



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 11:20 AM UTC

PDB ID : 8TEW / pdb_00008tew
EMDB ID : EMD-41204
Title : Human cytomegalovirus penton vertex, CVSC-bound configuration
Authors : Jih, J.; Liu, Y.T.; Liu, W.; Zhou, H.
Deposited on : 2023-07-07
Resolution : 3.02 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

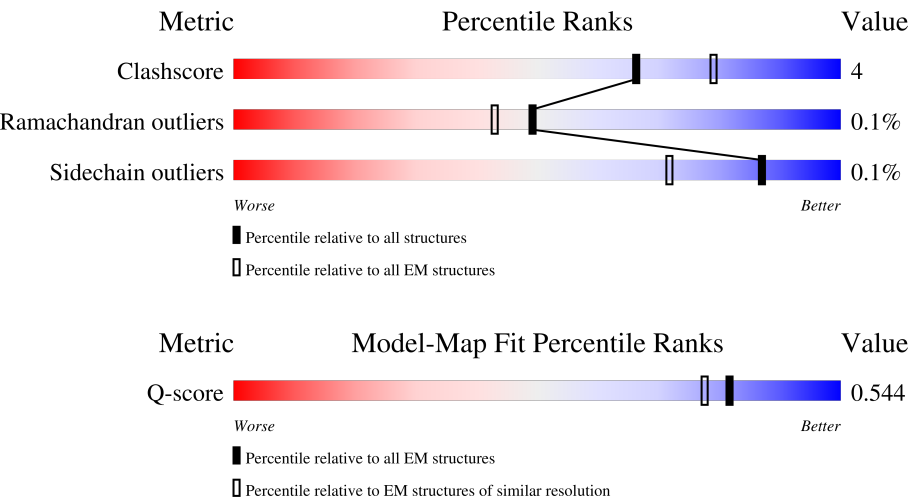
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.02 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.



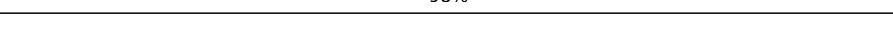
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13913 (2.52 - 3.52)

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

Mol	Chain	Length	Quality of chain
1	1	1370	88%8%5%
1	H	1370	90%8%
1	I	1370	89%9%
1	J	1370	86%10%

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Mol	Chain	Length	Quality of chain
1	K	1370	 90% 9%
1	L	1370	 89% 9%
1	M	1370	 88% 11%
2	2	75	 77% 7% 16%
2	N	75	 69% 13% 16%
2	O	75	 73% 11% 16%
2	P	75	 64% 20% 16%
2	Q	75	 76% 8% 16%
2	R	75	 65% 19% 16%
2	S	75	 73% 11% 16%
3	3	1048	 26% 73%
3	Z	1048	 22% 5% 73%
4	A	2241	 98%
4	C	2241	 98%
5	E	642	 11% 87%
5	F	642	 43% 53% 21% 26%
6	G	594	 71% 8% 21%
7	T	290	 37% 8% 56%
7	W	290	 88% 11%
8	U	306	 91% 8%
8	V	306	 87% 10%
8	X	306	 90% 7%
8	Y	306	 85% 8% 7%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 104261 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1306	Total	C	N	O	S	0	0
			10362	6608	1796	1899	59		
1	H	1335	Total	C	N	O	S	0	0
			10574	6733	1830	1950	61		
1	I	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
1	J	1317	Total	C	N	O	S	0	0
			10433	6641	1814	1919	59		
1	K	1351	Total	C	N	O	S	0	0
			10705	6816	1854	1974	61		
1	L	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
1	M	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
2	N	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
2	O	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
2	P	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
2	Q	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
2	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
2	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 3 is a protein called Large structural phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
3	Z	284	Total	C	N	O	S	0	0
			2320	1463	425	420	12		

- Molecule 4 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	43	Total	C	N	O	S	0	0
			354	228	63	62	1		
4	C	36	Total	C	N	O	S	0	0
			301	193	55	52	1		

- Molecule 5 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	82	Total	C	N	O	S	0	0
			681	419	133	125	4		
5	F	478	Total	C	N	O	S	0	0
			3893	2508	686	688	11		

- Molecule 6 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	472	Total	C	N	O	S	0	0
			3873	2422	744	693	14		

- Molecule 7 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	129	Total	C	N	O	S	0	0
			1067	691	185	186	5		
7	W	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 8 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	303	Total	C	N	O	S	0	0
			2406	1541	419	428	18		
8	V	298	Total	C	N	O	S	0	0
			2369	1517	414	421	17		

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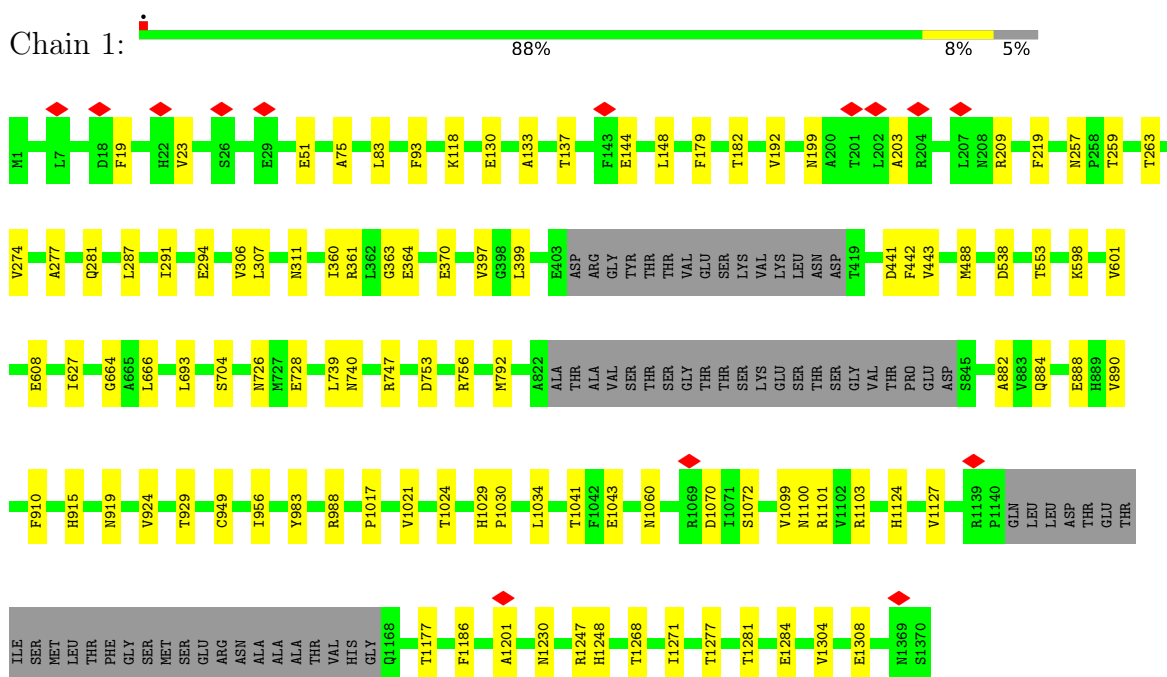
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Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
8	Y	285	Total	C	N	O	S	0	0
			2266	1456	387	405	18		

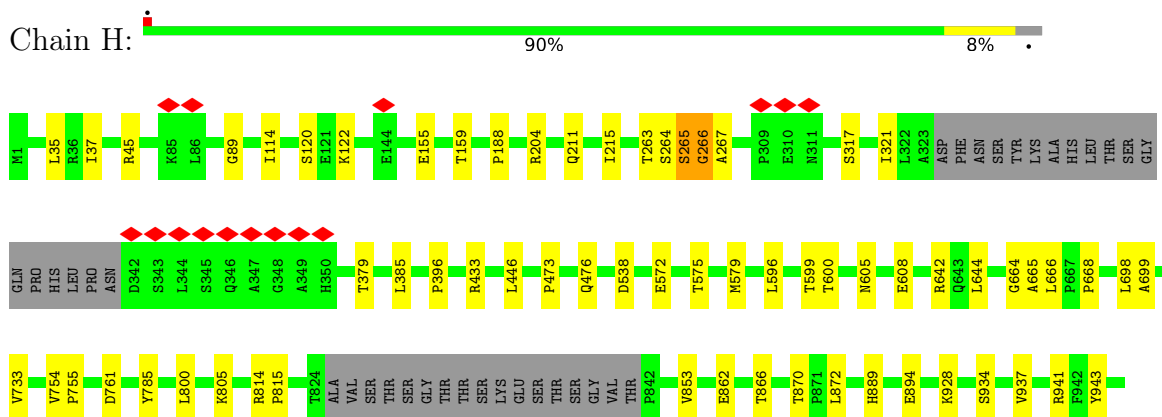
3 Residue-property plots

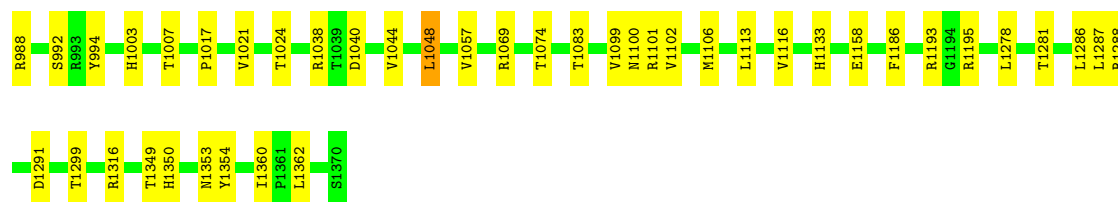
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Major capsid protein



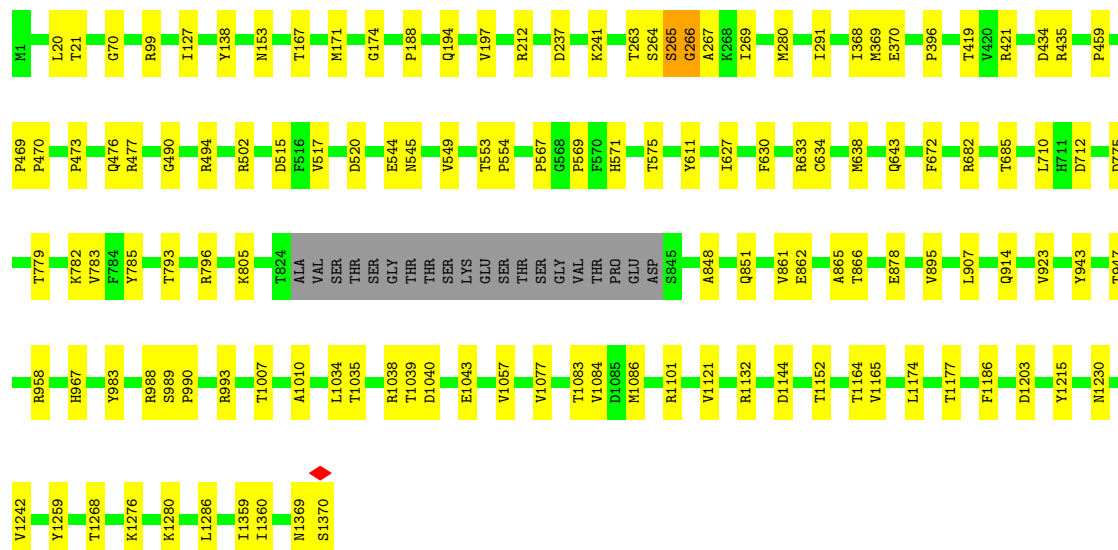
• Molecule 1: Major capsid protein





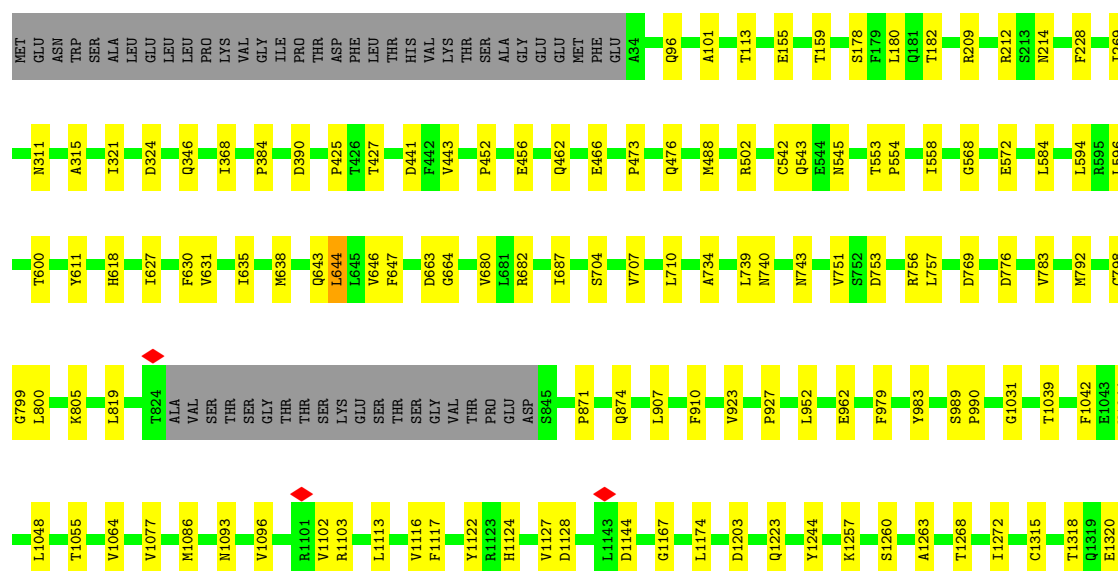
• Molecule 1: Major capsid protein

Chain I: 89% 9%



• Molecule 1: Major capsid protein

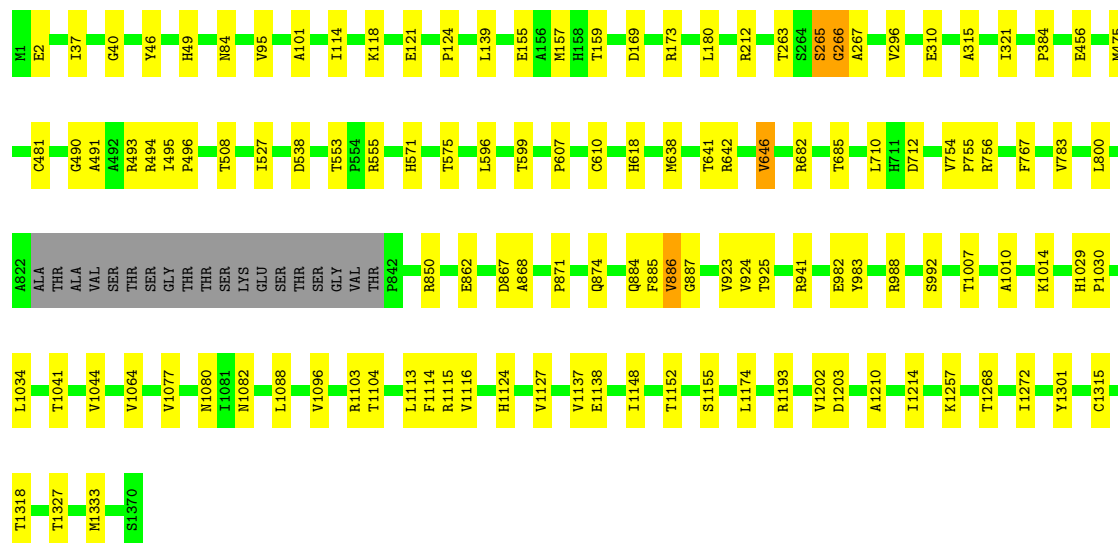
Chain J: 86% 10%





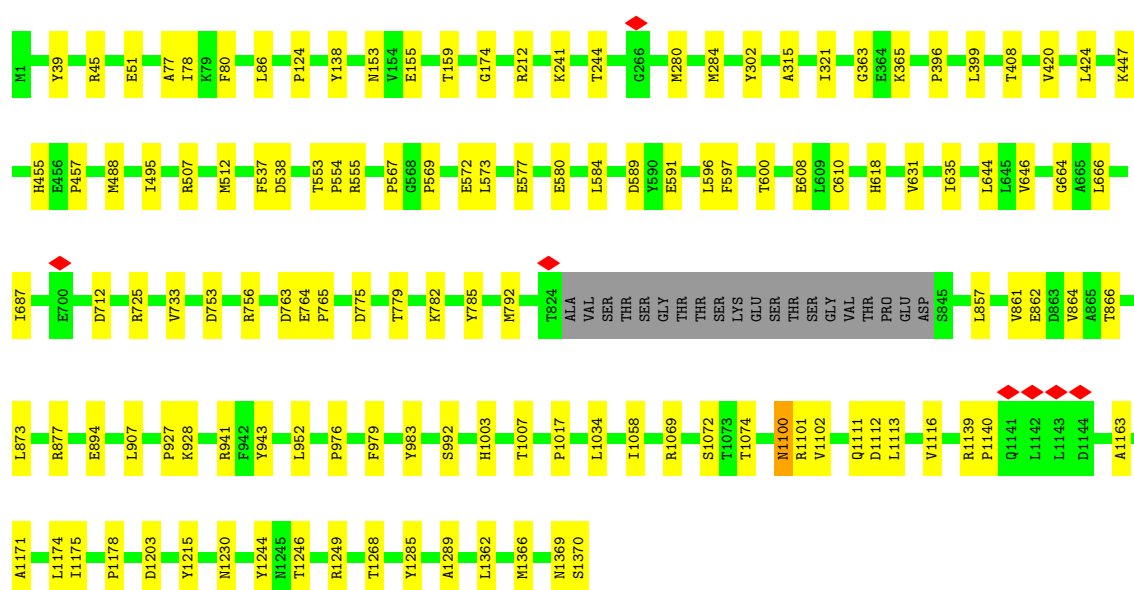
- Molecule 1: Major capsid protein

Chain K: 90% 9%



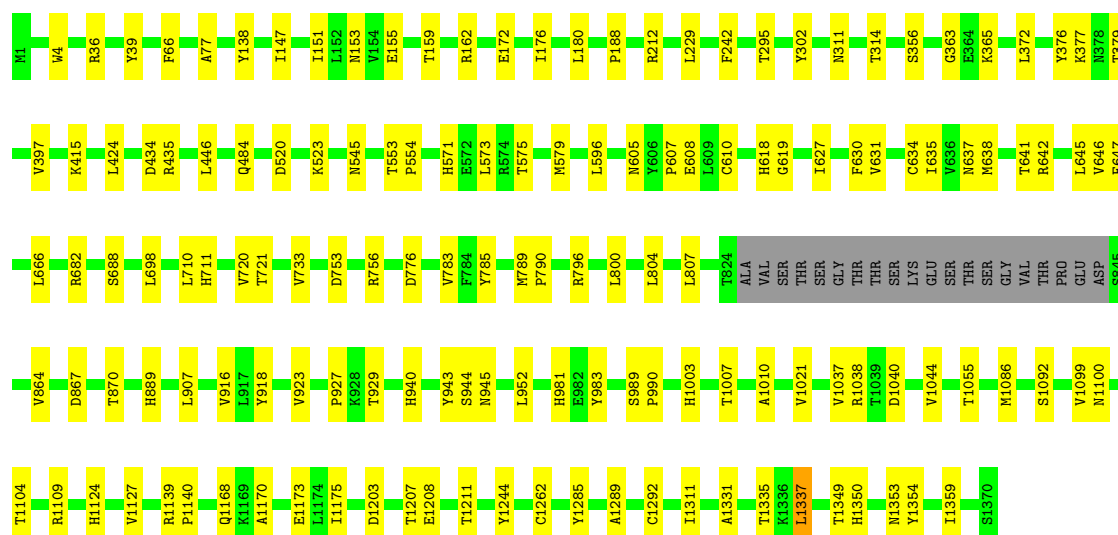
- Molecule 1: Major capsid protein

Chain L: 89% 9%



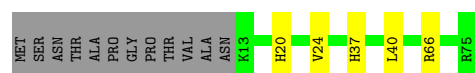
- Molecule 1: Major capsid protein

Chain M: 88% 11%



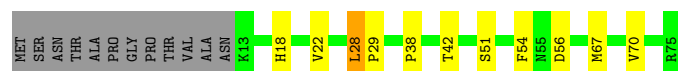
• Molecule 2: Small capsomere-interacting protein

Chain 2: 77% 7% 16%



• Molecule 2: Small capsomere-interacting protein

Chain N: 69% 13% 16%



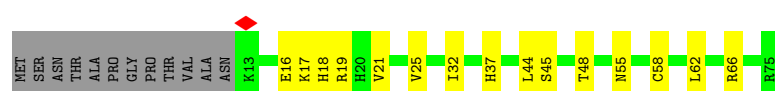
• Molecule 2: Small capsomere-interacting protein

Chain O: 73% 11% 16%



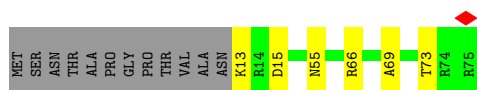
• Molecule 2: Small capsomere-interacting protein

Chain P: 64% 20% 16%



• Molecule 2: Small capsomere-interacting protein

Chain Q: 76% 8% 16%



- Molecule 2: Small capsomere-interacting protein



- Molecule 2: Small capsomere-interacting protein

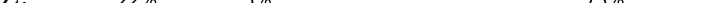


- Molecule 3: Large structural phosphoprotein



[illegible]

- Molecule 3: Large structural phosphoprotein

Chain Z:  22% 5% 73%

[illegible]

Chain A: 98%



T2231		L2238
I2232		Y2239
Q2233		L2240
		L2241

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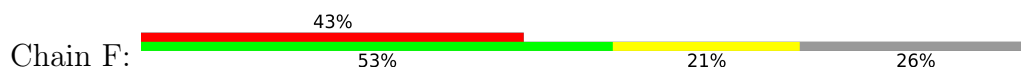
98%

[illegible]

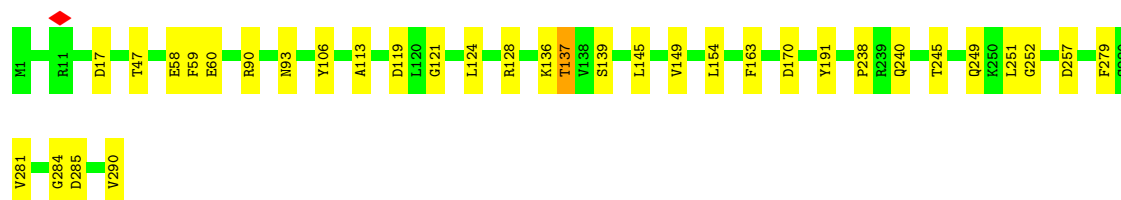
T2231		L2238
I2232		Y2239
Q2233		L2240
H2234		L2241

HIS	TYR	GLU	GLU	HIS	GLY	LEU	GLY	ARG	GLY	VAL	GLY	GLY	TYR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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● Molecule 5: Capsid vertex component 2



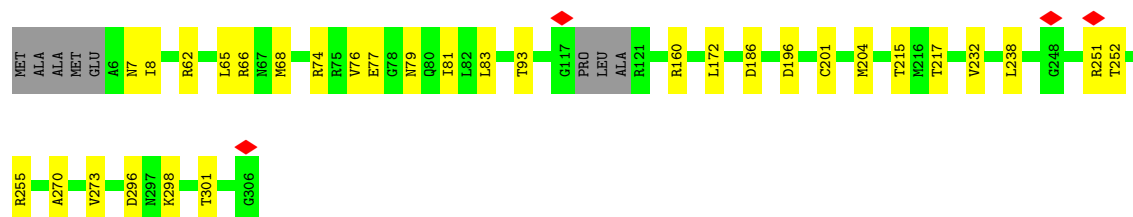
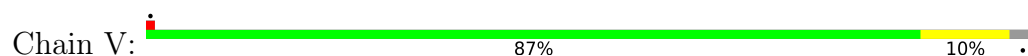
R340	D341	D344	Y348	K349	P350	LEU	SER	GLY	GLY	H356	Y357	H358	P359	F362	D363	R364	H365	V366	V368	R369	L370	F371	H372	K373	R374	I377	Q378	H379	L380	P381	G382	Y383	G384	THR	ILE	THR	GLU	GLU	LEU	VAL	GLN	GLU	ARG	D401	D402	V403	L404												
A280	A281	C282	L283	L284	A285	A286	Y287	G288	H289	A290	L291	W292	E293	G294	R295	D296	P297	P298	D299	S300	V301	A302	T303	V304	L305	G306	E307	L308	Q309	Q310	L311	L312	P313	R314	L315	A316	D317	D318	V319	S320	R321	E322	I323	A324	A325	W326	E327	G328	PRO	VAL	ALA	ALA	G333	N334	N335	Y336	Y337	A338	Y339
G219	I220	W221	Y222	Y223	R224	L225	K226	R227	G228	L229	Y230	T231	Q232	P233	R234	W235	K236	R237	V238	Y239	H240	L241	A242	Q243	M244	D245	N246	F247	S248	I249	S250	Q251	E252	L253	L254	L255	G256	V257	N258	N259	A260	L261	E262	N263	V264	T265	V266	Y267	P268	Y270	D271	C272	V273	L274	L277	E278	A279		
ALA	ALA	ALA	GLY	ALA	SER	THR	LEU	TRP	LEU	GLN	CYS	ALA	ALA	ARG	ARG	PRO	LEU	PRO	GLY	N179	V180	P181	S182	Y183	F184	G185	I186	T187	Q188	N189	D190	P191	F192	I193	R194	F195	H196	T197	D198	F199	R200	G201	E202	V203	V204	N205	T206	M207	F208	E209	N210	A211	S212	T213	W214	T215	F216	S217	F218
GLY	PRO	SER	PRO	THR	LEU	GLN	PRO	PRO	ARG	ARG	CYS	ARG	PRO	TRP	GLU	ARG	SER	SER	SER	ASP	VAL	PRO	GLY	THR	GLY	VAL	ALA	GLY	ALA	ALA	ALA	VAL	VAL	ASP	HIS	ASP	ILE	ALA	THR	GLY	PRO	ALA	ALA	PRO	ALA	VAL	PRO	SER	ASP	ALA	VAL	ALA	ALA	SER	GLU	LEU	ASP	GLU	
MET	S2	T6	P11	E17	M42	C45	GLY	TRP	GLU	GLU	ASP	VAL	LEU	MET	D54	R55	V56	K57	R59	Y60	E64	L65	L68	G69	H70	Q73	C76	E77	D78	L79	E80	G81	R82	V83	S84	E85	A86	E87	A88	L89	L90	N91	Q92	Q93	C94	GLU	LEU	ASP	GLU										



- Molecule 8: Triplex capsid protein 2



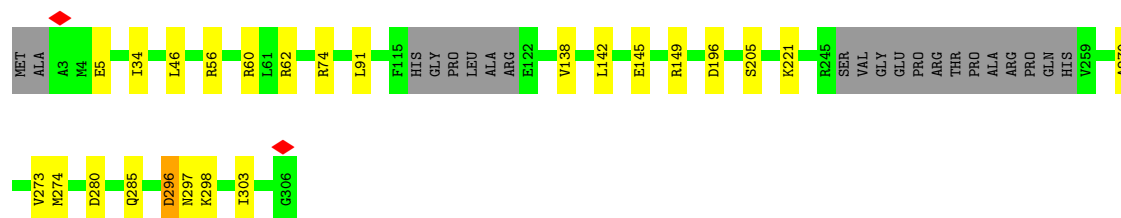
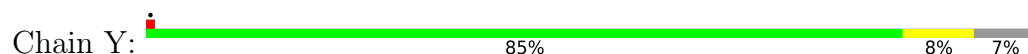
- Molecule 8: Triplex capsid protein 2



- Molecule 8: Triplex capsid protein 2



- Molecule 8: Triplex capsid protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	355778	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0045	Depositor
Map size (Å)	489.6, 489.6, 489.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	1	0.20	0/10613	0.39	2/14458 (0.0%)
1	H	0.21	0/10824	0.39	0/14743
1	I	0.21	0/10949	0.39	0/14916
1	J	0.19	0/10682	0.38	0/14553
1	K	0.21	0/10962	0.40	0/14933
1	L	0.20	0/10949	0.39	0/14916
1	M	0.19	0/10949	0.38	0/14916
2	2	0.16	0/520	0.39	0/697
2	N	0.16	0/520	0.32	0/697
2	O	0.16	0/520	0.29	0/697
2	P	0.15	0/520	0.34	0/697
2	Q	0.17	0/520	0.30	0/697
2	R	0.15	0/520	0.33	0/697
2	S	0.15	0/520	0.33	0/697
3	3	0.15	0/2366	0.32	0/3192
3	Z	0.17	0/2358	0.36	0/3182
4	A	0.14	0/357	0.28	0/482
4	C	0.13	0/303	0.27	0/407
5	E	0.15	0/690	0.26	0/927
5	F	0.11	0/3995	0.30	0/5426
6	G	0.20	0/3962	0.38	0/5371
7	T	0.18	0/1093	0.35	0/1481
7	W	0.22	0/2374	0.44	0/3221
8	U	0.21	0/2453	0.39	2/3332 (0.1%)
8	V	0.20	0/2414	0.40	0/3277
8	X	0.19	0/2379	0.39	0/3230
8	Y	0.19	0/2305	0.41	0/3126
All	All	0.20	0/106617	0.38	4/144968 (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	1	0	1
1	H	0	2
1	I	0	1
1	K	0	1
1	L	0	1
1	M	0	1
6	G	0	1
8	Y	0	1
All	All	0	9

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1099	VAL	CA-C-N	-5.23	114.73	123.04
1	1	1099	VAL	C-N-CA	-5.23	114.73	123.04
8	U	291	CYS	CA-C-N	5.06	131.21	121.54
8	U	291	CYS	C-N-CA	5.06	131.21	121.54

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	1100	ASN	Peptide
6	G	77	GLY	Peptide
1	H	1100	ASN	Peptide
1	H	265	SER	Peptide
1	I	265	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	10362	0	10310	56	0
1	H	10574	0	10522	61	0
1	I	10693	0	10635	75	0
1	J	10433	0	10379	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	10705	0	10641	74	0
1	L	10693	0	10635	77	0
1	M	10693	0	10635	86	0
2	2	513	0	539	3	0
2	N	513	0	539	6	0
2	O	513	0	539	5	0
2	P	513	0	539	15	0
2	Q	513	0	539	4	0
2	R	513	0	539	9	0
2	S	513	0	539	6	0
3	3	2328	0	2363	9	0
3	Z	2320	0	2351	27	0
4	A	354	0	384	11	0
4	C	301	0	323	8	0
5	E	681	0	674	11	0
5	F	3893	0	3823	102	0
6	G	3873	0	3792	31	0
7	T	1067	0	1076	15	0
7	W	2325	0	2363	22	0
8	U	2406	0	2495	15	0
8	V	2369	0	2456	19	0
8	X	2334	0	2431	14	0
8	Y	2266	0	2355	14	0
All	All	104261	0	104416	805	0

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

The worst 5 of 805 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:K:575:THR:HG21	1:K:1007:THR:HA	1.58	0.85
5:F:450:ASP:HB2	5:F:624:ILE:HG13	1.62	0.80
3:Z:230:GLU:OE2	3:Z:231:ARG:NH1	2.16	0.79
1:K:1193:ARG:NH2	1:K:1214:ILE:O	2.15	0.79
1:I:1152:THR:HG21	7:W:113:ALA:HB2	1.65	0.79

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1	1298/1370 (95%)	1238 (95%)	60 (5%)	0	100	100
1	H	1329/1370 (97%)	1264 (95%)	62 (5%)	3 (0%)	43	75
1	I	1346/1370 (98%)	1297 (96%)	48 (4%)	1 (0%)	48	79
1	J	1313/1370 (96%)	1263 (96%)	50 (4%)	0	100	100
1	K	1347/1370 (98%)	1300 (96%)	45 (3%)	2 (0%)	48	79
1	L	1346/1370 (98%)	1293 (96%)	51 (4%)	2 (0%)	48	79
1	M	1346/1370 (98%)	1291 (96%)	54 (4%)	1 (0%)	48	79
2	2	61/75 (81%)	61 (100%)	0	0	100	100
2	N	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
2	O	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
2	P	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
2	Q	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
2	R	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
2	S	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
3	3	283/1048 (27%)	276 (98%)	7 (2%)	0	100	100
3	Z	282/1048 (27%)	272 (96%)	9 (3%)	1 (0%)	30	63
4	A	41/2241 (2%)	40 (98%)	1 (2%)	0	100	100
4	C	34/2241 (2%)	34 (100%)	0	0	100	100
5	E	80/642 (12%)	79 (99%)	1 (1%)	0	100	100
5	F	462/642 (72%)	454 (98%)	8 (2%)	0	100	100
6	G	468/594 (79%)	452 (97%)	16 (3%)	0	100	100
7	T	127/290 (44%)	120 (94%)	7 (6%)	0	100	100
7	W	288/290 (99%)	272 (94%)	16 (6%)	0	100	100
8	U	301/306 (98%)	285 (95%)	15 (5%)	1 (0%)	36	68
8	V	294/306 (96%)	283 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	X	291/306 (95%)	281 (97%)	10 (3%)	0	100	100
8	Y	279/306 (91%)	265 (95%)	13 (5%)	1 (0%)	30	63
All	All	12982/20375 (64%)	12473 (96%)	497 (4%)	12 (0%)	49	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	266	GLY
1	I	266	GLY
1	K	266	GLY
1	K	886	VAL
1	L	764	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	1138/1192 (96%)	1138 (100%)	0	100	100
1	H	1162/1192 (98%)	1160 (100%)	2 (0%)	87	91
1	I	1175/1192 (99%)	1175 (100%)	0	100	100
1	J	1146/1192 (96%)	1145 (100%)	1 (0%)	88	92
1	K	1177/1192 (99%)	1175 (100%)	2 (0%)	87	91
1	L	1175/1192 (99%)	1174 (100%)	1 (0%)	88	92
1	M	1175/1192 (99%)	1172 (100%)	3 (0%)	86	90
2	2	59/68 (87%)	59 (100%)	0	100	100
2	N	59/68 (87%)	58 (98%)	1 (2%)	53	77
2	O	59/68 (87%)	59 (100%)	0	100	100
2	P	59/68 (87%)	59 (100%)	0	100	100
2	Q	59/68 (87%)	59 (100%)	0	100	100
2	R	59/68 (87%)	59 (100%)	0	100	100
2	S	59/68 (87%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	256/883 (29%)	255 (100%)	1 (0%)	84	89
3	Z	255/883 (29%)	255 (100%)	0	100	100
4	A	41/1941 (2%)	41 (100%)	0	100	100
4	C	34/1941 (2%)	34 (100%)	0	100	100
5	E	72/526 (14%)	72 (100%)	0	100	100
5	F	415/526 (79%)	414 (100%)	1 (0%)	87	91
6	G	398/500 (80%)	398 (100%)	0	100	100
7	T	117/252 (46%)	117 (100%)	0	100	100
7	W	252/252 (100%)	251 (100%)	1 (0%)	84	89
8	U	272/273 (100%)	272 (100%)	0	100	100
8	V	268/273 (98%)	268 (100%)	0	100	100
8	X	263/273 (96%)	263 (100%)	0	100	100
8	Y	257/273 (94%)	257 (100%)	0	100	100
All	All	11461/17616 (65%)	11448 (100%)	13 (0%)	87	92

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1102	VAL
1	M	397	VAL
7	W	137	THR
1	M	1337	LEU
2	N	28	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	722	HIS
8	V	258	HIS
1	K	1061	ASN
8	V	173	GLN
1	M	1309	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

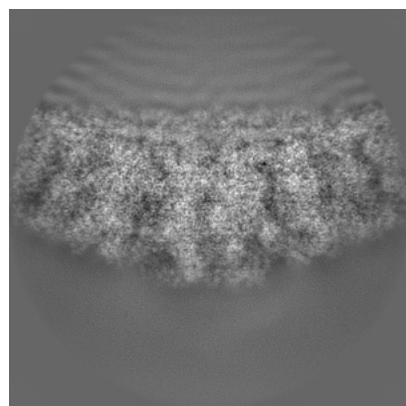
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41204. These allow visual inspection of the internal detail of the map and identification of artifacts.

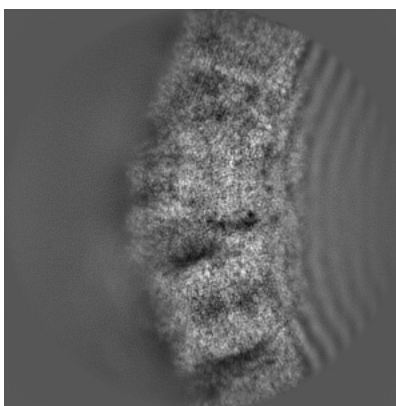
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

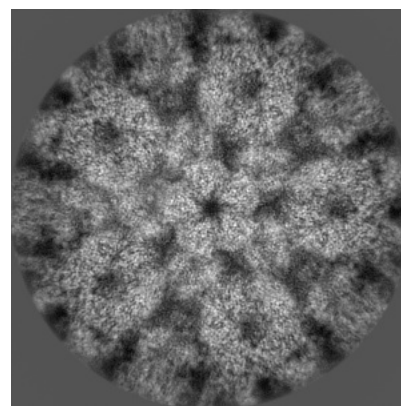
6.1.1 Primary map



X

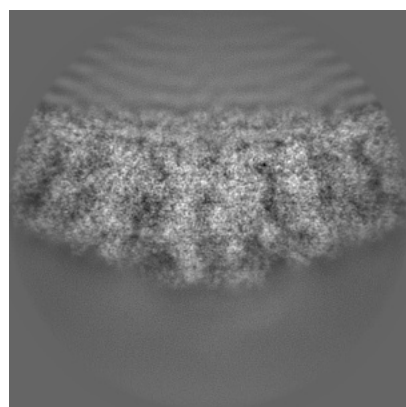


Y

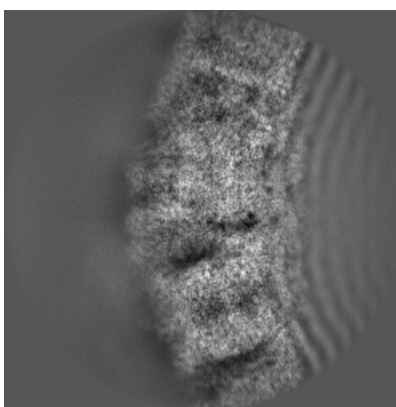


Z

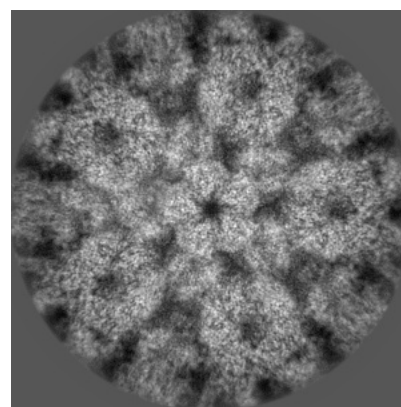
6.1.2 Raw map



X



Y

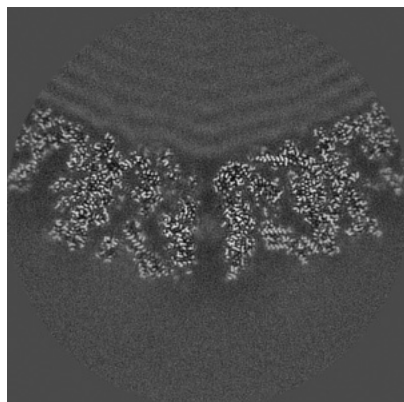


Z

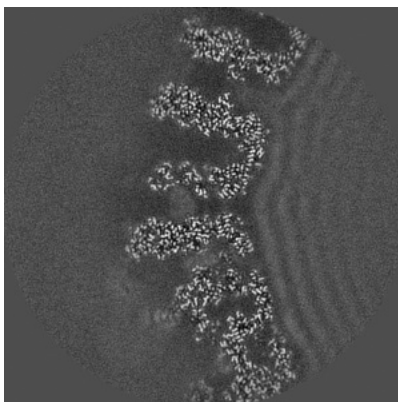
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

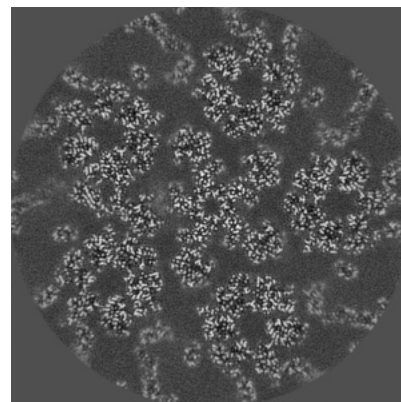
6.2.1 Primary map



X Index: 180

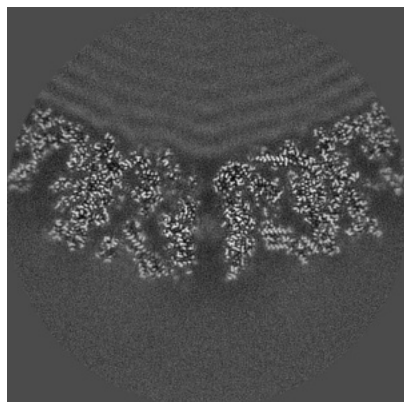


Y Index: 180

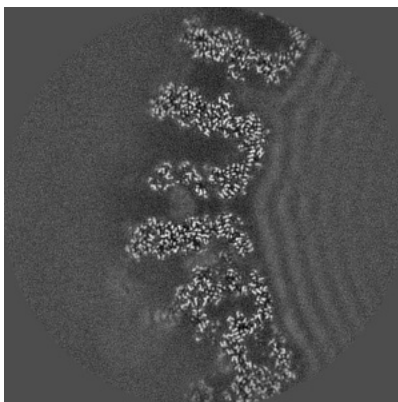


Z Index: 180

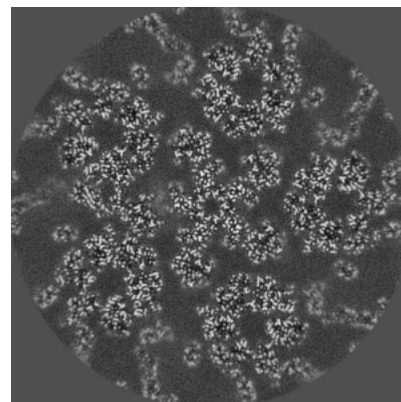
6.2.2 Raw map



X Index: 180



Y Index: 180

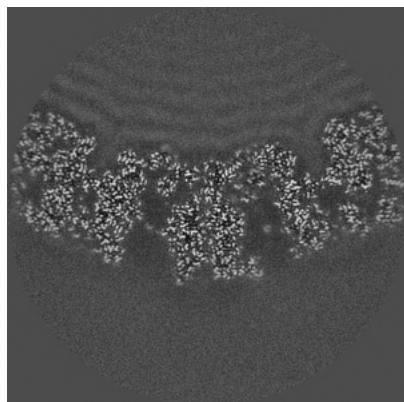


Z Index: 180

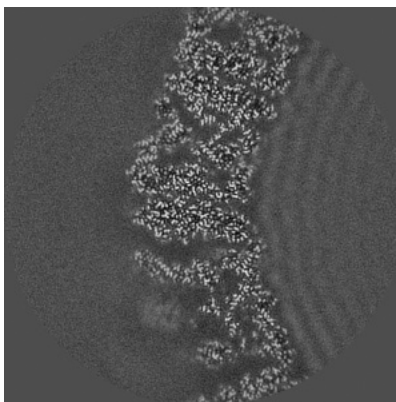
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

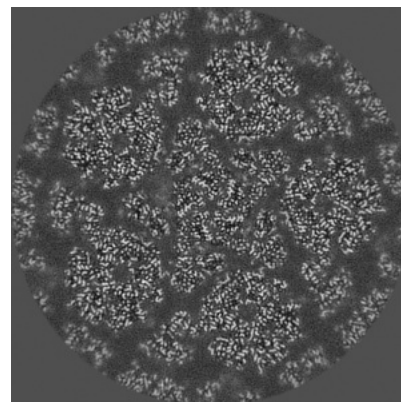
6.3.1 Primary map



X Index: 204

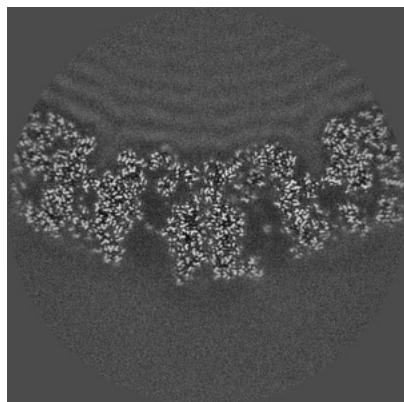


Y Index: 159

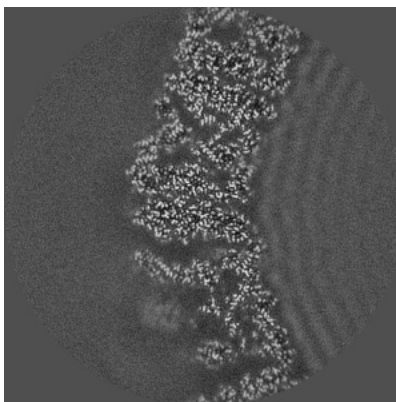


Z Index: 205

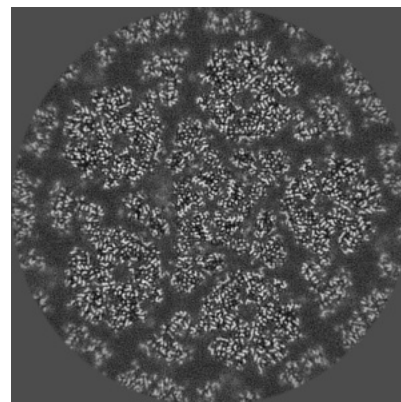
6.3.2 Raw map



X Index: 204



Y Index: 159

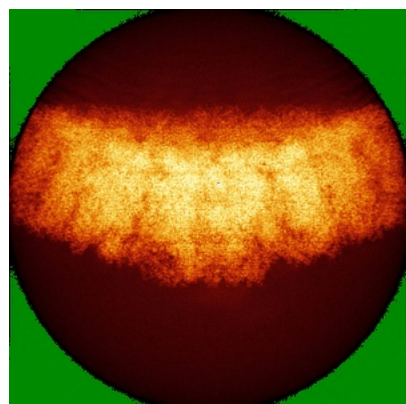


Z Index: 205

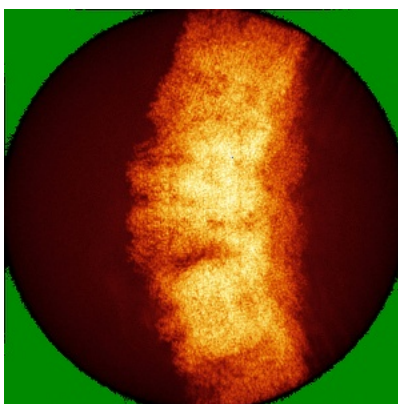
The images above show the largest variance slices of the map in three orthogonal directions.

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

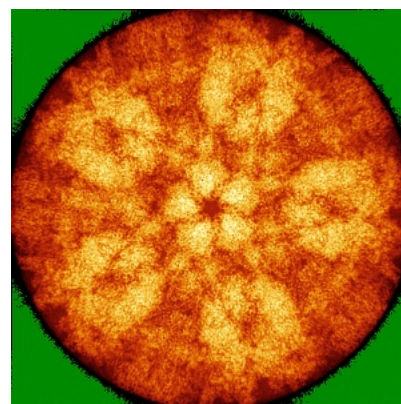
6.4.1 Primary map



X

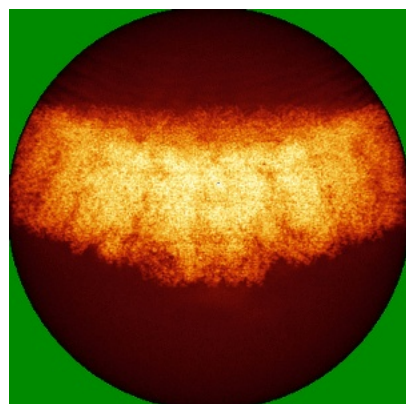


Y

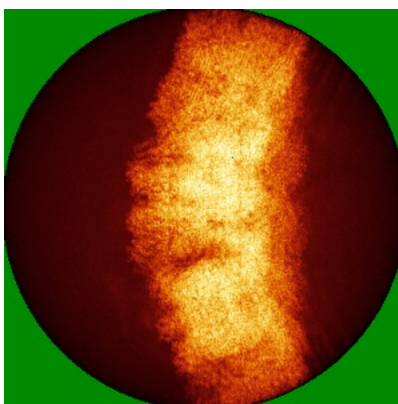


Z

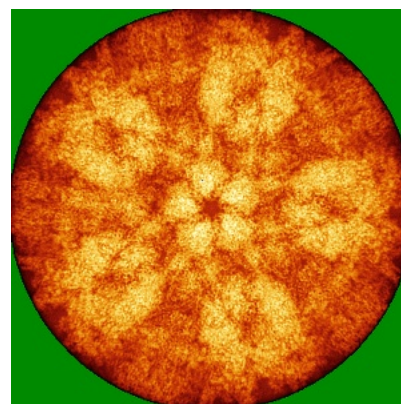
6.4.2 Raw map



X



Y

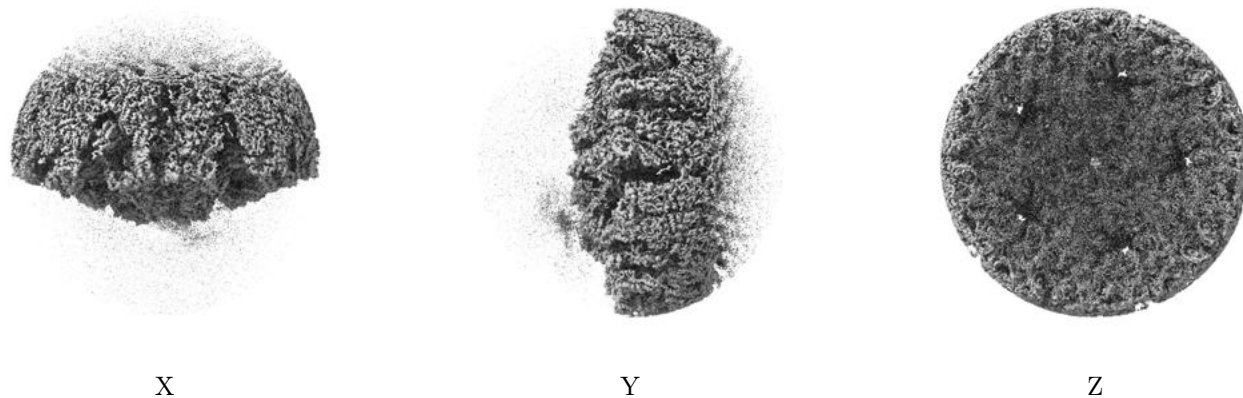


Z

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

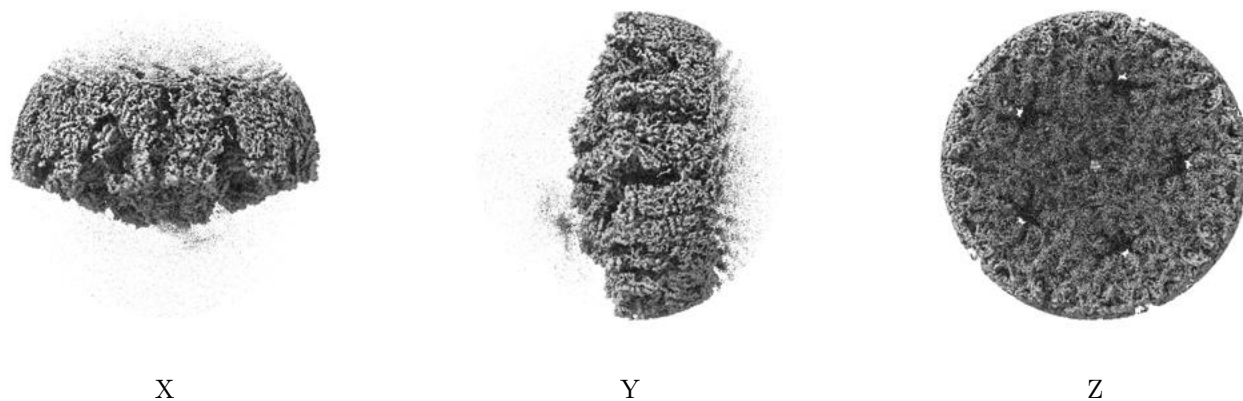
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

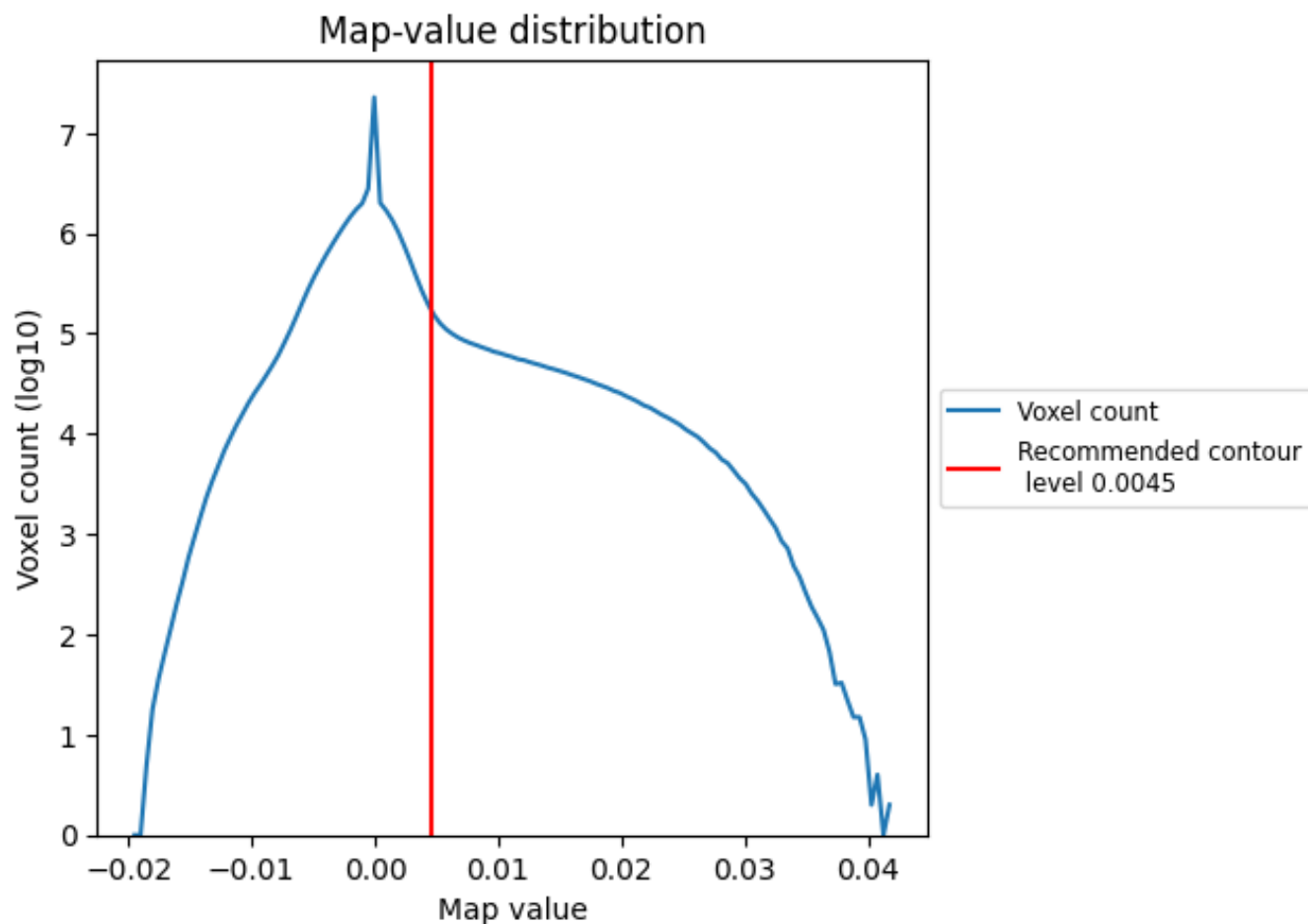
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

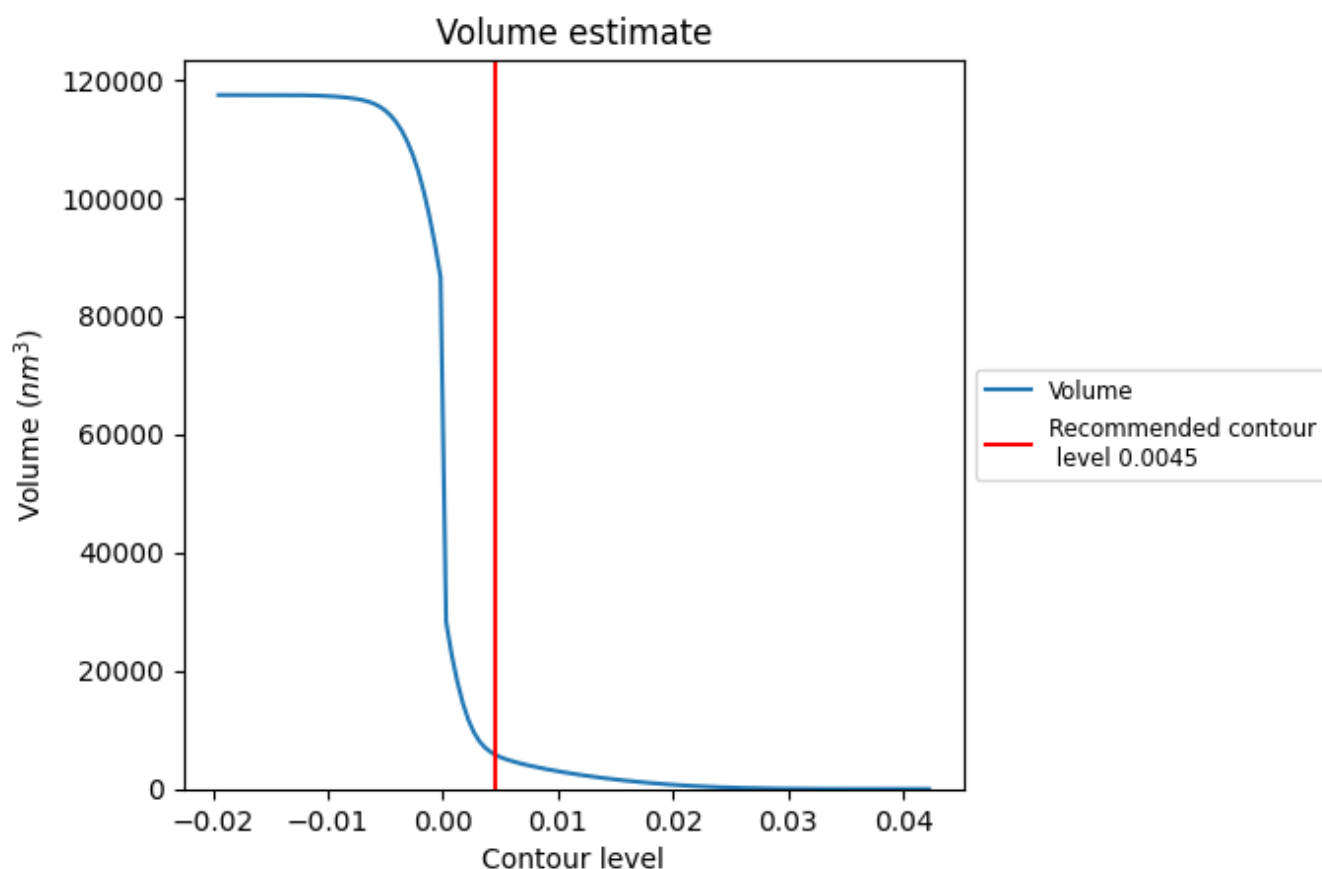
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

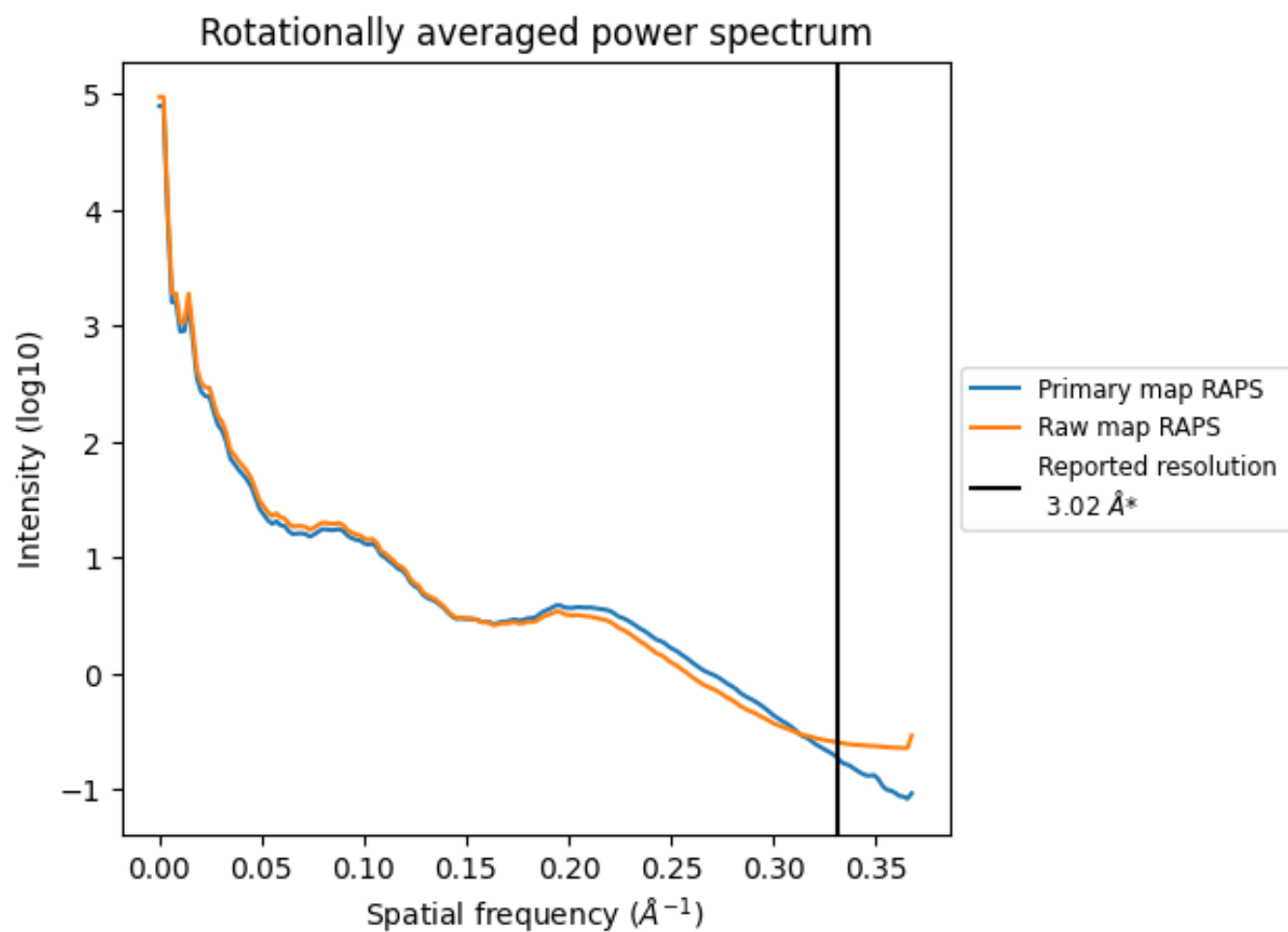
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5844 nm³; this corresponds to an approximate mass of 5279 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

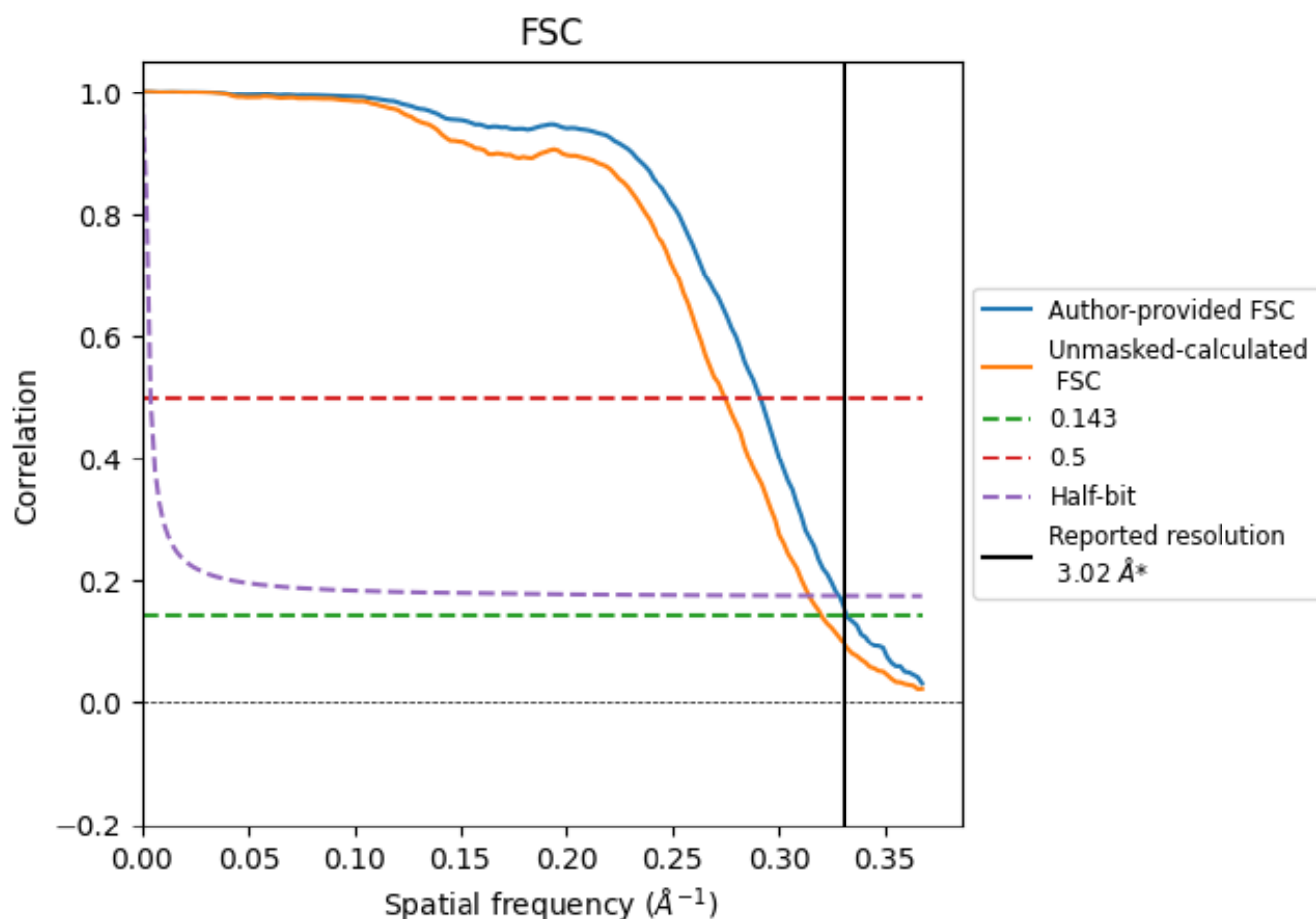


*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.01	3.44	3.05
Unmasked-calculated*	3.12	3.64	3.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

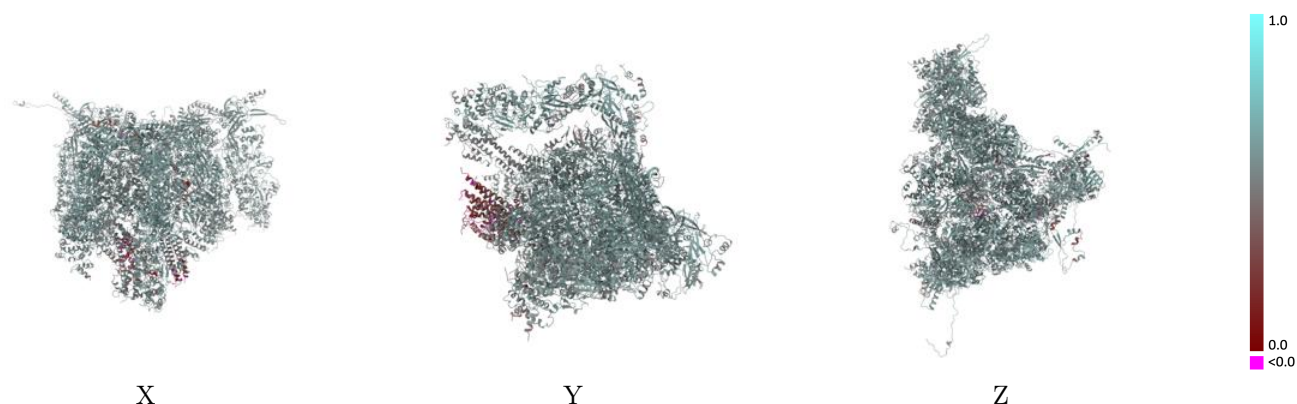
This section contains information regarding the fit between EMDB map EMD-41204 and PDB model 8TEW. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



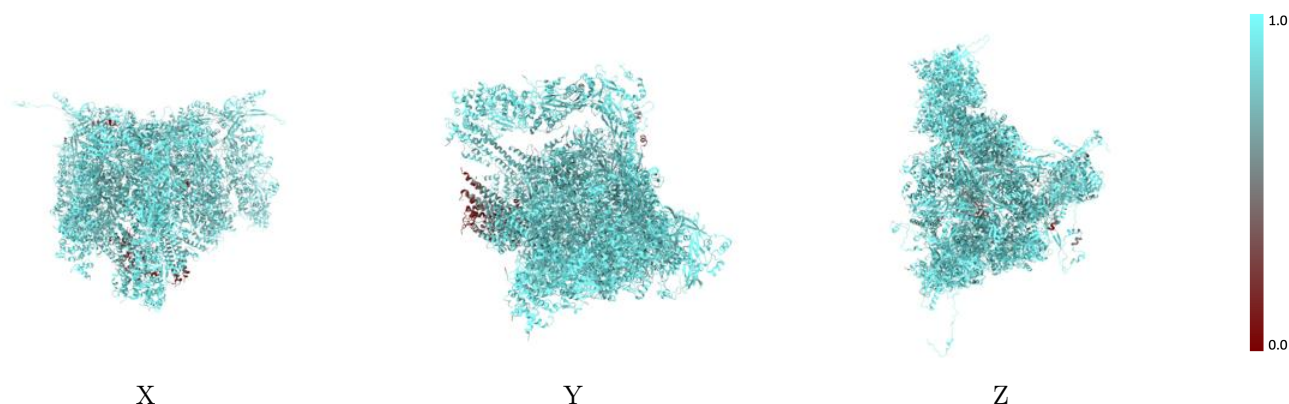
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



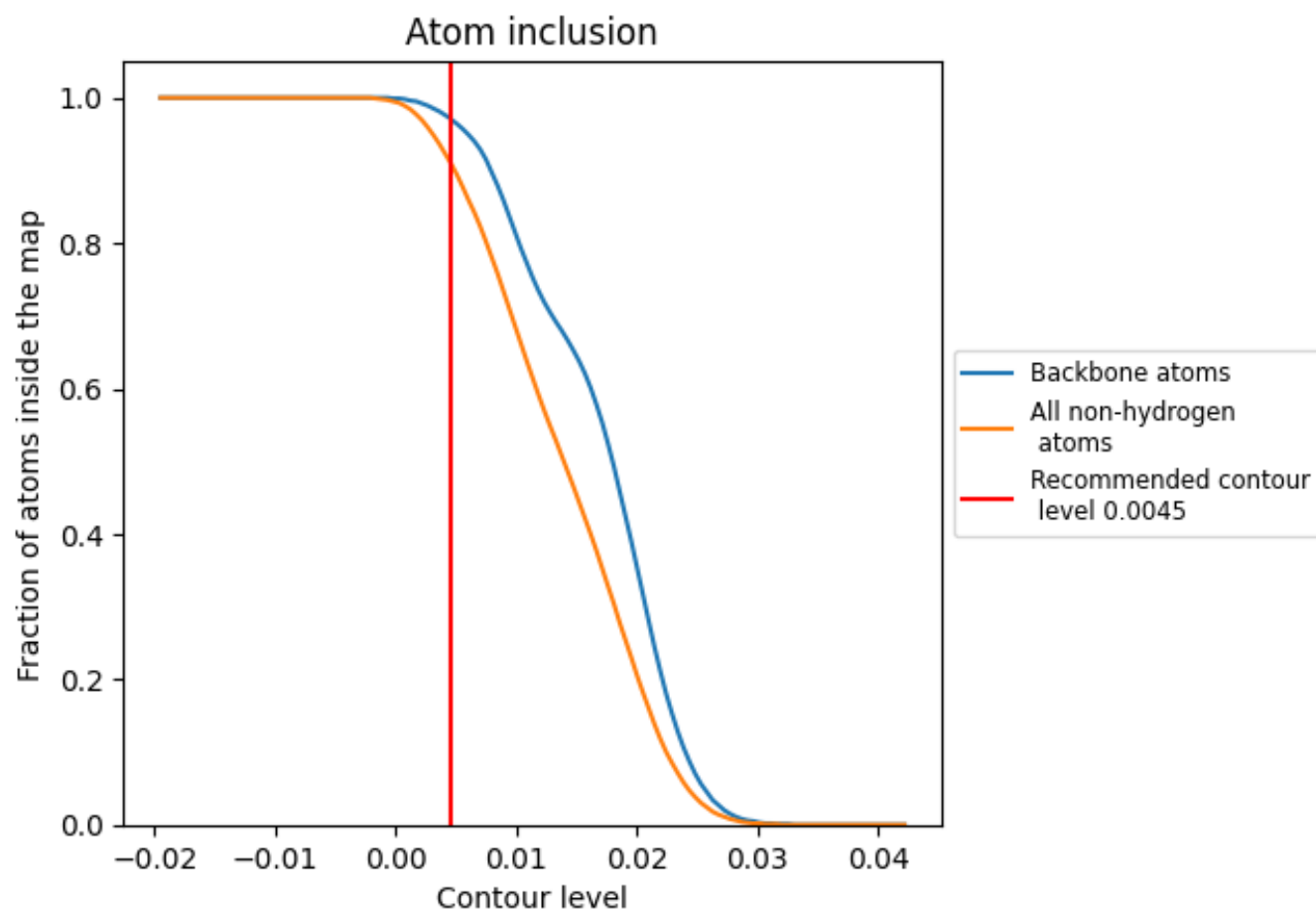
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9120	 0.5440
1	 0.9340	 0.5620
2	 0.9360	 0.5110
3	 0.8970	 0.5020
A	 0.6900	 0.3290
C	 0.6920	 0.3360
E	 0.8220	 0.4600
F	 0.3900	 0.2390
G	 0.9380	 0.5540
H	 0.9460	 0.5760
I	 0.9540	 0.5750
J	 0.9370	 0.5590
K	 0.9510	 0.5770
L	 0.9400	 0.5660
M	 0.9310	 0.5560
N	 0.9240	 0.4970
O	 0.9080	 0.5060
P	 0.8750	 0.4790
Q	 0.8980	 0.4990
R	 0.8900	 0.4920
S	 0.9000	 0.5010
T	 0.9030	 0.5300
U	 0.9140	 0.5570
V	 0.9060	 0.5430
W	 0.9290	 0.5610
X	 0.9000	 0.5420
Y	 0.9140	 0.5440
Z	 0.8930	 0.4980

