



## Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 02:05 PM EDT

PDB ID : 7RU3 / pdb\_00007ru3  
EMDB ID : EMD-24695  
Title : CC6.33 IgG in complex with SARS-CoV-2-6P-Mut7 S protein (non-uniform refinement)  
Authors : Ozorowski, G.; Turner, H.L.; Ward, A.B.  
Deposited on : 2021-08-16  
Resolution : 3.30 Å (reported)  
Based on initial model : 6VXX

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

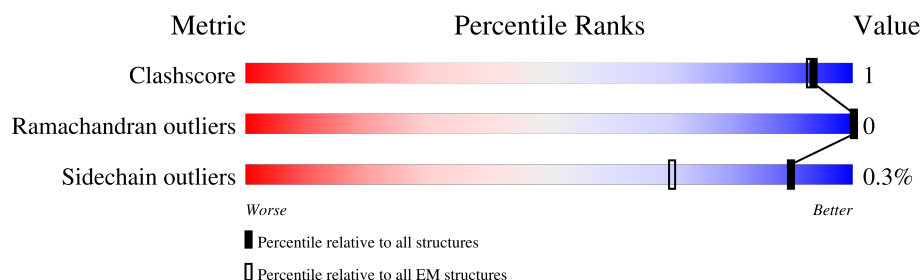
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	E	118	<div> <div>42%</div> <div>92%</div> <div>7%</div> </div>
1	H	118	<div> <div>21%</div> <div>95%</div> </div>
2	F	108	<div> <div>48%</div> <div>88%</div> <div>11%</div> </div>
2	L	108	<div> <div>44%</div> <div>94%</div> <div>6%</div> </div>
3	A	1280	<div> <div>76%</div> <div>6%</div> <div>17%</div> </div>
3	B	1280	<div> <div>75%</div> <div>6%</div> <div>19%</div> </div>
3	C	1280	<div> <div>8%</div> <div>71%</div> <div>6%</div> <div>23%</div> </div>
4	D	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	2	 100%
4	J	2	 100%
4	K	2	 100%
4	M	2	 100%
5	I	3	  33% 100%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28157 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 CC6.33 IgG heavy chain Fv.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	116	Total	C	N	O	S	0	0
			882	559	149	170	4		
1	E	116	Total	C	N	O	S	0	0
			882	559	149	170	4		

- Molecule 2 is a protein called CC6.33 IgG Kappa chain Fv.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	107	Total	C	N	O	S	0	0
			817	515	138	162	2		
2	F	107	Total	C	N	O	S	0	0
			817	515	138	162	2		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1062	Total	C	N	O	S	0	0
			8304	5297	1383	1583	41		
3	C	989	Total	C	N	O	S	0	0
			7737	4938	1290	1471	38		
3	B	1040	Total	C	N	O	S	0	0
			8134	5189	1356	1550	39		

There are 249 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	705	CYS	VAL	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	883	CYS	THR	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	ALA	-	expression tag	UNP P0DTC2
A	1252	TRP	-	expression tag	UNP P0DTC2
A	1253	SER	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	PRO	-	expression tag	UNP P0DTC2
A	1256	GLN	-	expression tag	UNP P0DTC2
A	1257	PHE	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	LYS	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	GLY	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	SER	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	GLY	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	ALA	-	expression tag	UNP P0DTC2
A	1273	TRP	-	expression tag	UNP P0DTC2
A	1274	SER	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	PRO	-	expression tag	UNP P0DTC2
A	1277	GLN	-	expression tag	UNP P0DTC2
A	1278	PHE	-	expression tag	UNP P0DTC2
A	1279	GLU	-	expression tag	UNP P0DTC2
A	1280	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	705	CYS	VAL	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	883	CYS	THR	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	ALA	-	expression tag	UNP P0DTC2
C	1252	TRP	-	expression tag	UNP P0DTC2
C	1253	SER	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	PRO	-	expression tag	UNP P0DTC2
C	1256	GLN	-	expression tag	UNP P0DTC2
C	1257	PHE	-	expression tag	UNP P0DTC2
C	1258	GLU	-	expression tag	UNP P0DTC2
C	1259	LYS	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	GLY	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	SER	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	GLY	-	expression tag	UNP P0DTC2
C	1266	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	ALA	-	expression tag	UNP P0DTC2
C	1273	TRP	-	expression tag	UNP P0DTC2
C	1274	SER	-	expression tag	UNP P0DTC2
C	1275	HIS	-	expression tag	UNP P0DTC2
C	1276	PRO	-	expression tag	UNP P0DTC2
C	1277	GLN	-	expression tag	UNP P0DTC2
C	1278	PHE	-	expression tag	UNP P0DTC2
C	1279	GLU	-	expression tag	UNP P0DTC2
C	1280	LYS	-	expression tag	UNP P0DTC2
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	705	CYS	VAL	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	883	CYS	THR	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	1248	PRO	-	expression tag	UNP P0DTC2

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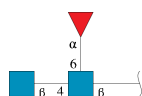
Chain	Residue	Modelled	Actual	Comment	Reference
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	ALA	-	expression tag	UNP P0DTC2
B	1252	TRP	-	expression tag	UNP P0DTC2
B	1253	SER	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	PRO	-	expression tag	UNP P0DTC2
B	1256	GLN	-	expression tag	UNP P0DTC2
B	1257	PHE	-	expression tag	UNP P0DTC2
B	1258	GLU	-	expression tag	UNP P0DTC2
B	1259	LYS	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	GLY	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	SER	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	GLY	-	expression tag	UNP P0DTC2
B	1266	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	ALA	-	expression tag	UNP P0DTC2
B	1273	TRP	-	expression tag	UNP P0DTC2
B	1274	SER	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	PRO	-	expression tag	UNP P0DTC2
B	1277	GLN	-	expression tag	UNP P0DTC2
B	1278	PHE	-	expression tag	UNP P0DTC2
B	1279	GLU	-	expression tag	UNP P0DTC2
B	1280	LYS	-	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.



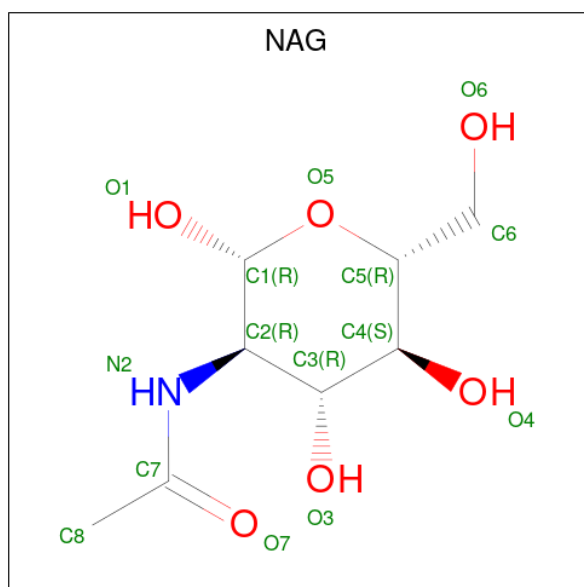
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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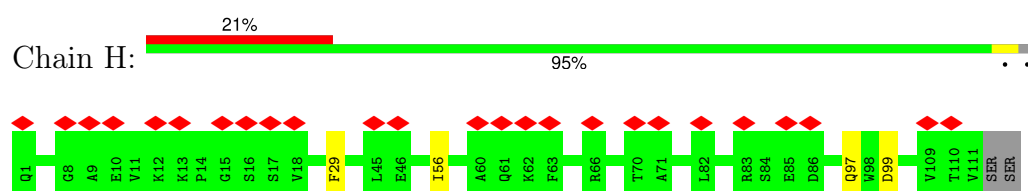
*Continued from previous page...*

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

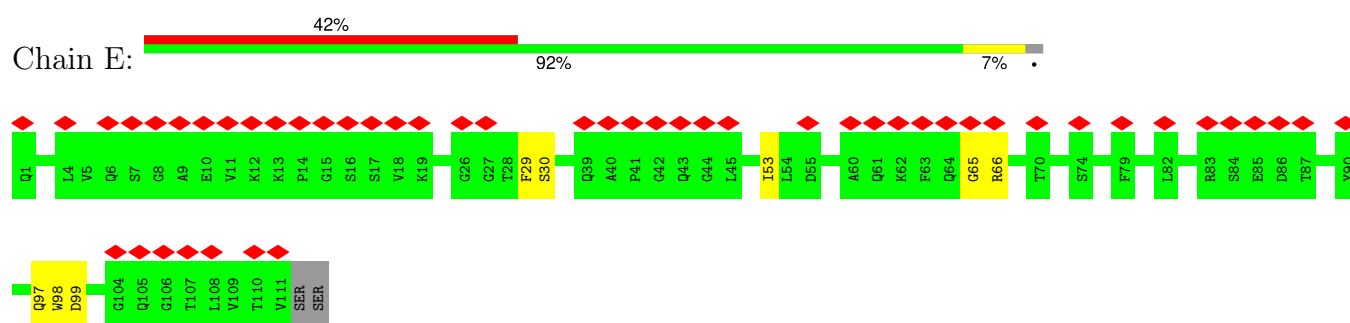
### 3 Residue-property plots [i](#)

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.

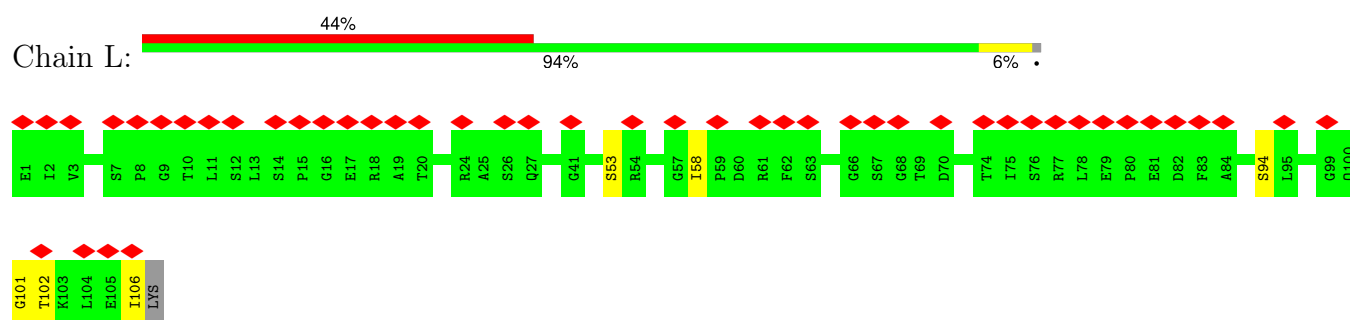
- Molecule 1: CC6.33 IgG heavy chain Fv



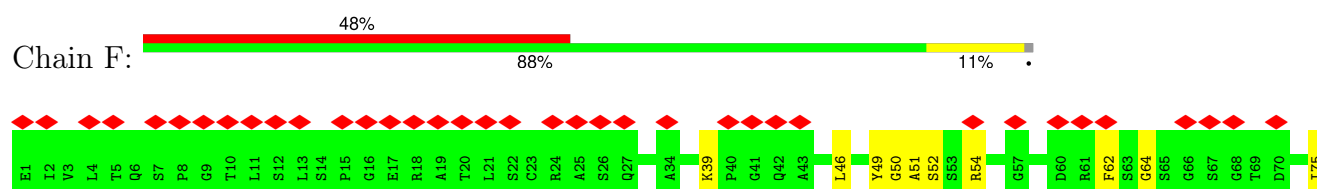
- Molecule 1: CC6.33 IgG heavy chain Fv



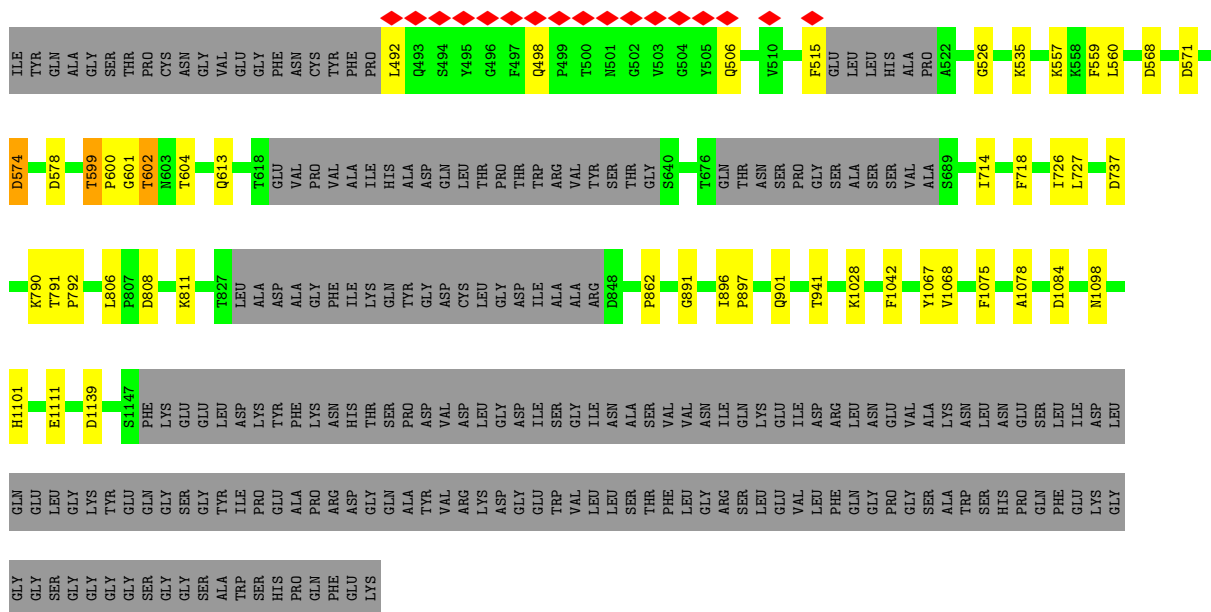
- Molecule 2: CC6.33 IgG Kappa chain Fv



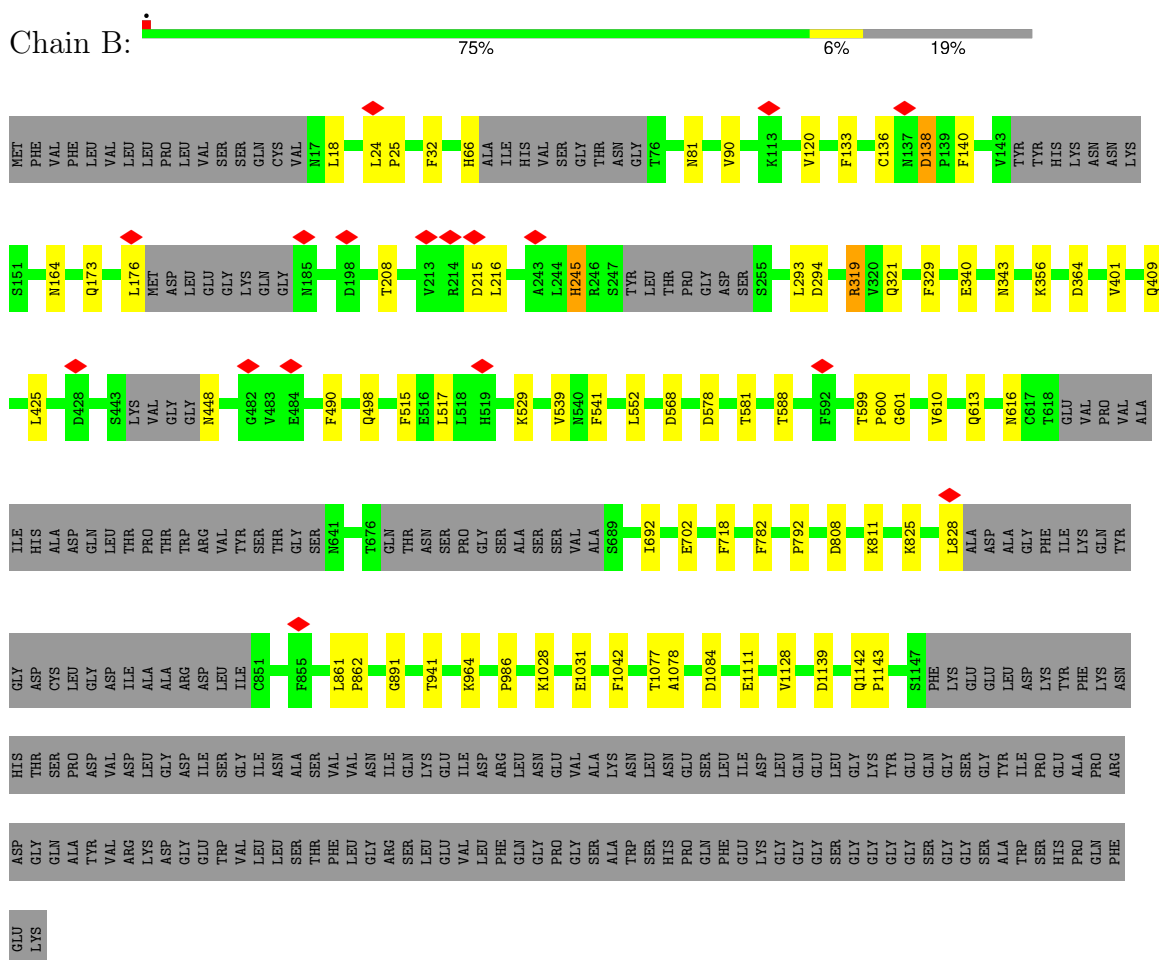
- Molecule 2: CC6.33 IgG Kappa chain Fv







- Molecule 3: Spike glycoprotein




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



Chain D:  100%


MAG1  
MAG2

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

Chain G:  100%


MAG1  
MAG2

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

Chain J:  100%


MAG1  
MAG2

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

Chain K:  100%

MAG1  
MAG2

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

Chain M:  100%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 100%

MAG1  
MAG2  
FUC3

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47461	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.033	Depositor
Minimum map value	-0.369	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	461.44, 461.44, 461.44	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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, FUC

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	E	0.97	0/899	1.20	4/1220 (0.3%)
1	H	0.97	0/899	1.22	4/1220 (0.3%)
2	F	1.07	2/837 (0.2%)	1.52	6/1137 (0.5%)
2	L	1.00	1/837 (0.1%)	1.23	3/1137 (0.3%)
3	A	1.16	11/8495 (0.1%)	1.31	81/11561 (0.7%)
3	B	1.13	5/8322 (0.1%)	1.29	81/11327 (0.7%)
3	C	1.14	12/7905 (0.2%)	1.30	77/10749 (0.7%)
All	All	1.13	31/28194 (0.1%)	1.30	256/38351 (0.7%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	828	LEU	CB-CG	7.48	1.68	1.53
3	C	466	ARG	NE-CZ	6.85	1.40	1.33
3	A	152	TRP	CZ2-CH2	6.68	1.50	1.37
3	C	1067	TYR	CB-CG	-6.67	1.36	1.51
2	F	49	TYR	CB-CG	-6.42	1.37	1.51
3	A	1083	HIS	CB-CG	-6.24	1.41	1.50
3	C	418	ILE	CB-CG1	6.21	1.65	1.53
3	B	692	ILE	CB-CG1	-6.14	1.41	1.53
3	C	454	ARG	NE-CZ	5.91	1.39	1.33
3	B	176	LEU	CB-CG	5.82	1.65	1.53
3	A	49	HIS	CB-CG	-5.74	1.42	1.50
3	A	828	LEU	CB-CG	5.73	1.65	1.53
3	A	152	TRP	CD2-CE3	5.70	1.49	1.40
3	C	441	LEU	CB-CG	5.68	1.64	1.53
3	A	312	ILE	CB-CG1	-5.55	1.42	1.53
3	A	37	TYR	CB-CG	-5.48	1.39	1.51
3	A	592	PHE	CB-CG	-5.43	1.38	1.50
2	L	106	ILE	CB-CG1	5.41	1.64	1.53
3	A	888	PHE	CB-CG	-5.40	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	90	HIS	CB-CG	-5.36	1.42	1.50
3	C	1067	TYR	CA-C	-5.31	1.46	1.52
3	B	66	HIS	CB-CG	5.23	1.57	1.50
3	C	79	PHE	CG-CD1	5.20	1.49	1.38
3	C	1075	PHE	CB-CG	-5.20	1.38	1.50
3	C	312	ILE	CB-CG1	-5.18	1.43	1.53
3	A	351	TYR	CB-CG	-5.18	1.40	1.51
3	C	396	TYR	CG-CD1	5.16	1.50	1.39
3	C	175	PHE	CG-CD1	5.14	1.49	1.38
3	C	492	LEU	CB-CG	5.13	1.63	1.53
3	B	448	ASN	CB-CG	5.10	1.64	1.52
3	A	454	ARG	CD-NE	-5.08	1.39	1.46

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	52	SER	N-CA-C	26.39	146.50	112.72
3	A	519	HIS	N-CA-C	-10.04	96.34	110.50
3	B	600	PRO	CA-C-N	-8.86	111.27	120.31
3	B	600	PRO	C-N-CA	-8.86	111.27	120.31
2	F	52	SER	CB-CA-C	-8.13	97.03	110.37
3	A	319	ARG	CA-C-N	7.97	132.33	120.69
3	A	319	ARG	C-N-CA	7.97	132.33	120.69
3	A	862	PRO	CA-C-N	7.96	127.89	119.85
3	A	862	PRO	C-N-CA	7.96	127.89	119.85
3	C	811	LYS	CA-C-N	7.89	127.61	119.56
3	C	811	LYS	C-N-CA	7.89	127.61	119.56
3	C	81	ASN	CA-C-N	7.88	127.83	120.03
3	C	81	ASN	C-N-CA	7.88	127.83	120.03
3	A	81	ASN	CA-C-N	7.79	127.74	120.03
3	A	81	ASN	C-N-CA	7.79	127.74	120.03
3	C	133	PHE	CA-CB-CG	7.55	121.35	113.80
3	C	574	ASP	CA-CB-CG	7.54	120.14	112.60
3	B	862	PRO	CA-C-N	7.54	127.47	119.85
3	B	862	PRO	C-N-CA	7.54	127.47	119.85
3	C	862	PRO	CA-C-N	7.46	127.42	120.03
3	C	862	PRO	C-N-CA	7.46	127.42	120.03
3	B	792	PRO	CA-C-N	7.40	128.03	120.04
3	B	792	PRO	C-N-CA	7.40	128.03	120.04
1	H	97	GLN	N-CA-C	-7.30	100.89	110.53
3	B	599	THR	CA-C-N	7.27	127.72	120.52
3	B	599	THR	C-N-CA	7.27	127.72	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	613	GLN	N-CA-C	7.14	119.07	111.28
3	C	714	ILE	CA-C-N	7.13	127.12	119.78
3	C	714	ILE	C-N-CA	7.13	127.12	119.78
3	A	235	ILE	N-CA-C	7.08	124.08	109.34
3	B	616	ASN	CA-C-N	7.02	132.40	122.08
3	B	616	ASN	C-N-CA	7.02	132.40	122.08
1	H	99	ASP	CA-CB-CG	6.98	119.58	112.60
3	C	383	SER	CA-C-N	6.97	128.56	119.84
3	C	383	SER	C-N-CA	6.97	128.56	119.84
3	C	602	THR	N-CA-C	-6.95	106.69	114.62
3	A	25	PRO	CA-C-N	6.95	126.91	120.03
3	A	25	PRO	C-N-CA	6.95	126.91	120.03
3	C	792	PRO	CA-C-N	6.95	127.55	120.04
3	C	792	PRO	C-N-CA	6.95	127.55	120.04
3	A	498	GLN	CA-C-N	6.94	126.64	119.56
3	A	498	GLN	C-N-CA	6.94	126.64	119.56
1	E	97	GLN	N-CA-C	-6.88	101.44	110.53
3	C	173	GLN	CA-C-N	6.84	126.83	119.78
3	C	173	GLN	C-N-CA	6.84	126.83	119.78
3	A	578	ASP	CA-C-N	6.83	126.52	119.56
3	A	578	ASP	C-N-CA	6.83	126.52	119.56
3	A	90	VAL	N-CA-C	6.73	117.54	108.11
3	B	1111	GLU	CA-C-N	6.72	126.68	119.76
3	B	1111	GLU	C-N-CA	6.72	126.68	119.76
3	C	559	PHE	CA-CB-CG	6.65	120.45	113.80
3	B	811	LYS	CA-C-N	6.64	126.26	119.56
3	B	811	LYS	C-N-CA	6.64	126.26	119.56
3	A	133	PHE	CA-CB-CG	6.63	120.43	113.80
3	A	120	VAL	N-CA-C	6.59	117.61	108.12
3	A	212	LEU	N-CA-C	6.59	119.19	109.24
3	C	1098	ASN	CA-CB-CG	6.57	119.17	112.60
3	B	1139	ASP	CA-C-N	6.57	126.70	119.87
3	B	1139	ASP	C-N-CA	6.57	126.70	119.87
3	B	133	PHE	CA-CB-CG	6.56	120.36	113.80
2	F	54	ARG	N-CA-C	-6.56	99.89	110.32
2	L	58	ILE	CA-C-N	6.56	126.25	119.56
2	L	58	ILE	C-N-CA	6.56	126.25	119.56
3	A	176	LEU	N-CA-C	6.54	118.20	111.14
3	A	122	ASN	CA-CB-CG	6.51	119.11	112.60
3	A	1111	GLU	CA-C-N	6.49	126.84	119.83
3	A	1111	GLU	C-N-CA	6.49	126.84	119.83
1	E	99	ASP	CA-CB-CG	6.49	119.09	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	891	GLY	CA-C-N	6.48	126.40	119.85
3	B	891	GLY	C-N-CA	6.48	126.40	119.85
3	B	539	VAL	N-CA-C	6.44	118.05	108.46
3	A	599	THR	CA-C-N	6.43	126.34	119.85
3	A	599	THR	C-N-CA	6.43	126.34	119.85
1	E	30	SER	N-CA-C	-6.42	101.45	110.50
3	B	216	LEU	CA-C-N	6.41	126.38	120.03
3	B	216	LEU	C-N-CA	6.41	126.38	120.03
3	B	517	LEU	N-CA-C	6.40	118.85	108.41
3	A	1139	ASP	CA-C-N	6.39	126.52	119.87
3	A	1139	ASP	C-N-CA	6.39	126.52	119.87
3	C	1111	GLU	CA-C-N	6.38	126.72	119.83
3	C	1111	GLU	C-N-CA	6.38	126.72	119.83
3	B	293	LEU	N-CA-C	6.36	118.30	111.36
3	C	301	CYS	N-CA-C	6.35	117.87	111.07
3	A	349	SER	N-CA-C	-6.30	102.21	110.53
3	C	90	VAL	N-CA-C	6.30	116.93	108.11
3	C	24	LEU	CA-C-N	6.22	126.79	120.38
3	C	24	LEU	C-N-CA	6.22	126.79	120.38
3	A	392	PHE	N-CA-C	6.19	119.12	109.52
3	C	498	GLN	CA-C-N	6.19	125.88	119.56
3	C	498	GLN	C-N-CA	6.19	125.88	119.56
3	B	164	ASN	N-CA-C	6.19	118.69	108.48
3	B	861	LEU	CA-C-N	6.19	124.12	119.66
3	B	861	LEU	C-N-CA	6.19	124.12	119.66
3	C	1078	ALA	CA-C-N	6.17	126.36	119.32
3	C	1078	ALA	C-N-CA	6.17	126.36	119.32
3	B	294	ASP	CA-C-N	6.16	126.62	119.47
3	B	294	ASP	C-N-CA	6.16	126.62	119.47
3	A	811	LYS	CA-C-N	6.16	125.78	119.56
3	A	811	LYS	C-N-CA	6.16	125.78	119.56
3	C	808	ASP	CA-C-N	6.14	126.26	119.87
3	C	808	ASP	C-N-CA	6.14	126.26	119.87
3	B	613	GLN	N-CA-C	6.12	117.95	111.28
3	B	409	GLN	CA-C-N	-6.11	115.91	121.65
3	B	409	GLN	C-N-CA	-6.11	115.91	121.65
3	C	1139	ASP	CA-C-N	6.09	127.46	119.84
3	C	1139	ASP	C-N-CA	6.09	127.46	119.84
3	B	498	GLN	CA-C-N	6.07	125.69	119.56
3	B	498	GLN	C-N-CA	6.07	125.69	119.56
3	B	1077	THR	N-CA-C	6.05	117.39	108.86
3	B	515	PHE	N-CA-C	6.04	118.24	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	120	VAL	N-CA-C	6.02	117.42	108.46
3	B	90	VAL	N-CA-C	6.00	116.50	108.11
3	C	941	THR	CA-C-N	5.98	125.60	119.56
3	C	941	THR	C-N-CA	5.98	125.60	119.56
3	A	481	ASN	N-CA-C	-5.97	99.98	109.23
3	C	231	ILE	N-CA-C	5.95	117.32	111.67
3	C	526	GLY	CA-C-N	5.95	125.86	119.85
3	C	526	GLY	C-N-CA	5.95	125.86	119.85
3	C	718	PHE	CA-CB-CG	5.94	119.74	113.80
3	B	578	ASP	CA-C-N	5.91	125.53	119.56
3	B	578	ASP	C-N-CA	5.91	125.53	119.56
3	A	706	ALA	CA-C-N	-5.89	112.71	120.95
3	A	706	ALA	C-N-CA	-5.89	112.71	120.95
3	C	97	LYS	N-CA-C	-5.89	105.69	114.64
3	C	891	GLY	CA-C-N	5.89	125.86	120.03
3	C	891	GLY	C-N-CA	5.89	125.86	120.03
3	B	173	GLN	CA-C-N	5.88	125.90	119.90
3	B	173	GLN	C-N-CA	5.88	125.90	119.90
3	A	164	ASN	N-CA-C	5.88	118.64	111.82
3	C	578	ASP	CA-C-N	5.87	126.28	119.47
3	C	578	ASP	C-N-CA	5.87	126.28	119.47
3	B	941	THR	CA-C-N	5.87	125.48	119.56
3	B	941	THR	C-N-CA	5.87	125.48	119.56
3	A	600	PRO	N-CA-C	-5.86	102.06	111.38
3	B	601	GLY	N-CA-C	-5.85	103.58	111.54
3	A	400	PHE	N-CA-C	5.84	117.02	108.14
3	C	335	LEU	CA-C-N	5.83	128.77	120.49
3	C	335	LEU	C-N-CA	5.83	128.77	120.49
3	C	727	LEU	CA-C-N	5.83	125.74	119.85
3	C	727	LEU	C-N-CA	5.83	125.74	119.85
3	A	520	ALA	CA-C-N	5.81	126.28	120.52
3	A	520	ALA	C-N-CA	5.81	126.28	120.52
3	A	425	LEU	CA-C-N	5.79	125.75	119.78
3	A	425	LEU	C-N-CA	5.79	125.75	119.78
3	A	294	ASP	CA-C-N	5.79	126.19	119.47
3	A	294	ASP	C-N-CA	5.79	126.19	119.47
3	B	32	PHE	CA-CB-CG	-5.74	108.06	113.80
3	A	887	THR	CA-C-N	5.74	127.91	120.44
3	A	887	THR	C-N-CA	5.74	127.91	120.44
3	C	294	ASP	CA-C-N	5.72	126.11	119.47
3	C	294	ASP	C-N-CA	5.72	126.11	119.47
3	A	861	LEU	CA-C-N	5.70	123.77	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	861	LEU	C-N-CA	5.70	123.77	119.66
3	C	613	GLN	N-CA-C	5.68	120.75	111.37
3	C	1068	VAL	CA-C-N	5.68	125.63	119.78
3	C	1068	VAL	C-N-CA	5.68	125.63	119.78
3	B	808	ASP	CA-C-N	5.68	125.78	119.87
3	B	808	ASP	C-N-CA	5.68	125.78	119.87
3	A	173	GLN	CA-C-N	5.68	125.69	119.90
3	A	173	GLN	C-N-CA	5.68	125.69	119.90
3	B	245	HIS	CA-CB-CG	-5.68	108.12	113.80
3	A	600	PRO	CA-C-N	-5.66	114.72	120.10
3	A	600	PRO	C-N-CA	-5.66	114.72	120.10
3	A	409	GLN	CA-C-N	-5.66	116.33	121.65
3	A	409	GLN	C-N-CA	-5.66	116.33	121.65
3	A	491	PRO	N-CA-C	5.63	121.25	113.65
3	B	120	VAL	N-CA-C	5.62	116.21	108.12
3	A	490	PHE	CA-C-N	5.61	125.45	119.28
3	A	490	PHE	C-N-CA	5.61	125.45	119.28
3	B	81	ASN	CA-C-N	5.60	125.58	120.03
3	B	81	ASN	C-N-CA	5.60	125.58	120.03
3	B	782	PHE	N-CA-C	5.56	120.17	113.17
3	A	1098	ASN	CA-CB-CG	5.55	118.15	112.60
3	A	214	ARG	CB-CA-C	-5.55	109.69	117.23
3	A	411	ALA	CA-C-N	5.54	126.77	119.84
3	A	411	ALA	C-N-CA	5.54	126.77	119.84
3	B	24	LEU	CA-C-N	5.54	126.08	120.38
3	B	24	LEU	C-N-CA	5.54	126.08	120.38
3	B	1128	VAL	N-CA-C	5.52	116.37	111.90
3	B	215	ASP	N-CA-C	5.51	117.81	110.53
3	C	80	ASP	CA-CB-CG	5.51	118.11	112.60
3	B	1078	ALA	CA-C-N	5.46	125.08	119.56
3	B	1078	ALA	C-N-CA	5.46	125.08	119.56
2	L	94	SER	N-CA-C	-5.45	106.48	114.39
2	F	39	LYS	N-CA-C	-5.44	103.21	110.07
3	C	1101	HIS	N-CA-C	5.43	118.31	109.24
3	C	462	LYS	CA-C-N	5.42	125.68	119.83
3	C	462	LYS	C-N-CA	5.42	125.68	119.83
3	B	588	THR	CA-C-N	5.41	125.35	119.78
3	B	588	THR	C-N-CA	5.41	125.35	119.78
3	B	136	CYS	N-CA-C	-5.38	102.52	110.48
3	C	515	PHE	CA-CB-CG	5.34	119.14	113.80
3	A	791	THR	CA-C-N	5.33	123.55	119.66
3	A	791	THR	C-N-CA	5.33	123.55	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	VAL	N-CA-C	5.33	115.63	108.17
3	B	208	THR	CA-C-N	5.32	125.24	119.76
3	B	208	THR	C-N-CA	5.32	125.24	119.76
3	C	791	THR	CA-C-N	5.31	123.54	119.66
3	C	791	THR	C-N-CA	5.31	123.54	119.66
3	B	490	PHE	N-CA-C	-5.31	101.69	109.50
3	A	595	VAL	N-CA-C	5.31	115.77	108.12
3	C	737	ASP	CA-C-N	5.30	127.34	120.44
3	C	737	ASP	C-N-CA	5.30	127.34	120.44
3	A	138	ASP	CA-C-N	5.29	125.21	119.76
3	A	138	ASP	C-N-CA	5.29	125.21	119.76
3	A	473	TYR	N-CA-C	5.29	116.83	108.96
2	F	79	GLU	CA-C-N	5.27	125.59	119.47
2	F	79	GLU	C-N-CA	5.27	125.59	119.47
3	A	216	LEU	CA-C-N	5.27	125.25	120.03
3	A	216	LEU	C-N-CA	5.27	125.25	120.03
3	B	138	ASP	CA-C-N	5.26	125.47	120.31
3	B	138	ASP	C-N-CA	5.26	125.47	120.31
3	A	229	LEU	N-CA-C	5.26	116.29	109.72
3	B	610	VAL	N-CA-C	5.25	115.46	108.11
3	C	901	GLN	N-CA-C	-5.25	105.64	111.36
3	C	806	LEU	CA-C-N	5.23	125.15	119.76
3	C	806	LEU	C-N-CA	5.23	125.15	119.76
3	A	1068	VAL	CA-C-N	5.22	125.14	119.76
3	A	1068	VAL	C-N-CA	5.22	125.14	119.76
3	B	329	PHE	CA-C-N	5.22	125.20	120.03
3	B	329	PHE	C-N-CA	5.22	125.20	120.03
3	C	506	GLN	CA-C-N	5.22	124.98	119.76
3	C	506	GLN	C-N-CA	5.22	124.98	119.76
3	A	1078	ALA	CA-C-N	5.21	124.82	119.56
3	A	1078	ALA	C-N-CA	5.21	124.82	119.56
3	A	487	ASN	N-CA-C	5.21	118.94	112.59
3	C	560	LEU	N-CA-C	-5.20	102.90	110.08
3	C	117	LEU	N-CA-C	5.18	117.18	108.73
3	A	808	ASP	CA-C-N	5.18	124.79	119.56
3	A	808	ASP	C-N-CA	5.18	124.79	119.56
3	B	1031	GLU	N-CA-C	5.17	117.82	111.82
3	A	233	ILE	CA-C-N	5.16	127.46	120.44
3	A	233	ILE	C-N-CA	5.16	127.46	120.44
3	B	321	GLN	CA-C-N	5.15	125.05	119.85
3	B	321	GLN	C-N-CA	5.15	125.05	119.85
3	B	825	LYS	CA-C-N	-5.12	115.97	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	825	LYS	C-N-CA	-5.12	115.97	122.43
3	C	208	THR	CA-C-N	5.10	124.86	119.76
3	C	208	THR	C-N-CA	5.10	124.86	119.76
3	B	581	THR	N-CA-C	-5.10	100.59	108.90
3	C	535	LYS	CA-C-N	5.09	129.78	122.40
3	C	535	LYS	C-N-CA	5.09	129.78	122.40
1	H	29	PHE	N-CA-C	-5.08	105.66	111.14
1	H	56	ILE	N-CA-C	5.08	115.22	108.11
3	C	726	ILE	N-CA-C	5.08	115.22	108.11
3	A	205	SER	N-CA-C	5.07	116.01	108.60
3	B	425	LEU	CA-C-N	5.06	125.00	119.78
3	B	425	LEU	C-N-CA	5.06	125.00	119.78
1	E	29	PHE	N-CA-C	-5.06	105.22	111.40
3	A	1074	ASN	CA-CB-CG	5.05	117.65	112.60
3	A	883	CYS	N-CA-C	5.03	116.84	111.36
3	C	53	ASP	CA-CB-CG	5.03	117.63	112.60
3	B	25	PRO	CA-C-N	5.01	124.91	119.85
3	B	25	PRO	C-N-CA	5.01	124.91	119.85
3	C	342	PHE	CA-CB-CG	-5.00	108.80	113.80
3	B	986	PRO	CB-CA-C	5.00	117.02	110.92

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	E	882	0	881	3	0
1	H	882	0	881	0	0
2	F	817	0	790	3	0
2	L	817	0	790	3	0
3	A	8304	0	8085	28	0
3	B	8134	0	7920	19	0
3	C	7737	0	7545	15	0
4	D	28	0	25	0	0
4	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
5	I	38	0	34	0	0
6	A	196	0	180	0	0
6	B	70	0	64	0	0
6	C	140	0	130	0	0
All	All	28157	0	27425	64	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 1.

All (64) 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:A:235:ILE:HG22	3:A:235:ILE:O	1.52	1.05
3:B:529:LYS:NZ	1:E:53:ILE:O	2.06	0.88
3:A:236:THR:HG23	3:A:237:ARG:HG3	1.55	0.87
3:A:235:ILE:O	3:A:235:ILE:CG2	2.26	0.83
3:A:319:ARG:NE	3:A:319:ARG:HA	2.00	0.77
3:C:308:VAL:HG12	3:C:599:THR:HG21	1.68	0.75
3:B:18:LEU:HD12	3:B:138:ASP:HB3	1.77	0.67
3:A:318:PHE:HB3	3:A:593:GLY:HA3	1.77	0.67
3:A:106:PHE:HB3	3:A:235:ILE:CG2	2.29	0.62
3:B:319:ARG:HG3	3:B:319:ARG:NH1	2.13	0.62
2:L:53:SER:HB2	3:A:345:THR:HG21	1.82	0.62
2:L:53:SER:HB2	3:A:345:THR:CG2	2.32	0.60
3:A:541:PHE:CZ	3:A:552:LEU:HB2	2.37	0.59
3:B:319:ARG:HG3	3:B:319:ARG:HH11	1.69	0.57
2:F:51:ALA:O	2:F:64:GLY:C	2.48	0.57
3:C:310:LYS:HA	3:C:601:GLY:H	1.69	0.56
3:A:106:PHE:HB3	3:A:235:ILE:HG23	1.87	0.56
3:A:557:LYS:NZ	3:A:574:ASP:OD2	2.38	0.56
3:B:541:PHE:CZ	3:B:552:LEU:HG	2.41	0.56
3:B:364:ASP:O	1:E:98:TRP:NE1	2.40	0.55
3:B:319:ARG:HH11	3:B:319:ARG:CG	2.19	0.55
3:C:308:VAL:CG1	3:C:599:THR:HG21	2.35	0.54
3:B:340:GLU:OE1	3:B:356:LYS:NZ	2.42	0.53
3:B:245:HIS:N	3:B:245:HIS:ND1	2.57	0.52
3:B:18:LEU:HD21	3:B:140:PHE:CD2	2.45	0.51
3:A:319:ARG:HG3	3:A:319:ARG:HH11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:790:LYS:NZ	3:B:702:GLU:OE2	2.44	0.50
3:A:541:PHE:HZ	3:A:552:LEU:HB2	1.75	0.49
3:A:986:PRO:HB2	3:A:987:PRO:HD3	1.95	0.49
3:B:18:LEU:HD21	3:B:140:PHE:CE2	2.48	0.49
3:A:106:PHE:HB3	3:A:235:ILE:HG21	1.95	0.49
3:A:233:ILE:HG13	3:A:235:ILE:HG13	1.95	0.49
3:A:233:ILE:HD11	3:A:235:ILE:HD11	1.95	0.48
3:C:299:THR:O	3:C:300:LYS:C	2.57	0.47
3:C:299:THR:O	3:C:302:THR:N	2.48	0.47
3:A:81:ASN:N	3:A:82:PRO:CD	2.78	0.46
3:A:236:THR:HG23	3:A:237:ARG:N	2.30	0.46
3:C:602:THR:C	3:C:604:THR:N	2.73	0.46
3:A:319:ARG:HA	3:A:319:ARG:HE	1.79	0.46
3:B:1028:LYS:NZ	3:B:1042:PHE:O	2.49	0.45
3:C:1084:ASP:N	3:C:1084:ASP:OD1	2.46	0.45
2:L:101:GLY:O	2:L:102:THR:C	2.60	0.45
3:A:318:PHE:CB	3:A:593:GLY:HA3	2.46	0.44
3:A:319:ARG:O	3:A:321:GLN:NE2	2.44	0.44
3:A:702:GLU:OE2	3:C:790:LYS:NZ	2.50	0.44
3:B:1084:ASP:N	3:B:1084:ASP:OD1	2.44	0.44
3:A:519:HIS:O	3:A:520:ALA:C	2.60	0.44
3:C:571:ASP:OD2	3:B:964:LYS:NZ	2.45	0.44
3:A:758:SER:O	3:A:759:PHE:C	2.62	0.43
3:C:193:VAL:HG12	3:C:204:TYR:HB2	2.02	0.42
1:E:65:GLY:O	1:E:66:ARG:HB2	2.20	0.42
3:C:599:THR:HA	3:C:600:PRO:HD3	1.88	0.42
3:B:718:PHE:CD1	3:B:718:PHE:C	2.98	0.42
3:A:908:GLY:O	3:A:1038:LYS:NZ	2.53	0.41
3:C:557:LYS:NZ	3:C:574:ASP:OD2	2.53	0.41
3:A:81:ASN:N	3:A:82:PRO:HD3	2.35	0.41
3:B:541:PHE:HZ	3:B:552:LEU:HG	1.83	0.41
3:C:896:ILE:O	3:C:897:PRO:C	2.63	0.41
3:C:568:ASP:OD1	3:C:568:ASP:C	2.63	0.41
2:F:62:PHE:CE2	2:F:75:ILE:HG12	2.56	0.41
3:C:1028:LYS:NZ	3:C:1042:PHE:O	2.54	0.41
2:F:50:GLY:O	2:F:51:ALA:HB3	2.21	0.41
3:B:568:ASP:OD1	3:B:568:ASP:C	2.64	0.40
3:B:1142:GLN:N	3:B:1143:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
1	H	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
2	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	L	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
3	A	1046/1280 (82%)	1012 (97%)	34 (3%)	0	100	100
3	B	1022/1280 (80%)	993 (97%)	29 (3%)	0	100	100
3	C	955/1280 (75%)	922 (96%)	33 (4%)	0	100	100
All	All	3461/4292 (81%)	3351 (97%)	110 (3%)	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	E	96/98 (98%)	96 (100%)	0	100	100
1	H	96/98 (98%)	96 (100%)	0	100	100
2	F	89/90 (99%)	88 (99%)	1 (1%)	70	82
2	L	89/90 (99%)	89 (100%)	0	100	100
3	A	933/1108 (84%)	928 (100%)	5 (0%)	86	91
3	B	914/1108 (82%)	912 (100%)	2 (0%)	92	95
3	C	873/1108 (79%)	871 (100%)	2 (0%)	92	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3090/3700 (84%)	3080 (100%)	10 (0%)	90	94

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	122	ASN
3	A	319	ARG
3	A	331	ASN
3	A	343	ASN
3	A	1074	ASN
3	C	300	LYS
3	C	599	THR
3	B	319	ARG
3	B	343	ASN
2	F	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
1	H	61	GLN
2	L	38	GLN
3	A	137	ASN
3	A	542	ASN
3	A	856	ASN
3	A	969	ASN
3	C	14	GLN
3	C	134	GLN
3	C	188	ASN
3	C	394	ASN
3	C	755	GLN
3	C	1005	GLN
3	B	134	GLN
3	B	173	GLN
3	B	185	ASN
3	B	188	ASN
3	B	334	ASN
3	B	493	GLN
3	B	580	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

13 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	D	1	3,4	14,14,15	2.12	5 (35%)	17,19,21	1.14	1 (5%)
4	NAG	D	2	4	14,14,15	2.00	6 (42%)	17,19,21	1.05	2 (11%)
4	NAG	G	1	3,4	14,14,15	1.95	5 (35%)	17,19,21	1.02	1 (5%)
4	NAG	G	2	4	14,14,15	1.99	6 (42%)	17,19,21	0.89	1 (5%)
5	NAG	I	1	3,5	14,14,15	1.57	2 (14%)	17,19,21	1.11	0
5	NAG	I	2	5	14,14,15	2.07	5 (35%)	17,19,21	0.91	1 (5%)
5	FUC	I	3	5	10,10,11	1.91	5 (50%)	14,14,16	0.78	0
4	NAG	J	1	3,4	14,14,15	1.99	4 (28%)	17,19,21	1.01	2 (11%)
4	NAG	J	2	4	14,14,15	1.98	5 (35%)	17,19,21	0.89	1 (5%)
4	NAG	K	1	3,4	14,14,15	2.04	4 (28%)	17,19,21	0.97	0
4	NAG	K	2	4	14,14,15	1.89	5 (35%)	17,19,21	0.91	1 (5%)
4	NAG	M	1	3,4	14,14,15	2.05	5 (35%)	17,19,21	1.15	2 (11%)
4	NAG	M	2	4	14,14,15	1.98	4 (28%)	17,19,21	0.84	1 (5%)

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	D	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
5	NAG	I	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	FUC	I	3	5	-	-	0/1/1/1
4	NAG	J	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	M	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	C1-C2	5.52	1.59	1.52
4	K	1	NAG	C1-C2	5.44	1.59	1.52
4	M	1	NAG	C1-C2	5.24	1.59	1.52
5	I	2	NAG	C1-C2	5.20	1.59	1.52
4	J	1	NAG	C1-C2	4.86	1.59	1.52
4	G	1	NAG	C1-C2	4.85	1.58	1.52
4	G	2	NAG	C1-C2	4.77	1.58	1.52
4	M	2	NAG	C1-C2	4.75	1.58	1.52
4	D	2	NAG	C1-C2	4.71	1.58	1.52
4	J	2	NAG	C1-C2	4.68	1.58	1.52
5	I	1	NAG	C1-C2	4.34	1.58	1.52
4	K	2	NAG	C1-C2	4.33	1.58	1.52
4	M	2	NAG	O5-C5	3.23	1.49	1.43
4	M	1	NAG	O5-C5	3.18	1.49	1.43
4	D	2	NAG	O5-C5	3.15	1.49	1.43
4	J	2	NAG	O5-C5	3.07	1.49	1.43
4	K	2	NAG	O5-C5	3.02	1.49	1.43
5	I	2	NAG	O5-C5	3.02	1.49	1.43
4	J	1	NAG	O5-C5	2.99	1.49	1.43
4	G	2	NAG	O5-C5	2.95	1.49	1.43
5	I	3	FUC	C2-C3	2.90	1.56	1.52
4	G	1	NAG	O5-C5	2.81	1.48	1.43
5	I	3	FUC	O5-C5	2.80	1.49	1.43
5	I	3	FUC	C4-C5	2.71	1.58	1.52
4	D	1	NAG	O5-C5	2.68	1.48	1.43
4	K	1	NAG	O5-C5	2.53	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	C3-C2	2.45	1.57	1.52
4	K	2	NAG	C3-C2	2.44	1.57	1.52
4	G	2	NAG	C3-C2	2.42	1.57	1.52
4	D	2	NAG	C3-C2	2.42	1.57	1.52
4	D	1	NAG	O5-C1	2.41	1.47	1.43
5	I	2	NAG	C3-C2	2.41	1.57	1.52
4	M	1	NAG	C4-C5	2.39	1.58	1.53
5	I	2	NAG	C4-C5	2.37	1.58	1.53
4	M	2	NAG	C3-C2	2.35	1.57	1.52
4	K	2	NAG	C4-C5	2.33	1.58	1.53
4	J	1	NAG	O5-C1	2.31	1.47	1.43
4	D	2	NAG	C4-C5	2.31	1.57	1.53
4	G	2	NAG	C2-N2	2.30	1.50	1.46
4	M	2	NAG	C4-C5	2.26	1.57	1.53
4	J	2	NAG	C2-N2	2.22	1.49	1.46
5	I	3	FUC	C4-C3	2.21	1.58	1.52
4	D	1	NAG	C3-C2	2.19	1.57	1.52
4	K	1	NAG	C3-C2	2.18	1.57	1.52
4	G	2	NAG	C4-C5	2.17	1.57	1.53
4	G	1	NAG	O5-C1	2.17	1.47	1.43
4	J	1	NAG	C4-C5	2.16	1.57	1.53
4	M	1	NAG	O5-C1	2.16	1.47	1.43
4	D	1	NAG	C4-C3	2.15	1.57	1.52
4	J	2	NAG	C4-C5	2.10	1.57	1.53
4	G	1	NAG	C4-C5	2.09	1.57	1.53
4	K	1	NAG	O5-C1	2.08	1.47	1.43
4	G	2	NAG	C4-C3	2.05	1.57	1.52
5	I	3	FUC	C1-C2	2.05	1.57	1.52
4	D	2	NAG	C4-C3	2.04	1.57	1.52
5	I	2	NAG	C2-N2	2.04	1.49	1.46
4	G	1	NAG	C3-C2	2.02	1.56	1.52
4	M	1	NAG	C3-C2	2.02	1.56	1.52
4	D	2	NAG	C2-N2	2.02	1.49	1.46
5	I	1	NAG	O5-C5	2.02	1.47	1.43
4	K	2	NAG	C4-C3	2.01	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C8-C7-N2	2.55	120.35	116.12
4	D	2	NAG	C8-C7-N2	2.55	120.35	116.12
4	D	2	NAG	O7-C7-C8	-2.47	117.66	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NAG	C8-C7-N2	2.34	119.99	116.12
4	J	2	NAG	C8-C7-N2	2.29	119.92	116.12
4	J	1	NAG	C1-C2-N2	-2.20	106.96	110.43
4	J	1	NAG	C8-C7-N2	2.19	119.75	116.12
4	G	1	NAG	C8-C7-N2	2.14	119.67	116.12
4	M	1	NAG	O4-C4-C3	-2.06	105.51	110.38
4	K	2	NAG	C8-C7-N2	2.06	119.54	116.12
4	M	1	NAG	C1-C2-N2	-2.03	107.24	110.43
4	M	2	NAG	C8-C7-N2	2.02	119.48	116.12
5	I	2	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

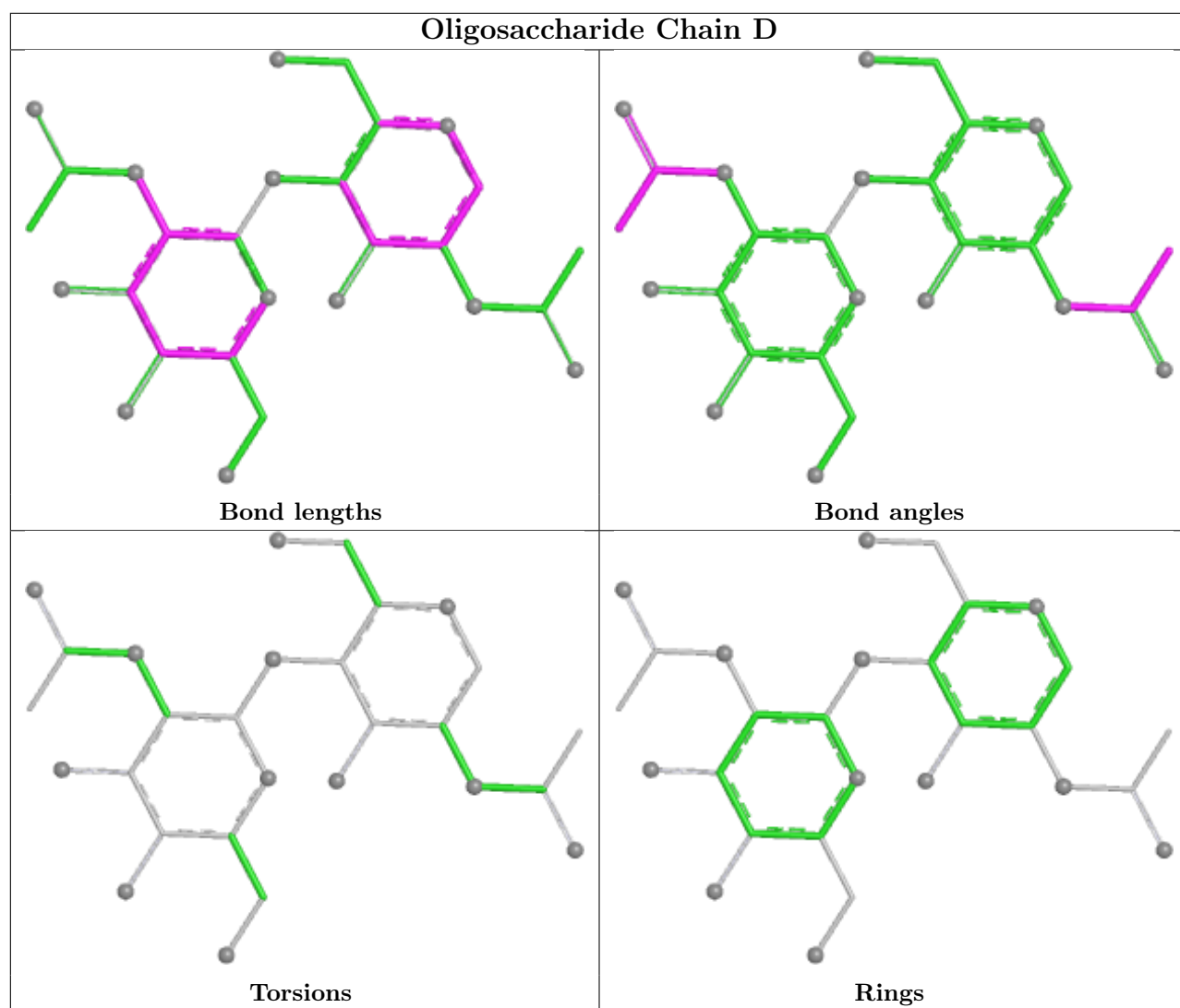
All (3) torsion outliers are listed below:

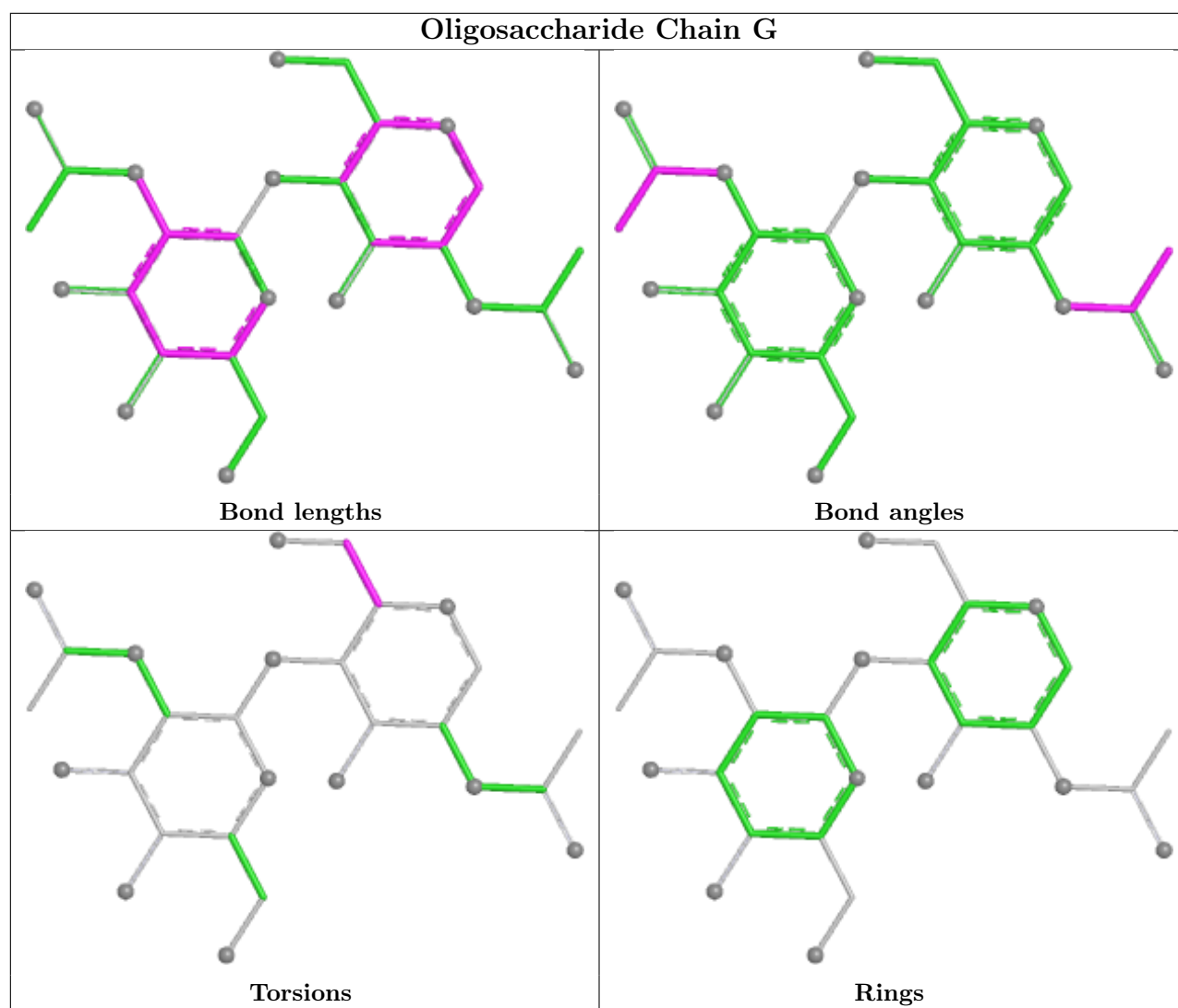
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C1-C2-N2-C7
5	I	1	NAG	C3-C2-N2-C7
4	G	1	NAG	C4-C5-C6-O6

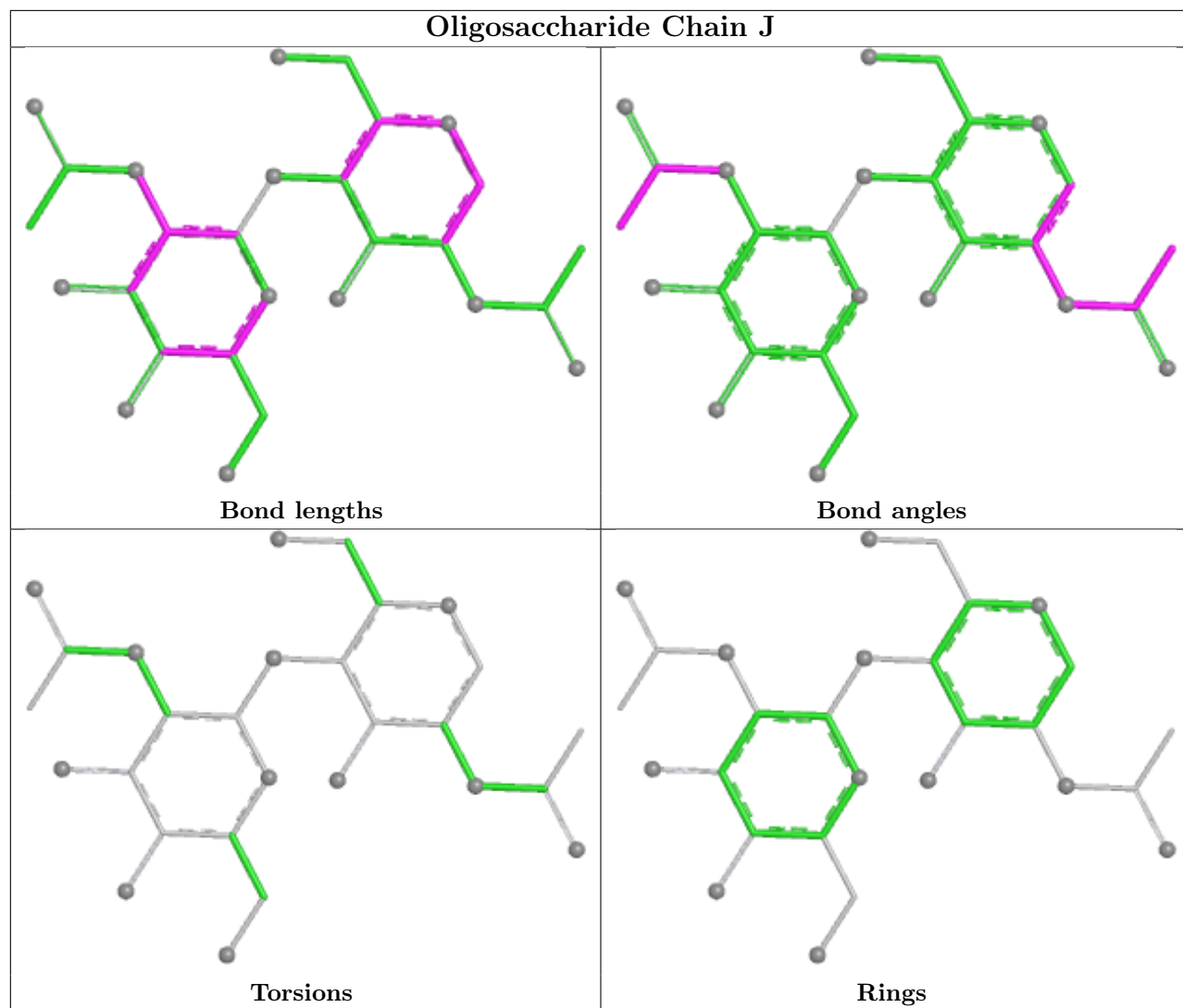
There are no ring outliers.

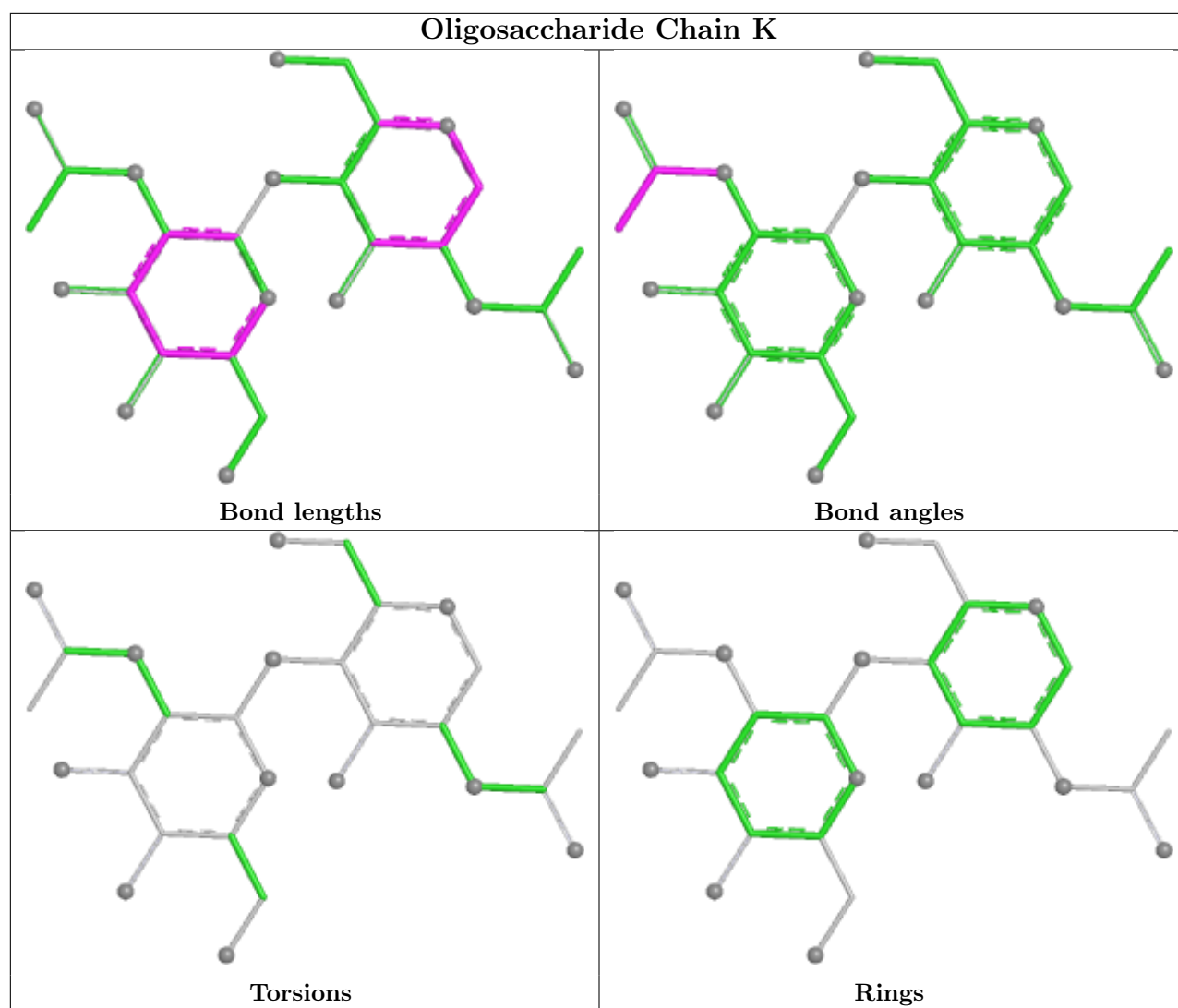
No monomer is involved in short contacts.

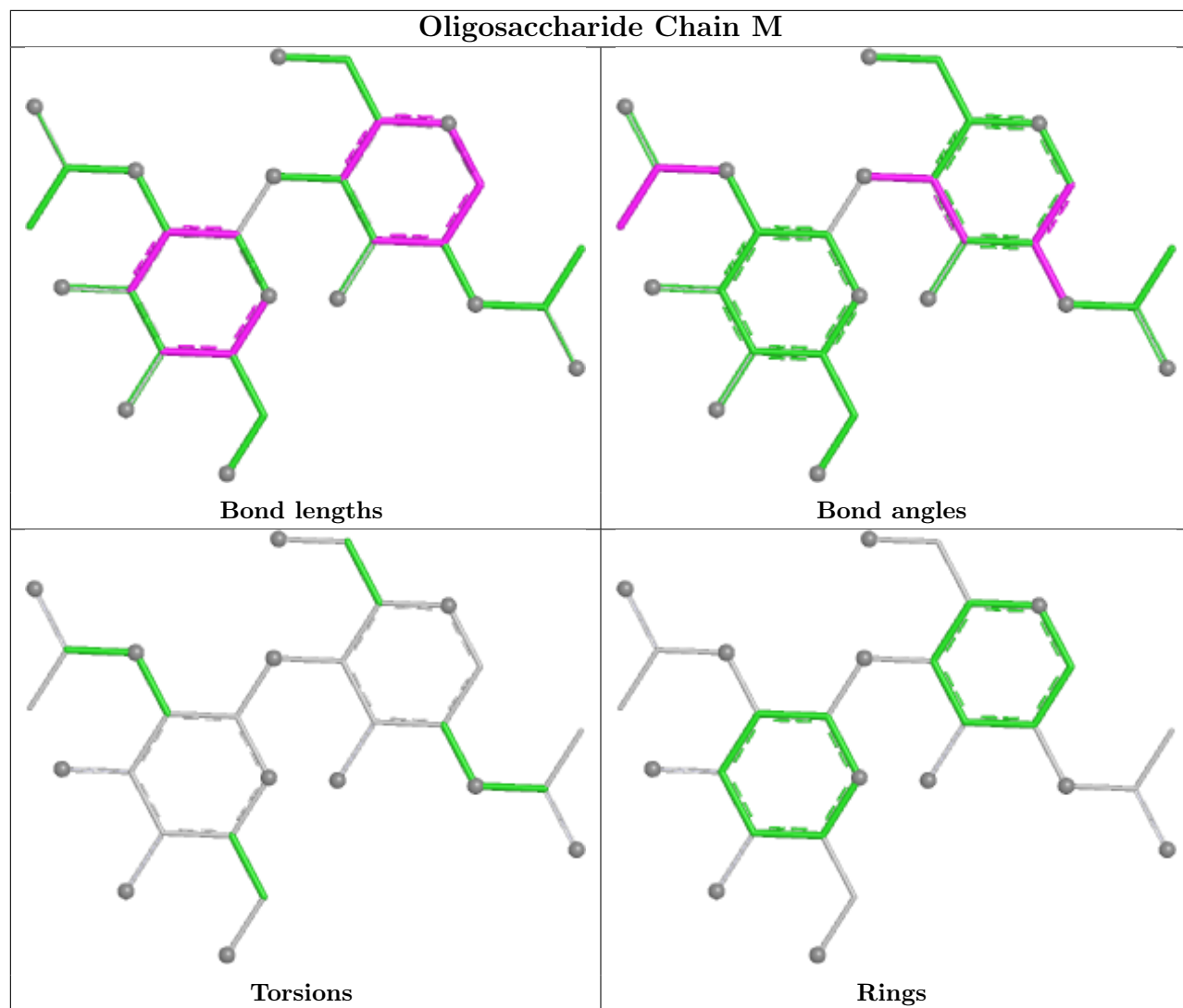
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

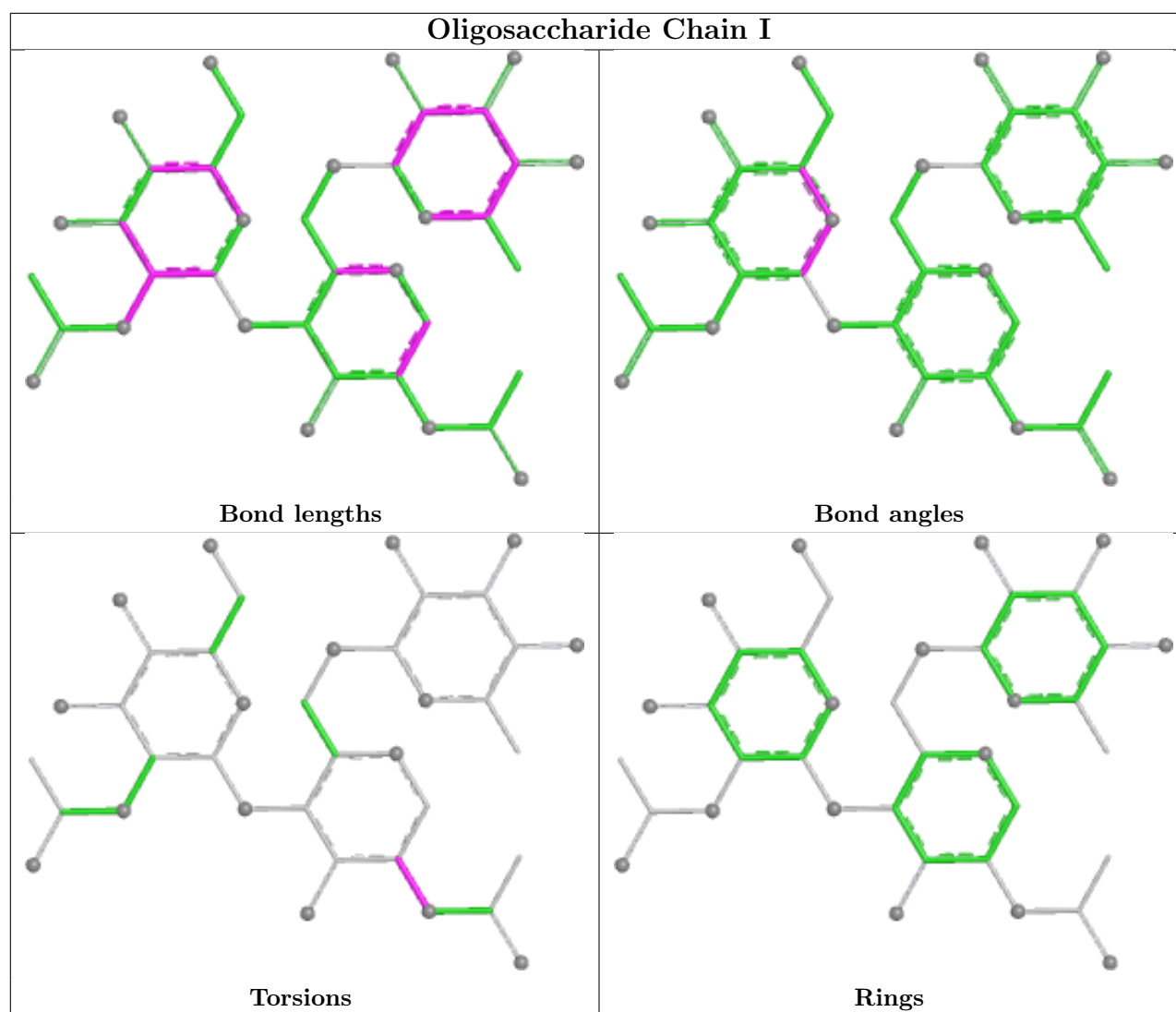












## 5.6 Ligand geometry [i](#)

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$
6	NAG	A	1305	3	14,14,15	2.19	5 (35%)	17,19,21	1.07	1 (5%)
6	NAG	A	1308	3	14,14,15	2.08	5 (35%)	17,19,21	6.80	3 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	B	1301	3	14,14,15	2.21	5 (35%)	17,19,21	0.97	1 (5%)
6	NAG	A	1310	3	14,14,15	2.23	7 (50%)	17,19,21	1.14	2 (11%)
6	NAG	A	1311	3	14,14,15	2.05	6 (42%)	17,19,21	0.95	1 (5%)
6	NAG	C	1308	3	14,14,15	2.13	5 (35%)	17,19,21	0.98	1 (5%)
6	NAG	C	1307	3	14,14,15	2.03	4 (28%)	17,19,21	0.89	0
6	NAG	C	1301	3	14,14,15	2.17	7 (50%)	17,19,21	0.99	1 (5%)
6	NAG	A	1301	3	14,14,15	2.24	5 (35%)	17,19,21	0.93	0
6	NAG	C	1305	3	14,14,15	2.10	5 (35%)	17,19,21	2.16	3 (17%)
6	NAG	A	1312	3	14,14,15	2.12	4 (28%)	17,19,21	1.03	1 (5%)
6	NAG	A	1306	3	14,14,15	2.06	5 (35%)	17,19,21	0.92	0
6	NAG	C	1309	3	14,14,15	2.17	4 (28%)	17,19,21	1.00	1 (5%)
6	NAG	C	1303	3	14,14,15	2.14	5 (35%)	17,19,21	1.10	1 (5%)
6	NAG	C	1310	3	14,14,15	2.17	5 (35%)	17,19,21	0.97	0
6	NAG	B	1305	3	14,14,15	2.16	4 (28%)	17,19,21	0.98	0
6	NAG	B	1304	3	14,14,15	2.28	7 (50%)	17,19,21	1.20	2 (11%)
6	NAG	A	1304	3	14,14,15	2.64	6 (42%)	17,19,21	11.65	4 (23%)
6	NAG	C	1302	3	14,14,15	2.22	5 (35%)	17,19,21	1.04	2 (11%)
6	NAG	A	1309	3	14,14,15	2.26	6 (42%)	17,19,21	0.94	1 (5%)
6	NAG	A	1302	3	14,14,15	2.10	6 (42%)	17,19,21	2.02	3 (17%)
6	NAG	A	1303	3	14,14,15	2.26	5 (35%)	17,19,21	1.09	1 (5%)
6	NAG	C	1304	3	14,14,15	2.11	6 (42%)	17,19,21	1.20	2 (11%)
6	NAG	B	1303	3	14,14,15	2.06	4 (28%)	17,19,21	6.68	2 (11%)
6	NAG	A	1313	3	14,14,15	2.10	3 (21%)	17,19,21	1.15	3 (17%)
6	NAG	A	1307	3	14,14,15	2.10	5 (35%)	17,19,21	2.00	2 (11%)
6	NAG	A	1314	3	14,14,15	2.17	5 (35%)	17,19,21	1.01	0
6	NAG	B	1302	3	14,14,15	2.17	7 (50%)	17,19,21	1.00	1 (5%)
6	NAG	C	1306	3	14,14,15	2.09	5 (35%)	17,19,21	0.98	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1305	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1308	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1301	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1310	3	-	3/6/23/26	0/1/1/1
6	NAG	A	1311	3	-	1/6/23/26	0/1/1/1
6	NAG	C	1308	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1307	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1301	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1301	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1305	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1312	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1306	3	-	1/6/23/26	0/1/1/1
6	NAG	C	1309	3	-	2/6/23/26	0/1/1/1
6	NAG	C	1303	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1310	3	-	0/6/23/26	0/1/1/1
6	NAG	B	1305	3	-	0/6/23/26	0/1/1/1
6	NAG	B	1304	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1304	3	-	2/6/23/26	0/1/1/1
6	NAG	C	1302	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1309	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1302	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1303	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1304	3	-	0/6/23/26	0/1/1/1
6	NAG	B	1303	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1313	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1307	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1314	3	-	1/6/23/26	0/1/1/1
6	NAG	B	1302	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1306	3	-	1/6/23/26	0/1/1/1

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1303	NAG	C1-C2	6.32	1.61	1.52
6	A	1304	NAG	C8-C7	6.27	1.63	1.50
6	A	1301	NAG	C1-C2	6.08	1.60	1.52
6	B	1301	NAG	C1-C2	5.91	1.60	1.52
6	A	1309	NAG	C1-C2	5.90	1.60	1.52
6	C	1309	NAG	C1-C2	5.82	1.60	1.52
6	B	1305	NAG	C1-C2	5.79	1.60	1.52
6	A	1313	NAG	C1-C2	5.76	1.60	1.52
6	B	1304	NAG	C1-C2	5.75	1.60	1.52
6	C	1302	NAG	C1-C2	5.74	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1310	NAG	C1-C2	5.70	1.60	1.52
6	A	1314	NAG	C1-C2	5.67	1.60	1.52
6	A	1305	NAG	C1-C2	5.65	1.60	1.52
6	C	1303	NAG	C1-C2	5.62	1.60	1.52
6	C	1301	NAG	C1-C2	5.59	1.60	1.52
6	A	1310	NAG	C1-C2	5.56	1.59	1.52
6	C	1305	NAG	C1-C2	5.54	1.59	1.52
6	C	1306	NAG	C1-C2	5.48	1.59	1.52
6	A	1312	NAG	C1-C2	5.41	1.59	1.52
6	B	1302	NAG	C1-C2	5.40	1.59	1.52
6	A	1302	NAG	C1-C2	5.39	1.59	1.52
6	A	1304	NAG	C1-C2	5.34	1.59	1.52
6	A	1307	NAG	C1-C2	5.34	1.59	1.52
6	C	1308	NAG	C1-C2	5.30	1.59	1.52
6	A	1308	NAG	C1-C2	5.26	1.59	1.52
6	C	1307	NAG	C1-C2	5.23	1.59	1.52
6	B	1303	NAG	C1-C2	5.12	1.59	1.52
6	A	1311	NAG	C1-C2	5.10	1.59	1.52
6	C	1304	NAG	C1-C2	5.06	1.59	1.52
6	A	1306	NAG	C1-C2	4.83	1.58	1.52
6	B	1303	NAG	O5-C5	3.53	1.50	1.43
6	C	1308	NAG	O5-C5	3.45	1.50	1.43
6	A	1306	NAG	O5-C5	3.40	1.50	1.43
6	A	1310	NAG	O5-C5	3.35	1.50	1.43
6	C	1304	NAG	O5-C5	3.33	1.49	1.43
6	A	1309	NAG	O5-C5	3.32	1.49	1.43
6	C	1309	NAG	O5-C5	3.31	1.49	1.43
6	A	1308	NAG	O5-C5	3.31	1.49	1.43
6	C	1306	NAG	O5-C5	3.29	1.49	1.43
6	C	1307	NAG	O5-C5	3.27	1.49	1.43
6	A	1305	NAG	O5-C5	3.25	1.49	1.43
6	C	1302	NAG	O5-C5	3.25	1.49	1.43
6	A	1301	NAG	O5-C5	3.23	1.49	1.43
6	A	1314	NAG	O5-C5	3.19	1.49	1.43
6	A	1312	NAG	O5-C5	3.18	1.49	1.43
6	C	1310	NAG	O5-C5	3.18	1.49	1.43
6	A	1307	NAG	O5-C5	3.17	1.49	1.43
6	A	1311	NAG	O5-C5	3.11	1.49	1.43
6	A	1302	NAG	O5-C5	3.09	1.49	1.43
6	B	1305	NAG	O5-C5	3.06	1.49	1.43
6	B	1301	NAG	O5-C5	3.05	1.49	1.43
6	C	1305	NAG	O5-C5	3.04	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1302	NAG	O5-C5	3.04	1.49	1.43
6	B	1304	NAG	O5-C5	3.03	1.49	1.43
6	C	1301	NAG	O5-C5	3.01	1.49	1.43
6	A	1304	NAG	O5-C5	2.97	1.49	1.43
6	C	1303	NAG	O5-C5	2.97	1.49	1.43
6	A	1303	NAG	C3-C2	2.85	1.58	1.52
6	A	1303	NAG	O5-C5	2.74	1.48	1.43
6	C	1302	NAG	O5-C1	2.69	1.48	1.43
6	C	1304	NAG	O5-C1	2.68	1.48	1.43
6	A	1306	NAG	O5-C1	2.68	1.48	1.43
6	A	1314	NAG	O5-C1	2.68	1.48	1.43
6	A	1309	NAG	O5-C1	2.64	1.48	1.43
6	B	1304	NAG	C2-N2	2.64	1.50	1.46
6	A	1313	NAG	O5-C5	2.63	1.48	1.43
6	C	1308	NAG	O5-C1	2.63	1.48	1.43
6	A	1305	NAG	O5-C1	2.63	1.48	1.43
6	C	1310	NAG	O5-C1	2.62	1.48	1.43
6	C	1309	NAG	O5-C1	2.60	1.48	1.43
6	B	1303	NAG	O5-C1	2.58	1.48	1.43
6	A	1310	NAG	O5-C1	2.57	1.48	1.43
6	A	1301	NAG	O5-C1	2.56	1.48	1.43
6	B	1301	NAG	O5-C1	2.56	1.48	1.43
6	A	1308	NAG	O5-C1	2.56	1.48	1.43
6	B	1304	NAG	O5-C1	2.55	1.48	1.43
6	A	1313	NAG	C3-C2	2.52	1.57	1.52
6	B	1305	NAG	O5-C1	2.48	1.47	1.43
6	C	1303	NAG	C3-C2	2.46	1.57	1.52
6	C	1306	NAG	O5-C1	2.45	1.47	1.43
6	B	1302	NAG	O5-C1	2.43	1.47	1.43
6	A	1307	NAG	O5-C1	2.42	1.47	1.43
6	A	1312	NAG	C4-C5	2.42	1.58	1.53
6	A	1301	NAG	C3-C2	2.42	1.57	1.52
6	A	1302	NAG	O5-C1	2.41	1.47	1.43
6	B	1302	NAG	C3-C2	2.41	1.57	1.52
6	A	1304	NAG	O5-C1	2.41	1.47	1.43
6	A	1311	NAG	O5-C1	2.40	1.47	1.43
6	C	1301	NAG	O5-C1	2.38	1.47	1.43
6	A	1312	NAG	O5-C1	2.36	1.47	1.43
6	C	1305	NAG	O5-C1	2.36	1.47	1.43
6	A	1310	NAG	C3-C2	2.36	1.57	1.52
6	A	1304	NAG	C3-C2	2.33	1.57	1.52
6	C	1309	NAG	C3-C2	2.33	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1310	NAG	C4-C5	2.32	1.58	1.53
6	C	1301	NAG	C3-C2	2.32	1.57	1.52
6	C	1307	NAG	O5-C1	2.32	1.47	1.43
6	A	1306	NAG	C4-C5	2.32	1.58	1.53
6	B	1304	NAG	C4-C5	2.30	1.57	1.53
6	A	1308	NAG	C4-C5	2.30	1.57	1.53
6	A	1309	NAG	C3-C2	2.27	1.57	1.52
6	B	1302	NAG	C4-C5	2.25	1.57	1.53
6	A	1304	NAG	C4-C5	2.25	1.57	1.53
6	B	1302	NAG	C2-N2	2.25	1.50	1.46
6	C	1303	NAG	O5-C1	2.24	1.47	1.43
6	A	1305	NAG	C3-C2	2.24	1.57	1.52
6	A	1310	NAG	C2-N2	2.24	1.50	1.46
6	B	1304	NAG	C3-C2	2.23	1.57	1.52
6	B	1303	NAG	C4-C5	2.22	1.57	1.53
6	C	1301	NAG	C4-C5	2.20	1.57	1.53
6	B	1305	NAG	C3-C2	2.20	1.57	1.52
6	B	1301	NAG	C4-C5	2.20	1.57	1.53
6	C	1302	NAG	C3-C2	2.19	1.57	1.52
6	A	1302	NAG	C4-C5	2.18	1.57	1.53
6	C	1304	NAG	C4-C5	2.17	1.57	1.53
6	B	1304	NAG	C4-C3	2.16	1.57	1.52
6	A	1306	NAG	C3-C2	2.16	1.57	1.52
6	C	1302	NAG	C4-C5	2.14	1.57	1.53
6	C	1310	NAG	C3-C2	2.14	1.57	1.52
6	B	1301	NAG	C3-C2	2.14	1.57	1.52
6	A	1314	NAG	C4-C5	2.13	1.57	1.53
6	C	1305	NAG	C3-C2	2.13	1.57	1.52
6	A	1307	NAG	C4-C5	2.12	1.57	1.53
6	A	1309	NAG	C4-C5	2.12	1.57	1.53
6	A	1307	NAG	C3-C2	2.11	1.56	1.52
6	A	1311	NAG	C2-N2	2.11	1.49	1.46
6	C	1308	NAG	C4-C5	2.10	1.57	1.53
6	C	1310	NAG	C4-C5	2.10	1.57	1.53
6	A	1301	NAG	C4-C5	2.09	1.57	1.53
6	A	1314	NAG	C3-C2	2.09	1.56	1.52
6	A	1308	NAG	C4-C3	2.08	1.57	1.52
6	C	1308	NAG	C3-C2	2.08	1.56	1.52
6	A	1311	NAG	C4-C5	2.08	1.57	1.53
6	A	1311	NAG	C3-C2	2.08	1.56	1.52
6	B	1302	NAG	C4-C3	2.07	1.57	1.52
6	C	1304	NAG	C2-N2	2.07	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1307	NAG	C4-C5	2.06	1.57	1.53
6	A	1303	NAG	C2-N2	2.06	1.49	1.46
6	C	1305	NAG	C4-C5	2.06	1.57	1.53
6	C	1304	NAG	C3-C2	2.06	1.56	1.52
6	A	1309	NAG	C2-N2	2.06	1.49	1.46
6	A	1302	NAG	C2-N2	2.05	1.49	1.46
6	A	1305	NAG	C4-C5	2.05	1.57	1.53
6	C	1306	NAG	C3-C2	2.04	1.56	1.52
6	C	1303	NAG	C4-C5	2.04	1.57	1.53
6	A	1302	NAG	C3-C2	2.04	1.56	1.52
6	C	1301	NAG	C4-C3	2.04	1.57	1.52
6	A	1303	NAG	O5-C1	2.02	1.47	1.43
6	C	1301	NAG	C2-N2	2.01	1.49	1.46
6	C	1306	NAG	C4-C5	2.01	1.57	1.53
6	A	1310	NAG	C4-C3	2.01	1.57	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1304	NAG	O7-C7-N2	28.75	172.78	121.98
6	A	1304	NAG	C2-N2-C7	27.37	159.58	122.90
6	A	1308	NAG	C2-N2-C7	27.24	159.41	122.90
6	B	1303	NAG	C2-N2-C7	27.11	159.22	122.90
6	A	1304	NAG	O7-C7-C8	-20.47	85.60	122.05
6	A	1304	NAG	C8-C7-N2	-17.45	87.18	116.12
6	C	1305	NAG	C8-C7-N2	6.72	127.26	116.12
6	A	1302	NAG	C8-C7-N2	6.28	126.54	116.12
6	A	1307	NAG	C8-C7-N2	6.14	126.29	116.12
6	A	1308	NAG	C8-C7-N2	4.85	124.17	116.12
6	C	1305	NAG	O7-C7-N2	-4.36	114.28	121.98
6	A	1302	NAG	O7-C7-N2	-3.94	115.01	121.98
6	A	1307	NAG	O7-C7-N2	-3.92	115.05	121.98
6	B	1303	NAG	C8-C7-N2	3.26	121.53	116.12
6	C	1304	NAG	C8-C7-N2	3.19	121.40	116.12
6	B	1304	NAG	C8-C7-N2	3.10	121.26	116.12
6	A	1308	NAG	O7-C7-N2	-3.09	116.51	121.98
6	B	1304	NAG	O7-C7-C8	-2.75	117.15	122.05
6	A	1303	NAG	C8-C7-N2	2.74	120.67	116.12
6	C	1304	NAG	O7-C7-C8	-2.52	117.57	122.05
6	A	1305	NAG	C8-C7-N2	2.48	120.23	116.12
6	A	1312	NAG	C8-C7-N2	2.46	120.20	116.12
6	A	1311	NAG	C8-C7-N2	2.40	120.11	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1302	NAG	C8-C7-N2	2.40	120.09	116.12
6	C	1302	NAG	C8-C7-N2	2.39	120.08	116.12
6	A	1313	NAG	C1-C2-N2	-2.25	106.89	110.43
6	A	1310	NAG	C2-N2-C7	2.21	125.86	122.90
6	A	1310	NAG	C8-C7-N2	2.20	119.77	116.12
6	C	1301	NAG	C8-C7-N2	2.19	119.75	116.12
6	B	1301	NAG	C8-C7-N2	2.13	119.65	116.12
6	C	1306	NAG	C8-C7-N2	2.08	119.57	116.12
6	C	1303	NAG	C8-C7-N2	2.05	119.52	116.12
6	C	1302	NAG	O7-C7-C8	-2.05	118.41	122.05
6	A	1309	NAG	C8-C7-N2	2.04	119.50	116.12
6	C	1308	NAG	O7-C7-C8	-2.03	118.44	122.05
6	A	1302	NAG	O7-C7-C8	-2.02	118.45	122.05
6	A	1313	NAG	C8-C7-N2	2.02	119.47	116.12
6	C	1305	NAG	O7-C7-C8	-2.02	118.47	122.05
6	C	1309	NAG	O5-C1-C2	-2.01	108.18	111.29
6	A	1313	NAG	C1-O5-C5	2.01	114.87	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1302	NAG	C8-C7-N2-C2
6	A	1302	NAG	O7-C7-N2-C2
6	A	1304	NAG	O7-C7-N2-C2
6	A	1307	NAG	C8-C7-N2-C2
6	A	1307	NAG	O7-C7-N2-C2
6	A	1308	NAG	C8-C7-N2-C2
6	A	1308	NAG	O7-C7-N2-C2
6	C	1305	NAG	C8-C7-N2-C2
6	C	1305	NAG	O7-C7-N2-C2
6	C	1309	NAG	O5-C5-C6-O6
6	A	1311	NAG	O5-C5-C6-O6
6	C	1306	NAG	O5-C5-C6-O6
6	A	1306	NAG	O5-C5-C6-O6
6	A	1310	NAG	O5-C5-C6-O6
6	A	1314	NAG	O5-C5-C6-O6
6	A	1310	NAG	C1-C2-N2-C7
6	A	1305	NAG	C4-C5-C6-O6
6	A	1304	NAG	C3-C2-N2-C7
6	A	1310	NAG	C3-C2-N2-C7
6	A	1305	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	C	1309	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.



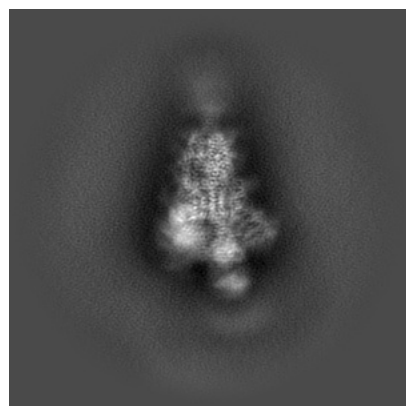
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24695. These allow visual inspection of the internal detail of the map and identification of artifacts.

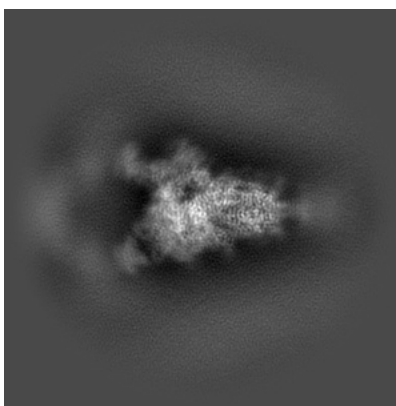
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

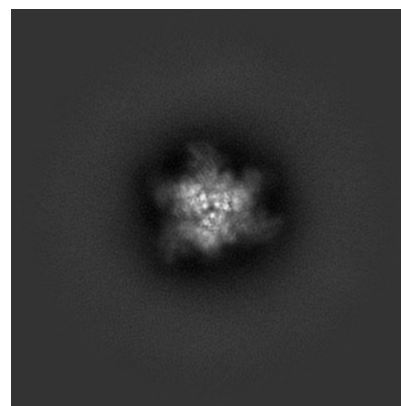
#### 6.1.1 Primary map



X

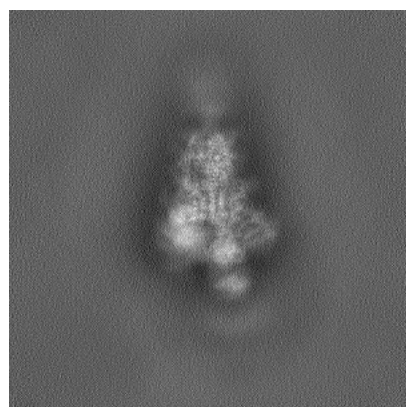


Y

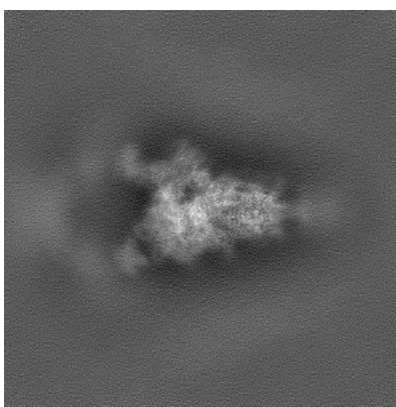


Z

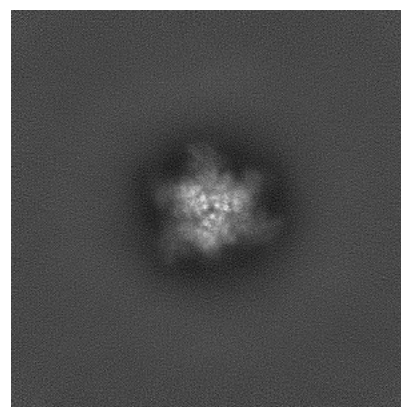
#### 6.1.2 Raw map



X



Y

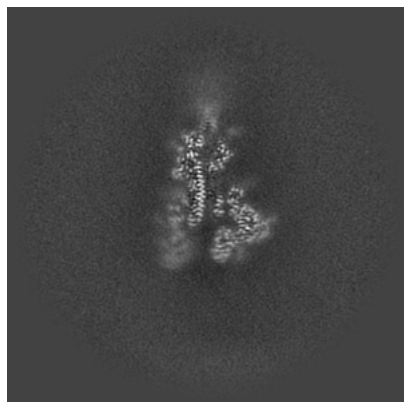


Z

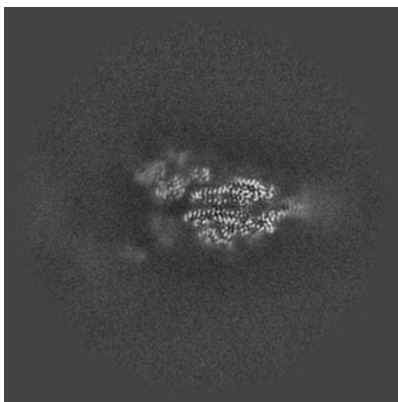
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

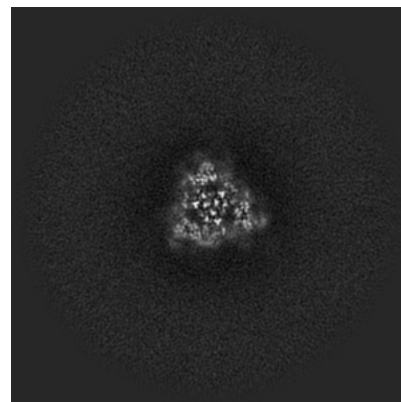
### 6.2.1 Primary map



X Index: 224

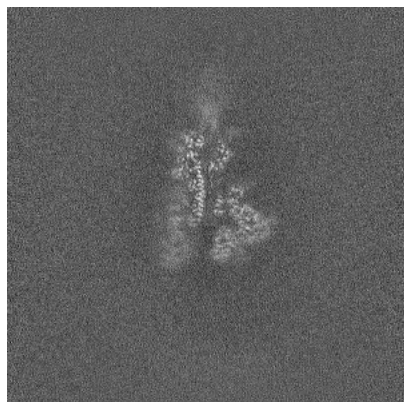


Y Index: 224



Z Index: 224

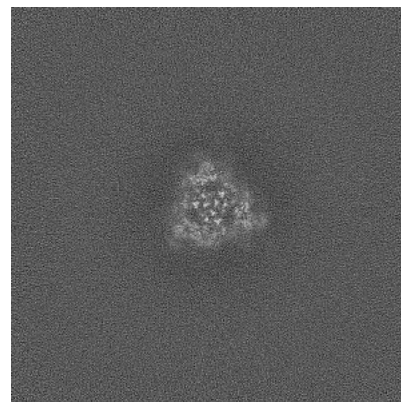
### 6.2.2 Raw map



X Index: 224



Y Index: 224

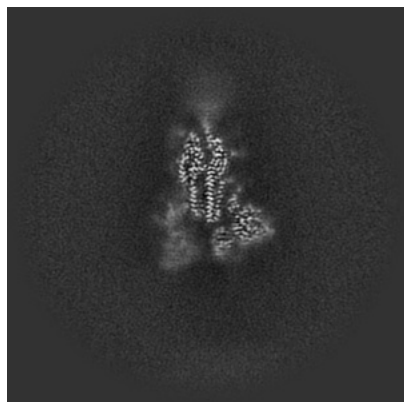


Z Index: 224

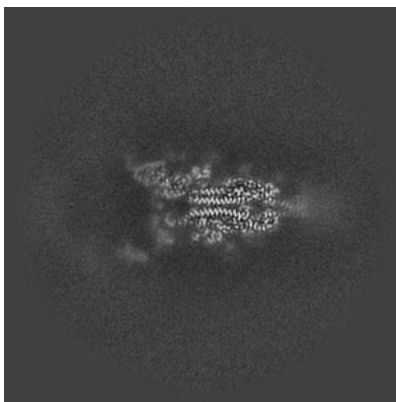
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

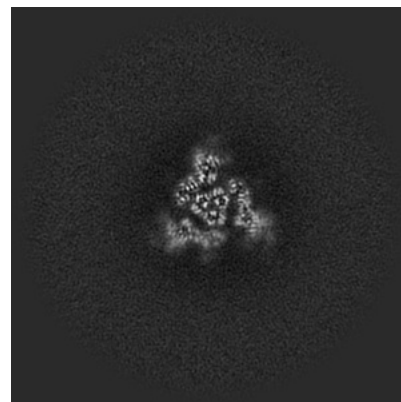
### 6.3.1 Primary map



X Index: 217

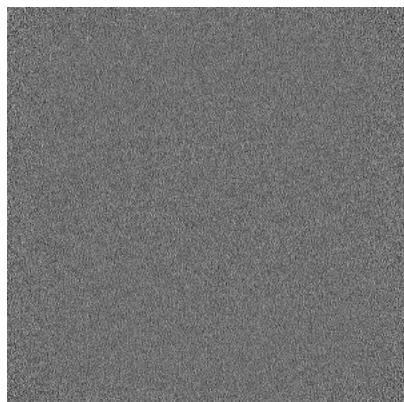


Y Index: 228

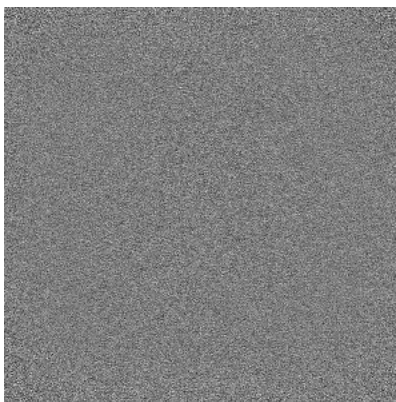


Z Index: 214

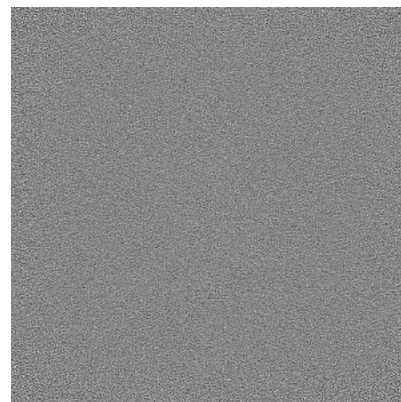
### 6.3.2 Raw map



X Index: 0



Y Index: 0



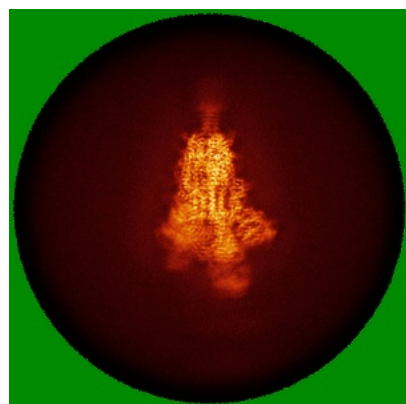
Z Index: 0

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

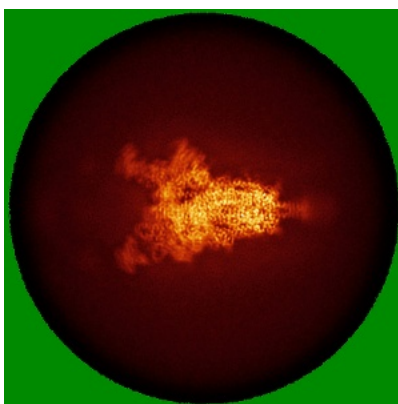


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

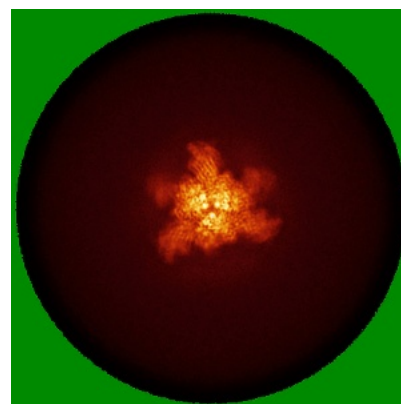
### 6.4.1 Primary map



X

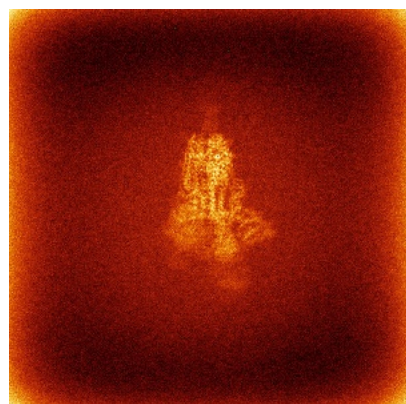


Y

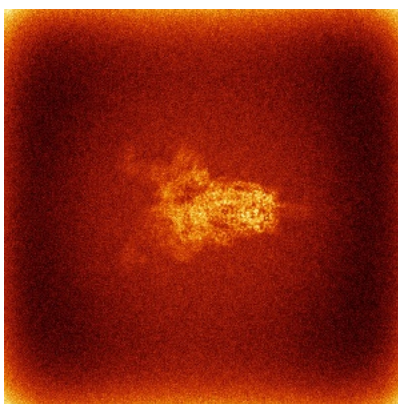


Z

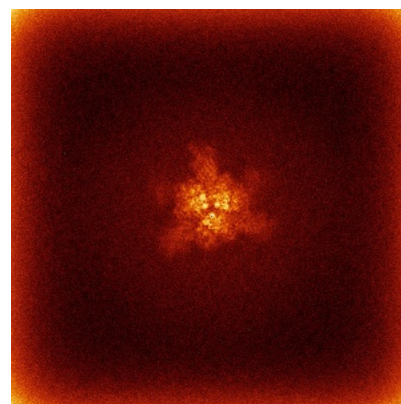
### 6.4.2 Raw map



X



Y

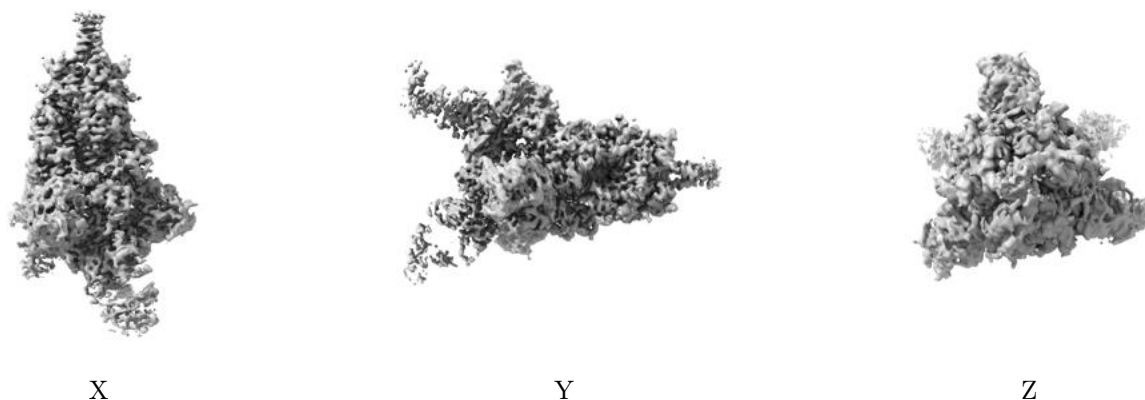


Z

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

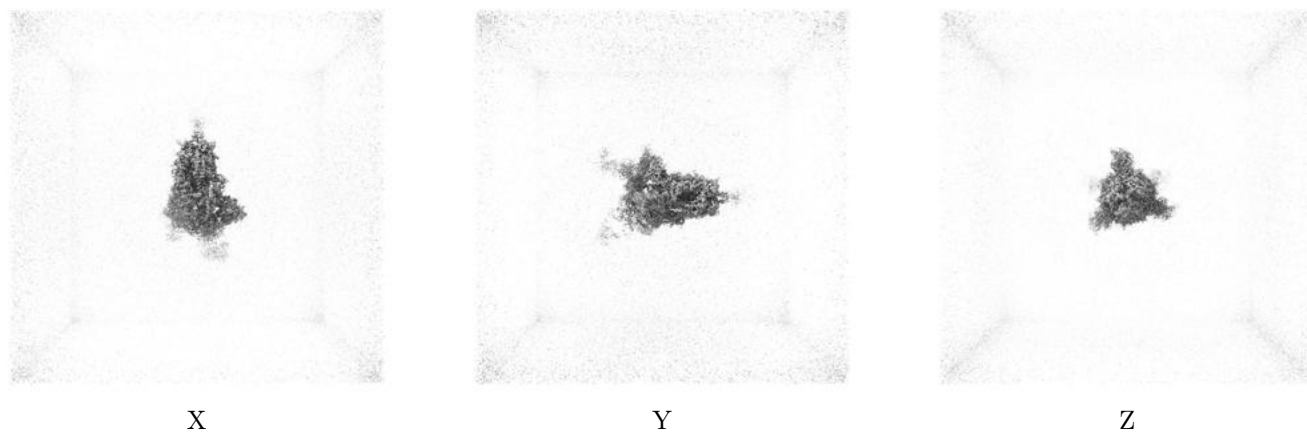
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

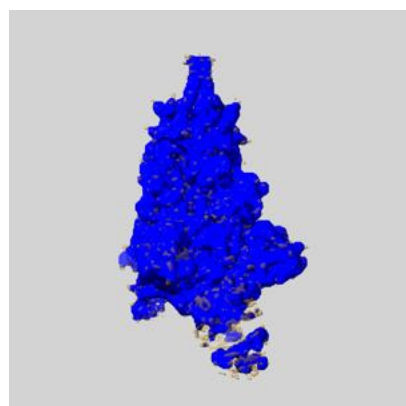
## 6.6 Mask visualisation [i](#)

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

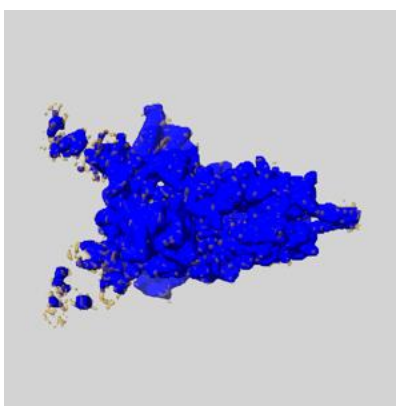
A mask typically either:

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

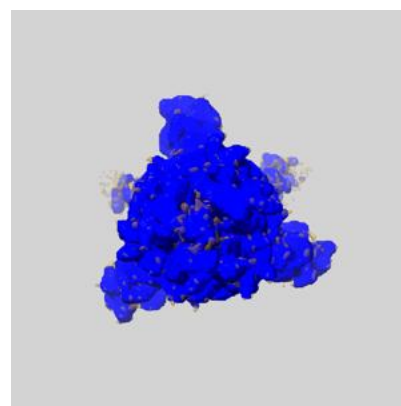
### 6.6.1 emd\_24695\_msk\_1.map [i](#)



X



Y

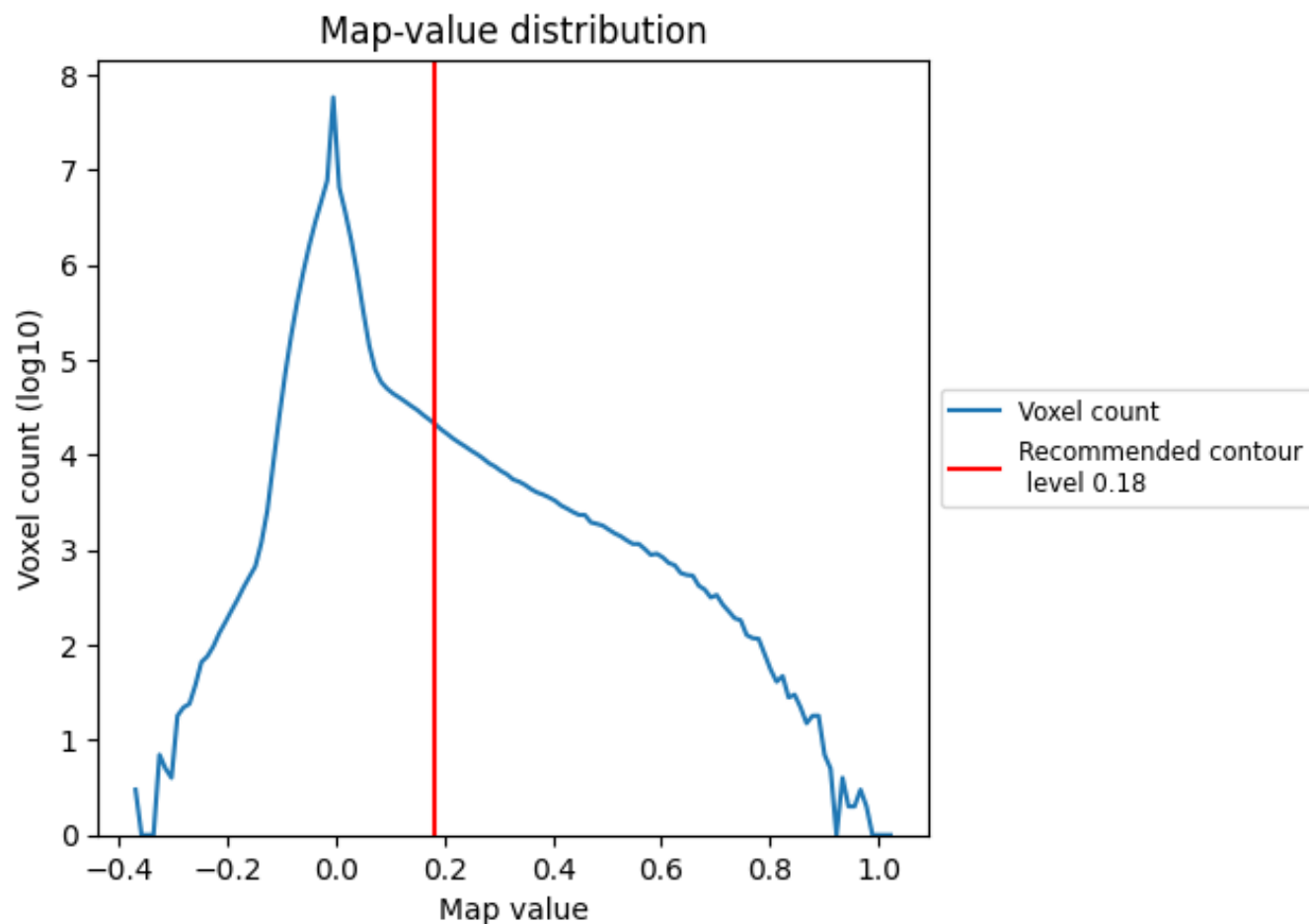


Z

## 7 Map analysis [i](#)

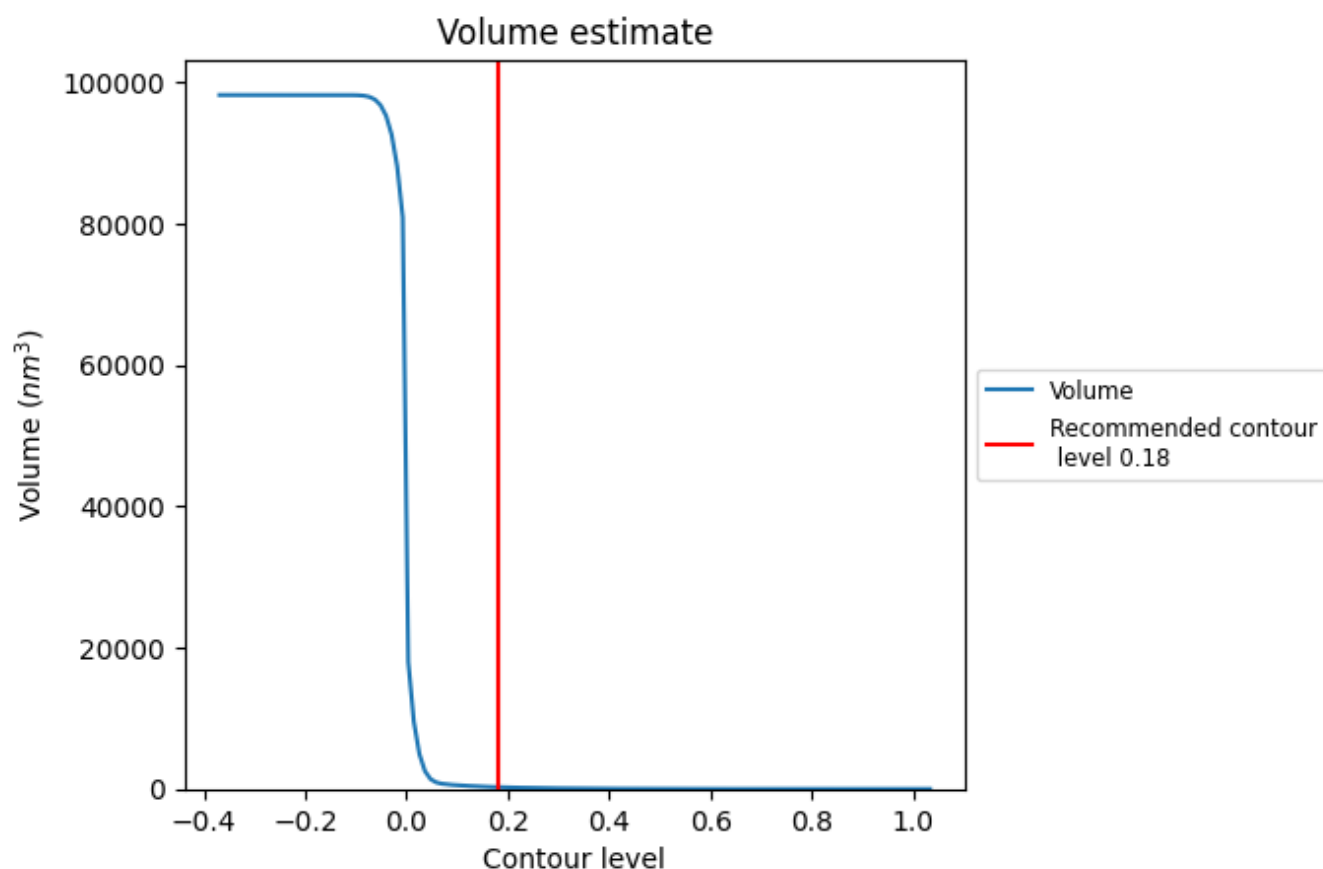
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

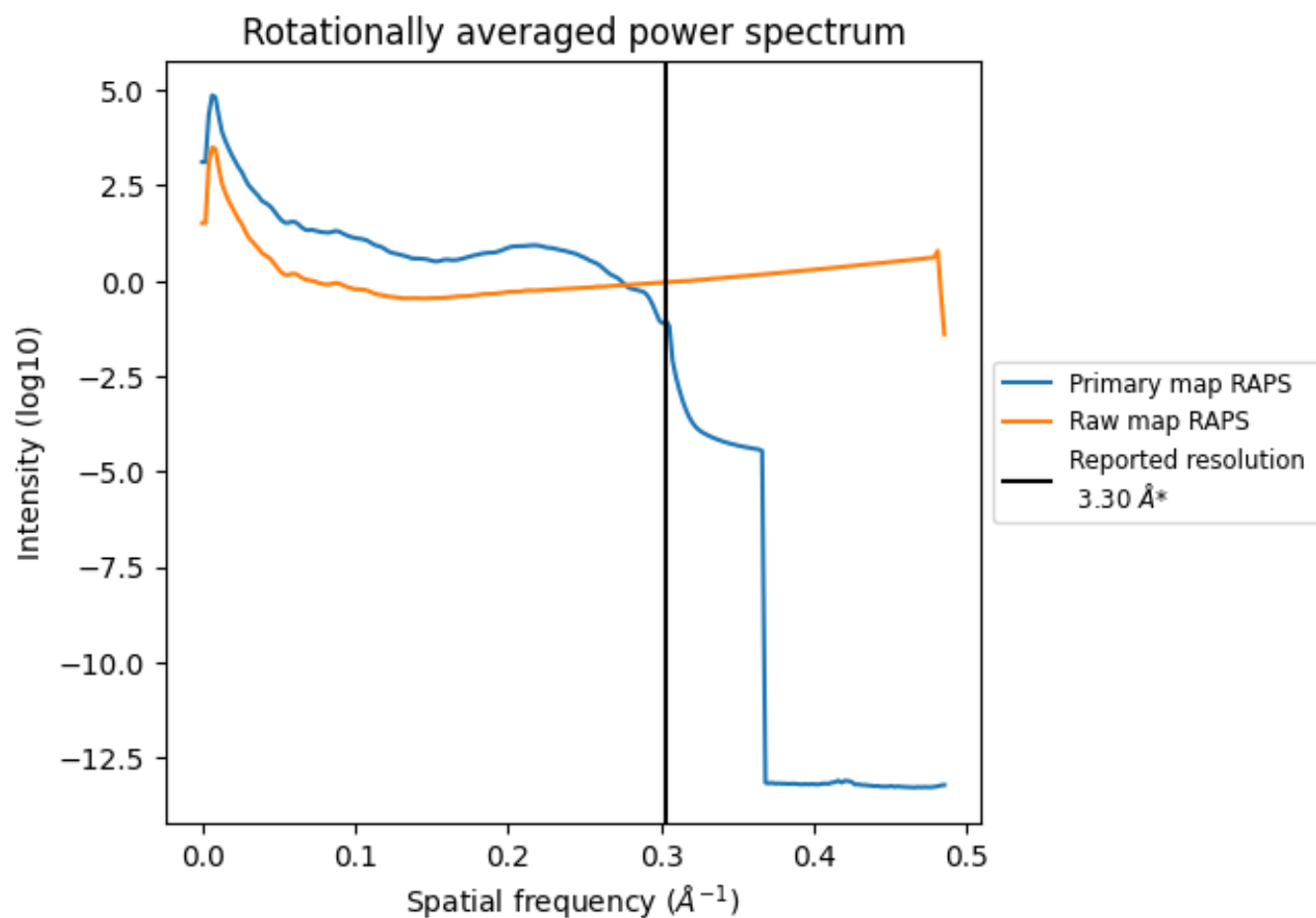


The volume at the recommended contour level is 255 nm<sup>3</sup>; this corresponds to an approximate mass of 230 kDa.

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 ⓘ

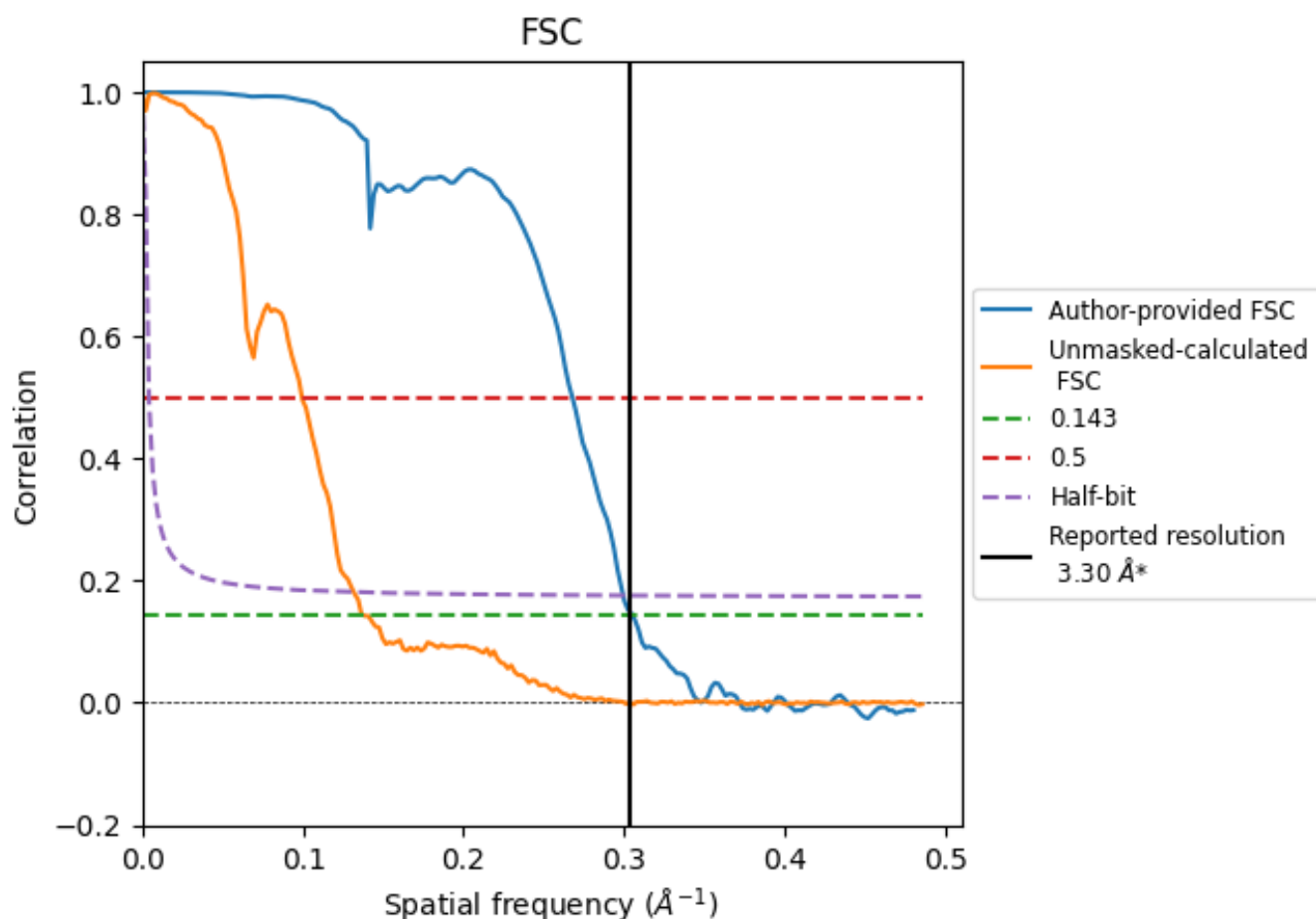


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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  $0.303 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

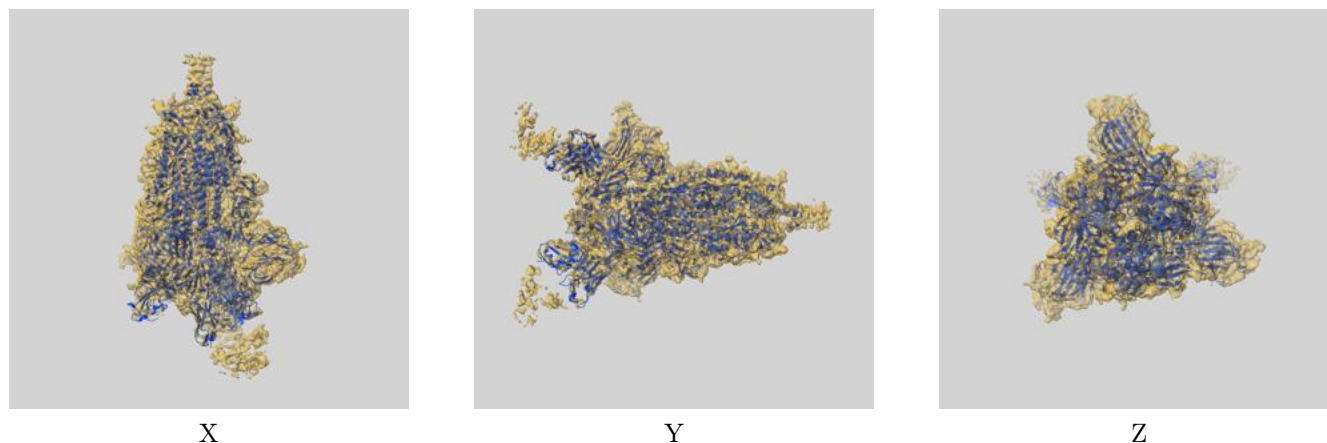
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	3.73	3.34
Unmasked-calculated*	7.24	10.06	7.59

\*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 7.24 differs from the reported value 3.3 by more than 10 %

## 9 Map-model fit ⓘ

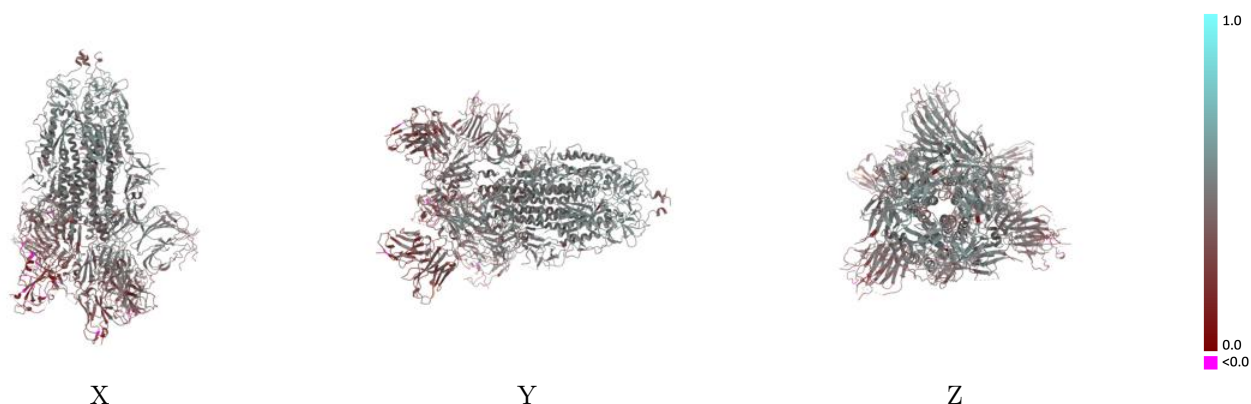
This section contains information regarding the fit between EMDB map EMD-24695 and PDB model 7RU3. Per-residue inclusion information can be found in section 3 on page 14.

### 9.1 Map-model overlay ⓘ



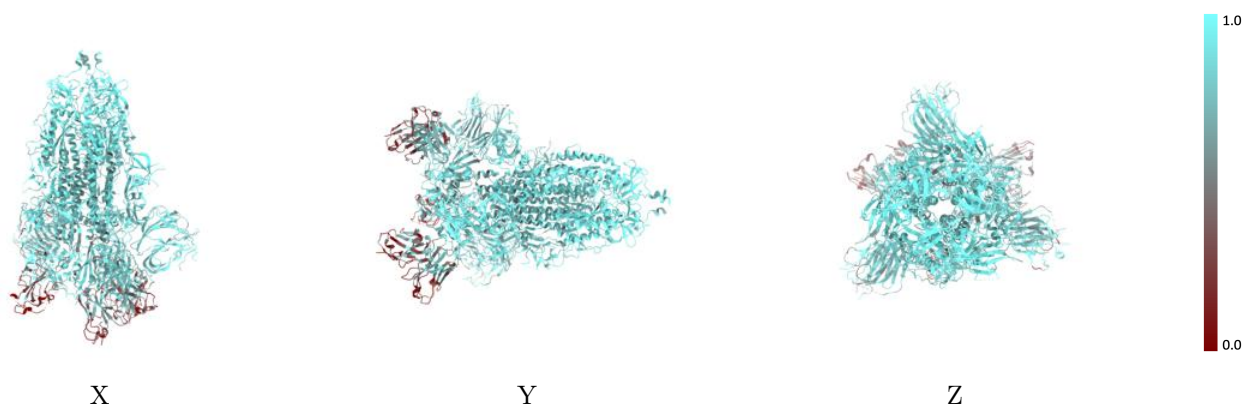
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



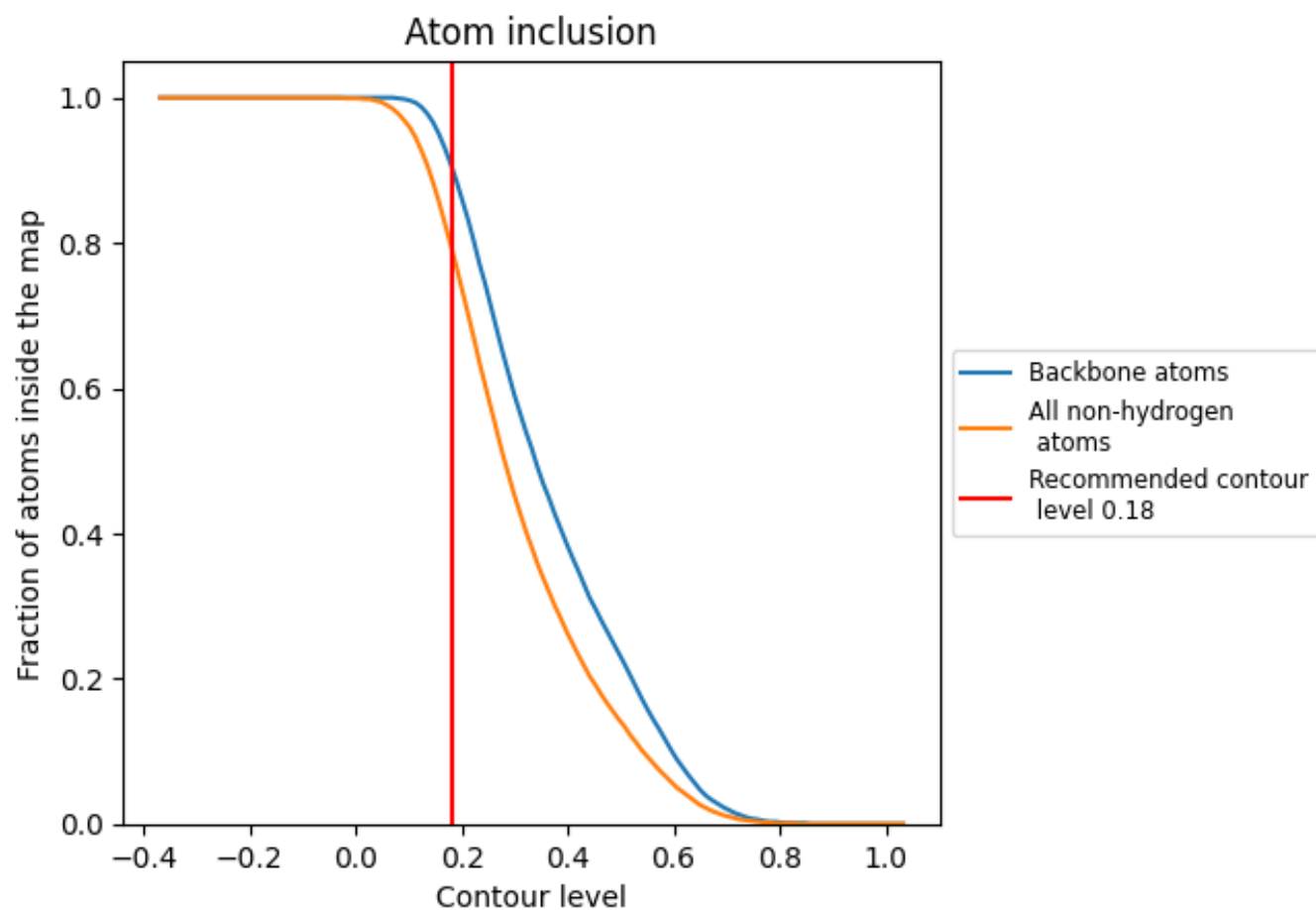
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7950</div>	<div><div></div>0.4130</div>
A	<div><div></div>0.8690</div>	<div><div></div>0.4490</div>
B	<div><div></div>0.8590</div>	<div><div></div>0.4280</div>
C	<div><div></div>0.7860</div>	<div><div></div>0.3960</div>
D	<div><div></div>0.7860</div>	<div><div></div>0.4720</div>
E	<div><div></div>0.4560</div>	<div><div></div>0.3150</div>
F	<div><div></div>0.4300</div>	<div><div></div>0.2970</div>
G	<div><div></div>0.7140</div>	<div><div></div>0.4320</div>
H	<div><div></div>0.5740</div>	<div><div></div>0.3710</div>
I	<div><div></div>0.7110</div>	<div><div></div>0.3880</div>
J	<div><div></div>0.7500</div>	<div><div></div>0.4620</div>
K	<div><div></div>0.6790</div>	<div><div></div>0.3580</div>
L	<div><div></div>0.4530</div>	<div><div></div>0.3230</div>
M	<div><div></div>0.7860</div>	<div><div></div>0.3530</div>

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