



## wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 04:16 PM EDT

PDB ID : 5W9N  
EMDB ID : EMD-8789  
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 : 5.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

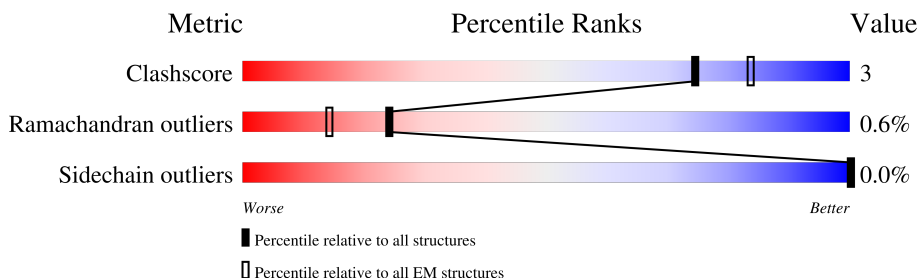
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1329	
1	D	1329	
1	G	1329	
1	H	1329	
1	I	1329	
1	J	1329	
2	B	233	
2	E	233	

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Mol	Chain	Length	Quality of chain
3	C	218	<div><div><div>11%</div><div>49%</div><div></div></div><div></div></div>
3	F	218	<div><div><div>9%</div><div>49%</div><div></div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31126 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 MERS S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	D	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	G	457	Total	C	N	O	S	0	0
			3496	2214	590	675	17		
1	H	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	I	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	J	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	1304	GLN	-	expression tag	UNP W5ZZF5

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
I	1300	PRO	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 2 is a protein called G4 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	E	119	Total	C	N	O	S	0	0
			948	602	156	185	5		

- Molecule 3 is a protein called G4 VL.

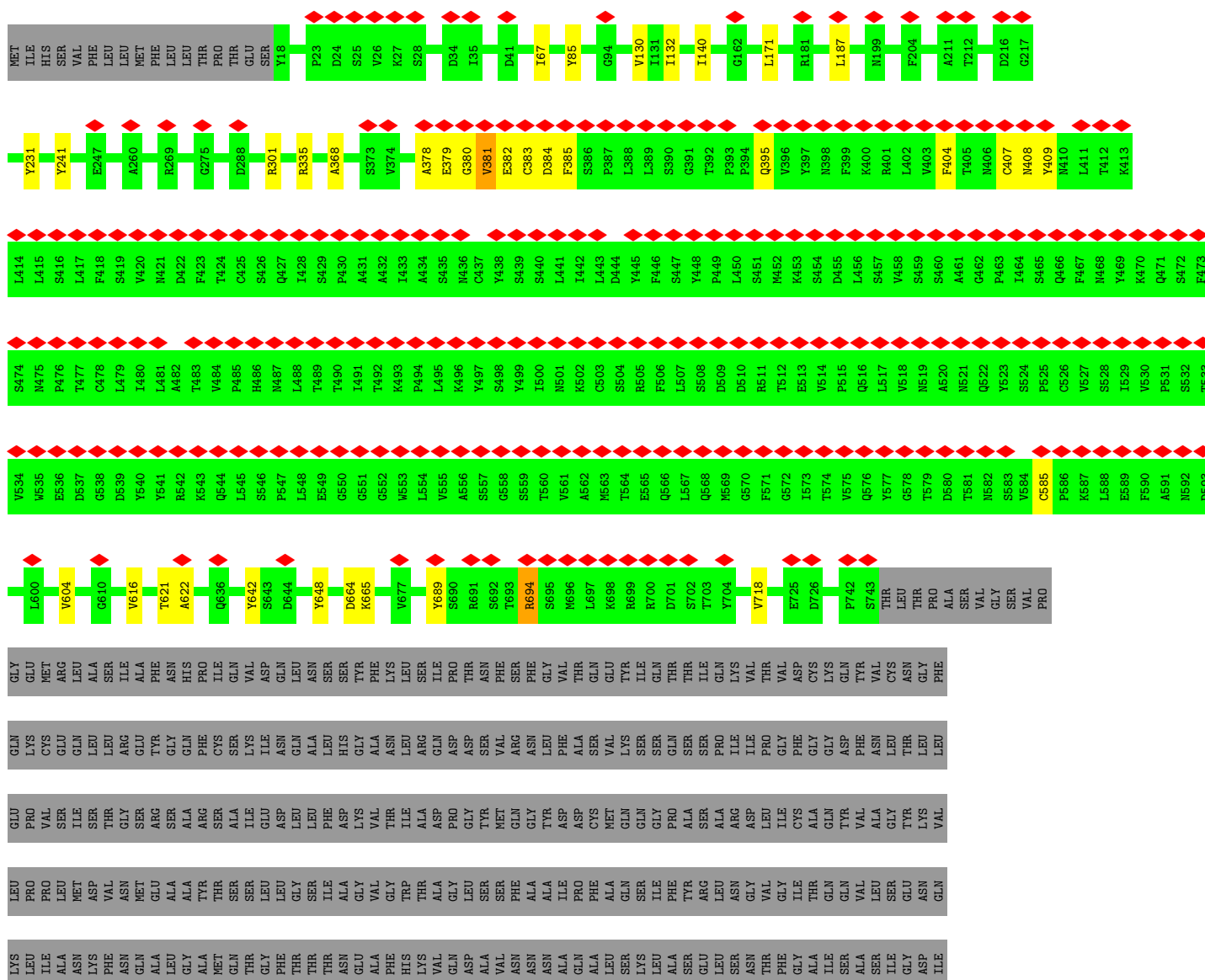
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	111	Total 835	C 522	N 143	O 166	S 4	0	0
3	F	111	Total 835	C 522	N 143	O 166	S 4	0	0







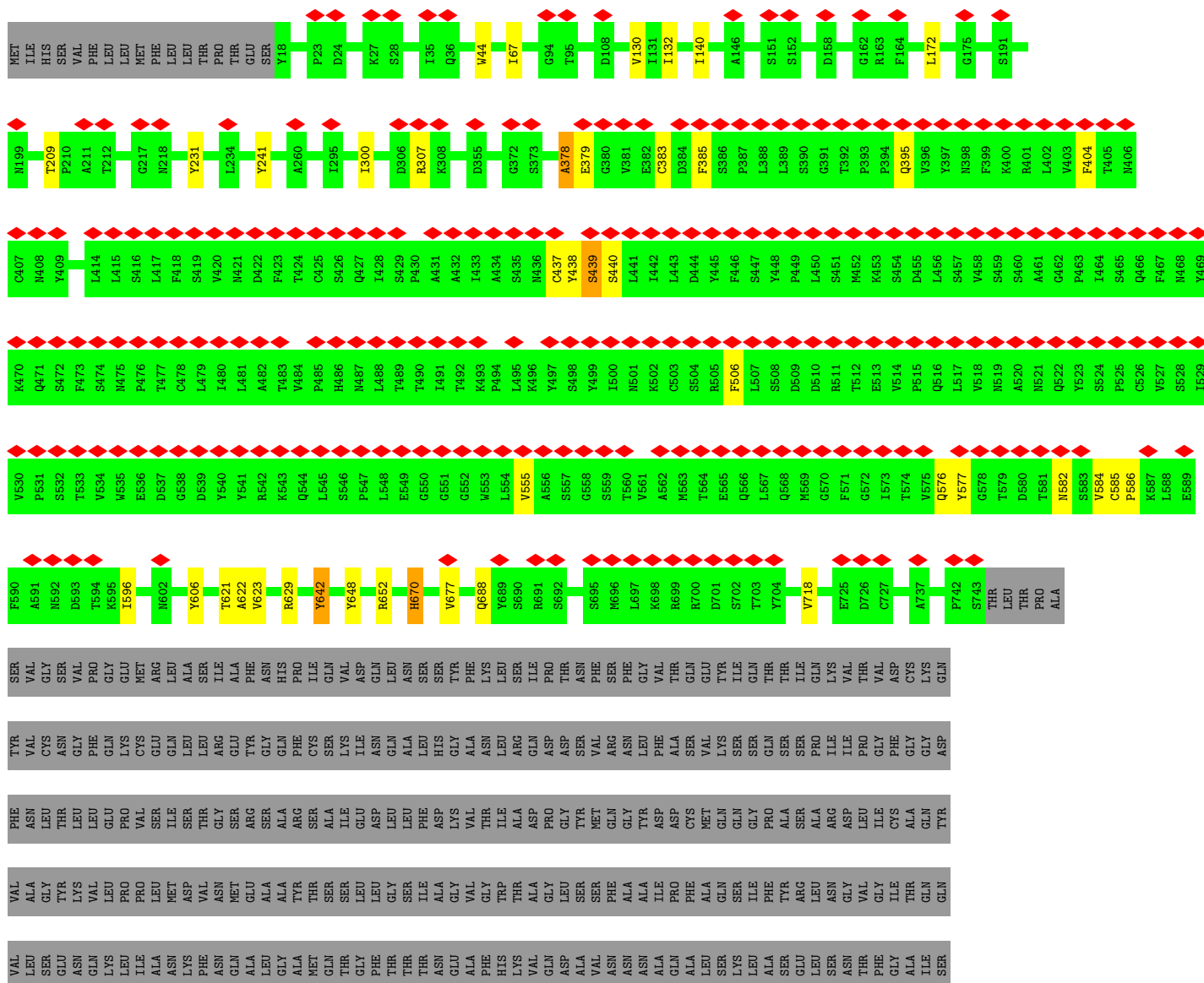
- Molecule 1: MERS S



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

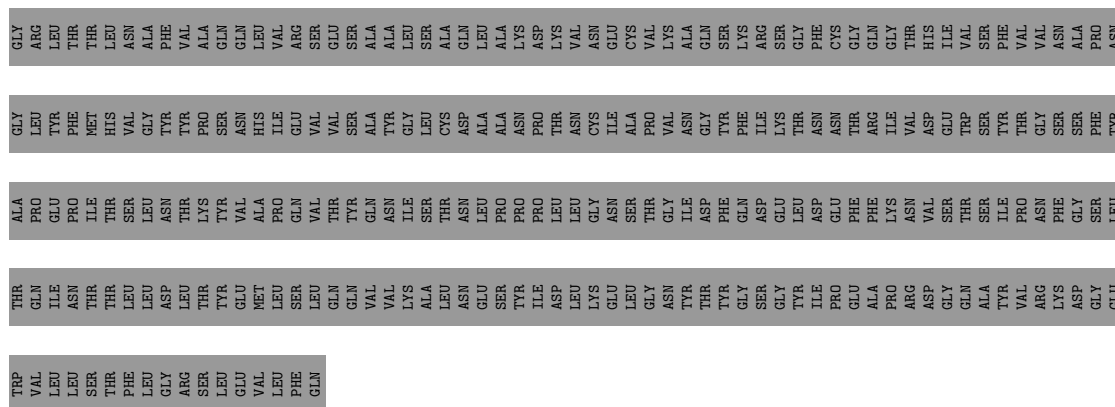
- Molecule 1: MERS S

Chain I:

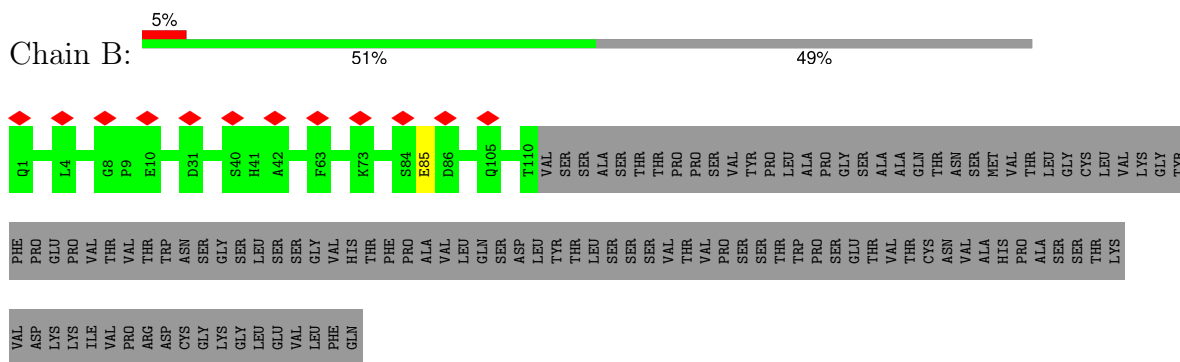




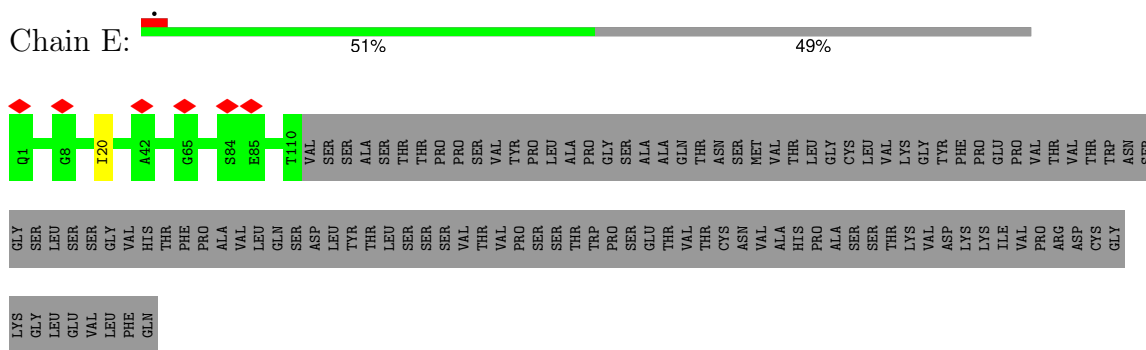




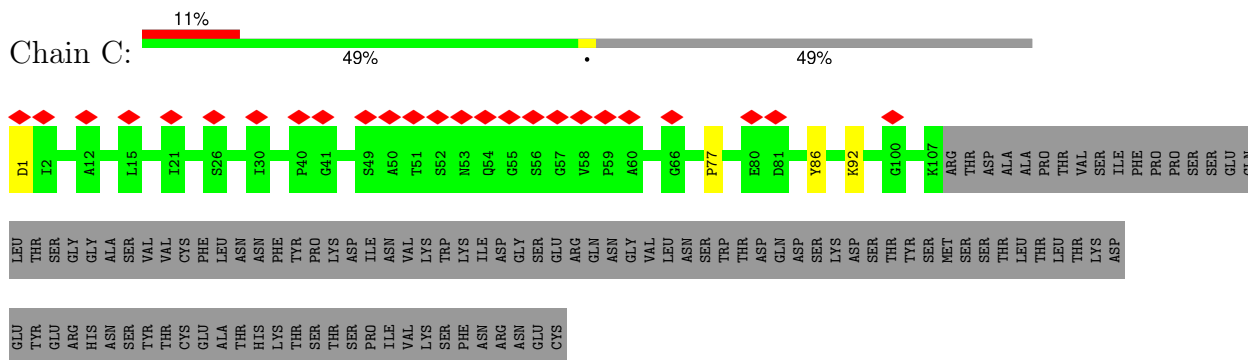
- Molecule 2: G4 VH



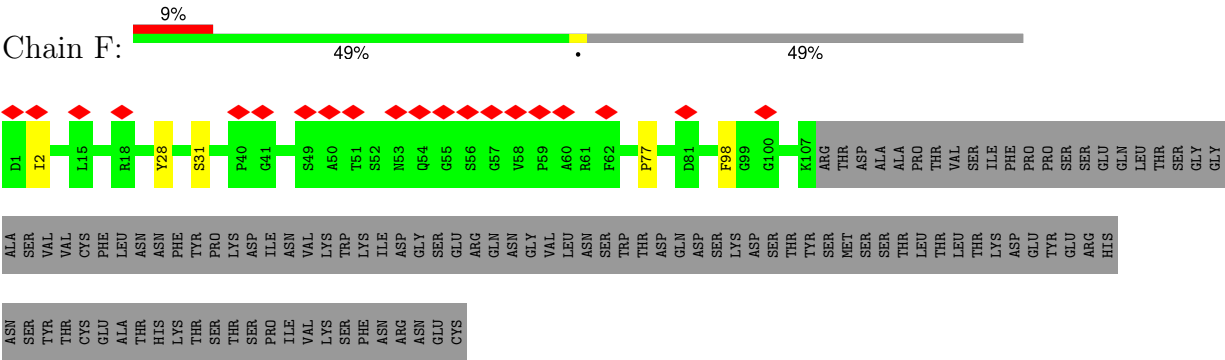
- Molecule 2: G4 VH



- Molecule 3: G4 VL



- Molecule 3: G4 VL



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	8133	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	0.041	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	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 [i](#)

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

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	0.72	0/3618	0.81	1/4921 (0.0%)
1	D	0.72	0/3618	0.81	1/4921 (0.0%)
1	G	0.72	0/3568	0.82	4/4851 (0.1%)
1	H	0.72	0/5803	0.89	8/7901 (0.1%)
1	I	0.72	0/5803	0.89	5/7901 (0.1%)
1	J	0.73	0/5803	0.91	11/7901 (0.1%)
2	B	0.71	0/972	0.83	0/1317
2	E	0.74	0/972	0.84	0/1317
3	C	0.76	0/852	0.81	1/1153 (0.1%)
3	F	0.80	0/852	0.87	1/1153 (0.1%)
All	All	0.73	0/31861	0.86	32/43336 (0.1%)

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1156	CYS	O-C-N	-9.22	107.94	122.70
1	I	642	TYR	CB-CG-CD1	-7.73	116.36	121.00
1	J	584	VAL	C-N-CA	7.44	140.30	121.70
1	G	1156	CYS	CA-C-O	7.40	135.64	120.10
1	H	642	TYR	CB-CG-CD2	-7.27	116.64	121.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3545	0	3470	14	0
1	D	3545	0	3471	27	0
1	G	3496	0	3420	14	0
1	H	5658	0	5425	34	0
1	I	5658	0	5425	57	0
1	J	5658	0	5423	26	0
2	B	948	0	904	1	0
2	E	948	0	904	2	0
3	C	835	0	816	2	0
3	F	835	0	816	2	0
All	All	31126	0	30074	179	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 3.

The worst 5 of 179 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:J:506:PHE:CE2	1:J:555:VAL:HG21	1.09	1.61
1:I:506:PHE:CE2	1:I:555:VAL:CG2	1.84	1.58
1:I:506:PHE:CE2	1:I:555:VAL:HG21	0.95	1.47
1:I:506:PHE:HE2	1:I:555:VAL:CG2	1.15	1.43
1:J:506:PHE:CE2	1:J:555:VAL:CG2	2.00	1.42

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	459/1329 (34%)	441 (96%)	15 (3%)	3 (1%)	19 56
1	D	459/1329 (34%)	440 (96%)	14 (3%)	5 (1%)	12 46

*Continued on next page...*

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	451/1329 (34%)	433 (96%)	17 (4%)	1 (0%)	44	78
1	H	724/1329 (54%)	693 (96%)	27 (4%)	4 (1%)	22	60
1	I	724/1329 (54%)	691 (95%)	29 (4%)	4 (1%)	22	60
1	J	724/1329 (54%)	695 (96%)	24 (3%)	5 (1%)	19	56
2	B	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
2	E	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
3	C	109/218 (50%)	103 (94%)	5 (5%)	1 (1%)	14	51
3	F	109/218 (50%)	105 (96%)	2 (2%)	2 (2%)	7	34
All	All	3993/8876 (45%)	3831 (96%)	137 (3%)	25 (1%)	24	60

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	961	THR
1	G	962	ALA
1	H	381	VAL
1	I	439	SER
1	J	378	ALA

### 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	388/1148 (34%)	388 (100%)	0	100	100
1	D	388/1148 (34%)	388 (100%)	0	100	100
1	G	382/1148 (33%)	382 (100%)	0	100	100
1	H	635/1148 (55%)	635 (100%)	0	100	100
1	I	635/1148 (55%)	634 (100%)	1 (0%)	92	94
1	J	635/1148 (55%)	635 (100%)	0	100	100
2	B	102/202 (50%)	102 (100%)	0	100	100
2	E	102/202 (50%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	93/192 (48%)	93 (100%)	0	100	100
3	F	93/192 (48%)	93 (100%)	0	100	100
All	All	3453/7676 (45%)	3452 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	670	HIS

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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.



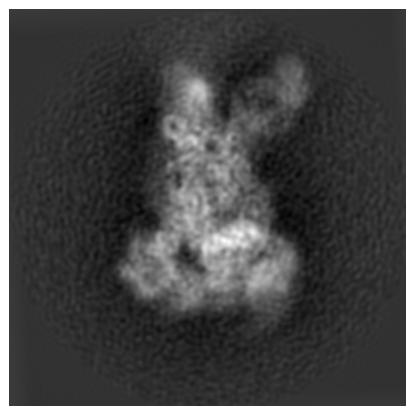
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8789. These allow visual inspection of the internal detail of the map and identification of artifacts.

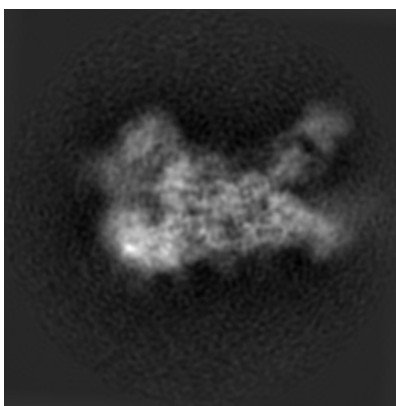
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

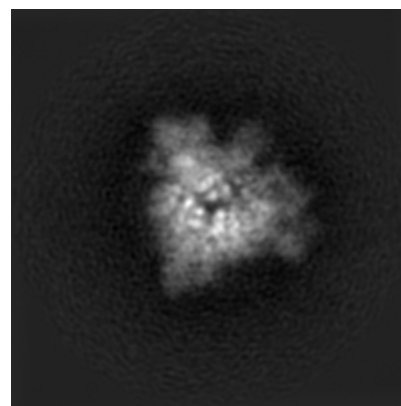
#### 6.1.1 Primary map



X

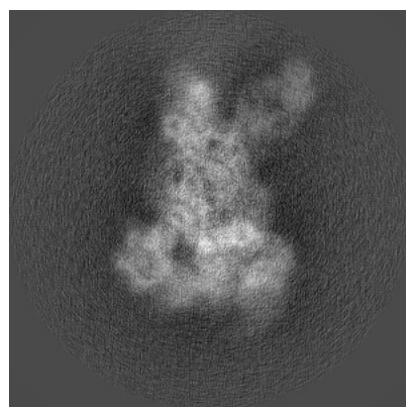


Y

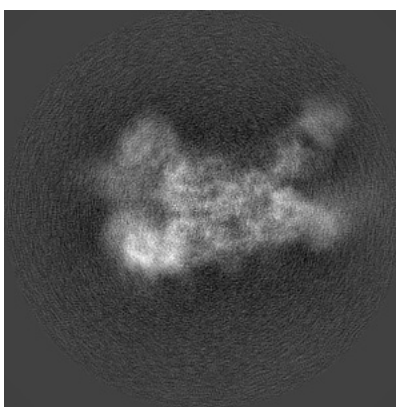


Z

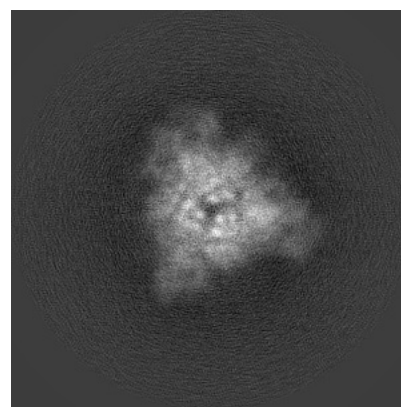
#### 6.1.2 Raw map



X



Y

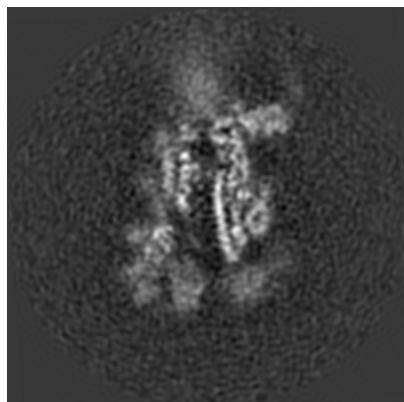


Z

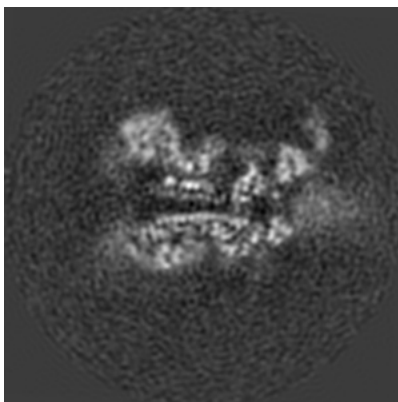
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

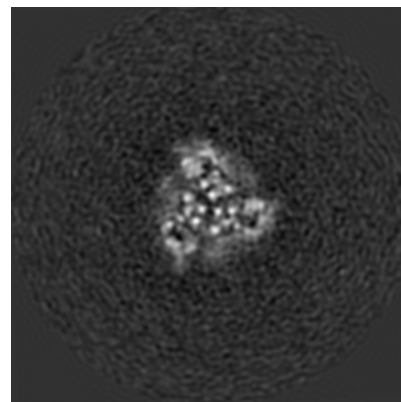
### 6.2.1 Primary map



X Index: 152

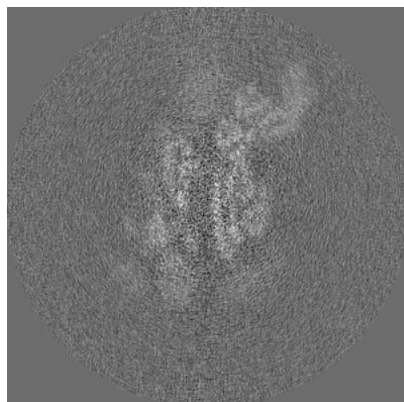


Y Index: 152

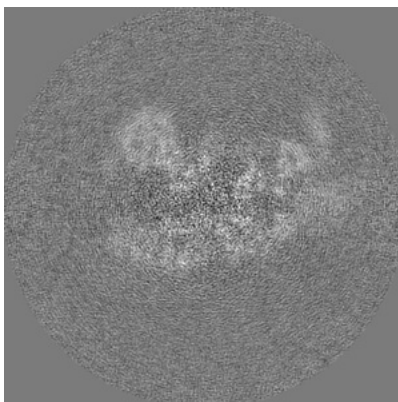


Z Index: 152

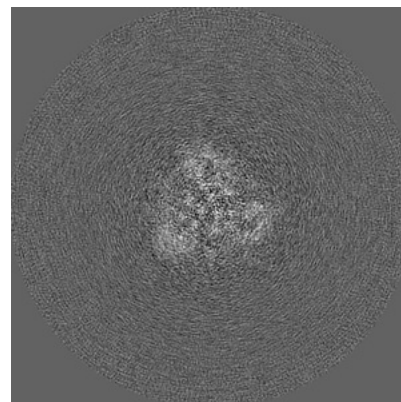
### 6.2.2 Raw map



X Index: 152



Y Index: 152

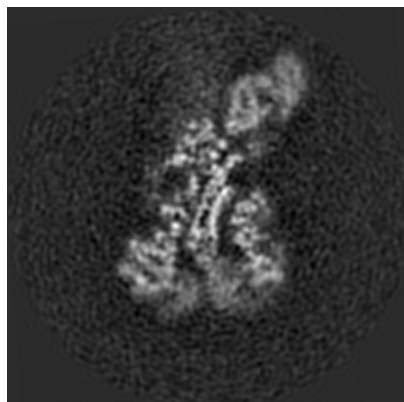


Z Index: 152

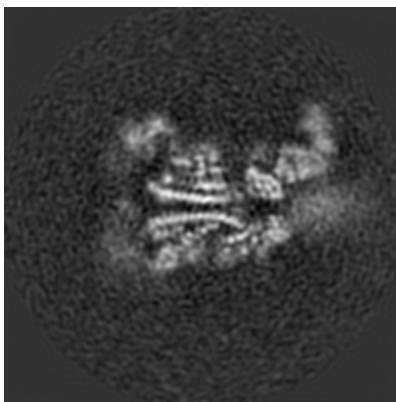
The images above show central slices of the map in three orthogonal directions.

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

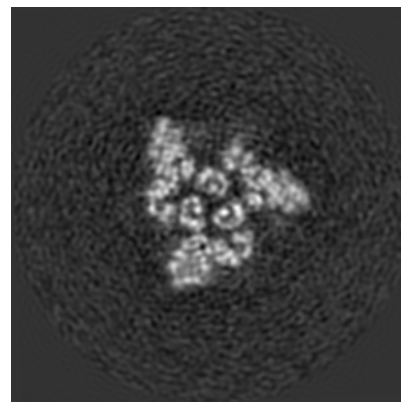
### 6.3.1 Primary map



X Index: 135

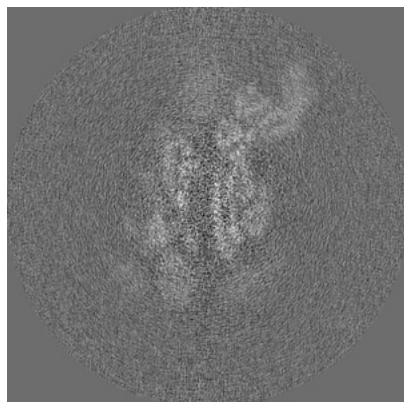


Y Index: 148

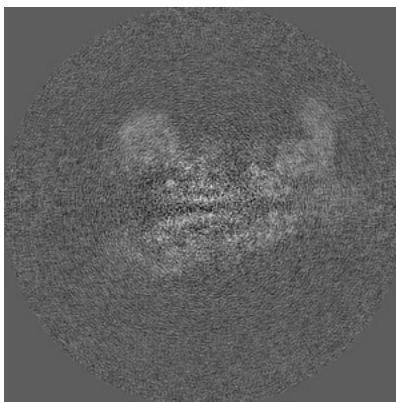


Z Index: 124

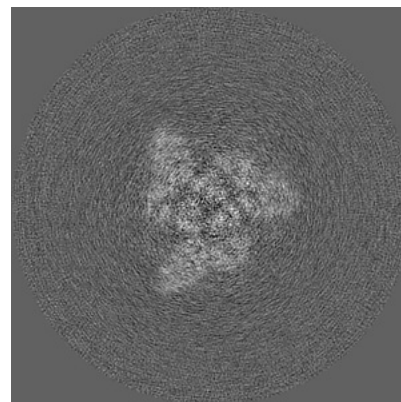
### 6.3.2 Raw map



X Index: 152



Y Index: 147

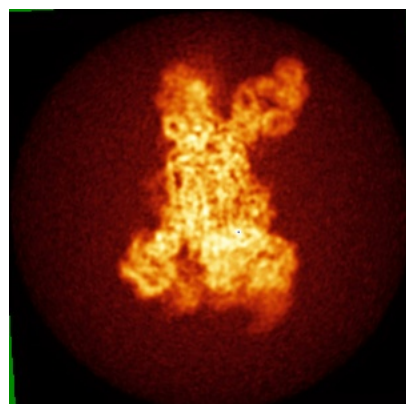


Z Index: 128

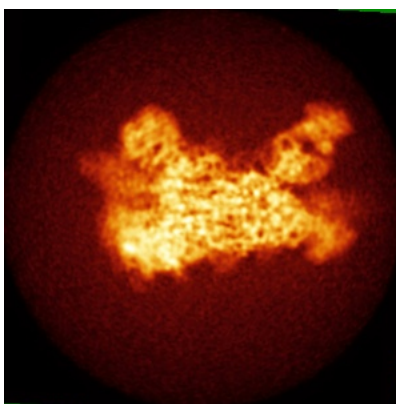
The images above show the largest variance slices of the map in three orthogonal directions.

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

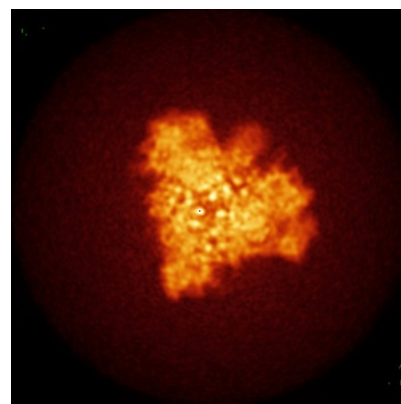
### 6.4.1 Primary map



X

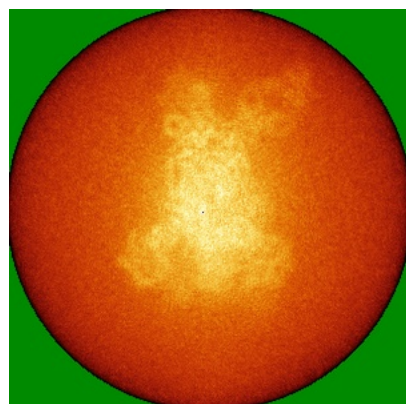


Y

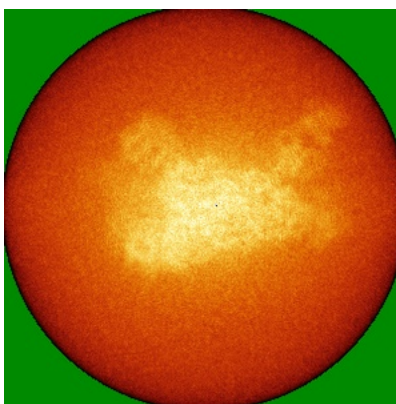


Z

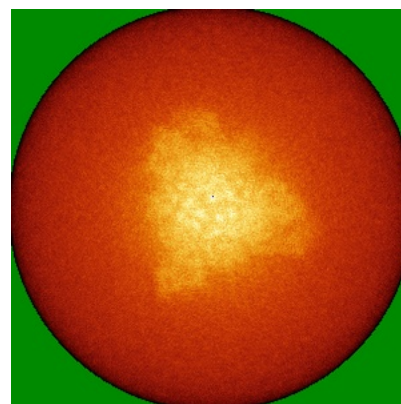
### 6.4.2 Raw map



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.

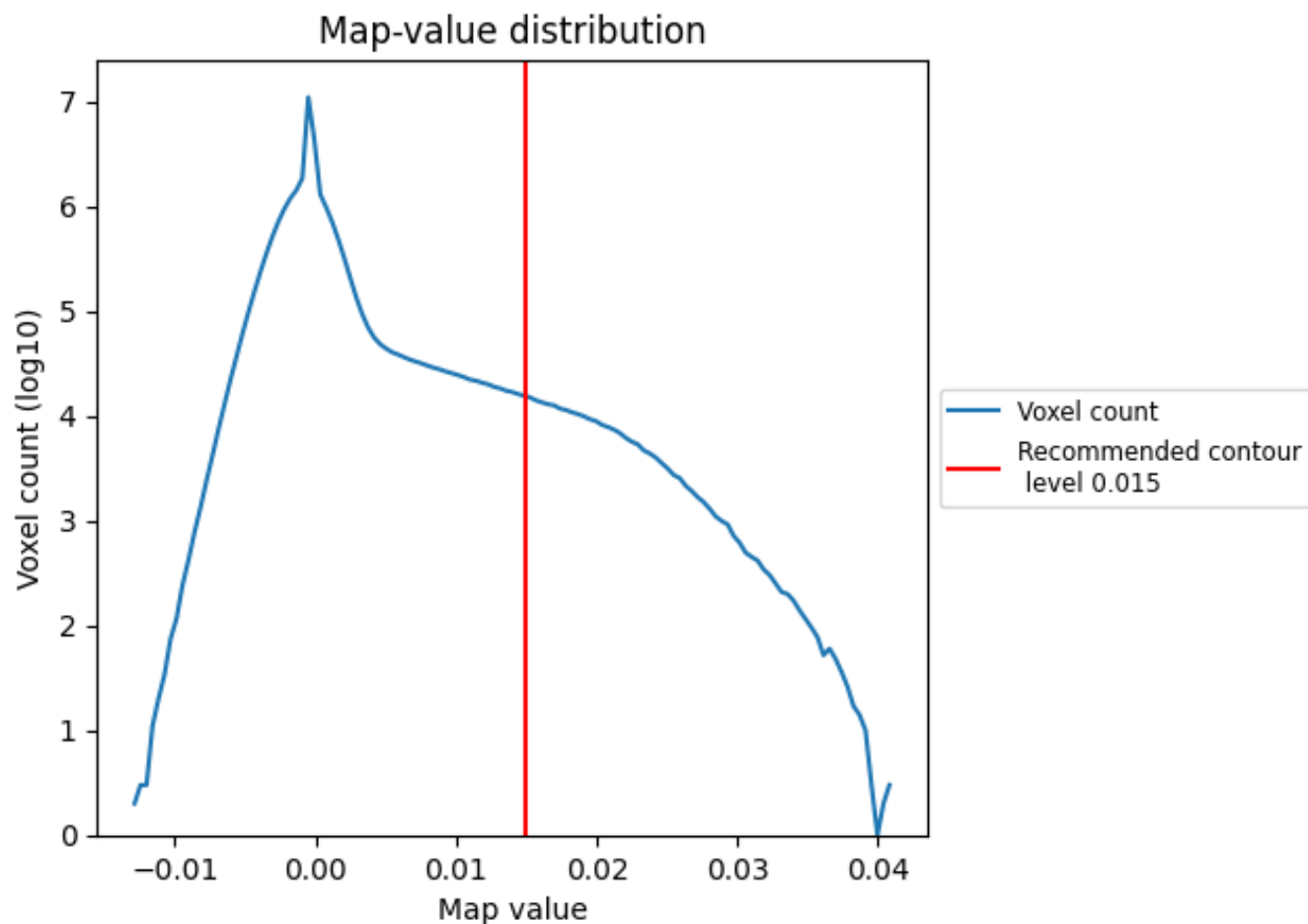
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

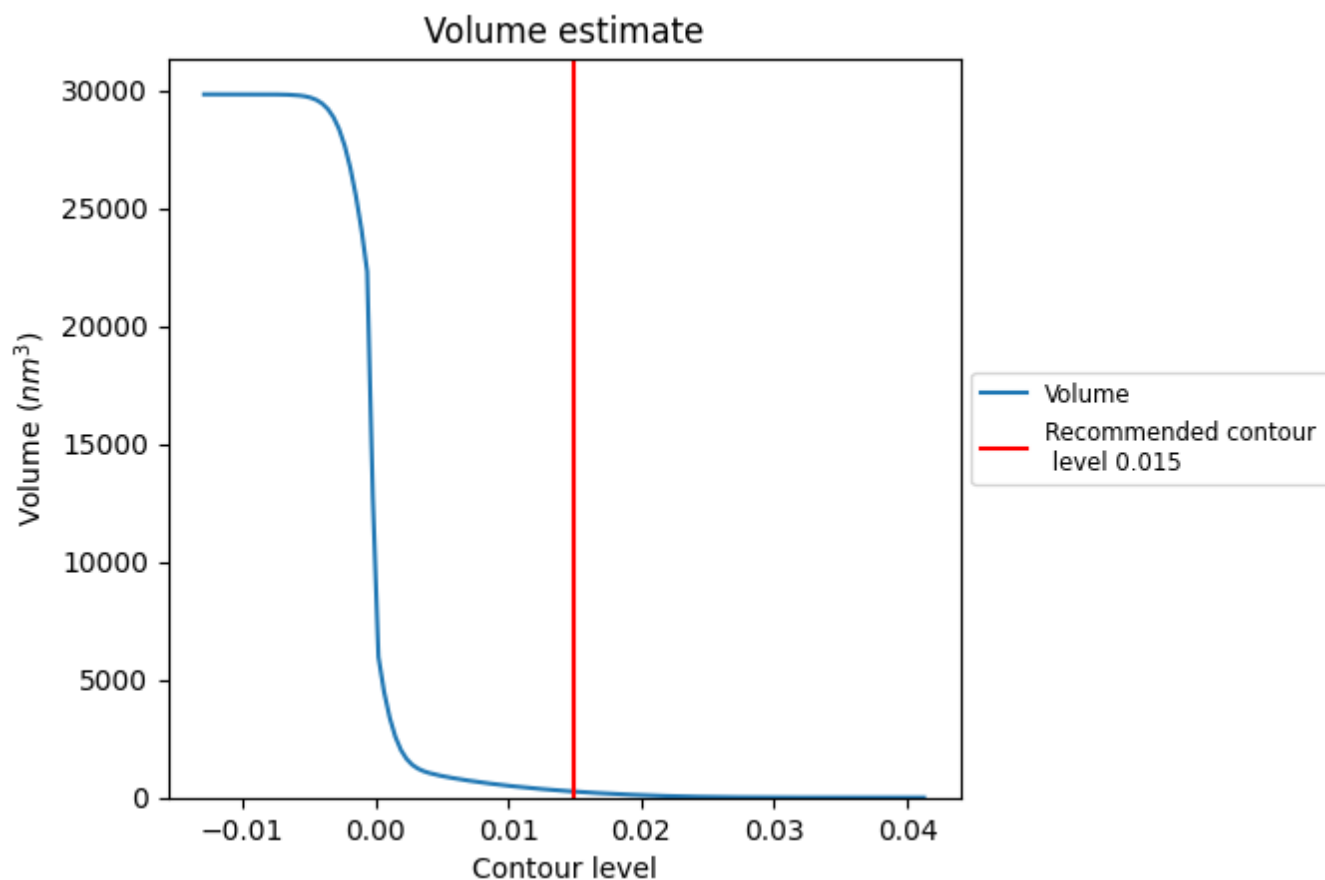
This section contains the results of statistical analysis of the map.

### 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.

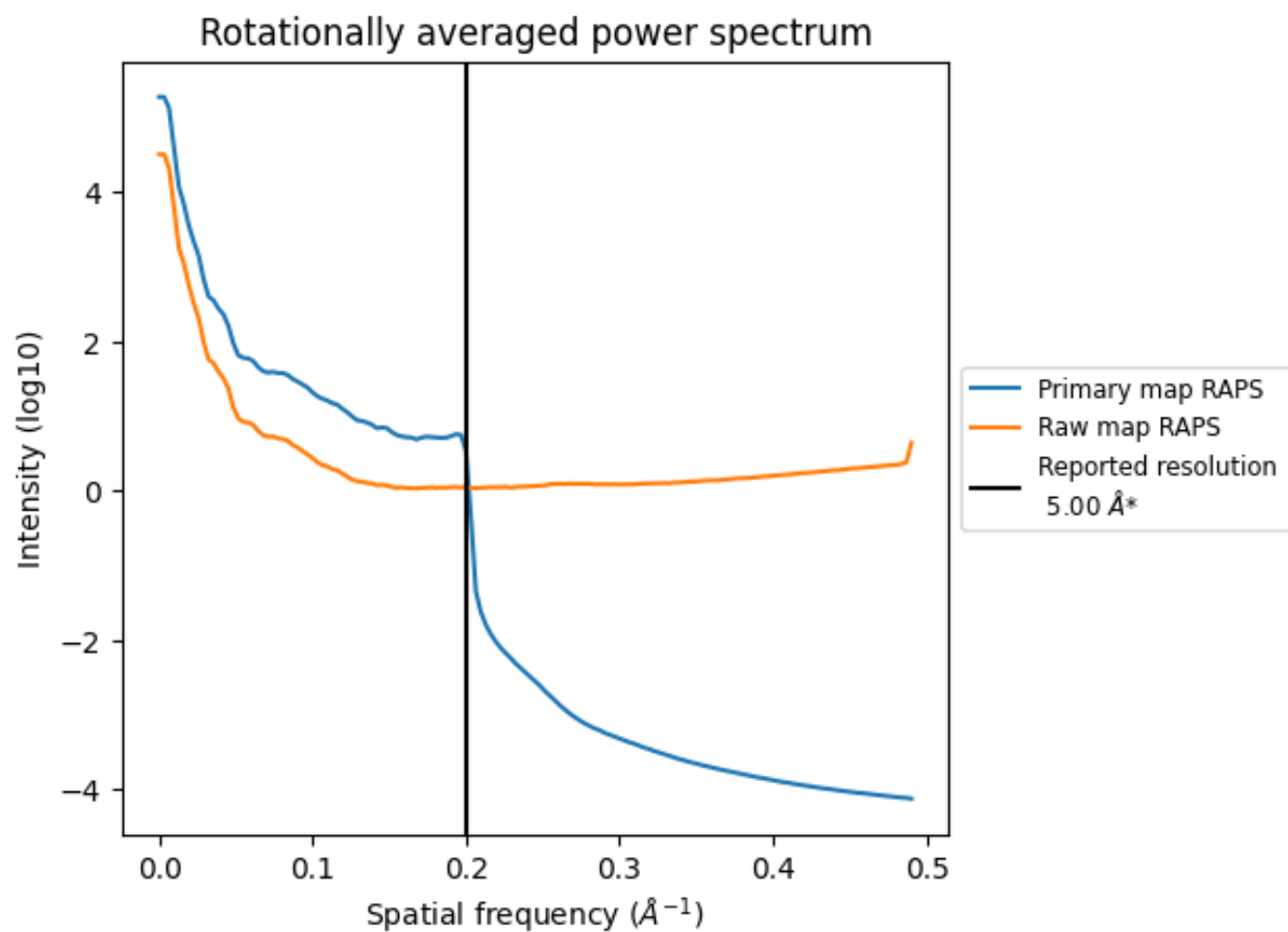
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 253 nm<sup>3</sup>; this corresponds to an approximate mass of 229 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 ⓘ



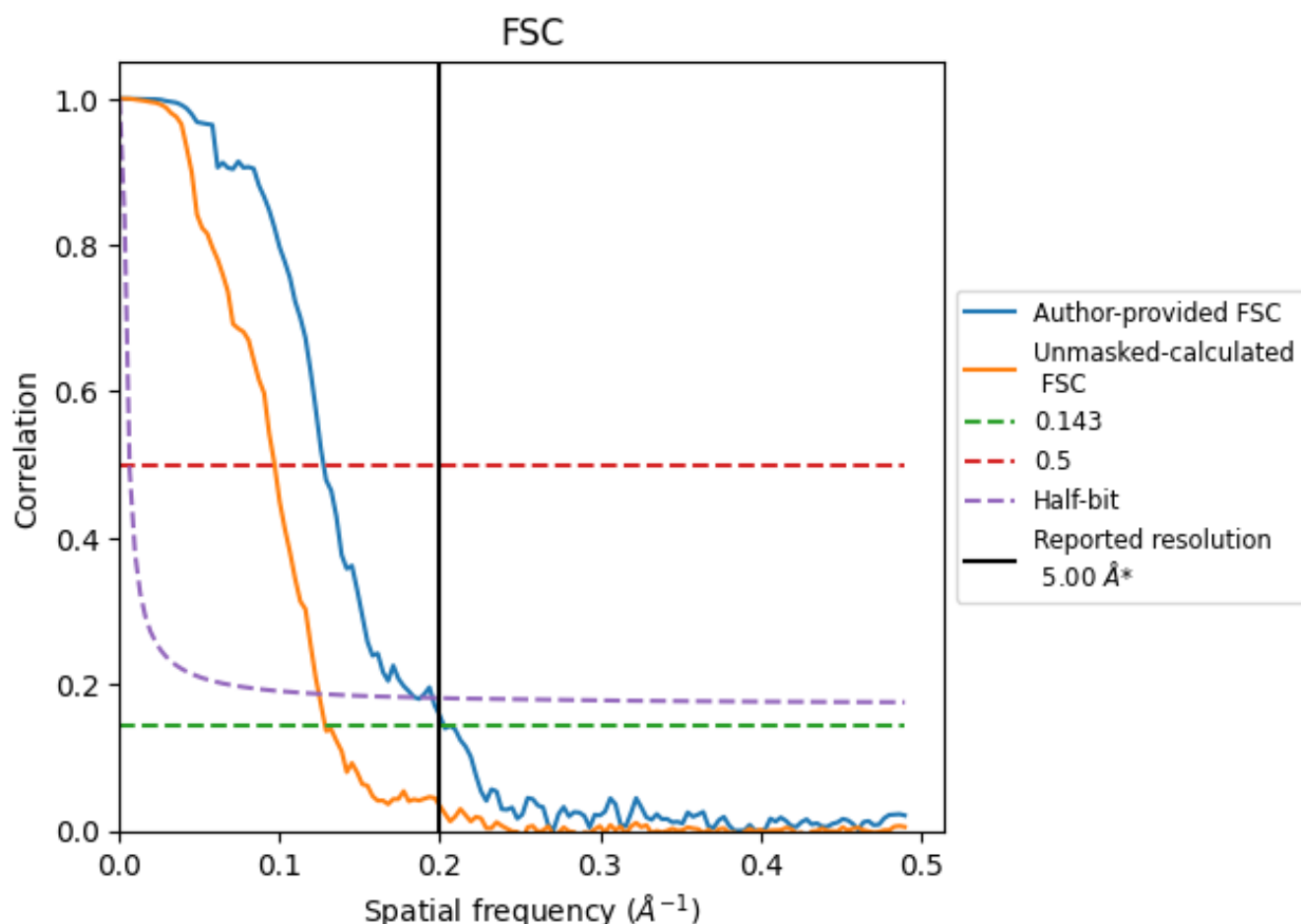
\*Reported resolution corresponds to spatial frequency of 0.200  $\text{\AA}^{-1}$



## 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 0.200 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

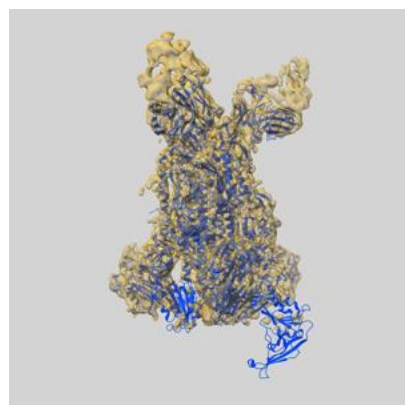
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	4.94	7.85	5.40
Unmasked-calculated*	7.79	10.32	8.04

\*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 7.79 differs from the reported value 5.0 by more than 10 %

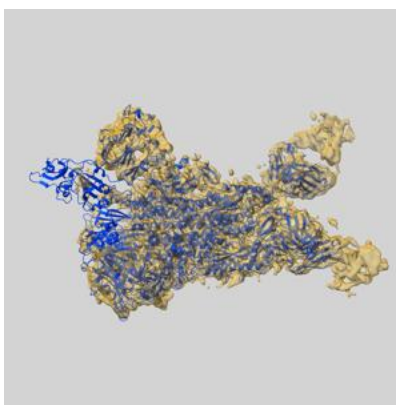
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8789 and PDB model 5W9N. Per-residue inclusion information can be found in section [3](#) on page [12](#).

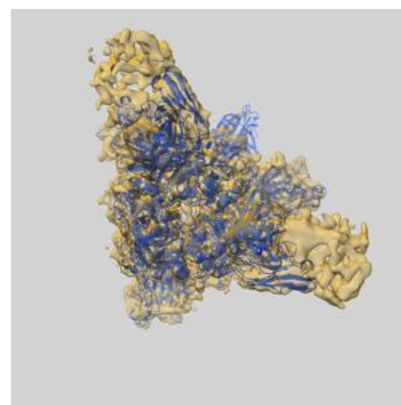
### 9.1 Map-model overlay [i](#)



X



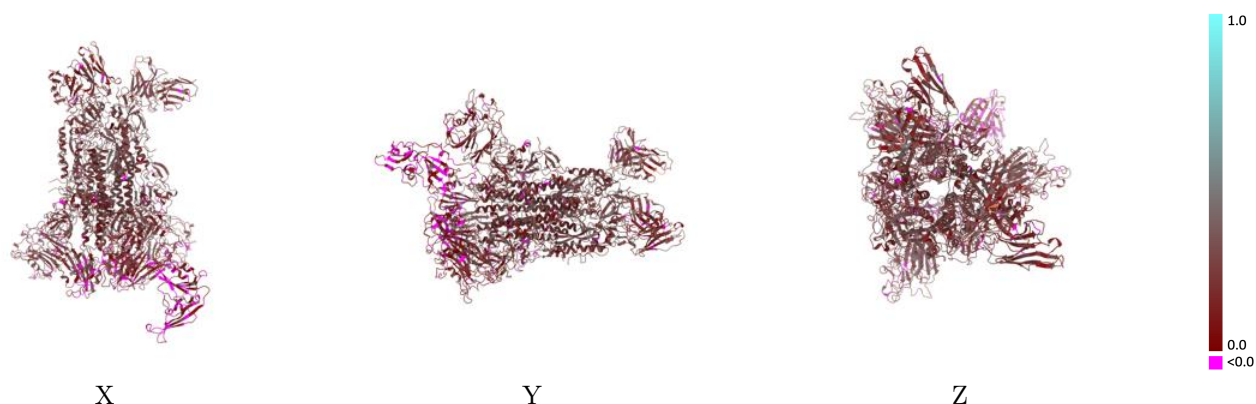
Y



Z

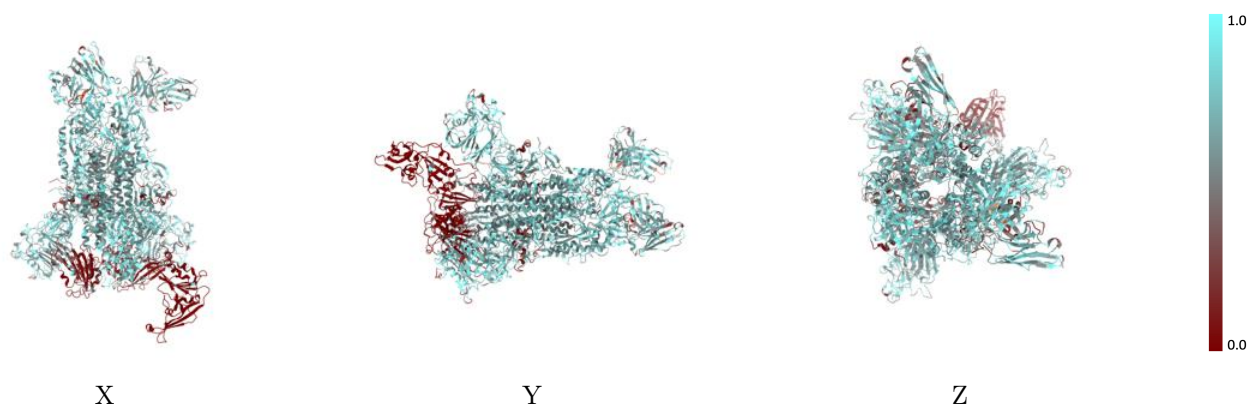
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



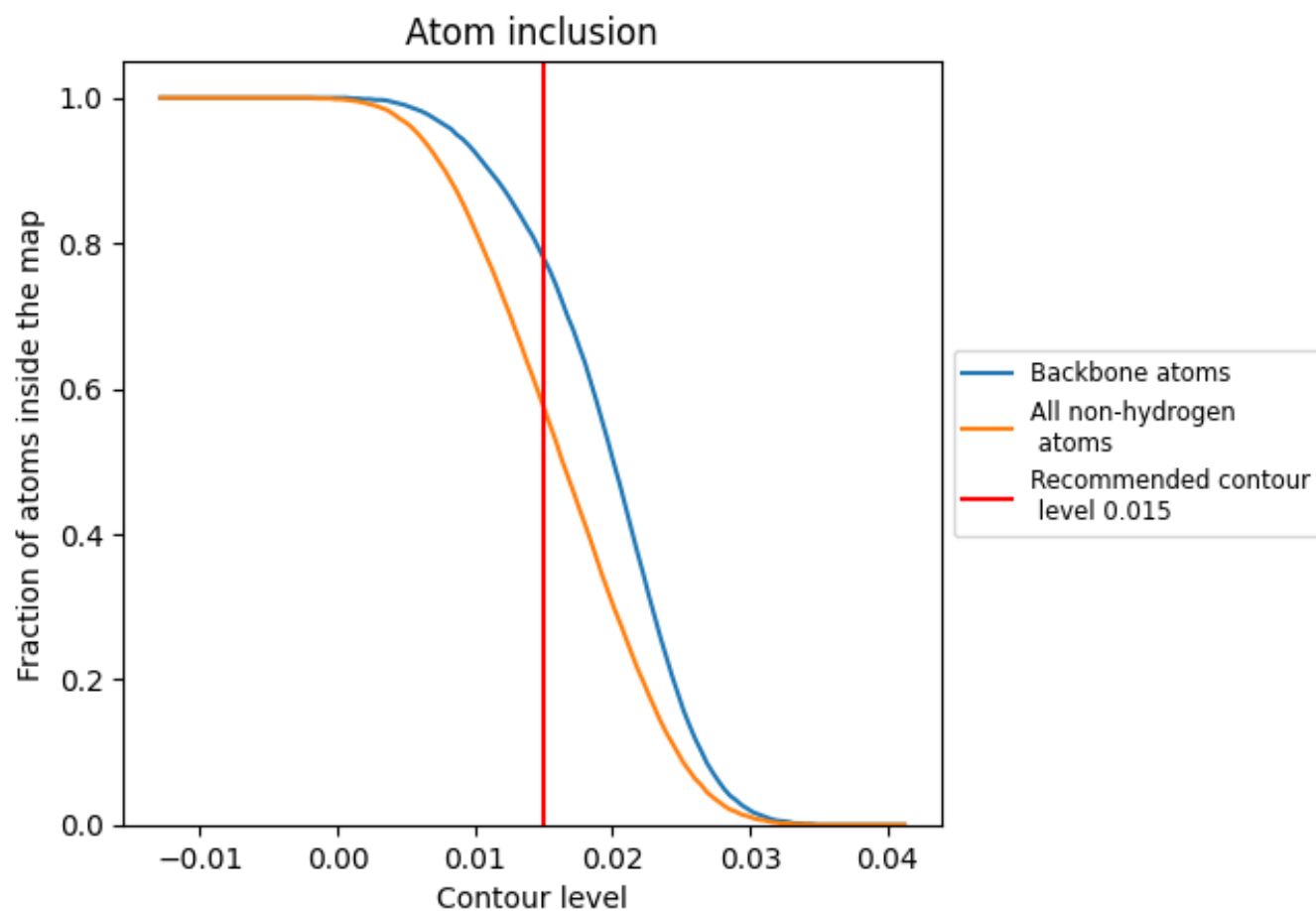
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.015).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 57% 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	<div></div> 0.5750	<div></div> 0.2140
A	<div></div> 0.6460	<div></div> 0.2520
B	<div></div> 0.6420	<div></div> 0.2350
C	<div></div> 0.5610	<div></div> 0.2110
D	<div></div> 0.6550	<div></div> 0.2600
E	<div></div> 0.7080	<div></div> 0.2320
F	<div></div> 0.5980	<div></div> 0.2000
G	<div></div> 0.6600	<div></div> 0.2490
H	<div></div> 0.4950	<div></div> 0.1720
I	<div></div> 0.5170	<div></div> 0.1920
J	<div></div> 0.5320	<div></div> 0.1970

1.0

0.0

<0.0