Full wwPDB EM Validation Report

Aug 16, 2026 – 02:30 PM EDT

PDB ID	:	9BHH / pdb_00009bhh
EMDB ID	:	EMD-44547
Title	:	Cryo-EM structure of Chikungunya virus asymmetric unit with Fab IM-CKV063
Authors	:	Su, G.C.; Galaz-Montoya, J.G.; Pintilie, G.; Jin, J.; Chiu, W.
Deposited on	:	2024-04-20
Resolution	:	3.50 Å(reported)
Based on initial model	:	8FCG

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 (i) 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 (i)) were used in the production of this report:

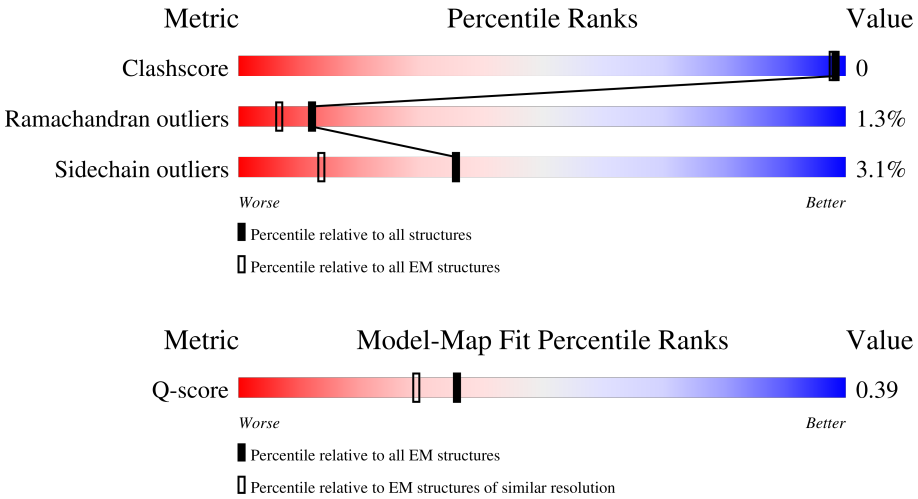
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	438	96%
1	B	438	95%
1	C	438	97%
1	D	438	96%

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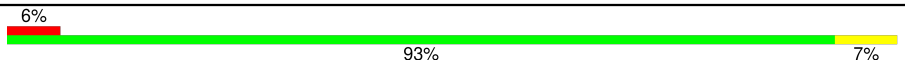
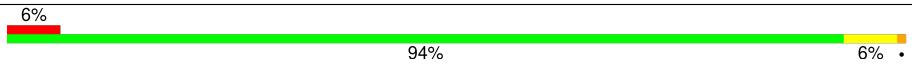
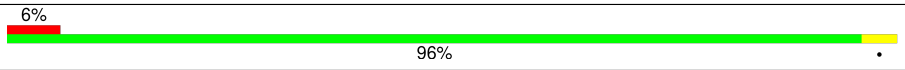
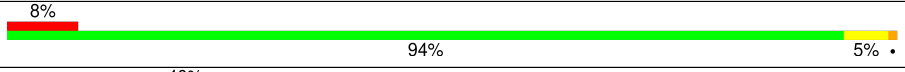
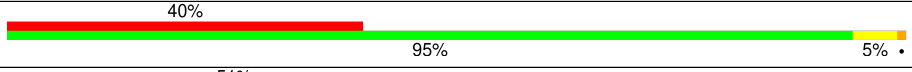
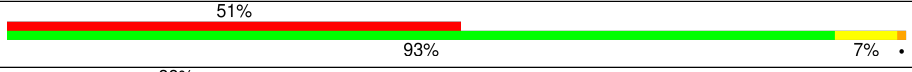
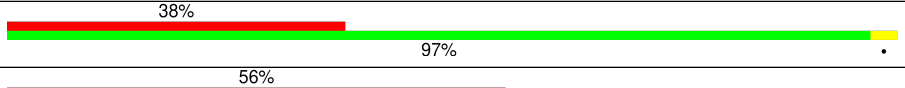
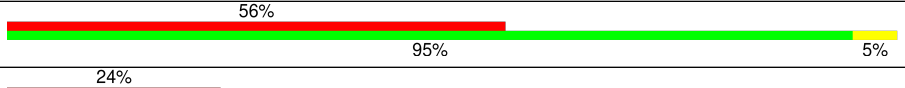
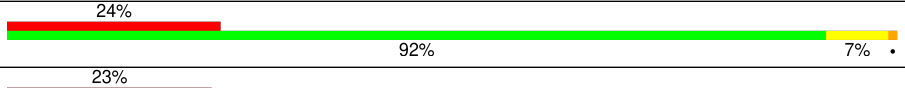
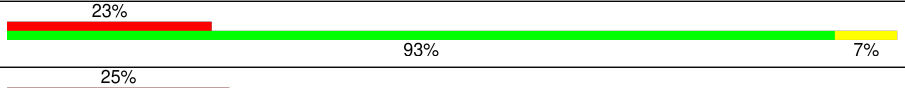
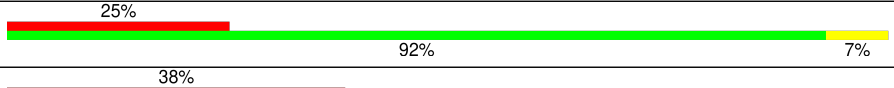
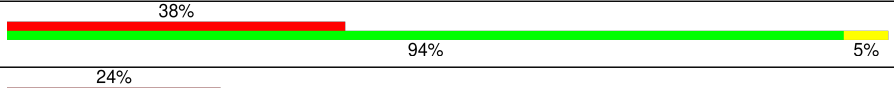
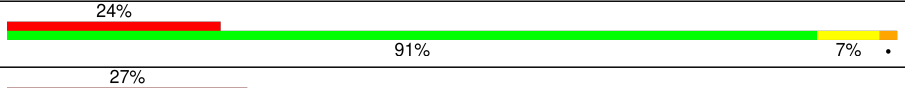
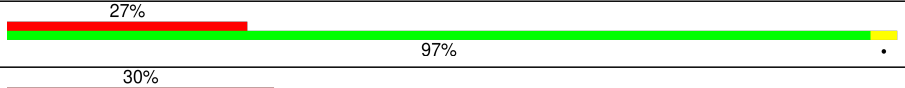
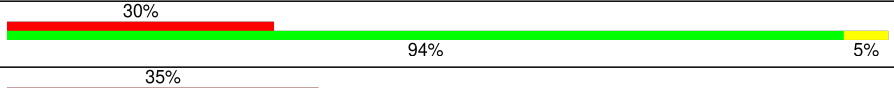
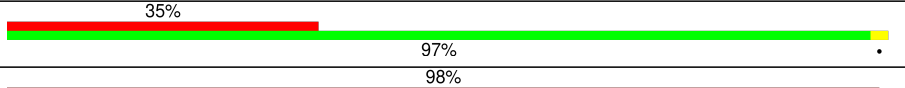
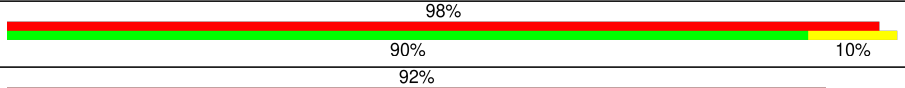
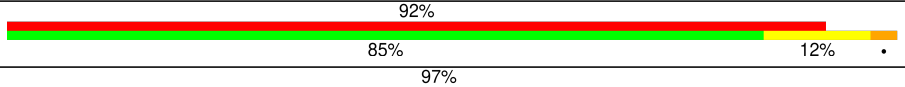
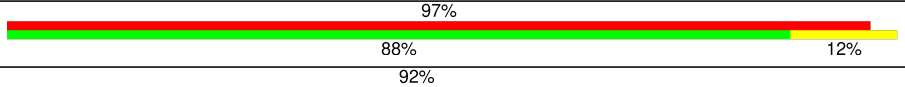
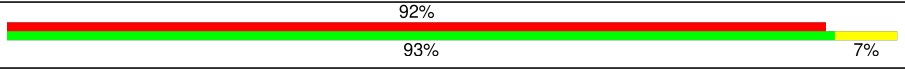
Mol	Chain	Length	Quality of chain
2	E	418	
2	F	418	
2	G	418	
2	H	418	
3	I	151	
3	J	151	
3	K	151	
3	L	151	
4	M	213	
4	O	213	
4	Q	213	
4	S	213	
5	N	242	
5	P	242	
5	R	242	
5	T	242	
6	U	60	
6	V	60	
6	W	60	
6	X	60	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 92756 atoms, of which 45956 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 E1 glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	438	Total	C	H	N	O	S	0	0
			6574	2100	3258	553	636	27		
1	B	438	Total	C	H	N	O	S	0	0
			6574	2100	3258	553	636	27		
1	C	438	Total	C	H	N	O	S	0	0
			6573	2100	3257	553	636	27		
1	D	438	Total	C	H	N	O	S	0	0
			6573	2100	3257	553	636	27		

- Molecule 2 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	418	Total	C	H	N	O	S	0	0
			6532	2064	3243	591	606	28		
2	F	418	Total	C	H	N	O	S	0	0
			6530	2064	3241	591	606	28		
2	G	418	Total	C	H	N	O	S	0	0
			6532	2064	3243	591	606	28		
2	H	418	Total	C	H	N	O	S	0	0
			6532	2064	3243	591	606	28		

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	J	151	Total	C	H	N	O	S	0	0
			2294	730	1138	204	217	5		
3	I	151	Total	C	H	N	O	S	0	0
			2294	730	1138	204	217	5		
3	K	151	Total	C	H	N	O	S	0	0
			2294	730	1138	204	217	5		
3	L	151	Total	C	H	N	O	S	0	0
			2294	730	1138	204	217	5		

- Molecule 4 is a protein called Light chain of IM-CKV063.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	M	213	Total	C	H	N	O	S	0	0
			3235	1026	1586	284	334	5		
4	O	213	Total	C	H	N	O	S	0	0
			3235	1026	1586	284	334	5		
4	Q	213	Total	C	H	N	O	S	0	0
			3242	1026	1593	284	334	5		
4	S	213	Total	C	H	N	O	S	0	0
			3254	1026	1605	284	334	5		

- Molecule 5 is a protein called Heavy Chain of IM-CKV063.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	N	242	Total	C	H	N	O	S	0	0
			3592	1146	1782	297	361	6		
5	P	242	Total	C	H	N	O	S	0	0
			3595	1146	1785	297	361	6		
5	R	242	Total	C	H	N	O	S	0	0
			3599	1146	1789	297	361	6		
5	T	242	Total	C	H	N	O	S	0	0
			3600	1146	1790	297	361	6		

- Molecule 6 is a protein called E3 glycoprotein.

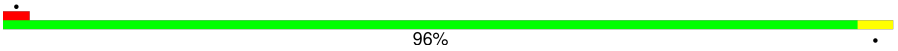
Mol	Chain	Residues	Atoms						AltConf	Trace
6	U	60	Total	C	H	N	O	S	0	0
			952	297	472	84	90	9		
6	V	60	Total	C	H	N	O	S	0	0
			952	297	472	84	90	9		
6	W	60	Total	C	H	N	O	S	0	0
			952	297	472	84	90	9		
6	X	60	Total	C	H	N	O	S	0	0
			952	297	472	84	90	9		

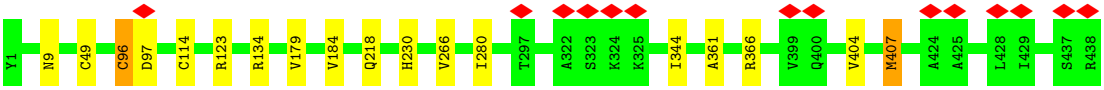
3 Residue-property plots (i)

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: E1 glycoprotein

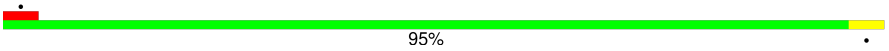
Chain A:

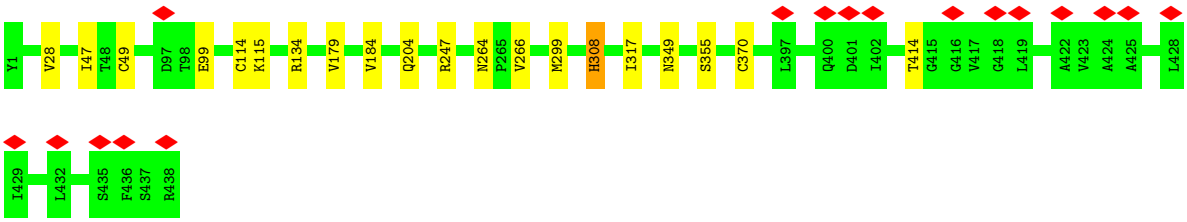




• Molecule 1: E1 glycoprotein

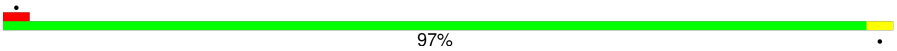
Chain B:

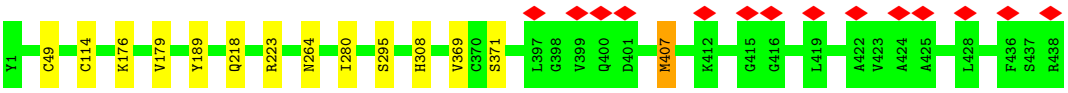




• Molecule 1: E1 glycoprotein

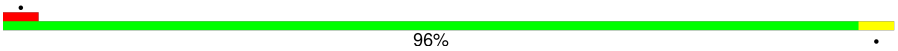
Chain C:

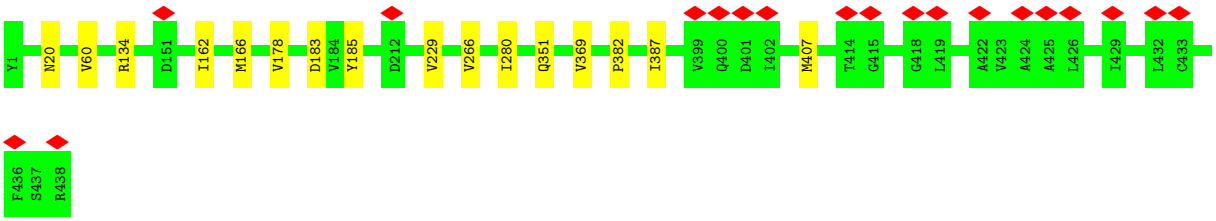




• Molecule 1: E1 glycoprotein

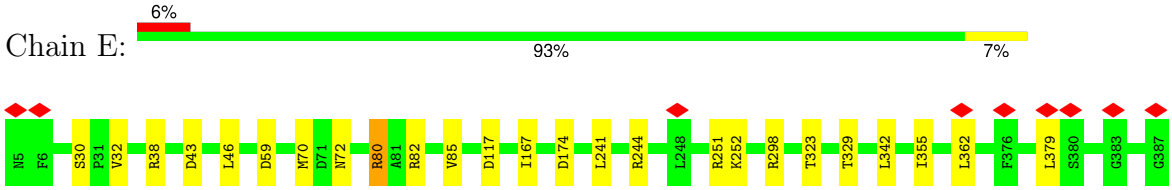
Chain D:





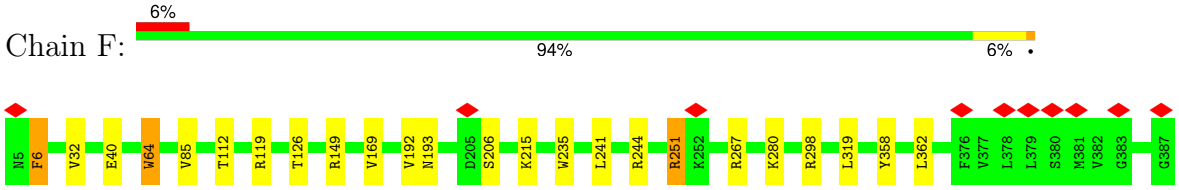
• Molecule 2: E2 glycoprotein

Chain E:



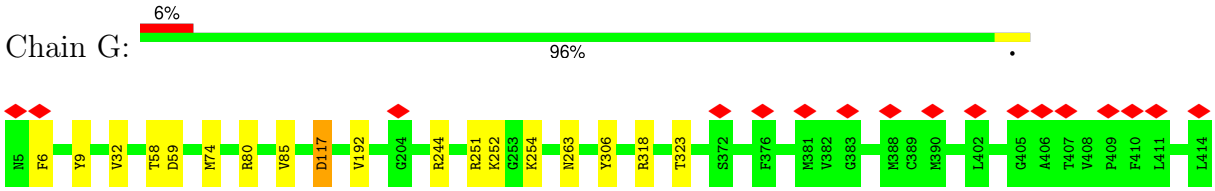
• Molecule 2: E2 glycoprotein

Chain F:



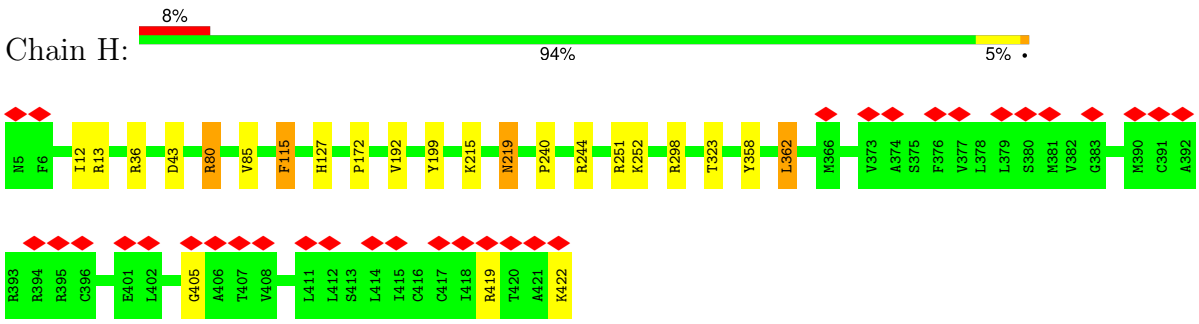
• Molecule 2: E2 glycoprotein

Chain G:



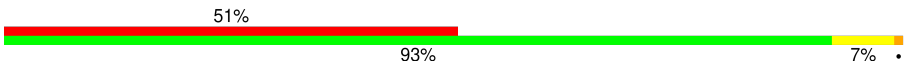
• Molecule 2: E2 glycoprotein

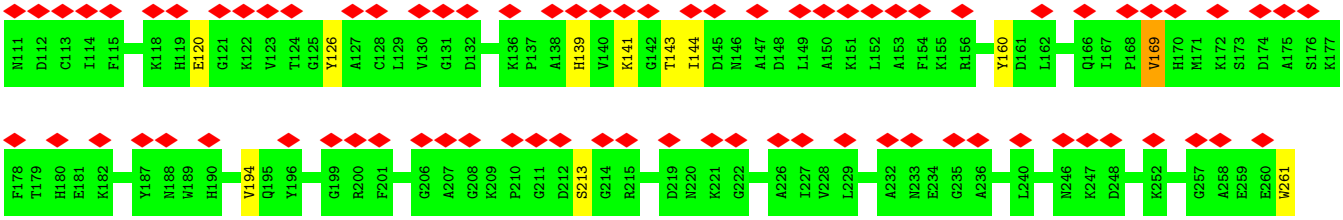
Chain H:



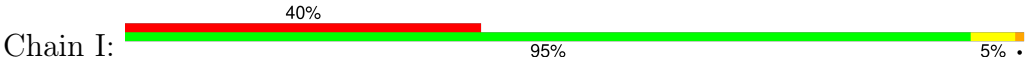
• Molecule 3: Capsid protein

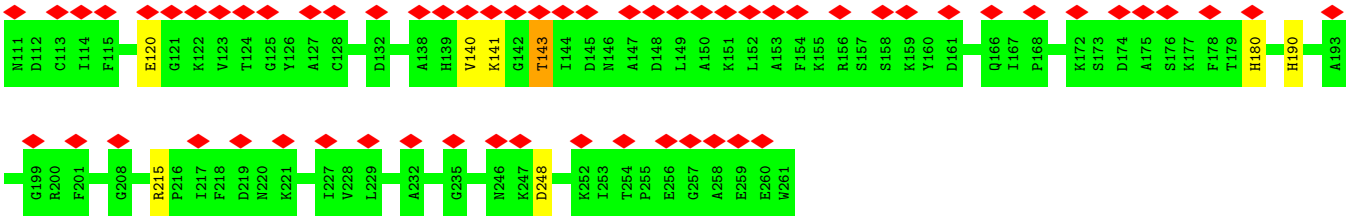
Chain J:





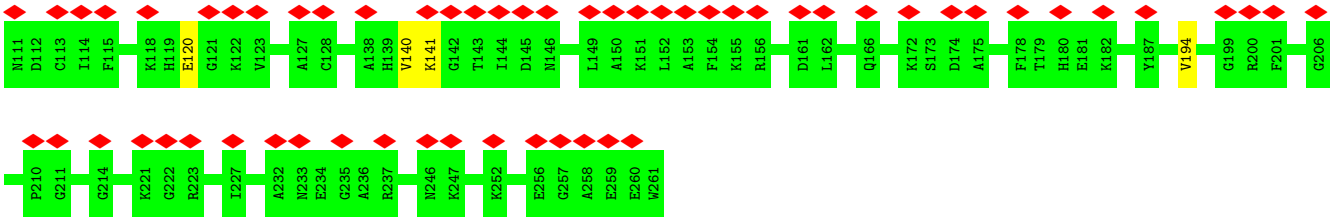
• Molecule 3: Capsid protein



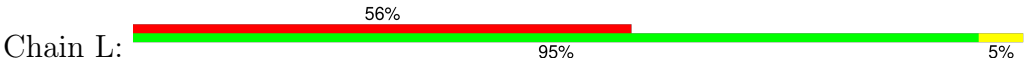


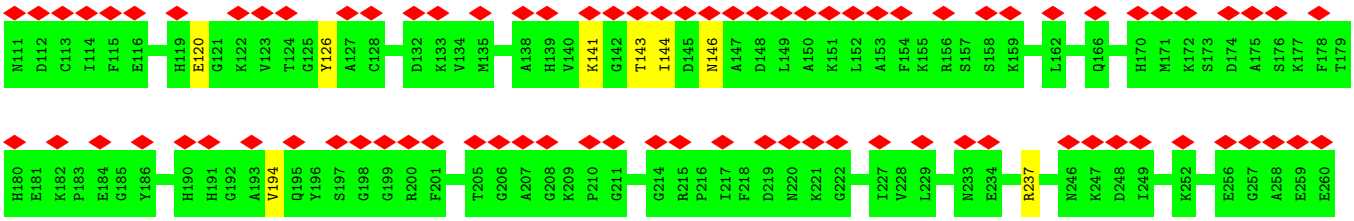
• Molecule 3: Capsid protein



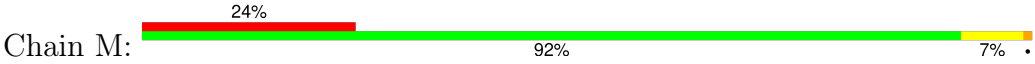


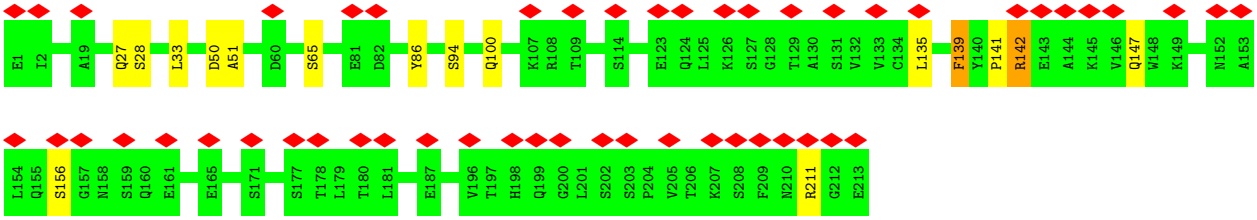
• Molecule 3: Capsid protein



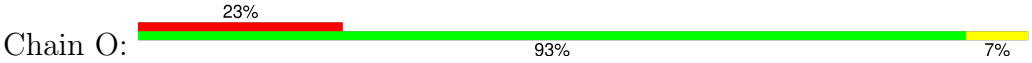


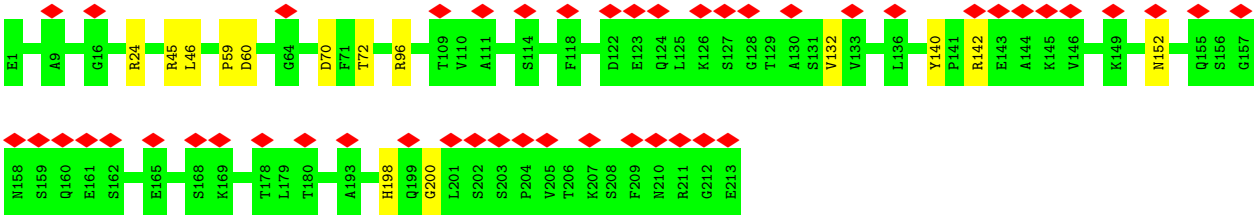
• Molecule 4: Light chain of IM-CKV063



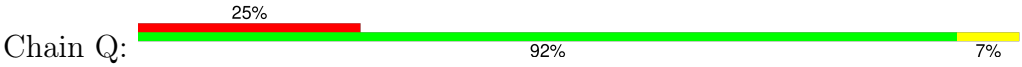


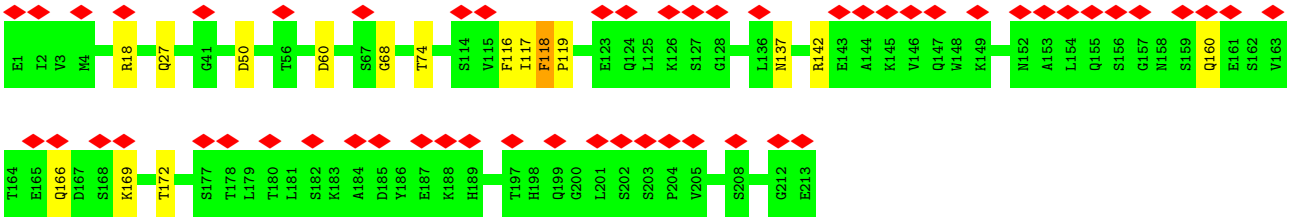
• Molecule 4: Light chain of IM-CKV063





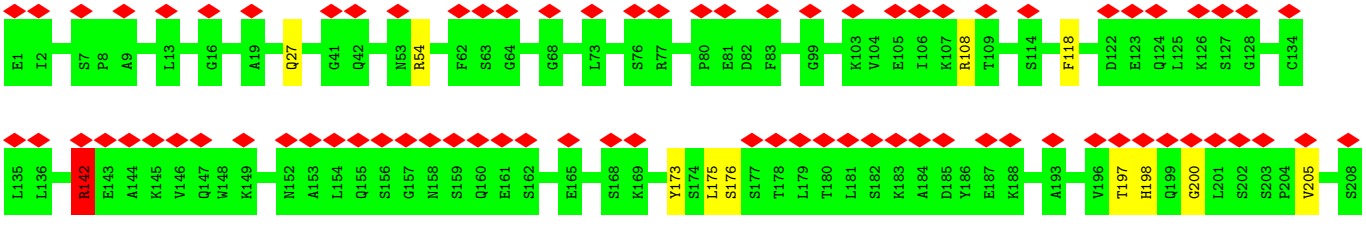
• Molecule 4: Light chain of IM-CKV063



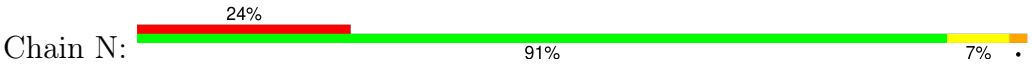


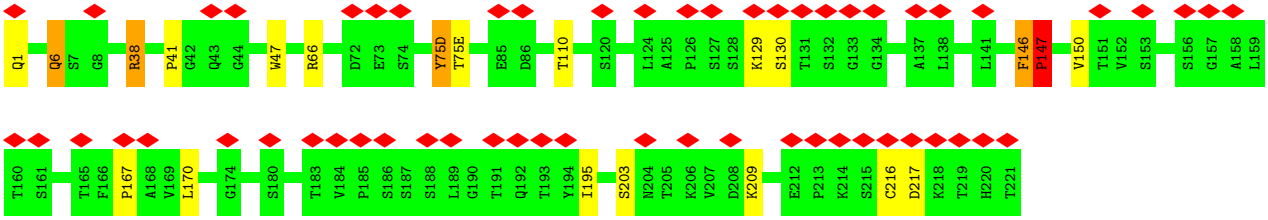
• Molecule 4: Light chain of IM-CKV063





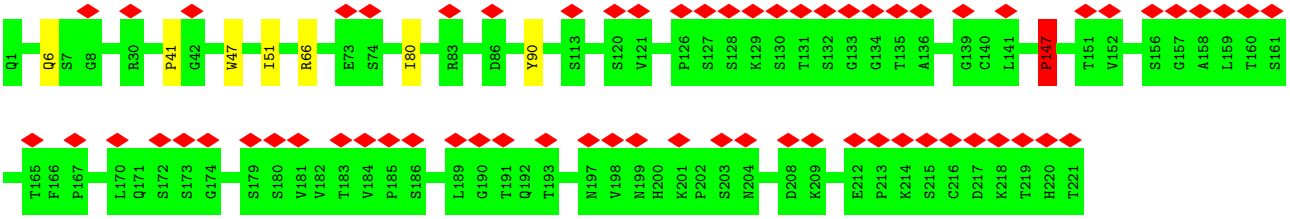
• Molecule 5: Heavy Chain of IM-CKV063





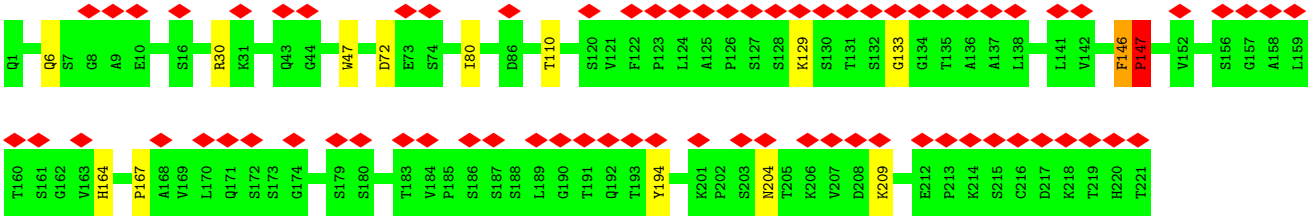
• Molecule 5: Heavy Chain of IM-CKV063





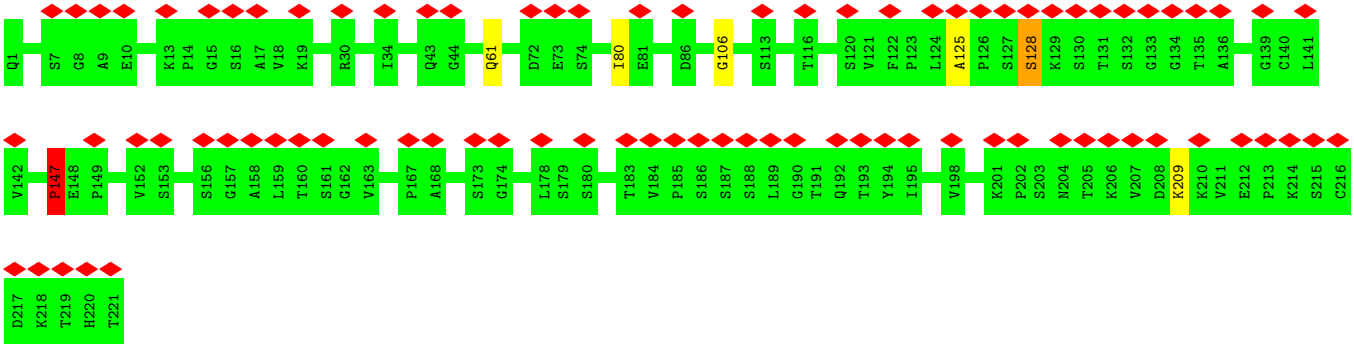
• Molecule 5: Heavy Chain of IM-CKV063



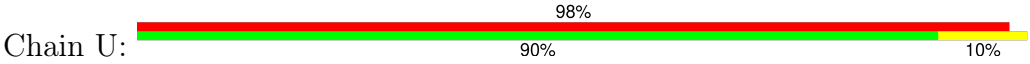


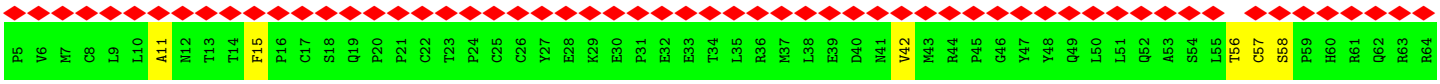
• Molecule 5: Heavy Chain of IM-CKV063





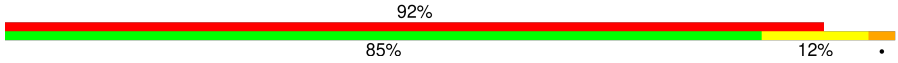
• Molecule 6: E3 glycoprotein

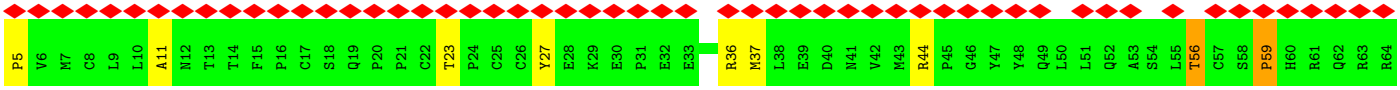




• Molecule 6: E3 glycoprotein

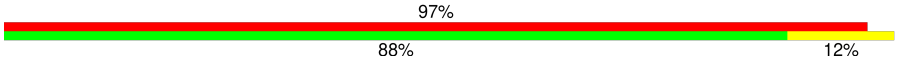
Chain V:

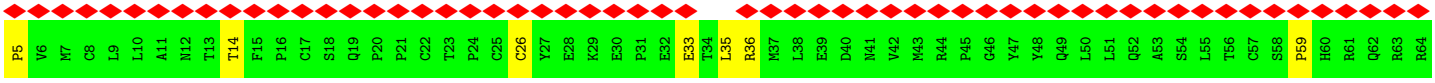




• Molecule 6: E3 glycoprotein

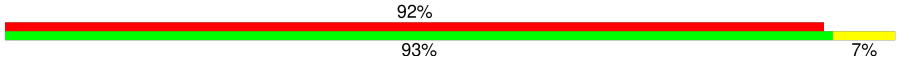
Chain W:

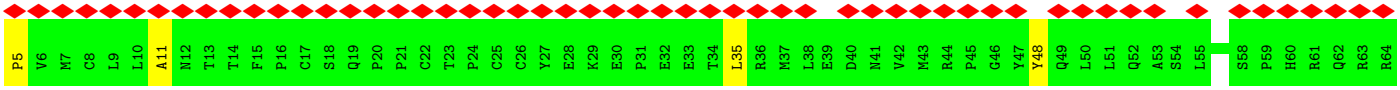




• Molecule 6: E3 glycoprotein

Chain X:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	401348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	106000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.133	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	473.2, 473.2, 473.2	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.352, 1.352, 1.352	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	0.71	0/3397	1.26	4/4636 (0.1%)
1	B	0.71	0/3397	1.26	4/4636 (0.1%)
1	C	0.70	0/3397	1.26	2/4636 (0.0%)
1	D	0.69	0/3397	1.24	4/4636 (0.1%)
2	E	0.78	0/3376	1.37	10/4599 (0.2%)
2	F	0.77	0/3376	1.34	5/4599 (0.1%)
2	G	0.78	0/3376	1.34	4/4599 (0.1%)
2	H	0.78	0/3376	1.36	6/4599 (0.1%)
3	I	0.77	0/1184	1.32	3/1599 (0.2%)
3	J	0.78	0/1184	1.33	1/1599 (0.1%)
3	K	0.77	0/1184	1.30	0/1599
3	L	0.80	0/1184	1.33	0/1599
4	M	0.79	0/1683	1.32	1/2282 (0.0%)
4	O	0.78	0/1683	1.32	3/2282 (0.1%)
4	Q	0.80	1/1683 (0.1%)	1.30	4/2282 (0.2%)
4	S	0.80	0/1683	1.34	4/2282 (0.2%)
5	N	0.78	0/1855	1.31	5/2532 (0.2%)
5	P	0.78	0/1855	1.35	2/2532 (0.1%)
5	R	0.79	0/1855	1.31	4/2532 (0.2%)
5	T	0.80	0/1855	1.34	4/2532 (0.2%)
6	U	0.89	0/492	1.51	1/667 (0.1%)
6	V	0.88	0/492	1.56	4/667 (0.6%)
6	W	0.88	0/492	1.48	1/667 (0.1%)
6	X	0.86	0/492	1.49	1/667 (0.1%)
All	All	0.77	1/47948 (0.0%)	1.32	77/65260 (0.1%)

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	B	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	E	0	1
2	F	0	3
2	G	0	3
2	H	0	4
3	J	0	1
4	M	0	1
4	O	0	2
4	S	0	2
5	N	0	1
5	P	0	1
5	R	0	1
6	V	0	2
6	X	0	1
All	All	0	26

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	119	PRO	CA-C	6.23	1.55	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	147	PRO	CA-N-CD	-8.77	99.72	112.00
5	R	147	PRO	CA-N-CD	-8.60	99.95	112.00
1	B	308	HIS	CA-CB-CG	8.57	122.37	113.80
5	T	147	PRO	CA-N-CD	-7.69	101.24	112.00
5	P	147	PRO	CA-N-CD	-7.54	101.44	112.00
1	D	183	ASP	CA-CB-CG	7.20	119.80	112.60
1	B	134	ARG	NE-CZ-NH2	7.11	125.59	119.20
6	X	5	PRO	CA-N-CD	-7.07	102.10	112.00
4	Q	119	PRO	N-CA-C	7.04	117.22	110.47
4	Q	118	PHE	CA-C-N	6.92	124.71	119.66
4	Q	118	PHE	C-N-CA	6.92	124.71	119.66
6	V	5	PRO	CA-N-CD	-6.91	102.32	112.00
1	B	308	HIS	CB-CG-CD2	-6.74	122.43	131.20
2	G	6	PHE	CA-CB-CG	6.64	120.44	113.80
6	W	5	PRO	CA-N-CD	-6.58	102.79	112.00
1	A	134	ARG	NE-CZ-NH2	6.47	125.02	119.20
2	H	219	ASN	CA-CB-CG	6.29	118.89	112.60
2	E	30	SER	N-CA-C	6.26	113.85	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	308	HIS	CA-CB-CG	6.21	120.01	113.80
2	E	298	ARG	NE-CZ-NH2	6.14	124.72	119.20
4	O	96	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	D	134	ARG	NE-CZ-NH2	6.08	124.67	119.20
2	E	251	ARG	NE-CZ-NH2	5.98	124.58	119.20
2	G	117	ASP	CA-CB-CG	5.96	118.56	112.60
4	O	70	ASP	CA-CB-CG	5.96	118.56	112.60
2	F	298	ARG	NE-CZ-NH2	5.93	124.54	119.20
2	E	244	ARG	NE-CZ-NH2	5.91	124.52	119.20
2	H	298	ARG	NE-CZ-NH2	5.87	124.48	119.20
5	R	72	ASP	CA-CB-CG	5.70	118.30	112.60
5	N	146	PHE	CB-CA-C	5.70	118.16	109.56
4	S	211	ARG	NE-CZ-NH2	5.66	124.29	119.20
6	V	59	PRO	CA-N-CD	-5.56	104.22	112.00
4	M	139	PHE	CA-CB-CG	5.54	119.33	113.80
2	H	172	PRO	N-CA-CB	5.50	106.27	103.19
2	F	169	VAL	N-CA-C	5.49	115.77	107.75
1	D	20	ASN	N-CA-CB	-5.49	103.04	110.95
2	F	119	ARG	NE-CZ-NH2	5.44	124.09	119.20
5	R	30	ARG	NE-CZ-NH2	5.43	124.08	119.20
3	I	215	ARG	NE-CZ-NH2	5.43	124.08	119.20
5	T	128	SER	CA-C-N	5.42	131.07	121.80
5	T	128	SER	C-N-CA	5.42	131.07	121.80
2	F	6	PHE	CA-CB-CG	5.38	119.18	113.80
6	V	56	THR	CA-CB-CG2	5.37	119.63	110.50
1	A	366	ARG	NE-CZ-NH2	5.36	124.03	119.20
5	N	66	ARG	NE-CZ-NH2	5.36	124.02	119.20
5	N	38	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	C	223	ARG	NE-CZ-NH2	5.32	123.98	119.20
1	A	97	ASP	CA-CB-CG	5.31	117.91	112.60
2	E	82	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	G	254	LYS	CA-C-N	5.31	130.44	122.58
2	G	254	LYS	C-N-CA	5.31	130.44	122.58
4	S	118	PHE	CA-C-N	5.31	125.85	120.38
4	S	118	PHE	C-N-CA	5.31	125.85	120.38
4	S	142	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	E	252	LYS	CA-C-N	5.29	129.01	121.03
2	E	252	LYS	C-N-CA	5.29	129.01	121.03
2	H	419	ARG	NE-CZ-NH2	5.28	123.95	119.20
3	I	190	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	D	382	PRO	N-CA-CB	5.24	105.94	103.22
6	V	36	ARG	NE-CZ-NH2	5.23	123.91	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	115	PHE	CA-CB-CG	5.22	119.02	113.80
5	P	66	ARG	NE-CZ-NH2	5.16	123.85	119.20
4	Q	142	ARG	NE-CZ-NH2	5.16	123.85	119.20
2	E	419	ARG	CA-C-N	5.16	131.39	121.54
2	E	419	ARG	C-N-CA	5.16	131.39	121.54
1	B	204	GLN	OE1-CD-NE2	-5.14	117.46	122.60
2	E	393	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	123	ARG	NE-CZ-NH2	5.10	123.79	119.20
5	T	125	ALA	N-CA-C	5.10	112.81	108.22
4	O	45	ARG	NE-CZ-NH2	5.08	123.77	119.20
3	J	139	HIS	CB-CG-CD2	-5.07	124.61	131.20
5	R	146	PHE	CB-CA-C	5.07	116.92	109.22
6	U	15	PHE	N-CA-C	5.06	114.12	108.25
5	N	6	GLN	OE1-CD-NE2	-5.05	117.55	122.60
2	F	267	ARG	NE-CZ-NH2	5.04	123.74	119.20
2	H	36	ARG	NE-CZ-NH2	5.04	123.73	119.20
3	I	180	HIS	CB-CG-CD2	-5.01	124.69	131.20

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	247	ARG	Sidechain
1	B	308	HIS	Sidechain
1	D	185	TYR	Sidechain
2	E	80	ARG	Sidechain
2	F	149	ARG	Sidechain
2	F	244	ARG	Sidechain
2	F	251	ARG	Sidechain
2	G	244	ARG	Sidechain
2	G	318	ARG	Sidechain
2	G	9	TYR	Sidechain
2	H	199	TYR	Sidechain
2	H	244	ARG	Sidechain
2	H	358	TYR	Sidechain
2	H	80	ARG	Sidechain
3	J	160	TYR	Sidechain
4	M	86	TYR	Sidechain
5	N	75(D)	TYR	Sidechain
4	O	140	TYR	Sidechain
4	O	24	ARG	Sidechain
5	P	90	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	R	194	TYR	Sidechain
4	S	173	TYR	Sidechain
4	S	54	ARG	Sidechain
6	V	27	TYR	Sidechain
6	V	44	ARG	Sidechain
6	X	48	TYR	Sidechain

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	3316	3258	3257	5	0
1	B	3316	3258	3257	2	0
1	C	3316	3257	3257	3	0
1	D	3316	3257	3257	0	0
2	E	3289	3243	3240	1	0
2	F	3289	3241	3240	5	0
2	G	3289	3243	3240	1	0
2	H	3289	3243	3240	0	0
3	I	1156	1138	1135	0	0
3	J	1156	1138	1135	1	0
3	K	1156	1138	1135	0	0
3	L	1156	1138	1135	0	0
4	M	1649	1586	1605	3	0
4	O	1649	1586	1605	1	0
4	Q	1649	1593	1605	1	0
4	S	1649	1605	1605	3	0
5	N	1810	1782	1789	2	0
5	P	1810	1785	1789	0	0
5	R	1810	1789	1789	1	0
5	T	1810	1790	1789	0	0
6	U	480	472	470	0	0
6	V	480	472	470	0	0
6	W	480	472	470	2	0
6	X	480	472	470	0	0
All	All	46800	45956	45984	28	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 0.

All (28) 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)
4:M:65:SER:OG	4:Q:27:GLN:NE2	2.26	0.69
1:B:49:CYS:HB2	1:B:114:CYS:HG	1.71	0.54
4:M:27:GLN:HG3	4:M:28:SER:N	2.23	0.54
4:S:142:ARG:H	4:S:142:ARG:HD3	1.73	0.53
2:F:235:TRP:HE1	6:W:35:LEU:HD11	1.73	0.53
2:F:112:THR:HG22	2:F:126:THR:HG23	1.91	0.53
1:B:49:CYS:CB	1:B:114:CYS:HG	2.23	0.51
1:A:49:CYS:HG	1:A:114:CYS:HG	1.60	0.49
1:C:176:LYS:HE3	1:C:189:TYR:CE1	2.47	0.49
5:R:146:PHE:CD2	5:R:147:PRO:HD2	2.48	0.49
2:G:58:THR:HG22	2:G:59:ASP:H	1.78	0.48
1:A:49:CYS:HB2	1:A:114:CYS:HG	1.80	0.46
4:O:198:HIS:CE1	4:O:200:GLY:H	2.34	0.45
1:A:49:CYS:CB	1:A:114:CYS:HG	2.29	0.45
1:C:49:CYS:HG	1:C:114:CYS:HG	1.65	0.45
4:S:175:LEU:HD23	4:S:176:SER:N	2.32	0.45
4:M:139:PHE:CE2	4:M:142:ARG:HA	2.53	0.44
1:A:407:MET:C	1:A:407:MET:SD	3.01	0.44
1:A:361:ALA:HB3	1:A:404:VAL:CG1	2.48	0.43
2:F:235:TRP:HE1	6:W:35:LEU:CD1	2.31	0.43
2:F:358:TYR:CD1	2:F:358:TYR:C	2.97	0.43
4:S:198:HIS:CD2	4:S:200:GLY:H	2.37	0.43
2:E:342:LEU:HD22	2:E:342:LEU:H	1.84	0.43
5:N:146:PHE:CD2	5:N:147:PRO:HD2	2.54	0.43
3:J:213:SER:HB2	3:J:261:TRP:C	2.44	0.42
1:C:407:MET:SD	1:C:407:MET:C	3.03	0.42
2:F:235:TRP:CD1	2:F:235:TRP:N	2.88	0.41
5:N:75(D):TYR:CG	5:N:75(E):THR:N	2.89	0.41

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	436/438 (100%)	404 (93%)	31 (7%)	1 (0%)	43	74
1	B	436/438 (100%)	407 (93%)	28 (6%)	1 (0%)	43	74
1	C	436/438 (100%)	409 (94%)	24 (6%)	3 (1%)	18	51
1	D	436/438 (100%)	403 (92%)	31 (7%)	2 (0%)	24	57
2	E	416/418 (100%)	382 (92%)	30 (7%)	4 (1%)	12	44
2	F	416/418 (100%)	382 (92%)	27 (6%)	7 (2%)	7	35
2	G	416/418 (100%)	386 (93%)	28 (7%)	2 (0%)	24	57
2	H	416/418 (100%)	377 (91%)	34 (8%)	5 (1%)	10	41
3	I	149/151 (99%)	140 (94%)	7 (5%)	2 (1%)	9	39
3	J	149/151 (99%)	137 (92%)	8 (5%)	4 (3%)	4	27
3	K	149/151 (99%)	136 (91%)	12 (8%)	1 (1%)	18	51
3	L	149/151 (99%)	135 (91%)	11 (7%)	3 (2%)	6	32
4	M	211/213 (99%)	189 (90%)	17 (8%)	5 (2%)	4	29
4	O	211/213 (99%)	193 (92%)	15 (7%)	3 (1%)	9	38
4	Q	211/213 (99%)	178 (84%)	26 (12%)	7 (3%)	3	23
4	S	211/213 (99%)	199 (94%)	9 (4%)	3 (1%)	9	38
5	N	240/242 (99%)	210 (88%)	21 (9%)	9 (4%)	2	20
5	P	240/242 (99%)	215 (90%)	23 (10%)	2 (1%)	16	49
5	R	240/242 (99%)	221 (92%)	16 (7%)	3 (1%)	9	39
5	T	240/242 (99%)	224 (93%)	13 (5%)	3 (1%)	9	39
6	U	58/60 (97%)	52 (90%)	3 (5%)	3 (5%)	1	14
6	V	58/60 (97%)	48 (83%)	8 (14%)	2 (3%)	3	23
6	W	58/60 (97%)	44 (76%)	13 (22%)	1 (2%)	7	35
6	X	58/60 (97%)	52 (90%)	5 (9%)	1 (2%)	7	35
All	All	6040/6088 (99%)	5523 (91%)	440 (7%)	77 (1%)	12	39

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	251	ARG
2	G	306	TYR
3	J	120	GLU

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Mol	Chain	Res	Type
4	M	141	PRO
5	N	147	PRO
5	P	147	PRO
5	R	147	PRO
5	T	147	PRO
6	V	59	PRO
3	L	143	THR
1	B	370	CYS
1	D	387	ILE
2	E	420	THR
2	F	362	LEU
2	H	362	LEU
3	J	143	THR
4	M	100	GLN
5	N	129	LYS
5	N	130	SER
5	N	167	PRO
5	N	217	ASP
5	R	167	PRO
4	S	142	ARG
3	L	144	ILE
1	C	295	SER
1	C	371	SER
3	J	169	VAL
4	M	50	ASP
4	M	51	ALA
4	O	59	PRO
4	O	60	ASP
4	S	27	GLN
5	T	128	SER
6	V	11	ALA
6	X	11	ALA
3	I	120	GLU
3	L	120	GLU
1	C	369	VAL
2	E	72	ASN
2	E	362	LEU
2	F	64	TRP
2	F	206	SER
2	F	280	LYS
2	H	192	VAL
5	N	203	SER

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Mol	Chain	Res	Type
5	N	216	CYS
4	O	152	ASN
4	Q	50	ASP
4	Q	68	GLY
4	Q	116	PHE
4	Q	166	GLN
5	R	133	GLY
6	U	11	ALA
6	U	42	VAL
3	I	143	THR
3	K	120	GLU
1	A	96	CYS
2	G	192	VAL
4	M	156	SER
4	Q	60	ASP
4	Q	118	PHE
6	U	57	CYS
6	W	59	PRO
1	D	369	VAL
2	E	406	ALA
2	F	192	VAL
2	H	252	LYS
5	N	150	VAL
4	Q	117	ILE
5	N	41	PRO
2	F	32	VAL
3	J	144	ILE
5	T	106	GLY
2	H	240	PRO
5	P	41	PRO
2	H	405	GLY
4	S	205	VAL

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	368/368 (100%)	358 (97%)	10 (3%)	39	62
1	B	368/368 (100%)	355 (96%)	13 (4%)	32	57
1	C	368/368 (100%)	363 (99%)	5 (1%)	59	71
1	D	368/368 (100%)	359 (98%)	9 (2%)	43	64
2	E	369/369 (100%)	352 (95%)	17 (5%)	24	50
2	F	369/369 (100%)	358 (97%)	11 (3%)	36	60
2	G	369/369 (100%)	360 (98%)	9 (2%)	43	64
2	H	369/369 (100%)	356 (96%)	13 (4%)	32	57
3	I	120/120 (100%)	116 (97%)	4 (3%)	33	58
3	J	120/120 (100%)	116 (97%)	4 (3%)	33	58
3	K	120/120 (100%)	117 (98%)	3 (2%)	42	63
3	L	120/120 (100%)	115 (96%)	5 (4%)	26	52
4	M	185/185 (100%)	179 (97%)	6 (3%)	34	59
4	O	185/185 (100%)	181 (98%)	4 (2%)	45	65
4	Q	185/185 (100%)	179 (97%)	6 (3%)	34	59
4	S	185/185 (100%)	181 (98%)	4 (2%)	45	65
5	N	203/203 (100%)	195 (96%)	8 (4%)	28	54
5	P	203/203 (100%)	198 (98%)	5 (2%)	42	63
5	R	203/203 (100%)	194 (96%)	9 (4%)	25	51
5	T	203/203 (100%)	199 (98%)	4 (2%)	48	67
6	U	57/57 (100%)	55 (96%)	2 (4%)	32	57
6	V	57/57 (100%)	54 (95%)	3 (5%)	20	47
6	W	57/57 (100%)	53 (93%)	4 (7%)	14	39
6	X	57/57 (100%)	56 (98%)	1 (2%)	51	69
All	All	5208/5208 (100%)	5049 (97%)	159 (3%)	36	59

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	96	CYS
1	A	179	VAL
1	A	184	VAL
1	A	218	GLN
1	A	230	HIS

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Mol	Chain	Res	Type
1	A	266	VAL
1	A	280	ILE
1	A	344	ILE
1	A	407	MET
1	B	28	VAL
1	B	47	ILE
1	B	99	GLU
1	B	115	LYS
1	B	179	VAL
1	B	184	VAL
1	B	264	ASN
1	B	266	VAL
1	B	299	MET
1	B	317	ILE
1	B	349	ASN
1	B	355	SER
1	B	414	THR
1	C	179	VAL
1	C	218	GLN
1	C	264	ASN
1	C	280	ILE
1	C	407	MET
1	D	60	VAL
1	D	162	ILE
1	D	166	MET
1	D	178	VAL
1	D	229	VAL
1	D	266	VAL
1	D	280	ILE
1	D	351	GLN
1	D	407	MET
2	E	32	VAL
2	E	38	ARG
2	E	43	ASP
2	E	46	LEU
2	E	59	ASP
2	E	70	MET
2	E	80	ARG
2	E	85	VAL
2	E	117	ASP
2	E	167	ILE
2	E	174	ASP

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Mol	Chain	Res	Type
2	E	241	LEU
2	E	323	THR
2	E	329	THR
2	E	355	ILE
2	E	379	LEU
2	E	412	LEU
2	F	6	PHE
2	F	40	GLU
2	F	64	TRP
2	F	85	VAL
2	F	193	ASN
2	F	215	LYS
2	F	241	LEU
2	F	319	LEU
2	F	398	THR
2	F	403	THR
2	F	419	ARG
2	G	32	VAL
2	G	74	MET
2	G	80	ARG
2	G	85	VAL
2	G	117	ASP
2	G	251	ARG
2	G	252	LYS
2	G	263	ASN
2	G	323	THR
2	H	12	ILE
2	H	13	ARG
2	H	43	ASP
2	H	80	ARG
2	H	85	VAL
2	H	115	PHE
2	H	127	HIS
2	H	215	LYS
2	H	219	ASN
2	H	251	ARG
2	H	323	THR
2	H	362	LEU
2	H	422	LYS
3	J	126	TYR
3	J	141	LYS
3	J	169	VAL

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Mol	Chain	Res	Type
3	J	194	VAL
4	M	33	LEU
4	M	94	SER
4	M	135	LEU
4	M	142	ARG
4	M	147	GLN
4	M	211	ARG
5	N	1	GLN
5	N	6	GLN
5	N	38	ARG
5	N	47	TRP
5	N	110	THR
5	N	170	LEU
5	N	195	ILE
5	N	209	LYS
4	O	46	LEU
4	O	72	THR
4	O	132	VAL
4	O	142	ARG
5	P	6	GLN
5	P	47	TRP
5	P	51	ILE
5	P	80	ILE
5	P	147	PRO
4	Q	18	ARG
4	Q	74	THR
4	Q	137	ASN
4	Q	160	GLN
4	Q	169	LYS
4	Q	172	THR
5	R	6	GLN
5	R	47	TRP
5	R	80	ILE
5	R	110	THR
5	R	129	LYS
5	R	147	PRO
5	R	164	HIS
5	R	204	ASN
5	R	209	LYS
4	S	108	ARG
4	S	142	ARG
4	S	197	THR

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Mol	Chain	Res	Type
4	S	211	ARG
5	T	61	GLN
5	T	80	ILE
5	T	147	PRO
5	T	209	LYS
6	U	56	THR
6	U	58	SER
6	V	23	THR
6	V	37	MET
6	V	56	THR
6	W	14	THR
6	W	26	CYS
6	W	33	GLU
6	W	36	ARG
6	X	35	LEU
3	I	140	VAL
3	I	141	LYS
3	I	143	THR
3	I	248	ASP
3	K	140	VAL
3	K	141	LYS
3	K	194	VAL
3	L	126	TYR
3	L	141	LYS
3	L	146	ASN
3	L	194	VAL
3	L	237	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	264	ASN
1	A	394	HIS
1	B	216	ASN
1	B	368	GLN
1	B	373	GLN
1	C	138	GLN
1	D	252	GLN
1	D	260	GLN
2	E	7	ASN
2	E	142	HIS

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Mol	Chain	Res	Type
2	E	281	ASN
2	F	5	ASN
2	F	49	GLN
2	F	72	ASN
2	F	123	HIS
2	F	142	HIS
2	F	219	ASN
2	F	232	HIS
2	G	72	ASN
2	G	218	ASN
2	G	299	ASN
2	G	305	ASN
2	G	307	GLN
2	H	72	ASN
2	H	127	HIS
2	H	158	GLN
2	H	207	ASN
2	H	232	HIS
2	H	282	GLN
4	M	38	GLN
4	M	137	ASN
5	N	39	GLN
4	O	137	ASN
5	P	43	GLN
5	P	58	ASN
5	P	171	GLN
4	Q	100	GLN
4	Q	137	ASN
4	Q	138	ASN
4	Q	160	GLN
4	Q	210	ASN
5	R	171	GLN
5	R	192	GLN
4	S	160	GLN
5	T	199	ASN
5	T	204	ASN
6	V	49	GLN
6	W	62	GLN
3	I	190	HIS
3	K	170	HIS
3	L	166	GLN
3	L	190	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

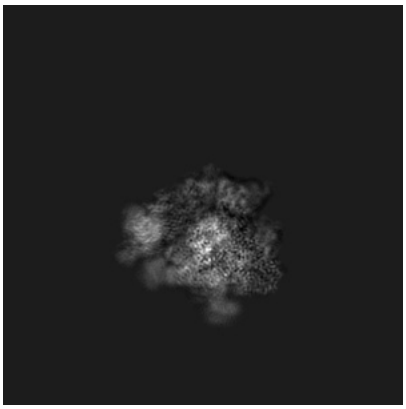
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44547. These allow visual inspection of the internal detail of the map and identification of artifacts.

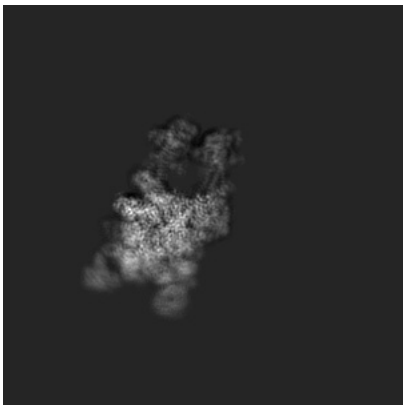
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

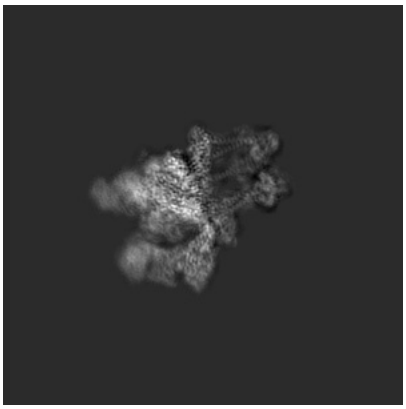
6.1.1 Primary map



X

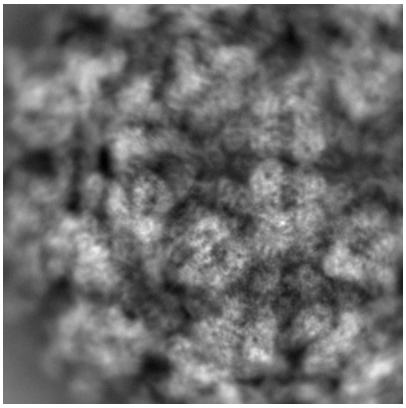


Y

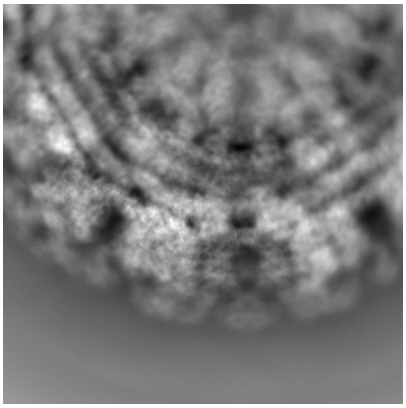


Z

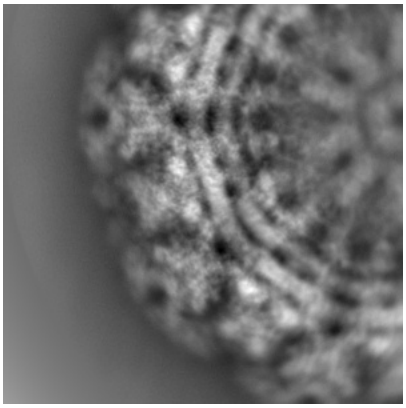
6.1.2 Raw map



X



Y

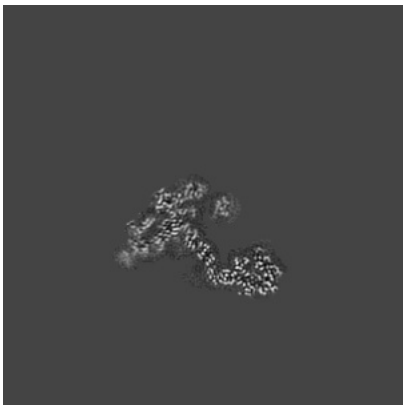


Z

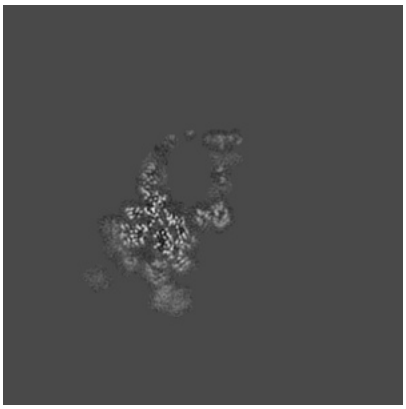
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

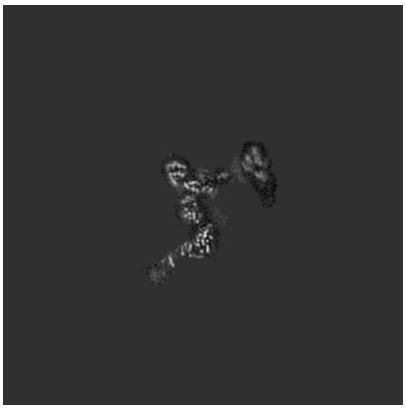
6.2.1 Primary map



X Index: 175

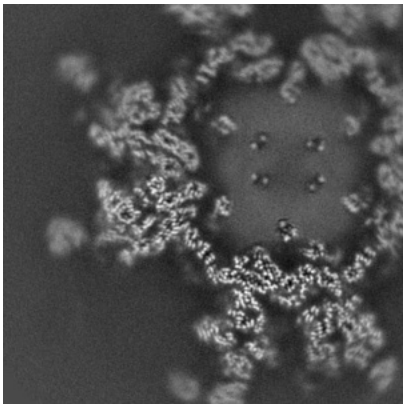


Y Index: 175

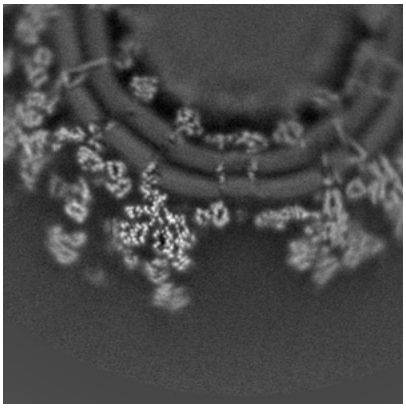


Z Index: 175

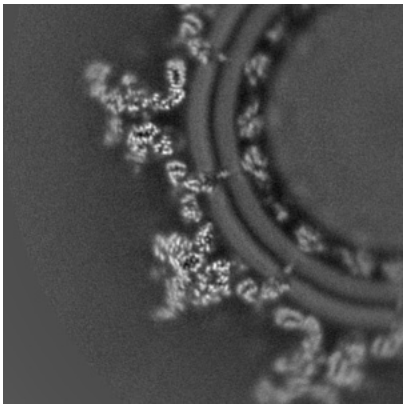
6.2.2 Raw map



X Index: 175



Y Index: 175

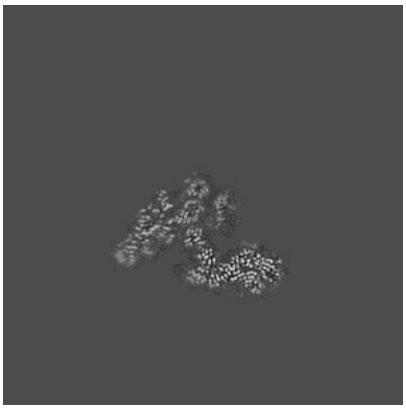


Z Index: 175

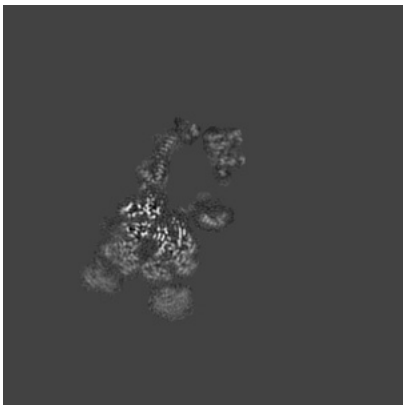
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 170

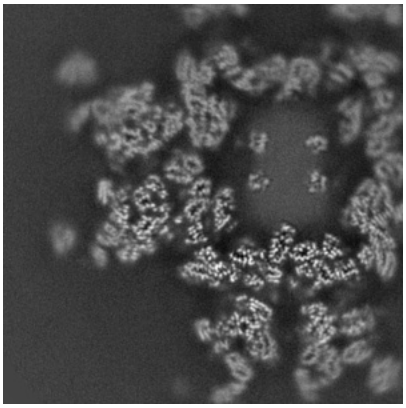


Y Index: 181

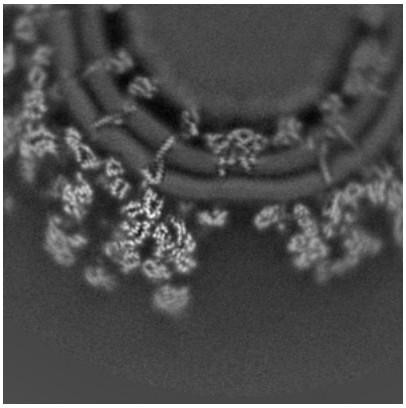


Z Index: 127

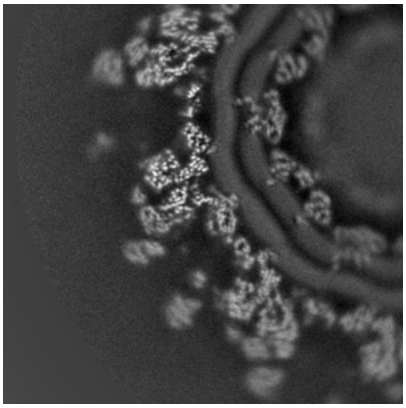
6.3.2 Raw map



X Index: 167



Y Index: 180

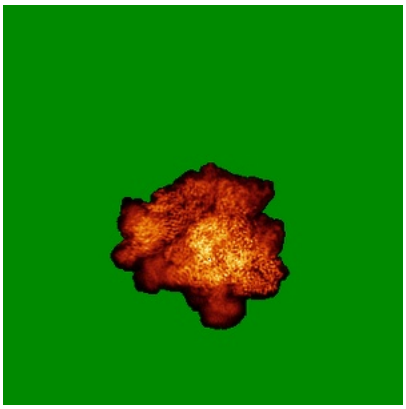


Z Index: 124

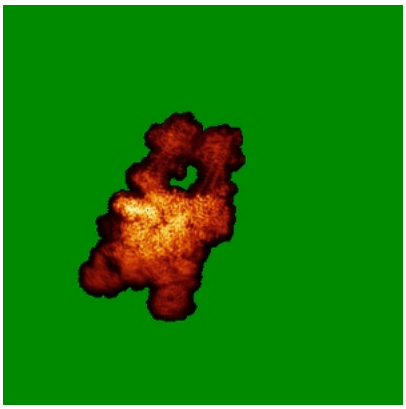
The images above show the largest variance slices of the map in three orthogonal directions.

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

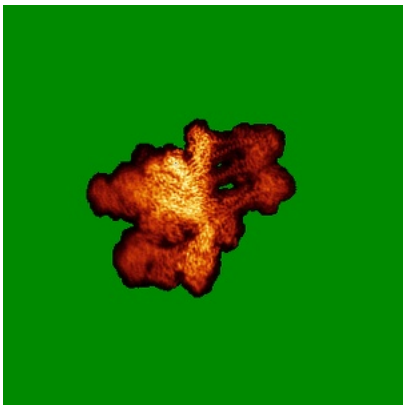
6.4.1 Primary map



X

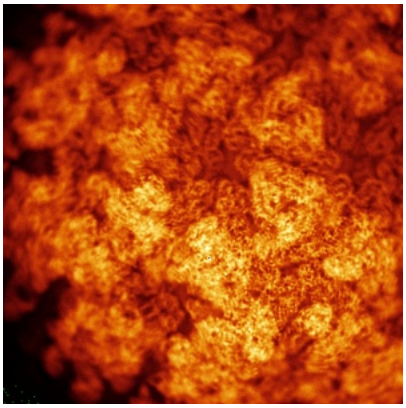


Y

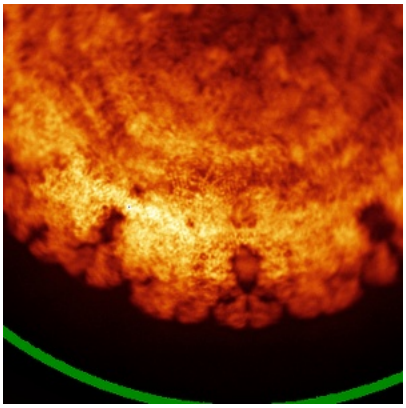


Z

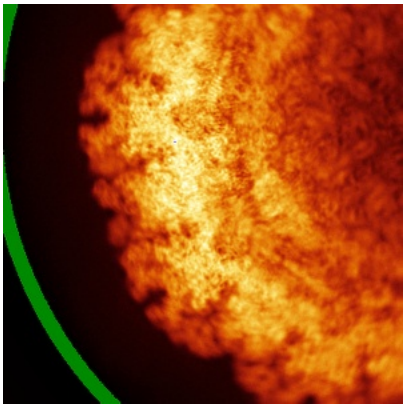
6.4.2 Raw map



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 0.02. 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.

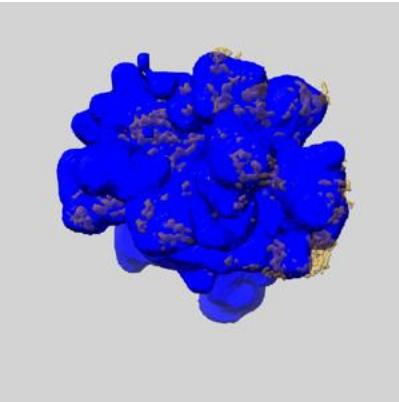
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

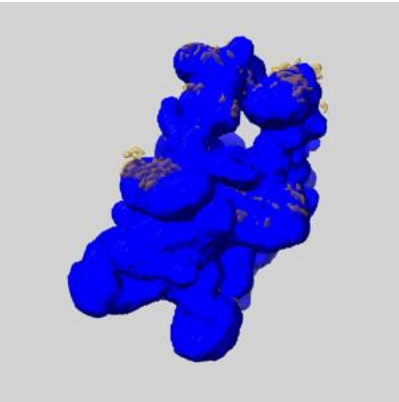
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

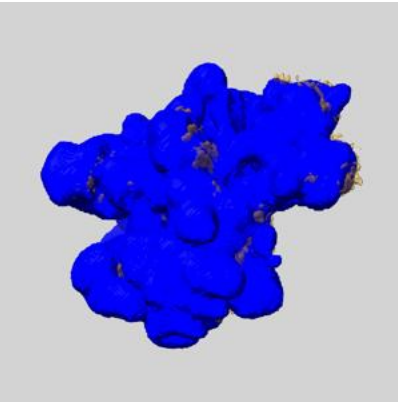
6.6.1 emd_44547_msk_1.map (i)



X



Y

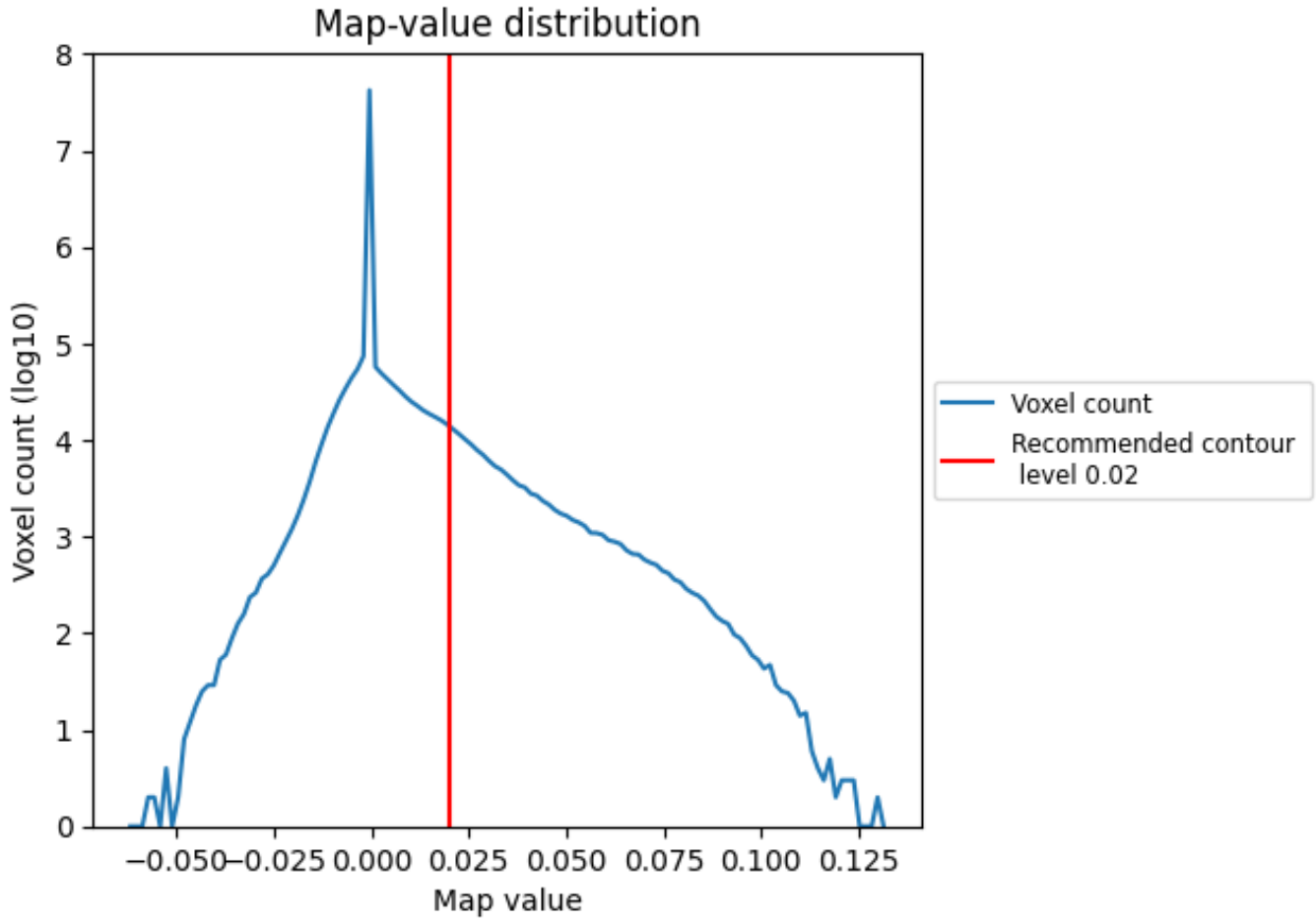


Z

7 Map analysis

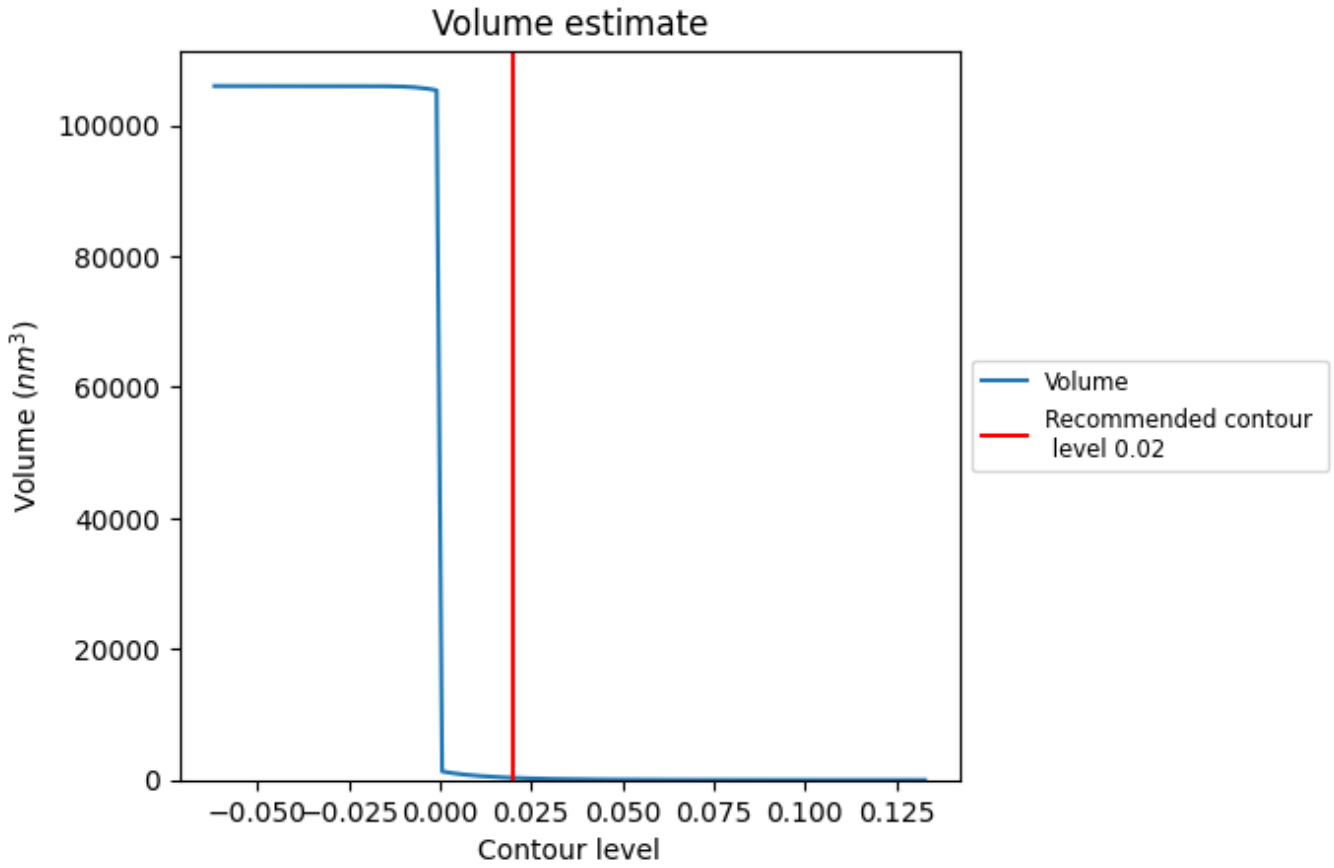
This section contains the results of statistical analysis of the map.

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.

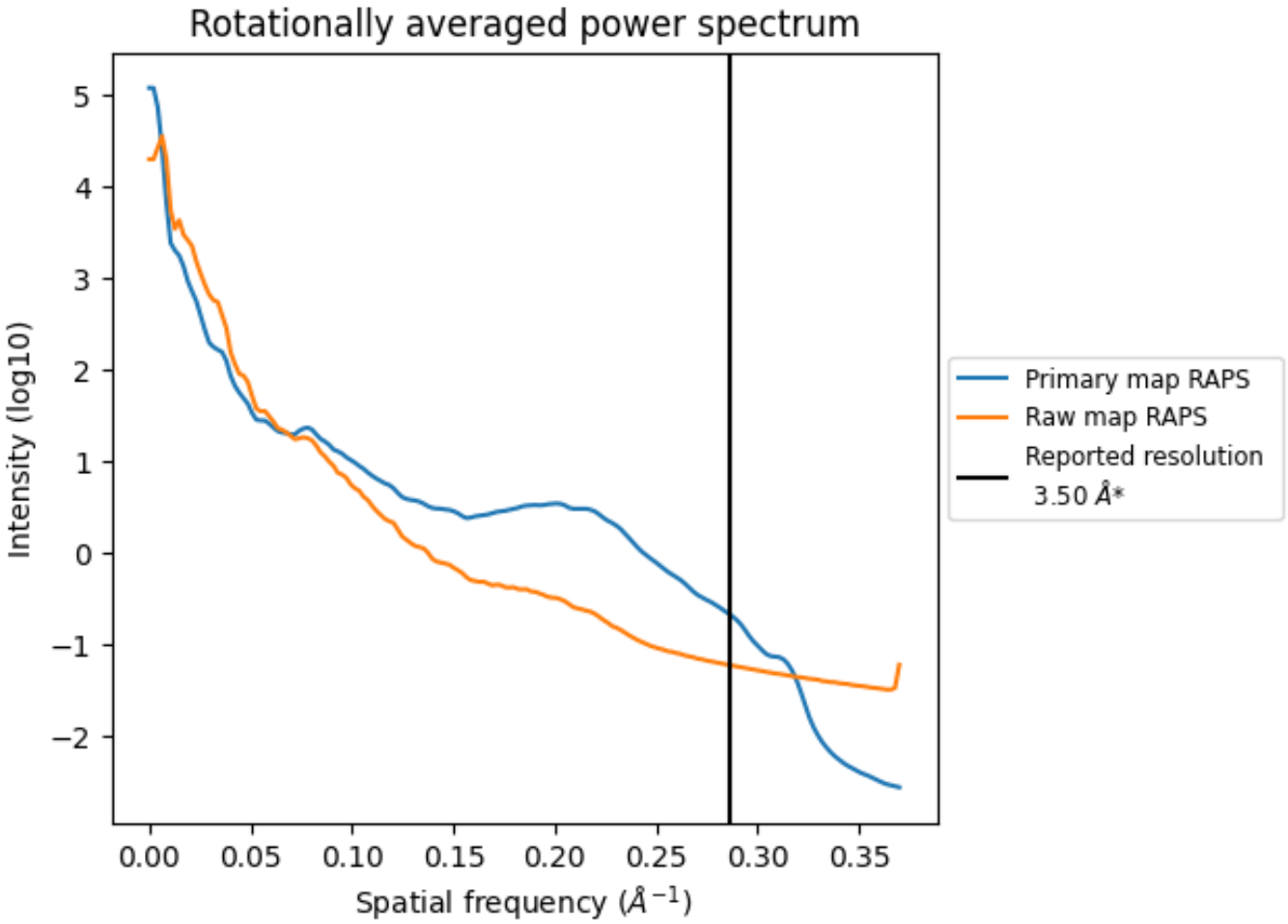
7.2 Volume estimate



The volume at the recommended contour level is 327 nm^3; this corresponds to an approximate mass of 296 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)

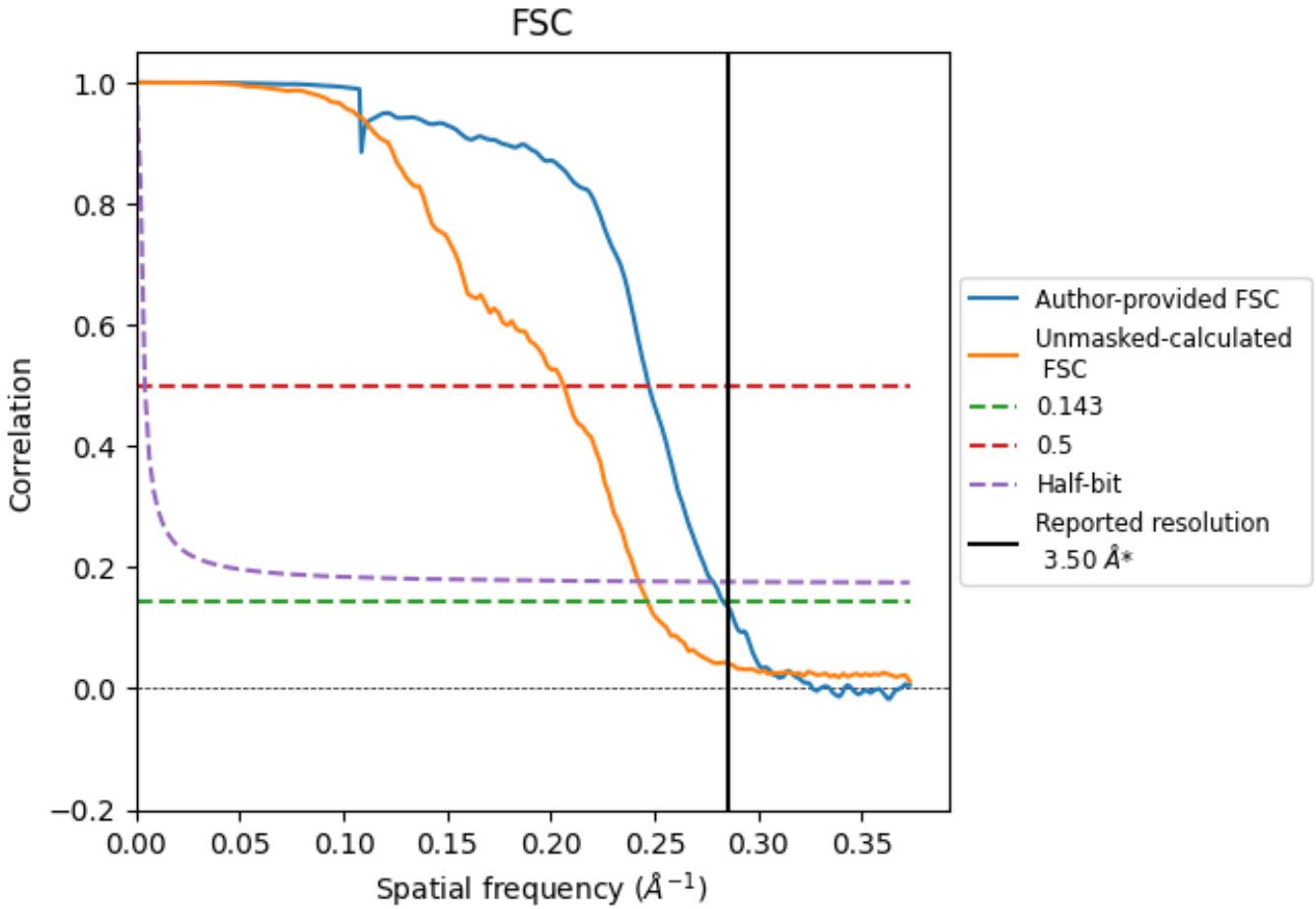


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

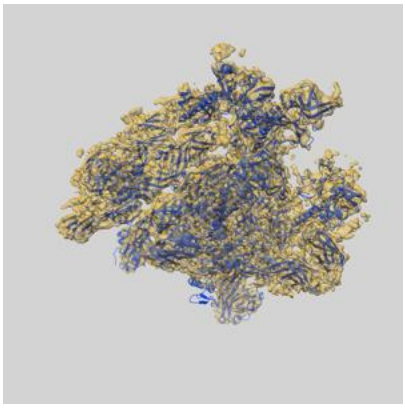
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.53	4.05	3.59
Unmasked-calculated*	4.05	4.85	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.5 by more than 10 %

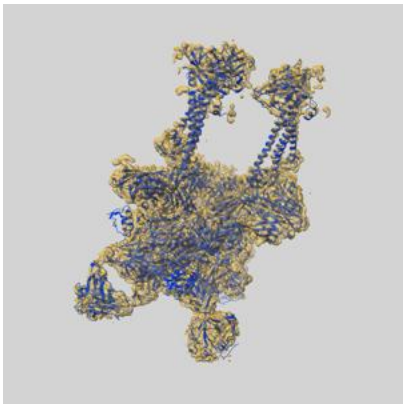
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44547 and PDB model 9BHH. Per-residue inclusion information can be found in section 3 on page 6.

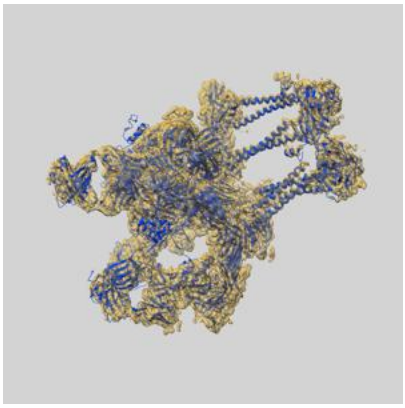
9.1 Map-model overlay



X



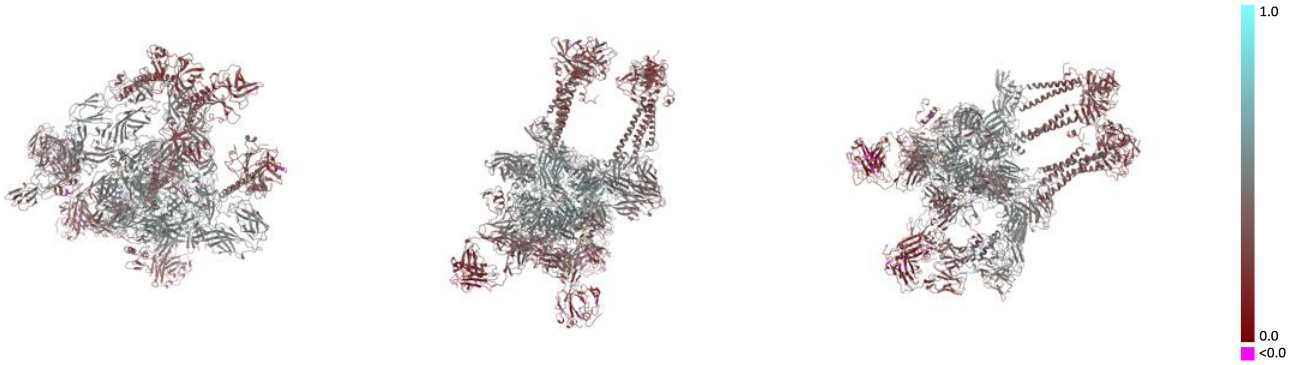
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

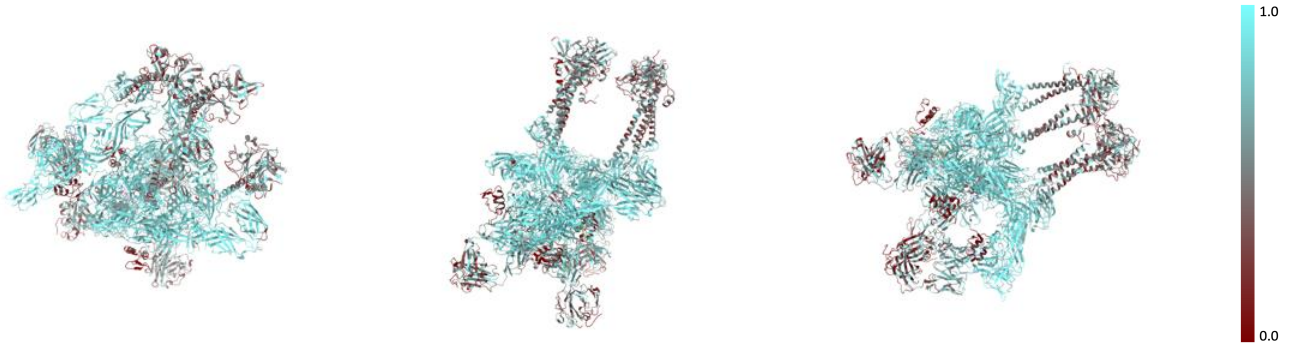
9.2 Q-score mapped to coordinate model



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.

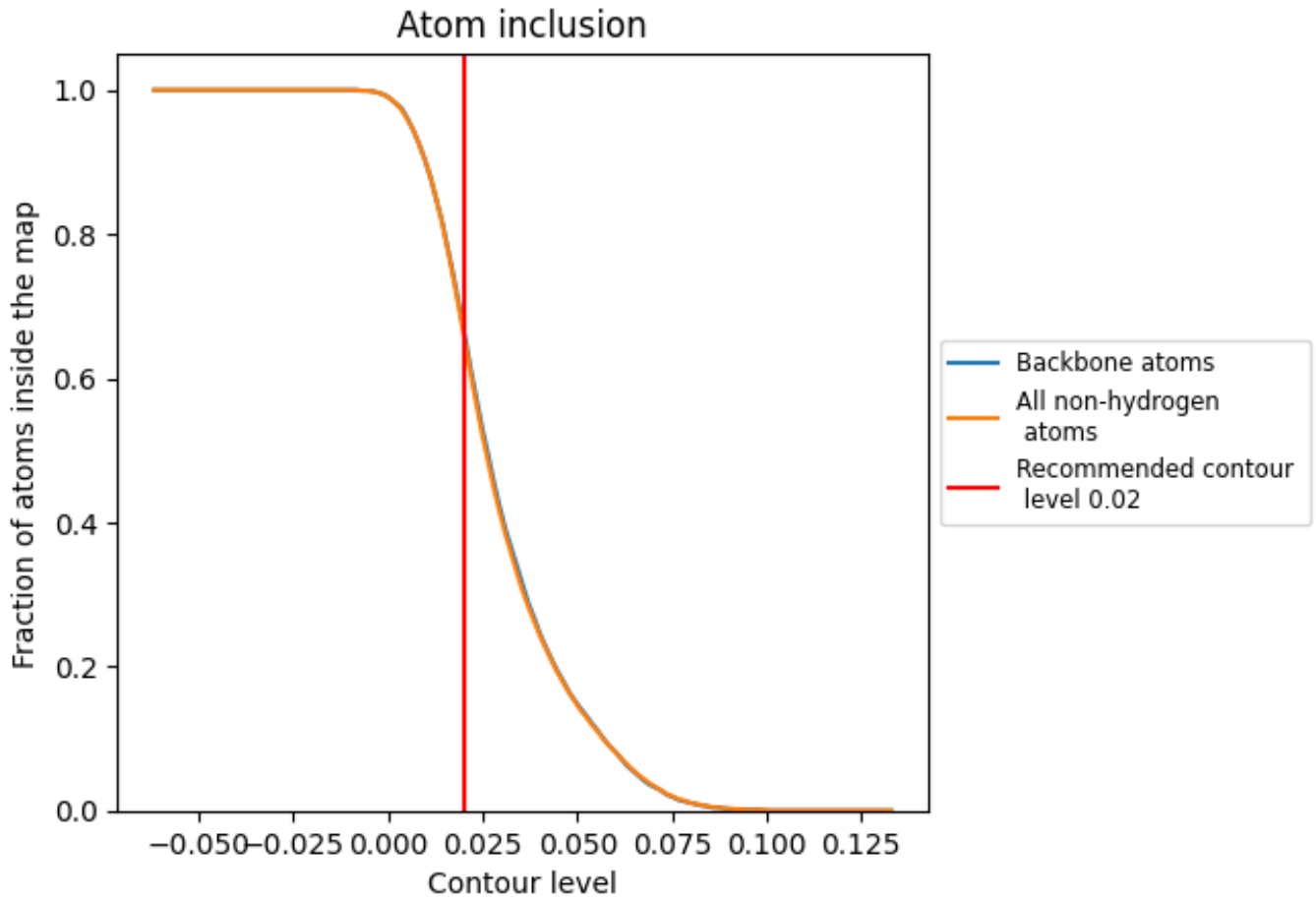
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 67% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6610	0.3900
A	0.8270	0.4800
B	0.8100	0.4600
C	0.7990	0.4650
D	0.7920	0.4440
E	0.8240	0.4720
F	0.8130	0.4610
G	0.8180	0.4630
H	0.7800	0.4230
I	0.4640	0.3020
J	0.4270	0.2820
K	0.4770	0.3100
L	0.3930	0.2740
M	0.6040	0.3110
N	0.5750	0.3360
O	0.5940	0.2960
P	0.5480	0.3210
Q	0.5620	0.2950
R	0.5410	0.3240
S	0.4970	0.2590
T	0.4970	0.3030
U	0.0490	0.2610
V	0.1050	0.3030
W	0.0600	0.2650
X	0.1200	0.2920

