



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 04:47 AM UTC

PDB ID : 9BNE / pdb_00009bne
EMDB ID : EMD-44725
Title : SARS-CoV-2 spike HexaPro protein in complex with T3A trimeric antagonist
Authors : Young, T.
Deposited on : 2024-05-02
Resolution : 3.43 Å(reported)
Based on initial models : 6VXX, 6M0J

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:

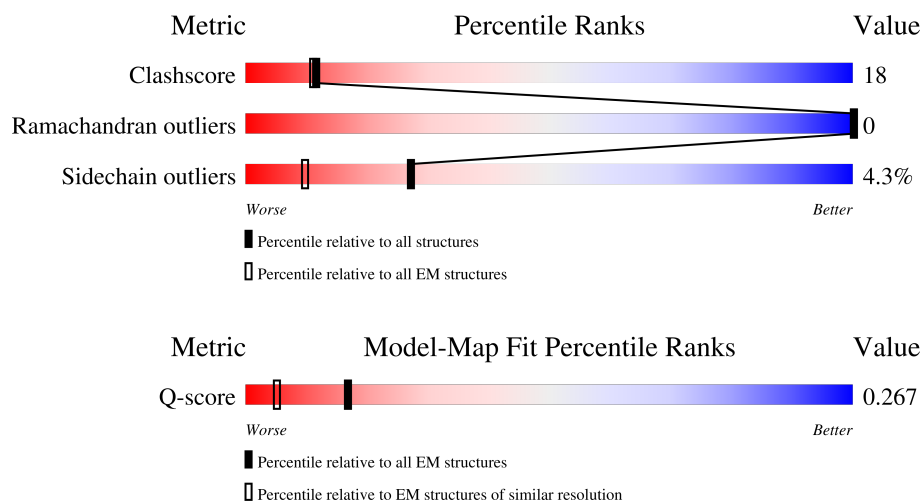
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 3.43 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	13927 (2.93 - 3.93)

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	680	
1	C	680	
1	E	680	
2	B	1288	

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Mol	Chain	Length	Quality of chain
2	D	1288	
2	F	1288	
3	G	2	
3	H	2	
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 40071 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 Collagen alpha-1(XVIII) chain, Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	647	Total	C	N	O	S	0	0
			5276	3374	882	991	29		
1	C	647	Total	C	N	O	S	0	0
			5266	3369	880	987	30		
1	E	647	Total	C	N	O	S	0	0
			5268	3369	879	990	30		

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP P39060
A	-24	GLY	-	expression tag	UNP P39060
A	-23	TRP	-	expression tag	UNP P39060
A	-22	SER	-	expression tag	UNP P39060
A	-21	LEU	-	expression tag	UNP P39060
A	-20	ILE	-	expression tag	UNP P39060
A	-19	LEU	-	expression tag	UNP P39060
A	-18	LEU	-	expression tag	UNP P39060
A	-17	PHE	-	expression tag	UNP P39060
A	-16	LEU	-	expression tag	UNP P39060
A	-15	VAL	-	expression tag	UNP P39060
A	-14	ALA	-	expression tag	UNP P39060
A	-13	VAL	-	expression tag	UNP P39060
A	-12	ALA	-	expression tag	UNP P39060
A	-11	THR	-	expression tag	UNP P39060
A	-10	ARG	-	expression tag	UNP P39060
A	-9	VAL	-	expression tag	UNP P39060
A	-8	LEU	-	expression tag	UNP P39060
A	-7	SER	-	expression tag	UNP P39060
A	-6	HIS	-	expression tag	UNP P39060
A	-5	HIS	-	expression tag	UNP P39060
A	-4	HIS	-	expression tag	UNP P39060
A	-3	HIS	-	expression tag	UNP P39060

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	HIS	-	expression tag	UNP P39060
A	-1	HIS	-	expression tag	UNP P39060
A	0	GLY	-	expression tag	UNP P39060
A	56	GLY	-	linker	UNP P39060
A	57	SER	-	linker	UNP P39060
A	58	GLY	-	linker	UNP P39060
C	-25	MET	-	initiating methionine	UNP P39060
C	-24	GLY	-	expression tag	UNP P39060
C	-23	TRP	-	expression tag	UNP P39060
C	-22	SER	-	expression tag	UNP P39060
C	-21	LEU	-	expression tag	UNP P39060
C	-20	ILE	-	expression tag	UNP P39060
C	-19	LEU	-	expression tag	UNP P39060
C	-18	LEU	-	expression tag	UNP P39060
C	-17	PHE	-	expression tag	UNP P39060
C	-16	LEU	-	expression tag	UNP P39060
C	-15	VAL	-	expression tag	UNP P39060
C	-14	ALA	-	expression tag	UNP P39060
C	-13	VAL	-	expression tag	UNP P39060
C	-12	ALA	-	expression tag	UNP P39060
C	-11	THR	-	expression tag	UNP P39060
C	-10	ARG	-	expression tag	UNP P39060
C	-9	VAL	-	expression tag	UNP P39060
C	-8	LEU	-	expression tag	UNP P39060
C	-7	SER	-	expression tag	UNP P39060
C	-6	HIS	-	expression tag	UNP P39060
C	-5	HIS	-	expression tag	UNP P39060
C	-4	HIS	-	expression tag	UNP P39060
C	-3	HIS	-	expression tag	UNP P39060
C	-2	HIS	-	expression tag	UNP P39060
C	-1	HIS	-	expression tag	UNP P39060
C	0	GLY	-	expression tag	UNP P39060
C	56	GLY	-	linker	UNP P39060
C	57	SER	-	linker	UNP P39060
C	58	GLY	-	linker	UNP P39060
E	-25	MET	-	initiating methionine	UNP P39060
E	-24	GLY	-	expression tag	UNP P39060
E	-23	TRP	-	expression tag	UNP P39060
E	-22	SER	-	expression tag	UNP P39060
E	-21	LEU	-	expression tag	UNP P39060
E	-20	ILE	-	expression tag	UNP P39060
E	-19	LEU	-	expression tag	UNP P39060

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	LEU	-	expression tag	UNP P39060
E	-17	PHE	-	expression tag	UNP P39060
E	-16	LEU	-	expression tag	UNP P39060
E	-15	VAL	-	expression tag	UNP P39060
E	-14	ALA	-	expression tag	UNP P39060
E	-13	VAL	-	expression tag	UNP P39060
E	-12	ALA	-	expression tag	UNP P39060
E	-11	THR	-	expression tag	UNP P39060
E	-10	ARG	-	expression tag	UNP P39060
E	-9	VAL	-	expression tag	UNP P39060
E	-8	LEU	-	expression tag	UNP P39060
E	-7	SER	-	expression tag	UNP P39060
E	-6	HIS	-	expression tag	UNP P39060
E	-5	HIS	-	expression tag	UNP P39060
E	-4	HIS	-	expression tag	UNP P39060
E	-3	HIS	-	expression tag	UNP P39060
E	-2	HIS	-	expression tag	UNP P39060
E	-1	HIS	-	expression tag	UNP P39060
E	0	GLY	-	expression tag	UNP P39060
E	56	GLY	-	linker	UNP P39060
E	57	SER	-	linker	UNP P39060
E	58	GLY	-	linker	UNP P39060

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1006	Total	C	N	O	S	0	0
			7825	5005	1300	1485	35		
2	D	1002	Total	C	N	O	S	0	0
			7801	4988	1293	1485	35		
2	F	1006	Total	C	N	O	S	0	0
			7837	5006	1302	1494	35		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
D	682	GLY	ARG	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	683	SER	ARG	engineered mutation	UNP P0DTC2
D	685	SER	ARG	engineered mutation	UNP P0DTC2
D	817	PRO	PHE	engineered mutation	UNP P0DTC2
D	892	PRO	ALA	engineered mutation	UNP P0DTC2
D	899	PRO	ALA	engineered mutation	UNP P0DTC2
D	942	PRO	ALA	engineered mutation	UNP P0DTC2
D	986	PRO	LYS	engineered mutation	UNP P0DTC2
D	987	PRO	VAL	engineered mutation	UNP P0DTC2
D	1209	GLY	-	expression tag	UNP P0DTC2
D	1210	SER	-	expression tag	UNP P0DTC2
D	1211	GLY	-	expression tag	UNP P0DTC2
D	1212	TYR	-	expression tag	UNP P0DTC2
D	1213	ILE	-	expression tag	UNP P0DTC2
D	1214	PRO	-	expression tag	UNP P0DTC2
D	1215	GLU	-	expression tag	UNP P0DTC2
D	1216	ALA	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	ARG	-	expression tag	UNP P0DTC2
D	1219	ASP	-	expression tag	UNP P0DTC2
D	1220	GLY	-	expression tag	UNP P0DTC2
D	1221	GLN	-	expression tag	UNP P0DTC2
D	1222	ALA	-	expression tag	UNP P0DTC2
D	1223	TYR	-	expression tag	UNP P0DTC2
D	1224	VAL	-	expression tag	UNP P0DTC2
D	1225	ARG	-	expression tag	UNP P0DTC2
D	1226	LYS	-	expression tag	UNP P0DTC2
D	1227	ASP	-	expression tag	UNP P0DTC2
D	1228	GLY	-	expression tag	UNP P0DTC2
D	1229	GLU	-	expression tag	UNP P0DTC2
D	1230	TRP	-	expression tag	UNP P0DTC2
D	1231	VAL	-	expression tag	UNP P0DTC2
D	1232	LEU	-	expression tag	UNP P0DTC2
D	1233	LEU	-	expression tag	UNP P0DTC2
D	1234	SER	-	expression tag	UNP P0DTC2
D	1235	THR	-	expression tag	UNP P0DTC2
D	1236	PHE	-	expression tag	UNP P0DTC2
D	1237	LEU	-	expression tag	UNP P0DTC2
D	1238	GLY	-	expression tag	UNP P0DTC2
D	1239	ARG	-	expression tag	UNP P0DTC2
D	1240	SER	-	expression tag	UNP P0DTC2
D	1241	LEU	-	expression tag	UNP P0DTC2
D	1242	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1243	VAL	-	expression tag	UNP P0DTC2
D	1244	LEU	-	expression tag	UNP P0DTC2
D	1245	PHE	-	expression tag	UNP P0DTC2
D	1246	GLN	-	expression tag	UNP P0DTC2
D	1247	GLY	-	expression tag	UNP P0DTC2
D	1248	PRO	-	expression tag	UNP P0DTC2
D	1249	GLY	-	expression tag	UNP P0DTC2
D	1250	HIS	-	expression tag	UNP P0DTC2
D	1251	HIS	-	expression tag	UNP P0DTC2
D	1252	HIS	-	expression tag	UNP P0DTC2
D	1253	HIS	-	expression tag	UNP P0DTC2
D	1254	HIS	-	expression tag	UNP P0DTC2
D	1255	HIS	-	expression tag	UNP P0DTC2
D	1256	HIS	-	expression tag	UNP P0DTC2
D	1257	HIS	-	expression tag	UNP P0DTC2
D	1258	SER	-	expression tag	UNP P0DTC2
D	1259	ALA	-	expression tag	UNP P0DTC2
D	1260	TRP	-	expression tag	UNP P0DTC2
D	1261	SER	-	expression tag	UNP P0DTC2
D	1262	HIS	-	expression tag	UNP P0DTC2
D	1263	PRO	-	expression tag	UNP P0DTC2
D	1264	GLN	-	expression tag	UNP P0DTC2
D	1265	PHE	-	expression tag	UNP P0DTC2
D	1266	GLU	-	expression tag	UNP P0DTC2
D	1267	LYS	-	expression tag	UNP P0DTC2
D	1268	GLY	-	expression tag	UNP P0DTC2
D	1269	GLY	-	expression tag	UNP P0DTC2
D	1270	GLY	-	expression tag	UNP P0DTC2
D	1271	SER	-	expression tag	UNP P0DTC2
D	1272	GLY	-	expression tag	UNP P0DTC2
D	1273	GLY	-	expression tag	UNP P0DTC2
D	1274	GLY	-	expression tag	UNP P0DTC2
D	1275	GLY	-	expression tag	UNP P0DTC2
D	1276	SER	-	expression tag	UNP P0DTC2
D	1277	GLY	-	expression tag	UNP P0DTC2
D	1278	GLY	-	expression tag	UNP P0DTC2
D	1279	SER	-	expression tag	UNP P0DTC2
D	1280	ALA	-	expression tag	UNP P0DTC2
D	1281	TRP	-	expression tag	UNP P0DTC2
D	1282	SER	-	expression tag	UNP P0DTC2
D	1283	HIS	-	expression tag	UNP P0DTC2
D	1284	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1285	GLN	-	expression tag	UNP P0DTC2
D	1286	PHE	-	expression tag	UNP P0DTC2
D	1287	GLU	-	expression tag	UNP P0DTC2
D	1288	LYS	-	expression tag	UNP P0DTC2
F	682	GLY	ARG	engineered mutation	UNP P0DTC2
F	683	SER	ARG	engineered mutation	UNP P0DTC2
F	685	SER	ARG	engineered mutation	UNP P0DTC2
F	817	PRO	PHE	engineered mutation	UNP P0DTC2
F	892	PRO	ALA	engineered mutation	UNP P0DTC2
F	899	PRO	ALA	engineered mutation	UNP P0DTC2
F	942	PRO	ALA	engineered mutation	UNP P0DTC2
F	986	PRO	LYS	engineered mutation	UNP P0DTC2
F	987	PRO	VAL	engineered mutation	UNP P0DTC2
F	1209	GLY	-	expression tag	UNP P0DTC2
F	1210	SER	-	expression tag	UNP P0DTC2
F	1211	GLY	-	expression tag	UNP P0DTC2
F	1212	TYR	-	expression tag	UNP P0DTC2
F	1213	ILE	-	expression tag	UNP P0DTC2
F	1214	PRO	-	expression tag	UNP P0DTC2
F	1215	GLU	-	expression tag	UNP P0DTC2
F	1216	ALA	-	expression tag	UNP P0DTC2
F	1217	PRO	-	expression tag	UNP P0DTC2
F	1218	ARG	-	expression tag	UNP P0DTC2
F	1219	ASP	-	expression tag	UNP P0DTC2
F	1220	GLY	-	expression tag	UNP P0DTC2
F	1221	GLN	-	expression tag	UNP P0DTC2
F	1222	ALA	-	expression tag	UNP P0DTC2
F	1223	TYR	-	expression tag	UNP P0DTC2
F	1224	VAL	-	expression tag	UNP P0DTC2
F	1225	ARG	-	expression tag	UNP P0DTC2
F	1226	LYS	-	expression tag	UNP P0DTC2
F	1227	ASP	-	expression tag	UNP P0DTC2
F	1228	GLY	-	expression tag	UNP P0DTC2
F	1229	GLU	-	expression tag	UNP P0DTC2
F	1230	TRP	-	expression tag	UNP P0DTC2
F	1231	VAL	-	expression tag	UNP P0DTC2
F	1232	LEU	-	expression tag	UNP P0DTC2
F	1233	LEU	-	expression tag	UNP P0DTC2
F	1234	SER	-	expression tag	UNP P0DTC2
F	1235	THR	-	expression tag	UNP P0DTC2
F	1236	PHE	-	expression tag	UNP P0DTC2
F	1237	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1238	GLY	-	expression tag	UNP P0DTC2
F	1239	ARG	-	expression tag	UNP P0DTC2
F	1240	SER	-	expression tag	UNP P0DTC2
F	1241	LEU	-	expression tag	UNP P0DTC2
F	1242	GLU	-	expression tag	UNP P0DTC2
F	1243	VAL	-	expression tag	UNP P0DTC2
F	1244	LEU	-	expression tag	UNP P0DTC2
F	1245	PHE	-	expression tag	UNP P0DTC2
F	1246	GLN	-	expression tag	UNP P0DTC2
F	1247	GLY	-	expression tag	UNP P0DTC2
F	1248	PRO	-	expression tag	UNP P0DTC2
F	1249	GLY	-	expression tag	UNP P0DTC2
F	1250	HIS	-	expression tag	UNP P0DTC2
F	1251	HIS	-	expression tag	UNP P0DTC2
F	1252	HIS	-	expression tag	UNP P0DTC2
F	1253	HIS	-	expression tag	UNP P0DTC2
F	1254	HIS	-	expression tag	UNP P0DTC2
F	1255	HIS	-	expression tag	UNP P0DTC2
F	1256	HIS	-	expression tag	UNP P0DTC2
F	1257	HIS	-	expression tag	UNP P0DTC2
F	1258	SER	-	expression tag	UNP P0DTC2
F	1259	ALA	-	expression tag	UNP P0DTC2
F	1260	TRP	-	expression tag	UNP P0DTC2
F	1261	SER	-	expression tag	UNP P0DTC2
F	1262	HIS	-	expression tag	UNP P0DTC2
F	1263	PRO	-	expression tag	UNP P0DTC2
F	1264	GLN	-	expression tag	UNP P0DTC2
F	1265	PHE	-	expression tag	UNP P0DTC2
F	1266	GLU	-	expression tag	UNP P0DTC2
F	1267	LYS	-	expression tag	UNP P0DTC2
F	1268	GLY	-	expression tag	UNP P0DTC2
F	1269	GLY	-	expression tag	UNP P0DTC2
F	1270	GLY	-	expression tag	UNP P0DTC2
F	1271	SER	-	expression tag	UNP P0DTC2
F	1272	GLY	-	expression tag	UNP P0DTC2
F	1273	GLY	-	expression tag	UNP P0DTC2
F	1274	GLY	-	expression tag	UNP P0DTC2
F	1275	GLY	-	expression tag	UNP P0DTC2
F	1276	SER	-	expression tag	UNP P0DTC2
F	1277	GLY	-	expression tag	UNP P0DTC2
F	1278	GLY	-	expression tag	UNP P0DTC2
F	1279	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1280	ALA	-	expression tag	UNP P0DTC2
F	1281	TRP	-	expression tag	UNP P0DTC2
F	1282	SER	-	expression tag	UNP P0DTC2
F	1283	HIS	-	expression tag	UNP P0DTC2
F	1284	PRO	-	expression tag	UNP P0DTC2
F	1285	GLN	-	expression tag	UNP P0DTC2
F	1286	PHE	-	expression tag	UNP P0DTC2
F	1287	GLU	-	expression tag	UNP P0DTC2
F	1288	LYS	-	expression tag	UNP P0DTC2

- 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	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	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		
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	J	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	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	B	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	

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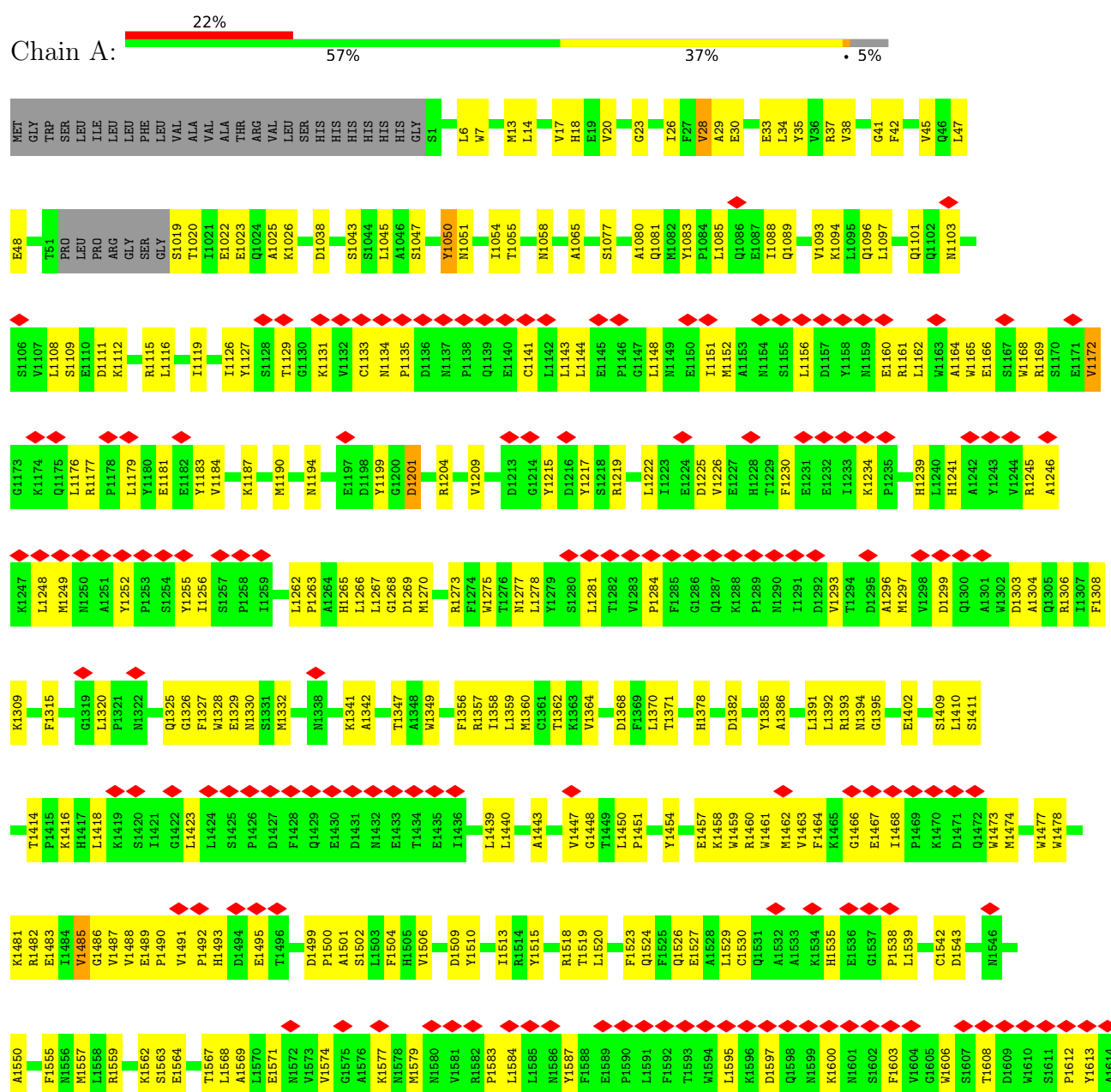
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Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total 14	C 8	N 1	O 5	0
4	D	1	Total 14	C 8	N 1	O 5	0
4	D	1	Total 14	C 8	N 1	O 5	0
4	D	1	Total 14	C 8	N 1	O 5	0
4	D	1	Total 14	C 8	N 1	O 5	0
4	D	1	Total 14	C 8	N 1	O 5	0
4	D	1	Total 14	C 8	N 1	O 5	0
4	D	1	Total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

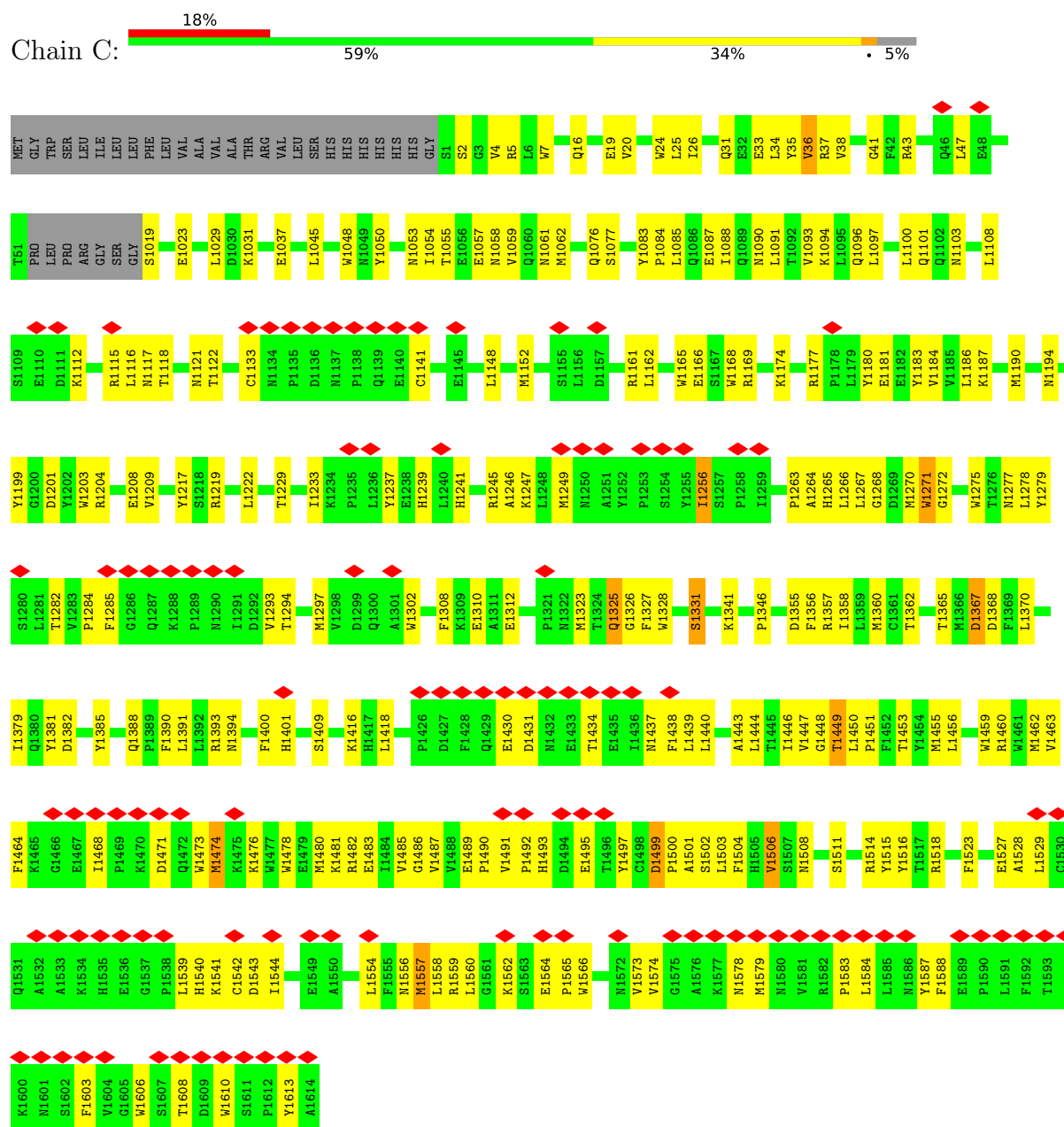
3 Residue-property plots

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: Collagen alpha-1(XVIII) chain, Processed angiotensin-converting enzyme 2



- Molecule 1: Collagen alpha-1(XVIII) chain, Processed angiotensin-converting enzyme 2

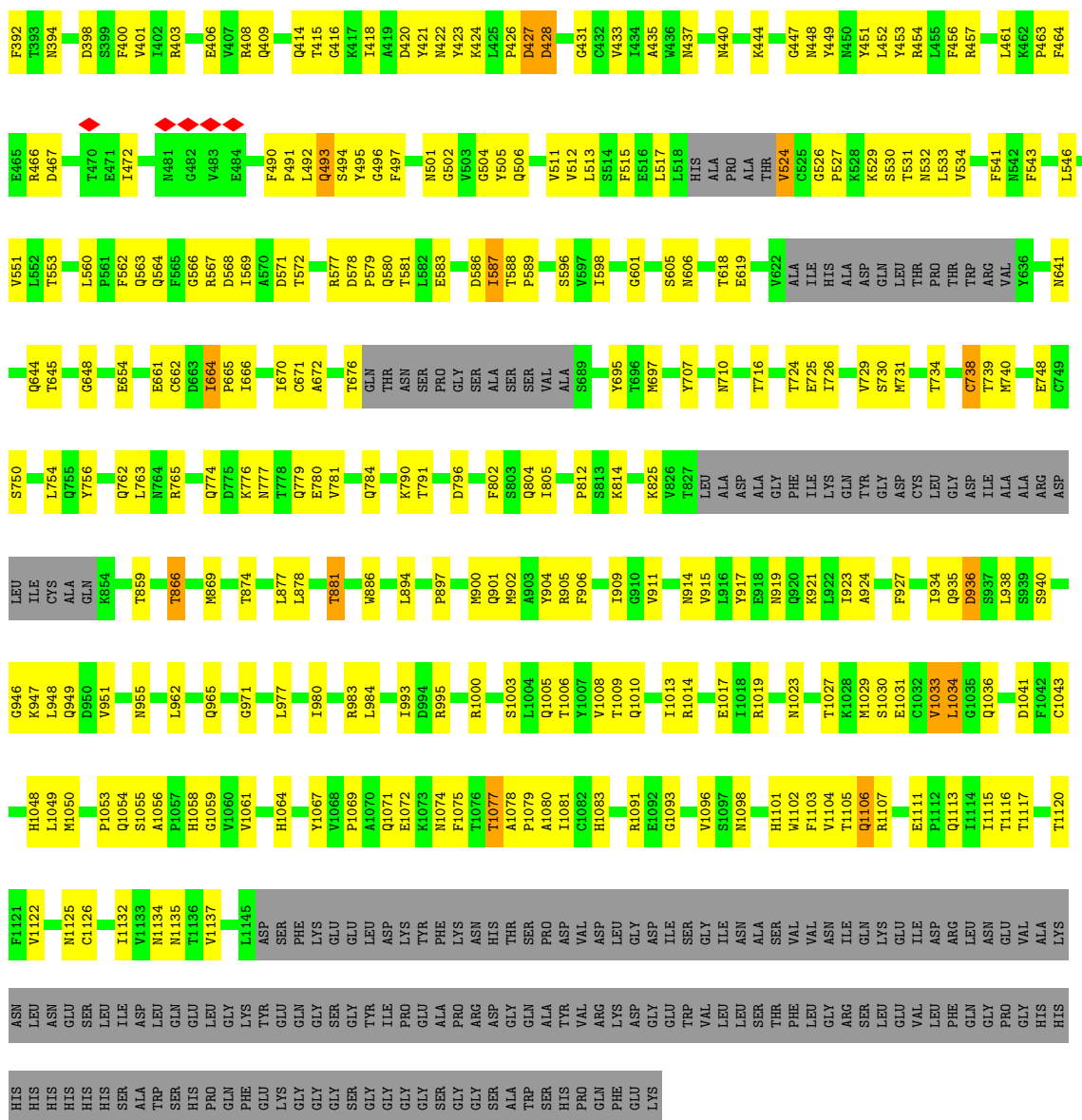




F306	F306	L223	GLU	D80	MET
E309	GLU	E224	GLU	N81	PHE
K310	PHE	P225	PHE	N82	VAL
G311	ARG	L226	ARG	N83	LEU
I312	VAL	V227	VAL	N87	VAL
Y313	THR		THR		LEU
G314	THR	P230	THR	F92	LEU
T315	ALA		ALA	F93	PRO
R319	ASN	N234	ASN	A93	VAL
	ASN	I235	ASN	S94	VAL
T323	N165	T236	N165	T95	SER
E324	C166	R237	C166	E96	SER
				K97	GLN
R328	E169	Q238	E169		
	Y170	Q239	Y170	N99	CYS
	T240	T240	T240	N100	ASN
N331	V171	L241	V171	I100	VAL
I332	S172	L242	S172	I101	LEU
T333	GLN	A243	GLN	R102	THR
N334	PRO	L244	PRO	G103	THR
L335	PHE	H245	PHE	W104	ARG
	LEU		LEU	I105	THR
	MET	ARG	MET	F106	THR
G339	ASP	THR	ASP	G107	LEU
E340	LEU	LEU	LEU	T108	PRO
F341	GLU	THR	GLU		PRO
F342	GLY	PRO	GLY	D111	A27
N343	LVS	GLY	LVS	S112	
A344	GLN	ASP	GLN	K113	R34
T345	GLY	SER	GLY	T114	
R346	ASN	SER	ASN	Q115	K41
F347	F186	SER	F186	S116	V42
A348	K187	GLY	K187	L117	F43
S349	L188	TRP	L188	L118	R44
V350	L189	THR	L189	I119	
Y351	R190	ALA	R190	V120	V47
A352	E191	GLY	E191	N121	L48
W353	F192	ALA	F192		
N354	V126	A263	V126	V127	D53
R355	K195	A264	K195	I128	L54
K356	R196		R196	K129	F58
R357	I197	V267	I197	C136	F59
L358	D198		D198		
S359	G199	L276	G199	P139	T63
N360	G278	L277	G278	Y200	W64
G361	F201	K279	F201	F140	F65
V362		N280		L141	
	Y204		Y204	G142	T68
Y365	T284		T284	V143	H69
F374	T208		T208	TVR	VAL
S375	TVR	D267	TVR	L15	SER
T376	L15	A268	L15	H15	GLY
	ASN	L212	ASN	L15	THR
V382	ASN	V213	ASN	ASN	ASN
	GLY	R214	GLY	GLY	GLY
K386	D215	S297	D215	LVS	THR
L387	L216		L216	LVS	LYS
N388	P217	K300	P217	TRP	ARG

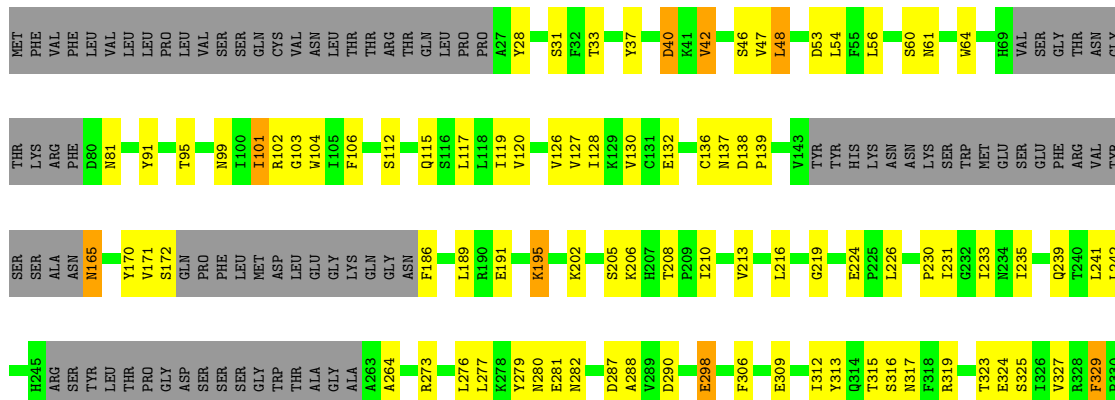


D294	D215	LYS	ARG	MET
K310	L216	SER	PHE	PHE
G311	L223	TRP	D80	VAL
L312		MET	N81	PHE
		GLU		LEU
N317	L226	SER	P85	VAL
F318	V227	GLU	F86	LEU
R319	D228	PHE	N87	
V320	L229	ARG	D88	PRO
	P230	VAL	G89	LEU
	I231	TYR	V90	VAL
T323	G232	SER	Y91	SER
E324	I233	SER	F92	SER
	N234	ALA	A93	SER
I326	L235	ASN	S94	CYS
V327	T236	H165	T95	VAL
R328	R237	C166	E96	ASN
F329	P238	T167	K97	ASN
P330	Q239	F168	S98	THR
	T240		N99	THR
C336	L241	V171	I100	THR
F337	L242	S172	I101	THR
F338	A243	GLN	R102	LEU
	L244	PRO	G103	LEU
F342	H245	PHE	W104	PRO
	ARG	LEU	I105	PRO
T345	SER	MET	F106	
R346	TYR	ASP	G107	A27
F347	LEU	LEU	T108	
	THR	GLU		Y37
	PRO	GLY		
V350	GLY	LYS	S112	D40
Y351	ASP	GLN	Q115	
A352	SER	GLY		S46
W353	ASP	ASN		V47
N354	SER		I119	
R355	SER	F186	V120	Q52
F356	GLY	K187	N121	D53
R357	THR	N188	N122	L54
L358	TRP	L189		F55
S359	ALA	R190	N125	
	GLY	E191	V126	F58
	ALA	F192	V127	F59
V362	A263	V193	I128	S60
A363	A264	F194	N129	N61
D364		K195	V130	V62
Y365	Y265	N196	C131	
S366		I197	E132	W64
		D198	F133	F85
Y269		G199		H66
L270	Q271	Y200	P139	A67
P272	T271	F201	L140	I68
			L141	H69
Y279		Y204	G142	VAL
N280			V143	SER
				GLY
		T208	TYR	THR
T284		P209	HIS	THR
		I210	ASN	
D287		N211	LYS	GLY
			THR	LYS
A288		P214	ASN	THR
				LYS



• Molecule 2: Spike glycoprotein

Chain F: 49% 27% 22%



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

Chain I:  50% 50%



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

Chain K:  50% 50%



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

Chain L:  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% 50%



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

Chain P:  100%

MAG1
MAG2

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

Chain Q:  50% 50%

MAG1
MAG2

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

Chain R:  50% 50%

MAG1
MAG2

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

Chain J:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	225636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch motion correction and Patch CTF applied after Import Movies and before Blob Picker	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.288	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	319.488, 319.488, 319.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.832, 0.832, 0.832	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	0.07	0/5421	0.19	0/7363
1	C	0.07	0/5409	0.19	0/7345
1	E	0.10	0/5413	0.22	0/7352
2	B	0.21	0/8006	0.33	0/10903
2	D	0.23	0/7979	0.33	0/10864
2	F	0.22	0/8017	0.32	0/10915
All	All	0.18	0/40245	0.28	0/54742

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	5276	0	5049	176	0
1	C	5266	0	5041	175	0
1	E	5268	0	5031	241	0
2	B	7825	0	7618	269	0
2	D	7801	0	7582	292	0
2	F	7837	0	7624	276	0
3	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	28	0	25	0	0
3	I	28	0	25	2	0
3	J	28	0	25	0	0
3	K	28	0	25	1	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	1	0
3	O	28	0	25	1	0
3	P	28	0	25	2	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
4	B	140	0	130	1	0
4	D	168	0	156	4	0
4	F	154	0	143	5	0
All	All	40071	0	38674	1392	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 18.

The worst 5 of 1392 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:431:GLY:HA3	2:D:513:LEU:O	1.50	1.10
2:F:431:GLY:HA3	2:F:513:LEU:O	1.62	0.98
2:F:448:ASN:H	2:F:497:PHE:H	1.18	0.90
2:B:360:ASN:H	2:B:523:THR:HB	1.39	0.87
2:F:1093:GLY:HA3	2:F:1105:THR:O	1.74	0.86

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	643/680 (95%)	633 (98%)	10 (2%)	0	100	100
1	C	643/680 (95%)	631 (98%)	12 (2%)	0	100	100
1	E	643/680 (95%)	632 (98%)	11 (2%)	0	100	100
2	B	990/1288 (77%)	930 (94%)	60 (6%)	0	100	100
2	D	984/1288 (76%)	907 (92%)	77 (8%)	0	100	100
2	F	990/1288 (77%)	933 (94%)	57 (6%)	0	100	100
All	All	4893/5904 (83%)	4666 (95%)	227 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	568/596 (95%)	558 (98%)	10 (2%)	51	68
1	C	565/596 (95%)	548 (97%)	17 (3%)	36	60
1	E	566/596 (95%)	554 (98%)	12 (2%)	47	66
2	B	873/1116 (78%)	817 (94%)	56 (6%)	16	43
2	D	871/1116 (78%)	826 (95%)	45 (5%)	21	48
2	F	877/1116 (79%)	830 (95%)	47 (5%)	20	47
All	All	4320/5136 (84%)	4133 (96%)	187 (4%)	27	52

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	859	THR
2	F	48	LEU
2	D	934	ILE
1	E	1201	ASP
2	F	298	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1340	GLN
2	F	188	ASN
2	F	777	ASN
2	B	536	ASN
2	B	360	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

24 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	G	1	3,2	14,14,15	0.82	1 (7%)	17,19,21	1.28	1 (5%)
3	NAG	G	2	3	14,14,15	0.76	1 (7%)	17,19,21	0.88	1 (5%)
3	NAG	H	1	3,2	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	H	2	3	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	I	1	3,2	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	I	2	3	14,14,15	0.44	0	17,19,21	1.33	2 (11%)
3	NAG	J	1	3,2	14,14,15	0.28	0	17,19,21	0.60	0
3	NAG	J	2	3	14,14,15	0.94	2 (14%)	17,19,21	1.00	1 (5%)
3	NAG	K	1	3,2	14,14,15	0.80	1 (7%)	17,19,21	1.37	1 (5%)
3	NAG	K	2	3	14,14,15	0.48	0	17,19,21	1.34	2 (11%)
3	NAG	L	1	3,2	14,14,15	0.31	0	17,19,21	0.43	0
3	NAG	L	2	3	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	M	1	3,2	14,14,15	0.77	1 (7%)	17,19,21	1.19	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	M	2	3	14,14,15	0.15	0	17,19,21	0.49	0
3	NAG	N	1	3,2	14,14,15	0.27	0	17,19,21	0.58	0
3	NAG	N	2	3	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	O	1	3,2	14,14,15	0.36	0	17,19,21	0.43	0
3	NAG	O	2	3	14,14,15	0.24	0	17,19,21	0.54	0
3	NAG	P	1	3,2	14,14,15	0.17	0	17,19,21	0.54	0
3	NAG	P	2	3	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	Q	1	3,2	14,14,15	1.32	1 (7%)	17,19,21	1.10	2 (11%)
3	NAG	Q	2	3	14,14,15	0.39	0	17,19,21	0.63	0
3	NAG	R	1	3,2	14,14,15	0.40	0	17,19,21	1.06	1 (5%)
3	NAG	R	2	3	14,14,15	0.23	0	17,19,21	0.56	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	G	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	6/6/23/26	0/1/1/1
3	NAG	J	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	NAG	K	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	4/6/23/26	0/1/1/1
3	NAG	L	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	M	2	3	-	4/6/23/26	0/1/1/1
3	NAG	N	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	NAG	O	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	O	2	3	-	4/6/23/26	0/1/1/1
3	NAG	P	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	4/6/23/26	0/1/1/1
3	NAG	R	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	1	NAG	O5-C1	-4.73	1.35	1.43
3	G	1	NAG	O5-C1	2.96	1.48	1.43
3	K	1	NAG	O5-C1	2.89	1.48	1.43
3	J	2	NAG	O5-C1	2.83	1.48	1.43
3	M	1	NAG	O5-C1	2.73	1.48	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	C1-O5-C5	5.15	119.09	112.19
3	G	1	NAG	C1-O5-C5	5.03	118.93	112.19
3	I	2	NAG	C2-N2-C7	4.55	129.00	122.90
3	K	2	NAG	C2-N2-C7	4.55	129.00	122.90
3	M	1	NAG	C1-O5-C5	4.55	118.28	112.19

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 7 short contacts:

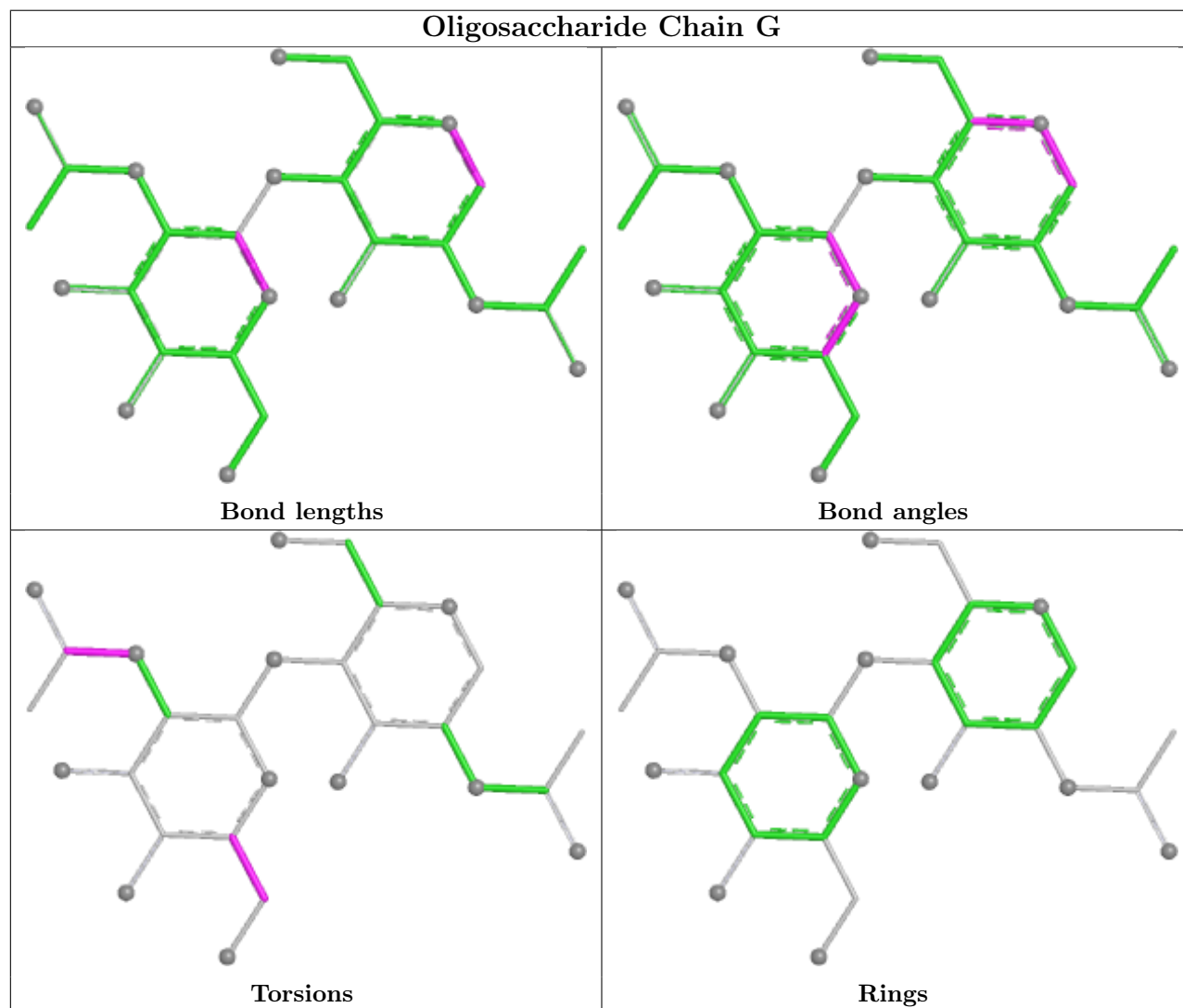
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1	NAG	1	0
3	I	2	NAG	1	0
3	K	2	NAG	1	0

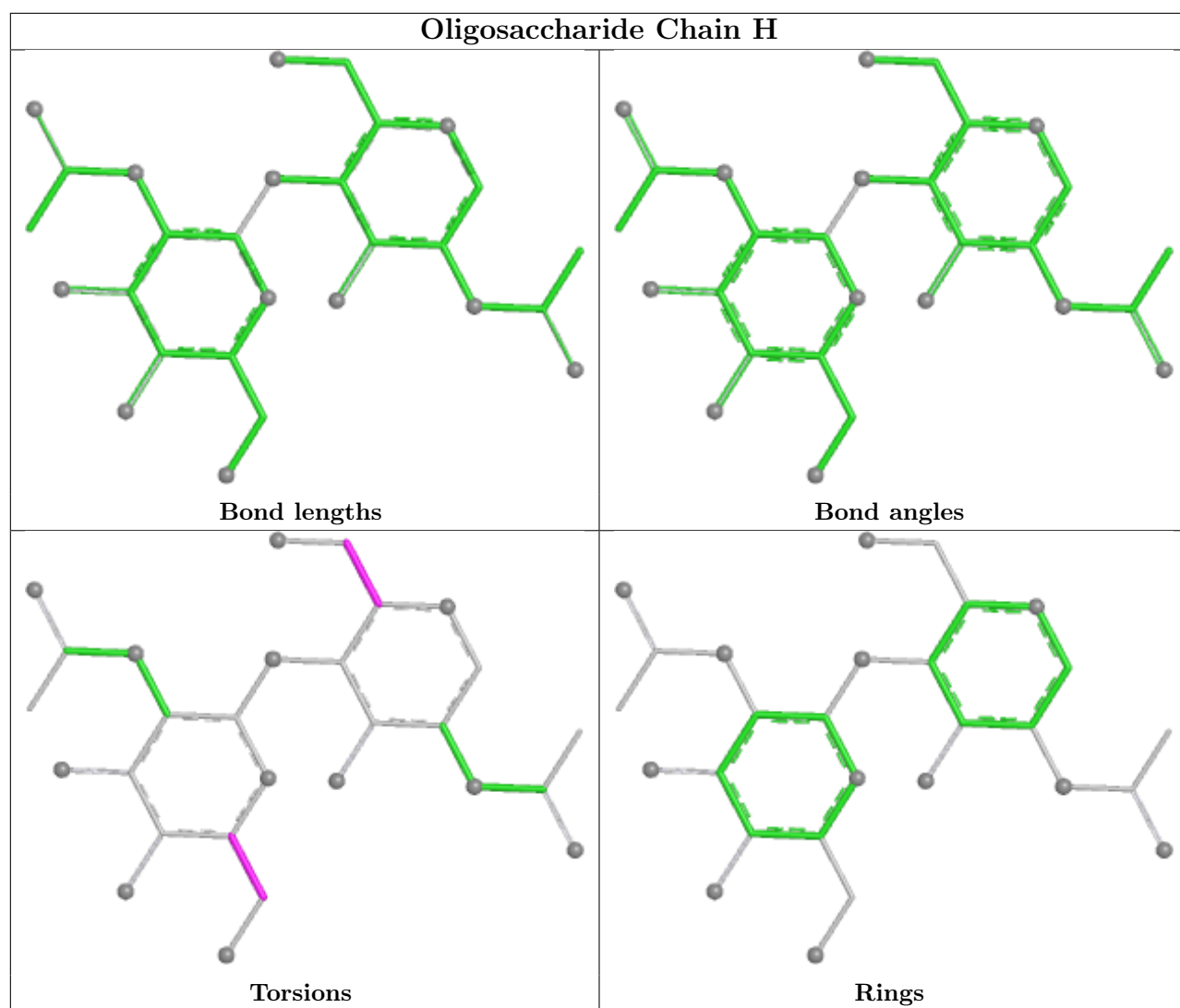
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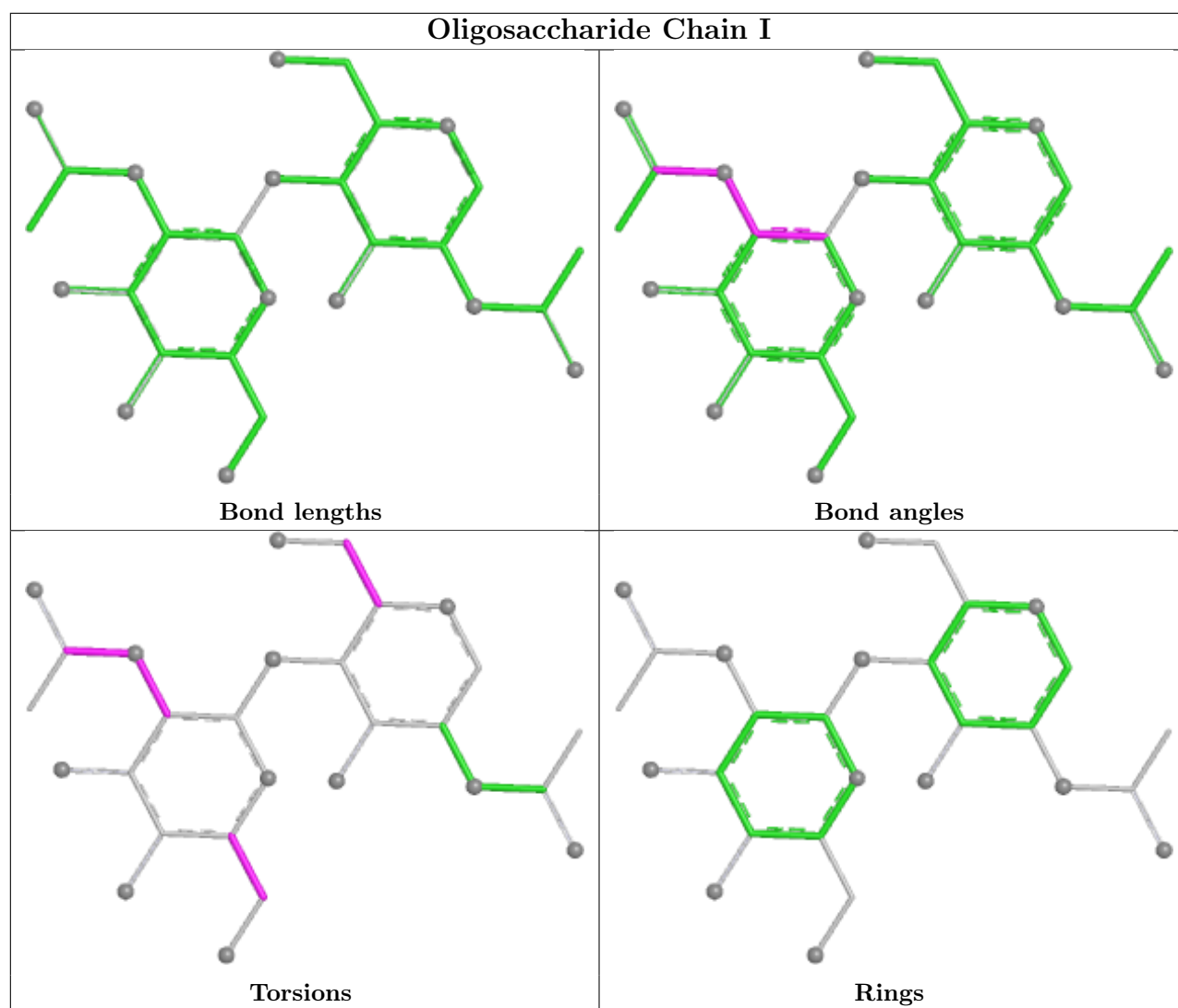
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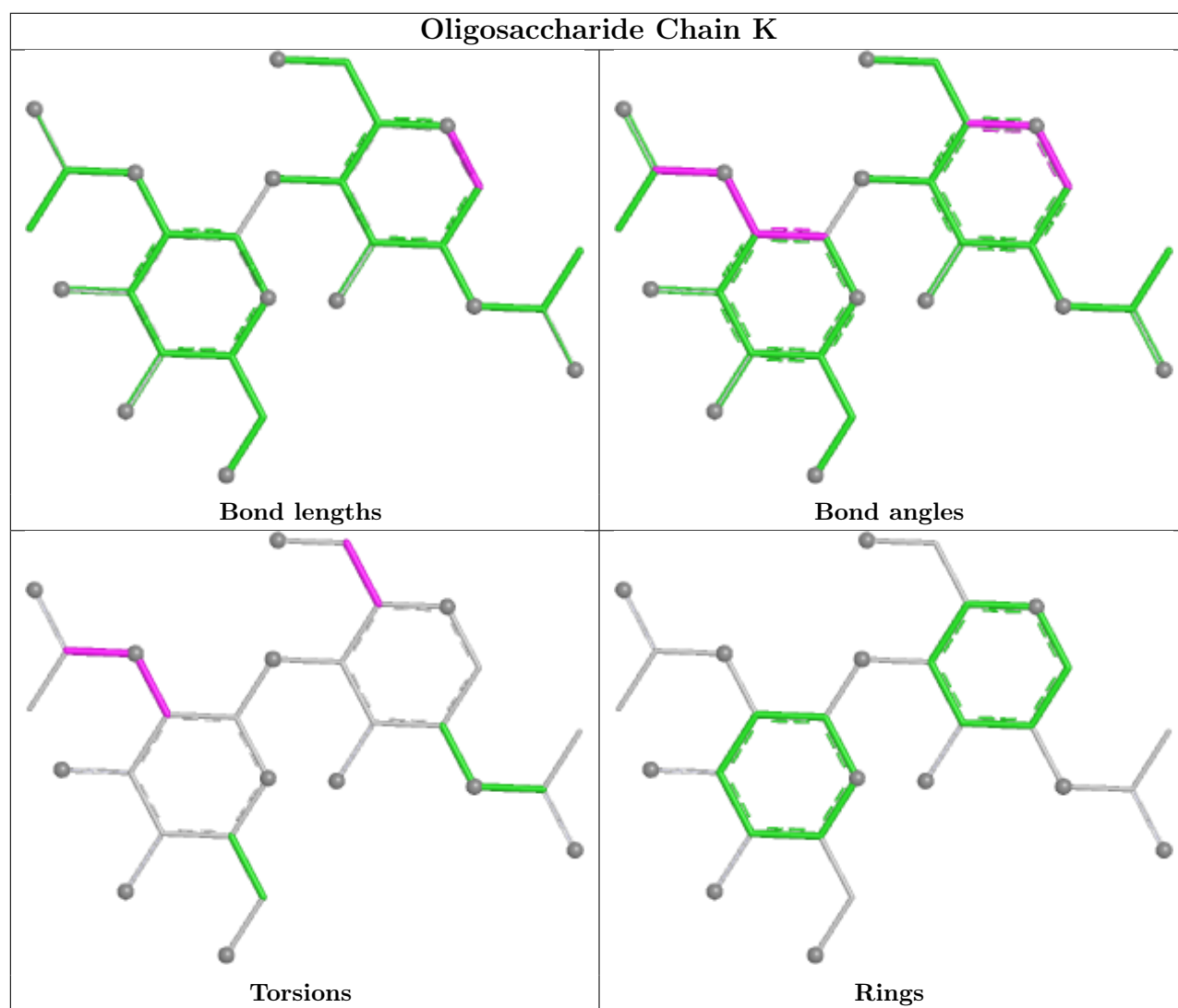
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	1	0
3	P	2	NAG	1	0
3	P	1	NAG	2	0
3	N	2	NAG	1	0

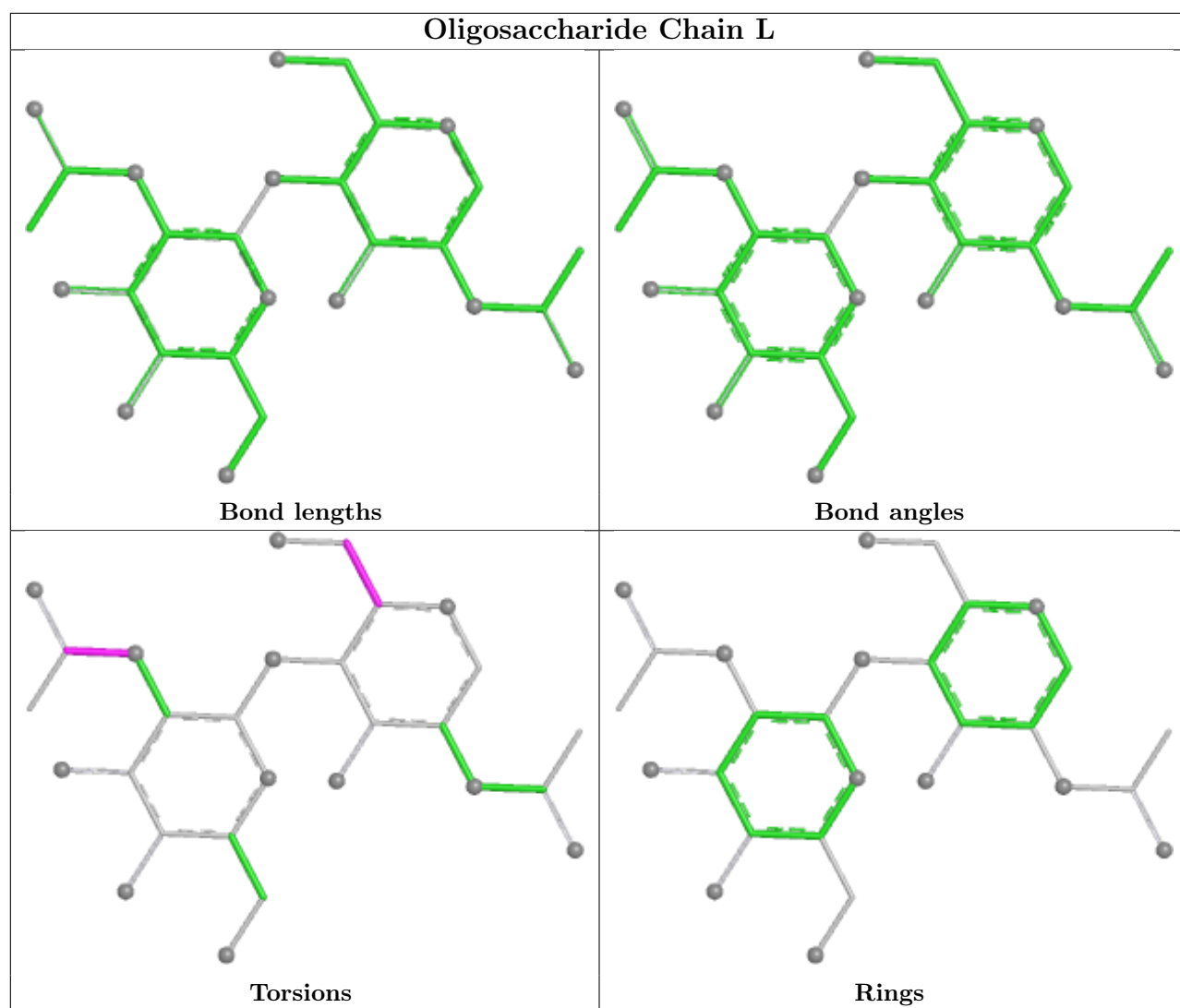
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

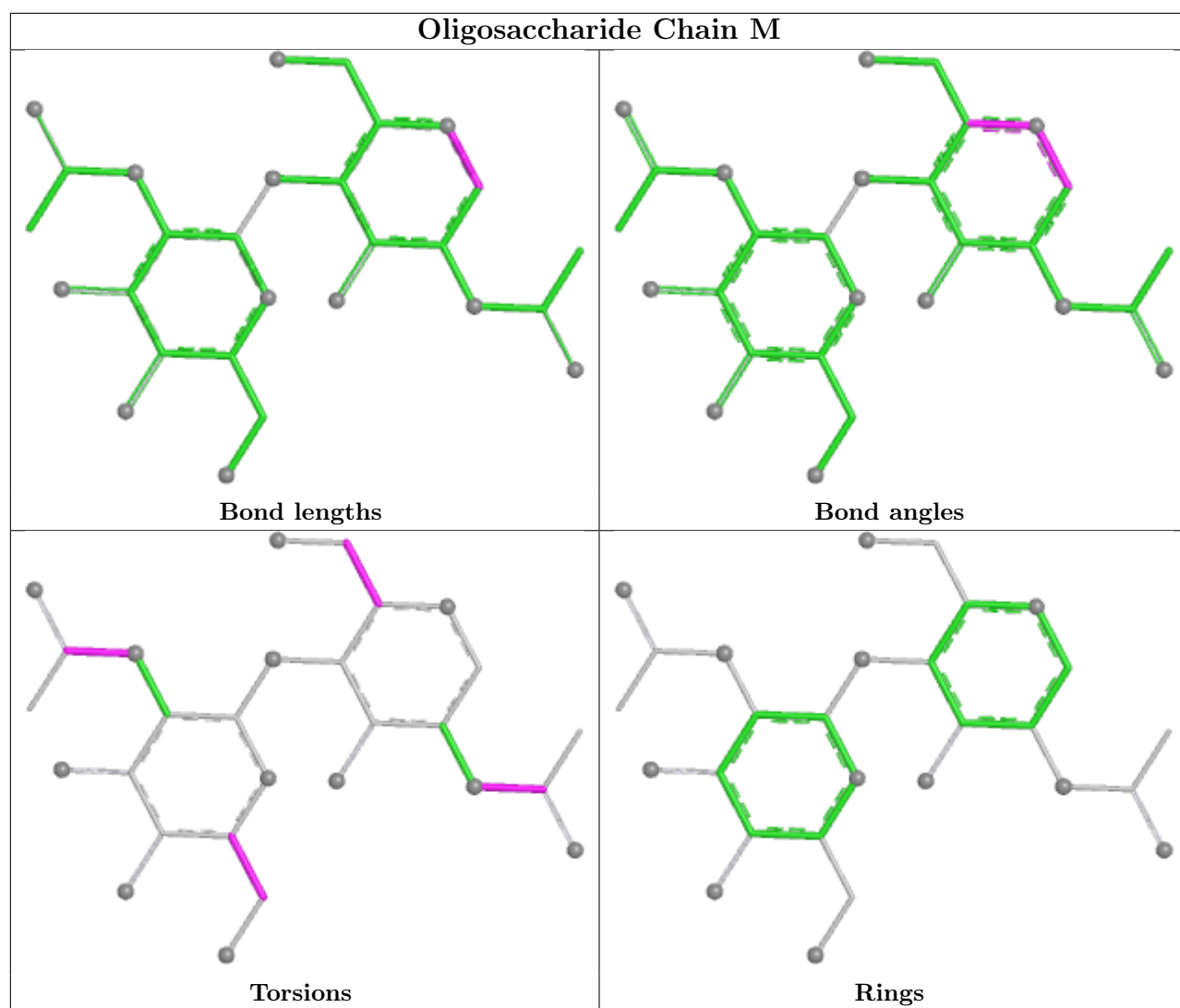


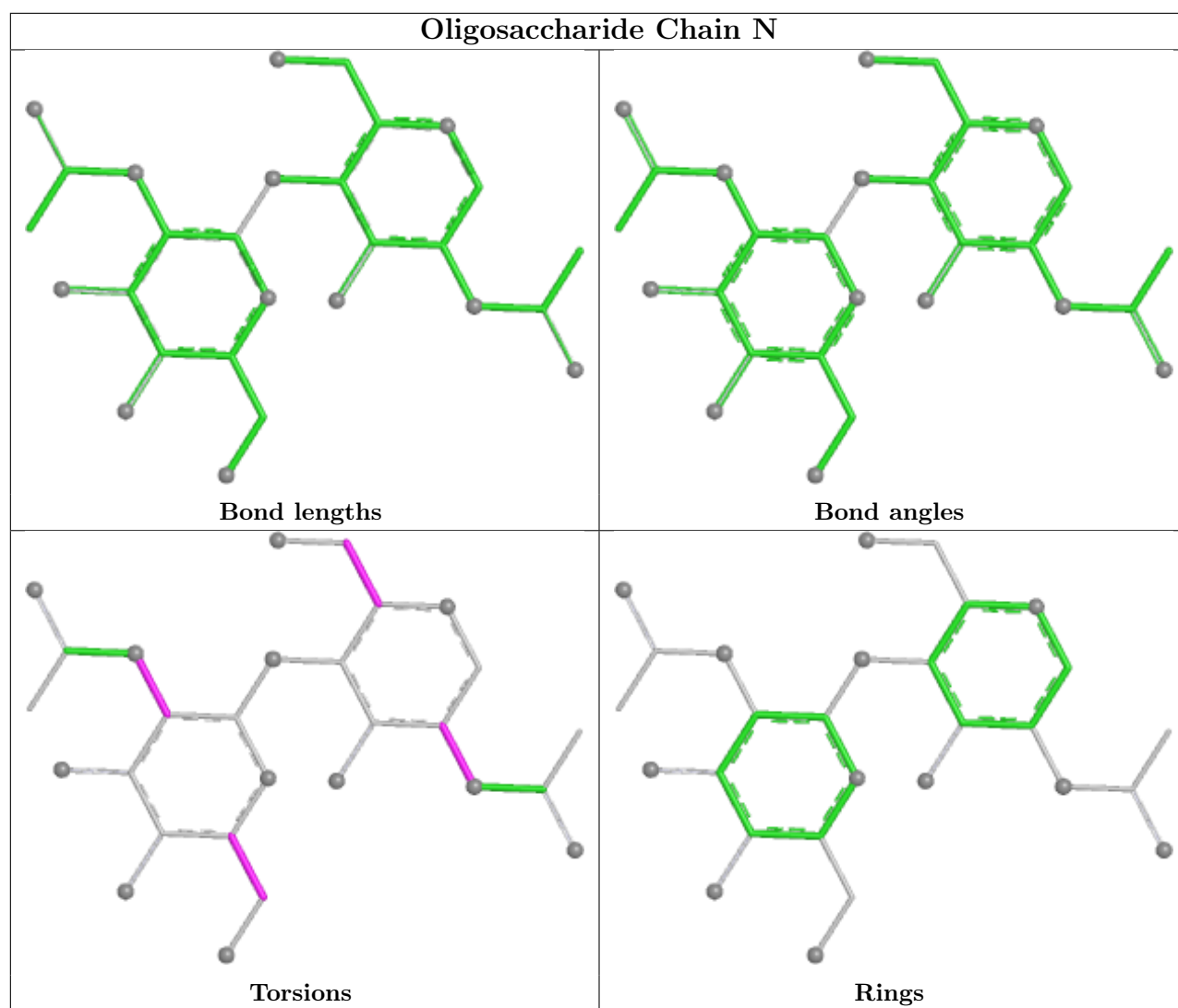


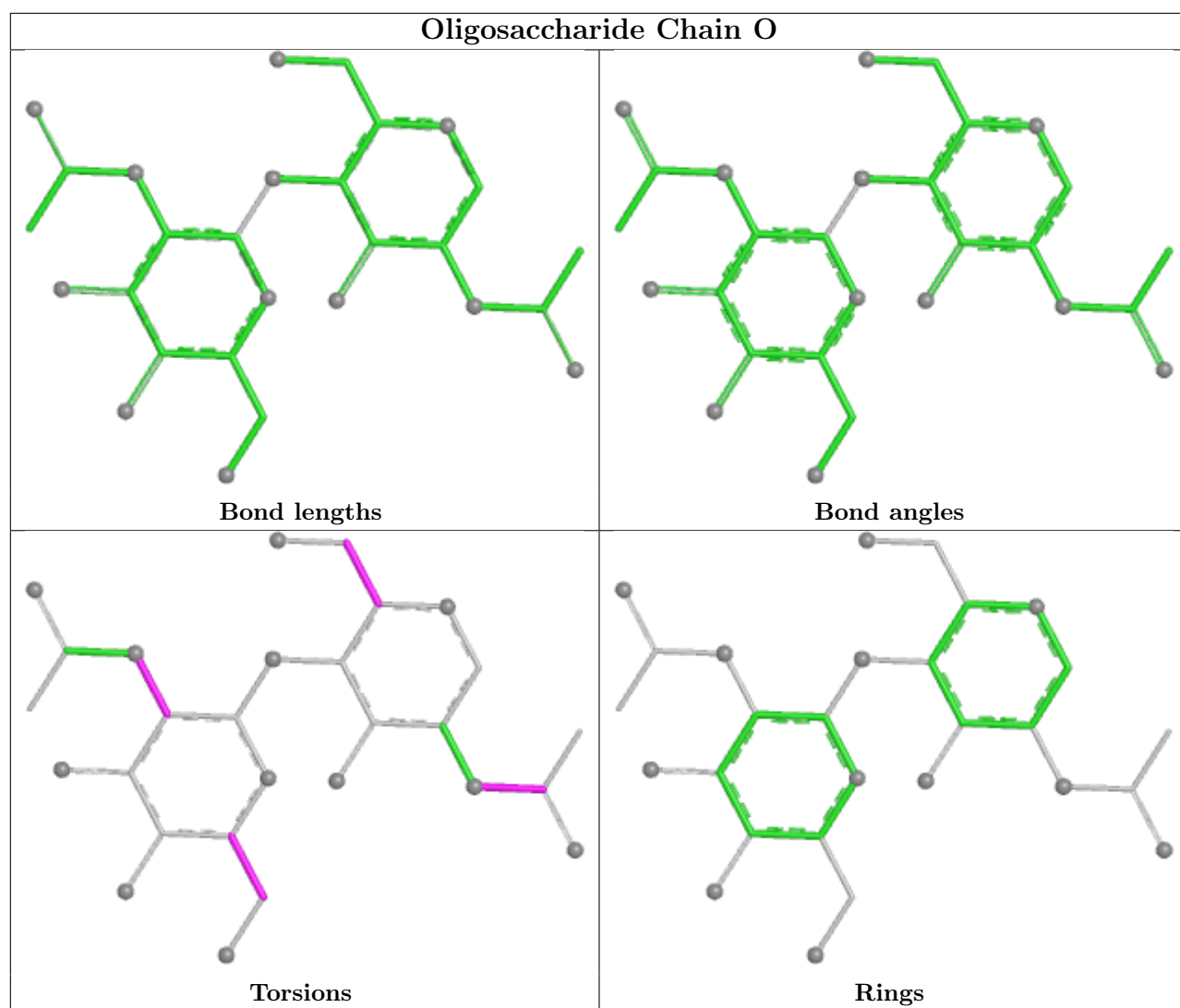


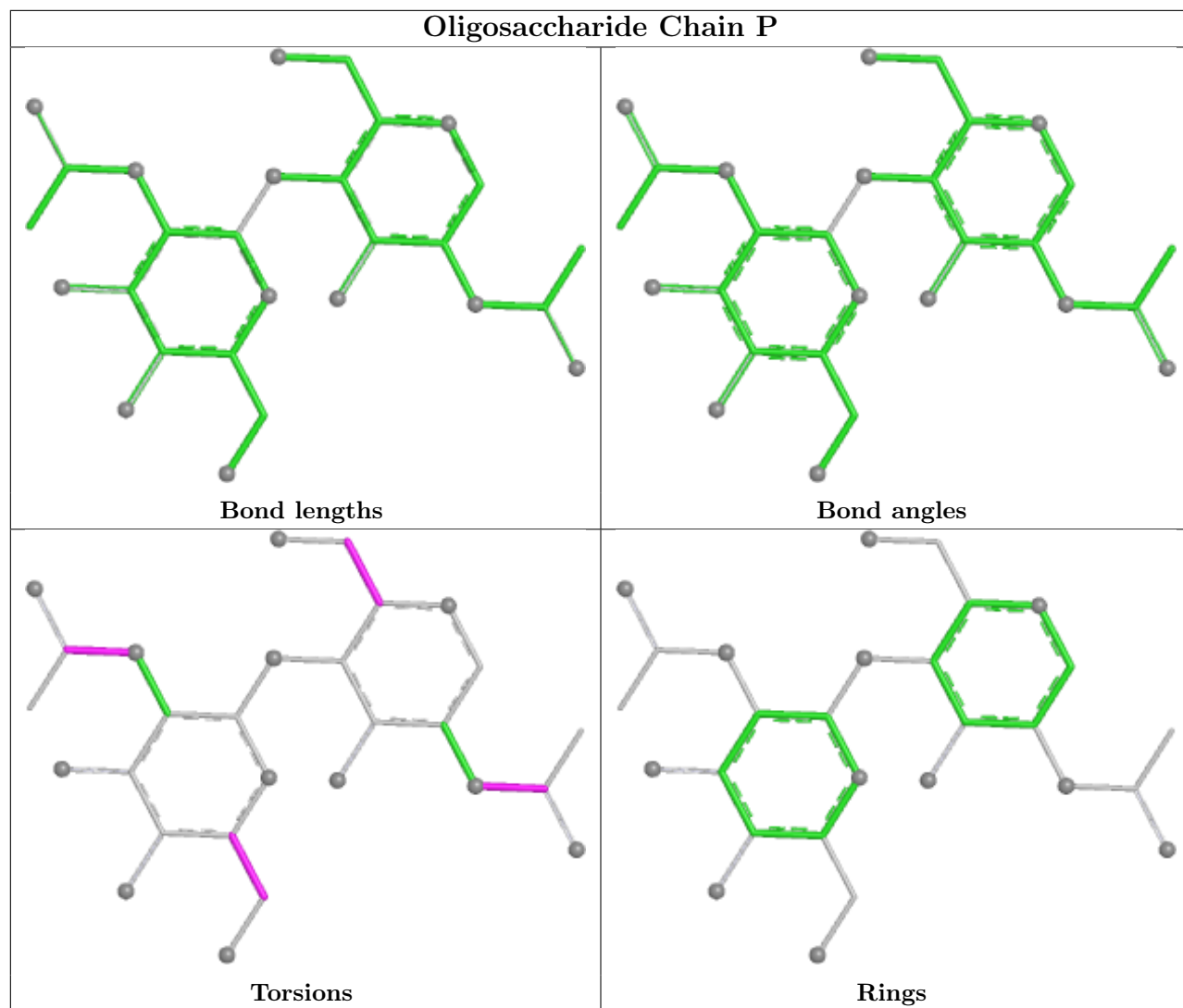


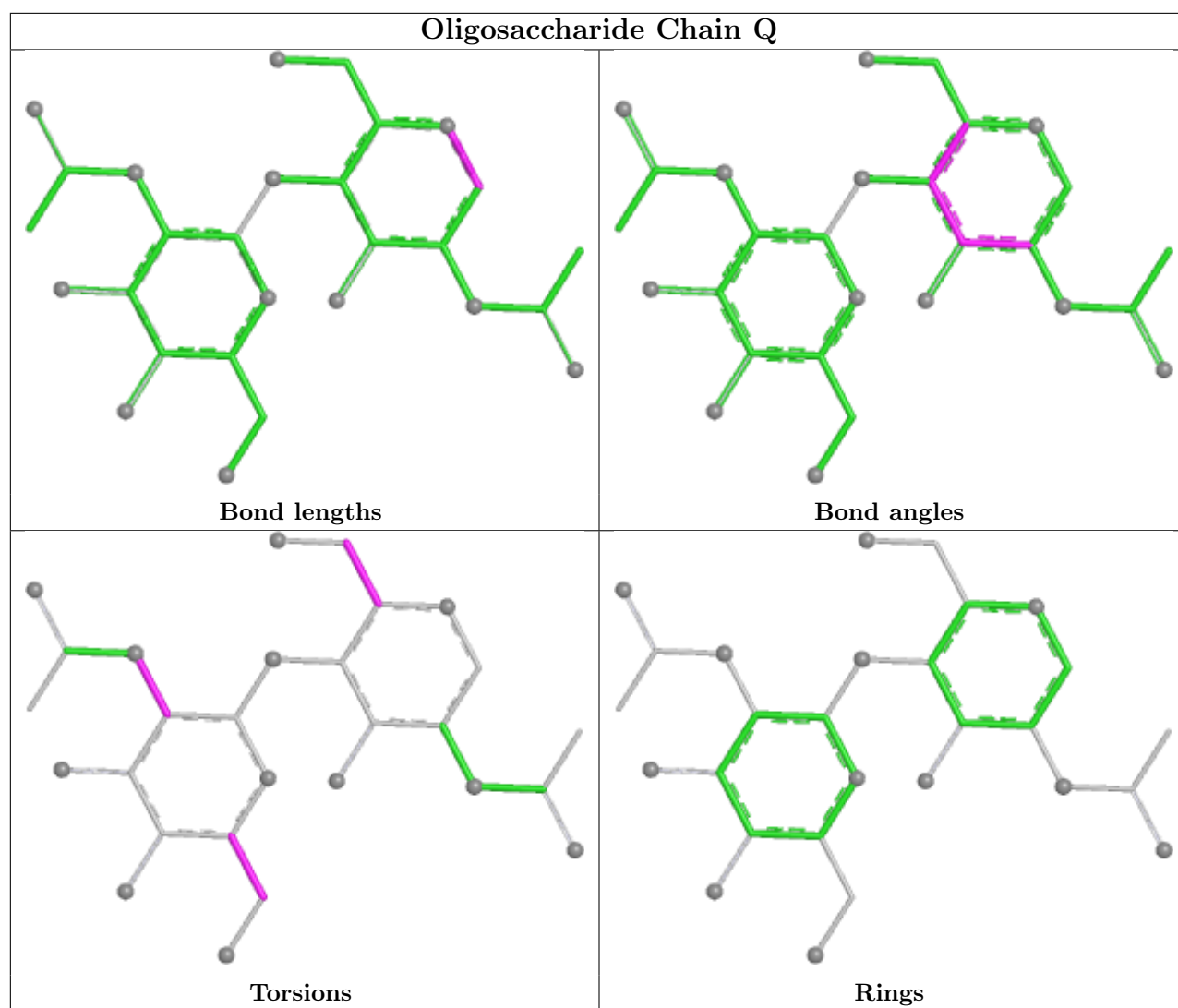


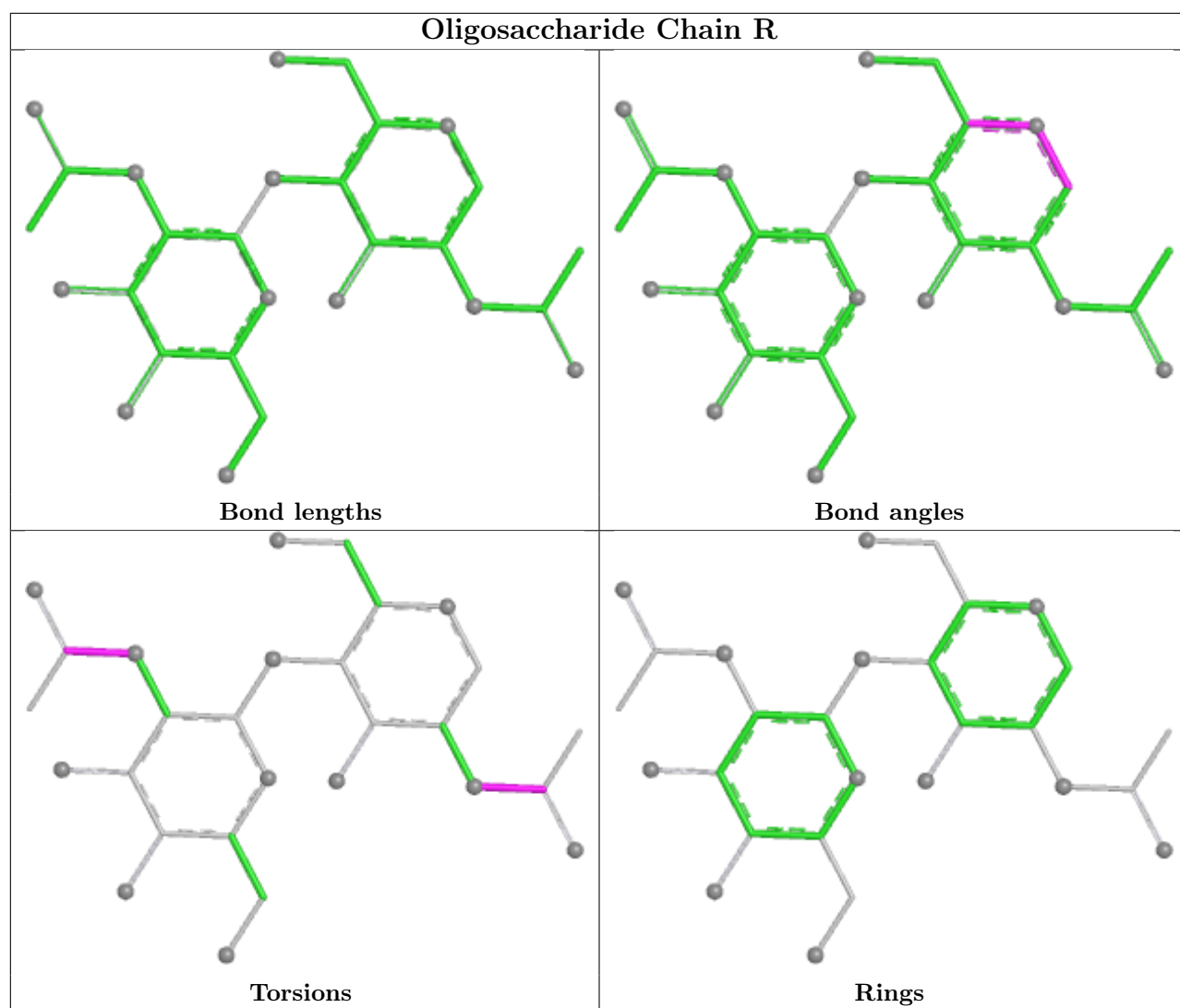


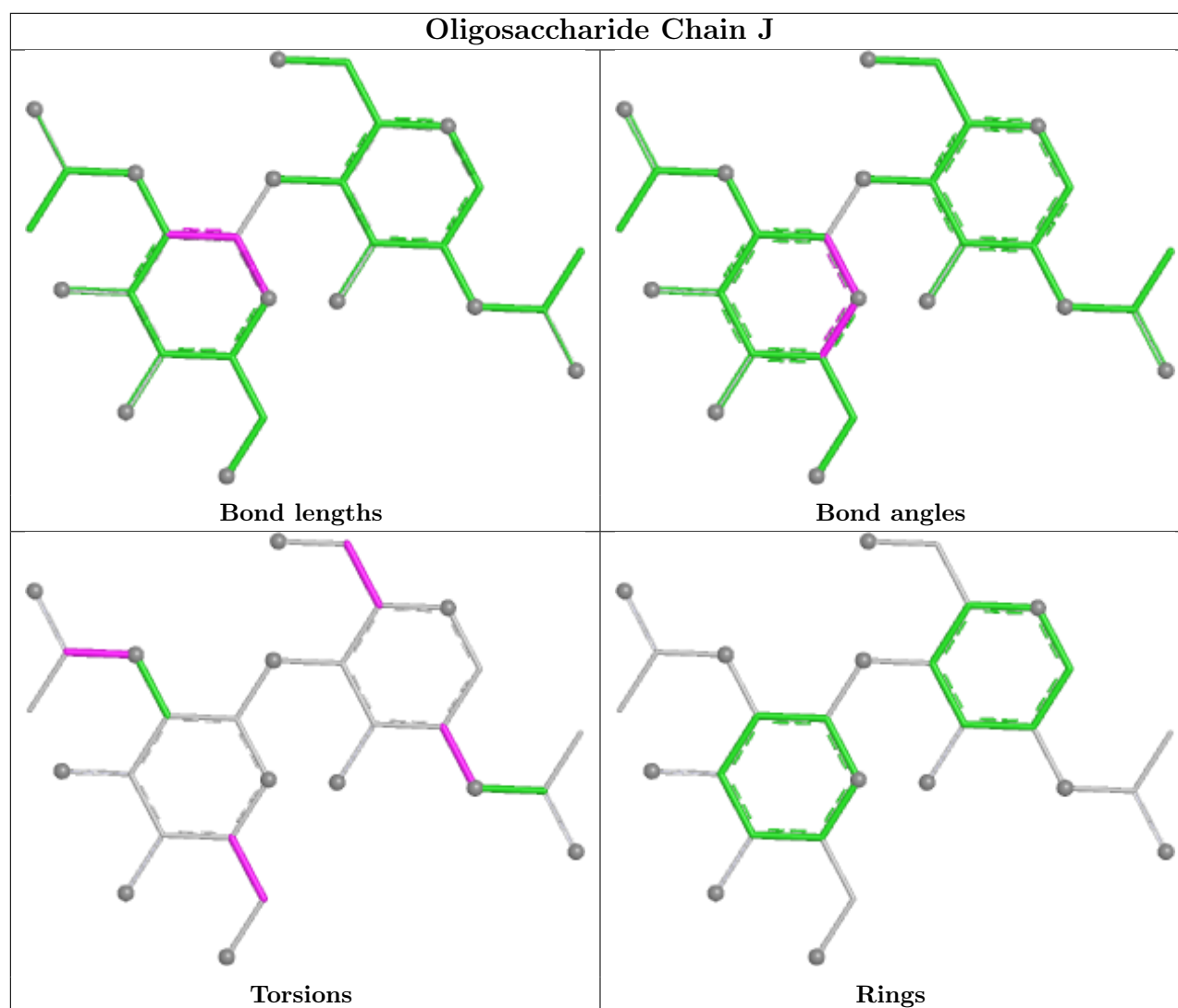












5.6 Ligand geometry [i](#)

33 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	F	1304	2	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	D	1310	2	14,14,15	0.85	1 (7%)	17,19,21	1.07	1 (5%)
4	NAG	B	1306	2	14,14,15	0.42	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	1310	2	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	F	1302	2	14,14,15	0.18	0	17,19,21	0.43	0
4	NAG	B	1304	2	14,14,15	0.43	0	17,19,21	1.32	1 (5%)
4	NAG	B	1307	2	14,14,15	0.75	1 (7%)	17,19,21	0.98	1 (5%)
4	NAG	F	1307	2	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	D	1306	2	14,14,15	0.65	1 (7%)	17,19,21	0.85	1 (5%)
4	NAG	D	1309	2	14,14,15	0.22	0	17,19,21	0.39	0
4	NAG	D	1307	2	14,14,15	0.20	0	17,19,21	0.46	0
4	NAG	B	1305	2	14,14,15	0.64	1 (7%)	17,19,21	0.71	0
4	NAG	D	1308	2	14,14,15	0.19	0	17,19,21	0.49	0
4	NAG	D	1312	2	14,14,15	0.35	0	17,19,21	0.34	0
4	NAG	F	1303	2	14,14,15	0.37	0	17,19,21	1.26	1 (5%)
4	NAG	B	1301	2	14,14,15	0.49	0	17,19,21	0.38	0
4	NAG	D	1302	2	14,14,15	0.90	2 (14%)	17,19,21	0.88	1 (5%)
4	NAG	D	1305	2	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	D	1301	2	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	D	1304	2	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	B	1310	2	14,14,15	0.22	0	17,19,21	0.58	0
4	NAG	F	1308	2	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	F	1311	2	14,14,15	0.91	1 (7%)	17,19,21	1.54	3 (17%)
4	NAG	B	1308	2	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	D	1311	2	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	B	1303	2	14,14,15	0.30	0	17,19,21	1.35	1 (5%)
4	NAG	F	1301	2	14,14,15	0.21	0	17,19,21	0.50	0
4	NAG	F	1309	2	14,14,15	0.28	0	17,19,21	0.49	0
4	NAG	B	1309	2	14,14,15	0.34	0	17,19,21	0.52	0
4	NAG	F	1305	2	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	F	1306	2	14,14,15	0.39	0	17,19,21	1.27	1 (5%)
4	NAG	D	1303	2	14,14,15	0.58	0	17,19,21	0.96	2 (11%)
4	NAG	B	1302	2	14,14,15	0.34	0	17,19,21	0.33	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	F	1304	2	-	2/6/23/26	0/1/1/1
4	NAG	D	1310	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1310	2	-	4/6/23/26	0/1/1/1
4	NAG	F	1302	2	-	3/6/23/26	0/1/1/1
4	NAG	B	1304	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	2	-	2/6/23/26	0/1/1/1
4	NAG	F	1307	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1306	2	-	2/6/23/26	0/1/1/1
4	NAG	D	1309	2	-	2/6/23/26	0/1/1/1
4	NAG	D	1307	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	2	-	4/6/23/26	0/1/1/1
4	NAG	D	1308	2	-	2/6/23/26	0/1/1/1
4	NAG	D	1312	2	-	2/6/23/26	0/1/1/1
4	NAG	F	1303	2	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	2	-	4/6/23/26	0/1/1/1
4	NAG	D	1302	2	-	3/6/23/26	0/1/1/1
4	NAG	D	1305	2	-	1/6/23/26	0/1/1/1
4	NAG	D	1301	2	-	2/6/23/26	0/1/1/1
4	NAG	D	1304	2	-	1/6/23/26	0/1/1/1
4	NAG	B	1310	2	-	2/6/23/26	0/1/1/1
4	NAG	F	1308	2	-	2/6/23/26	0/1/1/1
4	NAG	F	1311	2	-	3/6/23/26	0/1/1/1
4	NAG	B	1308	2	-	2/6/23/26	0/1/1/1
4	NAG	D	1311	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	2	-	0/6/23/26	0/1/1/1
4	NAG	F	1301	2	-	4/6/23/26	0/1/1/1
4	NAG	F	1309	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	2	-	2/6/23/26	0/1/1/1
4	NAG	F	1305	2	-	2/6/23/26	0/1/1/1
4	NAG	F	1306	2	-	1/6/23/26	0/1/1/1
4	NAG	D	1303	2	-	4/6/23/26	0/1/1/1
4	NAG	B	1302	2	-	2/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1310	NAG	O5-C1	2.76	1.48	1.43
4	F	1311	NAG	C1-C2	2.74	1.56	1.52
4	D	1302	NAG	O5-C1	2.52	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1307	NAG	O5-C1	2.42	1.47	1.43
4	B	1305	NAG	O5-C1	-2.27	1.39	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1304	NAG	C1-O5-C5	5.06	118.96	112.19
4	B	1303	NAG	C1-O5-C5	4.97	118.84	112.19
4	F	1306	NAG	C1-O5-C5	4.87	118.71	112.19
4	F	1311	NAG	C1-O5-C5	4.86	118.70	112.19
4	F	1303	NAG	C1-O5-C5	4.79	118.61	112.19

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1311	NAG	C1-C2-N2-C7
4	F	1309	NAG	C4-C5-C6-O6
4	D	1308	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1310	NAG	2	0
4	F	1302	NAG	1	0
4	B	1304	NAG	1	0
4	F	1307	NAG	2	0
4	D	1307	NAG	1	0
4	F	1311	NAG	2	0
4	D	1303	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

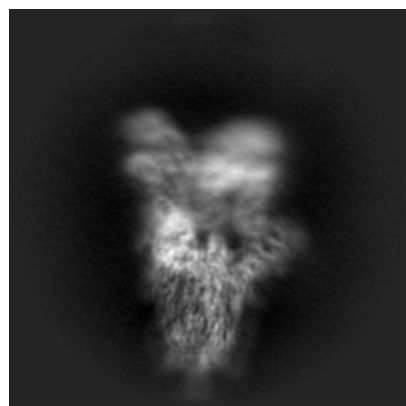
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44725. These allow visual inspection of the internal detail of the map and identification of artifacts.

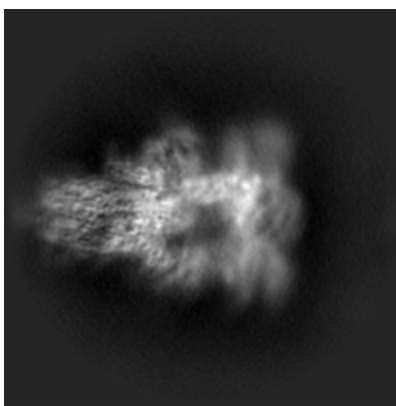
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

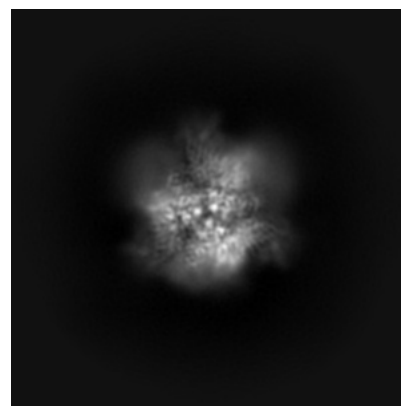
6.1.1 Primary map



X

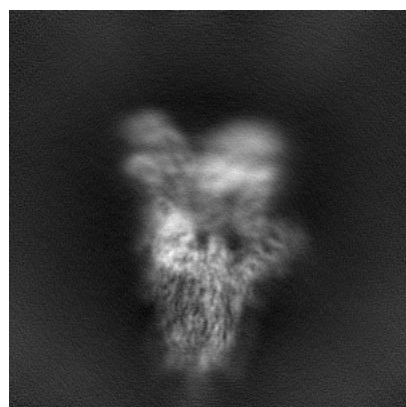


Y



Z

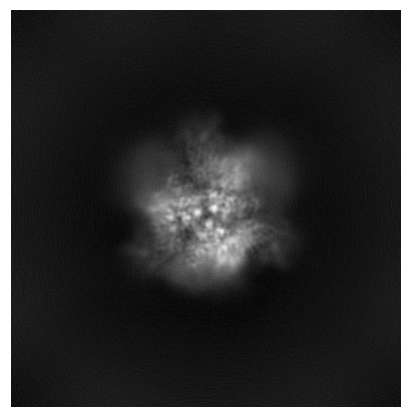
6.1.2 Raw map



X



Y

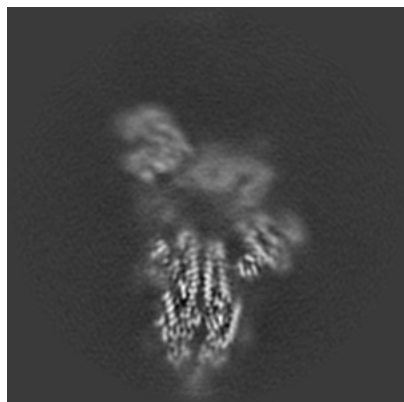


Z

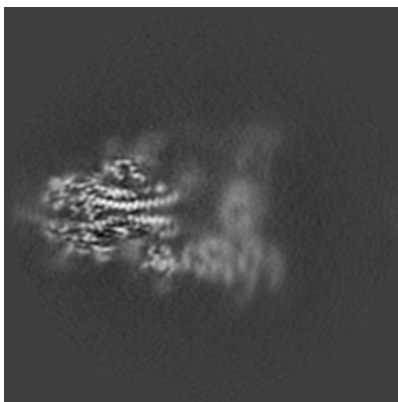
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

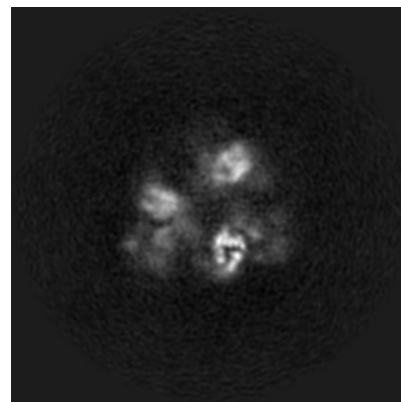
6.2.1 Primary map



X Index: 192

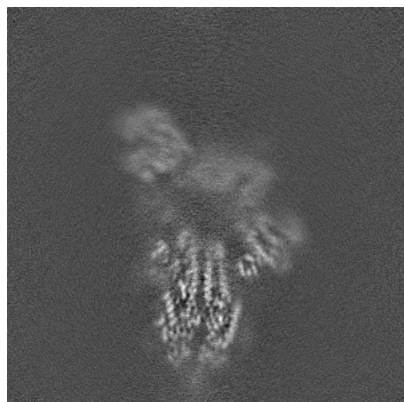


Y Index: 192

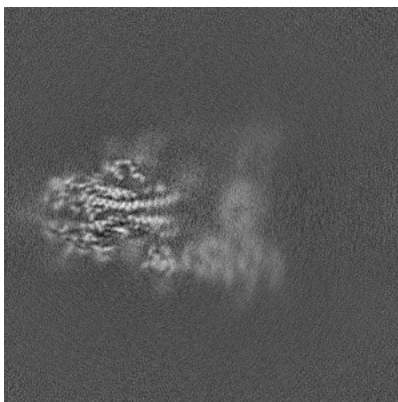


Z Index: 192

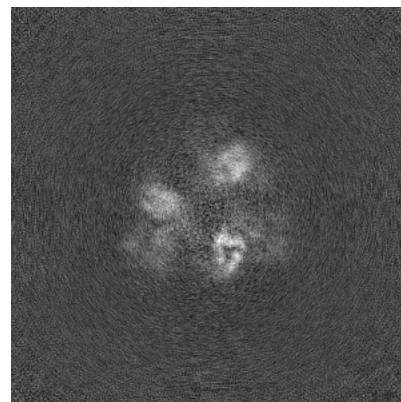
6.2.2 Raw map



X Index: 192



Y Index: 192

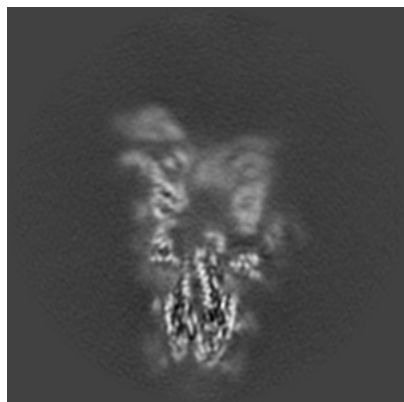


Z Index: 192

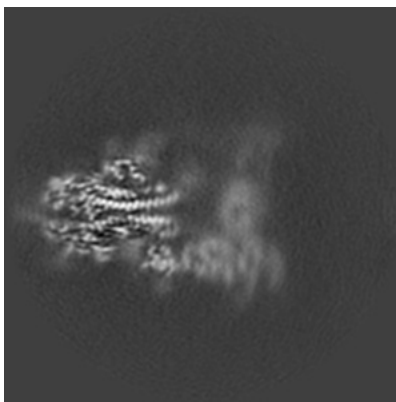
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

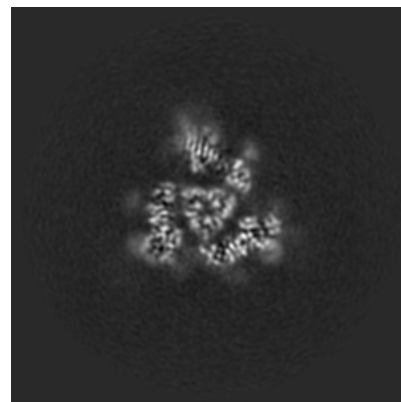
6.3.1 Primary map



X Index: 204

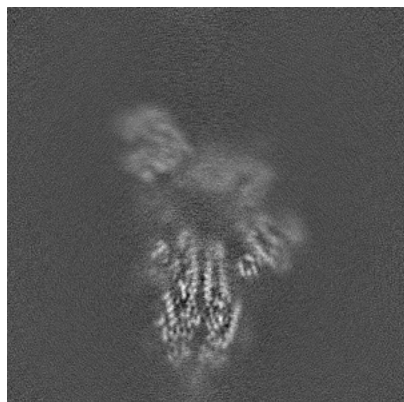


Y Index: 192

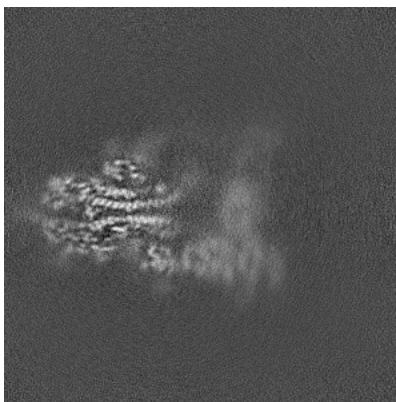


Z Index: 148

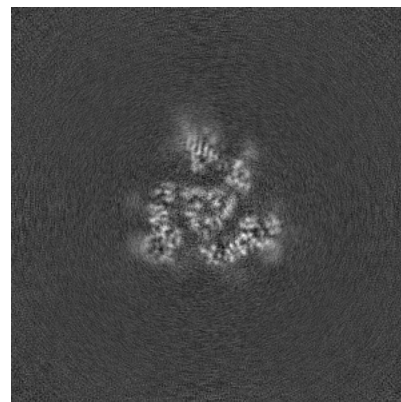
6.3.2 Raw map



X Index: 192



Y Index: 191



Z Index: 148

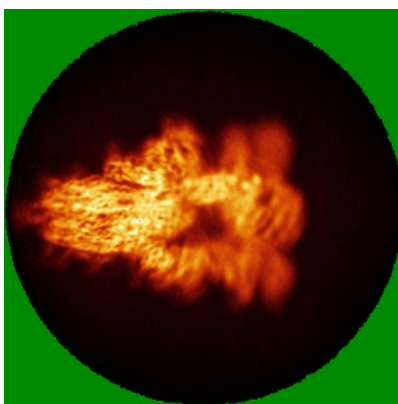
The images above show the largest variance slices of the map in three orthogonal directions.

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

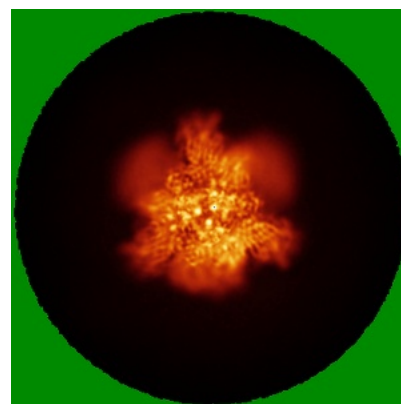
6.4.1 Primary map



X

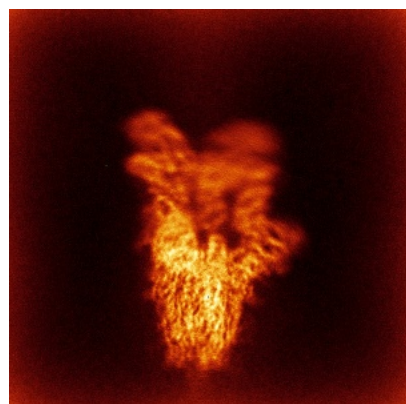


Y

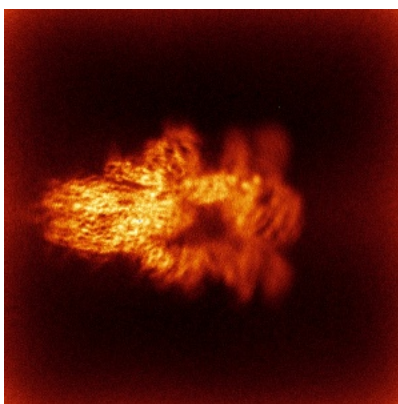


Z

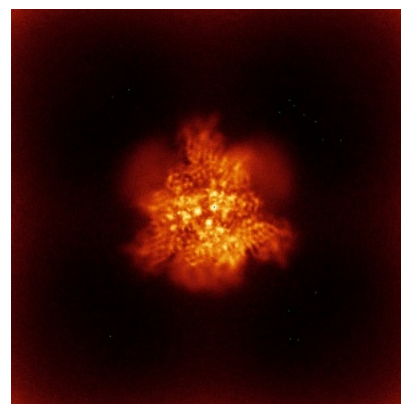
6.4.2 Raw map



X



Y



Z

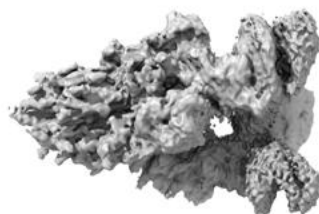
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



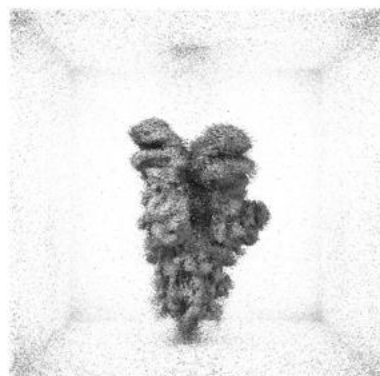
Y



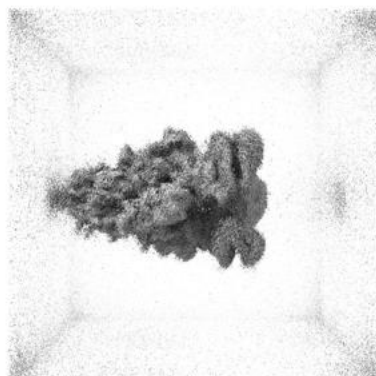
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

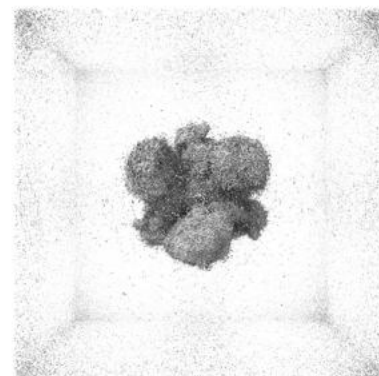
6.5.2 Raw map



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.

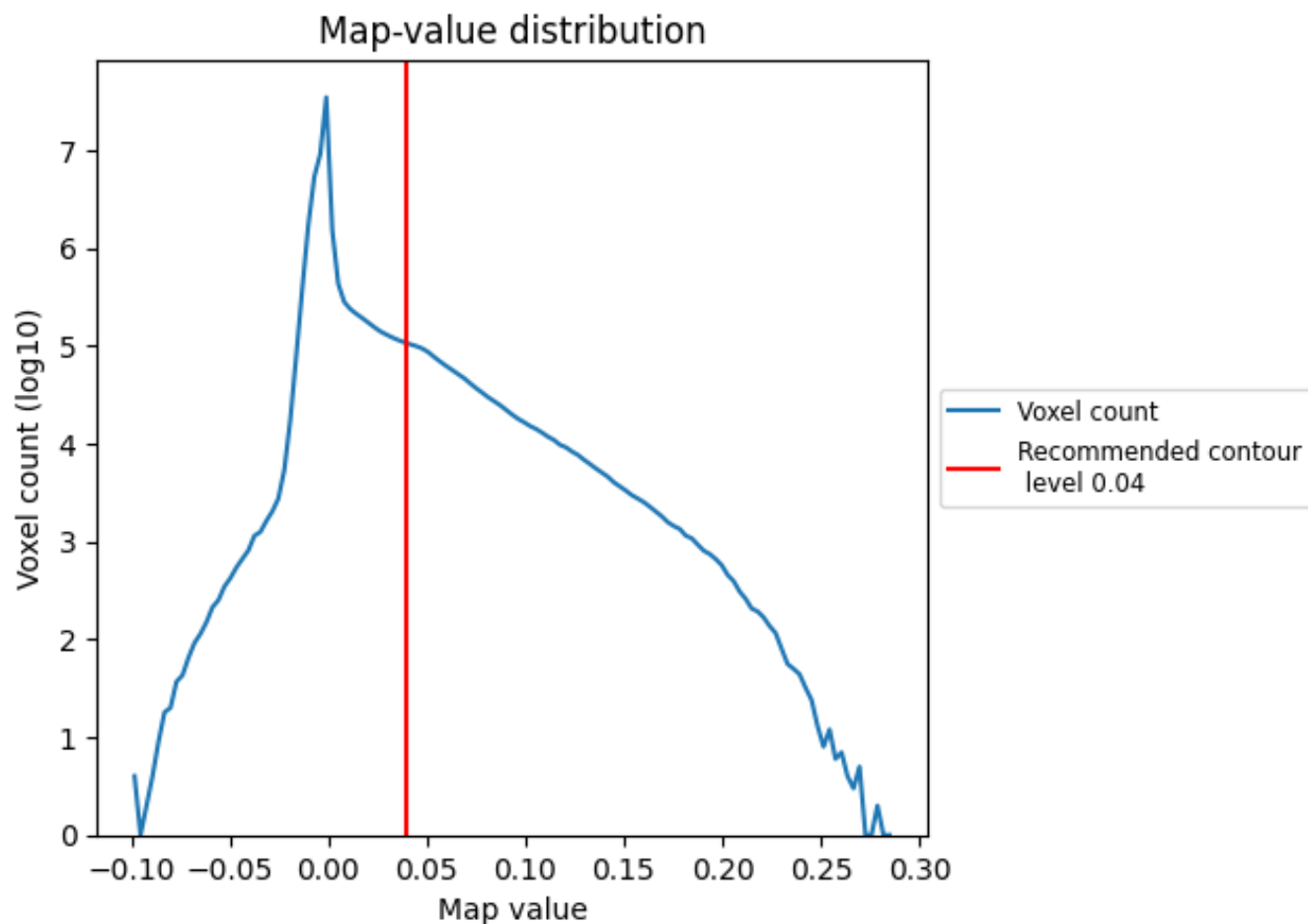
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

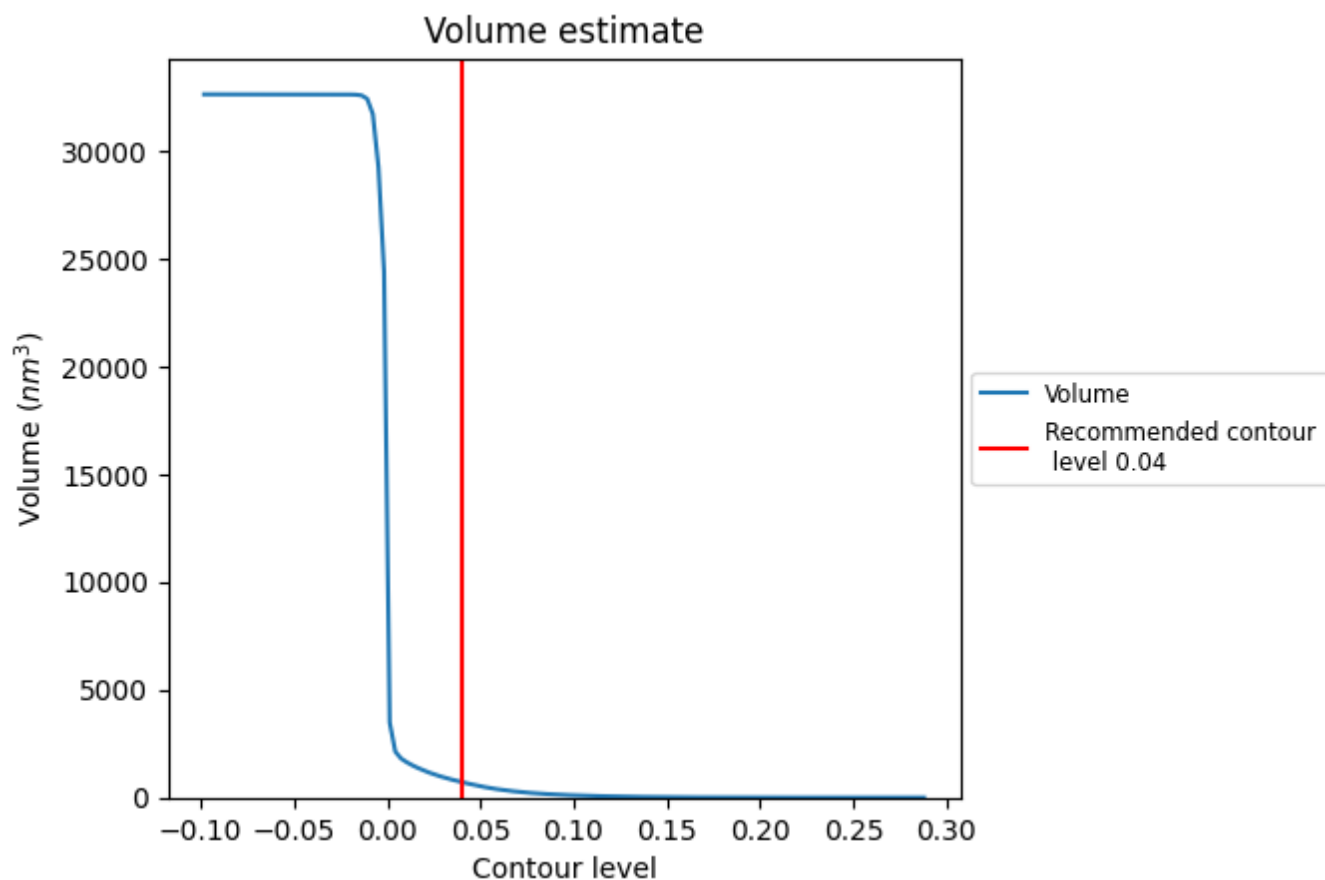
This section contains the results of statistical analysis of the map.

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.

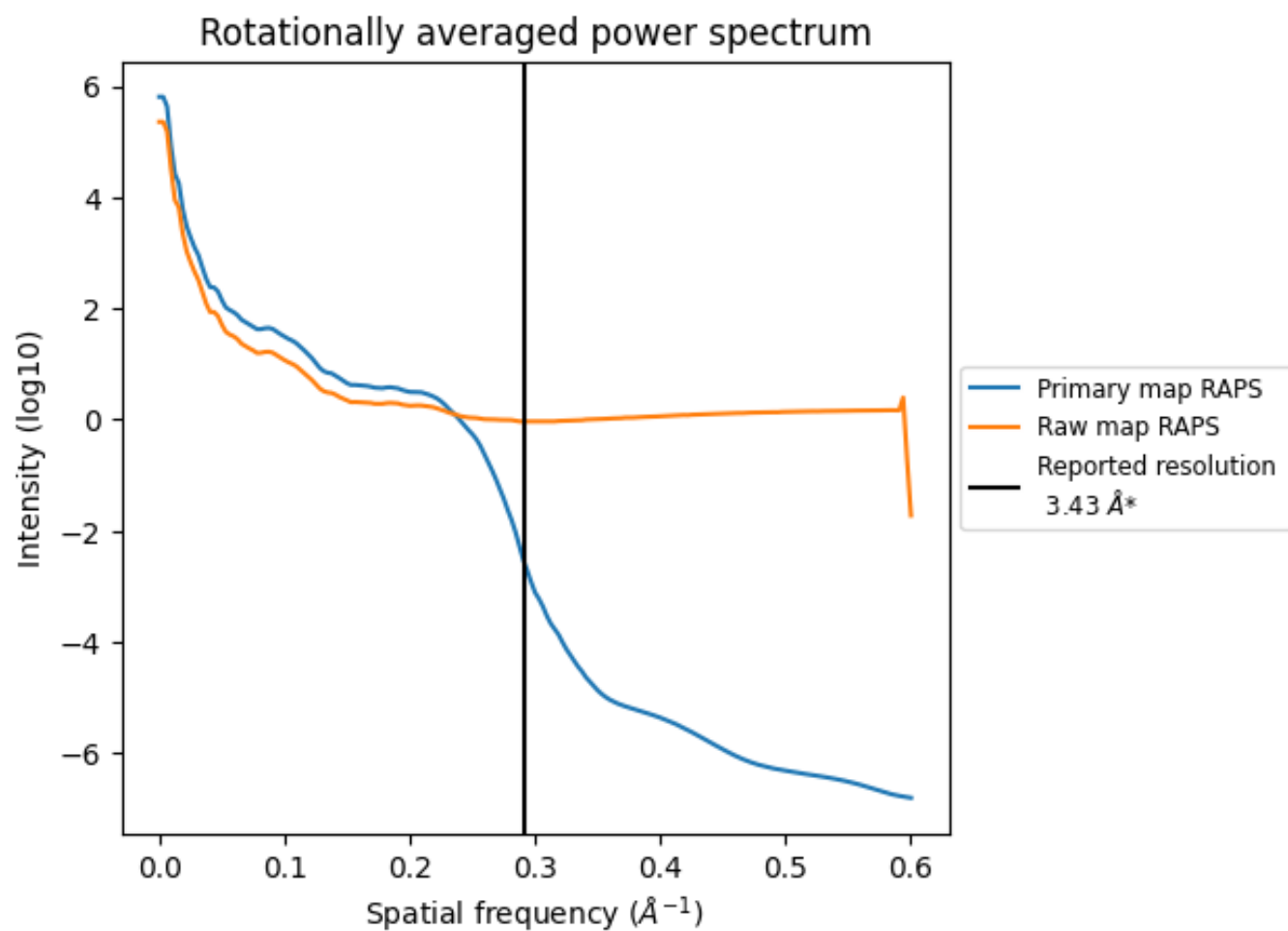
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 717 nm³; this corresponds to an approximate mass of 647 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 ⓘ

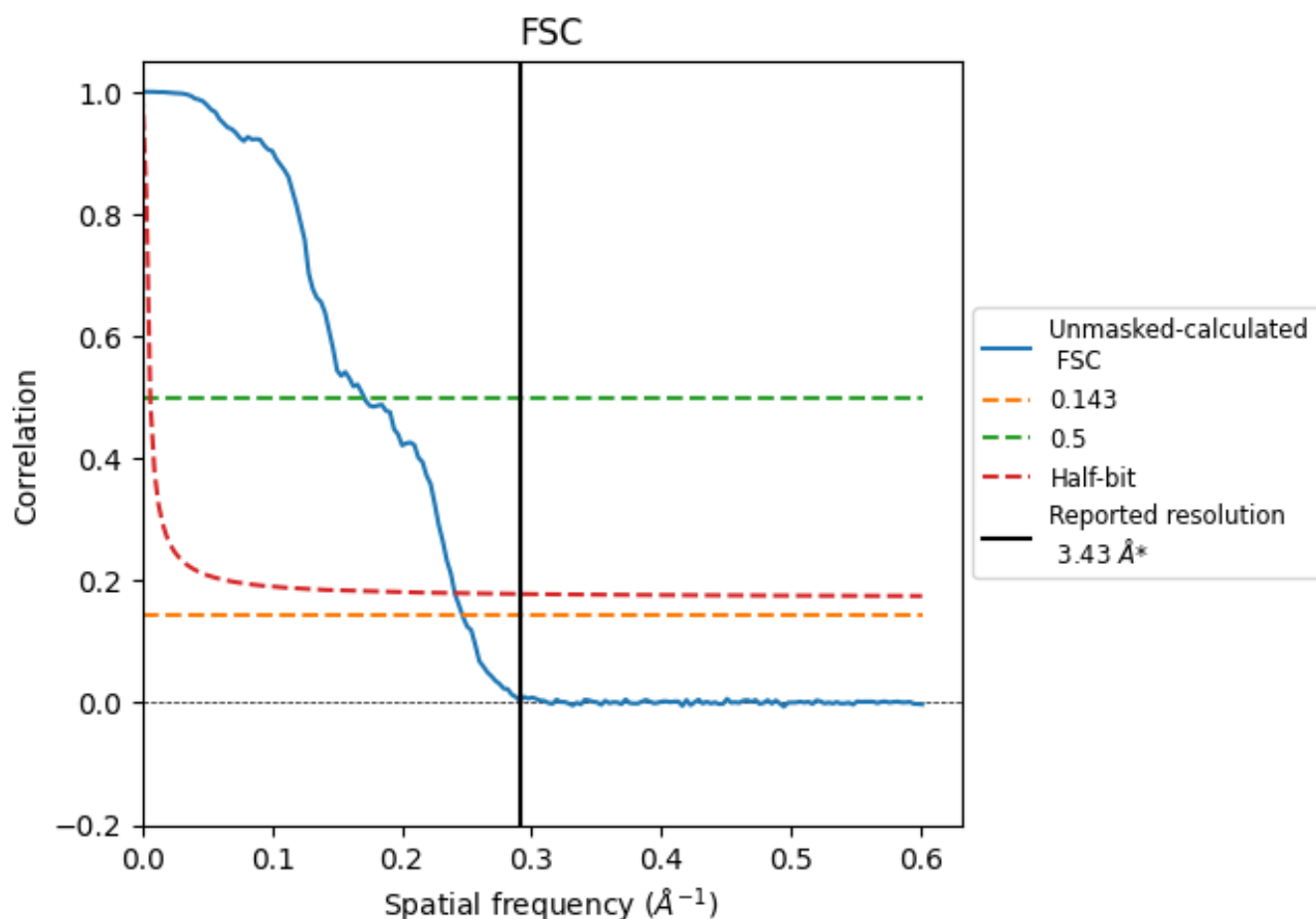


*Reported resolution corresponds to spatial frequency of 0.292 \AA^{-1}

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 0.292 Å⁻¹

8.2 Resolution estimates [i](#)

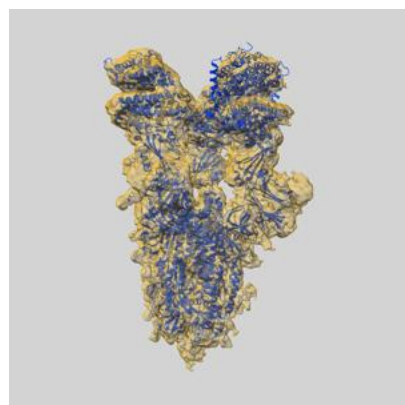
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.43	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.05	5.85	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.43 by more than 10 %

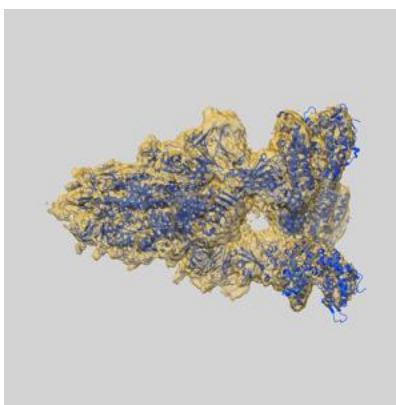
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44725 and PDB model 9BNE. Per-residue inclusion information can be found in section 3 on page 16.

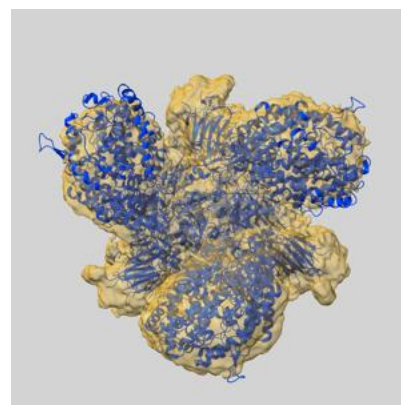
9.1 Map-model overlay [i](#)



X



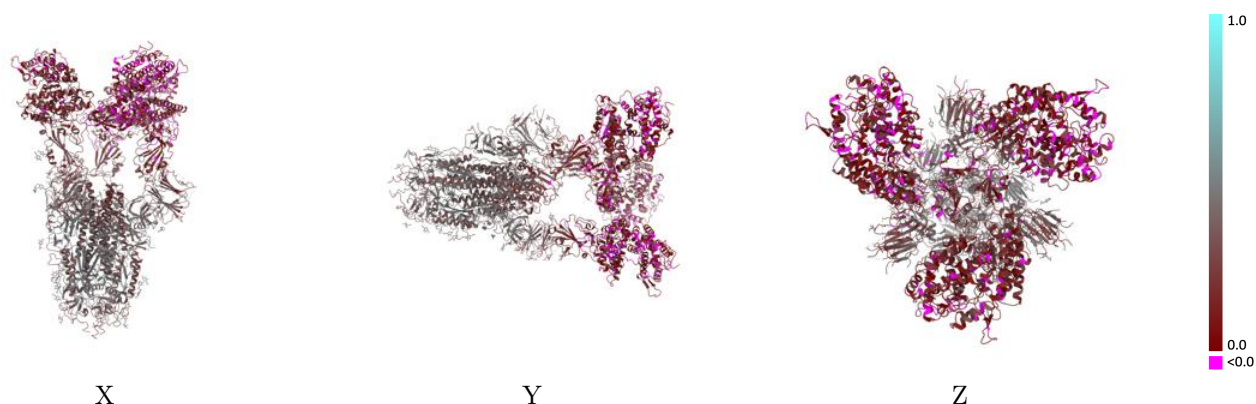
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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](#)

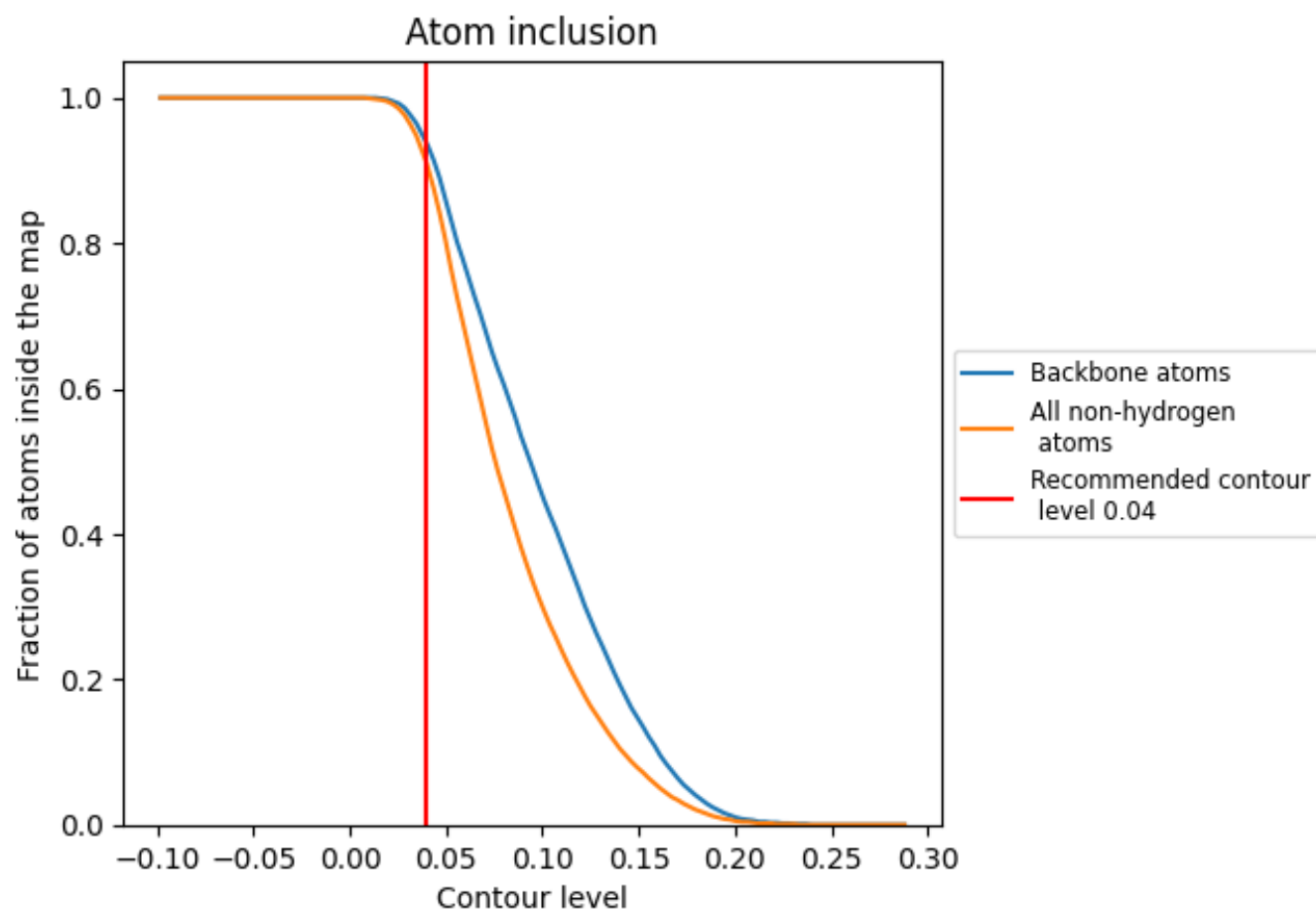


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.







































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.2670
A	 0.7190	 0.1040
B	 0.9730	 0.3440
C	 0.7660	 0.1100
D	 0.9730	 0.3550
E	 0.9480	 0.1680
F	 0.9720	 0.3730
G	 0.9640	 0.3980
H	 0.9640	 0.2580
I	 0.8570	 0.3360
J	 0.8570	 0.4060
K	 1.0000	 0.4580
L	 0.9640	 0.4830
M	 0.9640	 0.4050
N	 0.9290	 0.3690
O	 1.0000	 0.4030
P	 1.0000	 0.3690
Q	 0.8210	 0.3740
R	 0.9290	 0.3650

