



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 10:07 AM EST

PDB ID : 7KMK
EMDB ID : EMD-22925
Title : cryo-EM structure of SARS-CoV-2 spike in complex with Fab 15033-7, two RBDs bound
Authors : Li, Z.; Rini, J.M.
Deposited on : 2020-11-03
Resolution : 4.20 Å (reported)
Based on initial models : 7KML, 7KLH

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

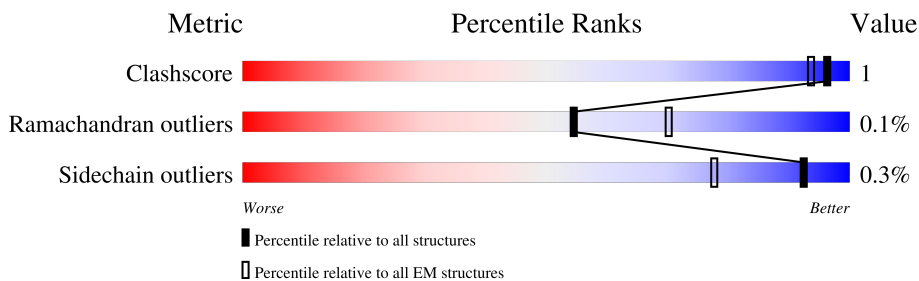
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1274	
1	B	1274	
1	C	1274	
2	L	214	
2	M	214	
3	H	225	
3	I	225	
4	D	2	

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Mol	Chain	Length	Quality of chain
4	G	2	 50% 50%
4	J	2	 100%
4	K	2	 50% 50%
4	N	2	 50% 50%
4	O	2	 100%
4	P	2	 100%
5	E	3	 67% 33%
5	F	3	 67% 33%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 31251 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1028	8039	5133	1339	1529	38	0	0
1	B	1025	8018	5121	1335	1524	38	0	0
1	C	1025	8018	5121	1335	1524	38	0	0

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	SER	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	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	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	ILE	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	GLU	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	ARG	-	expression tag	UNP P0DTC2
A	1222	ASP	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLN	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1269	GLU	-	expression tag	UNP P0DTC2
A	1270	ASP	-	expression tag	UNP P0DTC2
A	1271	THR	-	expression tag	UNP P0DTC2
A	1272	ALA	-	expression tag	UNP P0DTC2
A	1273	ALA	-	expression tag	UNP P0DTC2
A	1274	ALA	-	expression tag	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	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	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	ILE	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	GLU	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	ARG	-	expression tag	UNP P0DTC2
B	1222	ASP	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLN	-	expression tag	UNP P0DTC2
B	1225	ALA	-	expression tag	UNP P0DTC2
B	1226	TYR	-	expression tag	UNP P0DTC2
B	1227	VAL	-	expression tag	UNP P0DTC2
B	1228	ARG	-	expression tag	UNP P0DTC2
B	1229	LYS	-	expression tag	UNP P0DTC2
B	1230	ASP	-	expression tag	UNP P0DTC2
B	1231	GLY	-	expression tag	UNP P0DTC2
B	1232	GLU	-	expression tag	UNP P0DTC2
B	1233	TRP	-	expression tag	UNP P0DTC2
B	1234	VAL	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	PHE	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	ASN	-	expression tag	UNP P0DTC2
B	1242	SER	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	ARG	-	expression tag	UNP P0DTC2
B	1245	ALA	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	GLY	-	expression tag	UNP P0DTC2
B	1253	ALA	-	expression tag	UNP P0DTC2
B	1254	GLY	-	expression tag	UNP P0DTC2
B	1255	GLY	-	expression tag	UNP P0DTC2
B	1256	LEU	-	expression tag	UNP P0DTC2
B	1257	ASN	-	expression tag	UNP P0DTC2
B	1258	ASP	-	expression tag	UNP P0DTC2
B	1259	ILE	-	expression tag	UNP P0DTC2
B	1260	PHE	-	expression tag	UNP P0DTC2
B	1261	GLU	-	expression tag	UNP P0DTC2
B	1262	ALA	-	expression tag	UNP P0DTC2
B	1263	GLN	-	expression tag	UNP P0DTC2
B	1264	LYS	-	expression tag	UNP P0DTC2
B	1265	ILE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	TRP	-	expression tag	UNP P0DTC2
B	1268	HIS	-	expression tag	UNP P0DTC2
B	1269	GLU	-	expression tag	UNP P0DTC2
B	1270	ASP	-	expression tag	UNP P0DTC2
B	1271	THR	-	expression tag	UNP P0DTC2
B	1272	ALA	-	expression tag	UNP P0DTC2
B	1273	ALA	-	expression tag	UNP P0DTC2
B	1274	ALA	-	expression tag	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	TYR	-	expression tag	UNP P0DTC2
C	1216	ILE	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	GLU	-	expression tag	UNP P0DTC2
C	1219	ALA	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	ARG	-	expression tag	UNP P0DTC2
C	1222	ASP	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLN	-	expression tag	UNP P0DTC2
C	1225	ALA	-	expression tag	UNP P0DTC2
C	1226	TYR	-	expression tag	UNP P0DTC2
C	1227	VAL	-	expression tag	UNP P0DTC2
C	1228	ARG	-	expression tag	UNP P0DTC2
C	1229	LYS	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2
C	1232	GLU	-	expression tag	UNP P0DTC2
C	1233	TRP	-	expression tag	UNP P0DTC2
C	1234	VAL	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	THR	-	expression tag	UNP P0DTC2
C	1239	PHE	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	ASN	-	expression tag	UNP P0DTC2
C	1242	SER	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	ARG	-	expression tag	UNP P0DTC2
C	1245	ALA	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2

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

- Molecule 2 is a protein called Fab 15033-7 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	214	Total	C	N	O	S	0	0
			1641	1024	276	335	6		
2	M	214	Total	C	N	O	S	0	0
			1641	1024	276	335	6		

- Molecule 3 is a protein called Fab 15033-7 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	223	Total	C	N	O	S	0	0
			1635	1031	272	324	8		
3	I	223	Total	C	N	O	S	0	0
			1635	1031	272	324	8		

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

cetamido-2-deoxy-beta-D-glucopyranose.



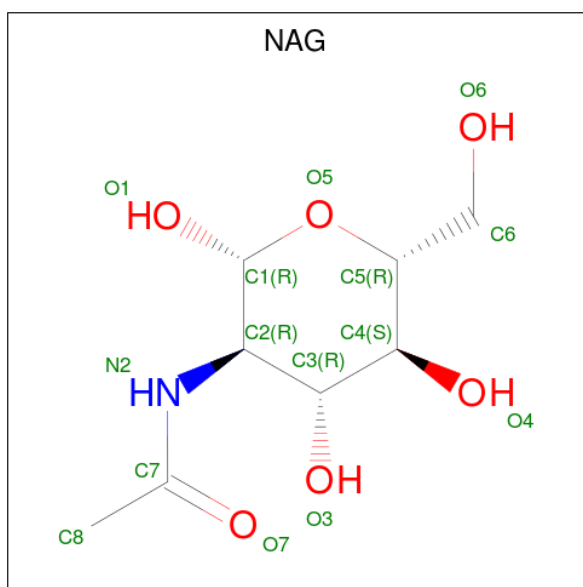
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
4	G	2	28	16	2	10	0	0
4	J	2	28	16	2	10	0	0
4	K	2	28	16	2	10	0	0
4	N	2	28	16	2	10	0	0
4	O	2	28	16	2	10	0	0
4	P	2	28	16	2	10	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	3	39	22	2	15	0	0
5	F	3	39	22	2	15	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	112	64	8	40	0
6	A	1	112	64	8	40	0
6	A	1	112	64	8	40	0
6	A	1	112	64	8	40	0
6	A	1	112	64	8	40	0
6	A	1	112	64	8	40	0
6	A	1	112	64	8	40	0
6	A	1	112	64	8	40	0
6	A	1	112	64	8	40	0
6	B	1	112	64	8	40	0
6	B	1	112	64	8	40	0
6	B	1	112	64	8	40	0
6	B	1	112	64	8	40	0
6	B	1	112	64	8	40	0
6	B	1	112	64	8	40	0

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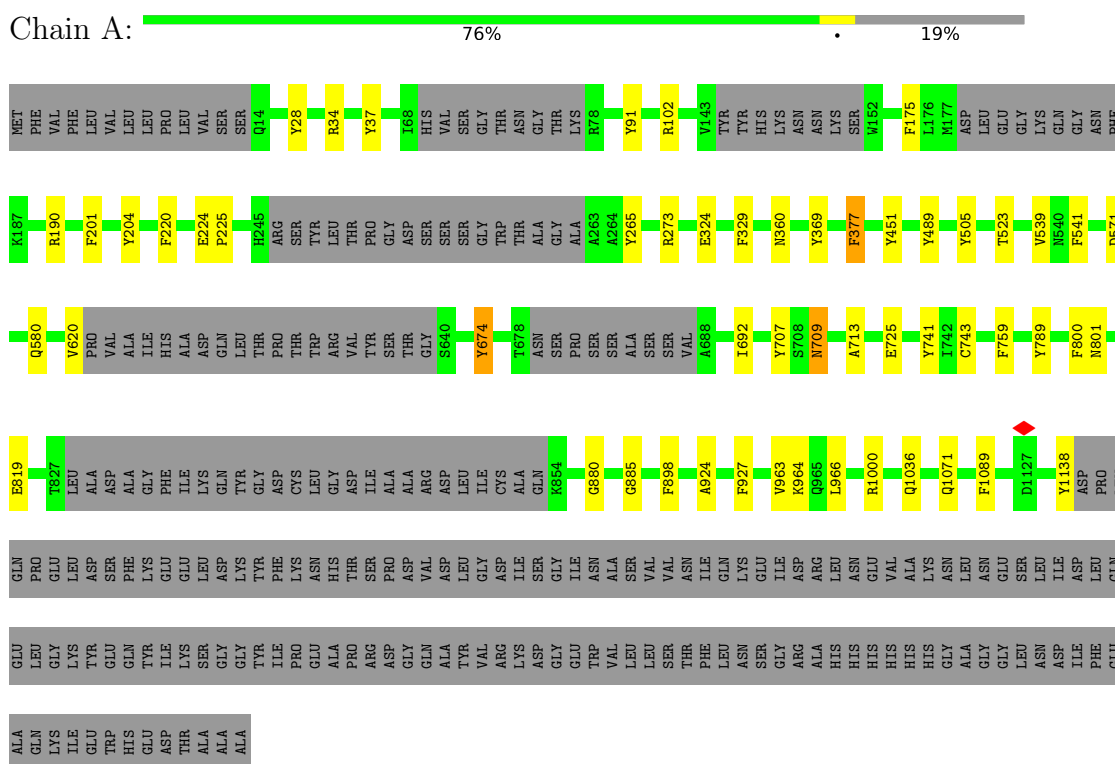
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	B	1	Total 112	C 64	N 8	O 40	0
6	B	1	Total 112	C 64	N 8	O 40	0
6	C	1	Total 126	C 72	N 9	O 45	0
6	C	1	Total 126	C 72	N 9	O 45	0
6	C	1	Total 126	C 72	N 9	O 45	0
6	C	1	Total 126	C 72	N 9	O 45	0
6	C	1	Total 126	C 72	N 9	O 45	0
6	C	1	Total 126	C 72	N 9	O 45	0
6	C	1	Total 126	C 72	N 9	O 45	0
6	C	1	Total 126	C 72	N 9	O 45	0
6	C	1	Total 126	C 72	N 9	O 45	0
6	C	1	Total 126	C 72	N 9	O 45	0

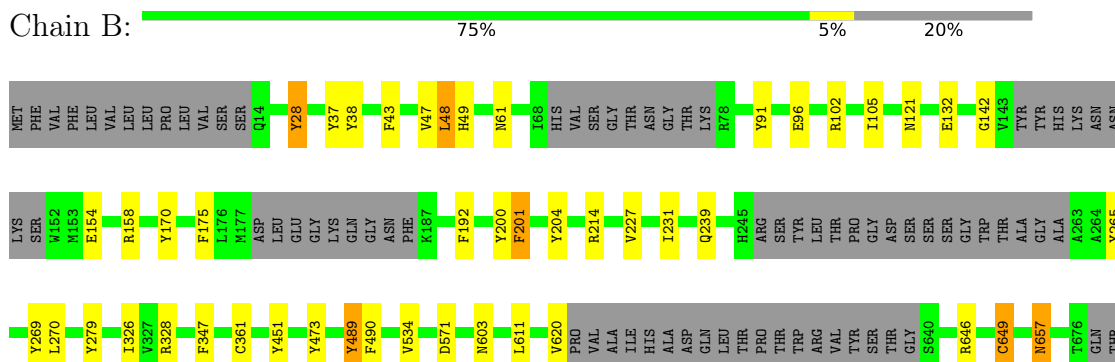
3 Residue-property plots [i](#)

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: Spike glycoprotein

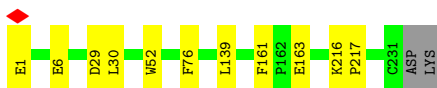


- Molecule 1: Spike glycoprotein



- Molecule 3: Fab 15033-7 heavy chain

Chain H:  94% 5%



- Molecule 3: Fab 15033-7 heavy chain

Chain I:  95%



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

Chain D:  50% 50%



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

Chain G:  50% 50%



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

Chain J:  100%



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

Chain K:  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:  100%



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

Chain P:  100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  67% 33%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	85843	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 ($e^-/\text{\AA}^2$)	38.08	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.745	Depositor
Minimum map value	-0.466	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.203	Depositor
Map size (Å)	412.0, 412.0, 412.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.01	21/8223 (0.3%)	0.95	17/11193 (0.2%)
1	B	1.02	26/8202 (0.3%)	0.96	22/11164 (0.2%)
1	C	0.99	17/8202 (0.2%)	0.95	14/11164 (0.1%)
2	L	1.01	2/1676 (0.1%)	0.97	3/2276 (0.1%)
2	M	1.00	3/1676 (0.2%)	0.99	3/2276 (0.1%)
3	H	1.00	7/1675 (0.4%)	0.91	1/2280 (0.0%)
3	I	0.98	5/1675 (0.3%)	0.95	2/2280 (0.1%)
All	All	1.01	81/31329 (0.3%)	0.95	62/42633 (0.1%)

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1072	GLU	CG-CD	-9.22	1.38	1.51
1	A	1138	TYR	CG-CD1	8.51	1.50	1.39
1	B	1138	TYR	CG-CD1	8.38	1.50	1.39
1	C	1138	TYR	CG-CD1	8.11	1.49	1.39
1	C	1138	TYR	CE1-CZ	7.96	1.49	1.38
1	B	1138	TYR	CE2-CZ	7.52	1.48	1.38
1	B	1138	TYR	CE1-CZ	7.51	1.48	1.38
1	B	1138	TYR	CG-CD2	7.51	1.49	1.39
1	A	1138	TYR	CG-CD2	7.47	1.48	1.39
1	C	1138	TYR	CG-CD2	7.44	1.48	1.39
1	B	37	TYR	CB-CG	7.41	1.62	1.51
1	A	1138	TYR	CE1-CZ	7.31	1.48	1.38
1	B	43	PHE	CB-CG	-7.24	1.39	1.51
1	A	1138	TYR	CE2-CZ	7.21	1.48	1.38
3	H	163	GLU	CG-CD	-7.07	1.41	1.51
3	I	163	GLU	CD-OE1	-6.91	1.18	1.25
1	C	1138	TYR	CE2-CZ	6.84	1.47	1.38
3	I	160	TYR	CB-CG	-6.78	1.41	1.51
1	B	707	TYR	CE2-CZ	-6.76	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	TYR	CB-CG	-6.39	1.42	1.51
3	H	1	GLU	CB-CG	6.35	1.64	1.52
3	H	161	PHE	CB-CG	-6.32	1.40	1.51
1	A	541	PHE	CB-CG	-6.28	1.40	1.51
1	C	154	GLU	CD-OE2	-6.26	1.18	1.25
1	B	170	TYR	CB-CG	-6.26	1.42	1.51
2	L	160	TYR	CB-CG	-6.25	1.42	1.51
1	B	489	TYR	CG-CD1	-6.22	1.31	1.39
1	B	154	GLU	CD-OE2	-6.18	1.18	1.25
1	A	1089	PHE	CB-CG	-6.13	1.41	1.51
1	A	91	TYR	CG-CD1	-6.07	1.31	1.39
1	B	649	CYS	CB-SG	-6.04	1.72	1.82
3	H	163	GLU	CD-OE2	-6.03	1.19	1.25
3	I	1	GLU	CB-CG	6.01	1.63	1.52
1	C	1103	PHE	CB-CG	-5.98	1.41	1.51
1	A	674	TYR	CB-CG	-5.96	1.42	1.51
1	A	1138	TYR	CB-CG	5.91	1.60	1.51
1	B	175	PHE	CB-CG	5.84	1.61	1.51
1	A	819	GLU	CD-OE1	-5.78	1.19	1.25
1	C	37	TYR	CB-CG	-5.77	1.43	1.51
1	B	695	TYR	CE2-CZ	-5.73	1.31	1.38
1	A	220	PHE	CB-CG	-5.71	1.41	1.51
1	B	1062	PHE	CB-CG	-5.53	1.42	1.51
1	A	725	GLU	CG-CD	-5.49	1.43	1.51
1	B	265	TYR	CG-CD2	-5.47	1.32	1.39
1	A	963	VAL	CB-CG2	-5.46	1.41	1.52
1	B	361	CYS	CB-SG	5.45	1.91	1.82
1	C	192	PHE	CB-CG	-5.45	1.42	1.51
1	C	488	CYS	CB-SG	-5.41	1.73	1.81
1	B	1095	PHE	CB-CG	-5.40	1.42	1.51
1	C	136	CYS	CB-SG	5.38	1.91	1.82
2	M	168	TRP	CB-CG	-5.37	1.40	1.50
1	B	1072	GLU	CD-OE1	-5.36	1.19	1.25
1	C	591	SER	CB-OG	-5.36	1.35	1.42
1	B	702	GLU	CD-OE2	-5.36	1.19	1.25
1	C	1072	GLU	CD-OE1	-5.30	1.19	1.25
1	A	489	TYR	CG-CD2	-5.29	1.32	1.39
1	A	1138	TYR	CD2-CE2	5.26	1.47	1.39
1	C	1138	TYR	CD1-CE1	5.25	1.47	1.39
1	B	1138	TYR	CD2-CE2	5.22	1.47	1.39
1	C	132	GLU	CD-OE2	-5.21	1.20	1.25
1	B	96	GLU	CD-OE2	-5.20	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	VAL	CB-CG2	-5.20	1.42	1.52
1	C	905	ARG	CZ-NH1	-5.20	1.26	1.33
1	A	898	PHE	CB-CG	-5.18	1.42	1.51
1	B	132	GLU	CD-OE2	-5.18	1.20	1.25
1	A	759	PHE	CB-CG	5.16	1.60	1.51
2	M	19	VAL	CB-CG2	-5.15	1.42	1.52
1	C	96	GLU	CD-OE1	-5.14	1.20	1.25
1	A	620	VAL	CB-CG2	5.12	1.63	1.52
1	B	620	VAL	CB-CG2	5.11	1.63	1.52
1	A	265	TYR	CB-CG	-5.08	1.44	1.51
2	L	125	GLU	CD-OE2	-5.07	1.20	1.25
2	M	42	TYR	CB-CG	-5.06	1.44	1.51
1	B	489	TYR	CG-CD2	-5.06	1.32	1.39
3	H	6	GLU	CD-OE2	-5.06	1.20	1.25
3	I	52	TRP	CZ3-CH2	-5.05	1.31	1.40
1	A	224	GLU	CD-OE2	-5.04	1.20	1.25
1	C	620	VAL	CB-CG2	5.04	1.63	1.52
3	H	163	GLU	CB-CG	-5.04	1.42	1.52
3	H	52	TRP	CZ3-CH2	-5.03	1.31	1.40
3	I	6	GLU	CD-OE2	-5.01	1.20	1.25

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1039	ARG	NE-CZ-NH2	-9.03	115.78	120.30
2	M	128	ARG	NE-CZ-NH2	-8.74	115.93	120.30
2	L	75	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	273	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	377	PHE	CB-CG-CD1	8.29	126.60	120.80
1	C	1000	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	C	454	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	B	214	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	B	1000	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	328	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	1000	ARG	NE-CZ-NH2	-7.34	116.63	120.30
3	I	76	PHE	CB-CG-CD1	7.30	125.91	120.80
1	C	273	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	505	TYR	CB-CG-CD1	-7.11	116.73	121.00
1	C	269	TYR	CB-CG-CD1	-7.06	116.76	121.00
3	H	76	PHE	CB-CG-CD1	7.03	125.72	120.80
1	B	269	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	A	34	ARG	NE-CZ-NH2	-6.91	116.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	646	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	377	PHE	CB-CG-CD2	-6.87	115.99	120.80
1	B	37	TYR	CB-CG-CD1	6.85	125.11	121.00
1	A	190	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	38	TYR	CB-CG-CD2	-6.61	117.03	121.00
1	C	351	TYR	CB-CG-CD1	-6.28	117.23	121.00
1	B	1000	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	192	PHE	CB-CG-CD2	-6.24	116.44	120.80
1	B	204	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	A	369	TYR	CB-CG-CD2	-6.15	117.31	121.00
2	L	128	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	C	1019	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	200	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	C	1000	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	M	75	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	789	TYR	CB-CG-CD2	-5.88	117.47	121.00
3	I	108	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	B	741	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	C	515	PHE	CB-CG-CD1	5.86	124.90	120.80
1	A	175	PHE	CB-CG-CD1	5.85	124.89	120.80
1	A	37	TYR	CB-CG-CD2	-5.84	117.50	121.00
1	A	707	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	C	1019	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	M	193	TYR	CB-CG-CD1	-5.71	117.58	121.00
1	A	28	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	B	451	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	B	28	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	A	201	PHE	CB-CA-C	5.50	121.39	110.40
2	L	114	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	C	451	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	C	44	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	347	PHE	CB-CG-CD1	5.31	124.52	120.80
1	B	201	PHE	CB-CG-CD1	5.30	124.51	120.80
1	B	37	TYR	CB-CG-CD2	-5.29	117.82	121.00
1	C	37	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	C	160	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	A	1000	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	489	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	B	192	PHE	CB-CG-CD1	5.11	124.38	120.80
1	A	102	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	266	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	B	473	TYR	CB-CG-CD2	-5.07	117.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	B	37	TYR	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8039	0	7847	14	0
1	B	8018	0	7825	19	0
1	C	8018	0	7825	11	0
2	L	1641	0	1594	3	0
2	M	1641	0	1594	1	0
3	H	1635	0	1586	3	0
3	I	1635	0	1586	1	0
4	D	28	0	25	0	0
4	G	28	0	25	1	0
4	J	28	0	25	0	0
4	K	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
5	E	39	0	34	0	0
5	F	39	0	34	0	0
6	A	112	0	104	1	0
6	B	112	0	104	0	0
6	C	126	0	117	1	0
All	All	31251	0	30425	48	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 (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLY:HA3	1:B:158:ARG:HD2	1.81	0.60
2:L:138:PHE:HB3	3:H:139:LEU:HB3	1.86	0.57
1:B:47:VAL:HG12	1:B:48:LEU:N	2.22	0.54
1:C:281:GLU:OE1	6:C:1302:NAG:H62	2.10	0.51
1:C:444:LYS:O	1:C:498:GLN:NE2	2.44	0.50
1:A:1071:GLN:HG3	6:A:1305:NAG:H5	1.94	0.50
1:A:709:ASN:N	1:A:709:ASN:OD1	2.45	0.50
1:A:571:ASP:OD2	1:C:964:LYS:NZ	2.44	0.50
1:B:47:VAL:CG1	1:B:48:LEU:N	2.76	0.49
1:B:326:ILE:HD11	1:B:534:VAL:H	1.79	0.48
1:C:48:LEU:HD23	1:C:278:LYS:HA	1.96	0.48
3:H:216:LYS:N	3:H:217:PRO:CD	2.77	0.47
1:A:964:LYS:NZ	1:B:571:ASP:OD2	2.48	0.47
1:A:800:PHE:CE2	1:A:927:PHE:HB3	2.50	0.47
1:B:49:HIS:HB3	1:B:279:TYR:HE1	1.79	0.47
1:B:489:TYR:CE2	1:B:490:PHE:O	2.68	0.47
1:B:28:TYR:HB3	1:B:61:ASN:HB3	1.98	0.46
1:C:1097:SER:HB2	1:C:1102:TRP:CE2	2.51	0.46
1:B:989:ALA:O	1:B:993:ILE:HG12	2.15	0.46
1:B:102:ARG:HB3	1:B:121:ASN:HB2	1.97	0.46
1:A:800:PHE:CE2	1:A:924:ALA:HA	2.52	0.45
1:B:657:ASN:N	1:B:657:ASN:OD1	2.49	0.45
1:A:324:GLU:HB2	1:A:539:VAL:HG22	1.98	0.45
3:H:29:ASP:OD1	3:H:30:LEU:N	2.50	0.45
1:A:880:GLY:O	1:A:885:GLY:N	2.50	0.45
2:M:41:TRP:HE1	2:M:102:TYR:HB3	1.82	0.45
1:B:201:PHE:CD2	1:B:231:ILE:HG13	2.53	0.44
1:C:47:VAL:HG12	1:C:48:LEU:N	2.33	0.44
1:C:578:ASP:HB3	1:C:581:THR:O	2.17	0.44
1:B:922:LEU:HD11	4:G:1:NAG:H5	2.00	0.43
1:C:102:ARG:HB3	1:C:121:ASN:HB3	2.01	0.43
1:B:818:ILE:HB	1:B:1054:GLN:HE22	1.85	0.42
1:C:342:PHE:O	1:C:509:ARG:NH1	2.53	0.42
1:B:91:TYR:CD1	1:B:270:LEU:HD21	2.55	0.42
1:B:714:ILE:HA	1:B:715:PRO:HD3	1.93	0.41
1:B:105:ILE:HG23	1:B:239:GLN:HB2	2.01	0.41
1:A:741:TYR:CE1	1:A:966:LEU:HD11	2.56	0.41
1:A:713:ALA:HB3	1:C:895:GLN:H	1.85	0.41
1:A:329:PHE:O	1:A:580:GLN:HG3	2.21	0.40
1:A:674:TYR:CE2	1:A:692:ILE:HG12	2.57	0.40
1:A:360:ASN:H	1:A:523:THR:HB	1.86	0.40
3:I:216:LYS:N	3:I:217:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:ASN:OD1	1:B:603:ASN:C	2.59	0.40
2:L:41:TRP:CD1	2:L:89:LEU:HB2	2.56	0.40
2:L:114:TYR:HA	2:L:115:PRO:C	2.41	0.40
1:B:611:LEU:HA	1:B:649:CYS:O	2.20	0.40
1:C:660:TYR:CD1	1:C:695:TYR:CD2	3.09	0.40
1:A:204:TYR:HA	1:A:225:PRO:HA	2.03	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	A	1012/1274 (79%)	989 (98%)	21 (2%)	2 (0%)	47	80
1	B	1009/1274 (79%)	991 (98%)	18 (2%)	0	100	100
1	C	1009/1274 (79%)	984 (98%)	24 (2%)	1 (0%)	51	85
2	L	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
2	M	212/214 (99%)	210 (99%)	2 (1%)	0	100	100
3	H	221/225 (98%)	216 (98%)	5 (2%)	0	100	100
3	I	221/225 (98%)	217 (98%)	4 (2%)	0	100	100
All	All	3896/4700 (83%)	3816 (98%)	77 (2%)	3 (0%)	54	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1036	GLN
1	A	743	CYS
1	C	743	CYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	903/1107 (82%)	900 (100%)	3 (0%)	92	95
1	B	901/1107 (81%)	898 (100%)	3 (0%)	92	95
1	C	901/1107 (81%)	899 (100%)	2 (0%)	93	96
2	L	189/189 (100%)	188 (100%)	1 (0%)	88	93
2	M	189/189 (100%)	189 (100%)	0	100	100
3	H	177/179 (99%)	177 (100%)	0	100	100
3	I	177/179 (99%)	177 (100%)	0	100	100
All	All	3437/4057 (85%)	3428 (100%)	9 (0%)	92	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	PHE
1	A	709	ASN
1	A	801	ASN
1	B	48	LEU
1	B	657	ASN
1	B	1134	ASN
1	C	457	ARG
1	C	657	ASN
2	L	104	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	580	GLN
1	B	1011	GLN
3	H	215	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	D	1	1,4	14,14,15	0.32	0	17,19,21	1.10	1 (5%)
4	NAG	D	2	4	14,14,15	0.32	0	17,19,21	0.66	0
5	NAG	E	1	1,5	14,14,15	0.32	0	17,19,21	0.52	0
5	NAG	E	2	5	14,14,15	0.32	0	17,19,21	0.83	1 (5%)
5	BMA	E	3	5	11,11,12	0.28	0	15,15,17	0.56	0
5	NAG	F	1	1,5	14,14,15	0.37	0	17,19,21	1.07	2 (11%)
5	NAG	F	2	5	14,14,15	0.34	0	17,19,21	0.65	0
5	BMA	F	3	5	11,11,12	0.28	0	15,15,17	0.65	0
4	NAG	G	1	1,4	14,14,15	0.36	0	17,19,21	0.80	0
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	0.69	0
4	NAG	J	1	1,4	14,14,15	0.36	0	17,19,21	0.81	0
4	NAG	J	2	4	14,14,15	0.32	0	17,19,21	0.74	0
4	NAG	K	1	1,4	14,14,15	0.35	0	17,19,21	1.41	3 (17%)
4	NAG	K	2	4	14,14,15	0.36	0	17,19,21	0.58	0
4	NAG	N	1	1,4	14,14,15	0.29	0	17,19,21	0.99	1 (5%)
4	NAG	N	2	4	14,14,15	0.37	0	17,19,21	0.62	0
4	NAG	O	1	1,4	14,14,15	0.34	0	17,19,21	0.66	0
4	NAG	O	2	4	14,14,15	0.32	0	17,19,21	0.65	0
4	NAG	P	1	1,4	14,14,15	0.35	0	17,19,21	0.54	0
4	NAG	P	2	4	14,14,15	0.32	0	17,19,21	0.62	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	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	4/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1	NAG	C4-C3-C2	-3.39	106.05	111.02
5	F	1	NAG	C4-C3-C2	-3.11	106.46	111.02
5	E	2	NAG	O5-C1-C2	-3.09	106.41	111.29
4	N	1	NAG	C4-C3-C2	-3.03	106.58	111.02
4	D	1	NAG	O5-C1-C2	-2.66	107.08	111.29
4	K	1	NAG	C3-C4-C5	-2.34	106.06	110.24
5	F	1	NAG	O5-C1-C2	-2.16	107.87	111.29
4	K	1	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

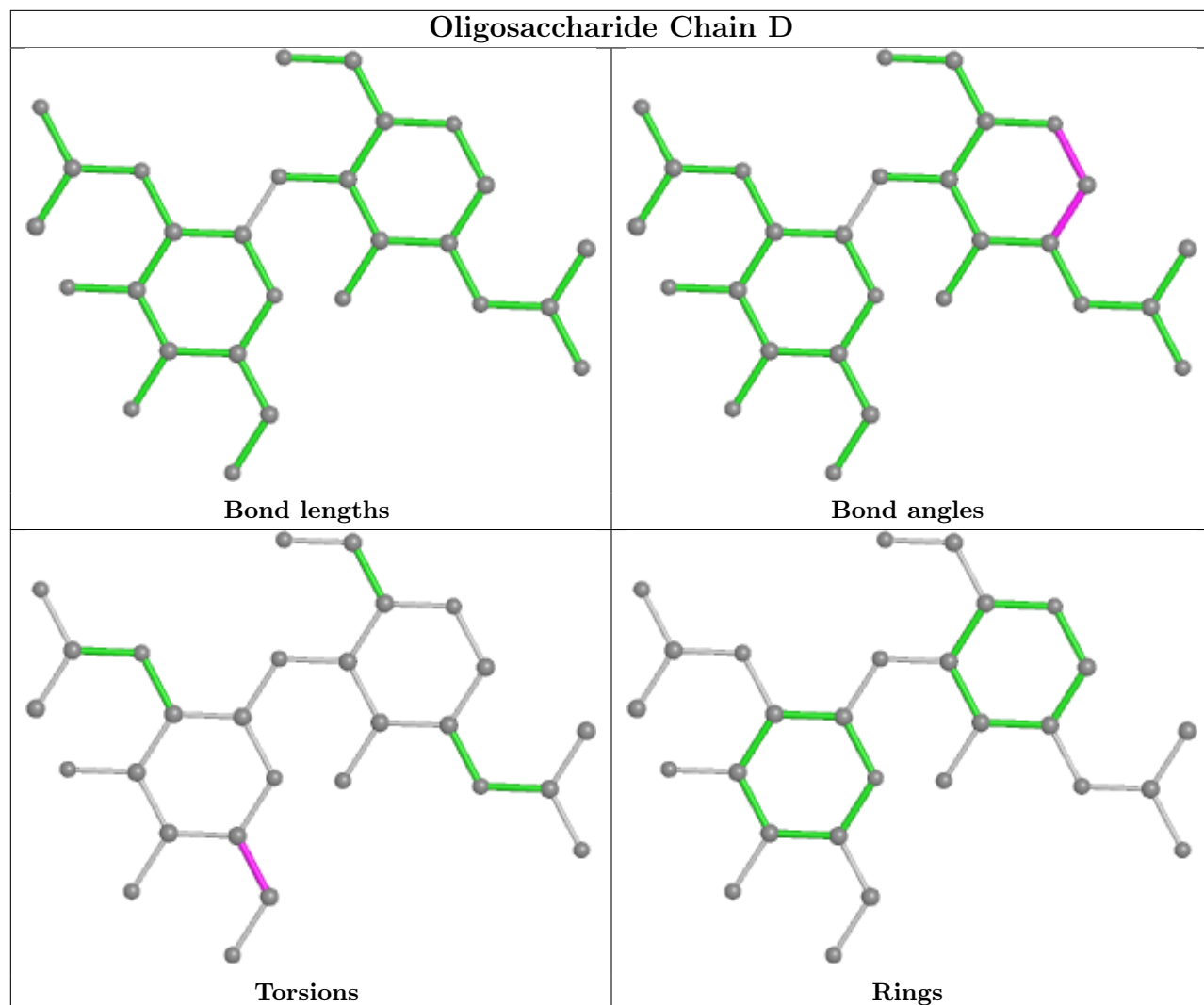
Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
4	O	1	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6

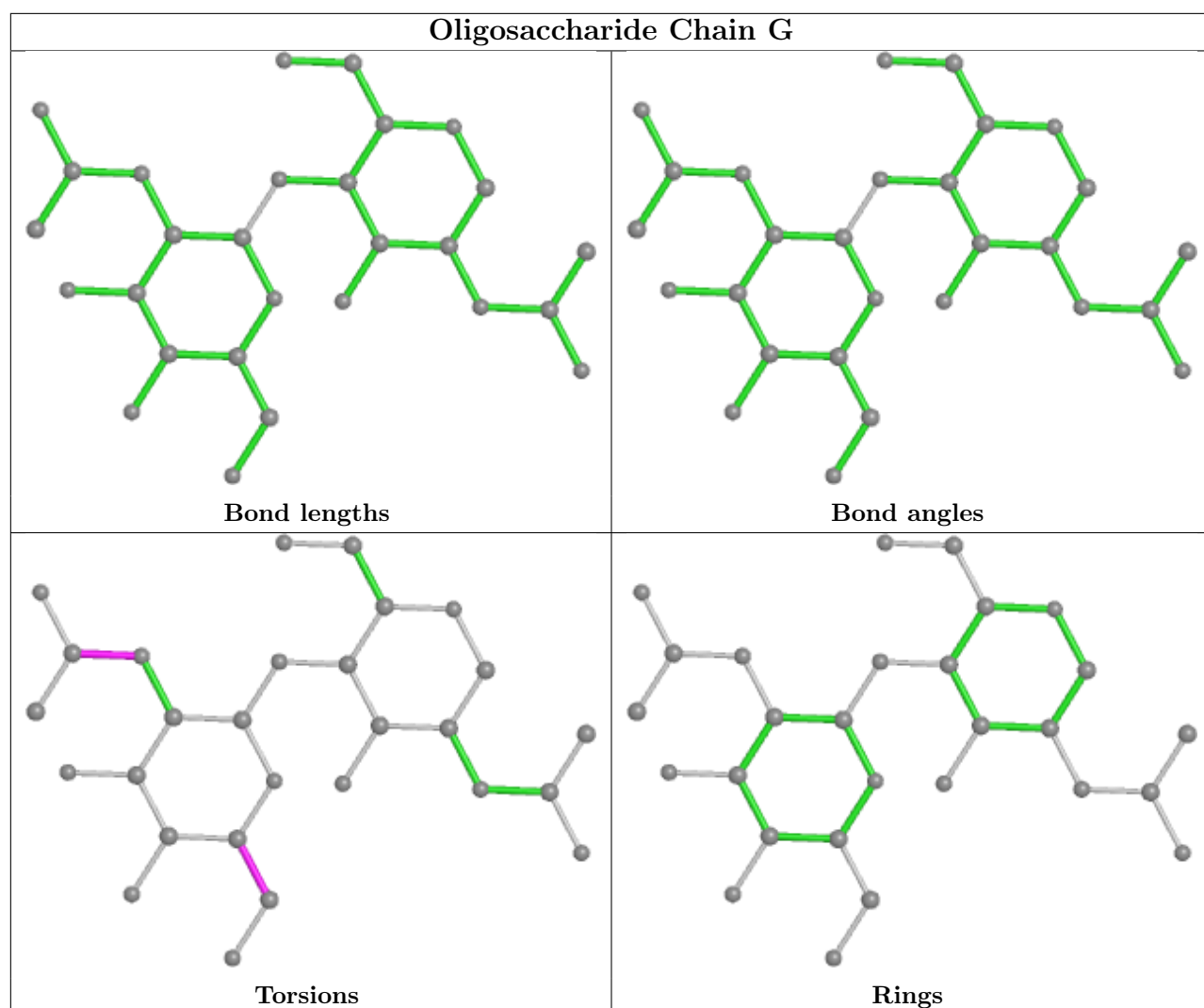
There are no ring outliers.

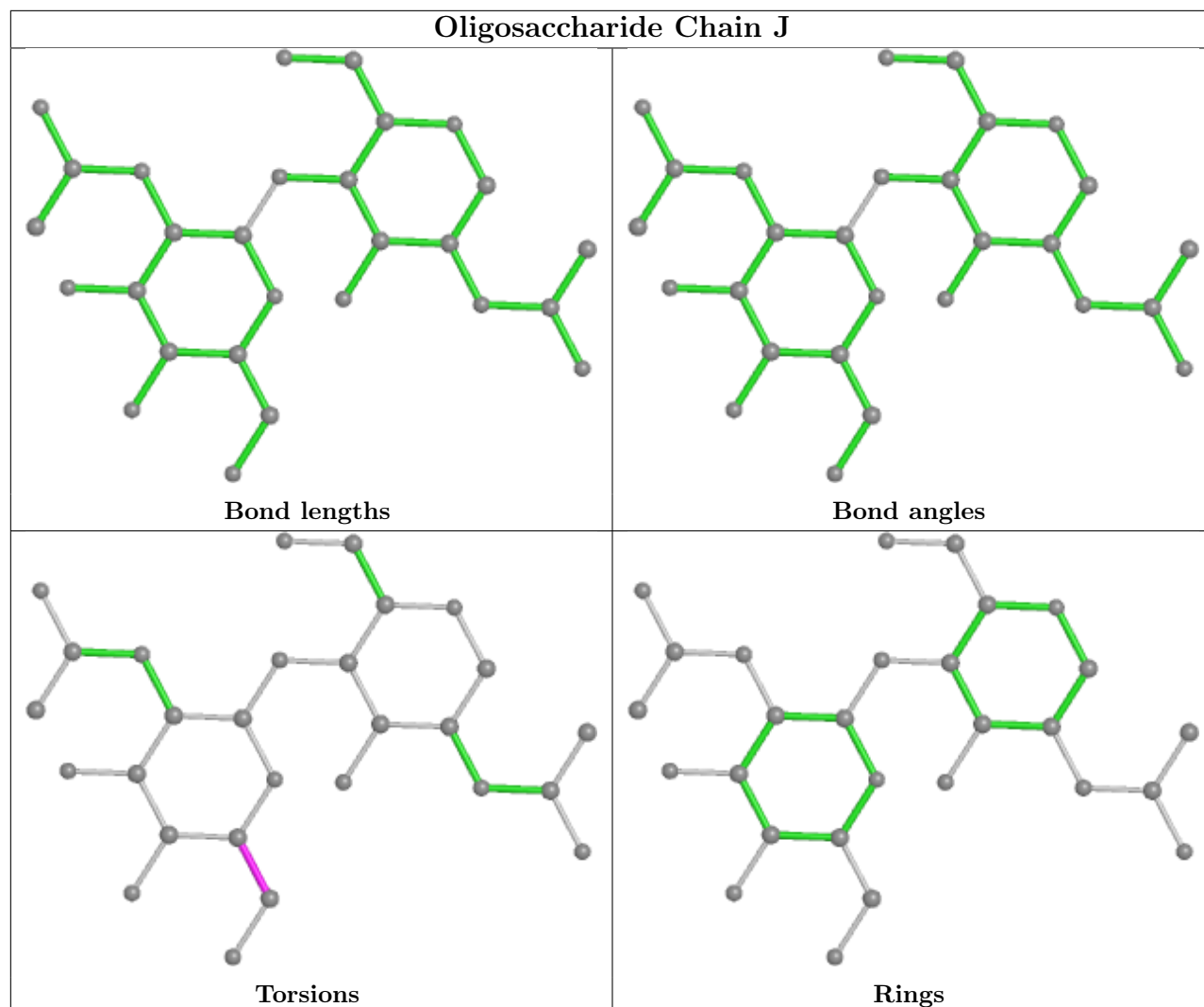
1 monomer is involved in 1 short contact:

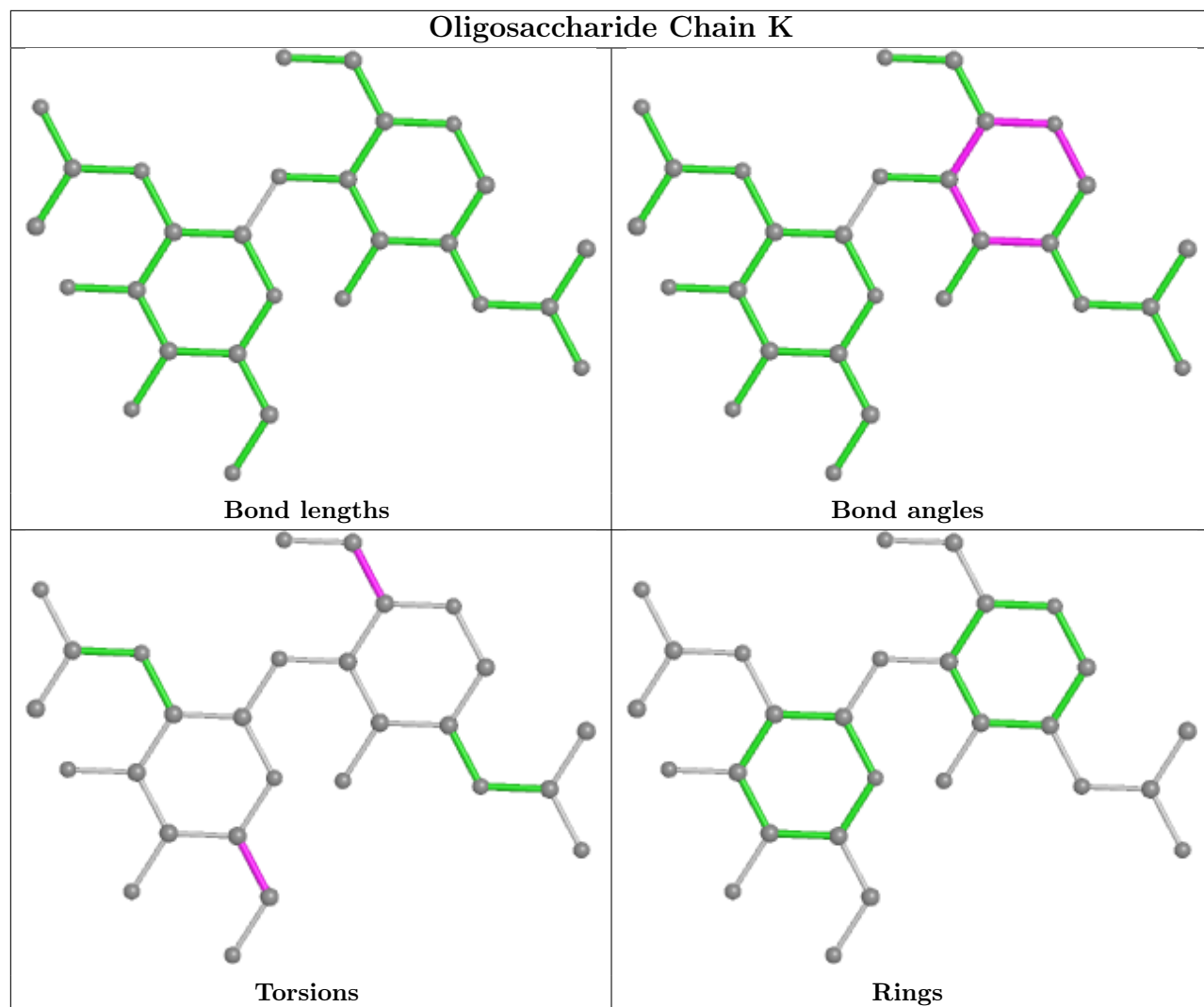
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0

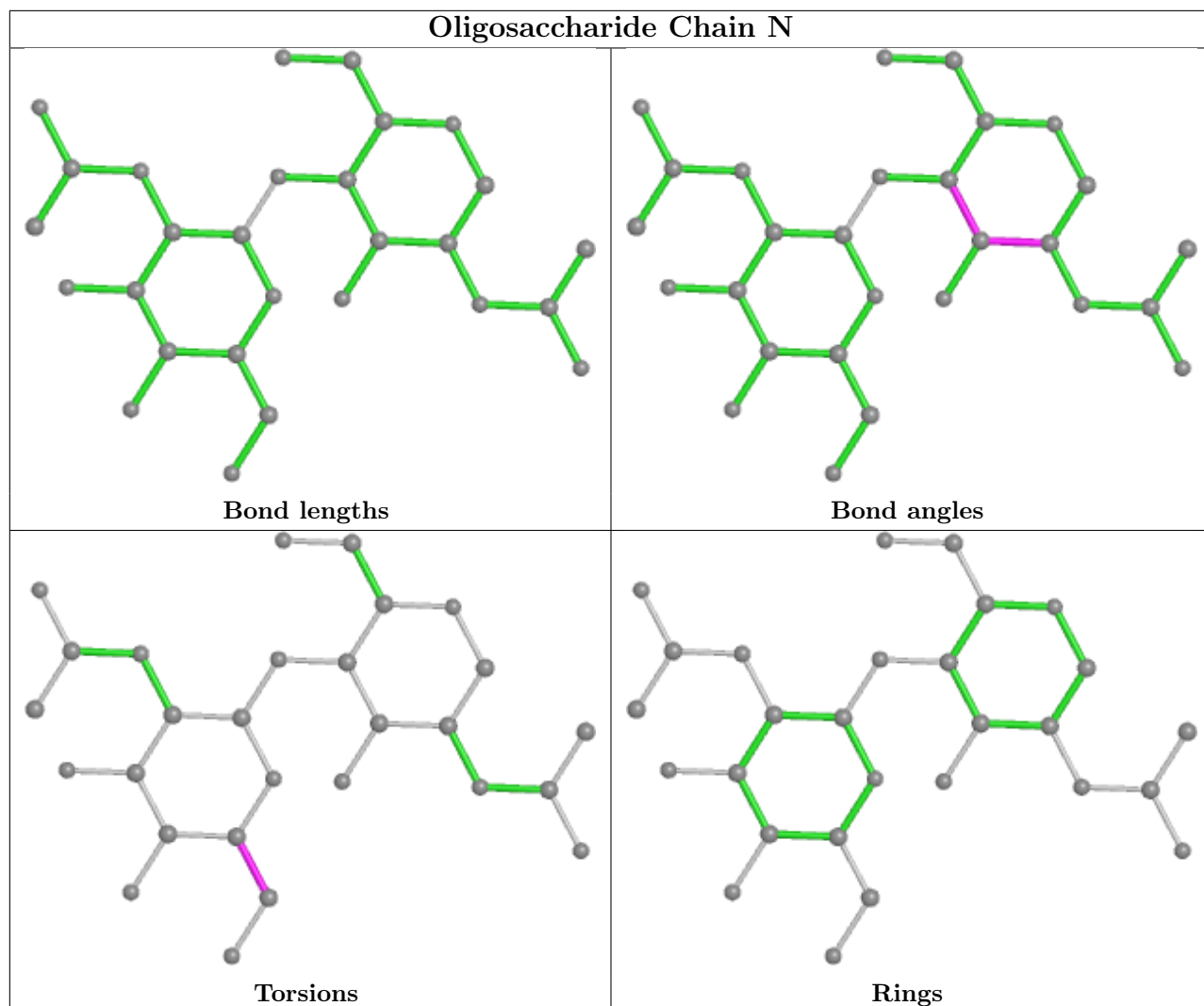
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

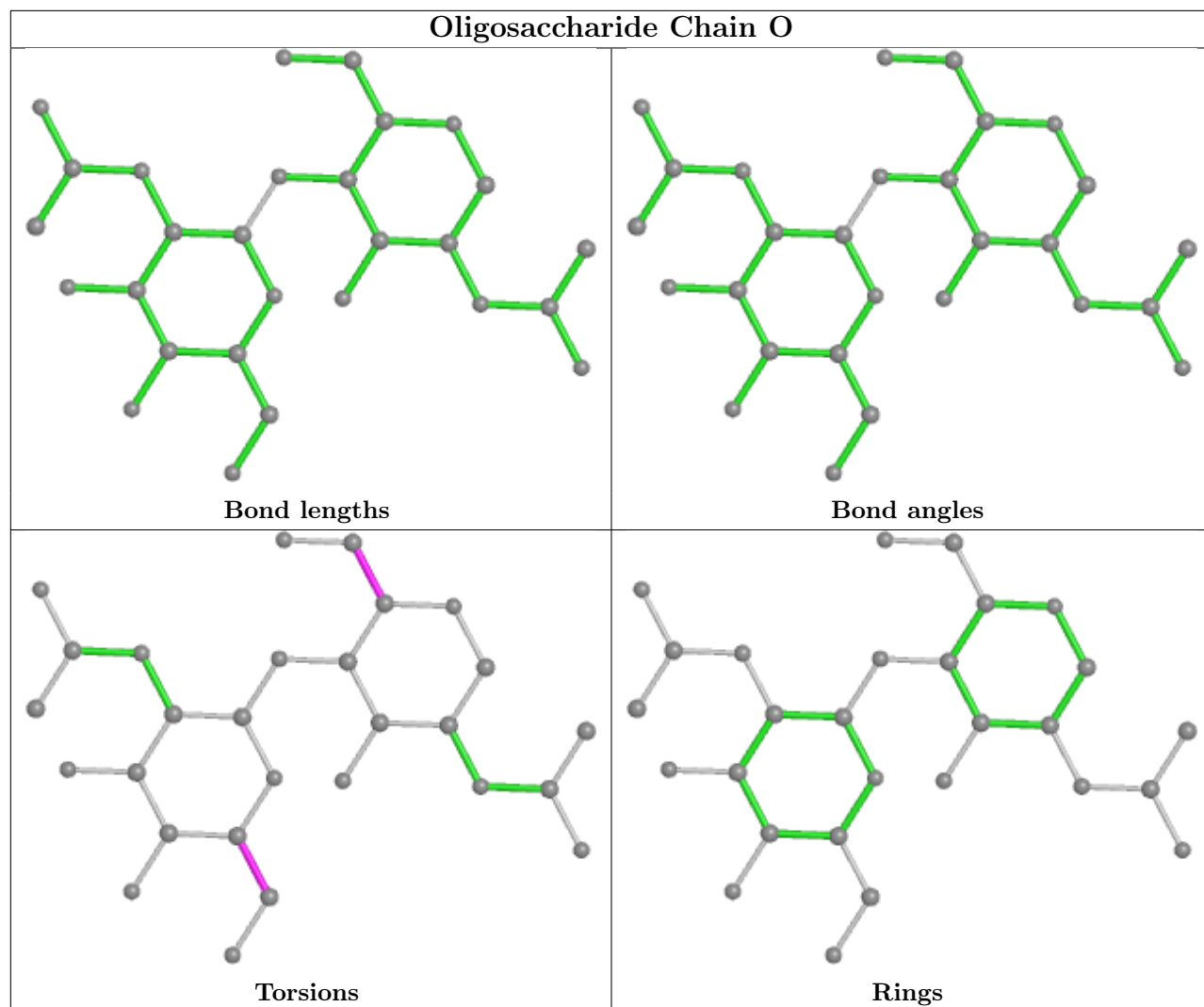


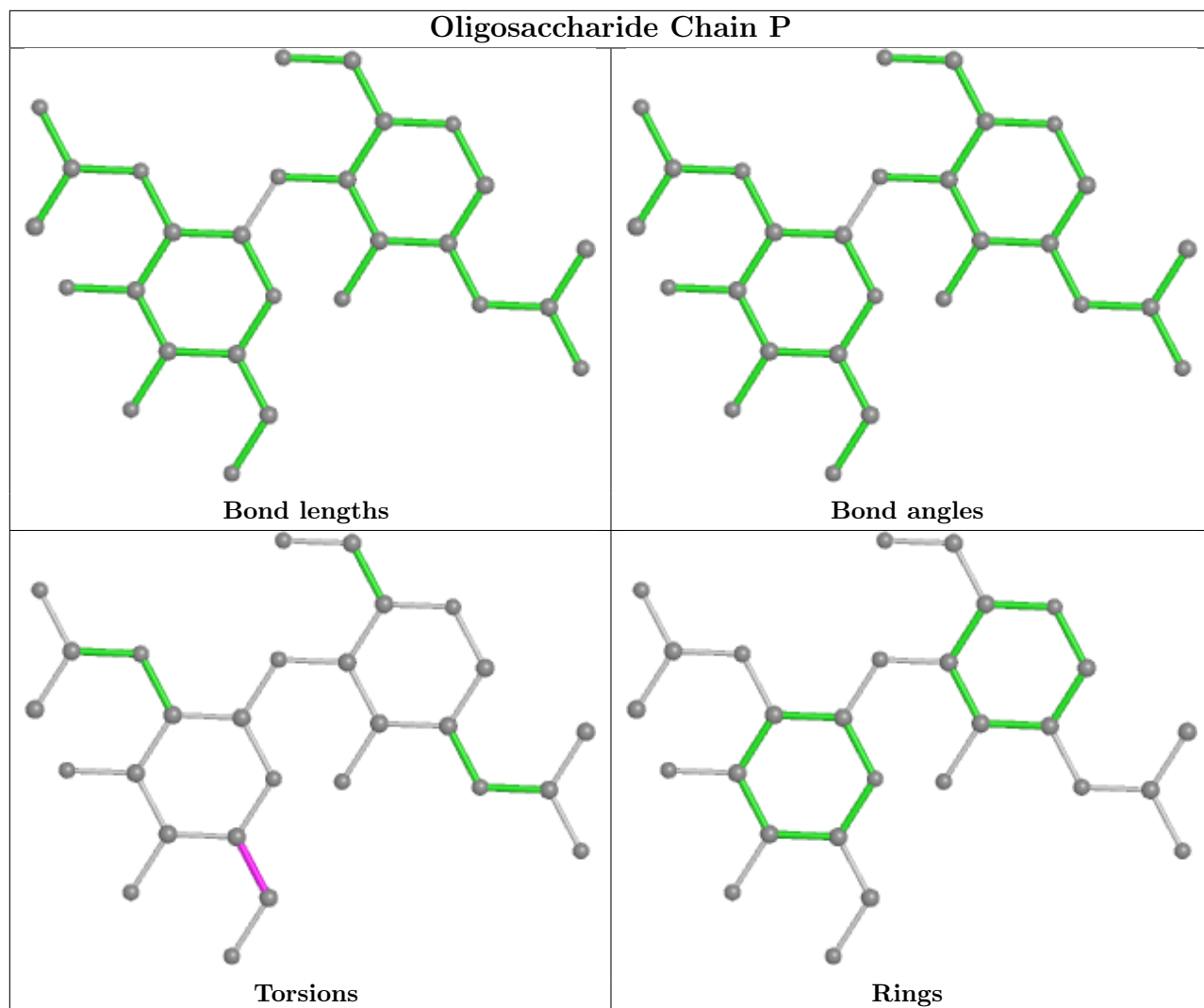


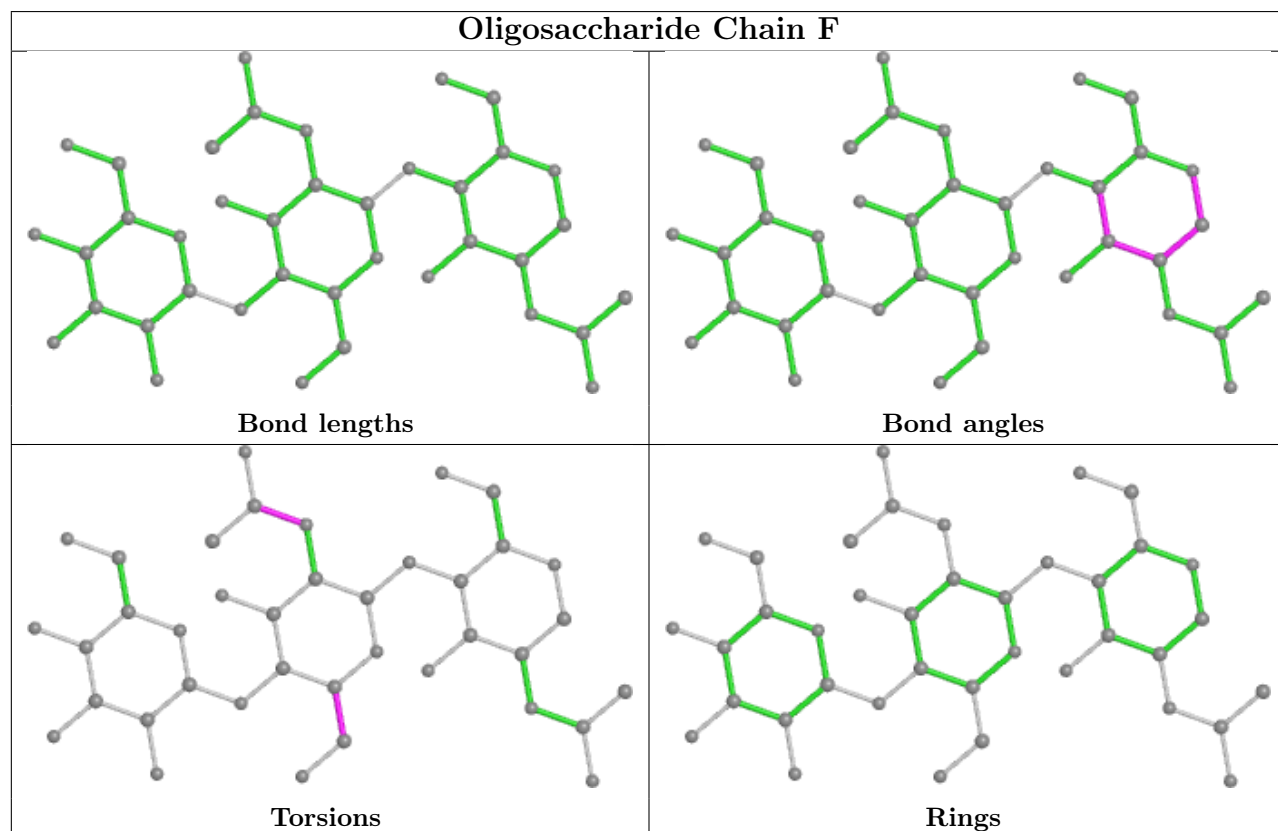
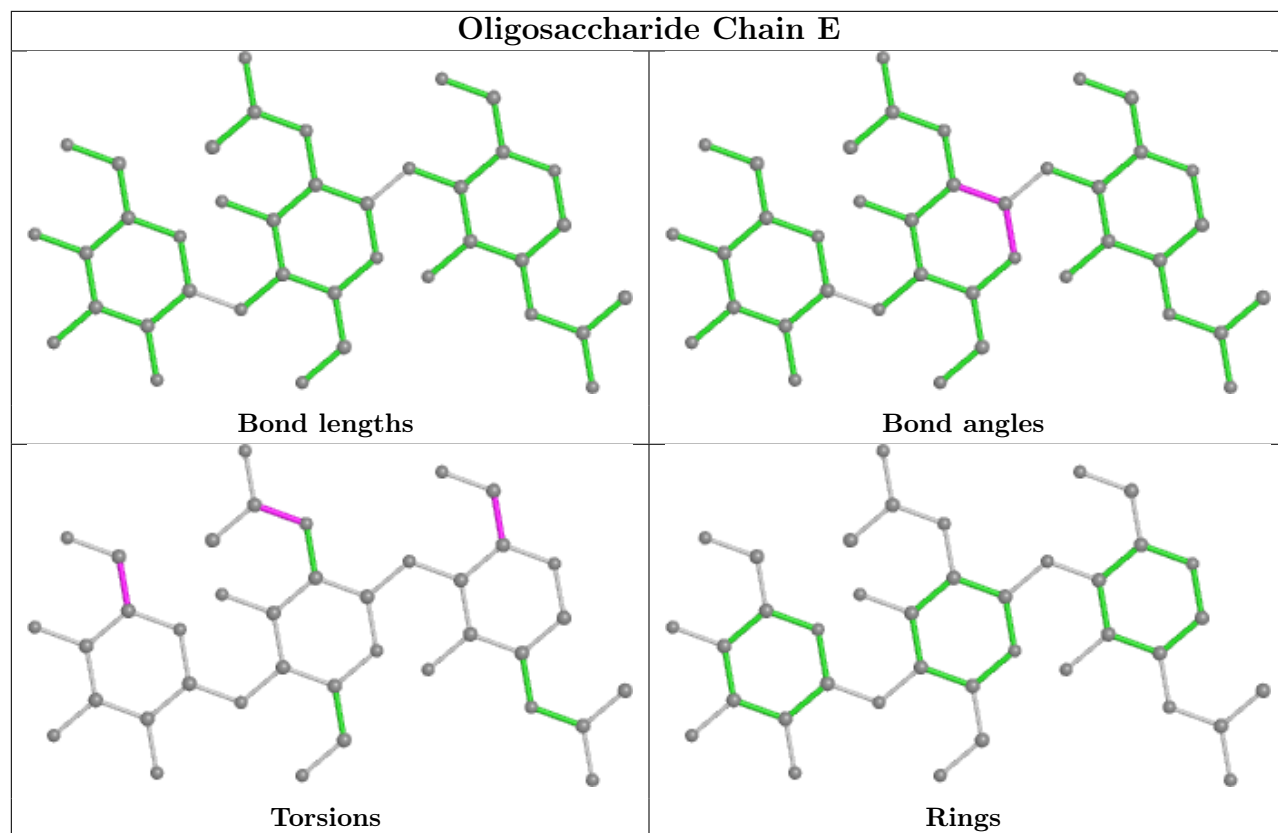












5.6 Ligand geometry

25 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	1304	1	14,14,15	0.33	0	17,19,21	0.56	0
6	NAG	C	1308	1	14,14,15	0.37	0	17,19,21	0.73	0
6	NAG	B	1307	1	14,14,15	0.28	0	17,19,21	0.92	1 (5%)
6	NAG	C	1301	1	14,14,15	0.28	0	17,19,21	0.76	1 (5%)
6	NAG	B	1305	1	14,14,15	0.33	0	17,19,21	0.57	0
6	NAG	A	1305	1	14,14,15	0.33	0	17,19,21	0.63	0
6	NAG	A	1301	1	14,14,15	0.32	0	17,19,21	0.64	0
6	NAG	C	1305	1	14,14,15	0.31	0	17,19,21	0.60	0
6	NAG	B	1302	1	14,14,15	0.31	0	17,19,21	0.60	0
6	NAG	B	1304	1	14,14,15	0.31	0	17,19,21	0.60	0
6	NAG	C	1307	1	14,14,15	0.34	0	17,19,21	0.64	0
6	NAG	A	1308	1	14,14,15	0.33	0	17,19,21	0.55	0
6	NAG	B	1301	1	14,14,15	0.29	0	17,19,21	0.98	1 (5%)
6	NAG	C	1302	1	14,14,15	0.34	0	17,19,21	0.64	0
6	NAG	A	1302	1	14,14,15	0.36	0	17,19,21	0.64	0
6	NAG	B	1303	1	14,14,15	0.38	0	17,19,21	0.79	0
6	NAG	C	1306	1	14,14,15	0.36	0	17,19,21	0.59	0
6	NAG	A	1303	1	14,14,15	0.33	0	17,19,21	0.73	0
6	NAG	A	1307	1	14,14,15	0.30	0	17,19,21	0.82	1 (5%)
6	NAG	C	1309	1	14,14,15	0.33	0	17,19,21	0.61	0
6	NAG	C	1303	1	14,14,15	0.28	0	17,19,21	0.62	0
6	NAG	A	1306	1	14,14,15	0.31	0	17,19,21	0.65	0
6	NAG	B	1308	1	14,14,15	0.32	0	17,19,21	0.64	0
6	NAG	B	1306	1	14,14,15	0.31	0	17,19,21	1.10	1 (5%)
6	NAG	C	1304	1	14,14,15	0.31	0	17,19,21	0.59	0

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1306	NAG	C2-N2-C7	2.95	127.11	122.90
6	B	1301	NAG	O5-C1-C2	-2.67	107.07	111.29
6	C	1301	NAG	O5-C1-C2	-2.44	107.43	111.29
6	B	1307	NAG	O5-C1-C2	-2.07	108.02	111.29
6	A	1307	NAG	O5-C1-C2	-2.03	108.08	111.29

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1301	NAG	O5-C5-C6-O6
6	A	1306	NAG	O5-C5-C6-O6
6	A	1307	NAG	O5-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	A	1302	NAG	O5-C5-C6-O6
6	B	1302	NAG	O5-C5-C6-O6
6	B	1306	NAG	O5-C5-C6-O6
6	B	1303	NAG	O5-C5-C6-O6
6	A	1308	NAG	C4-C5-C6-O6
6	C	1301	NAG	C4-C5-C6-O6
6	A	1307	NAG	C4-C5-C6-O6
6	B	1302	NAG	C4-C5-C6-O6
6	A	1304	NAG	O5-C5-C6-O6
6	A	1308	NAG	C8-C7-N2-C2
6	A	1308	NAG	O7-C7-N2-C2
6	B	1302	NAG	C8-C7-N2-C2
6	B	1302	NAG	O7-C7-N2-C2
6	C	1302	NAG	C8-C7-N2-C2
6	C	1302	NAG	O7-C7-N2-C2
6	C	1303	NAG	C8-C7-N2-C2
6	C	1303	NAG	O7-C7-N2-C2
6	C	1304	NAG	C8-C7-N2-C2
6	C	1304	NAG	O7-C7-N2-C2
6	C	1308	NAG	C8-C7-N2-C2
6	C	1308	NAG	O7-C7-N2-C2
6	B	1303	NAG	C4-C5-C6-O6
6	A	1308	NAG	O5-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	C	1305	NAG	O5-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6
6	A	1302	NAG	C4-C5-C6-O6
6	A	1304	NAG	C4-C5-C6-O6
6	A	1306	NAG	C4-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	C	1305	NAG	C4-C5-C6-O6
6	B	1306	NAG	C4-C5-C6-O6
6	A	1303	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	C	1309	NAG	C4-C5-C6-O6
6	C	1303	NAG	C4-C5-C6-O6
6	C	1309	NAG	O5-C5-C6-O6
6	C	1308	NAG	O5-C5-C6-O6
6	B	1307	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	1303	NAG	C4-C5-C6-O6
6	B	1307	NAG	O5-C5-C6-O6
6	B	1306	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1305	NAG	1	0
6	C	1302	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

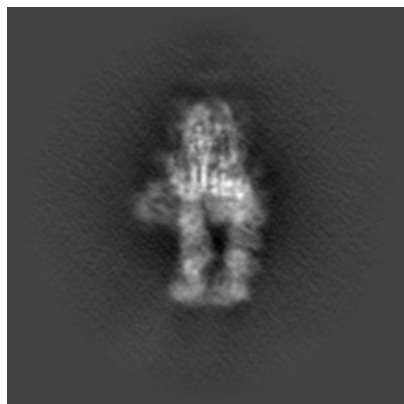
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22925. These allow visual inspection of the internal detail of the map and identification of artifacts.

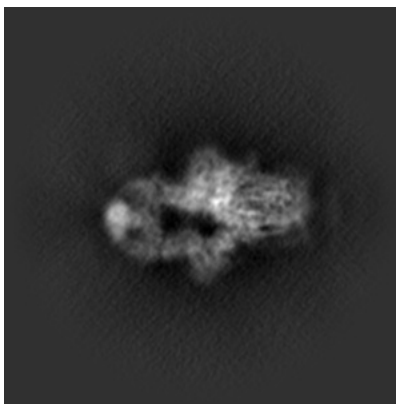
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

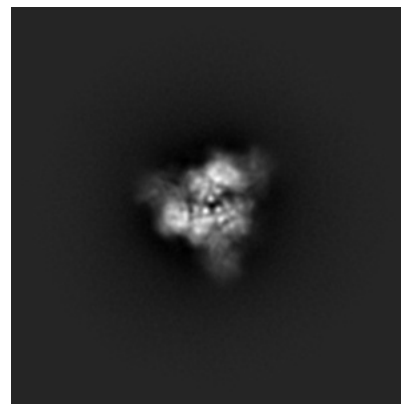
6.1.1 Primary map



X

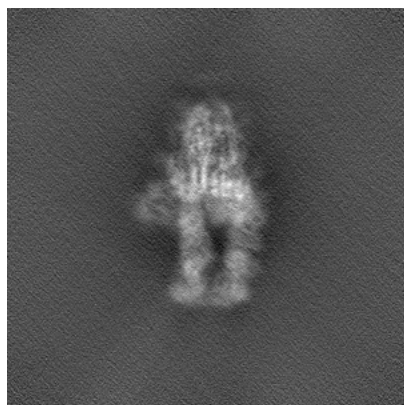


Y

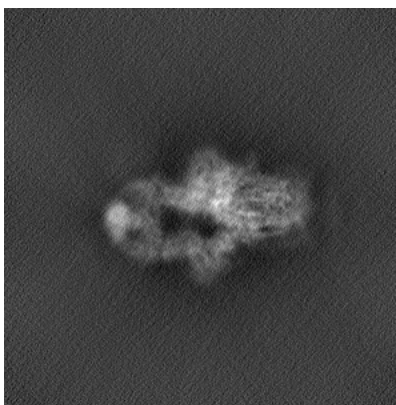


Z

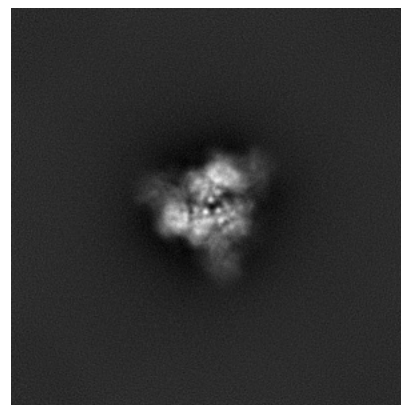
6.1.2 Raw map



X



Y

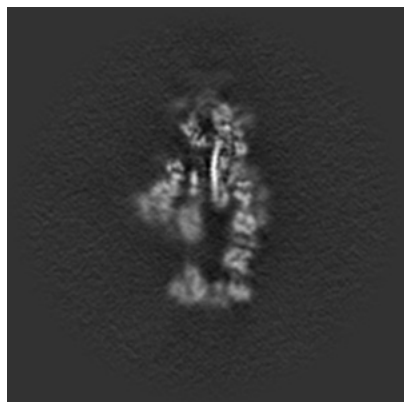


Z

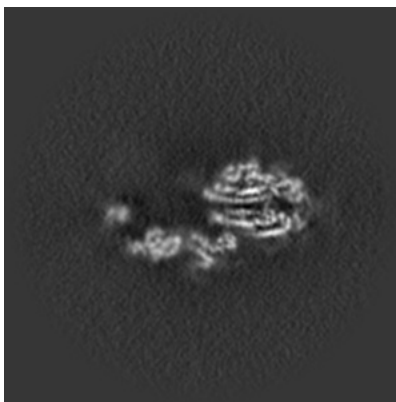
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

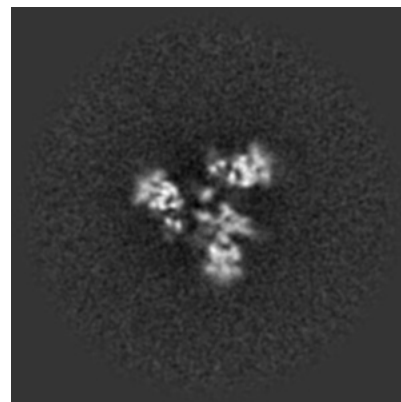
6.2.1 Primary map



X Index: 200

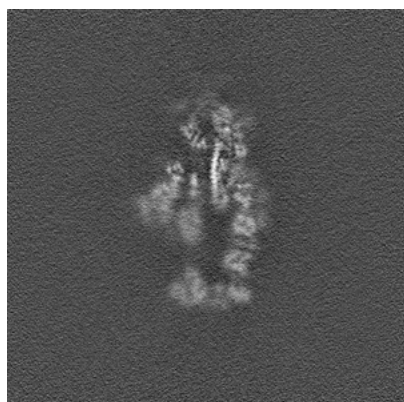


Y Index: 200

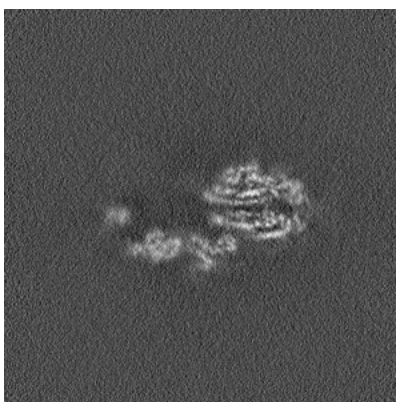


Z Index: 200

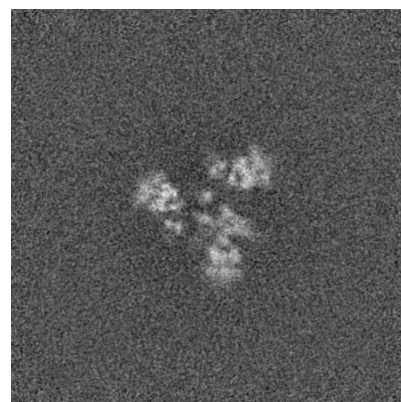
6.2.2 Raw map



X Index: 200



Y Index: 200

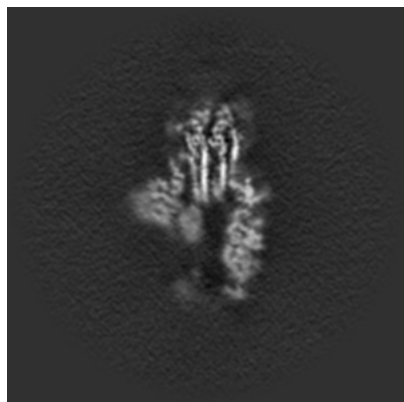


Z Index: 200

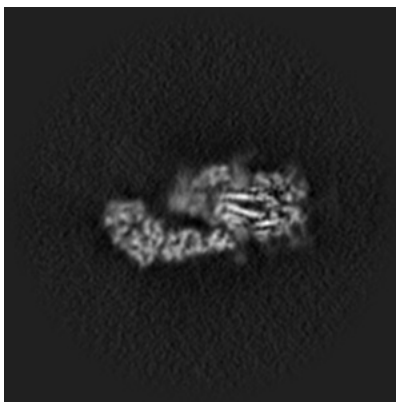
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

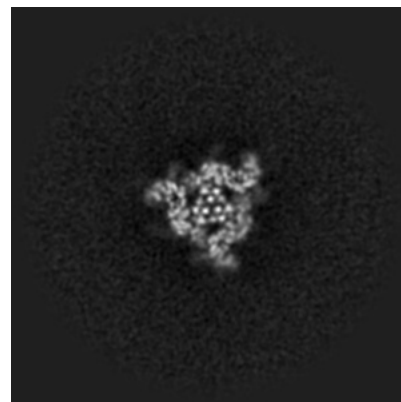
6.3.1 Primary map



X Index: 207



Y Index: 186

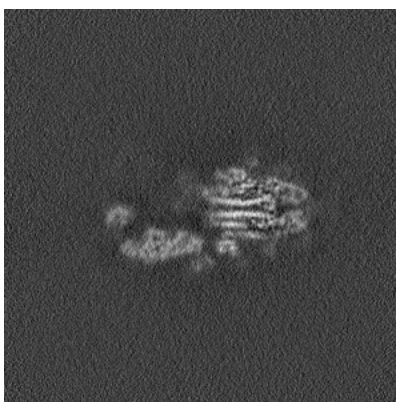


Z Index: 222

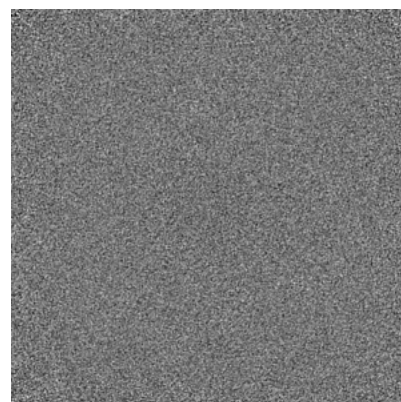
6.3.2 Raw map



X Index: 207



Y Index: 196



Z Index: 0

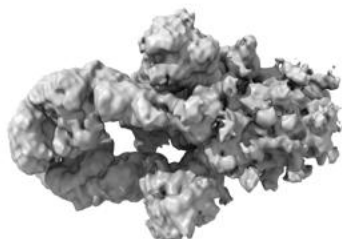
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

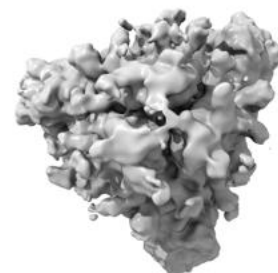
6.4.1 Primary map



X



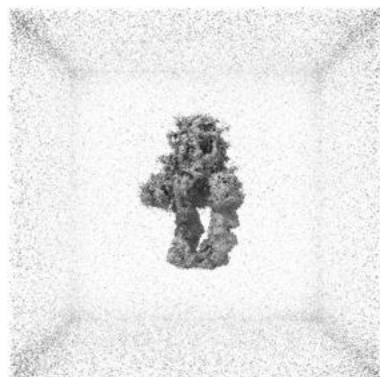
Y



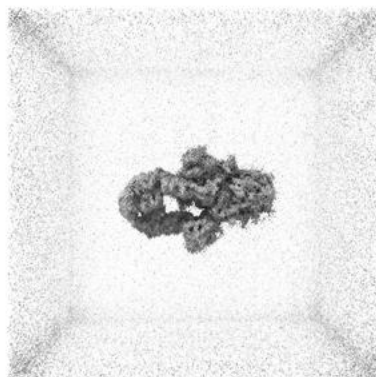
Z

The images above show the 3D surface view of the map at the recommended contour level 0.203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

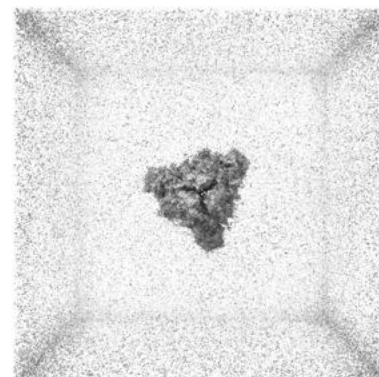
6.4.2 Raw map



X



Y



Z

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

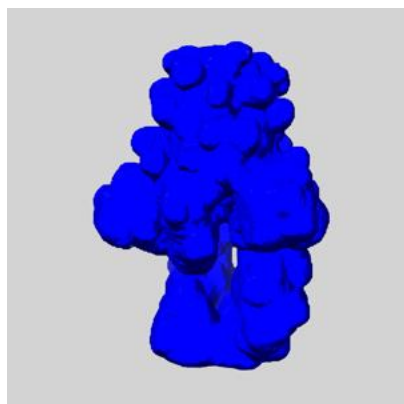
6.5 Mask visualisation [i](#)

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

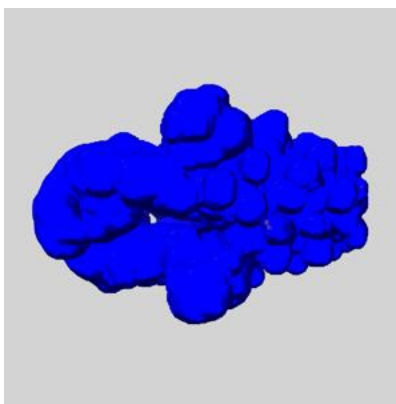
A mask typically either:

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

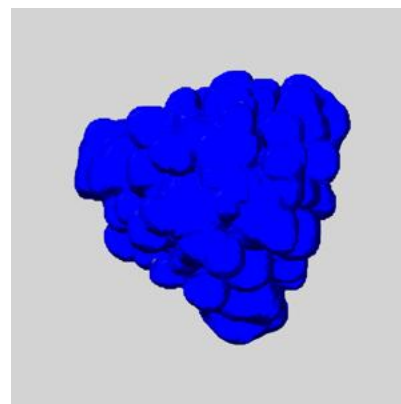
6.5.1 emd_22925_msk_1.map [i](#)



X



Y

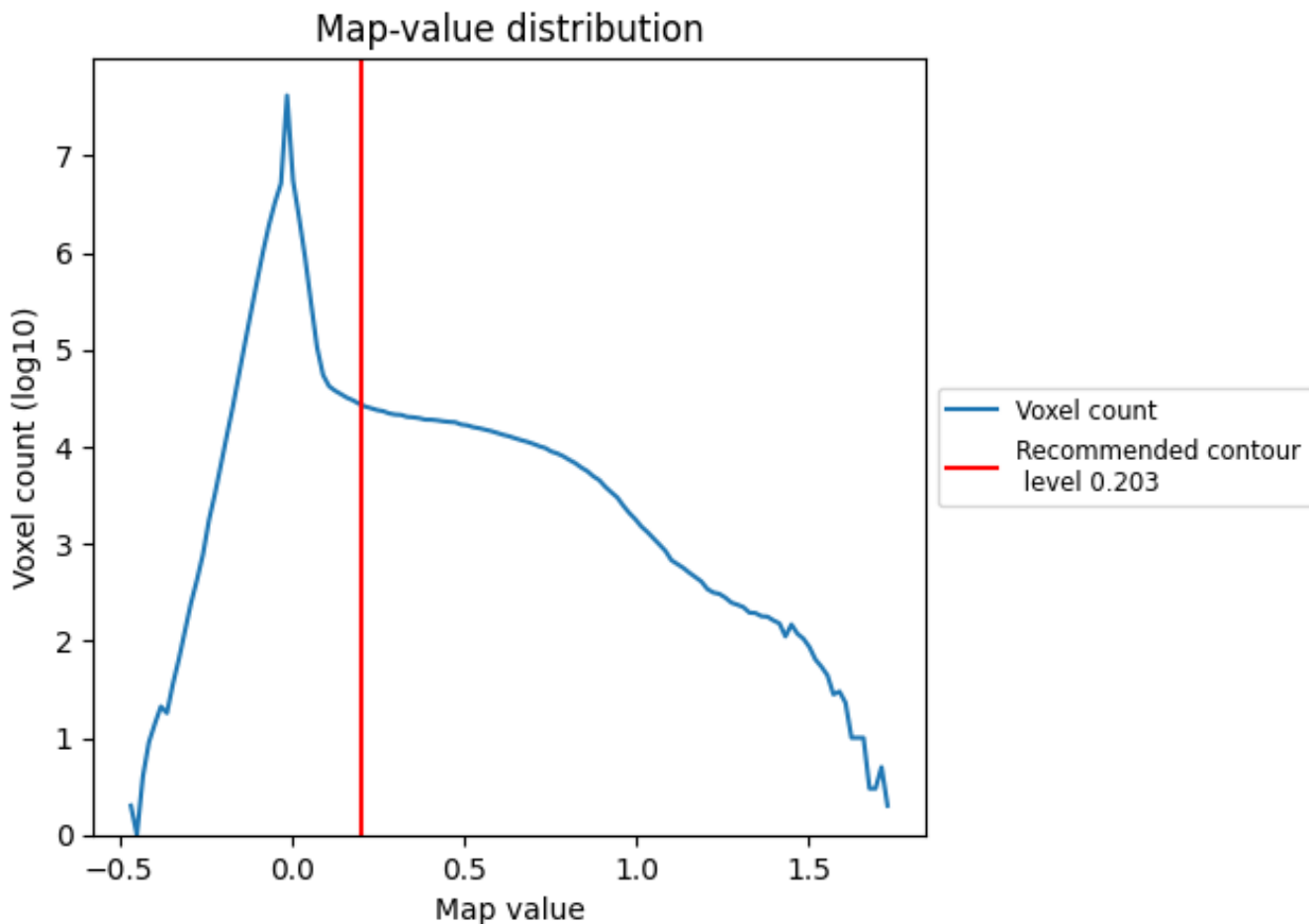


Z

7 Map analysis [i](#)

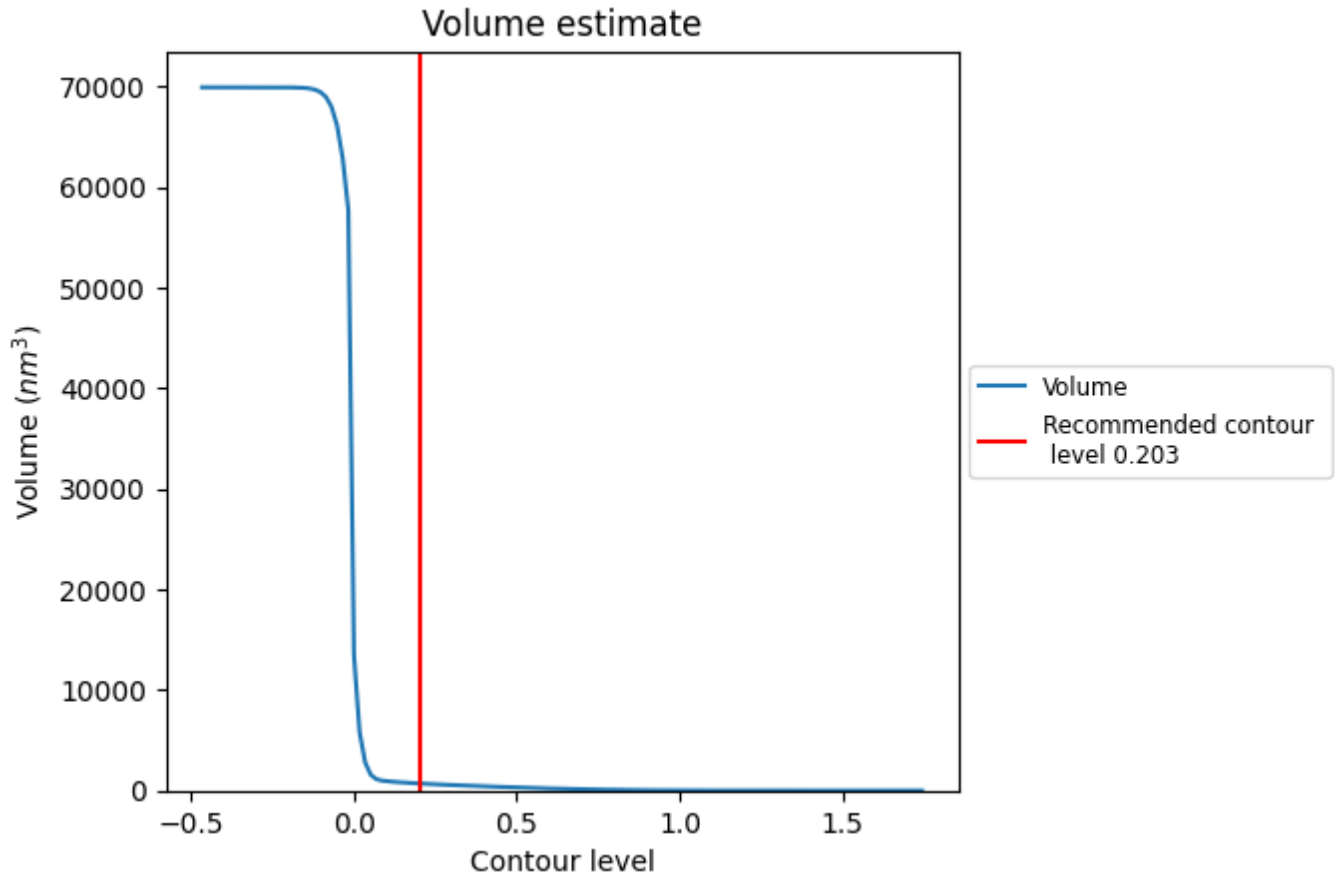
This section contains the results of statistical analysis of the map.

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.

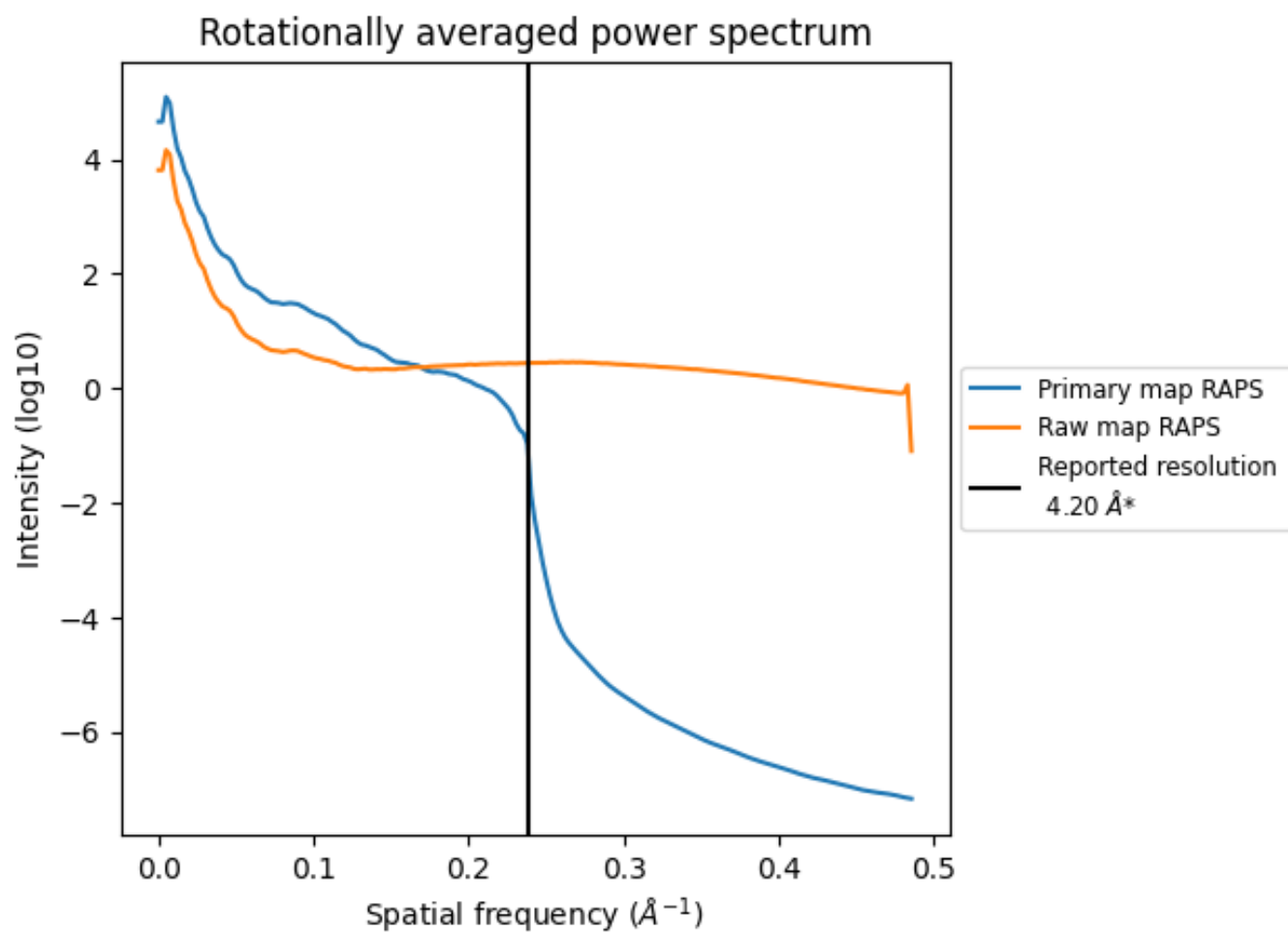
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm³; this corresponds to an approximate mass of 632 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

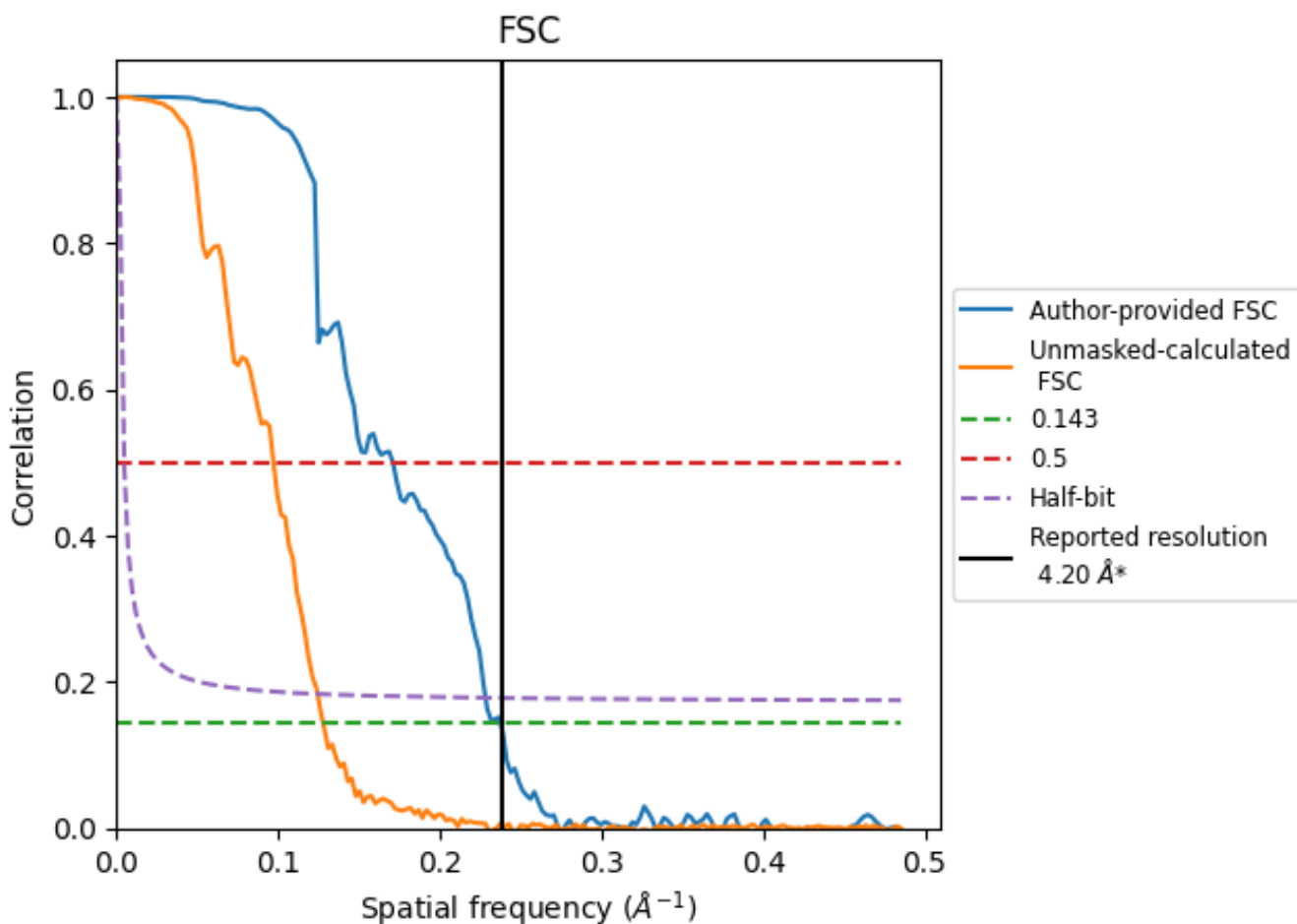


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

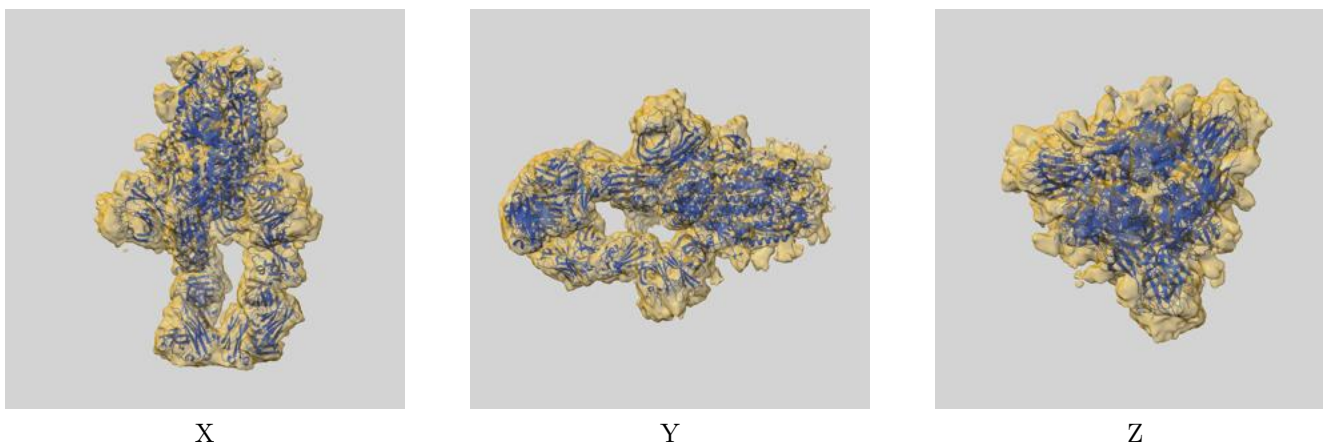
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.21	5.85	4.38
Unmasked-calculated*	7.82	10.30	8.04

*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 7.82 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

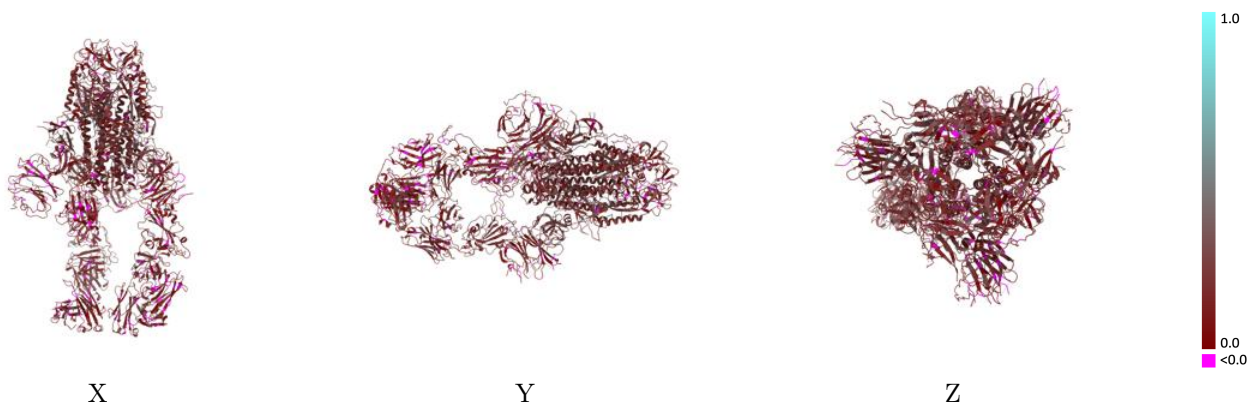
This section contains information regarding the fit between EMDB map EMD-22925 and PDB model 7KMK. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



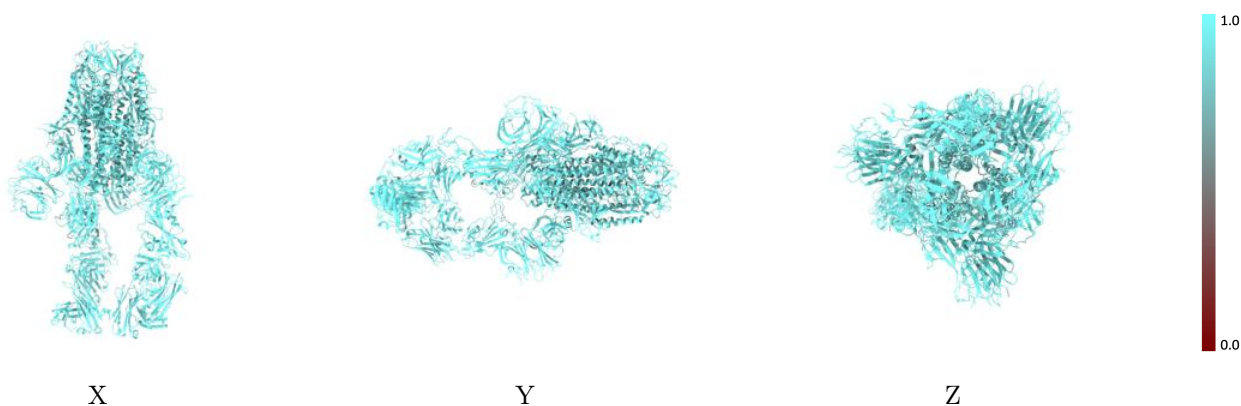
The images above show the 3D surface view of the map at the recommended contour level 0.203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



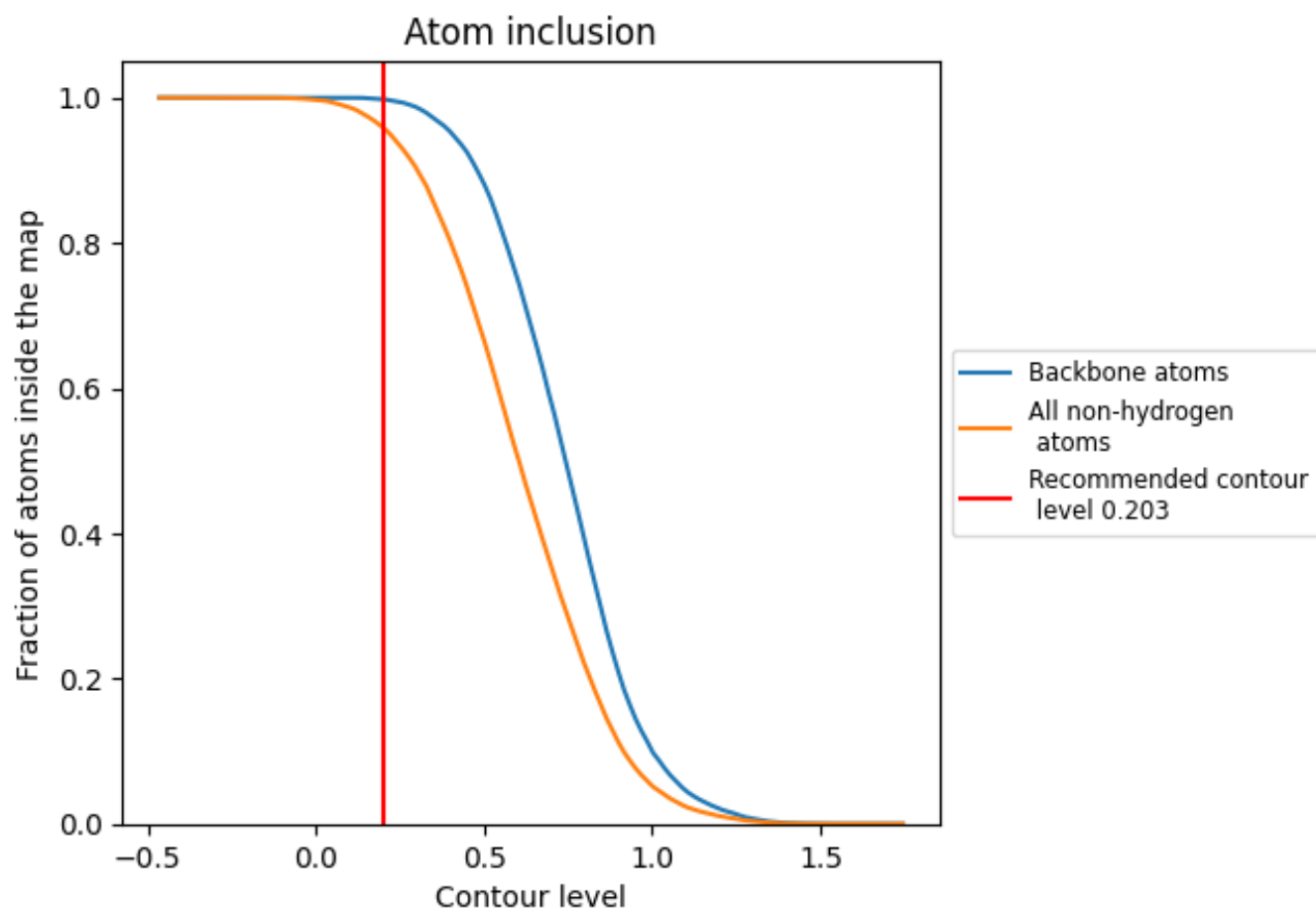
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.203).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 96% 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 (0.203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9571	 0.1910
A	 0.9558	 0.2070
B	 0.9552	 0.1950
C	 0.9413	 0.1860
D	 1.0000	 0.3020
E	 1.0000	 0.3860
F	 1.0000	 0.3900
G	 0.9286	 0.2960
H	 0.9757	 0.1530
I	 0.9770	 0.1580
J	 0.9643	 0.3610
K	 0.8929	 0.2060
L	 0.9864	 0.1840
M	 0.9833	 0.1650
N	 0.9643	 0.1540
O	 0.9286	 0.3140
P	 1.0000	 0.3710

