



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:29 AM UTC

PDB ID : 5W9P / pdb_00005w9p
EMDB ID : EMD-8791
Title : MERS S ectodomain trimer in complex with variable domain of neutralizing antibody G4
Authors : Pallesen, J.; Ward, A.B.
Deposited on : 2017-06-23
Resolution : 4.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

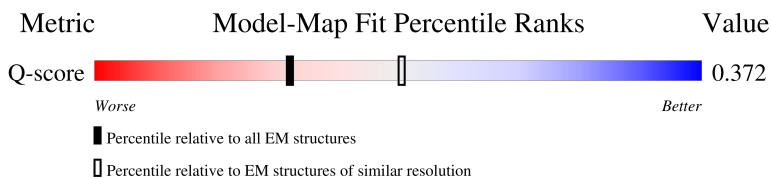
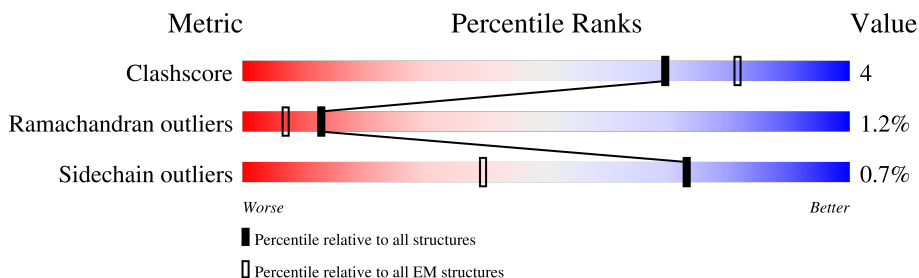
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



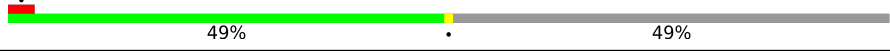
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	1329	
1	B	1329	
1	C	1329	
1	H	1329	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	1329	
1	J	1329	
2	D	233	
2	F	233	
2	K	233	
3	E	218	
3	G	218	
3	L	218	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28014 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	J	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	A	513	Total	C	N	O	S	0	0
			4010	2549	664	774	23		
1	B	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	C	513	Total	C	N	O	S	0	0
			4010	2549	664	774	23		
1	H	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	I	513	Total	C	N	O	S	0	0
			4010	2549	664	774	23		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	506	PHE	LEU	conflict	UNP W5ZZF5
J	748	ALA	ARG	conflict	UNP W5ZZF5
J	751	GLY	ARG	conflict	UNP W5ZZF5
J	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
J	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
J	1292	GLY	-	expression tag	UNP W5ZZF5
J	1293	SER	-	expression tag	UNP W5ZZF5
J	1294	GLY	-	expression tag	UNP W5ZZF5
J	1295	TYR	-	expression tag	UNP W5ZZF5
J	1296	ILE	-	expression tag	UNP W5ZZF5
J	1297	PRO	-	expression tag	UNP W5ZZF5
J	1298	GLU	-	expression tag	UNP W5ZZF5
J	1299	ALA	-	expression tag	UNP W5ZZF5
J	1300	PRO	-	expression tag	UNP W5ZZF5
J	1301	ARG	-	expression tag	UNP W5ZZF5
J	1302	ASP	-	expression tag	UNP W5ZZF5
J	1303	GLY	-	expression tag	UNP W5ZZF5
J	1304	GLN	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	1305	ALA	-	expression tag	UNP W5ZZF5
J	1306	TYR	-	expression tag	UNP W5ZZF5
J	1307	VAL	-	expression tag	UNP W5ZZF5
J	1308	ARG	-	expression tag	UNP W5ZZF5
J	1309	LYS	-	expression tag	UNP W5ZZF5
J	1310	ASP	-	expression tag	UNP W5ZZF5
J	1311	GLY	-	expression tag	UNP W5ZZF5
J	1312	GLU	-	expression tag	UNP W5ZZF5
J	1313	TRP	-	expression tag	UNP W5ZZF5
J	1314	VAL	-	expression tag	UNP W5ZZF5
J	1315	LEU	-	expression tag	UNP W5ZZF5
J	1316	LEU	-	expression tag	UNP W5ZZF5
J	1317	SER	-	expression tag	UNP W5ZZF5
J	1318	THR	-	expression tag	UNP W5ZZF5
J	1319	PHE	-	expression tag	UNP W5ZZF5
J	1320	LEU	-	expression tag	UNP W5ZZF5
J	1321	GLY	-	expression tag	UNP W5ZZF5
J	1322	ARG	-	expression tag	UNP W5ZZF5
J	1323	SER	-	expression tag	UNP W5ZZF5
J	1324	LEU	-	expression tag	UNP W5ZZF5
J	1325	GLU	-	expression tag	UNP W5ZZF5
J	1326	VAL	-	expression tag	UNP W5ZZF5
J	1327	LEU	-	expression tag	UNP W5ZZF5
J	1328	PHE	-	expression tag	UNP W5ZZF5
J	1329	GLN	-	expression tag	UNP W5ZZF5
A	506	PHE	LEU	conflict	UNP W5ZZF5
A	748	ALA	ARG	conflict	UNP W5ZZF5
A	751	GLY	ARG	conflict	UNP W5ZZF5
A	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
A	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
A	1292	GLY	-	expression tag	UNP W5ZZF5
A	1293	SER	-	expression tag	UNP W5ZZF5
A	1294	GLY	-	expression tag	UNP W5ZZF5
A	1295	TYR	-	expression tag	UNP W5ZZF5
A	1296	ILE	-	expression tag	UNP W5ZZF5
A	1297	PRO	-	expression tag	UNP W5ZZF5
A	1298	GLU	-	expression tag	UNP W5ZZF5
A	1299	ALA	-	expression tag	UNP W5ZZF5
A	1300	PRO	-	expression tag	UNP W5ZZF5
A	1301	ARG	-	expression tag	UNP W5ZZF5
A	1302	ASP	-	expression tag	UNP W5ZZF5
A	1303	GLY	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1304	GLN	-	expression tag	UNP W5ZZF5
A	1305	ALA	-	expression tag	UNP W5ZZF5
A	1306	TYR	-	expression tag	UNP W5ZZF5
A	1307	VAL	-	expression tag	UNP W5ZZF5
A	1308	ARG	-	expression tag	UNP W5ZZF5
A	1309	LYS	-	expression tag	UNP W5ZZF5
A	1310	ASP	-	expression tag	UNP W5ZZF5
A	1311	GLY	-	expression tag	UNP W5ZZF5
A	1312	GLU	-	expression tag	UNP W5ZZF5
A	1313	TRP	-	expression tag	UNP W5ZZF5
A	1314	VAL	-	expression tag	UNP W5ZZF5
A	1315	LEU	-	expression tag	UNP W5ZZF5
A	1316	LEU	-	expression tag	UNP W5ZZF5
A	1317	SER	-	expression tag	UNP W5ZZF5
A	1318	THR	-	expression tag	UNP W5ZZF5
A	1319	PHE	-	expression tag	UNP W5ZZF5
A	1320	LEU	-	expression tag	UNP W5ZZF5
A	1321	GLY	-	expression tag	UNP W5ZZF5
A	1322	ARG	-	expression tag	UNP W5ZZF5
A	1323	SER	-	expression tag	UNP W5ZZF5
A	1324	LEU	-	expression tag	UNP W5ZZF5
A	1325	GLU	-	expression tag	UNP W5ZZF5
A	1326	VAL	-	expression tag	UNP W5ZZF5
A	1327	LEU	-	expression tag	UNP W5ZZF5
A	1328	PHE	-	expression tag	UNP W5ZZF5
A	1329	GLN	-	expression tag	UNP W5ZZF5
B	506	PHE	LEU	conflict	UNP W5ZZF5
B	748	ALA	ARG	conflict	UNP W5ZZF5
B	751	GLY	ARG	conflict	UNP W5ZZF5
B	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
B	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
B	1292	GLY	-	expression tag	UNP W5ZZF5
B	1293	SER	-	expression tag	UNP W5ZZF5
B	1294	GLY	-	expression tag	UNP W5ZZF5
B	1295	TYR	-	expression tag	UNP W5ZZF5
B	1296	ILE	-	expression tag	UNP W5ZZF5
B	1297	PRO	-	expression tag	UNP W5ZZF5
B	1298	GLU	-	expression tag	UNP W5ZZF5
B	1299	ALA	-	expression tag	UNP W5ZZF5
B	1300	PRO	-	expression tag	UNP W5ZZF5
B	1301	ARG	-	expression tag	UNP W5ZZF5
B	1302	ASP	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1303	GLY	-	expression tag	UNP W5ZZF5
B	1304	GLN	-	expression tag	UNP W5ZZF5
B	1305	ALA	-	expression tag	UNP W5ZZF5
B	1306	TYR	-	expression tag	UNP W5ZZF5
B	1307	VAL	-	expression tag	UNP W5ZZF5
B	1308	ARG	-	expression tag	UNP W5ZZF5
B	1309	LYS	-	expression tag	UNP W5ZZF5
B	1310	ASP	-	expression tag	UNP W5ZZF5
B	1311	GLY	-	expression tag	UNP W5ZZF5
B	1312	GLU	-	expression tag	UNP W5ZZF5
B	1313	TRP	-	expression tag	UNP W5ZZF5
B	1314	VAL	-	expression tag	UNP W5ZZF5
B	1315	LEU	-	expression tag	UNP W5ZZF5
B	1316	LEU	-	expression tag	UNP W5ZZF5
B	1317	SER	-	expression tag	UNP W5ZZF5
B	1318	THR	-	expression tag	UNP W5ZZF5
B	1319	PHE	-	expression tag	UNP W5ZZF5
B	1320	LEU	-	expression tag	UNP W5ZZF5
B	1321	GLY	-	expression tag	UNP W5ZZF5
B	1322	ARG	-	expression tag	UNP W5ZZF5
B	1323	SER	-	expression tag	UNP W5ZZF5
B	1324	LEU	-	expression tag	UNP W5ZZF5
B	1325	GLU	-	expression tag	UNP W5ZZF5
B	1326	VAL	-	expression tag	UNP W5ZZF5
B	1327	LEU	-	expression tag	UNP W5ZZF5
B	1328	PHE	-	expression tag	UNP W5ZZF5
B	1329	GLN	-	expression tag	UNP W5ZZF5
C	506	PHE	LEU	conflict	UNP W5ZZF5
C	748	ALA	ARG	conflict	UNP W5ZZF5
C	751	GLY	ARG	conflict	UNP W5ZZF5
C	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
C	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
C	1292	GLY	-	expression tag	UNP W5ZZF5
C	1293	SER	-	expression tag	UNP W5ZZF5
C	1294	GLY	-	expression tag	UNP W5ZZF5
C	1295	TYR	-	expression tag	UNP W5ZZF5
C	1296	ILE	-	expression tag	UNP W5ZZF5
C	1297	PRO	-	expression tag	UNP W5ZZF5
C	1298	GLU	-	expression tag	UNP W5ZZF5
C	1299	ALA	-	expression tag	UNP W5ZZF5
C	1300	PRO	-	expression tag	UNP W5ZZF5
C	1301	ARG	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1302	ASP	-	expression tag	UNP W5ZZF5
C	1303	GLY	-	expression tag	UNP W5ZZF5
C	1304	GLN	-	expression tag	UNP W5ZZF5
C	1305	ALA	-	expression tag	UNP W5ZZF5
C	1306	TYR	-	expression tag	UNP W5ZZF5
C	1307	VAL	-	expression tag	UNP W5ZZF5
C	1308	ARG	-	expression tag	UNP W5ZZF5
C	1309	LYS	-	expression tag	UNP W5ZZF5
C	1310	ASP	-	expression tag	UNP W5ZZF5
C	1311	GLY	-	expression tag	UNP W5ZZF5
C	1312	GLU	-	expression tag	UNP W5ZZF5
C	1313	TRP	-	expression tag	UNP W5ZZF5
C	1314	VAL	-	expression tag	UNP W5ZZF5
C	1315	LEU	-	expression tag	UNP W5ZZF5
C	1316	LEU	-	expression tag	UNP W5ZZF5
C	1317	SER	-	expression tag	UNP W5ZZF5
C	1318	THR	-	expression tag	UNP W5ZZF5
C	1319	PHE	-	expression tag	UNP W5ZZF5
C	1320	LEU	-	expression tag	UNP W5ZZF5
C	1321	GLY	-	expression tag	UNP W5ZZF5
C	1322	ARG	-	expression tag	UNP W5ZZF5
C	1323	SER	-	expression tag	UNP W5ZZF5
C	1324	LEU	-	expression tag	UNP W5ZZF5
C	1325	GLU	-	expression tag	UNP W5ZZF5
C	1326	VAL	-	expression tag	UNP W5ZZF5
C	1327	LEU	-	expression tag	UNP W5ZZF5
C	1328	PHE	-	expression tag	UNP W5ZZF5
C	1329	GLN	-	expression tag	UNP W5ZZF5
H	506	PHE	LEU	conflict	UNP W5ZZF5
H	748	ALA	ARG	conflict	UNP W5ZZF5
H	751	GLY	ARG	conflict	UNP W5ZZF5
H	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
H	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
H	1292	GLY	-	expression tag	UNP W5ZZF5
H	1293	SER	-	expression tag	UNP W5ZZF5
H	1294	GLY	-	expression tag	UNP W5ZZF5
H	1295	TYR	-	expression tag	UNP W5ZZF5
H	1296	ILE	-	expression tag	UNP W5ZZF5
H	1297	PRO	-	expression tag	UNP W5ZZF5
H	1298	GLU	-	expression tag	UNP W5ZZF5
H	1299	ALA	-	expression tag	UNP W5ZZF5
H	1300	PRO	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	1301	ARG	-	expression tag	UNP W5ZZF5
H	1302	ASP	-	expression tag	UNP W5ZZF5
H	1303	GLY	-	expression tag	UNP W5ZZF5
H	1304	GLN	-	expression tag	UNP W5ZZF5
H	1305	ALA	-	expression tag	UNP W5ZZF5
H	1306	TYR	-	expression tag	UNP W5ZZF5
H	1307	VAL	-	expression tag	UNP W5ZZF5
H	1308	ARG	-	expression tag	UNP W5ZZF5
H	1309	LYS	-	expression tag	UNP W5ZZF5
H	1310	ASP	-	expression tag	UNP W5ZZF5
H	1311	GLY	-	expression tag	UNP W5ZZF5
H	1312	GLU	-	expression tag	UNP W5ZZF5
H	1313	TRP	-	expression tag	UNP W5ZZF5
H	1314	VAL	-	expression tag	UNP W5ZZF5
H	1315	LEU	-	expression tag	UNP W5ZZF5
H	1316	LEU	-	expression tag	UNP W5ZZF5
H	1317	SER	-	expression tag	UNP W5ZZF5
H	1318	THR	-	expression tag	UNP W5ZZF5
H	1319	PHE	-	expression tag	UNP W5ZZF5
H	1320	LEU	-	expression tag	UNP W5ZZF5
H	1321	GLY	-	expression tag	UNP W5ZZF5
H	1322	ARG	-	expression tag	UNP W5ZZF5
H	1323	SER	-	expression tag	UNP W5ZZF5
H	1324	LEU	-	expression tag	UNP W5ZZF5
H	1325	GLU	-	expression tag	UNP W5ZZF5
H	1326	VAL	-	expression tag	UNP W5ZZF5
H	1327	LEU	-	expression tag	UNP W5ZZF5
H	1328	PHE	-	expression tag	UNP W5ZZF5
H	1329	GLN	-	expression tag	UNP W5ZZF5
I	506	PHE	LEU	conflict	UNP W5ZZF5
I	748	ALA	ARG	conflict	UNP W5ZZF5
I	751	GLY	ARG	conflict	UNP W5ZZF5
I	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
I	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
I	1292	GLY	-	expression tag	UNP W5ZZF5
I	1293	SER	-	expression tag	UNP W5ZZF5
I	1294	GLY	-	expression tag	UNP W5ZZF5
I	1295	TYR	-	expression tag	UNP W5ZZF5
I	1296	ILE	-	expression tag	UNP W5ZZF5
I	1297	PRO	-	expression tag	UNP W5ZZF5
I	1298	GLU	-	expression tag	UNP W5ZZF5
I	1299	ALA	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

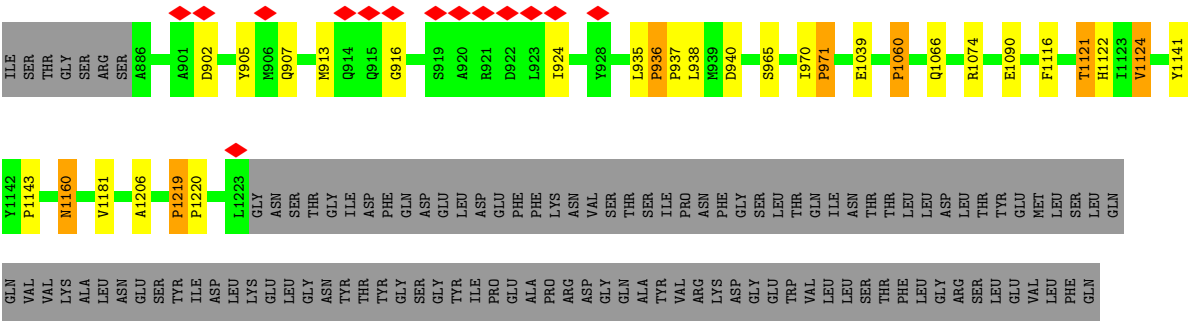
Chain	Residue	Modelled	Actual	Comment	Reference
I	1300	PRO	-	expression tag	UNP W5ZZF5
I	1301	ARG	-	expression tag	UNP W5ZZF5
I	1302	ASP	-	expression tag	UNP W5ZZF5
I	1303	GLY	-	expression tag	UNP W5ZZF5
I	1304	GLN	-	expression tag	UNP W5ZZF5
I	1305	ALA	-	expression tag	UNP W5ZZF5
I	1306	TYR	-	expression tag	UNP W5ZZF5
I	1307	VAL	-	expression tag	UNP W5ZZF5
I	1308	ARG	-	expression tag	UNP W5ZZF5
I	1309	LYS	-	expression tag	UNP W5ZZF5
I	1310	ASP	-	expression tag	UNP W5ZZF5
I	1311	GLY	-	expression tag	UNP W5ZZF5
I	1312	GLU	-	expression tag	UNP W5ZZF5
I	1313	TRP	-	expression tag	UNP W5ZZF5
I	1314	VAL	-	expression tag	UNP W5ZZF5
I	1315	LEU	-	expression tag	UNP W5ZZF5
I	1316	LEU	-	expression tag	UNP W5ZZF5
I	1317	SER	-	expression tag	UNP W5ZZF5
I	1318	THR	-	expression tag	UNP W5ZZF5
I	1319	PHE	-	expression tag	UNP W5ZZF5
I	1320	LEU	-	expression tag	UNP W5ZZF5
I	1321	GLY	-	expression tag	UNP W5ZZF5
I	1322	ARG	-	expression tag	UNP W5ZZF5
I	1323	SER	-	expression tag	UNP W5ZZF5
I	1324	LEU	-	expression tag	UNP W5ZZF5
I	1325	GLU	-	expression tag	UNP W5ZZF5
I	1326	VAL	-	expression tag	UNP W5ZZF5
I	1327	LEU	-	expression tag	UNP W5ZZF5
I	1328	PHE	-	expression tag	UNP W5ZZF5
I	1329	GLN	-	expression tag	UNP W5ZZF5

- Molecule 2 is a protein called G4 VH.

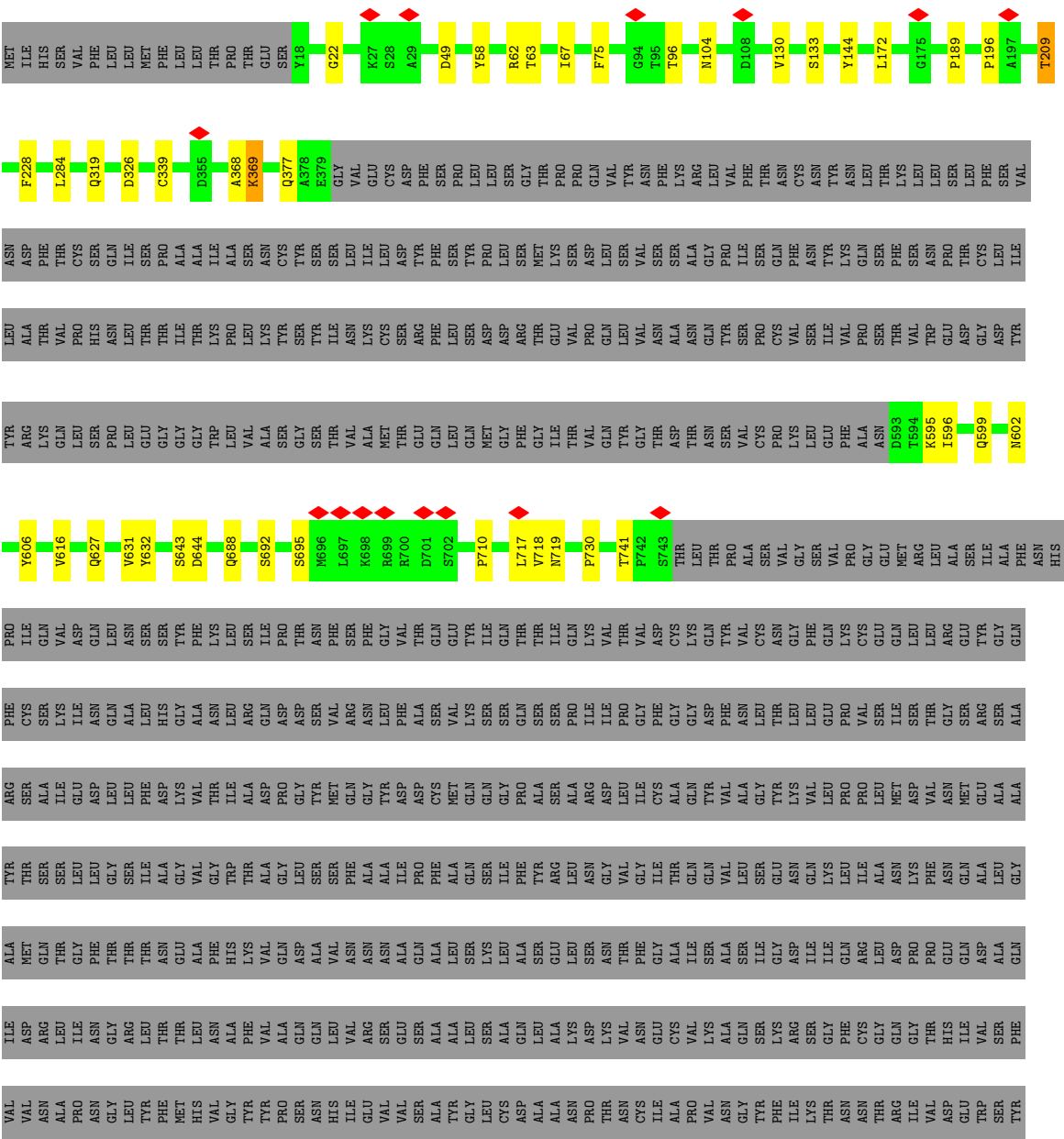
Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	D	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	K	119	Total	C	N	O	S	0	0
			948	602	156	185	5		

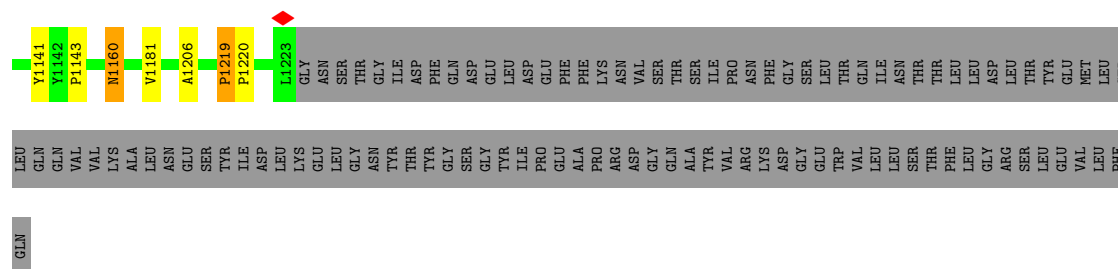
- Molecule 3 is a protein called G4 VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	111	Total 835	C 522	N 143	O 166	S 4	0	0
3	E	111	Total 835	C 522	N 143	O 166	S 4	0	0
3	L	111	Total 835	C 522	N 143	O 166	S 4	0	0

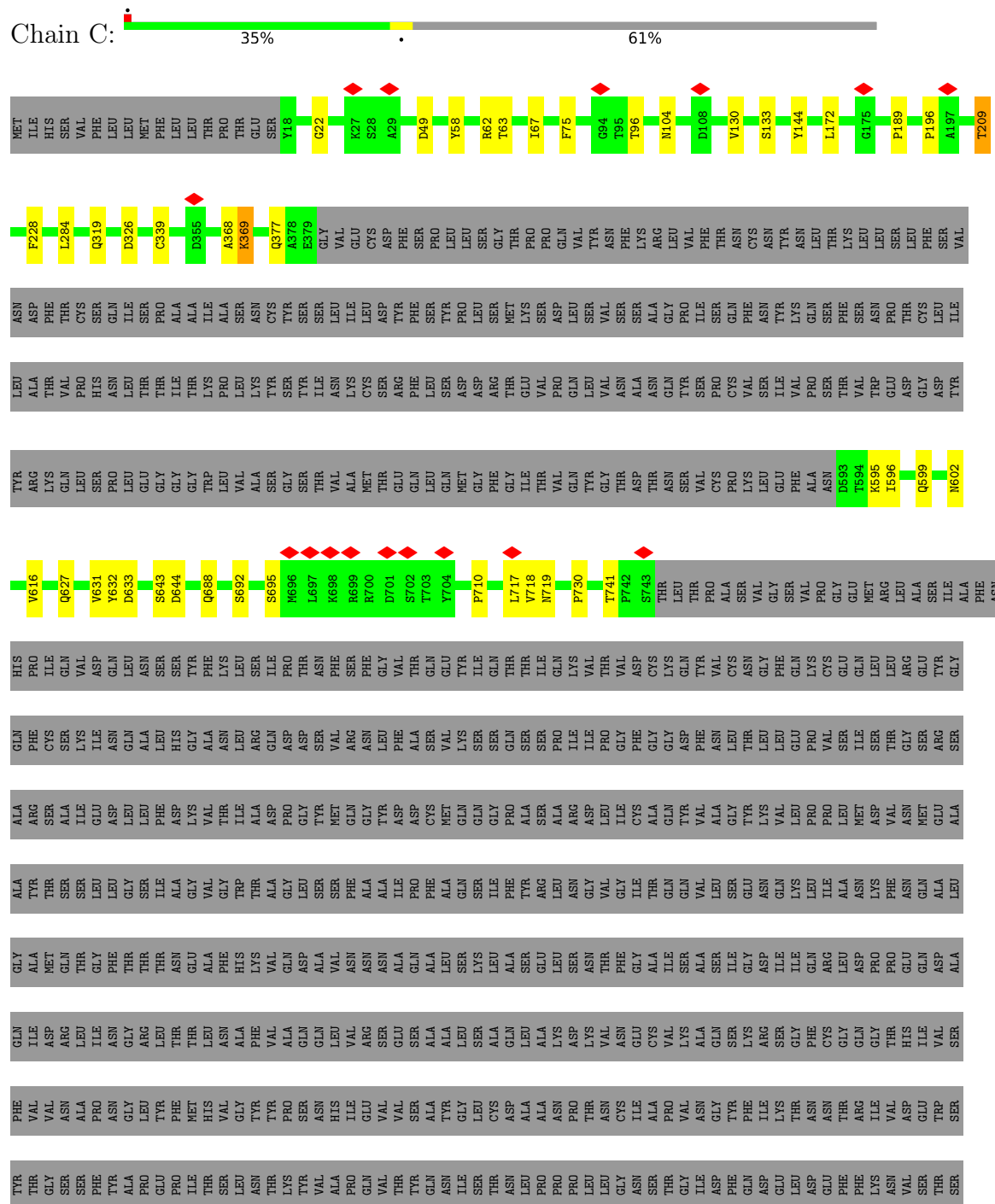


• Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein



[illegible]

- Molecule 1: Spike glycoprotein



H1122	V877	SER	VAL	GLY	TTR	LEU	ASN	TTR	ASN	TTR	ARG	TTR	ARG	GLY	MET
I1123	SER	LEU	ILE	ASN	ARG	ALA	ASP	VAL	ASP	SER	ILE	THR	ALA	THR	ILE
V1124	THR	PHE	TTR	ILE	LYS	THR	PHE	GLN	THR	VAL	GLN	THR	THR	THR	THR
Y1141	THR	VAL	ASP	VAL	GLN	VAL	GLY	LEU	CYS	SER	SER	ILE	CYS	ASN	VAL
Y1142	GLY	GLU	GLY	TTR	SER	HIS	TTR	SER	GLN	PHE	ASP	THR	ILE	ASN	PHE
P1143	SER	ASP	THR	SER	PRO	ASN	ASN	PRO	GLY	GLU	ARG	GLU	LEU	THR	LEU
N1160	ARG	CYS	LYS	LYS	LEU	LEU	LEU	LEU	ILE	ALA	ALA	ALA	SER	THR	LEU
V1181	SER	LEU	ALA	VAL	GLY	GLY	GLY	GLY	ALA	SER	SER	LEU	GLY	TTR	LEU
A1206	ASN	GLN	LEU	GLY	TRP	LYS	ILE	TRP	ILE	PHE	ALA	GLU	ASN	GLY	THR
P1219	ASN	LEU	PHE	ARG	LEU	PRO	ALA	LEU	ALA	VAL	HIS	PRO	HIS	PRO	THR
P1220	SER	LEU	GLY	GLY	VAL	LEU	SER	VAL	ASN	VAL	CYS	GLY	CYS	GLY	THR
L1223	GLY	CYS	VAL	ASN	ALA	LYS	ASN	ALA	CYS	LYS	LYS	THR	ALA	GLY	TTR
	ASN	LEU	ALA	GLN	GLY	SER	GLY	GLY	TTR	ALA	GLY	GLN	GLY	THR	VAL
	SER	PRO	CYS	ASN	SER	THR	ASN	SER	THR	THR	ALA	THR	ASP	PRO	ASP
	THR	THR	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	GLY	Q914	SER	VAL	GLY	GLY	VAL	GLY	LEU	PHE	SER	ILE	ASP	MET	ASP
	ILE	Q915	THR	GLY	THR	GLY	THR	GLY	THR	THR	LEU	THR	GLY	TTR	THR
	ASP	G916	THR	VAL	GLY	ARG	VAL	GLY	THR	PHE	LEU	LEU	ALA	PRO	TTR
	PHE		MET	THR	GLN	GLN	GLN	GLN	SER	THR	THR	THR	THR	VAL	VAL
	GLN	S919	SER	TTR	ARG	LEU	GLN	GLN	LEU	SER	SER	SER	HIS	LYS	LYS
	ASP	A920	THR	SER	THR	ASP	THR	THR	PRO	LEU	VAL	ARG	THR	LEU	ALA
	GLU	R921	VAL	SER	PHE	GLY	VAL	PHE	LEU	SER	ASP	THR	PRO	GLY	CYS
	LEU	D922	GLY	ARG	THR	THR	THR	THR	THR	THR	GLY	THR	ASP	ALA	ILE
	ASP	L923	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	PHE	I924	ARG	THR	THR	THR	THR	THR	VAL	VAL	ARG	GLY	CYS	GLY	GLY
	LYS	E756	SER	THR	GLN	GLN	GLN	GLN	PRO	GLN	ARG	GLY	SER	ASN	THR
	ASN	Y928	MET	THR	ASN	LEU	THR	THR	GLN	THR	ILE	ALA	ASP	PHE	GLN
	VAL	H766	LEU	LEU	LEU	VAL	VAL	VAL	LEU	THR	ILE	ALA	GLY	THR	THR
	SER	L935	LYS	ARG	THR	VAL	VAL	THR	ASN	ASP	CYS	THR	ASN	GLN	GLN
	THR	P936	ARG	THR	THR	THR	THR	THR	SER	THR	THR	THR	THR	THR	THR
	SER	P937	THR	THR	THR	THR	THR	THR	SER	PHE	GLY	GLN	ASN	LYS	THR
	ILE	L938	THR	THR	THR	THR	THR	THR	ALA	ARG	PHE	PHE	ARG	THR	PHE
	PRO	M939	SER	THR	ASN	GLN	GLY	ASN	ALA	ASN	ASN	ALA	ASN	GLY	THR
	ASN	D940	THR	THR	SER	THR	THR	SER	PRO	THR	THR	THR	THR	VAL	LYS
	PHE		TTR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA	THR
	GLY	L964	PRO	GLY	GLY	PRO	ASP	CYS	GLY	THR	THR	THR	THR	THR	THR
	SER	S965	LEU	ASN	LYS	LEU	ASN	LYS	VAL	PHE	LEU	THR	SER	GLN	ASP
	LEU														
	THR	C817	THR	THR	GLY	THR	THR	GLY	THR	THR	CYS	THR	THR	THR	THR
	GLN	P971	PRO	CYS	PHE	VAL	THR	PHE	ILE	LEU	SER	ILE	GLU	VAL	THR
	ILE	E818	VAL	LEU	ALA	VAL	VAL	ALA	GLN	THR	THR	THR	THR	GLN	VAL
	ASN		GLY	ARG	ASN	SER	THR	ASN	THR	THR	GLU	THR	THR	PHE	LYS
	THR	E1039	THR	THR	THR	CYS	ALA	ASP	PHE	LYS	SER	THR	THR	ALA	LYS
	THR		VAL	CYS	THR	VAL	SER	THR	SER	THR	PHE	SER	THR	ALA	THR
	THR	P1060	LEU	LEU	THR	VAL	VAL	THR	LEU	LEU	PHE	THR	THR	ASP	ASP
	LEU	Q1066	LEU	GLY	GLY	LEU	VAL	LYS	LEU	LEU	ASP	ILE	ARG	GLY	THR
	LEU		LEU	SER	THR	THR	VAL	ILE	SER	THR	VAL	ILE	THR	THR	THR
	THR	R1074	VAL	VAL	PRO	VAL	VAL	ALA	THR	PHE	GLY	THR	THR	VAL	THR
	TTR		ASN	SER	THR	THR	THR	GLN	SER	THR	THR	THR	THR	THR	THR
		E1090	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

[illegible]

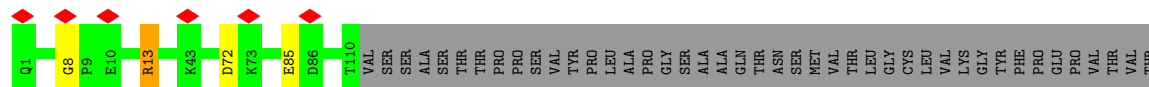
Chain I:

[illegible]

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

• Molecule 2: G4 VH

Chain F:  49%

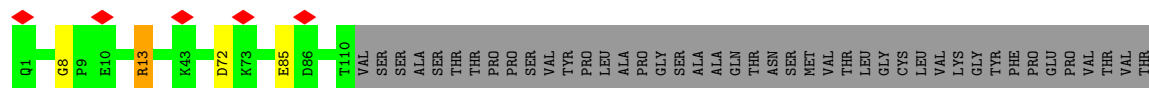
 Q1 G8 P9 E10 R13 K43 D72 K73 E85 D86 T110

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

ASP CYS GLY LYS GLY LEU GLU VAL PHE GLN

• Molecule 2: G4 VH

Chain D:  49%

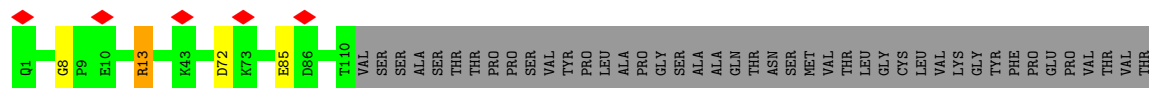
 Q1 G8 P9 E10 R13 K43 D72 K73 E85 D86 T110

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

ASP CYS GLY LYS GLY LEU GLU VAL PHE GLN

• Molecule 2: G4 VH

Chain K:  49%

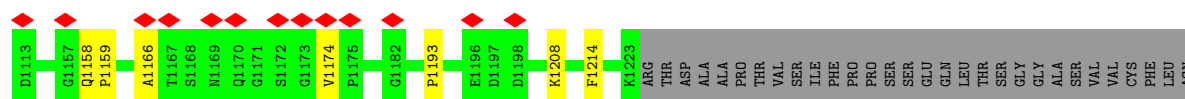
 Q1 G8 P9 E10 R13 K43 D72 K73 E85 D86 T110

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

ASP CYS GLY LYS GLY LEU GLU VAL PHE GLN

• Molecule 3: G4 VL

Chain G:  6% 48% 49%

 D1113 G1157 Q1158 P1159 A1166 T1167 S1168 N1169 Q1170 G1171 S1172 G1173 V1174 P1175 G1182 P1193 E1196 D1197 D1198 K1208 F1214 K1223

ASN PHE TYR PRO LYS ASP ASP ASN VAL VAL TRP LYS THR TLE ASP GLY SER GLU ARG GLN ASN GLY VAL LEU ASN SER TRP THR ASP GLN SER LYS ASP SER THR TYR ASP MET SER SER THR LEU THR THR ILE PHE PRO LYS ASP GLU TYR GLU ARG HIS ASN SER TYR GLY THR CYS GLU VAL VAL PHE CYS THR LEU ASN

HIS
LYS
THR
SER
THR
SER
PRO
ILE
VAL
LYS
SER
SER
PHE
ASN
ARG
ASN
GLU
CYS

● Molecule 3: G4 VL



D1113	G1157	Q1158	P1159	A1166	T1167	S1168	N1169	Q1170	G1171	S1172	G1173	V1174	P1175	G1182	P1193	E1196	D1197	D1198	K1208	F1214	K1223	ARG	THR	THR	ASP	ALA	ALA	PRO	THR	THR	VAL	LEU	SER	THR	ILE	PHE	PRO	LYS	ASP	GLU	TYR	SER	GLN	ARG	GLU	LEU	THR	ASN	THR	GLY	GLY	ALA	VAL	VAL	CYS	PHE	LEU	ASN
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASN	PHE	TYR	PRO	LYS	ASP	ILE	ASN	VAL	VAL	LYS	TRP	LYS	LYS	ILE	ASP	GLY	SER	GLU	ARG	GLN	ASN	GLY	VAL	LEU	ASN	SER	TRP	THR	THR	ASP	GLN	ASP	SER	LYS	ASP	SER	THR	TYR	ASP	THR	MET	SER	ALA	SER	PRO	THR	THR	VAL	LEU	THR	THR	ILE	LEU	THR	LYS	ASP	GLU	TYR	GLU	ARG	HIS	LEU	THR	ASN	SER	TYR	GLY	THR	CYS	ALA	GLU	VAL	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

HIS
LYS
THR
SER
THR
SER
PRO
ILE
VAL
LYS
SER
SER
PHE
ASN
ARG
ASN
GLU
CYS

● Molecule 3: G4 VL



D1113	G1157	Q1158	P1159	A1166	T1167	S1168	N1169	Q1170	G1171	S1172	G1173	V1174	P1175	G1182	P1193	E1196	D1197	D1198	K1208	F1214	K1223	ARG	THR	THR	ASP	ALA	ALA	PRO	THR	THR	VAL	LEU	SER	THR	ILE	PHE	PRO	LYS	ASP	GLU	TYR	SER	GLN	ARG	GLU	LEU	THR	ASN	THR	GLY	GLY	ALA	SER	VAL	VAL	CYS	PHE	LEU	ASN
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASN	PHE	TYR	PRO	LYS	ASP	ILE	ASN	VAL	VAL	LYS	TRP	LYS	LYS	ILE	ASP	GLY	SER	GLU	ARG	GLN	ASN	GLY	VAL	LEU	ASN	SER	TRP	THR	THR	ASP	GLN	ASP	SER	LYS	ASP	SER	THR	TYR	ASP	THR	MET	SER	ALA	SER	PRO	THR	THR	VAL	LEU	THR	THR	ILE	LEU	THR	LYS	ASP	GLU	TYR	GLU	ARG	HIS	LEU	THR	ASN	SER	TYR	GLY	THR	CYS	ALA	GLU	VAL	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

HIS
LYS
THR
SER
THR
SER
PRO
ILE
VAL
LYS
SER
SER
PHE
ASN
ARG
ASN
GLU
CYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	11218	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.89	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	310.08, 310.08, 310.08	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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	0.77	0/4112	1.15	25/5590 (0.4%)
1	B	0.87	0/3618	1.18	34/4921 (0.7%)
1	C	0.77	0/4112	1.15	25/5590 (0.4%)
1	H	0.87	0/3618	1.18	34/4921 (0.7%)
1	I	0.77	0/4112	1.15	25/5590 (0.4%)
1	J	0.87	0/3618	1.18	34/4921 (0.7%)
2	D	0.78	0/972	1.05	4/1317 (0.3%)
2	F	0.77	0/972	1.05	4/1317 (0.3%)
2	K	0.78	0/972	1.05	4/1317 (0.3%)
3	E	0.84	0/852	1.22	10/1153 (0.9%)
3	G	0.84	0/852	1.22	10/1153 (0.9%)
3	L	0.85	0/852	1.22	10/1153 (0.9%)
All	All	0.82	0/28662	1.16	219/38943 (0.6%)

There are no bond length outliers.

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	LEU	CA-C-N	9.00	129.23	119.87
1	A	284	LEU	C-N-CA	9.00	129.23	119.87
1	C	284	LEU	CA-C-N	8.92	129.15	119.87
1	C	284	LEU	C-N-CA	8.92	129.15	119.87
1	I	284	LEU	CA-C-N	8.92	129.15	119.87
1	I	284	LEU	C-N-CA	8.92	129.15	119.87
3	L	1174	VAL	CA-C-N	8.26	128.21	120.03
3	L	1174	VAL	C-N-CA	8.26	128.21	120.03
3	G	1174	VAL	CA-C-N	8.21	128.16	120.03
3	G	1174	VAL	C-N-CA	8.21	128.16	120.03
3	E	1174	VAL	CA-C-N	8.21	128.16	120.03
3	E	1174	VAL	C-N-CA	8.21	128.16	120.03
1	C	133	SER	CA-C-N	8.18	127.90	119.56
1	C	133	SER	C-N-CA	8.18	127.90	119.56
1	A	133	SER	CA-C-N	8.15	127.87	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	SER	C-N-CA	8.15	127.87	119.56
1	I	133	SER	CA-C-N	8.15	127.87	119.56
1	I	133	SER	C-N-CA	8.15	127.87	119.56
1	I	144	TYR	CA-C-N	8.02	127.95	119.85
1	I	144	TYR	C-N-CA	8.02	127.95	119.85
1	C	144	TYR	CA-C-N	8.00	127.93	119.85
1	C	144	TYR	C-N-CA	8.00	127.93	119.85
1	A	144	TYR	CA-C-N	7.99	127.92	119.85
1	A	144	TYR	C-N-CA	7.99	127.92	119.85
1	A	209	THR	CA-C-N	7.99	127.71	119.56
1	A	209	THR	C-N-CA	7.99	127.71	119.56
1	I	209	THR	CA-C-N	7.94	127.66	119.56
1	I	209	THR	C-N-CA	7.94	127.66	119.56
1	C	209	THR	CA-C-N	7.92	127.64	119.56
1	C	209	THR	C-N-CA	7.92	127.64	119.56
1	H	1160	ASN	CA-C-N	7.83	127.54	119.56
1	H	1160	ASN	C-N-CA	7.83	127.54	119.56
1	H	935	LEU	CA-C-N	7.80	125.28	119.66
1	H	935	LEU	C-N-CA	7.80	125.28	119.66
1	J	935	LEU	CA-C-N	7.80	125.27	119.66
1	J	935	LEU	C-N-CA	7.80	125.27	119.66
1	J	1160	ASN	CA-C-N	7.77	127.49	119.56
1	J	1160	ASN	C-N-CA	7.77	127.49	119.56
1	B	935	LEU	CA-C-N	7.74	125.23	119.66
1	B	935	LEU	C-N-CA	7.74	125.23	119.66
1	B	1160	ASN	CA-C-N	7.73	127.45	119.56
1	B	1160	ASN	C-N-CA	7.73	127.45	119.56
2	D	8	GLY	CA-C-N	7.53	127.46	119.85
2	D	8	GLY	C-N-CA	7.53	127.46	119.85
2	F	8	GLY	CA-C-N	7.52	127.45	119.85
2	F	8	GLY	C-N-CA	7.52	127.45	119.85
2	K	8	GLY	CA-C-N	7.50	127.43	119.85
2	K	8	GLY	C-N-CA	7.50	127.43	119.85
1	J	936	PRO	CA-C-N	7.36	127.36	119.78
1	J	936	PRO	C-N-CA	7.36	127.36	119.78
1	H	936	PRO	CA-C-N	7.35	127.35	119.78
1	H	936	PRO	C-N-CA	7.35	127.35	119.78
1	B	936	PRO	CA-C-N	7.32	127.32	119.78
1	B	936	PRO	C-N-CA	7.32	127.32	119.78
1	J	1060	PRO	N-CA-C	7.30	119.61	110.70
1	H	1060	PRO	N-CA-C	7.28	119.58	110.70
1	B	1060	PRO	N-CA-C	7.28	119.58	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1208	LYS	N-CA-C	6.98	118.88	111.28
3	G	1208	LYS	N-CA-C	6.94	118.84	111.28
3	E	1214	PHE	CA-CB-CG	6.94	120.74	113.80
3	G	1214	PHE	CA-CB-CG	6.94	120.74	113.80
3	L	1214	PHE	CA-CB-CG	6.94	120.74	113.80
3	L	1208	LYS	N-CA-C	6.92	118.82	111.28
1	A	96	THR	CA-C-N	6.80	126.72	119.85
1	A	96	THR	C-N-CA	6.80	126.72	119.85
1	I	96	THR	CA-C-N	6.79	126.71	119.85
1	I	96	THR	C-N-CA	6.79	126.71	119.85
1	C	96	THR	CA-C-N	6.75	126.66	119.85
1	C	96	THR	C-N-CA	6.75	126.66	119.85
1	H	1219	PRO	CA-C-N	6.50	127.08	120.38
1	H	1219	PRO	C-N-CA	6.50	127.08	120.38
1	J	1219	PRO	CA-C-N	6.50	127.08	120.38
1	J	1219	PRO	C-N-CA	6.50	127.08	120.38
1	B	1219	PRO	CA-C-N	6.49	127.07	120.38
1	B	1219	PRO	C-N-CA	6.49	127.07	120.38
1	H	902	ASP	CA-C-N	6.32	126.28	120.03
1	H	902	ASP	C-N-CA	6.32	126.28	120.03
1	B	902	ASP	CA-C-N	6.27	126.23	120.03
1	B	902	ASP	C-N-CA	6.27	126.23	120.03
1	J	902	ASP	CA-C-N	6.26	126.23	120.03
1	J	902	ASP	C-N-CA	6.26	126.23	120.03
1	J	1206	ALA	CA-C-N	6.22	126.14	119.85
1	J	1206	ALA	C-N-CA	6.22	126.14	119.85
1	B	1206	ALA	CA-C-N	6.22	126.13	119.85
1	B	1206	ALA	C-N-CA	6.22	126.13	119.85
1	C	75	PHE	CA-C-N	6.21	126.12	119.85
1	C	75	PHE	C-N-CA	6.21	126.12	119.85
1	H	1206	ALA	CA-C-N	6.19	126.10	119.85
1	H	1206	ALA	C-N-CA	6.19	126.10	119.85
1	I	75	PHE	CA-C-N	6.17	126.08	119.85
1	I	75	PHE	C-N-CA	6.17	126.08	119.85
1	A	75	PHE	CA-C-N	6.16	126.07	119.85
1	A	75	PHE	C-N-CA	6.16	126.07	119.85
1	J	753	VAL	CA-C-N	6.13	126.04	119.85
1	J	753	VAL	C-N-CA	6.13	126.04	119.85
1	J	782	ILE	CA-C-N	6.12	126.03	119.85
1	J	782	ILE	C-N-CA	6.12	126.03	119.85
1	H	753	VAL	CA-C-N	6.11	126.02	119.85
1	H	753	VAL	C-N-CA	6.11	126.02	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	753	VAL	CA-C-N	6.11	126.02	119.85
1	B	753	VAL	C-N-CA	6.11	126.02	119.85
1	H	782	ILE	CA-C-N	6.11	126.02	119.85
1	H	782	ILE	C-N-CA	6.11	126.02	119.85
1	H	924	ILE	CB-CA-C	-6.09	104.07	112.04
1	B	924	ILE	CB-CA-C	-6.08	104.07	112.04
1	J	924	ILE	CB-CA-C	-6.08	104.08	112.04
1	B	782	ILE	CA-C-N	6.08	125.99	119.85
1	B	782	ILE	C-N-CA	6.08	125.99	119.85
1	C	369	LYS	CA-C-N	6.06	126.02	119.78
1	C	369	LYS	C-N-CA	6.06	126.02	119.78
1	A	369	LYS	CA-C-N	6.04	126.01	119.78
1	A	369	LYS	C-N-CA	6.04	126.01	119.78
1	I	369	LYS	CA-C-N	6.04	126.00	119.78
1	I	369	LYS	C-N-CA	6.04	126.00	119.78
3	E	1158	GLN	CA-C-N	6.03	126.59	120.38
3	E	1158	GLN	C-N-CA	6.03	126.59	120.38
3	G	1158	GLN	CA-C-N	5.99	126.55	120.38
3	G	1158	GLN	C-N-CA	5.99	126.55	120.38
3	L	1158	GLN	CA-C-N	5.96	126.51	120.38
3	L	1158	GLN	C-N-CA	5.96	126.51	120.38
1	C	319	GLN	CA-C-N	5.92	127.23	119.84
1	C	319	GLN	C-N-CA	5.92	127.23	119.84
1	A	319	GLN	CA-C-N	5.91	127.23	119.84
1	A	319	GLN	C-N-CA	5.91	127.23	119.84
1	I	319	GLN	CA-C-N	5.87	127.18	119.84
1	I	319	GLN	C-N-CA	5.87	127.18	119.84
3	L	1174	VAL	N-CA-C	5.85	115.47	108.45
3	E	1174	VAL	N-CA-C	5.84	115.45	108.45
3	G	1174	VAL	N-CA-C	5.82	115.44	108.45
1	H	859	SER	CA-C-N	5.82	125.73	119.85
1	H	859	SER	C-N-CA	5.82	125.73	119.85
1	I	22	GLY	CA-C-N	5.79	125.70	119.85
1	I	22	GLY	C-N-CA	5.79	125.70	119.85
1	J	859	SER	CA-C-N	5.79	125.69	119.85
1	J	859	SER	C-N-CA	5.79	125.69	119.85
1	B	859	SER	CA-C-N	5.76	125.67	119.85
1	B	859	SER	C-N-CA	5.76	125.67	119.85
1	A	22	GLY	CA-C-N	5.76	125.67	119.85
1	A	22	GLY	C-N-CA	5.76	125.67	119.85
1	A	741	THR	CA-C-N	5.74	125.69	119.78
1	A	741	THR	C-N-CA	5.74	125.69	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	22	GLY	CA-C-N	5.73	125.63	119.85
1	C	22	GLY	C-N-CA	5.73	125.63	119.85
1	I	741	THR	CA-C-N	5.72	125.67	119.78
1	I	741	THR	C-N-CA	5.72	125.67	119.78
2	D	13	ARG	CA-C-N	5.70	125.61	119.85
2	D	13	ARG	C-N-CA	5.70	125.61	119.85
1	C	741	THR	CA-C-N	5.70	125.65	119.78
1	C	741	THR	C-N-CA	5.70	125.65	119.78
2	F	13	ARG	CA-C-N	5.69	125.60	119.85
2	F	13	ARG	C-N-CA	5.69	125.60	119.85
2	K	13	ARG	CA-C-N	5.66	125.57	119.85
2	K	13	ARG	C-N-CA	5.66	125.57	119.85
3	E	1159	PRO	CA-C-N	5.66	125.61	119.78
3	E	1159	PRO	C-N-CA	5.66	125.61	119.78
1	J	1124	VAL	N-CA-C	5.65	117.59	109.51
3	G	1159	PRO	CA-C-N	5.65	125.60	119.78
3	G	1159	PRO	C-N-CA	5.65	125.60	119.78
1	H	1124	VAL	N-CA-C	5.65	117.59	109.51
1	B	1124	VAL	N-CA-C	5.64	117.58	109.51
3	L	1159	PRO	CA-C-N	5.62	125.57	119.78
3	L	1159	PRO	C-N-CA	5.62	125.57	119.78
1	H	1219	PRO	N-CA-C	5.49	117.39	110.70
1	J	1219	PRO	N-CA-C	5.46	117.36	110.70
1	I	58	TYR	CA-C-N	5.45	125.40	119.78
1	I	58	TYR	C-N-CA	5.45	125.40	119.78
1	B	1219	PRO	N-CA-C	5.45	117.35	110.70
1	C	58	TYR	CA-C-N	5.44	125.39	119.78
1	C	58	TYR	C-N-CA	5.44	125.39	119.78
1	A	58	TYR	CA-C-N	5.44	125.38	119.78
1	A	58	TYR	C-N-CA	5.44	125.38	119.78
1	B	871	LEU	N-CA-C	5.41	117.24	110.91
1	J	871	LEU	N-CA-C	5.39	117.22	110.91
1	H	871	LEU	N-CA-C	5.37	117.19	110.91
1	B	1121	THR	CB-CA-C	-5.34	110.40	116.54
1	J	1121	THR	CB-CA-C	-5.33	110.41	116.54
1	H	1121	THR	CB-CA-C	-5.33	110.41	116.54
1	I	717	LEU	N-CA-C	5.27	119.77	113.23
1	A	717	LEU	N-CA-C	5.26	119.76	113.23
1	C	717	LEU	N-CA-C	5.25	119.73	113.23
1	B	850	PHE	CA-CB-CG	-5.24	108.56	113.80
1	H	850	PHE	CA-CB-CG	-5.22	108.58	113.80
1	B	916	GLY	CA-C-N	5.21	125.11	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	916	GLY	C-N-CA	5.21	125.11	119.85
1	I	339	CYS	N-CA-C	5.21	116.96	111.28
1	J	850	PHE	CA-CB-CG	-5.21	108.59	113.80
1	A	339	CYS	N-CA-C	5.21	116.96	111.28
1	H	971	PRO	CA-N-CD	-5.19	104.74	112.00
1	B	971	PRO	CA-N-CD	-5.18	104.75	112.00
1	J	916	GLY	CA-C-N	5.18	125.08	119.85
1	J	916	GLY	C-N-CA	5.18	125.08	119.85
1	B	970	ILE	CA-C-N	5.18	125.47	119.93
1	B	970	ILE	C-N-CA	5.18	125.47	119.93
1	H	970	ILE	CA-C-N	5.17	125.47	119.93
1	H	970	ILE	C-N-CA	5.17	125.47	119.93
1	C	339	CYS	N-CA-C	5.17	116.92	111.28
1	H	916	GLY	CA-C-N	5.17	125.07	119.85
1	H	916	GLY	C-N-CA	5.17	125.07	119.85
1	J	971	PRO	CA-N-CD	-5.17	104.77	112.00
1	J	970	ILE	CA-C-N	5.15	125.44	119.93
1	J	970	ILE	C-N-CA	5.15	125.44	119.93
1	C	695	SER	N-CA-C	5.10	117.58	111.71
1	B	1060	PRO	CA-C-N	5.09	124.88	119.28
1	B	1060	PRO	C-N-CA	5.09	124.88	119.28
3	L	1166	ALA	N-CA-C	5.09	117.49	111.33
3	E	1166	ALA	N-CA-C	5.08	117.47	111.33
3	G	1166	ALA	N-CA-C	5.08	117.47	111.33
1	J	1060	PRO	CA-C-N	5.06	124.85	119.28
1	J	1060	PRO	C-N-CA	5.06	124.85	119.28
1	H	1060	PRO	CA-C-N	5.06	124.85	119.28
1	H	1060	PRO	C-N-CA	5.06	124.85	119.28
1	A	695	SER	N-CA-C	5.06	117.53	111.71
1	I	695	SER	N-CA-C	5.05	117.52	111.71
1	J	766	HIS	CA-C-N	5.03	124.93	119.85
1	J	766	HIS	C-N-CA	5.03	124.93	119.85
1	B	766	HIS	CA-C-N	5.03	124.93	119.85
1	B	766	HIS	C-N-CA	5.03	124.93	119.85
1	H	766	HIS	CA-C-N	5.03	124.93	119.85
1	H	766	HIS	C-N-CA	5.03	124.93	119.85

There are no chirality outliers.

There are no planarity outliers.

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	4010	0	3820	28	0
1	B	3545	0	3472	37	0
1	C	4010	0	3820	28	0
1	H	3545	0	3472	40	0
1	I	4010	0	3820	29	0
1	J	3545	0	3472	39	0
2	D	948	0	904	3	0
2	F	948	0	904	3	0
2	K	948	0	904	3	0
3	E	835	0	813	0	0
3	G	835	0	813	0	0
3	L	835	0	813	0	0
All	All	28014	0	27027	198	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 4.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:TYR:CZ	1:B:936:PRO:HA	1.67	1.25
1:J:905:TYR:CZ	1:J:936:PRO:HA	1.67	1.25
1:H:905:TYR:CZ	1:H:936:PRO:HA	1.67	1.25
1:H:905:TYR:CE1	1:H:936:PRO:HD3	1.75	1.22
1:H:905:TYR:CZ	1:H:936:PRO:CA	2.20	1.21
1:B:905:TYR:CE1	1:B:936:PRO:HD3	1.75	1.21
1:J:905:TYR:CE1	1:J:936:PRO:HD3	1.75	1.20
1:B:905:TYR:CZ	1:B:936:PRO:CA	2.19	1.20
1:J:905:TYR:CZ	1:J:936:PRO:CA	2.19	1.15
1:J:905:TYR:CE2	1:J:936:PRO:HA	1.87	1.10
1:B:905:TYR:CE2	1:B:936:PRO:HA	1.87	1.10
1:H:905:TYR:CE2	1:H:936:PRO:HA	1.87	1.08
1:H:905:TYR:HE1	1:H:936:PRO:HD3	1.06	1.02
1:B:905:TYR:HE1	1:B:936:PRO:HD3	1.06	1.01
1:B:905:TYR:CE1	1:B:936:PRO:CD	2.45	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:905:TYR:HE1	1:J:936:PRO:HD3	1.06	0.98
1:H:905:TYR:CE1	1:H:936:PRO:CD	2.45	0.98
1:J:905:TYR:CE1	1:J:936:PRO:CD	2.45	0.98
1:B:1074:ARG:HG2	1:B:1074:ARG:HH11	1.35	0.90
1:H:1074:ARG:HH11	1:H:1074:ARG:HG2	1.35	0.90
1:J:1074:ARG:HG2	1:J:1074:ARG:HH11	1.35	0.88
1:I:377:GLN:OE1	1:I:377:GLN:O	1.94	0.85
1:A:377:GLN:OE1	1:A:377:GLN:O	1.94	0.85
1:C:377:GLN:O	1:C:377:GLN:OE1	1.94	0.84
1:C:63:THR:CG2	1:I:631:VAL:HG22	2.11	0.80
1:A:63:THR:CG2	1:C:631:VAL:HG22	2.11	0.80
1:A:631:VAL:HG22	1:I:63:THR:CG2	2.11	0.80
1:C:172:LEU:HD12	1:C:172:LEU:O	1.82	0.80
1:I:172:LEU:O	1:I:172:LEU:HD12	1.81	0.80
1:A:172:LEU:HD12	1:A:172:LEU:O	1.82	0.79
1:B:938:LEU:HG	1:B:938:LEU:O	1.89	0.72
1:H:818:GLU:HA	1:H:818:GLU:OE1	1.89	0.72
1:J:938:LEU:O	1:J:938:LEU:CG	2.38	0.72
1:B:818:GLU:HA	1:B:818:GLU:OE1	1.89	0.71
1:B:938:LEU:O	1:B:938:LEU:CG	2.38	0.71
1:H:938:LEU:O	1:H:938:LEU:HG	1.89	0.71
1:J:818:GLU:HA	1:J:818:GLU:OE1	1.89	0.70
1:J:938:LEU:O	1:J:938:LEU:HG	1.89	0.70
1:H:938:LEU:O	1:H:938:LEU:CG	2.38	0.70
1:I:616:VAL:HG13	1:I:616:VAL:O	1.92	0.70
1:A:616:VAL:HG13	1:A:616:VAL:O	1.92	0.69
1:C:616:VAL:O	1:C:616:VAL:HG13	1.92	0.69
1:J:1074:ARG:HG2	1:J:1074:ARG:NH1	2.11	0.65
1:B:1074:ARG:HG2	1:B:1074:ARG:NH1	2.11	0.63
1:H:938:LEU:O	1:H:938:LEU:HD12	1.99	0.63
1:B:938:LEU:O	1:B:938:LEU:HD12	1.98	0.63
1:J:938:LEU:O	1:J:938:LEU:HD12	1.99	0.62
1:H:1074:ARG:HG2	1:H:1074:ARG:NH1	2.11	0.62
1:B:938:LEU:O	1:B:938:LEU:CD1	2.50	0.60
1:H:938:LEU:O	1:H:938:LEU:CD1	2.50	0.60
1:J:938:LEU:O	1:J:938:LEU:CD1	2.50	0.60
1:H:1066:GLN:HA	1:H:1066:GLN:OE1	2.02	0.59
1:J:1066:GLN:HA	1:J:1066:GLN:OE1	2.02	0.58
2:K:13:ARG:HA	2:K:13:ARG:NE	2.19	0.58
1:B:1066:GLN:HA	1:B:1066:GLN:OE1	2.02	0.57
2:F:13:ARG:NE	2:F:13:ARG:HA	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:ARG:NE	2:D:13:ARG:HA	2.19	0.57
1:B:826:GLN:CD	1:B:826:GLN:H	2.13	0.57
1:H:826:GLN:H	1:H:826:GLN:CD	2.13	0.57
1:J:826:GLN:H	1:J:826:GLN:CD	2.13	0.57
1:A:172:LEU:HD12	1:A:172:LEU:C	2.31	0.56
1:I:172:LEU:HD12	1:I:172:LEU:C	2.31	0.55
1:A:63:THR:HG23	1:C:631:VAL:HG22	1.87	0.55
1:A:599:GLN:O	1:A:599:GLN:OE1	2.24	0.55
1:C:172:LEU:HD12	1:C:172:LEU:C	2.31	0.55
1:I:599:GLN:O	1:I:599:GLN:OE1	2.24	0.55
1:A:631:VAL:HG22	1:I:63:THR:HG23	1.87	0.54
2:F:85:GLU:OE1	2:F:85:GLU:N	2.39	0.54
1:I:130:VAL:O	1:I:130:VAL:HG12	2.07	0.54
1:A:62:ARG:HG2	1:C:632:TYR:CE2	2.43	0.54
1:A:130:VAL:HG12	1:A:130:VAL:O	2.07	0.54
1:C:62:ARG:HG2	1:I:632:TYR:CE2	2.43	0.54
1:C:599:GLN:O	1:C:599:GLN:OE1	2.25	0.54
1:A:632:TYR:CE2	1:I:62:ARG:HG2	2.43	0.53
1:H:1160:ASN:OD1	1:H:1160:ASN:C	2.52	0.53
1:J:1160:ASN:C	1:J:1160:ASN:OD1	2.52	0.53
1:B:1160:ASN:OD1	1:B:1160:ASN:C	2.52	0.53
1:C:63:THR:HG23	1:I:631:VAL:HG22	1.87	0.53
1:C:130:VAL:O	1:C:130:VAL:HG12	2.07	0.53
1:I:209:THR:O	1:I:209:THR:HG22	2.09	0.53
1:A:209:THR:O	1:A:209:THR:HG22	2.09	0.53
1:H:818:GLU:OE1	1:H:818:GLU:CA	2.57	0.53
1:B:905:TYR:HE2	1:B:937:PRO:HD3	1.75	0.52
1:C:209:THR:HG22	1:C:209:THR:O	2.09	0.52
1:J:905:TYR:HE2	1:J:937:PRO:HD3	1.75	0.51
1:H:905:TYR:CE1	1:H:936:PRO:CA	2.90	0.51
1:H:905:TYR:CZ	1:H:936:PRO:CB	2.92	0.51
1:I:719:ASN:OD1	1:I:719:ASN:C	2.54	0.51
2:K:72:ASP:OD1	2:K:72:ASP:C	2.54	0.51
1:C:643:SER:OG	1:C:644:ASP:N	2.44	0.51
1:H:1124:VAL:O	1:H:1124:VAL:HG13	2.11	0.51
2:D:72:ASP:C	2:D:72:ASP:OD1	2.54	0.50
1:H:905:TYR:HE2	1:H:937:PRO:HD3	1.75	0.50
1:J:1124:VAL:HG13	1:J:1124:VAL:O	2.11	0.50
1:A:67:ILE:O	1:A:67:ILE:HG13	2.12	0.50
1:A:616:VAL:O	1:A:616:VAL:CG1	2.58	0.50
1:I:616:VAL:O	1:I:616:VAL:CG1	2.58	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:ASN:OD1	1:A:719:ASN:C	2.54	0.49
2:D:85:GLU:OE1	2:D:85:GLU:N	2.39	0.49
1:A:596:ILE:HG22	1:A:596:ILE:O	2.12	0.49
1:H:1039:GLU:HA	1:H:1039:GLU:OE1	2.12	0.49
1:I:67:ILE:HG13	1:I:67:ILE:O	2.12	0.49
1:B:1124:VAL:HG13	1:B:1124:VAL:O	2.11	0.49
1:J:1121:THR:OG1	1:J:1122:HIS:N	2.45	0.49
1:A:643:SER:OG	1:A:644:ASP:N	2.44	0.49
1:C:67:ILE:O	1:C:67:ILE:HG13	2.12	0.49
1:A:130:VAL:O	1:A:130:VAL:CG1	2.61	0.49
1:B:1074:ARG:HH11	1:B:1074:ARG:CG	2.07	0.49
1:I:643:SER:OG	1:I:644:ASP:N	2.44	0.49
1:C:596:ILE:O	1:C:596:ILE:HG22	2.11	0.49
1:H:1121:THR:OG1	1:H:1122:HIS:N	2.45	0.49
1:C:130:VAL:O	1:C:130:VAL:CG1	2.61	0.49
1:B:1121:THR:OG1	1:B:1122:HIS:N	2.45	0.49
1:C:719:ASN:OD1	1:C:719:ASN:C	2.54	0.48
1:J:1039:GLU:OE1	1:J:1039:GLU:HA	2.12	0.48
1:B:905:TYR:CE1	1:B:936:PRO:CA	2.90	0.48
1:J:905:TYR:CE2	1:J:937:PRO:HD3	2.49	0.48
1:C:616:VAL:O	1:C:616:VAL:CG1	2.58	0.48
1:I:596:ILE:HG22	1:I:596:ILE:O	2.11	0.48
1:J:905:TYR:CZ	1:J:936:PRO:CB	2.92	0.48
1:B:1039:GLU:OE1	1:B:1039:GLU:HA	2.12	0.48
1:I:130:VAL:O	1:I:130:VAL:CG1	2.61	0.48
1:H:905:TYR:CE2	1:H:937:PRO:HD3	2.49	0.48
1:B:905:TYR:CZ	1:B:936:PRO:CB	2.92	0.48
1:B:905:TYR:CE2	1:B:937:PRO:HD3	2.49	0.48
1:H:1074:ARG:HH11	1:H:1074:ARG:CG	2.07	0.48
2:F:72:ASP:OD1	2:F:72:ASP:C	2.54	0.47
1:J:905:TYR:CE1	1:J:936:PRO:N	2.66	0.47
1:J:1090:GLU:HA	1:J:1090:GLU:OE1	2.15	0.47
1:J:905:TYR:CE1	1:J:936:PRO:CA	2.90	0.47
1:H:905:TYR:CE1	1:H:936:PRO:N	2.66	0.47
1:J:1074:ARG:HH11	1:J:1074:ARG:CG	2.07	0.46
1:A:688:GLN:OE1	1:A:688:GLN:N	2.42	0.46
1:H:1090:GLU:HA	1:H:1090:GLU:OE1	2.15	0.46
2:K:85:GLU:OE1	2:K:85:GLU:N	2.39	0.46
1:A:599:GLN:CD	1:A:599:GLN:C	2.84	0.46
1:C:599:GLN:CD	1:C:599:GLN:C	2.84	0.46
1:B:1074:ARG:NH1	1:B:1074:ARG:CG	2.70	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:817:CYS:SG	1:H:818:GLU:N	2.90	0.45
1:I:599:GLN:CD	1:I:599:GLN:C	2.84	0.45
1:J:817:CYS:SG	1:J:818:GLU:N	2.90	0.45
1:C:228:PHE:C	1:C:228:PHE:CD1	2.95	0.45
1:J:818:GLU:OE1	1:J:818:GLU:CA	2.57	0.45
1:B:1090:GLU:HA	1:B:1090:GLU:OE1	2.15	0.45
1:C:688:GLN:OE1	1:C:688:GLN:N	2.42	0.45
1:C:104:ASN:OD1	1:C:104:ASN:C	2.60	0.45
1:H:905:TYR:CE1	1:H:936:PRO:CB	3.00	0.45
1:I:228:PHE:C	1:I:228:PHE:CD1	2.95	0.44
1:J:905:TYR:CE1	1:J:936:PRO:CB	3.01	0.44
1:B:817:CYS:SG	1:B:818:GLU:N	2.89	0.44
1:A:228:PHE:CD1	1:A:228:PHE:C	2.95	0.44
1:A:63:THR:HG21	1:C:631:VAL:HG22	1.98	0.44
1:B:905:TYR:CE1	1:B:936:PRO:CB	3.01	0.44
1:C:326:ASP:OD1	1:C:326:ASP:C	2.59	0.44
1:H:1074:ARG:NH1	1:H:1074:ARG:CG	2.70	0.44
1:H:801:LYS:HB2	1:H:801:LYS:HE2	1.83	0.44
1:I:326:ASP:OD1	1:I:326:ASP:C	2.59	0.43
1:A:326:ASP:C	1:A:326:ASP:OD1	2.59	0.43
1:I:49:ASP:OD1	1:I:49:ASP:C	2.61	0.43
1:I:104:ASN:OD1	1:I:104:ASN:C	2.60	0.43
1:J:1074:ARG:NH1	1:J:1074:ARG:CG	2.70	0.43
1:B:801:LYS:HB2	1:B:801:LYS:HE2	1.83	0.43
1:J:756:GLU:OE1	1:J:756:GLU:N	2.42	0.43
1:H:1181:VAL:O	1:H:1181:VAL:HG23	2.18	0.43
1:C:49:ASP:C	1:C:49:ASP:OD1	2.61	0.43
1:A:49:ASP:OD1	1:A:49:ASP:C	2.61	0.43
1:J:805:ASP:OD1	1:J:805:ASP:C	2.62	0.43
1:B:805:ASP:OD1	1:B:805:ASP:C	2.62	0.43
1:J:1181:VAL:O	1:J:1181:VAL:HG23	2.18	0.42
1:B:809:TYR:CD1	1:B:809:TYR:C	2.97	0.42
1:C:62:ARG:HG2	1:I:632:TYR:HE2	1.84	0.42
1:J:826:GLN:OE1	1:J:826:GLN:N	2.37	0.42
1:A:104:ASN:OD1	1:A:104:ASN:C	2.60	0.42
1:C:633:ASP:OD1	1:C:633:ASP:C	2.62	0.42
1:A:632:TYR:HE2	1:I:62:ARG:HG2	1.84	0.42
1:J:809:TYR:CD1	1:J:809:TYR:C	2.97	0.42
1:B:1181:VAL:O	1:B:1181:VAL:HG23	2.18	0.42
1:J:1116:PHE:HD1	1:J:1116:PHE:H	1.66	0.42
1:H:809:TYR:CD1	1:H:809:TYR:C	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1116:PHE:H	1:H:1116:PHE:HD1	1.66	0.42
1:B:818:GLU:OE1	1:B:818:GLU:CA	2.57	0.42
1:H:805:ASP:C	1:H:805:ASP:OD1	2.62	0.42
1:H:1141:TYR:CD1	1:H:1141:TYR:C	2.98	0.41
1:J:774:ASN:OD1	1:J:774:ASN:C	2.63	0.41
1:H:774:ASN:C	1:H:774:ASN:OD1	2.63	0.41
1:B:1116:PHE:HD1	1:B:1116:PHE:H	1.66	0.41
1:B:774:ASN:OD1	1:B:774:ASN:C	2.63	0.41
1:H:913:MET:HE2	1:H:913:MET:HB3	1.95	0.41
1:B:909:TYR:N	1:B:909:TYR:CD1	2.89	0.41
1:J:913:MET:HE2	1:J:913:MET:HB3	1.95	0.41
1:H:756:GLU:OE1	1:H:756:GLU:N	2.42	0.41
1:J:1141:TYR:CD1	1:J:1141:TYR:C	2.98	0.41
1:A:606:TYR:CD1	1:A:606:TYR:C	2.99	0.41
1:B:1141:TYR:CD1	1:B:1141:TYR:C	2.98	0.41
1:I:606:TYR:CD1	1:I:606:TYR:C	2.99	0.41
1:I:633:ASP:OD1	1:I:633:ASP:C	2.62	0.40
1:I:688:GLN:OE1	1:I:688:GLN:N	2.42	0.40
1:H:909:TYR:N	1:H:909:TYR:CD1	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/1329 (38%)	474 (93%)	28 (6%)	7 (1%)	9	39
1	B	459/1329 (34%)	435 (95%)	18 (4%)	6 (1%)	9	41
1	C	509/1329 (38%)	474 (93%)	28 (6%)	7 (1%)	9	39
1	H	459/1329 (34%)	435 (95%)	18 (4%)	6 (1%)	9	41
1	I	509/1329 (38%)	474 (93%)	28 (6%)	7 (1%)	9	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	459/1329 (34%)	435 (95%)	18 (4%)	6 (1%)	9	41
2	D	117/233 (50%)	114 (97%)	3 (3%)	0	100	100
2	F	117/233 (50%)	114 (97%)	3 (3%)	0	100	100
2	K	117/233 (50%)	114 (97%)	3 (3%)	0	100	100
3	E	109/218 (50%)	105 (96%)	3 (3%)	1 (1%)	14	48
3	G	109/218 (50%)	105 (96%)	3 (3%)	1 (1%)	14	48
3	L	109/218 (50%)	105 (96%)	3 (3%)	1 (1%)	14	48
All	All	3582/9327 (38%)	3384 (94%)	156 (4%)	42 (1%)	13	42

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	1193	PRO
3	E	1193	PRO
3	L	1193	PRO
1	A	368	ALA
1	A	627	GLN
1	A	692	SER
1	A	718	VAL
1	C	368	ALA
1	C	627	GLN
1	C	692	SER
1	C	718	VAL
1	I	368	ALA
1	I	627	GLN
1	I	692	SER
1	I	718	VAL
1	J	1220	PRO
1	A	602	ASN
1	B	1220	PRO
1	C	602	ASN
1	H	1220	PRO
1	I	602	ASN
1	A	595	LYS
1	C	595	LYS
1	I	595	LYS
1	J	876	PRO
1	J	907	GLN
1	J	940	ASP
1	J	965	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	876	PRO
1	B	907	GLN
1	B	940	ASP
1	B	965	SER
1	H	876	PRO
1	H	907	GLN
1	H	940	ASP
1	H	965	SER
1	A	369	LYS
1	C	369	LYS
1	I	369	LYS
1	J	1219	PRO
1	B	1219	PRO
1	H	1219	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	442/1148 (38%)	438 (99%)	4 (1%)	70	76
1	B	388/1148 (34%)	385 (99%)	3 (1%)	73	77
1	C	442/1148 (38%)	438 (99%)	4 (1%)	70	76
1	H	388/1148 (34%)	385 (99%)	3 (1%)	73	77
1	I	442/1148 (38%)	438 (99%)	4 (1%)	70	76
1	J	388/1148 (34%)	385 (99%)	3 (1%)	73	77
2	D	102/202 (50%)	102 (100%)	0	100	100
2	F	102/202 (50%)	102 (100%)	0	100	100
2	K	102/202 (50%)	102 (100%)	0	100	100
3	E	93/192 (48%)	93 (100%)	0	100	100
3	G	93/192 (48%)	93 (100%)	0	100	100
3	L	93/192 (48%)	93 (100%)	0	100	100
All	All	3075/8070 (38%)	3054 (99%)	21 (1%)	73	79

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	971	PRO
1	J	1060	PRO
1	J	1143	PRO
1	A	189	PRO
1	A	196	PRO
1	A	710	PRO
1	A	730	PRO
1	B	971	PRO
1	B	1060	PRO
1	B	1143	PRO
1	C	189	PRO
1	C	196	PRO
1	C	710	PRO
1	C	730	PRO
1	H	971	PRO
1	H	1060	PRO
1	H	1143	PRO
1	I	189	PRO
1	I	196	PRO
1	I	710	PRO
1	I	730	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	772	GLN
1	J	836	HIS
1	J	981	ASN
1	J	987	GLN
1	J	1129	ASN
1	J	1208	GLN
3	G	1192	HIS
3	G	1206	GLN
1	B	772	GLN
1	B	836	HIS
1	B	981	ASN
1	B	987	GLN
1	B	1063	GLN
1	B	1208	GLN
3	E	1192	HIS
3	E	1205	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	1206	GLN
1	H	772	GLN
1	H	836	HIS
1	H	981	ASN
1	H	987	GLN
1	H	1063	GLN
1	H	1208	GLN
3	L	1192	HIS
3	L	1206	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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.

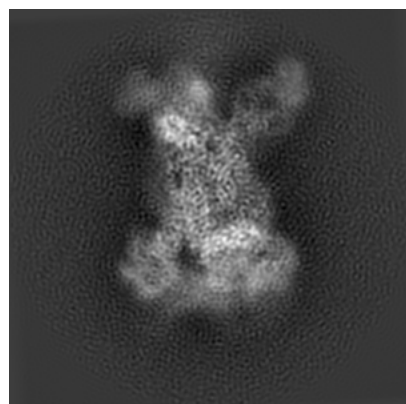
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8791. These allow visual inspection of the internal detail of the map and identification of artifacts.

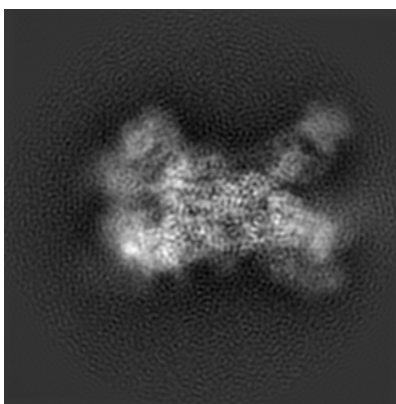
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

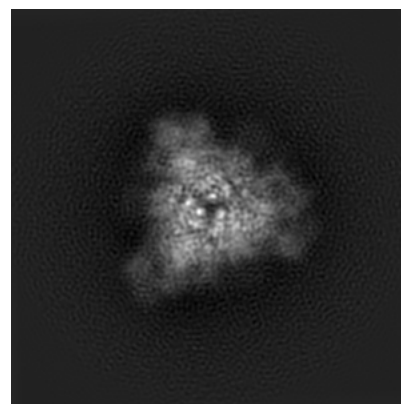
6.1.1 Primary map



X

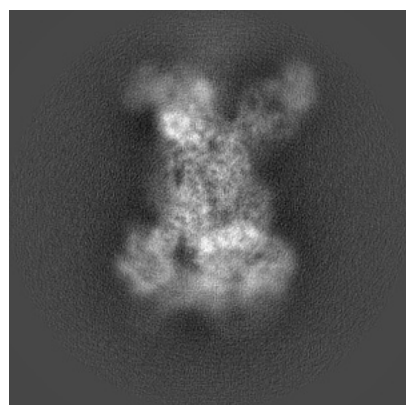


Y

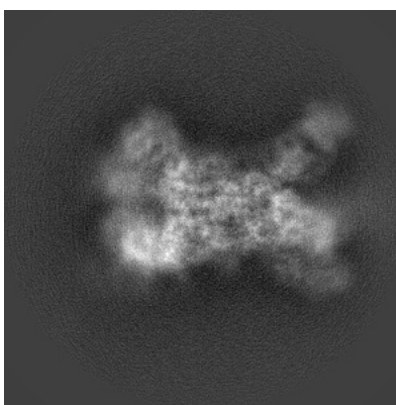


Z

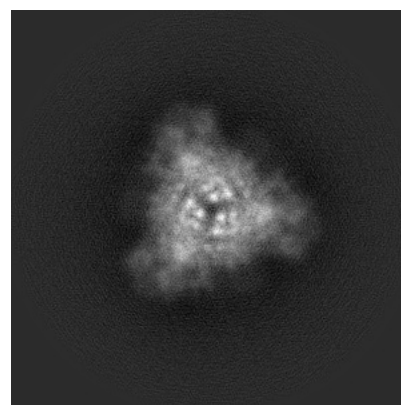
6.1.2 Raw map



X



Y

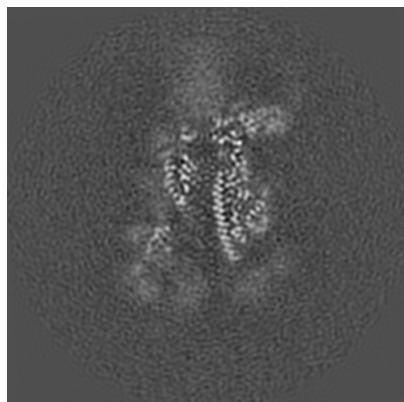


Z

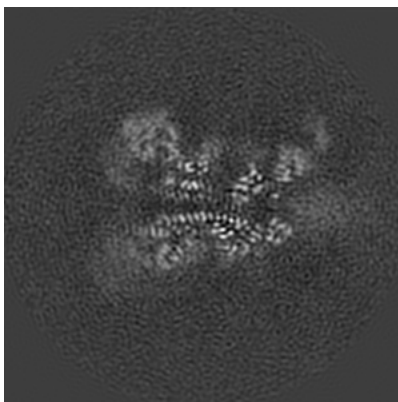
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

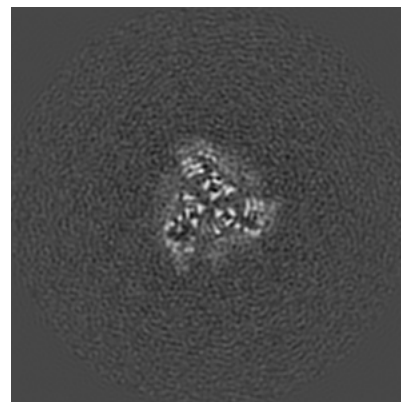
6.2.1 Primary map



X Index: 152

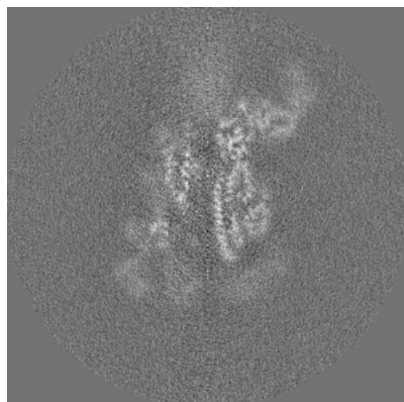


Y Index: 152

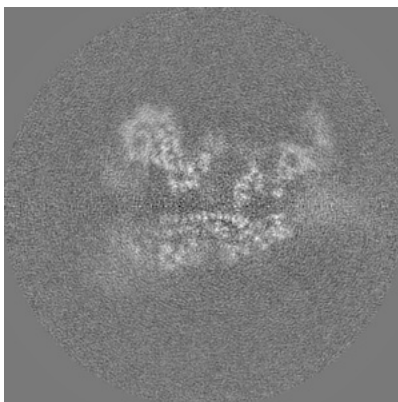


Z Index: 152

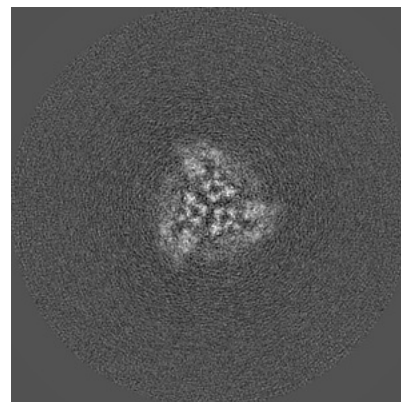
6.2.2 Raw map



X Index: 152



Y Index: 152

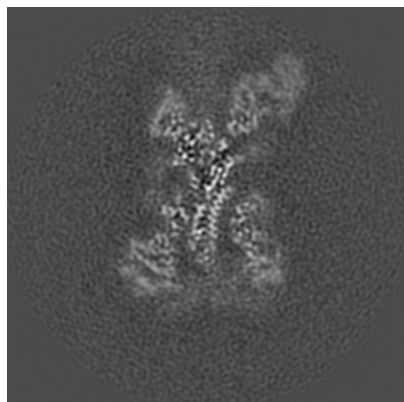


Z Index: 152

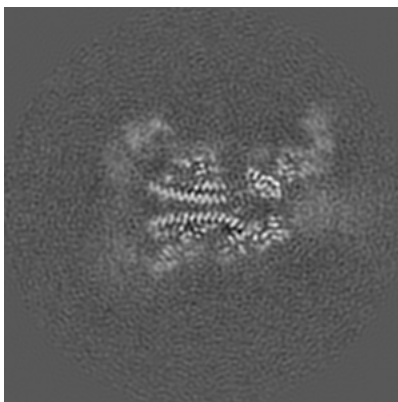
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

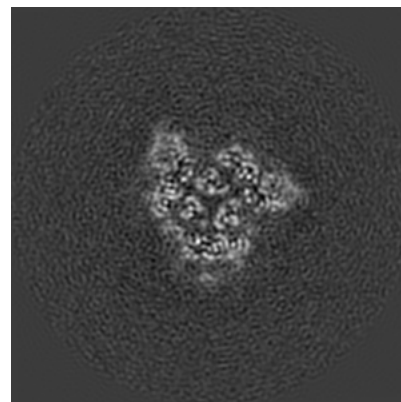
6.3.1 Primary map



X Index: 134

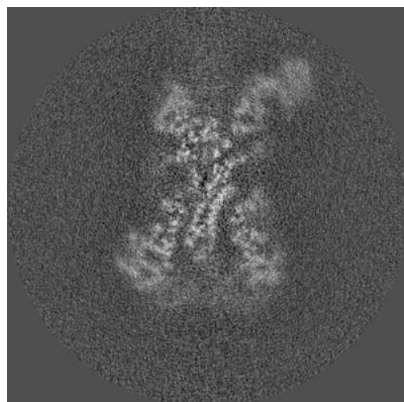


Y Index: 148

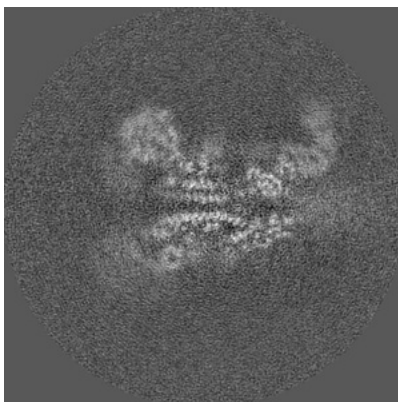


Z Index: 129

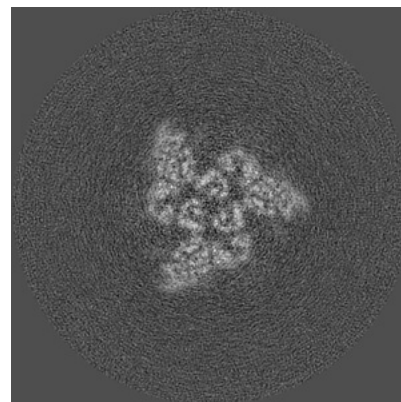
6.3.2 Raw map



X Index: 135



Y Index: 149

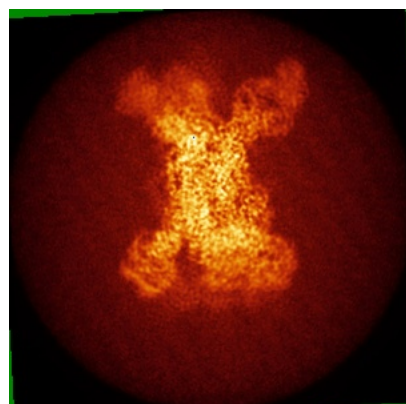


Z Index: 126

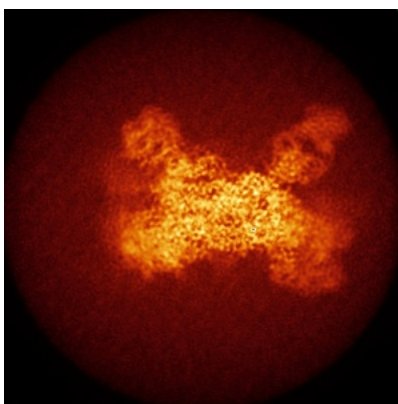
The images above show the largest variance slices of the map in three orthogonal directions.

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

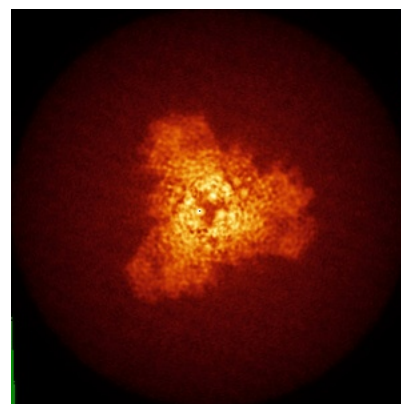
6.4.1 Primary map



X

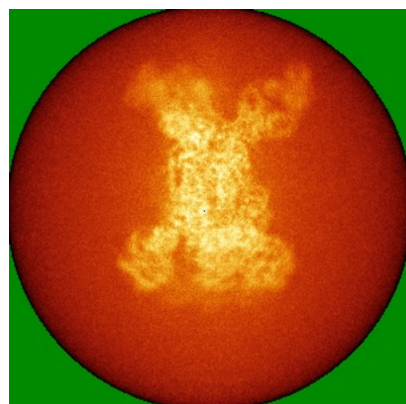


Y

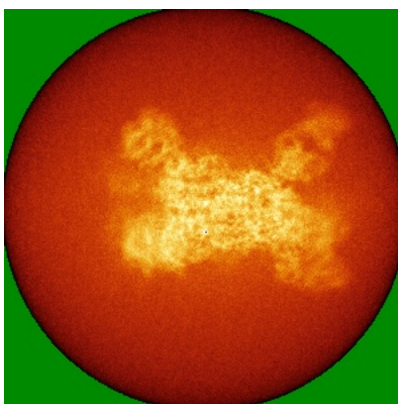


Z

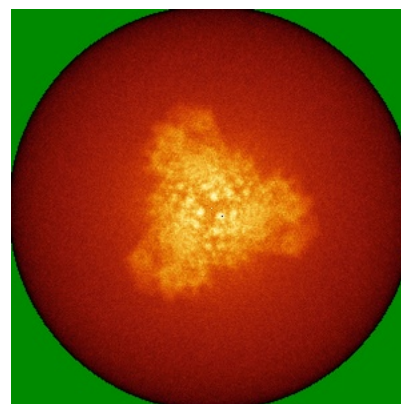
6.4.2 Raw map



X



Y

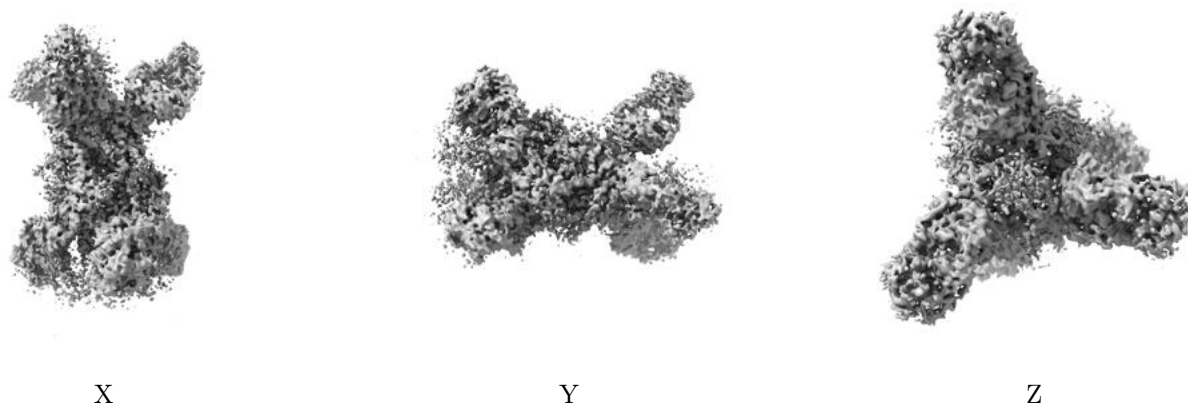


Z

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.

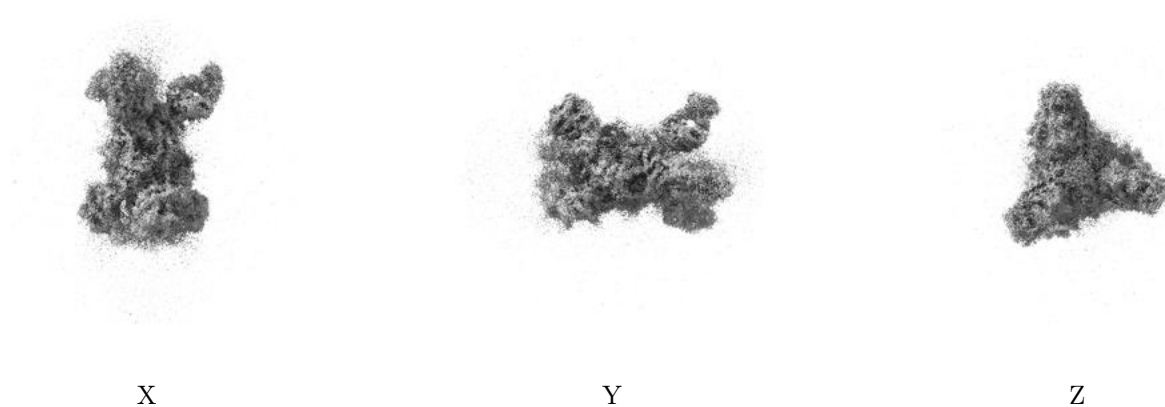
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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



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.

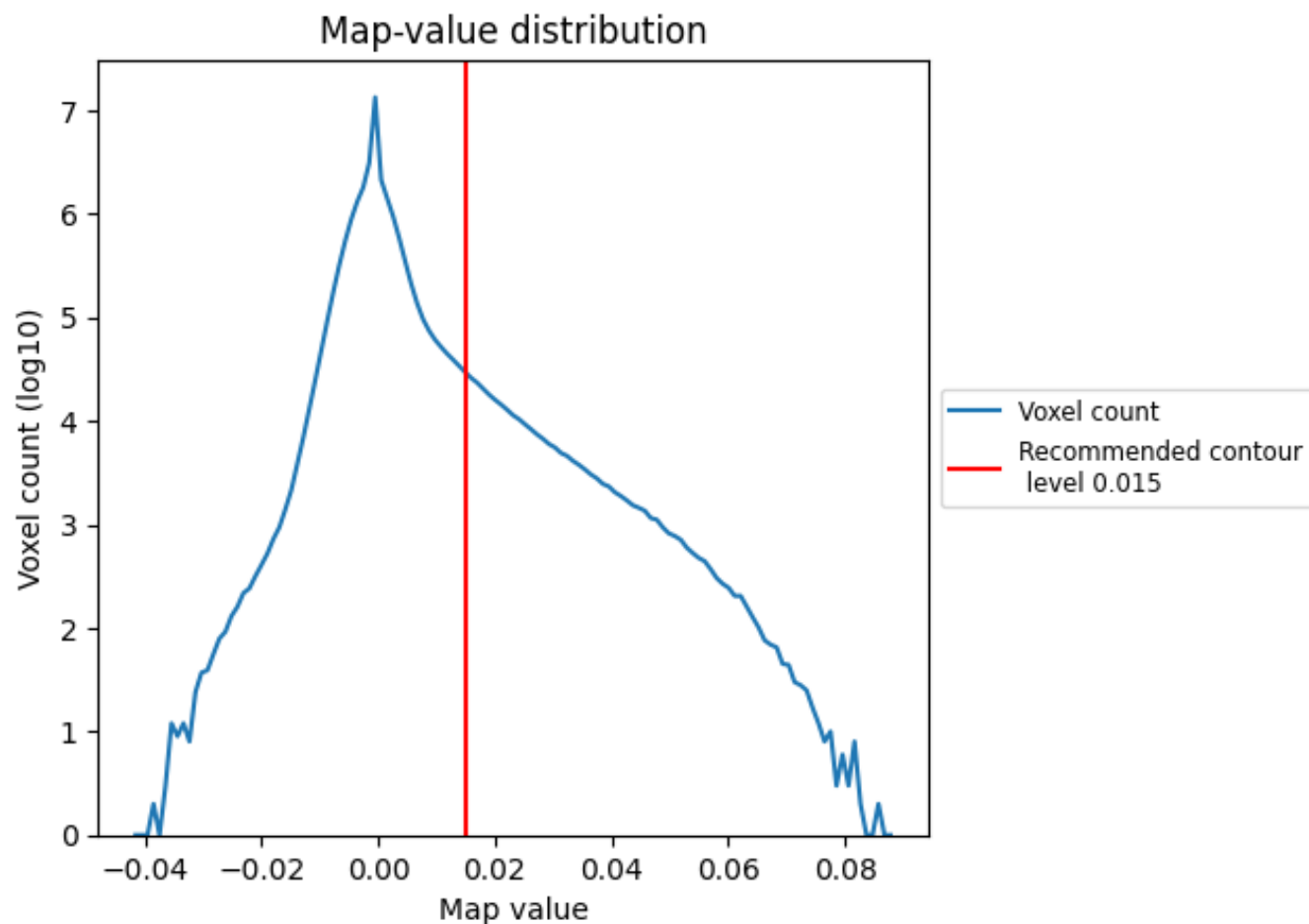
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

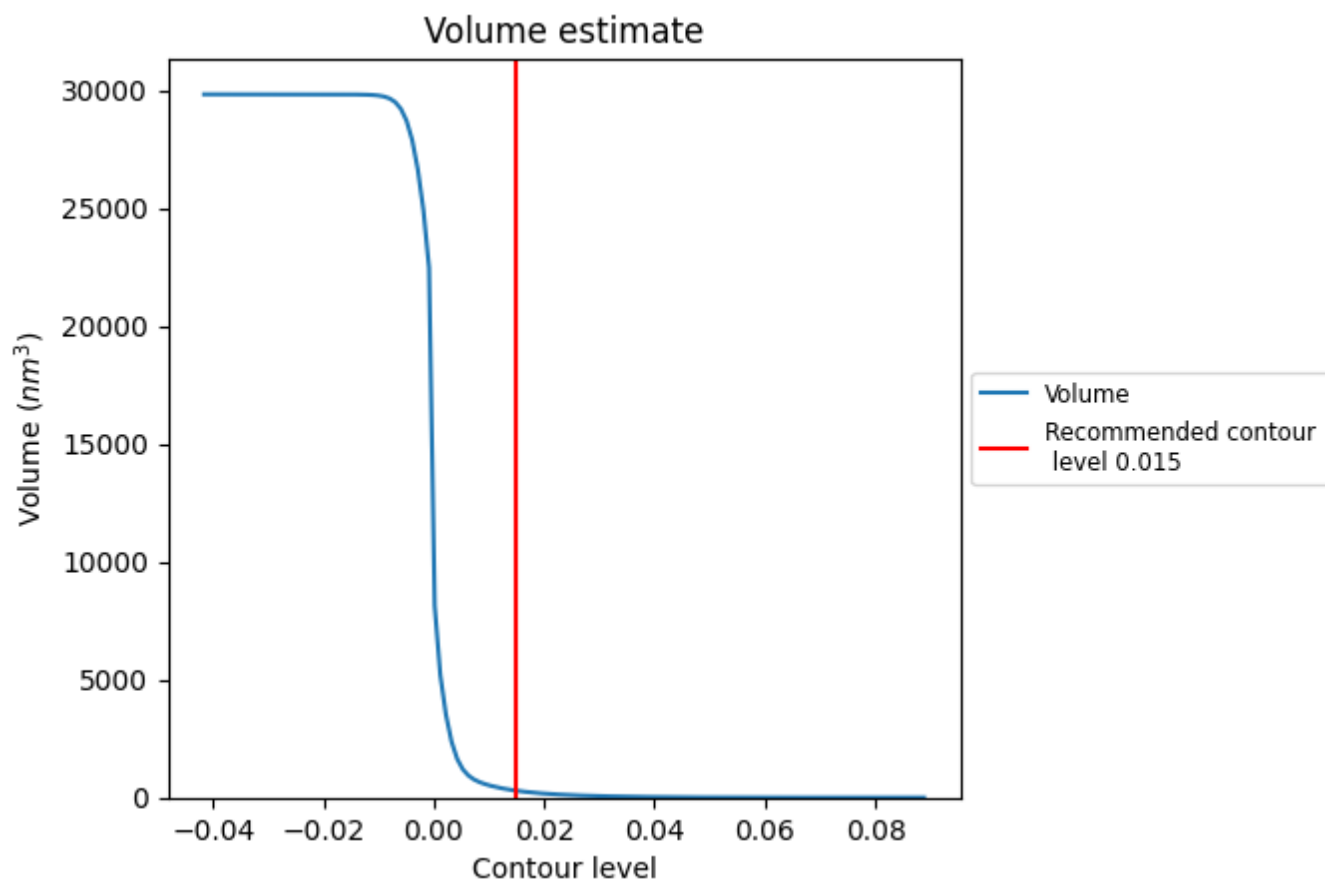
This section contains the results of statistical analysis of the map.

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.

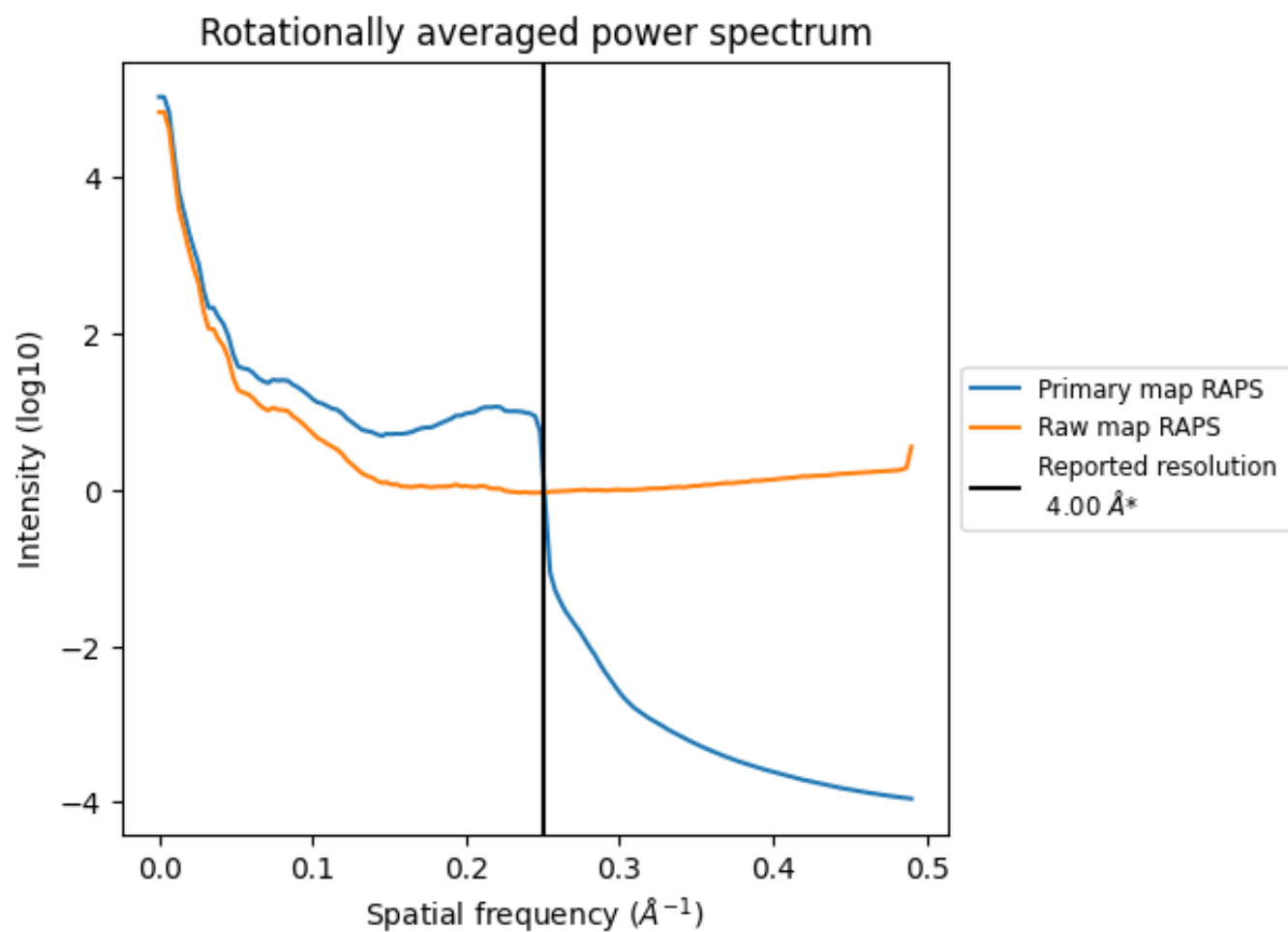
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 291 nm^3 ; this corresponds to an approximate mass of 263 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 ⓘ

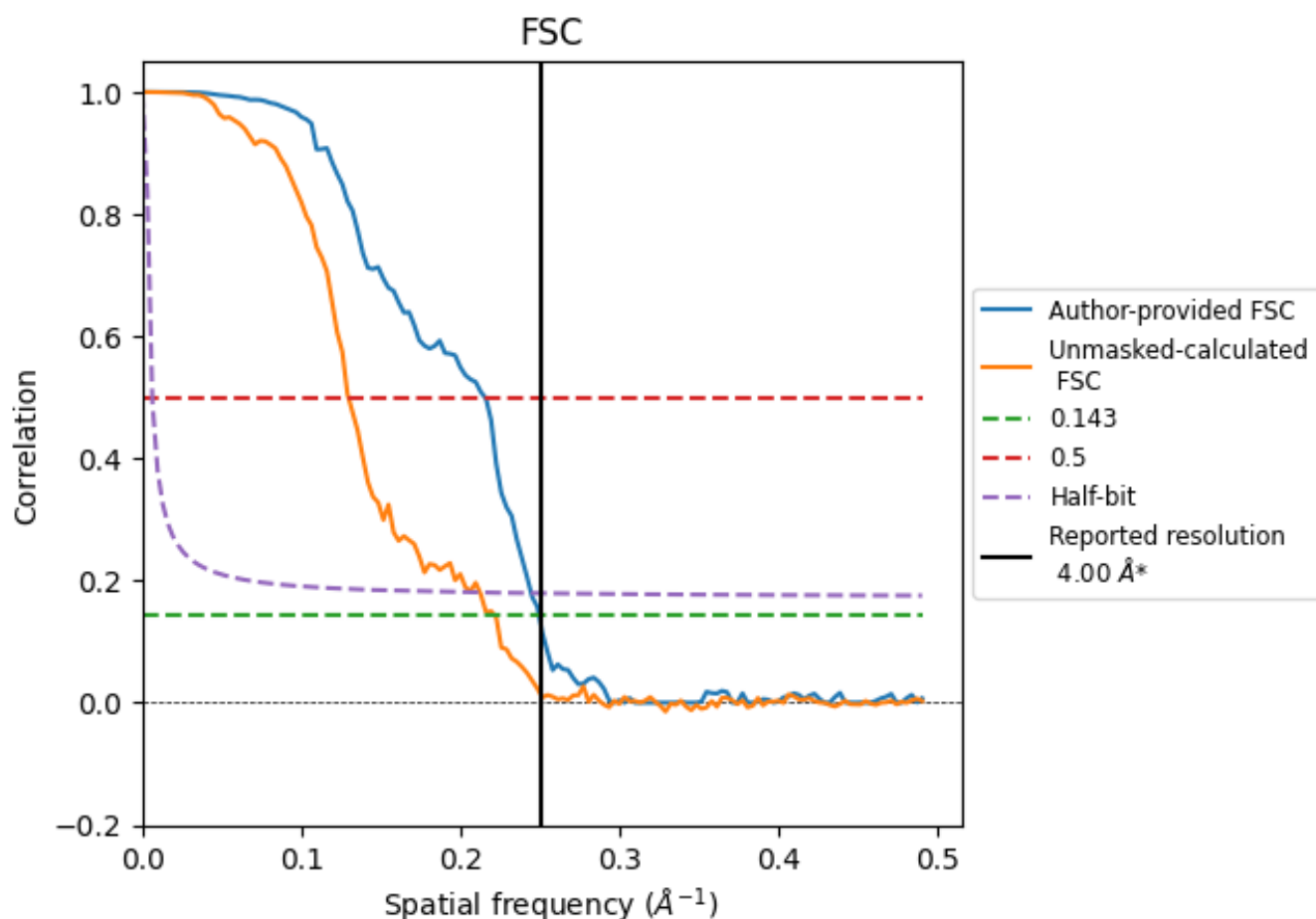


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

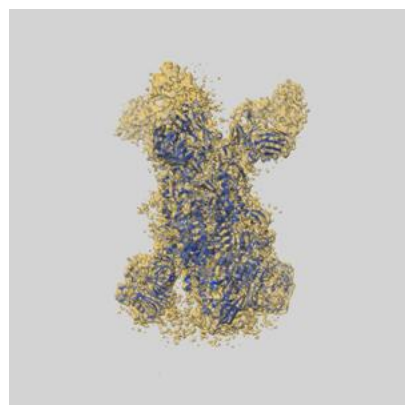
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.01	4.64	4.09
Unmasked-calculated*	4.51	7.72	4.71

*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 4.51 differs from the reported value 4.0 by more than 10 %

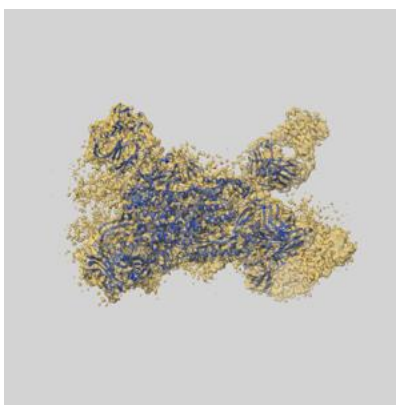
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8791 and PDB model 5W9P. Per-residue inclusion information can be found in section [3](#) on page [12](#).

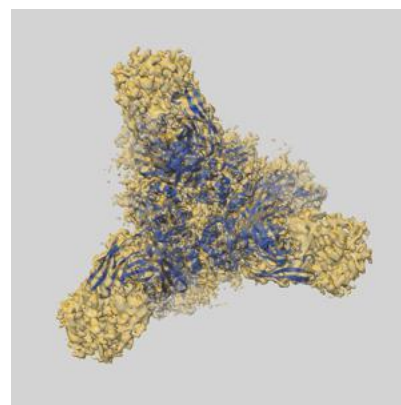
9.1 Map-model overlay [i](#)



X



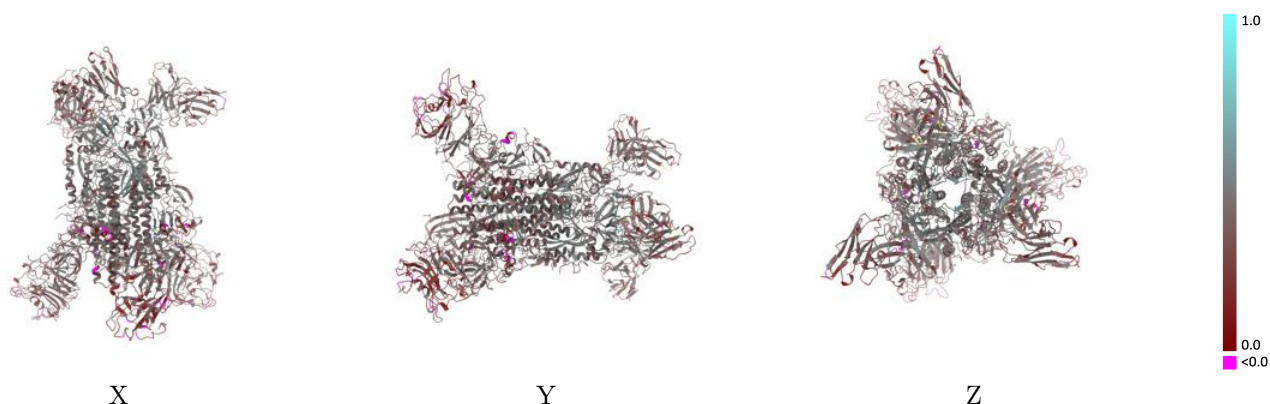
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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](#)

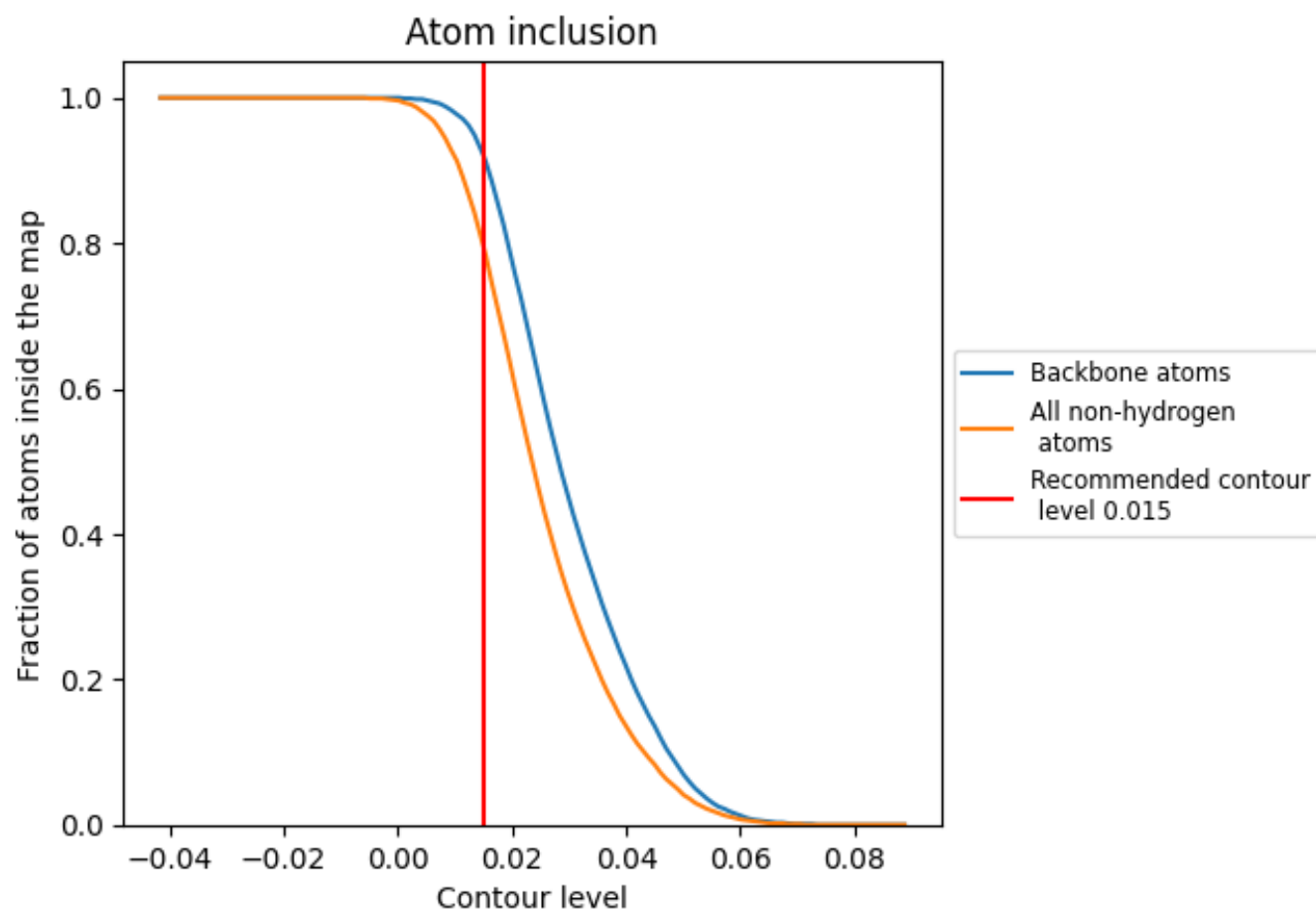


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7960	0.3720
A	0.7930	0.3420
B	0.8210	0.4150
C	0.7920	0.3420
D	0.7930	0.3780
E	0.7000	0.3230
F	0.7990	0.3800
G	0.7000	0.3240
H	0.8200	0.4160
I	0.7960	0.3430
J	0.8230	0.4160
K	0.7920	0.3800
L	0.7000	0.3200

1.0

0.0

<0.0