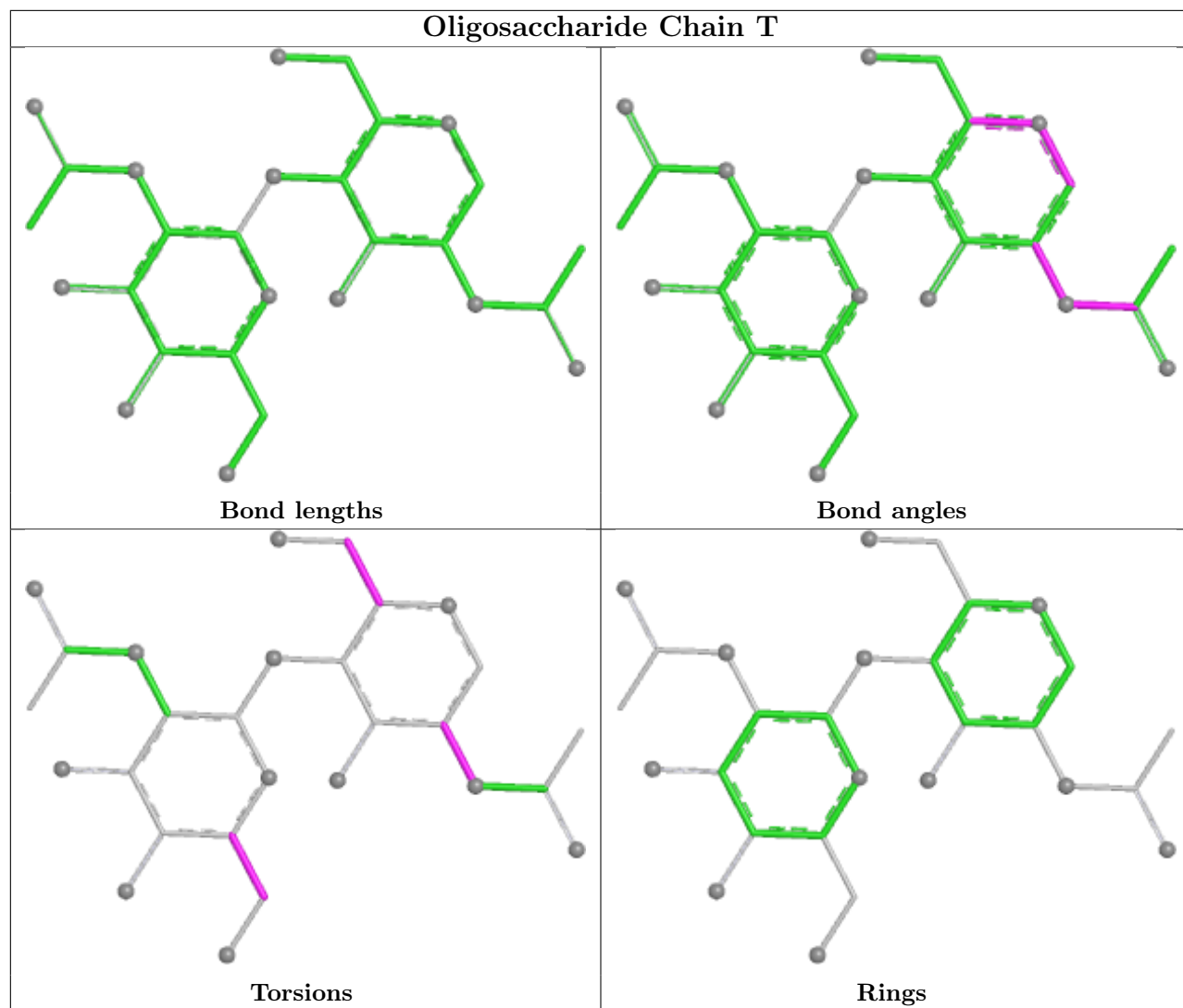


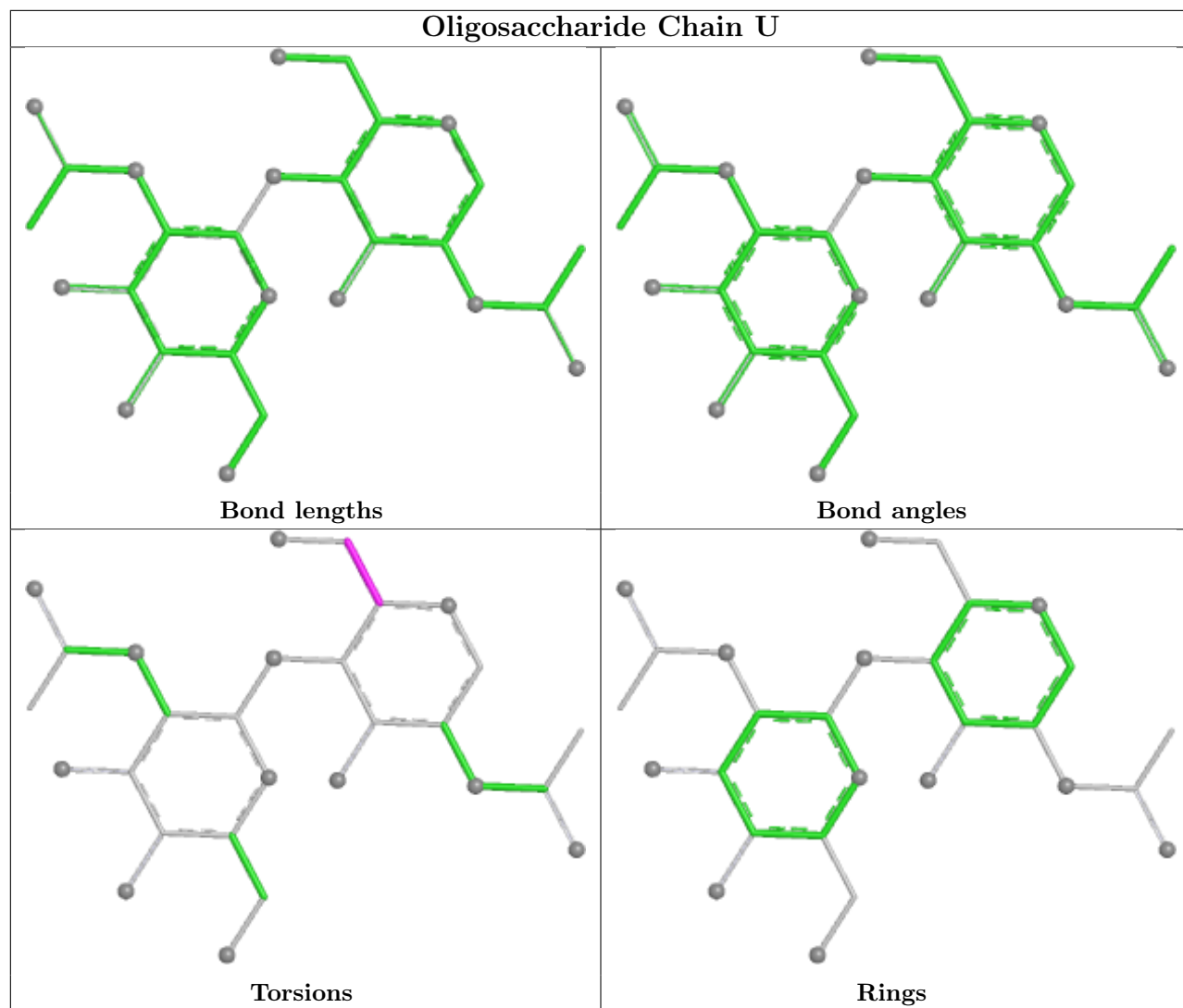


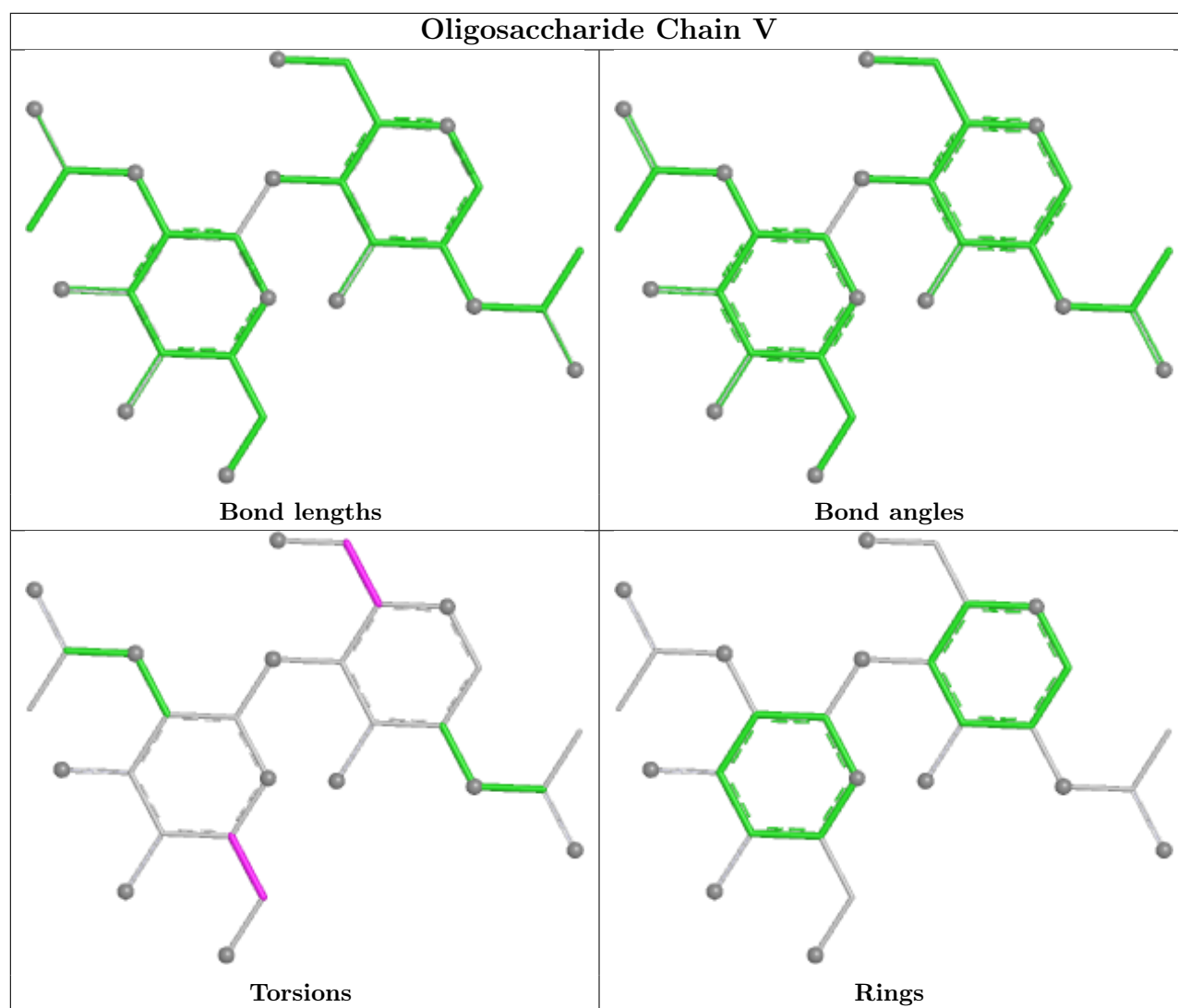


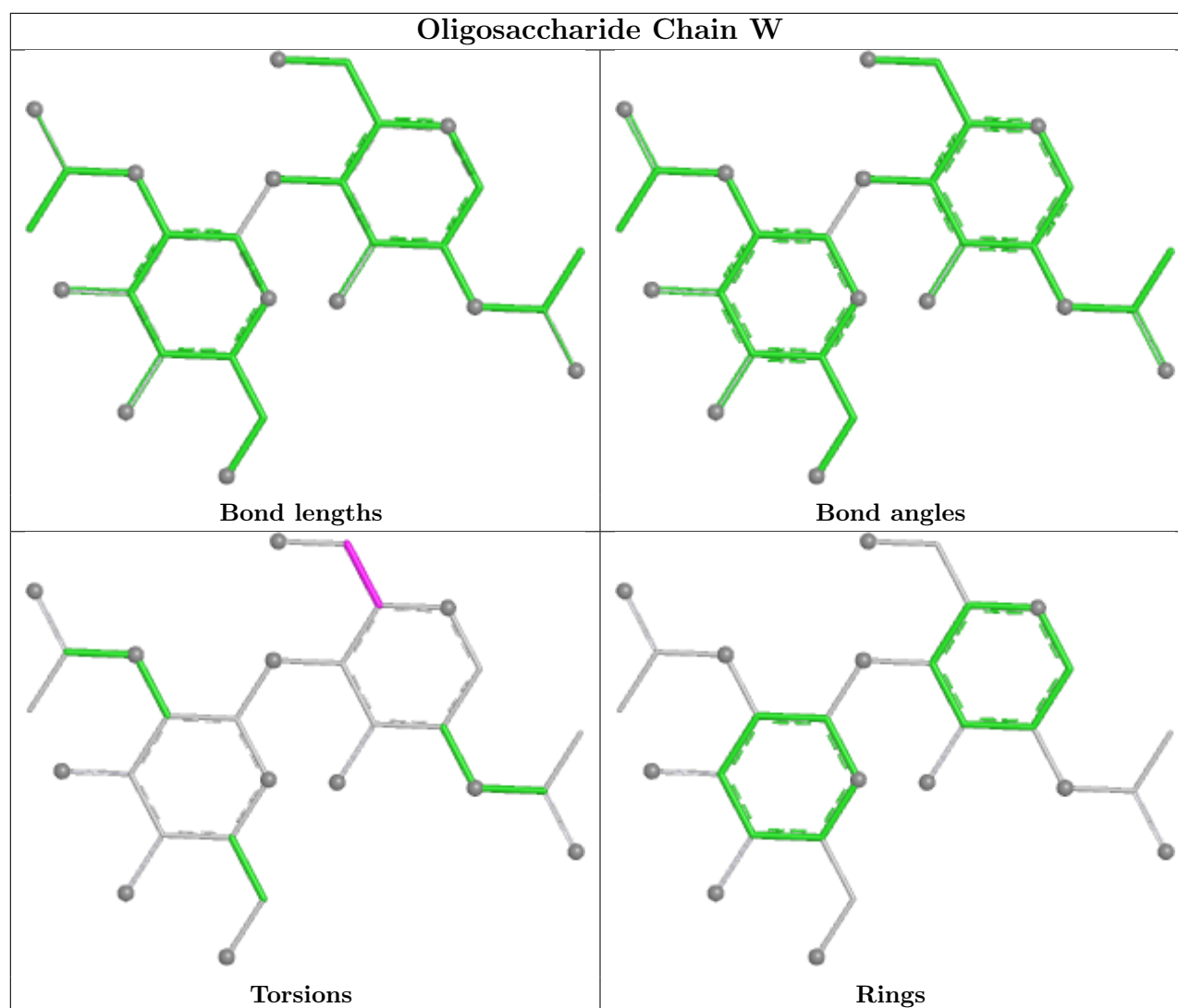












5.6 Ligand geometry [i](#)

34 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	$\# Z > 2$
4	NAG	A	1308	1	14,14,15	0.32	0	17,19,21	0.60	0
4	NAG	D	702	2	14,14,15	0.49	0	17,19,21	0.55	0
4	NAG	E	704	2	14,14,15	0.33	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1304	1	14,14,15	1.25	2 (14%)	17,19,21	0.97	1 (5%)
4	NAG	A	1305	1	14,14,15	0.39	0	17,19,21	0.48	0
4	NAG	A	1303	1	14,14,15	0.61	0	17,19,21	0.63	1 (5%)
4	NAG	C	1304	1	14,14,15	0.54	0	17,19,21	0.59	1 (5%)
4	NAG	D	701	2	14,14,15	0.38	0	17,19,21	0.52	0
4	NAG	C	1303	1	14,14,15	0.64	0	17,19,21	0.65	1 (5%)
4	NAG	B	1302	1	14,14,15	0.34	0	17,19,21	0.56	0
4	NAG	E	702	2	14,14,15	0.47	0	17,19,21	0.55	0
4	NAG	B	1301	1	14,14,15	0.43	0	17,19,21	0.61	1 (5%)
4	NAG	B	1307	1	14,14,15	0.57	0	17,19,21	1.03	1 (5%)
4	NAG	C	1306	1	14,14,15	0.38	0	17,19,21	0.53	0
4	NAG	B	1303	1	14,14,15	0.67	1 (7%)	17,19,21	0.70	1 (5%)
4	NAG	B	1306	1	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	C	1301	1	14,14,15	0.54	0	17,19,21	0.62	1 (5%)
4	NAG	C	1305	1	14,14,15	0.40	0	17,19,21	0.46	0
4	NAG	B	1304	1	14,14,15	0.47	0	17,19,21	0.59	1 (5%)
4	NAG	A	1307	1	14,14,15	0.54	0	17,19,21	1.04	1 (5%)
4	NAG	E	705	2	14,14,15	0.40	0	17,19,21	0.51	0
4	NAG	D	704	2	14,14,15	0.35	0	17,19,21	0.54	0
4	NAG	D	705	2	14,14,15	0.41	0	17,19,21	0.50	0
4	NAG	E	701	2	14,14,15	0.39	0	17,19,21	0.53	0
4	NAG	A	1306	1	14,14,15	0.31	0	17,19,21	0.40	0
4	NAG	D	706	2	14,14,15	0.58	0	17,19,21	0.64	1 (5%)
4	NAG	B	1305	1	14,14,15	0.40	0	17,19,21	0.59	1 (5%)
4	NAG	C	1302	1	14,14,15	0.33	0	17,19,21	0.57	0
4	NAG	A	1301	1	14,14,15	0.45	0	17,19,21	0.66	1 (5%)
4	NAG	A	1302	1	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	E	703	2	14,14,15	0.33	0	17,19,21	0.50	0
4	NAG	E	706	2	14,14,15	0.62	0	17,19,21	0.62	1 (5%)
4	NAG	B	1308	1	14,14,15	0.20	0	17,19,21	0.50	0
4	NAG	D	703	2	14,14,15	0.34	0	17,19,21	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1308	1	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	702	2	-	1/6/23/26	0/1/1/1
4	NAG	E	704	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	D	701	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	E	702	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	4/6/23/26	0/1/1/1
4	NAG	E	705	2	-	1/6/23/26	0/1/1/1
4	NAG	D	704	2	-	2/6/23/26	0/1/1/1
4	NAG	D	705	2	-	2/6/23/26	0/1/1/1
4	NAG	E	701	2	-	0/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	D	706	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	E	703	2	-	0/6/23/26	0/1/1/1
4	NAG	E	706	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	D	703	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1304	NAG	O5-C1	3.42	1.49	1.43
4	A	1304	NAG	C1-C2	3.08	1.56	1.52
4	B	1303	NAG	O5-C1	2.01	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1304	NAG	C1-O5-C5	3.57	116.97	112.19
4	B	1307	NAG	C2-N2-C7	3.22	127.22	122.90
4	A	1307	NAG	C2-N2-C7	3.20	127.19	122.90
4	B	1303	NAG	C1-O5-C5	2.62	115.69	112.19
4	C	1303	NAG	C1-O5-C5	2.40	115.40	112.19
4	A	1301	NAG	C1-O5-C5	2.34	115.33	112.19
4	A	1303	NAG	C1-O5-C5	2.30	115.27	112.19
4	D	706	NAG	C1-O5-C5	2.22	115.16	112.19
4	E	706	NAG	C1-O5-C5	2.16	115.08	112.19
4	B	1301	NAG	C1-O5-C5	2.15	115.07	112.19
4	C	1301	NAG	C1-O5-C5	2.15	115.07	112.19
4	B	1305	NAG	C1-O5-C5	2.11	115.01	112.19
4	C	1304	NAG	C1-O5-C5	2.07	114.97	112.19
4	B	1304	NAG	C1-O5-C5	2.03	114.90	112.19

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	701	NAG	C4-C5-C6-O6
4	E	706	NAG	C4-C5-C6-O6
4	D	704	NAG	O5-C5-C6-O6
4	D	701	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	E	706	NAG	O5-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	1303	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	D	704	NAG	C4-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	D	705	NAG	C4-C5-C6-O6
4	E	704	NAG	O5-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	D	705	NAG	O5-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6
4	E	704	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	A	1307	NAG	C1-C2-N2-C7
4	A	1308	NAG	C1-C2-N2-C7
4	B	1307	NAG	C1-C2-N2-C7
4	C	1306	NAG	C1-C2-N2-C7
4	A	1307	NAG	C3-C2-N2-C7
4	B	1307	NAG	C3-C2-N2-C7
4	B	1306	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	E	705	NAG	C4-C5-C6-O6
4	D	702	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1302	NAG	1	0
4	C	1302	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.

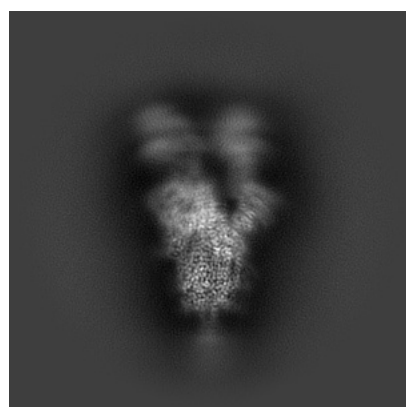
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25760. These allow visual inspection of the internal detail of the map and identification of artifacts.

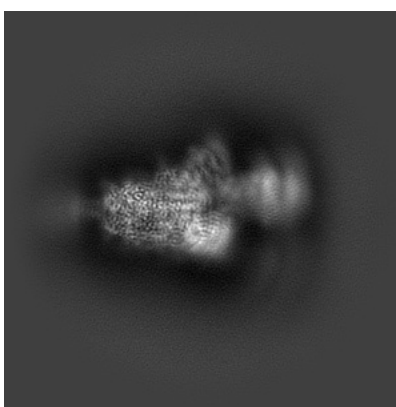
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

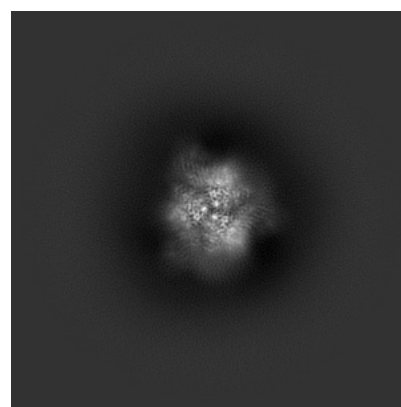
6.1.1 Primary map



X



Y

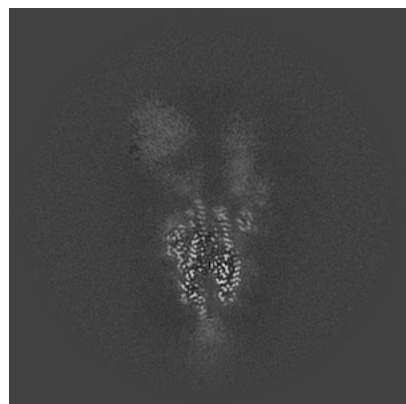


Z

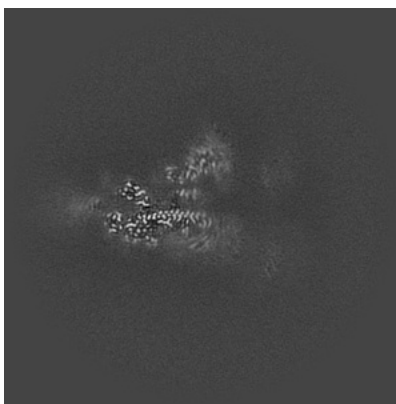
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

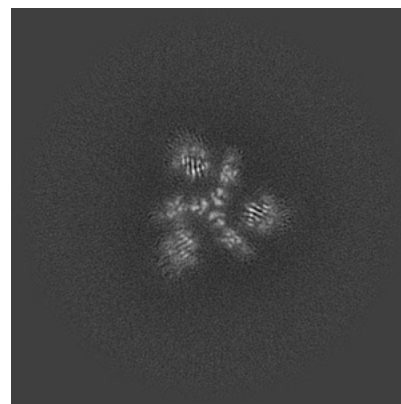
6.2.1 Primary map



X Index: 200



Y Index: 200

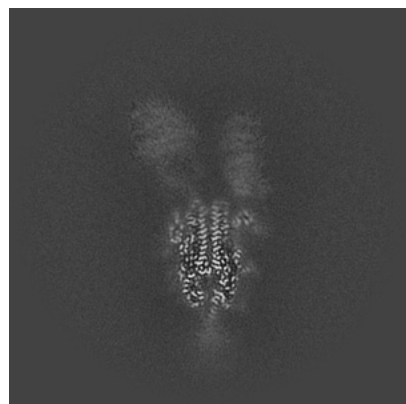


Z Index: 200

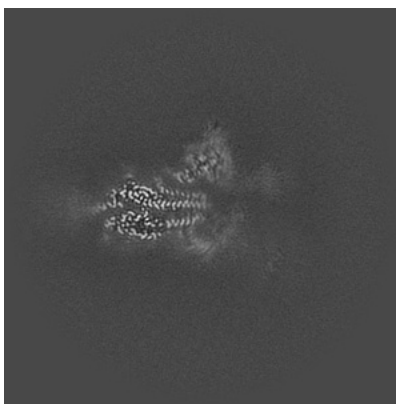
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

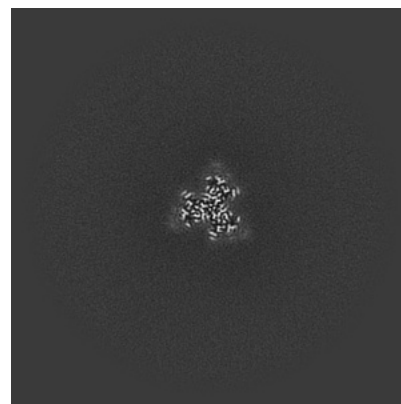
6.3.1 Primary map



X Index: 205



Y Index: 193

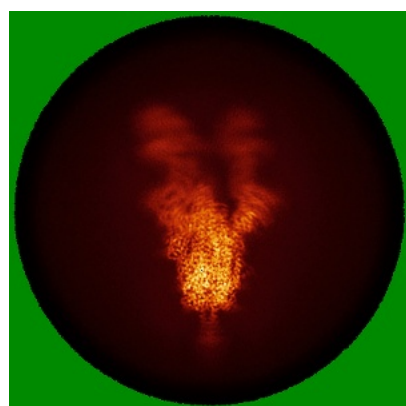


Z Index: 141

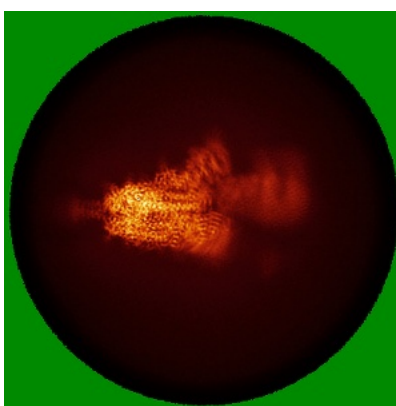
The images above show the largest variance slices of the map in three orthogonal directions.

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

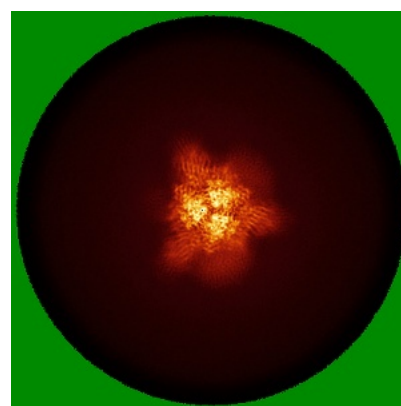
6.4.1 Primary map



X



Y

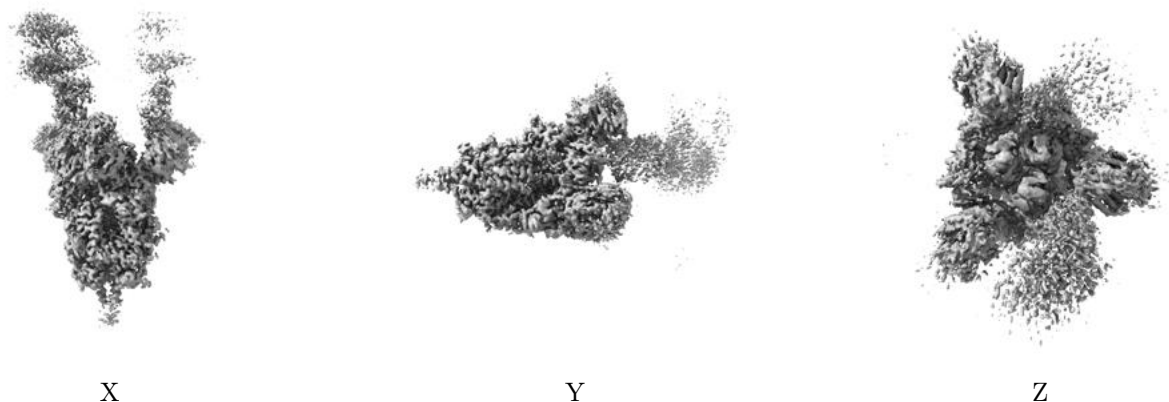


Z

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 0.152. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

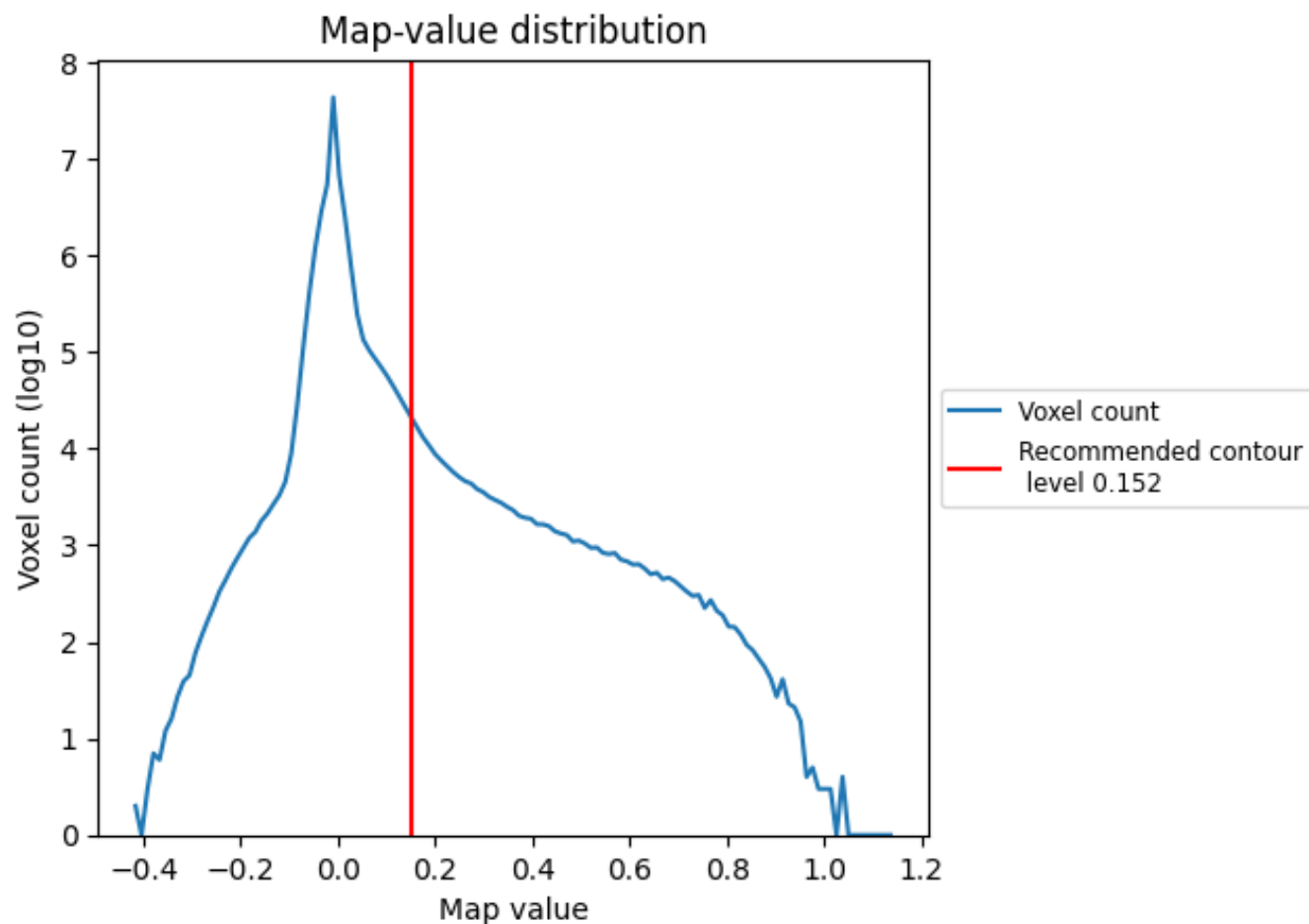
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

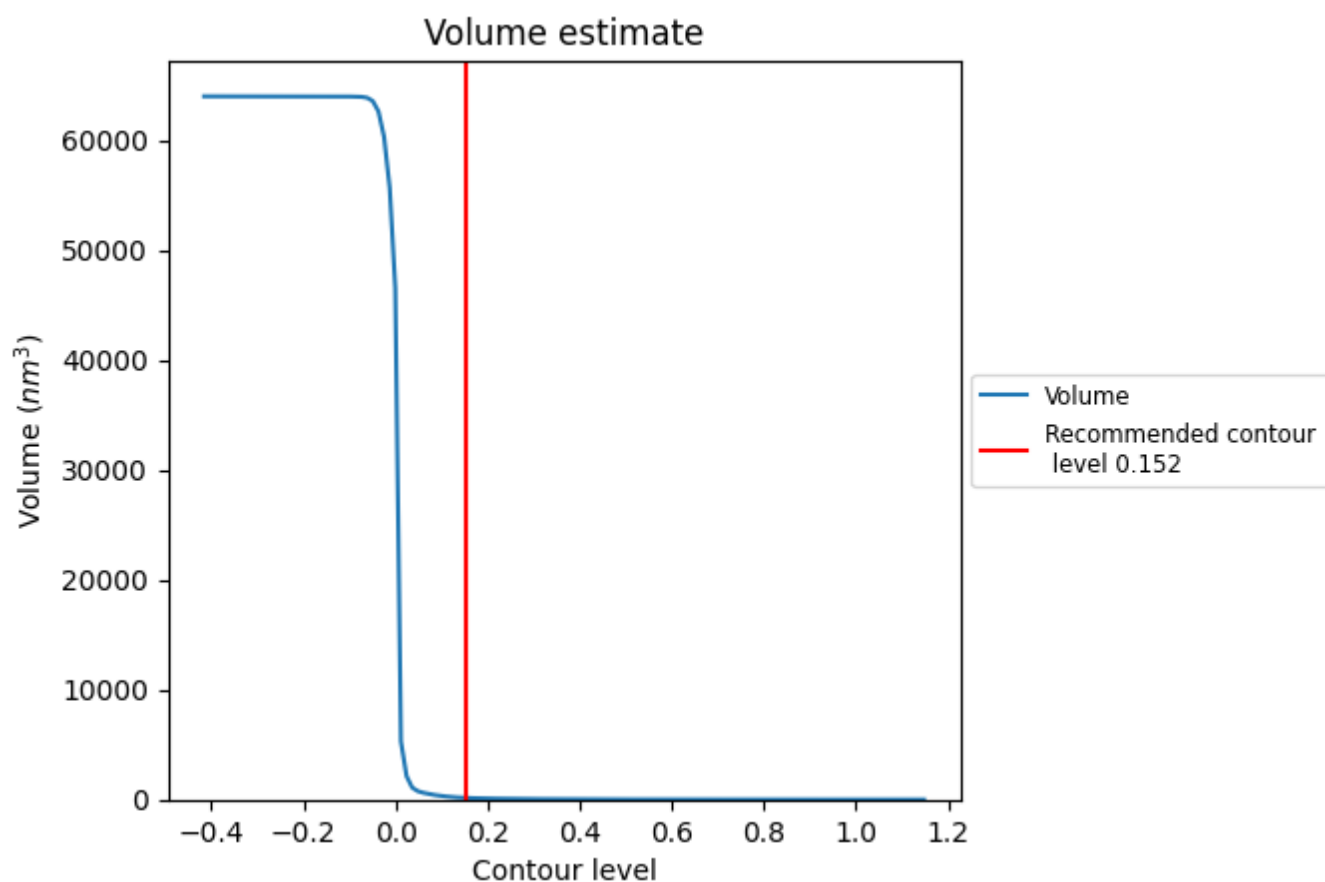
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

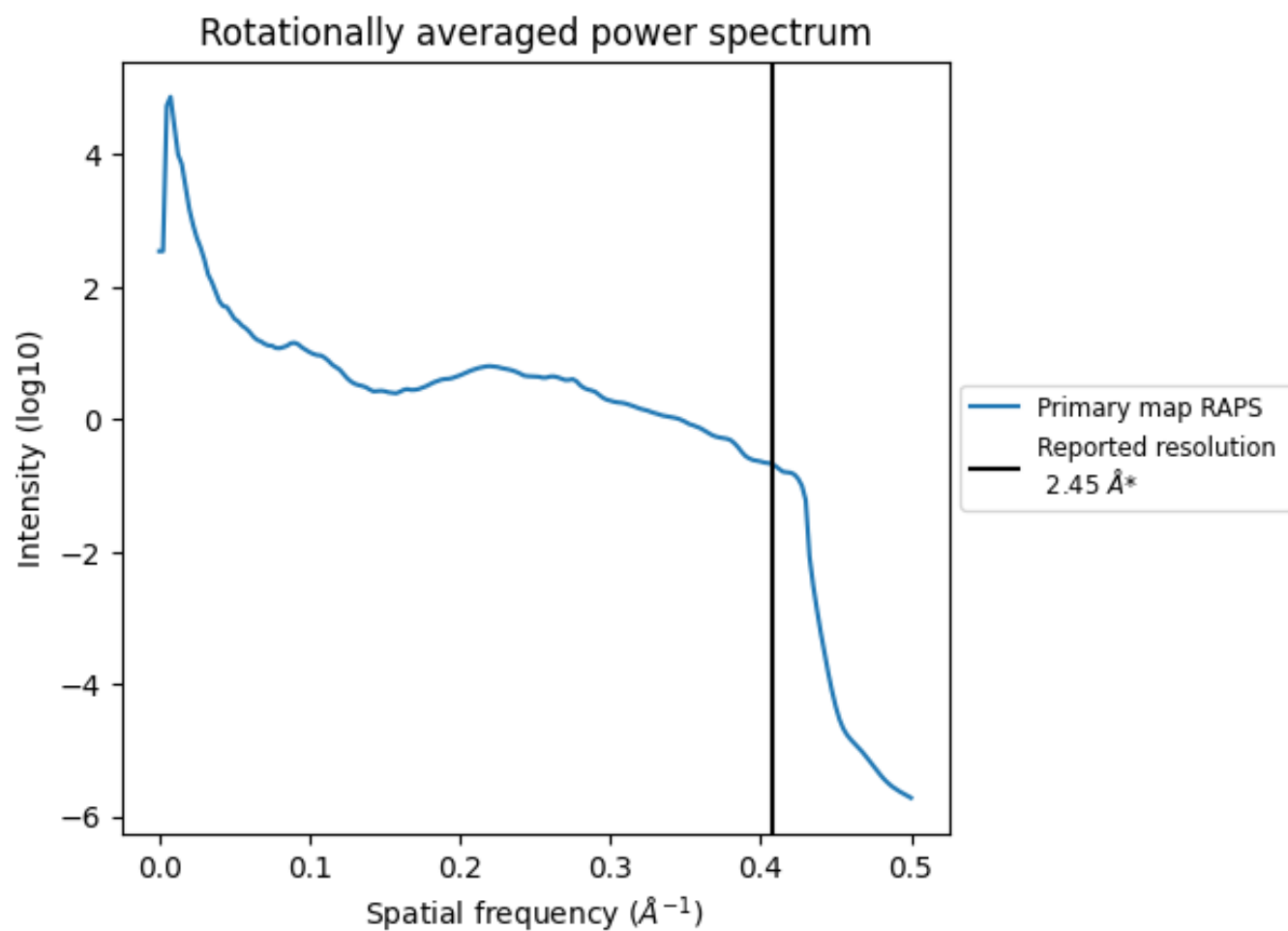
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; this corresponds to an approximate mass of 139 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 ⓘ

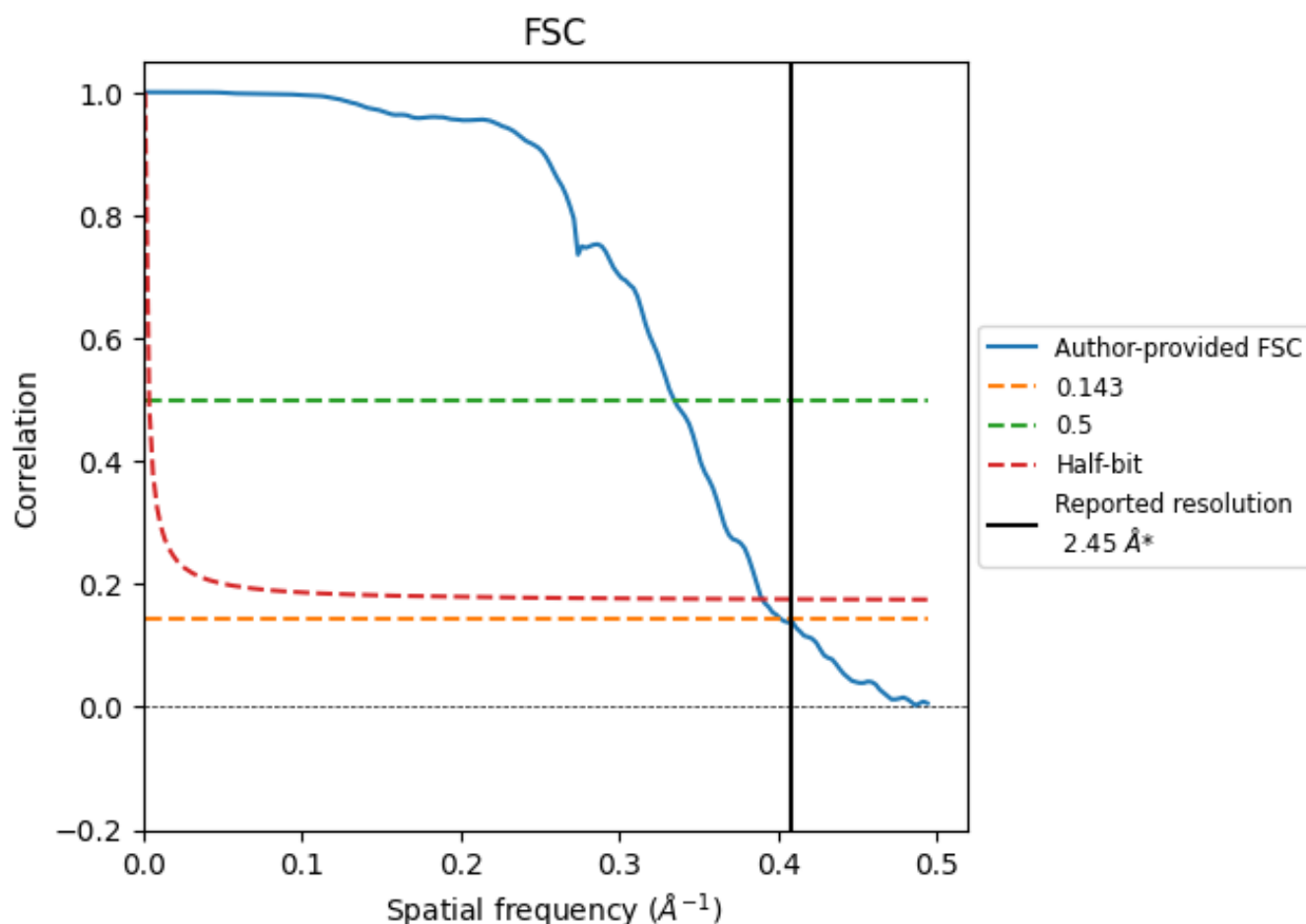


*Reported resolution corresponds to spatial frequency of 0.408 Å⁻¹

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 0.408 Å⁻¹

8.2 Resolution estimates [i](#)

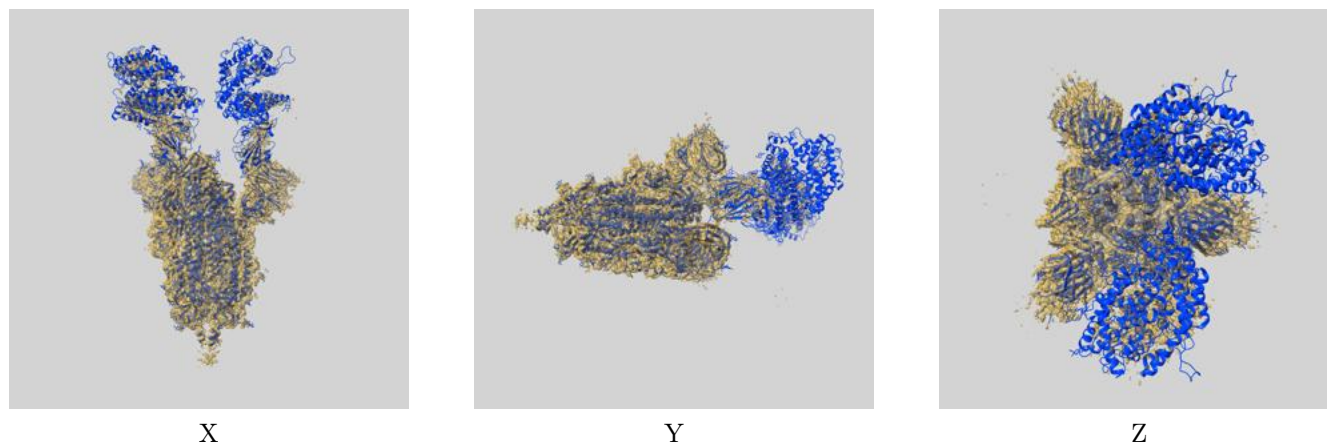
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.45	-	-
Author-provided FSC curve	2.49	2.99	2.57
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

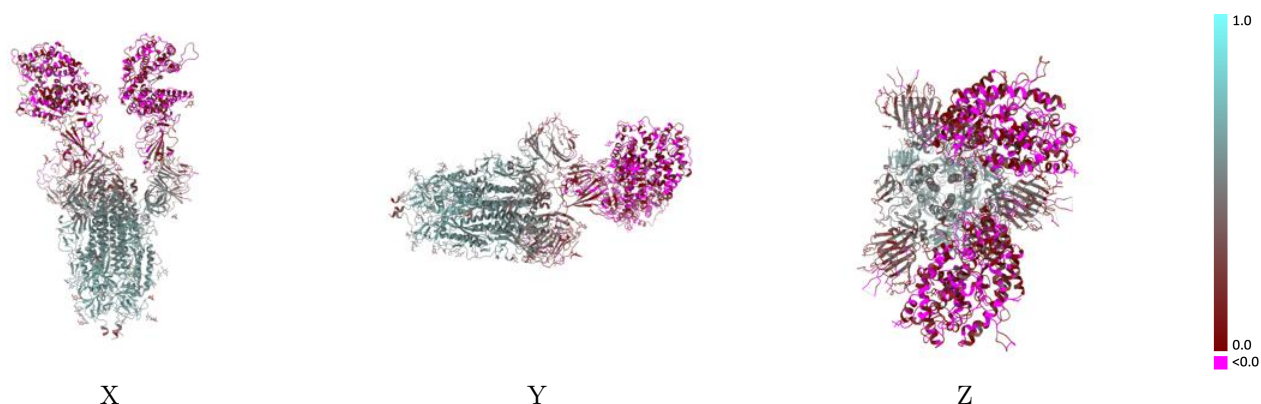
This section contains information regarding the fit between EMDB map EMD-25760 and PDB model 7T9K. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



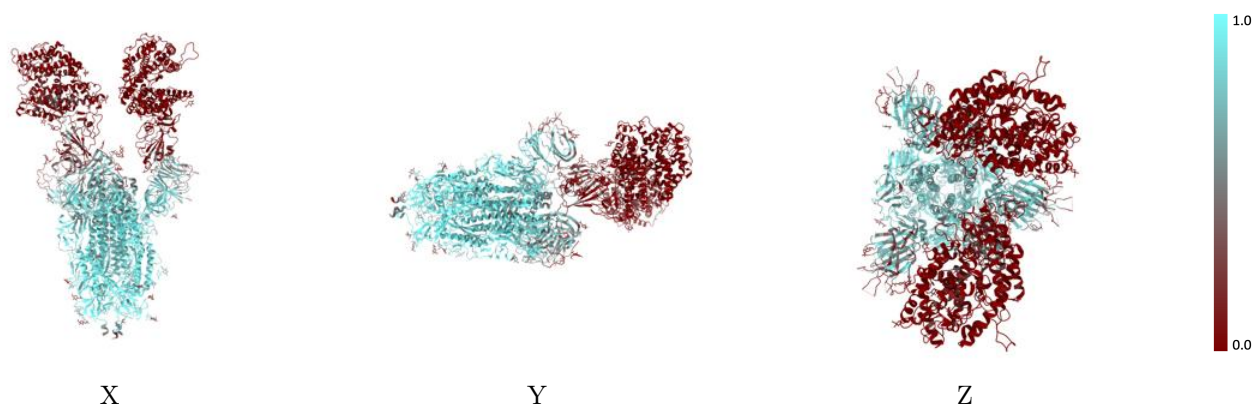
The images above show the 3D surface view of the map at the recommended contour level 0.152 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



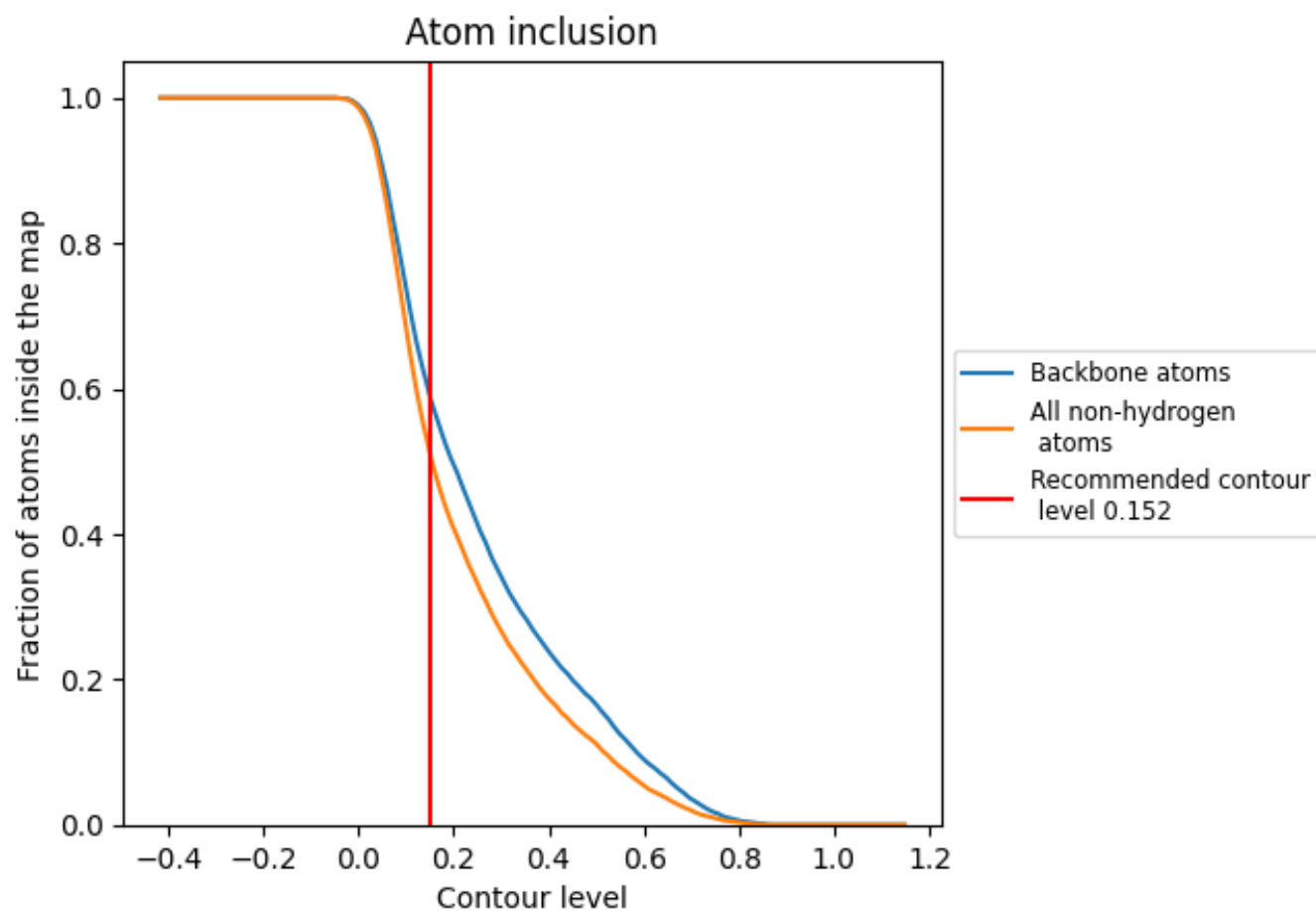
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.152).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 51% 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 (0.152) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5060	 0.3230
A	 0.6600	 0.4060
B	 0.6790	 0.4280
C	 0.8200	 0.4970
D	 0.0420	 0.0530
E	 0.0060	 0.0410
F	 0.0360	 0.0850
G	 0.7500	 0.5070
H	 0.7500	 0.4640
I	 0.3570	 0.5200
J	 0.5360	 0.3920
K	 0.4290	 0.3910
L	 0.0360	 0.0900
M	 0.7140	 0.4950
N	 0.7860	 0.5270
O	 0.3570	 0.4480
P	 0.5000	 0.4530
Q	 0.4640	 0.3650
R	 0.0360	 0.0650
S	 0.7140	 0.5110
T	 0.7140	 0.4870
U	 0.3570	 0.4580
V	 0.5360	 0.4350
W	 0.5000	 0.4240

