



# wwPDB EM Validation Summary Report ⓘ

Nov 23, 2022 – 03:29 PM JST

PDB ID : 7V7T  
EMDB ID : EMD-31781  
Title : Cryo-EM structure of SARS-CoV-2 S-Delta variant (B.1.617.2), two RBD-up conformation 1  
Authors : Yang, T.J.; Yu, P.Y.; Chang, Y.C.; Hsu, S.T.D.  
Deposited on : 2021-08-21  
Resolution : 3.00 Å(reported)

This is a wwPDB EM Validation Summary 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.dev43  
Mogul : **FAILED**  
MolProbity : 4.02b-467  
buster-report : **FAILED**  
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) : 2.31.3

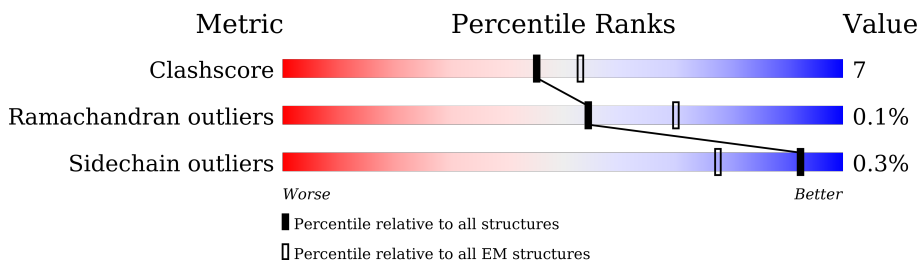
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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  $\geq 3$ , 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	A	1281	
1	B	1281	
1	C	1281	
2	D	2	
2	E	2	
2	F	2	
2	G	2	
2	H	2	

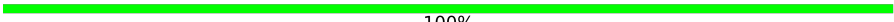


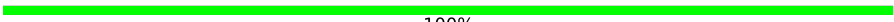
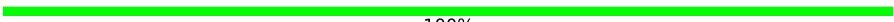
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Mol	Chain	Length	Quality of chain
2	I	2	100%
2	J	2	50% 50%
2	K	2	50% 50%
2	L	2	50% 50%
2	M	2	100%
2	N	2	100%
2	O	2	100%
2	P	2	100%
2	Q	2	50% 50%
2	R	2	100%
2	S	2	100%
2	T	2	100%
2	U	2	100%
2	V	2	100%
2	W	2	100%
2	X	2	100%
2	Y	2	100%
2	Z	2	100%
2	a	2	100%
2	b	2	50% 100%
2	c	2	50% 100%
2	d	2	50% 100%
2	e	2	100%
2	f	2	100%
2	g	2	100%

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Mol	Chain	Length	Quality of chain
2	h	2	 100%
2	i	2	 100%
2	j	2	 100%
2	k	2	 100%
2	l	2	 100%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 25290 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	1027	8016	5113	1340	1527	36	0	0
1	B	1033	8077	5156	1351	1534	36	0	0
1	C	1029	8035	5127	1342	1530	36	0	0

There are 270 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ARG	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	156	GLY	GLU	variant	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	450	ARG	LEU	variant	UNP P0DTC2
A	476	LYS	THR	variant	UNP P0DTC2
A	612	GLY	ASP	variant	UNP P0DTC2
A	679	ARG	PRO	engineered mutation	UNP P0DTC2
A	680	GLY	ARG	engineered mutation	UNP P0DTC2
A	681	SER	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	948	ASN	ASP	variant	UNP P0DTC2
A	984	PRO	LYS	engineered mutation	UNP P0DTC2
A	985	PRO	VAL	engineered mutation	UNP P0DTC2
A	1207	GLU	-	expression tag	UNP P0DTC2
A	1208	PHE	-	expression tag	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	GLY	-	expression tag	UNP P0DTC2
A	1213	TYR	-	expression tag	UNP P0DTC2
A	1214	ILE	-	expression tag	UNP P0DTC2
A	1215	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ALA	-	expression tag	UNP P0DTC2
A	1218	PRO	-	expression tag	UNP P0DTC2
A	1219	ARG	-	expression tag	UNP P0DTC2
A	1220	ASP	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	GLN	-	expression tag	UNP P0DTC2
A	1223	ALA	-	expression tag	UNP P0DTC2
A	1224	TYR	-	expression tag	UNP P0DTC2
A	1225	VAL	-	expression tag	UNP P0DTC2
A	1226	ARG	-	expression tag	UNP P0DTC2
A	1227	LYS	-	expression tag	UNP P0DTC2
A	1228	ASP	-	expression tag	UNP P0DTC2
A	1229	GLY	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	TRP	-	expression tag	UNP P0DTC2
A	1232	VAL	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	LEU	-	expression tag	UNP P0DTC2
A	1235	SER	-	expression tag	UNP P0DTC2
A	1236	THR	-	expression tag	UNP P0DTC2
A	1237	PHE	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	LYS	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	GLN	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	ASN	-	expression tag	UNP P0DTC2
A	1244	SER	-	expression tag	UNP P0DTC2
A	1245	ALA	-	expression tag	UNP P0DTC2
A	1246	ASP	-	expression tag	UNP P0DTC2
A	1247	ILE	-	expression tag	UNP P0DTC2
A	1248	GLN	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	GLY	-	expression tag	UNP P0DTC2
A	1252	ARG	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	LEU	-	expression tag	UNP P0DTC2
A	1255	GLU	-	expression tag	UNP P0DTC2
A	1256	SER	-	expression tag	UNP P0DTC2
A	1257	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	PRO	-	expression tag	UNP P0DTC2
A	1260	PHE	-	expression tag	UNP P0DTC2
A	1261	GLU	-	expression tag	UNP P0DTC2
A	1262	GLN	-	expression tag	UNP P0DTC2
A	1263	LYS	-	expression tag	UNP P0DTC2
A	1264	LEU	-	expression tag	UNP P0DTC2
A	1265	ILE	-	expression tag	UNP P0DTC2
A	1266	SER	-	expression tag	UNP P0DTC2
A	1267	GLU	-	expression tag	UNP P0DTC2
A	1268	GLU	-	expression tag	UNP P0DTC2
A	1269	ASP	-	expression tag	UNP P0DTC2
A	1270	LEU	-	expression tag	UNP P0DTC2
A	1271	ASN	-	expression tag	UNP P0DTC2
A	1272	MET	-	expression tag	UNP P0DTC2
A	1273	HIS	-	expression tag	UNP P0DTC2
A	1274	THR	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2
A	1278	HIS	-	expression tag	UNP P0DTC2
A	1279	HIS	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
B	19	ARG	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	156	GLY	GLU	variant	UNP P0DTC2
B	?	-	PHE	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	450	ARG	LEU	variant	UNP P0DTC2
B	476	LYS	THR	variant	UNP P0DTC2
B	612	GLY	ASP	variant	UNP P0DTC2
B	679	ARG	PRO	engineered mutation	UNP P0DTC2
B	680	GLY	ARG	engineered mutation	UNP P0DTC2
B	681	SER	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	948	ASN	ASP	variant	UNP P0DTC2
B	984	PRO	LYS	engineered mutation	UNP P0DTC2
B	985	PRO	VAL	engineered mutation	UNP P0DTC2
B	1207	GLU	-	expression tag	UNP P0DTC2
B	1208	PHE	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	TYR	-	expression tag	UNP P0DTC2
B	1214	ILE	-	expression tag	UNP P0DTC2
B	1215	PRO	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ALA	-	expression tag	UNP P0DTC2
B	1218	PRO	-	expression tag	UNP P0DTC2
B	1219	ARG	-	expression tag	UNP P0DTC2
B	1220	ASP	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	GLN	-	expression tag	UNP P0DTC2
B	1223	ALA	-	expression tag	UNP P0DTC2
B	1224	TYR	-	expression tag	UNP P0DTC2
B	1225	VAL	-	expression tag	UNP P0DTC2
B	1226	ARG	-	expression tag	UNP P0DTC2
B	1227	LYS	-	expression tag	UNP P0DTC2
B	1228	ASP	-	expression tag	UNP P0DTC2
B	1229	GLY	-	expression tag	UNP P0DTC2
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	TRP	-	expression tag	UNP P0DTC2
B	1232	VAL	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	SER	-	expression tag	UNP P0DTC2
B	1236	THR	-	expression tag	UNP P0DTC2
B	1237	PHE	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	LYS	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	GLN	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	ASN	-	expression tag	UNP P0DTC2
B	1244	SER	-	expression tag	UNP P0DTC2
B	1245	ALA	-	expression tag	UNP P0DTC2
B	1246	ASP	-	expression tag	UNP P0DTC2
B	1247	ILE	-	expression tag	UNP P0DTC2
B	1248	GLN	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1252	ARG	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	LEU	-	expression tag	UNP P0DTC2
B	1255	GLU	-	expression tag	UNP P0DTC2
B	1256	SER	-	expression tag	UNP P0DTC2
B	1257	ARG	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	PRO	-	expression tag	UNP P0DTC2
B	1260	PHE	-	expression tag	UNP P0DTC2
B	1261	GLU	-	expression tag	UNP P0DTC2
B	1262	GLN	-	expression tag	UNP P0DTC2
B	1263	LYS	-	expression tag	UNP P0DTC2
B	1264	LEU	-	expression tag	UNP P0DTC2
B	1265	ILE	-	expression tag	UNP P0DTC2
B	1266	SER	-	expression tag	UNP P0DTC2
B	1267	GLU	-	expression tag	UNP P0DTC2
B	1268	GLU	-	expression tag	UNP P0DTC2
B	1269	ASP	-	expression tag	UNP P0DTC2
B	1270	LEU	-	expression tag	UNP P0DTC2
B	1271	ASN	-	expression tag	UNP P0DTC2
B	1272	MET	-	expression tag	UNP P0DTC2
B	1273	HIS	-	expression tag	UNP P0DTC2
B	1274	THR	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	HIS	-	expression tag	UNP P0DTC2
B	1277	HIS	-	expression tag	UNP P0DTC2
B	1278	HIS	-	expression tag	UNP P0DTC2
B	1279	HIS	-	expression tag	UNP P0DTC2
B	1280	HIS	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
C	19	ARG	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	156	GLY	GLU	variant	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	450	ARG	LEU	variant	UNP P0DTC2
C	476	LYS	THR	variant	UNP P0DTC2
C	612	GLY	ASP	variant	UNP P0DTC2
C	679	ARG	PRO	engineered mutation	UNP P0DTC2
C	680	GLY	ARG	engineered mutation	UNP P0DTC2
C	681	SER	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	948	ASN	ASP	variant	UNP P0DTC2
C	984	PRO	LYS	engineered mutation	UNP P0DTC2
C	985	PRO	VAL	engineered mutation	UNP P0DTC2
C	1207	GLU	-	expression tag	UNP P0DTC2
C	1208	PHE	-	expression tag	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	GLY	-	expression tag	UNP P0DTC2
C	1213	TYR	-	expression tag	UNP P0DTC2
C	1214	ILE	-	expression tag	UNP P0DTC2
C	1215	PRO	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ALA	-	expression tag	UNP P0DTC2
C	1218	PRO	-	expression tag	UNP P0DTC2
C	1219	ARG	-	expression tag	UNP P0DTC2
C	1220	ASP	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	GLN	-	expression tag	UNP P0DTC2
C	1223	ALA	-	expression tag	UNP P0DTC2
C	1224	TYR	-	expression tag	UNP P0DTC2
C	1225	VAL	-	expression tag	UNP P0DTC2
C	1226	ARG	-	expression tag	UNP P0DTC2
C	1227	LYS	-	expression tag	UNP P0DTC2
C	1228	ASP	-	expression tag	UNP P0DTC2
C	1229	GLY	-	expression tag	UNP P0DTC2
C	1230	GLU	-	expression tag	UNP P0DTC2
C	1231	TRP	-	expression tag	UNP P0DTC2
C	1232	VAL	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	SER	-	expression tag	UNP P0DTC2
C	1236	THR	-	expression tag	UNP P0DTC2
C	1237	PHE	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	LYS	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	GLN	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	ASN	-	expression tag	UNP P0DTC2
C	1244	SER	-	expression tag	UNP P0DTC2
C	1245	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1246	ASP	-	expression tag	UNP P0DTC2
C	1247	ILE	-	expression tag	UNP P0DTC2
C	1248	GLN	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	GLY	-	expression tag	UNP P0DTC2
C	1252	ARG	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	LEU	-	expression tag	UNP P0DTC2
C	1255	GLU	-	expression tag	UNP P0DTC2
C	1256	SER	-	expression tag	UNP P0DTC2
C	1257	ARG	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	PRO	-	expression tag	UNP P0DTC2
C	1260	PHE	-	expression tag	UNP P0DTC2
C	1261	GLU	-	expression tag	UNP P0DTC2
C	1262	GLN	-	expression tag	UNP P0DTC2
C	1263	LYS	-	expression tag	UNP P0DTC2
C	1264	LEU	-	expression tag	UNP P0DTC2
C	1265	ILE	-	expression tag	UNP P0DTC2
C	1266	SER	-	expression tag	UNP P0DTC2
C	1267	GLU	-	expression tag	UNP P0DTC2
C	1268	GLU	-	expression tag	UNP P0DTC2
C	1269	ASP	-	expression tag	UNP P0DTC2
C	1270	LEU	-	expression tag	UNP P0DTC2
C	1271	ASN	-	expression tag	UNP P0DTC2
C	1272	MET	-	expression tag	UNP P0DTC2
C	1273	HIS	-	expression tag	UNP P0DTC2
C	1274	THR	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	HIS	-	expression tag	UNP P0DTC2
C	1277	HIS	-	expression tag	UNP P0DTC2
C	1278	HIS	-	expression tag	UNP P0DTC2
C	1279	HIS	-	expression tag	UNP P0DTC2
C	1280	HIS	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		

*Continued on next page...*

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	W	2	28	16	2	10	0	0
2	X	2	28	16	2	10	0	0
2	Y	2	28	16	2	10	0	0
2	Z	2	28	16	2	10	0	0
2	a	2	28	16	2	10	0	0
2	b	2	28	16	2	10	0	0
2	c	2	28	16	2	10	0	0
2	d	2	28	16	2	10	0	0
2	e	2	28	16	2	10	0	0
2	f	2	28	16	2	10	0	0
2	g	2	28	16	2	10	0	0
2	h	2	28	16	2	10	0	0
2	i	2	28	16	2	10	0	0
2	j	2	28	16	2	10	0	0
2	k	2	28	16	2	10	0	0
2	l	2	28	16	2	10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

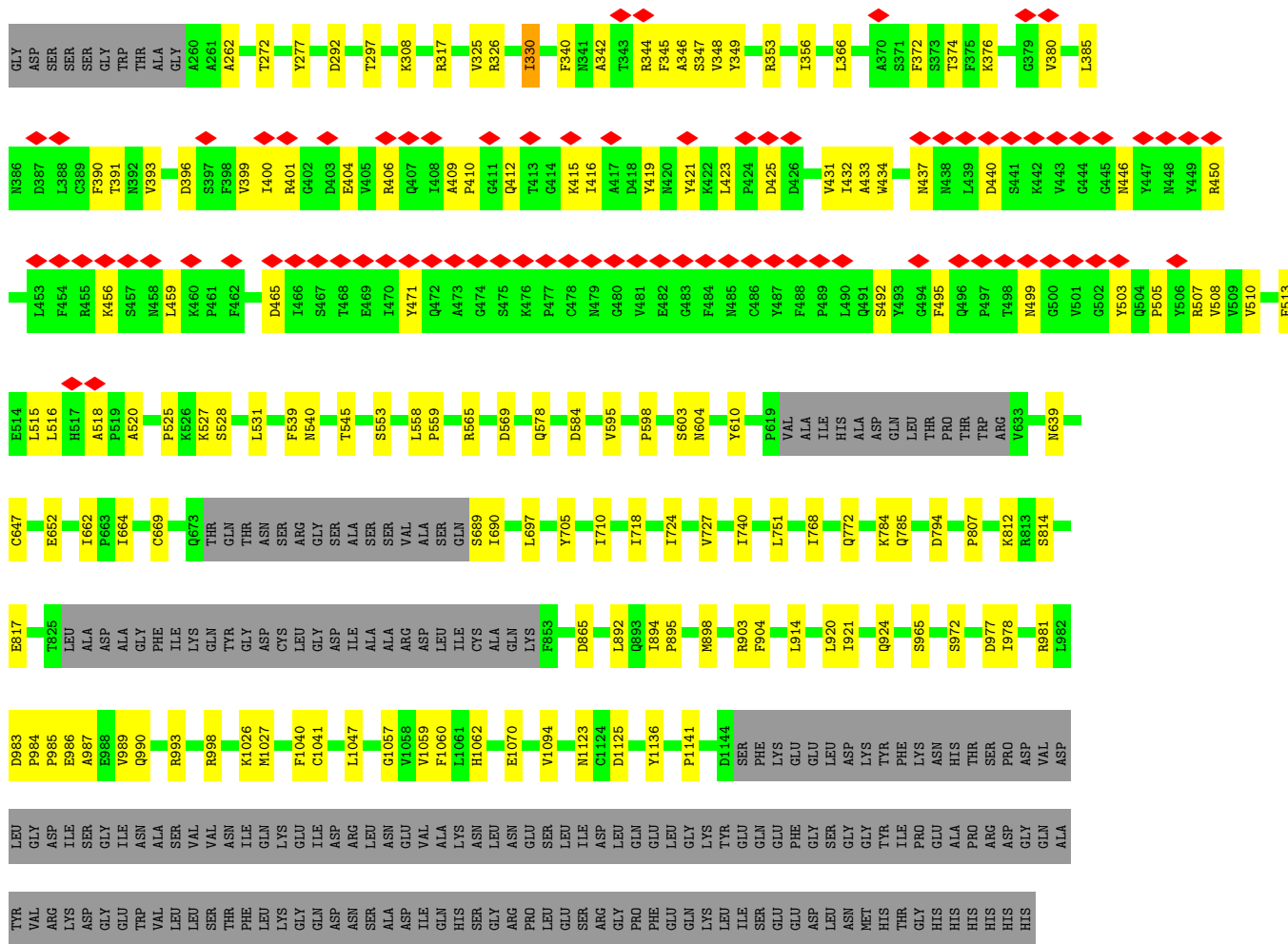


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	56	32	4	20	0
3	A	1	56	32	4	20	0
3	A	1	56	32	4	20	0
3	A	1	56	32	4	20	0
3	B	1	70	40	5	25	0
3	B	1	70	40	5	25	0
3	B	1	70	40	5	25	0
3	B	1	70	40	5	25	0
3	B	1	70	40	5	25	0
3	C	1	56	32	4	20	0
3	C	1	56	32	4	20	0
3	C	1	56	32	4	20	0
3	C	1	56	32	4	20	0









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

Chain D: 100%



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

Chain E: 100%



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

Chain F: 100%



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

Chain G:  50% 50%



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

Chain H:  100%



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

Chain I:  100%



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

Chain J:  50% 50%



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

Chain K:  50% 50%



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

Chain L:  50% 50%



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

Chain M:  100%



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

Chain N:  100%



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

Chain O:  100%



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

Chain P:  100%



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

Chain Q:  50% 50%



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

Chain R:  100%



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

Chain S:  100%

WAG1  
WAG2

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

Chain T:  100%

WAG1  
WAG2

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

Chain U:  100%

WAG1  
WAG2

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

Chain V:  100%

WAG1  
WAG2

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

Chain W:  100%

WAG1  
WAG2

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

Chain X:  100%

WAG1  
WAG2

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

Chain Y:  100%

WAG1  
WAG2

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

Chain Z:  100%



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

Chain a:  100%



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

Chain b:  50%  
 100%



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

Chain c:  50%  
 100%



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

Chain d:  50%  
 100%



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

Chain e:  100%



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

Chain f:  100%

MAG1  
MAG2

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

Chain g:  100%

MAG1  
MAG2

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

Chain h:  100%

MAG1  
MAG2

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

Chain i:  100%

MAG1  
MAG2

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

Chain j:  100%

MAG1  
MAG2

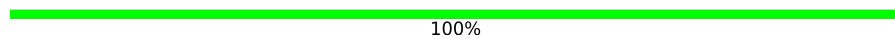
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  100%

MAG1  
MAG2

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

Chain 1:



100%

3AK2  
3AK2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	119914	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 ( $e^-/\text{\AA}^2$ )	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.955	Depositor
Minimum map value	-1.172	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/8197	0.48	0/11155
1	B	0.26	0/8261	0.48	0/11242
1	C	0.26	0/8217	0.48	0/11183
All	All	0.26	0/24675	0.48	0/33580

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8016	0	7819	117	0
1	B	8077	0	7882	101	0
1	C	8035	0	7837	120	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	1	0
2	L	28	0	25	1	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	1	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	W	28	0	25	0	0
2	X	28	0	25	0	0
2	Y	28	0	25	0	0
2	Z	28	0	25	0	0
2	a	28	0	25	0	0
2	b	28	0	25	0	0
2	c	28	0	25	0	0
2	d	28	0	25	0	0
2	e	28	0	25	0	0
2	f	28	0	25	0	0
2	g	28	0	25	0	0
2	h	28	0	25	0	0
2	i	28	0	25	0	0
2	j	28	0	25	0	0
2	k	28	0	25	0	0
2	l	28	0	25	0	0
3	A	56	0	52	0	0
3	B	70	0	65	0	0
3	C	56	0	52	1	0
All	All	25290	0	24582	332	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 7.

The worst 5 of 332 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:PHE:O	1:C:262:ALA:HA	1.69	0.92
1:A:65:PHE:O	1:A:262:ALA:HA	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:PHE:O	1:B:262:ALA:HA	1.82	0.78
1:B:126:VAL:HG13	1:B:172:PRO:HA	1.68	0.74
1:B:46:SER:HA	1:B:277:TYR:O	1.88	0.73

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	1011/1281 (79%)	969 (96%)	41 (4%)	1 (0%)	51 85
1	B	1017/1281 (79%)	971 (96%)	45 (4%)	1 (0%)	51 85
1	C	1013/1281 (79%)	972 (96%)	40 (4%)	1 (0%)	51 85
All	All	3041/3843 (79%)	2912 (96%)	126 (4%)	3 (0%)	54 85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	ILE
1	B	142	ASP
1	C	330	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	898/1113 (81%)	895 (100%)	3 (0%)	92	97
1	B	904/1113 (81%)	902 (100%)	2 (0%)	93	98
1	C	900/1113 (81%)	898 (100%)	2 (0%)	93	98
All	All	2702/3339 (81%)	2695 (100%)	7 (0%)	92	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	406	ARG
1	B	774	LYS
1	C	406	ARG
1	C	212	ARG
1	A	450	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

Mogul failed to run properly - this section is therefore empty.

## 5.5 Carbohydrates [i](#)

Mogul failed to run properly - this section is therefore empty.

## 5.6 Ligand geometry [i](#)

Mogul failed to run properly - this section is therefore empty.

## 5.7 Other polymers [i](#)

Mogul failed to run properly - this section is therefore empty.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

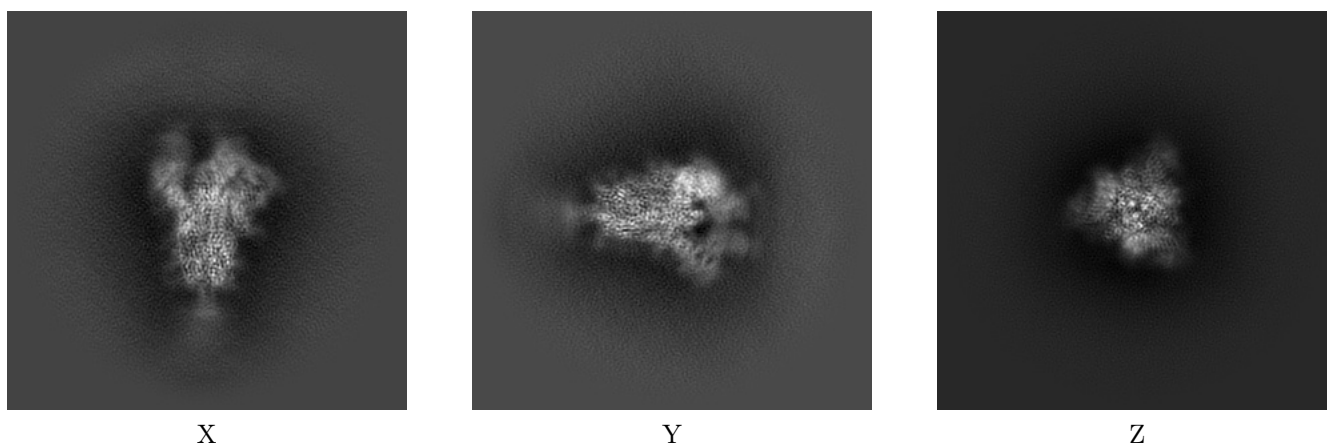
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31781. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

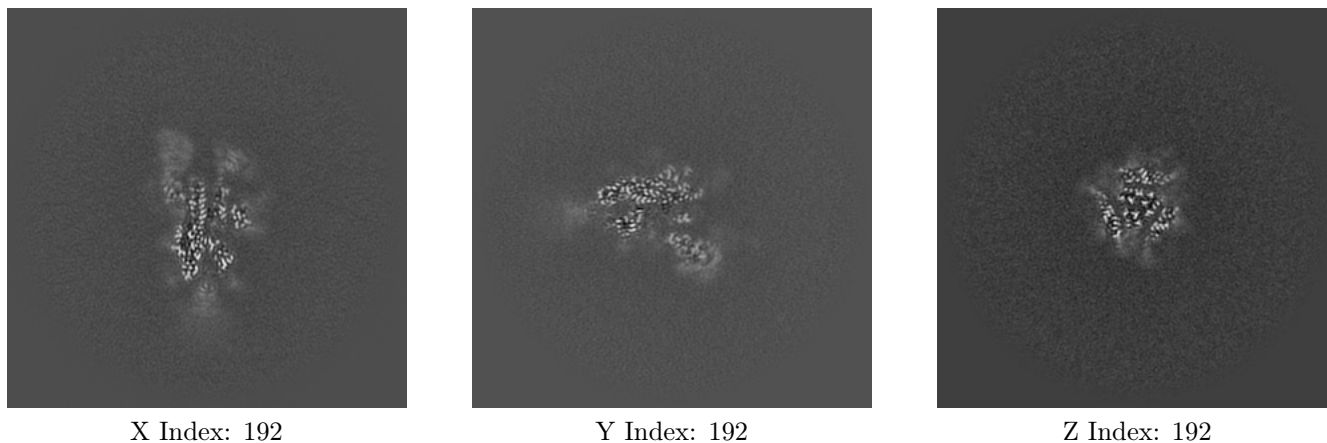
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

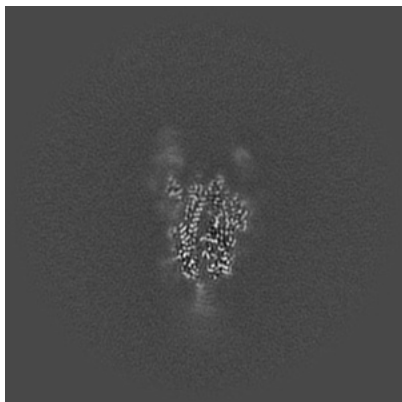
#### 6.2.1 Primary map



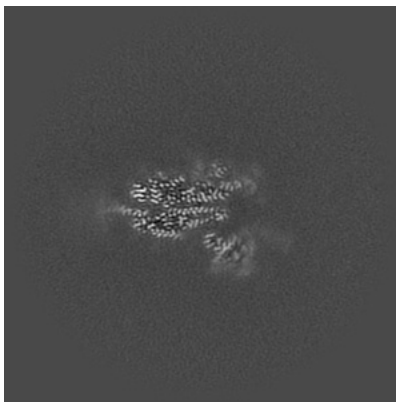
The images above show central slices of the map in three orthogonal directions.

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

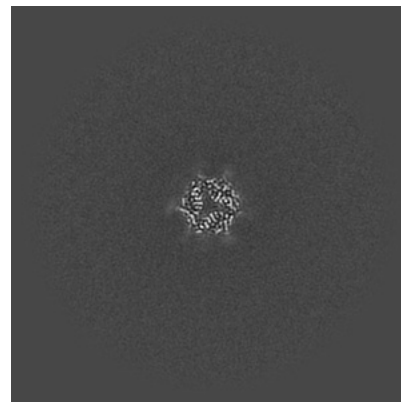
### 6.3.1 Primary map



X Index: 182



Y Index: 197



Z Index: 144

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

## 6.5 Mask visualisation

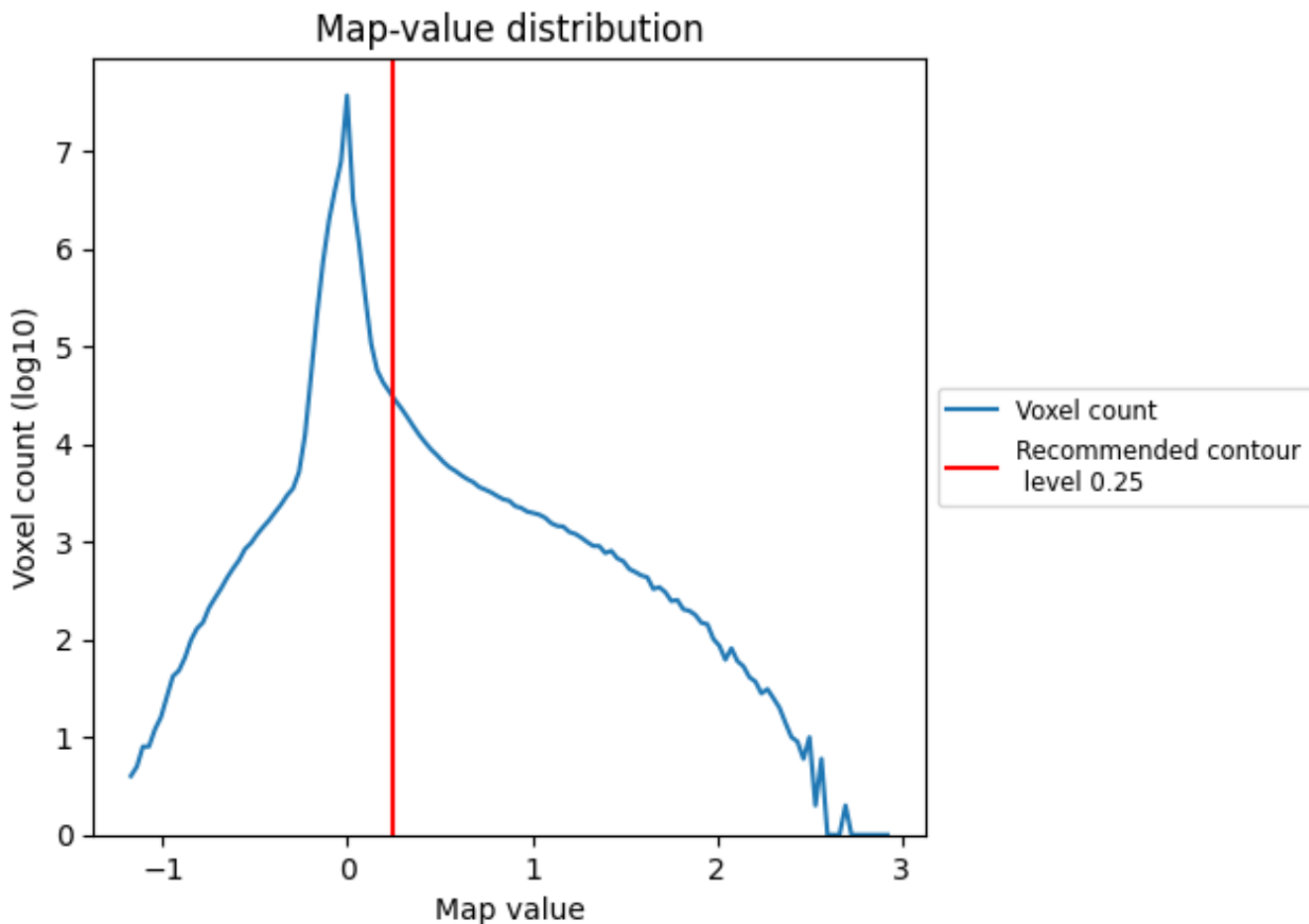
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

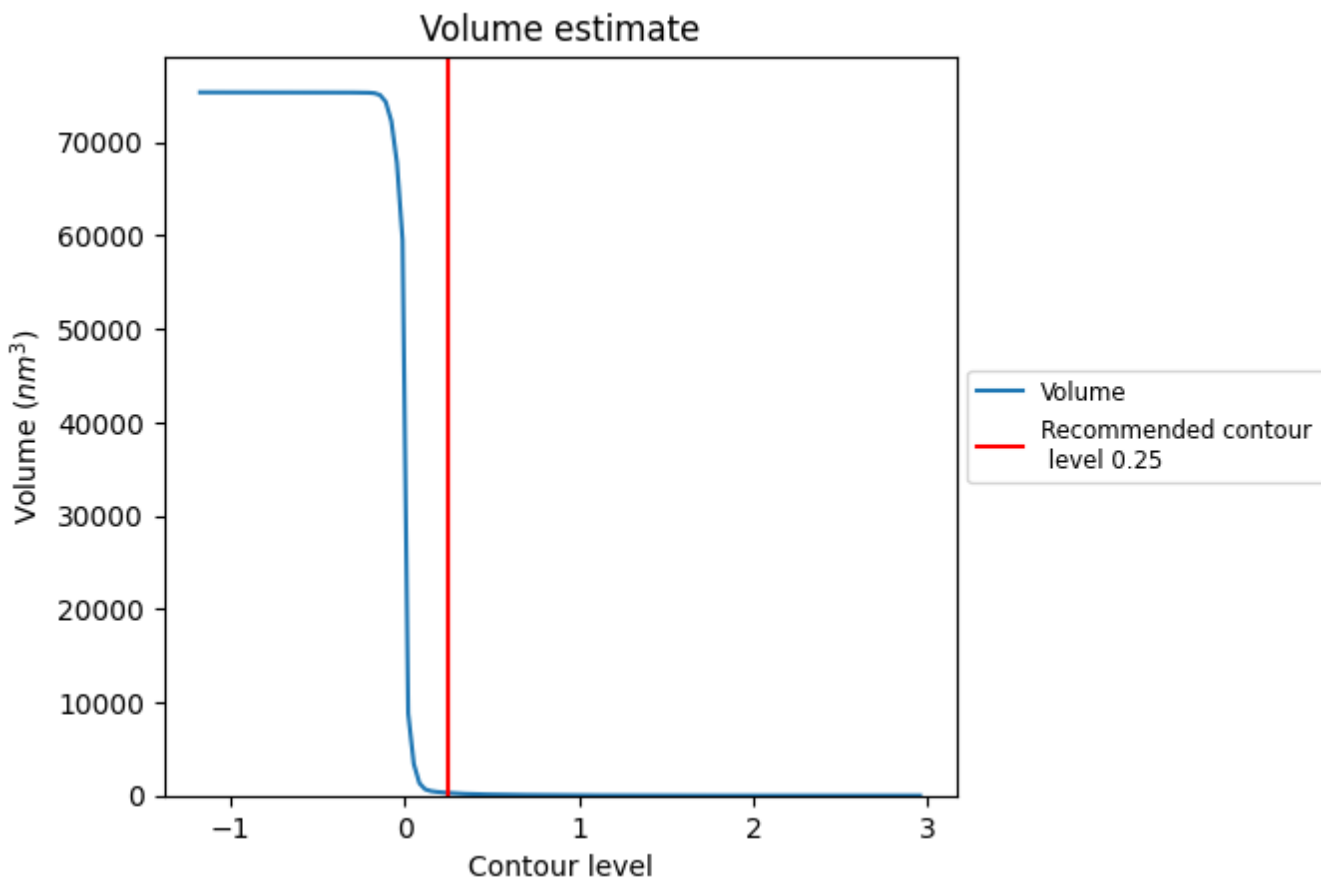
This section contains the results of statistical analysis of the map.

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



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

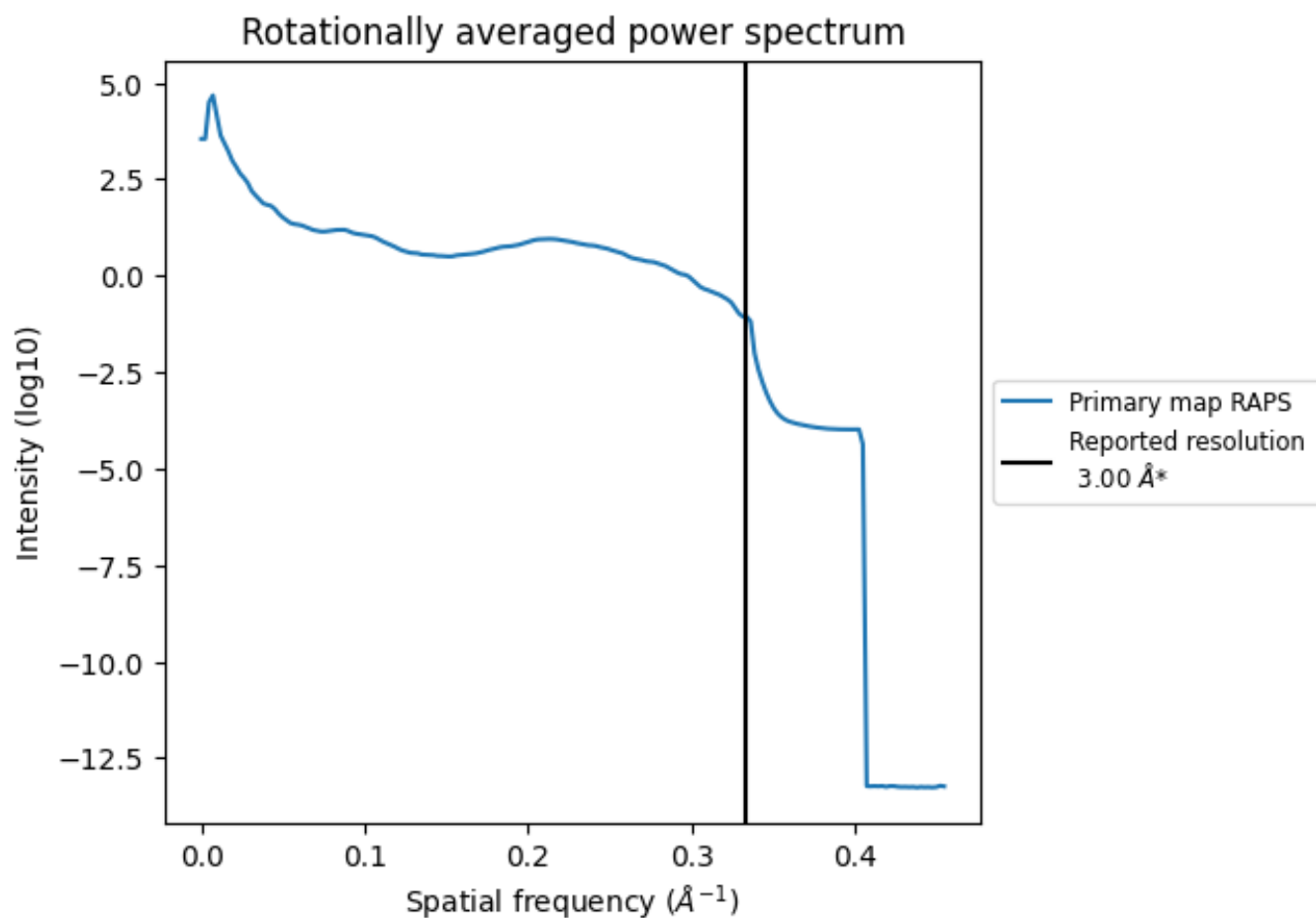
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 283 nm<sup>3</sup>; this corresponds to an approximate mass of 256 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  $0.333 \text{\AA}^{-1}$

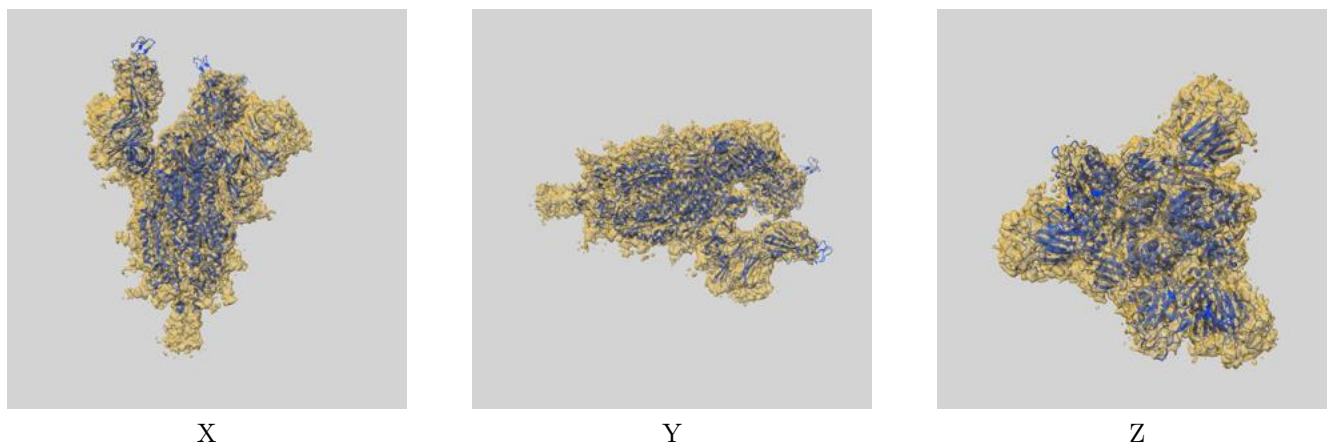
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

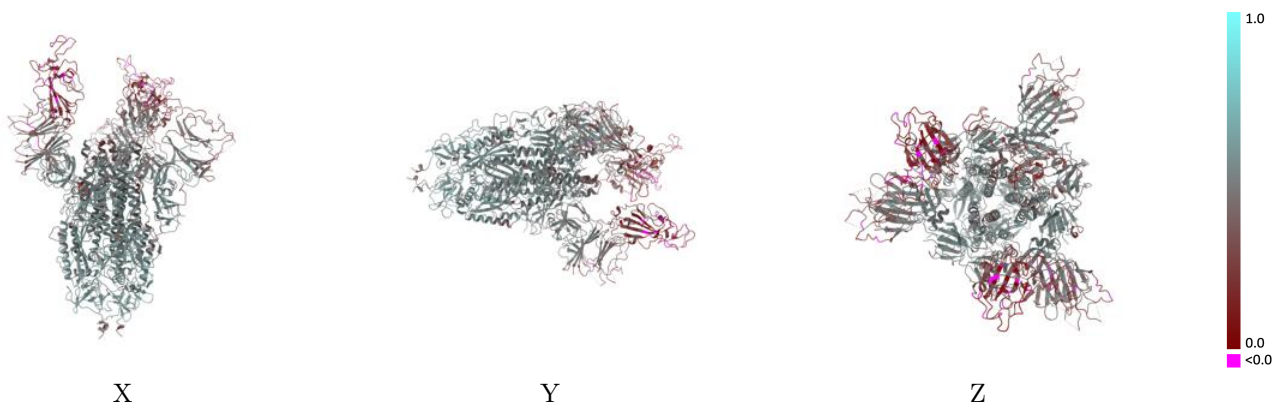
This section contains information regarding the fit between EMDB map EMD-31781 and PDB model 7V7T. Per-residue inclusion information can be found in section 3 on page 15.

### 9.1 Map-model overlay [i](#)



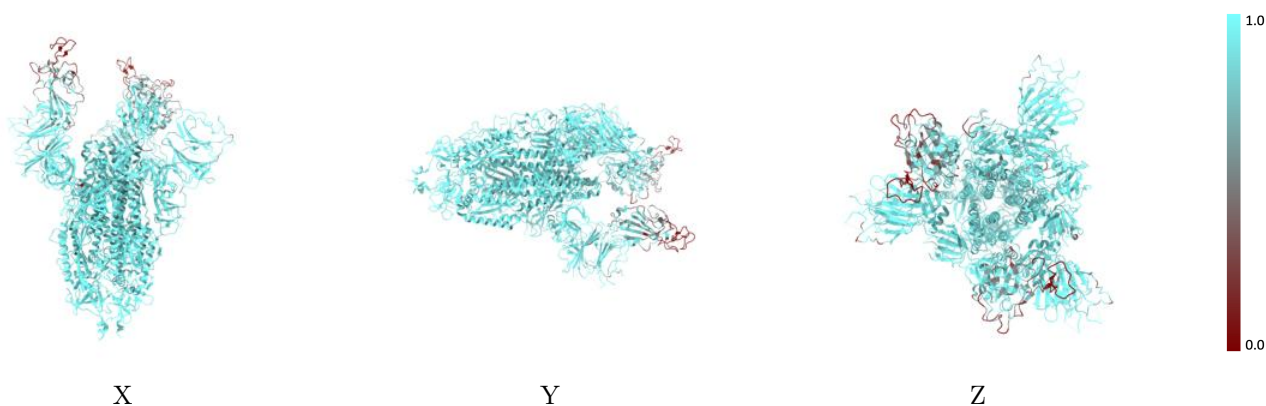
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



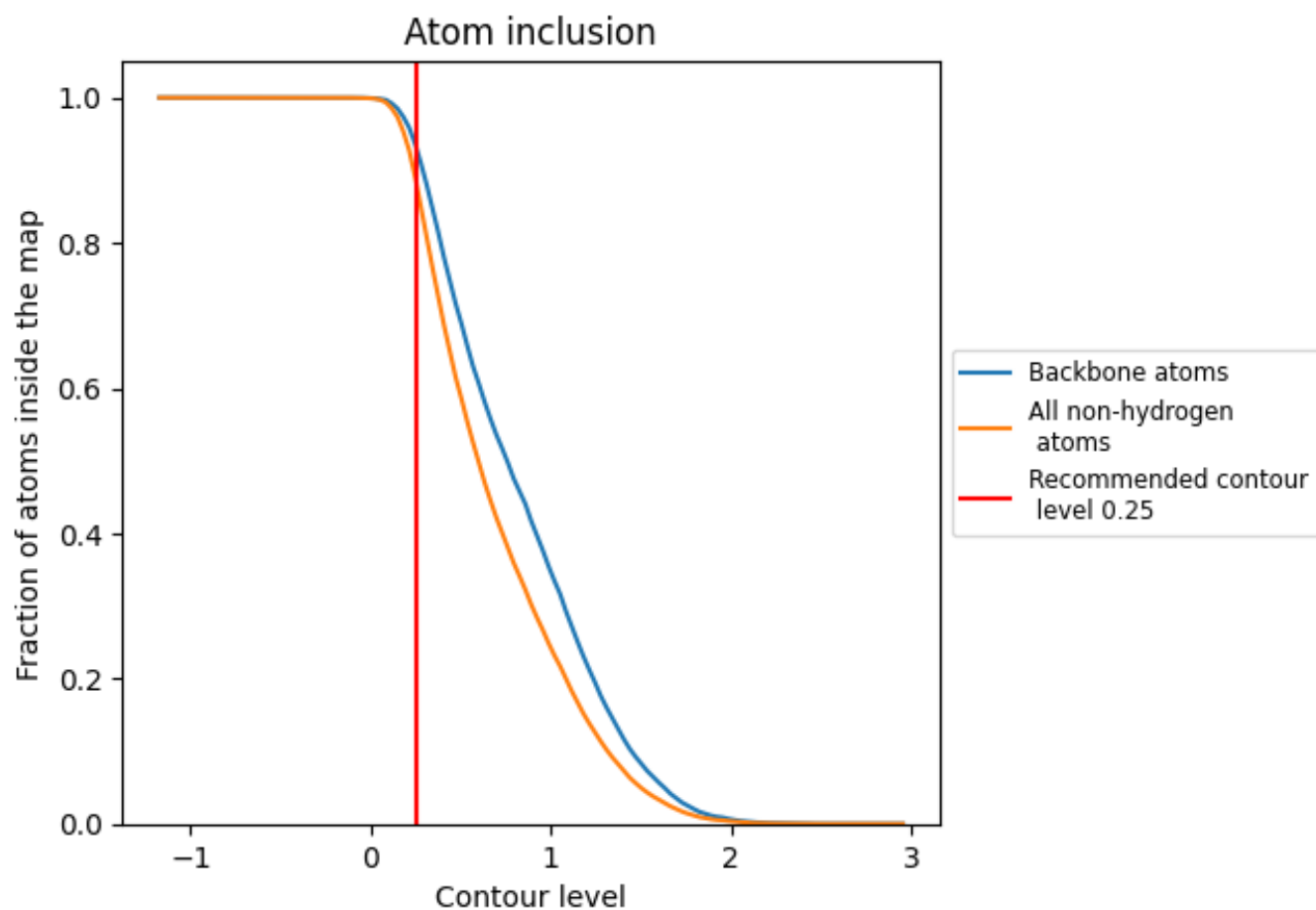
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.25) and Q-score for the entire model and for each chain.









Chain	Atom inclusion	Q-score
All	 0.8873	 0.4440
A	 0.8809	 0.4340
B	 0.9304	 0.4680
C	 0.8643	 0.4370
D	 0.7857	 0.3250
E	 0.5357	 0.3330
F	 0.0714	 0.0920
G	 0.7500	 0.3470
H	 0.9643	 0.3710
I	 0.8929	 0.4770
J	 0.7857	 0.3790
K	 1.0000	 0.5080
L	 0.9643	 0.4780
M	 0.7143	 0.3280
N	 0.8929	 0.4890
O	 0.8571	 0.4780
P	 0.8214	 0.4030
Q	 0.5357	 0.2210
R	 0.6429	 0.3610
S	 0.7857	 0.4030
T	 0.6071	 0.3940
U	 0.8214	 0.4820
V	 0.9286	 0.4710
W	 0.8929	 0.4540
X	 0.6786	 0.3220
Y	 0.9643	 0.4700
Z	 0.8929	 0.4210
a	 0.8929	 0.3260
b	 0.3929	 0.1340
c	 0.4643	 0.2990
d	 0.5714	 0.2350
e	 0.8929	 0.3840
f	 0.6786	 0.3920
g	 0.8929	 0.4550
h	 0.9643	 0.4990



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Chain	Atom inclusion	Q-score
i	 0.8929	 0.4570
j	 0.7857	 0.3600
k	 0.9643	 0.5230
l	 0.9286	 0.4920