



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:53 PM UTC

PDB ID : 9AU2 / pdb_00009au2
EMDB ID : EMD-43842
Title : VIR-7229 Fab fragment bound the BA.2.86 spike trimer (global refinement)
Authors : Tortorici, M.A.; Park, Y.J.; Veelser, D.; Seattle Structural Genomics Center
for Infectious Disease (SSGCID)
Deposited on : 2024-02-28
Resolution : 3.10 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:

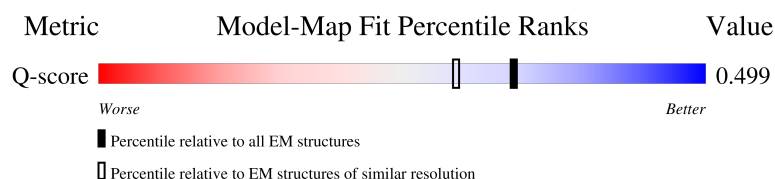
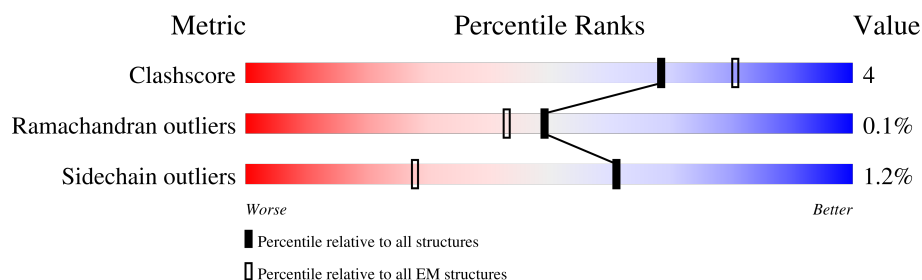
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.10 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.



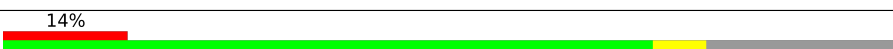
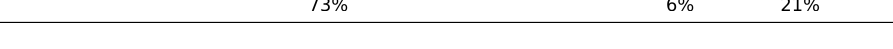
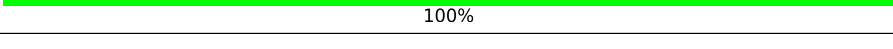
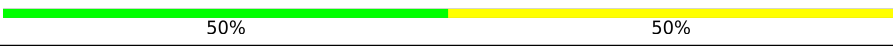
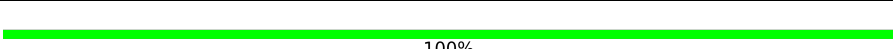
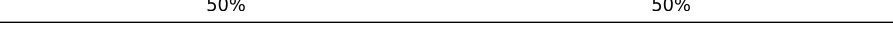
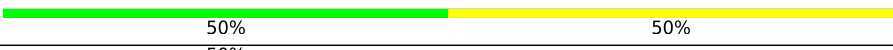
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	D	226	
1	F	226	
2	I	216	
2	J	216	

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Mol	Chain	Length	Quality of chain
3	A	1273	
3	B	1273	
3	C	1273	
4	E	2	
4	G	2	
4	H	2	
4	K	2	
4	L	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23745 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 VIR-7229 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	120	Total	C	N	O	S	0	0
			595	353	120	120	2		
1	F	120	Total	C	N	O	S	0	0
			596	353	120	121	2		

- Molecule 2 is a protein called VIR-7229 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	108	Total	C	N	O	S	0	0
			541	323	108	108	2		
2	J	108	Total	C	N	O	S	0	0
			545	326	108	109	2		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	978	Total	C	N	O	S	0	0
			7064	4572	1214	1245	33		
3	B	977	Total	C	N	O	S	0	0
			6854	4409	1188	1223	34		
3	C	1008	Total	C	N	O	S	0	0
			6864	4402	1208	1220	34		

There are 429 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	insertion	UNP P0DTC2
A	18	PRO	ASN	conflict	UNP P0DTC2
A	20	PHE	THR	conflict	UNP P0DTC2
A	21	ASN	THR	conflict	UNP P0DTC2
A	22	LEU	ARG	conflict	UNP P0DTC2
A	23	ILE	THR	conflict	UNP P0DTC2
A	24	THR	GLN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	THR	LEU	conflict	UNP P0DTC2
A	26	THR	PRO	conflict	UNP P0DTC2
A	27	GLN	PRO	conflict	UNP P0DTC2
A	28	SER	ALA	conflict	UNP P0DTC2
A	51	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	conflict	UNP P0DTC2
A	143	ASP	GLY	conflict	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	conflict	UNP P0DTC2
A	158	GLY	ARG	conflict	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	conflict	UNP P0DTC2
A	213	GLY	VAL	conflict	UNP P0DTC2
A	216	PHE	LEU	conflict	UNP P0DTC2
A	245	ASN	HIS	conflict	UNP P0DTC2
A	264	ASP	ALA	conflict	UNP P0DTC2
A	332	VAL	ILE	conflict	UNP P0DTC2
A	339	HIS	GLY	conflict	UNP P0DTC2
A	356	THR	LYS	conflict	UNP P0DTC2
A	371	PHE	SER	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	376	ALA	THR	conflict	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2
A	405	ASN	ASP	conflict	UNP P0DTC2
A	408	SER	ARG	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	445	HIS	VAL	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	450	ASP	ASN	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	conflict	UNP P0DTC2
A	478	ASN	SER	conflict	UNP P0DTC2
A	479	LYS	THR	conflict	UNP P0DTC2
A	482	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	484	LYS	GLU	conflict	UNP P0DTC2
A	486	PRO	PHE	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2
A	554	LYS	GLU	conflict	UNP P0DTC2
A	570	VAL	ALA	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	621	SER	PRO	conflict	UNP P0DTC2
A	655	TYR	HIS	conflict	UNP P0DTC2
A	670	VAL	ILE	conflict	UNP P0DTC2
A	679	LYS	ASN	conflict	UNP P0DTC2
A	681	ARG	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	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	939	PHE	SER	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	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1143	LEU	PRO	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

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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	SER	-	expression tag	UNP P0DTC2
A	1251	GLY	-	expression tag	UNP P0DTC2
A	1252	GLY	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	ASN	-	expression tag	UNP P0DTC2
A	1255	ASP	-	expression tag	UNP P0DTC2
A	1256	ILE	-	expression tag	UNP P0DTC2
A	1257	PHE	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	GLN	-	expression tag	UNP P0DTC2
A	1261	LYS	-	expression tag	UNP P0DTC2
A	1262	ILE	-	expression tag	UNP P0DTC2
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	TRP	-	expression tag	UNP P0DTC2
A	1265	HIS	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	HIS	-	expression tag	UNP P0DTC2
A	1271	HIS	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	HIS	-	expression tag	UNP P0DTC2
A	1274	HIS	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2
B	17	MET	-	insertion	UNP P0DTC2
B	18	PRO	ASN	conflict	UNP P0DTC2
B	20	PHE	THR	conflict	UNP P0DTC2
B	21	ASN	THR	conflict	UNP P0DTC2
B	22	LEU	ARG	conflict	UNP P0DTC2
B	23	ILE	THR	conflict	UNP P0DTC2
B	24	THR	GLN	conflict	UNP P0DTC2
B	25	THR	LEU	conflict	UNP P0DTC2
B	26	THR	PRO	conflict	UNP P0DTC2
B	27	GLN	PRO	conflict	UNP P0DTC2
B	28	SER	ALA	conflict	UNP P0DTC2
B	51	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	conflict	UNP P0DTC2
B	143	ASP	GLY	conflict	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	158	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	conflict	UNP P0DTC2
B	213	GLY	VAL	conflict	UNP P0DTC2
B	216	PHE	LEU	conflict	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2
B	332	VAL	ILE	conflict	UNP P0DTC2
B	339	HIS	GLY	conflict	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2
B	375	PHE	SER	conflict	UNP P0DTC2
B	376	ALA	THR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	conflict	UNP P0DTC2
B	408	SER	ARG	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	445	HIS	VAL	conflict	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2
B	452	TRP	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2
B	482	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	conflict	UNP P0DTC2
B	486	PRO	PHE	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	554	LYS	GLU	conflict	UNP P0DTC2
B	570	VAL	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	621	SER	PRO	conflict	UNP P0DTC2
B	655	TYR	HIS	conflict	UNP P0DTC2
B	670	VAL	ILE	conflict	UNP P0DTC2
B	679	LYS	ASN	conflict	UNP P0DTC2
B	681	ARG	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	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	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	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1251	GLY	-	expression tag	UNP P0DTC2
B	1252	GLY	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	ASN	-	expression tag	UNP P0DTC2
B	1255	ASP	-	expression tag	UNP P0DTC2
B	1256	ILE	-	expression tag	UNP P0DTC2
B	1257	PHE	-	expression tag	UNP P0DTC2
B	1258	GLU	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	GLN	-	expression tag	UNP P0DTC2
B	1261	LYS	-	expression tag	UNP P0DTC2
B	1262	ILE	-	expression tag	UNP P0DTC2
B	1263	GLU	-	expression tag	UNP P0DTC2
B	1264	TRP	-	expression tag	UNP P0DTC2
B	1265	HIS	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	HIS	-	expression tag	UNP P0DTC2
B	1271	HIS	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	HIS	-	expression tag	UNP P0DTC2
B	1274	HIS	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	HIS	-	expression tag	UNP P0DTC2
B	1277	HIS	-	expression tag	UNP P0DTC2
C	17	MET	-	insertion	UNP P0DTC2
C	18	PRO	ASN	conflict	UNP P0DTC2
C	20	PHE	THR	conflict	UNP P0DTC2
C	21	ASN	THR	conflict	UNP P0DTC2
C	22	LEU	ARG	conflict	UNP P0DTC2
C	23	ILE	THR	conflict	UNP P0DTC2
C	24	THR	GLN	conflict	UNP P0DTC2
C	25	THR	LEU	conflict	UNP P0DTC2
C	26	THR	PRO	conflict	UNP P0DTC2
C	27	GLN	PRO	conflict	UNP P0DTC2
C	28	SER	ALA	conflict	UNP P0DTC2
C	51	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	142	ASP	GLY	conflict	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	conflict	UNP P0DTC2
C	158	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	conflict	UNP P0DTC2
C	213	GLY	VAL	conflict	UNP P0DTC2
C	216	PHE	LEU	conflict	UNP P0DTC2
C	245	ASN	HIS	conflict	UNP P0DTC2
C	264	ASP	ALA	conflict	UNP P0DTC2
C	332	VAL	ILE	conflict	UNP P0DTC2
C	339	HIS	GLY	conflict	UNP P0DTC2
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	376	ALA	THR	conflict	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	conflict	UNP P0DTC2
C	408	SER	ARG	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	445	HIS	VAL	conflict	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	conflict	UNP P0DTC2
C	478	ASN	SER	conflict	UNP P0DTC2
C	479	LYS	THR	conflict	UNP P0DTC2
C	482	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	conflict	UNP P0DTC2
C	486	PRO	PHE	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	554	LYS	GLU	conflict	UNP P0DTC2
C	570	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2
C	670	VAL	ILE	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	ARG	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	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	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	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1143	LEU	PRO	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
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

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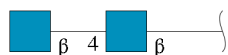
Chain	Residue	Modelled	Actual	Comment	Reference
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression 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	SER	-	expression tag	UNP P0DTC2
C	1251	GLY	-	expression tag	UNP P0DTC2
C	1252	GLY	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	ASN	-	expression tag	UNP P0DTC2
C	1255	ASP	-	expression tag	UNP P0DTC2
C	1256	ILE	-	expression tag	UNP P0DTC2
C	1257	PHE	-	expression tag	UNP P0DTC2
C	1258	GLU	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	GLN	-	expression tag	UNP P0DTC2
C	1261	LYS	-	expression tag	UNP P0DTC2
C	1262	ILE	-	expression tag	UNP P0DTC2
C	1263	GLU	-	expression tag	UNP P0DTC2
C	1264	TRP	-	expression tag	UNP P0DTC2
C	1265	HIS	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	HIS	-	expression tag	UNP P0DTC2
C	1271	HIS	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	HIS	-	expression tag	UNP P0DTC2
C	1274	HIS	-	expression tag	UNP P0DTC2
C	1275	HIS	-	expression tag	UNP P0DTC2

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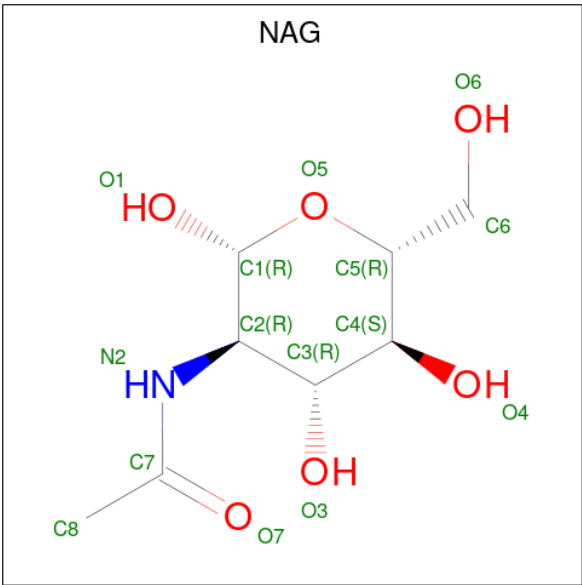
Chain	Residue	Modelled	Actual	Comment	Reference
C	1276	HIS	-	expression tag	UNP P0DTC2
C	1277	HIS	-	expression tag	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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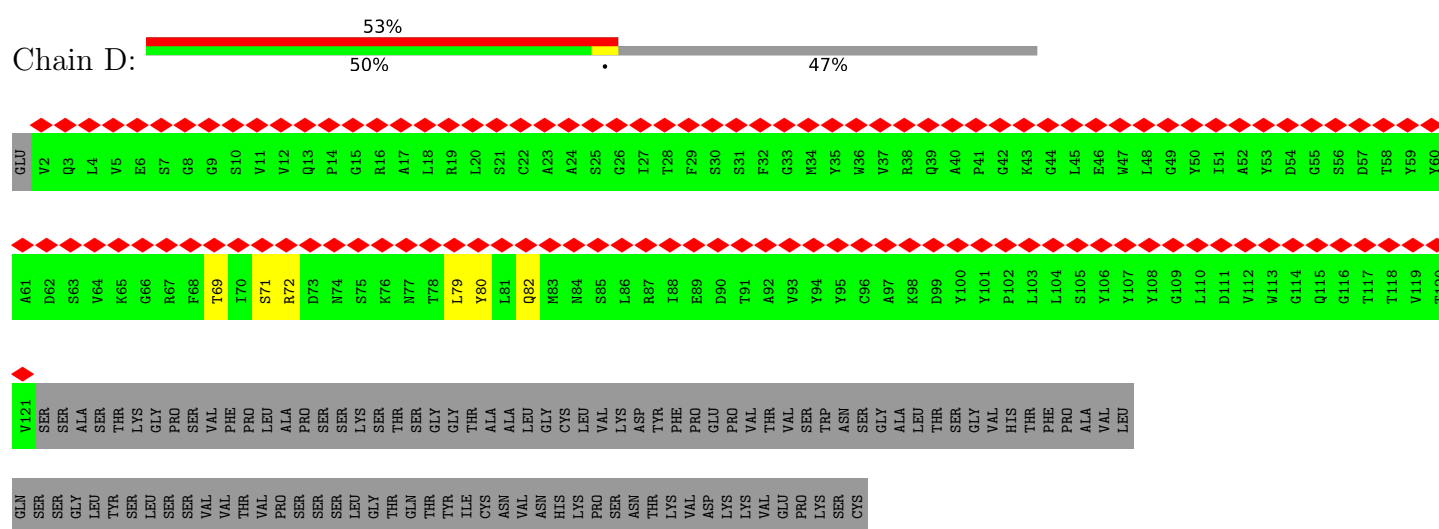
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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C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

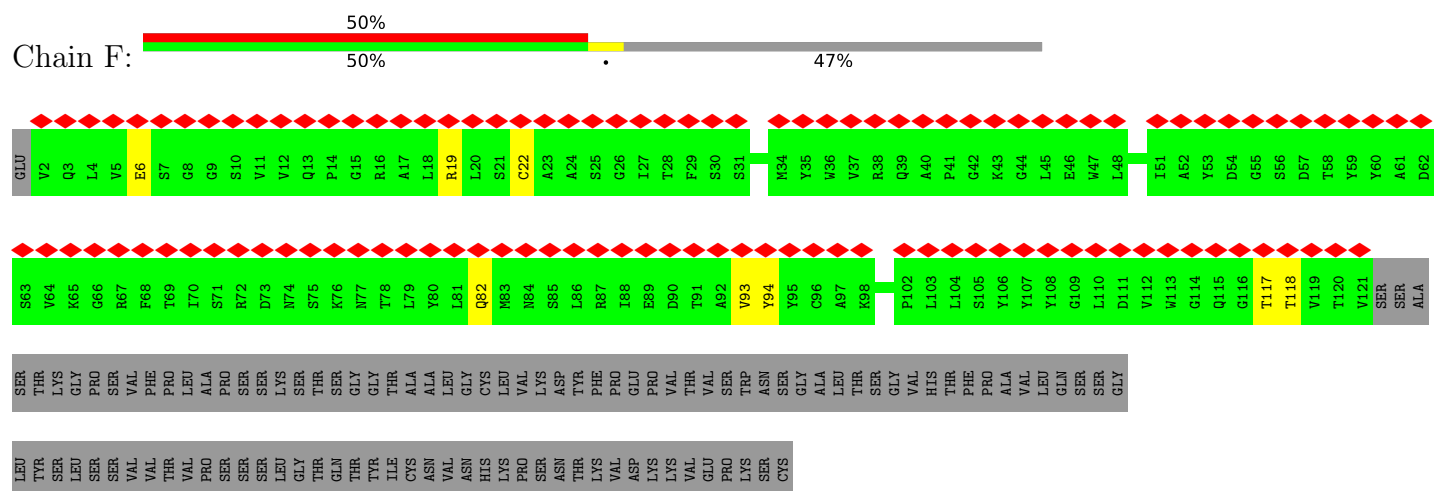
3 Residue-property plots

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: VIR-7229 Fab heavy chain

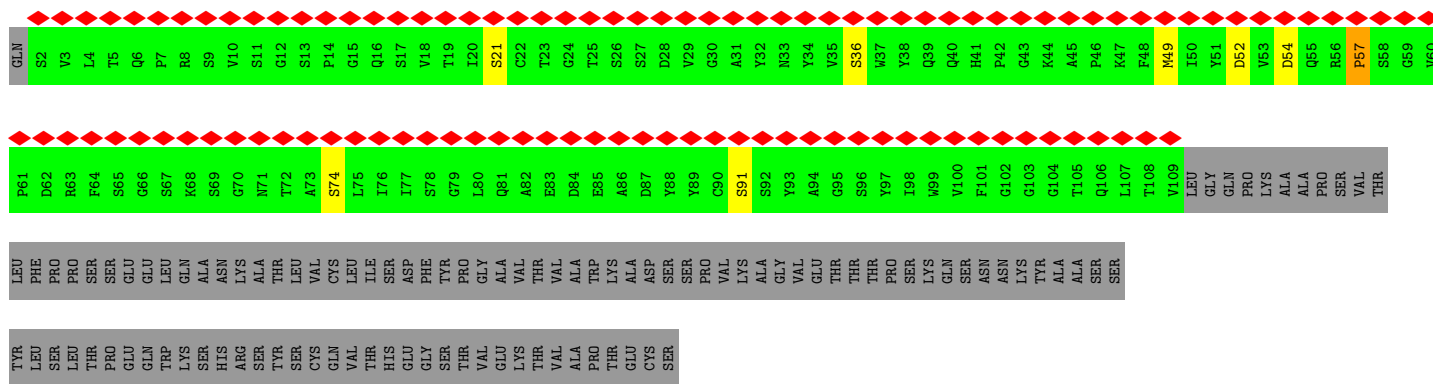


• Molecule 1: VIR-7229 Fab heavy chain

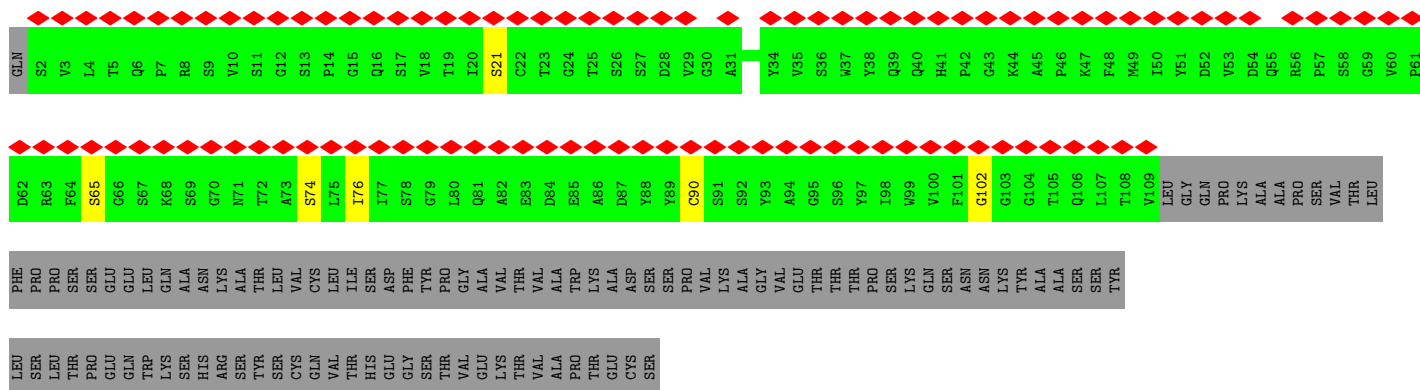


• Molecule 2: VIR-7229 Fab light chain

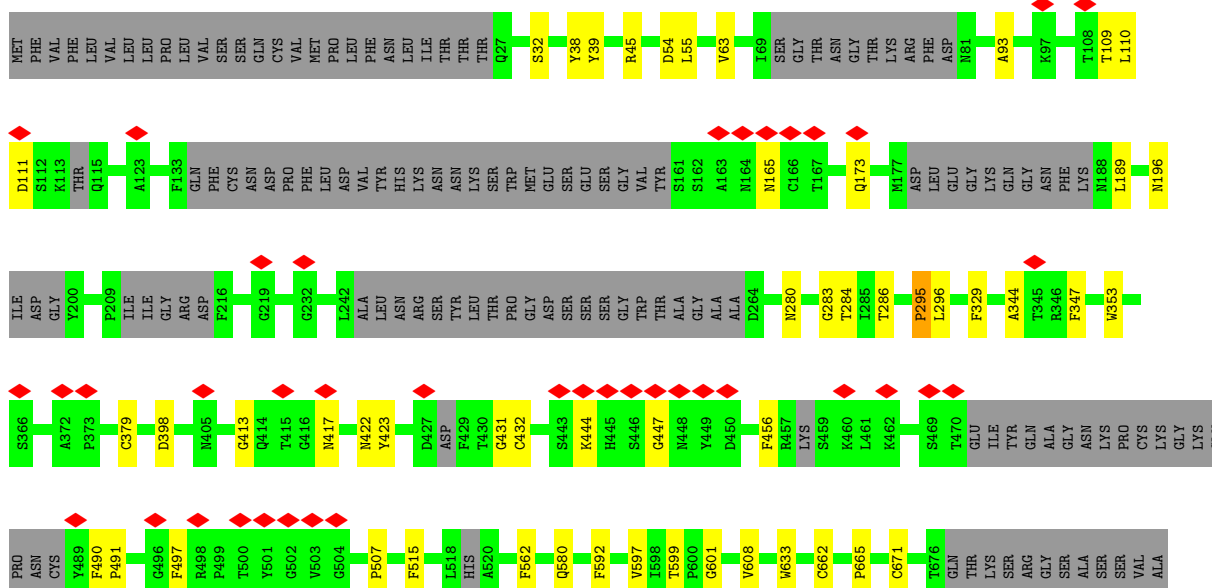


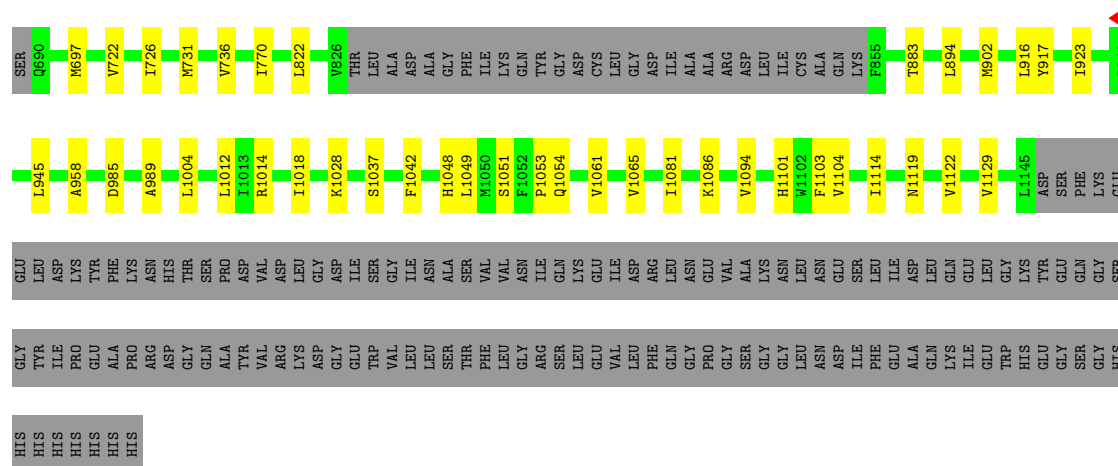


- Molecule 2: VIR-7229 Fab light chain

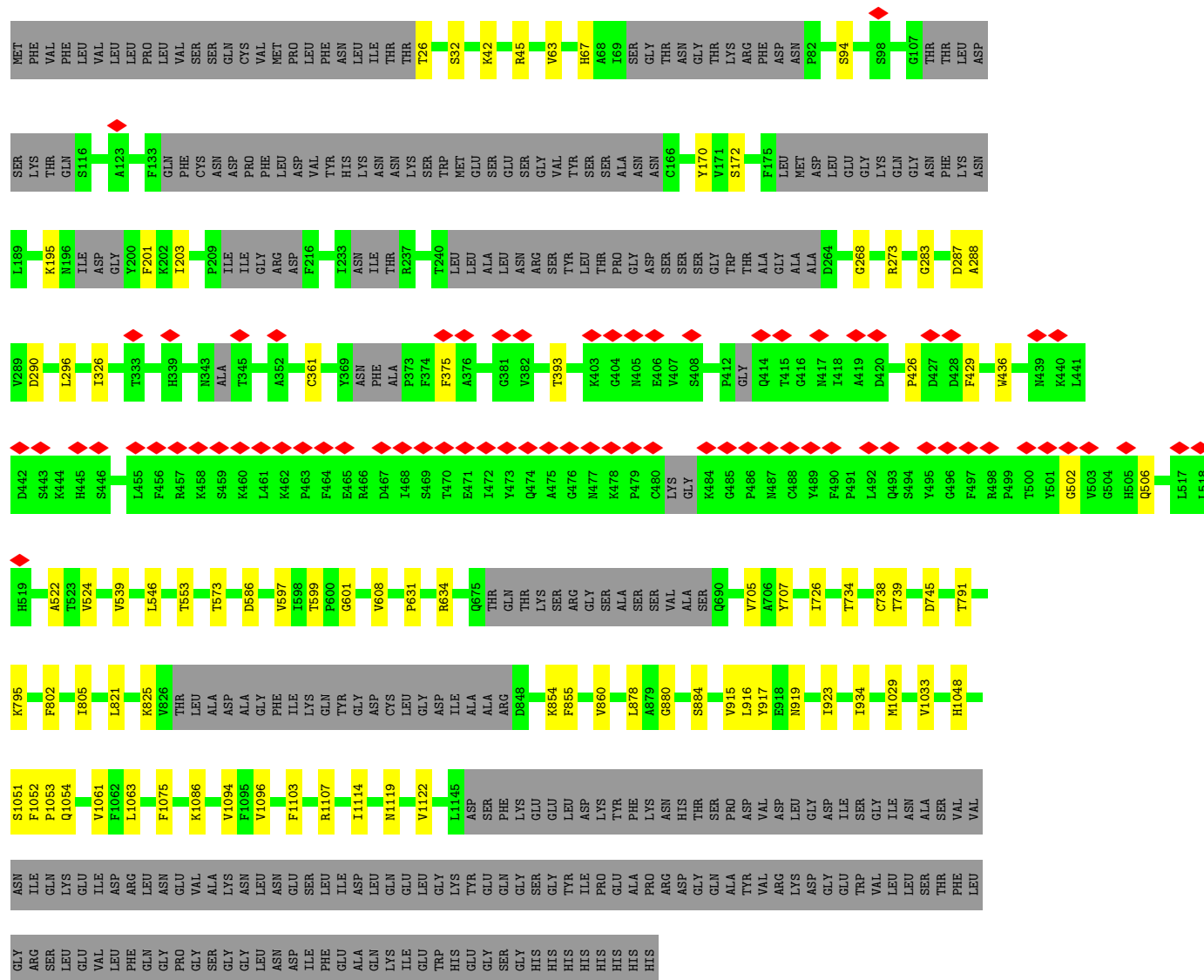


- Molecule 3: Spike glycoprotein

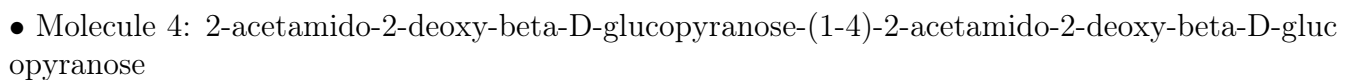




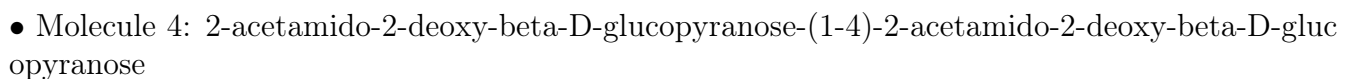
• Molecule 3: Spike glycoprotein



Chain C:



Chain E: 100%



Chain G:  50% 50%



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

Chain H:  100%



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

Chain K:  100%



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

Chain L:  50% 50%



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

Chain M:  50% 50%



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

Chain N:  50% 50%

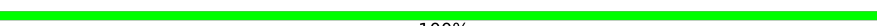


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 100%



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

Chain P:  100%



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

Chain Q:  50%  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	314440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.714	Depositor
Minimum map value	-3.256	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	512.0, 512.0, 512.0	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

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	D	0.05	0/597	0.20	0/828
1	F	0.06	0/598	0.22	0/829
2	I	0.16	0/546	0.40	1/759 (0.1%)
2	J	0.05	0/550	0.22	0/764
3	A	0.27	1/7233 (0.0%)	0.38	0/9890
3	B	0.25	0/7009	0.36	1/9593 (0.0%)
3	C	0.34	1/7005 (0.0%)	0.45	3/9599 (0.0%)
All	All	0.28	2/23538 (0.0%)	0.39	5/32262 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	295	PRO	N-CD	7.00	1.57	1.47
3	A	295	PRO	N-CD	6.81	1.57	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	57	PRO	CA-N-CD	-9.12	99.23	112.00
3	C	86	PHE	CB-CA-C	-6.74	99.39	110.85
3	C	92	PHE	CA-CB-CG	5.29	119.08	113.80
3	B	268	GLY	CA-C-O	-5.15	117.09	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	92	PHE	N-CA-CB	-5.11	102.34	111.08

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	102	ARG	Sidechain
3	C	35	ARG	Sidechain
3	C	634	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	595	0	295	3	0
1	F	596	0	298	4	0
2	I	541	0	280	5	0
2	J	545	0	292	3	0
3	A	7064	0	6326	55	0
3	B	6854	0	5953	61	0
3	C	6864	0	5799	43	0
4	E	28	0	25	0	0
4	G	28	0	25	2	0
4	H	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	2	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
5	A	196	0	182	0	0
5	B	56	0	52	0	0
5	C	154	0	143	0	0
All	All	23745	0	19870	163	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 (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:201:PHE:CE2	3:B:203:ILE:HD11	1.83	1.12
3:B:201:PHE:HE2	3:B:203:ILE:HD11	1.16	1.02
3:B:201:PHE:HE2	3:B:203:ILE:CD1	1.81	0.93
3:B:201:PHE:CE2	3:B:203:ILE:CD1	2.56	0.88
3:A:32:SER:HB3	3:A:63:VAL:HG23	1.62	0.80
3:B:201:PHE:CE2	3:B:203:ILE:CG1	2.66	0.79
3:A:295:PRO:HG3	3:A:633:TRP:CZ3	2.17	0.78
3:B:170:TYR:CE2	3:B:172:SER:CB	2.67	0.77
3:A:770:ILE:HD11	3:A:1012:LEU:HD12	1.66	0.77
3:B:26:THR:OG1	3:B:67:HIS:O	2.03	0.76
3:A:295:PRO:HG3	3:A:633:TRP:CE3	2.21	0.76
2:I:49:MET:O	2:I:57:PRO:HD3	1.86	0.74
3:C:599:THR:HG22	3:C:601:GLY:H	1.54	0.72
3:A:280:ASN:HB3	3:A:286:THR:HG21	1.72	0.71
3:B:599:THR:HG22	3:B:601:GLY:H	1.56	0.69
3:A:1037:SER:H	3:A:1048:HIS:HD2	1.41	0.69
3:C:295:PRO:HG3	3:C:633:TRP:CE3	2.28	0.69
3:B:201:PHE:CD2	3:B:203:ILE:HD11	2.28	0.69
3:A:599:THR:HG22	3:A:601:GLY:H	1.60	0.66
3:A:883:THR:HG23	3:C:707:TYR:HB2	1.78	0.64
3:B:296:LEU:HB2	3:B:608:VAL:HG21	1.79	0.63
3:C:731:MET:HG3	3:C:1018:ILE:HG13	1.81	0.62
3:B:707:TYR:HB2	3:C:883:THR:HG23	1.81	0.62
3:B:631:PRO:O	3:B:634:ARG:NH1	2.31	0.61
3:B:705:VAL:HB	3:C:883:THR:HG21	1.82	0.61
3:B:273:ARG:NH2	3:B:290:ASP:OD2	2.34	0.61
3:B:915:VAL:O	3:B:919:ASN:ND2	2.31	0.60
3:B:802:PHE:HD1	3:B:805:ILE:HD11	1.67	0.60
3:B:738:CYS:SG	3:B:739:THR:N	2.77	0.58
3:B:201:PHE:HE2	3:B:203:ILE:CG1	2.14	0.57
3:C:902:MET:HE1	3:C:1049:LEU:HD13	1.87	0.57
3:B:1086:LYS:HD2	3:B:1122:VAL:HG11	1.87	0.56
3:C:819:GLU:OE2	3:C:1055:SER:OG	2.20	0.56
3:A:883:THR:HG21	3:C:705:VAL:HB	1.86	0.56
3:B:745:ASP:N	3:B:745:ASP:OD1	2.38	0.55
3:A:280:ASN:HB3	3:A:286:THR:CG2	2.36	0.55
3:A:456:PHE:HD2	3:A:491:PRO:HA	1.72	0.55
3:C:595:VAL:HG11	3:C:633:TRP:HH2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:VAL:HA	1:F:118:THR:HA	1.88	0.54
3:C:1037:SER:H	3:C:1048:HIS:HD2	1.54	0.54
1:D:72:ARG:HA	1:D:79:LEU:HA	1.90	0.54
3:A:32:SER:HB3	3:A:63:VAL:CG2	2.37	0.54
3:C:722:VAL:HG22	3:C:1065:VAL:HG22	1.89	0.54
3:A:497:PHE:CG	3:A:507:PRO:HG3	2.43	0.54
3:A:731:MET:HG3	3:A:1018:ILE:HG13	1.90	0.54
1:F:19:ARG:HA	1:F:82:GLN:HA	1.89	0.53
3:B:1075:PHE:HB3	3:B:1096:VAL:HG13	1.91	0.53
1:D:69:THR:O	1:D:82:GLN:N	2.39	0.53
3:C:336:CYS:SG	3:C:362:VAL:N	2.82	0.53
3:C:726:ILE:HG12	3:C:1061:VAL:HG22	1.90	0.53
3:B:880:GLY:O	3:B:884:SER:OG	2.25	0.52
3:A:39:TYR:OH	3:A:284:THR:HG23	2.10	0.52
3:A:398:ASP:OD2	3:A:423:TYR:OH	2.27	0.52
3:C:914:ASN:O	3:C:918:GLU:HG2	2.10	0.52
3:B:726:ILE:HG12	3:B:1061:VAL:HG22	1.92	0.51
3:A:1037:SER:H	3:A:1048:HIS:CD2	2.25	0.51
3:A:958:ALA:HB2	3:A:1014:ARG:HH12	1.74	0.51
3:B:426:PRO:HB2	3:B:429:PHE:HB3	1.93	0.51
3:A:93:ALA:HB1	3:A:189:LEU:HD11	1.93	0.51
3:B:916:LEU:HD12	3:B:923:ILE:HD12	1.92	0.51
3:B:201:PHE:CE2	3:B:203:ILE:HG12	2.44	0.51
3:B:201:PHE:CD2	3:B:203:ILE:HG13	2.45	0.51
3:A:417:ASN:O	3:A:422:ASN:ND2	2.42	0.50
3:B:1053:PRO:O	3:B:1054:GLN:NE2	2.36	0.50
3:A:894:LEU:HD13	3:C:715:PRO:HD3	1.93	0.50
3:A:490:PHE:HD1	3:A:491:PRO:HD2	1.76	0.50
3:C:289:VAL:HG23	3:C:306:PHE:CE2	2.47	0.50
3:C:909:ILE:HG13	3:C:911:VAL:HG23	1.94	0.50
3:C:358:ILE:N	3:C:395:VAL:O	2.41	0.49
3:A:902:MET:HE1	3:A:1049:LEU:HD13	1.93	0.49
3:A:592:PHE:HZ	3:B:855:PHE:HA	1.77	0.49
3:B:170:TYR:HE2	3:B:172:SER:CB	2.24	0.49
1:F:94:TYR:N	1:F:117:THR:O	2.43	0.49
3:A:916:LEU:HD12	3:A:923:ILE:HD12	1.94	0.49
3:C:1006:THR:O	3:C:1010:GLN:NE2	2.42	0.49
2:J:21:SER:HA	2:J:74:SER:HA	1.93	0.49
2:I:57:PRO:HD2	2:I:57:PRO:O	2.13	0.48
3:B:393:THR:HA	3:B:522:ALA:HA	1.94	0.48
3:B:546:LEU:HD21	3:B:573:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1114:ILE:O	3:B:1119:ASN:ND2	2.46	0.48
3:B:32:SER:HB3	3:B:63:VAL:HG23	1.94	0.48
3:C:289:VAL:HG23	3:C:306:PHE:CZ	2.49	0.48
3:B:878:LEU:HD11	3:B:1054:GLN:HE22	1.78	0.48
3:B:201:PHE:CD2	3:B:203:ILE:CD1	2.93	0.48
3:B:1094:VAL:HG23	3:B:1107:ARG:HG2	1.94	0.48
3:B:878:LEU:HD21	3:B:1052:PHE:HB3	1.95	0.48
3:B:1048:HIS:HE1	3:B:1051:SER:HB2	1.79	0.48
3:A:1053:PRO:O	3:A:1054:GLN:NE2	2.37	0.47
3:C:736:VAL:HG11	3:C:1004:LEU:HD21	1.96	0.47
3:C:319:ARG:H	3:C:630:THR:HB	1.79	0.47
3:B:287:ASP:OD1	3:B:288:ALA:N	2.46	0.47
2:J:65:SER:O	2:J:76:ILE:N	2.42	0.47
3:A:431:GLY:HA2	3:A:515:PHE:CD2	2.50	0.47
3:A:665:PRO:HA	3:A:671:CYS:SG	2.55	0.47
3:A:726:ILE:HG13	3:A:1061:VAL:HG22	1.97	0.47
3:A:1028:LYS:NZ	3:A:1042:PHE:O	2.48	0.47
3:A:1103:PHE:HZ	4:G:1:NAG:H62	1.79	0.47
3:B:45:ARG:O	3:B:283:GLY:HA2	2.15	0.47
3:B:361:CYS:O	3:B:524:VAL:HA	2.14	0.47
3:C:104:TRP:CD1	3:C:238:PHE:HE1	2.34	0.46
3:C:105:ILE:HD13	3:C:135:PHE:CE1	2.51	0.46
3:B:934:ILE:HD13	3:B:1063:LEU:HD22	1.96	0.46
3:C:295:PRO:HG3	3:C:633:TRP:CZ3	2.51	0.46
3:A:296:LEU:HB2	3:A:608:VAL:HG21	1.97	0.46
3:B:734:THR:HG22	3:B:860:VAL:HG22	1.97	0.46
3:C:878:LEU:HD11	3:C:1054:GLN:HE22	1.81	0.45
3:A:344:ALA:HB3	3:A:347:PHE:HE1	1.81	0.45
3:C:822:LEU:HD21	3:C:938:LEU:HD21	1.98	0.45
3:A:38:TYR:OH	3:A:55:LEU:O	2.24	0.45
3:B:201:PHE:CD2	3:B:203:ILE:CG1	2.99	0.45
3:B:375:PHE:H	3:B:436:TRP:HA	1.83	0.44
3:A:1114:ILE:O	3:A:1119:ASN:ND2	2.50	0.44
3:A:985:ASP:O	3:A:989:ALA:N	2.44	0.44
3:A:1048:HIS:HE1	3:A:1051:SER:OG	1.99	0.44
3:B:597:VAL:HG13	3:B:608:VAL:HG13	2.00	0.44
2:I:21:SER:HA	2:I:74:SER:HA	1.99	0.44
3:A:413:GLY:HA3	3:C:987:PRO:HD3	1.99	0.43
1:F:6:GLU:HA	1:F:22:CYS:HA	1.99	0.43
3:B:878:LEU:HD11	3:B:1054:GLN:NE2	2.34	0.43
3:C:85:PRO:O	3:C:269:TYR:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:109:THR:C	3:A:111:ASP:N	2.75	0.43
3:B:802:PHE:CD1	3:B:805:ILE:HD11	2.50	0.43
3:B:326:ILE:HG13	3:B:539:VAL:HG11	2.01	0.43
3:A:444:LYS:HG3	3:A:447:GLY:H	1.82	0.42
3:A:353:TRP:H	3:A:353:TRP:CD1	2.36	0.42
3:A:822:LEU:HD22	3:A:945:LEU:HD21	2.01	0.42
3:C:1053:PRO:O	3:C:1054:GLN:NE2	2.41	0.42
1:D:71:SER:O	1:D:80:TYR:N	2.36	0.42
3:A:597:VAL:HG13	3:A:608:VAL:CG1	2.50	0.42
3:A:662:CYS:SG	3:A:697:MET:HB3	2.59	0.42
3:C:396:TYR:O	3:C:514:SER:N	2.50	0.42
3:B:502:GLY:O	3:B:506:GLN:HG3	2.19	0.42
3:B:707:TYR:HB3	3:C:792:PRO:HG2	2.01	0.41
3:C:1086:LYS:HB3	3:C:1122:VAL:HG13	2.01	0.41
3:B:821:LEU:O	3:B:825:LYS:HG3	2.20	0.41
3:A:722:VAL:HG22	3:A:1065:VAL:HG22	2.01	0.41
3:B:854:LYS:HE2	3:B:854:LYS:HB3	1.88	0.41
3:C:136:CYS:SG	3:C:137:ASN:N	2.94	0.41
3:B:553:THR:O	3:B:586:ASP:N	2.50	0.41
2:I:36:SER:O	2:I:91:SER:N	2.48	0.41
3:A:562:PHE:O	3:B:42:LYS:HE2	2.21	0.41
3:A:736:VAL:HG11	3:A:1004:LEU:HD11	2.03	0.41
3:A:329:PHE:O	3:A:580:GLN:NE2	2.36	0.41
3:A:379:CYS:HA	3:A:432:CYS:HA	2.02	0.41
3:C:319:ARG:HB2	3:C:630:THR:OG1	2.20	0.41
3:C:770:ILE:O	3:C:774:GLN:HG2	2.21	0.41
3:A:1101:HIS:CD2	4:G:1:NAG:H5	2.56	0.41
3:B:1103:PHE:HZ	4:L:1:NAG:H62	1.85	0.41
3:C:234:ASN:N	3:C:234:ASN:OD1	2.53	0.41
3:C:1073:LYS:HD3	3:C:1075:PHE:CZ	2.56	0.41
3:A:45:ARG:O	3:A:283:GLY:HA2	2.20	0.40
3:A:1129:VAL:HG13	3:B:917:TYR:HB3	2.03	0.40
2:I:52:ASP:O	2:I:54:ASP:N	2.51	0.40
2:J:90:CYS:O	2:J:102:GLY:N	2.49	0.40
3:A:917:TYR:HB3	3:C:1129:VAL:HG13	2.03	0.40
3:C:45:ARG:O	3:C:283:GLY:HA2	2.21	0.40
3:C:805:ILE:HG22	3:C:878:LEU:HD13	2.03	0.40
3:A:1086:LYS:HD2	3:A:1122:VAL:HG11	2.03	0.40
3:B:1029:MET:O	3:B:1033:VAL:HB	2.22	0.40
3:C:25:THR:HA	3:C:68:ALA:HA	2.02	0.40
3:A:54:ASP:CG	3:A:55:LEU:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:791:THR:OG1	3:B:795:LYS:HE3	2.21	0.40
3:B:1103:PHE:CZ	4:L:1:NAG:H62	2.57	0.40

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	D	118/226 (52%)	117 (99%)	1 (1%)	0	100	100
1	F	118/226 (52%)	115 (98%)	3 (2%)	0	100	100
2	I	106/216 (49%)	105 (99%)	1 (1%)	0	100	100
2	J	106/216 (49%)	105 (99%)	1 (1%)	0	100	100
3	A	950/1273 (75%)	918 (97%)	30 (3%)	2 (0%)	43	73
3	B	947/1273 (74%)	910 (96%)	37 (4%)	0	100	100
3	C	980/1273 (77%)	953 (97%)	26 (3%)	1 (0%)	48	78
All	All	3325/4703 (71%)	3223 (97%)	99 (3%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	165	ASN
3	A	110	LEU
3	C	100	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	5/191 (3%)	5 (100%)	0	100	100
1	F	6/191 (3%)	6 (100%)	0	100	100
2	I	8/182 (4%)	8 (100%)	0	100	100
2	J	10/182 (6%)	10 (100%)	0	100	100
3	A	642/1109 (58%)	637 (99%)	5 (1%)	73	81
3	B	589/1109 (53%)	587 (100%)	2 (0%)	86	87
3	C	546/1109 (49%)	532 (97%)	14 (3%)	40	68
All	All	1806/4073 (44%)	1785 (99%)	21 (1%)	61	78

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	173	GLN
3	A	196	ASN
3	A	1081	ILE
3	A	1094	VAL
3	A	1104	VAL
3	B	94	SER
3	B	195	LYS
3	C	90	VAL
3	C	190	ARG
3	C	216	PHE
3	C	234	ASN
3	C	238	PHE
3	C	635	VAL
3	C	738	CYS
3	C	785	VAL
3	C	791	THR
3	C	938	LEU
3	C	1010	GLN
3	C	1096	VAL
3	C	1104	VAL
3	C	1105	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	173	GLN
3	A	606	ASN
3	A	856	ASN
3	A	901	GLN
3	A	1048	HIS
3	B	774	GLN
3	B	901	GLN
3	B	949	GLN
3	B	992	GLN
3	B	1048	HIS
3	B	1058	HIS
3	B	1083	HIS
3	B	1101	HIS
3	C	321	GLN
3	C	542	ASN
3	C	949	GLN
3	C	992	GLN
3	C	1011	GLN
3	C	1048	HIS
3	C	1054	GLN
3	C	1101	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

20 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	1	4,3	14,14,15	0.77	0	17,19,21	0.86	0
4	NAG	E	2	4	14,14,15	0.72	0	17,19,21	0.80	0
4	NAG	G	1	4,3	14,14,15	0.73	0	17,19,21	0.81	0
4	NAG	G	2	4	14,14,15	0.71	0	17,19,21	0.85	0
4	NAG	H	1	4,3	14,14,15	0.77	0	17,19,21	0.86	0
4	NAG	H	2	4	14,14,15	0.73	0	17,19,21	0.82	0
4	NAG	K	1	4,3	14,14,15	0.78	0	17,19,21	0.91	0
4	NAG	K	2	4	14,14,15	0.72	0	17,19,21	0.85	0
4	NAG	L	1	4,3	14,14,15	0.74	0	17,19,21	1.12	3 (17%)
4	NAG	L	2	4	14,14,15	0.73	0	17,19,21	0.84	1 (5%)
4	NAG	M	1	4,3	14,14,15	0.74	0	17,19,21	0.98	1 (5%)
4	NAG	M	2	4	14,14,15	0.71	0	17,19,21	0.82	0
4	NAG	N	1	4,3	14,14,15	0.77	0	17,19,21	0.96	0
4	NAG	N	2	4	14,14,15	0.74	0	17,19,21	0.91	1 (5%)
4	NAG	O	1	4,3	14,14,15	0.72	0	17,19,21	0.85	0
4	NAG	O	2	4	14,14,15	0.74	0	17,19,21	0.82	0
4	NAG	P	1	4,3	14,14,15	0.78	0	17,19,21	0.95	0
4	NAG	P	2	4	14,14,15	0.73	0	17,19,21	0.83	0
4	NAG	Q	1	4,3	14,14,15	0.74	0	17,19,21	0.86	0
4	NAG	Q	2	4	14,14,15	0.69	0	17,19,21	0.81	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	E	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	NAG	G	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	NAG	M	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,3	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1	NAG	O5-C1-C2	-2.65	107.20	111.29
4	N	2	NAG	C2-N2-C7	2.31	126.00	122.90
4	M	1	NAG	C2-N2-C7	2.14	125.77	122.90
4	L	1	NAG	C2-N2-C7	2.14	125.77	122.90
4	L	1	NAG	O4-C4-C3	-2.09	105.45	110.38
4	L	2	NAG	O5-C1-C2	-2.04	108.13	111.29

There are no chirality outliers.

All (14) torsion outliers are listed below:

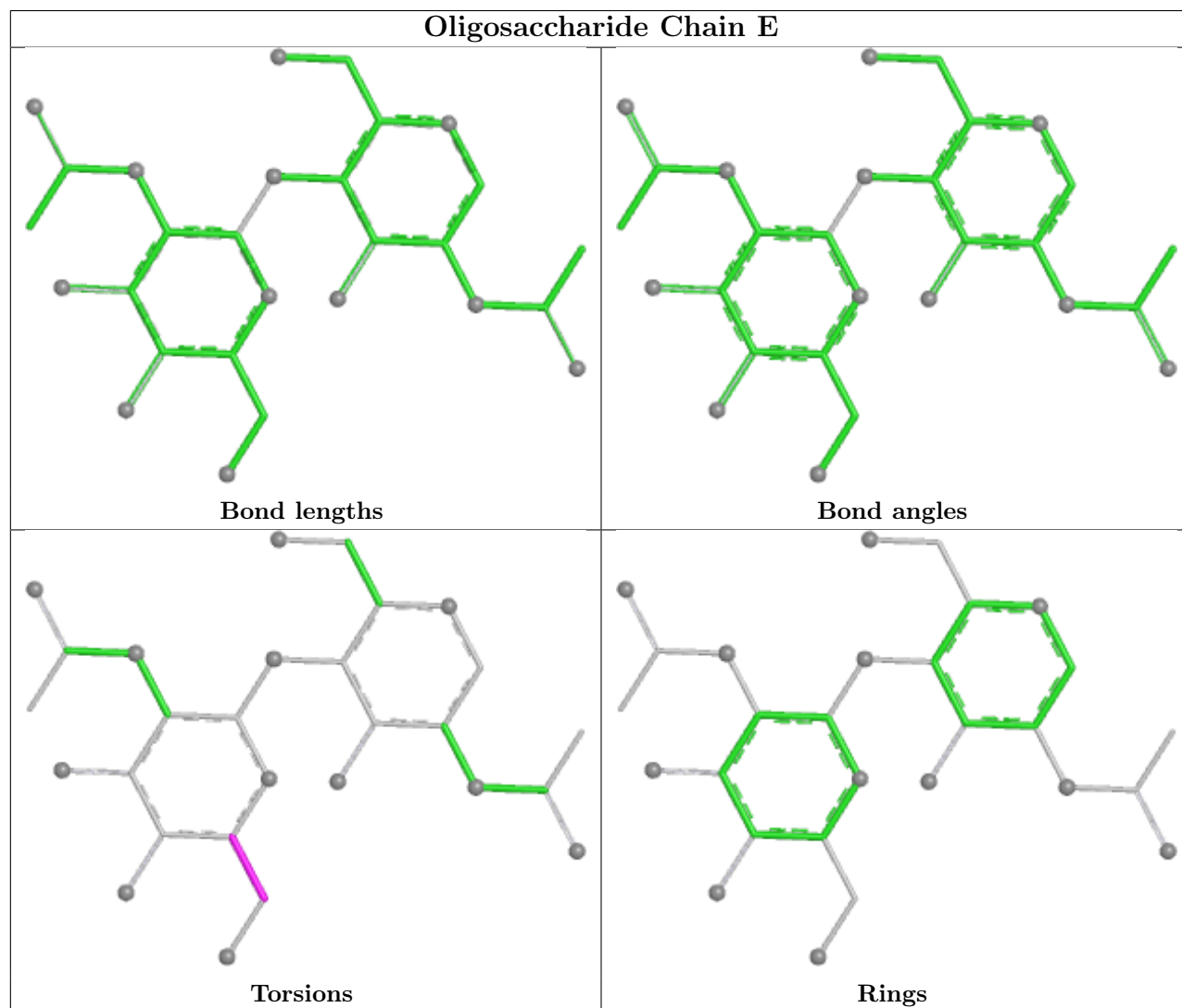
Mol	Chain	Res	Type	Atoms
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6

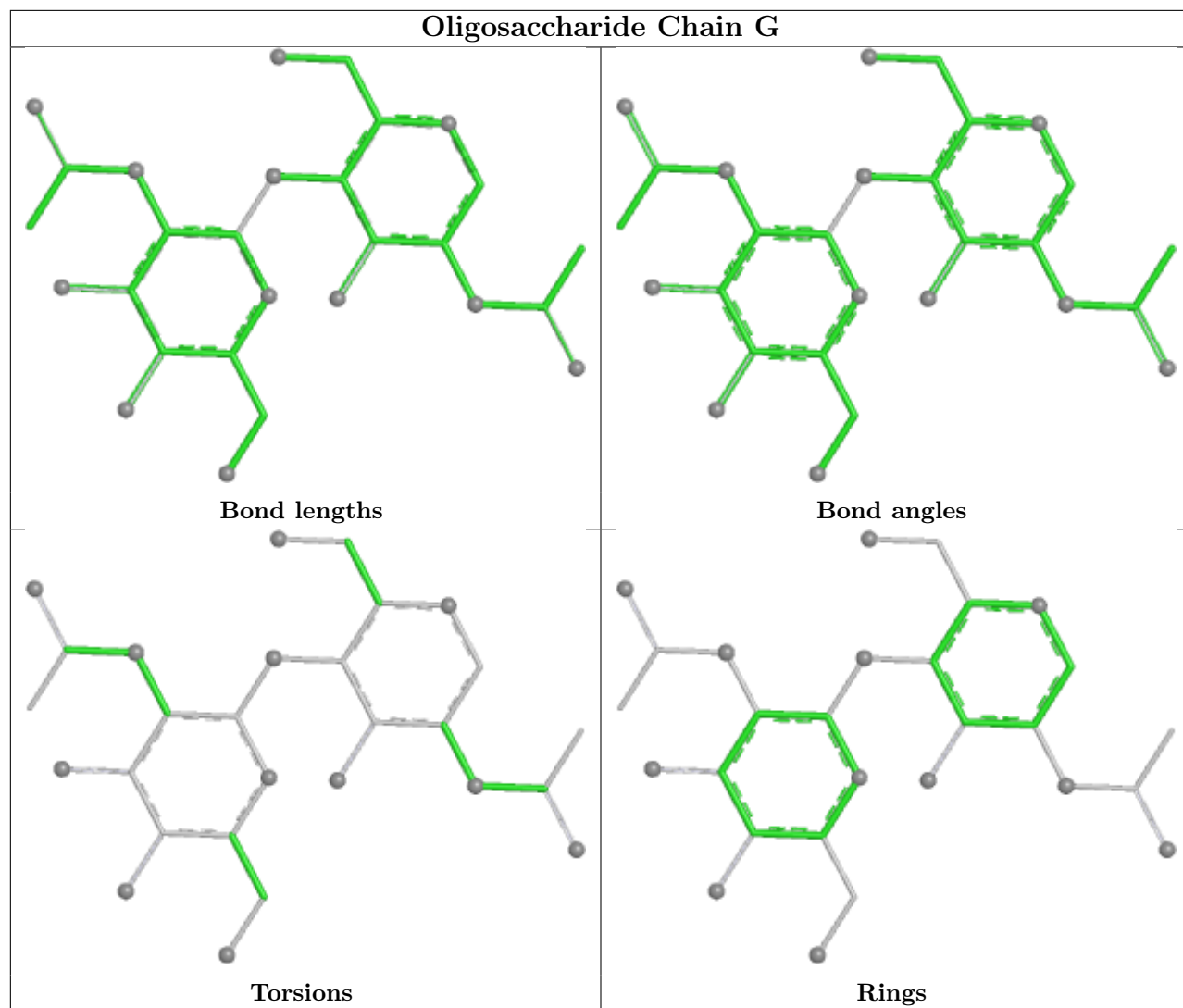
There are no ring outliers.

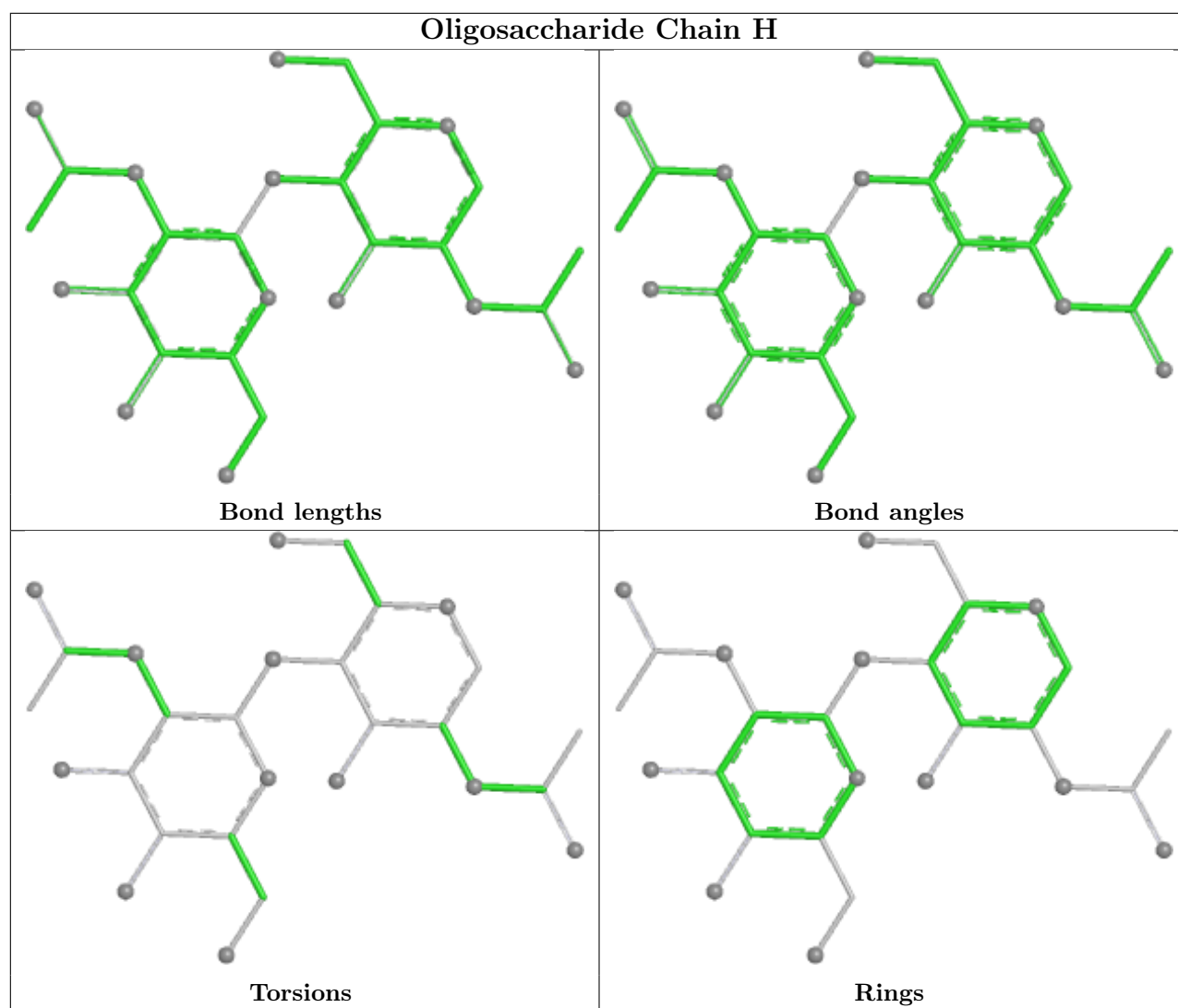
2 monomers are involved in 4 short contacts:

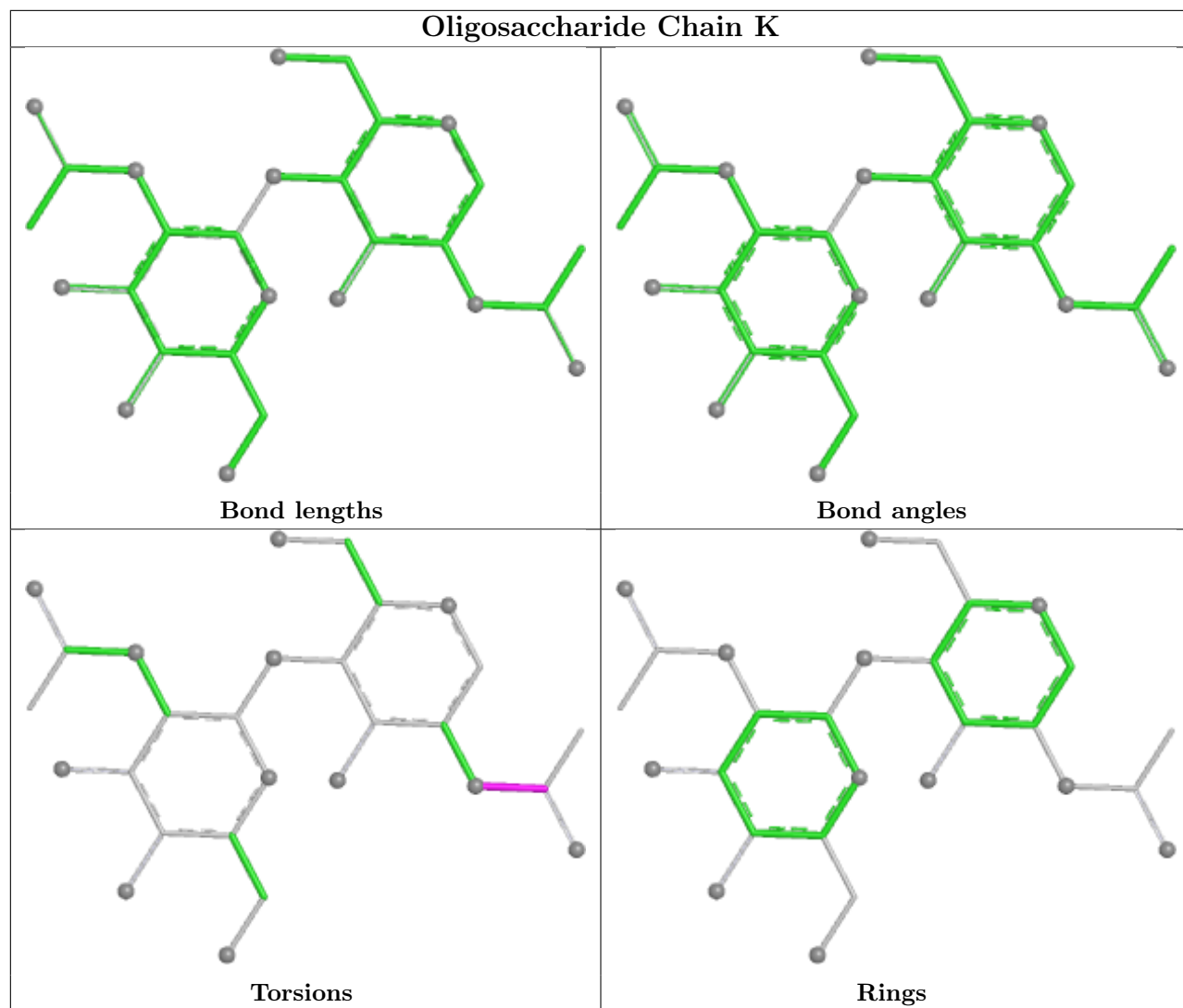
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	2	0
4	L	1	NAG	2	0

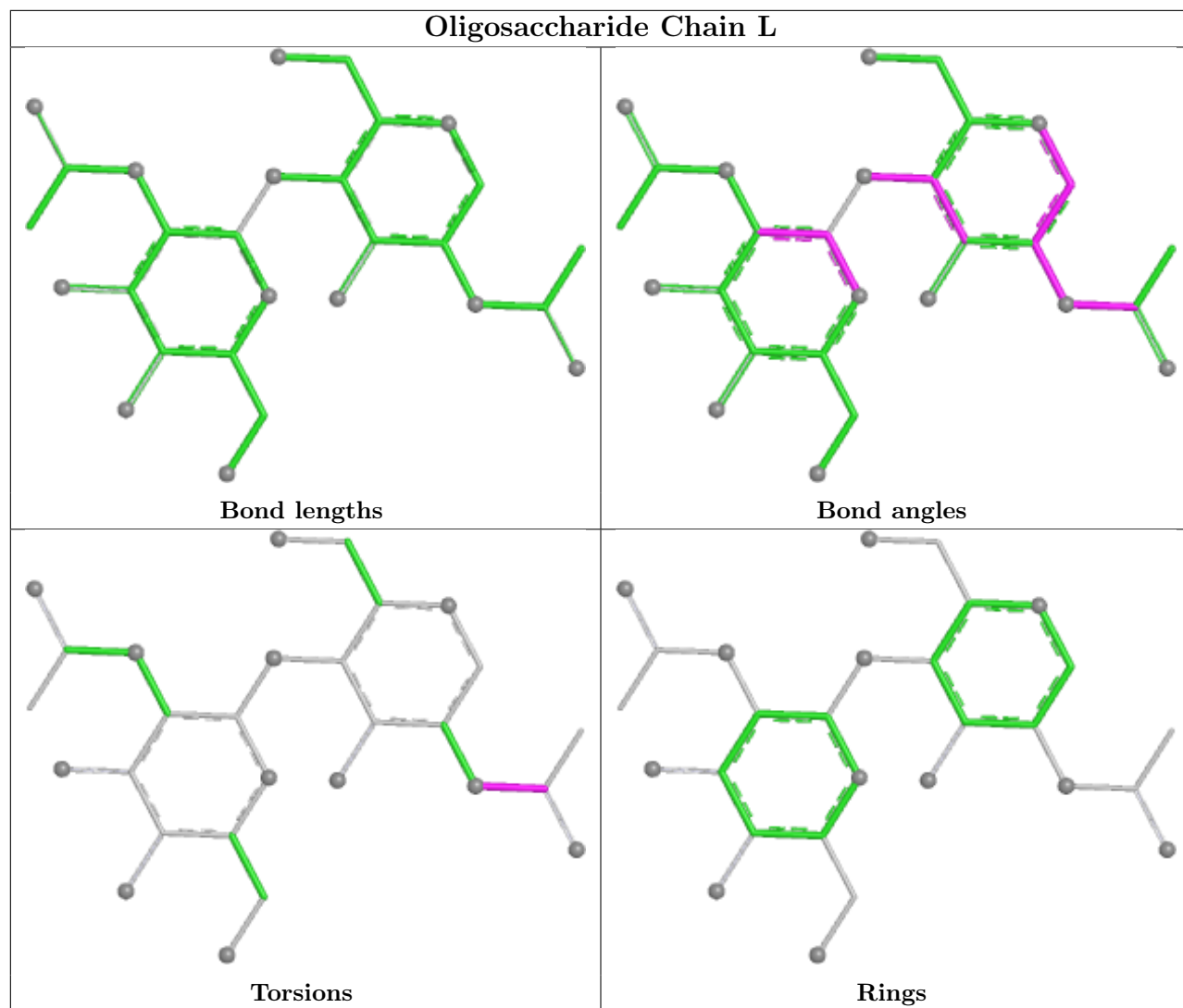
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

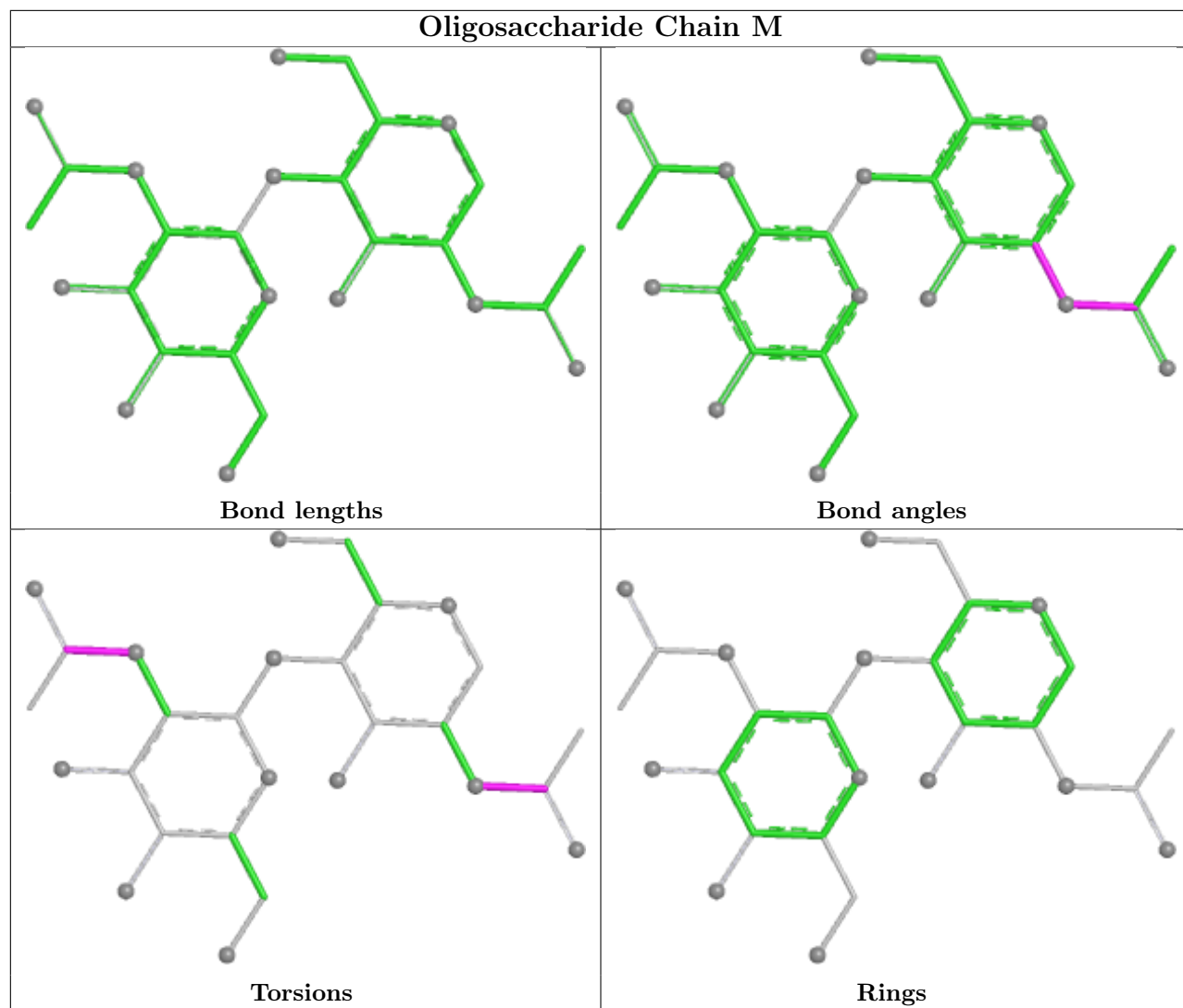


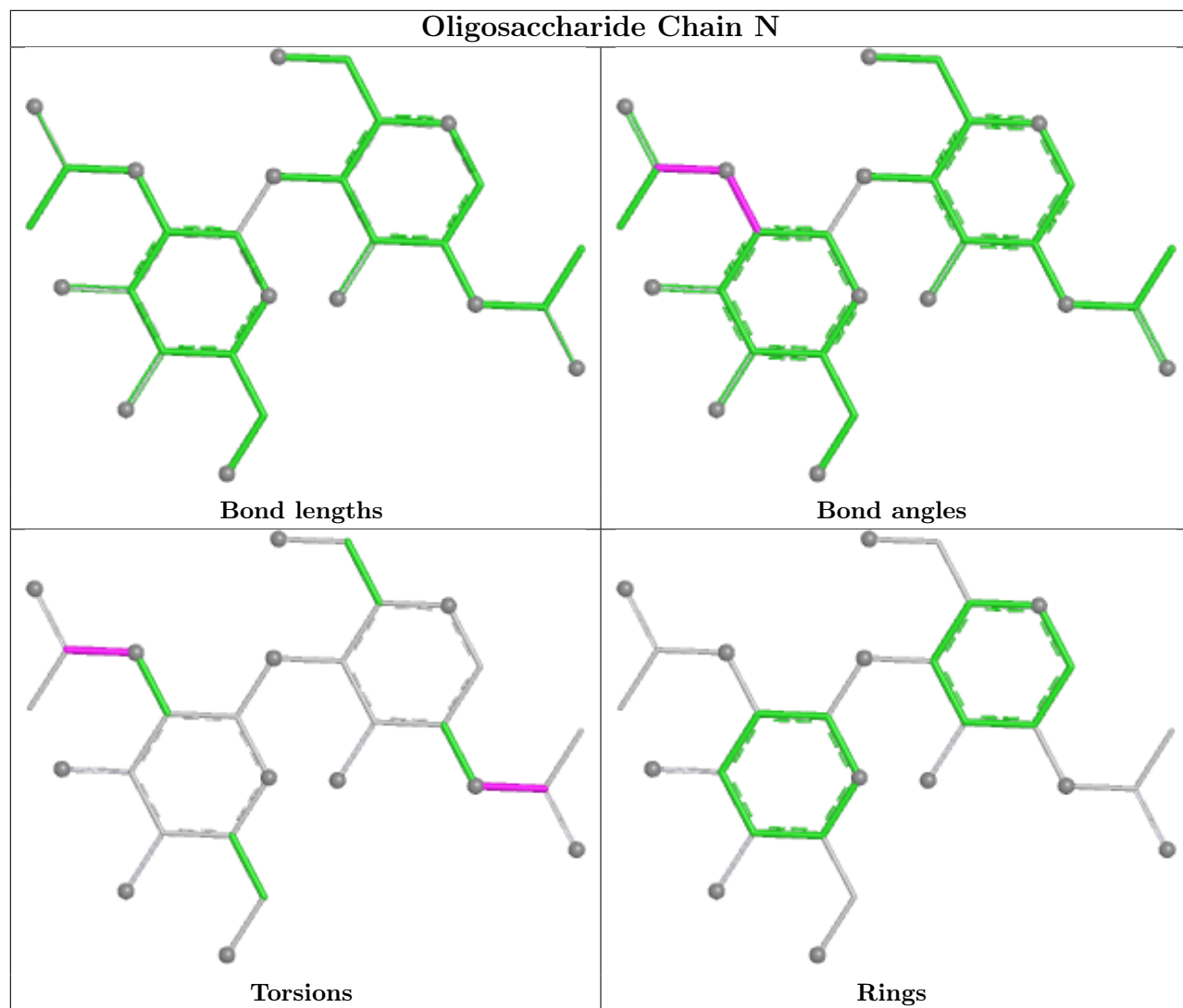


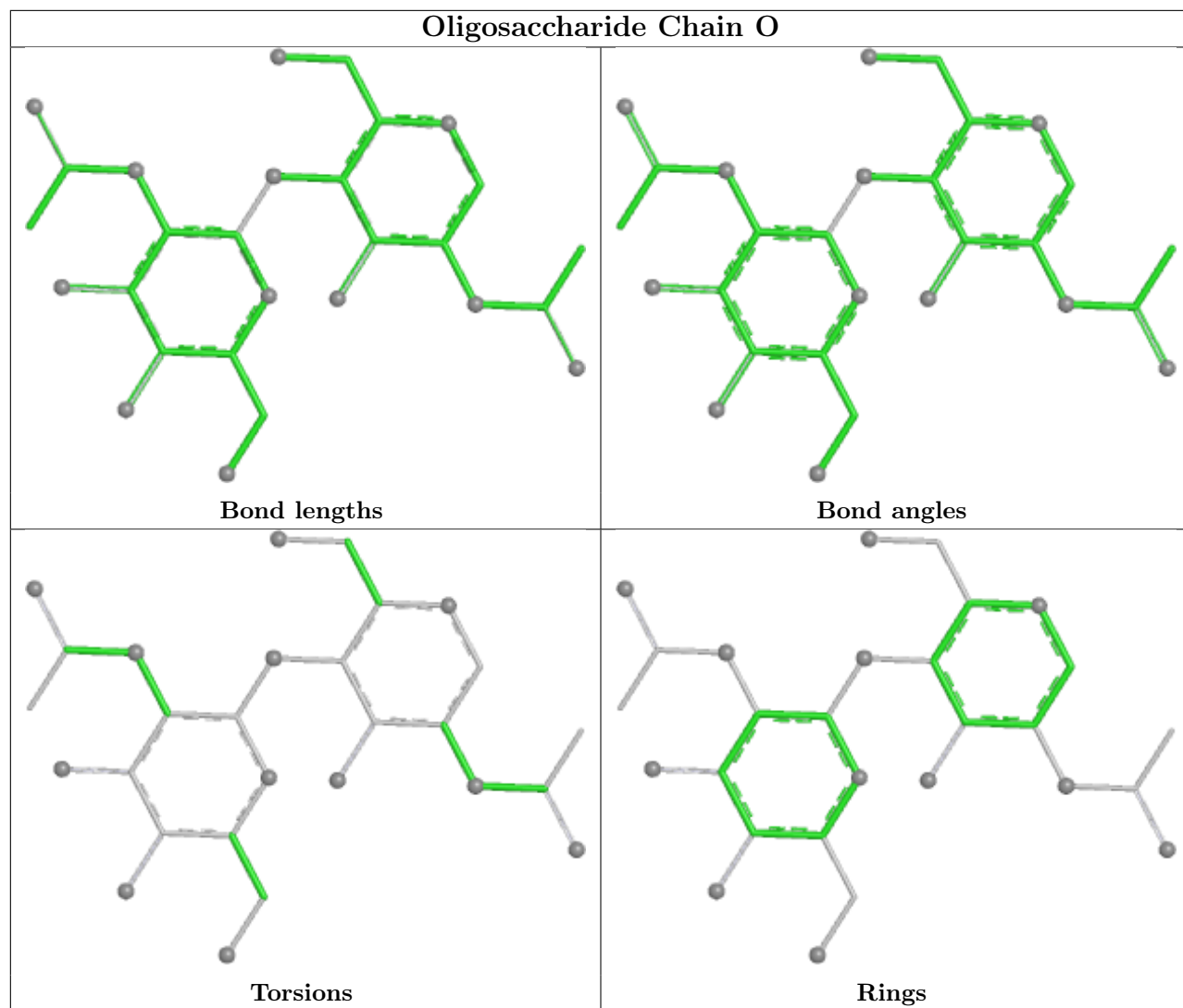


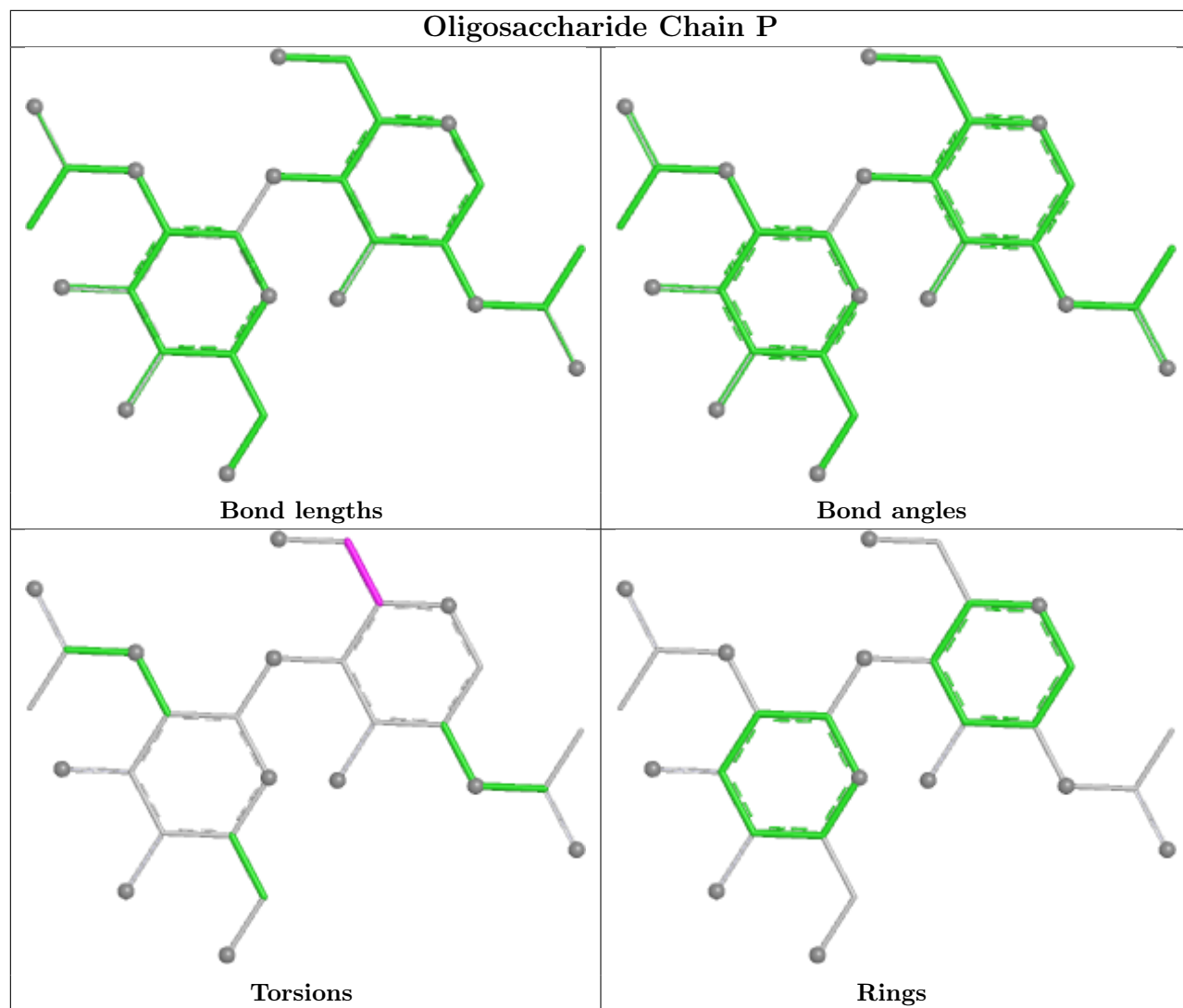


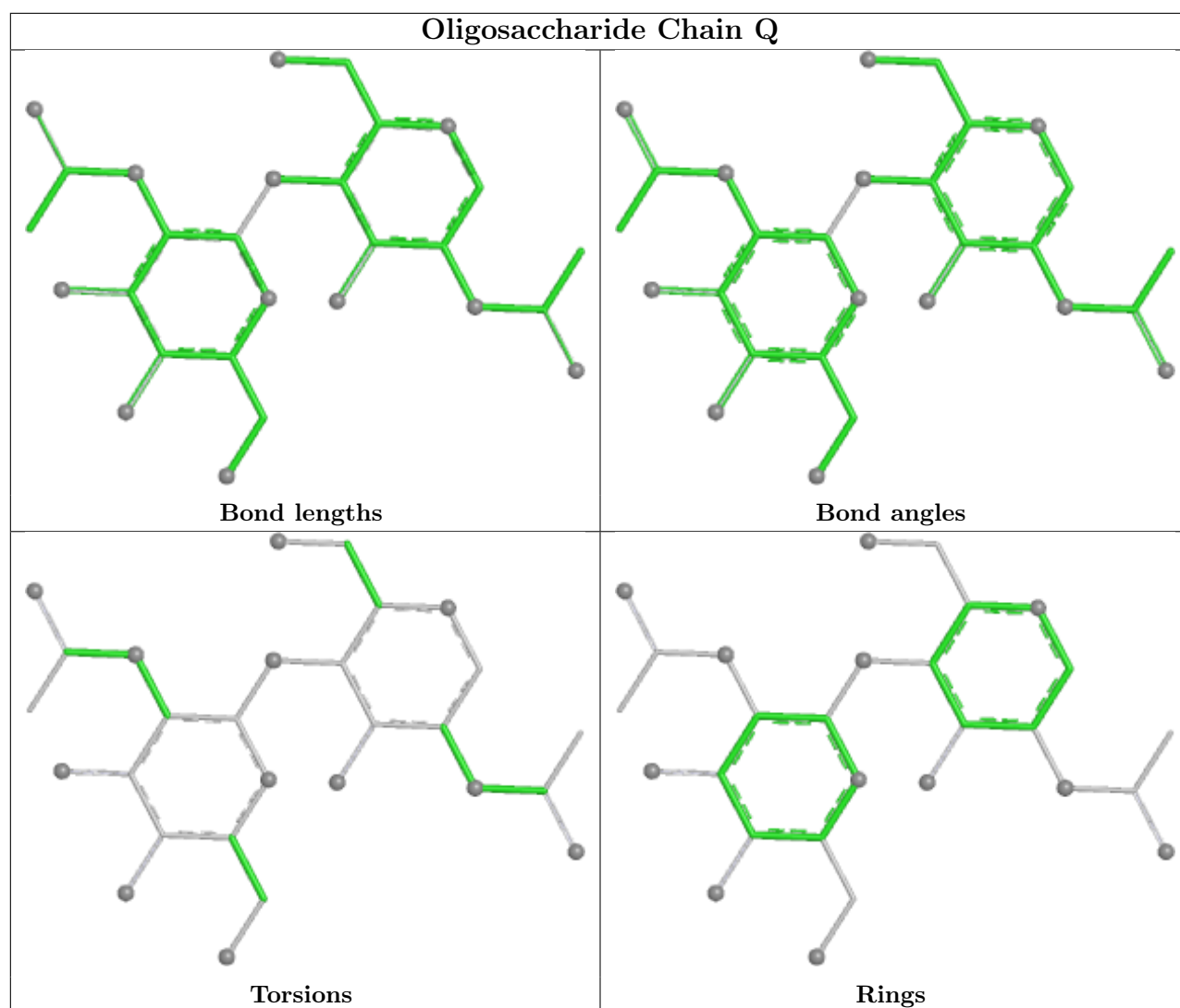












5.6 Ligand geometry [i](#)

29 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	$\# Z > 2$
5	NAG	A	1504	3	14,14,15	0.75	0	17,19,21	0.92	1 (5%)
5	NAG	B	1503	3	14,14,15	0.73	0	17,19,21	0.83	0
5	NAG	A	1505	3	14,14,15	0.73	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1508	3	14,14,15	0.75	0	17,19,21	0.79	0
5	NAG	C	1502	3	14,14,15	0.73	0	17,19,21	0.96	1 (5%)
5	NAG	C	1504	3	14,14,15	0.75	0	17,19,21	0.86	0
5	NAG	C	1509	3	14,14,15	0.73	0	17,19,21	0.83	0
5	NAG	A	1502	3	14,14,15	0.41	0	17,19,21	0.62	0
5	NAG	C	1505	3	14,14,15	0.75	0	17,19,21	0.82	0
5	NAG	C	1501	3	14,14,15	0.74	0	17,19,21	0.82	0
5	NAG	A	1509	3	14,14,15	0.71	0	17,19,21	0.86	0
5	NAG	A	1511	3	14,14,15	0.73	0	17,19,21	0.90	0
5	NAG	A	1514	3	14,14,15	0.71	0	17,19,21	0.76	0
5	NAG	A	1510	3	14,14,15	0.72	0	17,19,21	0.83	0
5	NAG	A	1506	3	14,14,15	0.74	0	17,19,21	1.16	2 (11%)
5	NAG	C	1508	3	14,14,15	0.71	0	17,19,21	0.87	0
5	NAG	C	1510	3	14,14,15	0.72	0	17,19,21	2.29	4 (23%)
5	NAG	C	1503	3	14,14,15	0.69	0	17,19,21	0.82	0
5	NAG	B	1502	3	14,14,15	0.76	0	17,19,21	0.97	1 (5%)
5	NAG	A	1513	3	14,14,15	0.75	0	17,19,21	0.92	0
5	NAG	A	1503	3	14,14,15	0.74	0	17,19,21	0.81	0
5	NAG	C	1506	3	14,14,15	0.74	0	17,19,21	0.87	0
5	NAG	A	1501	3	14,14,15	0.75	0	17,19,21	0.93	1 (5%)
5	NAG	C	1507	3	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
5	NAG	B	1501	3	14,14,15	0.74	0	17,19,21	0.76	0
5	NAG	B	1504	3	14,14,15	0.74	0	17,19,21	0.87	0
5	NAG	A	1507	3	14,14,15	0.76	0	17,19,21	0.86	0
5	NAG	A	1512	3	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
5	NAG	C	1511	3	14,14,15	0.74	0	17,19,21	0.79	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
5	NAG	A	1504	3	-	1/6/23/26	0/1/1/1
5	NAG	B	1503	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1505	3	-	2/6/23/26	0/1/1/1
5	NAG	A	1508	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1502	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1504	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1509	3	-	2/6/23/26	0/1/1/1
5	NAG	A	1502	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1505	3	-	2/6/23/26	0/1/1/1
5	NAG	C	1501	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1509	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1511	3	-	2/6/23/26	0/1/1/1
5	NAG	A	1514	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1510	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1506	3	-	3/6/23/26	0/1/1/1
5	NAG	C	1508	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1510	3	-	4/6/23/26	0/1/1/1
5	NAG	C	1503	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1502	3	-	1/6/23/26	0/1/1/1
5	NAG	A	1513	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1503	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1506	3	-	3/6/23/26	0/1/1/1
5	NAG	A	1501	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1507	3	-	2/6/23/26	0/1/1/1
5	NAG	B	1501	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1504	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1507	3	-	1/6/23/26	0/1/1/1
5	NAG	A	1512	3	-	2/6/23/26	0/1/1/1
5	NAG	C	1511	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(°)
5	C	1510	NAG	C1-O5-C5	7.63	122.41	112.19
5	C	1510	NAG	O5-C1-C2	3.57	116.82	111.29
5	A	1506	NAG	C1-O5-C5	3.07	116.31	112.19
5	C	1510	NAG	C3-C4-C5	-2.80	105.15	110.23
5	A	1506	NAG	C2-N2-C7	2.58	126.36	122.90
5	B	1502	NAG	C1-O5-C5	2.54	115.59	112.19
5	A	1505	NAG	O5-C1-C2	-2.42	107.55	111.29
5	A	1504	NAG	O5-C1-C2	-2.18	107.92	111.29
5	C	1502	NAG	C1-O5-C5	2.10	115.01	112.19
5	C	1510	NAG	C4-C3-C2	-2.07	107.98	111.02
5	A	1512	NAG	O5-C1-C2	-2.04	108.14	111.29
5	A	1501	NAG	C1-O5-C5	2.03	114.91	112.19
5	C	1507	NAG	O5-C1-C2	-2.00	108.19	111.29

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1510	NAG	O5-C5-C6-O6
5	A	1506	NAG	C8-C7-N2-C2
5	A	1506	NAG	O7-C7-N2-C2
5	A	1511	NAG	C8-C7-N2-C2
5	A	1511	NAG	O7-C7-N2-C2
5	A	1512	NAG	C8-C7-N2-C2
5	A	1512	NAG	O7-C7-N2-C2
5	C	1506	NAG	C8-C7-N2-C2
5	C	1506	NAG	O7-C7-N2-C2
5	C	1507	NAG	C8-C7-N2-C2
5	C	1507	NAG	O7-C7-N2-C2
5	C	1509	NAG	C8-C7-N2-C2
5	C	1509	NAG	O7-C7-N2-C2
5	C	1510	NAG	C8-C7-N2-C2
5	C	1510	NAG	O7-C7-N2-C2
5	C	1510	NAG	C4-C5-C6-O6
5	A	1506	NAG	O5-C5-C6-O6
5	A	1505	NAG	C4-C5-C6-O6
5	A	1507	NAG	O5-C5-C6-O6
5	A	1505	NAG	O5-C5-C6-O6
5	C	1505	NAG	C1-C2-N2-C7
5	C	1505	NAG	O5-C5-C6-O6
5	A	1504	NAG	O5-C5-C6-O6
5	B	1502	NAG	O5-C5-C6-O6
5	C	1506	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

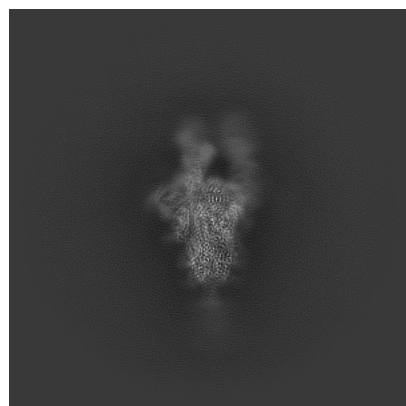
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43842. These allow visual inspection of the internal detail of the map and identification of artifacts.

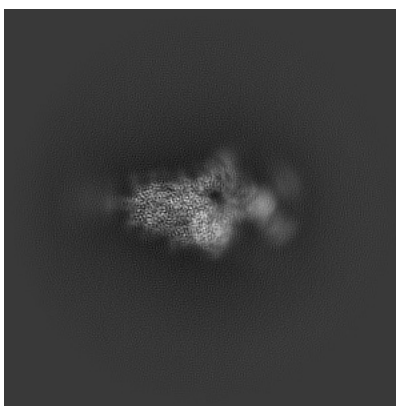
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

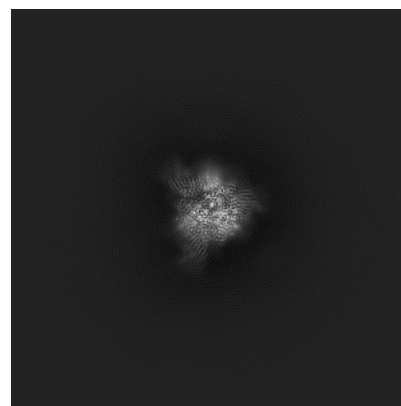
6.1.1 Primary map



X

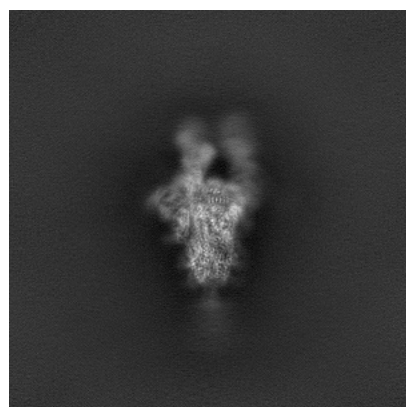


Y

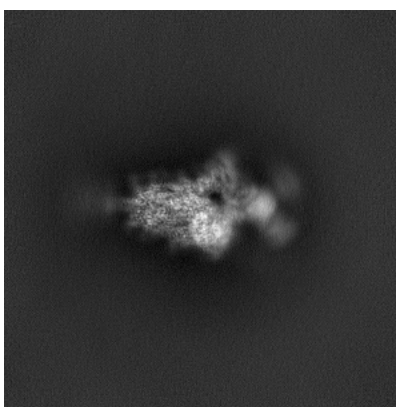


Z

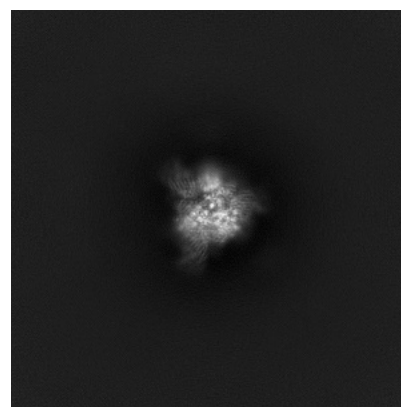
6.1.2 Raw map



X



Y



Z

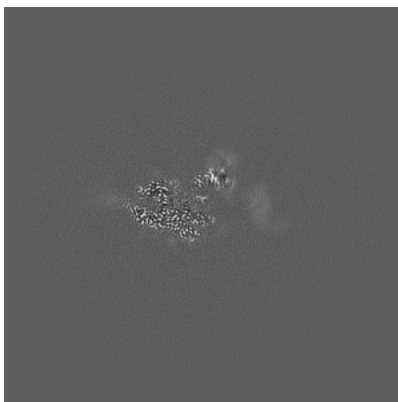
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

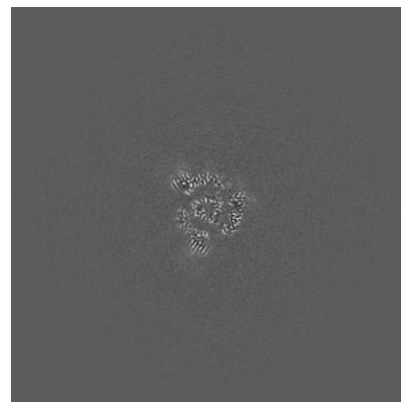
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

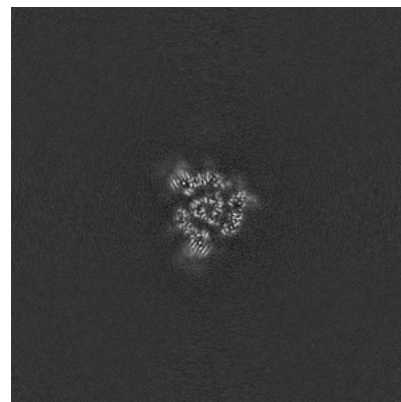
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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

6.3 Largest variance slices [i](#)

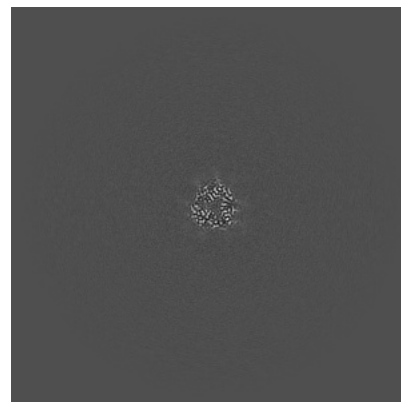
6.3.1 Primary map



X Index: 268



Y Index: 250



Z Index: 188

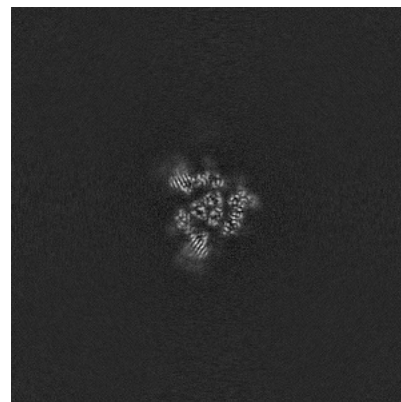
6.3.2 Raw map



X Index: 267



Y Index: 250



Z Index: 258

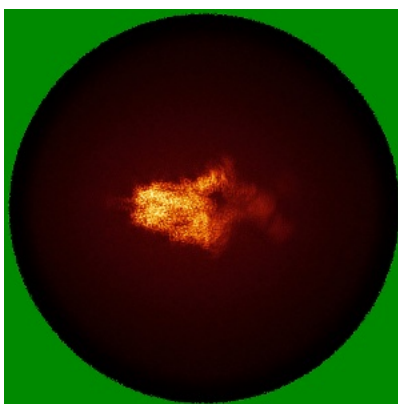
The images above show the largest variance slices of the map in three orthogonal directions.

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

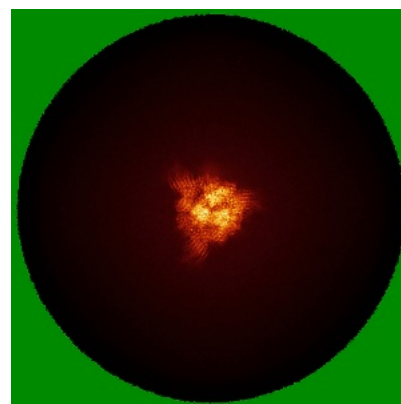
6.4.1 Primary map



X



Y

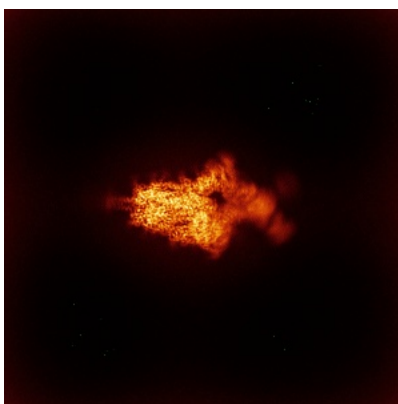


Z

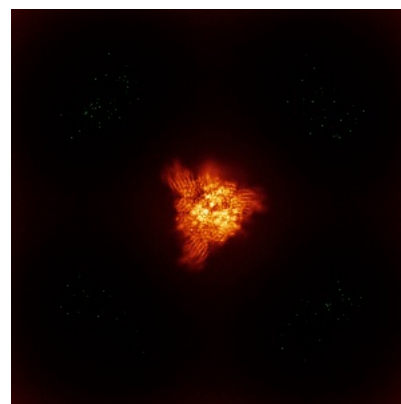
6.4.2 Raw map



X



Y

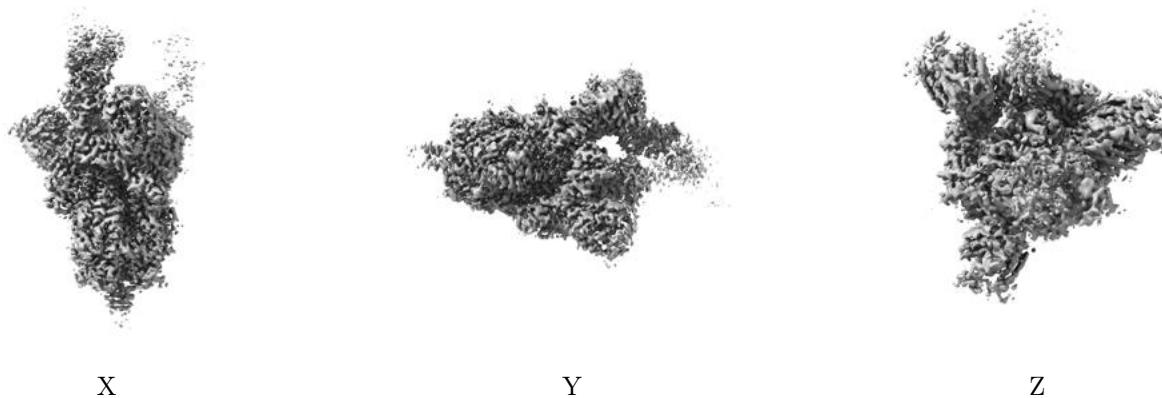


Z

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

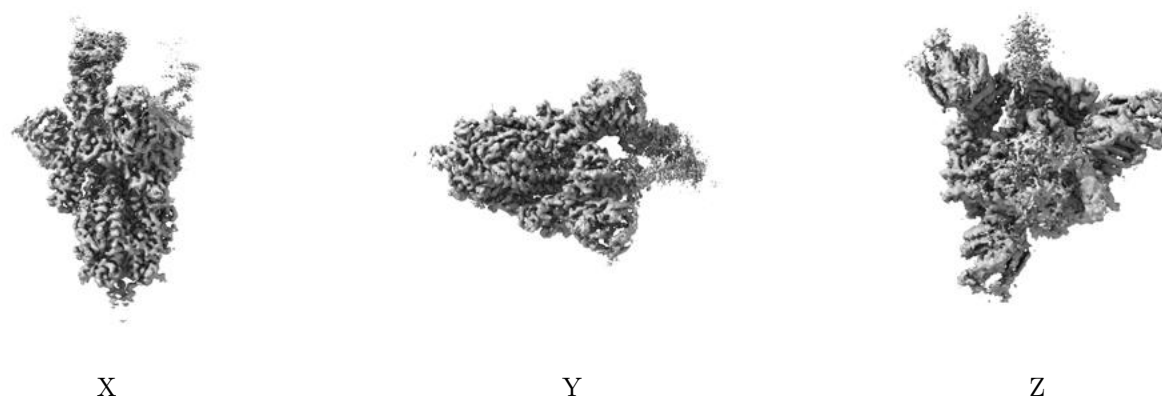
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

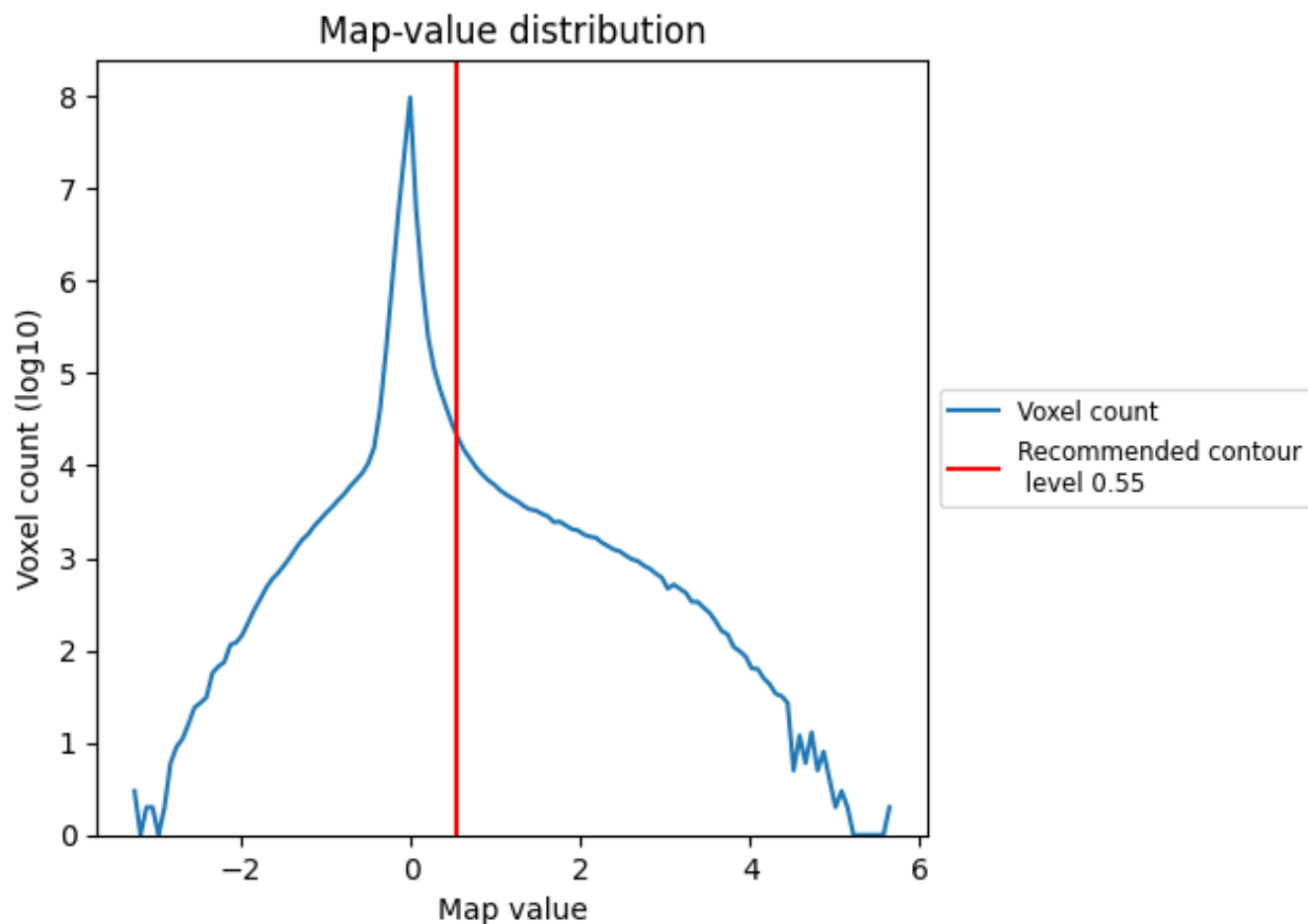
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

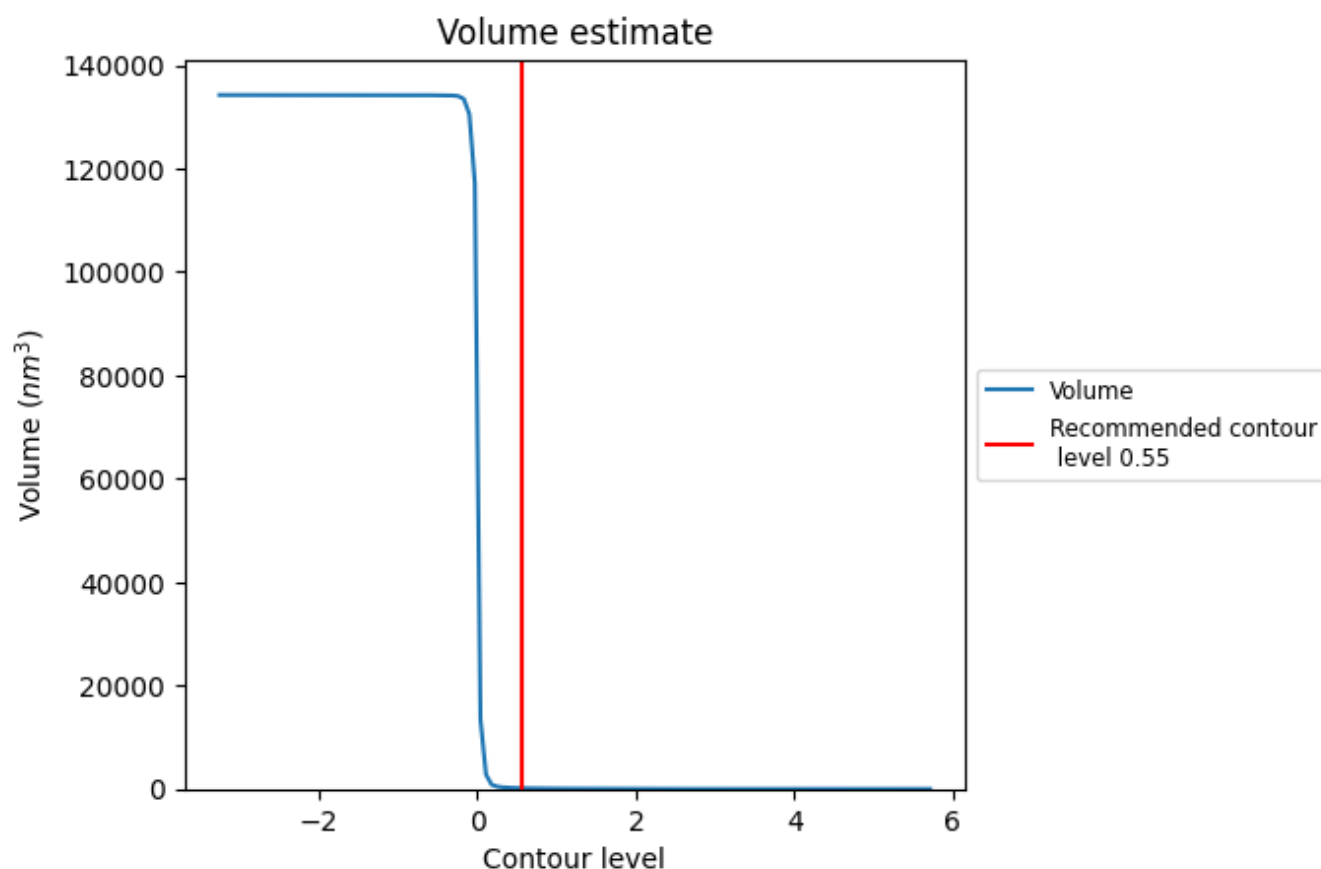
This section contains the results of statistical analysis of the map.

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.

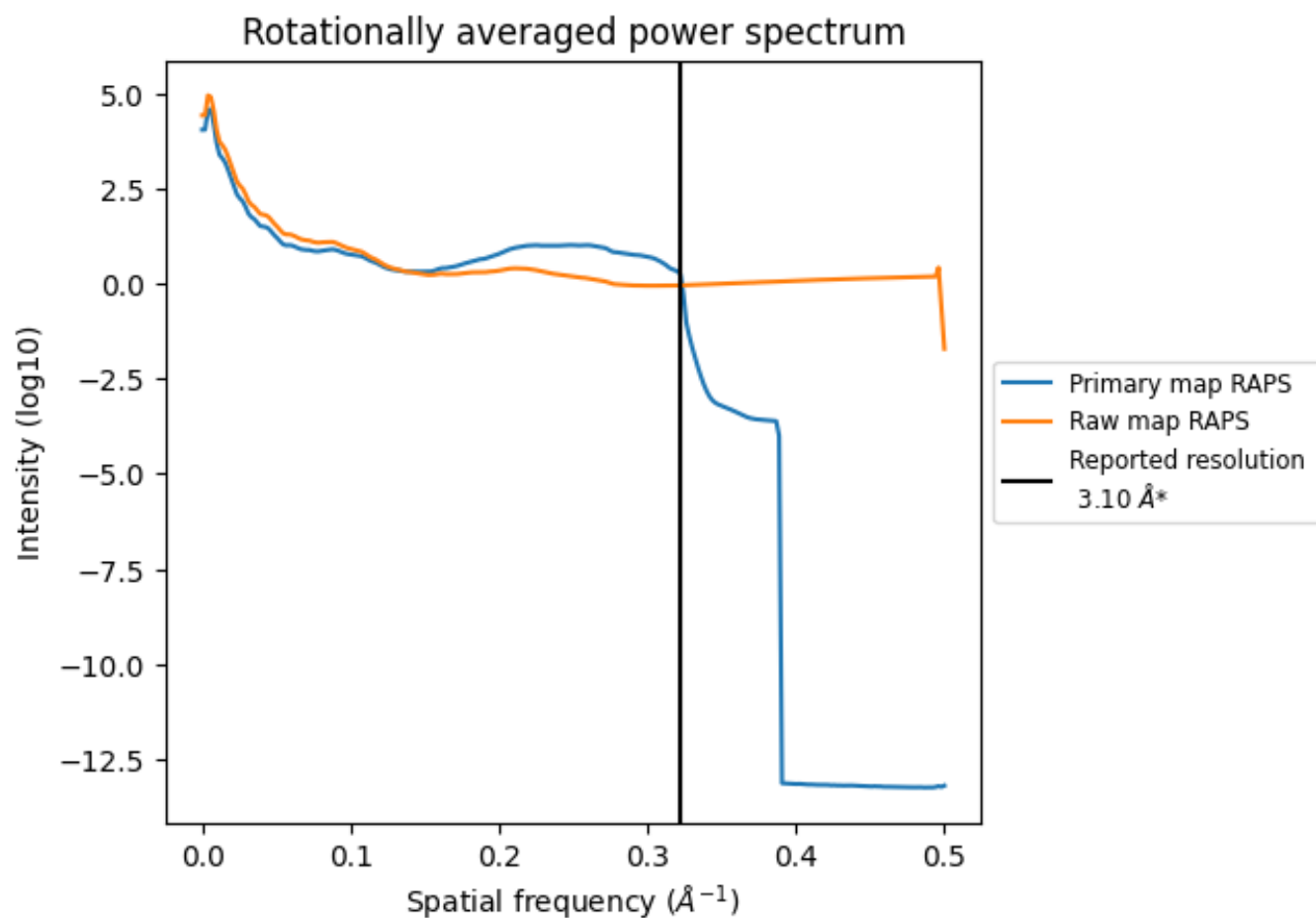
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 148 nm³; this corresponds to an approximate mass of 133 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 ⓘ

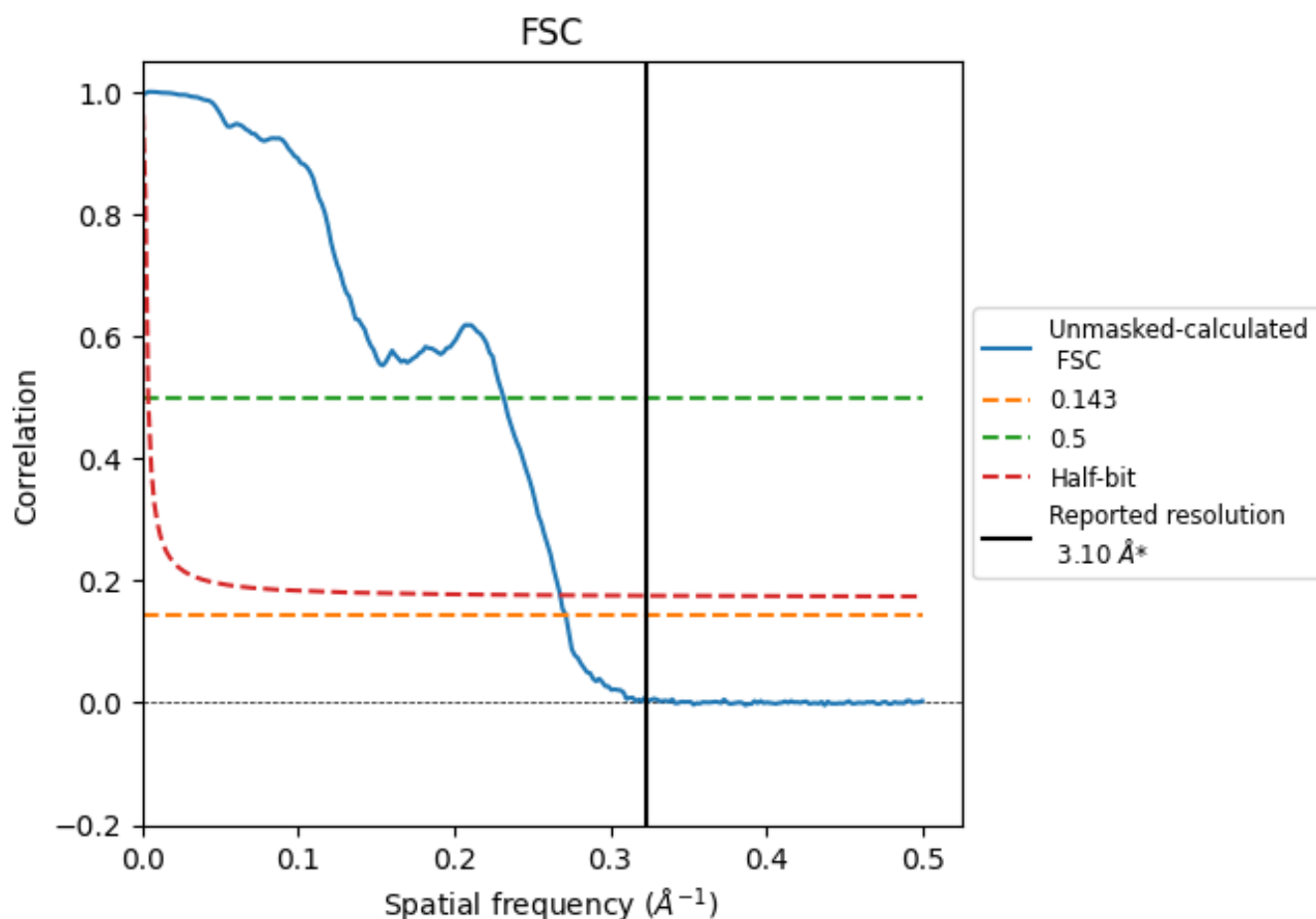


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

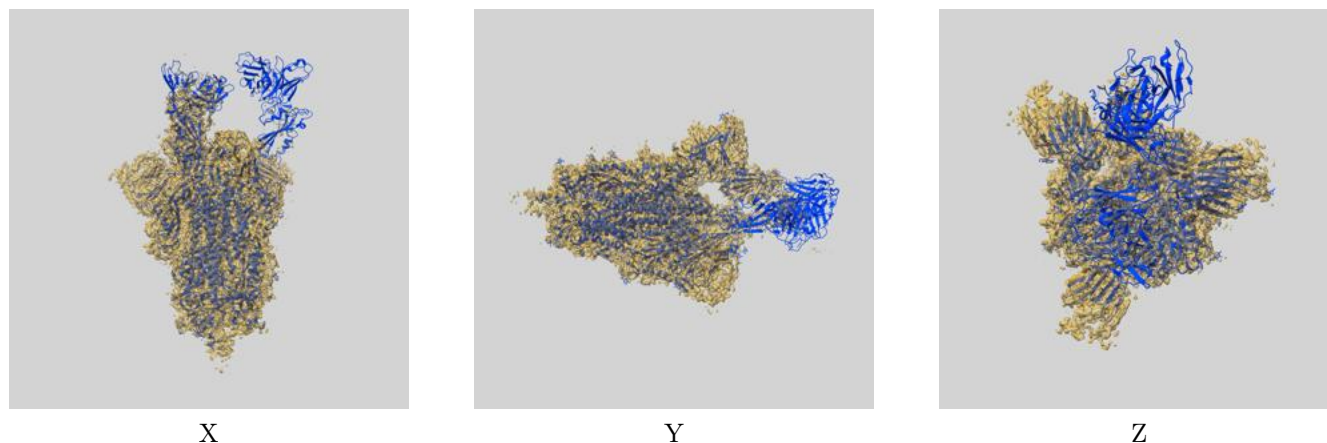
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.68	4.32	3.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.68 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

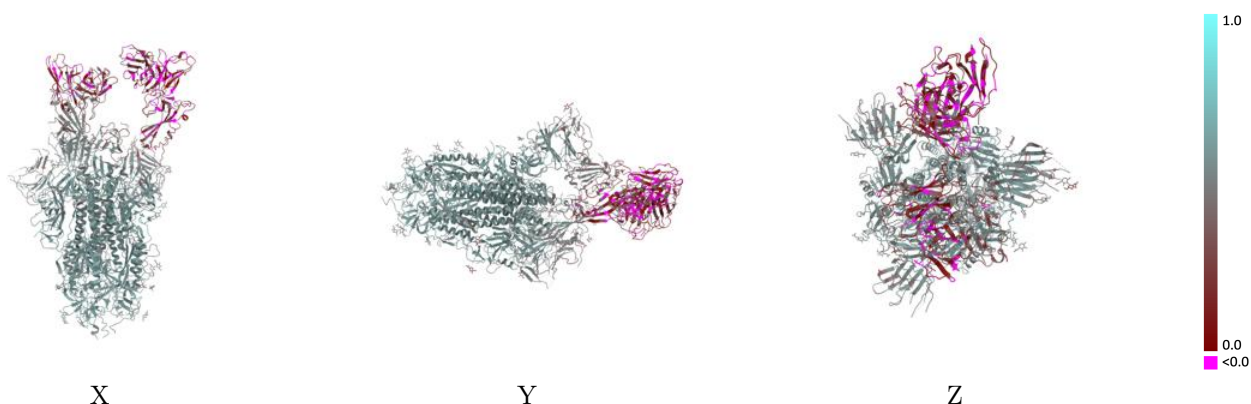
This section contains information regarding the fit between EMDB map EMD-43842 and PDB model 9AU2. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



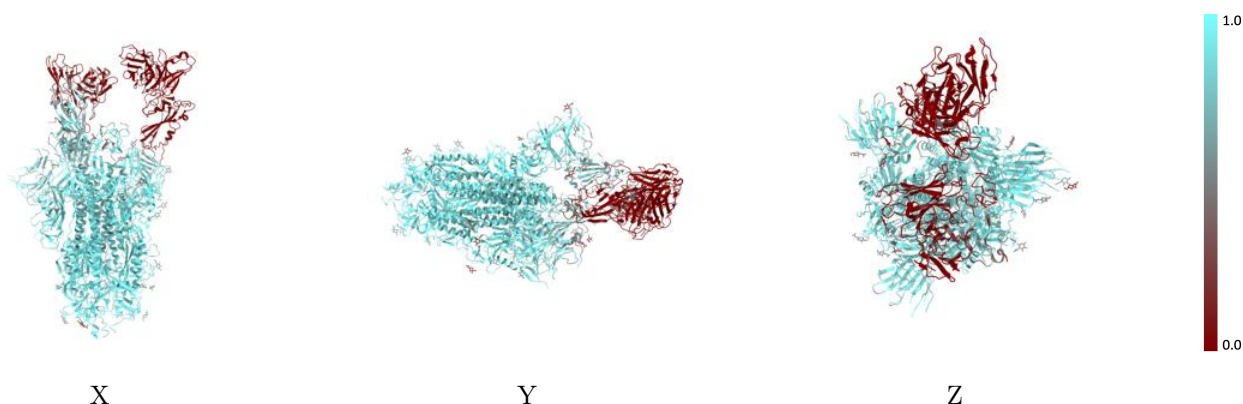
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



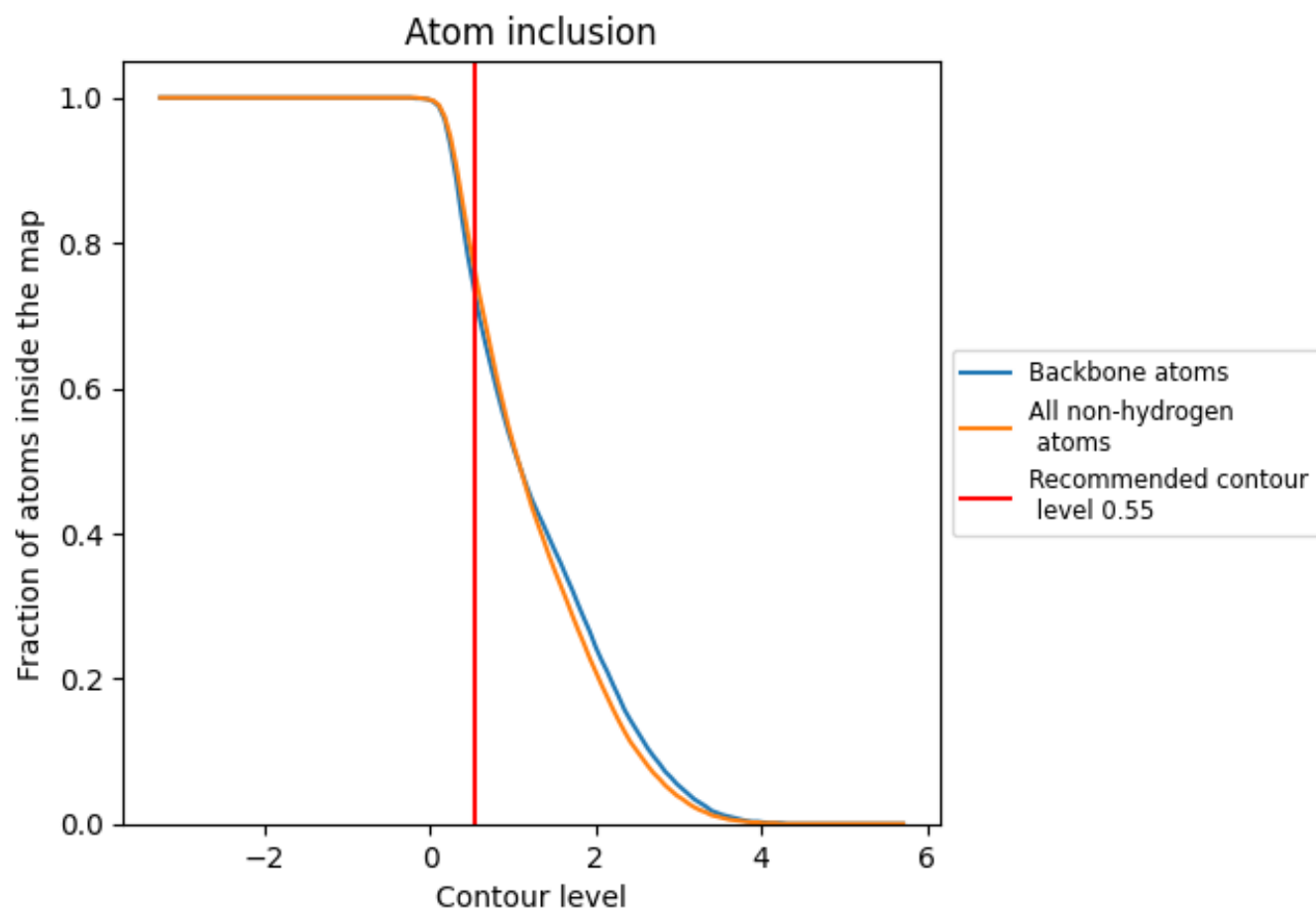
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 76% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7560	 0.4990
A	 0.8600	 0.5540
B	 0.8530	 0.5440
C	 0.7950	 0.5180
D	 0.0030	 0.1360
E	 0.7140	 0.4880
F	 0.0700	 0.1840
G	 0.6790	 0.4970
H	 0.6790	 0.4640
I	 0.0000	 0.0900
J	 0.0790	 0.1250
K	 0.7500	 0.5310
L	 0.7140	 0.4970
M	 0.6430	 0.4920
N	 0.7860	 0.5250
O	 0.3570	 0.4720
P	 0.7140	 0.4930
Q	 0.3210	 0.3390

