W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Nov 16, 2022 – 04:24 PM EST

PDB ID	:	7LQV
EMDB ID	:	EMD-23489
Title	:	Cryo-EM structure of NTD-directed neutralizing antibody 4-8 Fab in complex with SARS-CoV-2 S2P spike
Authors	:	Gorman, J.; Rapp, M.; Kwong, P.D.; Shapiro, L.
Deposited on	:	2021-02-15
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 (i) 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 (i)) 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 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.0%
Sidechain outliers		0.1%

Worse   *Better*

■ Percentile relative to all structures

▯ Percentile relative to all EM structures
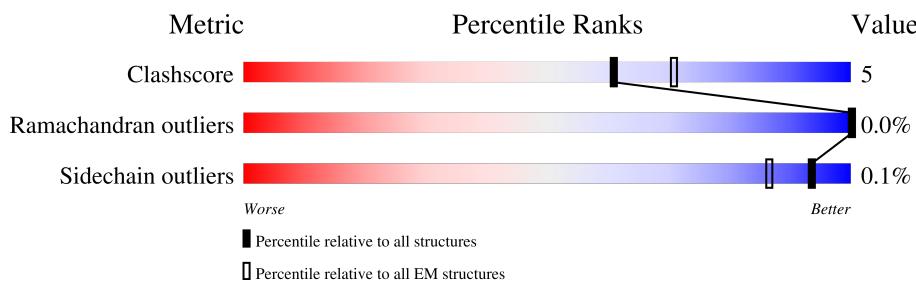
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1307	· 75% · 9% 16%
1	B	1307	5% · 75% · 10% 15%
1	C	1307	· 73% · 10% 17%
2	H	125	54% · 88% 12%
2	W	125	39% · 90% 10%
2	Y	125	55% · 88% 12%
3	L	106	56% · 92% 7% ·
3	X	106	44% · 91% 8% ·

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WORLDWIDE
wwPDB
PROTEIN DATA BANK
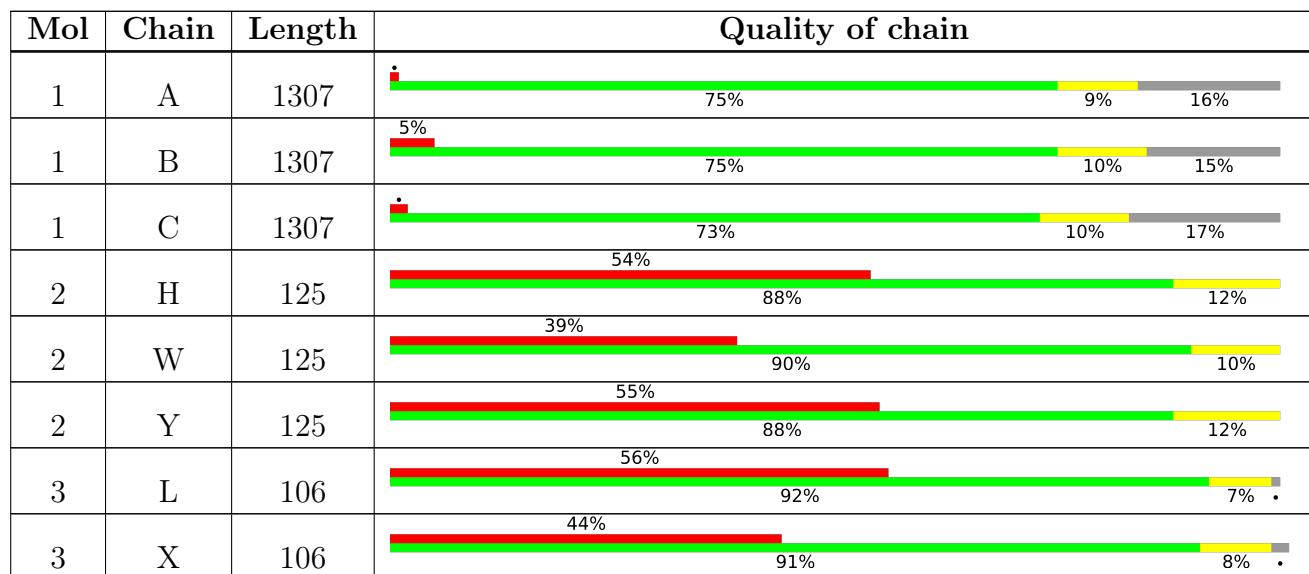
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Mol	Chain	Length	Quality of chain
3	Z	106	53% ... 92% ... 7%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 31274 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
1	A	1092	Total 8535	C 5445	N 1425	O 1626	S 39	0	0
1	B	1112	Total 8681	C 5535	N 1450	O 1656	S 40	0	0
1	C	1087	Total 8500	C 5421	N 1420	O 1621	S 38	0	0

There are 351 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP P0DTC2
A	-17	GLY	-	expression tag	UNP P0DTC2
A	-16	ILE	-	expression tag	UNP P0DTC2
A	-15	LEU	-	expression tag	UNP P0DTC2
A	-14	PRO	-	expression tag	UNP P0DTC2
A	-13	SER	-	expression tag	UNP P0DTC2
A	-12	PRO	-	expression tag	UNP P0DTC2
A	-11	GLY	-	expression tag	UNP P0DTC2
A	-10	MET	-	expression tag	UNP P0DTC2
A	-9	PRO	-	expression tag	UNP P0DTC2
A	-8	ALA	-	expression tag	UNP P0DTC2
A	-7	LEU	-	expression tag	UNP P0DTC2
A	-6	LEU	-	expression tag	UNP P0DTC2
A	-5	SER	-	expression tag	UNP P0DTC2
A	-4	LEU	-	expression tag	UNP P0DTC2
A	-3	VAL	-	expression tag	UNP P0DTC2
A	-2	SER	-	expression tag	UNP P0DTC2
A	-1	LEU	-	expression tag	UNP P0DTC2
A	0	LEU	-	expression tag	UNP P0DTC2
A	1	SER	-	expression tag	UNP P0DTC2
A	2	VAL	-	expression tag	UNP P0DTC2
A	3	LEU	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	MET	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	expression tag	UNP P0DTC2
A	7	CYS	-	expression tag	UNP P0DTC2
A	8	VAL	-	expression tag	UNP P0DTC2
A	9	ALA	-	expression tag	UNP P0DTC2
A	10	GLU	-	expression tag	UNP P0DTC2
A	11	THR	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	-18	MET	-	expression tag	UNP P0DTC2
B	-17	GLY	-	expression tag	UNP P0DTC2
B	-16	ILE	-	expression tag	UNP P0DTC2
B	-15	LEU	-	expression tag	UNP P0DTC2
B	-14	PRO	-	expression tag	UNP P0DTC2
B	-13	SER	-	expression tag	UNP P0DTC2
B	-12	PRO	-	expression tag	UNP P0DTC2
B	-11	GLY	-	expression tag	UNP P0DTC2
B	-10	MET	-	expression tag	UNP P0DTC2
B	-9	PRO	-	expression tag	UNP P0DTC2
B	-8	ALA	-	expression tag	UNP P0DTC2
B	-7	LEU	-	expression tag	UNP P0DTC2
B	-6	LEU	-	expression tag	UNP P0DTC2
B	-5	SER	-	expression tag	UNP P0DTC2
B	-4	LEU	-	expression tag	UNP P0DTC2
B	-3	VAL	-	expression tag	UNP P0DTC2
B	-2	SER	-	expression tag	UNP P0DTC2
B	-1	LEU	-	expression tag	UNP P0DTC2
B	0	LEU	-	expression tag	UNP P0DTC2
B	1	SER	-	expression tag	UNP P0DTC2
B	2	VAL	-	expression tag	UNP P0DTC2
B	3	LEU	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	MET	-	expression tag	UNP P0DTC2
B	6	GLY	-	expression tag	UNP P0DTC2
B	7	CYS	-	expression tag	UNP P0DTC2
B	8	VAL	-	expression tag	UNP P0DTC2
B	9	ALA	-	expression tag	UNP P0DTC2
B	10	GLU	-	expression tag	UNP P0DTC2
B	11	THR	-	expression tag	UNP P0DTC2
B	12	GLY	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	MET	-	expression tag	UNP P0DTC2
C	-17	GLY	-	expression tag	UNP P0DTC2
C	-16	ILE	-	expression tag	UNP P0DTC2
C	-15	LEU	-	expression tag	UNP P0DTC2
C	-14	PRO	-	expression tag	UNP P0DTC2
C	-13	SER	-	expression tag	UNP P0DTC2
C	-12	PRO	-	expression tag	UNP P0DTC2
C	-11	GLY	-	expression tag	UNP P0DTC2
C	-10	MET	-	expression tag	UNP P0DTC2
C	-9	PRO	-	expression tag	UNP P0DTC2
C	-8	ALA	-	expression tag	UNP P0DTC2
C	-7	LEU	-	expression tag	UNP P0DTC2
C	-6	LEU	-	expression tag	UNP P0DTC2
C	-5	SER	-	expression tag	UNP P0DTC2
C	-4	LEU	-	expression tag	UNP P0DTC2
C	-3	VAL	-	expression tag	UNP P0DTC2
C	-2	SER	-	expression tag	UNP P0DTC2
C	-1	LEU	-	expression tag	UNP P0DTC2
C	0	LEU	-	expression tag	UNP P0DTC2
C	1	SER	-	expression tag	UNP P0DTC2
C	2	VAL	-	expression tag	UNP P0DTC2
C	3	LEU	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	MET	-	expression tag	UNP P0DTC2
C	6	GLY	-	expression tag	UNP P0DTC2
C	7	CYS	-	expression tag	UNP P0DTC2
C	8	VAL	-	expression tag	UNP P0DTC2
C	9	ALA	-	expression tag	UNP P0DTC2
C	10	GLU	-	expression tag	UNP P0DTC2
C	11	THR	-	expression tag	UNP P0DTC2
C	12	GLY	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called 4-8 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	125	Total	C	N	O	S	0	0
			941	590	159	187	5		
2	W	125	Total	C	N	O	S	0	0
			941	590	159	187	5		
2	Y	125	Total	C	N	O	S	0	0
			941	590	159	187	5		

- Molecule 3 is a protein called 4-8 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	105	Total	C	N	O	S	0	0
			784	488	129	163	4		
3	X	104	Total	C	N	O	S	0	0
			775	483	127	161	4		
3	Z	105	Total	C	N	O	S	0	0
			784	488	129	163	4		

- 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
			154	88	11	55	
4	A	1	Total	C	N	O	0
			154	88	11	55	
4	A	1	Total	C	N	O	0
			154	88	11	55	
4	A	1	Total	C	N	O	0
			154	88	11	55	
4	A	1	Total	C	N	O	0
			154	88	11	55	
4	A	1	Total	C	N	O	0
			154	88	11	55	
4	A	1	Total	C	N	O	0
			154	88	11	55	

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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			154	88	11	55	
4	A	1	Total	C	N	O	0
			154	88	11	55	
4	A	1	Total	C	N	O	0
			154	88	11	55	
4	A	1	Total	C	N	O	0
			154	88	11	55	
4	B	1	Total	C	N	O	0
			126	72	9	45	
4	B	1	Total	C	N	O	0
			126	72	9	45	
4	B	1	Total	C	N	O	0
			126	72	9	45	
4	B	1	Total	C	N	O	0
			126	72	9	45	
4	B	1	Total	C	N	O	0
			126	72	9	45	
4	B	1	Total	C	N	O	0
			126	72	9	45	
4	B	1	Total	C	N	O	0
			126	72	9	45	
4	B	1	Total	C	N	O	0
			126	72	9	45	
4	B	1	Total	C	N	O	0
			126	72	9	45	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Spike glycoprotein
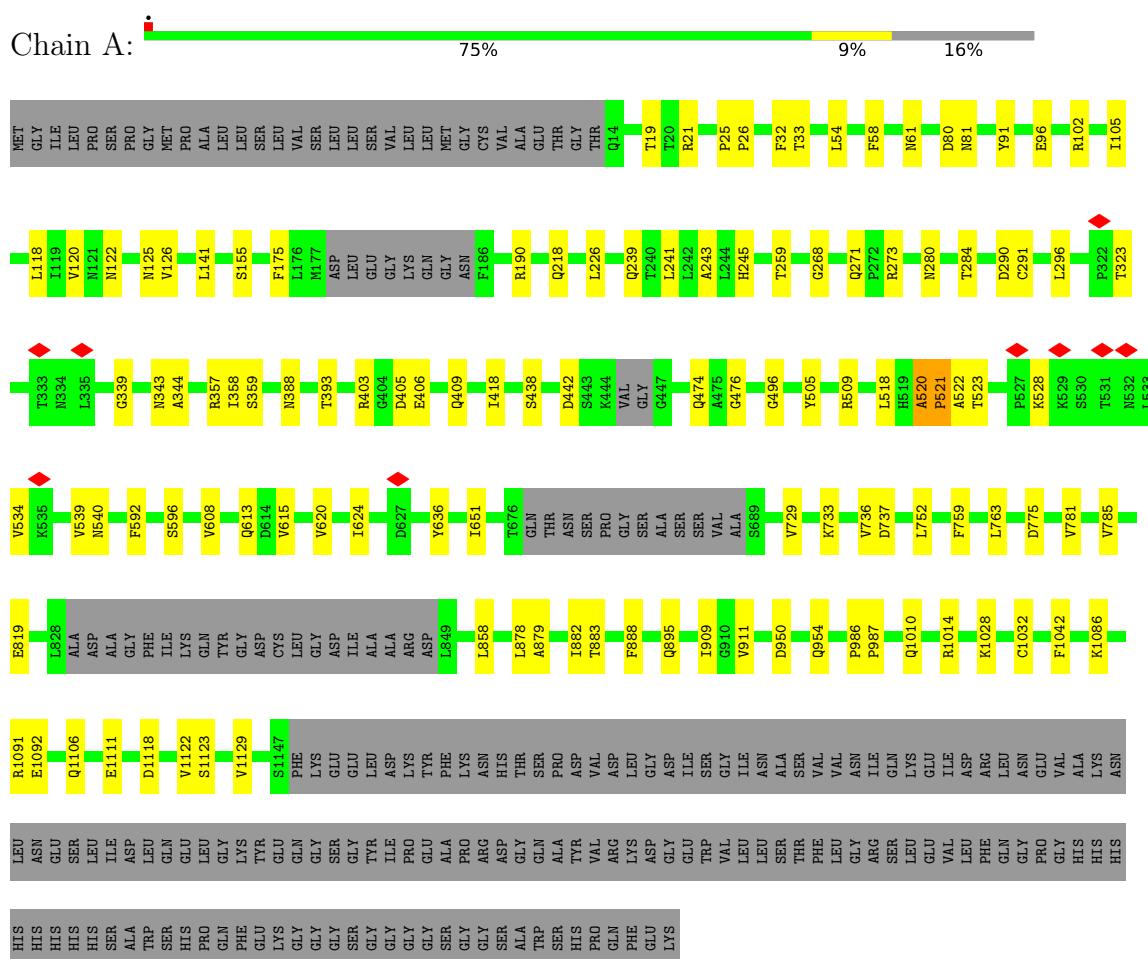
Chain A:

- Molecule 1: Spike glycoprotein
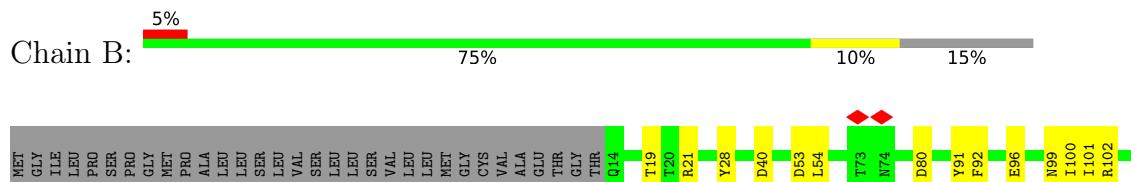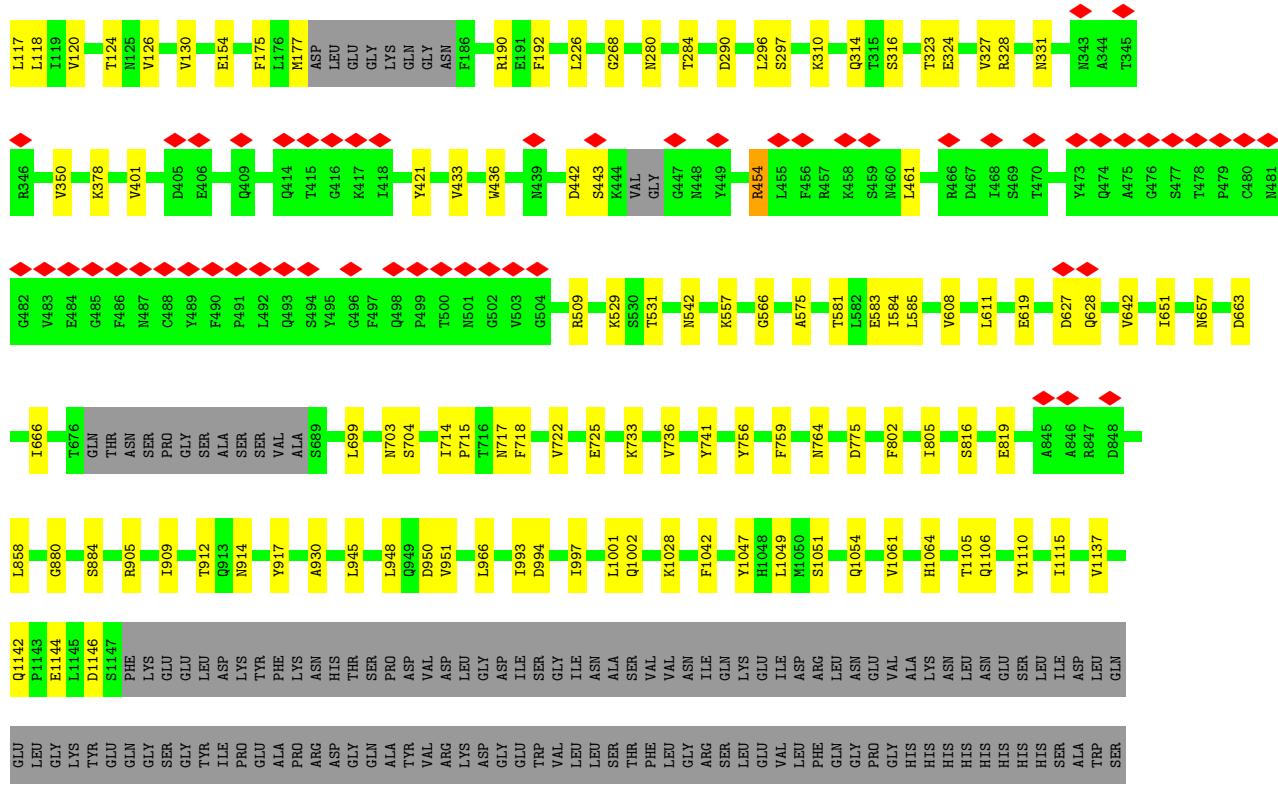
Chain B:

• Molecule 1: Spike glycoprotein

Chain C:

73%   10%   17%

ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA

TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN GLY PRO GLY HIS HIS HIS HIS HIS HIS SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY SER ALA TRP SER

HIS PRO GLN PHE GLU LYS

• Molecule 2: 4-8 Heavy Chain

Chain H:

54%
88% 12%

Q1 V5 Q6 S7 G8 A9 E10 V11 K12 K13 A14 G15 S16 S17 V18 K19 V20 A24 S25 G26 G27 T28 F29 S30 T33 R38 Q39 A40 P41 G42 Q43 G44 L45 E46 I53 L54 G55 I56 A57 N58 Y59 A60 Q61 K62 F63 Q64 G65 R66 V67 T68 I69 T70 A71 D72 K73

S74 T75 S76 T77 A78 Y79 M80 E81 L82 S82A S82B L82C R83 S84 E85 D86 T87 A88 V89 Y90 Y91 C92 A93 S94 L95 Q96 T97 V98 D99 E100C K100D Y100E T108 V109 T110 V111 S112 S113

• Molecule 2: 4-8 Heavy Chain

Chain W:

39%
90% 10%

Q1 Q6 S7 G8 A9 E10 V11 K12 K13 A14 G15 S16 S17 V18 K19 V20 G26 R38 Q39 A40 P41 G42 Q43 E46 W47 M48 G49 L54 G55 I56 A57 N58 Y59 A60 Q61 K62 F63 Q64 G65 R66 V67 T68 I69 T70 A71 D72 K73 S74 T75 Y79 M80 E81 L82 S82A

S82B L82C R83 S84 E85 D86 T87 A88 L95 A100A I100B E100C K100D T108 V109 T110 V111 S112 S113

• Molecule 2: 4-8 Heavy Chain

Chain Y:

55%
88% 12%

Q1 V2 Q3 L4 V5 Q6 S7 G8 A9 E10 V11 K12 K13 A14 G15 S16 S17 V18 K19 V20 S21 C22 K23 A24 S31 H32 T33 R38 Q39 A40 P41 G42 Q43 R50 I51 I53 L54 G55 I56 A57 N58 Y59 A60 Q61 K62 F63 Q64 G65 R66 V67 T68 I69 T70 A71 D72 K73

S74 T75 S76 T77 A78 Y79 M80 E81 L82 S82A S82B L82C R83 S84 E85 D86 T87 A88 V89 Y90 A93 T97 A100A I100B E100C K100D Y100E Y100F G104 T108 V109 T110 V111 S112 S113

• Molecule 3: 4-8 Light chain

Chain L:

56%
92% 7% •

SER Y2 E3 L4 T5 Q6 P7 P8 S9 V11 S12 V13 S14 P15 G16 Q17 T18 A19 S20 I21 T22 C23 S24 G25 D26 K27 L28 G29 D30 K31 G41 Q42 S43 P44 I48 Y49 Q50 D51 N52 K53 R54 E60 R61 F62 S63 G64 S65 N66 S67 G68 N69 T70 A71 T72 L73 T74 I75

• Molecule 3: 4-8 Light chain

Chain X:

• Molecule 3: 4-8 Light chain

Chain Z:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	88375	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 $(e^-/Å^2)$	52.56	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	1.931	Depositor
Minimum map value	-0.827	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	402.03998, 402.03998, 402.03998	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z|>5$	RMSZ	$\#|Z|>5$
1	A	0.27	0/8736	0.46	0/11897
1	B	0.25	0/8885	0.45	0/12099
1	C	0.25	0/8701	0.45	0/11849
2	H	0.25	0/957	0.48	0/1297
2	W	0.25	0/957	0.47	0/1297
2	Y	0.25	0/957	0.46	0/1297
3	L	0.25	0/802	0.47	0/1093
3	X	0.25	0/792	0.46	0/1078
3	Z	0.25	0/802	0.47	0/1093
All	All	0.26	0/31589	0.46	0/43000

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	520	ALA	Peptide

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	8535	0	8324	77	0
1	B	8681	0	8458	83	0
1	C	8500	0	8283	89	0
2	H	941	0	935	10	0
2	W	941	0	935	9	0
2	Y	941	0	935	10	0
3	L	784	0	744	5	0
3	X	775	0	735	5	0
3	Z	784	0	744	4	0
4	A	154	0	143	4	0
4	B	126	0	117	3	0
4	C	112	0	104	2	0
All	All	31274	0	30457	284	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 5.

The worst 5 of 284 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:175:PHE:CD1	1:C:226:LEU:HD13	1.96	0.99
1:C:175:PHE:HD1	1:C:226:LEU:HD13	1.23	0.98
1:A:126:VAL:HG21	1:A:175:PHE:CE2	2.10	0.87
1:B:175:PHE:HD1	1:B:226:LEU:HD13	1.40	0.83
1:C:175:PHE:HD1	1:C:226:LEU:CD1	1.97	0.78

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	1082/1307 (83%)	1017 (94%)	64 (6%)	1 (0%)	51	82
1	B	1104/1307 (84%)	1041 (94%)	63 (6%)	0	100	100
1	C	1077/1307 (82%)	1018 (94%)	59 (6%)	0	100	100
2	H	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
2	W	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
2	Y	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
3	L	103/106 (97%)	96 (93%)	7 (7%)	0	100	100
3	X	100/106 (94%)	96 (96%)	4 (4%)	0	100	100
3	Z	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
All	All	3938/4614 (85%)	3726 (95%)	211 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	521	PRO

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	955/1126 (85%)	954 (100%)	1 (0%)	93	97
1	B	968/1126 (86%)	966 (100%)	2 (0%)	93	96
1	C	951/1126 (84%)	949 (100%)	2 (0%)	93	96
2	H	102/102 (100%)	102 (100%)	0	100	100
2	W	102/102 (100%)	102 (100%)	0	100	100
2	Y	102/102 (100%)	102 (100%)	0	100	100
3	L	87/88 (99%)	87 (100%)	0	100	100
3	X	86/88 (98%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Z	87/88 (99%)	87 (100%)	0	100	100
All	All	3440/3948 (87%)	3435 (100%)	5 (0%)	93	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	819	GLU
1	B	454	ARG
1	B	529	LYS
1	C	709	ASN
1	C	935	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	914	ASN
1	B	1106	GLN
3	L	50	GLN
1	B	1134	ASN
1	B	804	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

28 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	B	1307	-	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	B	1303	1	14,14,15	0.39	0	17,19,21	0.70	0
4	NAG	B	1302	-	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	1305	-	14,14,15	0.14	0	17,19,21	0.63	0
4	NAG	B	1308	-	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	A	1302	-	14,14,15	0.29	0	17,19,21	0.55	0
4	NAG	B	1306	1	14,14,15	0.53	0	17,19,21	0.51	0
4	NAG	C	1304	-	14,14,15	0.17	0	17,19,21	0.58	0
4	NAG	A	1311	-	14,14,15	0.19	0	17,19,21	0.52	0
4	NAG	C	1305	-	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	C	1306	-	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	A	1305	-	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	A	1307	-	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	A	1306	1	14,14,15	0.31	0	17,19,21	0.42	0
4	NAG	C	1302	-	14,14,15	0.31	0	17,19,21	1.05	1 (5%)
4	NAG	A	1303	-	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	B	1304	-	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	A	1304	-	14,14,15	0.18	0	17,19,21	0.60	0
4	NAG	A	1310	-	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	B	1309	-	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	C	1301	-	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	C	1307	-	14,14,15	0.52	0	17,19,21	0.35	0
4	NAG	A	1309	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	C	1303	-	14,14,15	0.18	0	17,19,21	0.60	0
4	NAG	B	1301	-	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	C	1308	-	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	A	1301	-	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	A	1308	-	14,14,15	0.25	0	17,19,21	0.47	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	B	1307	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1302	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1311	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1305	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	-	-	5/6/23/26	0/1/1/1
4	NAG	A	1303	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1310	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1307	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1301	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1308	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1308	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1302	NAG	C2-N2-C7	3.37	127.71	122.90

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1303	NAG	O5-C5-C6-O6
4	A	1310	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	A	1309	NAG	C4-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1303	NAG	1	0
4	A	1302	NAG	1	0
4	B	1306	NAG	1	0
4	A	1311	NAG	1	0
4	C	1302	NAG	2	0
4	B	1301	NAG	1	0
4	A	1301	NAG	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

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-23489. 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
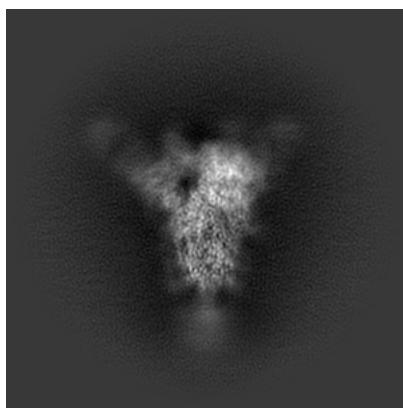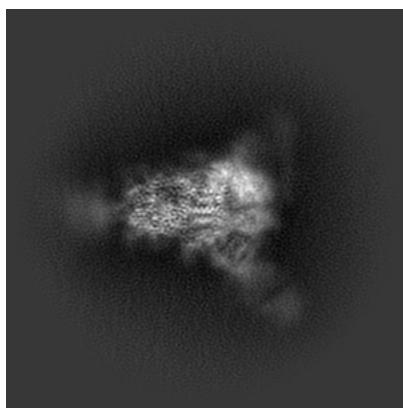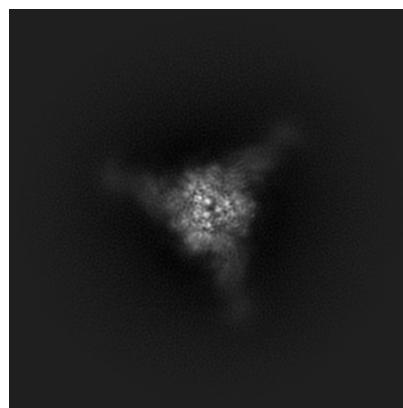
X   Y   Z

6.1.2 Raw map

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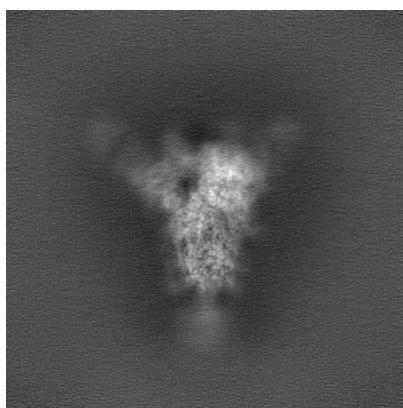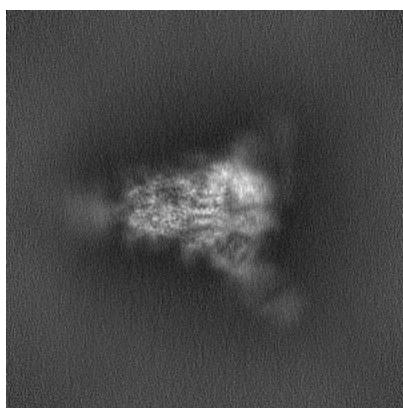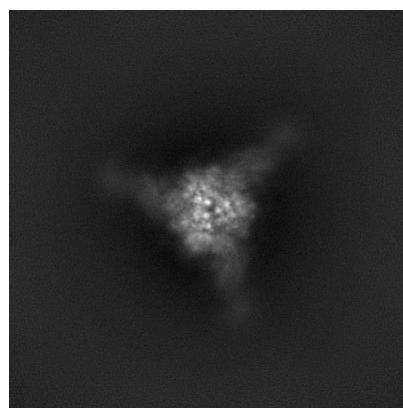
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
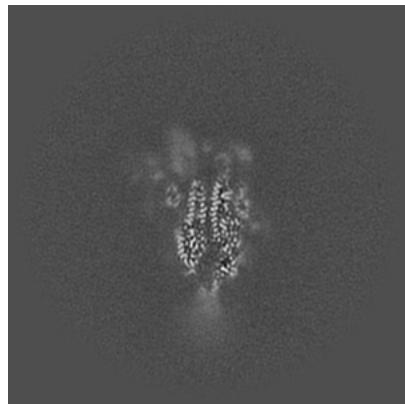
6.2.1 Primary map
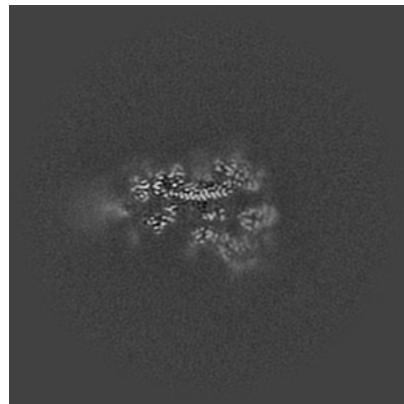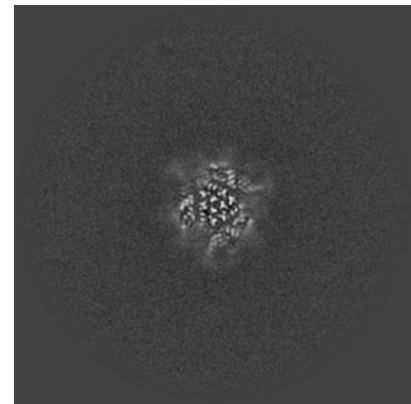
| X Index: 190 | Y Index: 190 | Z Index: 190 |

6.2.2 Raw map
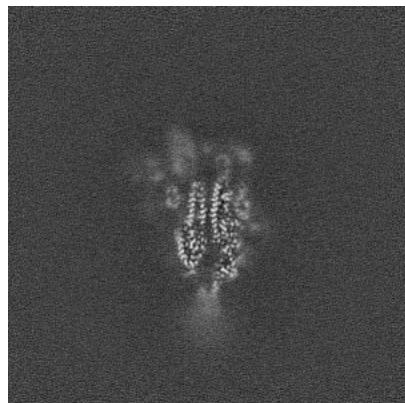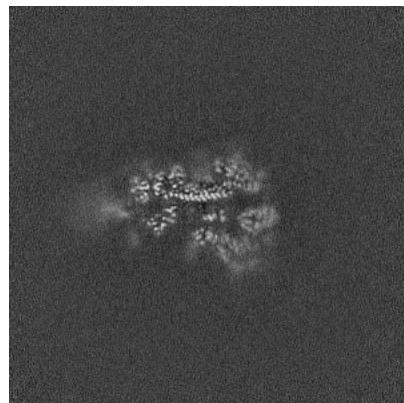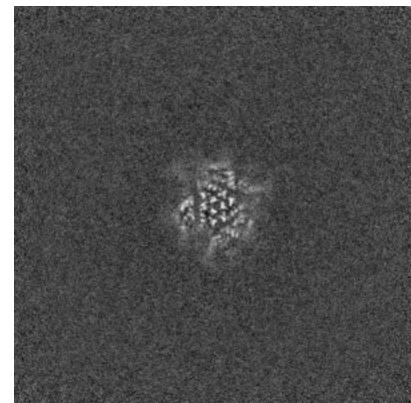
| X Index: 190 | Y Index: 190 | Z Index: 190 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
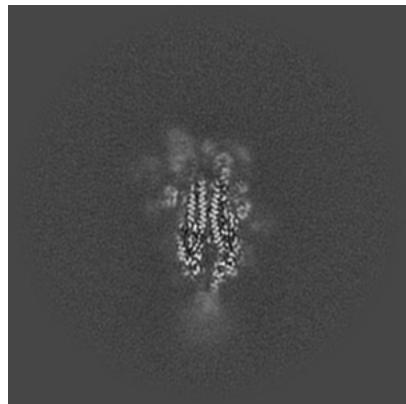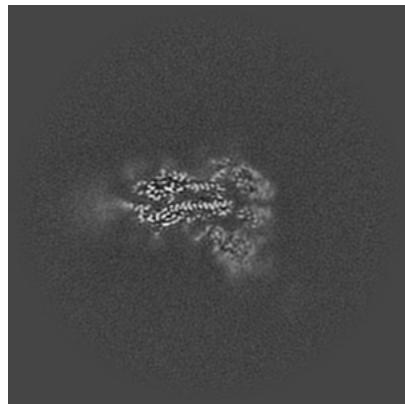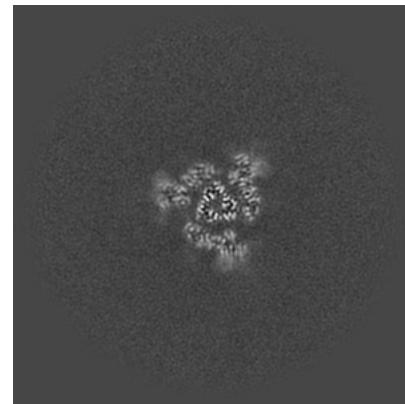
X Index: 188	Y Index: 197	Z Index: 204

6.3.2 Raw map
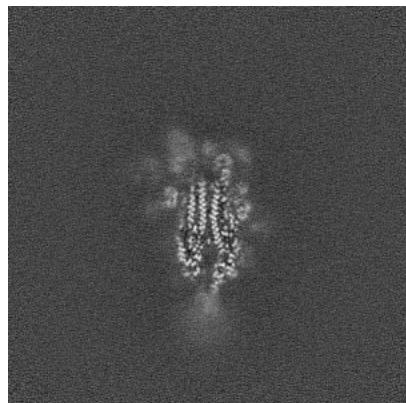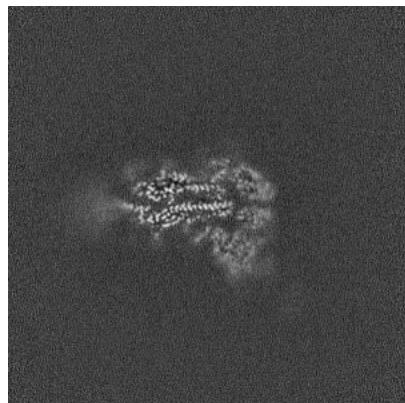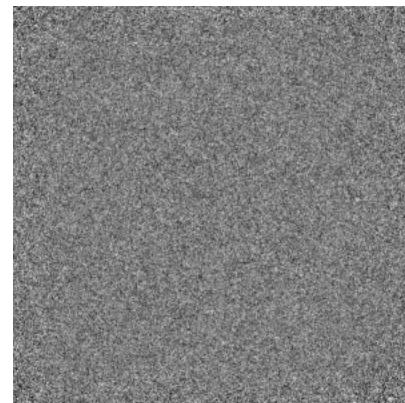
X Index: 188	Y Index: 197	Z Index: 0

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
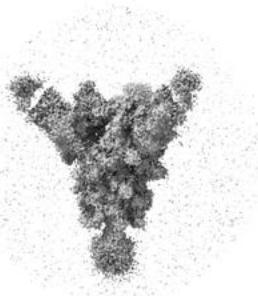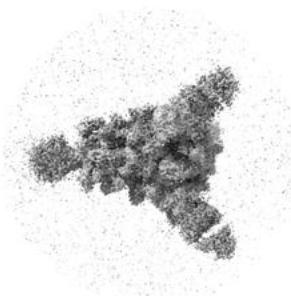
The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map
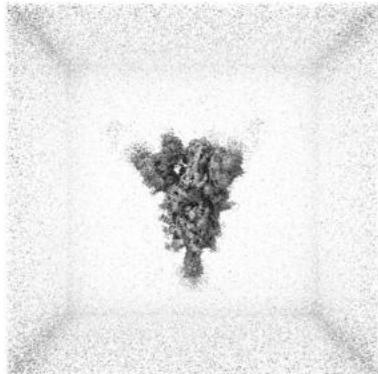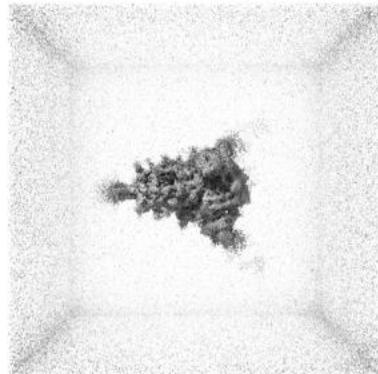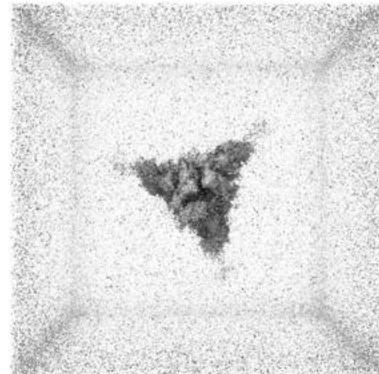
| X | Y | Z |

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 ⓘ

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_23489_msk_1.map ⓘ

X   Y   Z
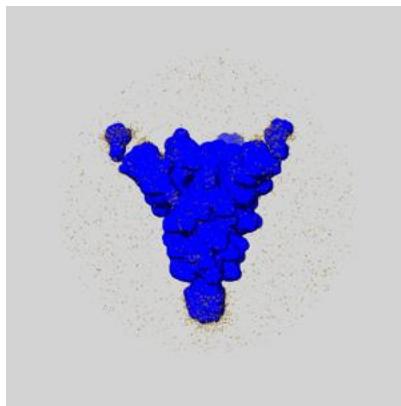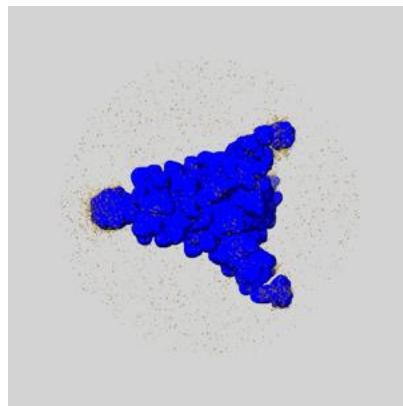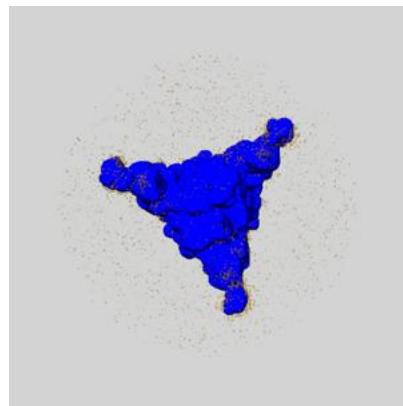
7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

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 ⓘ
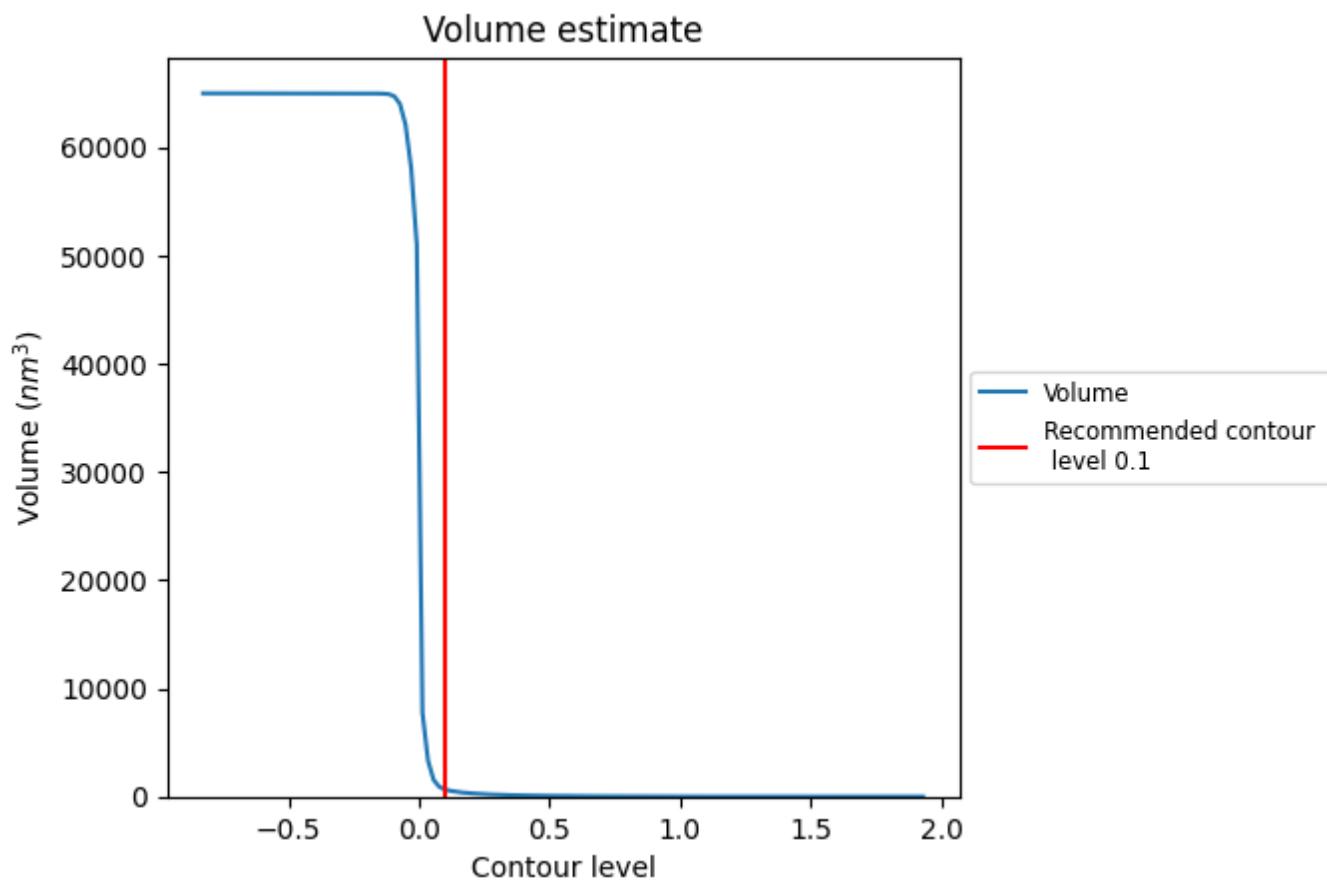
The volume at the recommended contour level is 654 nm^3; this corresponds to an approximate mass of 591 kDa.

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 ⓘ
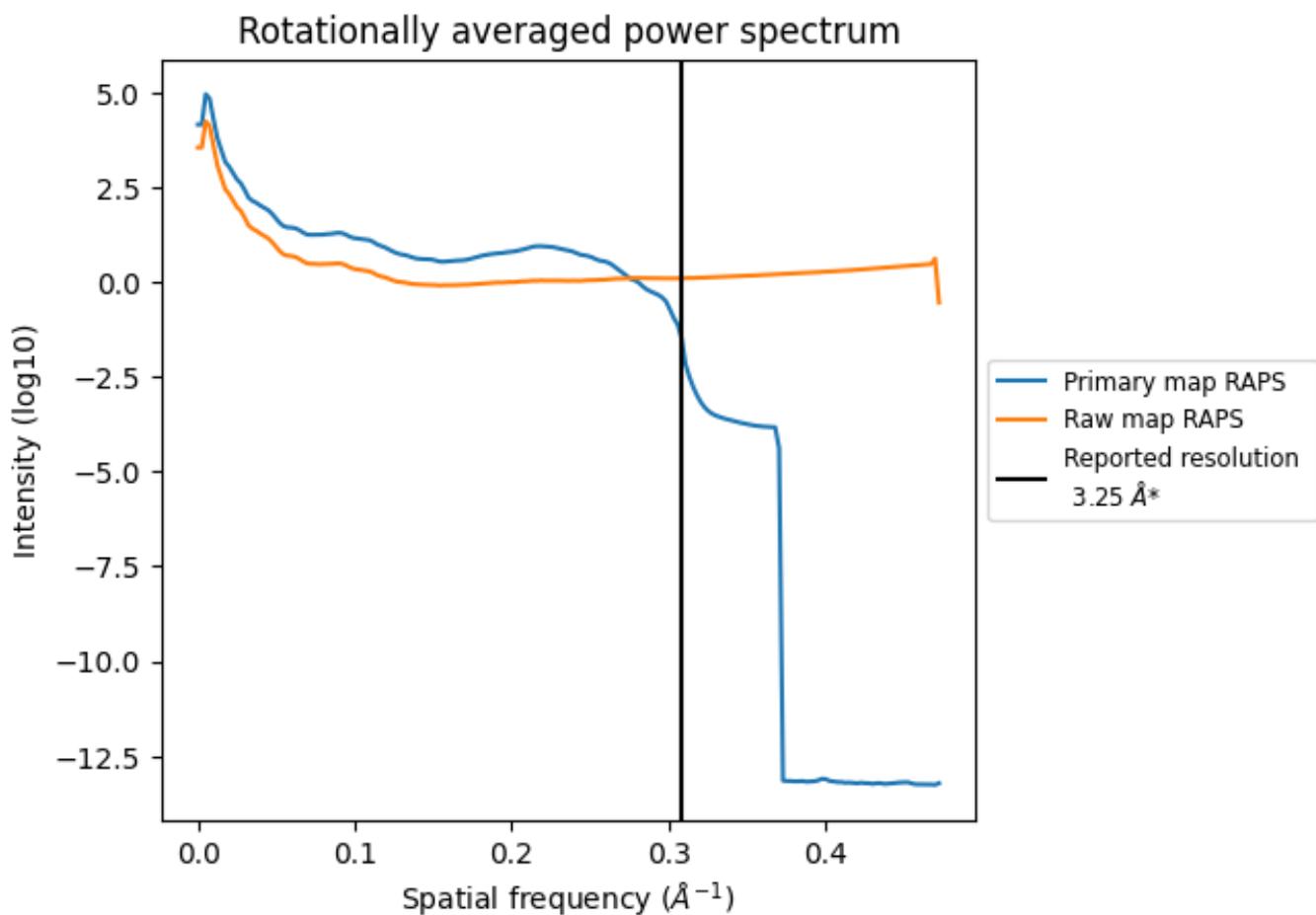
*Reported resolution corresponds to spatial frequency of 0.308 Å^{-1}

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)
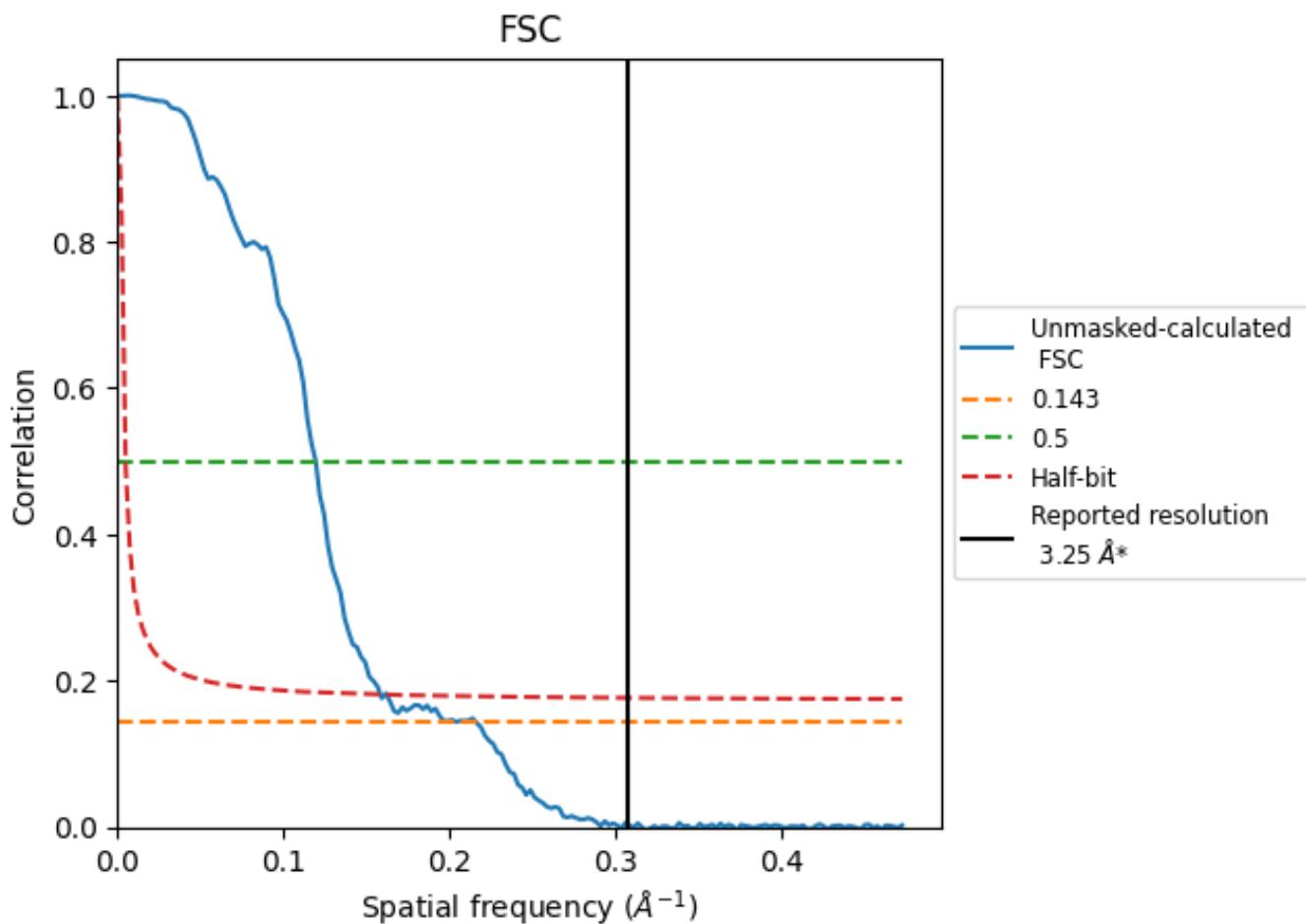
*Reported resolution corresponds to spatial frequency of 0.308 Å^{-1}

8.2   Resolution estimates   (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.63	8.38	6.31

*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 4.63 differs from the reported value 3.25 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-23489 and PDB model 7LQV. Per-residue inclusion information can be found in section 3 on page 15.

9.1   Map-model overlay ⓘ

X   Y   Z
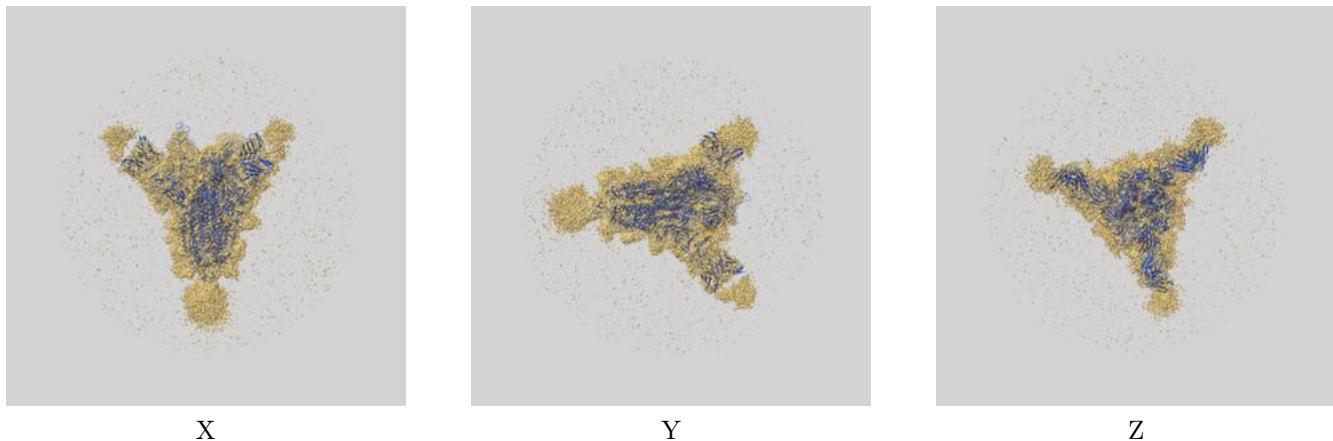
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model   ⓘ

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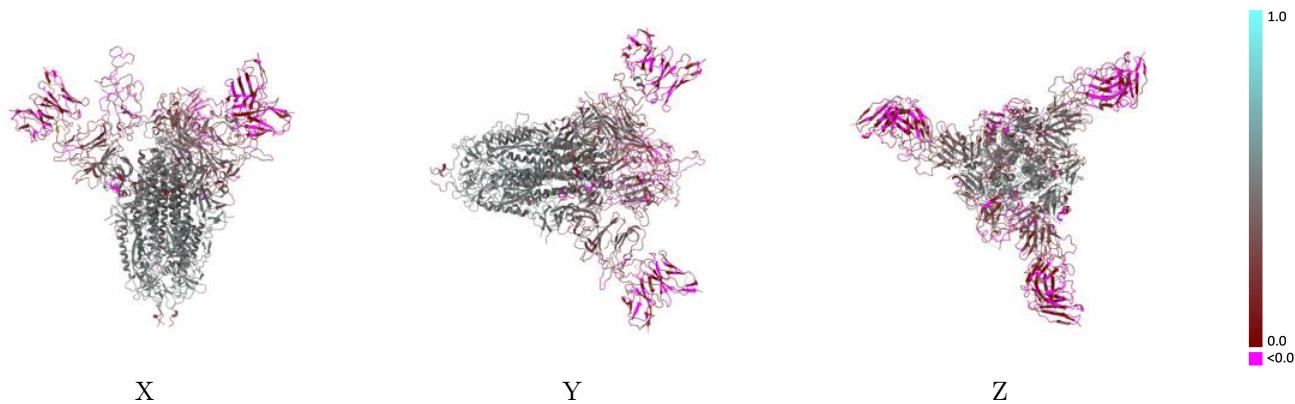
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
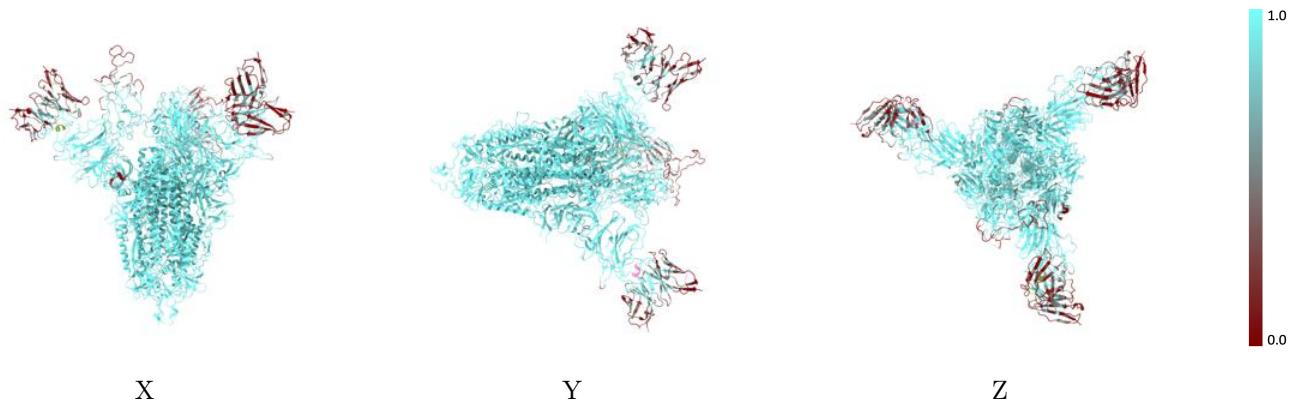
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)
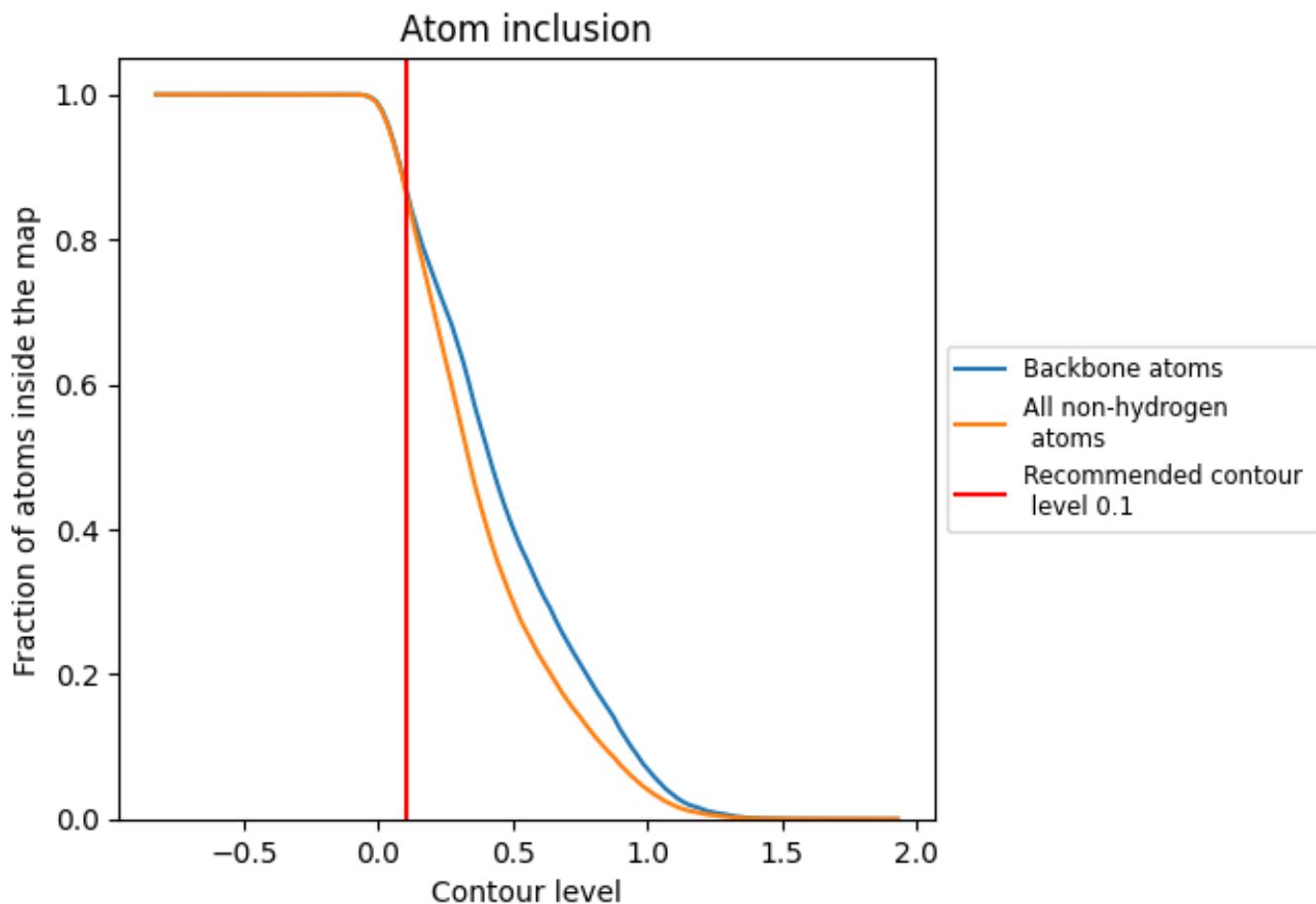
At the recommended contour level, 87% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary   ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8685	0.3180
A	0.9702	0.3810
B	0.9276	0.3570
C	0.9664	0.3830
H	0.3820	0.0100
L	0.3731	0.0090
W	0.5141	0.0520
X	0.4980	0.0870
Y	0.4048	0.0490
Z	0.4236	0.0280

1.0

0.0
<0.0