



wwPDB EM Validation Summary Report ⓘ

Oct 22, 2024 – 02:51 AM JST

PDB ID : 7FJN
EMDB ID : EMD-31624
Title : Cryo-EM structure of South African (B.1.351) SARS-CoV-2 spike glycoprotein
in complex with two T6 Fab
Authors : Wang, X.; Zhang, L.; Zhang, S.; Liang, Q.
Deposited on : 2021-08-04
Resolution : 3.25 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

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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

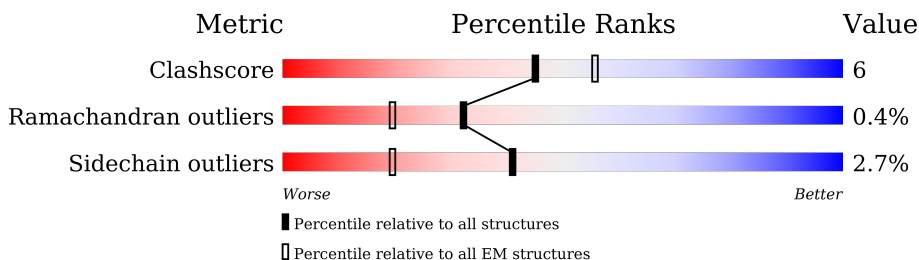
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1280	 6% 71% 6% 22%
1	B	1280	 5% 72% 5% 22%
1	C	1280	 5% 72% 5% 22%
2	H	117	 61% 59% 30% 9%
2	I	117	 86% 61% 30% 9%
3	J	113	 84% 65% 30% .
3	L	113	 52% 66% 29% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26824 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,Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	993	Total	C	N	O	S	0	0
			7687	4917	1277	1458	35		
1	B	993	Total	C	N	O	S	0	0
			7691	4921	1277	1458	35		
1	C	992	Total	C	N	O	S	0	0
			7678	4916	1279	1448	35		

There are 237 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	variant	UNP P0DTC2
A	80	ALA	ASP	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	305	THR	SER	engineered mutation	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	701	VAL	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP M1E1E4
A	1240	SER	-	expression tag	UNP M1E1E4
A	1241	LEU	-	expression tag	UNP M1E1E4
A	1242	GLU	-	expression tag	UNP M1E1E4
A	1243	VAL	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1244	LEU	-	expression tag	UNP M1E1E4
A	1245	PHE	-	expression tag	UNP M1E1E4
A	1246	GLN	-	expression tag	UNP M1E1E4
A	1247	GLY	-	expression tag	UNP M1E1E4
A	1248	PRO	-	expression tag	UNP M1E1E4
A	1249	GLY	-	expression tag	UNP M1E1E4
A	1250	HIS	-	expression tag	UNP M1E1E4
A	1251	HIS	-	expression tag	UNP M1E1E4
A	1252	HIS	-	expression tag	UNP M1E1E4
A	1253	HIS	-	expression tag	UNP M1E1E4
A	1254	HIS	-	expression tag	UNP M1E1E4
A	1255	HIS	-	expression tag	UNP M1E1E4
A	1256	HIS	-	expression tag	UNP M1E1E4
A	1257	HIS	-	expression tag	UNP M1E1E4
A	1258	SER	-	expression tag	UNP M1E1E4
A	1259	ALA	-	expression tag	UNP M1E1E4
A	1260	TRP	-	expression tag	UNP M1E1E4
A	1261	SER	-	expression tag	UNP M1E1E4
A	1262	HIS	-	expression tag	UNP M1E1E4
A	1263	PRO	-	expression tag	UNP M1E1E4
A	1264	GLN	-	expression tag	UNP M1E1E4
A	1265	PHE	-	expression tag	UNP M1E1E4
A	1266	GLU	-	expression tag	UNP M1E1E4
A	1267	LYS	-	expression tag	UNP M1E1E4
A	1268	GLY	-	expression tag	UNP M1E1E4
A	1269	GLY	-	expression tag	UNP M1E1E4
A	1270	GLY	-	expression tag	UNP M1E1E4
A	1271	SER	-	expression tag	UNP M1E1E4
A	1272	GLY	-	expression tag	UNP M1E1E4
A	1273	GLY	-	expression tag	UNP M1E1E4
A	1274	GLY	-	expression tag	UNP M1E1E4
A	1275	GLY	-	expression tag	UNP M1E1E4
A	1276	SER	-	expression tag	UNP M1E1E4
A	1277	GLY	-	expression tag	UNP M1E1E4
A	1278	GLY	-	expression tag	UNP M1E1E4
A	1279	SER	-	expression tag	UNP M1E1E4
A	1280	ALA	-	expression tag	UNP M1E1E4
A	1281	TRP	-	expression tag	UNP M1E1E4
A	1282	SER	-	expression tag	UNP M1E1E4
A	1283	HIS	-	expression tag	UNP M1E1E4
A	1284	PRO	-	expression tag	UNP M1E1E4
A	1285	GLN	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1286	PHE	-	expression tag	UNP M1E1E4
A	1287	GLU	-	expression tag	UNP M1E1E4
A	1288	LYS	-	expression tag	UNP M1E1E4
A	1289	GLY	-	expression tag	UNP M1E1E4
A	1290	SER	-	expression tag	UNP M1E1E4
A	1291	ASP	-	expression tag	UNP M1E1E4
A	1292	TYR	-	expression tag	UNP M1E1E4
A	1293	LYS	-	expression tag	UNP M1E1E4
A	1294	ASP	-	expression tag	UNP M1E1E4
A	1295	ASP	-	expression tag	UNP M1E1E4
A	1296	ASP	-	expression tag	UNP M1E1E4
A	1297	ASP	-	expression tag	UNP M1E1E4
A	1298	LYS	-	expression tag	UNP M1E1E4
B	18	PHE	LEU	variant	UNP P0DTC2
B	80	ALA	ASP	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	305	THR	SER	engineered mutation	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	701	VAL	ALA	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP M1E1E4
B	1240	SER	-	expression tag	UNP M1E1E4
B	1241	LEU	-	expression tag	UNP M1E1E4
B	1242	GLU	-	expression tag	UNP M1E1E4
B	1243	VAL	-	expression tag	UNP M1E1E4
B	1244	LEU	-	expression tag	UNP M1E1E4
B	1245	PHE	-	expression tag	UNP M1E1E4
B	1246	GLN	-	expression tag	UNP M1E1E4
B	1247	GLY	-	expression tag	UNP M1E1E4
B	1248	PRO	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1249	GLY	-	expression tag	UNP M1E1E4
B	1250	HIS	-	expression tag	UNP M1E1E4
B	1251	HIS	-	expression tag	UNP M1E1E4
B	1252	HIS	-	expression tag	UNP M1E1E4
B	1253	HIS	-	expression tag	UNP M1E1E4
B	1254	HIS	-	expression tag	UNP M1E1E4
B	1255	HIS	-	expression tag	UNP M1E1E4
B	1256	HIS	-	expression tag	UNP M1E1E4
B	1257	HIS	-	expression tag	UNP M1E1E4
B	1258	SER	-	expression tag	UNP M1E1E4
B	1259	ALA	-	expression tag	UNP M1E1E4
B	1260	TRP	-	expression tag	UNP M1E1E4
B	1261	SER	-	expression tag	UNP M1E1E4
B	1262	HIS	-	expression tag	UNP M1E1E4
B	1263	PRO	-	expression tag	UNP M1E1E4
B	1264	GLN	-	expression tag	UNP M1E1E4
B	1265	PHE	-	expression tag	UNP M1E1E4
B	1266	GLU	-	expression tag	UNP M1E1E4
B	1267	LYS	-	expression tag	UNP M1E1E4
B	1268	GLY	-	expression tag	UNP M1E1E4
B	1269	GLY	-	expression tag	UNP M1E1E4
B	1270	GLY	-	expression tag	UNP M1E1E4
B	1271	SER	-	expression tag	UNP M1E1E4
B	1272	GLY	-	expression tag	UNP M1E1E4
B	1273	GLY	-	expression tag	UNP M1E1E4
B	1274	GLY	-	expression tag	UNP M1E1E4
B	1275	GLY	-	expression tag	UNP M1E1E4
B	1276	SER	-	expression tag	UNP M1E1E4
B	1277	GLY	-	expression tag	UNP M1E1E4
B	1278	GLY	-	expression tag	UNP M1E1E4
B	1279	SER	-	expression tag	UNP M1E1E4
B	1280	ALA	-	expression tag	UNP M1E1E4
B	1281	TRP	-	expression tag	UNP M1E1E4
B	1282	SER	-	expression tag	UNP M1E1E4
B	1283	HIS	-	expression tag	UNP M1E1E4
B	1284	PRO	-	expression tag	UNP M1E1E4
B	1285	GLN	-	expression tag	UNP M1E1E4
B	1286	PHE	-	expression tag	UNP M1E1E4
B	1287	GLU	-	expression tag	UNP M1E1E4
B	1288	LYS	-	expression tag	UNP M1E1E4
B	1289	GLY	-	expression tag	UNP M1E1E4
B	1290	SER	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1291	ASP	-	expression tag	UNP M1E1E4
B	1292	TYR	-	expression tag	UNP M1E1E4
B	1293	LYS	-	expression tag	UNP M1E1E4
B	1294	ASP	-	expression tag	UNP M1E1E4
B	1295	ASP	-	expression tag	UNP M1E1E4
B	1296	ASP	-	expression tag	UNP M1E1E4
B	1297	ASP	-	expression tag	UNP M1E1E4
B	1298	LYS	-	expression tag	UNP M1E1E4
C	18	PHE	LEU	variant	UNP P0DTC2
C	80	ALA	ASP	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	305	THR	SER	engineered mutation	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	701	VAL	ALA	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP M1E1E4
C	1240	SER	-	expression tag	UNP M1E1E4
C	1241	LEU	-	expression tag	UNP M1E1E4
C	1242	GLU	-	expression tag	UNP M1E1E4
C	1243	VAL	-	expression tag	UNP M1E1E4
C	1244	LEU	-	expression tag	UNP M1E1E4
C	1245	PHE	-	expression tag	UNP M1E1E4
C	1246	GLN	-	expression tag	UNP M1E1E4
C	1247	GLY	-	expression tag	UNP M1E1E4
C	1248	PRO	-	expression tag	UNP M1E1E4
C	1249	GLY	-	expression tag	UNP M1E1E4
C	1250	HIS	-	expression tag	UNP M1E1E4
C	1251	HIS	-	expression tag	UNP M1E1E4
C	1252	HIS	-	expression tag	UNP M1E1E4
C	1253	HIS	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1254	HIS	-	expression tag	UNP M1E1E4
C	1255	HIS	-	expression tag	UNP M1E1E4
C	1256	HIS	-	expression tag	UNP M1E1E4
C	1257	HIS	-	expression tag	UNP M1E1E4
C	1258	SER	-	expression tag	UNP M1E1E4
C	1259	ALA	-	expression tag	UNP M1E1E4
C	1260	TRP	-	expression tag	UNP M1E1E4
C	1261	SER	-	expression tag	UNP M1E1E4
C	1262	HIS	-	expression tag	UNP M1E1E4
C	1263	PRO	-	expression tag	UNP M1E1E4
C	1264	GLN	-	expression tag	UNP M1E1E4
C	1265	PHE	-	expression tag	UNP M1E1E4
C	1266	GLU	-	expression tag	UNP M1E1E4
C	1267	LYS	-	expression tag	UNP M1E1E4
C	1268	GLY	-	expression tag	UNP M1E1E4
C	1269	GLY	-	expression tag	UNP M1E1E4
C	1270	GLY	-	expression tag	UNP M1E1E4
C	1271	SER	-	expression tag	UNP M1E1E4
C	1272	GLY	-	expression tag	UNP M1E1E4
C	1273	GLY	-	expression tag	UNP M1E1E4
C	1274	GLY	-	expression tag	UNP M1E1E4
C	1275	GLY	-	expression tag	UNP M1E1E4
C	1276	SER	-	expression tag	UNP M1E1E4
C	1277	GLY	-	expression tag	UNP M1E1E4
C	1278	GLY	-	expression tag	UNP M1E1E4
C	1279	SER	-	expression tag	UNP M1E1E4
C	1280	ALA	-	expression tag	UNP M1E1E4
C	1281	TRP	-	expression tag	UNP M1E1E4
C	1282	SER	-	expression tag	UNP M1E1E4
C	1283	HIS	-	expression tag	UNP M1E1E4
C	1284	PRO	-	expression tag	UNP M1E1E4
C	1285	GLN	-	expression tag	UNP M1E1E4
C	1286	PHE	-	expression tag	UNP M1E1E4
C	1287	GLU	-	expression tag	UNP M1E1E4
C	1288	LYS	-	expression tag	UNP M1E1E4
C	1289	GLY	-	expression tag	UNP M1E1E4
C	1290	SER	-	expression tag	UNP M1E1E4
C	1291	ASP	-	expression tag	UNP M1E1E4
C	1292	TYR	-	expression tag	UNP M1E1E4
C	1293	LYS	-	expression tag	UNP M1E1E4
C	1294	ASP	-	expression tag	UNP M1E1E4
C	1295	ASP	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1296	ASP	-	expression tag	UNP M1E1E4
C	1297	ASP	-	expression tag	UNP M1E1E4
C	1298	LYS	-	expression tag	UNP M1E1E4

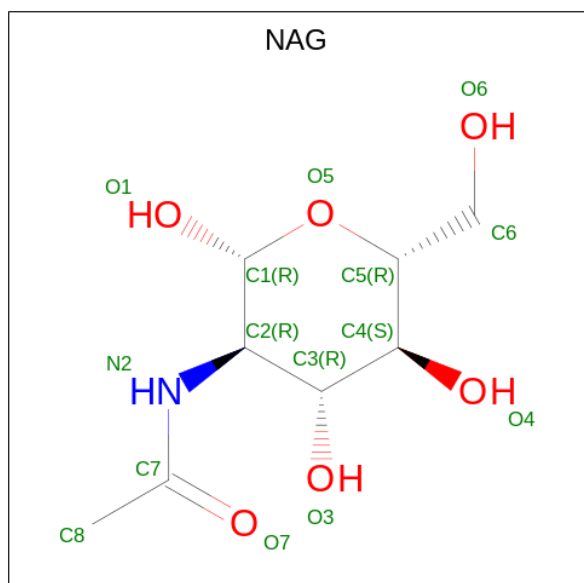
- Molecule 2 is a protein called T6 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	107	Total	C	N	O	S	0	0
			823	517	132	170	4		
2	I	107	Total	C	N	O	S	0	0
			823	517	132	170	4		

- Molecule 3 is a protein called T6 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	113	Total	C	N	O	S	0	0
			886	564	146	174	2		
3	L	113	Total	C	N	O	S	0	0
			886	564	146	174	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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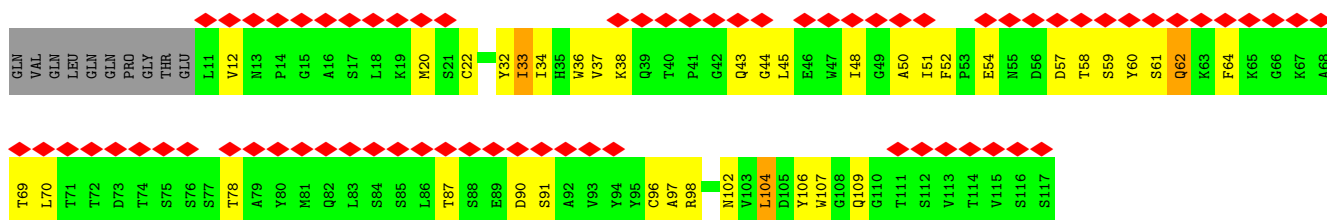
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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

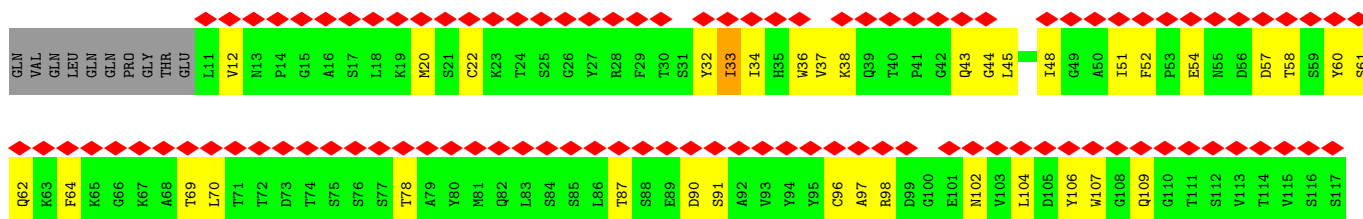
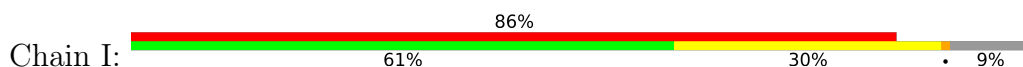


[illegible]

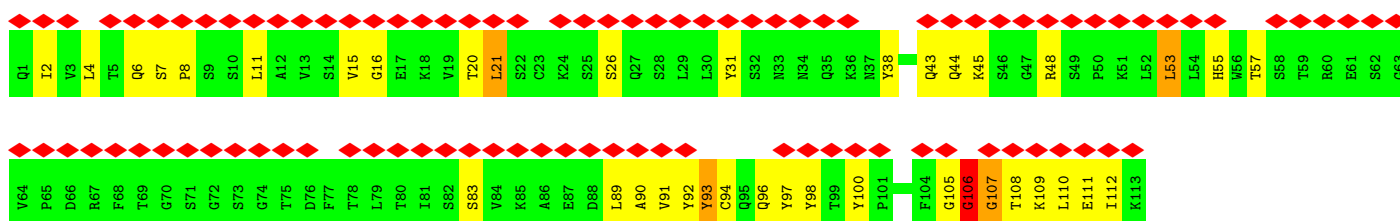
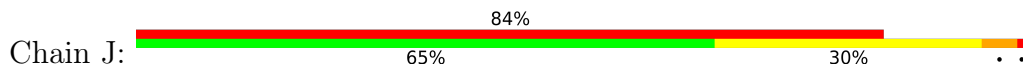
- Molecule 2: T6 heavy chain



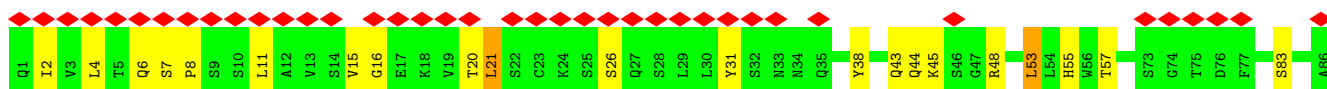
- Molecule 2: T6 heavy chain

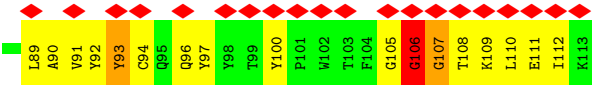


- Molecule 3: T6 light chain



- Molecule 3: T6 light chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	286245	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (\AA)	351.328, 351.328, 351.328	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0979, 1.0979, 1.0979	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	0.58	0/7858	0.81	11/10696 (0.1%)
1	B	0.59	0/7864	0.84	13/10706 (0.1%)
1	C	0.57	0/7853	0.82	14/10696 (0.1%)
2	H	0.66	0/842	0.65	0/1144
2	I	0.66	0/842	0.65	0/1144
3	J	0.70	1/907 (0.1%)	0.65	0/1231
3	L	0.70	1/907 (0.1%)	0.65	0/1231
All	All	0.59	2/27073 (0.0%)	0.80	38/36848 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
3	J	0	1
3	L	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	106	GLY	CA-C	6.98	1.63	1.51
3	J	106	GLY	CA-C	6.96	1.62	1.51

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	B	904	TYR	CB-CG-CD2	-8.19	116.09	121.00
1	C	1014	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	B	1014	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	34	ARG	NE-CZ-NH1	7.66	124.13	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	ILE	Peptide
1	A	34	ARG	Sidechain
1	B	577	ARG	Sidechain
3	J	106	GLY	Mainchain
3	L	106	GLY	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7687	0	7472	86	0
1	B	7691	0	7484	90	0
1	C	7678	0	7478	50	0
2	H	823	0	779	43	0
2	I	823	0	779	33	0
3	J	886	0	872	57	0
3	L	886	0	872	57	0
4	A	112	0	104	0	0
4	B	112	0	104	0	0
4	C	126	0	117	0	0
All	All	26824	0	26061	321	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 6.

The worst 5 of 321 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:A:521:PRO:CG	1:B:230:PRO:HB2	1.18	1.62
1:C:498:GLN:CB	1:C:501:TYR:CE2	1.75	1.60
1:B:456:PHE:CZ	2:H:54:GLU:HG2	1.32	1.59
1:A:521:PRO:HG2	1:B:230:PRO:CB	1.14	1.58
1:A:498:GLN:HB2	1:A:501:TYR:CE2	1.42	1.52

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	975/1280 (76%)	893 (92%)	78 (8%)	4 (0%)	30	60
1	B	975/1280 (76%)	891 (91%)	80 (8%)	4 (0%)	30	60
1	C	976/1280 (76%)	899 (92%)	74 (8%)	3 (0%)	37	66
2	H	105/117 (90%)	97 (92%)	8 (8%)	0	100	100
2	I	105/117 (90%)	97 (92%)	8 (8%)	0	100	100
3	J	111/113 (98%)	108 (97%)	2 (2%)	1 (1%)	14	43
3	L	111/113 (98%)	108 (97%)	2 (2%)	1 (1%)	14	43
All	All	3358/4300 (78%)	3093 (92%)	252 (8%)	13 (0%)	32	60

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	986	PRO
1	A	197	ILE
1	C	112	SER
1	B	137	ASN
1	B	334	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	849/1103 (77%)	834 (98%)	15 (2%)	54	72
1	B	851/1103 (77%)	843 (99%)	8 (1%)	75	84
1	C	848/1103 (77%)	839 (99%)	9 (1%)	70	81
2	H	92/101 (91%)	78 (85%)	14 (15%)	2	10
2	I	92/101 (91%)	78 (85%)	14 (15%)	2	10
3	J	100/100 (100%)	91 (91%)	9 (9%)	8	27
3	L	100/100 (100%)	91 (91%)	9 (9%)	8	27
All	All	2932/3711 (79%)	2854 (97%)	78 (3%)	41	63

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	102	ASN
3	L	21	LEU
2	I	109	GLN
3	J	108	THR
3	L	109	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	334	ASN
1	C	414	GLN
1	C	1135	ASN
1	C	474	GLN
1	A	474	GLN

5.3.3 RNA ⓘ

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	NAG	A	1304	1	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	A	1306	1	14,14,15	0.28	0	17,19,21	0.69	0
4	NAG	A	1301	1	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
4	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.62	0
4	NAG	A	1308	1	14,14,15	0.30	0	17,19,21	0.68	1 (5%)
4	NAG	A	1307	1	14,14,15	0.28	0	17,19,21	0.68	0
4	NAG	C	1306	1	14,14,15	0.25	0	17,19,21	1.00	1 (5%)
4	NAG	C	1307	1	14,14,15	0.28	0	17,19,21	0.51	0
4	NAG	A	1302	1	14,14,15	0.28	0	17,19,21	0.81	1 (5%)
4	NAG	C	1309	1	14,14,15	0.29	0	17,19,21	0.65	0
4	NAG	B	1302	1	14,14,15	0.25	0	17,19,21	0.94	1 (5%)
4	NAG	B	1305	1	14,14,15	0.25	0	17,19,21	0.95	0
4	NAG	B	1308	1	14,14,15	0.29	0	17,19,21	0.59	0
4	NAG	B	1304	1	14,14,15	0.28	0	17,19,21	0.58	0
4	NAG	C	1305	1	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	C	1308	1	14,14,15	0.29	0	17,19,21	1.15	2 (11%)
4	NAG	B	1306	1	14,14,15	0.25	0	17,19,21	0.98	1 (5%)
4	NAG	B	1303	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	B	1307	1	14,14,15	0.29	0	17,19,21	0.72	0
4	NAG	A	1303	1	14,14,15	0.27	0	17,19,21	0.63	0
4	NAG	C	1302	1	14,14,15	0.30	0	17,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1301	1	14,14,15	0.27	0	17,19,21	0.67	0
4	NAG	C	1303	1	14,14,15	0.27	0	17,19,21	1.10	2 (11%)
4	NAG	C	1301	1	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	A	1305	1	14,14,15	0.28	0	17,19,21	0.69	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	A	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	NAG	C2-N2-C7	2.99	127.17	122.90
4	C	1308	NAG	C1-O5-C5	2.66	115.80	112.19
4	C	1303	NAG	C2-N2-C7	2.61	126.62	122.90
4	C	1308	NAG	C2-N2-C7	2.57	126.57	122.90
4	C	1303	NAG	C1-O5-C5	2.34	115.36	112.19

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	C8-C7-N2-C2
4	A	1301	NAG	O7-C7-N2-C2
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	A	1307	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

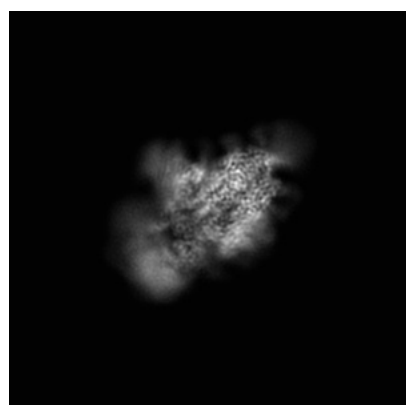
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31624. These allow visual inspection of the internal detail of the map and identification of artifacts.

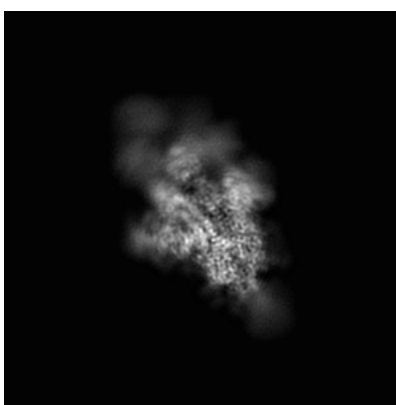
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

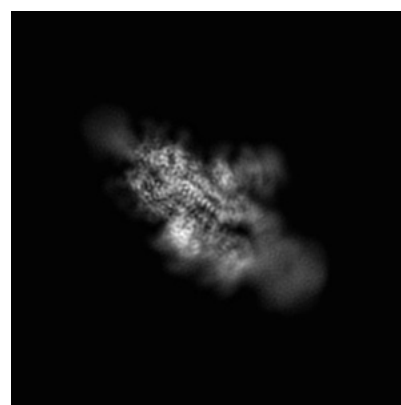
6.1.1 Primary map



X



Y

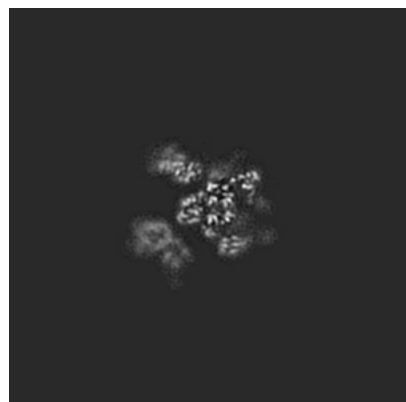


Z

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

6.2 Central slices [i](#)

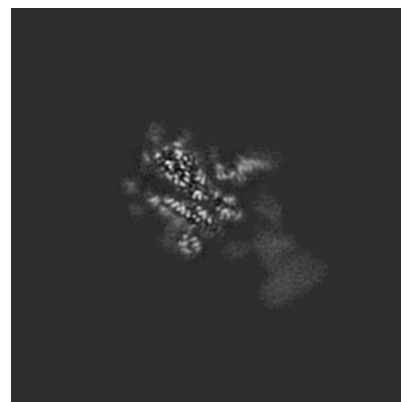
6.2.1 Primary map



X Index: 160



Y Index: 160

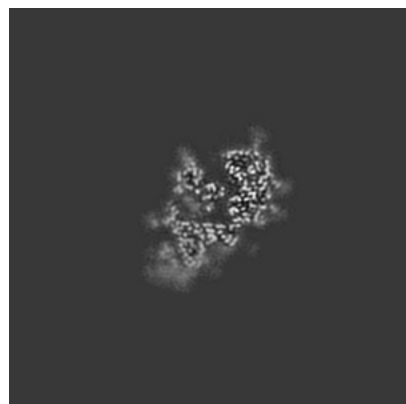


Z Index: 160

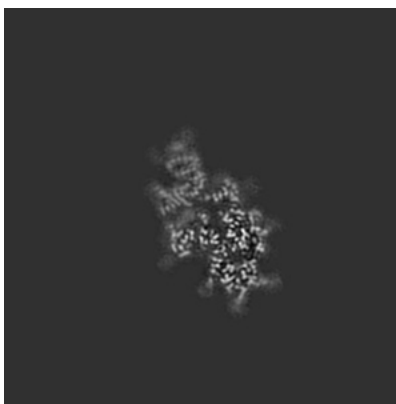
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

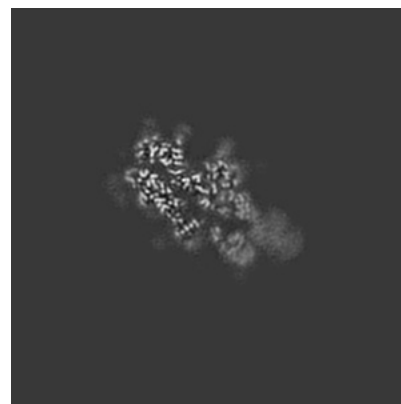
6.3.1 Primary map



X Index: 135



Y Index: 182

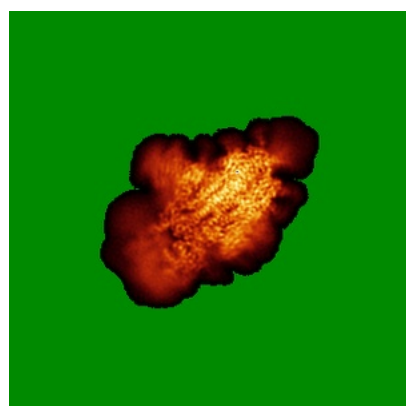


Z Index: 180

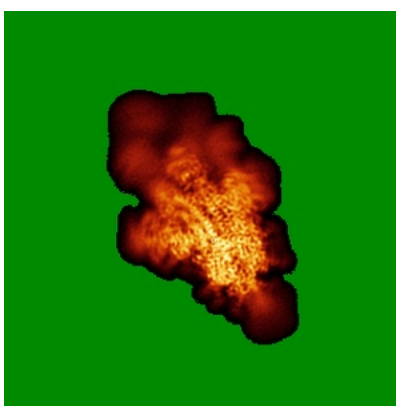
The images above show the largest variance slices of the map in three orthogonal directions.

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

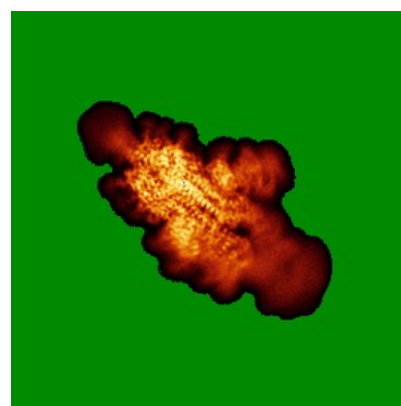
6.4.1 Primary map



X



Y

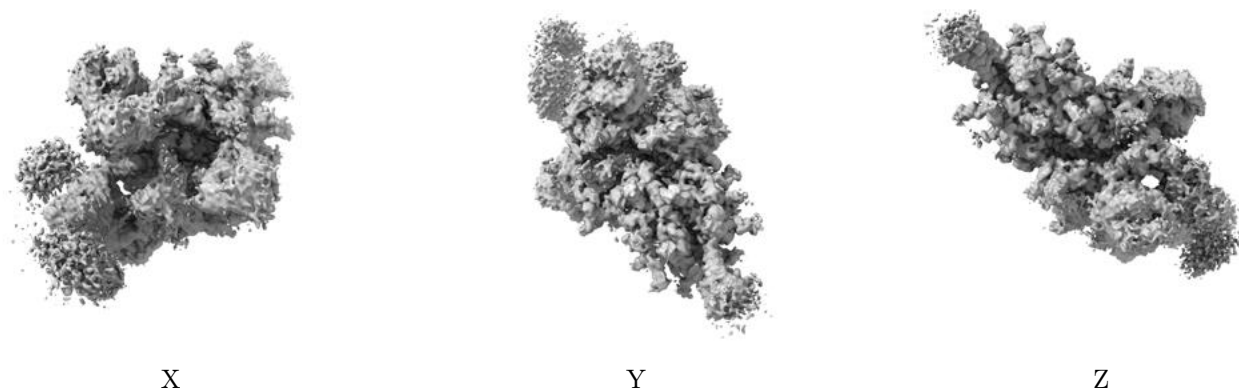


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

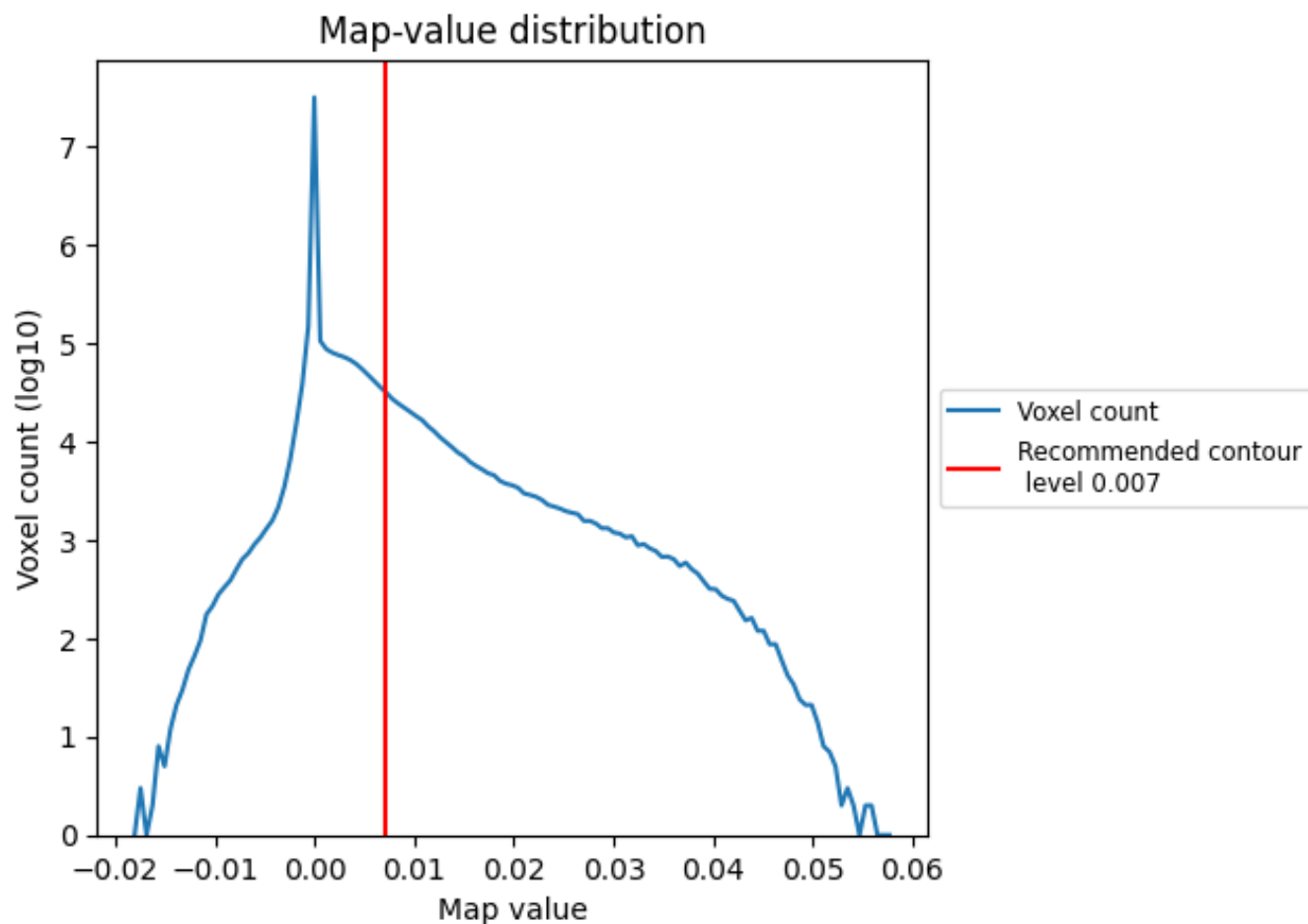
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

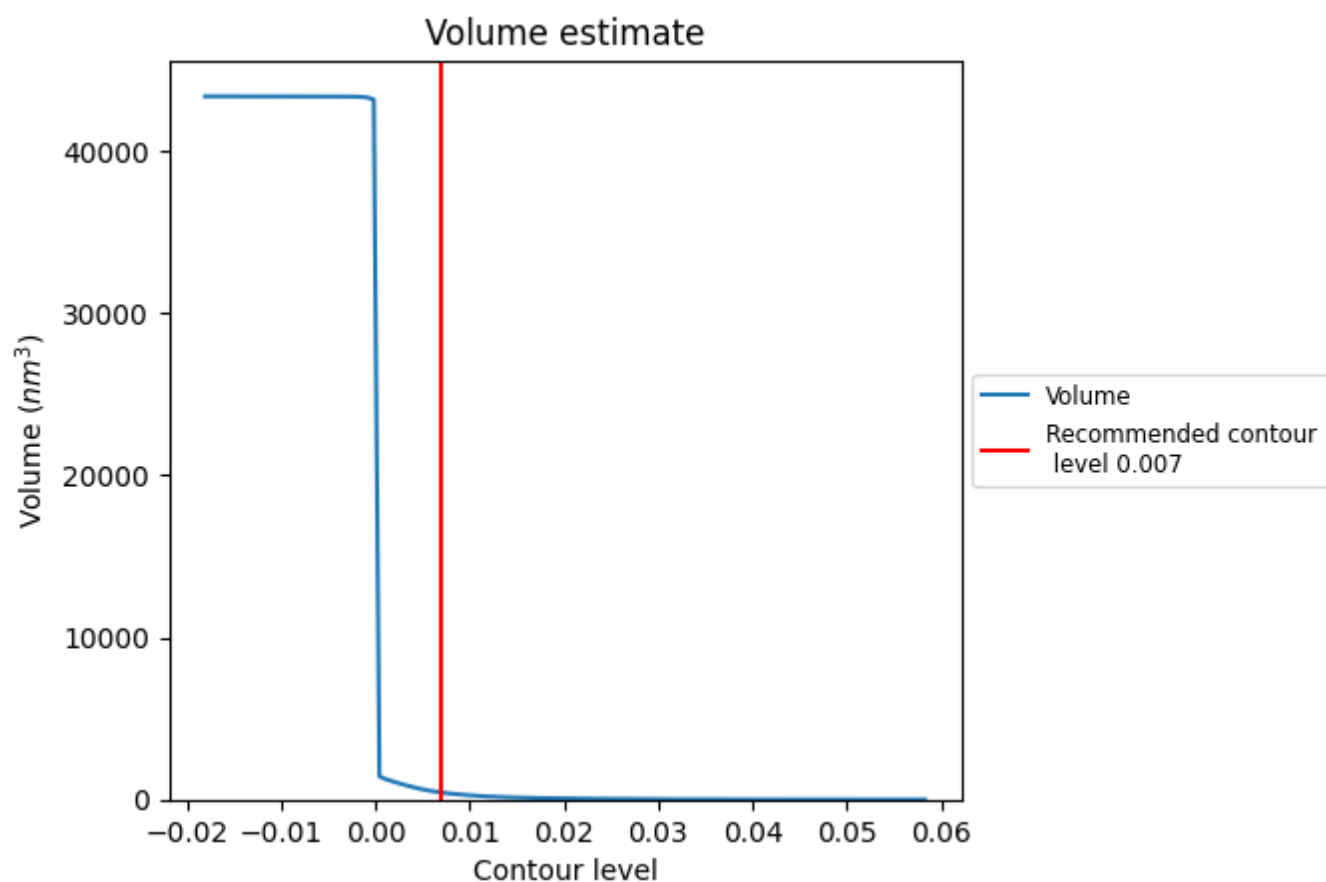
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

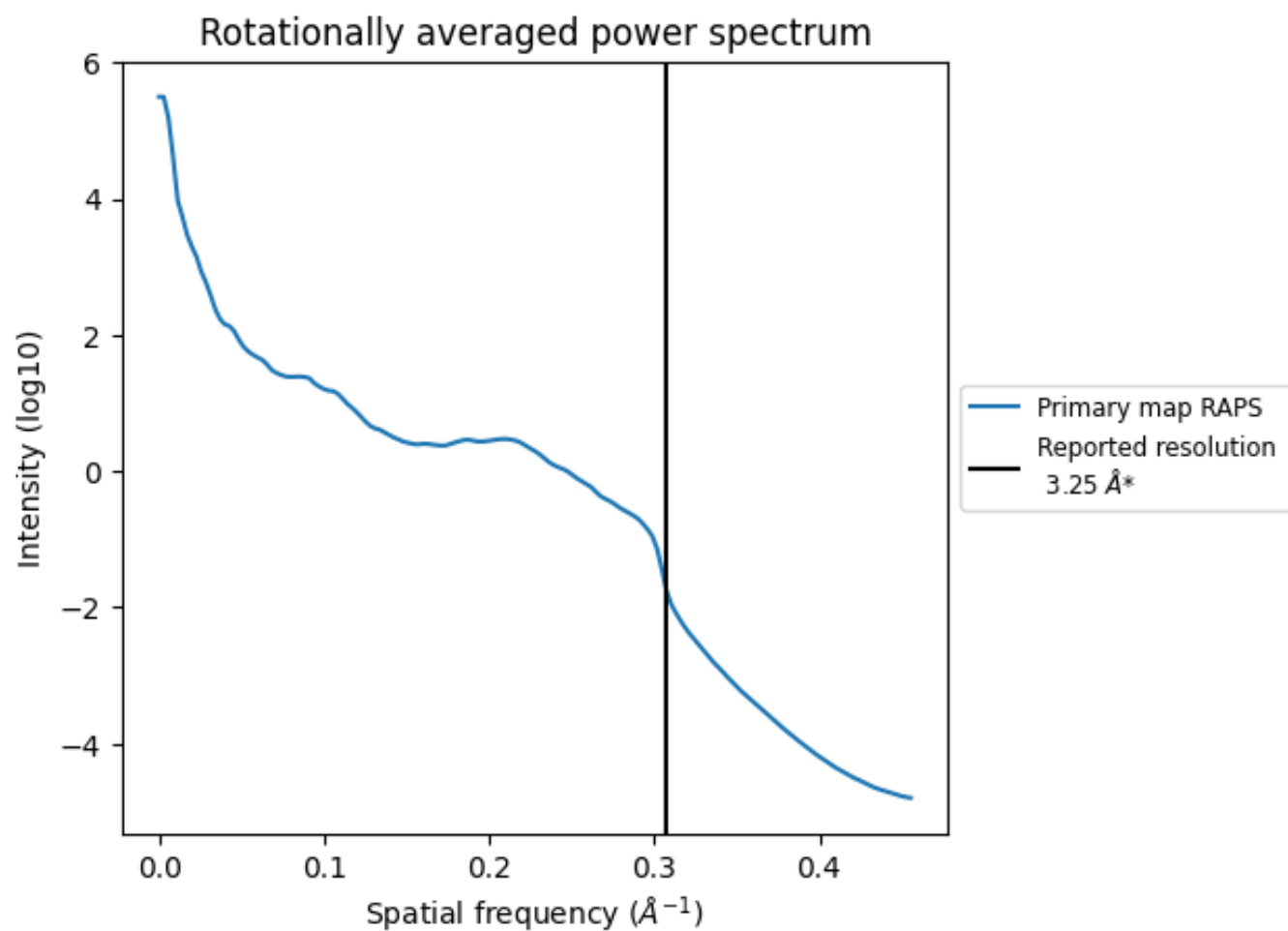
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 433 nm^3 ; this corresponds to an approximate mass of 391 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.308 \AA^{-1}

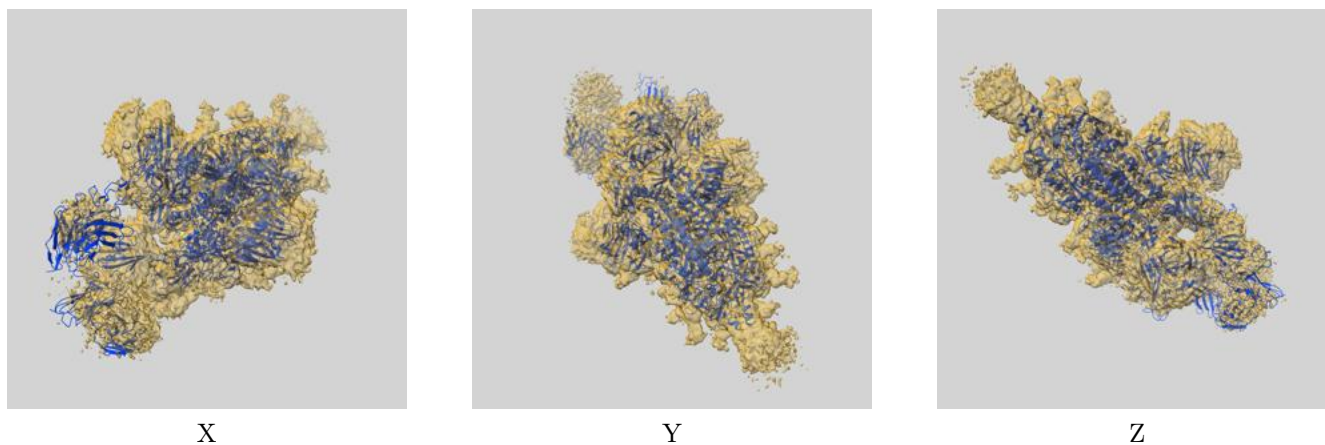
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

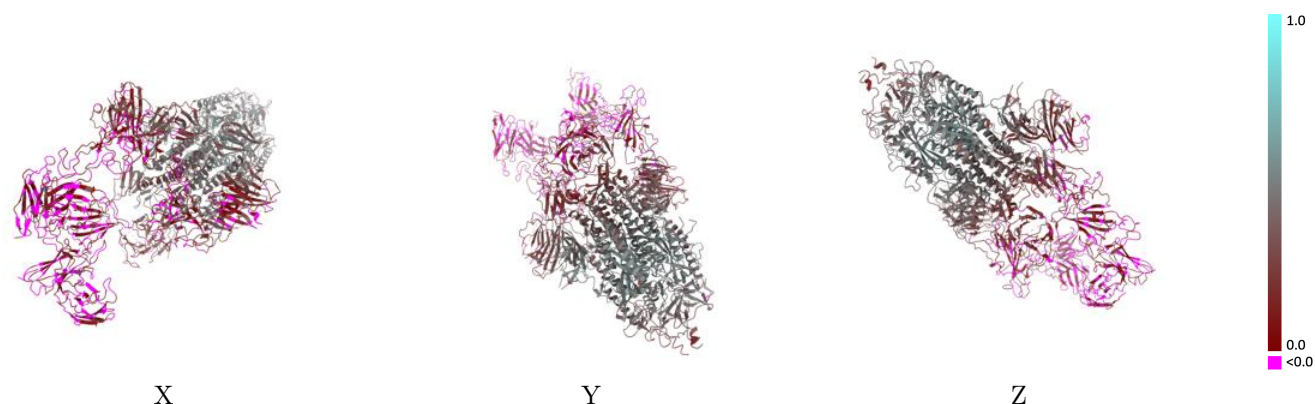
This section contains information regarding the fit between EMDB map EMD-31624 and PDB model 7FJN. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



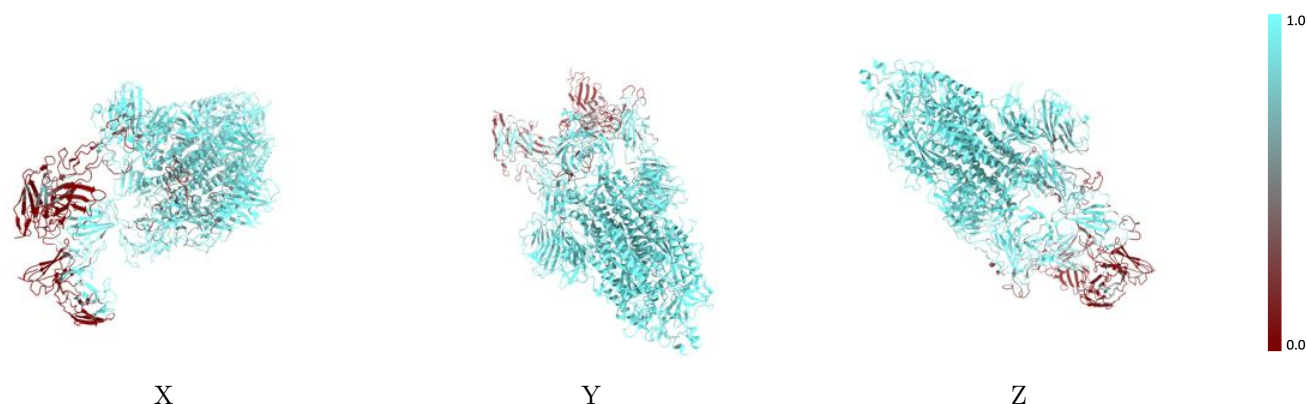
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



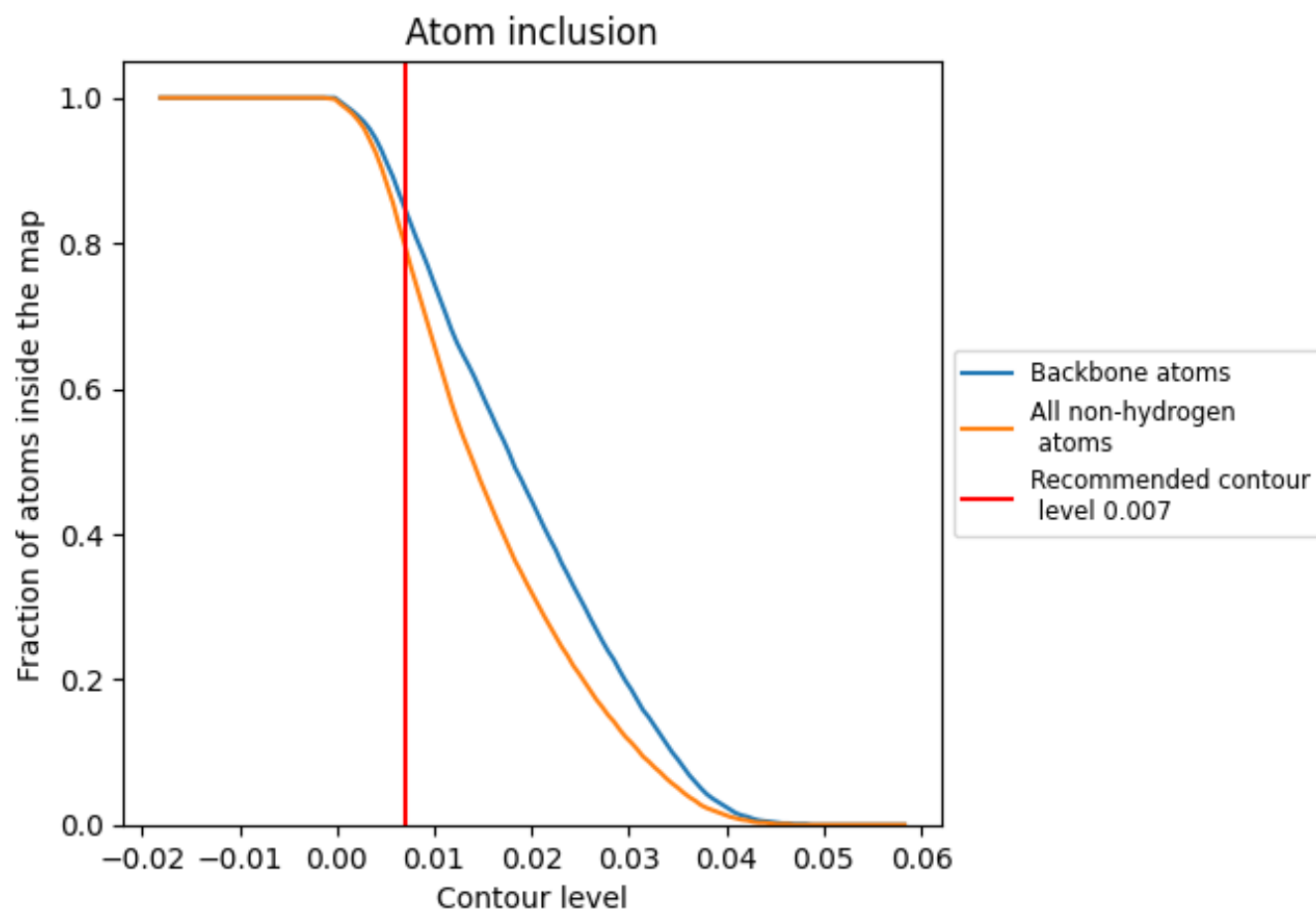
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7970	<div></div> 0.2700
A	<div></div> 0.8620	<div></div> 0.2910
B	<div></div> 0.8880	<div></div> 0.3010
C	<div></div> 0.8720	<div></div> 0.3260
H	<div></div> 0.3470	<div></div> 0.0260
I	<div></div> 0.0950	<div></div> 0.0320
J	<div></div> 0.1480	<div></div> 0.0060
L	<div></div> 0.4780	<div></div> 0.0100

1.0

0.0

<0.0