Full wwPDB EM Validation Report ⓘ

Aug 5, 2024 – 02:28 pm BST

PDB ID	:	9FJK
EMDB ID	:	EMD-50503
Title	:	Omicron BA.1 Spike protein with neutralizing NTD specific mAb K501SP6
Authors	:	Bjoernsson, K.H.; Walker, M.R.; Raghavan, S.S.R.; Ward, A.B.; Barfod, L.K.
Deposited on	:	2024-05-31
Resolution	:	2.84 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:

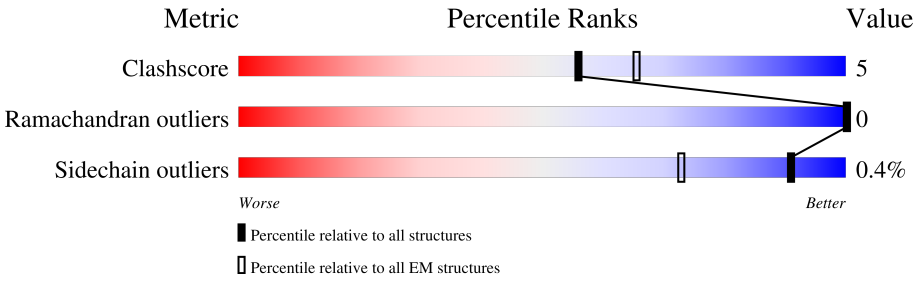
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1277	24% 72% 9% • 19%
1	B	1277	30% 72% 10% 18%
1	C	1277	32% 74% 8% 17%
2	H	129	78% 82% 17% •
3	L	134	75% 72% 10% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26529 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1040	Total	C	N	O	S	0	0
			8185	5244	1361	1543	37		
1	B	1047	Total	C	N	O	S	0	0
			8226	5265	1369	1555	37		
1	C	1055	Total	C	N	O	S	0	0
			8288	5307	1379	1565	37		

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	93	ILE	THR	variant	UNP P0DTC2
A	140	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	206	LEU	ASN	variant	UNP P0DTC2
A	207	VAL	LEU	variant	UNP P0DTC2
A	208	ARG	VAL	variant	UNP P0DTC2
A	209	GLU	ARG	variant	UNP P0DTC2
A	210	PRO	-	insertion	UNP P0DTC2
A	211	GLU	-	insertion	UNP P0DTC2
A	336	ASP	GLY	variant	UNP P0DTC2
A	368	LEU	SER	variant	UNP P0DTC2
A	370	PRO	SER	variant	UNP P0DTC2
A	372	PHE	SER	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	variant	UNP P0DTC2
A	443	SER	GLY	variant	UNP P0DTC2
A	474	ASN	SER	variant	UNP P0DTC2
A	475	LYS	THR	variant	UNP P0DTC2
A	481	ALA	GLU	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	490	ARG	GLN	variant	UNP P0DTC2
A	493	SER	GLY	variant	UNP P0DTC2
A	495	ARG	GLN	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	502	HIS	TYR	variant	UNP P0DTC2
A	544	LYS	THR	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	652	TYR	HIS	variant	UNP P0DTC2
A	676	LYS	ASN	variant	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	679	GLY	ARG	engineered mutation	UNP P0DTC2
A	680	SER	ARG	engineered mutation	UNP P0DTC2
A	682	SER	ARG	engineered mutation	UNP P0DTC2
A	761	LYS	ASN	variant	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	814	PRO	PHE	conflict	UNP P0DTC2
A	853	LYS	ASN	variant	UNP P0DTC2
A	889	PRO	ALA	engineered mutation	UNP P0DTC2
A	896	PRO	ALA	engineered mutation	UNP P0DTC2
A	939	PRO	ALA	engineered mutation	UNP P0DTC2
A	951	HIS	GLN	variant	UNP P0DTC2
A	966	LYS	ASN	variant	UNP P0DTC2
A	978	PHE	LEU	variant	UNP P0DTC2
A	983	PRO	LYS	engineered mutation	UNP P0DTC2
A	984	PRO	VAL	engineered mutation	UNP P0DTC2
A	1205	GLN	-	linker	UNP P0DTC2
A	1206	GLY	-	linker	UNP P0DTC2
A	1207	SER	-	linker	UNP P0DTC2
A	1229	LEU	PHE	engineered mutation	UNP P10104
A	1235	GLY	-	expression tag	UNP P10104
A	1236	ARG	-	expression tag	UNP P10104
A	1237	SER	-	expression tag	UNP P10104
A	1238	LEU	-	expression tag	UNP P10104
A	1239	GLU	-	expression tag	UNP P10104
A	1240	VAL	-	expression tag	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	PHE	-	expression tag	UNP P10104
A	1243	GLN	-	expression tag	UNP P10104
A	1244	GLY	-	expression tag	UNP P10104
A	1245	PRO	-	expression tag	UNP P10104
A	1246	GLY	-	expression tag	UNP P10104
A	1247	SER	-	expression tag	UNP P10104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1248	ALA	-	expression tag	UNP P10104
A	1249	TRP	-	expression tag	UNP P10104
A	1250	SER	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	PRO	-	expression tag	UNP P10104
A	1253	GLN	-	expression tag	UNP P10104
A	1254	PHE	-	expression tag	UNP P10104
A	1255	GLU	-	expression tag	UNP P10104
A	1256	LYS	-	expression tag	UNP P10104
A	1257	GLY	-	expression tag	UNP P10104
A	1258	GLY	-	expression tag	UNP P10104
A	1259	GLY	-	expression tag	UNP P10104
A	1260	SER	-	expression tag	UNP P10104
A	1261	GLY	-	expression tag	UNP P10104
A	1262	GLY	-	expression tag	UNP P10104
A	1263	GLY	-	expression tag	UNP P10104
A	1264	GLY	-	expression tag	UNP P10104
A	1265	SER	-	expression tag	UNP P10104
A	1266	GLY	-	expression tag	UNP P10104
A	1267	GLY	-	expression tag	UNP P10104
A	1268	SER	-	expression tag	UNP P10104
A	1269	ALA	-	expression tag	UNP P10104
A	1270	TRP	-	expression tag	UNP P10104
A	1271	SER	-	expression tag	UNP P10104
A	1272	HIS	-	expression tag	UNP P10104
A	1273	PRO	-	expression tag	UNP P10104
A	1274	GLN	-	expression tag	UNP P10104
A	1275	PHE	-	expression tag	UNP P10104
A	1276	GLU	-	expression tag	UNP P10104
A	1277	LYS	-	expression tag	UNP P10104
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	93	ILE	THR	variant	UNP P0DTC2
B	140	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	206	LEU	ASN	variant	UNP P0DTC2
B	207	VAL	LEU	variant	UNP P0DTC2
B	208	ARG	VAL	variant	UNP P0DTC2
B	209	GLU	ARG	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	210	PRO	-	insertion	UNP P0DTC2
B	211	GLU	-	insertion	UNP P0DTC2
B	336	ASP	GLY	variant	UNP P0DTC2
B	368	LEU	SER	variant	UNP P0DTC2
B	370	PRO	SER	variant	UNP P0DTC2
B	372	PHE	SER	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	437	LYS	ASN	variant	UNP P0DTC2
B	443	SER	GLY	variant	UNP P0DTC2
B	474	ASN	SER	variant	UNP P0DTC2
B	475	LYS	THR	variant	UNP P0DTC2
B	481	ALA	GLU	variant	UNP P0DTC2
B	490	ARG	GLN	variant	UNP P0DTC2
B	493	SER	GLY	variant	UNP P0DTC2
B	495	ARG	GLN	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	502	HIS	TYR	variant	UNP P0DTC2
B	544	LYS	THR	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	652	TYR	HIS	variant	UNP P0DTC2
B	676	LYS	ASN	variant	UNP P0DTC2
B	678	HIS	PRO	variant	UNP P0DTC2
B	679	GLY	ARG	engineered mutation	UNP P0DTC2
B	680	SER	ARG	engineered mutation	UNP P0DTC2
B	682	SER	ARG	engineered mutation	UNP P0DTC2
B	761	LYS	ASN	variant	UNP P0DTC2
B	793	TYR	ASP	variant	UNP P0DTC2
B	814	PRO	PHE	conflict	UNP P0DTC2
B	853	LYS	ASN	variant	UNP P0DTC2
B	889	PRO	ALA	engineered mutation	UNP P0DTC2
B	896	PRO	ALA	engineered mutation	UNP P0DTC2
B	939	PRO	ALA	engineered mutation	UNP P0DTC2
B	951	HIS	GLN	variant	UNP P0DTC2
B	966	LYS	ASN	variant	UNP P0DTC2
B	978	PHE	LEU	variant	UNP P0DTC2
B	983	PRO	LYS	engineered mutation	UNP P0DTC2
B	984	PRO	VAL	engineered mutation	UNP P0DTC2
B	1205	GLN	-	linker	UNP P0DTC2
B	1206	GLY	-	linker	UNP P0DTC2
B	1207	SER	-	linker	UNP P0DTC2
B	1229	LEU	PHE	engineered mutation	UNP P10104
B	1235	GLY	-	expression tag	UNP P10104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1236	ARG	-	expression tag	UNP P10104
B	1237	SER	-	expression tag	UNP P10104
B	1238	LEU	-	expression tag	UNP P10104
B	1239	GLU	-	expression tag	UNP P10104
B	1240	VAL	-	expression tag	UNP P10104
B	1241	LEU	-	expression tag	UNP P10104
B	1242	PHE	-	expression tag	UNP P10104
B	1243	GLN	-	expression tag	UNP P10104
B	1244	GLY	-	expression tag	UNP P10104
B	1245	PRO	-	expression tag	UNP P10104
B	1246	GLY	-	expression tag	UNP P10104
B	1247	SER	-	expression tag	UNP P10104
B	1248	ALA	-	expression tag	UNP P10104
B	1249	TRP	-	expression tag	UNP P10104
B	1250	SER	-	expression tag	UNP P10104
B	1251	HIS	-	expression tag	UNP P10104
B	1252	PRO	-	expression tag	UNP P10104
B	1253	GLN	-	expression tag	UNP P10104
B	1254	PHE	-	expression tag	UNP P10104
B	1255	GLU	-	expression tag	UNP P10104
B	1256	LYS	-	expression tag	UNP P10104
B	1257	GLY	-	expression tag	UNP P10104
B	1258	GLY	-	expression tag	UNP P10104
B	1259	GLY	-	expression tag	UNP P10104
B	1260	SER	-	expression tag	UNP P10104
B	1261	GLY	-	expression tag	UNP P10104
B	1262	GLY	-	expression tag	UNP P10104
B	1263	GLY	-	expression tag	UNP P10104
B	1264	GLY	-	expression tag	UNP P10104
B	1265	SER	-	expression tag	UNP P10104
B	1266	GLY	-	expression tag	UNP P10104
B	1267	GLY	-	expression tag	UNP P10104
B	1268	SER	-	expression tag	UNP P10104
B	1269	ALA	-	expression tag	UNP P10104
B	1270	TRP	-	expression tag	UNP P10104
B	1271	SER	-	expression tag	UNP P10104
B	1272	HIS	-	expression tag	UNP P10104
B	1273	PRO	-	expression tag	UNP P10104
B	1274	GLN	-	expression tag	UNP P10104
B	1275	PHE	-	expression tag	UNP P10104
B	1276	GLU	-	expression tag	UNP P10104
B	1277	LYS	-	expression tag	UNP P10104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	93	ILE	THR	variant	UNP P0DTC2
C	140	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	206	LEU	ASN	variant	UNP P0DTC2
C	207	VAL	LEU	variant	UNP P0DTC2
C	208	ARG	VAL	variant	UNP P0DTC2
C	209	GLU	ARG	variant	UNP P0DTC2
C	210	PRO	-	insertion	UNP P0DTC2
C	211	GLU	-	insertion	UNP P0DTC2
C	336	ASP	GLY	variant	UNP P0DTC2
C	368	LEU	SER	variant	UNP P0DTC2
C	370	PRO	SER	variant	UNP P0DTC2
C	372	PHE	SER	variant	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2
C	437	LYS	ASN	variant	UNP P0DTC2
C	443	SER	GLY	variant	UNP P0DTC2
C	474	ASN	SER	variant	UNP P0DTC2
C	475	LYS	THR	variant	UNP P0DTC2
C	481	ALA	GLU	variant	UNP P0DTC2
C	490	ARG	GLN	variant	UNP P0DTC2
C	493	SER	GLY	variant	UNP P0DTC2
C	495	ARG	GLN	variant	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	502	HIS	TYR	variant	UNP P0DTC2
C	544	LYS	THR	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	652	TYR	HIS	variant	UNP P0DTC2
C	676	LYS	ASN	variant	UNP P0DTC2
C	678	HIS	PRO	variant	UNP P0DTC2
C	679	GLY	ARG	engineered mutation	UNP P0DTC2
C	680	SER	ARG	engineered mutation	UNP P0DTC2
C	682	SER	ARG	engineered mutation	UNP P0DTC2
C	761	LYS	ASN	variant	UNP P0DTC2
C	793	TYR	ASP	variant	UNP P0DTC2
C	814	PRO	PHE	conflict	UNP P0DTC2
C	853	LYS	ASN	variant	UNP P0DTC2
C	889	PRO	ALA	engineered mutation	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	896	PRO	ALA	engineered mutation	UNP P0DTC2
C	939	PRO	ALA	engineered mutation	UNP P0DTC2
C	951	HIS	GLN	variant	UNP P0DTC2
C	966	LYS	ASN	variant	UNP P0DTC2
C	978	PHE	LEU	variant	UNP P0DTC2
C	983	PRO	LYS	engineered mutation	UNP P0DTC2
C	984	PRO	VAL	engineered mutation	UNP P0DTC2
C	1205	GLN	-	linker	UNP P0DTC2
C	1206	GLY	-	linker	UNP P0DTC2
C	1207	SER	-	linker	UNP P0DTC2
C	1229	LEU	PHE	engineered mutation	UNP P10104
C	1235	GLY	-	expression tag	UNP P10104
C	1236	ARG	-	expression tag	UNP P10104
C	1237	SER	-	expression tag	UNP P10104
C	1238	LEU	-	expression tag	UNP P10104
C	1239	GLU	-	expression tag	UNP P10104
C	1240	VAL	-	expression tag	UNP P10104
C	1241	LEU	-	expression tag	UNP P10104
C	1242	PHE	-	expression tag	UNP P10104
C	1243	GLN	-	expression tag	UNP P10104
C	1244	GLY	-	expression tag	UNP P10104
C	1245	PRO	-	expression tag	UNP P10104
C	1246	GLY	-	expression tag	UNP P10104
C	1247	SER	-	expression tag	UNP P10104
C	1248	ALA	-	expression tag	UNP P10104
C	1249	TRP	-	expression tag	UNP P10104
C	1250	SER	-	expression tag	UNP P10104
C	1251	HIS	-	expression tag	UNP P10104
C	1252	PRO	-	expression tag	UNP P10104
C	1253	GLN	-	expression tag	UNP P10104
C	1254	PHE	-	expression tag	UNP P10104
C	1255	GLU	-	expression tag	UNP P10104
C	1256	LYS	-	expression tag	UNP P10104
C	1257	GLY	-	expression tag	UNP P10104
C	1258	GLY	-	expression tag	UNP P10104
C	1259	GLY	-	expression tag	UNP P10104
C	1260	SER	-	expression tag	UNP P10104
C	1261	GLY	-	expression tag	UNP P10104
C	1262	GLY	-	expression tag	UNP P10104
C	1263	GLY	-	expression tag	UNP P10104
C	1264	GLY	-	expression tag	UNP P10104
C	1265	SER	-	expression tag	UNP P10104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1266	GLY	-	expression tag	UNP P10104
C	1267	GLY	-	expression tag	UNP P10104
C	1268	SER	-	expression tag	UNP P10104
C	1269	ALA	-	expression tag	UNP P10104
C	1270	TRP	-	expression tag	UNP P10104
C	1271	SER	-	expression tag	UNP P10104
C	1272	HIS	-	expression tag	UNP P10104
C	1273	PRO	-	expression tag	UNP P10104
C	1274	GLN	-	expression tag	UNP P10104
C	1275	PHE	-	expression tag	UNP P10104
C	1276	GLU	-	expression tag	UNP P10104
C	1277	LYS	-	expression tag	UNP P10104

- Molecule 2 is a protein called K501SP6 Fv Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	129	Total	C	N	O	S	0	0
			1014	646	162	202	4		

- Molecule 3 is a protein called K501SP6 Fv Light Chain.

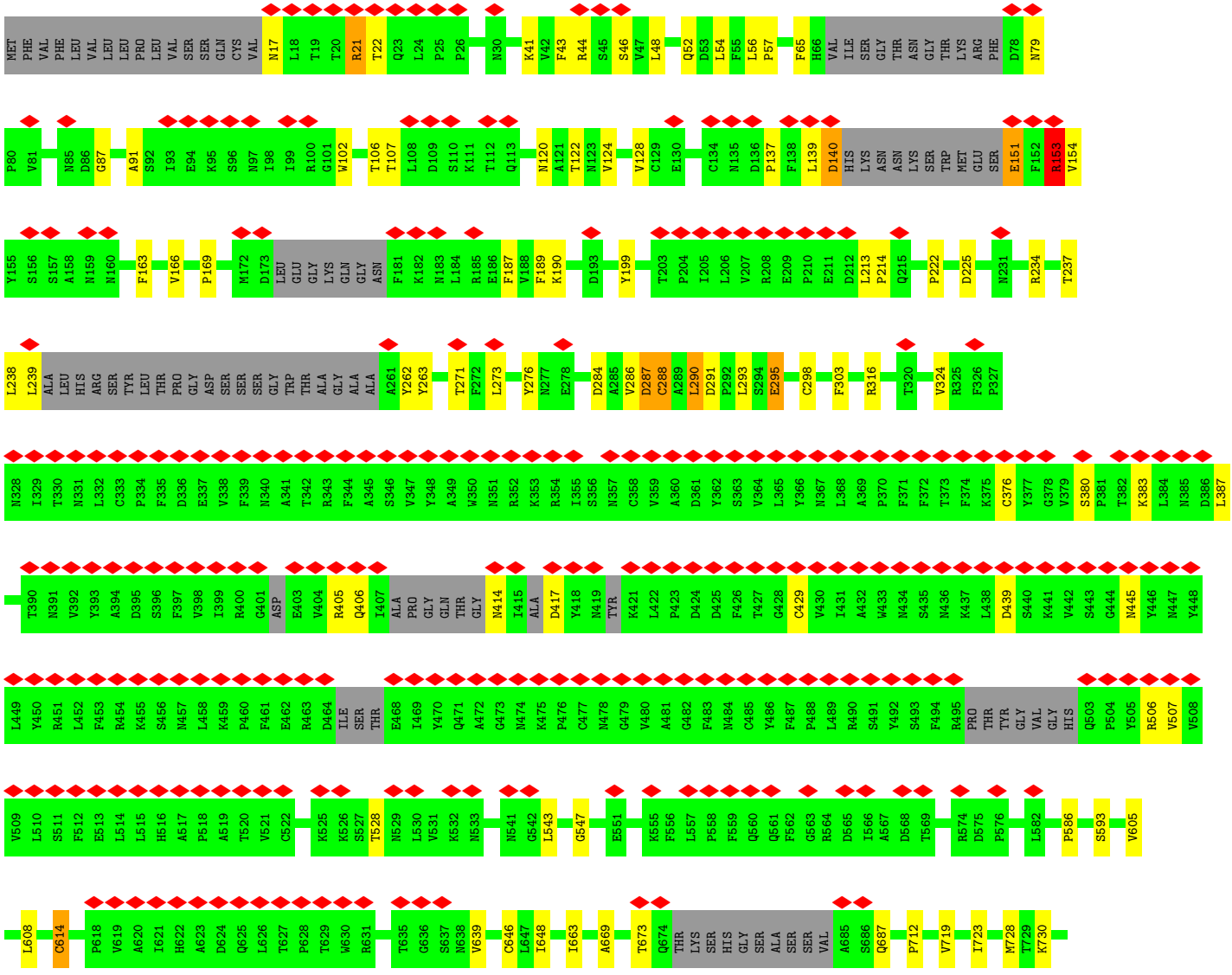
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	111	Total	C	N	O	S	0	0
			816	505	140	169	2		

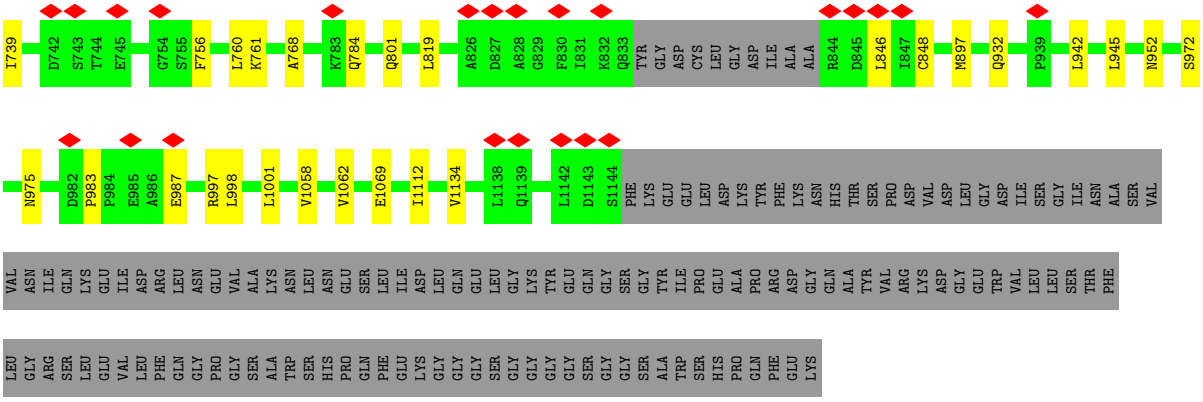
3 Residue-property plots (i)

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,Fibritin

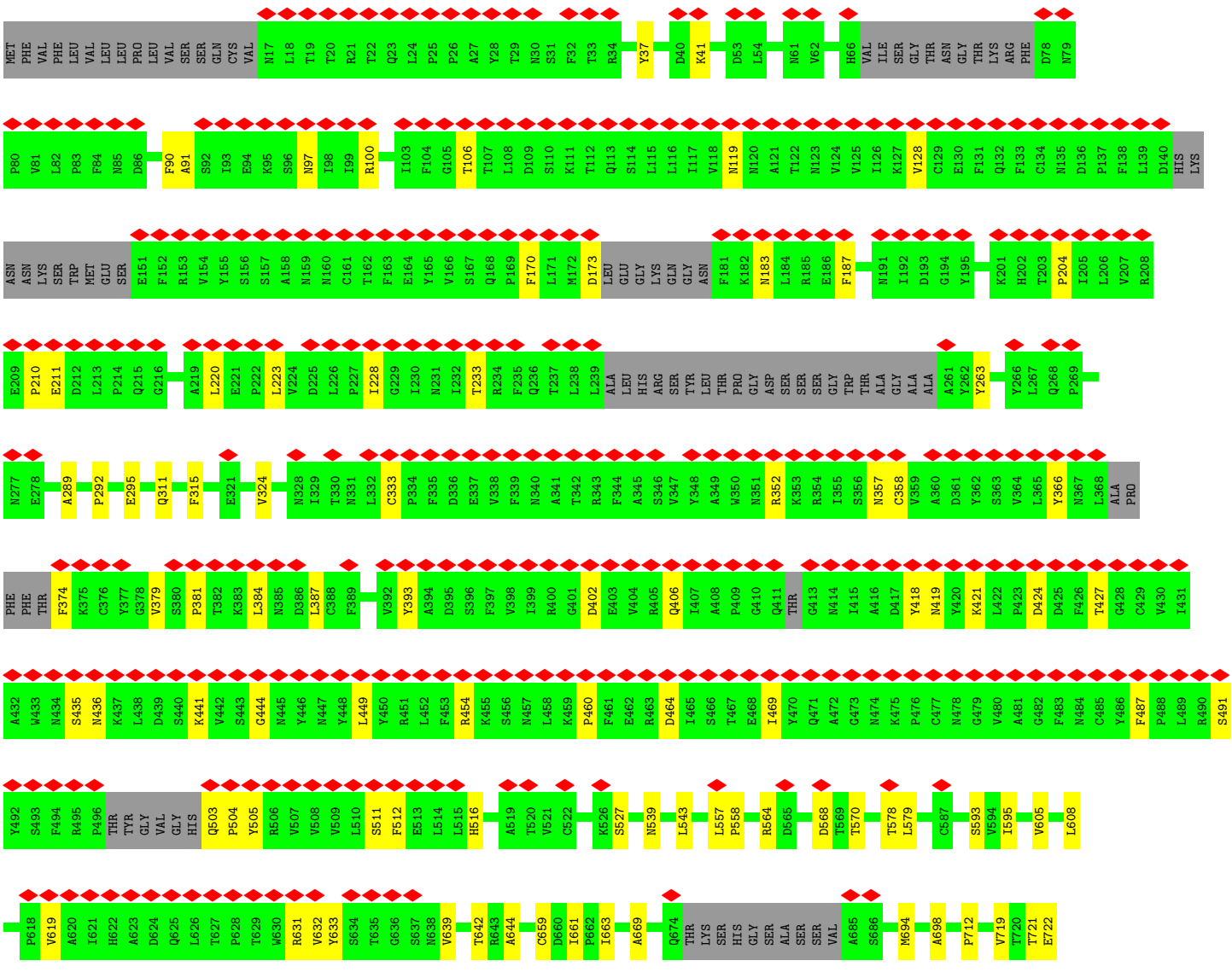
Chain A:

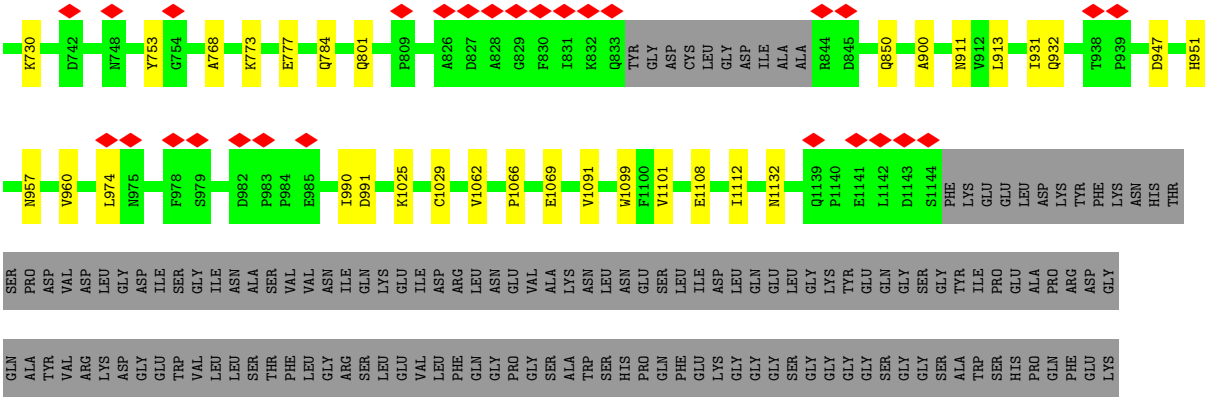




• Molecule 1: Spike glycoprotein,Fibritin

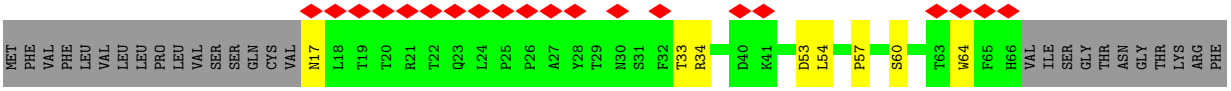
Chain B:

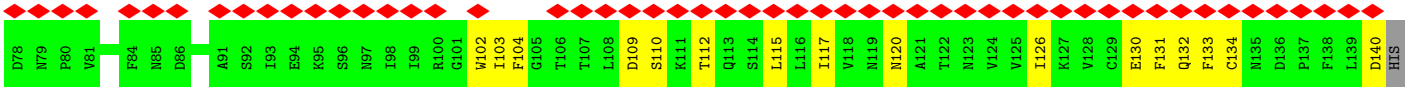


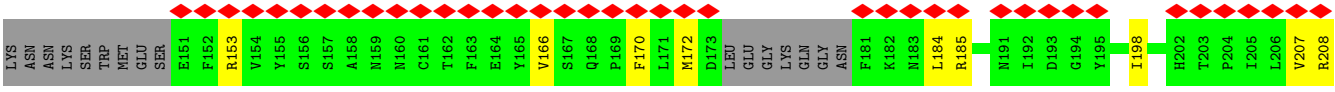


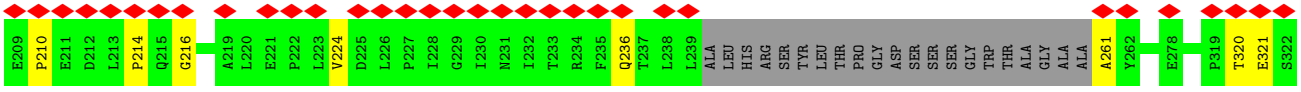
- Molecule 1: Spike glycoprotein,Fibritin

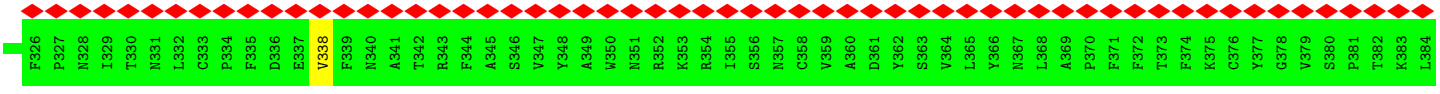
Chain C:

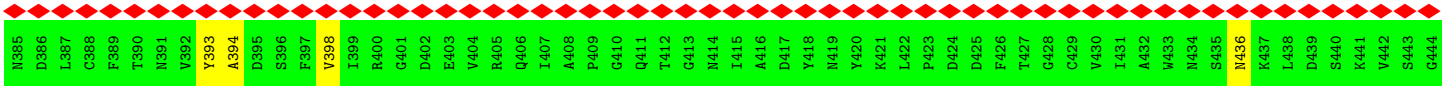


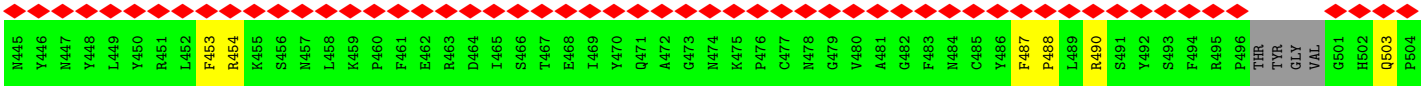


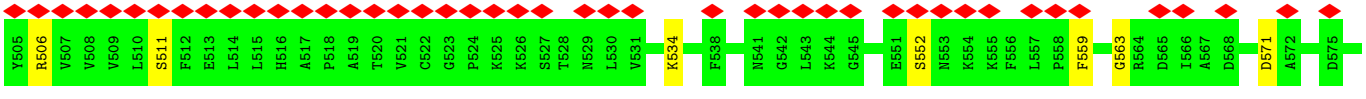


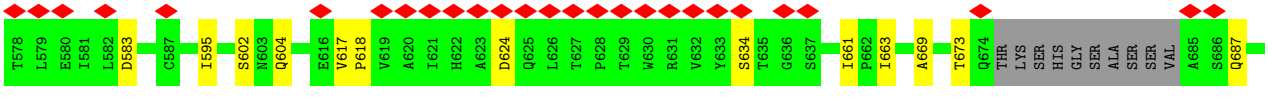


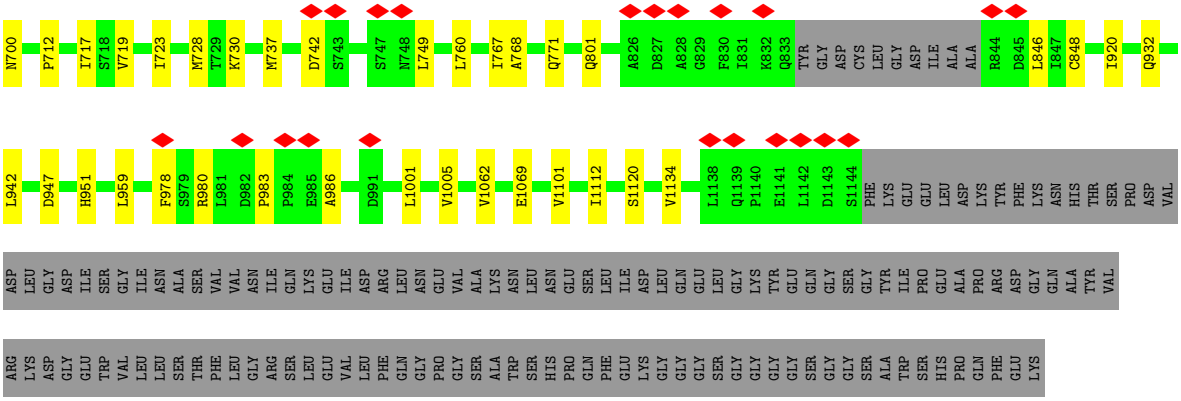






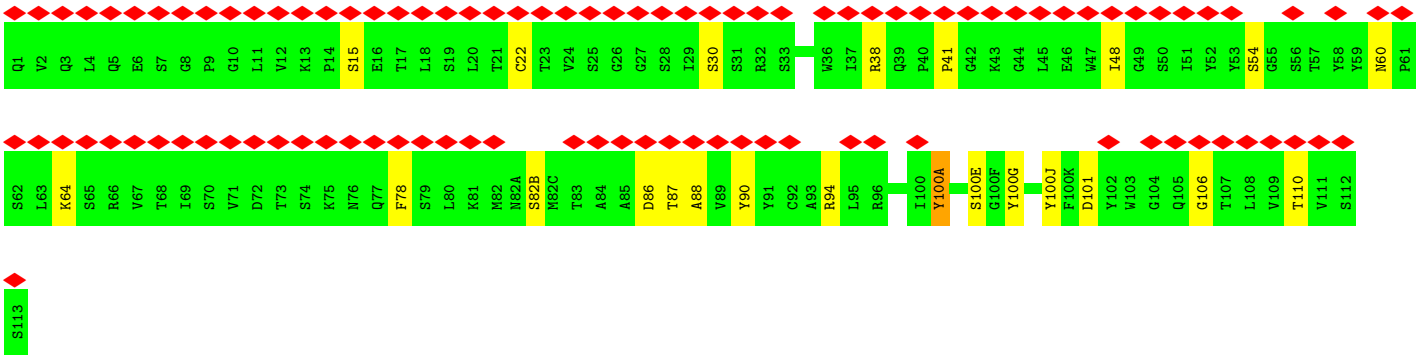






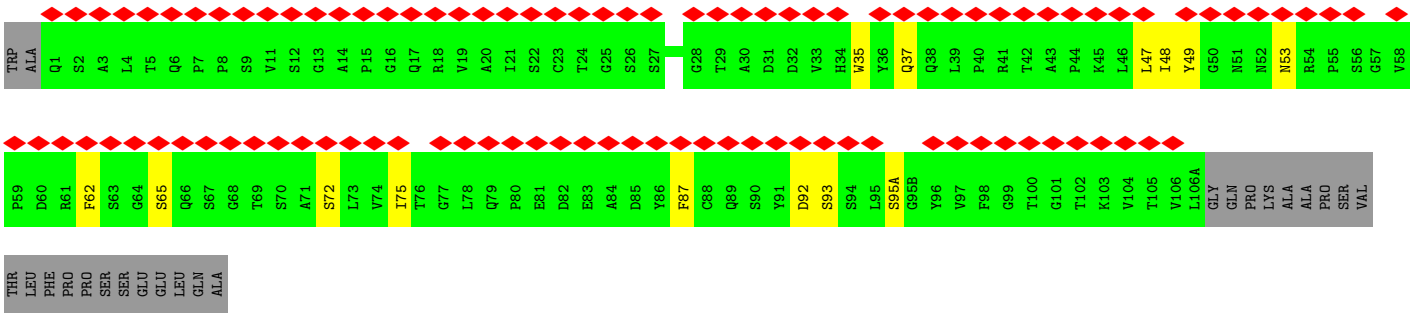
• Molecule 2: K501SP6 Fv Heavy Chain

Chain H:



• Molecule 3: K501SP6 Fv Light Chain

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87875	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	195000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.017	Depositor
Minimum map value	-0.614	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	367.616, 367.616, 367.616	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.718, 0.718, 0.718	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/8372	0.60	4/11383 (0.0%)
1	B	0.29	0/8416	0.58	0/11449
1	C	0.30	0/8484	0.59	1/11546 (0.0%)
2	H	0.34	0/1042	0.78	2/1417 (0.1%)
3	L	0.30	0/834	0.61	0/1139
All	All	0.30	0/27148	0.60	7/36934 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	H	0	1
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	101	ASP	CB-CG-OD1	8.76	126.19	118.30
1	A	998	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	756	PHE	CB-CG-CD1	5.35	124.55	120.80
1	C	184	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	756	PHE	CB-CG-CD2	-5.16	117.19	120.80
2	H	100(A)	TYR	CA-CB-CG	5.06	123.02	113.40
1	A	543	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	ARG	Sidechain
1	A	614	CYS	Peptide
2	H	100(J)	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8185	0	8036	107	0
1	B	8226	0	8074	120	0
1	C	8288	0	8131	64	0
2	H	1014	0	964	37	0
3	L	816	0	780	11	0
All	All	26529	0	25985	274	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 5.

All (274) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:LEU:HB2	2:H:64:LYS:CE	1.23	1.64
1:A:44:ARG:HH22	1:B:564:ARG:CA	1.18	1.52
1:A:48:LEU:CD1	1:A:303:PHE:HE1	1.21	1.50
1:A:48:LEU:HD11	1:A:303:PHE:CE1	1.51	1.45
1:A:44:ARG:HH22	1:B:564:ARG:N	1.09	1.44
1:A:44:ARG:NH2	1:B:564:ARG:H	1.10	1.43
1:B:579:LEU:CB	2:H:64:LYS:HE3	1.49	1.39
1:A:48:LEU:CD1	1:A:303:PHE:CE1	2.03	1.38
1:A:44:ARG:NH2	1:B:564:ARG:N	1.65	1.38
1:A:284:ASP:OD2	1:A:303:PHE:CE2	1.76	1.38
1:B:579:LEU:CB	2:H:64:LYS:CE	2.02	1.35
1:B:352:ARG:NH2	2:H:100(A):TYR:HE1	1.28	1.29
1:B:579:LEU:HB2	2:H:64:LYS:NZ	1.47	1.26
1:A:44:ARG:NH2	1:B:564:ARG:CA	1.97	1.25
1:B:558:PRO:HD3	3:L:93:SER:O	1.36	1.23
1:A:273:LEU:HD11	1:A:298:CYS:CA	1.70	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ARG:NH2	2:H:100(A):TYR:CE1	2.12	1.16
1:A:48:LEU:HD12	1:A:303:PHE:HE1	1.05	1.15
1:A:273:LEU:HD11	1:A:298:CYS:HA	1.14	1.13
1:B:579:LEU:CG	2:H:64:LYS:HE3	1.81	1.11
1:A:273:LEU:HG	1:A:298:CYS:SG	1.92	1.09
1:A:284:ASP:OD2	1:A:303:PHE:HE2	1.12	1.08
1:A:48:LEU:HD11	1:A:303:PHE:CD1	1.91	1.04
1:B:579:LEU:CB	2:H:64:LYS:NZ	2.15	1.04
1:A:44:ARG:NH2	1:B:564:ARG:CB	2.19	1.03
1:A:44:ARG:NH2	1:B:564:ARG:HB2	1.72	1.03
1:B:579:LEU:CA	2:H:64:LYS:NZ	2.25	0.99
1:A:273:LEU:CD1	1:A:298:CYS:HA	1.93	0.98
1:A:43:PHE:HE1	1:B:557:LEU:HD12	1.30	0.96
1:A:284:ASP:OD2	1:A:303:PHE:CD2	2.18	0.95
1:A:273:LEU:CG	1:A:298:CYS:SG	2.54	0.95
1:A:44:ARG:HH21	1:B:564:ARG:H	1.16	0.94
1:A:43:PHE:CZ	1:B:557:LEU:HB2	2.04	0.92
1:A:273:LEU:CD1	1:A:298:CYS:SG	2.59	0.91
1:A:43:PHE:CE1	1:B:557:LEU:HB2	2.08	0.89
1:B:579:LEU:CD1	2:H:64:LYS:HE3	2.04	0.88
1:A:43:PHE:CE1	1:B:557:LEU:HD12	2.09	0.87
1:B:579:LEU:HB2	2:H:64:LYS:HE3	0.89	0.87
1:B:579:LEU:HB2	2:H:64:LYS:HZ1	1.41	0.85
1:A:273:LEU:HD11	1:A:298:CYS:SG	2.16	0.84
1:A:44:ARG:HH22	1:B:564:ARG:C	1.76	0.83
1:B:558:PRO:CD	3:L:93:SER:O	2.26	0.80
1:A:44:ARG:CZ	1:B:564:ARG:HB2	2.12	0.79
1:C:17:ASN:N	1:C:134:CYS:HG	1.82	0.78
1:A:48:LEU:HD12	1:A:303:PHE:CE1	1.91	0.77
1:B:579:LEU:CG	2:H:64:LYS:CE	2.53	0.77
1:A:273:LEU:HD11	1:A:298:CYS:CB	2.16	0.76
1:B:579:LEU:HD12	2:H:64:LYS:HE3	1.67	0.76
1:B:579:LEU:C	2:H:64:LYS:NZ	2.43	0.72
1:A:293:LEU:HB2	1:A:605:VAL:HG11	1.73	0.70
1:C:110:SER:H	1:C:132:GLN:HE22	1.39	0.70
1:C:801:GLN:NE2	1:C:932:GLN:OE1	2.26	0.66
1:A:151:GLU:HB2	1:A:153:ARG:HE	1.62	0.65
1:A:761:LYS:HE3	1:B:311:GLN:HB3	1.79	0.65
1:B:579:LEU:CA	2:H:64:LYS:CE	2.75	0.63
1:A:41:LYS:NZ	1:B:516:HIS:O	2.32	0.63
1:B:436:ASN:HB3	1:B:505:TYR:HE1	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:MET:O	1:C:185:ARG:NH2	2.33	0.61
1:C:947:ASP:O	1:C:951:HIS:ND1	2.29	0.61
1:B:579:LEU:CB	2:H:64:LYS:HZ1	2.02	0.61
1:A:137:PRO:HB3	1:A:154:VAL:HA	1.83	0.60
1:B:170:PHE:HA	1:B:223:LEU:HD21	1.83	0.60
1:A:846:LEU:HG	1:A:848:CYS:H	1.66	0.60
1:C:624:ASP:HB3	1:C:634:SER:HB2	1.84	0.60
1:B:333:CYS:HA	1:B:358:CYS:HB3	1.84	0.60
1:A:43:PHE:CE1	1:B:557:LEU:CB	2.85	0.59
1:A:52:GLN:HG2	1:A:271:THR:HG22	1.85	0.59
1:C:109:ASP:OD1	1:C:132:GLN:NE2	2.36	0.58
2:H:22:CYS:HB3	2:H:78:PHE:HB3	1.84	0.58
1:B:947:ASP:O	1:B:951:HIS:ND1	2.31	0.58
1:C:104:PHE:HB2	1:C:115:LEU:HB3	1.85	0.58
1:B:564:ARG:NH2	1:B:568:ASP:OD1	2.35	0.58
1:C:198:ILE:HB	1:C:224:VAL:HB	1.85	0.58
1:A:222:PRO:HB2	2:H:100(G):TYR:HE2	1.68	0.57
1:A:293:LEU:HB2	1:A:605:VAL:CG1	2.35	0.57
1:B:441:LYS:O	1:B:503:GLN:N	2.38	0.57
1:B:379:VAL:HG21	1:B:387:LEU:HD11	1.87	0.57
1:C:393:TYR:HB2	1:C:511:SER:HB3	1.86	0.57
1:B:578:THR:O	2:H:64:LYS:HG2	2.05	0.57
1:B:289:ALA:HB1	1:B:632:VAL:HG11	1.87	0.56
1:A:760:LEU:HD21	1:A:1001:LEU:HB3	1.86	0.56
1:A:187:PHE:HA	1:A:199:TYR:O	2.06	0.56
1:A:784:GLN:HG2	1:B:698:ALA:HB3	1.85	0.56
1:A:719:VAL:HG22	1:A:1062:VAL:HG22	1.88	0.56
1:C:34:ARG:NH1	1:C:216:GLY:O	2.38	0.56
1:C:1112:ILE:HG22	1:C:1134:VAL:HG13	1.89	0.55
1:B:712:PRO:HG3	1:B:1066:PRO:HB3	1.88	0.55
1:B:381:PRO:HA	1:B:384:LEU:HD23	1.89	0.55
1:B:631:ARG:NH2	1:B:633:TYR:OH	2.40	0.55
1:A:380:SER:N	1:C:980:ARG:O	2.39	0.55
1:C:338:VAL:HG21	1:C:394:ALA:HB1	1.89	0.55
1:C:846:LEU:HG	1:C:848:CYS:H	1.71	0.54
1:B:557:LEU:HD22	3:L:93:SER:HB2	1.89	0.54
1:C:120:ASN:HB2	1:C:166:VAL:HG11	1.90	0.54
1:B:900:ALA:HB2	1:B:913:LEU:HD22	1.88	0.54
1:A:43:PHE:HE1	1:B:557:LEU:CD1	2.12	0.54
1:C:320:THR:OG1	1:C:534:LYS:NZ	2.38	0.54
1:A:43:PHE:CE1	1:B:557:LEU:CD1	2.86	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ARG:O	1:B:119:ASN:ND2	2.39	0.54
1:C:53:ASP:OD1	1:C:54:LEU:N	2.41	0.54
1:B:850:GLN:HG2	1:B:960:VAL:HG21	1.90	0.53
1:C:1101:VAL:HG23	1:C:1112:ILE:HG12	1.91	0.53
1:B:558:PRO:HG2	3:L:95(A):SER:OG	2.08	0.53
1:C:321:GLU:HG2	1:C:534:LYS:HZ2	1.72	0.53
1:B:441:LYS:HE3	1:B:444:GLY:HA2	1.89	0.53
1:A:44:ARG:HH21	1:B:564:ARG:N	1.80	0.53
1:A:225:ASP:HB2	2:H:100(E):SER:HB3	1.91	0.53
1:C:760:LEU:HD21	1:C:1001:LEU:HB3	1.91	0.53
1:B:579:LEU:N	2:H:64:LYS:CE	2.66	0.52
1:B:722:GLU:OE2	1:B:1025:LYS:NZ	2.34	0.52
1:C:115:LEU:HD12	1:C:126:ILE:HD13	1.92	0.52
1:A:46:SER:HA	1:A:276:TYR:O	2.09	0.52
2:H:38:ARG:NH1	2:H:86:ASP:OD1	2.42	0.52
1:B:357:ASN:ND2	2:H:54:SER:HB2	2.25	0.52
1:B:324:VAL:HG13	1:B:527:SER:HA	1.92	0.52
1:A:723:ILE:HG12	1:A:1058:VAL:HG22	1.91	0.52
1:C:617:VAL:HG22	1:C:618:PRO:HD2	1.92	0.52
1:A:287:ASP:HB2	1:A:290:LEU:HB3	1.92	0.51
1:B:1099:TRP:HB2	1:B:1132:ASN:HD22	1.75	0.51
1:B:619:VAL:HG13	1:B:639:VAL:HG21	1.92	0.51
1:B:974:LEU:HD13	1:B:990:ILE:HD12	1.93	0.51
1:A:44:ARG:CZ	1:B:564:ARG:CB	2.81	0.51
1:A:273:LEU:HD11	1:A:298:CYS:N	2.24	0.51
1:B:659:CYS:HB2	1:B:694:MET:HE3	1.92	0.51
2:H:87:THR:HG23	2:H:110:THR:HA	1.92	0.51
1:C:602:SER:OG	1:C:604:GLN:OE1	2.25	0.51
1:A:21:ARG:HD3	1:A:22:THR:H	1.76	0.50
1:B:753:TYR:OH	1:B:991:ASP:OD1	2.29	0.50
1:A:124:VAL:HB	1:A:169:PRO:HA	1.93	0.50
1:A:739:ILE:O	1:A:997:ARG:NH1	2.45	0.50
1:A:439:ASP:OD1	1:A:445:ASN:ND2	2.41	0.50
1:A:897:MET:HE1	1:B:1091:VAL:HG23	1.94	0.50
1:A:1112:ILE:HG22	1:A:1134:VAL:HG13	1.93	0.50
1:A:639:VAL:HG22	1:A:648:ILE:HG12	1.93	0.50
1:C:103:ILE:HB	1:C:236:GLN:HB2	1.93	0.50
1:B:850:GLN:NE2	1:B:957:ASN:OD1	2.45	0.50
1:C:983:PRO:HA	1:C:986:ALA:HB3	1.94	0.50
2:H:41:PRO:HD3	2:H:88:ALA:HA	1.92	0.50
1:A:213:LEU:HD12	1:A:214:PRO:HD2	1.92	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:THR:O	2:H:64:LYS:CG	2.60	0.49
1:B:419:ASN:ND2	1:B:464:ASP:O	2.41	0.49
1:C:208:ARG:HB3	1:C:210:PRO:HD2	1.93	0.49
1:A:288:CYS:HB3	1:A:295:GLU:HA	1.94	0.49
1:B:210:PRO:HG2	1:B:211:GLU:HG3	1.94	0.49
1:C:552:SER:HA	1:C:583:ASP:HB2	1.93	0.49
1:A:124:VAL:O	1:A:166:VAL:HA	2.12	0.49
1:B:90:PHE:HB3	1:B:187:PHE:HB2	1.95	0.49
1:C:719:VAL:HG22	1:C:1062:VAL:HG22	1.95	0.49
1:A:65:PHE:O	1:A:262:TYR:HB3	2.13	0.49
1:A:286:VAL:HG23	1:A:303:PHE:CE2	2.48	0.49
1:B:719:VAL:HG22	1:B:1062:VAL:HG22	1.95	0.49
1:C:33:THR:OG1	1:C:216:GLY:O	2.30	0.49
1:B:1101:VAL:HG23	1:B:1112:ILE:HG12	1.95	0.48
1:C:487:PHE:O	1:C:490:ARG:NH1	2.38	0.48
3:L:37:GLN:HB2	3:L:47:LEU:HD22	1.94	0.48
1:A:801:GLN:NE2	1:A:932:GLN:OE1	2.36	0.48
1:B:393:TYR:HB3	1:B:511:SER:HB2	1.95	0.48
1:C:207:VAL:HG12	1:C:208:ARG:HG2	1.96	0.48
1:B:366:TYR:HH	1:B:374:PHE:N	2.12	0.48
1:A:712:PRO:HA	1:A:1069:GLU:HA	1.96	0.48
1:C:140:ASP:OD2	1:C:153:ARG:NH2	2.40	0.48
3:L:65:SER:HG	3:L:72:SER:HG	1.61	0.48
1:A:128:VAL:HB	1:A:163:PHE:HB3	1.96	0.47
3:L:35:TRP:HA	3:L:87:PHE:O	2.14	0.47
1:A:46:SER:CA	1:A:276:TYR:O	2.63	0.47
1:A:54:LEU:HD12	1:A:190:LYS:HE3	1.96	0.47
1:A:739:ILE:HG12	1:A:997:ARG:HB3	1.96	0.47
1:B:91:ALA:HB3	1:B:263:TYR:HB2	1.96	0.47
1:B:579:LEU:HG	2:H:64:LYS:CE	2.40	0.47
1:B:784:GLN:OE1	1:C:700:ASN:ND2	2.43	0.47
1:A:79:ASN:HB3	1:A:239:LEU:HD23	1.97	0.47
1:A:983:PRO:O	1:A:987:GLU:HB2	2.14	0.47
1:C:728:MET:H	1:C:771:GLN:HG2	1.80	0.47
1:A:376:CYS:HA	1:A:429:CYS:HA	1.96	0.47
1:C:64:TRP:HE1	1:C:261:ALA:HA	1.80	0.47
1:C:742:ASP:OD1	1:C:742:ASP:N	2.48	0.47
1:A:43:PHE:CE1	1:B:557:LEU:CG	2.97	0.47
1:A:972:SER:OG	1:B:568:ASP:OD2	2.33	0.47
1:B:801:GLN:OE1	1:B:932:GLN:NE2	2.42	0.47
1:A:316:ARG:HH21	1:C:737:MET:HG2	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ALA:HB3	1:A:263:TYR:HB2	1.97	0.46
1:A:324:VAL:H	1:A:528:THR:HB	1.79	0.46
1:B:578:THR:HA	2:H:64:LYS:HG3	1.98	0.46
1:B:402:ASP:O	1:B:406:GLN:NE2	2.48	0.46
1:B:642:THR:HG22	1:B:644:ALA:H	1.81	0.46
1:C:57:PRO:HB2	1:C:60:SER:HB2	1.97	0.46
1:C:453:PHE:HB2	1:C:488:PRO:HB3	1.98	0.46
2:H:15:SER:HA	2:H:82(B):SER:HA	1.96	0.46
1:A:405:ARG:HG3	1:A:406:GLN:HG3	1.98	0.46
1:B:418:TYR:HB3	1:B:454:ARG:HD3	1.98	0.46
1:A:673:THR:HG22	1:A:687:GLN:HG2	1.97	0.46
1:A:287:ASP:OD1	1:A:287:ASP:N	2.49	0.46
1:B:324:VAL:HG23	1:B:539:ASN:HB3	1.97	0.45
2:H:48:ILE:HA	2:H:60:ASN:HB2	1.97	0.45
1:A:506:ARG:NH1	1:A:507:VAL:O	2.50	0.45
1:C:563:GLY:O	1:C:571:ASP:N	2.47	0.45
2:H:90:TYR:O	2:H:106:GLY:HA2	2.16	0.45
1:C:170:PHE:HE1	1:C:198:ILE:HG21	1.82	0.45
1:A:380:SER:HB3	1:A:383:LYS:HB2	1.98	0.45
1:B:579:LEU:C	2:H:64:LYS:HZ1	2.18	0.45
1:C:712:PRO:HA	1:C:1069:GLU:HA	1.98	0.45
1:C:102:TRP:HB2	1:C:117:ILE:HB	1.98	0.45
1:B:315:PHE:HA	1:B:631:ARG:HD3	1.99	0.45
1:B:37:TYR:HA	1:B:220:LEU:H	1.81	0.45
2:H:30:SER:OG	2:H:94:ARG:NE	2.41	0.45
1:B:543:LEU:HD11	1:B:570:THR:HG21	1.97	0.45
1:C:959:LEU:HD11	1:C:1001:LEU:HD23	1.98	0.45
1:A:87:GLY:HA2	1:A:189:PHE:O	2.17	0.44
1:C:436:ASN:HD21	1:C:503:GLN:HG2	1.82	0.44
1:A:728:MET:HG3	1:A:952:ASN:HD21	1.82	0.44
1:B:41:LYS:HG2	1:C:559:PHE:HD2	1.82	0.44
1:B:579:LEU:HD12	2:H:64:LYS:CE	2.44	0.44
1:B:579:LEU:N	2:H:64:LYS:HE2	2.23	0.44
1:A:106:THR:O	1:A:234:ARG:NH2	2.51	0.44
1:A:593:SER:HB2	1:A:608:LEU:HB3	2.00	0.44
1:A:723:ILE:HD13	1:A:942:LEU:HD13	1.99	0.44
1:C:730:LYS:HD2	1:C:768:ALA:HB1	2.00	0.44
1:C:398:VAL:HG22	1:C:506:ARG:HG2	2.00	0.44
3:L:35:TRP:HB2	3:L:48:ILE:HG22	2.00	0.44
1:B:595:ILE:HG23	1:B:661:ILE:HG21	2.00	0.44
1:B:97:ASN:ND2	1:B:173:ASP:OD1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HD11	1:C:980:ARG:HA	2.00	0.43
1:A:730:LYS:HD2	1:A:768:ALA:HB1	2.01	0.43
1:B:712:PRO:HA	1:B:1069:GLU:HA	2.00	0.43
1:B:721:THR:HG23	1:B:931:ILE:HD12	2.00	0.43
1:B:911:ASN:ND2	1:B:1108:GLU:OE2	2.47	0.43
3:L:49:TYR:O	3:L:53:ASN:N	2.49	0.43
1:A:614:CYS:HB3	1:A:646:CYS:HB3	1.88	0.43
1:B:579:LEU:HG	2:H:64:LYS:HE2	1.99	0.43
1:C:767:ILE:O	1:C:771:GLN:OE1	2.37	0.43
1:A:120:ASN:O	1:A:122:THR:N	2.51	0.43
1:A:663:ILE:HD11	1:A:669:ALA:HB2	2.01	0.43
1:B:730:LYS:HD2	1:B:768:ALA:HB1	2.00	0.43
1:B:593:SER:HB2	1:B:608:LEU:HB3	1.99	0.43
1:C:673:THR:HG22	1:C:687:GLN:HG2	1.99	0.43
1:A:46:SER:N	1:A:276:TYR:O	2.52	0.43
1:B:773:LYS:NZ	1:B:777:GLU:OE2	2.43	0.43
1:B:469:ILE:HG12	1:B:487:PHE:HB2	1.99	0.42
1:A:140:ASP:OD2	1:A:140:ASP:N	2.52	0.42
1:A:106:THR:OG1	1:A:107:THR:N	2.52	0.42
1:B:295:GLU:OE1	1:B:633:TYR:OH	2.31	0.42
1:C:112:THR:HA	1:C:130:GLU:HA	2.00	0.42
1:A:102:TRP:CD1	1:A:237:THR:HG22	2.55	0.42
1:A:139:LEU:HD23	1:A:238:LEU:HB3	2.02	0.42
1:A:383:LYS:NZ	1:C:978:PHE:O	2.43	0.42
1:B:128:VAL:HG21	1:B:228:ILE:HG21	2.02	0.42
1:B:608:LEU:HD22	1:B:663:ILE:HG23	2.02	0.42
1:B:435:SER:OG	1:B:504:PRO:O	2.31	0.41
1:C:760:LEU:HG	1:C:1005:VAL:HG21	2.02	0.41
1:C:595:ILE:HG23	1:C:661:ILE:HG21	2.02	0.41
1:C:723:ILE:HD13	1:C:942:LEU:HD23	2.01	0.41
1:A:56:LEU:HD12	1:A:57:PRO:HD2	2.02	0.41
1:B:424:ASP:OD1	1:B:424:ASP:N	2.53	0.41
1:A:414:ASN:O	1:A:417:ASP:N	2.53	0.41
1:B:292:PRO:HG2	1:B:605:VAL:HG21	2.02	0.41
1:C:131:PHE:HB3	1:C:133:PHE:CZ	2.55	0.41
1:C:749:LEU:HD11	1:C:978:PHE:HZ	1.86	0.41
3:L:92:ASP:OD2	3:L:95(A):SER:N	2.53	0.41
1:B:106:THR:HA	1:B:233:THR:H	1.86	0.41
3:L:62:PHE:CD1	3:L:75:ILE:HG12	2.56	0.41
1:A:942:LEU:HD12	1:A:945:LEU:HD12	2.02	0.41
1:B:421:LYS:HB3	1:B:460:PRO:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:GLY:HA2	1:A:586:PRO:HA	2.03	0.41
1:A:819:LEU:HD22	1:A:942:LEU:HD11	2.02	0.41
1:B:183:ASN:HA	1:B:204:PRO:HA	2.02	0.41
1:B:1025:LYS:O	1:B:1029:CYS:HB2	2.21	0.41
1:C:17:ASN:N	1:C:134:CYS:SG	2.91	0.41
1:C:663:ILE:HD11	1:C:669:ALA:HB2	2.03	0.41
1:B:427:THR:OG1	1:B:512:PHE:O	2.34	0.40
1:B:449:LEU:HA	1:B:491:SER:HA	2.03	0.40
1:C:717:ILE:HG13	1:C:920:ILE:HG23	2.03	0.40
1:B:911:ASN:ND2	1:C:1120:SER:OG	2.54	0.40
1:C:34:ARG:HH21	1:C:214:PRO:HG2	1.87	0.40
1:B:663:ILE:HD11	1:B:669:ALA:HB2	2.03	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	1014/1277 (79%)	976 (96%)	38 (4%)	0	100	100
1	B	1027/1277 (80%)	986 (96%)	41 (4%)	0	100	100
1	C	1039/1277 (81%)	989 (95%)	50 (5%)	0	100	100
2	H	127/129 (98%)	114 (90%)	13 (10%)	0	100	100
3	L	109/134 (81%)	99 (91%)	10 (9%)	0	100	100
All	All	3316/4094 (81%)	3164 (95%)	152 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	919/1108 (83%)	908 (99%)	11 (1%)	71 85
1	B	923/1108 (83%)	923 (100%)	0	100 100
1	C	929/1108 (84%)	928 (100%)	1 (0%)	93 97
2	H	112/112 (100%)	112 (100%)	0	100 100
3	L	91/109 (84%)	91 (100%)	0	100 100
All	All	2974/3545 (84%)	2962 (100%)	12 (0%)	91 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	21	ARG
1	A	140	ASP
1	A	151	GLU
1	A	153	ARG
1	A	287	ASP
1	A	288	CYS
1	A	290	LEU
1	A	291	ASP
1	A	295	GLU
1	A	975	ASN
1	C	454	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	132	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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.

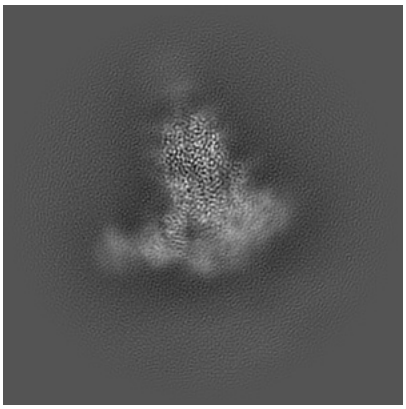
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50503. These allow visual inspection of the internal detail of the map and identification of artifacts.

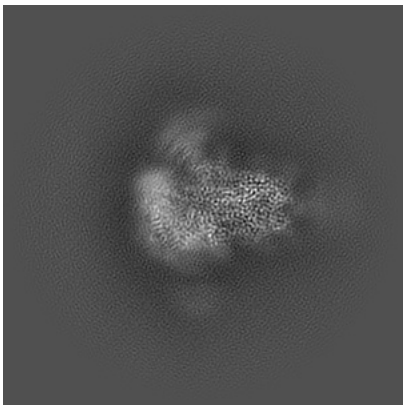
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

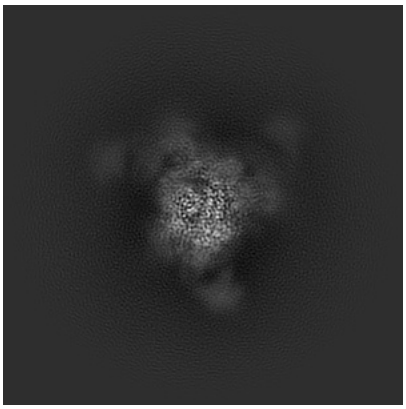
6.1.1 Primary map



X

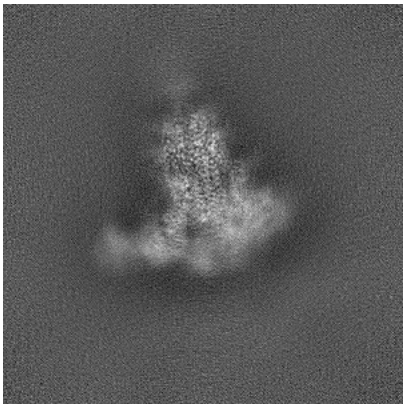


Y

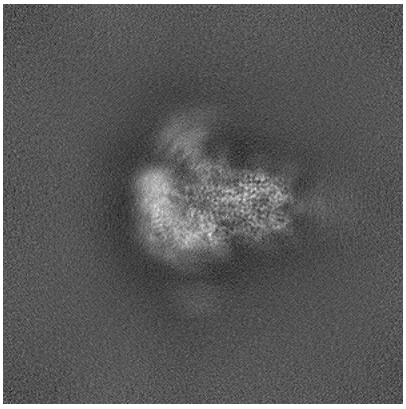


Z

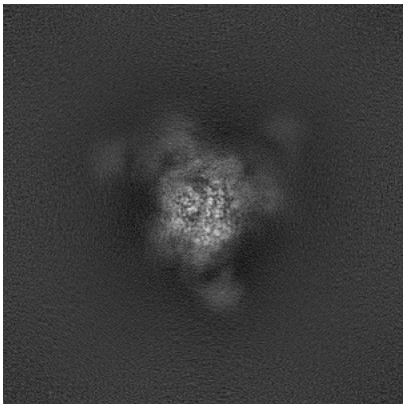
6.1.2 Raw map



X



Y

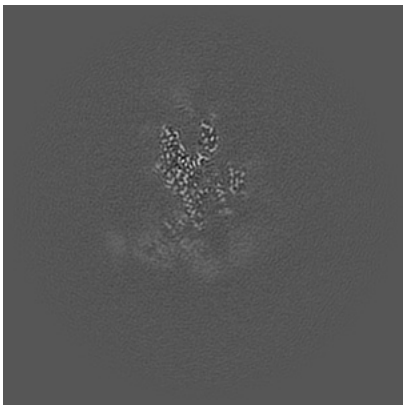


Z

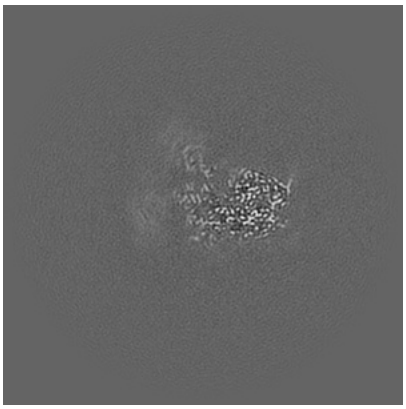
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

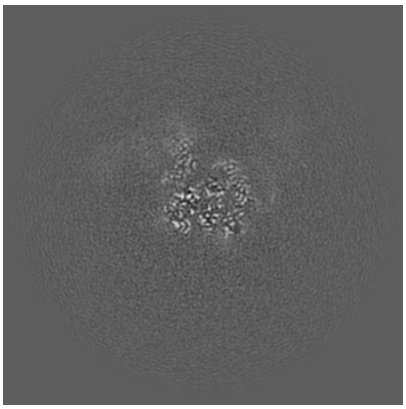
6.2.1 Primary map



X Index: 256

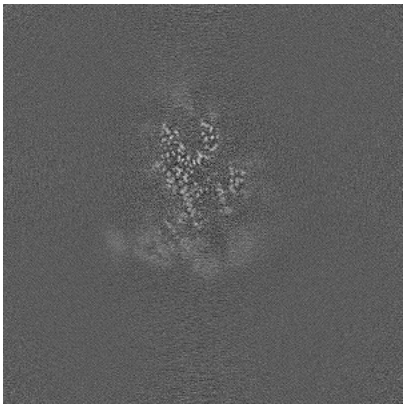


Y Index: 256

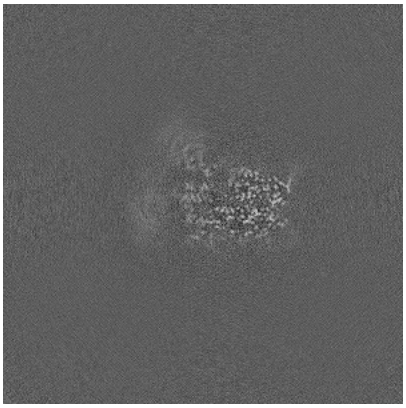


Z Index: 256

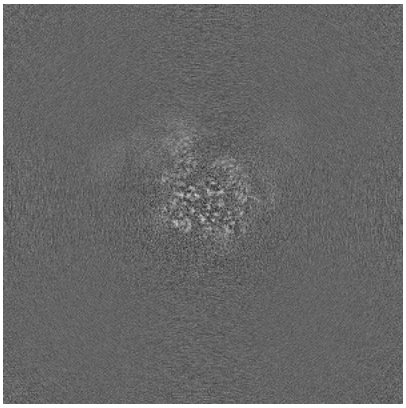
6.2.2 Raw map



X Index: 256



Y Index: 256

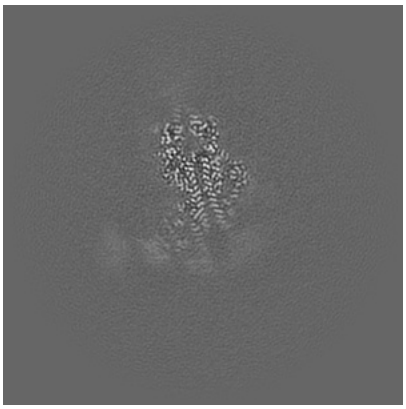


Z Index: 256

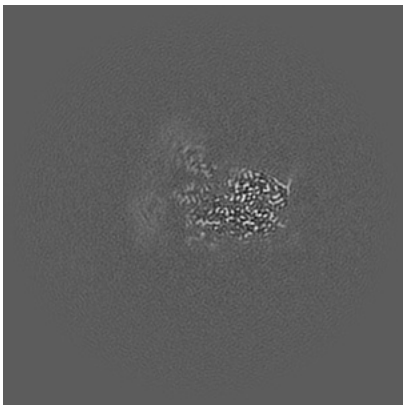
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

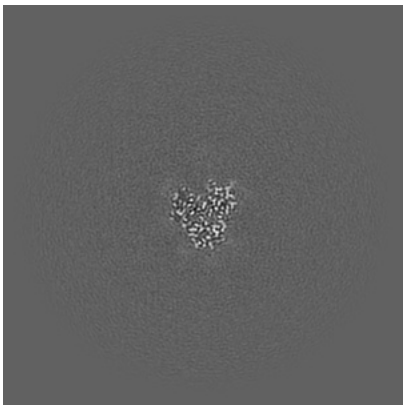
6.3.1 Primary map



X Index: 263

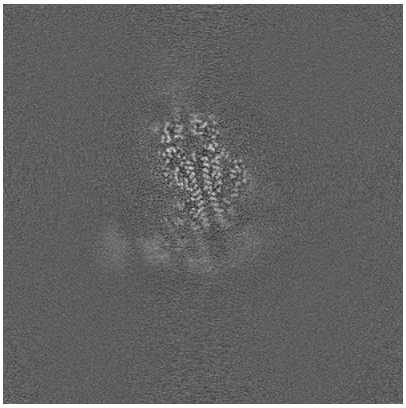


Y Index: 257

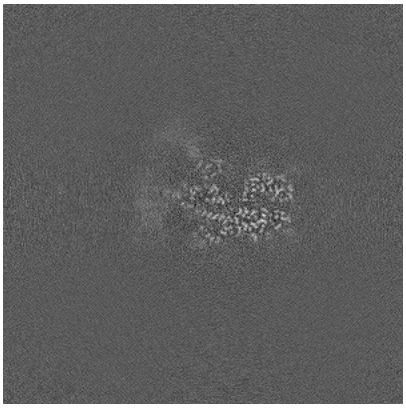


Z Index: 317

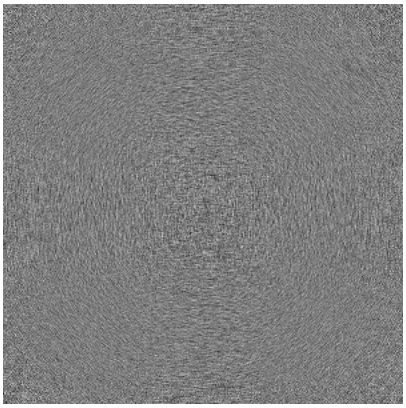
6.3.2 Raw map



X Index: 263



Y Index: 247

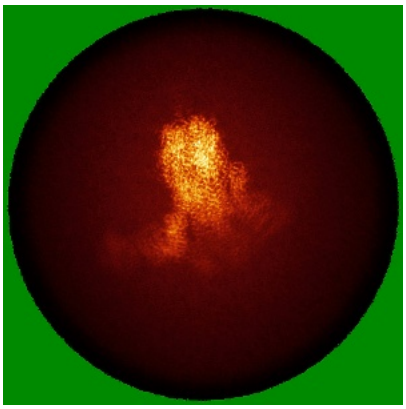


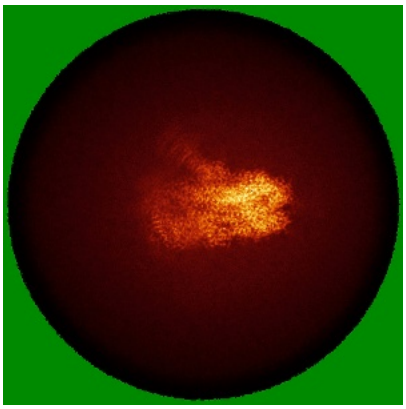
Z Index: 0

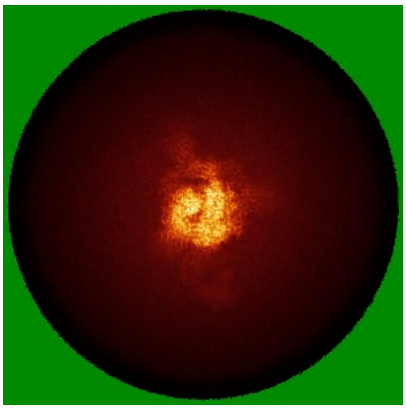
The images above show the largest variance slices of the map in three orthogonal directions.

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

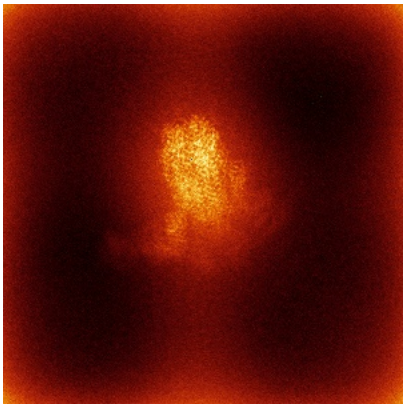
6.4.1 Primary map

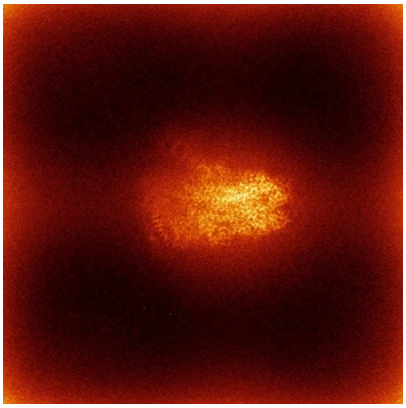

X

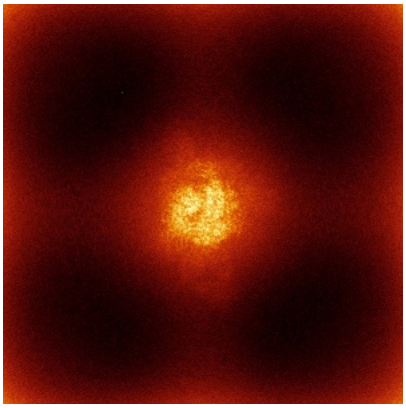

Y


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 0.1. 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.

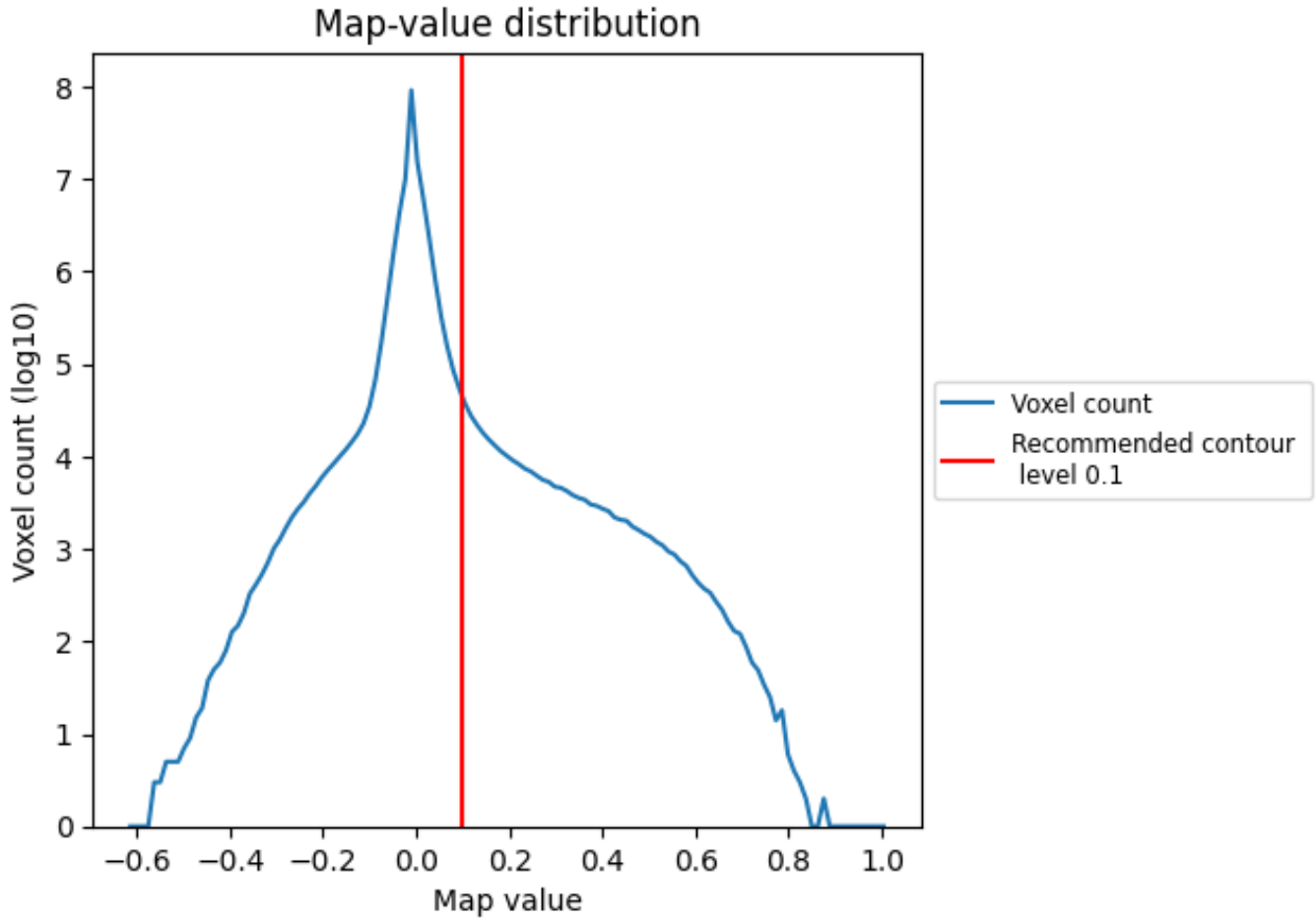
6.6 Mask visualisation (i)

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

7 Map analysis

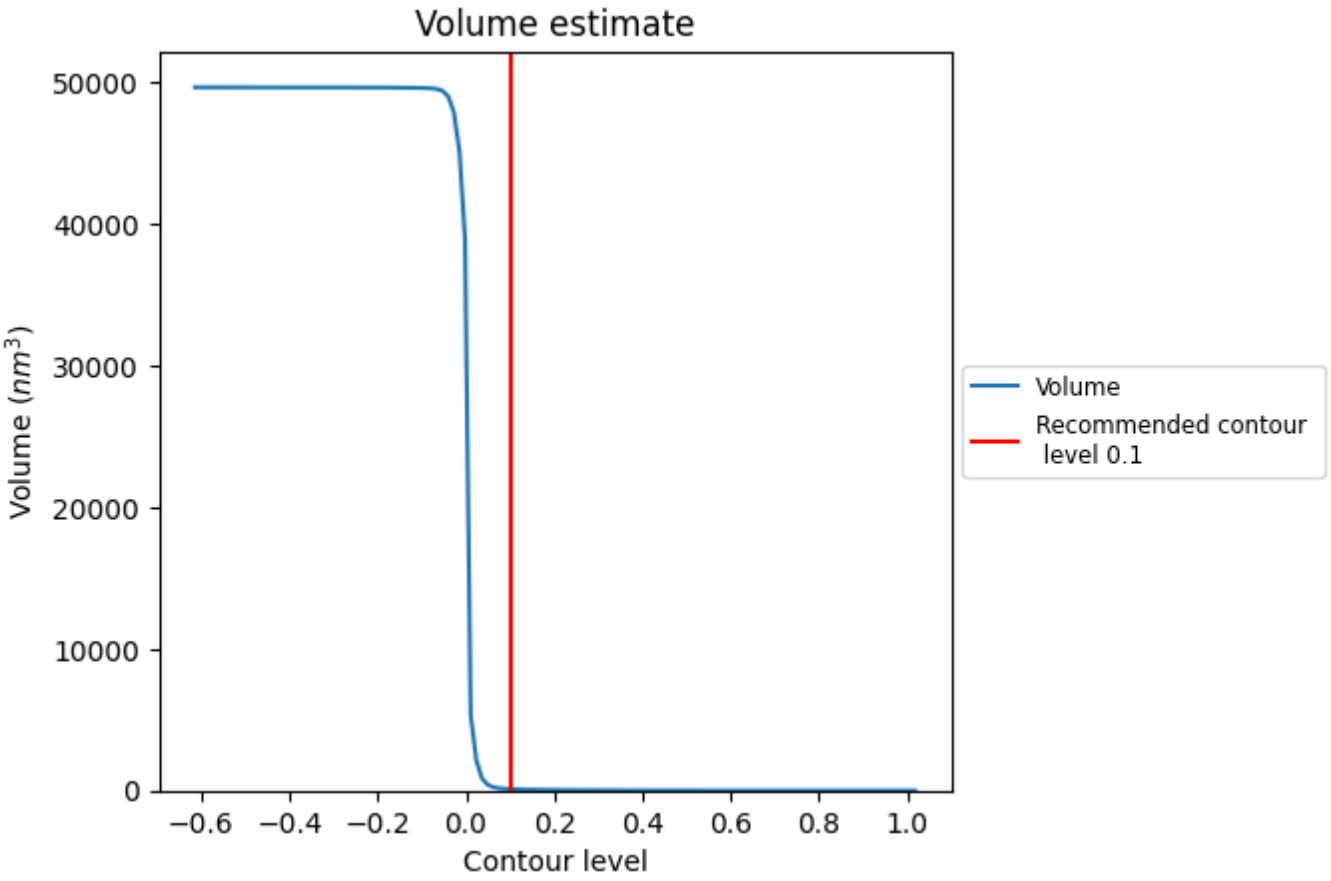
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

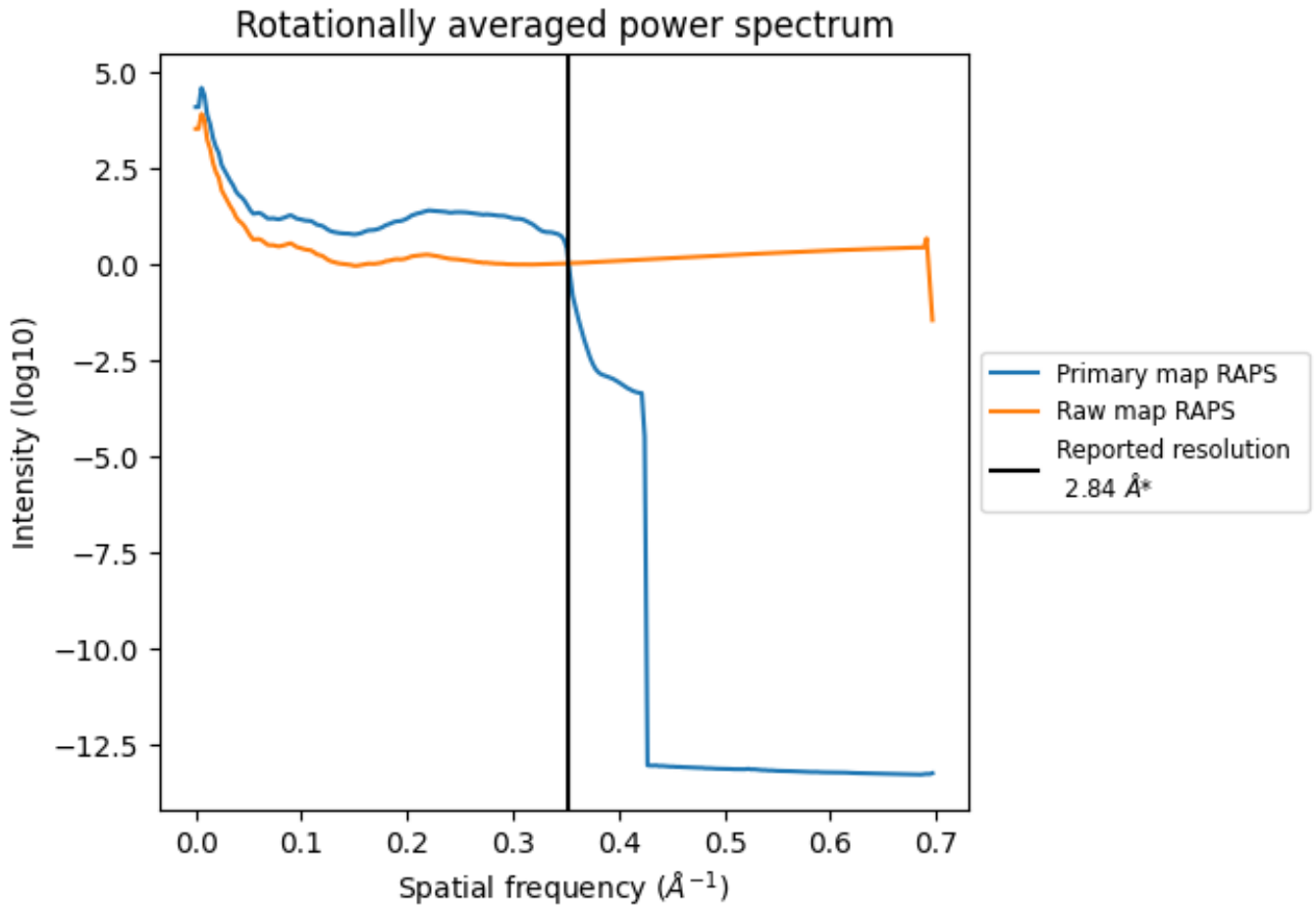
7.2 Volume estimate



The volume at the recommended contour level is 104 nm^3; this corresponds to an approximate mass of 94 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 (i)

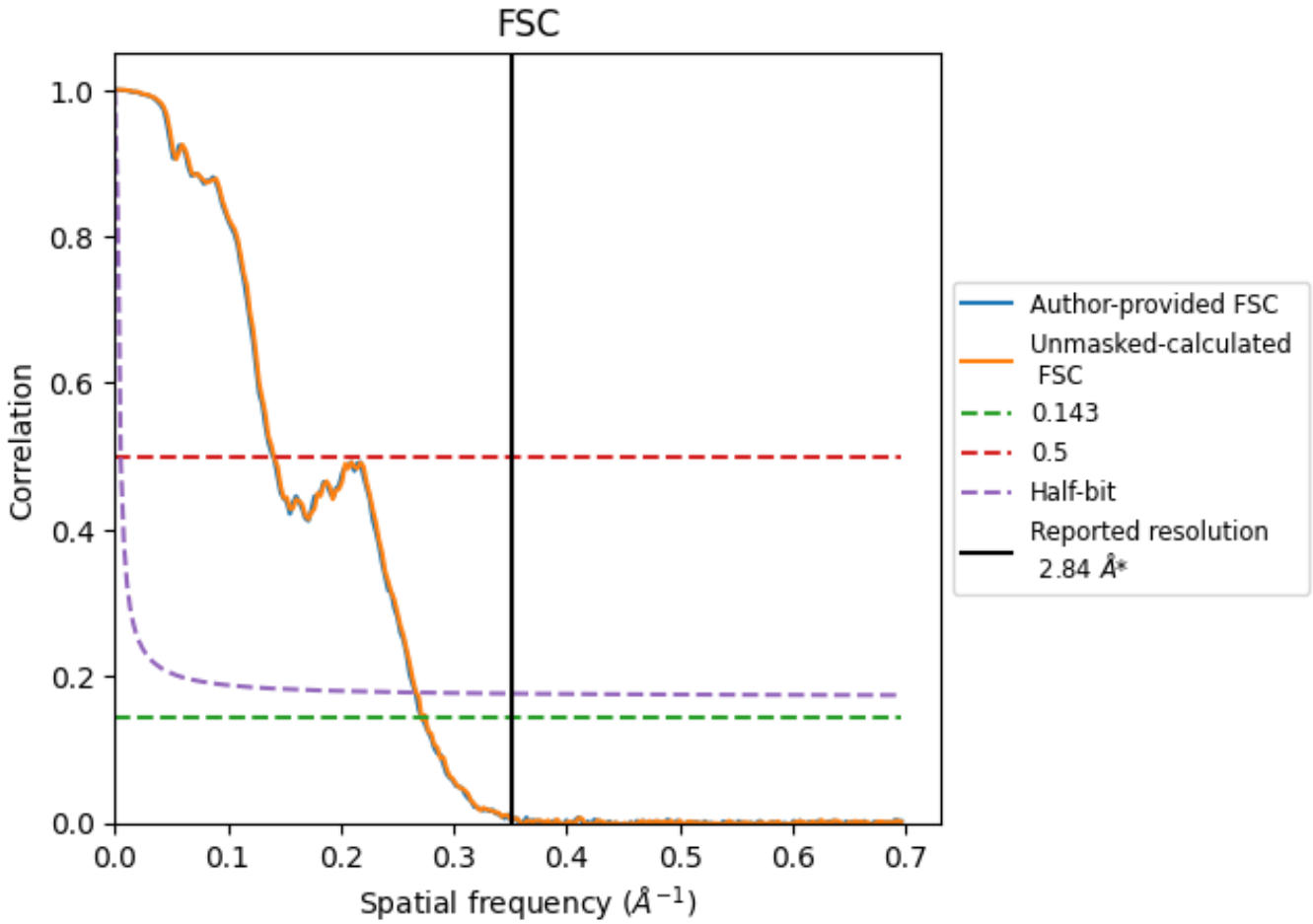


*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	2.84	-
Author-provided FSC curve	3.67	7.14	3.76
Unmasked-calculated*	3.68	7.10	3.75

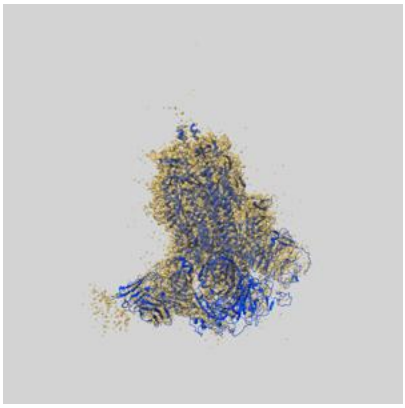
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.5 CUT-OFF 7.14 differs from the reported value 2.84 by more than 10 %

The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 7.10 differs from the reported value 2.84 by more than 10 %

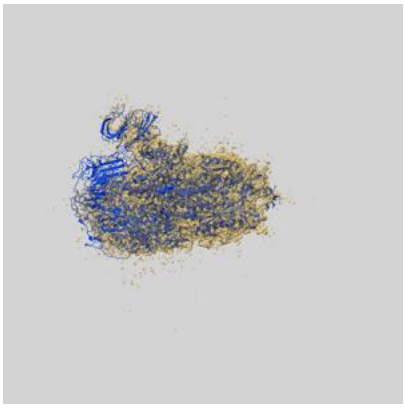
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50503 and PDB model 9FJK. Per-residue inclusion information can be found in section 3 on page 11.

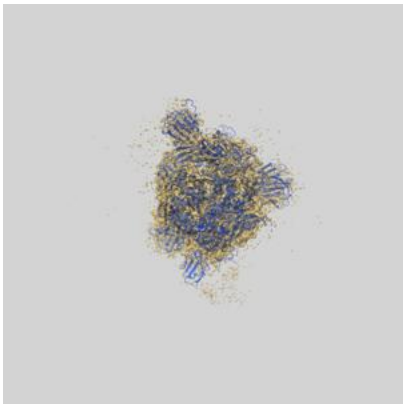
9.1 Map-model overlay



X



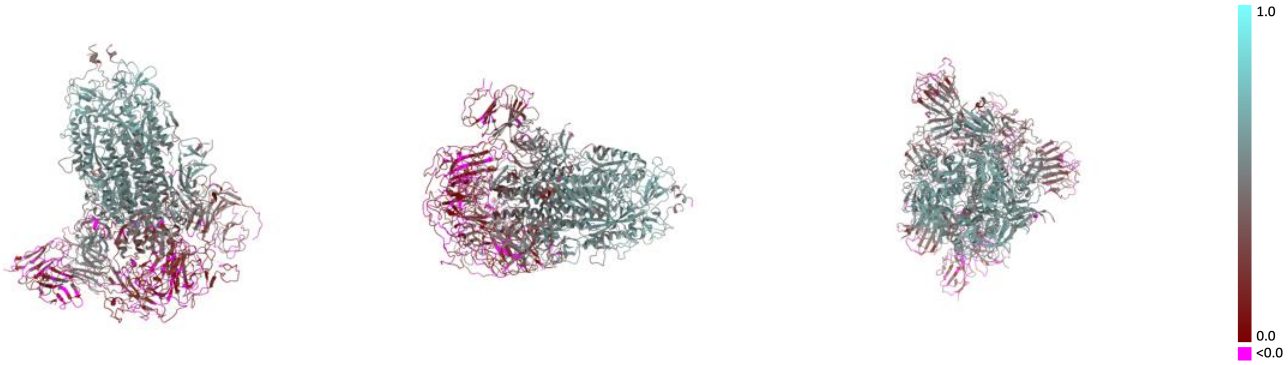
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

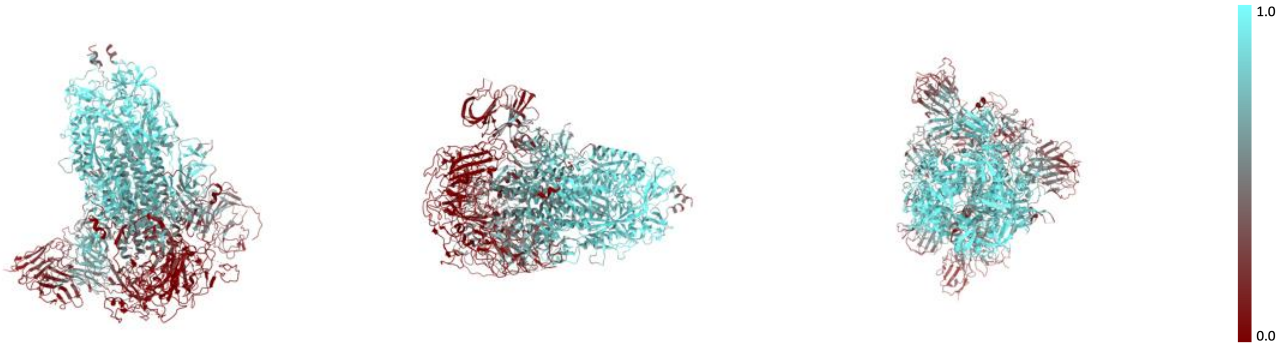
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

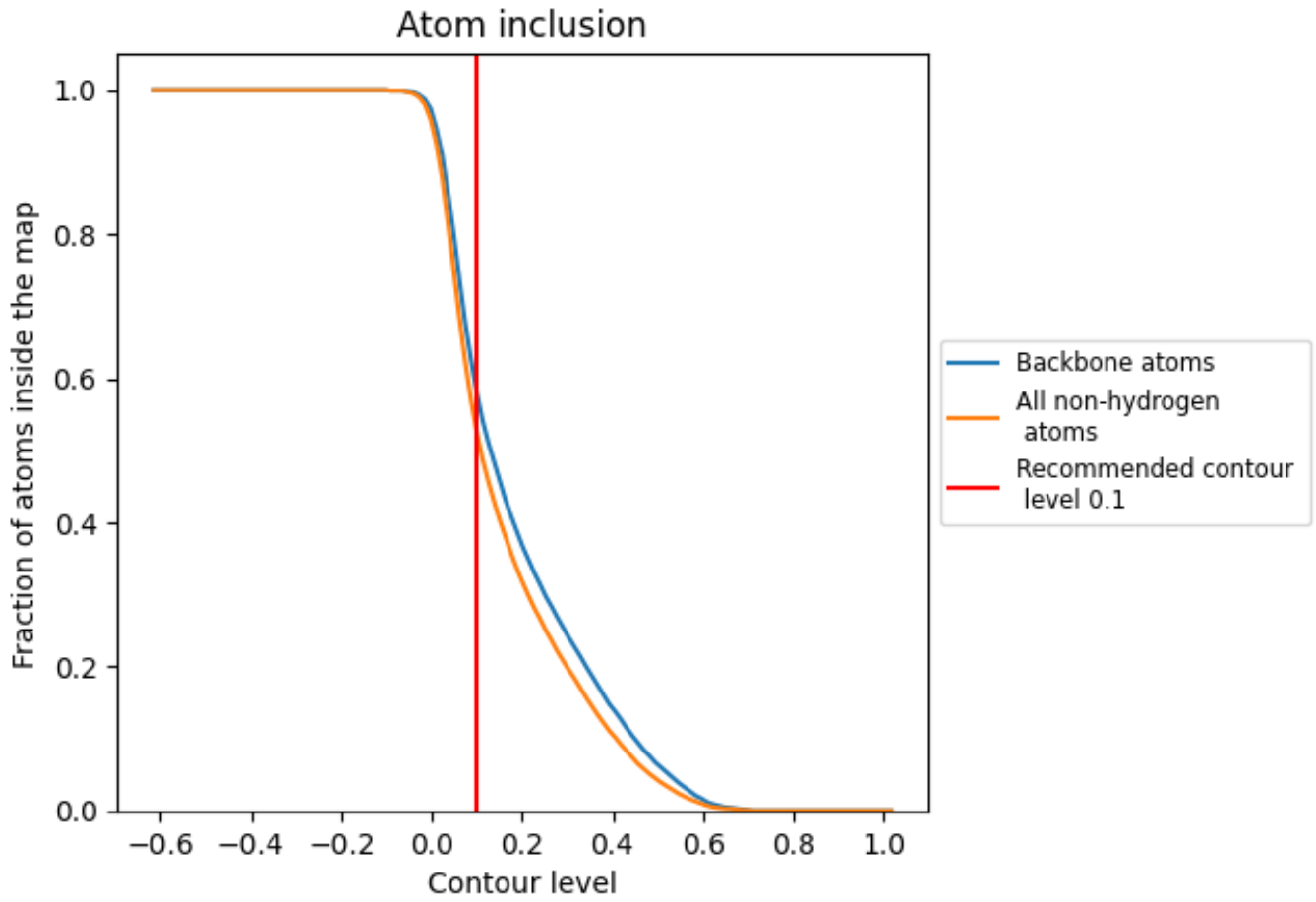
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 52% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5250	0.3730
A	0.5980	0.4060
B	0.5420	0.3950
C	0.5170	0.3770
H	0.1860	0.1120
L	0.1020	0.0960