



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:02 PM UTC

PDB ID : 5W9M / pdb_00005w9m
EMDB ID : EMD-8788
Title : MERS S ectodomain trimer in complex with variable domain of neutralizing antibody G4
Authors : Pallesen, J.; Ward, A.B.
Deposited on : 2017-06-23
Resolution : 4.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

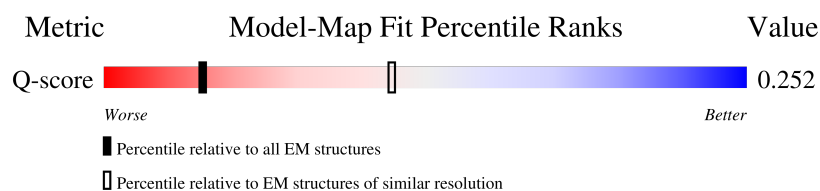
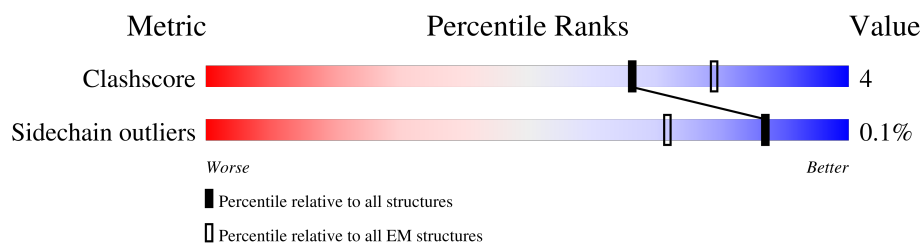
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1989 (4.20 - 5.20)

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	 32% 65%
1	D	1329	 31% 66%
1	E	1329	 14% 48% 6% 45%
1	F	1329	 16% 48% 6% 45%
1	G	1329	 32% 65%

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Mol	Chain	Length	Quality of chain
1	J	1329	13% 49% 6% 45%
2	B	233	48% 49%
2	H	233	48% 49%
3	C	218	9% 46% 5% 49%
3	I	218	7% 47% 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	D	457	Total	C	N	O	S	0	0
			3496	2214	590	675	17		
1	G	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	E	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	F	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
E	506	PHE	LEU	conflict	UNP W5ZZF5
E	748	ALA	ARG	conflict	UNP W5ZZF5
E	751	GLY	ARG	conflict	UNP W5ZZF5
E	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
E	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
E	1292	GLY	-	expression tag	UNP W5ZZF5
E	1293	SER	-	expression tag	UNP W5ZZF5
E	1294	GLY	-	expression tag	UNP W5ZZF5
E	1295	TYR	-	expression tag	UNP W5ZZF5
E	1296	ILE	-	expression tag	UNP W5ZZF5
E	1297	PRO	-	expression tag	UNP W5ZZF5
E	1298	GLU	-	expression tag	UNP W5ZZF5
E	1299	ALA	-	expression tag	UNP W5ZZF5
E	1300	PRO	-	expression tag	UNP W5ZZF5
E	1301	ARG	-	expression tag	UNP W5ZZF5

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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1301	ARG	-	expression tag	UNP W5ZZF5
F	1302	ASP	-	expression tag	UNP W5ZZF5
F	1303	GLY	-	expression tag	UNP W5ZZF5
F	1304	GLN	-	expression tag	UNP W5ZZF5
F	1305	ALA	-	expression tag	UNP W5ZZF5
F	1306	TYR	-	expression tag	UNP W5ZZF5
F	1307	VAL	-	expression tag	UNP W5ZZF5
F	1308	ARG	-	expression tag	UNP W5ZZF5
F	1309	LYS	-	expression tag	UNP W5ZZF5
F	1310	ASP	-	expression tag	UNP W5ZZF5
F	1311	GLY	-	expression tag	UNP W5ZZF5
F	1312	GLU	-	expression tag	UNP W5ZZF5
F	1313	TRP	-	expression tag	UNP W5ZZF5
F	1314	VAL	-	expression tag	UNP W5ZZF5
F	1315	LEU	-	expression tag	UNP W5ZZF5
F	1316	LEU	-	expression tag	UNP W5ZZF5
F	1317	SER	-	expression tag	UNP W5ZZF5
F	1318	THR	-	expression tag	UNP W5ZZF5
F	1319	PHE	-	expression tag	UNP W5ZZF5
F	1320	LEU	-	expression tag	UNP W5ZZF5
F	1321	GLY	-	expression tag	UNP W5ZZF5
F	1322	ARG	-	expression tag	UNP W5ZZF5
F	1323	SER	-	expression tag	UNP W5ZZF5
F	1324	LEU	-	expression tag	UNP W5ZZF5
F	1325	GLU	-	expression tag	UNP W5ZZF5
F	1326	VAL	-	expression tag	UNP W5ZZF5
F	1327	LEU	-	expression tag	UNP W5ZZF5
F	1328	PHE	-	expression tag	UNP W5ZZF5
F	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	H	119	Total	C	N	O	S	0	0
			948	602	156	185	5		

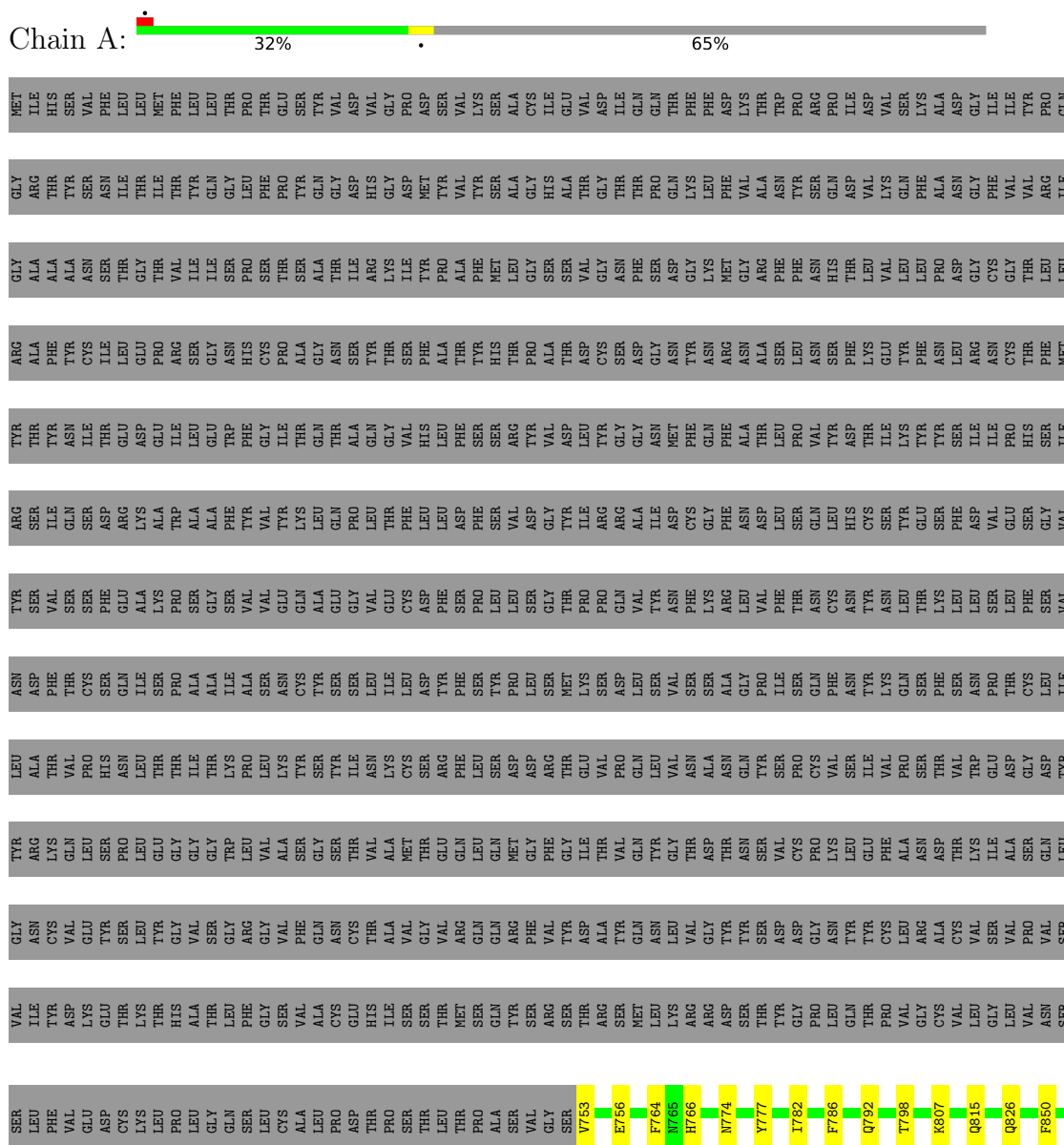
- Molecule 3 is a protein called G4 VL.

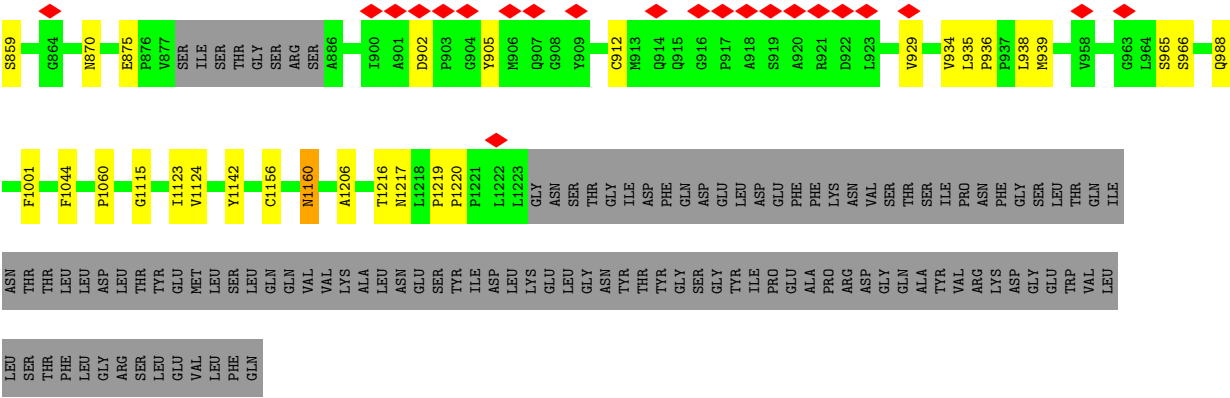
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	111	Total 835	C 522	N 143	O 166	S 4	0	0
3	I	111	Total 835	C 522	N 143	O 166	S 4	0	0

3 Residue-property plots

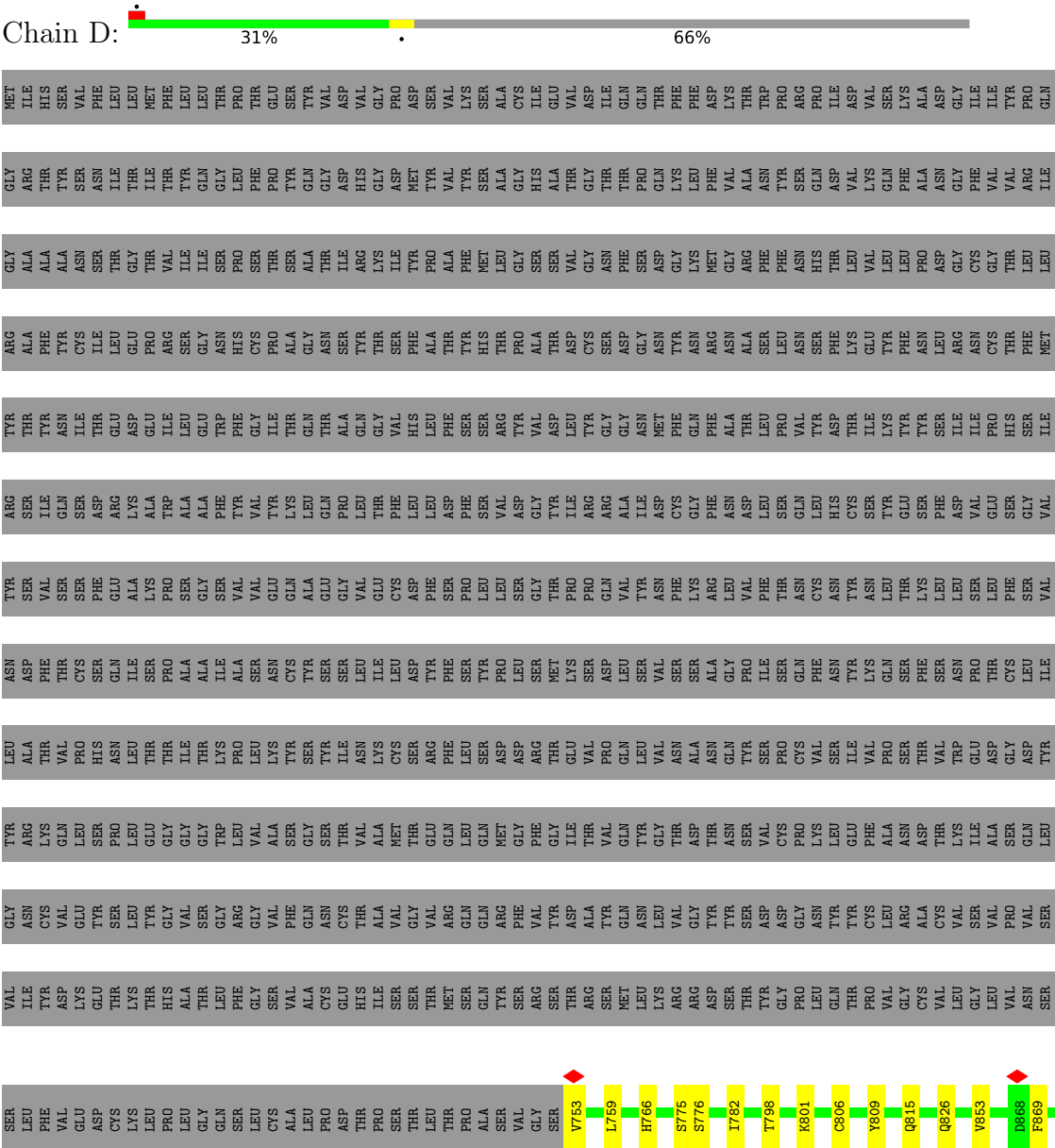
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein

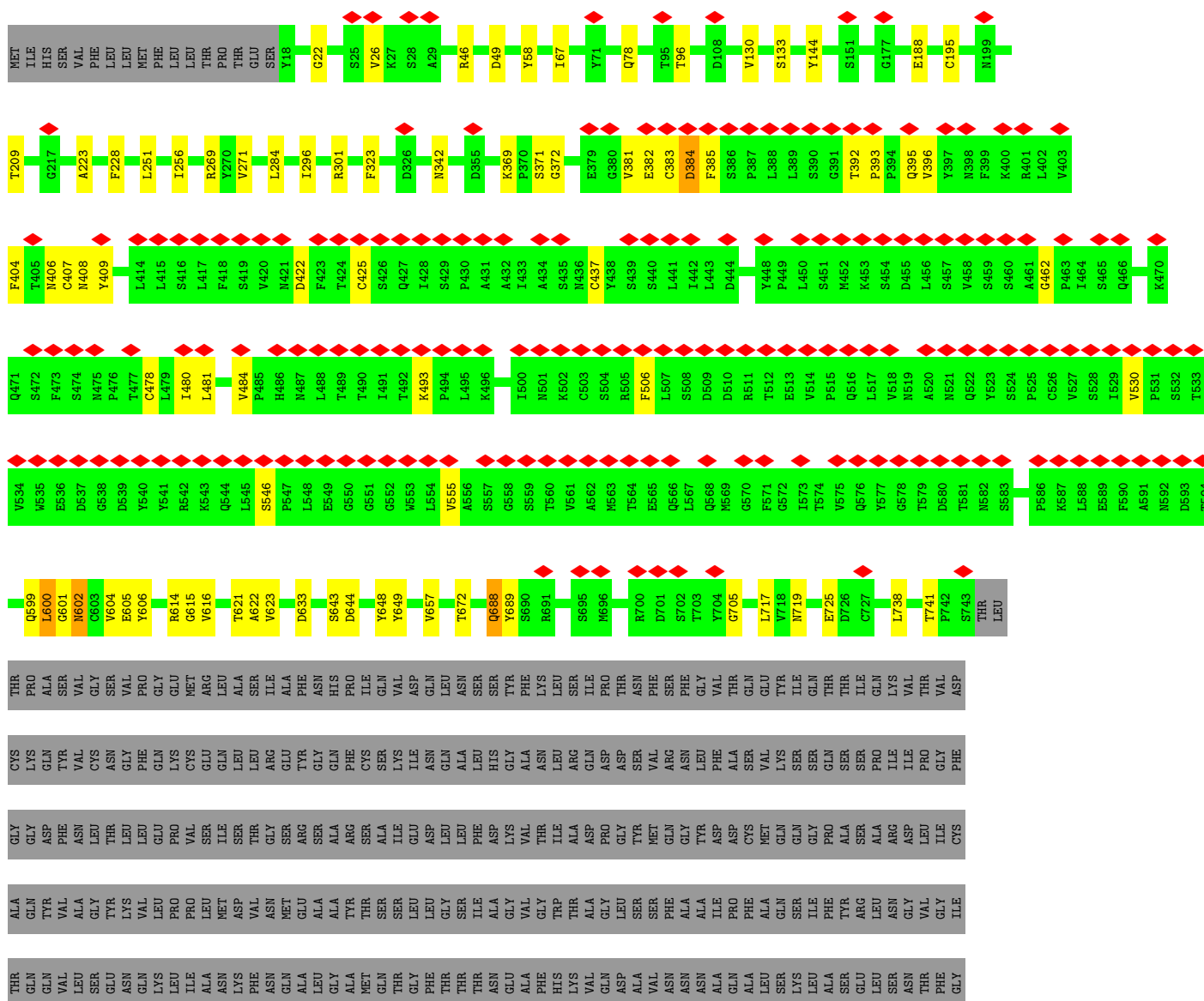




● Molecule 1: Spike glycoprotein

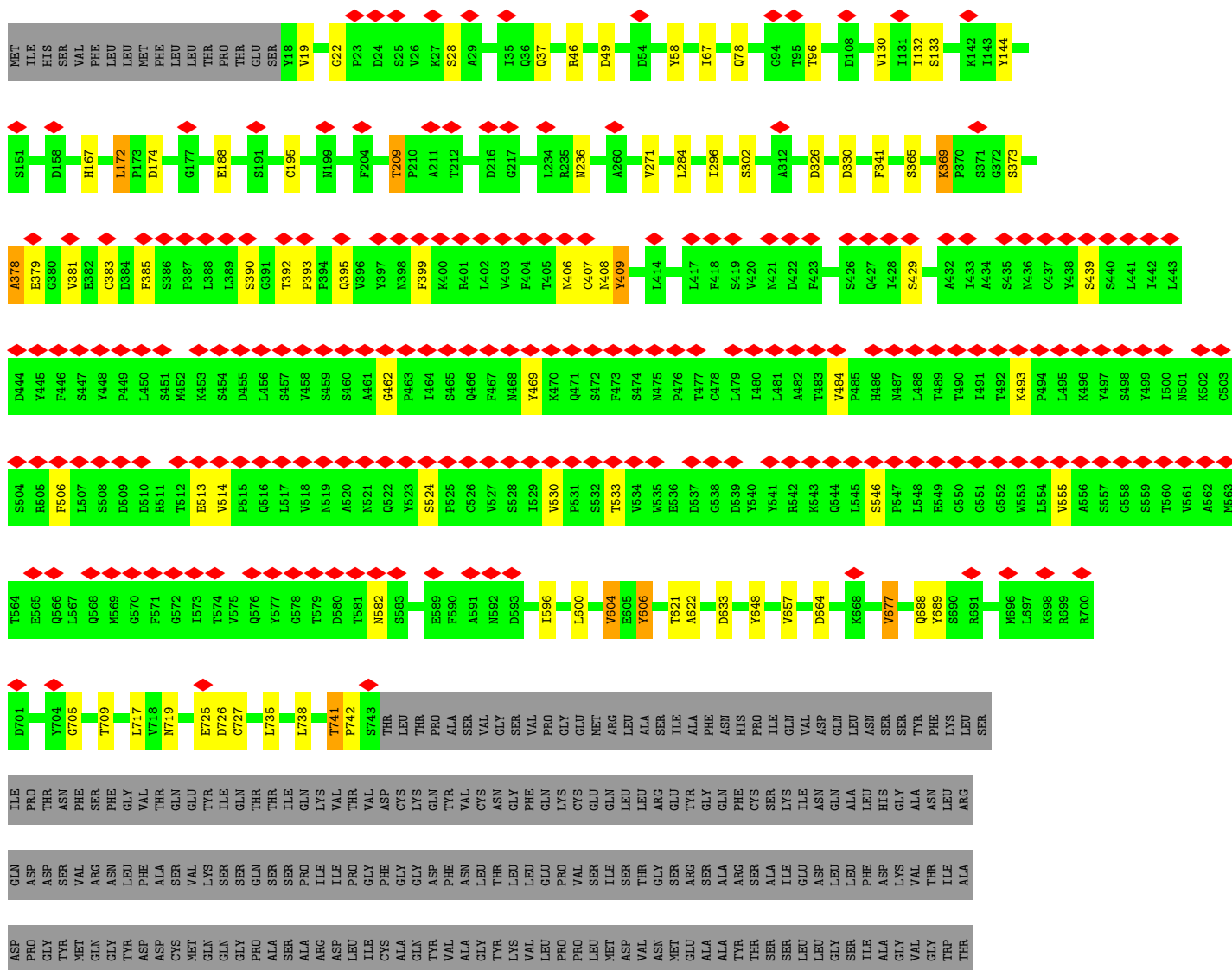


- Molecule 1: Spike glycoprotein



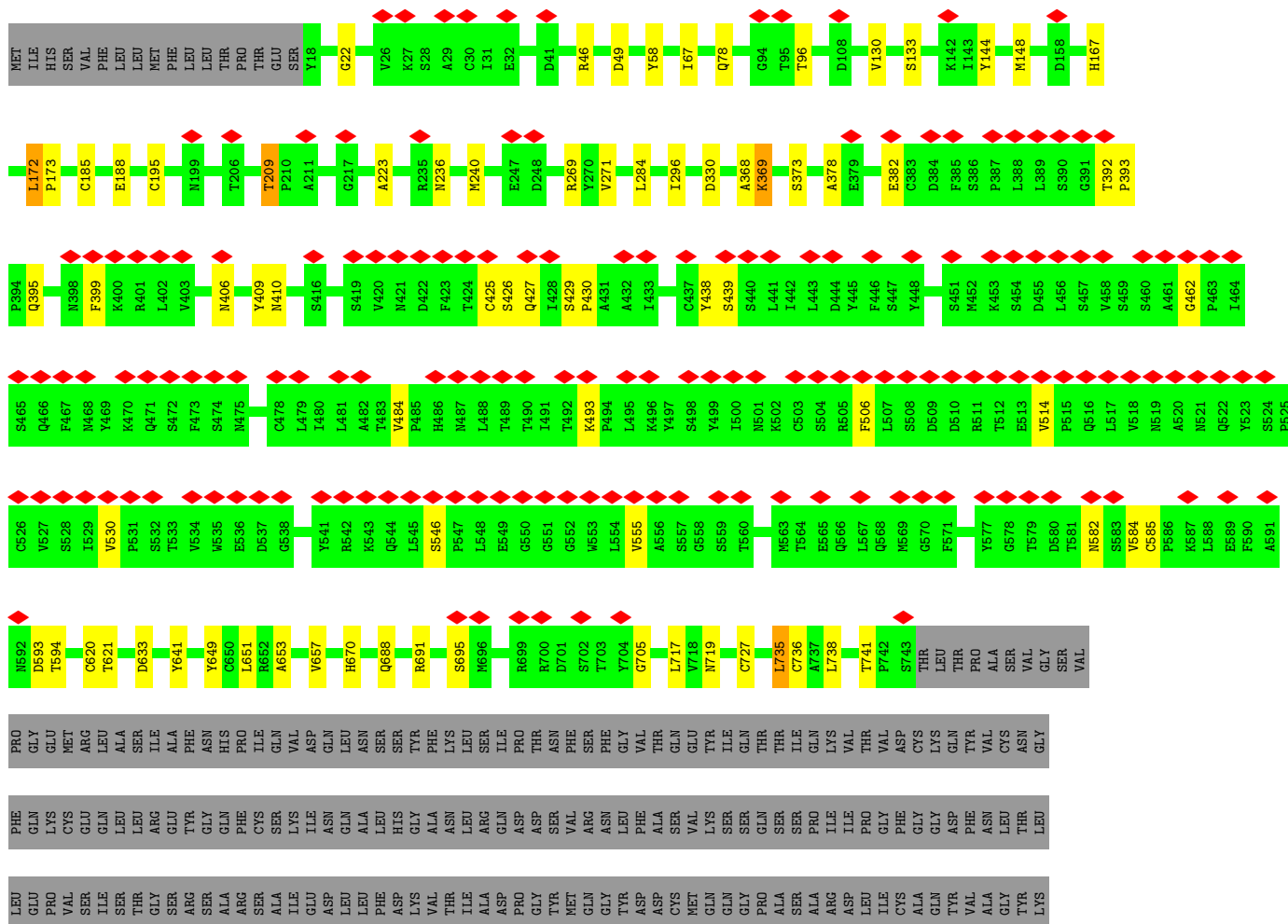
[illegible]

- Molecule 1: Spike glycoprotein



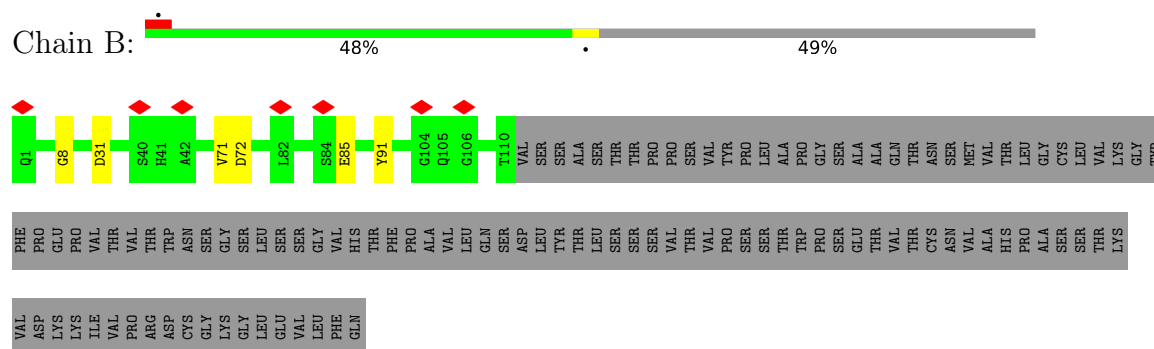
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- Molecule 1: Spike glycoprotein

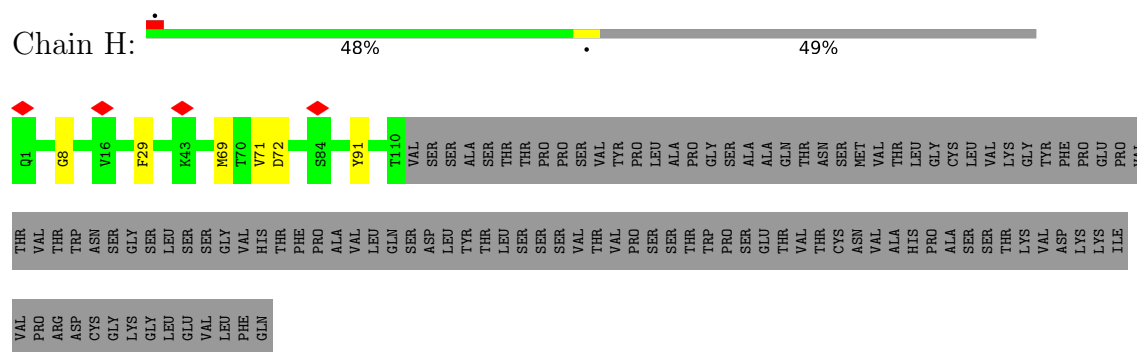


GLY	TYR	LEU	GLU	LYS	SER	ILE	GLN	VAL
ILE	ASP	LEU	ASN	THR	GLY	ILE	LEU	LEU
PRO	GLU	GLU	ASN	THR	CYS	ARG	GLN	PRO
GLU	PHE	THR	THR	ARG	GLN	ASP	ASN	MET
ALA	PHE	THR	ARG	ILE	GLY	PRO	LYS	ASP
PRO	ASN	VAL	VAL	ASP	HIS	THR	PRO	VAL
ARG	VAL	VAL	VAL	ASP	ILE	GLN	ASN	MET
ASP	GLY	THR	THR	THR	VAL	ASP	ALA	GLU
GLN	THR	THR	SER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

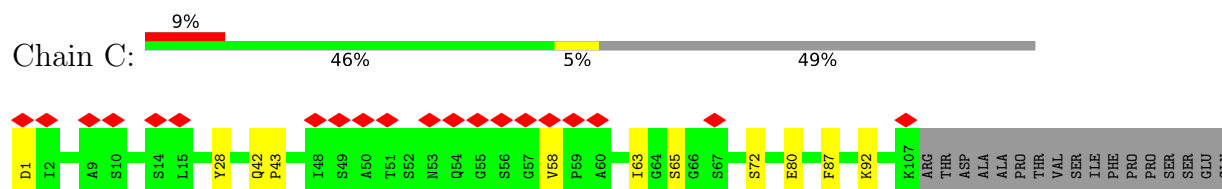
- Molecule 2: G4 VH



- Molecule 2: G4 VH



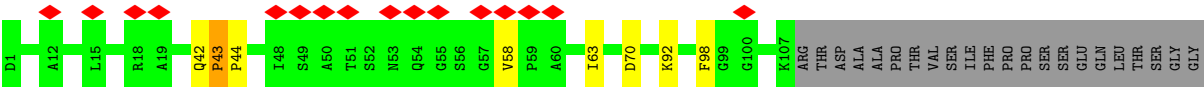
- Molecule 3: G4 VL



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

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

● Molecule 3: G4 VL



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

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9333	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	0.058	Depositor
Minimum map value	-0.025	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	0.93	1/3618 (0.0%)	1.25	42/4921 (0.9%)
1	D	0.91	0/3568	1.25	40/4851 (0.8%)
1	E	0.83	0/5803	1.32	70/7901 (0.9%)
1	F	0.84	0/5803	1.35	89/7901 (1.1%)
1	G	0.93	1/3618 (0.0%)	1.30	44/4921 (0.9%)
1	J	0.86	3/5803 (0.1%)	1.38	91/7901 (1.2%)
2	B	0.81	0/972	1.20	5/1317 (0.4%)
2	H	0.83	0/972	1.18	5/1317 (0.4%)
3	C	0.84	0/852	1.37	9/1153 (0.8%)
3	I	0.87	0/852	1.44	11/1153 (1.0%)
All	All	0.87	5/31861 (0.0%)	1.32	406/43336 (0.9%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	185	CYS	C-O	5.76	1.30	1.23
1	A	807	LYS	CA-C	-5.34	1.47	1.52
1	G	1219	PRO	CA-C	5.34	1.57	1.52
1	J	185	CYS	N-CA	-5.28	1.40	1.46
1	J	236	ASN	C-N	5.26	1.40	1.33

All (406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1220	PRO	N-CA-C	11.81	125.11	110.70
1	G	1219	PRO	N-CA-C	11.71	124.98	110.70
3	I	42	GLN	CA-C-N	10.80	127.44	119.66
3	I	42	GLN	C-N-CA	10.80	127.44	119.66
3	C	42	GLN	CA-C-N	10.80	127.54	119.66
3	C	42	GLN	C-N-CA	10.80	127.54	119.66
1	A	935	LEU	CA-C-N	9.96	126.83	119.66
1	A	935	LEU	C-N-CA	9.96	126.83	119.66
1	J	688	GLN	N-CA-C	9.84	122.00	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	144	TYR	CA-C-N	9.73	129.67	119.85
1	J	144	TYR	C-N-CA	9.73	129.67	119.85
3	C	58	VAL	CA-C-N	9.67	130.27	119.92
3	C	58	VAL	C-N-CA	9.67	130.27	119.92
1	F	284	LEU	CA-C-N	9.65	129.31	119.56
1	F	284	LEU	C-N-CA	9.65	129.31	119.56
1	J	284	LEU	CA-C-N	9.40	129.65	119.87
1	J	284	LEU	C-N-CA	9.40	129.65	119.87
1	E	144	TYR	CA-C-N	9.39	129.33	119.85
1	E	144	TYR	C-N-CA	9.39	129.33	119.85
1	D	935	LEU	CA-C-N	9.32	126.37	119.66
1	D	935	LEU	C-N-CA	9.32	126.37	119.66
1	F	144	TYR	CA-C-N	9.26	129.21	119.85
1	F	144	TYR	C-N-CA	9.26	129.21	119.85
1	F	741	THR	CA-C-N	9.12	129.18	119.78
1	F	741	THR	C-N-CA	9.12	129.18	119.78
1	J	530	VAL	CA-C-N	9.09	129.02	120.03
1	J	530	VAL	C-N-CA	9.09	129.02	120.03
1	E	462	GLY	CA-C-N	9.01	128.75	119.56
1	E	462	GLY	C-N-CA	9.01	128.75	119.56
3	I	58	VAL	CA-C-N	8.94	128.88	120.03
3	I	58	VAL	C-N-CA	8.94	128.88	120.03
3	I	58	VAL	N-CA-C	8.89	119.12	108.45
1	G	902	ASP	CA-C-N	8.77	128.71	120.03
1	G	902	ASP	C-N-CA	8.77	128.71	120.03
1	F	373	SER	N-CA-C	8.72	122.79	110.50
1	F	393	PRO	CA-C-N	8.60	128.55	120.03
1	F	393	PRO	C-N-CA	8.60	128.55	120.03
1	J	484	VAL	CA-C-N	8.60	128.63	119.78
1	J	484	VAL	C-N-CA	8.60	128.63	119.78
1	G	1218	LEU	CA-C-N	8.58	129.22	120.38
1	G	1218	LEU	C-N-CA	8.58	129.22	120.38
1	G	1156	CYS	N-CA-C	8.57	123.55	112.41
1	J	209	THR	CA-C-N	8.51	128.24	119.56
1	J	209	THR	C-N-CA	8.51	128.24	119.56
1	J	393	PRO	CA-C-N	8.47	128.42	120.03
1	J	393	PRO	C-N-CA	8.47	128.42	120.03
1	J	741	THR	CA-C-N	8.40	128.43	119.78
1	J	741	THR	C-N-CA	8.40	128.43	119.78
1	G	935	LEU	CA-C-N	8.40	125.71	119.66
1	G	935	LEU	C-N-CA	8.40	125.71	119.66
1	J	705	GLY	CA-C-N	8.39	128.33	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	705	GLY	C-N-CA	8.39	128.33	119.85
1	D	902	ASP	CA-C-N	8.32	128.35	119.78
1	D	902	ASP	C-N-CA	8.32	128.35	119.78
1	F	133	SER	CA-C-N	8.28	128.01	119.56
1	F	133	SER	C-N-CA	8.28	128.01	119.56
1	J	22	GLY	CA-C-N	8.22	128.25	119.78
1	J	22	GLY	C-N-CA	8.22	128.25	119.78
1	E	284	LEU	CA-C-N	8.20	127.92	119.56
1	E	284	LEU	C-N-CA	8.20	127.92	119.56
1	J	96	THR	CA-C-N	8.20	128.22	119.78
1	J	96	THR	C-N-CA	8.20	128.22	119.78
1	G	766	HIS	CA-C-N	8.11	128.04	119.85
1	G	766	HIS	C-N-CA	8.11	128.04	119.85
1	F	462	GLY	CA-C-N	8.02	127.74	119.56
1	F	462	GLY	C-N-CA	8.02	127.74	119.56
1	E	393	PRO	CA-C-N	7.94	127.86	119.85
1	E	393	PRO	C-N-CA	7.94	127.86	119.85
1	J	462	GLY	CA-C-N	7.93	127.65	119.56
1	J	462	GLY	C-N-CA	7.93	127.65	119.56
1	E	530	VAL	CA-C-N	7.89	128.36	119.92
1	E	530	VAL	C-N-CA	7.89	128.36	119.92
1	J	399	PHE	N-CA-C	7.89	121.36	110.24
1	F	493	LYS	CA-C-N	7.81	127.74	119.85
1	F	493	LYS	C-N-CA	7.81	127.74	119.85
2	B	8	GLY	CA-C-N	7.80	127.82	119.78
2	B	8	GLY	C-N-CA	7.80	127.82	119.78
1	J	493	LYS	CA-C-N	7.80	127.73	119.85
1	J	493	LYS	C-N-CA	7.80	127.73	119.85
2	H	8	GLY	CA-C-N	7.79	127.80	119.78
2	H	8	GLY	C-N-CA	7.79	127.80	119.78
1	J	236	ASN	CA-C-N	-7.79	110.05	120.95
1	J	236	ASN	C-N-CA	-7.79	110.05	120.95
1	F	378	ALA	CA-C-N	7.77	135.68	121.70
1	F	378	ALA	C-N-CA	7.77	135.68	121.70
1	G	1219	PRO	CA-C-N	7.76	128.38	120.38
1	G	1219	PRO	C-N-CA	7.76	128.38	120.38
1	F	96	THR	CA-C-N	7.75	127.68	119.85
1	F	96	THR	C-N-CA	7.75	127.68	119.85
1	J	133	SER	CA-C-N	7.75	127.47	119.56
1	J	133	SER	C-N-CA	7.75	127.47	119.56
1	J	738	LEU	CA-C-N	7.75	127.70	120.03
1	J	738	LEU	C-N-CA	7.75	127.70	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	96	THR	CA-C-N	7.75	127.67	119.85
1	E	96	THR	C-N-CA	7.75	127.67	119.85
1	F	530	VAL	CA-C-N	7.74	127.75	119.78
1	F	530	VAL	C-N-CA	7.74	127.75	119.78
1	F	209	THR	CA-C-N	7.73	127.45	119.56
1	F	209	THR	C-N-CA	7.73	127.45	119.56
1	D	753	VAL	CA-C-N	7.59	127.60	119.78
1	D	753	VAL	C-N-CA	7.59	127.60	119.78
1	J	649	TYR	CA-C-N	-7.55	109.48	121.87
1	J	649	TYR	C-N-CA	-7.55	109.48	121.87
1	A	1219	PRO	CA-C-N	7.55	128.15	120.38
1	A	1219	PRO	C-N-CA	7.55	128.15	120.38
1	J	392	THR	CA-C-N	7.54	125.17	119.66
1	J	392	THR	C-N-CA	7.54	125.17	119.66
1	A	939	MET	N-CA-C	7.49	120.51	111.82
1	E	369	LYS	CA-C-N	7.48	127.40	119.85
1	E	369	LYS	C-N-CA	7.48	127.40	119.85
1	D	766	HIS	CA-C-N	7.44	127.44	119.78
1	D	766	HIS	C-N-CA	7.44	127.44	119.78
1	E	484	VAL	N-CA-C	7.44	115.03	108.63
1	D	1219	PRO	CA-C-N	7.42	128.02	120.38
1	D	1219	PRO	C-N-CA	7.42	128.02	120.38
1	E	26	VAL	N-CA-C	7.39	117.99	110.82
1	E	493	LYS	CA-C-N	7.35	127.27	119.85
1	E	493	LYS	C-N-CA	7.35	127.27	119.85
1	E	741	THR	CA-C-N	7.35	127.35	119.78
1	E	741	THR	C-N-CA	7.35	127.35	119.78
1	J	373	SER	N-CA-C	7.34	120.86	110.50
1	E	738	LEU	CA-C-N	7.29	127.22	119.85
1	E	738	LEU	C-N-CA	7.29	127.22	119.85
1	A	766	HIS	CA-C-N	7.19	127.12	119.85
1	A	766	HIS	C-N-CA	7.19	127.12	119.85
1	A	1142	TYR	CA-C-N	7.19	127.19	119.78
1	A	1142	TYR	C-N-CA	7.19	127.19	119.78
1	E	717	LEU	N-CA-C	7.17	120.13	111.82
1	E	188	GLU	CA-C-N	7.16	127.16	119.78
1	E	188	GLU	C-N-CA	7.16	127.16	119.78
1	F	392	THR	CA-C-N	7.15	124.81	119.66
1	F	392	THR	C-N-CA	7.15	124.81	119.66
1	D	1160	ASN	CA-C-N	7.12	128.74	119.84
1	D	1160	ASN	C-N-CA	7.12	128.74	119.84
1	A	902	ASP	CA-C-N	7.11	127.10	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	902	ASP	C-N-CA	7.11	127.10	119.78
1	J	657	VAL	CA-C-N	7.10	127.09	119.78
1	J	657	VAL	C-N-CA	7.10	127.09	119.78
1	G	1160	ASN	CA-C-N	7.08	128.69	119.84
1	G	1160	ASN	C-N-CA	7.08	128.69	119.84
1	J	438	TYR	N-CA-C	6.95	119.74	109.24
1	D	1142	TYR	CA-C-N	6.95	126.94	119.78
1	D	1142	TYR	C-N-CA	6.95	126.94	119.78
1	G	1193	ALA	CA-C-N	6.93	126.92	119.78
1	G	1193	ALA	C-N-CA	6.93	126.92	119.78
1	G	1058	LEU	N-CA-C	6.90	120.76	109.72
1	F	406	ASN	CA-C-N	-6.88	110.59	121.87
1	F	406	ASN	C-N-CA	-6.88	110.59	121.87
1	G	912	CYS	CA-C-N	6.84	133.42	120.97
1	G	912	CYS	C-N-CA	6.84	133.42	120.97
1	G	1142	TYR	CA-C-N	6.82	126.74	119.85
1	G	1142	TYR	C-N-CA	6.82	126.74	119.85
1	E	209	THR	CA-C-N	6.80	128.34	119.84
1	E	209	THR	C-N-CA	6.80	128.34	119.84
1	E	688	GLN	N-CA-C	6.77	119.97	111.24
1	J	406	ASN	CA-C-N	-6.70	110.88	121.87
1	J	406	ASN	C-N-CA	-6.70	110.88	121.87
3	I	92	LYS	N-CA-C	6.67	118.55	111.28
1	D	1156	CYS	O-C-N	-6.67	114.56	122.96
1	E	546	SER	CA-C-N	6.63	126.58	119.28
1	E	546	SER	C-N-CA	6.63	126.58	119.28
1	E	600	LEU	N-CA-C	6.61	121.19	111.87
1	E	688	GLN	CA-C-N	6.61	133.59	121.70
1	E	688	GLN	C-N-CA	6.61	133.59	121.70
3	C	43	PRO	CA-C-N	6.60	126.52	119.85
3	C	43	PRO	C-N-CA	6.60	126.52	119.85
1	A	1220	PRO	N-CA-C	6.59	118.74	110.70
1	G	1115	GLY	CA-C-N	6.59	130.70	120.75
1	G	1115	GLY	C-N-CA	6.59	130.70	120.75
1	F	188	GLU	CA-C-N	6.57	126.55	119.78
1	F	188	GLU	C-N-CA	6.57	126.55	119.78
1	F	600	LEU	N-CA-C	6.55	120.45	111.54
1	F	236	ASN	CA-C-N	-6.54	112.97	122.19
1	F	236	ASN	C-N-CA	-6.54	112.97	122.19
1	G	912	CYS	N-CA-C	-6.54	104.95	113.12
1	D	782	ILE	CA-C-N	6.53	126.45	119.85
1	D	782	ILE	C-N-CA	6.53	126.45	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	369	LYS	CA-C-N	6.52	126.49	119.78
1	J	369	LYS	C-N-CA	6.52	126.49	119.78
1	A	859	SER	CA-C-N	6.49	126.47	119.78
1	A	859	SER	C-N-CA	6.49	126.47	119.78
1	G	753	VAL	CA-C-N	6.47	126.45	119.78
1	G	753	VAL	C-N-CA	6.47	126.45	119.78
1	F	399	PHE	N-CA-C	6.47	119.36	110.24
1	F	484	VAL	CA-C-N	6.45	126.42	119.78
1	F	484	VAL	C-N-CA	6.45	126.42	119.78
1	J	188	GLU	CA-C-N	6.45	126.42	119.78
1	J	188	GLU	C-N-CA	6.45	126.42	119.78
1	F	514	VAL	CA-C-N	6.44	126.42	119.78
1	F	514	VAL	C-N-CA	6.44	126.42	119.78
1	J	688	GLN	CA-C-N	6.44	133.29	121.70
1	J	688	GLN	C-N-CA	6.44	133.29	121.70
3	I	43	PRO	CA-C-N	6.43	126.40	119.78
3	I	43	PRO	C-N-CA	6.43	126.40	119.78
1	F	705	GLY	CA-C-N	6.41	126.39	119.78
1	F	705	GLY	C-N-CA	6.41	126.39	119.78
1	D	936	PRO	CA-C-N	6.40	126.31	119.85
1	D	936	PRO	C-N-CA	6.40	126.31	119.85
1	J	368	ALA	N-CA-C	6.40	120.39	112.58
1	F	409	TYR	N-CA-C	6.38	118.88	109.24
1	A	1044	PHE	CA-CB-CG	-6.32	107.48	113.80
1	A	938	LEU	N-CA-C	6.30	118.22	111.36
1	A	1160	ASN	CA-C-N	6.29	125.98	119.56
1	A	1160	ASN	C-N-CA	6.29	125.98	119.56
1	D	1193	ALA	CA-C-N	6.28	126.24	119.78
1	D	1193	ALA	C-N-CA	6.28	126.24	119.78
1	E	484	VAL	CA-C-N	6.27	126.24	119.78
1	E	484	VAL	C-N-CA	6.27	126.24	119.78
1	J	185	CYS	O-C-N	-6.25	116.69	123.26
1	D	1220	PRO	N-CA-C	6.23	118.31	110.70
1	E	195	CYS	CA-C-N	6.22	125.96	119.05
1	E	195	CYS	C-N-CA	6.22	125.96	119.05
1	F	22	GLY	CA-C-N	6.22	126.19	119.78
1	F	22	GLY	C-N-CA	6.22	126.19	119.78
1	J	172	LEU	CA-C-N	6.22	126.14	119.85
1	J	172	LEU	C-N-CA	6.22	126.14	119.85
1	F	341	PHE	N-CA-C	6.22	118.06	111.28
1	A	1060	PRO	N-CA-C	6.20	118.26	110.70
1	J	167	HIS	CA-CB-CG	6.19	119.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	850	PHE	CA-CB-CG	-6.14	107.66	113.80
1	A	1206	ALA	CA-C-N	6.12	126.08	119.78
1	A	1206	ALA	C-N-CA	6.12	126.08	119.78
1	D	970	ILE	CA-C-N	6.11	126.08	119.78
1	D	970	ILE	C-N-CA	6.11	126.08	119.78
1	J	269	ARG	N-CA-C	6.08	117.91	111.28
1	J	296	ILE	CA-C-N	6.06	125.97	119.85
1	J	296	ILE	C-N-CA	6.06	125.97	119.85
1	E	46	ARG	CA-C-N	6.06	126.02	119.78
1	E	46	ARG	C-N-CA	6.06	126.02	119.78
1	F	296	ILE	CA-C-N	6.06	125.97	119.85
1	F	296	ILE	C-N-CA	6.06	125.97	119.85
1	F	709	THR	CA-C-N	6.06	125.74	119.56
1	F	709	THR	C-N-CA	6.06	125.74	119.56
3	C	87	PHE	N-CA-C	6.01	118.19	108.34
1	J	695	SER	N-CA-C	6.01	118.62	111.71
1	J	585	CYS	CA-C-N	6.00	125.96	119.78
1	J	585	CYS	C-N-CA	6.00	125.96	119.78
1	G	782	ILE	CA-C-N	6.00	125.91	119.85
1	G	782	ILE	C-N-CA	6.00	125.91	119.85
1	F	28	SER	CA-C-N	6.00	129.81	120.75
1	F	28	SER	C-N-CA	6.00	129.81	120.75
1	F	37	GLN	N-CA-C	6.00	119.43	111.75
1	E	437	CYS	O-C-N	-5.99	115.94	123.01
1	D	1206	ALA	CA-C-N	5.99	125.95	119.78
1	D	1206	ALA	C-N-CA	5.99	125.95	119.78
1	J	727	CYS	N-CA-C	5.98	119.83	112.54
1	E	623	VAL	CA-C-N	-5.97	114.78	121.83
1	E	623	VAL	C-N-CA	-5.97	114.78	121.83
1	E	58	TYR	CA-C-N	5.97	125.93	119.78
1	E	58	TYR	C-N-CA	5.97	125.93	119.78
1	A	912	CYS	CA-C-N	5.97	130.96	120.87
1	A	912	CYS	C-N-CA	5.97	130.96	120.87
1	J	185	CYS	N-CA-C	5.97	117.31	108.60
1	E	271	VAL	N-CA-C	5.97	116.69	111.56
1	D	1115	GLY	CA-C-N	5.91	129.67	120.75
1	D	1115	GLY	C-N-CA	5.91	129.67	120.75
1	G	936	PRO	CA-C-N	5.89	125.85	119.78
1	G	936	PRO	C-N-CA	5.89	125.85	119.78
1	J	409	TYR	N-CA-C	5.89	118.14	109.24
1	E	705	GLY	CA-C-N	5.88	125.84	119.78
1	E	705	GLY	C-N-CA	5.88	125.84	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1060	PRO	N-CA-C	5.87	117.86	110.70
1	F	271	VAL	N-CA-C	5.86	117.04	112.12
1	G	1195	GLU	CA-C-N	5.84	125.80	119.78
1	G	1195	GLU	C-N-CA	5.84	125.80	119.78
1	J	736	CYS	N-CA-C	-5.84	100.19	109.07
1	J	271	VAL	N-CA-C	5.84	116.58	111.56
1	F	600	LEU	CA-C-N	5.83	132.20	121.70
1	F	600	LEU	C-N-CA	5.83	132.20	121.70
1	J	546	SER	CA-C-N	5.83	125.69	119.28
1	J	546	SER	C-N-CA	5.83	125.69	119.28
2	H	29	PHE	N-CA-C	5.83	117.63	111.28
1	E	296	ILE	CA-C-N	5.82	125.73	119.85
1	E	296	ILE	C-N-CA	5.82	125.73	119.85
1	F	46	ARG	CA-C-N	5.82	125.78	119.78
1	F	46	ARG	C-N-CA	5.82	125.78	119.78
1	E	725	GLU	N-CA-C	5.81	117.61	111.28
1	F	78	GLN	N-CA-C	5.81	117.61	111.28
1	F	657	VAL	CA-C-N	5.79	125.74	119.78
1	F	657	VAL	C-N-CA	5.79	125.74	119.78
1	E	133	SER	CA-C-N	5.78	127.06	119.84
1	E	133	SER	C-N-CA	5.78	127.06	119.84
1	F	58	TYR	CA-C-N	5.78	125.73	119.78
1	F	58	TYR	C-N-CA	5.78	125.73	119.78
1	J	717	LEU	N-CA-C	5.77	120.32	113.16
1	A	753	VAL	CA-C-N	5.77	125.72	119.78
1	A	753	VAL	C-N-CA	5.77	125.72	119.78
1	G	1044	PHE	CA-CB-CG	-5.77	108.03	113.80
1	E	657	VAL	CA-C-N	5.72	125.68	119.78
1	E	657	VAL	C-N-CA	5.72	125.68	119.78
1	J	735	LEU	CA-C-N	-5.71	111.87	121.75
1	J	735	LEU	C-N-CA	-5.71	111.87	121.75
3	I	98	PHE	CA-CB-CG	5.71	119.51	113.80
1	F	195	CYS	CA-C-N	5.69	125.37	119.05
1	F	195	CYS	C-N-CA	5.69	125.37	119.05
1	F	546	SER	CA-C-N	5.69	125.54	119.28
1	F	546	SER	C-N-CA	5.69	125.54	119.28
1	A	1156	CYS	CA-C-O	5.68	127.47	121.33
1	D	924	ILE	CA-C-N	-5.66	113.26	122.26
1	D	924	ILE	C-N-CA	-5.66	113.26	122.26
2	B	71	VAL	N-CA-C	5.65	116.25	108.12
1	D	1060	PRO	N-CA-C	5.63	117.57	110.70
1	F	172	LEU	CA-C-N	5.63	125.53	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	172	LEU	C-N-CA	5.63	125.53	119.85
1	J	651	LEU	N-CA-C	5.63	118.65	109.59
1	F	606	TYR	N-CA-C	5.62	117.61	109.07
1	E	22	GLY	CA-C-N	5.61	125.56	119.78
1	E	22	GLY	C-N-CA	5.61	125.56	119.78
3	C	92	LYS	N-CA-C	5.60	117.39	111.28
1	G	1156	CYS	CB-CA-C	-5.60	101.95	111.02
1	D	1113	ARG	N-CA-C	5.59	117.38	111.28
1	E	78	GLN	N-CA-C	5.58	117.36	111.28
1	A	807	LYS	N-CA-C	-5.57	105.52	112.93
1	E	396	VAL	N-CA-C	5.57	118.85	111.17
3	I	58	VAL	CB-CA-C	-5.56	103.08	110.97
1	J	223	ALA	N-CA-C	5.56	117.02	111.07
1	F	677	VAL	N-CA-C	5.55	117.98	111.05
1	J	378	ALA	CA-C-N	5.52	131.64	121.70
1	J	378	ALA	C-N-CA	5.52	131.64	121.70
1	J	429	SER	CA-C-N	5.52	125.35	119.28
1	J	429	SER	C-N-CA	5.52	125.35	119.28
2	B	91	TYR	N-CA-C	5.51	117.37	108.34
1	D	929	VAL	N-CA-C	-5.48	106.47	111.67
1	J	399	PHE	CB-CA-C	-5.47	100.89	109.70
1	G	938	LEU	N-CA-C	5.45	117.98	111.71
1	G	859	SER	CA-C-N	5.45	125.39	119.78
1	G	859	SER	C-N-CA	5.45	125.39	119.78
1	J	653	ALA	CA-C-N	-5.43	113.67	122.36
1	J	653	ALA	C-N-CA	-5.43	113.67	122.36
3	I	63	ILE	N-CA-C	5.42	115.12	106.88
1	F	604	VAL	N-CA-C	5.42	117.43	109.63
1	A	1217	ASN	N-CA-C	5.41	117.12	108.41
1	A	1123	ILE	N-CA-C	-5.39	102.25	108.82
1	E	649	TYR	CA-C-N	-5.38	113.50	122.64
1	E	649	TYR	C-N-CA	-5.38	113.50	122.64
1	J	195	CYS	CA-C-N	5.37	125.44	119.32
1	J	195	CYS	C-N-CA	5.37	125.44	119.32
1	J	584	VAL	CB-CA-C	-5.36	104.47	110.96
1	E	406	ASN	CA-C-N	-5.35	113.09	121.87
1	E	406	ASN	C-N-CA	-5.35	113.09	121.87
1	A	1115	GLY	CA-C-N	5.35	128.83	120.75
1	A	1115	GLY	C-N-CA	5.35	128.83	120.75
1	A	1124	VAL	N-CA-C	5.35	117.16	109.51
1	F	167	HIS	CA-CB-CG	5.33	119.14	113.80
1	A	929	VAL	N-CA-C	-5.33	106.60	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1156	CYS	O-C-N	-5.31	117.20	123.25
1	F	429	SER	CA-C-N	5.31	125.12	119.28
1	F	429	SER	C-N-CA	5.31	125.12	119.28
1	A	798	THR	N-CA-C	5.30	117.25	109.24
1	E	323	PHE	N-CA-C	5.30	117.45	109.23
1	D	869	PHE	CA-CB-CG	-5.30	108.50	113.80
1	F	302	SER	CA-C-N	5.30	127.60	120.50
1	F	302	SER	C-N-CA	5.30	127.60	120.50
1	A	870	ASN	N-CA-C	5.28	117.11	111.36
2	H	71	VAL	N-CA-C	5.28	115.72	108.12
1	A	912	CYS	N-CA-C	-5.28	105.66	112.68
1	J	58	TYR	CA-C-N	5.25	125.19	119.78
1	J	58	TYR	C-N-CA	5.25	125.19	119.78
1	J	173	PRO	CA-C-N	-5.25	115.37	122.77
1	J	173	PRO	C-N-CA	-5.25	115.37	122.77
1	E	392	THR	CA-C-N	5.24	123.43	119.66
1	E	392	THR	C-N-CA	5.24	123.43	119.66
1	E	369	LYS	N-CA-C	5.23	114.32	108.25
1	J	46	ARG	CA-C-N	5.23	125.16	119.78
1	J	46	ARG	C-N-CA	5.23	125.16	119.78
1	G	1206	ALA	CA-C-N	5.22	125.16	119.78
1	G	1206	ALA	C-N-CA	5.22	125.16	119.78
1	F	399	PHE	CB-CA-C	-5.22	101.30	109.70
1	D	798	THR	N-CA-C	5.21	117.11	109.24
1	E	271	VAL	CB-CA-C	-5.21	106.49	111.44
2	H	91	TYR	N-CA-C	5.19	116.86	108.34
1	D	853	VAL	N-CA-C	5.19	115.96	110.72
1	F	727	CYS	N-CA-C	5.17	117.81	111.82
1	F	533	THR	CA-C-N	-5.16	115.92	122.37
1	F	533	THR	C-N-CA	-5.16	115.92	122.37
1	D	815	GLN	N-CA-C	5.16	117.64	111.71
1	D	968	ALA	N-CA-C	5.16	117.64	111.71
1	F	390	SER	N-CA-C	5.15	116.90	109.07
1	G	807	LYS	N-CA-C	-5.13	107.08	113.55
1	E	269	ARG	N-CA-C	5.13	116.87	111.28
1	J	514	VAL	CA-C-N	5.12	125.05	119.78
1	J	514	VAL	C-N-CA	5.12	125.05	119.78
1	G	1220	PRO	CB-CA-C	-5.11	104.68	110.92
1	F	19	VAL	N-CA-C	5.11	116.17	109.58
2	B	31	ASP	N-CA-C	5.10	119.14	113.02
1	F	365	SER	N-CA-C	5.10	117.69	110.50
1	G	966	SER	N-CA-C	5.10	116.82	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	641	TYR	N-CA-C	5.10	116.82	109.07
1	F	369	LYS	CB-CA-C	-5.10	107.58	111.20
1	E	672	THR	N-CA-C	5.09	116.93	109.24
1	A	782	ILE	CA-C-N	5.09	124.99	119.85
1	A	782	ILE	C-N-CA	5.09	124.99	119.85
1	J	78	GLN	N-CA-C	5.09	116.83	111.28
1	E	223	ALA	N-CA-C	5.08	116.51	111.07
1	A	1216	THR	N-CA-C	5.08	116.22	108.30
1	A	786	PHE	CA-CB-CG	-5.08	108.72	113.80
1	D	1219	PRO	N-CA-C	5.06	116.88	110.70
1	F	688	GLN	CA-C-N	5.06	130.81	121.70
1	F	688	GLN	C-N-CA	5.06	130.81	121.70
3	C	63	ILE	N-CA-C	5.05	115.04	107.51
1	F	524	SER	CA-C-N	5.03	124.82	119.28
1	F	524	SER	C-N-CA	5.03	124.82	119.28
1	F	469	TYR	N-CA-C	5.03	117.35	108.75
1	F	738	LEU	CA-C-N	5.02	124.95	119.78
1	F	738	LEU	C-N-CA	5.02	124.95	119.78
1	D	958	VAL	N-CA-C	-5.00	107.26	111.56

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	14	0
1	D	3496	0	3420	23	0
1	E	5658	0	5423	89	0
1	F	5658	0	5423	54	0
1	G	3545	0	3471	16	0
1	J	5658	0	5425	33	0
2	B	948	0	904	2	0
2	H	948	0	904	2	0
3	C	835	0	816	4	0
3	I	835	0	816	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31126	0	30072	238	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (238) 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:F:506:PHE:HE2	1:F:555:VAL:CG2	0.99	1.62
1:J:506:PHE:CE2	1:J:555:VAL:HG21	1.13	1.60
1:E:506:PHE:CE2	1:E:555:VAL:CG2	1.76	1.58
1:J:506:PHE:CE2	1:J:555:VAL:CG2	1.94	1.51
1:F:506:PHE:CE2	1:F:555:VAL:CG2	1.74	1.43
1:E:371:SER:CB	1:E:604:VAL:HG12	1.48	1.40
1:E:506:PHE:CD2	1:E:555:VAL:HG21	1.55	1.39
1:F:506:PHE:CE2	1:F:555:VAL:HG21	0.86	1.37
1:E:506:PHE:CE2	1:E:555:VAL:HG21	0.83	1.36
1:E:506:PHE:CD2	1:E:555:VAL:CG2	2.10	1.34
1:E:371:SER:CB	1:E:604:VAL:CG1	2.05	1.30
1:D:905:TYR:OH	1:D:936:PRO:N	1.70	1.24
1:E:371:SER:HB3	1:E:604:VAL:CG1	1.66	1.20
1:E:371:SER:C	1:E:604:VAL:HG12	1.64	1.20
1:G:905:TYR:OH	1:G:934:VAL:O	1.60	1.18
1:E:506:PHE:HE2	1:E:555:VAL:CG2	1.26	1.18
1:E:384:ASP:O	1:E:404:PHE:CZ	1.98	1.16
1:E:372:GLY:O	1:E:604:VAL:HB	1.44	1.15
1:E:371:SER:CA	1:E:604:VAL:HG12	1.77	1.14
1:E:384:ASP:O	1:E:404:PHE:HZ	1.27	1.14
1:F:506:PHE:CE1	1:F:513:GLU:OE2	2.01	1.13
1:F:506:PHE:CD2	1:F:555:VAL:CG2	2.31	1.12
1:E:371:SER:OG	1:E:604:VAL:CG1	1.96	1.12
1:F:506:PHE:CD2	1:F:555:VAL:HG21	1.85	1.09
1:J:506:PHE:HE2	1:J:555:VAL:CG2	1.41	1.08
1:J:506:PHE:CD2	1:J:555:VAL:HG21	1.89	1.05
1:E:371:SER:HB3	1:E:604:VAL:HG13	1.39	1.03
1:D:905:TYR:OH	1:D:936:PRO:CA	2.07	1.02
1:J:506:PHE:CD2	1:J:555:VAL:CG2	2.41	1.02
1:E:372:GLY:O	1:E:604:VAL:CB	2.07	1.02
1:F:506:PHE:CD2	1:F:555:VAL:HG23	1.99	0.96
1:E:506:PHE:CD2	1:E:555:VAL:HG23	1.99	0.94
1:E:371:SER:CB	1:E:604:VAL:HG13	1.92	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:CYS:HG	1:E:407:CYS:HG	1.09	0.93
1:J:506:PHE:HE2	1:J:555:VAL:HG22	1.36	0.89
1:F:506:PHE:CE2	1:F:555:VAL:HG23	2.05	0.87
1:E:371:SER:C	1:E:604:VAL:CG1	2.47	0.86
1:F:506:PHE:CZ	1:F:513:GLU:OE2	2.28	0.85
1:F:621:THR:HG22	1:F:622:ALA:H	1.42	0.83
1:E:602:ASN:HB3	1:E:604:VAL:HG13	1.64	0.80
1:E:506:PHE:HE2	1:E:555:VAL:HG22	1.41	0.80
1:F:506:PHE:HE2	1:F:555:VAL:CB	1.94	0.78
1:E:301:ARG:O	1:E:301:ARG:HG2	1.81	0.78
1:E:506:PHE:CE2	1:E:555:VAL:HG22	2.13	0.77
1:D:905:TYR:OH	1:D:936:PRO:CD	2.32	0.77
1:E:600:LEU:N	1:E:601:GLY:HA2	1.99	0.76
1:F:506:PHE:CE2	1:F:555:VAL:CB	2.69	0.74
1:E:372:GLY:C	1:E:604:VAL:HB	2.13	0.73
1:J:506:PHE:CD2	1:J:555:VAL:HG23	2.23	0.73
1:D:905:TYR:OH	1:D:935:LEU:C	2.32	0.73
1:E:381:VAL:H	1:E:408:ASN:HD22	1.37	0.73
1:F:383:CYS:HB2	1:F:385:PHE:CE2	2.24	0.72
1:E:372:GLY:N	1:E:604:VAL:HG12	2.05	0.71
1:E:384:ASP:O	1:E:404:PHE:CE1	2.42	0.71
1:F:506:PHE:CD1	1:F:513:GLU:OE2	2.44	0.70
1:J:240:MET:O	1:J:240:MET:SD	2.50	0.70
1:E:371:SER:OG	1:E:604:VAL:HG13	1.85	0.70
1:D:905:TYR:HH	1:D:936:PRO:N	1.91	0.69
1:F:369:LYS:O	1:F:369:LYS:HG2	1.94	0.68
1:E:506:PHE:HD2	1:E:555:VAL:HG23	1.50	0.67
1:D:905:TYR:CZ	1:D:936:PRO:HB3	2.28	0.67
1:E:506:PHE:HD2	1:E:555:VAL:CG2	1.93	0.67
1:F:506:PHE:HD2	1:F:555:VAL:HG23	1.54	0.66
1:E:371:SER:OG	1:E:604:VAL:HG12	1.73	0.66
1:E:381:VAL:HG12	1:E:407:CYS:HB2	1.78	0.66
1:J:426:SER:O	1:J:427:GLN:HB2	1.96	0.66
1:E:621:THR:O	1:E:648:TYR:HD2	1.80	0.65
1:J:691:ARG:HA	1:J:691:ARG:NE	2.10	0.65
1:E:616:VAL:HG13	1:E:616:VAL:O	1.95	0.64
1:E:422:ASP:HB3	1:E:481:LEU:HB2	1.79	0.64
1:E:371:SER:HB3	1:E:604:VAL:HG12	1.41	0.63
1:J:172:LEU:HD12	1:J:172:LEU:O	1.98	0.63
1:J:240:MET:SD	1:J:240:MET:C	2.82	0.63
1:E:372:GLY:N	1:E:604:VAL:CG1	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:372:GLY:O	1:E:604:VAL:CG2	2.47	0.62
1:D:905:TYR:OH	1:D:936:PRO:HA	1.99	0.60
1:E:384:ASP:CB	1:E:404:PHE:HE1	2.14	0.60
1:E:621:THR:HG22	1:E:622:ALA:N	2.16	0.60
1:D:905:TYR:HH	1:D:935:LEU:C	2.09	0.59
1:J:506:PHE:CZ	1:J:555:VAL:HG21	2.13	0.59
1:E:600:LEU:N	1:E:601:GLY:CA	2.66	0.58
1:F:621:THR:O	1:F:648:TYR:HD2	1.86	0.58
1:J:691:ARG:HA	1:J:691:ARG:HE	1.67	0.58
1:E:383:CYS:SG	1:E:409:TYR:HB3	2.45	0.57
1:G:875:GLU:OE1	1:G:875:GLU:N	2.35	0.56
1:F:621:THR:O	1:F:648:TYR:HB3	2.06	0.56
1:D:826:GLN:OE1	1:D:826:GLN:N	2.27	0.56
1:D:905:TYR:CE2	1:D:936:PRO:HB3	2.41	0.56
1:J:425:CYS:SG	1:J:430:PRO:HA	2.46	0.56
1:G:875:GLU:O	1:G:875:GLU:HG2	2.05	0.55
1:A:1001:PHE:CD1	1:A:1001:PHE:C	2.83	0.55
1:E:372:GLY:O	1:E:604:VAL:CG1	2.55	0.55
1:E:256:ILE:HG23	1:E:256:ILE:O	2.07	0.54
1:E:383:CYS:O	1:E:385:PHE:N	2.40	0.54
1:J:67:ILE:HG13	1:J:67:ILE:O	2.08	0.54
1:E:67:ILE:O	1:E:67:ILE:HG13	2.08	0.54
2:B:85:GLU:OE1	2:B:85:GLU:N	2.35	0.54
1:G:1160:ASN:C	1:G:1160:ASN:OD1	2.51	0.54
1:E:602:ASN:O	1:E:615:GLY:O	2.26	0.53
1:E:383:CYS:HB3	1:E:385:PHE:CD2	2.43	0.53
1:F:621:THR:HG22	1:F:622:ALA:N	2.19	0.53
1:E:384:ASP:CA	1:E:404:PHE:HE1	2.22	0.53
1:G:823:GLU:OE1	1:G:823:GLU:N	2.37	0.53
1:E:381:VAL:N	1:E:408:ASN:HD22	2.07	0.52
2:B:72:ASP:C	2:B:72:ASP:OD1	2.51	0.52
1:F:606:TYR:CD1	1:F:606:TYR:C	2.88	0.51
1:A:826:GLN:OE1	1:A:826:GLN:N	2.27	0.51
1:D:905:TYR:CZ	1:D:936:PRO:CB	2.92	0.51
1:E:251:LEU:C	1:E:251:LEU:HD23	2.36	0.51
1:D:905:TYR:OH	1:D:936:PRO:CB	2.57	0.50
1:E:689:TYR:CD1	1:E:689:TYR:C	2.89	0.50
1:F:172:LEU:N	1:F:172:LEU:HD23	2.26	0.50
1:G:826:GLN:OE1	1:G:826:GLN:N	2.27	0.50
1:F:596:ILE:HD12	1:F:596:ILE:C	2.36	0.50
1:A:934:VAL:O	1:A:934:VAL:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:GLU:O	1:E:407:CYS:HB2	2.11	0.50
1:J:395:GLN:HA	1:J:395:GLN:OE1	2.12	0.50
1:E:422:ASP:CB	1:E:481:LEU:HB2	2.41	0.50
1:E:130:VAL:HG12	1:E:130:VAL:O	2.12	0.50
1:F:689:TYR:C	1:F:689:TYR:CD1	2.91	0.49
1:E:506:PHE:CE2	1:E:555:VAL:CB	2.83	0.49
1:A:815:GLN:OE1	1:A:815:GLN:N	2.33	0.48
1:F:381:VAL:O	1:F:407:CYS:HB2	2.13	0.48
1:F:381:VAL:O	1:F:407:CYS:HA	2.12	0.48
1:F:172:LEU:HD23	1:F:172:LEU:H	1.79	0.48
1:F:664:ASP:OD1	1:F:664:ASP:C	2.56	0.48
1:G:1120:GLY:O	1:G:1121:THR:OG1	2.26	0.47
1:J:719:ASN:C	1:J:719:ASN:OD1	2.57	0.47
1:E:719:ASN:C	1:E:719:ASN:OD1	2.57	0.47
1:F:409:TYR:CD1	1:F:409:TYR:C	2.93	0.47
3:C:80:GLU:OE1	3:C:80:GLU:N	2.36	0.47
1:G:906:MET:N	1:G:907:GLN:HA	2.30	0.47
1:E:383:CYS:HB3	1:E:385:PHE:CE2	2.50	0.47
1:A:777:TYR:CD1	1:A:777:TYR:N	2.82	0.47
1:F:633:ASP:OD1	1:F:633:ASP:C	2.57	0.47
1:G:938:LEU:O	1:G:938:LEU:HG	2.16	0.46
3:C:1:ASP:C	3:C:1:ASP:OD1	2.55	0.46
1:F:725:GLU:OE1	1:F:725:GLU:N	2.32	0.46
1:F:735:LEU:N	1:F:735:LEU:HD12	2.31	0.46
1:E:616:VAL:O	1:E:616:VAL:CG1	2.62	0.46
1:F:67:ILE:HG13	1:F:67:ILE:O	2.15	0.46
1:E:384:ASP:C	1:E:404:PHE:CE1	2.94	0.46
1:E:601:GLY:O	1:E:602:ASN:HB2	2.16	0.46
1:A:905:TYR:CE2	1:A:936:PRO:HB3	2.30	0.45
1:E:621:THR:CG2	1:E:622:ALA:N	2.78	0.45
1:F:395:GLN:OE1	1:F:395:GLN:HA	2.15	0.45
3:I:70:ASP:C	3:I:70:ASP:OD1	2.58	0.45
1:E:371:SER:HB3	1:E:604:VAL:N	2.32	0.45
1:E:599:GLN:C	1:E:601:GLY:HA2	2.42	0.45
1:E:633:ASP:C	1:E:633:ASP:OD1	2.60	0.45
1:F:381:VAL:O	1:F:407:CYS:CA	2.64	0.45
1:G:1173:ILE:HG13	1:G:1185:SER:OG	2.16	0.45
1:E:372:GLY:O	1:E:604:VAL:HG21	2.16	0.45
1:F:174:ASP:OD1	1:F:174:ASP:C	2.59	0.45
3:C:65:SER:OG	3:C:72:SER:OG	2.32	0.45
1:E:425:CYS:HA	1:E:478:CYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:621:THR:O	1:E:648:TYR:CD2	2.65	0.44
1:F:383:CYS:CB	1:F:385:PHE:CE2	2.98	0.44
1:F:439:SER:HA	1:F:582:ASN:HA	1.99	0.44
1:J:633:ASP:C	1:J:633:ASP:OD1	2.60	0.44
1:J:735:LEU:N	1:J:735:LEU:HD22	2.32	0.44
1:E:228:PHE:C	1:E:228:PHE:CD1	2.95	0.44
1:E:49:ASP:C	1:E:49:ASP:OD1	2.60	0.44
1:J:49:ASP:C	1:J:49:ASP:OD1	2.59	0.44
1:E:371:SER:CB	1:E:602:ASN:OD1	2.65	0.44
1:J:369:LYS:O	1:J:369:LYS:HG2	2.18	0.44
2:H:72:ASP:OD1	2:H:72:ASP:C	2.57	0.44
1:E:342:ASN:C	1:E:342:ASN:OD1	2.61	0.44
1:J:439:SER:HA	1:J:582:ASN:HA	1.98	0.44
1:E:130:VAL:O	1:E:130:VAL:CG1	2.66	0.44
1:F:677:VAL:O	1:F:677:VAL:HG22	2.17	0.44
1:J:130:VAL:O	1:J:130:VAL:HG12	2.17	0.44
2:H:69:MET:HE2	2:H:69:MET:HB3	1.85	0.44
1:F:381:VAL:O	1:F:408:ASN:N	2.46	0.44
1:J:620:CYS:O	1:J:621:THR:C	2.60	0.44
1:A:875:GLU:O	1:A:875:GLU:HG2	2.18	0.43
1:D:801:LYS:HB2	1:D:801:LYS:HE2	1.87	0.43
1:G:774:ASN:C	1:G:774:ASN:OD1	2.59	0.43
1:F:326:ASP:C	1:F:326:ASP:OD1	2.59	0.43
1:E:422:ASP:O	1:E:480:ILE:HA	2.17	0.43
1:J:735:LEU:HD13	1:J:735:LEU:HA	1.80	0.43
1:D:905:TYR:CZ	1:D:936:PRO:CA	2.98	0.43
1:D:1001:PHE:CD1	1:D:1001:PHE:C	2.97	0.43
1:G:1124:VAL:O	1:G:1124:VAL:HG13	2.18	0.43
1:E:602:ASN:C	1:E:604:VAL:H	2.26	0.43
1:F:719:ASN:OD1	1:F:719:ASN:C	2.60	0.43
1:D:1183:GLU:O	1:D:1183:GLU:HG3	2.19	0.43
3:C:28:TYR:CD1	3:C:28:TYR:N	2.85	0.43
1:F:383:CYS:CB	1:F:385:PHE:CZ	3.02	0.42
1:J:172:LEU:HD12	1:J:172:LEU:C	2.43	0.42
1:E:422:ASP:HB3	1:E:481:LEU:CB	2.47	0.42
1:E:605:GLU:HB2	1:E:614:ARG:HG2	2.00	0.42
1:F:130:VAL:O	1:F:130:VAL:HG12	2.18	0.42
3:I:43:PRO:HA	3:I:44:PRO:HD3	1.93	0.42
1:E:688:GLN:HA	1:E:688:GLN:OE1	2.19	0.42
1:J:593:ASP:N	1:J:594:THR:HA	2.35	0.42
1:A:1160:ASN:OD1	1:A:1160:ASN:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:741:THR:HA	1:F:742:PRO:HD3	1.87	0.42
1:J:410:ASN:OD1	1:J:410:ASN:C	2.63	0.42
1:D:988:GLN:HB3	1:D:1195:GLU:OE2	2.20	0.42
1:D:806:CYS:O	1:D:806:CYS:SG	2.78	0.42
1:G:906:MET:O	1:G:906:MET:HG3	2.20	0.42
1:E:606:TYR:CD1	1:E:606:TYR:C	2.97	0.42
1:D:759:LEU:N	1:F:717:LEU:O	2.53	0.41
1:E:381:VAL:HG13	1:E:407:CYS:HA	1.25	0.41
1:G:801:LYS:HB2	1:G:801:LYS:HE2	1.93	0.41
1:E:371:SER:HB2	1:E:602:ASN:OD1	2.20	0.41
1:F:369:LYS:O	1:F:369:LYS:CG	2.60	0.41
1:J:330:ASP:OD1	1:J:330:ASP:C	2.62	0.41
1:E:371:SER:HB3	1:E:604:VAL:CA	2.50	0.41
1:J:670:HIS:CD2	1:J:670:HIS:N	2.86	0.41
1:A:756:GLU:OE1	1:A:756:GLU:N	2.49	0.41
1:F:49:ASP:OD1	1:F:49:ASP:C	2.62	0.41
1:F:689:TYR:CD1	1:F:689:TYR:O	2.74	0.41
1:E:395:GLN:HA	1:E:395:GLN:OE1	2.21	0.41
1:F:726:ASP:C	1:F:726:ASP:OD1	2.63	0.41
1:F:378:ALA:HB1	1:F:379:GLU:HA	2.03	0.41
1:F:604:VAL:O	1:F:604:VAL:HG13	2.21	0.41
1:J:209:THR:O	1:J:209:THR:HG22	2.20	0.41
1:A:965:SER:OG	1:A:966:SER:N	2.51	0.41
1:F:132:ILE:HD12	1:F:132:ILE:HA	1.83	0.41
1:A:988:GLN:CD	1:A:988:GLN:C	2.89	0.41
1:G:1060:PRO:HA	1:G:1063:GLN:HB3	2.03	0.41
1:E:371:SER:OG	1:E:604:VAL:HG11	2.04	0.41
1:E:384:ASP:N	1:E:404:PHE:CE1	2.89	0.41
1:F:330:ASP:OD1	1:F:330:ASP:C	2.64	0.41
1:A:774:ASN:OD1	1:A:774:ASN:C	2.64	0.40
1:D:905:TYR:OH	1:D:936:PRO:HD3	2.18	0.40
1:A:764:PHE:CD1	1:A:764:PHE:C	3.00	0.40
1:E:643:SER:OG	1:E:644:ASP:N	2.54	0.40
1:A:792:GLN:N	1:A:792:GLN:CD	2.80	0.40
1:D:927:GLN:HB2	1:D:932:TYR:HB2	2.03	0.40
1:D:775:SER:OG	1:D:776:SER:N	2.53	0.40
1:F:209:THR:O	1:F:209:THR:HG22	2.21	0.40
1:J:148:MET:HE3	1:J:148:MET:HB2	1.95	0.40
1:D:809:TYR:CD2	1:D:809:TYR:C	3.00	0.40
1:G:873:LEU:C	1:G:873:LEU:HD12	2.46	0.40
1:E:384:ASP:N	1:E:404:PHE:HE1	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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	382/1148 (33%)	382 (100%)	0	100	100
1	E	635/1148 (55%)	633 (100%)	2 (0%)	86	84
1	F	635/1148 (55%)	635 (100%)	0	100	100
1	G	388/1148 (34%)	388 (100%)	0	100	100
1	J	635/1148 (55%)	634 (100%)	1 (0%)	87	86
2	B	102/202 (50%)	102 (100%)	0	100	100
2	H	102/202 (50%)	102 (100%)	0	100	100
3	C	93/192 (48%)	93 (100%)	0	100	100
3	I	93/192 (48%)	93 (100%)	0	100	100
All	All	3453/7676 (45%)	3450 (100%)	3 (0%)	87	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	384	ASP
1	E	602	ASN
1	J	382	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	766	HIS
1	A	769	GLN
1	A	772	GLN
1	A	833	GLN
1	A	836	HIS
1	A	914	GLN
1	A	1009	GLN
1	D	766	HIS
1	D	769	GLN
1	D	833	GLN
1	D	914	GLN
1	D	1132	ASN
1	G	836	HIS
1	G	914	GLN
1	G	1023	GLN
3	I	34	ASN
1	E	36	GLN
1	E	78	GLN
1	E	91	HIS
1	E	125	ASN
1	E	471	GLN
1	F	36	GLN
1	F	60	GLN
1	F	78	GLN
1	F	104	ASN
1	F	107	GLN
1	F	194	HIS
1	F	475	ASN
1	F	516	GLN
1	F	628	GLN
1	J	37	GLN
1	J	78	GLN
1	J	167	HIS
1	J	471	GLN
1	J	618	GLN
1	J	688	GLN

5.3.3 RNA ⓘ

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.

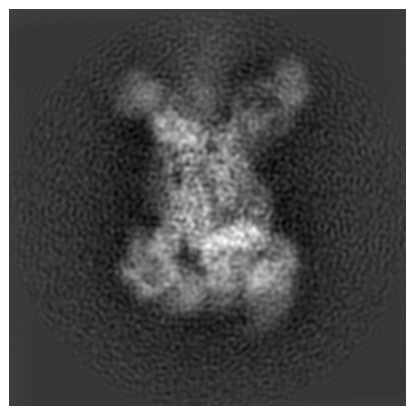
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8788. These allow visual inspection of the internal detail of the map and identification of artifacts.

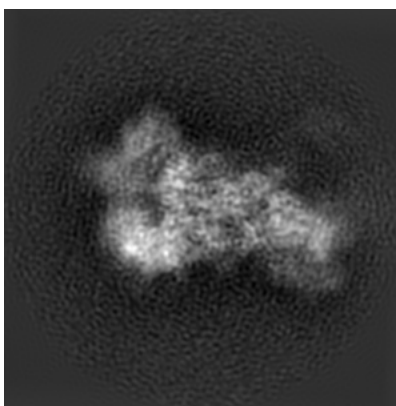
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

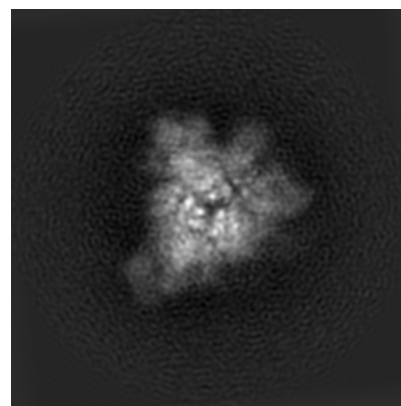
6.1.1 Primary map



X

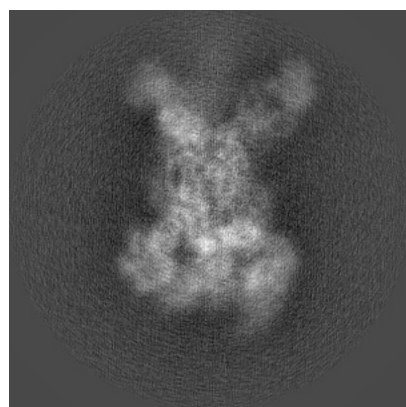


Y

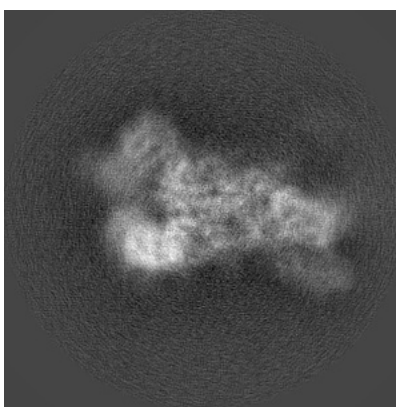


Z

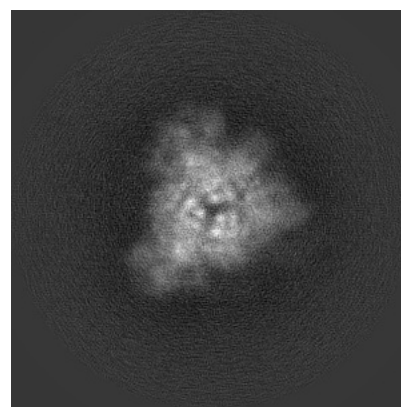
6.1.2 Raw map



X



Y

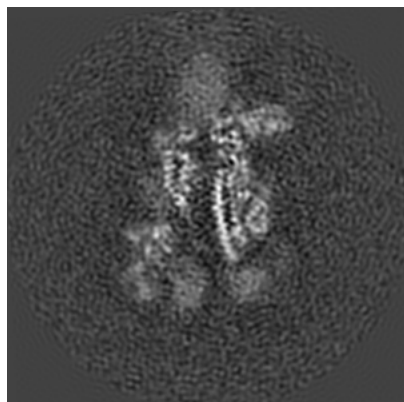


Z

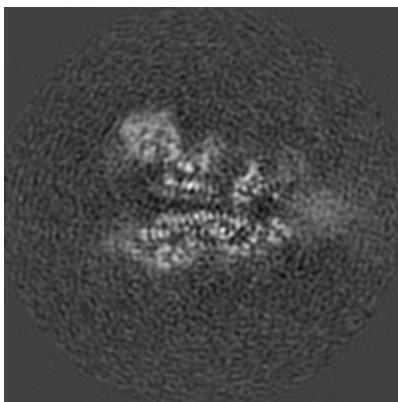
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

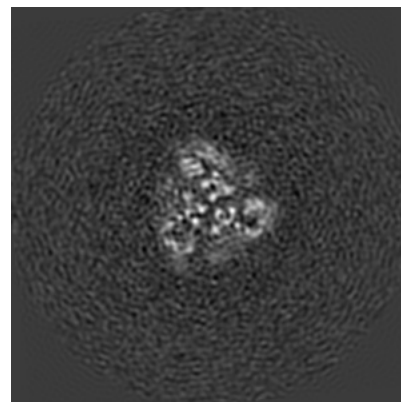
6.2.1 Primary map



X Index: 152

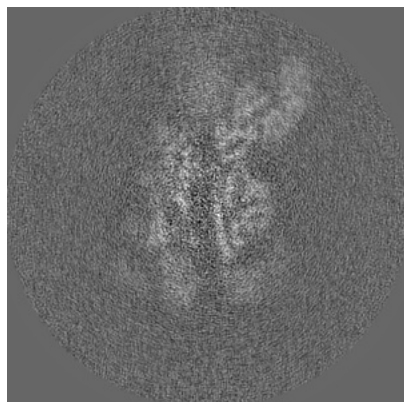


Y Index: 152

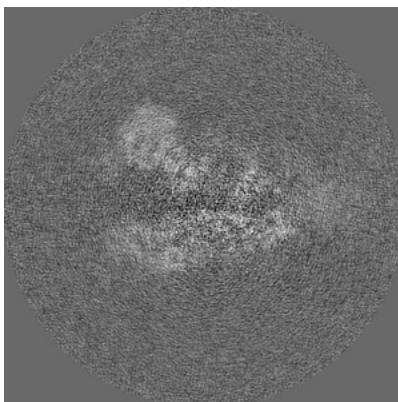


Z Index: 152

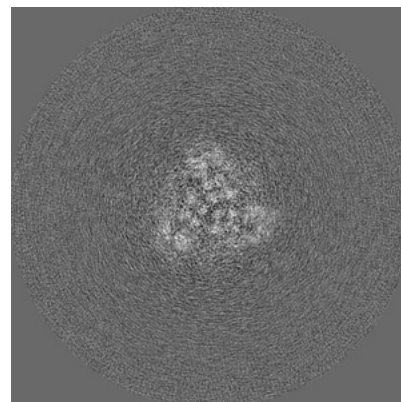
6.2.2 Raw map



X Index: 152



Y Index: 152

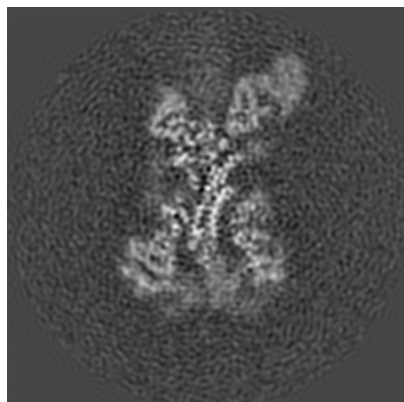


Z Index: 152

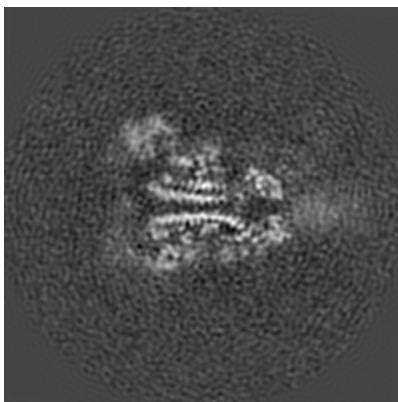
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

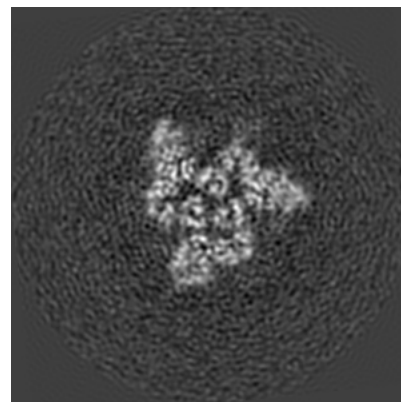
6.3.1 Primary map



X Index: 134

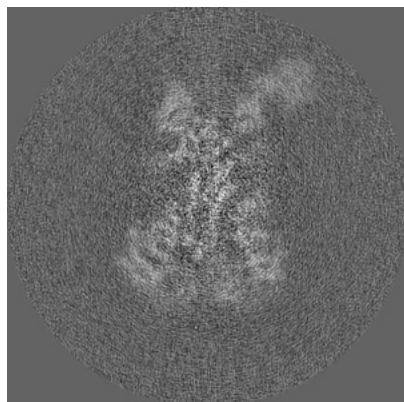


Y Index: 149

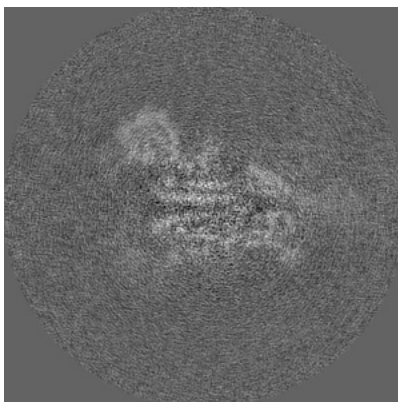


Z Index: 125

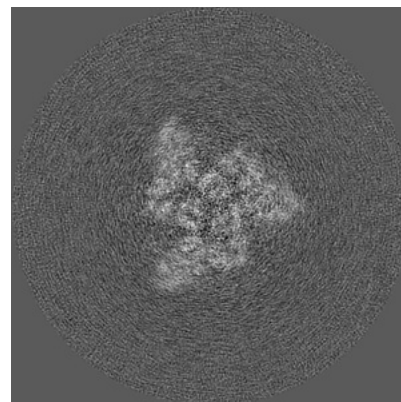
6.3.2 Raw map



X Index: 137



Y Index: 146

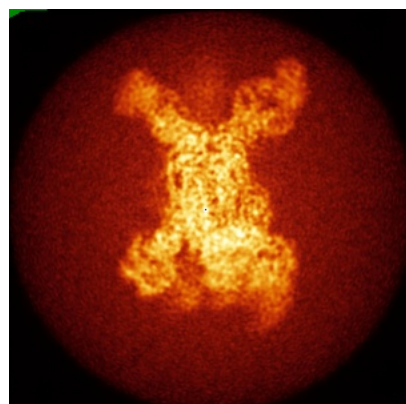


Z Index: 127

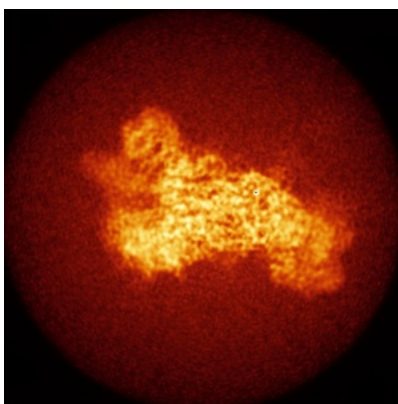
The images above show the largest variance slices of the map in three orthogonal directions.

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

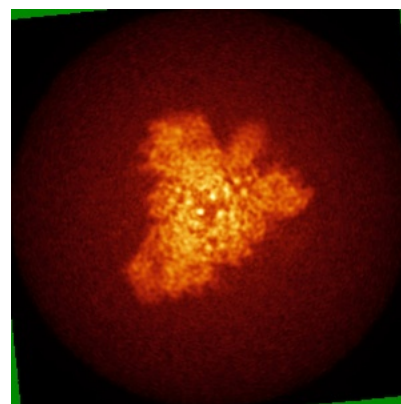
6.4.1 Primary map



X

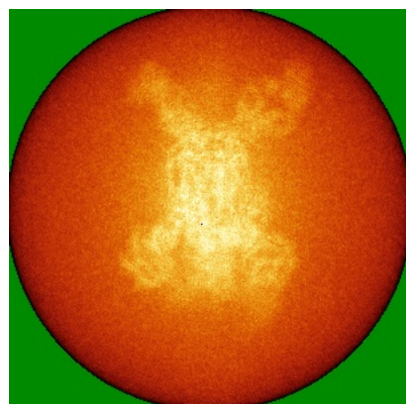


Y

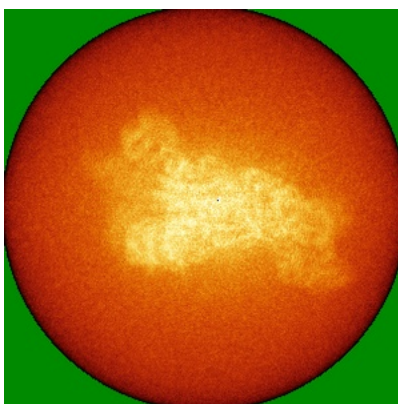


Z

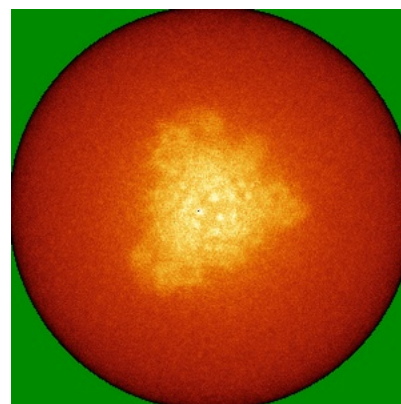
6.4.2 Raw map



X



Y

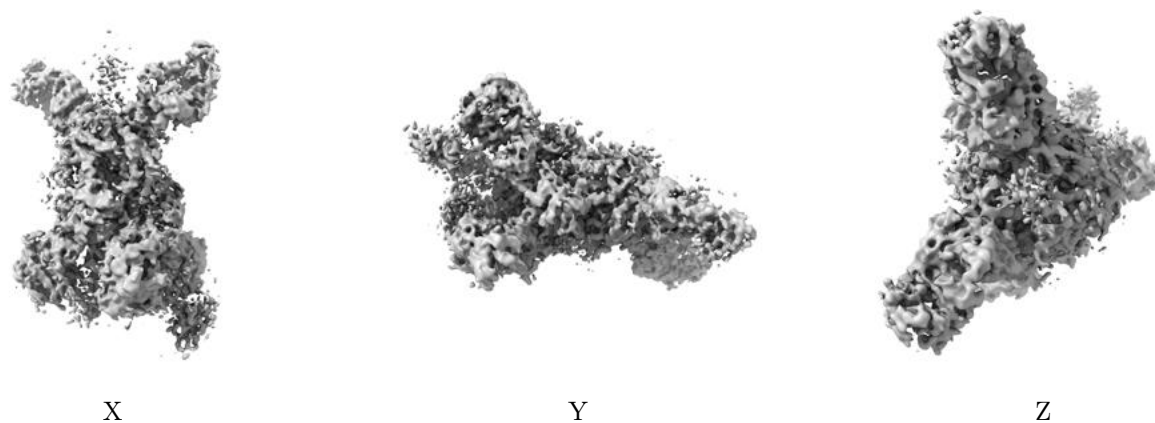


Z

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.

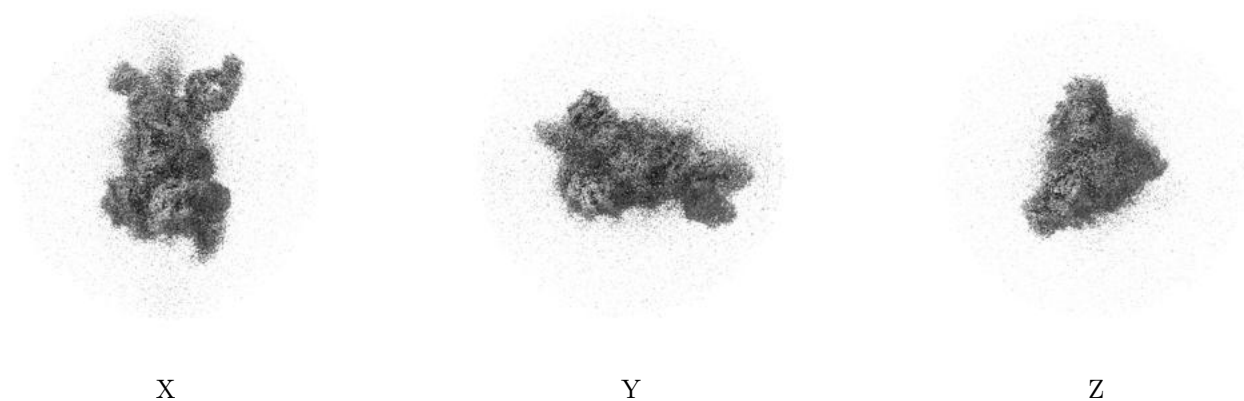
6.5 Orthogonal surface views [i](#)

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.

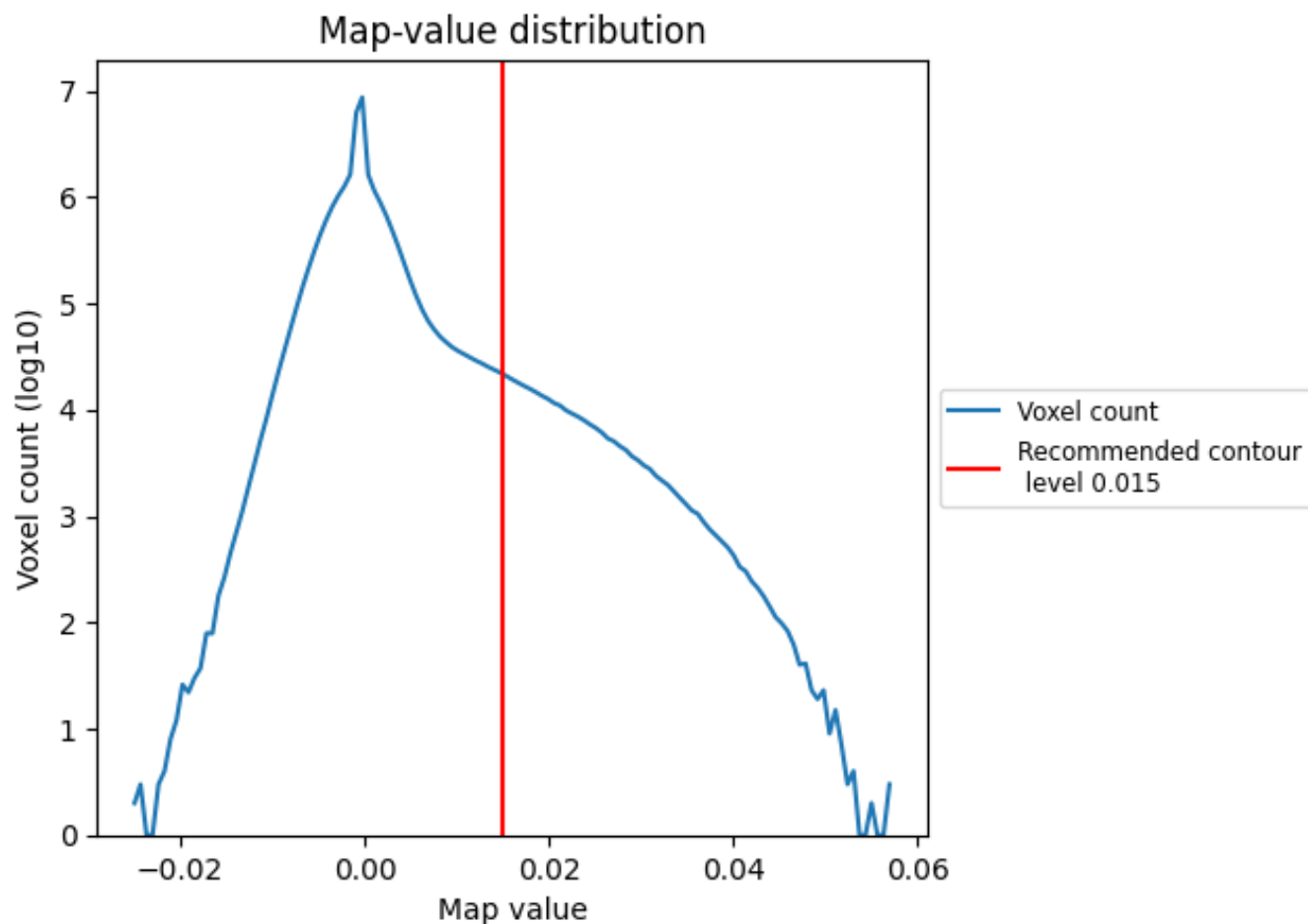
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

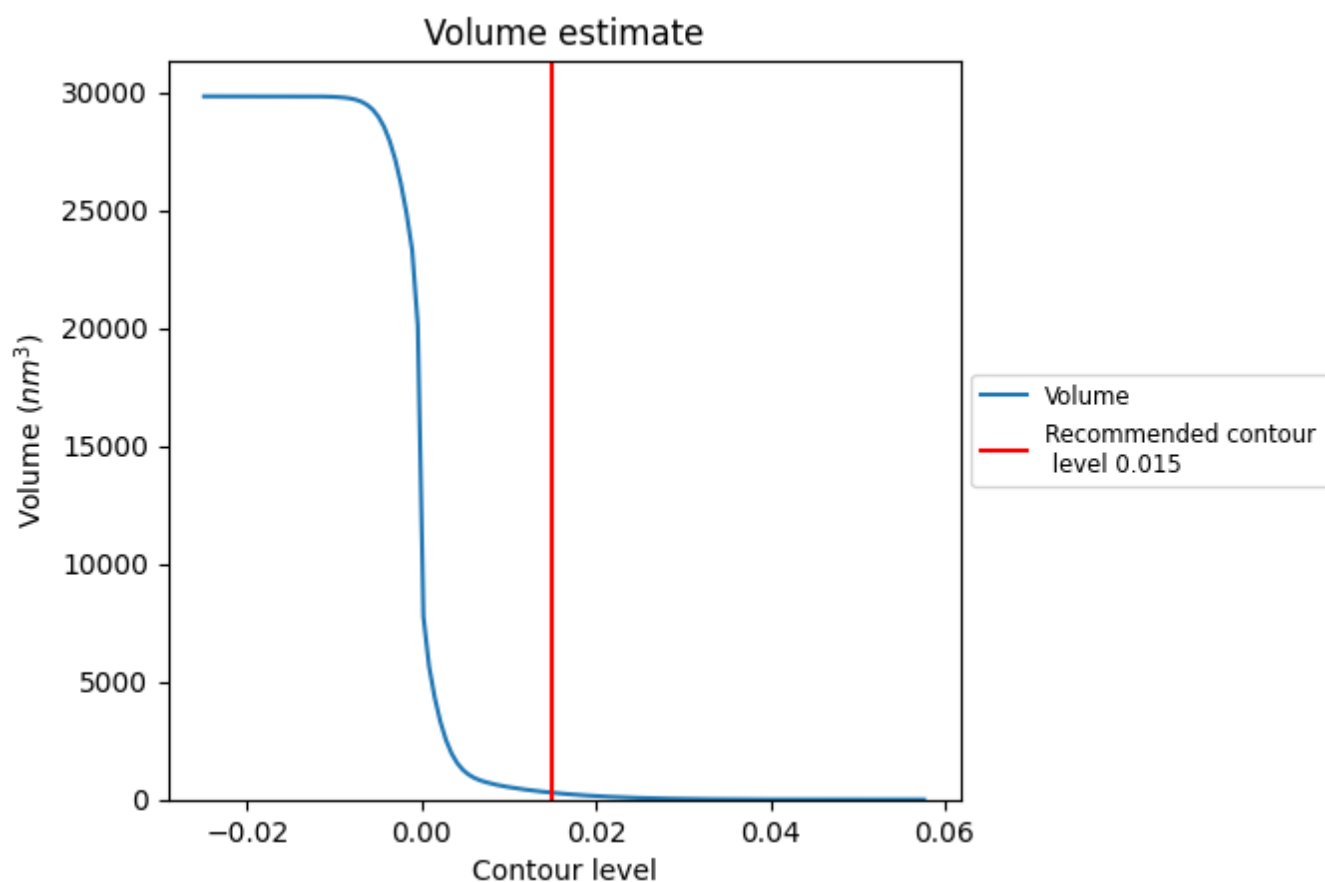
This section contains the results of statistical analysis of the map.

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.

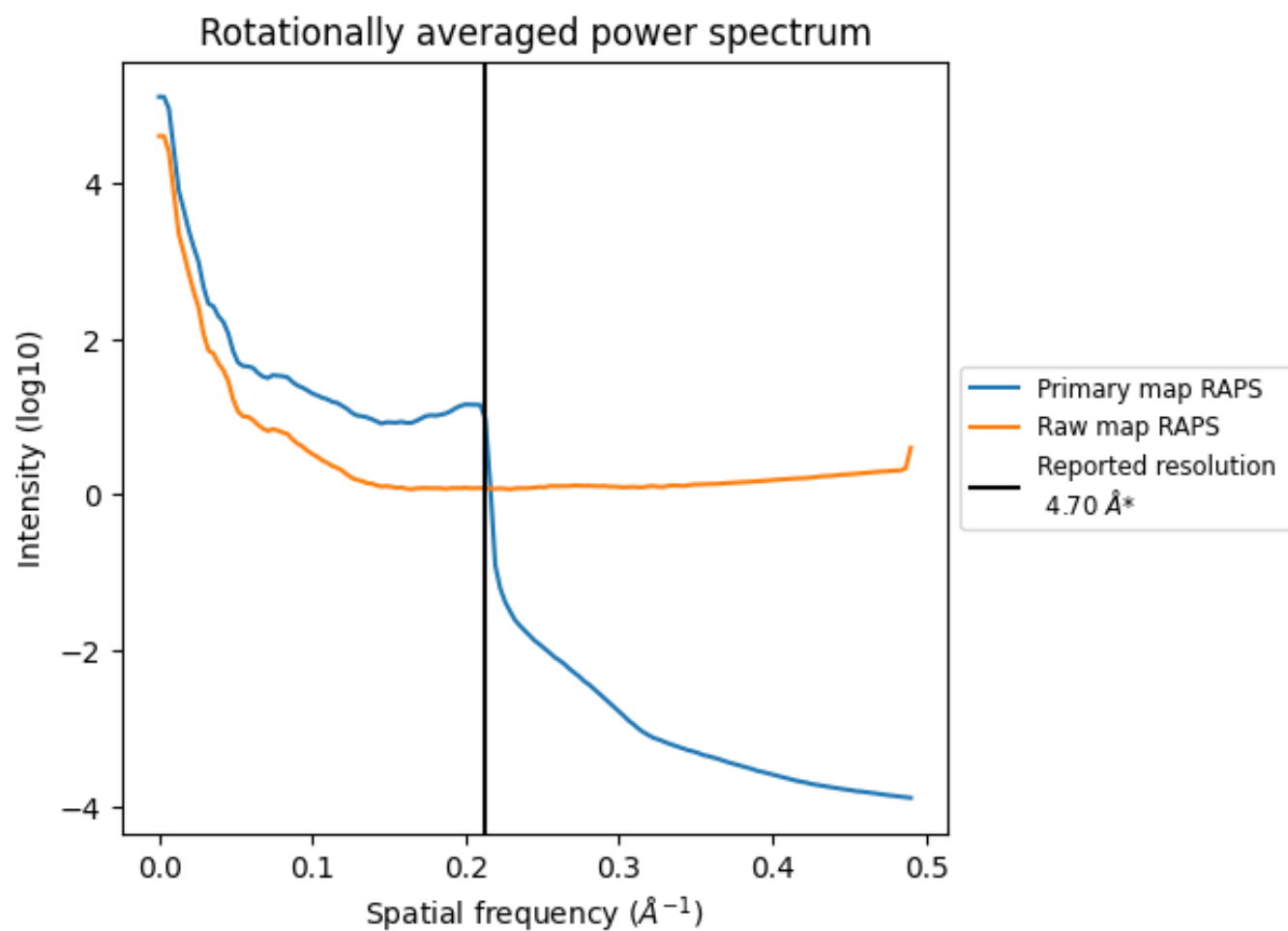
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 289 nm³; this corresponds to an approximate mass of 261 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 ⓘ

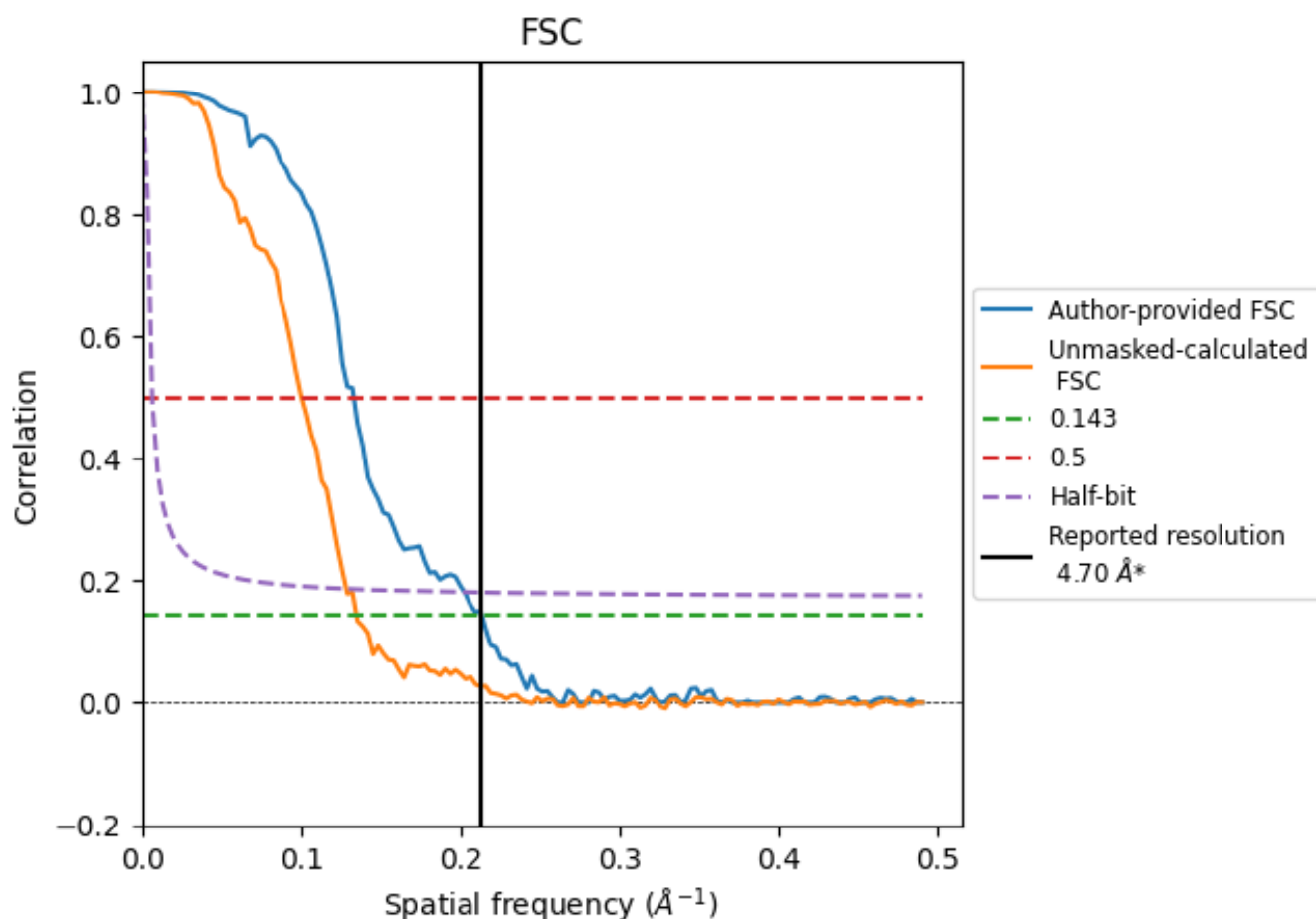


*Reported resolution corresponds to spatial frequency of 0.213 $\text{\AA}^{-1}$

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 0.213 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

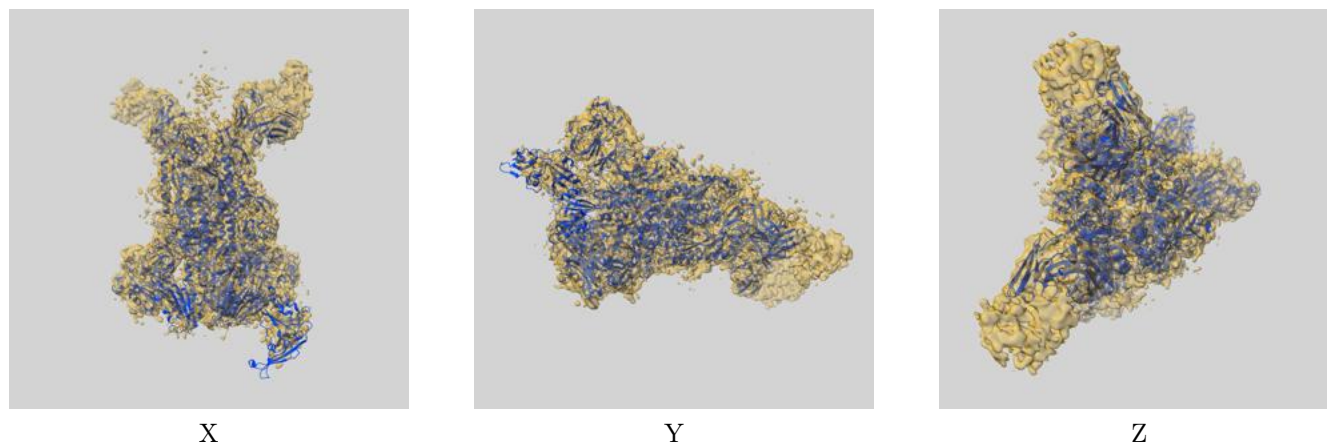
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.68	7.51	4.94
Unmasked-calculated*	7.42	9.97	7.79

*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 7.42 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

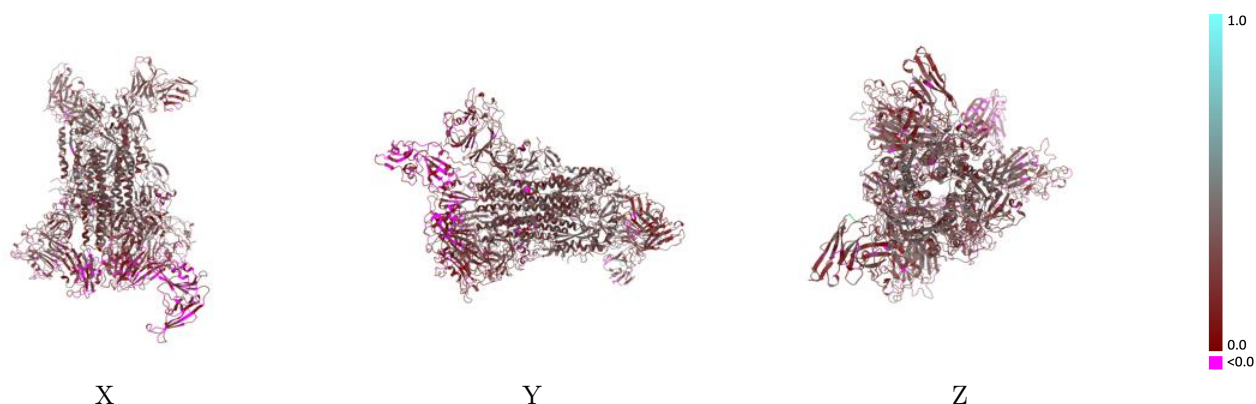
This section contains information regarding the fit between EMDB map EMD-8788 and PDB model 5W9M. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



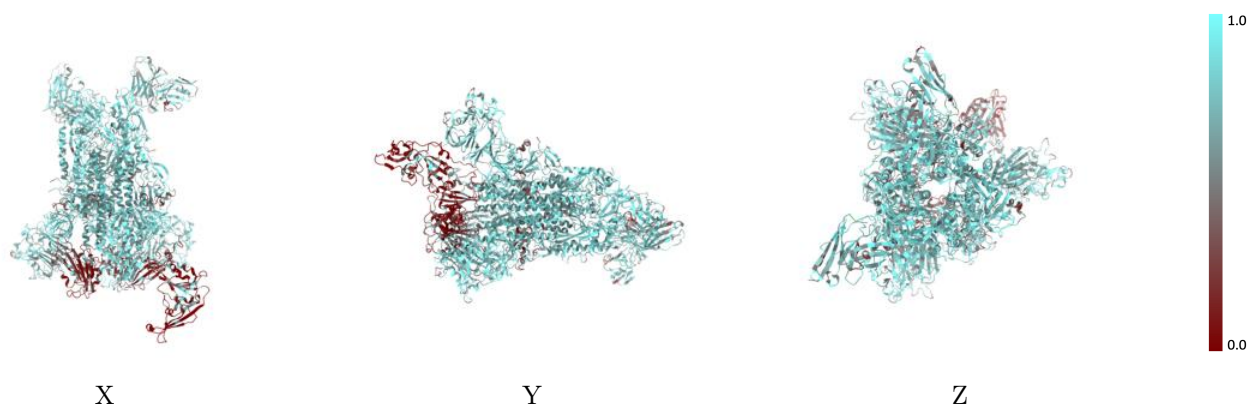
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



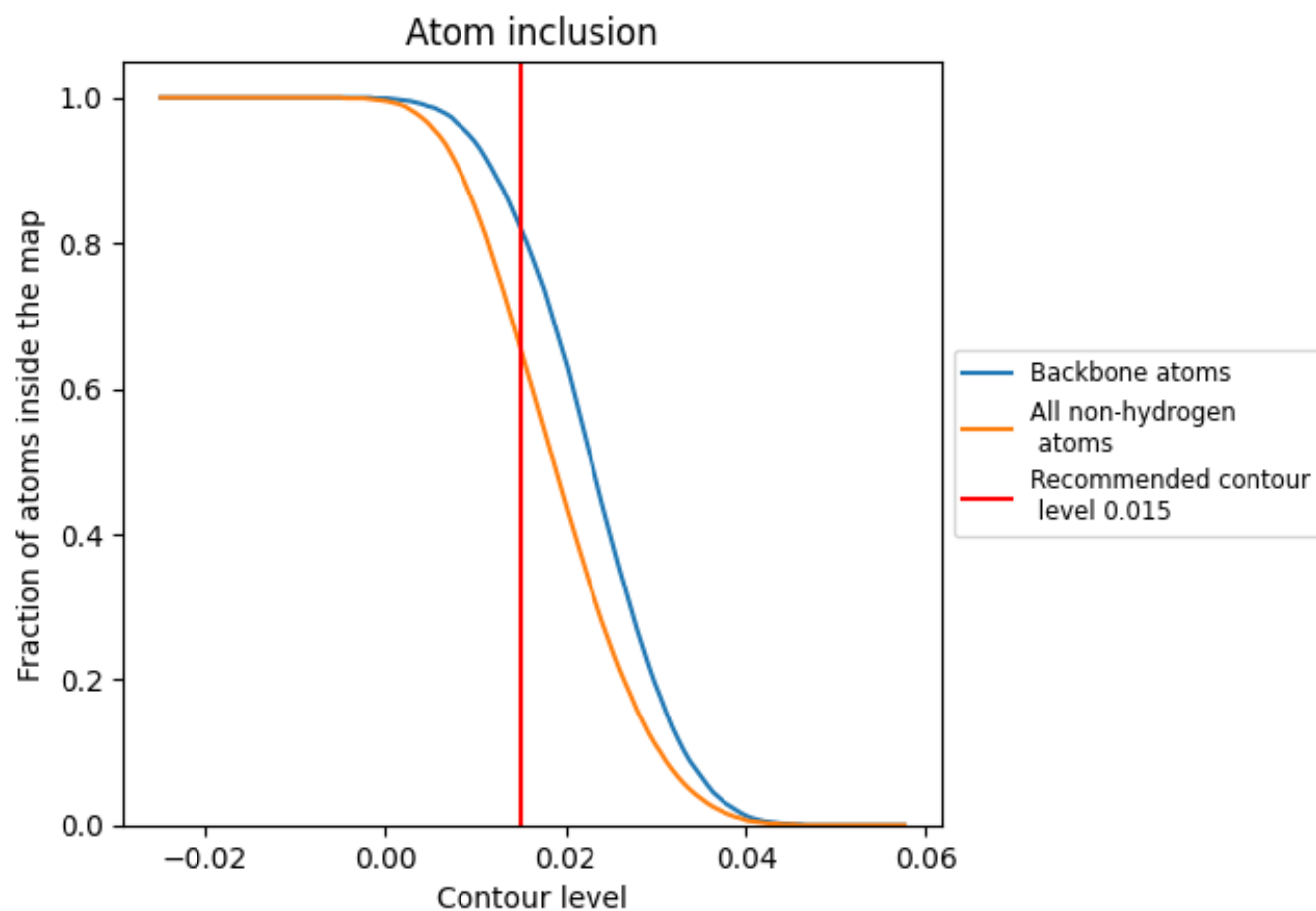
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 82% of all backbone atoms, 66% 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	 0.6560	 0.2520
A	 0.7460	 0.3180
B	 0.6920	 0.2630
C	 0.6350	 0.2240
D	 0.7380	 0.3060
E	 0.5980	 0.2090
F	 0.5740	 0.2130
G	 0.7450	 0.3110
H	 0.7410	 0.2870
I	 0.6400	 0.2110
J	 0.6160	 0.2220

