



Full wwPDB EM Validation Report ⓘ

Dec 28, 2024 – 03:16 PM EST

PDB ID : 7BW6
EMDB ID : EMD-30228
Title : Varicella-zoster virus capsid
Authors : Wang, P.Y.; Qi, J.X.; Liu, C.C.; Sun, J.Q.
Deposited on : 2020-04-13
Resolution : 3.70 Å (reported)
Based on initial model : 5ZZ8

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:

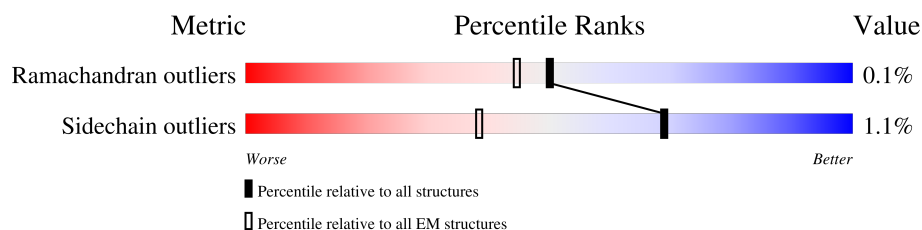
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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


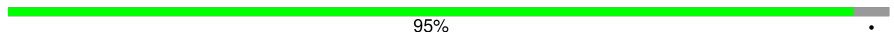
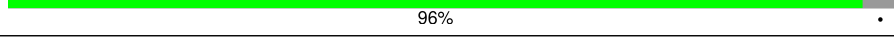
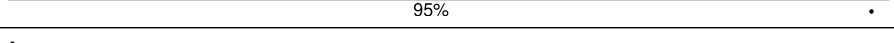
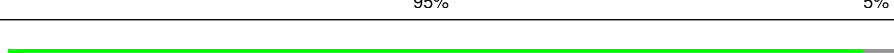

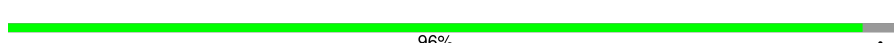
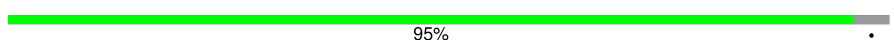

The reported resolution of this entry is 3.70 Å.

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.



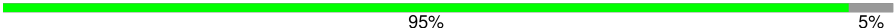





















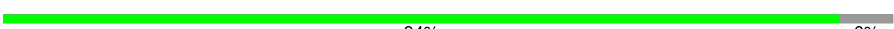


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1396	
1	B	1396	
1	D	1396	
1	F	1396	
1	H	1396	
1	J	1396	
1	L	1396	
1	N	1396	
1	P	1396	


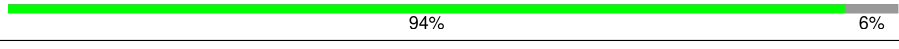
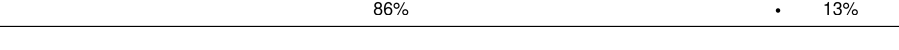
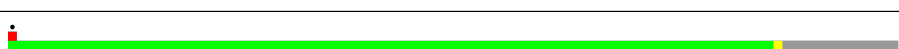
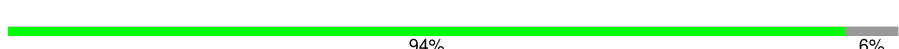


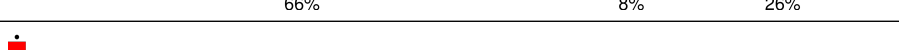




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Mol	Chain	Length	Quality of chain
1	R	1396	
1	T	1396	
1	V	1396	
1	X	1396	
1	a	1396	
1	c	1396	
1	e	1396	
2	C	235	
2	E	235	
2	G	235	
2	I	235	
2	K	235	
2	M	235	
2	O	235	
2	Q	235	
2	S	235	
2	U	235	
2	W	235	
2	Y	235	
2	b	235	
2	d	235	
2	f	235	
3	g	316	
3	h	316	
3	j	316	

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Mol	Chain	Length	Quality of chain
3	k	316	
3	m	316	
3	n	316	
3	p	316	
3	q	316	
3	s	316	
3	t	316	
4	i	483	
4	l	483	
4	o	483	
4	r	483	
4	w	483	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 208818 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	1166	Total	C	N	O	S	0	0
			9043	5744	1576	1664	59		
1	B	1336	Total	C	N	O	S	0	0
			10251	6516	1767	1900	68		
1	D	1337	Total	C	N	O	S	0	0
			10365	6574	1804	1919	68		
1	F	1337	Total	C	N	O	S	0	0
			10350	6566	1801	1915	68		
1	H	1333	Total	C	N	O	S	0	0
			10319	6550	1794	1907	68		
1	J	1337	Total	C	N	O	S	0	0
			10331	6557	1793	1913	68		
1	L	1336	Total	C	N	O	S	0	0
			10293	6537	1778	1912	66		
1	N	1337	Total	C	N	O	S	0	0
			10328	6558	1786	1916	68		
1	P	1337	Total	C	N	O	S	0	0
			10245	6510	1760	1909	66		
1	R	1332	Total	C	N	O	S	0	0
			10280	6528	1784	1900	68		
1	T	1281	Total	C	N	O	S	0	0
			9821	6246	1690	1819	66		
1	V	1280	Total	C	N	O	S	0	0
			9861	6251	1715	1830	65		
1	X	1314	Total	C	N	O	S	0	0
			10178	6460	1764	1888	66		
1	a	1335	Total	C	N	O	S	0	0
			10276	6528	1766	1915	67		
1	c	1298	Total	C	N	O	S	0	0
			10039	6363	1754	1856	66		
1	e	1298	Total	C	N	O	S	0	0
			10113	6402	1780	1865	66		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	101	Total	C	N	O	S	0	0
			736	467	129	138	2		
2	E	101	Total	C	N	O	S	0	0
			748	473	135	138	2		
2	G	101	Total	C	N	O	S	0	0
			733	466	129	136	2		
2	I	101	Total	C	N	O	S	0	0
			742	470	132	138	2		
2	K	100	Total	C	N	O	S	0	0
			729	462	128	137	2		
2	M	101	Total	C	N	O	S	0	0
			742	470	132	138	2		
2	O	101	Total	C	N	O	S	0	0
			736	467	129	138	2		
2	Q	97	Total	C	N	O	S	0	0
			712	452	126	132	2		
2	S	101	Total	C	N	O	S	0	0
			724	461	123	138	2		
2	U	101	Total	C	N	O	S	0	0
			742	470	132	138	2		
2	W	101	Total	C	N	O	S	0	0
			742	470	132	138	2		
2	Y	101	Total	C	N	O	S	0	0
			721	459	122	138	2		
2	b	101	Total	C	N	O	S	0	0
			742	470	132	138	2		
2	d	101	Total	C	N	O	S	0	0
			748	473	135	138	2		
2	f	101	Total	C	N	O	S	0	0
			742	470	132	138	2		

- Molecule 3 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	g	298	Total	C	N	O	S	0	0
			2284	1457	394	422	11		
3	h	275	Total	C	N	O	S	0	0
			2083	1334	354	386	9		
3	j	298	Total	C	N	O	S	0	0
			2288	1458	397	422	11		
3	k	275	Total	C	N	O	S	0	0
			2083	1334	354	386	9		
3	m	298	Total	C	N	O	S	0	0
			2288	1458	397	422	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	n	275	Total	C	N	O	S	0	0
			2080	1333	354	384	9		
3	p	298	Total	C	N	O	S	0	0
			2288	1458	397	422	11		
3	q	275	Total	C	N	O	S	0	0
			2083	1334	354	386	9		
3	s	298	Total	C	N	O	S	0	0
			2283	1456	394	422	11		
3	t	275	Total	C	N	O	S	0	0
			2079	1332	354	384	9		

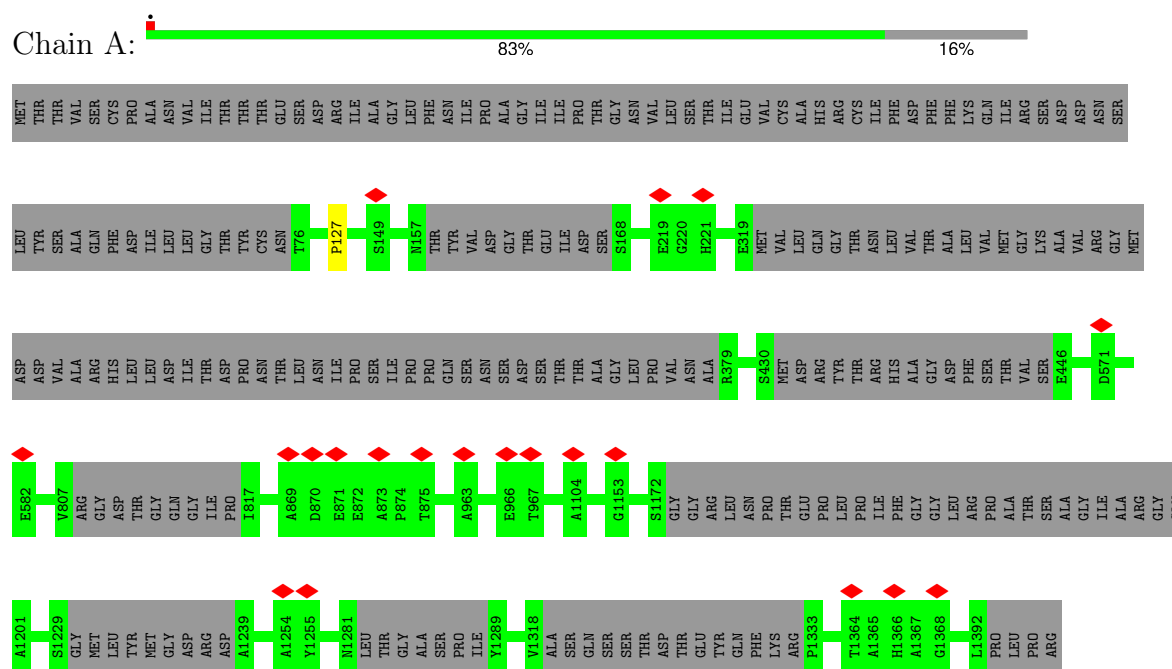
- Molecule 4 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	i	357	Total	C	N	O	S	0	0
			2770	1754	484	516	16		
4	l	357	Total	C	N	O	S	0	0
			2770	1754	484	516	16		
4	o	357	Total	C	N	O	S	0	0
			2767	1753	483	515	16		
4	r	357	Total	C	N	O	S	0	0
			2770	1754	484	516	16		
4	w	357	Total	C	N	O	S	0	0
			2770	1754	484	516	16		

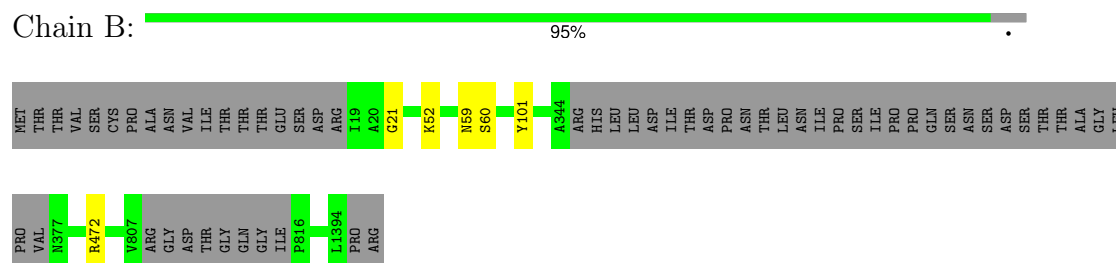
3 Residue-property plots

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

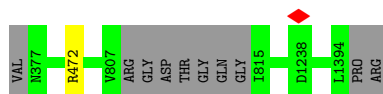


- Molecule 1: Major capsid protein

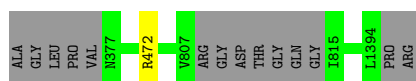


- Molecule 1: Major capsid protein

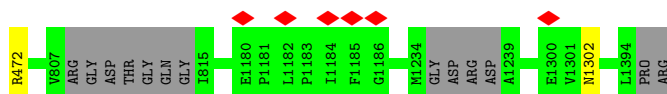




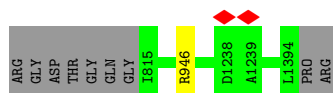
- Chain F:  95% .



- Chain H:  95% 5%



- Chain J:  96%

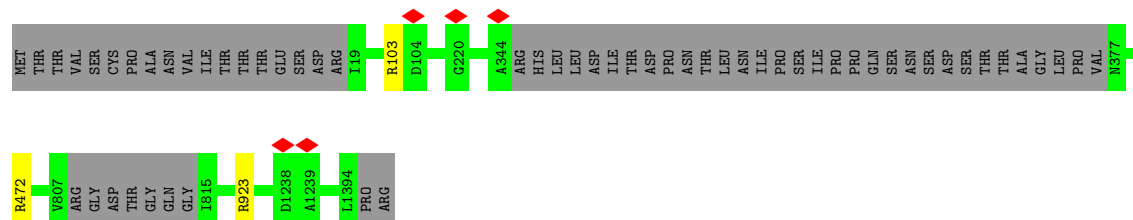


- Chain L: 95% .



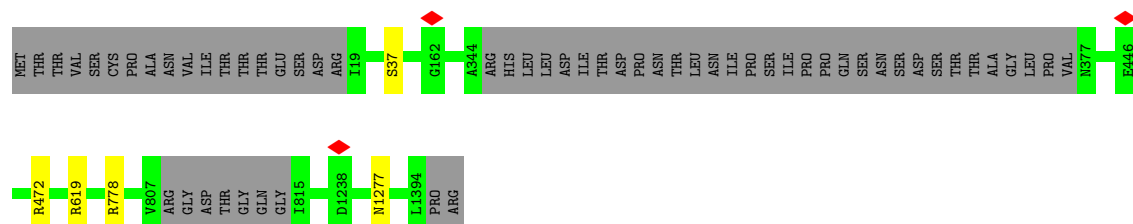
- Molecule 1: Major capsid protein

Chain N: 96%



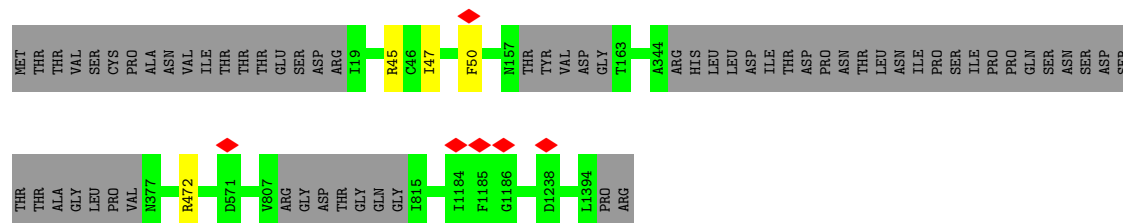
- Molecule 1: Major capsid protein

Chain P: 95% .



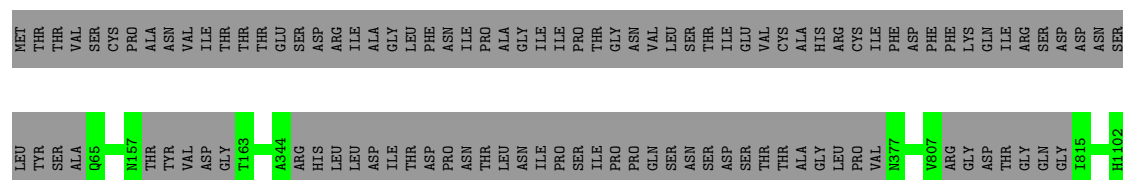
- Molecule 1: Major capsid protein

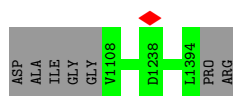
Chain R:  95% 5%



- Molecule 1: Major capsid protein

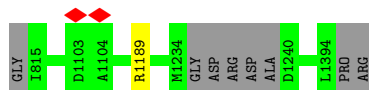
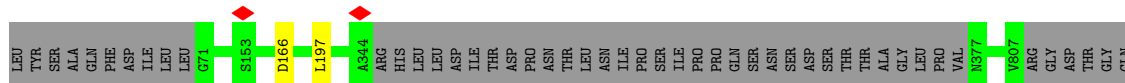
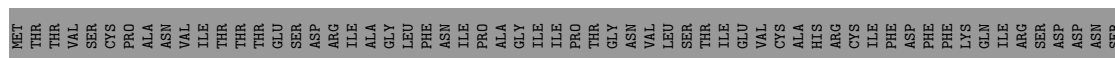
Chain T:  92% 8%





- Molecule 1: Major capsid protein

Chain V: 91% 8%



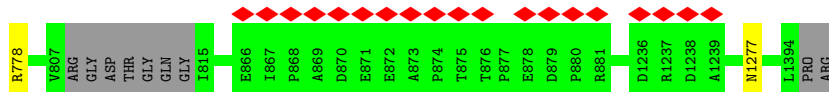
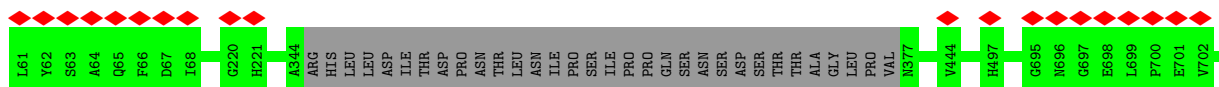
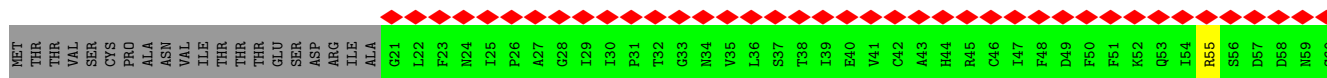
- Molecule 1: Major capsid protein

Chain X: 94% 6%



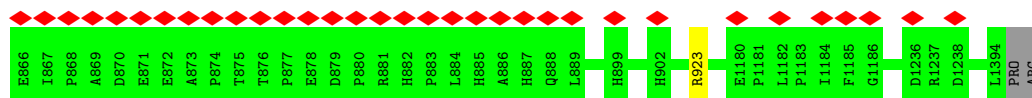
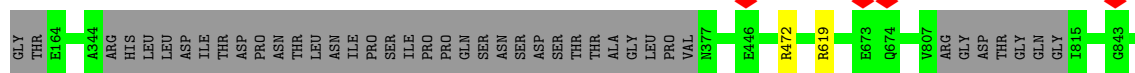
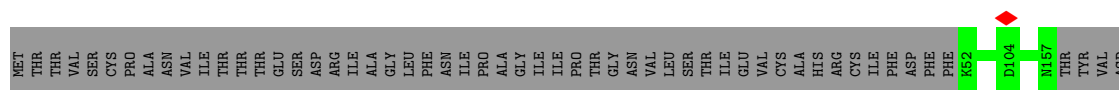
- Molecule 1: Major capsid protein

Chain a: 6% 95%

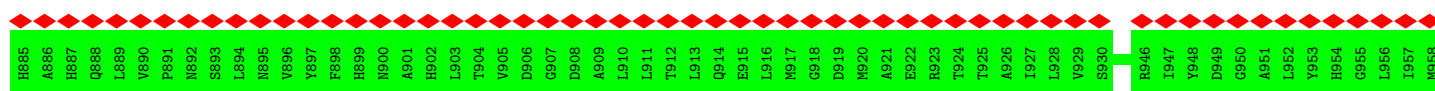
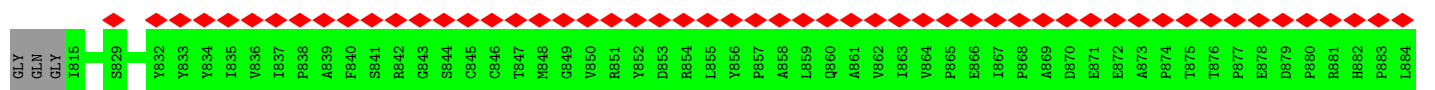
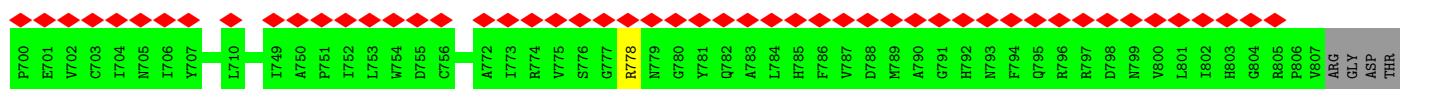
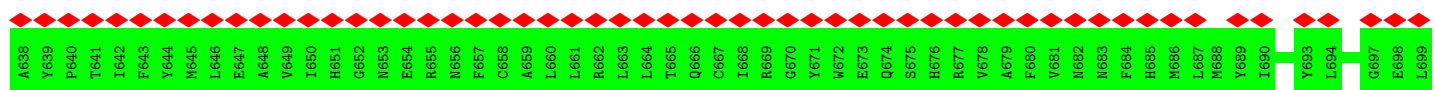
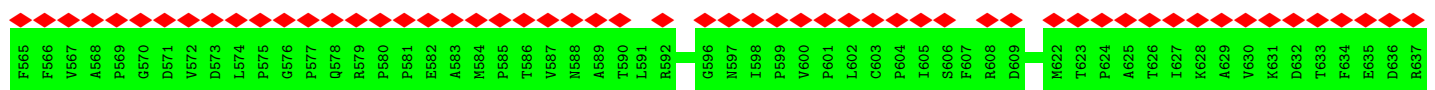
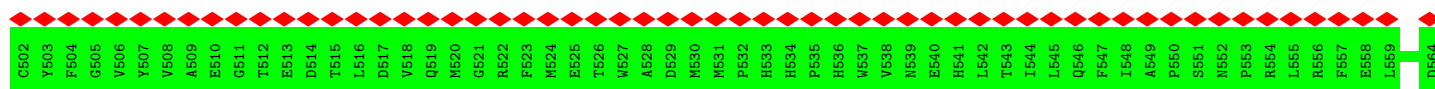
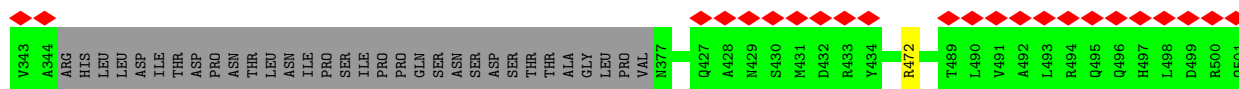
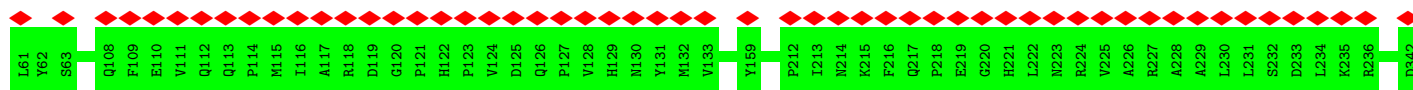
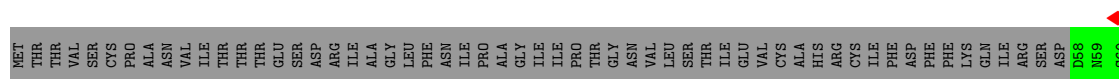
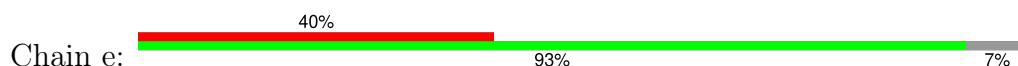


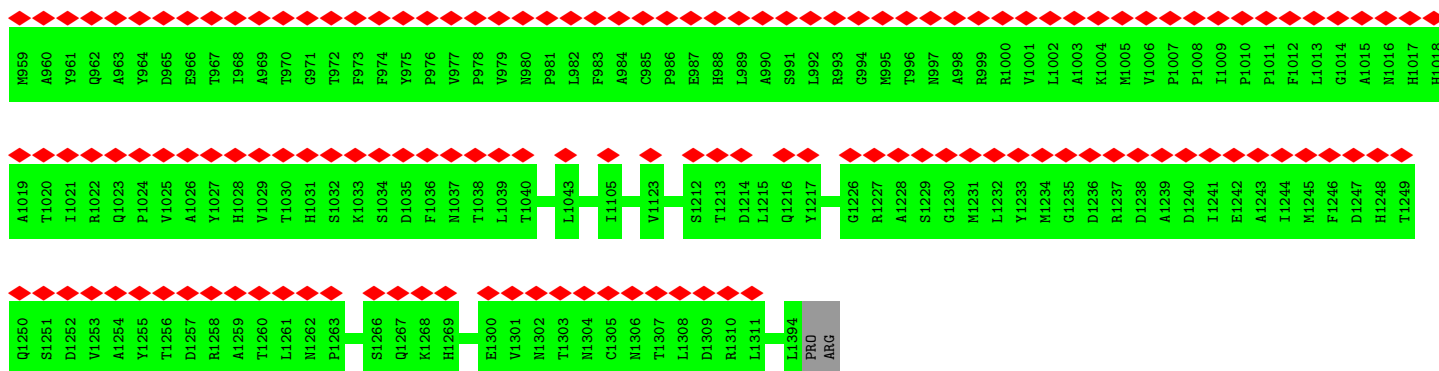
- Molecule 1: Major capsid protein

Chain c: 93% 7%

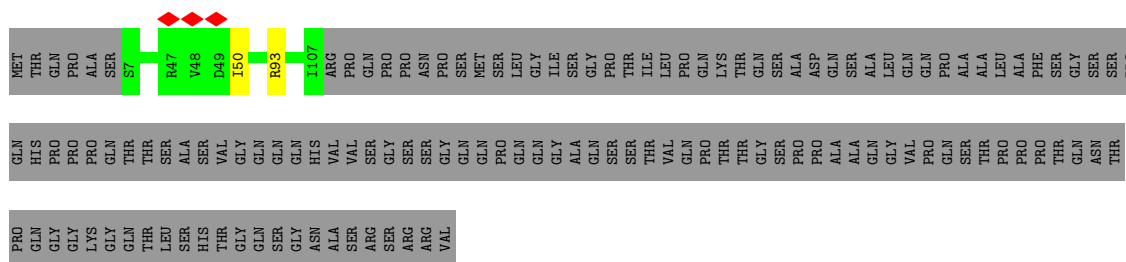


• Molecule 1: Major capsid protein

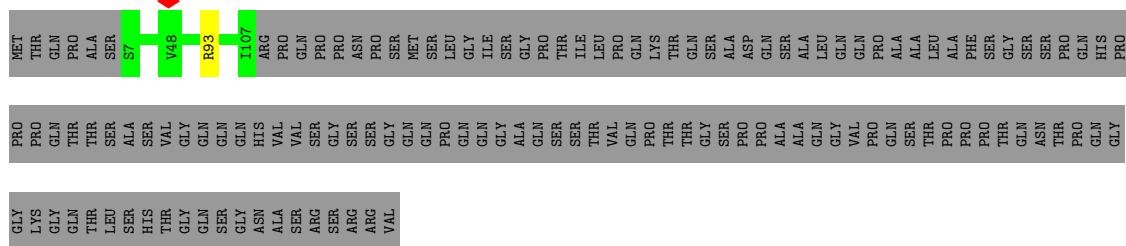
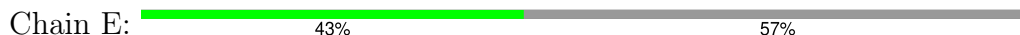




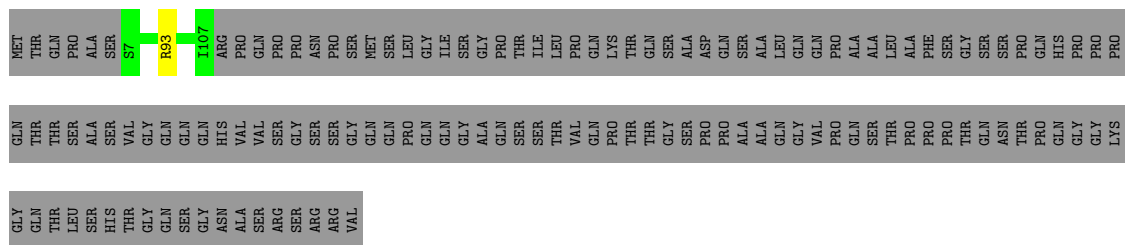
- Molecule 2: Small capsomere-interacting protein



- Molecule 2: Small capsomere-interacting protein



- Molecule 2: Small capsomere-interacting protein



- Molecule 2: Small capsomere-interacting protein

[illegible]

- Chain K:  42% 57%

THR	PRO	THR	GLN	GLN	GLY	PRO	PRO	ALA	LYS	GLY	GLN	THR	THR	LEU	SER	SER	ALA	THR	THR	GLY	GLN	GLN	GLN	GLN	GLN	ASN	GLY	VAL	ARG	ARG	SER	ARG	THR	GLN	THR	THR	PRO	ALA	ALA	GLN	GLY	VAL	PRO	PRO	PRO	PRO	ASP	ALA	SER	SER	GLN	LEU	ALA	ALA	GLN	GLN	LEU	ALA	ALA	PHE	LEU	GLY	SER	GLN	SER	GLN	THR	GLN	ASN
MET	THR	GLN	PRO	PRO	ALA	SER	87	847	848	849	150	893	1106	ILE	ARG	PRO	GLN	PRO	PRO	PRO	ASN	PRO	SER	SER	MET	SER	LEU	GLY	ILE	SER	GLY	PRO	THR	THR	ILE	LEU	PRO	GLN	LYS	THR	GLN	SER	SER	ALA	ASP	GLN	SER	SER	LEU	ALA	ALA	GLN	GLN	LEU	ALA	ALA	PHE	LEU	GLY	SER	GLN	SER	GLN	THR	GLN	ASN			

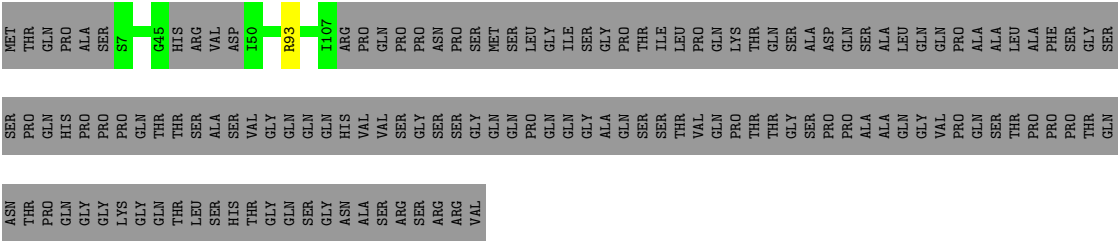
- Chain M:  42% . 57%

[illegible]

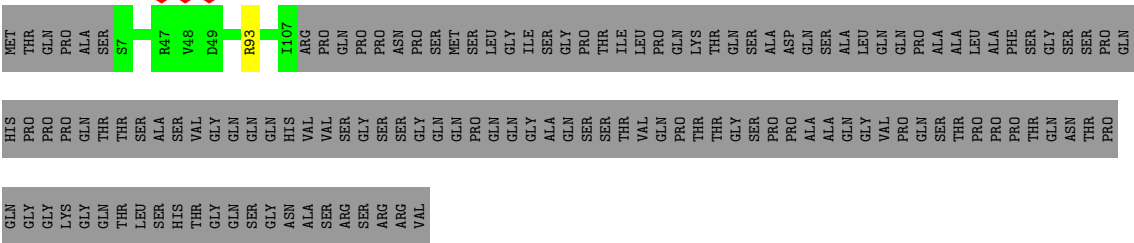
- Chain O: 43% 57%

[illegible]

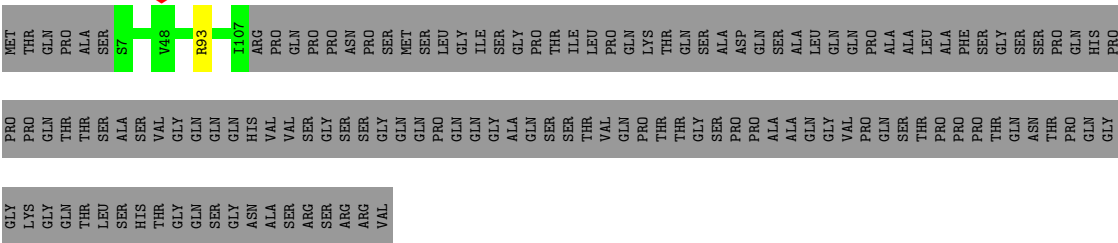
- Chain Q: 41% 59%



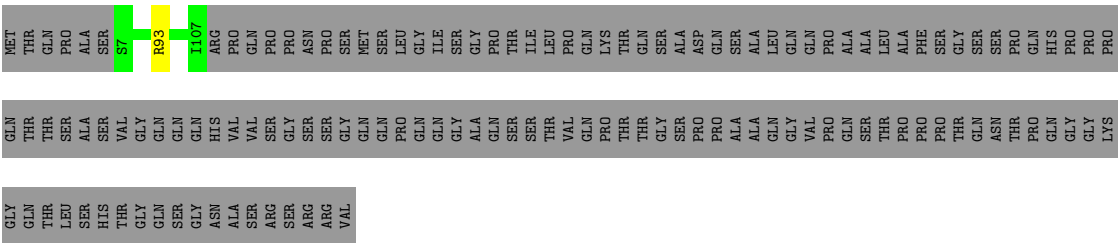
• Molecule 2: Small capsomere-interacting protein



• Molecule 2: Small capsomere-interacting protein



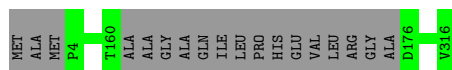
• Molecule 2: Small capsomere-interacting protein




• Molecule 2: Small capsomere-interacting protein

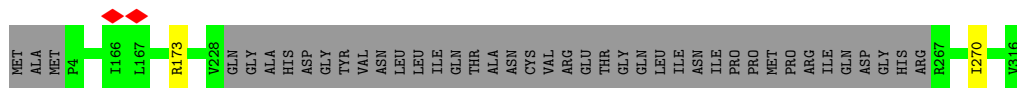


Chain g:  94% 6%



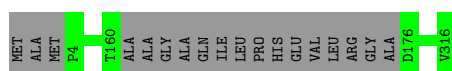
- Molecule 3: Triplex capsid protein 2

Chain h:  86% 13%




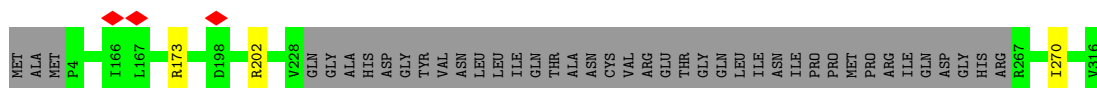
- Molecule 3: Triplex capsid protein 2

Chain j:  94% 6%



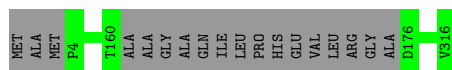
- Molecule 3: Triplex capsid protein 2

Chain k:  86% 13%




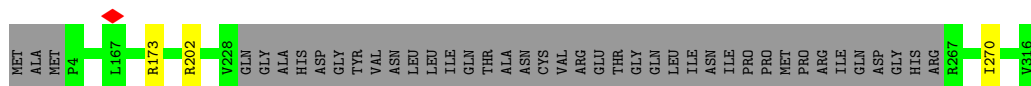
- Molecule 3: Triplex capsid protein 2

Chain m:  94% 6%



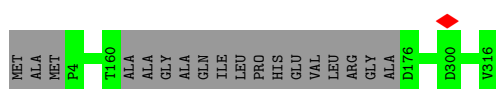
- Molecule 3: Triplex capsid protein 2

Chain n:  86% 13%




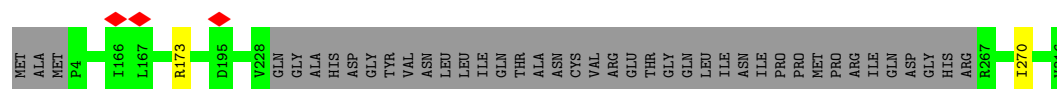
- Molecule 3: Triplex capsid protein 2

Chain p:  94% 6%



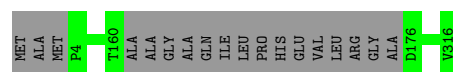
- Molecule 3: Triplex capsid protein 2

Chain q:  86% 13%




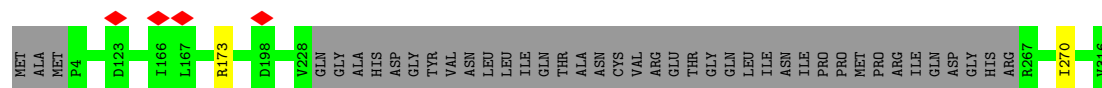
- Molecule 3: Triplex capsid protein 2

Chain s:  94% 6%



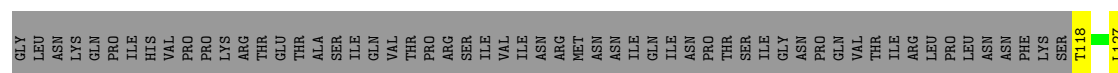
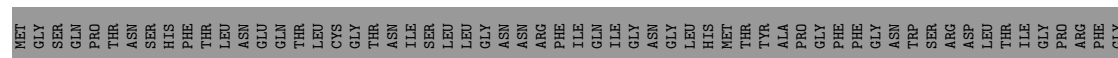
- Molecule 3: Triplex capsid protein 2

Chain t:  86% 13%



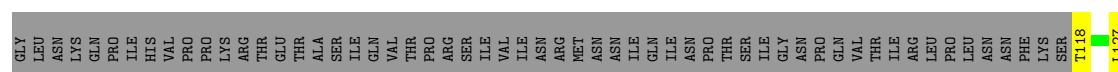
- Molecule 4: Triplex capsid protein 1

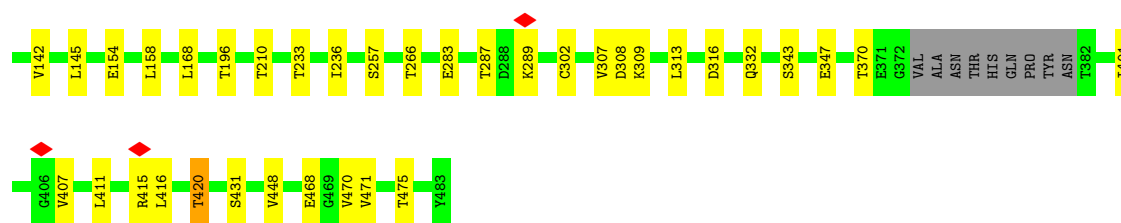
Chain i:  66% 8% 26%



- Molecule 4: Triplex capsid protein 1

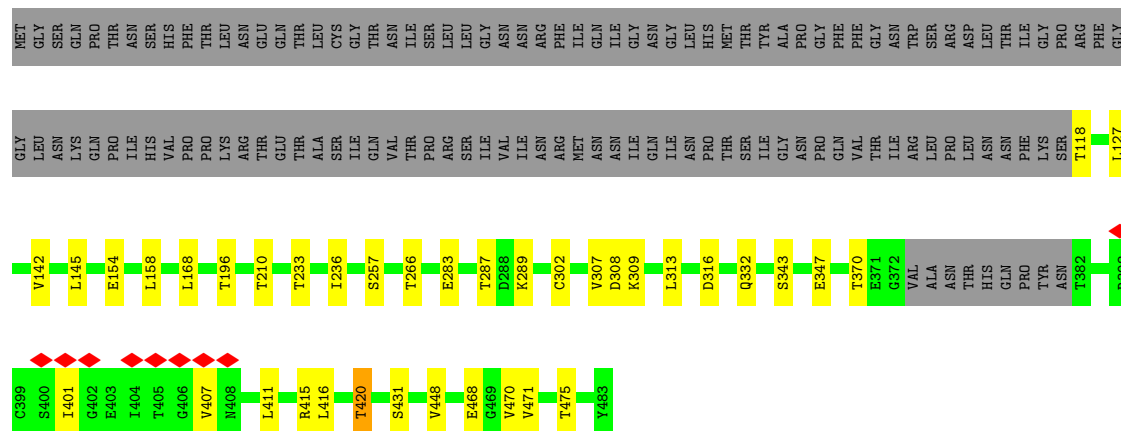
Chain l:  66% 8% 26%





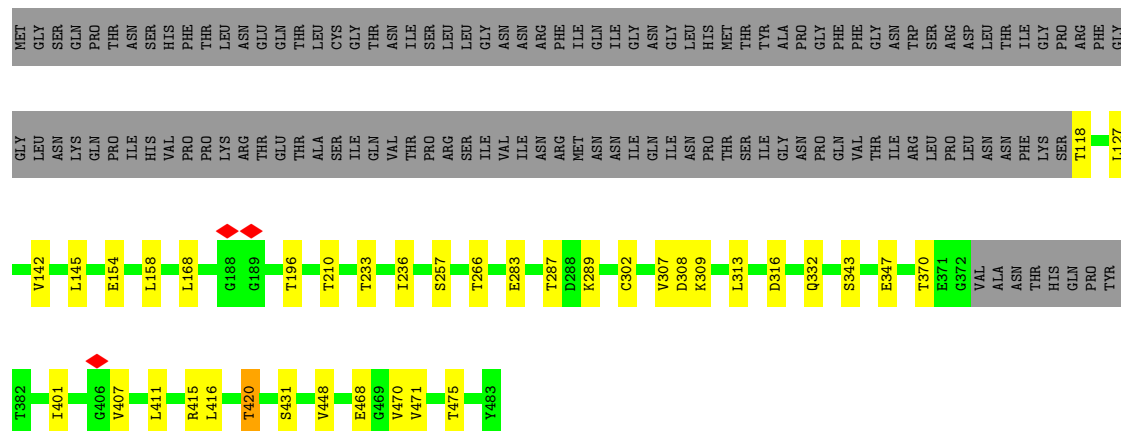
• Molecule 4: Triplex capsid protein 1

Chain o: 66% 8% 26%



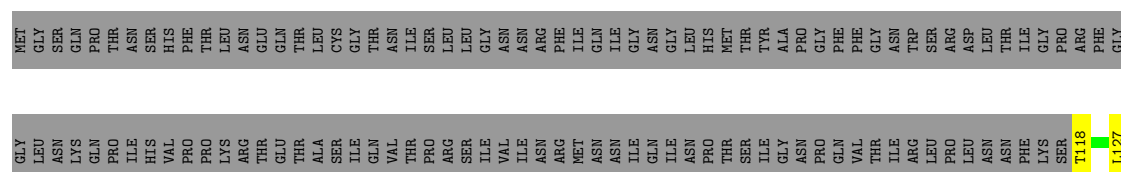
• Molecule 4: Triplex capsid protein 1

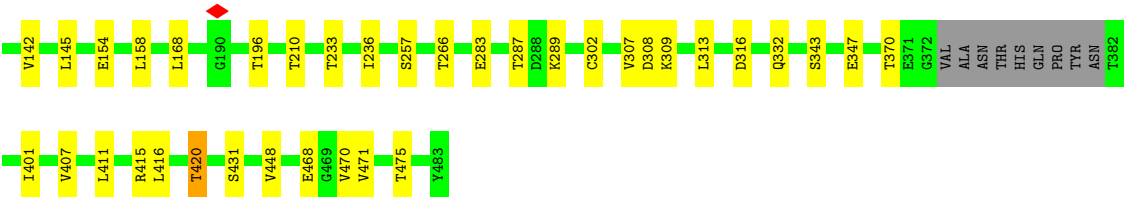
Chain r: 66% 8% 26%



• Molecule 4: Triplex capsid protein 1

Chain w: 66% 8% 26%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	311236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	386.3	Depositor
Maximum defocus (nm)	5116	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	564.0, 564.0, 564.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.41, 1.41, 1.41	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	0.25	0/9259	0.44	0/12619
1	B	0.27	0/10500	0.43	0/14329
1	D	0.27	0/10614	0.43	0/14468
1	F	0.27	0/10599	0.43	0/14450
1	H	0.27	0/10567	0.43	0/14406
1	J	0.26	0/10580	0.42	0/14428
1	L	0.27	0/10542	0.43	0/14381
1	N	0.26	0/10575	0.43	0/14419
1	P	0.27	0/10493	0.44	0/14326
1	R	0.27	0/10527	0.43	0/14354
1	T	0.26	0/10059	0.42	0/13730
1	V	0.26	0/10098	0.43	0/13777
1	X	0.26	0/10427	0.43	0/14221
1	a	0.26	0/10525	0.43	0/14360
1	c	0.26	0/10278	0.43	0/14011
1	e	0.26	0/10355	0.43	0/14107
2	C	0.25	0/753	0.43	0/1036
2	E	0.26	0/765	0.45	0/1050
2	G	0.26	0/750	0.43	0/1032
2	I	0.25	0/759	0.44	0/1043
2	K	0.26	0/746	0.44	0/1026
2	M	0.25	0/759	0.43	0/1043
2	O	0.25	0/753	0.44	0/1036
2	Q	0.26	0/727	0.42	0/997
2	S	0.25	0/741	0.44	0/1022
2	U	0.25	0/759	0.43	0/1043
2	W	0.25	0/759	0.44	0/1043
2	Y	0.26	0/738	0.45	0/1019
2	b	0.25	0/759	0.44	0/1043
2	d	0.25	0/765	0.43	0/1050
2	f	0.30	0/759	0.47	0/1043
3	g	0.26	0/2327	0.42	0/3173
3	h	0.27	0/2122	0.44	0/2896
3	j	0.26	0/2331	0.42	0/3178

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	k	0.27	0/2122	0.45	0/2896
3	m	0.25	0/2331	0.44	0/3178
3	n	0.25	0/2119	0.44	0/2892
3	p	0.26	0/2331	0.43	0/3178
3	q	0.27	0/2122	0.44	0/2896
3	s	0.27	0/2326	0.45	0/3172
3	t	0.27	0/2118	0.47	0/2891
4	i	0.28	0/2832	0.48	0/3854
4	l	0.28	0/2832	0.48	0/3854
4	o	0.28	0/2829	0.48	0/3850
4	r	0.28	0/2832	0.48	0/3854
4	w	0.28	0/2832	0.48	0/3854
All	All	0.27	0/213696	0.44	0/291528

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1148/1396 (82%)	1047 (91%)	100 (9%)	1 (0%)	48	78
1	B	1330/1396 (95%)	1207 (91%)	121 (9%)	2 (0%)	44	72
1	D	1331/1396 (95%)	1214 (91%)	117 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	1331/1396 (95%)	1219 (92%)	111 (8%)	1 (0%)	48	78
1	H	1325/1396 (95%)	1212 (92%)	113 (8%)	0	100	100
1	J	1331/1396 (95%)	1225 (92%)	106 (8%)	0	100	100
1	L	1330/1396 (95%)	1212 (91%)	115 (9%)	3 (0%)	44	72
1	N	1331/1396 (95%)	1228 (92%)	103 (8%)	0	100	100
1	P	1331/1396 (95%)	1205 (90%)	125 (9%)	1 (0%)	48	78
1	R	1324/1396 (95%)	1202 (91%)	122 (9%)	0	100	100
1	T	1271/1396 (91%)	1174 (92%)	97 (8%)	0	100	100
1	V	1272/1396 (91%)	1157 (91%)	114 (9%)	1 (0%)	48	78
1	X	1308/1396 (94%)	1192 (91%)	116 (9%)	0	100	100
1	a	1329/1396 (95%)	1229 (92%)	100 (8%)	0	100	100
1	c	1290/1396 (92%)	1188 (92%)	102 (8%)	0	100	100
1	e	1292/1396 (93%)	1188 (92%)	104 (8%)	0	100	100
2	C	99/235 (42%)	91 (92%)	7 (7%)	1 (1%)	13	44
2	E	99/235 (42%)	89 (90%)	10 (10%)	0	100	100
2	G	99/235 (42%)	91 (92%)	8 (8%)	0	100	100
2	I	99/235 (42%)	88 (89%)	10 (10%)	1 (1%)	13	44
2	K	98/235 (42%)	91 (93%)	6 (6%)	1 (1%)	13	44
2	M	99/235 (42%)	91 (92%)	7 (7%)	1 (1%)	13	44
2	O	99/235 (42%)	92 (93%)	7 (7%)	0	100	100
2	Q	93/235 (40%)	88 (95%)	5 (5%)	0	100	100
2	S	99/235 (42%)	92 (93%)	7 (7%)	0	100	100
2	U	99/235 (42%)	92 (93%)	7 (7%)	0	100	100
2	W	99/235 (42%)	91 (92%)	8 (8%)	0	100	100
2	Y	99/235 (42%)	92 (93%)	6 (6%)	1 (1%)	13	44
2	b	99/235 (42%)	91 (92%)	8 (8%)	0	100	100
2	d	99/235 (42%)	92 (93%)	7 (7%)	0	100	100
2	f	99/235 (42%)	93 (94%)	6 (6%)	0	100	100
3	g	294/316 (93%)	276 (94%)	18 (6%)	0	100	100
3	h	271/316 (86%)	248 (92%)	22 (8%)	1 (0%)	30	62
3	j	294/316 (93%)	275 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	k	271/316 (86%)	244 (90%)	26 (10%)	1 (0%)	30	62
3	m	294/316 (93%)	273 (93%)	21 (7%)	0	100	100
3	n	271/316 (86%)	247 (91%)	23 (8%)	1 (0%)	30	62
3	p	294/316 (93%)	275 (94%)	19 (6%)	0	100	100
3	q	271/316 (86%)	247 (91%)	23 (8%)	1 (0%)	30	62
3	s	294/316 (93%)	271 (92%)	23 (8%)	0	100	100
3	t	271/316 (86%)	247 (91%)	23 (8%)	1 (0%)	30	62
4	i	353/483 (73%)	318 (90%)	33 (9%)	2 (1%)	22	54
4	l	353/483 (73%)	318 (90%)	33 (9%)	2 (1%)	22	54
4	o	353/483 (73%)	318 (90%)	33 (9%)	2 (1%)	22	54
4	r	353/483 (73%)	317 (90%)	34 (10%)	2 (1%)	22	54
4	w	353/483 (73%)	317 (90%)	34 (10%)	2 (1%)	22	54
All	All	26942/31436 (86%)	24654 (92%)	2259 (8%)	29 (0%)	50	78

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	h	270	ILE
4	i	420	THR
3	k	270	ILE
4	l	420	THR
3	n	270	ILE
4	o	420	THR
3	q	270	ILE
3	t	270	ILE
4	w	420	THR
1	B	21	GLY
1	B	60	SER
4	i	416	LEU
4	l	416	LEU
4	o	416	LEU
4	r	416	LEU
4	r	420	THR
4	w	416	LEU
1	L	270	VAL
1	F	60	SER
1	L	47	ILE
1	L	49	ASP

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Mol	Chain	Res	Type
1	P	37	SER
1	V	166	ASP
1	A	127	PRO
2	I	50	ILE
2	K	50	ILE
2	M	50	ILE
2	C	50	ILE
2	Y	50	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	964/1182 (82%)	964 (100%)	0	100	100
1	B	1088/1182 (92%)	1084 (100%)	4 (0%)	89	93
1	D	1111/1182 (94%)	1110 (100%)	1 (0%)	92	96
1	F	1108/1182 (94%)	1104 (100%)	4 (0%)	89	93
1	H	1105/1182 (94%)	1103 (100%)	2 (0%)	92	96
1	J	1103/1182 (93%)	1100 (100%)	3 (0%)	91	94
1	L	1096/1182 (93%)	1089 (99%)	7 (1%)	84	90
1	N	1102/1182 (93%)	1099 (100%)	3 (0%)	91	94
1	P	1087/1182 (92%)	1083 (100%)	4 (0%)	89	93
1	R	1096/1182 (93%)	1092 (100%)	4 (0%)	89	93
1	T	1040/1182 (88%)	1040 (100%)	0	100	100
1	V	1051/1182 (89%)	1049 (100%)	2 (0%)	92	96
1	X	1088/1182 (92%)	1084 (100%)	4 (0%)	89	93
1	a	1095/1182 (93%)	1092 (100%)	3 (0%)	91	94
1	c	1070/1182 (90%)	1067 (100%)	3 (0%)	91	94
1	e	1086/1182 (92%)	1084 (100%)	2 (0%)	92	96
2	C	74/189 (39%)	73 (99%)	1 (1%)	62	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	76/189 (40%)	75 (99%)	1 (1%)	65	77
2	G	73/189 (39%)	72 (99%)	1 (1%)	62	76
2	I	75/189 (40%)	74 (99%)	1 (1%)	65	77
2	K	73/189 (39%)	72 (99%)	1 (1%)	62	76
2	M	75/189 (40%)	74 (99%)	1 (1%)	65	77
2	O	74/189 (39%)	73 (99%)	1 (1%)	62	76
2	Q	72/189 (38%)	71 (99%)	1 (1%)	62	76
2	S	72/189 (38%)	71 (99%)	1 (1%)	62	76
2	U	75/189 (40%)	74 (99%)	1 (1%)	65	77
2	W	75/189 (40%)	74 (99%)	1 (1%)	65	77
2	Y	71/189 (38%)	70 (99%)	1 (1%)	62	76
2	b	75/189 (40%)	74 (99%)	1 (1%)	65	77
2	d	76/189 (40%)	75 (99%)	1 (1%)	65	77
2	f	75/189 (40%)	73 (97%)	2 (3%)	40	61
3	g	255/267 (96%)	255 (100%)	0	100	100
3	h	230/267 (86%)	229 (100%)	1 (0%)	89	93
3	j	256/267 (96%)	256 (100%)	0	100	100
3	k	230/267 (86%)	228 (99%)	2 (1%)	75	84
3	m	256/267 (96%)	256 (100%)	0	100	100
3	n	229/267 (86%)	227 (99%)	2 (1%)	75	84
3	p	256/267 (96%)	256 (100%)	0	100	100
3	q	230/267 (86%)	229 (100%)	1 (0%)	89	93
3	s	255/267 (96%)	255 (100%)	0	100	100
3	t	229/267 (86%)	228 (100%)	1 (0%)	89	93
4	i	289/410 (70%)	251 (87%)	38 (13%)	3	18
4	l	289/410 (70%)	252 (87%)	37 (13%)	3	19
4	o	288/410 (70%)	251 (87%)	37 (13%)	3	19
4	r	289/410 (70%)	252 (87%)	37 (13%)	3	19
4	w	289/410 (70%)	252 (87%)	37 (13%)	3	19
All	All	22271/26467 (84%)	22016 (99%)	255 (1%)	69	80

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	52	LYS
1	B	59	ASN
1	B	101	TYR
1	B	472	ARG
2	C	93	ARG
1	D	472	ARG
2	E	93	ARG
1	F	52	LYS
1	F	58	ASP
1	F	60	SER
1	F	472	ARG
2	G	93	ARG
1	H	472	ARG
1	H	1302	ASN
2	I	93	ARG
1	J	45	ARG
1	J	52	LYS
1	J	946	ARG
2	K	93	ARG
1	L	47	ILE
1	L	49	ASP
1	L	50	PHE
1	L	619	ARG
1	L	769	ARG
1	L	923	ARG
1	L	1277	ASN
2	M	93	ARG
1	N	103	ARG
1	N	472	ARG
1	N	923	ARG
2	O	93	ARG
1	P	472	ARG
1	P	619	ARG
1	P	778	ARG
1	P	1277	ASN
2	Q	93	ARG
1	R	45	ARG
1	R	47	ILE
1	R	50	PHE
1	R	472	ARG
2	S	93	ARG
2	U	93	ARG
1	V	197	LEU

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Mol	Chain	Res	Type
1	V	1189	ARG
2	W	93	ARG
1	X	45	ARG
1	X	281	ARG
1	X	472	ARG
1	X	619	ARG
2	Y	93	ARG
1	a	55	ARG
1	a	778	ARG
1	a	1277	ASN
2	b	93	ARG
1	c	472	ARG
1	c	619	ARG
1	c	923	ARG
2	d	93	ARG
1	e	472	ARG
1	e	778	ARG
2	f	50	ILE
2	f	93	ARG
3	h	173	ARG
4	i	118	THR
4	i	127	LEU
4	i	142	VAL
4	i	145	LEU
4	i	154	GLU
4	i	158	LEU
4	i	168	LEU
4	i	196	THR
4	i	210	THR
4	i	233	THR
4	i	236	ILE
4	i	241	CYS
4	i	257	SER
4	i	266	THR
4	i	283	GLU
4	i	287	THR
4	i	289	LYS
4	i	302	CYS
4	i	307	VAL
4	i	308	ASP
4	i	309	LYS
4	i	313	LEU

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Mol	Chain	Res	Type
4	i	316	ASP
4	i	332	GLN
4	i	343	SER
4	i	347	GLU
4	i	370	THR
4	i	401	ILE
4	i	407	VAL
4	i	411	LEU
4	i	415	ARG
4	i	420	THR
4	i	431	SER
4	i	448	VAL
4	i	468	GLU
4	i	470	VAL
4	i	471	VAL
4	i	475	THR
3	k	173	ARG
3	k	202	ARG
4	l	118	THR
4	l	127	LEU
4	l	142	VAL
4	l	145	LEU
4	l	154	GLU
4	l	158	LEU
4	l	168	LEU
4	l	196	THR
4	l	210	THR
4	l	233	THR
4	l	236	ILE
4	l	257	SER
4	l	266	THR
4	l	283	GLU
4	l	287	THR
4	l	289	LYS
4	l	302	CYS
4	l	307	VAL
4	l	308	ASP
4	l	309	LYS
4	l	313	LEU
4	l	316	ASP
4	l	332	GLN
4	l	343	SER

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Mol	Chain	Res	Type
4	l	347	GLU
4	l	370	THR
4	l	401	ILE
4	l	407	VAL
4	l	411	LEU
4	l	415	ARG
4	l	420	THR
4	l	431	SER
4	l	448	VAL
4	l	468	GLU
4	l	470	VAL
4	l	471	VAL
4	l	475	THR
3	n	173	ARG
3	n	202	ARG
4	o	118	THR
4	o	127	LEU
4	o	142	VAL
4	o	145	LEU
4	o	154	GLU
4	o	158	LEU
4	o	168	LEU
4	o	196	THR
4	o	210	THR
4	o	233	THR
4	o	236	ILE
4	o	257	SER
4	o	266	THR
4	o	283	GLU
4	o	287	THR
4	o	289	LYS
4	o	302	CYS
4	o	307	VAL
4	o	308	ASP
4	o	309	LYS
4	o	313	LEU
4	o	316	ASP
4	o	332	GLN
4	o	343	SER
4	o	347	GLU
4	o	370	THR
4	o	401	ILE

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Mol	Chain	Res	Type
4	o	407	VAL
4	o	411	LEU
4	o	415	ARG
4	o	420	THR
4	o	431	SER
4	o	448	VAL
4	o	468	GLU
4	o	470	VAL
4	o	471	VAL
4	o	475	THR
3	q	173	ARG
4	r	118	THR
4	r	127	LEU
4	r	142	VAL
4	r	145	LEU
4	r	154	GLU
4	r	158	LEU
4	r	168	LEU
4	r	196	THR
4	r	210	THR
4	r	233	THR
4	r	236	ILE
4	r	257	SER
4	r	266	THR
4	r	283	GLU
4	r	287	THR
4	r	289	LYS
4	r	302	CYS
4	r	307	VAL
4	r	308	ASP
4	r	309	LYS
4	r	313	LEU
4	r	316	ASP
4	r	332	GLN
4	r	343	SER
4	r	347	GLU
4	r	370	THR
4	r	401	ILE
4	r	407	VAL
4	r	411	LEU
4	r	415	ARG
4	r	420	THR

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Mol	Chain	Res	Type
4	r	431	SER
4	r	448	VAL
4	r	468	GLU
4	r	470	VAL
4	r	471	VAL
4	r	475	THR
3	t	173	ARG
4	w	118	THR
4	w	127	LEU
4	w	142	VAL
4	w	145	LEU
4	w	154	GLU
4	w	158	LEU
4	w	168	LEU
4	w	196	THR
4	w	210	THR
4	w	233	THR
4	w	236	ILE
4	w	257	SER
4	w	266	THR
4	w	283	GLU
4	w	287	THR
4	w	289	LYS
4	w	302	CYS
4	w	307	VAL
4	w	308	ASP
4	w	309	LYS
4	w	313	LEU
4	w	316	ASP
4	w	332	GLN
4	w	343	SER
4	w	347	GLU
4	w	370	THR
4	w	401	ILE
4	w	407	VAL
4	w	411	LEU
4	w	415	ARG
4	w	420	THR
4	w	431	SER
4	w	448	VAL
4	w	468	GLU
4	w	470	VAL

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Mol	Chain	Res	Type
4	w	471	VAL
4	w	475	THR

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	221	HIS
1	A	1267	GLN
1	A	1348	GLN
1	B	683	ASN
1	D	24	ASN
1	D	157	ASN
1	D	685	HIS
1	D	696	ASN
1	F	130	ASN
1	F	157	ASN
1	F	305	GLN
1	F	533	HIS
1	F	1074	GLN
2	G	15	ASN
1	H	682	ASN
1	H	1304	ASN
1	J	533	HIS
1	J	656	ASN
1	L	427	GLN
1	L	533	HIS
1	L	1058	GLN
1	N	24	ASN
1	N	656	ASN
1	N	696	ASN
1	N	1102	HIS
1	P	217	GLN
1	P	682	ASN
1	R	305	GLN
1	R	533	HIS
1	R	656	ASN
1	R	1057	HIS
1	T	495	GLN
1	T	1057	HIS
2	U	71	ASN
1	V	656	ASN
1	X	129	HIS

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Mol	Chain	Res	Type
1	X	305	GLN
1	X	533	HIS
1	X	656	ASN
1	c	305	GLN
1	c	656	ASN
1	c	696	ASN
1	e	157	ASN
1	e	305	GLN
1	e	495	GLN
1	e	533	HIS
1	e	656	ASN
1	e	696	ASN
3	g	193	HIS
3	j	193	HIS
3	p	193	HIS
3	q	85	HIS
4	w	429	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 ⓘ

There are no chain breaks in this entry.

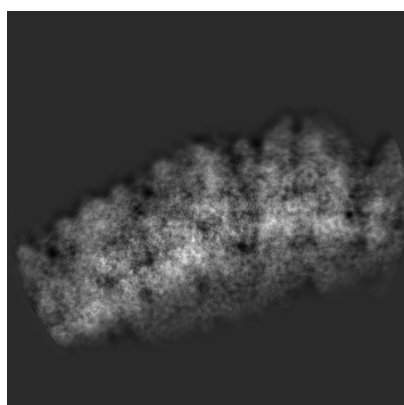
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30228. These allow visual inspection of the internal detail of the map and identification of artifacts.

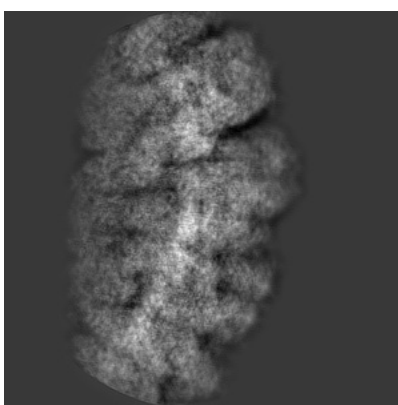
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

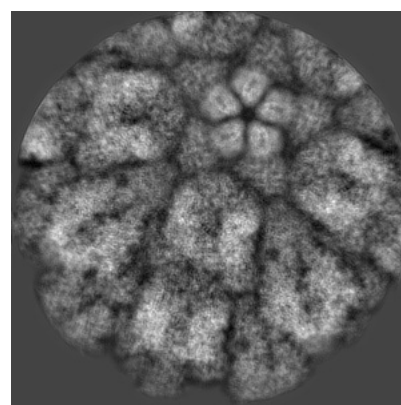
6.1.1 Primary map



X



Y

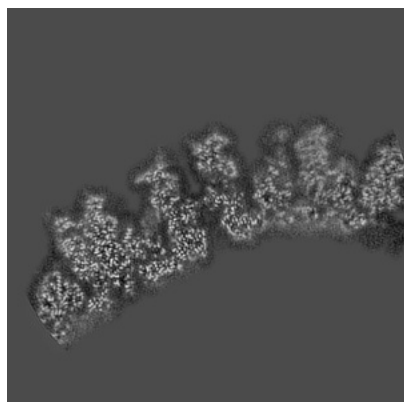


Z

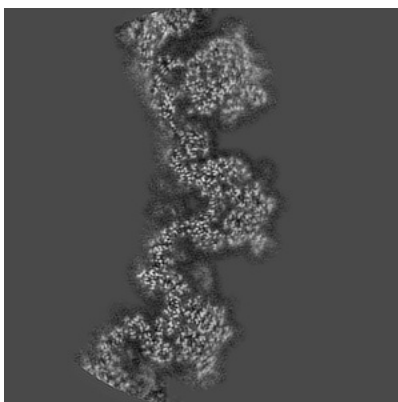
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

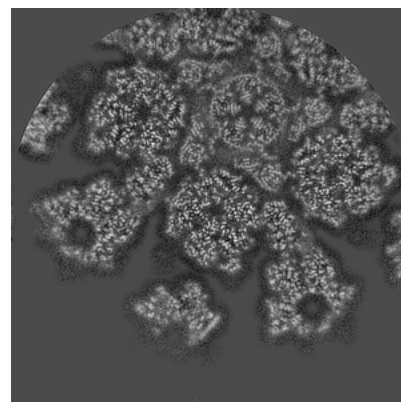
6.2.1 Primary map



X Index: 200



Y Index: 200

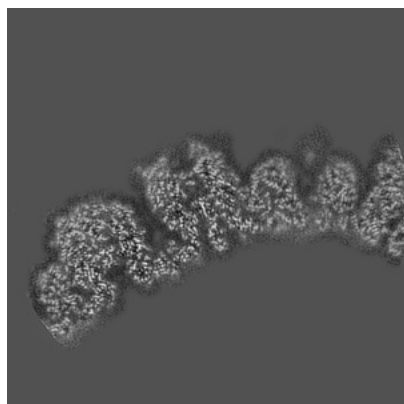


Z Index: 200

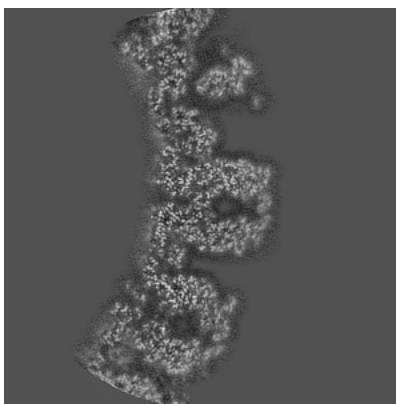
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

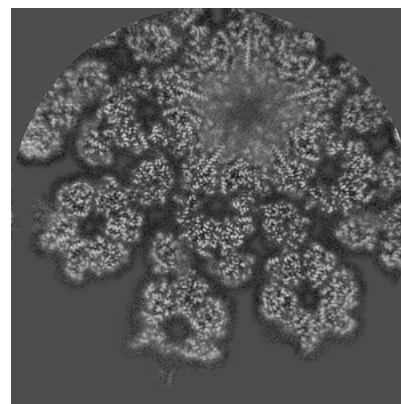
6.3.1 Primary map



X Index: 187



Y Index: 187

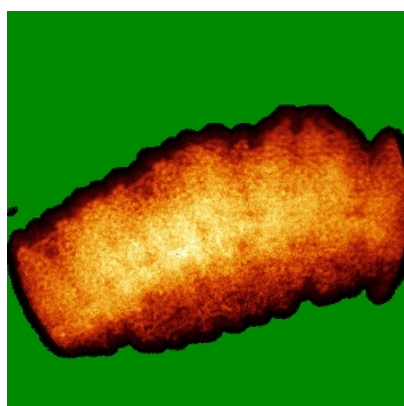


Z Index: 186

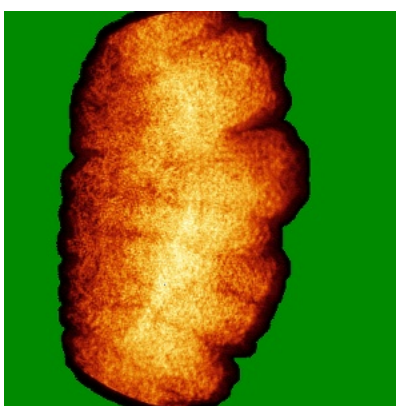
The images above show the largest variance slices of the map in three orthogonal directions.

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

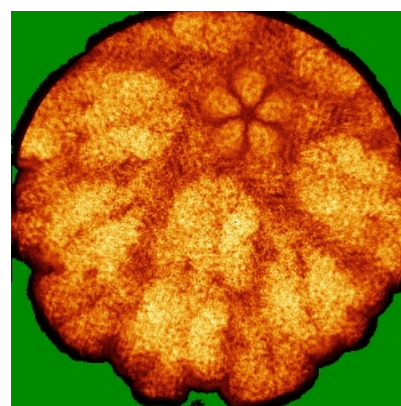
6.4.1 Primary map



X



Y

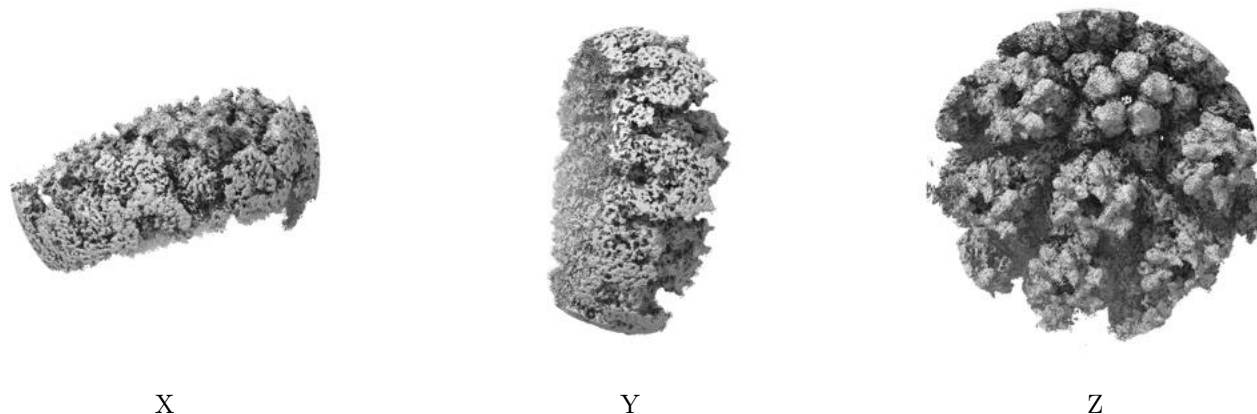


Z

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

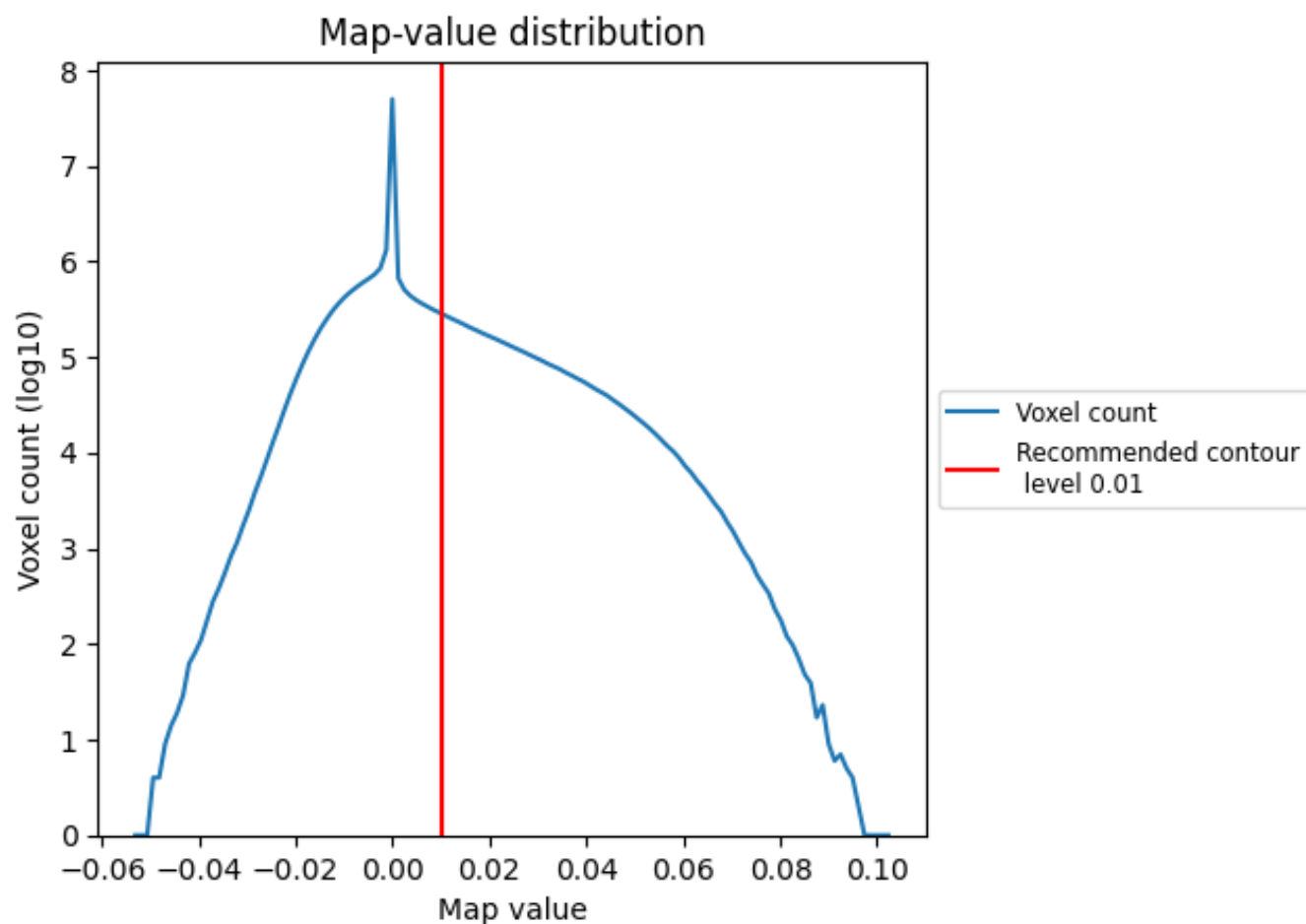
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

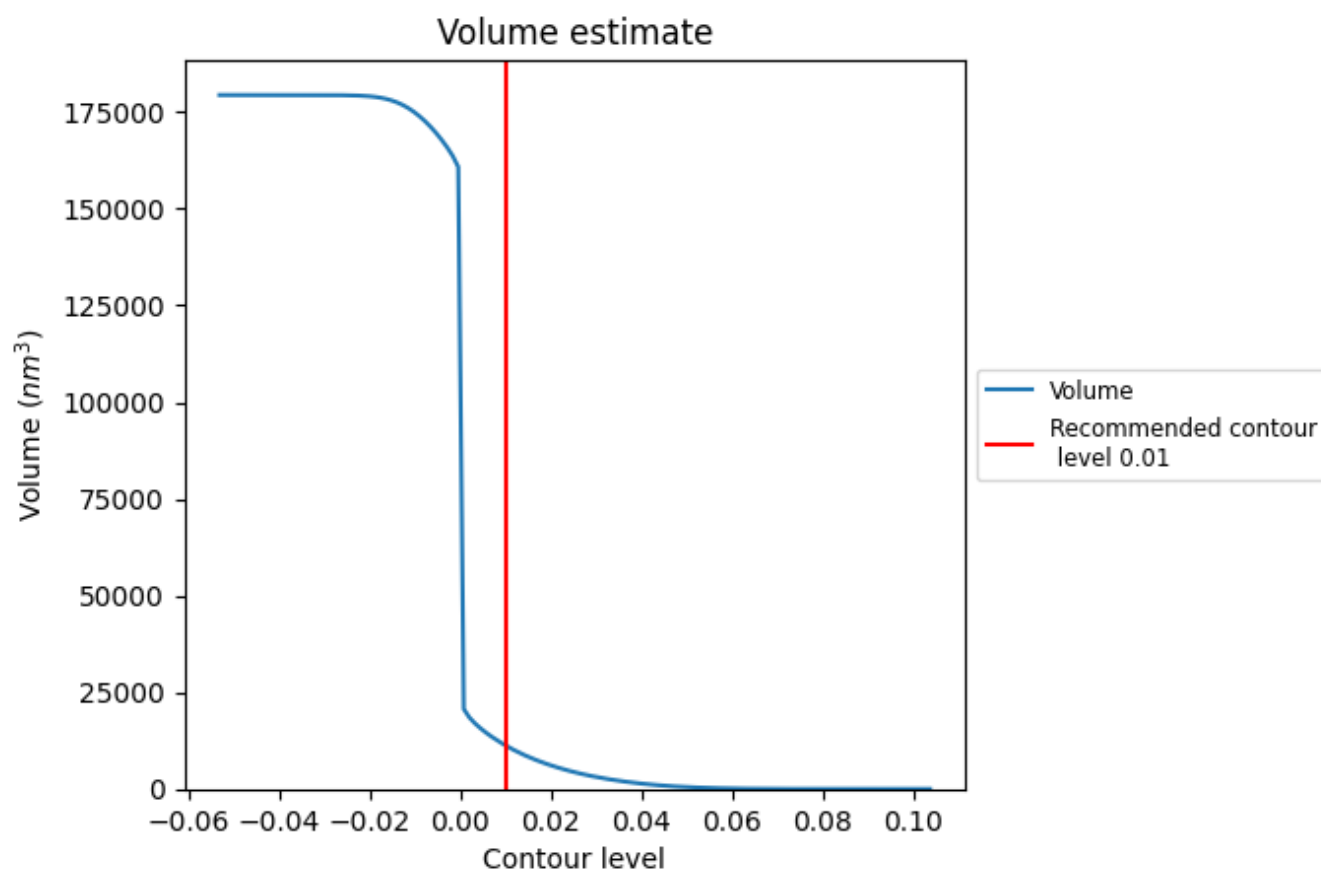
This section contains the results of statistical analysis of the map.

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.

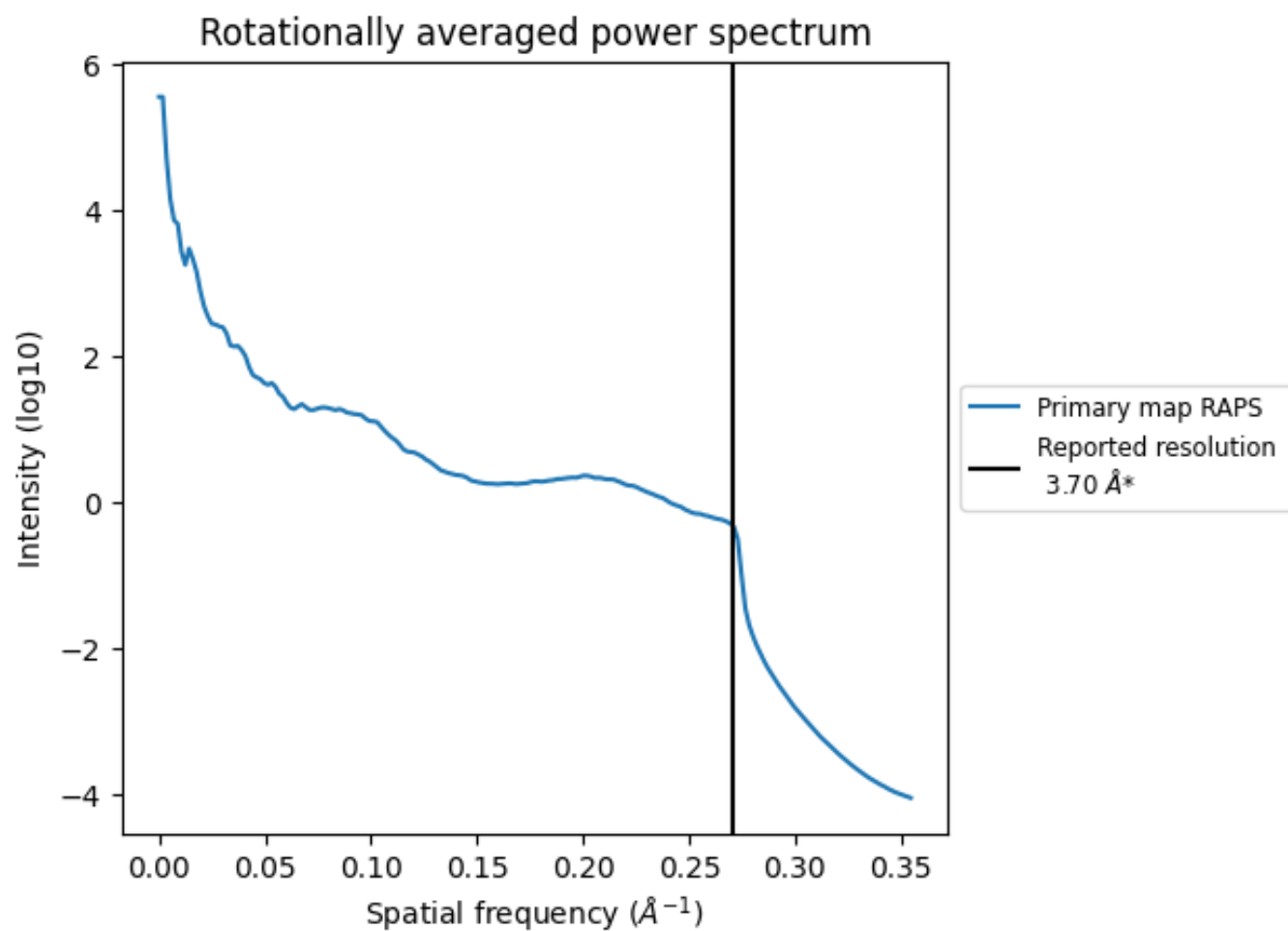
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11233 nm³; this corresponds to an approximate mass of 10147 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 ⓘ

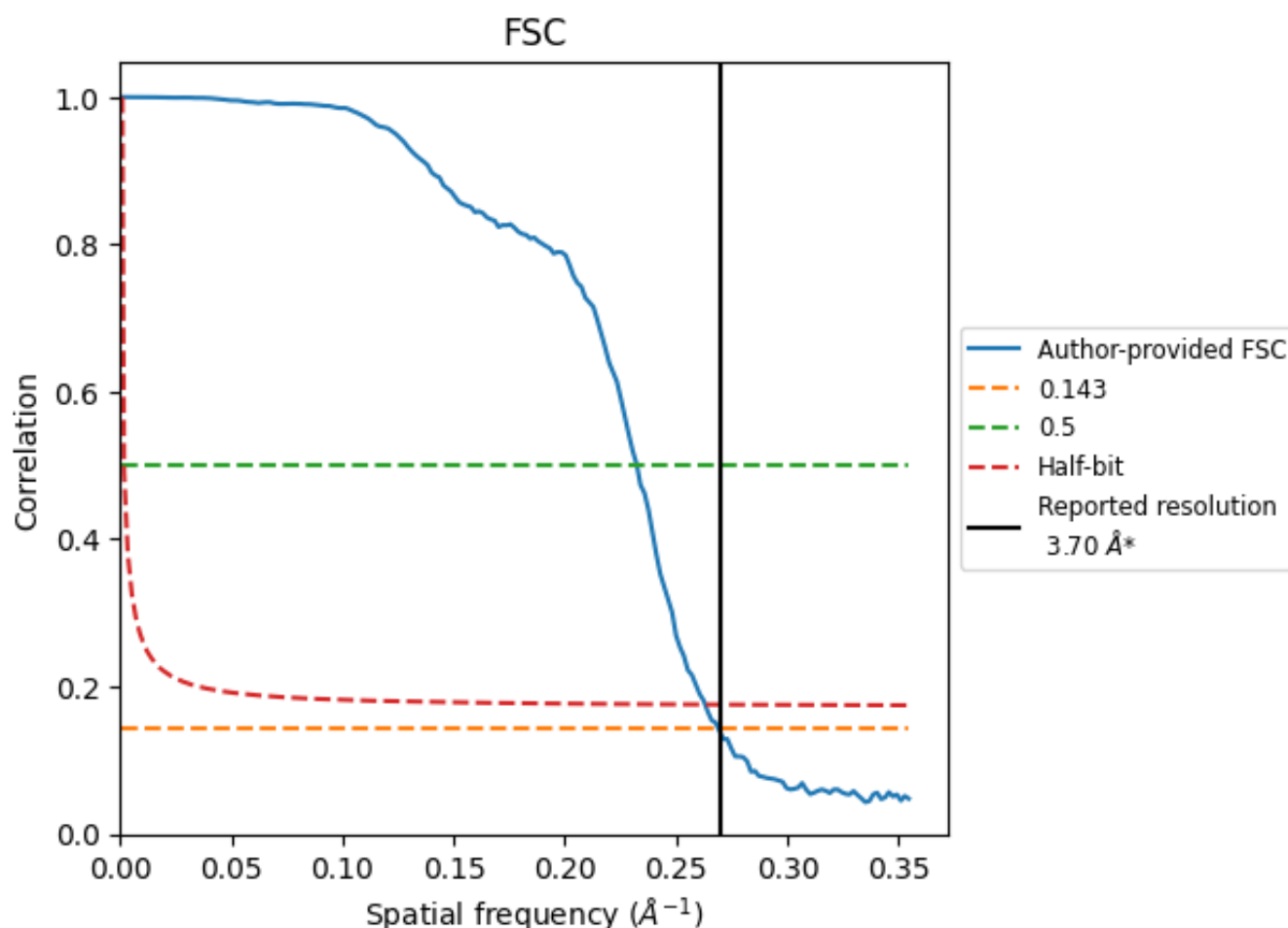


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 \AA^{-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	3.72	4.30	3.80
Unmasked-calculated*	-	-	-

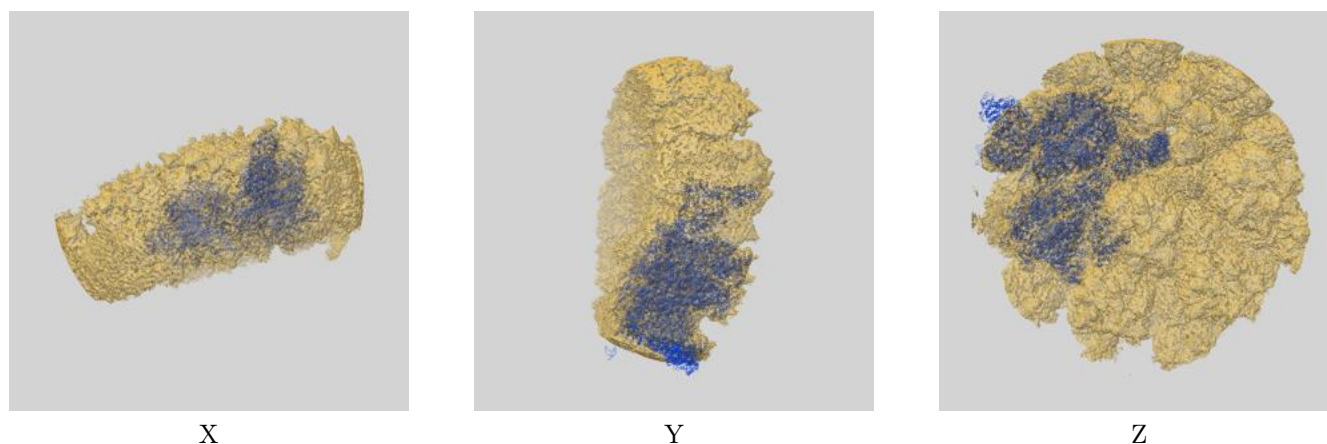
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

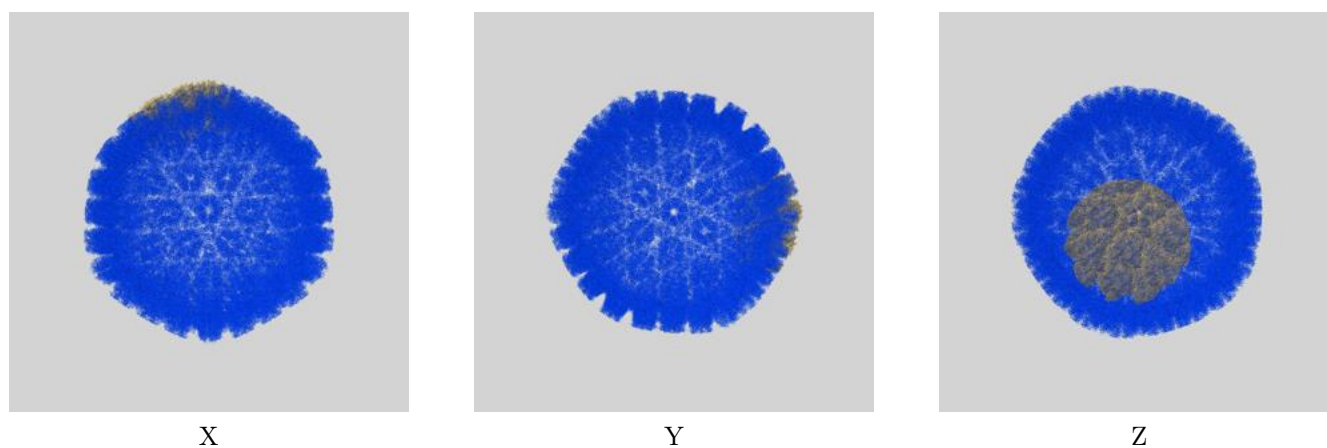
This section contains information regarding the fit between EMDB map EMD-30228 and PDB model 7BW6. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

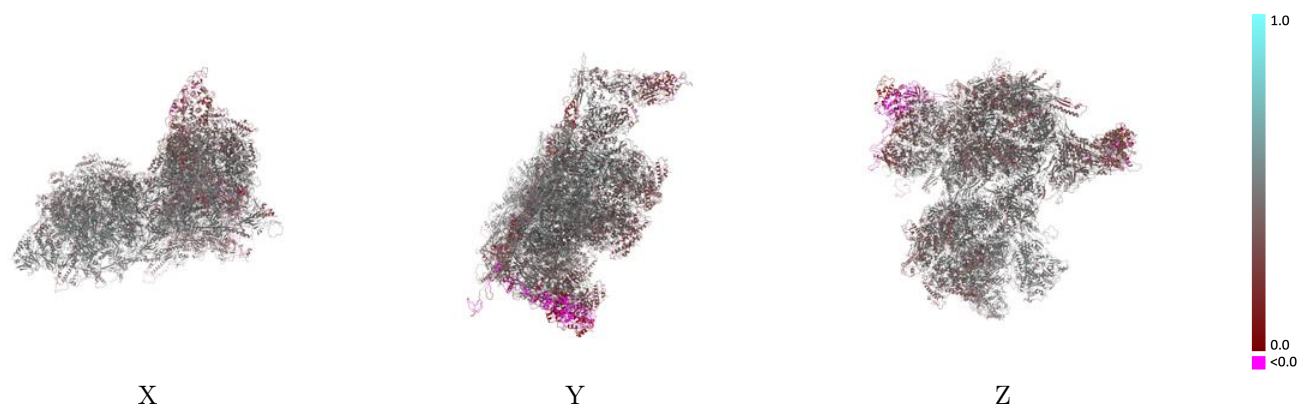


9.1.2 Map-model assembly overlay [i](#)



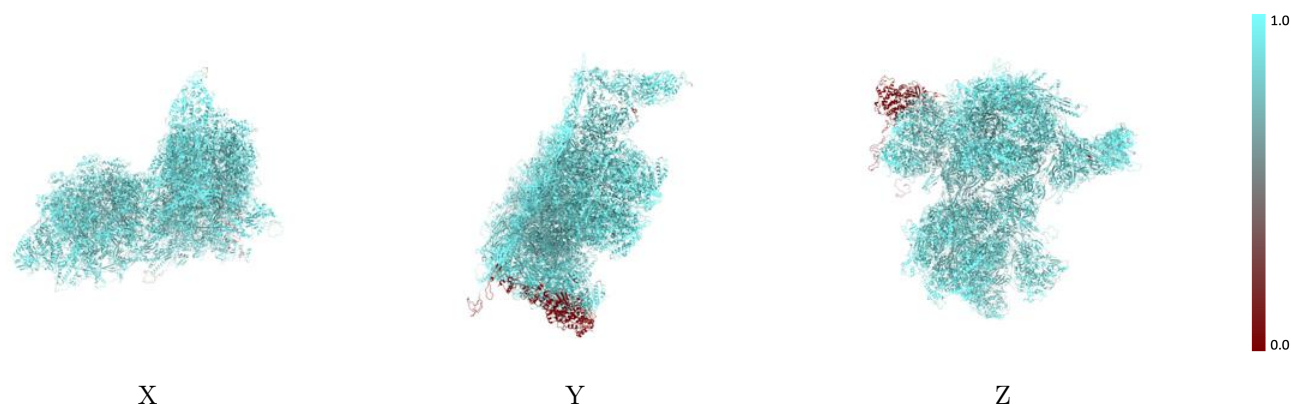
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



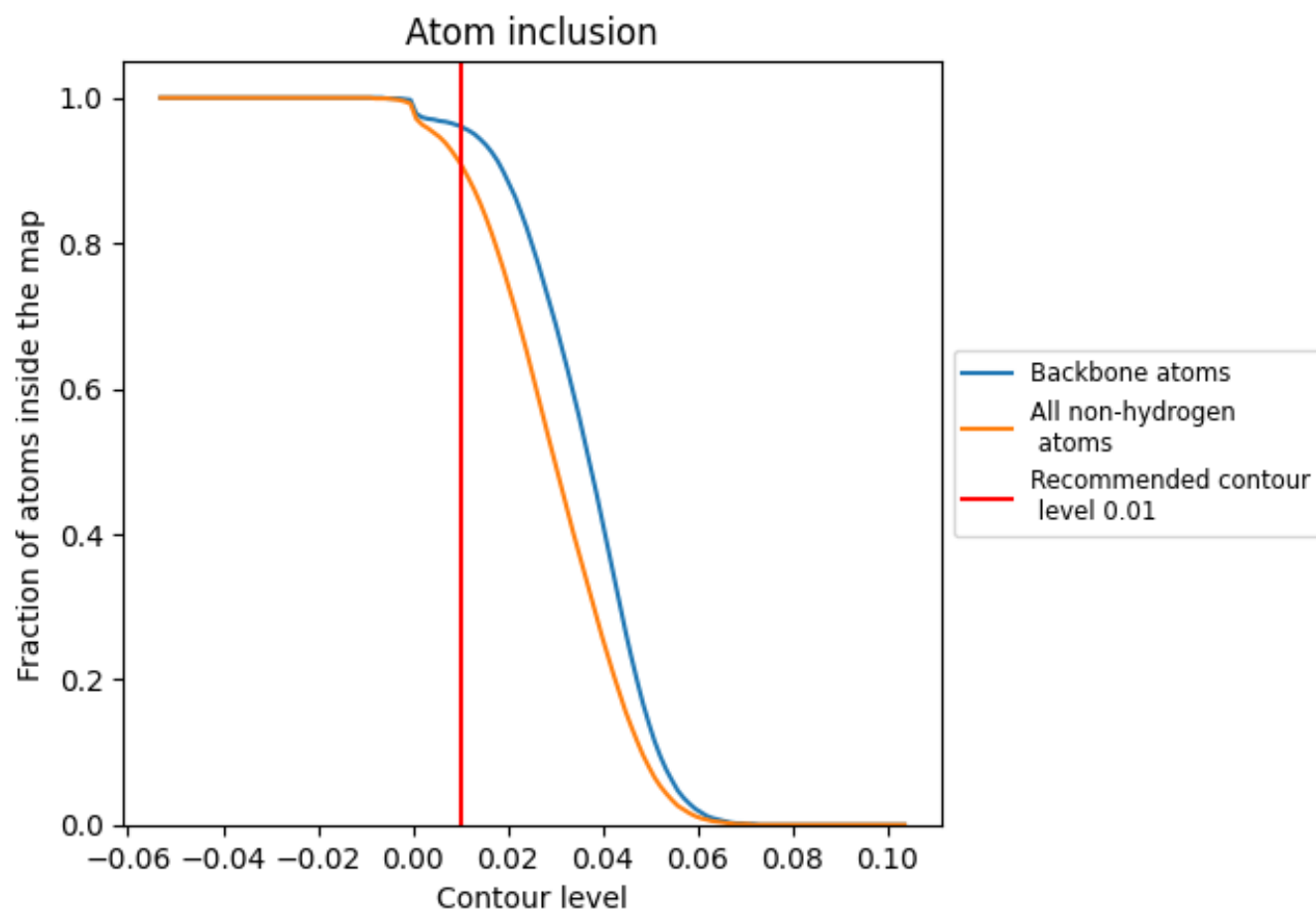
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9100	 0.4090
A	 0.9160	 0.3270
B	 0.9630	 0.4660
C	 0.9460	 0.3180
D	 0.9450	 0.4490
E	 0.9490	 0.3130
F	 0.9450	 0.4410
G	 0.9530	 0.3020
H	 0.9440	 0.4280
I	 0.9530	 0.3000
J	 0.9570	 0.4500
K	 0.9530	 0.3000
L	 0.9560	 0.4540
M	 0.9490	 0.3340
N	 0.9530	 0.4510
O	 0.9490	 0.2950
P	 0.9520	 0.4490
Q	 0.9670	 0.3240
R	 0.9350	 0.4360
S	 0.9620	 0.3170
T	 0.9530	 0.4310
U	 0.9590	 0.3030
V	 0.9500	 0.4200
W	 0.9510	 0.2890
X	 0.9240	 0.4280
Y	 0.9110	 0.3020
a	 0.8830	 0.3670
b	 0.6310	 0.1390
c	 0.9010	 0.3810
d	 0.9180	 0.2420
e	 0.5150	 0.1900
f	 0.1500	 0.0280
g	 0.9150	 0.4490
h	 0.9290	 0.4470
i	 0.9090	 0.4410



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Chain	Atom inclusion	Q-score
j	 0.9350	 0.4520
k	 0.9230	 0.4400
l	 0.9230	 0.4360
m	 0.9230	 0.4150
n	 0.8990	 0.4040
o	 0.8740	 0.4060
p	 0.9080	 0.4610
q	 0.9100	 0.4490
r	 0.9170	 0.4540
s	 0.9140	 0.4520
t	 0.8720	 0.4430
w	 0.9310	 0.4400