



Full wwPDB EM Validation Report ⓘ

Apr 21, 2025 – 03:19 PM JST

PDB ID : 8XA3 / pdb_00008xa3
EMDB ID : EMD-38193
Title : C-hexon capsomer of the VZV B-Capsid
Authors : Wang, N.; Cao, L.; Wang, X.
Deposited on : 2023-12-01
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

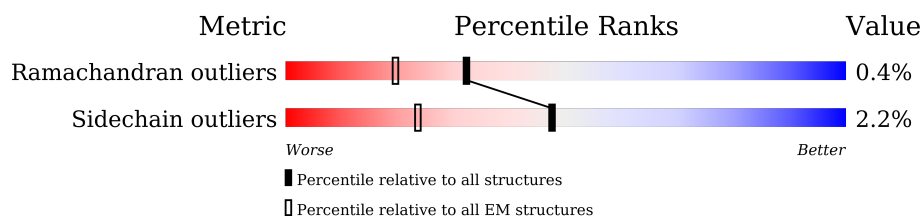
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

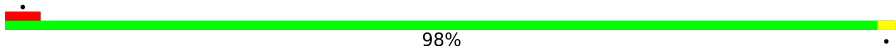
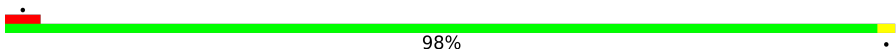
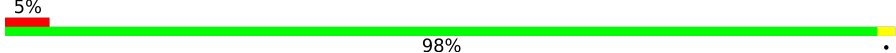
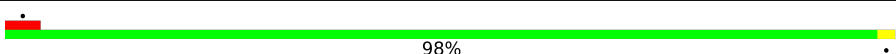
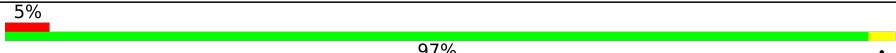
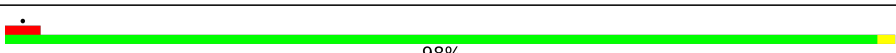
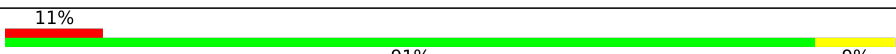
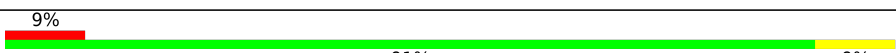
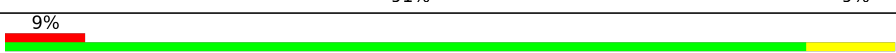
The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1381	
1	C	1381	
1	D	1381	
1	E	1381	
1	F	1381	
1	H	1381	
2	B	94	
2	G	94	
2	L	94	

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Mol	Chain	Length	Quality of chain
2	Q	94	
2	V	94	
2	g	94	
3	I	256	
3	K	256	
4	N	263	
4	P	263	
5	S	392	
5	U	392	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 81795 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	A	1381	Total 10675	C 6757	N 1870	O 1981	S 67	0	0
1	C	1381	Total 10675	C 6757	N 1870	O 1981	S 67	0	0
1	D	1381	Total 10680	C 6759	N 1873	O 1981	S 67	0	0
1	E	1381	Total 10675	C 6757	N 1870	O 1981	S 67	0	0
1	F	1381	Total 10675	C 6757	N 1870	O 1981	S 67	0	0
1	H	1381	Total 10675	C 6757	N 1870	O 1981	S 67	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	LEU	conflict	UNP Q6QCL5
A	814	ALA	GLY	conflict	UNP Q6QCL5
C	22	ILE	LEU	conflict	UNP Q6QCL5
C	814	ALA	GLY	conflict	UNP Q6QCL5
D	22	ILE	LEU	conflict	UNP Q6QCL5
D	814	ALA	GLY	conflict	UNP Q6QCL5
E	22	ILE	LEU	conflict	UNP Q6QCL5
E	814	ALA	GLY	conflict	UNP Q6QCL5
F	22	ILE	LEU	conflict	UNP Q6QCL5
F	814	ALA	GLY	conflict	UNP Q6QCL5
H	22	ILE	LEU	conflict	UNP Q6QCL5
H	814	ALA	GLY	conflict	UNP Q6QCL5

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	G	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	B	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	g	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	V	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	Q	94	Total	C	N	O	S	0	0
			699	437	135	125	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	95	ARG	LYS	conflict	UNP U5NQG6
G	95	ARG	LYS	conflict	UNP U5NQG6
B	95	ARG	LYS	conflict	UNP U5NQG6
g	95	ARG	LYS	conflict	UNP U5NQG6
V	95	ARG	LYS	conflict	UNP U5NQG6
Q	95	ARG	LYS	conflict	UNP U5NQG6

- Molecule 3 is a protein called Tri2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	256	Total	C	N	O	S	0	0
			1847	1191	315	333	8		
3	K	256	Total	C	N	O	S	0	0
			1847	1191	315	333	8		

- Molecule 4 is a protein called Tri2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	263	Total	C	N	O	S	0	0
			1975	1269	339	358	9		
4	P	263	Total	C	N	O	S	0	0
			1975	1269	339	358	9		

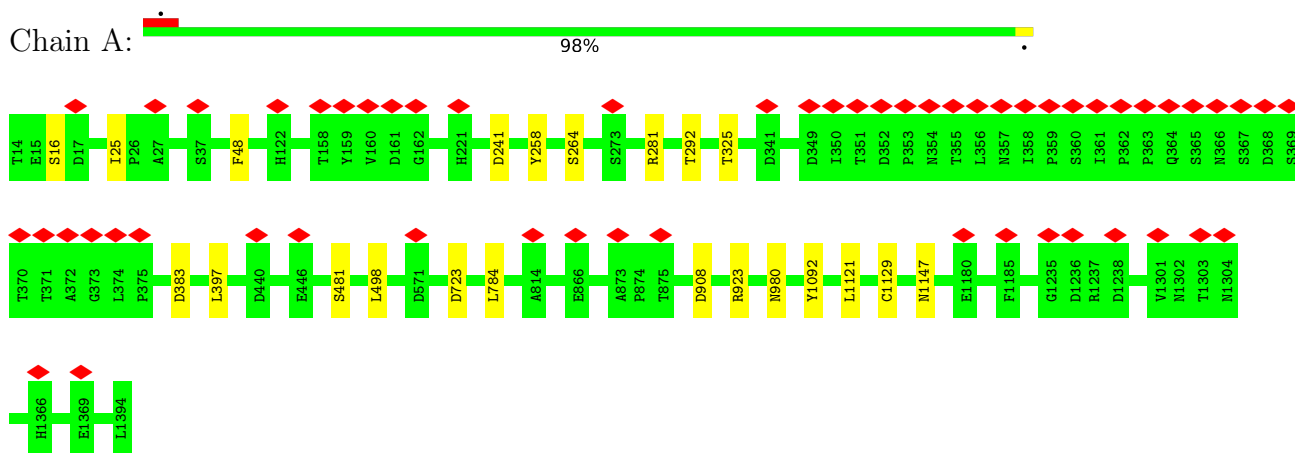
- Molecule 5 is a protein called Tri1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	392	Total 2951	C 1854	N 552	O 529	S 16	0	0
5	U	392	Total 2951	C 1854	N 552	O 529	S 16	0	0

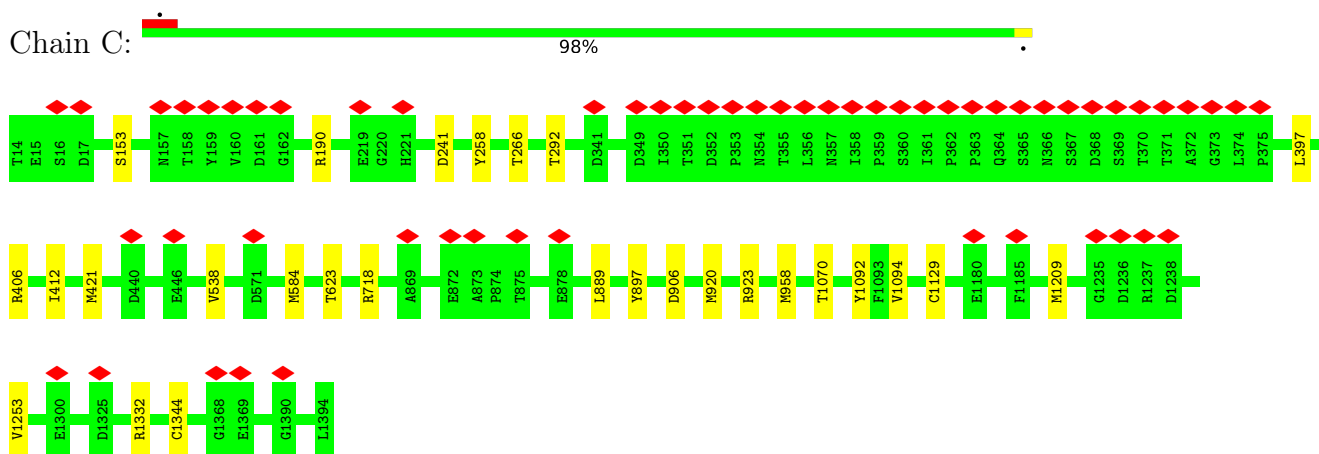
3 Residue-property plots

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

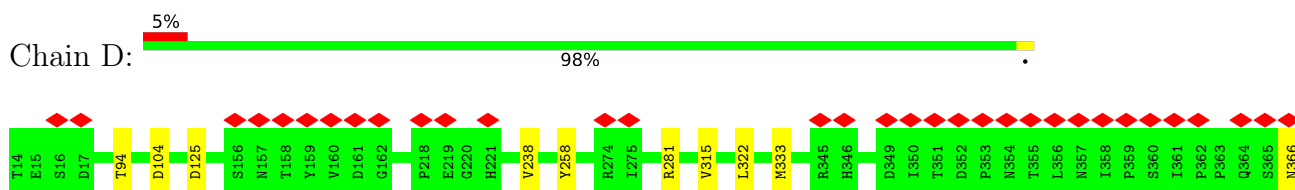
- Molecule 1: Major capsid protein

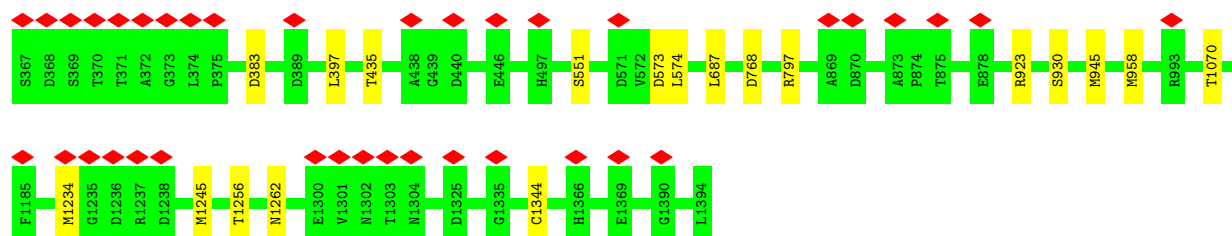


- Molecule 1: Major capsid protein



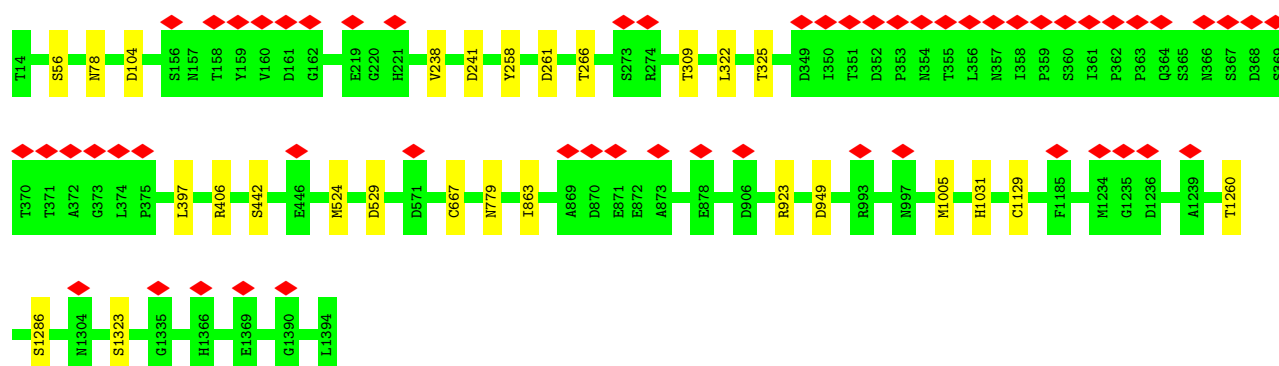
- Molecule 1: Major capsid protein





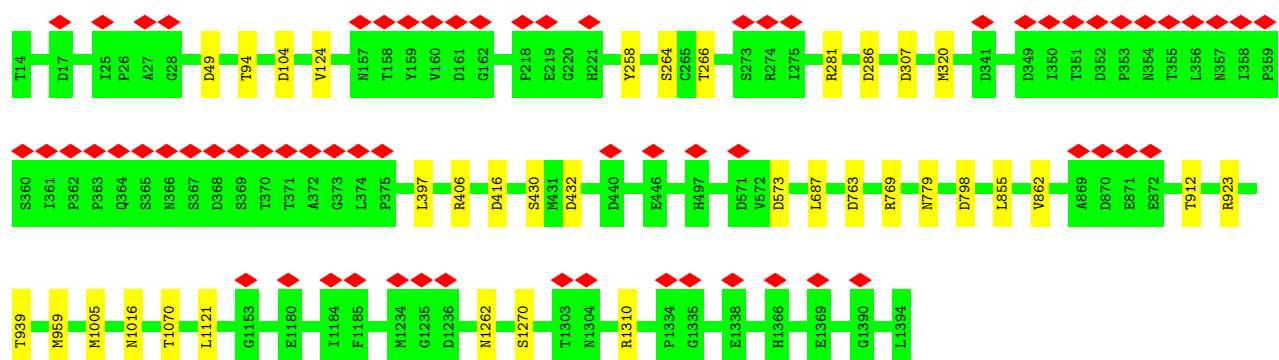
- Molecule 1: Major capsid protein

Chain E: 98%



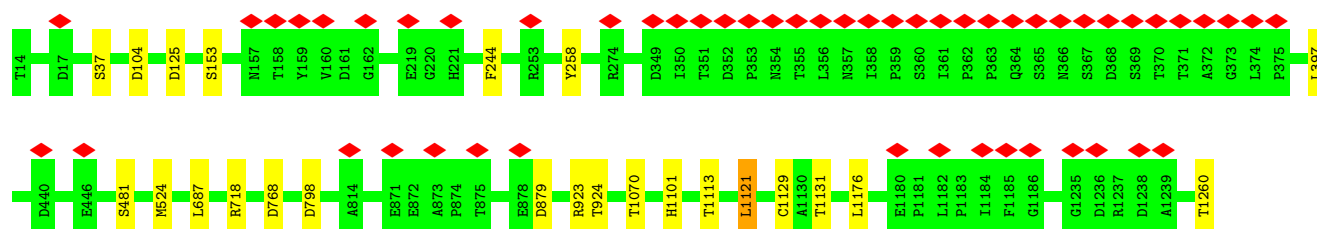
- Molecule 1: Major capsid protein

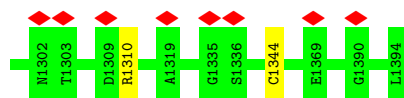
Chain F: 5% 97%



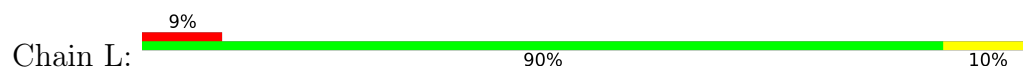
- Molecule 1: Major capsid protein

Chain H: 98%

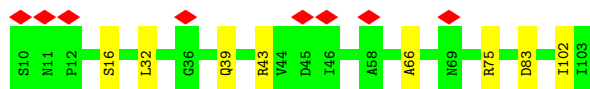




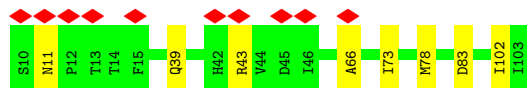
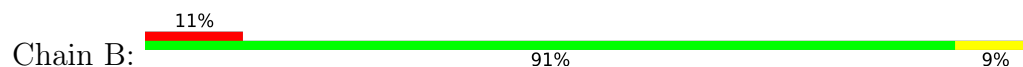
- Molecule 2: Small capsomere-interacting protein



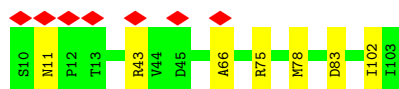
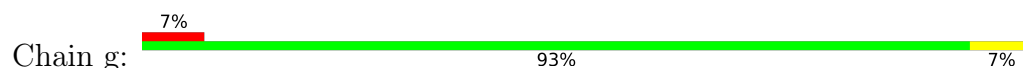
- Molecule 2: Small capsomere-interacting protein



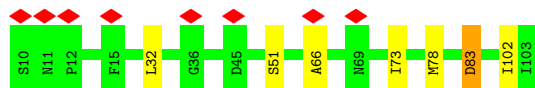
- Molecule 2: Small capsomere-interacting protein



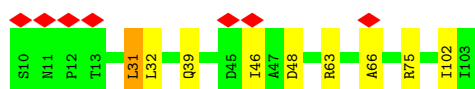
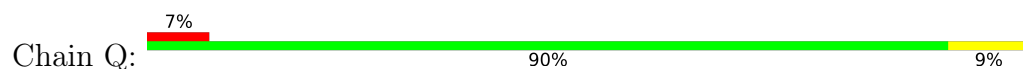
- Molecule 2: Small capsomere-interacting protein



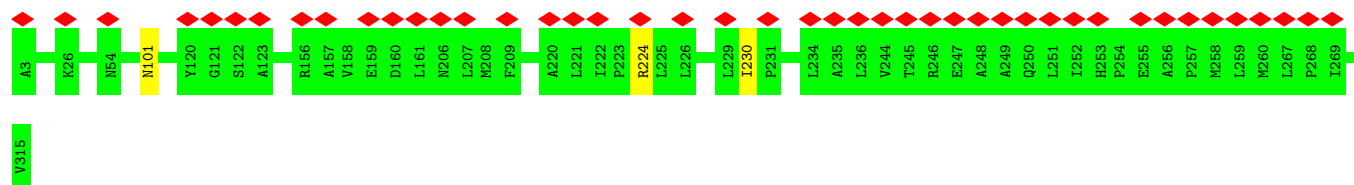
- Molecule 2: Small capsomere-interacting protein



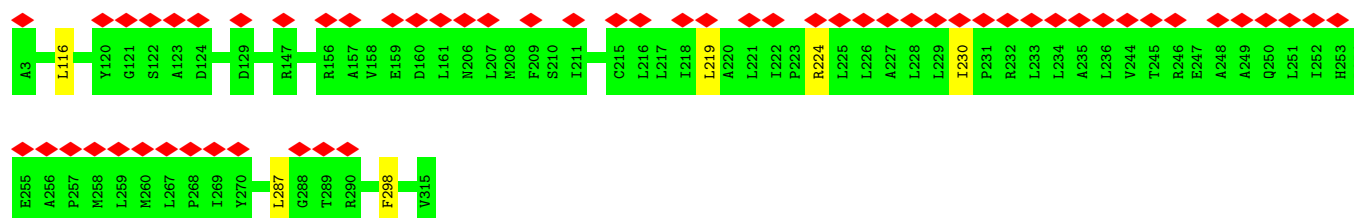
- Molecule 2: Small capsomere-interacting protein



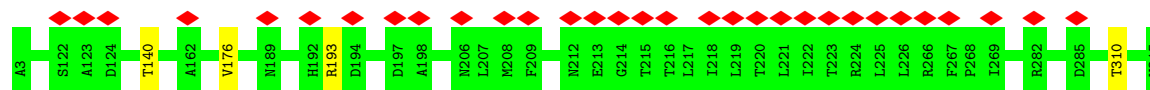
- Molecule 3: Tri2A



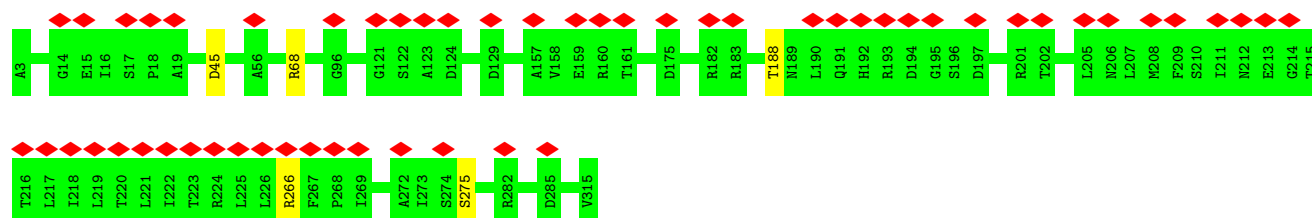
• Molecule 3: Tri2A



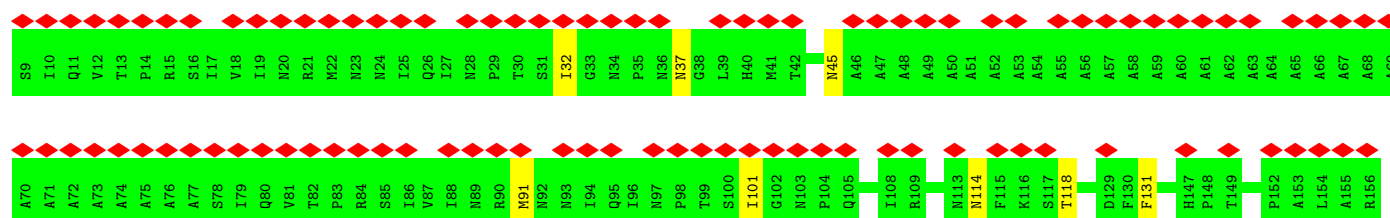
• Molecule 4: Tri2B

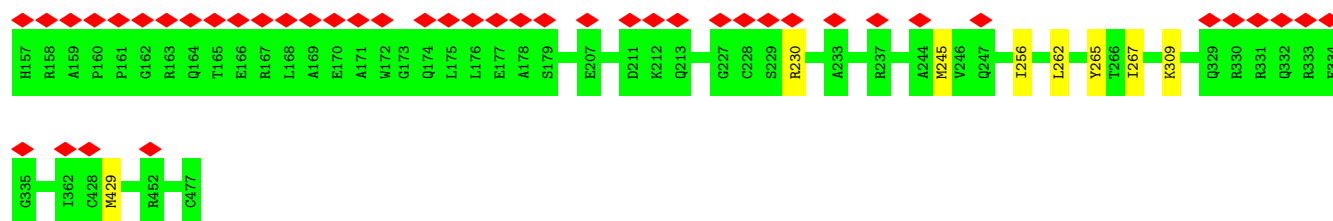


• Molecule 4: Tri2B

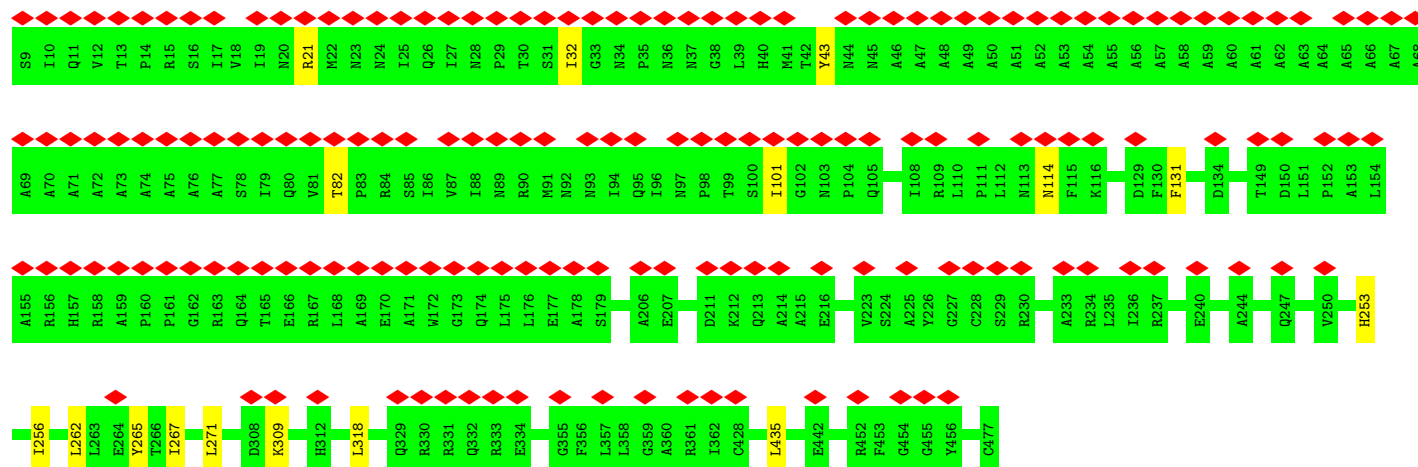
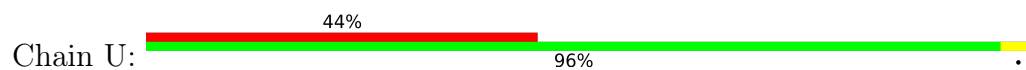


• Molecule 5: Tri1





• Molecule 5: Tri1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1442742	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.267	Depositor
Minimum map value	-0.201	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/10933	0.58	4/14911 (0.0%)
1	C	0.27	0/10933	0.57	3/14911 (0.0%)
1	D	0.27	0/10938	0.57	1/14917 (0.0%)
1	E	0.27	0/10933	0.58	6/14911 (0.0%)
1	F	0.27	0/10933	0.58	4/14911 (0.0%)
1	H	0.28	0/10933	0.59	6/14911 (0.0%)
2	B	0.29	0/714	0.71	0/978
2	G	0.30	0/714	0.73	0/978
2	L	0.31	0/714	0.73	1/978 (0.1%)
2	Q	0.31	0/714	0.82	2/978 (0.2%)
2	V	0.32	0/714	0.80	2/978 (0.2%)
2	g	0.29	0/714	0.67	0/978
3	I	0.26	0/1878	0.56	0/2568
3	K	0.26	0/1878	0.60	2/2568 (0.1%)
4	N	0.26	0/2010	0.55	0/2743
4	P	0.26	0/2010	0.55	0/2743
5	S	0.31	0/3008	0.64	0/4097
5	U	0.31	1/3008 (0.0%)	0.66	3/4097 (0.1%)
All	All	0.27	1/83679 (0.0%)	0.59	34/114156 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
2	B	0	1
2	G	0	1
2	Q	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	82	THR	C-N	5.05	1.43	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	83	ASP	CB-CG-OD1	10.34	127.61	118.30
2	Q	48	ASP	CB-CG-OD2	9.58	126.92	118.30
1	C	397	LEU	CA-CB-CG	8.25	134.27	115.30
1	E	261	ASP	CB-CG-OD2	8.12	125.60	118.30
1	C	412	ILE	CG1-CB-CG2	-8.05	93.69	111.40
1	A	723	ASP	CB-CG-OD1	7.58	125.12	118.30
1	F	307	ASP	CB-CG-OD1	7.49	125.05	118.30
1	H	768	ASP	CB-CG-OD1	7.05	124.65	118.30
1	F	397	LEU	CA-CB-CG	7.02	131.44	115.30
1	H	1121	LEU	CA-CB-CG	6.91	131.19	115.30
1	H	879	ASP	CB-CG-OD2	6.83	124.45	118.30
1	E	397	LEU	CA-CB-CG	6.73	130.77	115.30
1	A	1121	LEU	CA-CB-CG	6.65	130.60	115.30
3	K	287	LEU	CA-CB-CG	6.46	130.16	115.30
1	H	397	LEU	CA-CB-CG	6.45	130.15	115.30
1	E	241	ASP	CB-CG-OD2	6.39	124.05	118.30
1	F	1121	LEU	CA-CB-CG	6.37	129.95	115.30
1	A	397	LEU	CA-CB-CG	6.22	129.61	115.30
2	L	31	LEU	CA-CB-CG	6.04	129.19	115.30
3	K	219	LEU	CA-CB-CG	6.01	129.12	115.30
5	U	271	LEU	CA-CB-CG	5.98	129.06	115.30
5	U	253	HIS	C-N-CA	5.86	136.34	121.70
1	C	397	LEU	CB-CG-CD1	5.73	120.73	111.00
1	F	855	LEU	CA-CB-CG	5.67	128.33	115.30
1	D	104	ASP	CB-CG-OD1	5.57	123.31	118.30
5	U	318	LEU	CA-CB-CG	5.44	127.81	115.30
2	Q	31	LEU	CA-CB-CG	5.42	127.78	115.30
1	E	322	LEU	CA-CB-CG	5.39	127.70	115.30
1	H	1176	LEU	CA-CB-CG	5.38	127.69	115.30
1	A	784	LEU	CA-CB-CG	5.25	127.38	115.30
2	V	83	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	E	863	ILE	CG1-CB-CG2	-5.21	99.94	111.40
1	H	687	LEU	CA-CB-CG	5.13	127.09	115.30
1	E	104	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	ILE	Peptide
2	B	39	GLN	Peptide
1	F	573	ASP	Peptide
2	G	39	GLN	Peptide
2	Q	39	GLN	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1379/1381 (100%)	1278 (93%)	101 (7%)	0	100	100
1	C	1379/1381 (100%)	1271 (92%)	108 (8%)	0	100	100
1	D	1379/1381 (100%)	1281 (93%)	97 (7%)	1 (0%)	48	78
1	E	1379/1381 (100%)	1276 (92%)	103 (8%)	0	100	100
1	F	1379/1381 (100%)	1261 (91%)	118 (9%)	0	100	100
1	H	1379/1381 (100%)	1268 (92%)	111 (8%)	0	100	100
2	B	92/94 (98%)	72 (78%)	17 (18%)	3 (3%)	3	26
2	G	92/94 (98%)	72 (78%)	18 (20%)	2 (2%)	5	32
2	L	92/94 (98%)	69 (75%)	19 (21%)	4 (4%)	2	20
2	Q	92/94 (98%)	70 (76%)	19 (21%)	3 (3%)	3	26
2	V	92/94 (98%)	72 (78%)	17 (18%)	3 (3%)	3	26
2	g	92/94 (98%)	71 (77%)	18 (20%)	3 (3%)	3	26
3	I	248/256 (97%)	234 (94%)	13 (5%)	1 (0%)	30	62
3	K	248/256 (97%)	232 (94%)	15 (6%)	1 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	N	257/263 (98%)	238 (93%)	19 (7%)	0	100	100
4	P	257/263 (98%)	241 (94%)	16 (6%)	0	100	100
5	S	386/392 (98%)	322 (83%)	55 (14%)	9 (2%)	5	31
5	U	386/392 (98%)	320 (83%)	58 (15%)	8 (2%)	5	33
All	All	10608/10672 (99%)	9648 (91%)	922 (9%)	38 (0%)	32	62

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	46	ILE
2	L	66	ALA
2	L	102	ILE
5	S	267	ILE
5	U	267	ILE
2	G	102	ILE
2	B	102	ILE
2	g	66	ALA
2	g	102	ILE
2	V	66	ALA
2	V	102	ILE
2	Q	46	ILE
2	Q	66	ALA
2	Q	102	ILE
3	I	230	ILE
5	S	265	TYR
3	K	230	ILE
5	U	265	TYR
2	G	66	ALA
2	B	66	ALA
5	U	131	PHE
2	V	78	MET
5	S	131	PHE
5	S	114	ASN
5	S	262	LEU
5	U	114	ASN
2	g	78	MET
1	D	366	ASN
2	L	78	MET
5	S	118	THR
5	U	262	LEU
2	B	78	MET

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Mol	Chain	Res	Type
5	U	101	ILE
5	U	256	ILE
5	S	101	ILE
5	S	256	ILE
5	U	32	ILE
5	S	32	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1141/1168 (98%)	1124 (98%)	17 (2%)	60	75
1	C	1141/1168 (98%)	1115 (98%)	26 (2%)	45	64
1	D	1142/1168 (98%)	1115 (98%)	27 (2%)	44	63
1	E	1141/1168 (98%)	1120 (98%)	21 (2%)	54	71
1	F	1141/1168 (98%)	1111 (97%)	30 (3%)	41	61
1	H	1141/1168 (98%)	1120 (98%)	21 (2%)	54	71
2	B	69/73 (94%)	65 (94%)	4 (6%)	17	44
2	G	69/73 (94%)	64 (93%)	5 (7%)	12	38
2	L	69/73 (94%)	65 (94%)	4 (6%)	17	44
2	Q	69/73 (94%)	65 (94%)	4 (6%)	17	44
2	V	69/73 (94%)	65 (94%)	4 (6%)	17	44
2	g	69/73 (94%)	65 (94%)	4 (6%)	17	44
3	I	188/218 (86%)	186 (99%)	2 (1%)	70	80
3	K	188/218 (86%)	185 (98%)	3 (2%)	58	74
4	N	214/224 (96%)	210 (98%)	4 (2%)	52	70
4	P	214/224 (96%)	209 (98%)	5 (2%)	45	64
5	S	295/309 (96%)	288 (98%)	7 (2%)	44	63
5	U	295/309 (96%)	291 (99%)	4 (1%)	62	76
All	All	8655/8948 (97%)	8463 (98%)	192 (2%)	47	65

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	48	PHE
1	A	241	ASP
1	A	258	TYR
1	A	264	SER
1	A	281	ARG
1	A	292	THR
1	A	325	THR
1	A	383	ASP
1	A	481	SER
1	A	498	LEU
1	A	908	ASP
1	A	923	ARG
1	A	980	ASN
1	A	1092	TYR
1	A	1129	CYS
1	A	1147	ASN
1	C	153	SER
1	C	190	ARG
1	C	241	ASP
1	C	258	TYR
1	C	266	THR
1	C	292	THR
1	C	406	ARG
1	C	421	MET
1	C	538	VAL
1	C	584	MET
1	C	623	THR
1	C	718	ARG
1	C	889	LEU
1	C	897	TYR
1	C	906	ASP
1	C	920	MET
1	C	923	ARG
1	C	958	MET
1	C	1070	THR
1	C	1092	TYR
1	C	1094	VAL
1	C	1129	CYS
1	C	1209	MET
1	C	1253	VAL
1	C	1332	ARG

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Mol	Chain	Res	Type
1	C	1344	CYS
1	D	94	THR
1	D	125	ASP
1	D	238	VAL
1	D	258	TYR
1	D	281	ARG
1	D	315	VAL
1	D	322	LEU
1	D	333	MET
1	D	383	ASP
1	D	397	LEU
1	D	435	THR
1	D	551	SER
1	D	573	ASP
1	D	574	LEU
1	D	687	LEU
1	D	768	ASP
1	D	797	ARG
1	D	923	ARG
1	D	930	SER
1	D	945	MET
1	D	958	MET
1	D	1070	THR
1	D	1234	MET
1	D	1245	MET
1	D	1256	THR
1	D	1262	ASN
1	D	1344	CYS
1	E	56	SER
1	E	78	ASN
1	E	238	VAL
1	E	258	TYR
1	E	266	THR
1	E	309	THR
1	E	325	THR
1	E	406	ARG
1	E	442	SER
1	E	524	MET
1	E	529	ASP
1	E	667	CYS
1	E	779	ASN
1	E	923	ARG

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Mol	Chain	Res	Type
1	E	949	ASP
1	E	1005	MET
1	E	1031	HIS
1	E	1129	CYS
1	E	1260	THR
1	E	1286	SER
1	E	1323	SER
1	F	49	ASP
1	F	94	THR
1	F	104	ASP
1	F	124	VAL
1	F	258	TYR
1	F	264	SER
1	F	266	THR
1	F	281	ARG
1	F	286	ASP
1	F	320	MET
1	F	406	ARG
1	F	416	ASP
1	F	430	SER
1	F	432	ASP
1	F	687	LEU
1	F	763	ASP
1	F	769	ARG
1	F	779	ASN
1	F	798	ASP
1	F	862	VAL
1	F	912	THR
1	F	923	ARG
1	F	939	THR
1	F	959	MET
1	F	1005	MET
1	F	1016	ASN
1	F	1070	THR
1	F	1262	ASN
1	F	1270	SER
1	F	1310	ARG
1	H	37	SER
1	H	104	ASP
1	H	125	ASP
1	H	153	SER
1	H	244	PHE

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Mol	Chain	Res	Type
1	H	258	TYR
1	H	481	SER
1	H	524	MET
1	H	718	ARG
1	H	798	ASP
1	H	923	ARG
1	H	924	THR
1	H	1070	THR
1	H	1101	HIS
1	H	1113	THR
1	H	1121	LEU
1	H	1129	CYS
1	H	1131	THR
1	H	1260	THR
1	H	1310	ARG
1	H	1344	CYS
2	L	23	TYR
2	L	32	LEU
2	L	43	ARG
2	L	75	ARG
3	I	101	ASN
3	I	224	ARG
4	N	140	THR
4	N	176	VAL
4	N	193	ARG
4	N	310	THR
5	S	37	ASN
5	S	45	ASN
5	S	91	MET
5	S	230	ARG
5	S	245	MET
5	S	309	LYS
5	S	429	MET
3	K	116	LEU
3	K	224	ARG
3	K	298	PHE
4	P	45	ASP
4	P	68	ARG
4	P	188	THR
4	P	266	ARG
4	P	275	SER
5	U	21	ARG

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Mol	Chain	Res	Type
5	U	43	TYR
5	U	309	LYS
5	U	435	LEU
2	G	16	SER
2	G	32	LEU
2	G	43	ARG
2	G	75	ARG
2	G	83	ASP
2	B	11	ASN
2	B	43	ARG
2	B	73	ILE
2	B	83	ASP
2	g	11	ASN
2	g	43	ARG
2	g	75	ARG
2	g	83	ASP
2	V	32	LEU
2	V	51	SER
2	V	73	ILE
2	V	83	ASP
2	Q	31	LEU
2	Q	32	LEU
2	Q	63	ARG
2	Q	75	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1147	ASN
1	A	1177	ASN
1	C	614	GLN
1	C	892	ASN
1	F	195	GLN
1	H	113	GLN
1	H	130	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	K	3
3	I	3
4	N	2
4	P	2
5	U	2
5	S	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	226:LEU	C	266:ARG	N	28.83
1	P	226:LEU	C	266:ARG	N	28.15
1	K	236:LEU	C	244:VAL	N	20.36
1	I	236:LEU	C	244:VAL	N	20.15
1	K	260:MET	C	267:LEU	N	18.69
1	I	260:MET	C	267:LEU	N	18.64
1	P	163:ALA	C	175:ASP	N	17.41
1	N	163:ALA	C	175:ASP	N	16.34
1	U	362:ILE	C	428:CYS	N	13.65
1	U	179:SER	C	192:ARG	N	12.91
1	S	179:SER	C	192:ARG	N	12.72

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	161:LEU	C	206:ASN	N	12.20
1	K	161:LEU	C	206:ASN	N	12.13
1	S	362:ILE	C	428:CYS	N	12.04

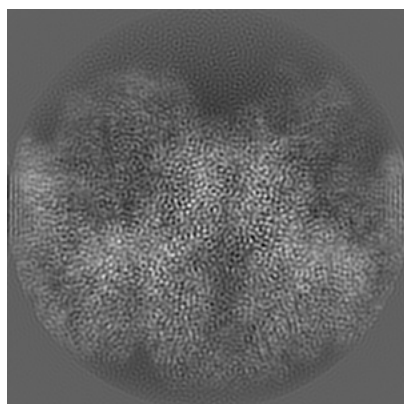
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38193. These allow visual inspection of the internal detail of the map and identification of artifacts.

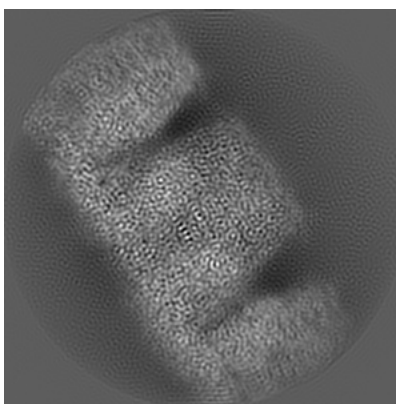
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

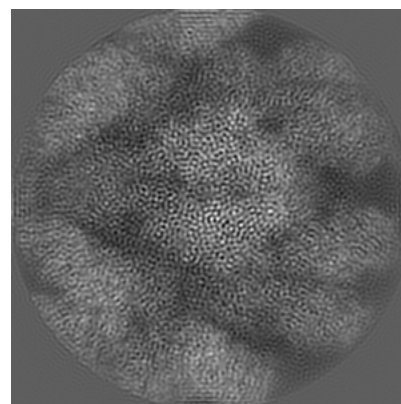
6.1.1 Primary map



X

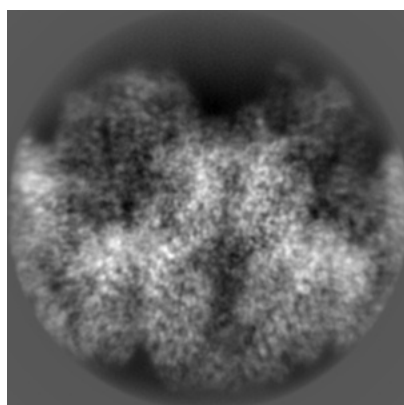


Y

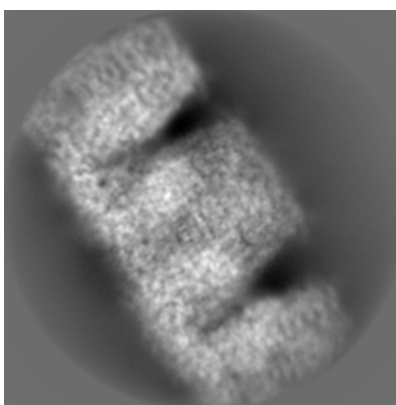


Z

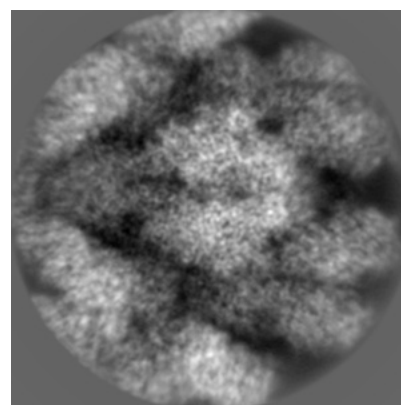
6.1.2 Raw map



X



Y

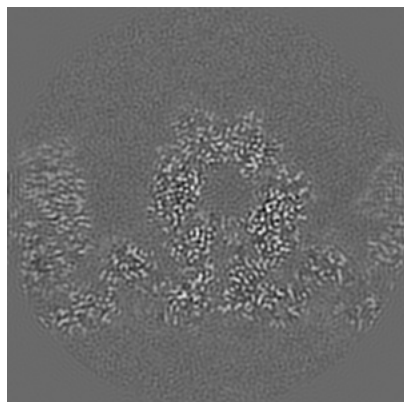


Z

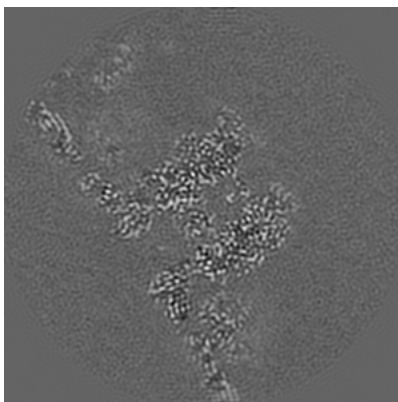
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

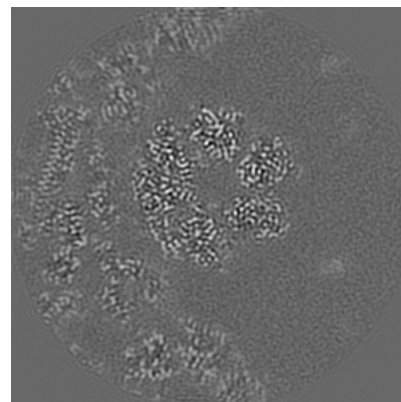
6.2.1 Primary map



X Index: 120

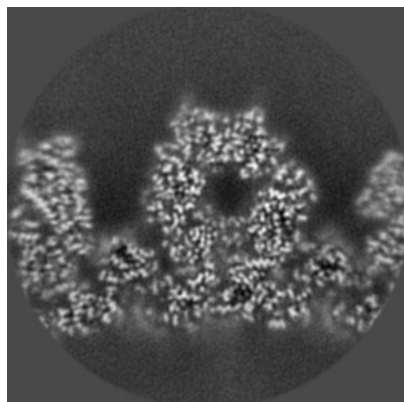


Y Index: 120

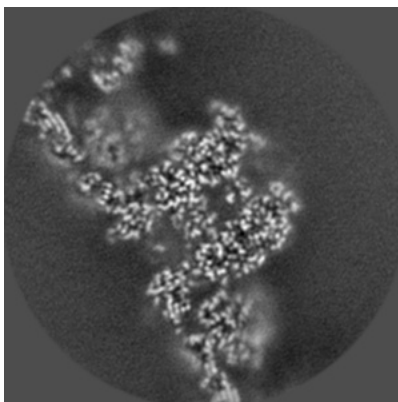


Z Index: 120

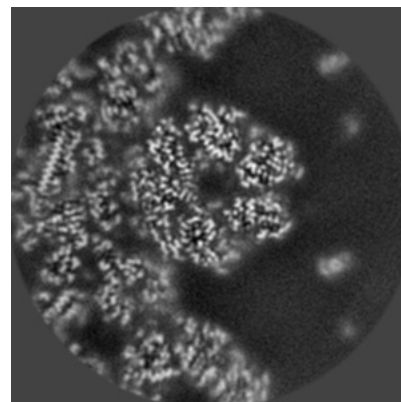
6.2.2 Raw map



X Index: 120



Y Index: 120

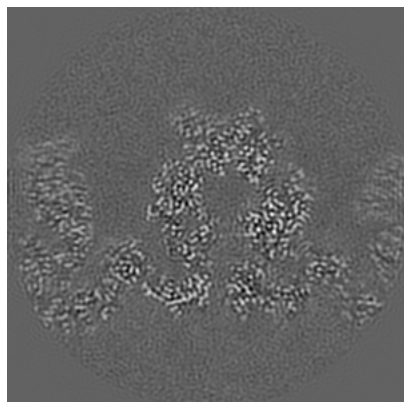


Z Index: 120

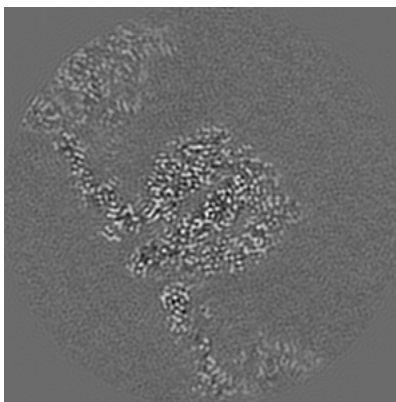
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

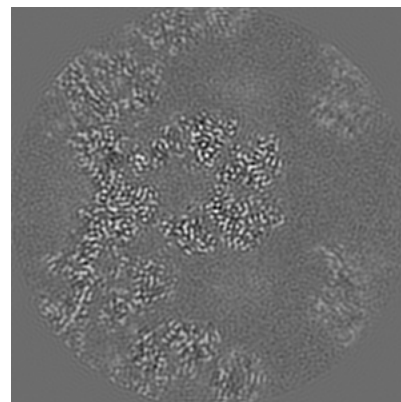
6.3.1 Primary map



X Index: 117

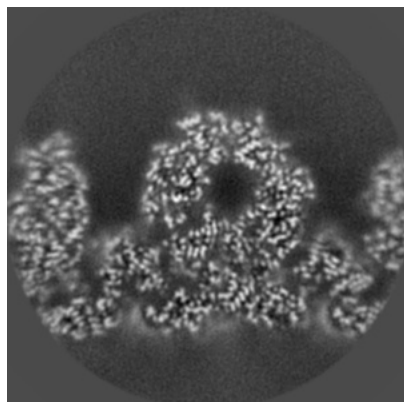


Y Index: 109

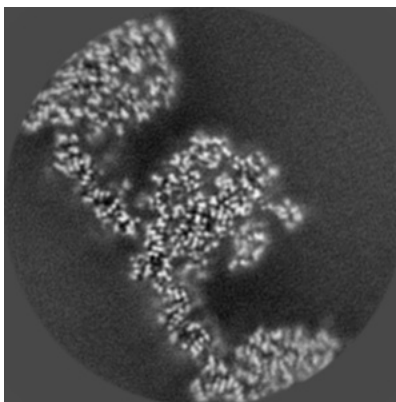


Z Index: 106

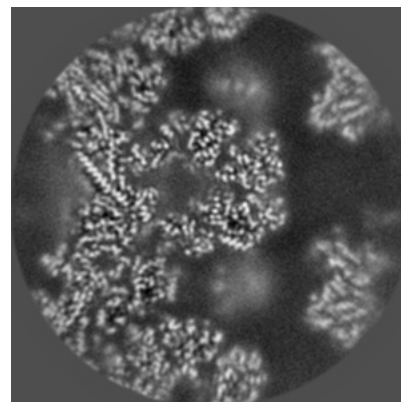
6.3.2 Raw map



X Index: 123



Y Index: 103

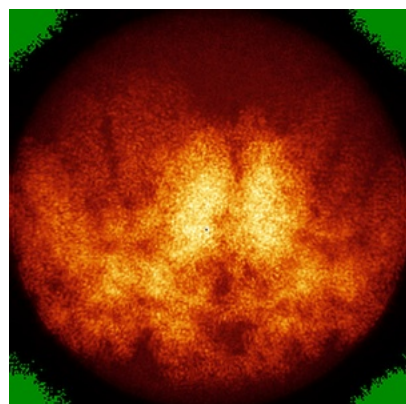


Z Index: 105

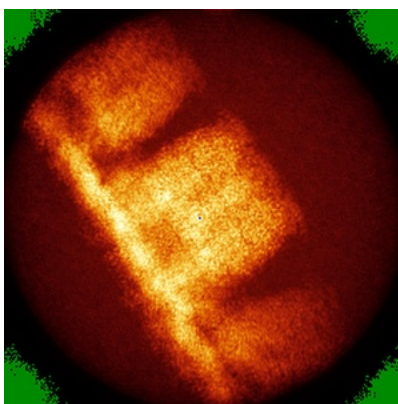
The images above show the largest variance slices of the map in three orthogonal directions.

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

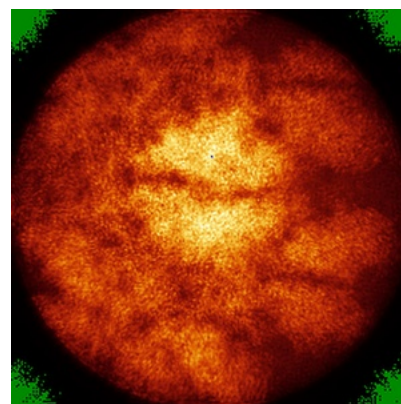
6.4.1 Primary map



X

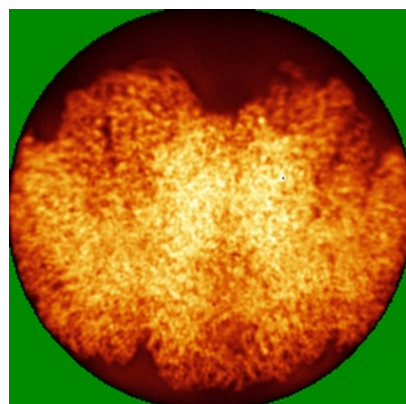


Y

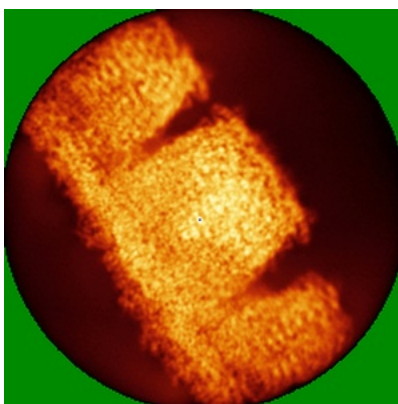


Z

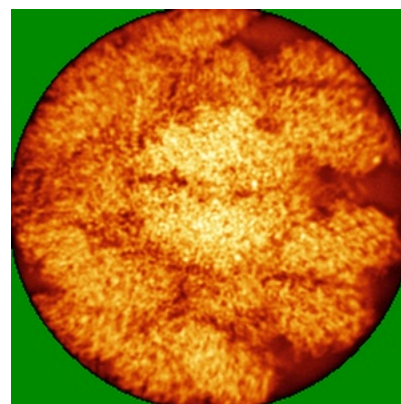
6.4.2 Raw map



X



Y

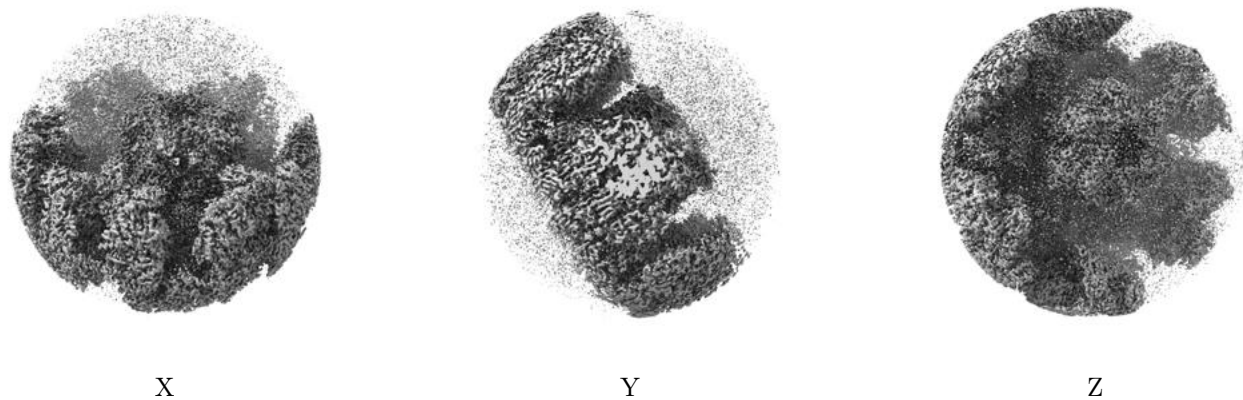


Z

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

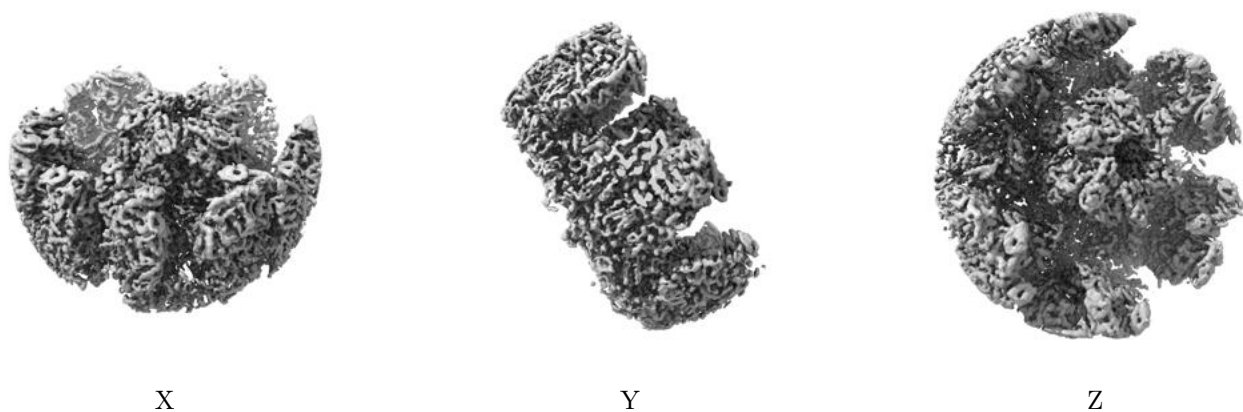
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

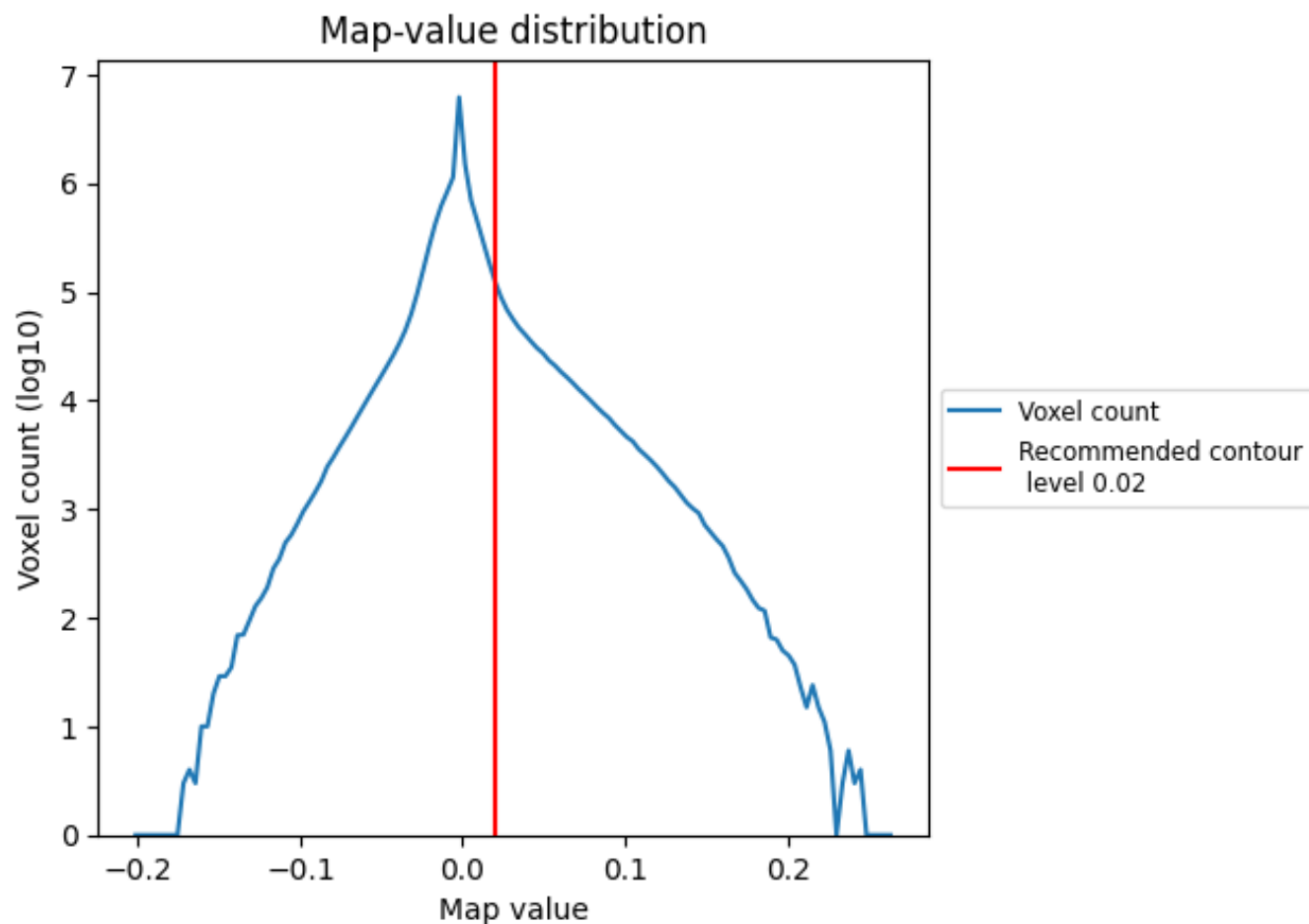
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

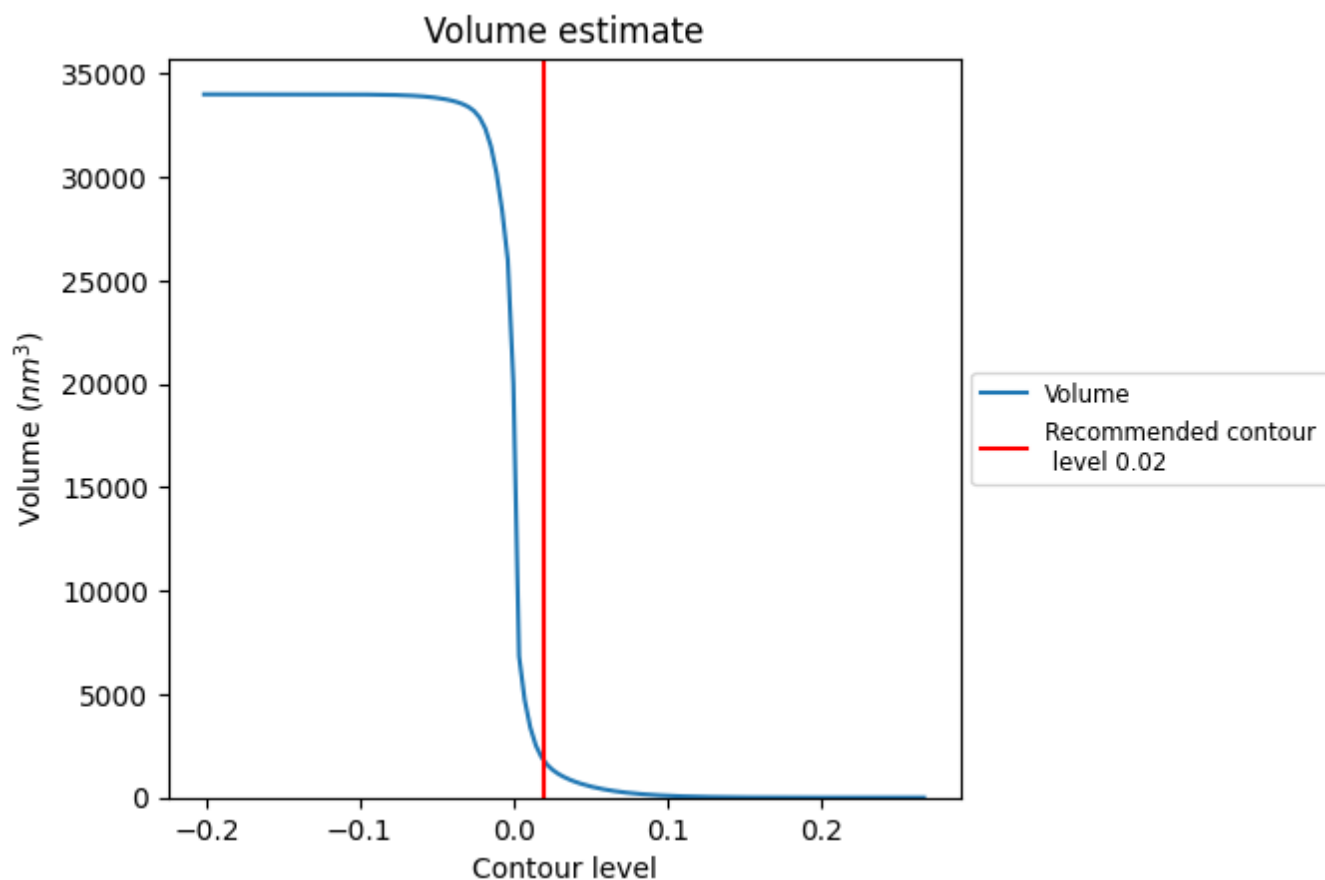
This section contains the results of statistical analysis of the map.

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.

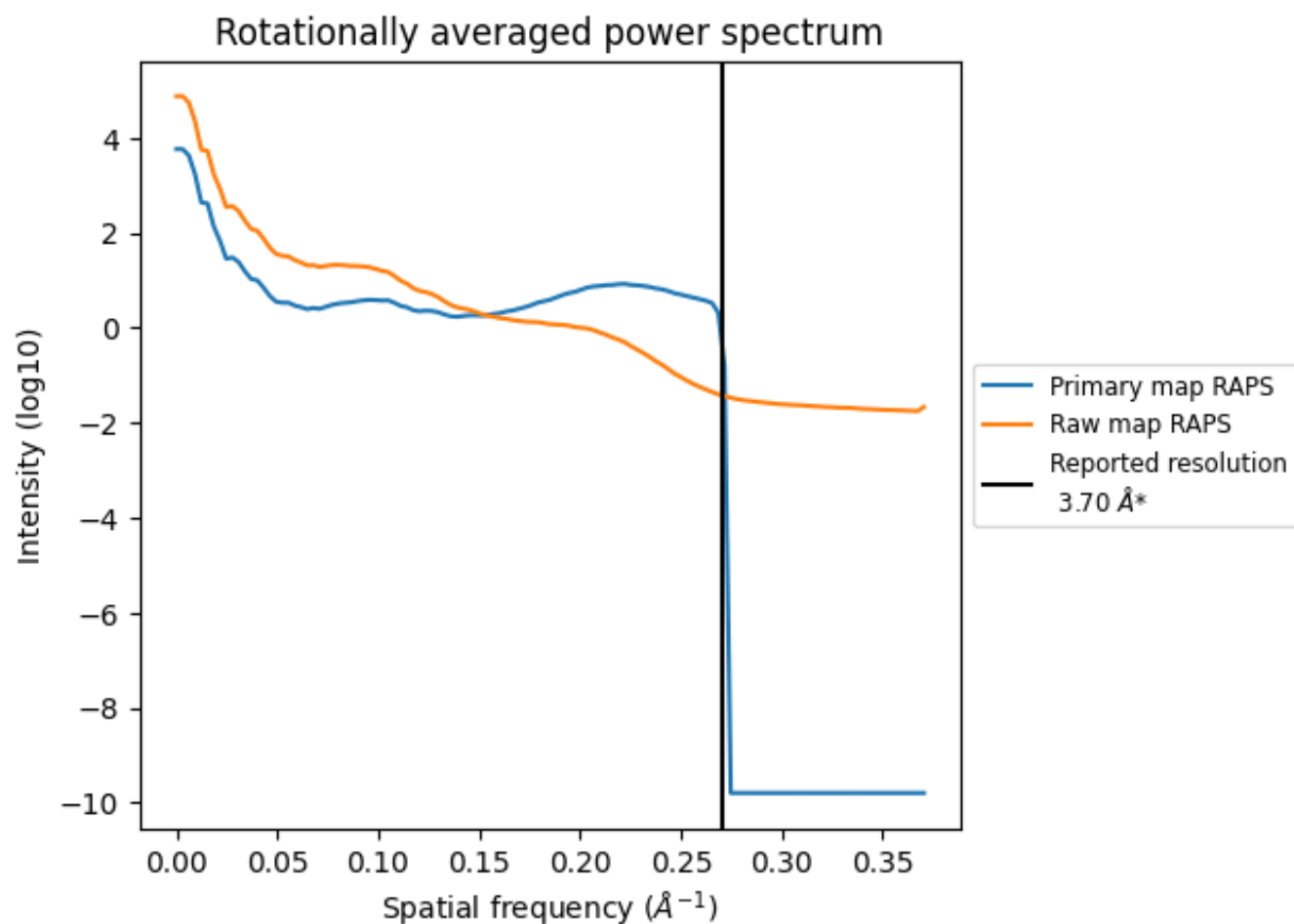
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1774 nm³; this corresponds to an approximate mass of 1603 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 ⓘ

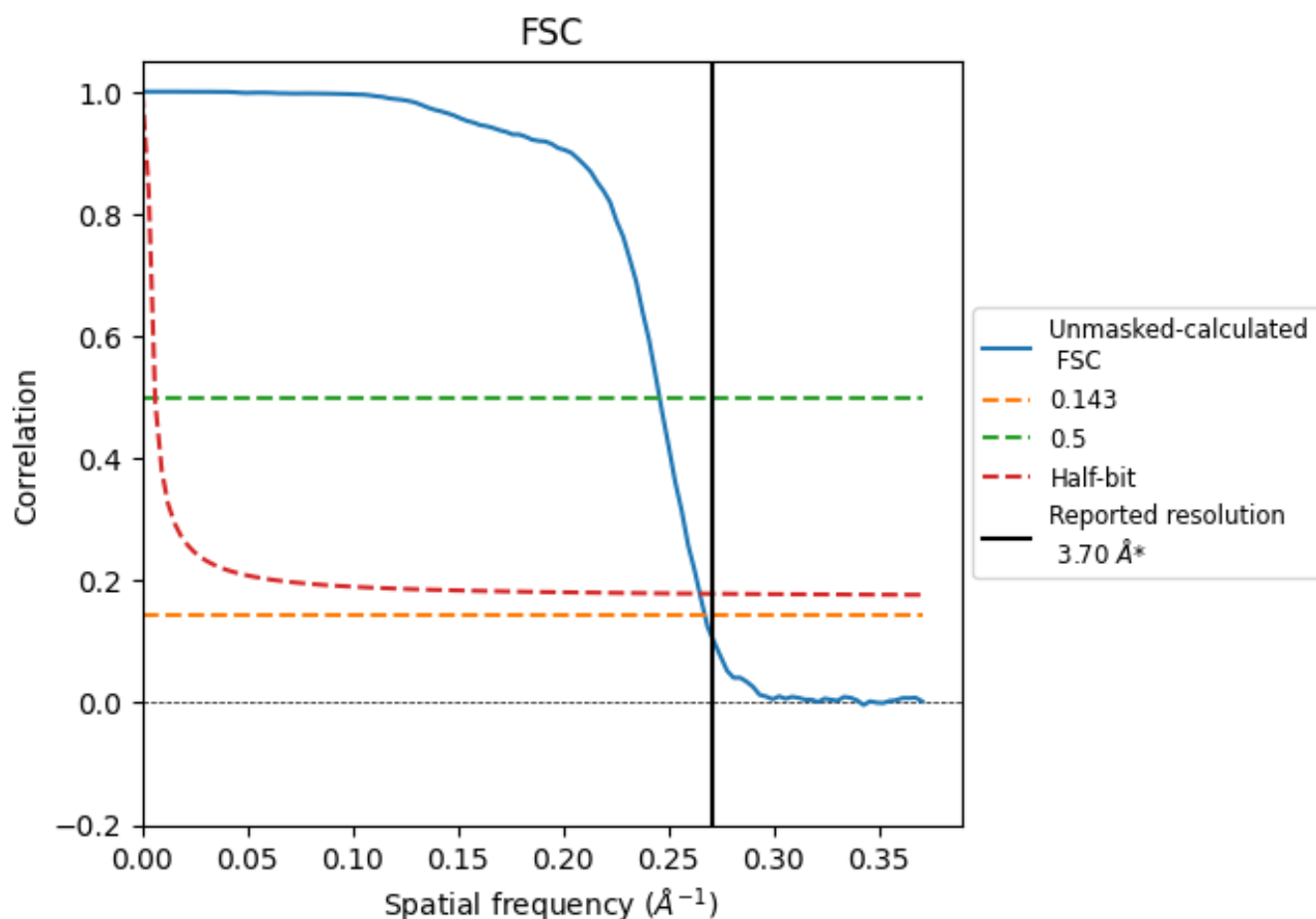


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

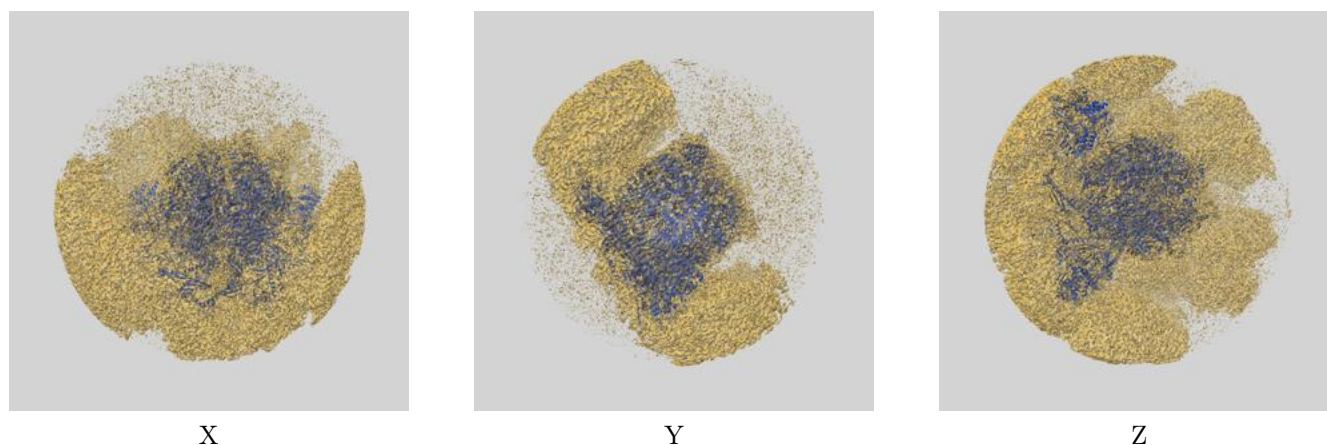
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	4.07	3.78

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

9 Map-model fit [i](#)

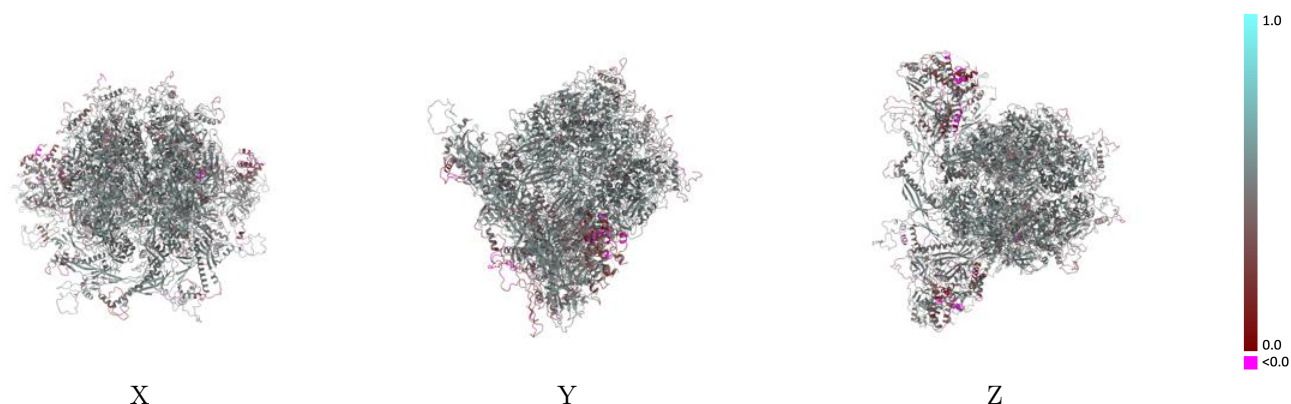
This section contains information regarding the fit between EMDB map EMD-38193 and PDB model 8XA3. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



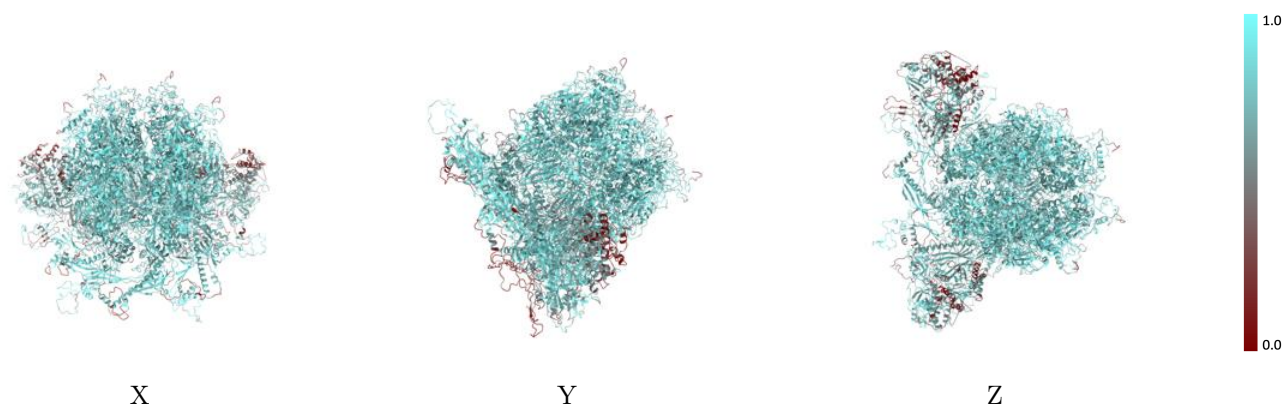
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



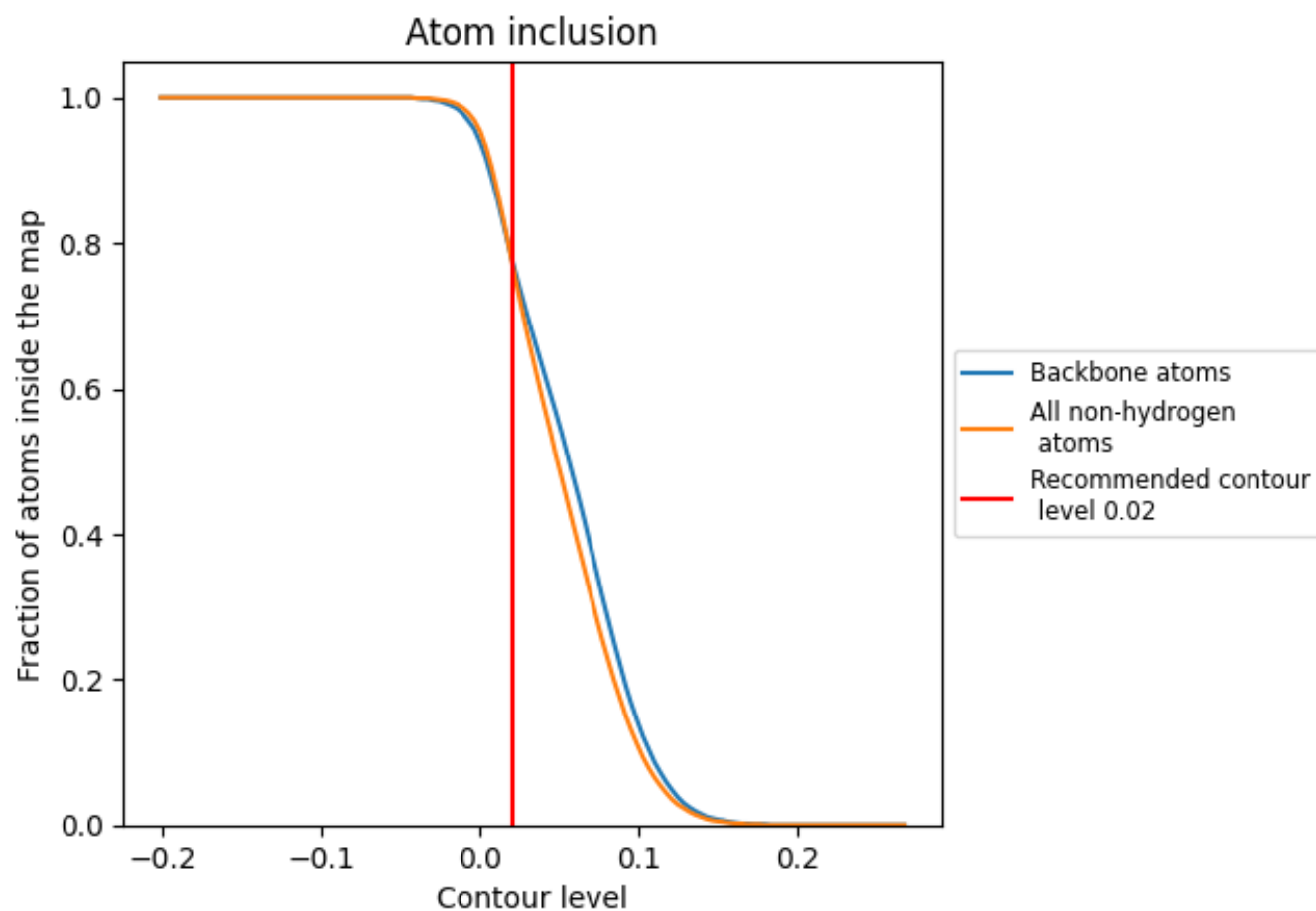
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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	 0.7730	 0.4760
A	 0.8180	 0.5000
B	 0.7340	 0.4090
C	 0.8190	 0.4980
D	 0.8140	 0.4980
E	 0.8150	 0.4970
F	 0.8090	 0.4940
G	 0.7310	 0.4020
H	 0.8120	 0.4970
I	 0.6900	 0.4310
K	 0.6190	 0.4160
L	 0.7370	 0.4280
N	 0.6960	 0.4470
P	 0.6010	 0.4120
Q	 0.7310	 0.4230
S	 0.5390	 0.3640
U	 0.4770	 0.3320
V	 0.7400	 0.4200
g	 0.7600	 0.4070

