WORLDWIDE PDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Feb 3, 2025 – 12:22 PM JST

PDB ID	:	8XSD
EMDB ID	:	EMD-38616
Title	:	BA.5 Spike complex with CR9
Authors	:	Feng, L.L.
Deposited on	:	2024-01-09
Resolution	:	3.55 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.

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 3.55 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.
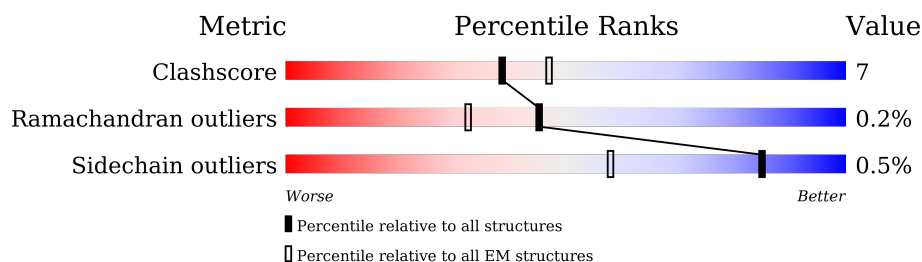
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	1289	58% / 67% 13% • 19%
1	B	1289	69% / 70% 11% 18%
1	C	1289	58% / 71% 11% 19%
2	G	115	100% / 70% 30%
2	H	115	91% / 70% 30%
2	I	115	97% / 74% 26%
3	J	107	100% / 71% 28% •
3	K	107	99% / 77% 22% •

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Mol	Chain	Length	Quality of chain
3	L	107	96% / 78% / 21%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 29708 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	1048	Total 8201	C 5249	N 1363	O 1551	S 38	0	0
1	B	1055	Total 8255	C 5280	N 1373	O 1564	S 38	0	0
1	C	1050	Total 8215	C 5254	N 1367	O 1557	S 37	0	0

There are 372 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	140	ASP	GLY	variant	UNP P0DTC2
A	211	GLY	VAL	variant	UNP P0DTC2
A	337	ASP	GLY	variant	UNP P0DTC2
A	369	PHE	SER	variant	UNP P0DTC2
A	371	PRO	SER	variant	UNP P0DTC2
A	373	PHE	SER	variant	UNP P0DTC2
A	374	ALA	THR	variant	UNP P0DTC2
A	403	ASN	ASP	variant	UNP P0DTC2
A	406	SER	ARG	variant	UNP P0DTC2
A	415	ASN	LYS	variant	UNP P0DTC2
A	438	LYS	ASN	variant	UNP P0DTC2
A	450	ARG	LEU	variant	UNP P0DTC2
A	475	ASN	SER	variant	UNP P0DTC2
A	476	LYS	THR	variant	UNP P0DTC2
A	482	ALA	GLU	variant	UNP P0DTC2
A	484	VAL	PHE	variant	UNP P0DTC2
A	496	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	499	TYR	ASN	variant	UNP P0DTC2
A	503	HIS	TYR	variant	UNP P0DTC2
A	612	GLY	ASP	variant	UNP P0DTC2
A	653	TYR	HIS	variant	UNP P0DTC2
A	656	SER	ASN	variant	UNP P0DTC2
A	677	LYS	ASN	variant	UNP P0DTC2
A	679	HIS	PRO	variant	UNP P0DTC2
A	681	ALA	ARG	variant	UNP P0DTC2
A	683	ALA	ARG	variant	UNP P0DTC2
A	762	LYS	ASN	variant	UNP P0DTC2
A	794	TYR	ASP	variant	UNP P0DTC2
A	815	PRO	PHE	variant	UNP P0DTC2
A	890	PRO	ALA	variant	UNP P0DTC2
A	897	PRO	ALA	variant	UNP P0DTC2
A	940	PRO	ALA	variant	UNP P0DTC2
A	952	HIS	GLN	variant	UNP P0DTC2
A	967	LYS	ASN	variant	UNP P0DTC2
A	984	PRO	LYS	variant	UNP P0DTC2
A	985	PRO	VAL	variant	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	GLY	-	expression tag	UNP P0DTC2
A	1217	SER	-	expression tag	UNP P0DTC2
A	1218	TYR	-	expression tag	UNP P0DTC2
A	1219	ILE	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	GLU	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	ARG	-	expression tag	UNP P0DTC2
A	1225	ASP	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	GLN	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	TYR	-	expression tag	UNP P0DTC2
A	1230	VAL	-	expression tag	UNP P0DTC2
A	1231	ARG	-	expression tag	UNP P0DTC2
A	1232	LYS	-	expression tag	UNP P0DTC2
A	1233	ASP	-	expression tag	UNP P0DTC2
A	1234	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1235	GLU	-	expression tag	UNP P0DTC2
A	1236	TRP	-	expression tag	UNP P0DTC2
A	1237	VAL	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	THR	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	ARG	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	GLU	-	expression tag	UNP P0DTC2
A	1249	VAL	-	expression tag	UNP P0DTC2
A	1250	LEU	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	GLN	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	PRO	-	expression tag	UNP P0DTC2
A	1255	GLY	-	expression tag	UNP P0DTC2
A	1256	TRP	-	expression tag	UNP P0DTC2
A	1257	SER	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	PRO	-	expression tag	UNP P0DTC2
A	1260	GLN	-	expression tag	UNP P0DTC2
A	1261	PHE	-	expression tag	UNP P0DTC2
A	1262	GLU	-	expression tag	UNP P0DTC2
A	1263	LYS	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	GLY	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	SER	-	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	SER	-	expression tag	UNP P0DTC2
A	1275	SER	-	expression tag	UNP P0DTC2
A	1276	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	TRP	-	expression tag	UNP P0DTC2
A	1278	SER	-	expression tag	UNP P0DTC2
A	1279	HIS	-	expression tag	UNP P0DTC2
A	1280	PRO	-	expression tag	UNP P0DTC2
A	1281	GLN	-	expression tag	UNP P0DTC2
A	1282	PHE	-	expression tag	UNP P0DTC2
A	1283	GLU	-	expression tag	UNP P0DTC2
A	1284	LYS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
A	1289	HIS	-	expression tag	UNP P0DTC2
A	1290	HIS	-	expression tag	UNP P0DTC2
A	1291	HIS	-	expression tag	UNP P0DTC2
A	1292	HIS	-	expression tag	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	140	ASP	GLY	variant	UNP P0DTC2
B	211	GLY	VAL	variant	UNP P0DTC2
B	337	ASP	GLY	variant	UNP P0DTC2
B	369	PHE	SER	variant	UNP P0DTC2
B	371	PRO	SER	variant	UNP P0DTC2
B	373	PHE	SER	variant	UNP P0DTC2
B	374	ALA	THR	variant	UNP P0DTC2
B	403	ASN	ASP	variant	UNP P0DTC2
B	406	SER	ARG	variant	UNP P0DTC2
B	415	ASN	LYS	variant	UNP P0DTC2
B	438	LYS	ASN	variant	UNP P0DTC2
B	450	ARG	LEU	variant	UNP P0DTC2
B	475	ASN	SER	variant	UNP P0DTC2
B	476	LYS	THR	variant	UNP P0DTC2
B	482	ALA	GLU	variant	UNP P0DTC2
B	484	VAL	PHE	variant	UNP P0DTC2
B	496	ARG	GLN	variant	UNP P0DTC2
B	499	TYR	ASN	variant	UNP P0DTC2
B	503	HIS	TYR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	612	GLY	ASP	variant	UNP P0DTC2
B	653	TYR	HIS	variant	UNP P0DTC2
B	656	SER	ASN	variant	UNP P0DTC2
B	677	LYS	ASN	variant	UNP P0DTC2
B	679	HIS	PRO	variant	UNP P0DTC2
B	681	ALA	ARG	variant	UNP P0DTC2
B	683	ALA	ARG	variant	UNP P0DTC2
B	762	LYS	ASN	variant	UNP P0DTC2
B	794	TYR	ASP	variant	UNP P0DTC2
B	815	PRO	PHE	variant	UNP P0DTC2
B	890	PRO	ALA	variant	UNP P0DTC2
B	897	PRO	ALA	variant	UNP P0DTC2
B	940	PRO	ALA	variant	UNP P0DTC2
B	952	HIS	GLN	variant	UNP P0DTC2
B	967	LYS	ASN	variant	UNP P0DTC2
B	984	PRO	LYS	variant	UNP P0DTC2
B	985	PRO	VAL	variant	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	GLY	-	expression tag	UNP P0DTC2
B	1217	SER	-	expression tag	UNP P0DTC2
B	1218	TYR	-	expression tag	UNP P0DTC2
B	1219	ILE	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	GLU	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	ARG	-	expression tag	UNP P0DTC2
B	1225	ASP	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	GLN	-	expression tag	UNP P0DTC2
B	1228	ALA	-	expression tag	UNP P0DTC2
B	1229	TYR	-	expression tag	UNP P0DTC2
B	1230	VAL	-	expression tag	UNP P0DTC2
B	1231	ARG	-	expression tag	UNP P0DTC2
B	1232	LYS	-	expression tag	UNP P0DTC2
B	1233	ASP	-	expression tag	UNP P0DTC2
B	1234	GLY	-	expression tag	UNP P0DTC2
B	1235	GLU	-	expression tag	UNP P0DTC2
B	1236	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1237	VAL	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	LEU	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	THR	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	ARG	-	expression tag	UNP P0DTC2
B	1246	SER	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	GLU	-	expression tag	UNP P0DTC2
B	1249	VAL	-	expression tag	UNP P0DTC2
B	1250	LEU	-	expression tag	UNP P0DTC2
B	1251	PHE	-	expression tag	UNP P0DTC2
B	1252	GLN	-	expression tag	UNP P0DTC2
B	1253	GLY	-	expression tag	UNP P0DTC2
B	1254	PRO	-	expression tag	UNP P0DTC2
B	1255	GLY	-	expression tag	UNP P0DTC2
B	1256	TRP	-	expression tag	UNP P0DTC2
B	1257	SER	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	PRO	-	expression tag	UNP P0DTC2
B	1260	GLN	-	expression tag	UNP P0DTC2
B	1261	PHE	-	expression tag	UNP P0DTC2
B	1262	GLU	-	expression tag	UNP P0DTC2
B	1263	LYS	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	GLY	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	SER	-	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	SER	-	expression tag	UNP P0DTC2
B	1275	SER	-	expression tag	UNP P0DTC2
B	1276	ALA	-	expression tag	UNP P0DTC2
B	1277	TRP	-	expression tag	UNP P0DTC2
B	1278	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1279	HIS	-	expression tag	UNP P0DTC2
B	1280	PRO	-	expression tag	UNP P0DTC2
B	1281	GLN	-	expression tag	UNP P0DTC2
B	1282	PHE	-	expression tag	UNP P0DTC2
B	1283	GLU	-	expression tag	UNP P0DTC2
B	1284	LYS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
B	1289	HIS	-	expression tag	UNP P0DTC2
B	1290	HIS	-	expression tag	UNP P0DTC2
B	1291	HIS	-	expression tag	UNP P0DTC2
B	1292	HIS	-	expression tag	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	140	ASP	GLY	variant	UNP P0DTC2
C	211	GLY	VAL	variant	UNP P0DTC2
C	337	ASP	GLY	variant	UNP P0DTC2
C	369	PHE	SER	variant	UNP P0DTC2
C	371	PRO	SER	variant	UNP P0DTC2
C	373	PHE	SER	variant	UNP P0DTC2
C	374	ALA	THR	variant	UNP P0DTC2
C	403	ASN	ASP	variant	UNP P0DTC2
C	406	SER	ARG	variant	UNP P0DTC2
C	415	ASN	LYS	variant	UNP P0DTC2
C	438	LYS	ASN	variant	UNP P0DTC2
C	450	ARG	LEU	variant	UNP P0DTC2
C	475	ASN	SER	variant	UNP P0DTC2
C	476	LYS	THR	variant	UNP P0DTC2
C	482	ALA	GLU	variant	UNP P0DTC2
C	484	VAL	PHE	variant	UNP P0DTC2
C	496	ARG	GLN	variant	UNP P0DTC2
C	499	TYR	ASN	variant	UNP P0DTC2
C	503	HIS	TYR	variant	UNP P0DTC2
C	612	GLY	ASP	variant	UNP P0DTC2
C	653	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	656	SER	ASN	variant	UNP P0DTC2
C	677	LYS	ASN	variant	UNP P0DTC2
C	679	HIS	PRO	variant	UNP P0DTC2
C	681	ALA	ARG	variant	UNP P0DTC2
C	683	ALA	ARG	variant	UNP P0DTC2
C	762	LYS	ASN	variant	UNP P0DTC2
C	794	TYR	ASP	variant	UNP P0DTC2
C	815	PRO	PHE	variant	UNP P0DTC2
C	890	PRO	ALA	variant	UNP P0DTC2
C	897	PRO	ALA	variant	UNP P0DTC2
C	940	PRO	ALA	variant	UNP P0DTC2
C	952	HIS	GLN	variant	UNP P0DTC2
C	967	LYS	ASN	variant	UNP P0DTC2
C	984	PRO	LYS	variant	UNP P0DTC2
C	985	PRO	VAL	variant	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	GLY	-	expression tag	UNP P0DTC2
C	1217	SER	-	expression tag	UNP P0DTC2
C	1218	TYR	-	expression tag	UNP P0DTC2
C	1219	ILE	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	GLU	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	ARG	-	expression tag	UNP P0DTC2
C	1225	ASP	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	GLN	-	expression tag	UNP P0DTC2
C	1228	ALA	-	expression tag	UNP P0DTC2
C	1229	TYR	-	expression tag	UNP P0DTC2
C	1230	VAL	-	expression tag	UNP P0DTC2
C	1231	ARG	-	expression tag	UNP P0DTC2
C	1232	LYS	-	expression tag	UNP P0DTC2
C	1233	ASP	-	expression tag	UNP P0DTC2
C	1234	GLY	-	expression tag	UNP P0DTC2
C	1235	GLU	-	expression tag	UNP P0DTC2
C	1236	TRP	-	expression tag	UNP P0DTC2
C	1237	VAL	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	THR	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	ARG	-	expression tag	UNP P0DTC2
C	1246	SER	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	GLU	-	expression tag	UNP P0DTC2
C	1249	VAL	-	expression tag	UNP P0DTC2
C	1250	LEU	-	expression tag	UNP P0DTC2
C	1251	PHE	-	expression tag	UNP P0DTC2
C	1252	GLN	-	expression tag	UNP P0DTC2
C	1253	GLY	-	expression tag	UNP P0DTC2
C	1254	PRO	-	expression tag	UNP P0DTC2
C	1255	GLY	-	expression tag	UNP P0DTC2
C	1256	TRP	-	expression tag	UNP P0DTC2
C	1257	SER	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	PRO	-	expression tag	UNP P0DTC2
C	1260	GLN	-	expression tag	UNP P0DTC2
C	1261	PHE	-	expression tag	UNP P0DTC2
C	1262	GLU	-	expression tag	UNP P0DTC2
C	1263	LYS	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	GLY	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	SER	-	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	SER	-	expression tag	UNP P0DTC2
C	1275	SER	-	expression tag	UNP P0DTC2
C	1276	ALA	-	expression tag	UNP P0DTC2
C	1277	TRP	-	expression tag	UNP P0DTC2
C	1278	SER	-	expression tag	UNP P0DTC2
C	1279	HIS	-	expression tag	UNP P0DTC2
C	1280	PRO	-	expression tag	UNP P0DTC2

Continued on next page...

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1281	GLN	-	expression tag	UNP P0DTC2
C	1282	PHE	-	expression tag	UNP P0DTC2
C	1283	GLU	-	expression tag	UNP P0DTC2
C	1284	LYS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	HIS	-	expression tag	UNP P0DTC2
C	1289	HIS	-	expression tag	UNP P0DTC2
C	1290	HIS	-	expression tag	UNP P0DTC2
C	1291	HIS	-	expression tag	UNP P0DTC2
C	1292	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called CR9 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	115	Total	C	N	O	S	0	0
			863	540	152	165	6		
2	G	115	Total	C	N	O	S	0	0
			863	540	152	165	6		
2	I	115	Total	C	N	O	S	0	0
			863	540	152	165	6		

- Molecule 3 is a protein called CR9 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	0	0
			816	510	139	165	2		
3	J	107	Total	C	N	O	S	0	0
			816	510	139	165	2		
3	K	107	Total	C	N	O	S	0	0
			816	510	139	165	2		

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

• Molecule 1: Spike glycoprotein

Chain B:

69%

70%   11%   18%

• Molecule 1: Spike glycoprotein

Chain C:

• Molecule 2: CR9 heavy chain

Chain H:

91%

70%   30%

K64 G65 R66 F67 T68 I69 S70 R71 H72 N73 S74 N75 N76 T77 L78 Y79 L80 Q81 M82 N83 S84 L85 R86 P87 E88 D89 T90 A91 M92 Y93 Y94 C95 A96 R97 D98 L99 L100 E101 A102 G103 G104 M105 D106 V107 W108 G109 Q110 G111 T112 A113 V114 T115 V116

• Molecule 2: CR9 heavy chain

Chain G:

100%
70% 30%

V2 Q3 L4 V5 Q6 S7 G8 G9 G10 L11 V12 Q13 P14 G15 G16 S17 L18 R19 L20 S21 C22 A23 A24 S25 G26 I27 T28 V29 S30 A31 N32 Y33 M34 N35 W36 V37 R38 Q39 A40 P41 G42 K43 G44 L45 E46 W47 V48 S49 L50 I51 Y52 A53 G54 G55 S56 T57 F58 Y59 A60 D61

S62 V63 K64 G65 R66 F67 T68 I69 S70 R71 H72 N73 S74 N75 N76 T77 L78 Y79 L80 Q81 M82 N83 S84 L85 R86 P87 E88 D89 T90 A91 M92 Y93 Y94 C95 A96 R97 D98 L99 L100 E101 A102 G103 G104 M105 D106 V107 W108 G109 Q110 G111 T112 A113 V114 T115 V116

• Molecule 2: CR9 heavy chain

Chain I:

97%
74% 26%

V2 Q3 L4 V5 Q6 S7 G8 G9 G10 L11 V12 Q13 P14 G15 G16 S17 L18 R19 L20 S21 C22 A23 A24 S25 G26 I27 T28 V29 S30 A31 N32 Y33 M34 N35 W36 V37 R38 Q39 A40 P41 G42 K43 G44 L45 E46 W47 V48 S49 L50 I51 Y52 A53 G54 G55 Y59 A60 D61 S62 V63

K64 G65 R66 F67 T68 I69 S70 R71 H72 N73 S74 N75 N76 T77 L78 Y79 L80 Q81 M82 N83 S84 L85 R86 P87 E88 D89 T90 A91 M92 Y93 Y94 C95 A96 R97 D98 L99 L100 E101 A102 G103 G104 M105 D106 V107 W108 G109 Q110 G111 T112 A113 V114 T115 V116

• Molecule 3: CR9 light chain

Chain L:

96%
78% 21%

E1 L2 V3 L4 T5 Q6 S7 P8 G9 T10 L11 S12 L13 S14 P15 G16 E17 R18 A19 T20 L21 S22 C23 R24 A25 S26 L27 S28 V29 S30 S31 N32 F33 L34 A35 W36 Y37 Q38 Q39 K40 P41 G42 Q43 A44 P45 R46 L47 L48 V49 Y50 G51 A52 S53 S54 R55 A56 T57 D58 I59 P60

D61 R62 I63 S64 G65 S66 G67 S68 G69 T70 D71 F72 T73 L74 N75 I76 S77 R78 L79 E80 P81 E82 D83 F84 A85 V86 Y87 Y88 C89 Q90 Y91 S92 D93 G94 S95 S96 W97 T98 F99 G100 Q101 G102 T103 R104 L105 E106 I107

• Molecule 3: CR9 light chain

Chain J:

100%
71% 28%

E1 L2 V3 L4 T5 Q6 S7 P8 G9 T10 L11 S12 L13 S14 P15 G16 E17 R18 A19 T20 L21 S22 C23 R24 A25 S26 L27 S28 V29 S30 S31 N32 F33 L34 A35 W36 Y37 Q38 Q39 K40 P41 G42 Q43 A44 P45 R46 L47 L48 V49 Y50 G51 A52 S53 S54 R55 A56 T57 D58 I59 P60

D61 R62 I63 S64 G65 S66 G67 S68 G69 T70 D71 F72 T73 L74 N75 I76 S77 R78 L79 E80 P81 E82 D83 F84 A85 V86 Y87 Y88 C89 Q90 Y91 S92 D93 G94 S95 S96 W97 T98 F99 G100 Q101 G102 T103 R104 L105 E106 I107

• Molecule 3: CR9 light chain

Chain K:

99%

77%   22%   •

E1 L2 V3 L4 T5 Q6 S7 P8 G9 T10 L11 S12 L13 S14 P15 G16 E17 R18 A19 T20 L21 S22 C23 R24 A25 S26 L27 S28 V29 S30 S31 N32 F33 L34 A35 W36 Y37 Q38 Q39 K40 P41 G42 Q43 A44 P45 R46 L47 L48 V49 Y50 G51 A52 S53 S54 R55 A56 T57 D58 I59 P60

D61 R62 I63 S64 G65 S66 G67 S68 G69 T70 D71 F72 T73 L74 N75 I76 S77 R78 L79 E80 P81 E82 D83 F84 A85 V86 Y87 Y88 C89 Q90 Y91 S92 D93 G94 S95 S96 W97 T98 F99 G100 Q101 G102 T103 R104 L105 E106 I107

4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	282590	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	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	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.716	Depositor
Minimum map value	-1.480	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.30	0/8397	0.55	1/11428 (0.0%)
1	B	0.28	0/8452	0.54	0/11502
1	C	0.27	0/8412	0.54	0/11448
2	G	0.26	0/880	0.62	0/1194
2	H	0.27	0/880	0.63	0/1194
2	I	0.26	0/880	0.59	0/1194
3	J	0.26	0/834	0.63	0/1134
3	K	0.26	0/834	0.63	0/1134
3	L	0.27	0/834	0.62	0/1134
All	All	0.28	0/30403	0.56	1/41362 (0.0%)

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	4
1	B	0	1
1	C	0	1
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	LEU	CA-CB-CG	6.75	130.83	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	ARG	Sidechain
1	A	329	ASN	Peptide
1	A	344	ARG	Sidechain
1	A	353	ARG	Sidechain
1	B	326	ARG	Sidechain

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	8201	0	8008	142	0
1	B	8255	0	8060	102	0
1	C	8215	0	8009	88	0
2	G	863	0	838	23	0
2	H	863	0	838	21	0
2	I	863	0	838	19	0
3	J	816	0	785	18	0
3	K	816	0	785	16	0
3	L	816	0	785	13	0
All	All	29708	0	28946	418	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 418 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:348:VAL:HG21	1:A:493:TYR:HE2	1.27	1.00
1:A:329:ASN:HB2	1:A:578:GLN:HA	1.41	0.97
1:A:348:VAL:HB	1:A:451:TYR:HB3	1.45	0.96
1:B:331:THR:HG21	1:B:525:PRO:HG3	1.54	0.89
1:A:348:VAL:HB	1:A:451:TYR:CB	2.05	0.86

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1036/1289 (80%)	956 (92%)	74 (7%)	6 (1%)	22	56
1	B	1045/1289 (81%)	978 (94%)	65 (6%)	2 (0%)	44	74
1	C	1040/1289 (81%)	963 (93%)	76 (7%)	1 (0%)	48	79
2	G	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
2	H	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
2	I	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
3	J	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
3	K	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
3	L	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
All	All	3775/4533 (83%)	3520 (93%)	246 (6%)	9 (0%)	45	74

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	ALA
1	A	343	THR
1	B	579	THR
1	A	331	THR
1	C	330	ILE

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	916/1115 (82%)	907 (99%)	9 (1%)	73	85
1	B	922/1115 (83%)	920 (100%)	2 (0%)	92	97
1	C	916/1115 (82%)	914 (100%)	2 (0%)	92	97
2	G	90/90 (100%)	90 (100%)	0	100	100
2	H	90/90 (100%)	90 (100%)	0	100	100
2	I	90/90 (100%)	90 (100%)	0	100	100
3	J	90/90 (100%)	88 (98%)	2 (2%)	47	70
3	K	90/90 (100%)	88 (98%)	2 (2%)	47	70
3	L	90/90 (100%)	89 (99%)	1 (1%)	70	84
All	All	3294/3885 (85%)	3276 (100%)	18 (0%)	85	93

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	24	ARG
3	K	62	ARG
3	K	24	ARG
1	A	360	VAL
3	L	62	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	578	GLN
1	C	329	ASN
2	H	6	GLN
1	A	407	GLN
1	A	332	ASN

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 (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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-38616. 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
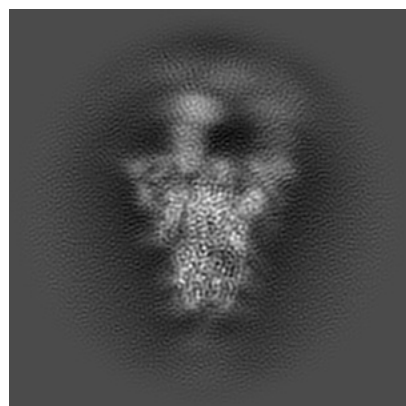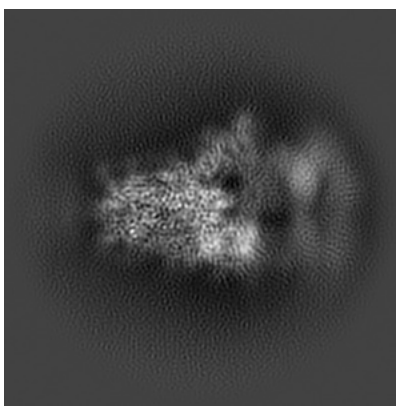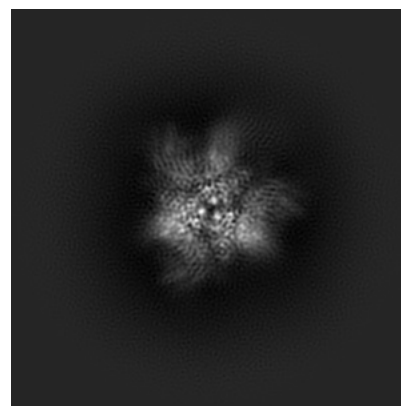
| X | Y | Z |

6.1.2 Raw map

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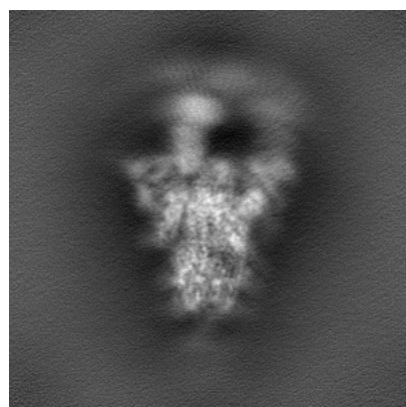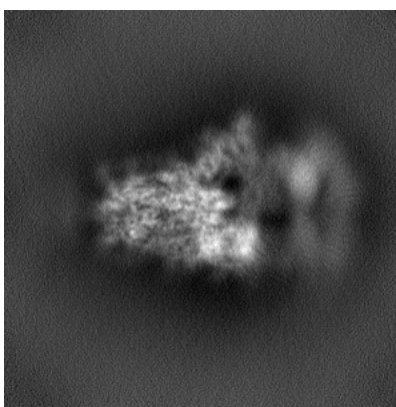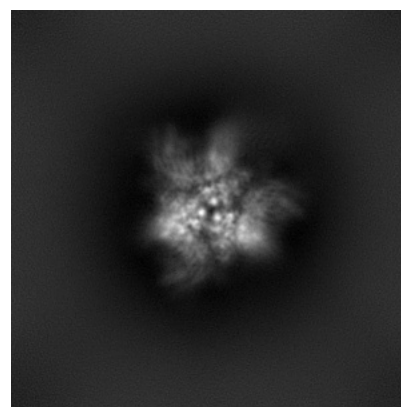
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
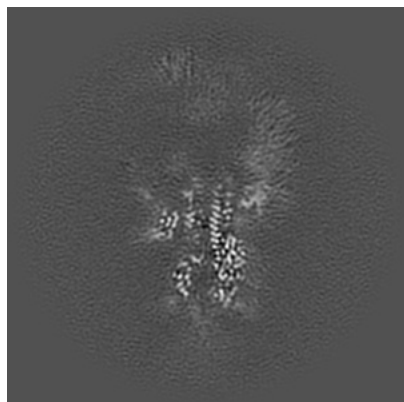
6.2.1 Primary map
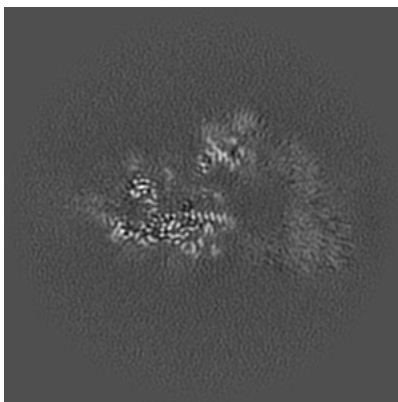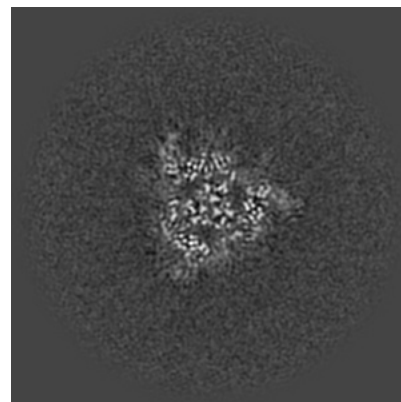
| X Index: 160 | Y Index: 160 | Z Index: 160 |

6.2.2 Raw map
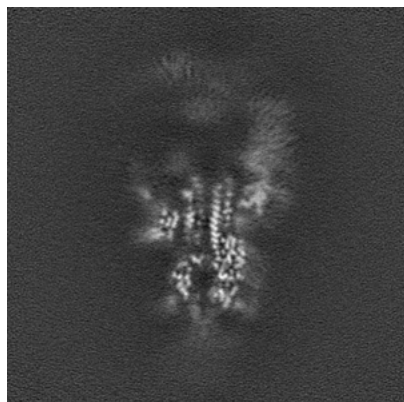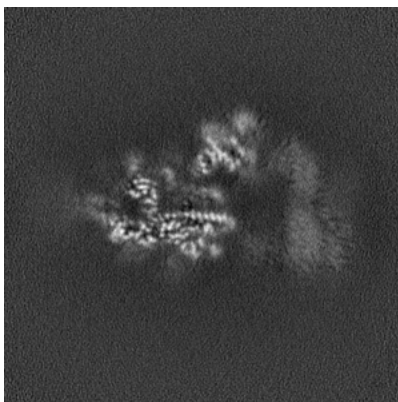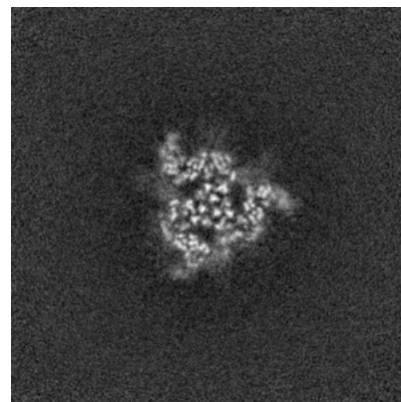
| X Index: 160 | Y Index: 160 | Z Index: 160 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
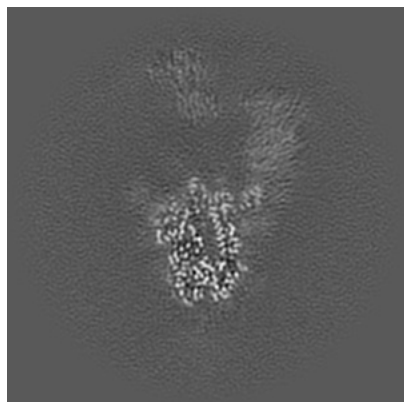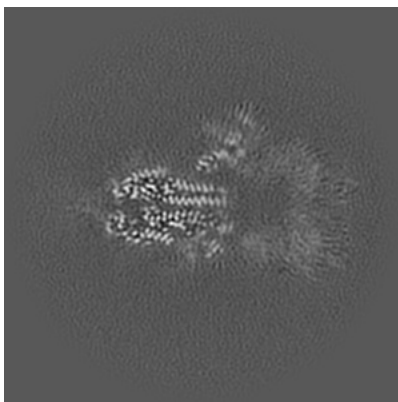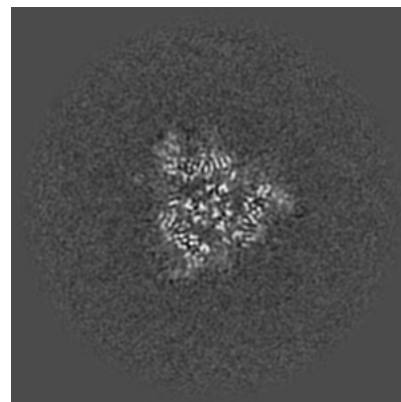
| X Index: 171 | Y Index: 155 | Z Index: 161 |

6.3.2 Raw map
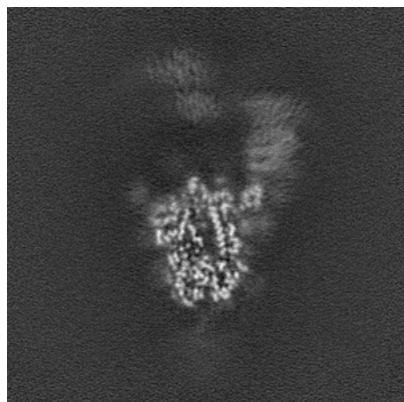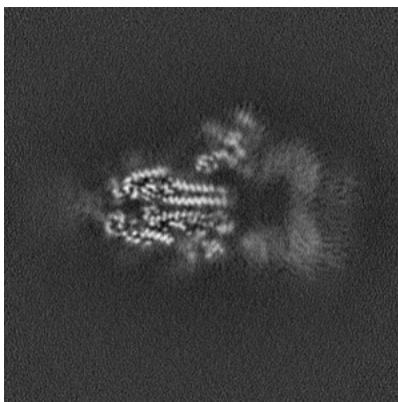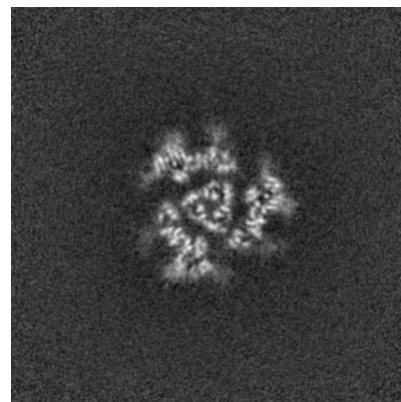
| X Index: 171 | Y Index: 155 | Z Index: 169 |

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map
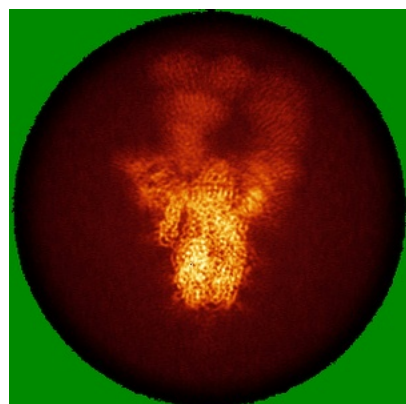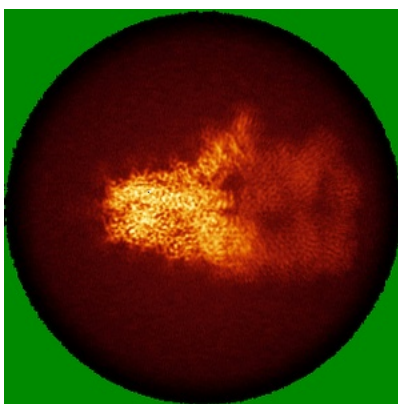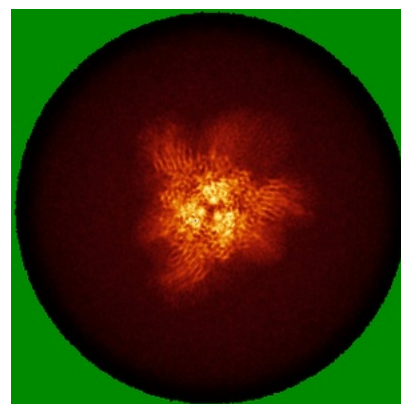
X   Y   Z

6.4.2 Raw map

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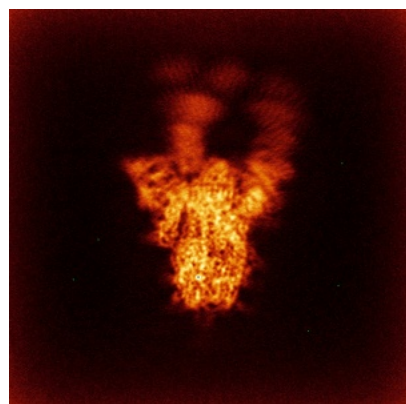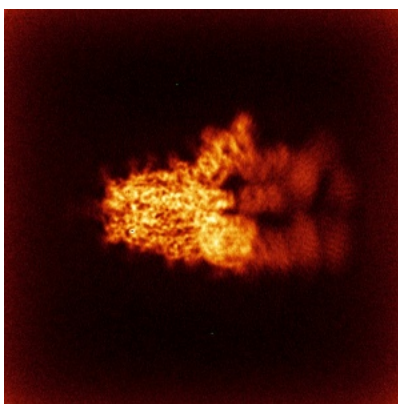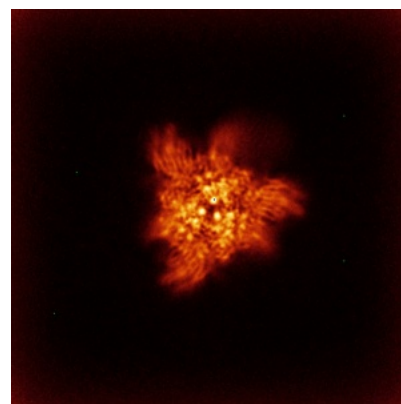
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X　　　　　　　　　　　Y　　　　　　　　　　　Z
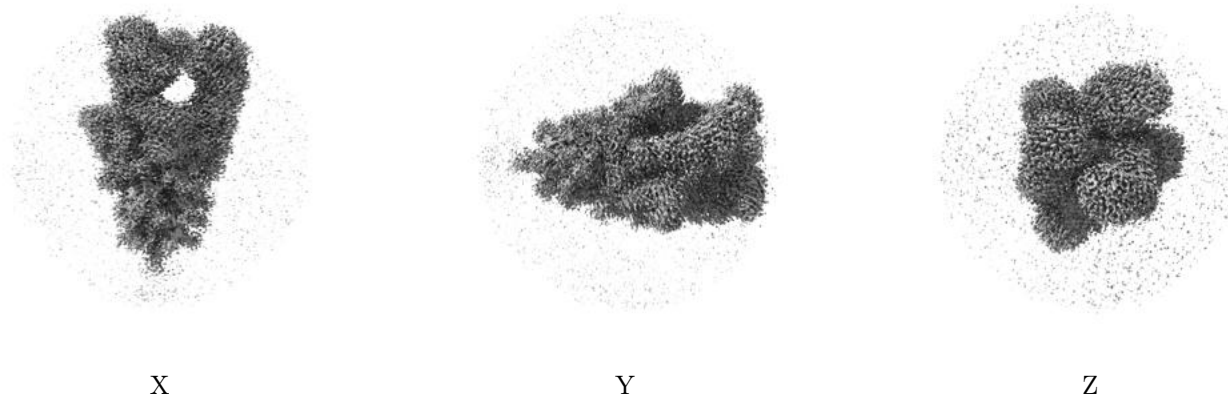
The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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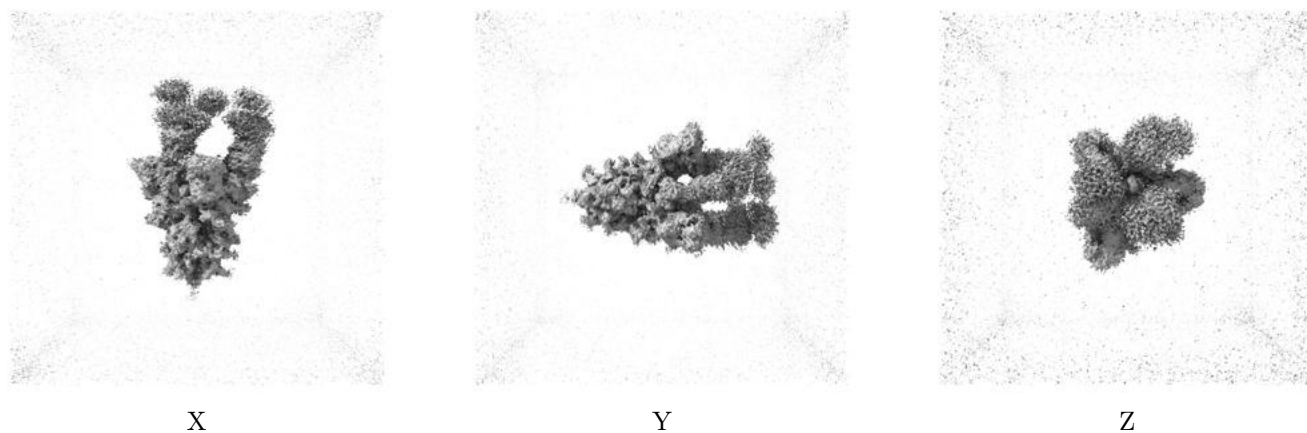
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 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)
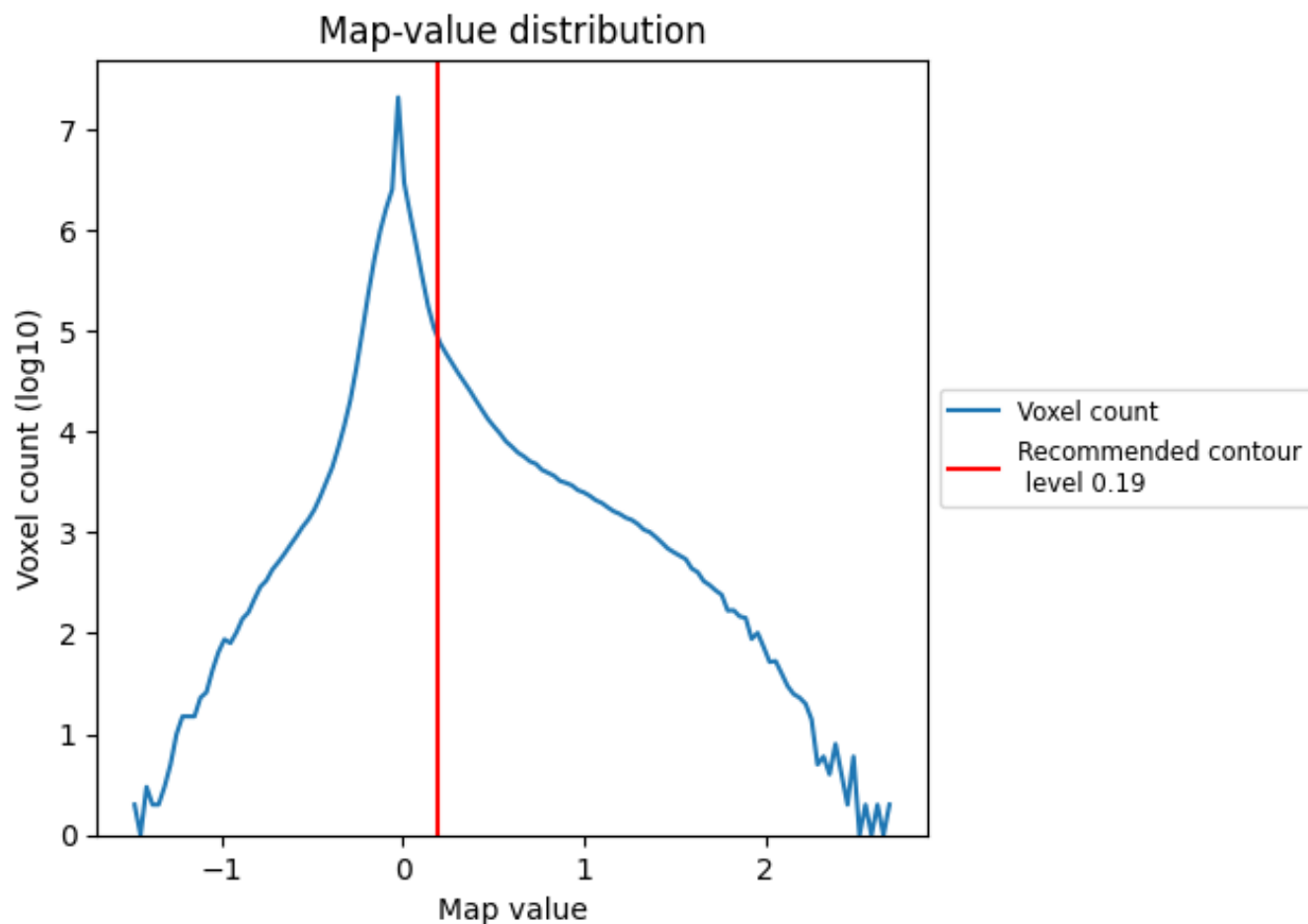
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
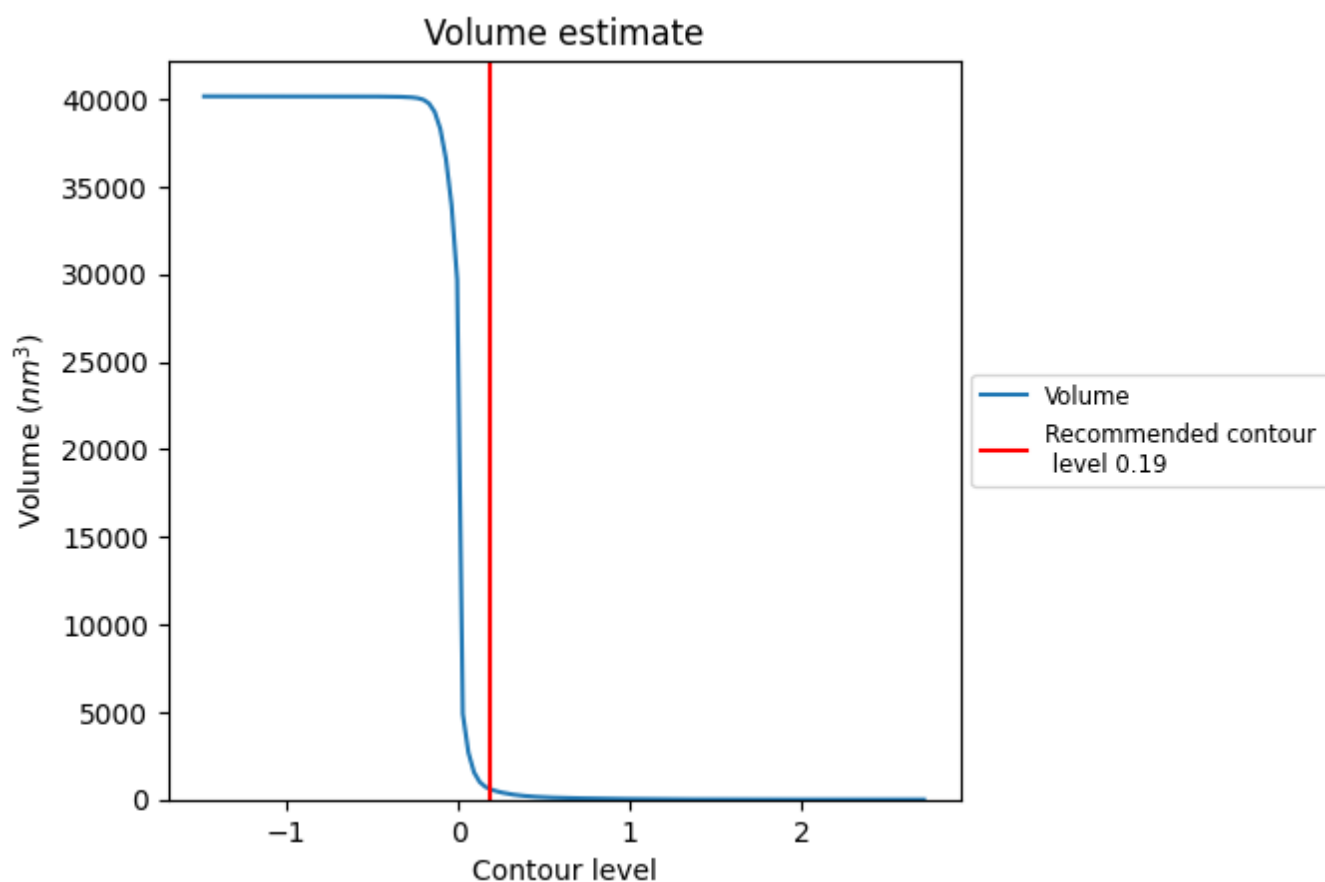
The volume at the recommended contour level is 587 nm^3; this corresponds to an approximate mass of 530 kDa.

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 ⓘ
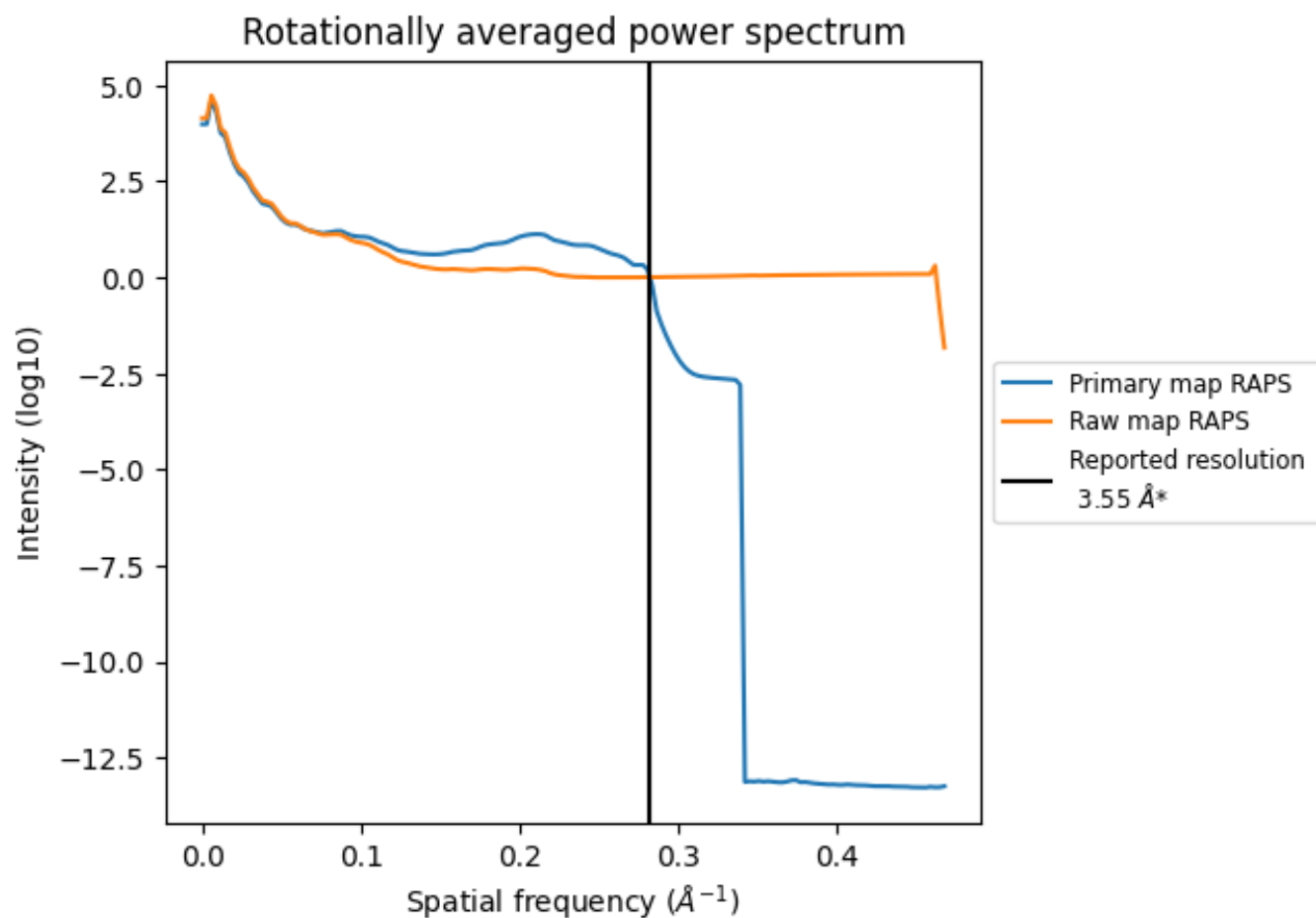
*Reported resolution corresponds to spatial frequency of 0.282 Å^{-1}

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)
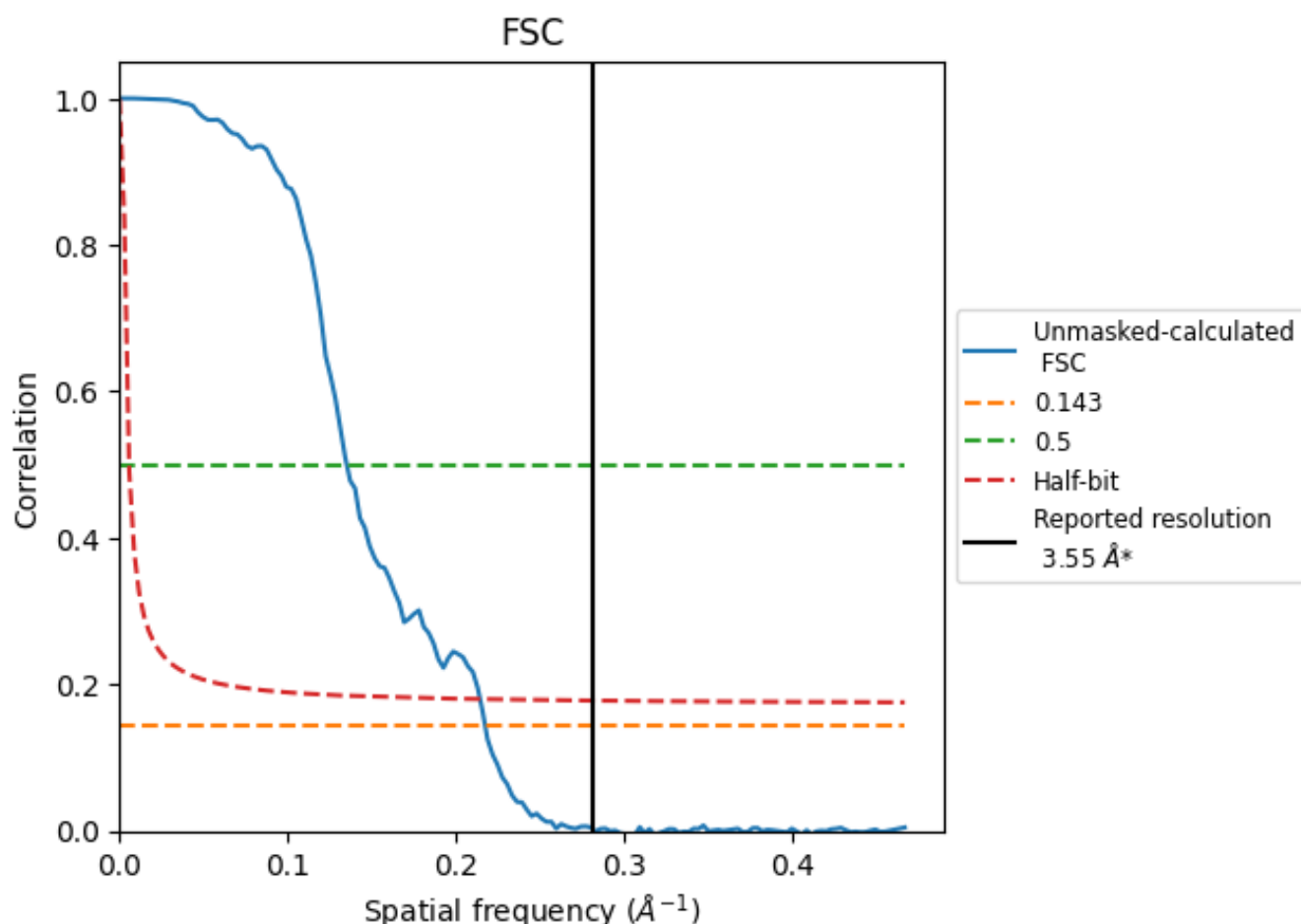
*Reported resolution corresponds to spatial frequency of 0.282 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.60	7.39	4.66

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-38616 and PDB model 8XSD. Per-residue inclusion information can be found in section 3 on page 14.

## 9.1   Map-model overlay ⓘ

| X | Y | Z |
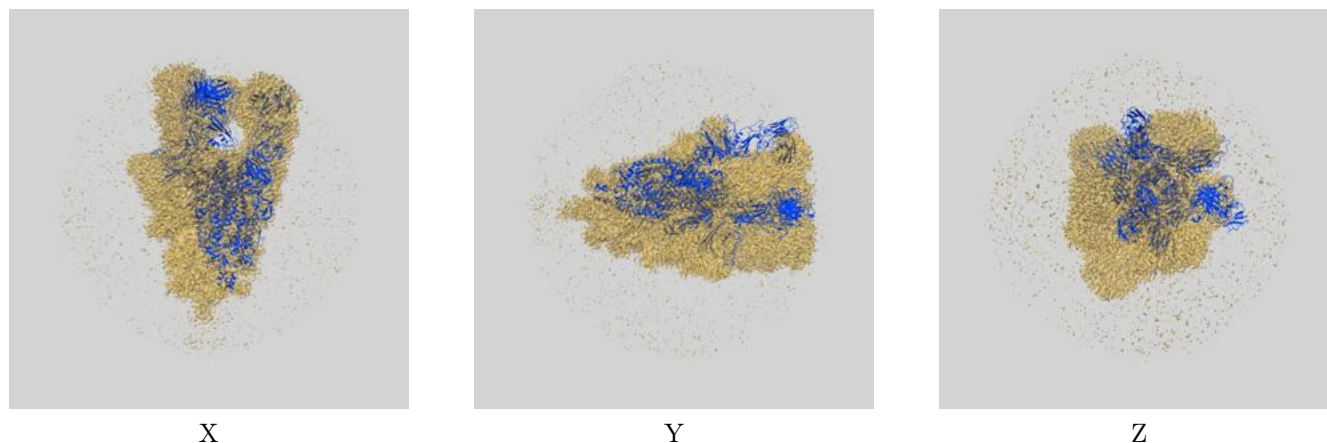
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2   Q-score mapped to coordinate model ⓘ

X   Y   Z
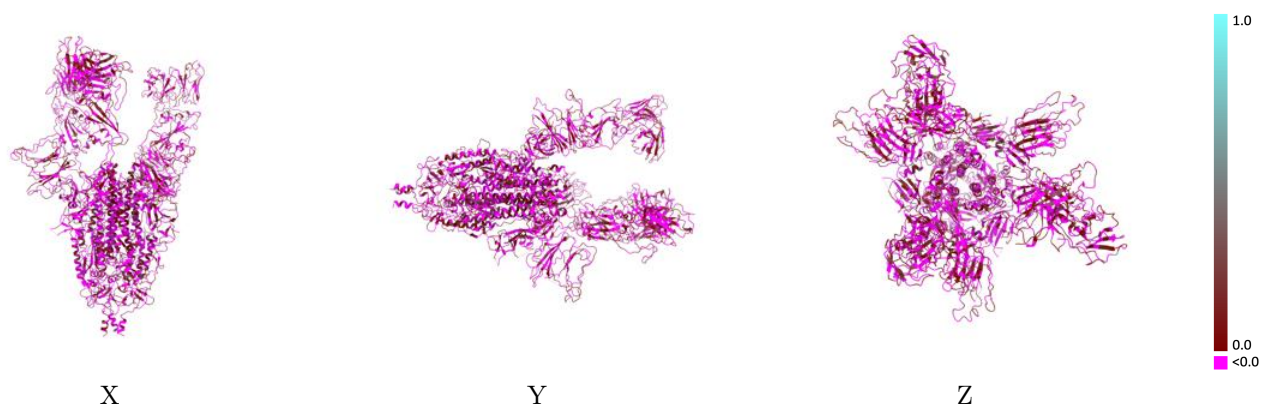
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
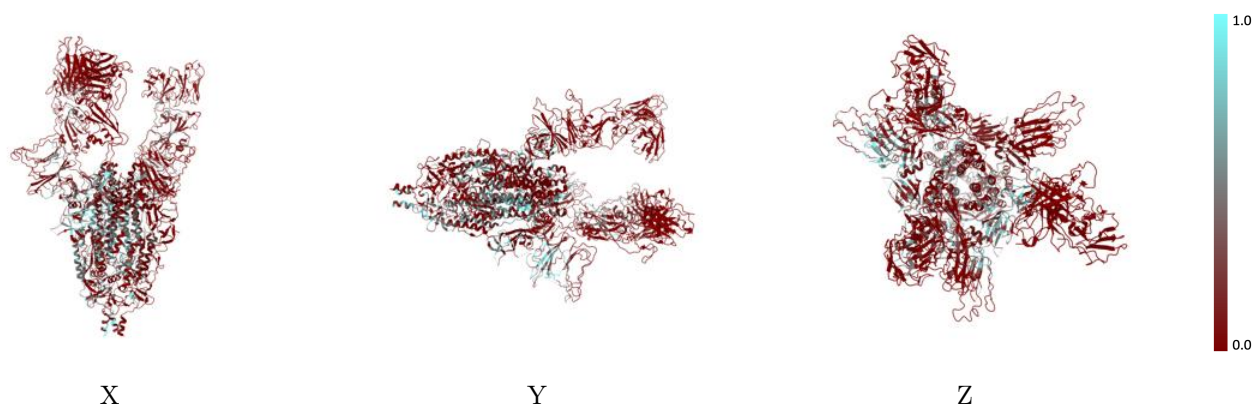
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.19).

9.4 Atom inclusion (i)
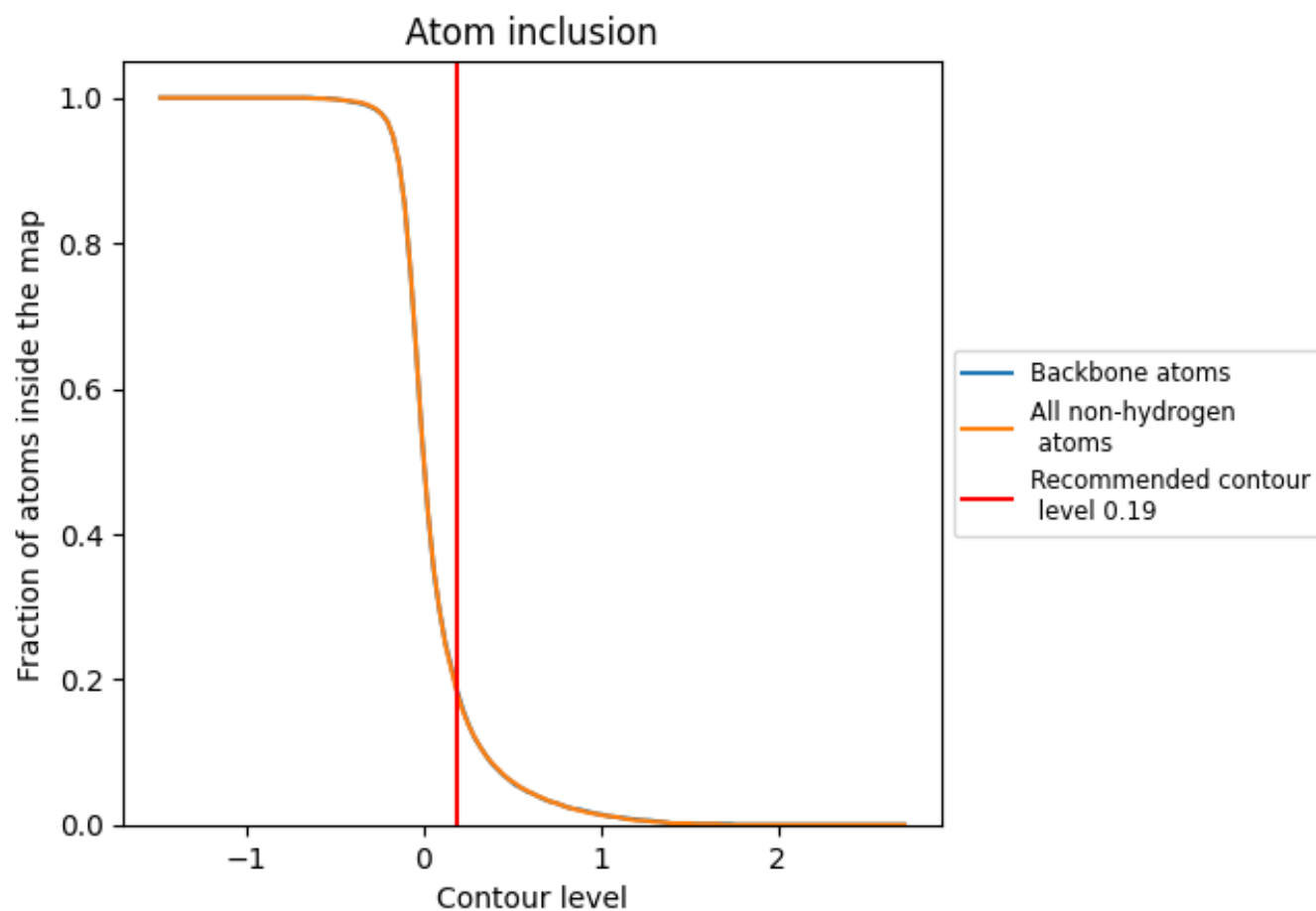
At the recommended contour level, 19% of all backbone atoms, 18% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary　ⓘ

The table lists the average atom inclusion at the recommended contour level (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	▬ 0.1830	▬ -0.0080
A	▬ 0.2390	▬ -0.0080
B	▬ 0.1410	▬ -0.0070
C	▬ 0.2580	▬ -0.0140
G	▬ 0.0020	▬ 0.0170
H	▬ 0.1140	▬ 0.0000
I	▬ 0.0380	▬ -0.0250
J	▬ 0.0000	▬ -0.0120
K	▬ 0.0060	▬ 0.0260
L	▬ 0.0620	▬ 0.0110

1.0

0.0
<0.0