



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:51 AM UTC

PDB ID : 5W9N / pdb_00005w9n
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 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

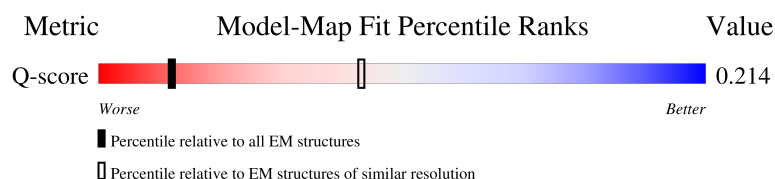
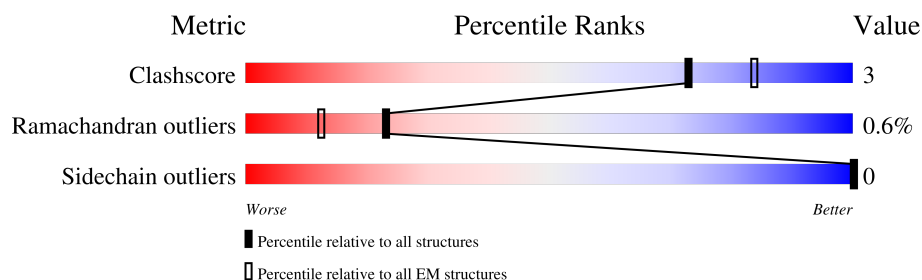
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1057 (4.50 - 5.50)

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	D	1329	
1	G	1329	
1	H	1329	

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Mol	Chain	Length	Quality of chain
1	I	1329	19% 48% 6% 45%
1	J	1329	17% 49% 6% 45%
2	B	233	5% 50% 49%
2	E	233	50% 49%
3	C	218	11% 48% 49%
3	F	218	9% 46% 5% 49%

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		

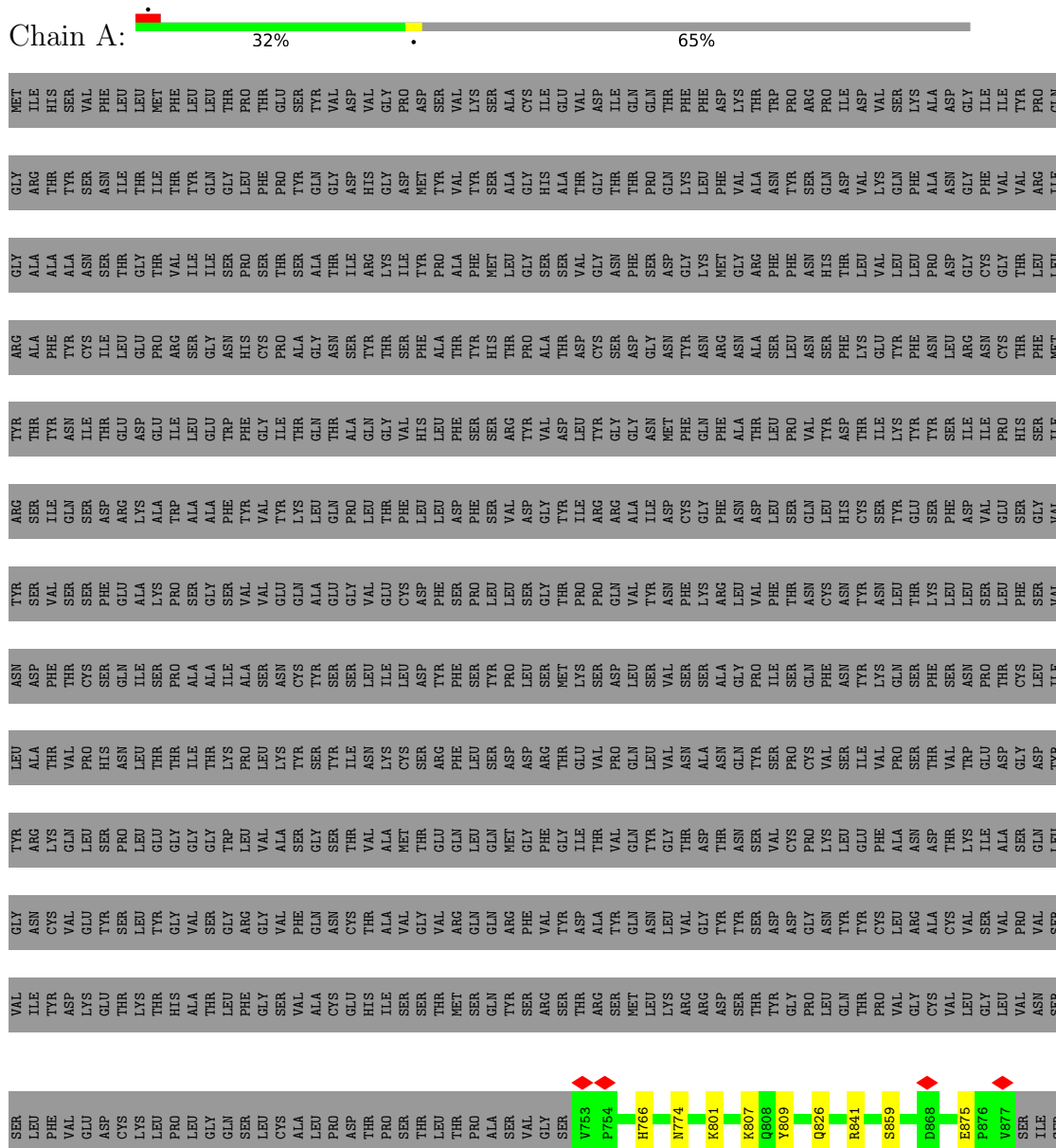
- Molecule 3 is a protein called G4 VL.

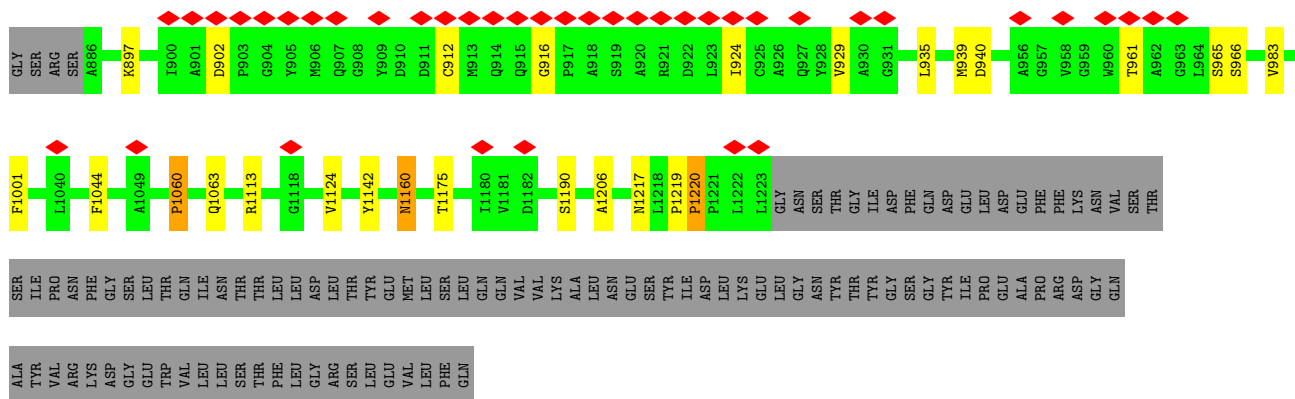
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	111	Total 835	C 522	N 143	O 166	S 4	0	0
3	F	111	Total 835	C 522	N 143	O 166	S 4	0	0

3 Residue-property plots

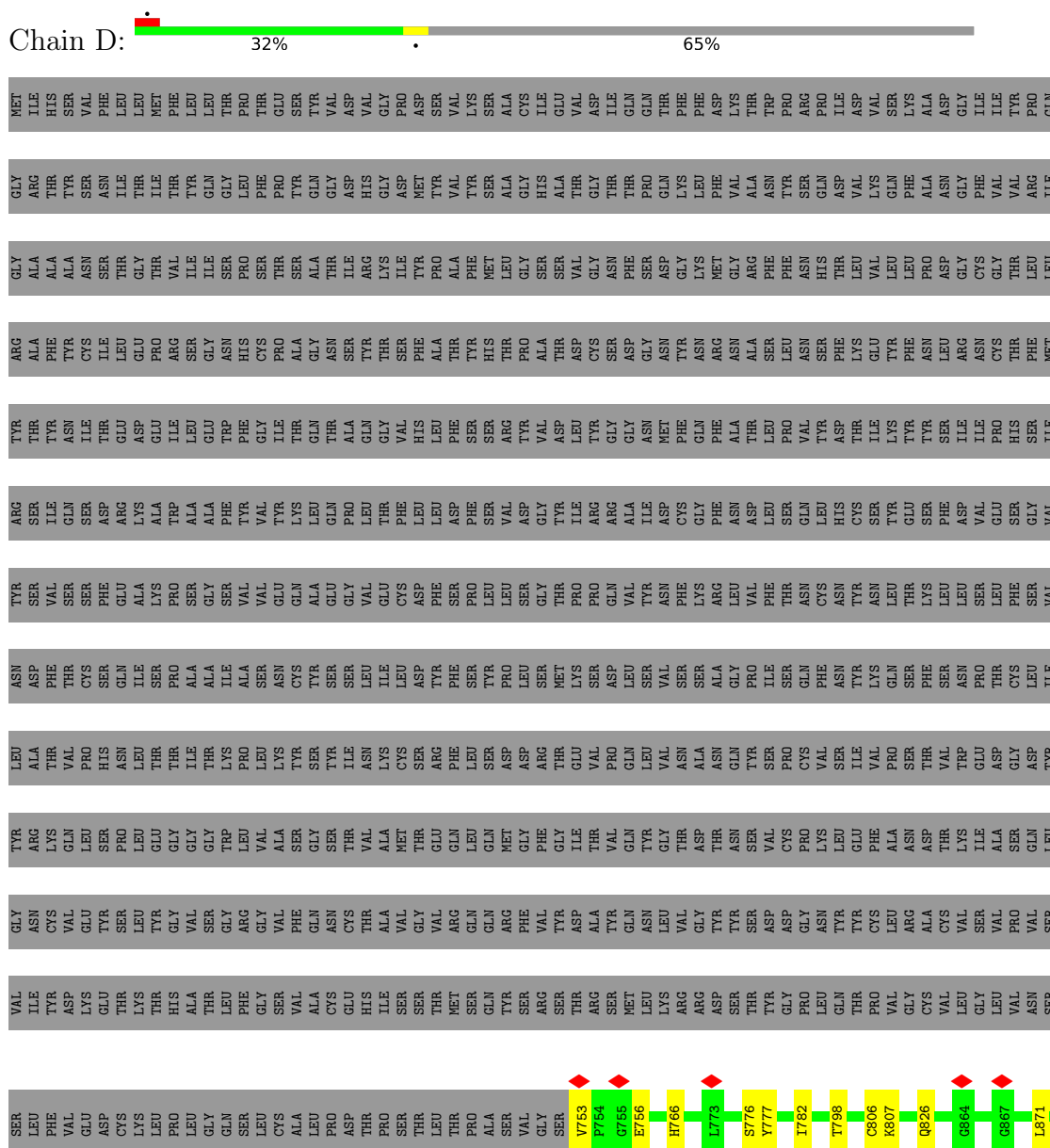
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: MERS S

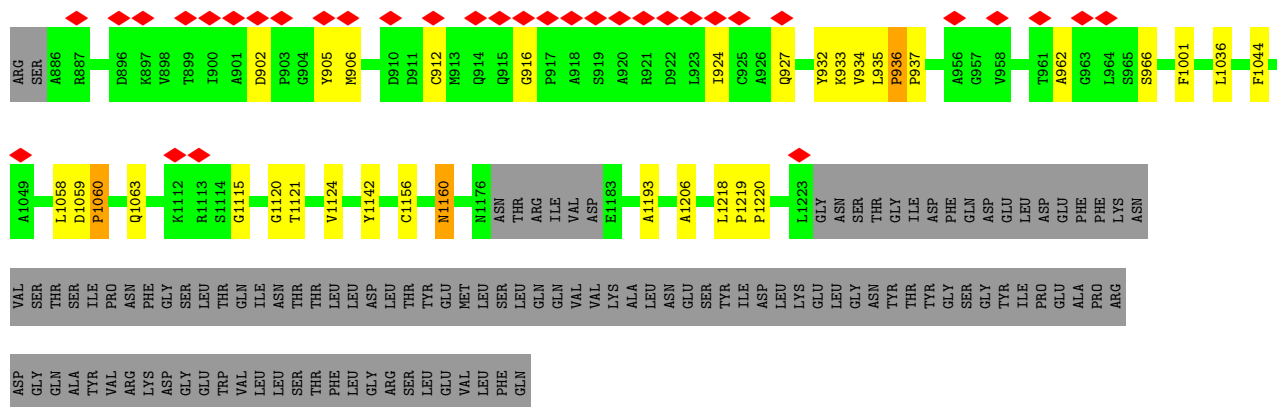




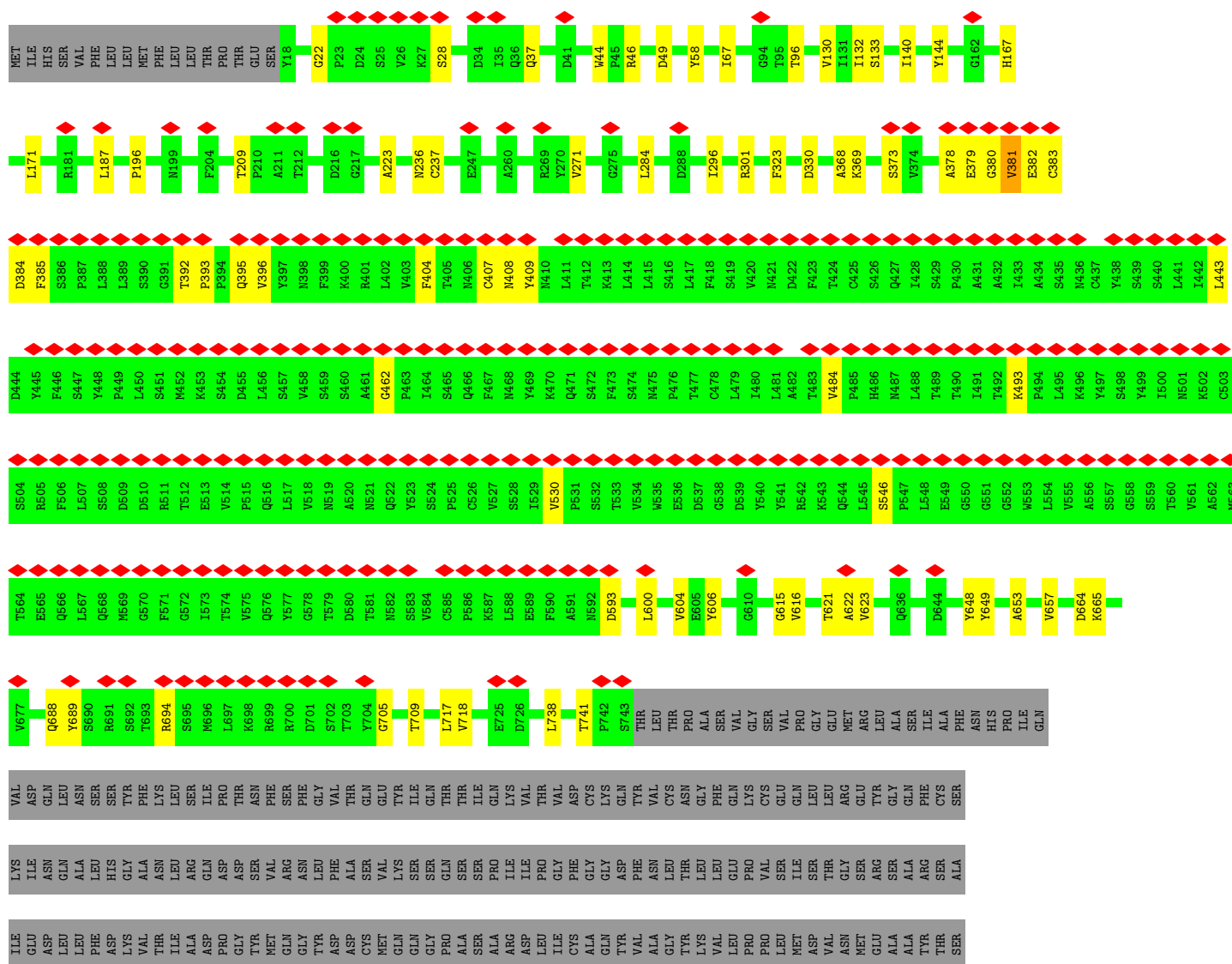
- Molecule 1: MERS S





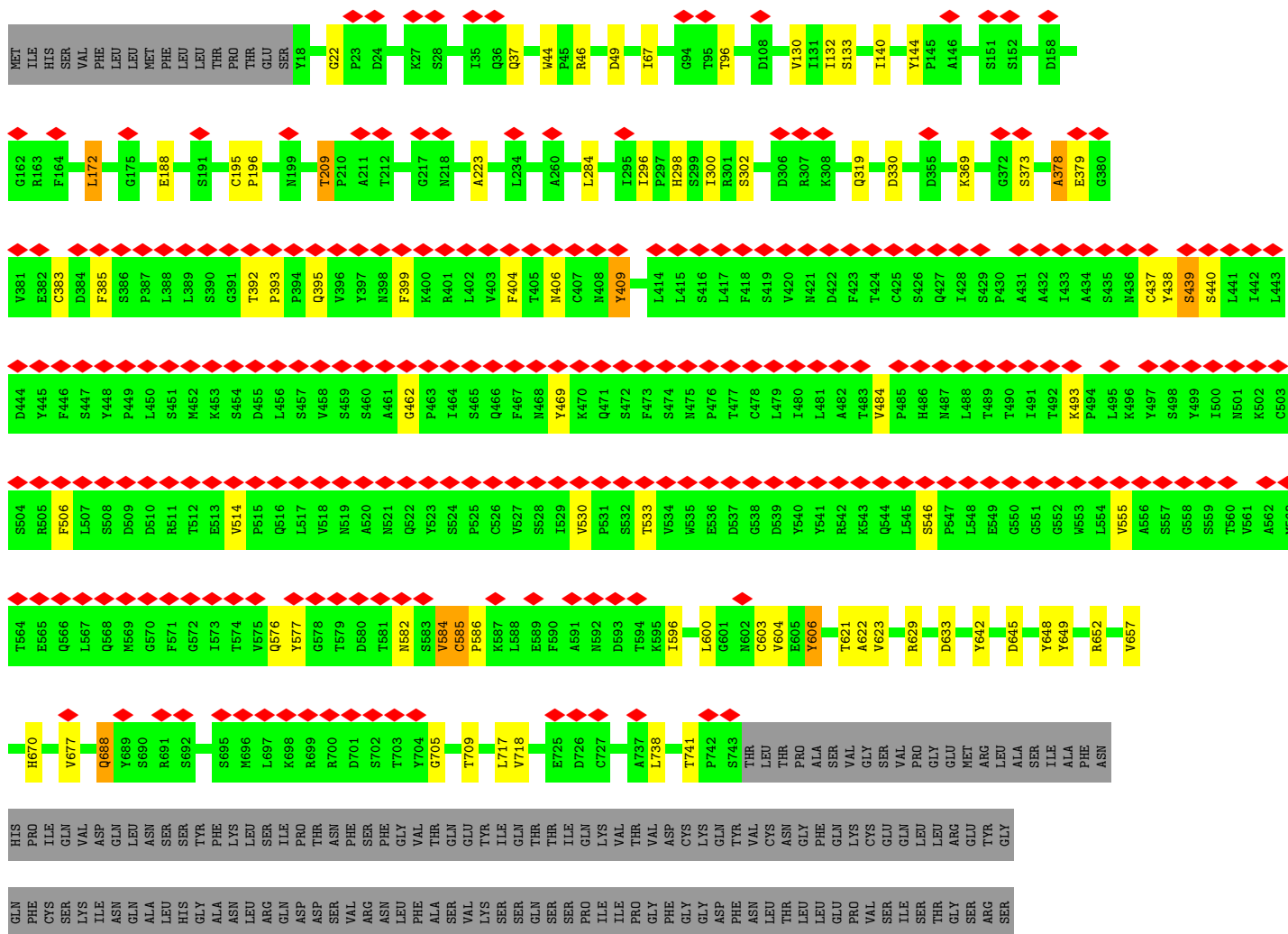


• Molecule 1: MERS S



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

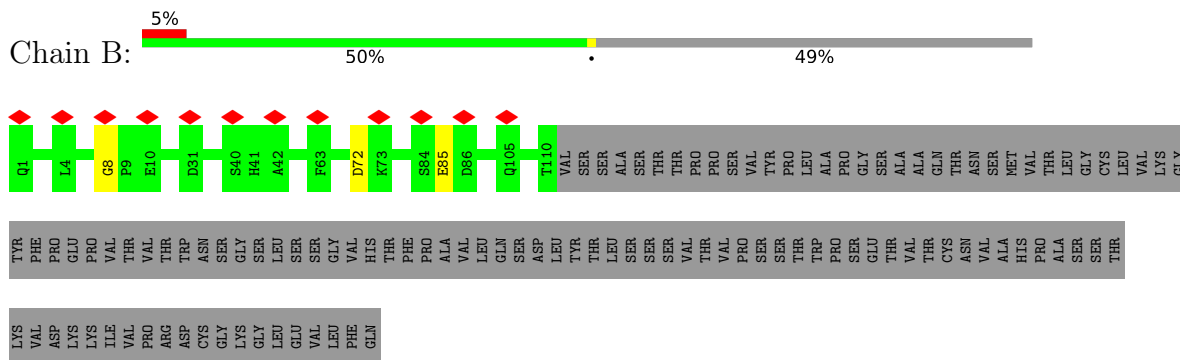
- Molecule 1: MERS S



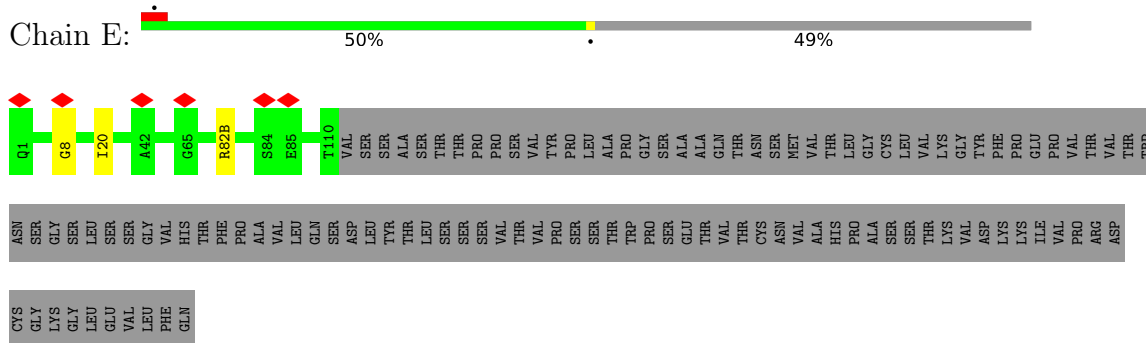


[illegible]

- Molecule 2: G4 VH



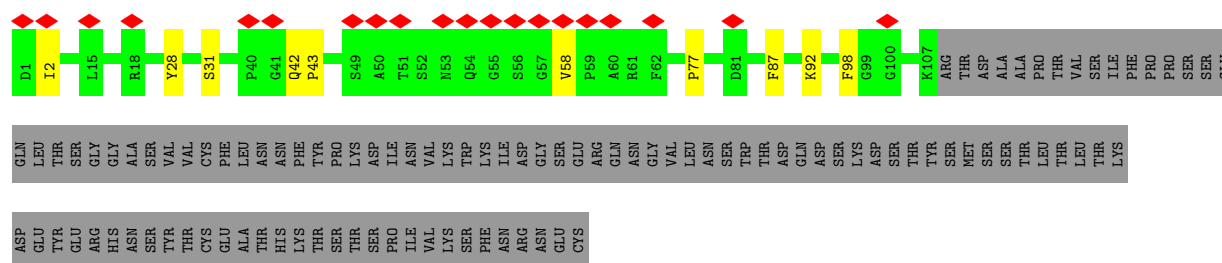
- Molecule 2: G4 VH



- 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

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	0.85	1/3618 (0.0%)	1.23	32/4921 (0.7%)
1	D	0.85	1/3618 (0.0%)	1.22	33/4921 (0.7%)
1	G	0.86	1/3568 (0.0%)	1.24	41/4851 (0.8%)
1	H	0.85	1/5803 (0.0%)	1.34	75/7901 (0.9%)
1	I	0.85	1/5803 (0.0%)	1.35	84/7901 (1.1%)
1	J	0.85	1/5803 (0.0%)	1.38	93/7901 (1.2%)
2	B	0.77	0/972	1.13	2/1317 (0.2%)
2	E	0.80	0/972	1.17	3/1317 (0.2%)
3	C	0.83	0/852	1.33	8/1153 (0.7%)
3	F	0.90	0/852	1.42	10/1153 (0.9%)
All	All	0.85	6/31861 (0.0%)	1.30	381/43336 (0.9%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	237	CYS	N-CA	6.05	1.53	1.46
1	G	1156	CYS	CA-C	-6.01	1.45	1.52
1	D	1219	PRO	CA-C	5.59	1.57	1.52
1	I	584	VAL	CA-C	-5.50	1.45	1.52
1	A	1219	PRO	CA-C	5.37	1.57	1.52
1	J	339	CYS	C-O	-5.01	1.17	1.24

All (381) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1156	CYS	CA-C-O	12.62	135.64	121.51
1	G	1156	CYS	O-C-N	-11.92	107.94	122.96
3	C	42	GLN	CA-C-N	10.24	127.03	119.66
3	C	42	GLN	C-N-CA	10.24	127.03	119.66
1	J	688	GLN	N-CA-C	10.24	122.44	111.28
1	H	144	TYR	CA-C-N	10.12	130.05	120.03
1	H	144	TYR	C-N-CA	10.12	130.05	120.03
3	C	58	VAL	CA-C-N	9.76	130.36	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	58	VAL	C-N-CA	9.76	130.36	119.92
3	F	42	GLN	CA-C-N	9.58	126.65	119.66
3	F	42	GLN	C-N-CA	9.58	126.65	119.66
1	J	284	LEU	CA-C-N	9.57	129.83	119.87
1	J	284	LEU	C-N-CA	9.57	129.83	119.87
1	H	369	LYS	CA-C-N	9.52	129.45	120.03
1	H	369	LYS	C-N-CA	9.52	129.45	120.03
1	J	585	CYS	CA-C-N	9.47	130.06	119.92
1	J	585	CYS	C-N-CA	9.47	130.06	119.92
1	I	284	LEU	CA-C-N	9.26	129.50	119.87
1	I	284	LEU	C-N-CA	9.26	129.50	119.87
3	F	98	PHE	CA-CB-CG	9.00	122.80	113.80
1	I	369	LYS	CA-C-N	8.92	128.86	119.85
1	I	369	LYS	C-N-CA	8.92	128.86	119.85
1	J	144	TYR	CA-C-N	8.80	128.74	119.85
1	J	144	TYR	C-N-CA	8.80	128.74	119.85
1	J	437	CYS	O-C-N	-8.77	112.99	123.16
1	J	741	THR	CA-C-N	8.77	128.81	119.78
1	J	741	THR	C-N-CA	8.77	128.81	119.78
1	H	462	GLY	CA-C-N	8.69	128.42	119.56
1	H	462	GLY	C-N-CA	8.69	128.42	119.56
1	A	902	ASP	CA-C-N	8.68	128.72	119.78
1	A	902	ASP	C-N-CA	8.68	128.72	119.78
1	H	393	PRO	CA-C-N	8.58	128.52	120.03
1	H	393	PRO	C-N-CA	8.58	128.52	120.03
1	D	902	ASP	CA-C-N	8.56	128.50	119.85
1	D	902	ASP	C-N-CA	8.56	128.50	119.85
1	G	935	LEU	CA-C-N	8.47	125.76	119.66
1	G	935	LEU	C-N-CA	8.47	125.76	119.66
3	F	58	VAL	CA-C-N	8.44	128.39	120.03
3	F	58	VAL	C-N-CA	8.44	128.39	120.03
1	J	530	VAL	CA-C-N	8.44	128.38	120.03
1	J	530	VAL	C-N-CA	8.44	128.38	120.03
1	I	393	PRO	CA-C-N	8.41	128.34	119.85
1	I	393	PRO	C-N-CA	8.41	128.34	119.85
2	E	8	GLY	CA-C-N	8.39	128.32	119.85
2	E	8	GLY	C-N-CA	8.39	128.32	119.85
1	J	22	GLY	CA-C-N	8.25	128.28	119.78
1	J	22	GLY	C-N-CA	8.25	128.28	119.78
1	I	144	TYR	CA-C-N	8.22	128.15	119.85
1	I	144	TYR	C-N-CA	8.22	128.15	119.85
1	H	530	VAL	CA-C-N	8.12	128.61	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	530	VAL	C-N-CA	8.12	128.61	119.92
1	J	209	THR	CA-C-N	8.10	127.83	119.56
1	J	209	THR	C-N-CA	8.10	127.83	119.56
1	I	462	GLY	CA-C-N	8.09	127.81	119.56
1	I	462	GLY	C-N-CA	8.09	127.81	119.56
1	J	462	GLY	CA-C-N	8.08	127.80	119.56
1	J	462	GLY	C-N-CA	8.08	127.80	119.56
1	H	741	THR	CA-C-N	8.06	128.08	119.78
1	H	741	THR	C-N-CA	8.06	128.08	119.78
1	A	1219	PRO	CA-C-N	8.05	128.68	120.38
1	A	1219	PRO	C-N-CA	8.05	128.68	120.38
1	J	96	THR	CA-C-N	8.05	127.98	119.85
1	J	96	THR	C-N-CA	8.05	127.98	119.85
1	H	209	THR	CA-C-N	8.04	127.76	119.56
1	H	209	THR	C-N-CA	8.04	127.76	119.56
1	J	493	LYS	CA-C-N	8.04	127.97	119.85
1	J	493	LYS	C-N-CA	8.04	127.97	119.85
1	G	1220	PRO	N-CA-C	8.01	120.48	110.70
1	H	284	LEU	CA-C-N	8.01	127.73	119.56
1	H	284	LEU	C-N-CA	8.01	127.73	119.56
1	J	399	PHE	N-CA-C	7.94	121.44	110.24
1	I	373	SER	N-CA-C	7.93	121.14	110.35
1	H	738	LEU	CA-C-N	7.89	127.82	119.85
1	H	738	LEU	C-N-CA	7.89	127.82	119.85
1	J	705	GLY	CA-C-N	7.85	127.78	119.85
1	J	705	GLY	C-N-CA	7.85	127.78	119.85
1	D	935	LEU	CA-C-N	7.79	125.27	119.66
1	D	935	LEU	C-N-CA	7.79	125.27	119.66
1	A	935	LEU	CA-C-N	7.78	125.26	119.66
1	A	935	LEU	C-N-CA	7.78	125.26	119.66
1	I	493	LYS	CA-C-N	7.75	127.68	119.85
1	I	493	LYS	C-N-CA	7.75	127.68	119.85
1	I	741	THR	CA-C-N	7.75	127.76	119.78
1	I	741	THR	C-N-CA	7.75	127.76	119.78
1	I	96	THR	CA-C-N	7.74	127.67	119.85
1	I	96	THR	C-N-CA	7.74	127.67	119.85
1	J	393	PRO	CA-C-N	7.72	127.68	120.03
1	J	393	PRO	C-N-CA	7.72	127.68	120.03
1	H	484	VAL	CA-C-N	7.67	127.68	119.78
1	H	484	VAL	C-N-CA	7.67	127.68	119.78
1	I	378	ALA	CA-C-N	7.63	135.44	121.70
1	I	378	ALA	C-N-CA	7.63	135.44	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1219	PRO	CA-C-N	7.61	128.22	120.38
1	D	1219	PRO	C-N-CA	7.61	128.22	120.38
1	J	584	VAL	CA-C-N	7.58	140.30	121.80
1	J	584	VAL	C-N-CA	7.58	140.30	121.80
1	J	392	THR	CA-C-N	7.57	125.18	119.66
1	J	392	THR	C-N-CA	7.57	125.18	119.66
1	H	493	LYS	CA-C-N	7.54	127.47	119.85
1	H	493	LYS	C-N-CA	7.54	127.47	119.85
3	F	43	PRO	CA-C-N	7.52	127.45	119.85
3	F	43	PRO	C-N-CA	7.52	127.45	119.85
1	G	1219	PRO	N-CA-C	7.46	119.81	110.70
1	J	484	VAL	N-CA-C	7.45	115.03	108.63
1	I	530	VAL	CA-C-N	7.43	127.43	119.78
1	I	530	VAL	C-N-CA	7.43	127.43	119.78
1	H	600	LEU	N-CA-C	7.40	121.88	111.30
2	B	8	GLY	CA-C-N	7.39	127.40	119.78
2	B	8	GLY	C-N-CA	7.39	127.40	119.78
1	I	392	THR	CA-C-N	7.37	124.97	119.66
1	I	392	THR	C-N-CA	7.37	124.97	119.66
3	F	58	VAL	N-CA-C	7.37	117.29	108.45
1	J	484	VAL	CA-C-N	7.36	127.36	119.78
1	J	484	VAL	C-N-CA	7.36	127.36	119.78
1	A	939	MET	N-CA-C	7.28	121.27	112.38
1	J	373	SER	N-CA-C	7.27	120.75	110.50
1	I	514	VAL	CA-C-N	7.22	127.22	119.78
1	I	514	VAL	C-N-CA	7.22	127.22	119.78
1	G	1044	PHE	CA-CB-CG	-7.20	106.60	113.80
1	I	209	THR	CA-C-N	7.17	126.88	119.56
1	I	209	THR	C-N-CA	7.17	126.88	119.56
1	G	912	CYS	CA-C-N	7.13	132.93	120.87
1	G	912	CYS	C-N-CA	7.13	132.93	120.87
1	H	22	GLY	CA-C-N	7.12	127.11	119.78
1	H	22	GLY	C-N-CA	7.12	127.11	119.78
1	G	1219	PRO	CA-C-N	7.09	127.68	120.38
1	G	1219	PRO	C-N-CA	7.09	127.68	120.38
1	G	753	VAL	CA-C-N	7.06	127.05	119.78
1	G	753	VAL	C-N-CA	7.06	127.05	119.78
1	A	1142	TYR	CA-C-N	7.04	127.04	119.78
1	A	1142	TYR	C-N-CA	7.04	127.04	119.78
1	G	766	HIS	CA-C-N	7.01	127.00	119.78
1	G	766	HIS	C-N-CA	7.01	127.00	119.78
1	I	406	ASN	CA-C-N	-6.92	110.52	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	406	ASN	C-N-CA	-6.92	110.52	121.87
1	J	406	ASN	CA-C-N	-6.92	110.53	121.87
1	J	406	ASN	C-N-CA	-6.92	110.53	121.87
1	D	1219	PRO	N-CA-C	6.89	119.11	110.70
1	J	438	TYR	N-CA-C	6.88	119.63	109.24
1	H	96	THR	CA-C-N	6.85	126.84	119.78
1	H	96	THR	C-N-CA	6.85	126.84	119.78
1	G	1218	LEU	CA-C-N	6.83	127.41	120.38
1	G	1218	LEU	C-N-CA	6.83	127.41	120.38
1	I	399	PHE	N-CA-C	6.82	119.86	110.24
1	J	369	LYS	CA-C-N	6.78	126.76	119.78
1	J	369	LYS	C-N-CA	6.78	126.76	119.78
1	D	1142	TYR	CA-C-N	6.72	126.70	119.78
1	D	1142	TYR	C-N-CA	6.72	126.70	119.78
1	J	688	GLN	CA-C-N	6.70	133.76	121.70
1	J	688	GLN	C-N-CA	6.70	133.76	121.70
1	G	1142	TYR	CA-C-N	6.69	126.61	119.85
1	G	1142	TYR	C-N-CA	6.69	126.61	119.85
1	G	902	ASP	CA-C-N	6.68	126.66	119.78
1	G	902	ASP	C-N-CA	6.68	126.66	119.78
1	H	223	ALA	N-CA-C	6.67	118.56	111.28
1	D	912	CYS	CA-C-N	6.62	130.75	120.75
1	D	912	CYS	C-N-CA	6.62	130.75	120.75
1	H	546	SER	CA-C-N	6.62	126.56	119.28
1	H	546	SER	C-N-CA	6.62	126.56	119.28
1	A	912	CYS	CA-C-N	6.60	130.71	120.75
1	A	912	CYS	C-N-CA	6.60	130.71	120.75
1	D	766	HIS	CA-C-N	6.60	126.58	119.78
1	D	766	HIS	C-N-CA	6.60	126.58	119.78
1	I	604	VAL	N-CA-C	6.58	119.10	109.63
1	I	705	GLY	CA-C-N	6.57	126.54	119.78
1	I	705	GLY	C-N-CA	6.57	126.54	119.78
1	A	1220	PRO	N-CA-C	6.55	118.70	110.70
1	J	319	GLN	CA-C-N	6.55	128.03	119.84
1	J	319	GLN	C-N-CA	6.55	128.03	119.84
1	D	1160	ASN	CA-C-N	6.54	128.01	119.84
1	D	1160	ASN	C-N-CA	6.54	128.01	119.84
1	J	133	SER	CA-C-N	6.50	126.19	119.56
1	J	133	SER	C-N-CA	6.50	126.19	119.56
1	A	1160	ASN	CA-C-N	6.49	127.95	119.84
1	A	1160	ASN	C-N-CA	6.49	127.95	119.84
1	G	1058	LEU	N-CA-C	6.45	119.68	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	688	GLN	CA-C-N	6.44	133.29	121.70
1	H	688	GLN	C-N-CA	6.44	133.29	121.70
1	I	484	VAL	CA-C-N	6.43	126.41	119.78
1	I	484	VAL	C-N-CA	6.43	126.41	119.78
3	C	58	VAL	N-CA-C	6.43	116.16	108.45
1	I	409	TYR	N-CA-C	6.42	118.94	109.24
3	C	92	LYS	N-CA-C	6.39	118.25	111.28
1	D	1220	PRO	N-CA-C	6.38	118.48	110.70
1	J	236	ASN	CA-C-N	-6.37	112.31	121.42
1	J	236	ASN	C-N-CA	-6.37	112.31	121.42
1	H	709	THR	CA-C-N	6.34	126.26	119.28
1	H	709	THR	C-N-CA	6.34	126.26	119.28
1	I	223	ALA	N-CA-C	6.32	117.83	111.07
1	J	657	VAL	CA-C-N	6.29	126.26	119.78
1	J	657	VAL	C-N-CA	6.29	126.26	119.78
1	G	1160	ASN	CA-C-N	6.28	127.69	119.84
1	G	1160	ASN	C-N-CA	6.28	127.69	119.84
1	H	133	SER	CA-C-N	6.28	125.96	119.56
1	H	133	SER	C-N-CA	6.28	125.96	119.56
1	H	705	GLY	CA-C-N	6.26	126.22	119.78
1	H	705	GLY	C-N-CA	6.26	126.22	119.78
1	I	649	TYR	CA-C-N	-6.22	113.38	122.65
1	I	649	TYR	C-N-CA	-6.22	113.38	122.65
1	I	600	LEU	N-CA-C	6.20	119.94	111.39
3	C	43	PRO	CA-C-N	6.18	126.09	119.85
3	C	43	PRO	C-N-CA	6.18	126.09	119.85
1	I	369	LYS	N-CA-C	6.18	117.17	109.57
1	H	688	GLN	N-CA-C	6.17	119.19	111.24
1	I	319	GLN	CA-C-N	6.13	127.51	119.84
1	I	319	GLN	C-N-CA	6.13	127.51	119.84
1	D	1193	ALA	CA-C-N	6.13	126.10	119.78
1	D	1193	ALA	C-N-CA	6.13	126.10	119.78
1	A	1113	ARG	N-CA-C	6.11	120.00	112.54
1	A	859	SER	CA-C-N	6.11	126.07	119.78
1	A	859	SER	C-N-CA	6.11	126.07	119.78
1	G	1060	PRO	N-CA-C	6.10	118.14	110.70
1	A	766	HIS	CA-C-N	6.09	126.05	119.78
1	A	766	HIS	C-N-CA	6.09	126.05	119.78
1	H	657	VAL	CA-C-N	6.09	126.05	119.78
1	H	657	VAL	C-N-CA	6.09	126.05	119.78
1	J	546	SER	CA-C-N	6.02	125.90	119.28
1	J	546	SER	C-N-CA	6.02	125.90	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	623	VAL	CA-C-N	-6.02	114.73	121.83
1	H	623	VAL	C-N-CA	-6.02	114.73	121.83
1	G	924	ILE	CA-C-N	-6.01	111.08	121.66
1	G	924	ILE	C-N-CA	-6.01	111.08	121.66
1	J	223	ALA	N-CA-C	6.00	117.49	111.07
1	I	46	ARG	CA-C-N	6.00	125.96	119.78
1	I	46	ARG	C-N-CA	6.00	125.96	119.78
1	D	924	ILE	CA-C-N	-5.98	110.93	122.06
1	D	924	ILE	C-N-CA	-5.98	110.93	122.06
1	I	22	GLY	CA-C-N	5.95	125.91	119.78
1	I	22	GLY	C-N-CA	5.95	125.91	119.78
1	J	717	LEU	N-CA-C	5.95	120.54	113.28
1	H	271	VAL	N-CA-C	5.94	116.67	111.56
1	D	1113	ARG	N-CA-C	5.92	118.52	111.71
1	J	164	PHE	CA-CB-CG	5.90	119.70	113.80
1	J	738	LEU	CA-C-N	5.90	125.81	119.85
1	J	738	LEU	C-N-CA	5.90	125.81	119.85
1	J	378	ALA	CA-C-N	5.88	132.29	121.70
1	J	378	ALA	C-N-CA	5.88	132.29	121.70
1	A	1060	PRO	N-CA-C	5.88	117.87	110.70
1	J	409	TYR	N-CA-C	5.84	118.06	109.24
1	D	1044	PHE	CA-CB-CG	-5.83	107.97	113.80
1	A	807	LYS	N-CA-C	-5.83	105.83	113.12
3	F	87	PHE	N-CA-C	5.83	117.90	108.34
1	I	738	LEU	CA-C-N	5.82	125.78	119.78
1	I	738	LEU	C-N-CA	5.82	125.78	119.78
1	G	1206	ALA	CA-C-N	5.81	125.76	119.78
1	G	1206	ALA	C-N-CA	5.81	125.76	119.78
1	I	603	CYS	CA-C-N	5.80	128.27	120.50
1	I	603	CYS	C-N-CA	5.80	128.27	120.50
1	I	296	ILE	CA-C-N	5.79	125.69	119.85
1	I	296	ILE	C-N-CA	5.79	125.69	119.85
1	I	133	SER	CA-C-N	5.78	125.46	119.56
1	I	133	SER	C-N-CA	5.78	125.46	119.56
1	I	195	CYS	CA-C-N	5.78	125.47	119.05
1	I	195	CYS	C-N-CA	5.78	125.47	119.05
1	H	46	ARG	CA-C-N	5.77	125.73	119.78
1	H	46	ARG	C-N-CA	5.77	125.73	119.78
1	H	392	THR	CA-C-N	5.73	123.79	119.66
1	H	392	THR	C-N-CA	5.73	123.79	119.66
1	G	916	GLY	CA-C-N	5.73	125.68	119.78
1	G	916	GLY	C-N-CA	5.73	125.68	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	302	SER	CA-C-N	5.71	128.15	120.50
1	I	302	SER	C-N-CA	5.71	128.15	120.50
1	H	649	TYR	CA-C-N	-5.70	113.23	122.81
1	H	649	TYR	C-N-CA	-5.70	113.23	122.81
1	D	936	PRO	CA-C-N	5.70	125.61	119.85
1	D	936	PRO	C-N-CA	5.70	125.61	119.85
1	D	1060	PRO	N-CA-C	5.70	117.65	110.70
1	H	373	SER	N-CA-C	5.68	118.08	110.35
1	J	188	GLU	CA-C-N	5.65	125.60	119.78
1	J	188	GLU	C-N-CA	5.65	125.60	119.78
1	A	924	ILE	CA-C-N	-5.65	112.27	120.29
1	A	924	ILE	C-N-CA	-5.65	112.27	120.29
1	G	1193	ALA	CA-C-N	5.65	125.60	119.78
1	G	1193	ALA	C-N-CA	5.65	125.60	119.78
1	J	296	ILE	CA-C-N	5.64	125.55	119.85
1	J	296	ILE	C-N-CA	5.64	125.55	119.85
1	H	717	LEU	N-CA-C	5.62	118.34	111.82
1	A	916	GLY	CA-C-N	5.62	125.52	119.85
1	A	916	GLY	C-N-CA	5.62	125.52	119.85
1	A	1219	PRO	N-CA-C	5.62	117.55	110.70
1	I	399	PHE	CB-CA-C	-5.61	100.66	109.70
1	D	753	VAL	CA-C-N	5.61	125.56	119.78
1	D	753	VAL	C-N-CA	5.61	125.56	119.78
1	I	688	GLN	CA-C-N	5.61	131.80	121.70
1	I	688	GLN	C-N-CA	5.61	131.80	121.70
1	A	1044	PHE	CA-CB-CG	-5.61	108.19	113.80
1	J	37	GLN	N-CA-C	5.57	118.87	111.75
1	D	807	LYS	N-CA-C	-5.56	106.54	113.55
1	I	188	GLU	CA-C-N	5.54	125.48	119.78
1	I	188	GLU	C-N-CA	5.54	125.48	119.78
1	J	302	SER	CA-C-N	5.53	127.91	120.50
1	J	302	SER	C-N-CA	5.53	127.91	120.50
1	J	46	ARG	CA-C-N	5.52	125.46	119.78
1	J	46	ARG	C-N-CA	5.52	125.46	119.78
1	A	929	VAL	N-CA-C	-5.51	106.43	111.67
1	D	782	ILE	CA-C-N	5.51	125.42	119.85
1	D	782	ILE	C-N-CA	5.51	125.42	119.85
1	H	196	PRO	N-CA-C	5.51	121.09	113.65
1	J	514	VAL	CA-C-N	5.50	125.45	119.78
1	J	514	VAL	C-N-CA	5.50	125.45	119.78
1	G	966	SER	N-CA-C	5.50	117.43	109.07
1	H	44	TRP	CA-C-N	5.50	125.40	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	44	TRP	C-N-CA	5.50	125.40	119.85
1	H	167	HIS	CA-CB-CG	5.46	119.26	113.80
1	D	1123	ILE	N-CA-C	-5.45	101.88	108.53
1	I	533	THR	CA-C-N	-5.45	115.56	122.37
1	I	533	THR	C-N-CA	-5.45	115.56	122.37
1	J	368	ALA	N-CA-C	5.44	119.21	112.58
1	I	600	LEU	CA-C-N	5.41	131.44	121.70
1	I	600	LEU	C-N-CA	5.41	131.44	121.70
1	I	717	LEU	N-CA-C	5.41	119.88	113.28
1	H	615	GLY	N-CA-C	5.40	118.46	110.42
1	J	195	CYS	CA-C-N	5.38	125.02	119.05
1	J	195	CYS	C-N-CA	5.38	125.02	119.05
1	I	298	HIS	CA-CB-CG	5.38	119.18	113.80
1	J	78	GLN	N-CA-C	5.38	117.14	111.28
1	J	196	PRO	N-CA-C	5.37	120.99	113.53
1	J	271	VAL	N-CA-C	5.36	116.17	111.56
1	G	1115	GLY	CA-C-N	5.36	128.84	120.75
1	G	1115	GLY	C-N-CA	5.36	128.84	120.75
1	H	296	ILE	CA-C-N	5.34	125.28	119.78
1	H	296	ILE	C-N-CA	5.34	125.28	119.78
1	G	912	CYS	N-CA-C	-5.30	105.63	112.68
1	H	653	ALA	CA-C-N	-5.30	113.89	122.36
1	H	653	ALA	C-N-CA	-5.30	113.89	122.36
1	J	173	PRO	CA-C-N	-5.29	115.53	122.99
1	J	173	PRO	C-N-CA	-5.29	115.53	122.99
1	H	396	VAL	N-CA-C	5.28	118.45	111.17
1	J	399	PHE	CB-CA-C	-5.28	101.21	109.70
1	I	196	PRO	N-CA-C	5.27	120.86	113.53
1	J	44	TRP	CA-C-N	5.27	125.17	119.85
1	J	44	TRP	C-N-CA	5.27	125.17	119.85
1	I	585	CYS	CA-C-N	5.26	125.20	119.78
1	I	585	CYS	C-N-CA	5.26	125.20	119.78
1	I	37	GLN	N-CA-C	5.25	118.47	111.75
3	F	92	LYS	N-CA-C	5.25	117.00	111.28
1	I	657	VAL	CA-C-N	5.25	125.19	119.78
1	I	657	VAL	C-N-CA	5.25	125.19	119.78
1	I	709	THR	CA-C-N	5.24	125.04	119.28
1	I	709	THR	C-N-CA	5.24	125.04	119.28
1	H	657	VAL	N-CA-C	5.24	112.73	107.55
1	I	546	SER	CA-C-N	5.24	125.04	119.28
1	I	546	SER	C-N-CA	5.24	125.04	119.28
1	I	606	TYR	N-CA-C	5.23	117.02	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	37	GLN	N-CA-C	5.22	118.44	111.75
1	J	709	THR	CA-C-N	5.21	125.01	119.28
1	J	709	THR	C-N-CA	5.21	125.01	119.28
1	J	269	ARG	N-CA-C	5.21	116.96	111.28
1	J	58	TYR	CA-C-N	5.20	125.13	119.78
1	J	58	TYR	C-N-CA	5.20	125.13	119.78
2	E	82(B)	ARG	N-CA-C	5.17	116.96	110.91
1	H	58	TYR	CA-C-N	5.16	125.09	119.78
1	H	58	TYR	C-N-CA	5.16	125.09	119.78
1	A	1206	ALA	CA-C-N	5.15	125.09	119.78
1	A	1206	ALA	C-N-CA	5.15	125.09	119.78
1	J	429	SER	CA-C-N	5.14	124.94	119.28
1	J	429	SER	C-N-CA	5.14	124.94	119.28
1	H	236	ASN	CA-C-N	-5.13	113.58	120.87
1	H	236	ASN	C-N-CA	-5.13	113.58	120.87
1	G	1059	ASP	CA-C-N	5.13	125.66	120.38
1	G	1059	ASP	C-N-CA	5.13	125.66	120.38
1	D	798	THR	N-CA-C	5.12	116.97	109.24
1	H	28	SER	CA-C-N	5.12	128.48	120.75
1	H	28	SER	C-N-CA	5.12	128.48	120.75
1	A	1124	VAL	N-CA-C	5.11	116.82	109.51
1	H	606	TYR	N-CA-C	5.11	116.83	109.07
1	J	524	SER	CA-C-N	5.10	124.89	119.28
1	J	524	SER	C-N-CA	5.10	124.89	119.28
1	J	437	CYS	CA-C-O	5.05	126.73	120.92
1	I	469	TYR	N-CA-C	5.04	117.37	108.75
1	H	593	ASP	CA-CB-CG	5.04	117.64	112.60
1	H	600	LEU	CA-C-N	5.04	130.76	121.70
1	H	600	LEU	C-N-CA	5.04	130.76	121.70
1	J	503	CYS	CA-C-O	5.03	125.86	119.98
1	H	323	PHE	N-CA-C	5.02	117.02	109.23
1	I	172	LEU	CA-C-N	5.02	124.92	119.85
1	I	172	LEU	C-N-CA	5.02	124.92	119.85
1	G	936	PRO	CA-C-N	5.02	124.95	119.78
1	G	936	PRO	C-N-CA	5.02	124.95	119.78
1	D	776	SER	N-CA-C	5.02	119.16	113.19
1	A	1217	ASN	N-CA-C	5.00	116.80	107.99

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	3545	0	3470	15	0
1	D	3545	0	3471	30	0
1	G	3496	0	3420	16	0
1	H	5658	0	5425	37	0
1	I	5658	0	5425	63	0
1	J	5658	0	5423	32	0
2	B	948	0	904	2	0
2	E	948	0	904	3	0
3	C	835	0	816	2	0
3	F	835	0	816	2	0
All	All	31126	0	30074	202	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.

All (202) 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
1:D:905:TYR:OH	1:D:936:PRO:CA	1.80	1.30
1:I:437:CYS:CB	1:I:584:VAL:O	1.80	1.27
1:D:905:TYR:OH	1:D:936:PRO:HA	1.26	1.23
1:I:506:PHE:CD2	1:I:555:VAL:HG21	1.75	1.21
1:I:437:CYS:CB	1:I:585:CYS:HA	1.72	1.17
1:I:506:PHE:CD2	1:I:555:VAL:CG2	2.28	1.15
1:J:506:PHE:CD2	1:J:555:VAL:HG21	1.82	1.15
1:J:506:PHE:HE2	1:J:555:VAL:CG2	1.43	1.14
1:I:437:CYS:HB3	1:I:585:CYS:HA	1.20	1.14
1:H:381:VAL:HG11	1:H:407:CYS:HA	1.28	1.10
1:I:437:CYS:HB2	1:I:584:VAL:O	0.89	1.06
1:J:621:THR:HG22	1:J:622:ALA:H	1.21	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:905:TYR:OH	1:G:934:VAL:O	1.75	1.03
1:J:506:PHE:CD2	1:J:555:VAL:CG2	2.42	0.99
1:J:621:THR:HG22	1:J:622:ALA:N	1.77	0.98
1:I:506:PHE:CD2	1:I:555:VAL:HG23	2.04	0.92
1:I:621:THR:O	1:I:648:TYR:HD2	1.53	0.90
1:H:384:ASP:O	1:H:404:PHE:CZ	2.24	0.90
1:J:621:THR:CG2	1:J:622:ALA:H	1.84	0.89
1:H:621:THR:O	1:H:648:TYR:HD2	1.55	0.89
1:J:621:THR:O	1:J:648:TYR:HD2	1.55	0.89
1:I:437:CYS:HB2	1:I:584:VAL:C	1.98	0.89
1:I:506:PHE:HE2	1:I:555:VAL:CB	1.87	0.88
1:D:927:GLN:HA	1:D:932:TYR:HB2	1.58	0.86
1:H:378:ALA:O	1:H:379:GLU:HG2	1.75	0.86
1:G:871:LEU:O	1:G:871:LEU:HG	1.75	0.85
1:I:621:THR:HG22	1:I:622:ALA:N	1.91	0.85
1:D:905:TYR:OH	1:D:936:PRO:N	2.12	0.82
1:H:381:VAL:CG1	1:H:407:CYS:HA	2.09	0.82
1:I:438:TYR:O	1:I:440:SER:N	2.14	0.80
1:D:871:LEU:O	1:D:871:LEU:HG	1.81	0.80
1:D:905:TYR:CZ	1:D:936:PRO:HB3	2.17	0.80
1:D:932:TYR:OH	1:D:1036:LEU:HB2	1.83	0.78
2:E:20:ILE:C	2:E:20:ILE:HD12	2.08	0.78
1:I:506:PHE:CE2	1:I:555:VAL:CB	2.63	0.77
1:H:384:ASP:O	1:H:404:PHE:HZ	1.66	0.77
1:H:621:THR:O	1:H:648:TYR:CD2	2.37	0.77
1:I:437:CYS:SG	1:I:585:CYS:CB	2.73	0.76
1:J:621:THR:O	1:J:648:TYR:CD2	2.42	0.73
1:A:983:VAL:O	1:A:1190:SER:OG	2.05	0.73
1:I:621:THR:HG22	1:I:622:ALA:H	1.53	0.73
1:I:621:THR:O	1:I:648:TYR:CD2	2.40	0.73
1:I:506:PHE:HD2	1:I:555:VAL:HG23	1.50	0.72
1:H:621:THR:HG22	1:H:622:ALA:N	2.06	0.70
1:I:621:THR:CG2	1:I:622:ALA:H	2.05	0.70
1:I:621:THR:CG2	1:I:622:ALA:N	2.55	0.69
1:I:437:CYS:CB	1:I:585:CYS:CA	2.63	0.69
1:D:983:VAL:O	1:D:1190:SER:OG	2.10	0.68
1:H:616:VAL:HG13	1:H:616:VAL:O	1.93	0.68
1:I:438:TYR:HB3	1:I:576:GLN:O	1.92	0.68
1:J:506:PHE:CD2	1:J:555:VAL:HG23	2.28	0.68
1:I:437:CYS:SG	1:I:585:CYS:HA	2.35	0.67
1:J:172:LEU:HD12	1:J:172:LEU:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:437:CYS:HG	1:I:585:CYS:HG	1.27	0.67
1:D:927:GLN:CA	1:D:932:TYR:HB2	2.24	0.66
2:E:20:ILE:HD12	2:E:20:ILE:O	1.96	0.66
1:I:437:CYS:HB3	1:I:586:PRO:HD3	1.79	0.65
1:J:506:PHE:HE2	1:J:555:VAL:HG22	1.53	0.65
1:G:927:GLN:HG2	1:G:932:TYR:HB2	1.79	0.63
1:H:384:ASP:O	1:H:404:PHE:CE2	2.50	0.63
1:G:932:TYR:OH	1:G:1036:LEU:HB2	1.98	0.62
1:I:172:LEU:O	1:I:172:LEU:HD12	2.00	0.62
1:D:927:GLN:HG3	1:D:932:TYR:HB3	1.81	0.62
1:H:378:ALA:C	1:H:379:GLU:HG2	2.23	0.62
1:J:506:PHE:HE2	1:J:555:VAL:HG21	0.80	0.61
1:G:932:TYR:OH	1:G:1036:LEU:CB	2.49	0.60
1:I:437:CYS:SG	1:I:585:CYS:CA	2.89	0.60
1:D:905:TYR:OH	1:D:936:PRO:CB	2.49	0.60
1:D:905:TYR:CZ	1:D:936:PRO:CB	2.85	0.59
1:D:905:TYR:CZ	1:D:936:PRO:CA	2.84	0.59
1:H:381:VAL:O	1:H:382:GLU:HB3	2.03	0.59
1:D:905:TYR:CZ	1:D:936:PRO:HA	2.31	0.59
1:I:67:ILE:HG13	1:I:67:ILE:O	2.03	0.59
2:B:85:GLU:OE1	2:B:85:GLU:N	2.35	0.58
1:I:438:TYR:C	1:I:440:SER:N	2.61	0.57
1:H:385:PHE:CE2	1:H:404:PHE:CE1	2.92	0.57
1:H:382:GLU:HA	1:H:408:ASN:O	2.04	0.57
1:J:67:ILE:HG13	1:J:67:ILE:O	2.05	0.57
1:H:621:THR:CG2	1:H:622:ALA:N	2.67	0.56
1:D:932:TYR:OH	1:D:1036:LEU:CB	2.53	0.56
1:D:1175:THR:HG23	1:D:1175:THR:O	2.05	0.56
1:I:383:CYS:HB2	1:I:385:PHE:CE1	2.41	0.56
1:H:604:VAL:O	1:H:604:VAL:HG23	2.07	0.55
1:I:438:TYR:O	1:I:439:SER:C	2.50	0.55
1:I:383:CYS:CB	1:I:385:PHE:CE1	2.91	0.54
1:I:438:TYR:HB3	1:I:576:GLN:C	2.33	0.54
1:A:1175:THR:HG23	1:A:1175:THR:O	2.08	0.54
1:A:897:LYS:HE2	1:A:897:LYS:HA	1.90	0.53
3:F:28:TYR:N	3:F:28:TYR:CD1	2.71	0.53
3:C:1:ASP:OD1	3:C:1:ASP:C	2.52	0.53
1:D:927:GLN:HG3	1:D:932:TYR:CB	2.38	0.53
1:I:437:CYS:SG	1:I:584:VAL:O	2.67	0.53
1:G:933:LYS:O	1:G:934:VAL:C	2.52	0.52
1:H:664:ASP:OD1	1:H:664:ASP:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1001:PHE:C	1:G:1001:PHE:CD2	2.89	0.51
1:D:905:TYR:HH	1:D:936:PRO:HA	1.63	0.51
1:H:395:GLN:HA	1:H:395:GLN:OE1	2.11	0.51
1:H:171:LEU:C	1:H:171:LEU:HD23	2.36	0.50
1:H:67:ILE:O	1:H:67:ILE:HG13	2.10	0.50
1:G:932:TYR:N	1:G:932:TYR:CD1	2.78	0.50
1:A:809:TYR:C	1:A:809:TYR:CD2	2.90	0.50
1:A:1001:PHE:C	1:A:1001:PHE:CD2	2.90	0.49
1:I:623:VAL:O	1:I:642:TYR:OH	2.27	0.49
1:I:606:TYR:C	1:I:606:TYR:CD1	2.90	0.49
1:J:369:LYS:HG2	1:J:369:LYS:O	2.12	0.49
1:I:385:PHE:CE2	1:I:404:PHE:CE1	3.01	0.48
1:H:616:VAL:O	1:H:616:VAL:CG1	2.59	0.48
1:D:756:GLU:H	1:D:756:GLU:CD	2.21	0.48
1:D:777:TYR:N	1:D:777:TYR:CD2	2.81	0.48
1:I:596:ILE:HD12	1:I:596:ILE:C	2.38	0.48
1:A:875:GLU:O	1:A:875:GLU:HG2	2.13	0.48
1:G:906:MET:HG2	1:G:906:MET:O	2.14	0.48
1:H:621:THR:CG2	1:H:622:ALA:H	2.26	0.47
1:D:1173:ILE:HG13	1:D:1185:SER:OG	2.14	0.47
1:A:1160:ASN:OD1	1:A:1160:ASN:C	2.58	0.47
2:E:20:ILE:C	2:E:20:ILE:CD1	2.80	0.47
1:G:1160:ASN:OD1	1:G:1160:ASN:C	2.57	0.47
1:A:875:GLU:OE1	1:A:875:GLU:N	2.38	0.47
1:J:172:LEU:HD12	1:J:172:LEU:C	2.39	0.47
1:J:139:THR:OG1	1:J:141:ARG:NH1	2.48	0.47
1:H:301:ARG:O	1:H:301:ARG:HG2	2.14	0.46
1:J:439:SER:HA	1:J:582:ASN:HA	1.98	0.46
1:J:330:ASP:OD1	1:J:330:ASP:C	2.58	0.46
3:C:92:LYS:HD3	3:C:92:LYS:C	2.41	0.45
1:H:665:LYS:C	1:H:665:LYS:HD3	2.41	0.45
1:H:689:TYR:CD1	1:H:689:TYR:C	2.94	0.45
1:D:904:GLY:O	1:D:905:TYR:HB2	2.16	0.45
1:J:633:ASP:OD1	1:J:633:ASP:C	2.58	0.45
1:I:130:VAL:O	1:I:130:VAL:HG12	2.16	0.45
1:D:875:GLU:HB3	1:D:886:ALA:HB3	1.99	0.45
1:A:1060:PRO:HA	1:A:1063:GLN:HB3	1.98	0.45
1:D:1001:PHE:C	1:D:1001:PHE:CD2	2.95	0.44
1:G:1060:PRO:HA	1:G:1063:GLN:HB3	1.98	0.44
1:J:621:THR:CG2	1:J:622:ALA:N	2.45	0.44
1:I:300:ILE:HD12	1:I:300:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:409:TYR:CD1	1:I:409:TYR:C	2.96	0.44
1:I:677:VAL:HG22	1:I:677:VAL:O	2.16	0.44
1:I:438:TYR:HD2	1:I:577:TYR:HB2	1.83	0.44
1:I:633:ASP:OD1	1:I:633:ASP:C	2.60	0.44
1:J:240:MET:SD	1:J:240:MET:C	3.01	0.44
1:I:670:HIS:CD2	1:I:670:HIS:N	2.84	0.44
1:H:694:ARG:NE	1:H:694:ARG:HA	2.33	0.43
1:I:395:GLN:HA	1:I:395:GLN:OE1	2.17	0.43
1:D:905:TYR:CE1	1:D:936:PRO:HB3	2.54	0.43
1:D:1175:THR:O	1:D:1175:THR:CG2	2.67	0.43
1:H:49:ASP:OD1	1:H:49:ASP:C	2.61	0.43
1:I:209:THR:O	1:I:209:THR:HG22	2.18	0.43
1:I:439:SER:HA	1:I:582:ASN:HA	2.00	0.43
1:A:801:LYS:HE3	1:A:801:LYS:HB2	1.85	0.43
3:F:2:ILE:HD12	3:F:2:ILE:N	2.33	0.43
1:I:132:ILE:HD12	1:I:132:ILE:HA	1.73	0.43
1:I:652:ARG:NE	1:I:652:ARG:HA	2.34	0.43
1:I:438:TYR:CB	1:I:576:GLN:O	2.63	0.43
1:A:826:GLN:OE1	1:A:826:GLN:N	2.32	0.43
1:H:330:ASP:OD1	1:H:330:ASP:C	2.62	0.43
1:I:330:ASP:C	1:I:330:ASP:OD1	2.61	0.43
1:J:37:GLN:CD	1:J:37:GLN:C	2.86	0.43
1:J:643:SER:OG	1:J:644:ASP:N	2.50	0.42
1:H:383:CYS:HB3	1:H:385:PHE:CE1	2.55	0.42
1:H:694:ARG:HA	1:H:694:ARG:HE	1.85	0.42
1:I:383:CYS:HB3	1:I:385:PHE:CE1	2.54	0.42
1:I:172:LEU:HD12	1:I:172:LEU:C	2.44	0.42
1:G:1124:VAL:O	1:G:1124:VAL:HG13	2.19	0.42
1:I:49:ASP:OD1	1:I:49:ASP:C	2.62	0.42
1:I:688:GLN:HA	1:I:688:GLN:OE1	2.20	0.42
1:H:621:THR:HG22	1:H:622:ALA:H	1.80	0.42
1:A:774:ASN:OD1	1:A:774:ASN:C	2.62	0.41
1:D:806:CYS:SG	1:D:806:CYS:O	2.77	0.41
1:G:841:ARG:NE	1:G:841:ARG:HA	2.34	0.41
1:D:930:ALA:HB2	1:D:1040:LEU:HD11	2.01	0.41
1:I:140:ILE:HG21	1:I:140:ILE:HD13	1.77	0.41
1:I:378:ALA:HB1	1:I:379:GLU:HA	2.03	0.41
1:A:965:SER:OG	1:A:966:SER:N	2.52	0.41
1:G:819:GLN:CD	1:G:819:GLN:C	2.88	0.41
1:H:383:CYS:SG	1:H:409:TYR:HB3	2.60	0.41
1:J:593:ASP:N	1:J:594:THR:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:506:PHE:HD2	1:J:555:VAL:HG23	1.81	0.41
1:D:826:GLN:OE1	1:D:826:GLN:N	2.28	0.41
1:D:909:TYR:CD2	1:D:909:TYR:C	2.98	0.41
1:H:130:VAL:O	1:H:130:VAL:HG12	2.21	0.41
1:H:140:ILE:HD13	1:H:140:ILE:HG21	1.83	0.41
1:I:130:VAL:O	1:I:130:VAL:CG1	2.66	0.41
1:I:506:PHE:HE2	1:I:555:VAL:CG1	2.31	0.41
1:J:410:ASN:OD1	1:J:410:ASN:C	2.64	0.41
1:A:826:GLN:H	1:A:826:GLN:CD	2.23	0.41
1:A:841:ARG:NE	1:A:841:ARG:HA	2.35	0.41
1:J:409:TYR:CD1	1:J:409:TYR:C	2.98	0.41
1:G:1120:GLY:O	1:G:1121:THR:OG1	2.31	0.40
1:J:719:ASN:OD1	1:J:719:ASN:C	2.63	0.40
1:G:936:PRO:HA	1:G:937:PRO:HD3	1.96	0.40
1:H:443:LEU:C	1:H:443:LEU:HD23	2.47	0.40
1:J:228:PHE:CD2	1:J:228:PHE:C	2.99	0.40
2:B:72:ASP:OD1	2:B:72:ASP:C	2.64	0.40
1:H:187:LEU:HD23	1:H:187:LEU:HA	1.87	0.40
1:I:645:ASP:OD1	1:I:645:ASP:C	2.64	0.40
1:J:395:GLN:HA	1:J:395:GLN:OE1	2.22	0.40
1:H:132:ILE:HA	1:H:132:ILE:HD12	1.87	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	459/1329 (34%)	441 (96%)	15 (3%)	3 (1%)	18	55
1	D	459/1329 (34%)	440 (96%)	14 (3%)	5 (1%)	11	45
1	G	451/1329 (34%)	433 (96%)	17 (4%)	1 (0%)	43	77
1	H	724/1329 (54%)	693 (96%)	27 (4%)	4 (1%)	21	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	724/1329 (54%)	691 (95%)	29 (4%)	4 (1%)	21	58
1	J	724/1329 (54%)	695 (96%)	24 (3%)	5 (1%)	18	55
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	50
3	F	109/218 (50%)	105 (96%)	2 (2%)	2 (2%)	6	32
All	All	3993/8876 (45%)	3831 (96%)	137 (3%)	25 (1%)	23	58

All (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
1	A	940	ASP
1	D	961	THR
1	D	965	SER
1	H	718	VAL
1	I	718	VAL
1	J	602	ASN
1	J	718	VAL
3	C	77	PRO
1	D	905	TYR
1	A	1220	PRO
1	D	1220	PRO
3	F	31	SER
3	F	77	PRO
1	J	596	ILE
1	J	629	ARG
1	D	956	ALA
1	H	368	ALA
1	H	380	GLY
1	I	629	ARG
1	I	44	TRP

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%)	635 (100%)	0	100	100
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
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%)	3453 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	808	GLN
1	A	812	ASN
1	A	836	HIS
1	A	914	GLN
1	A	981	ASN
1	A	1009	GLN
2	B	35	HIS
3	C	37	GLN
1	D	769	GLN
1	D	836	HIS
1	D	914	GLN
1	D	1020	HIS
3	F	34	ASN
3	F	89	GLN

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Mol	Chain	Res	Type
1	G	769	GLN
1	G	833	GLN
1	G	914	GLN
1	G	1031	GLN
1	G	1212	GLN
1	G	1213	ASN
1	H	78	GLN
1	H	155	ASN
1	H	167	HIS
1	H	194	HIS
1	H	261	GLN
1	H	319	GLN
1	H	566	GLN
1	H	618	GLN
1	I	81	HIS
1	I	104	ASN
1	I	107	GLN
1	I	566	GLN
1	I	627	GLN
1	I	628	GLN
1	J	78	GLN
1	J	104	ASN
1	J	107	GLN
1	J	194	HIS
1	J	208	HIS
1	J	244	ASN
1	J	436	ASN
1	J	636	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

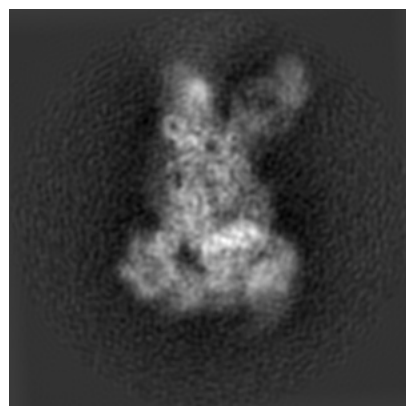
6 Map visualisation [i](#)

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

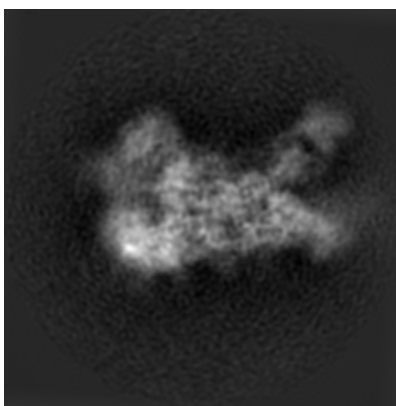
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

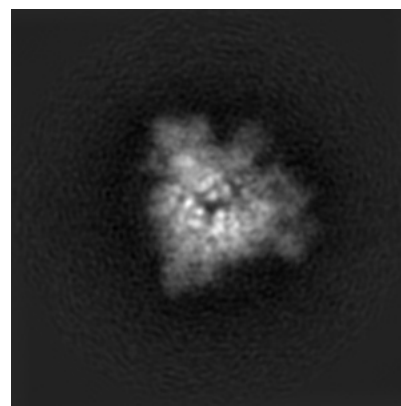
6.1.1 Primary map



X

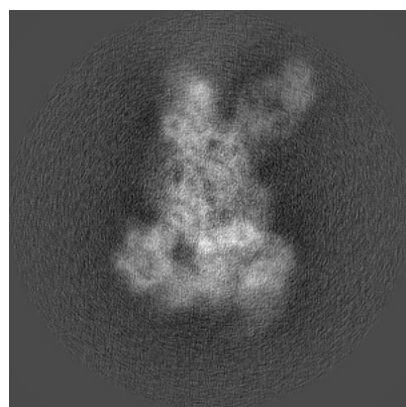


Y

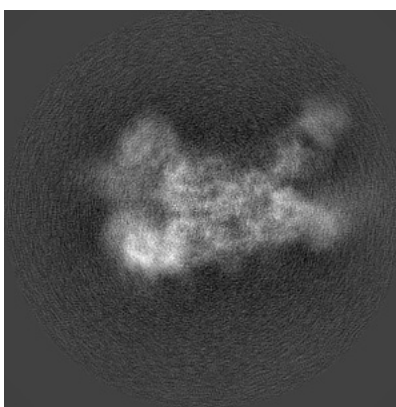


Z

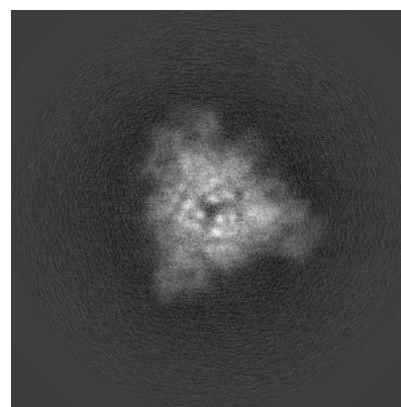
6.1.2 Raw map



X



Y

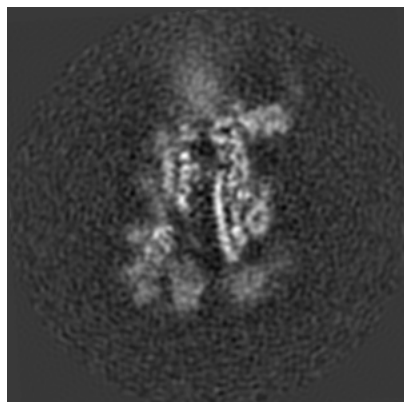


Z

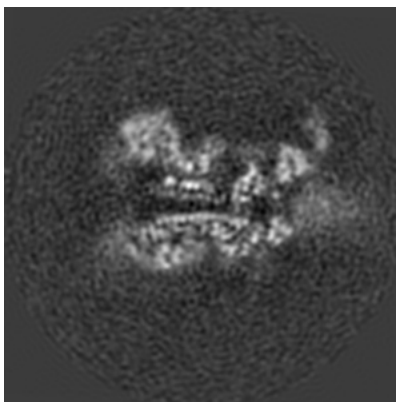
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

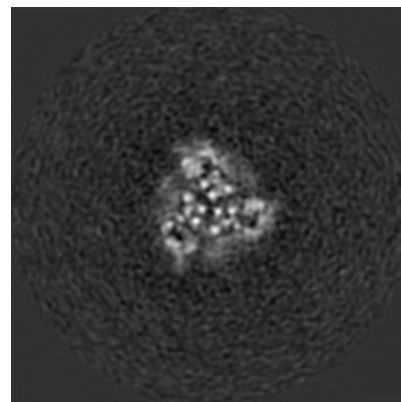
6.2.1 Primary map



X Index: 152

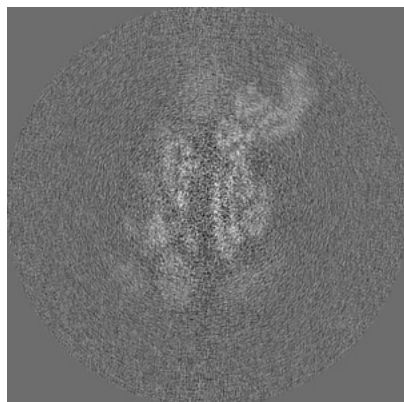


Y Index: 152

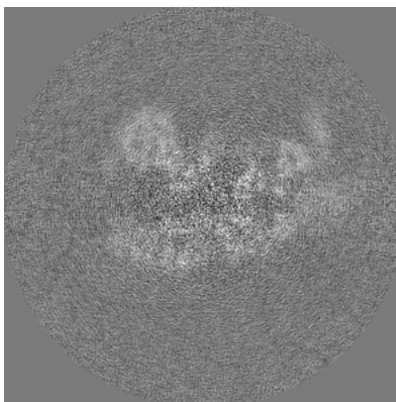


Z Index: 152

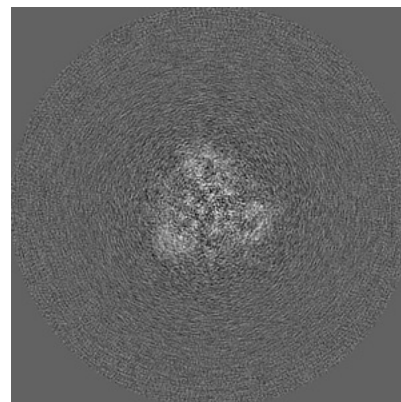
6.2.2 Raw map



X Index: 152



Y Index: 152

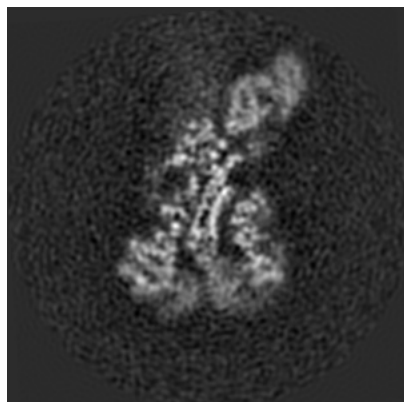


Z Index: 152

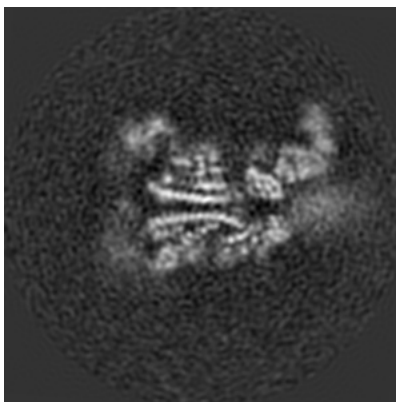
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

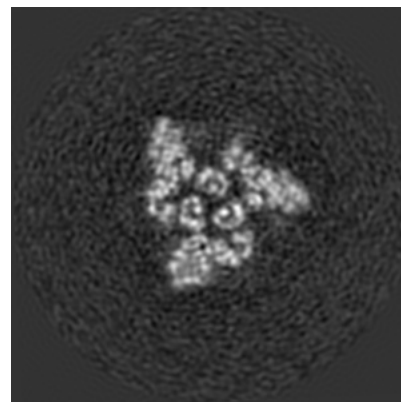
6.3.1 Primary map



X Index: 135

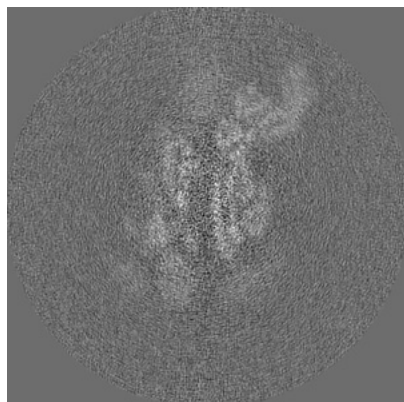


Y Index: 148

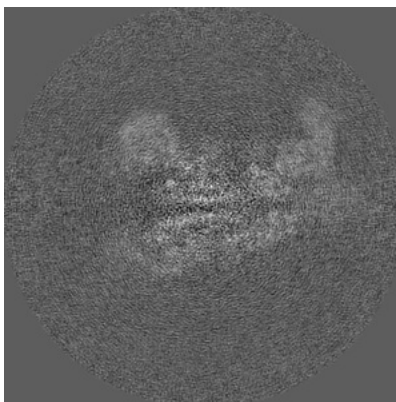


Z Index: 124

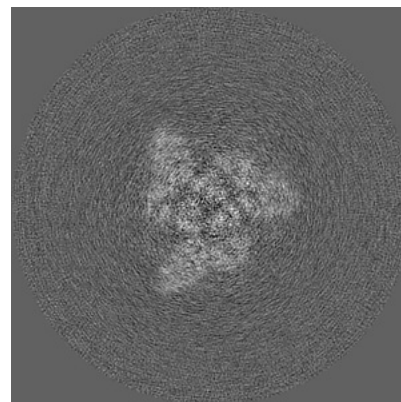
6.3.2 Raw map



X Index: 152



Y Index: 147

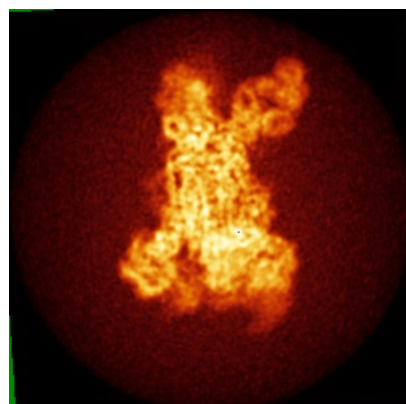


Z Index: 128

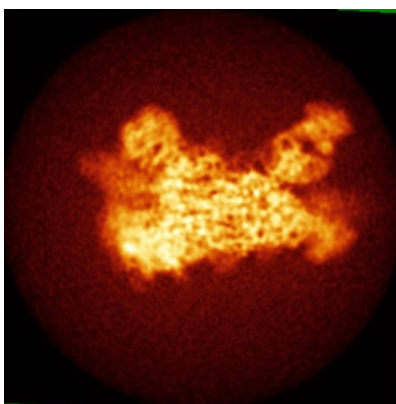
The images above show the largest variance slices of the map in three orthogonal directions.

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

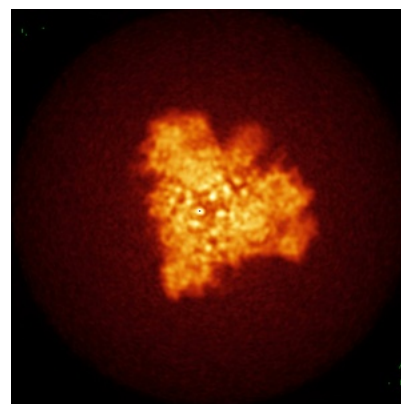
6.4.1 Primary map



X

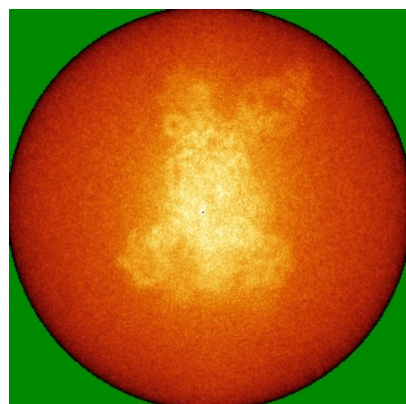


Y

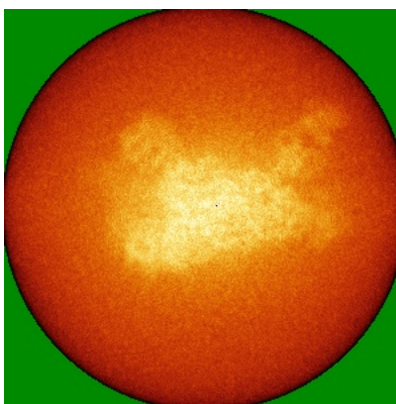


Z

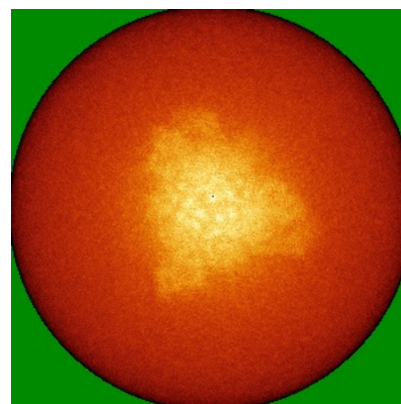
6.4.2 Raw map



X



Y



Z

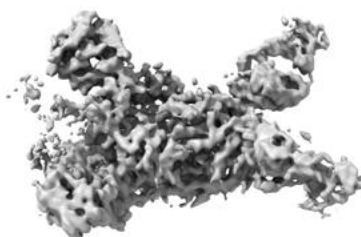
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

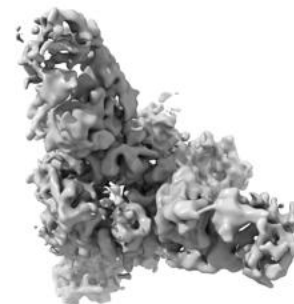
6.5.1 Primary map



X



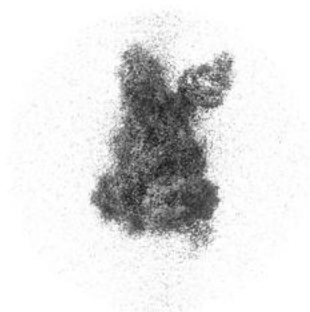
Y



Z

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.

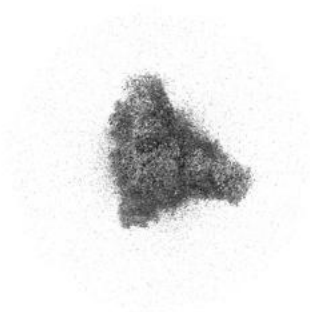
6.5.2 Raw map



X



Y



Z

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

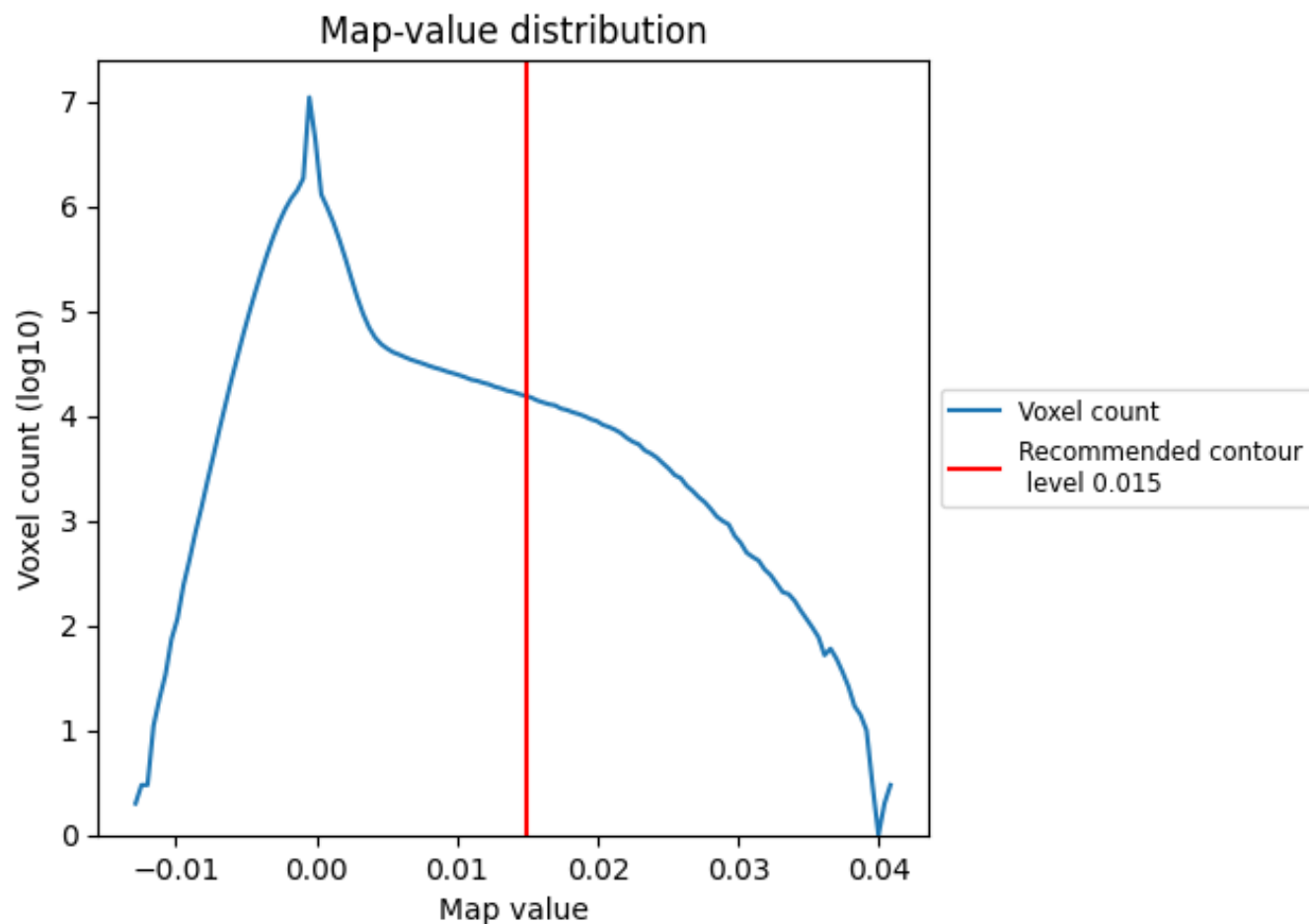
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

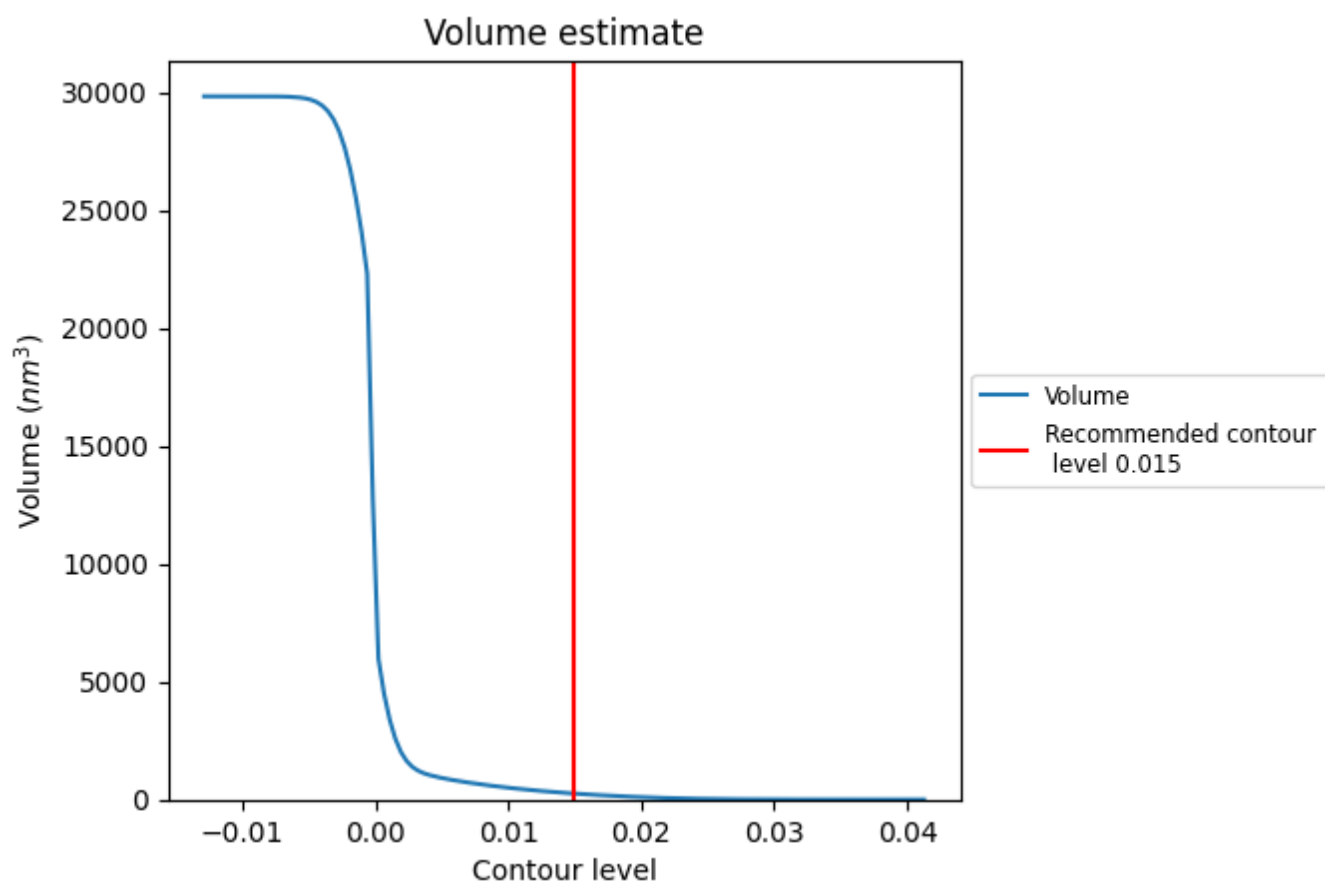
This section contains the results of statistical analysis of the map.

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.

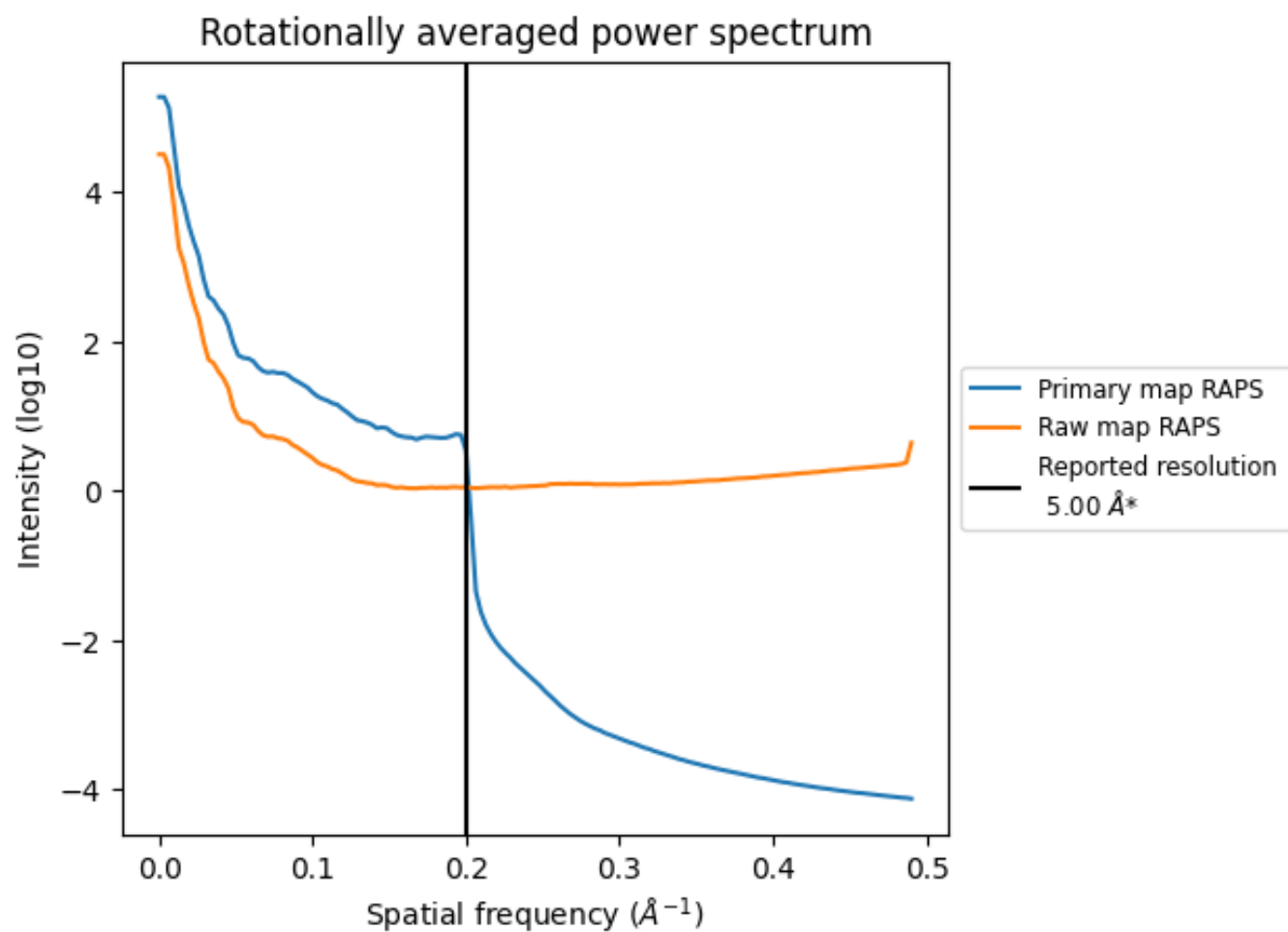
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 253 nm³; 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 ⓘ

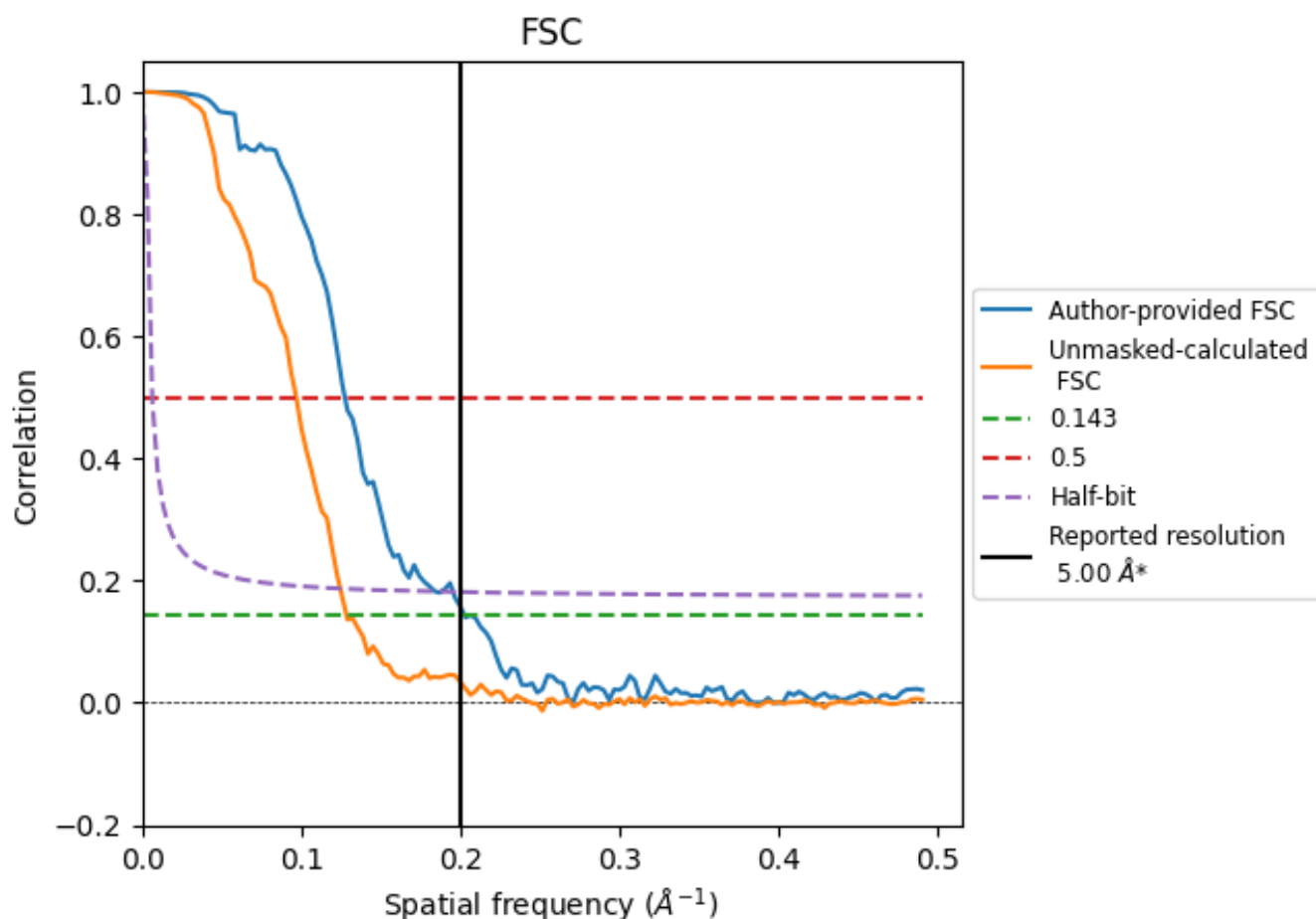


*Reported resolution corresponds to spatial frequency of 0.200 Å⁻¹

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 0.200 Å⁻¹

8.2 Resolution estimates [i](#)

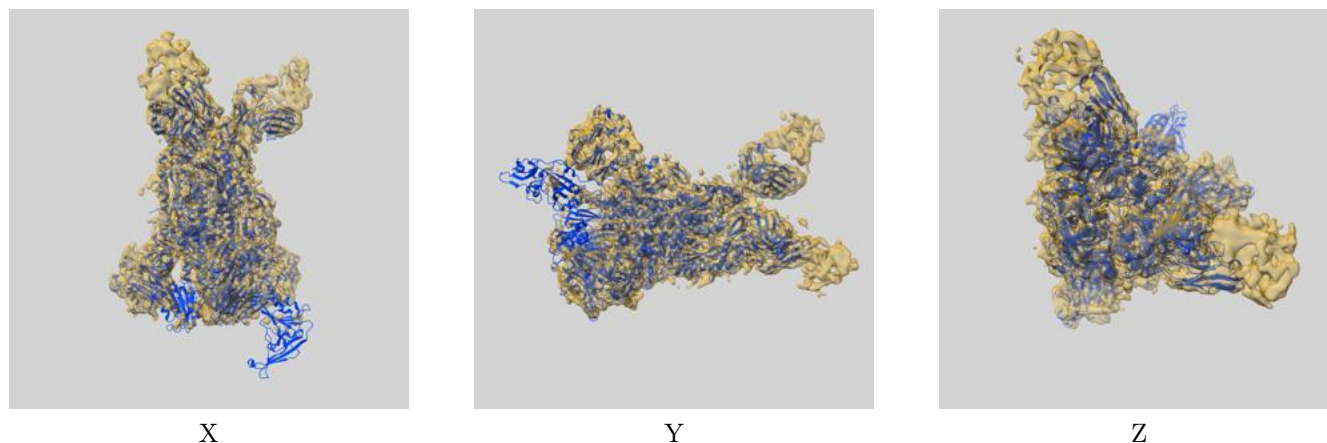
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	4.94	7.85	5.40
Unmasked-calculated*	7.79	10.32	8.04

*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](#)

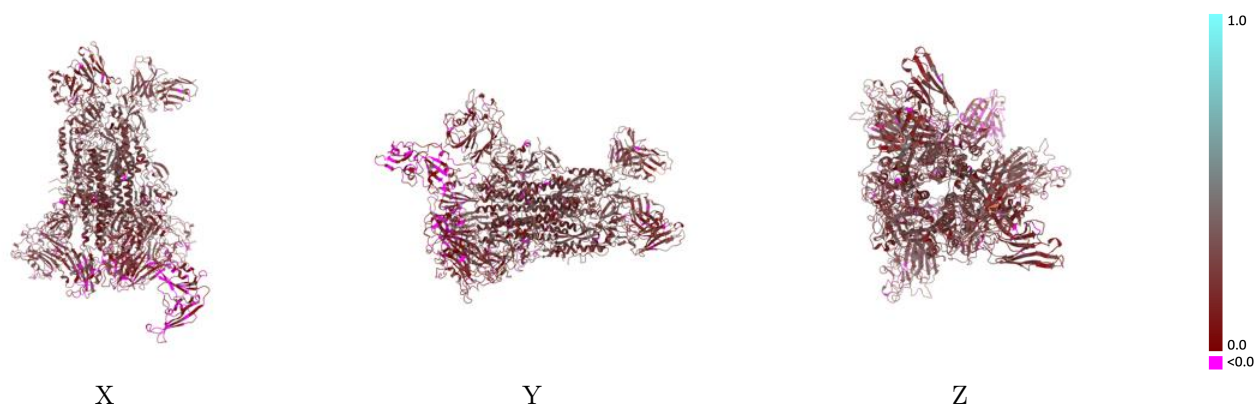
This section contains information regarding the fit between EMDB map EMD-8789 and PDB model 5W9N. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



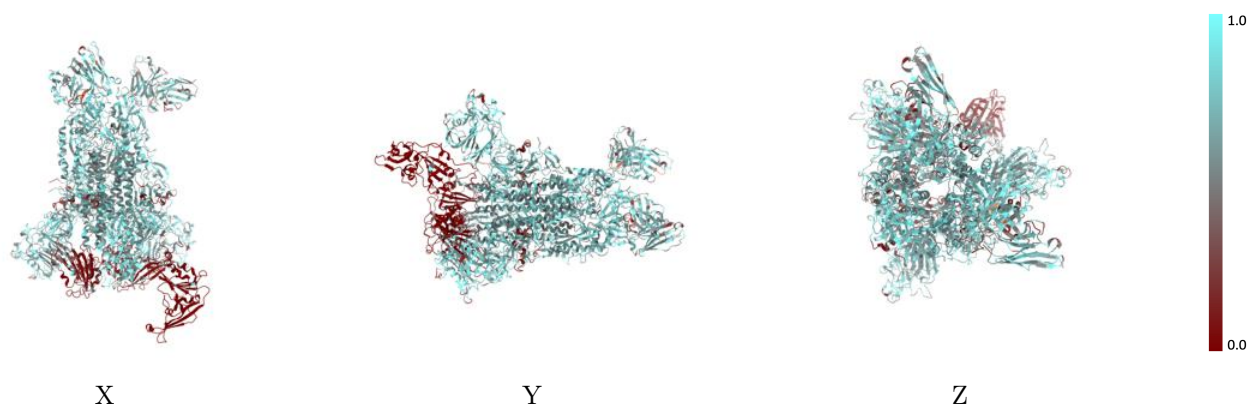
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



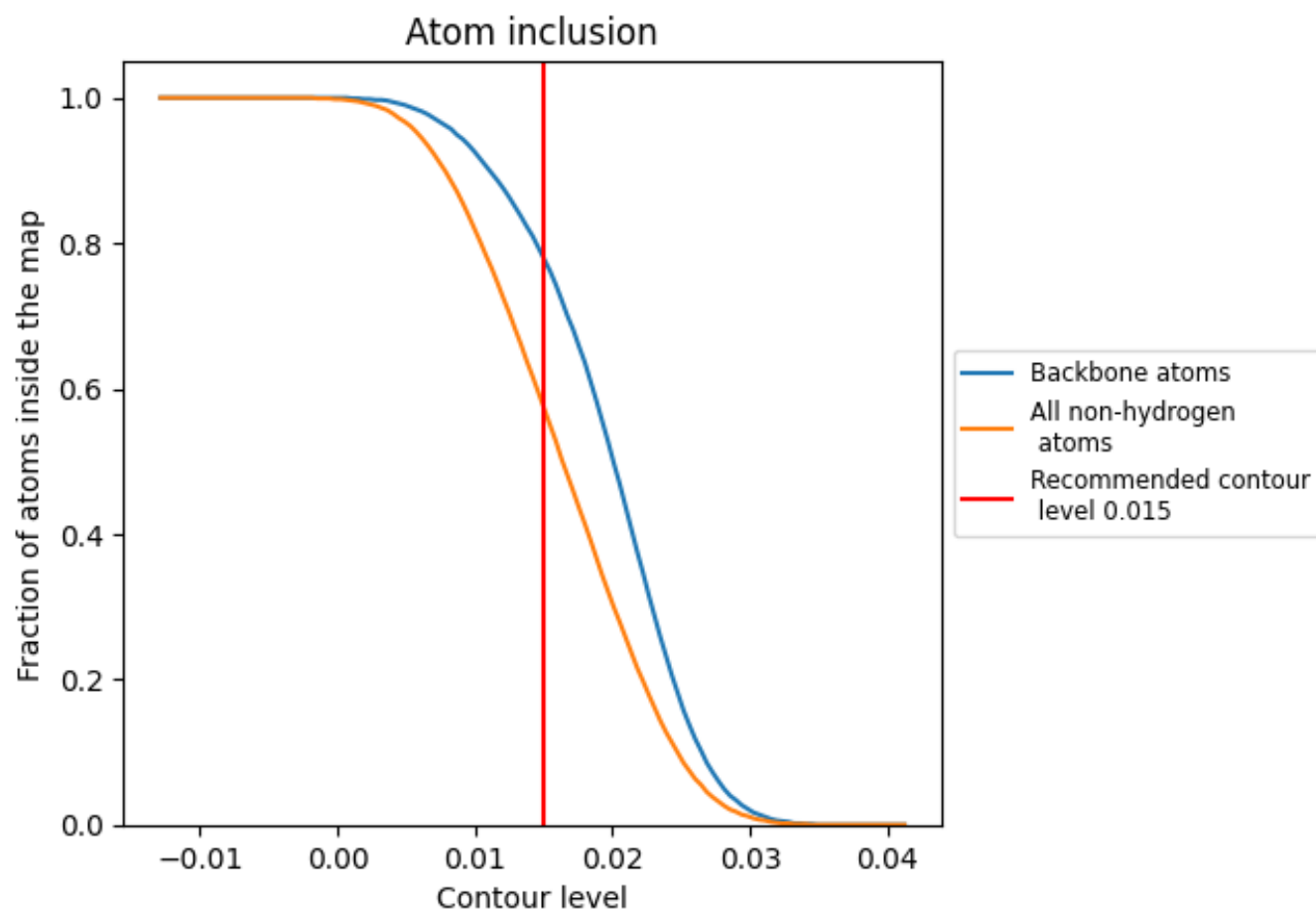
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.5750	0.2140
A	0.6460	0.2520
B	0.6420	0.2350
C	0.5610	0.2110
D	0.6550	0.2600
E	0.7080	0.2320
F	0.5980	0.2000
G	0.6600	0.2490
H	0.4950	0.1720
I	0.5170	0.1920
J	0.5320	0.1970

1.0

0.0

<0.0