Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 12:00 PM EDT

PDB ID	:	8VWI
EMDB ID	:	EMD-43588
Title	:	The base complex of the AcMNPV baculovirus nucleocapsid (Class 1, localised reconstruction)
Authors	:	Johnstone, B.A.; Koszalka, P.; Ha, J.; Venugopal, H.; Coulibaly, F.
Deposited on	:	2024-02-01
Resolution	:	4.71 Å(reported)
Based on initial model	:	.

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:

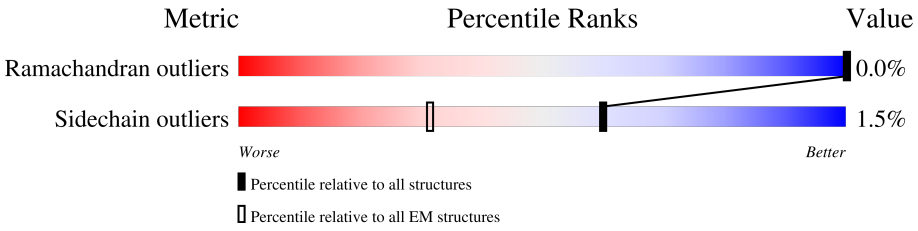
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.71 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 <=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	347	13% 76% 21%
1	B	347	19% 79% 20%
1	C	347	10% 81% 18%
1	D	347	80% 18%
1	E	347	5% 80% 18%
1	F	347	7% 82% 18%
1	V	347	17% 79% 21%
1	W	347	19% 80% 20%
1	X	347	11% 82% 18%

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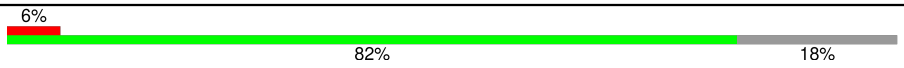
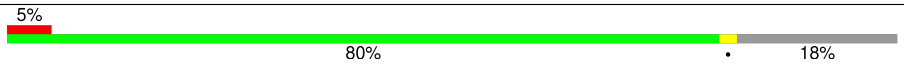
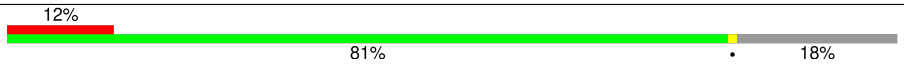
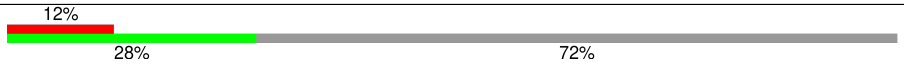
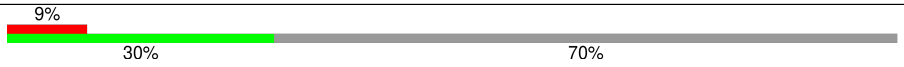
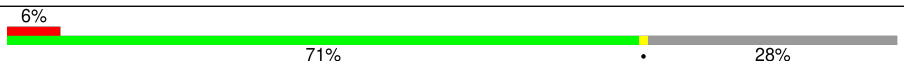
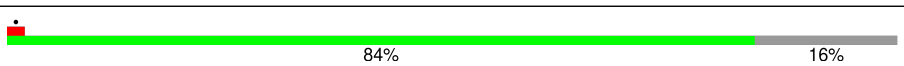
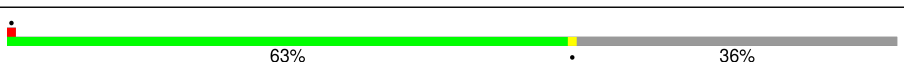
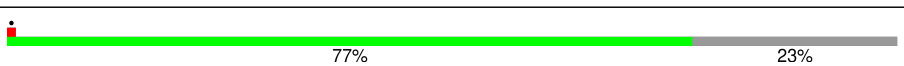
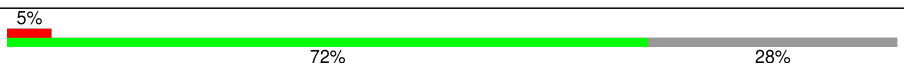
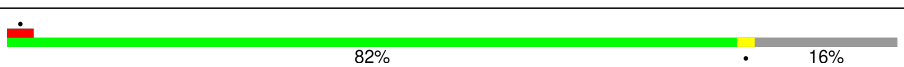
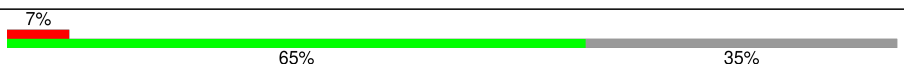
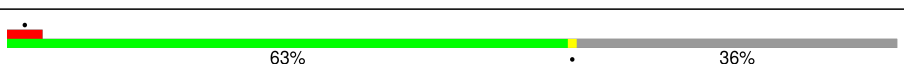
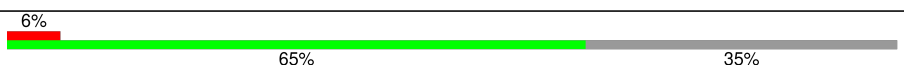
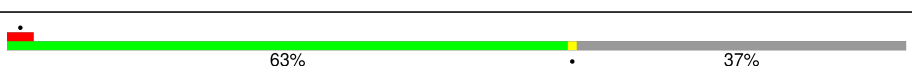
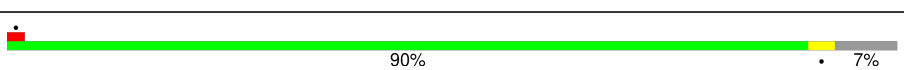
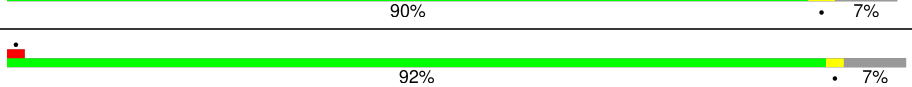
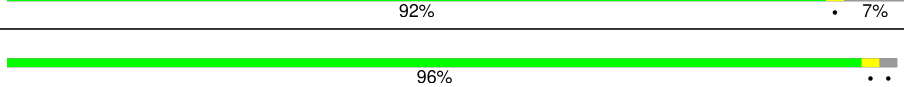
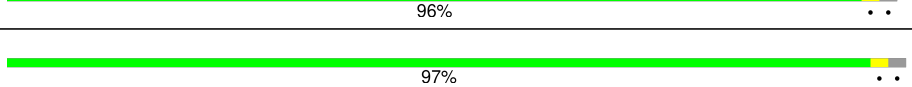
Mol	Chain	Length	Quality of chain
1	Y	347	
1	Z	347	
1	a	347	
2	G	691	
2	H	691	
2	I	691	
2	b	691	
2	c	691	
2	d	691	
3	J	290	
3	M	290	
3	Q	290	
3	S	290	
3	e	290	
3	h	290	
4	K	361	
4	L	361	
4	R	361	
4	T	361	
4	f	361	
4	g	361	
5	N	390	
5	i	390	
6	O	477	
6	j	477	

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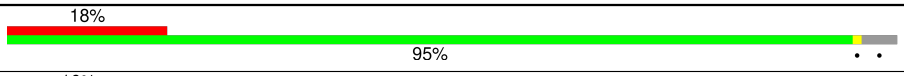
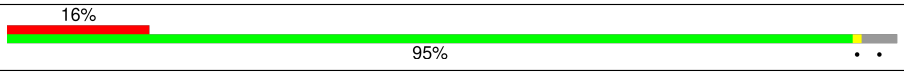
Mol	Chain	Length	Quality of chain
7	P	320	
7	k	320	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 156266 atoms, of which 77619 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	274	Total	C	H	N	O	S	0	0
			4371	1396	2157	387	419	12		
1	B	279	Total	C	H	N	O	S	0	0
			4449	1417	2195	396	429	12		
1	C	285	Total	C	H	N	O	S	0	0
			4564	1459	2252	406	435	12		
1	D	285	Total	C	H	N	O	S	0	0
			4550	1451	2244	404	439	12		
1	E	283	Total	C	H	N	O	S	0	0
			4506	1443	2220	398	432	13		
1	F	285	Total	C	H	N	O	S	0	0
			4538	1454	2234	402	435	13		
1	V	274	Total	C	H	N	O	S	0	0
			4371	1396	2157	387	419	12		
1	W	279	Total	C	H	N	O	S	0	0
			4449	1417	2195	396	429	12		
1	X	285	Total	C	H	N	O	S	0	0
			4564	1459	2252	406	435	12		
1	Y	285	Total	C	H	N	O	S	0	0
			4554	1455	2244	404	439	12		
1	Z	283	Total	C	H	N	O	S	0	0
			4507	1440	2224	398	432	13		
1	a	286	Total	C	H	N	O	S	0	0
			4550	1454	2243	403	437	13		

- Molecule 2 is a protein called Capsid-associated protein VP80.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	194	Total	C	H	N	O	S	0	0
			3228	1049	1612	265	290	12		
2	H	210	Total	C	H	N	O	S	0	0
			3513	1133	1760	293	314	13		
2	I	224	Total	C	H	N	O	S	0	0
			3740	1209	1862	315	340	14		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	197	Total	C	H	N	O	S	0	0
			3289	1066	1647	269	295	12		
2	c	206	Total	C	H	N	O	S	0	0
			3452	1113	1733	289	304	13		
2	d	223	Total	C	H	N	O	S	0	0
			3743	1206	1871	314	338	14		

- Molecule 3 is a protein called Occlusion-derived virus envelope protein E27.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	J	210	Total	C	H	N	O	S	0	0
			3389	1095	1690	270	325	9		
3	M	244	Total	C	H	N	O	S	0	0
			3956	1269	1979	317	381	10		
3	Q	185	Total	C	H	N	O	S	0	0
			3010	972	1508	237	285	8		
3	S	223	Total	C	H	N	O	S	0	0
			3619	1169	1807	285	350	8		
3	e	210	Total	C	H	N	O	S	0	0
			3384	1095	1685	270	325	9		
3	h	243	Total	C	H	N	O	S	0	0
			3933	1263	1965	315	380	10		

- Molecule 4 is a protein called Protein C42.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	K	234	Total	C	H	N	O	S	0	0
			3842	1217	1908	332	369	16		
4	L	231	Total	C	H	N	O	S	0	0
			3809	1203	1903	327	360	16		
4	R	220	Total	C	H	N	O	S	0	0
			3607	1150	1789	307	345	16		
4	T	222	Total	C	H	N	O	S	0	0
			3658	1161	1822	315	344	16		
4	f	234	Total	C	H	N	O	S	0	0
			3841	1217	1907	332	369	16		
4	g	229	Total	C	H	N	O	S	0	0
			3782	1195	1890	324	357	16		

- Molecule 5 is a protein called Protein AC109.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	N	364	Total	C	H	N	O	S	0	0
			5917	1913	2953	494	541	16		
5	i	364	Total	C	H	N	O	S	0	0
			5917	1913	2953	494	541	16		

- Molecule 6 is a protein called Protein AC142.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	O	469	Total	C	H	N	O	S	0	0
			7709	2507	3852	634	693	23		
6	j	469	Total	C	H	N	O	S	0	0
			7709	2507	3852	634	693	23		

- Molecule 7 is a protein called 38K (AC98) protein in P143-LEF5 intergenic region.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	P	307	Total	C	H	N	O	S	0	0
			5118	1682	2528	424	470	14		
7	k	307	Total	C	H	N	O	S	0	0
			5116	1682	2526	424	470	14		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Zn	0
			1	1	
8	B	1	Total	Zn	0
			1	1	
8	C	1	Total	Zn	0
			1	1	
8	D	1	Total	Zn	0
			1	1	
8	E	1	Total	Zn	0
			1	1	
8	F	1	Total	Zn	0
			1	1	
8	V	1	Total	Zn	0
			1	1	
8	W	1	Total	Zn	0
			1	1	
8	X	1	Total	Zn	0
			1	1	

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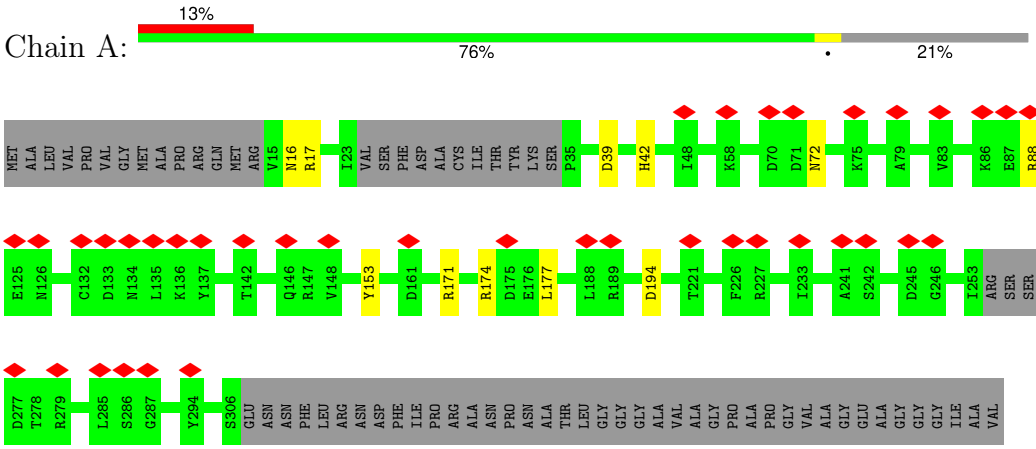
Mol	Chain	Residues	Atoms	AltConf
8	Y	1	Total Zn 1 1	0
8	Z	1	Total Zn 1 1	0
8	a	1	Total Zn 1 1	0

3 Residue-property plots (i)

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

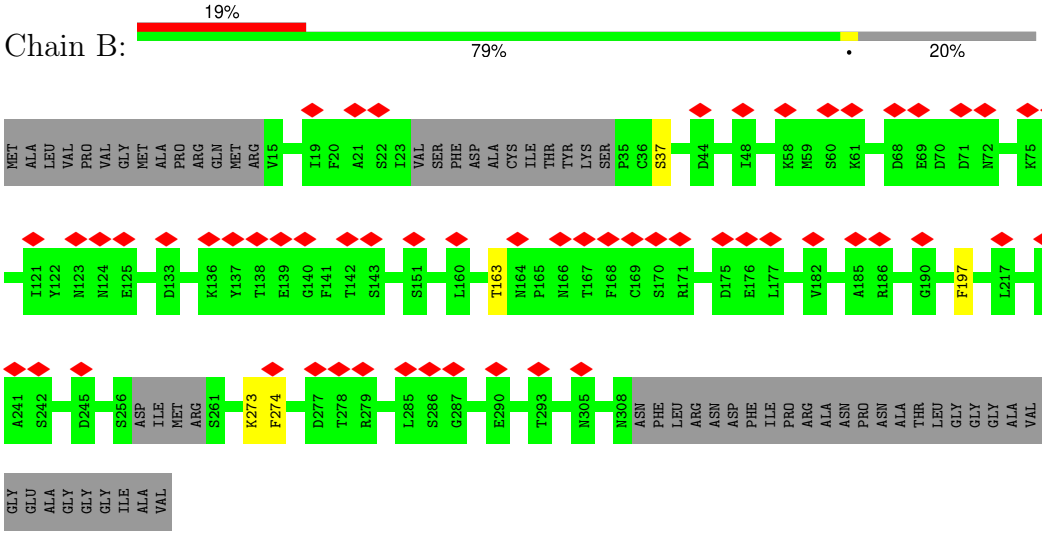
• Molecule 1: Major capsid protein

Chain A:



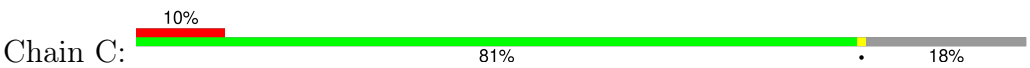
• Molecule 1: Major capsid protein

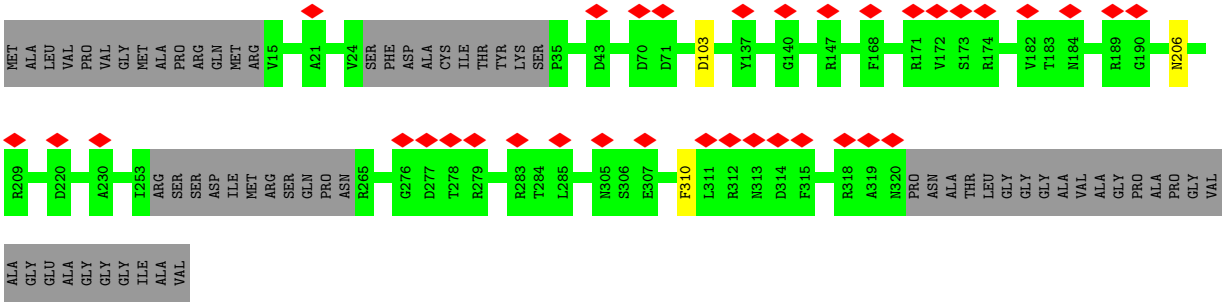
Chain B:



• Molecule 1: Major capsid protein

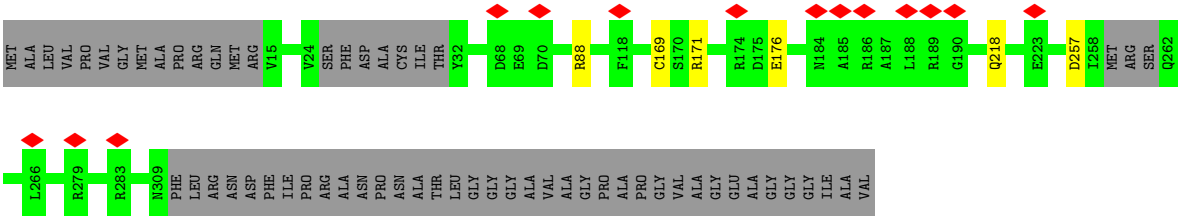
Chain C:





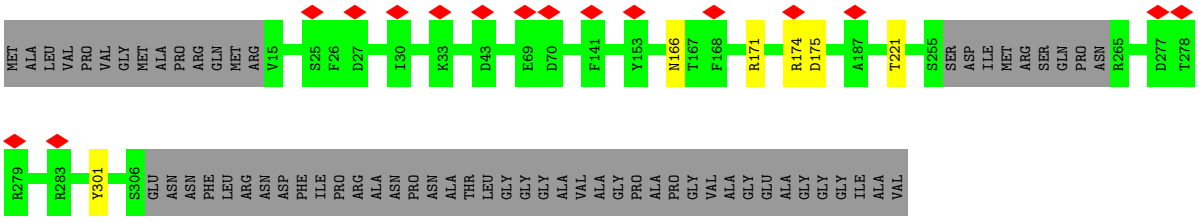
• Molecule 1: Major capsid protein

Chain D:



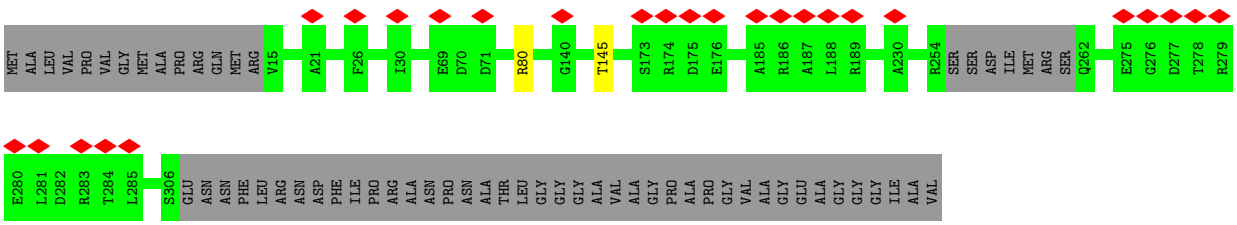
• Molecule 1: Major capsid protein

Chain E:



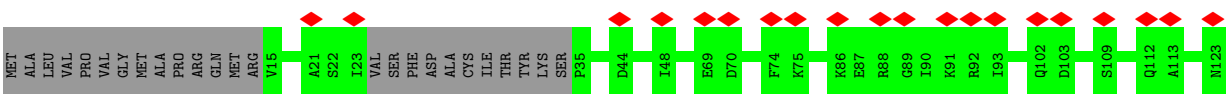
• Molecule 1: Major capsid protein

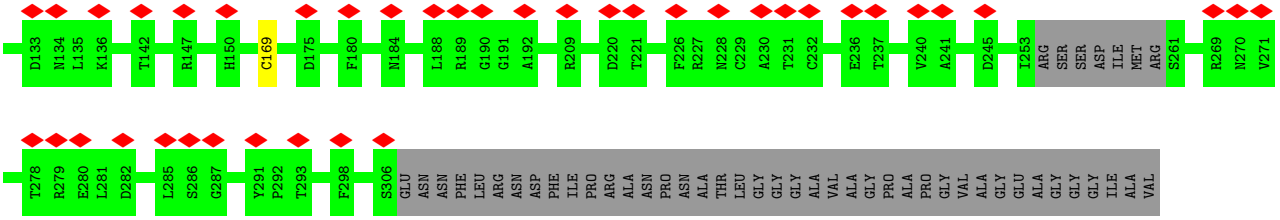
Chain F:



• Molecule 1: Major capsid protein

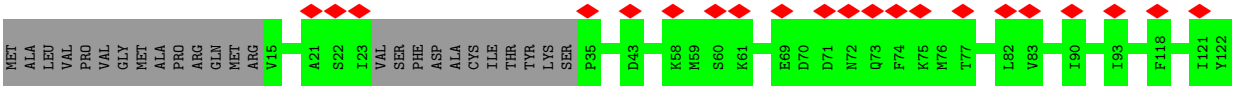
Chain V:

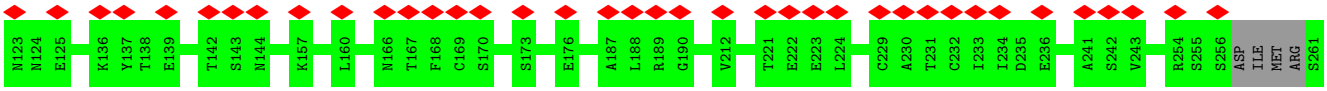


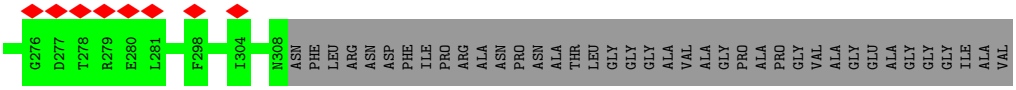


• Molecule 1: Major capsid protein

Chain W:

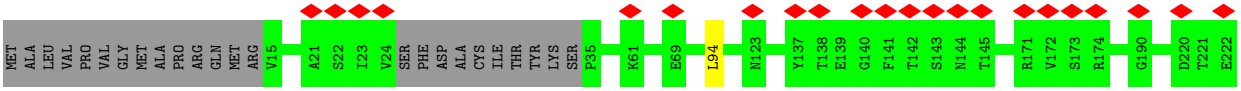


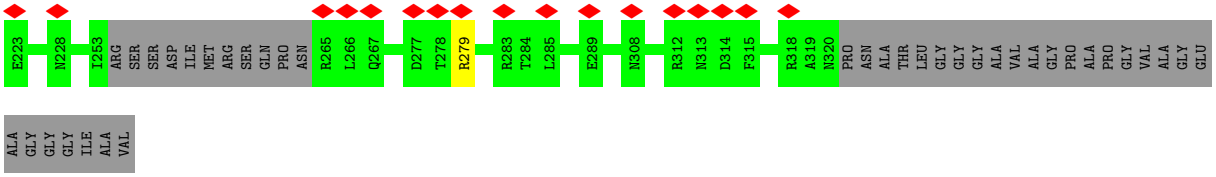




• Molecule 1: Major capsid protein

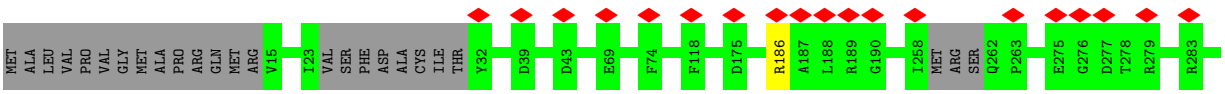
Chain X:

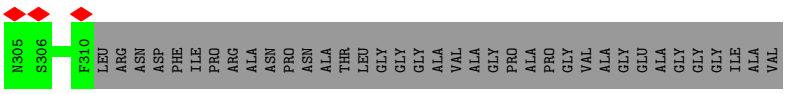




• Molecule 1: Major capsid protein

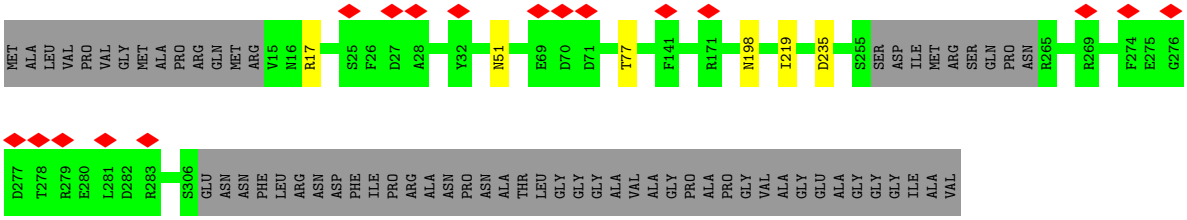
Chain Y:





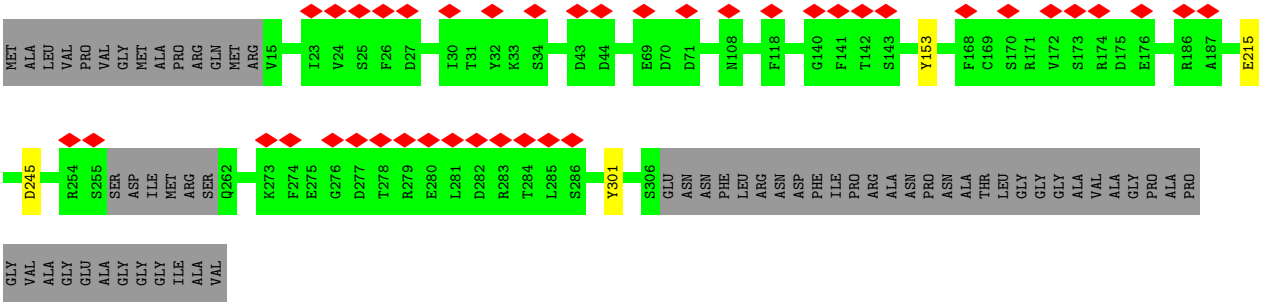
• Molecule 1: Major capsid protein

Chain Z:



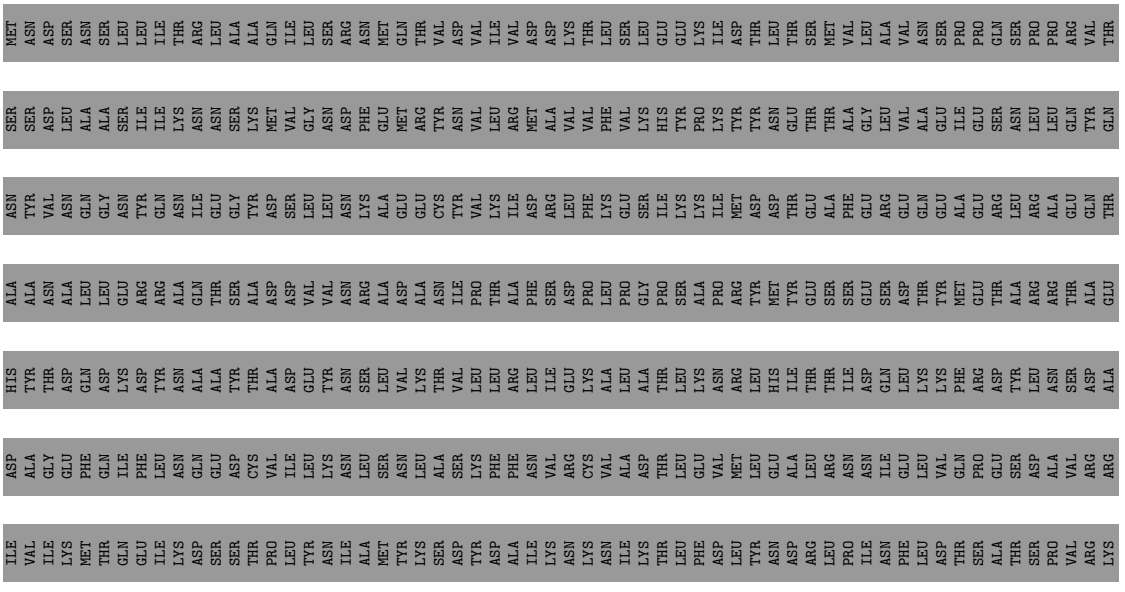
• Molecule 1: Major capsid protein

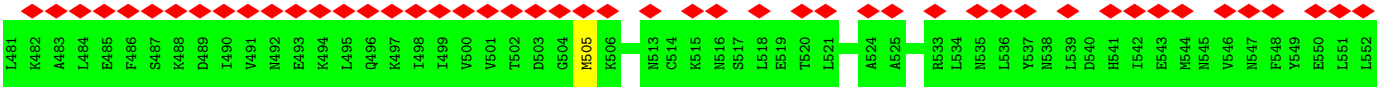
Chain a:

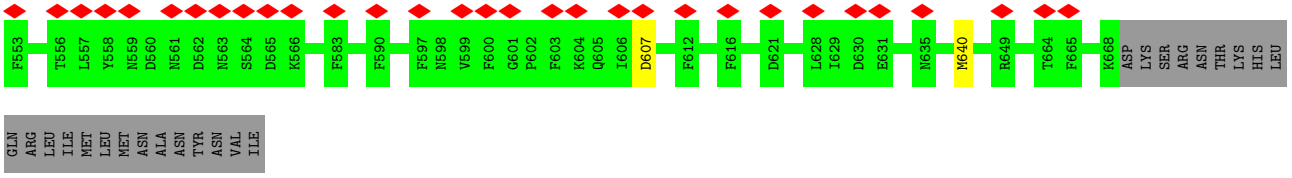


• Molecule 2: Capsid-associated protein VP80

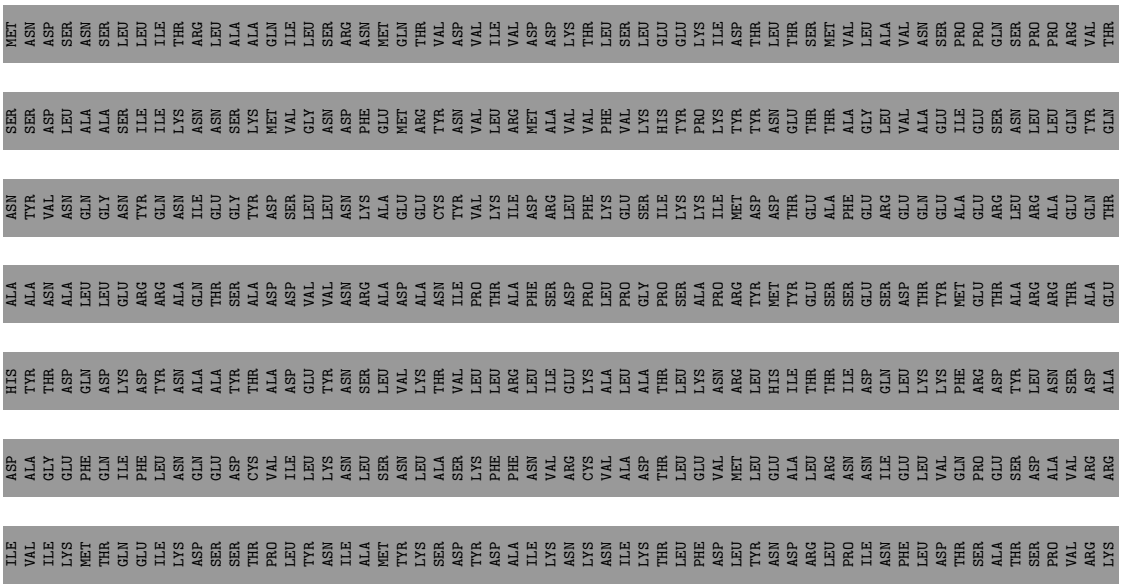
Chain G:



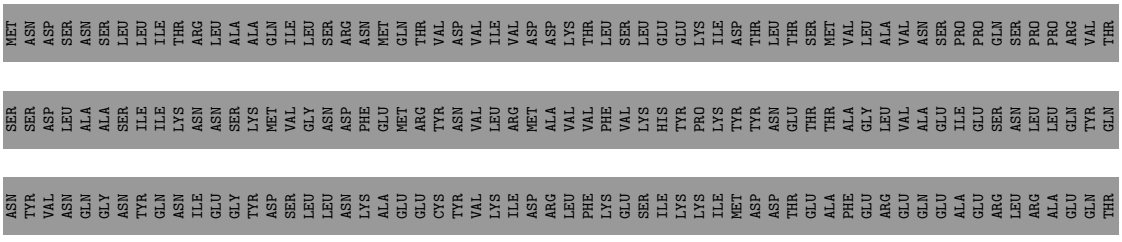


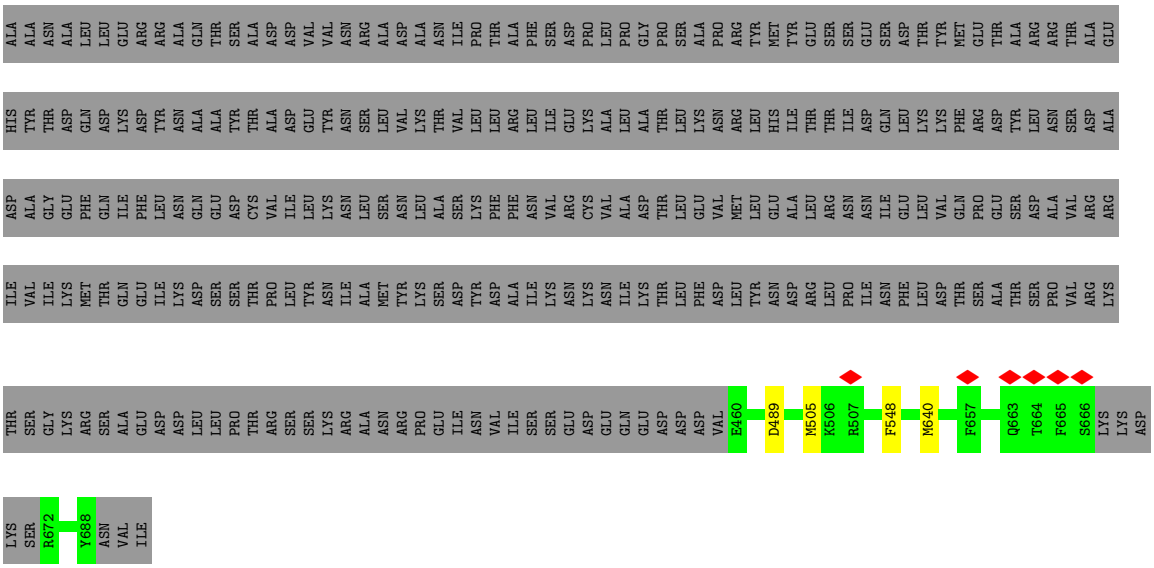


• Molecule 2: Capsid-associated protein VP80



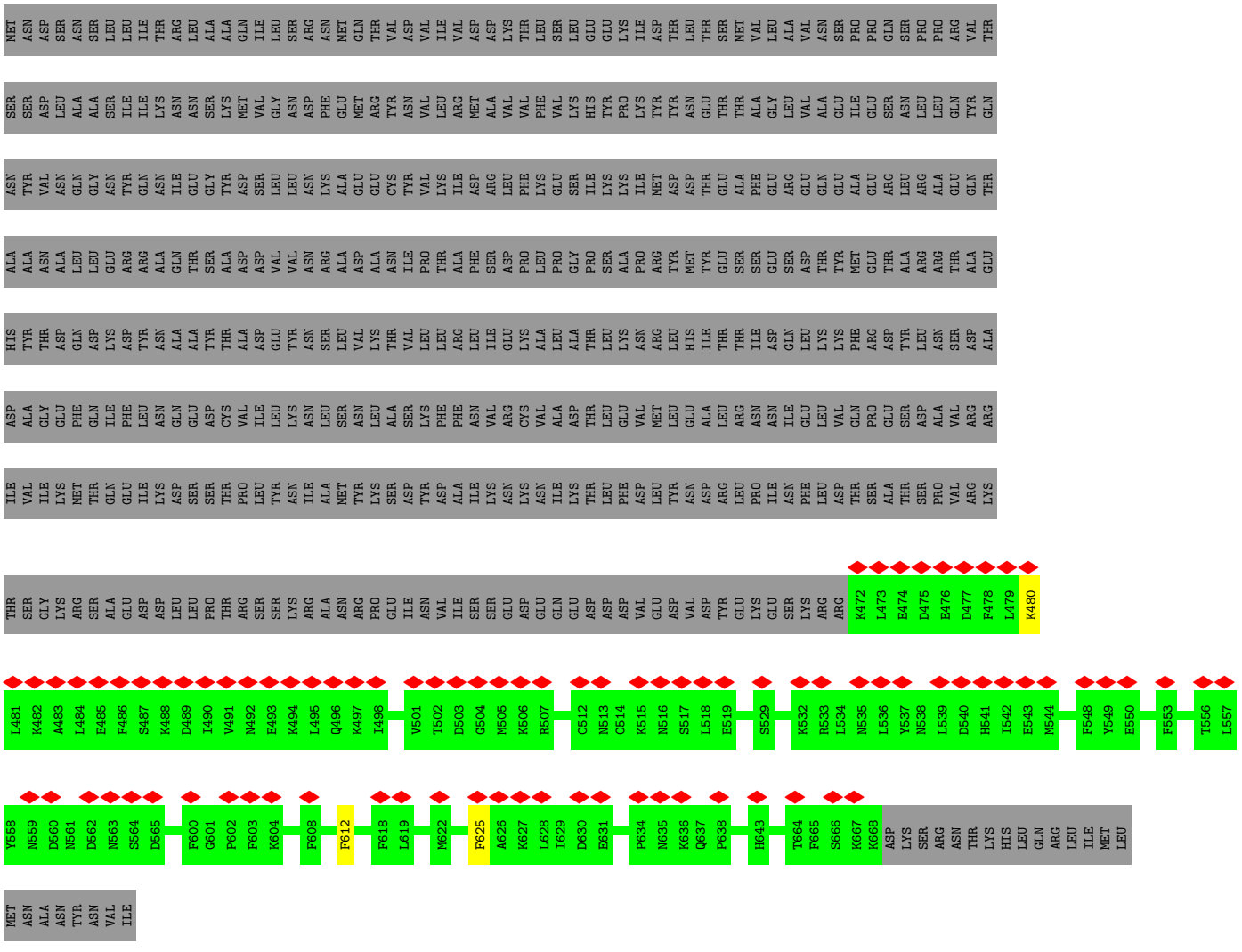
• Molecule 2: Capsid-associated protein VP80





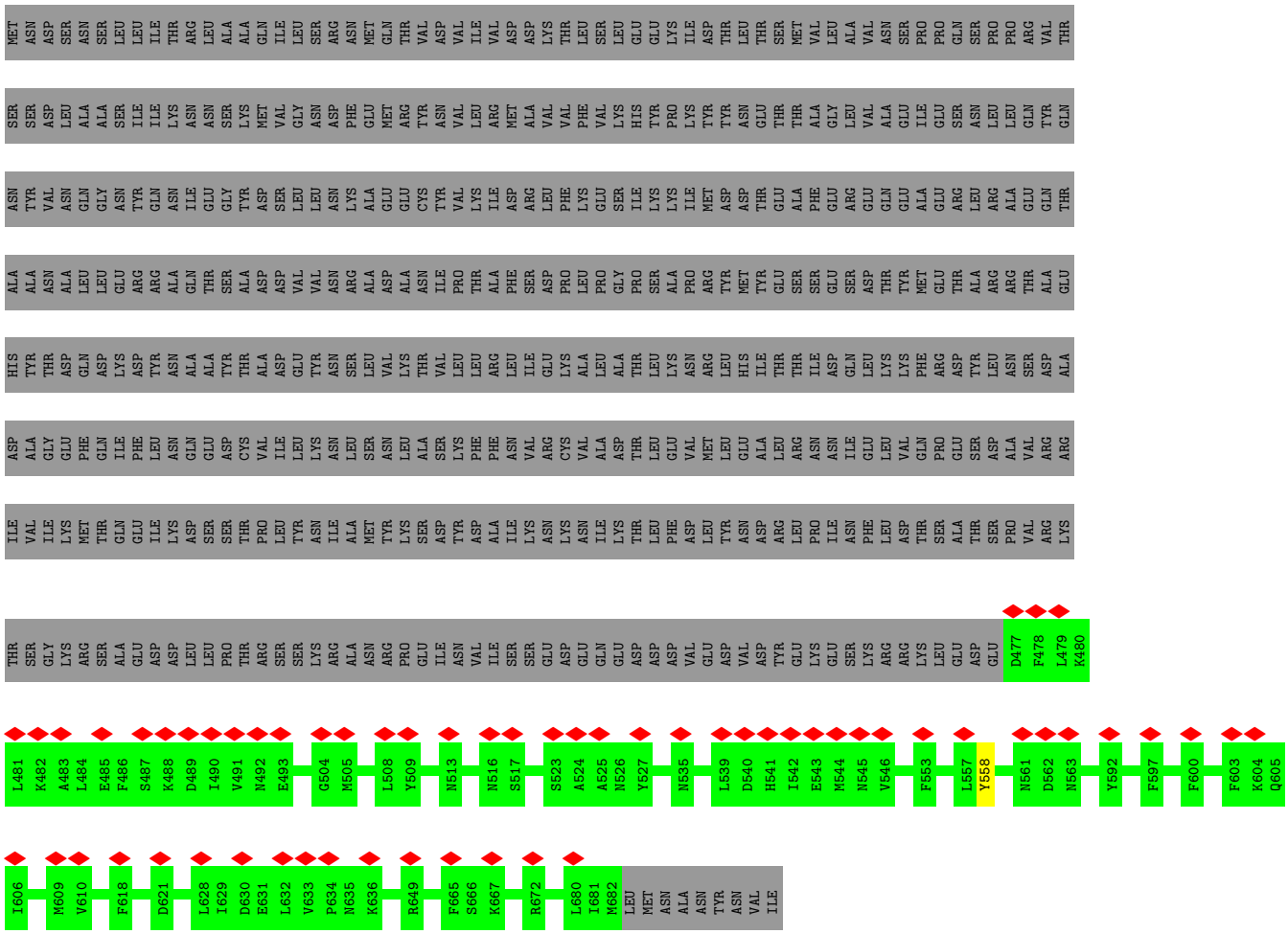
• Molecule 2: Capsid-associated protein VP80

Chain b:



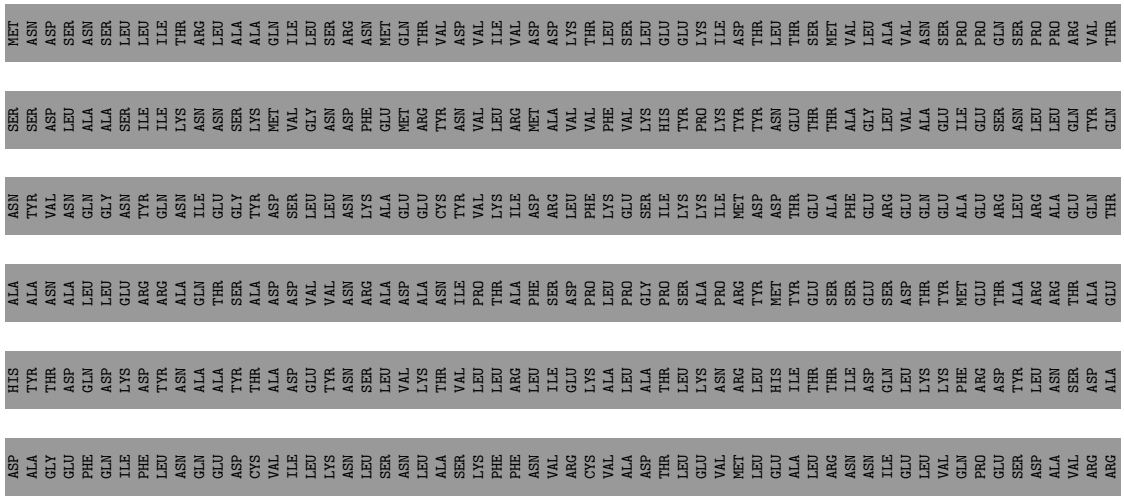
• Molecule 2: Capsid-associated protein VP80

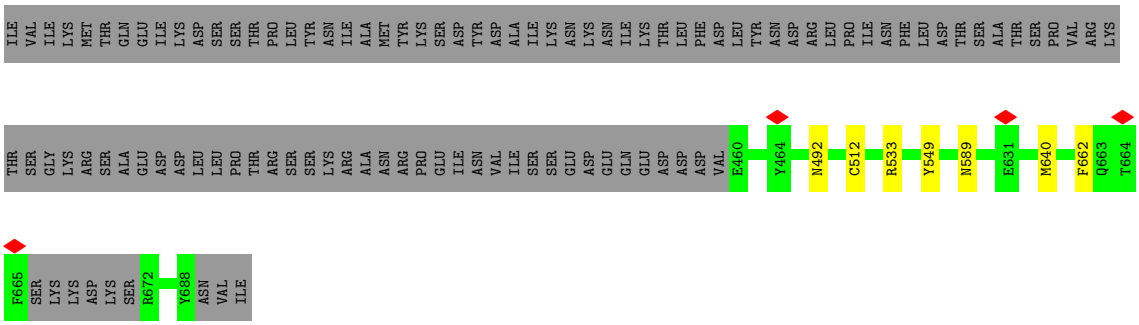
Chain c:



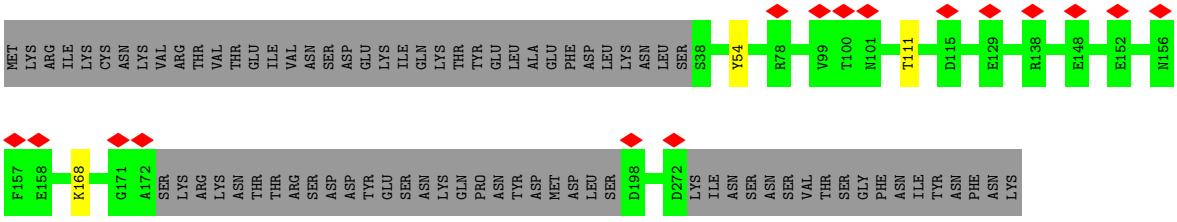
• Molecule 2: Capsid-associated protein VP80

Chain d:

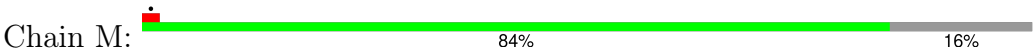


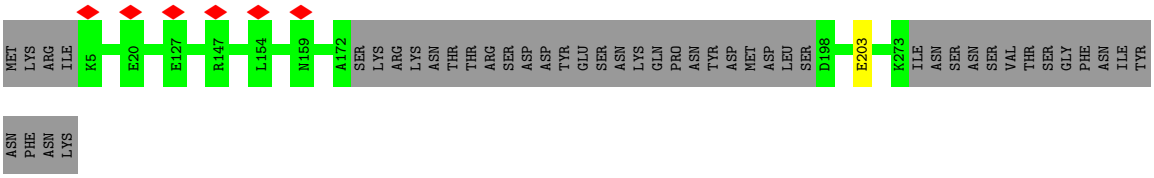


• Molecule 3: Occlusion-derived virus envelope protein E27

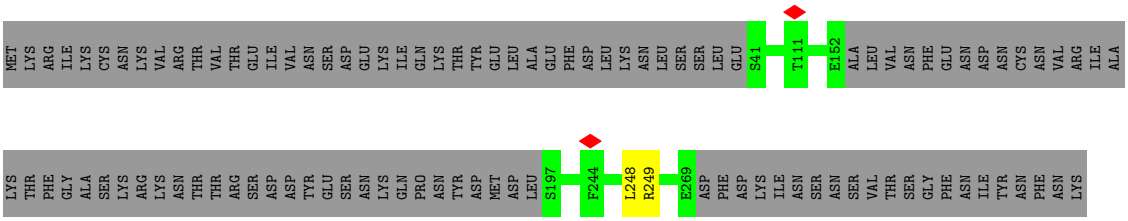


• Molecule 3: Occlusion-derived virus envelope protein E27

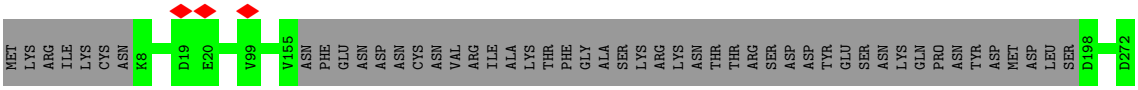




• Molecule 3: Occlusion-derived virus envelope protein E27

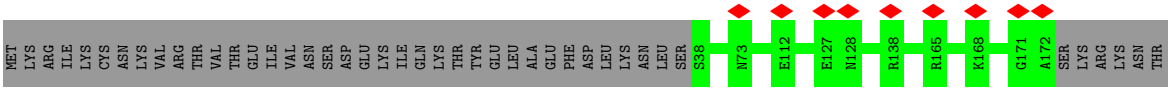


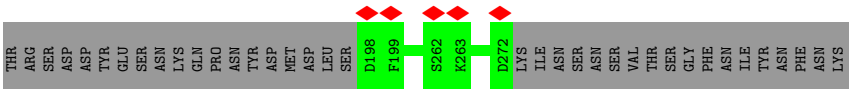
• Molecule 3: Occlusion-derived virus envelope protein E27



• Molecule 3: Occlusion-derived virus envelope protein E27

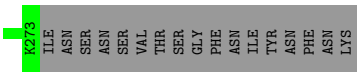
Chain e:





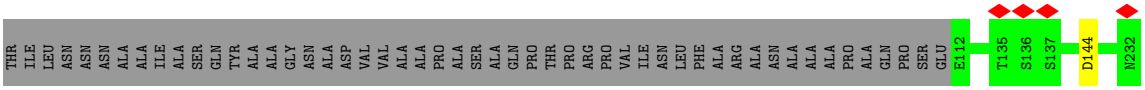
• Molecule 3: Occlusion-derived virus envelope protein E27

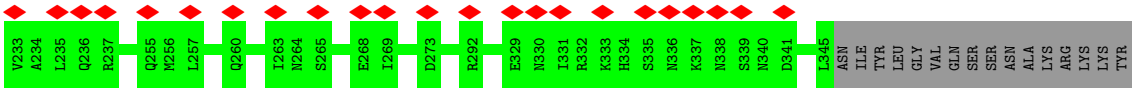
Chain h:



• Molecule 4: Protein C42

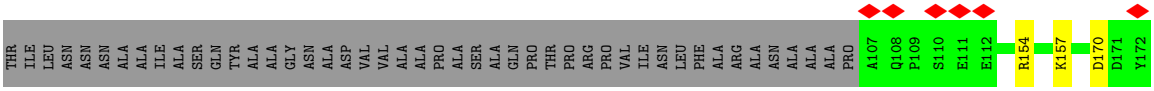
Chain K:

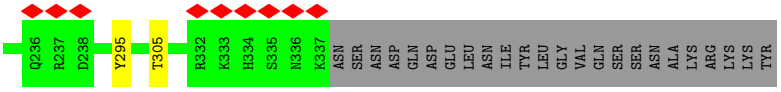




• Molecule 4: Protein C42

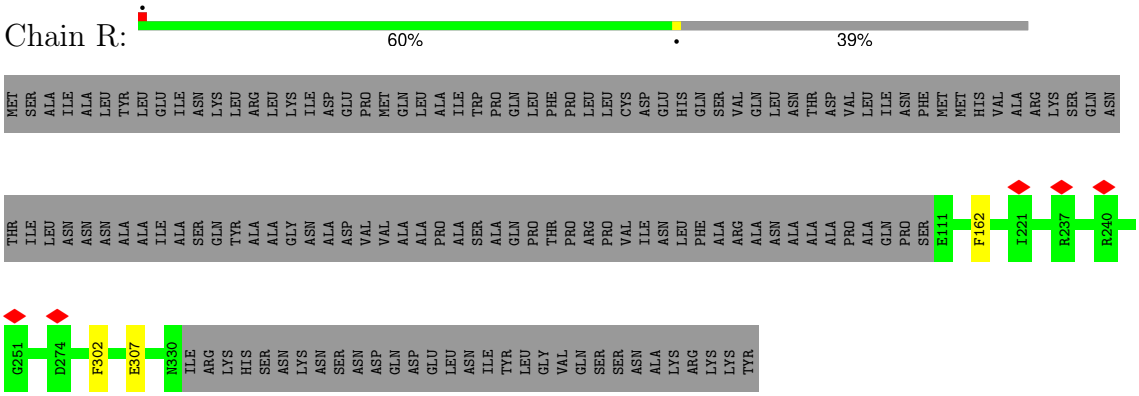
Chain L:





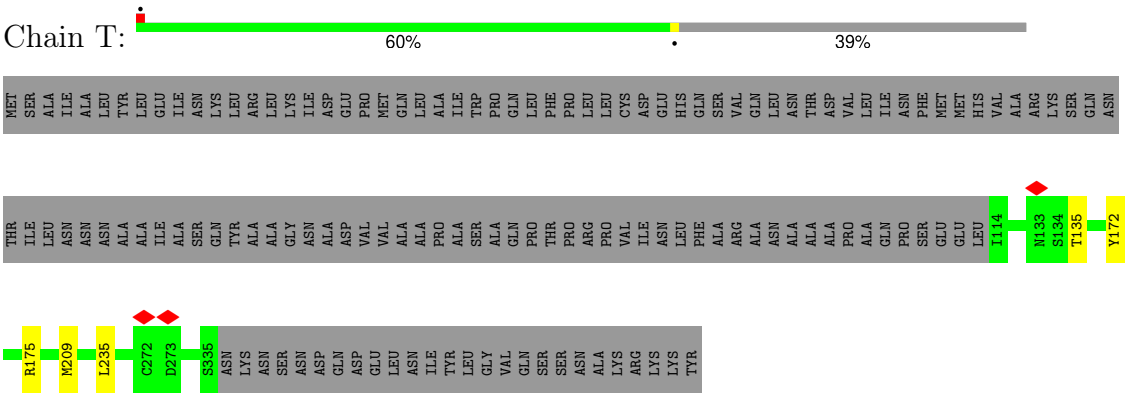
• Molecule 4: Protein C42

Chain R:



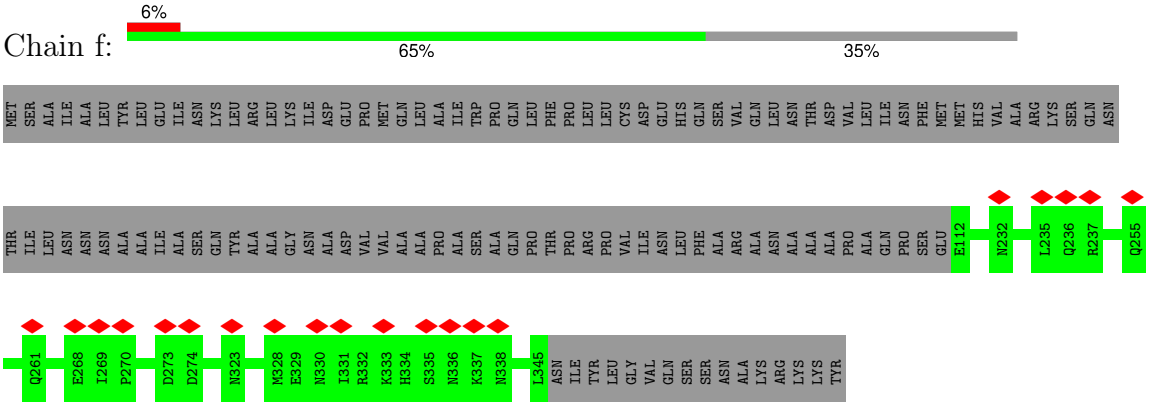
• Molecule 4: Protein C42

Chain T:



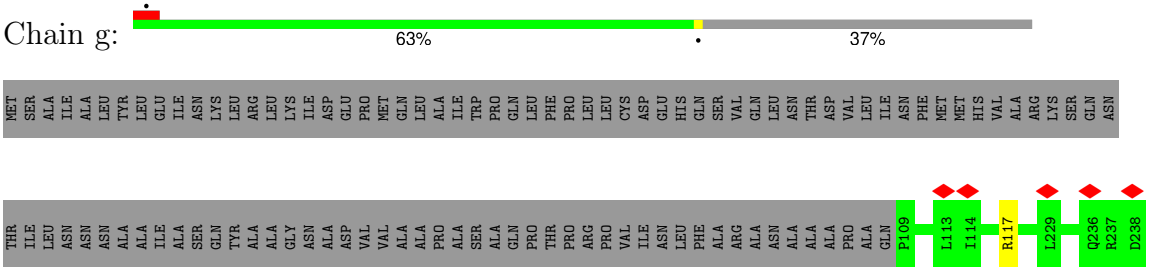
• Molecule 4: Protein C42

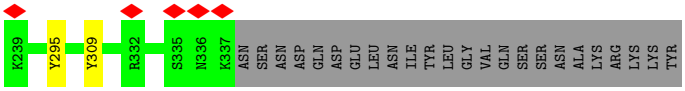
Chain f:



• Molecule 4: Protein C42

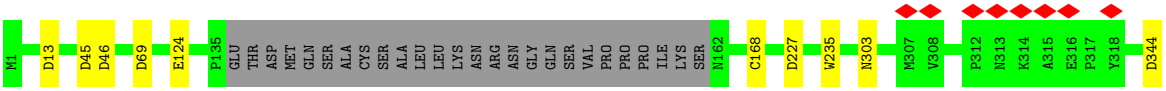
Chain g:





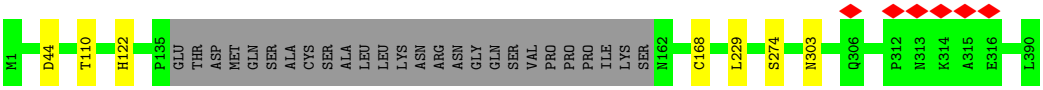
• Molecule 5: Protein AC109

Chain N:



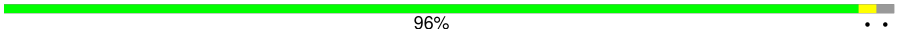
• Molecule 5: Protein AC109

Chain i:



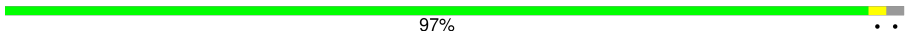
• Molecule 6: Protein AC142

Chain O:



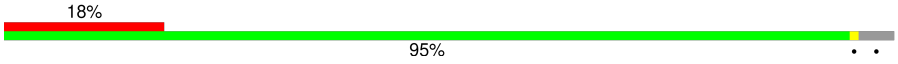
• Molecule 6: Protein AC142

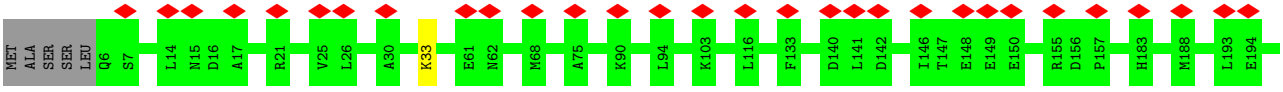
Chain j:

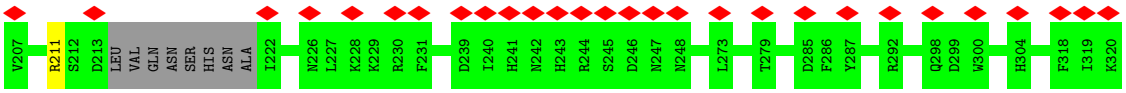


• Molecule 7: 38K (AC98) protein in P143-LEF5 intergenic region

Chain P:

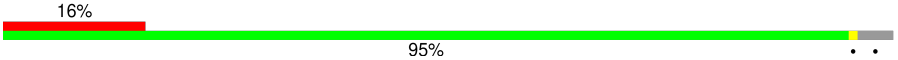


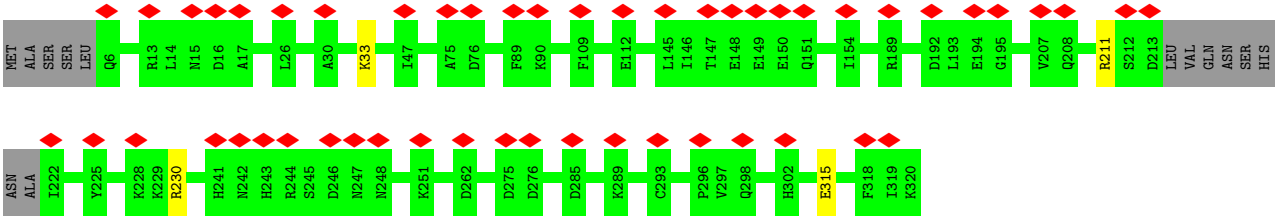




• Molecule 7: 38K (AC98) protein in P143-LEF5 intergenic region

Chain k:




MET ALA SER SER LEU Q6 R13 L14 N15 D16 A17 L26 A30 K33 I47 A75 D76 F89 K90 F109 E112 L145 I146 T147 E148 E149 E150 Q151 I154 R189 D192 L193 E194 G195 V207 Q208 R211 S212 D213 LEU VAL GLN ASN SER HIS
ASN ALA I222 Y225 K228 K229 R230 H241 N242 H243 R244 S245 D246 N247 N248 K251 D262 D275 D276 D285 K289 C293 P296 V297 Q298 H302 E315 F318 I319 K320

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53750	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.584	Depositor
Minimum map value	-0.880	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.298	Depositor
Map size (Å)	541.44, 541.44, 541.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.41, 1.41, 1.41	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0/2258	0.51	0/3058
1	B	0.25	0/2298	0.53	0/3111
1	C	0.25	0/2358	0.52	0/3193
1	D	0.25	0/2351	0.53	0/3184
1	E	0.27	0/2332	0.53	0/3159
1	F	0.26	0/2351	0.54	0/3186
1	V	0.25	0/2258	0.52	0/3058
1	W	0.25	0/2298	0.51	0/3111
1	X	0.26	0/2358	0.53	0/3193
1	Y	0.25	0/2356	0.52	0/3190
1	Z	0.27	0/2329	0.53	0/3155
1	a	0.26	0/2354	0.53	0/3190
2	G	0.26	0/1650	0.45	0/2221
2	H	0.25	0/1788	0.46	0/2404
2	I	0.26	0/1914	0.49	0/2572
2	b	0.26	0/1676	0.45	0/2255
2	c	0.25	0/1754	0.47	0/2358
2	d	0.26	0/1908	0.46	0/2564
3	J	0.26	0/1732	0.48	0/2344
3	M	0.27	0/2012	0.50	0/2719
3	Q	0.28	0/1532	0.49	0/2073
3	S	0.26	0/1845	0.48	0/2496
3	e	0.26	0/1732	0.47	0/2344
3	h	0.27	0/2003	0.51	0/2708
4	K	0.27	0/1968	0.53	0/2657
4	L	0.27	0/1941	0.54	0/2621
4	R	0.25	0/1851	0.52	0/2501
4	T	0.27	0/1870	0.51	0/2525
4	f	0.27	0/1968	0.53	0/2657
4	g	0.27	0/1927	0.52	0/2601
5	N	0.27	0/3040	0.48	0/4132
5	i	0.27	0/3040	0.50	0/4132

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
6	O	0.28	0/3956	0.50	0/5357
6	j	0.28	0/3956	0.50	0/5357
7	P	0.26	0/2662	0.48	0/3603
7	k	0.26	0/2662	0.47	0/3603
All	All	0.26	0/80288	0.50	0/108592

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	E	0	1
1	X	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	171	ARG	Sidechain
1	X	279	ARG	Sidechain

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	268/347 (77%)	243 (91%)	25 (9%)	0	100	100
1	B	273/347 (79%)	253 (93%)	20 (7%)	0	100	100
1	C	279/347 (80%)	243 (87%)	36 (13%)	0	100	100
1	D	279/347 (80%)	256 (92%)	23 (8%)	0	100	100
1	E	279/347 (80%)	257 (92%)	21 (8%)	1 (0%)	30	68
1	F	281/347 (81%)	253 (90%)	28 (10%)	0	100	100
1	V	268/347 (77%)	252 (94%)	16 (6%)	0	100	100
1	W	273/347 (79%)	260 (95%)	13 (5%)	0	100	100
1	X	279/347 (80%)	253 (91%)	26 (9%)	0	100	100
1	Y	279/347 (80%)	254 (91%)	25 (9%)	0	100	100
1	Z	279/347 (80%)	249 (89%)	30 (11%)	0	100	100
1	a	282/347 (81%)	257 (91%)	25 (9%)	0	100	100
2	G	192/691 (28%)	164 (85%)	28 (15%)	0	100	100
2	H	208/691 (30%)	185 (89%)	23 (11%)	0	100	100
2	I	220/691 (32%)	199 (90%)	21 (10%)	0	100	100
2	b	195/691 (28%)	171 (88%)	24 (12%)	0	100	100
2	c	204/691 (30%)	166 (81%)	38 (19%)	0	100	100
2	d	219/691 (32%)	206 (94%)	13 (6%)	0	100	100
3	J	206/290 (71%)	192 (93%)	14 (7%)	0	100	100
3	M	240/290 (83%)	213 (89%)	27 (11%)	0	100	100
3	Q	181/290 (62%)	165 (91%)	16 (9%)	0	100	100
3	S	219/290 (76%)	204 (93%)	15 (7%)	0	100	100
3	e	206/290 (71%)	193 (94%)	13 (6%)	0	100	100
3	h	239/290 (82%)	206 (86%)	33 (14%)	0	100	100
4	K	232/361 (64%)	207 (89%)	25 (11%)	0	100	100
4	L	229/361 (63%)	198 (86%)	31 (14%)	0	100	100
4	R	218/361 (60%)	192 (88%)	26 (12%)	0	100	100
4	T	220/361 (61%)	190 (86%)	30 (14%)	0	100	100
4	f	232/361 (64%)	210 (90%)	22 (10%)	0	100	100
4	g	227/361 (63%)	199 (88%)	28 (12%)	0	100	100
5	N	360/390 (92%)	329 (91%)	31 (9%)	0	100	100
5	i	360/390 (92%)	319 (89%)	41 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	O	467/477 (98%)	425 (91%)	42 (9%)	0	100	100
6	j	467/477 (98%)	435 (93%)	32 (7%)	0	100	100
7	P	303/320 (95%)	274 (90%)	29 (10%)	0	100	100
7	k	303/320 (95%)	273 (90%)	30 (10%)	0	100	100
All	All	9466/14590 (65%)	8545 (90%)	920 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	175	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/299 (83%)	236 (96%)	11 (4%)	23	46
1	B	252/299 (84%)	246 (98%)	6 (2%)	44	63
1	C	257/299 (86%)	254 (99%)	3 (1%)	67	79
1	D	258/299 (86%)	252 (98%)	6 (2%)	45	64
1	E	255/299 (85%)	251 (98%)	4 (2%)	58	74
1	F	257/299 (86%)	255 (99%)	2 (1%)	79	85
1	V	247/299 (83%)	246 (100%)	1 (0%)	89	91
1	W	252/299 (84%)	252 (100%)	0	100	100
1	X	257/299 (86%)	256 (100%)	1 (0%)	89	91
1	Y	258/299 (86%)	257 (100%)	1 (0%)	89	91
1	Z	254/299 (85%)	248 (98%)	6 (2%)	44	63
1	a	257/299 (86%)	253 (98%)	4 (2%)	58	74
2	G	184/634 (29%)	181 (98%)	3 (2%)	58	74
2	H	200/634 (32%)	198 (99%)	2 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	I	213/634 (34%)	209 (98%)	4 (2%)	52 70
2	b	187/634 (30%)	184 (98%)	3 (2%)	58 74
2	c	196/634 (31%)	195 (100%)	1 (0%)	86 90
2	d	212/634 (33%)	205 (97%)	7 (3%)	33 54
3	J	195/273 (71%)	192 (98%)	3 (2%)	60 75
3	M	228/273 (84%)	227 (100%)	1 (0%)	89 91
3	Q	174/273 (64%)	172 (99%)	2 (1%)	70 80
3	S	210/273 (77%)	210 (100%)	0	100 100
3	e	195/273 (71%)	195 (100%)	0	100 100
3	h	227/273 (83%)	221 (97%)	6 (3%)	41 60
4	K	222/326 (68%)	221 (100%)	1 (0%)	86 90
4	L	218/326 (67%)	213 (98%)	5 (2%)	45 64
4	R	208/326 (64%)	205 (99%)	3 (1%)	62 76
4	T	210/326 (64%)	205 (98%)	5 (2%)	44 63
4	f	222/326 (68%)	222 (100%)	0	100 100
4	g	217/326 (67%)	214 (99%)	3 (1%)	62 76
5	N	343/366 (94%)	330 (96%)	13 (4%)	28 49
5	i	343/366 (94%)	336 (98%)	7 (2%)	50 69
6	O	435/440 (99%)	426 (98%)	9 (2%)	48 67
6	j	435/440 (99%)	427 (98%)	8 (2%)	54 71
7	P	293/304 (96%)	291 (99%)	2 (1%)	81 87
7	k	293/304 (96%)	289 (99%)	4 (1%)	62 76
All	All	8911/13206 (68%)	8774 (98%)	137 (2%)	60 75

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	17	ARG
1	A	39	ASP
1	A	42	HIS
1	A	72	ASN
1	A	88	ARG
1	A	153	TYR

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Mol	Chain	Res	Type
1	A	171	ARG
1	A	174	ARG
1	A	177	LEU
1	A	194	ASP
1	B	37	SER
1	B	81	HIS
1	B	163	THR
1	B	197	PHE
1	B	273	LYS
1	B	274	PHE
1	C	103	ASP
1	C	206	ASN
1	C	310	PHE
1	D	88	ARG
1	D	169	CYS
1	D	171	ARG
1	D	176	GLU
1	D	218	GLN
1	D	257	ASP
1	E	166	ASN
1	E	174	ARG
1	E	221	THR
1	E	301	TYR
1	F	80	ARG
1	F	145	THR
2	G	505	MET
2	G	607	ASP
2	G	640	MET
2	H	558	TYR
2	H	559	ASN
2	I	489	ASP
2	I	505	MET
2	I	548	PHE
2	I	640	MET
3	J	54	TYR
3	J	111	THR
3	J	168	LYS
4	K	144	ASP
4	L	154	ARG
4	L	157	LYS
4	L	170	ASP
4	L	295	TYR

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Mol	Chain	Res	Type
4	L	305	THR
3	M	203	GLU
5	N	13	ASP
5	N	45	ASP
5	N	46	ASP
5	N	69	ASP
5	N	124	GLU
5	N	168	CYS
5	N	227	ASP
5	N	235	TRP
5	N	303	ASN
5	N	344	ASP
5	N	345	PHE
5	N	356	TYR
5	N	360	THR
6	O	62	TYR
6	O	92	ASP
6	O	94	THR
6	O	101	PHE
6	O	167	ASP
6	O	174	CYS
6	O	202	ASN
6	O	318	MET
6	O	458	ASP
7	P	33	LYS
7	P	211	ARG
3	Q	248	LEU
3	Q	249	ARG
4	R	162	PHE
4	R	302	PHE
4	R	307	GLU
4	T	135	THR
4	T	172	TYR
4	T	175	ARG
4	T	209	MET
4	T	235	LEU
1	V	169	CYS
1	X	94	LEU
1	Y	186	ARG
1	Z	17	ARG
1	Z	51	ASN
1	Z	77	THR

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Mol	Chain	Res	Type
1	Z	198	ASN
1	Z	219	ILE
1	Z	235	ASP
1	a	153	TYR
1	a	215	GLU
1	a	245	ASP
1	a	301	TYR
2	b	480	LYS
2	b	612	PHE
2	b	625	PHE
2	c	558	TYR
2	d	492	ASN
2	d	512	CYS
2	d	533	ARG
2	d	549	TYR
2	d	589	ASN
2	d	640	MET
2	d	662	PHE
4	g	117	ARG
4	g	295	TYR
4	g	309	TYR
3	h	28	LEU
3	h	42	TYR
3	h	87	THR
3	h	144	MET
3	h	165	ARG
3	h	258	ASN
5	i	44	ASP
5	i	110	THR
5	i	122	HIS
5	i	168	CYS
5	i	229	LEU
5	i	274	SER
5	i	303	ASN
6	j	74	SER
6	j	101	PHE
6	j	173	MET
6	j	260	LYS
6	j	281	GLN
6	j	303	ILE
6	j	435	ASN
6	j	458	ASP

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Mol	Chain	Res	Type
7	k	33	LYS
7	k	211	ARG
7	k	230	ARG
7	k	315	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	B	102	GLN
1	B	150	HIS
1	B	164	ASN
1	D	119	HIS
1	D	124	ASN
1	D	129	ASN
1	F	51	ASN
1	F	150	HIS
2	H	678	GLN
2	I	571	GLN
2	I	589	ASN
2	I	659	ASN
4	K	159	HIS
4	L	133	ASN
4	L	159	HIS
4	L	296	ASN
4	L	308	ASN
4	L	317	ASN
3	M	163	ASN
5	N	122	HIS
5	N	174	HIS
6	O	14	HIS
6	O	169	ASN
6	O	202	ASN
6	O	263	ASN
6	O	351	HIS
6	O	406	GLN
7	P	65	ASN
7	P	83	HIS
7	P	96	HIS
7	P	264	ASN
3	Q	218	HIS
4	R	129	HIS

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Mol	Chain	Res	Type
4	R	296	ASN
3	S	92	HIS
3	S	93	ASN
4	T	232	ASN
1	V	16	ASN
1	V	108	ASN
1	V	218	GLN
1	W	206	ASN
1	W	262	GLN
1	X	205	GLN
1	Y	264	ASN
1	Y	308	ASN
1	Z	72	ASN
1	Z	164	ASN
1	a	115	GLN
2	b	516	ASN
2	b	643	HIS
2	d	570	HIS
2	d	589	ASN
2	d	661	GLN
3	e	241	HIS
4	f	159	HIS
4	g	218	ASN
4	g	255	GLN
3	h	218	HIS
3	h	228	ASN
5	i	249	ASN
5	i	254	ASN
5	i	302	ASN
6	j	14	HIS
6	j	169	ASN
6	j	181	ASN
6	j	198	HIS
6	j	331	ASN
6	j	431	HIS

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)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

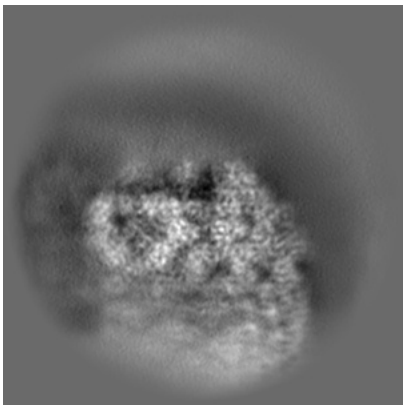
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43588. These allow visual inspection of the internal detail of the map and identification of artifacts.

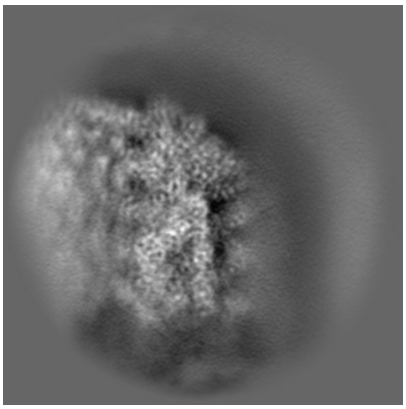
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

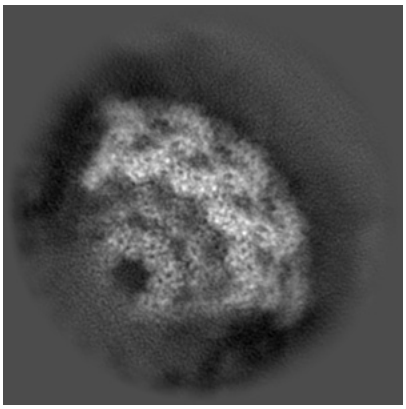
6.1.1 Primary map



X

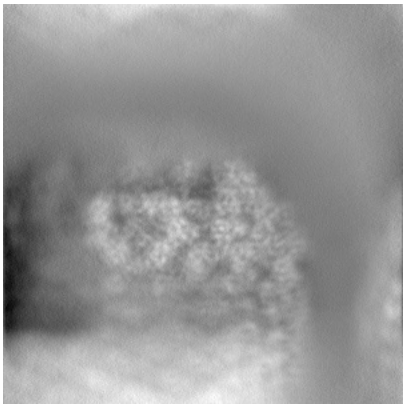


Y

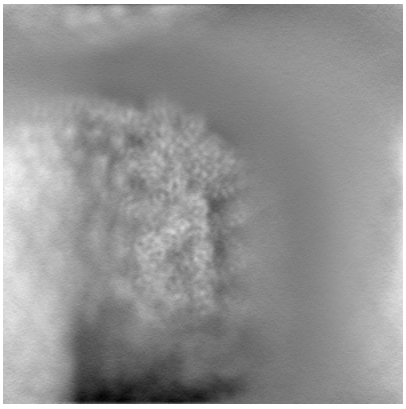


Z

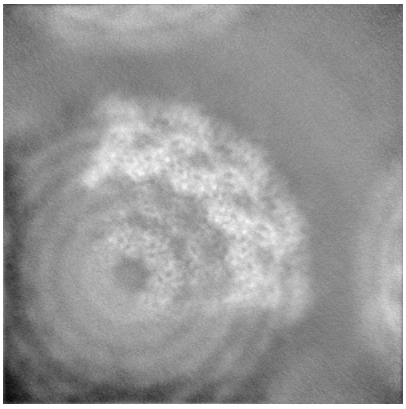
6.1.2 Raw map



X



Y

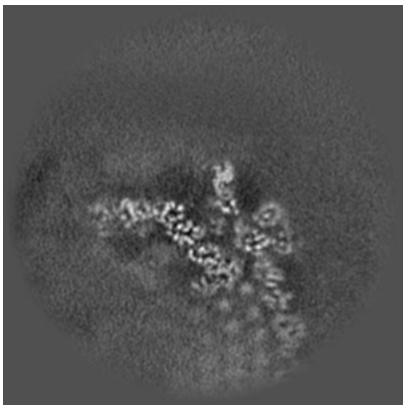


Z

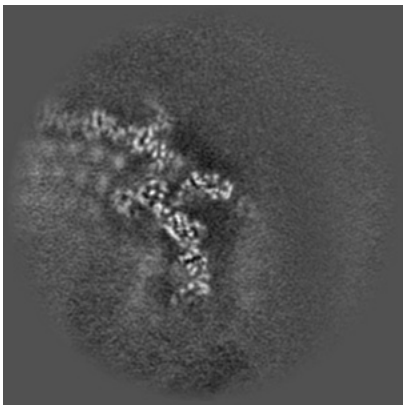
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

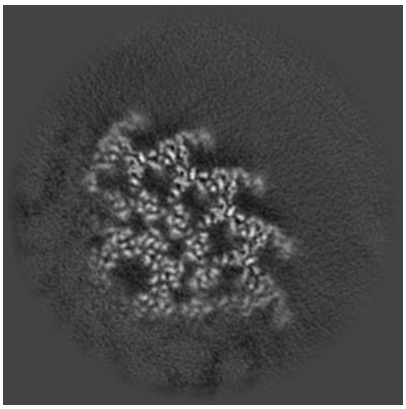
6.2.1 Primary map



X Index: 192

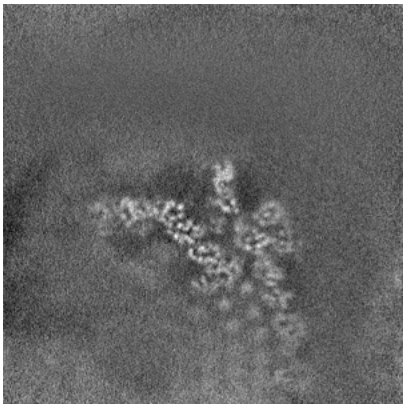


Y Index: 192

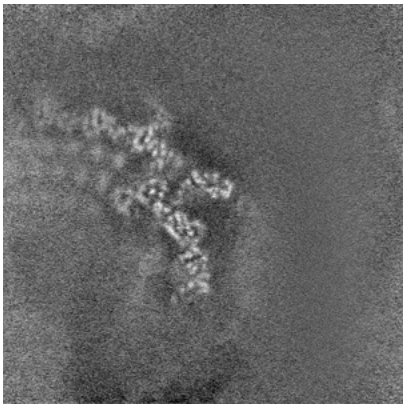


Z Index: 192

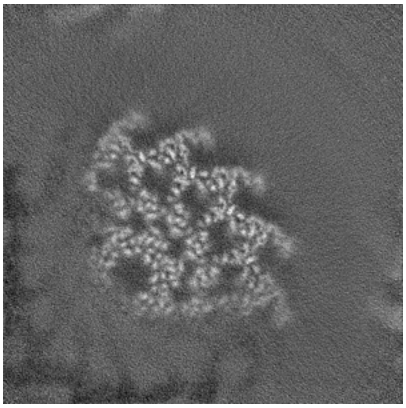
6.2.2 Raw map



X Index: 192



Y Index: 192

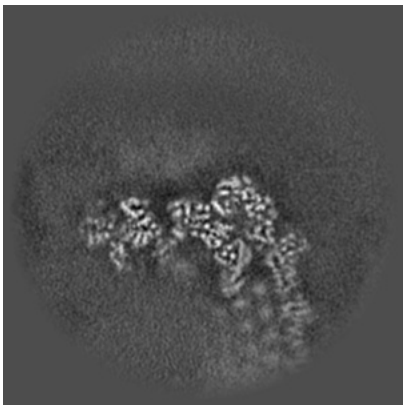


Z Index: 192

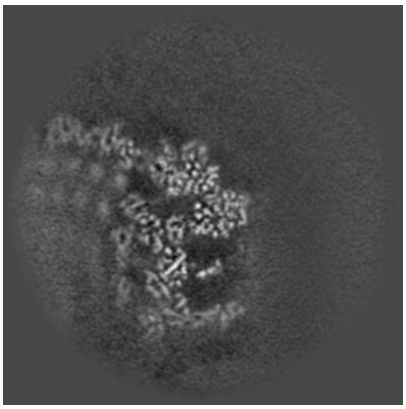
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

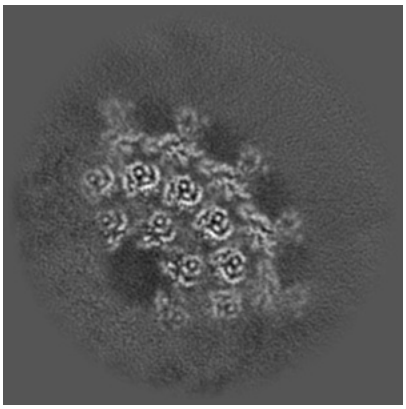
6.3.1 Primary map



X Index: 165

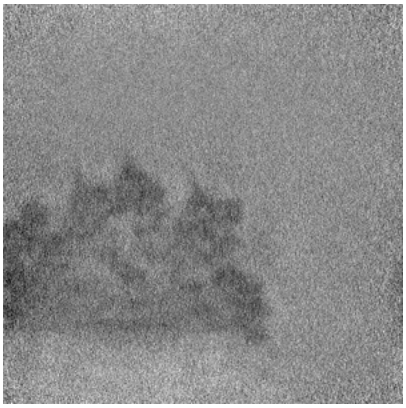


Y Index: 215

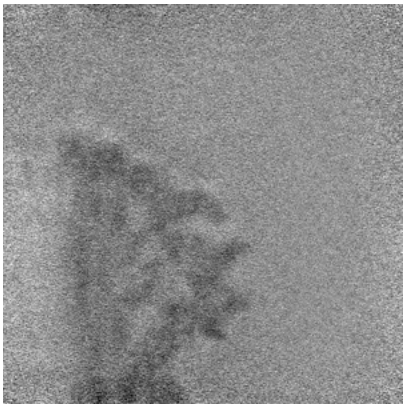


Z Index: 168

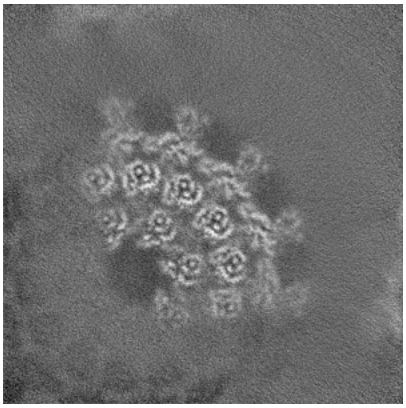
6.3.2 Raw map



X Index: 4



Y Index: 3

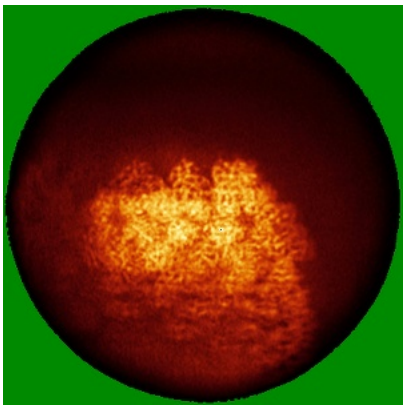


Z Index: 168

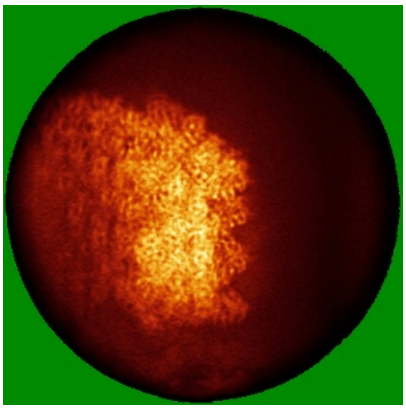
The images above show the largest variance slices of the map in three orthogonal directions.

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

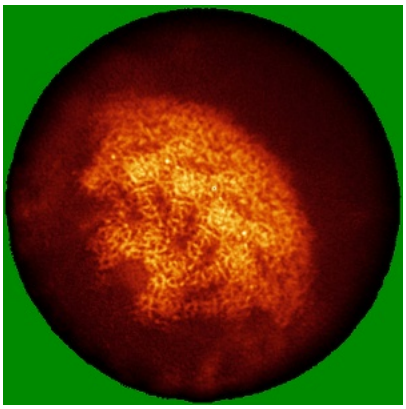
6.4.1 Primary map



X

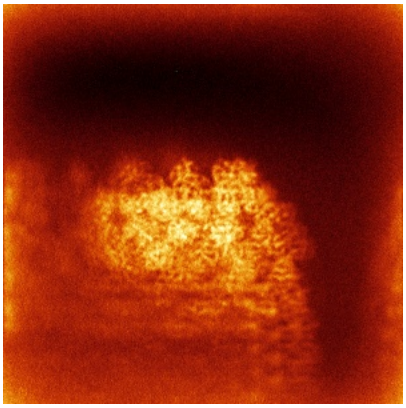


Y

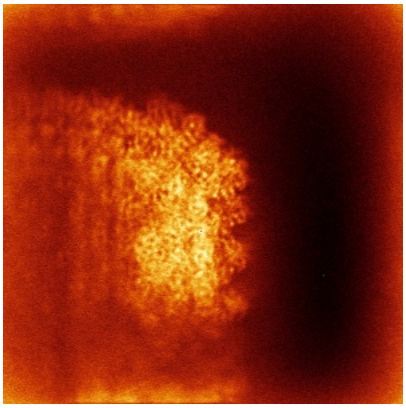


Z

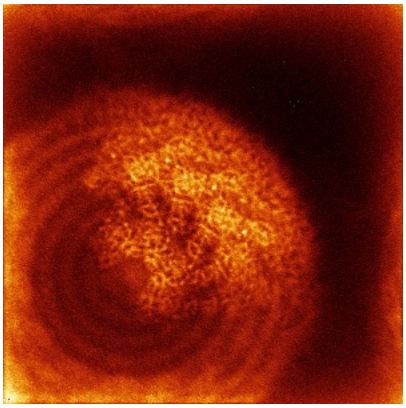
6.4.2 Raw map



X



Y

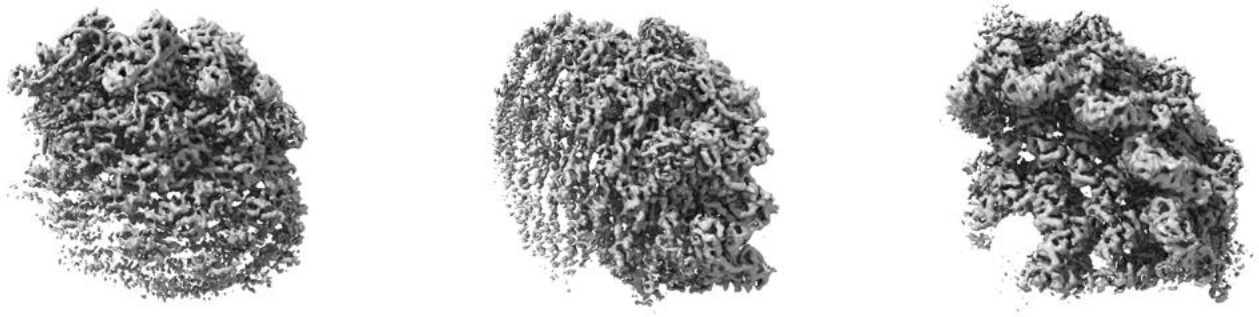


Z

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

6.5 Orthogonal surface views (i)

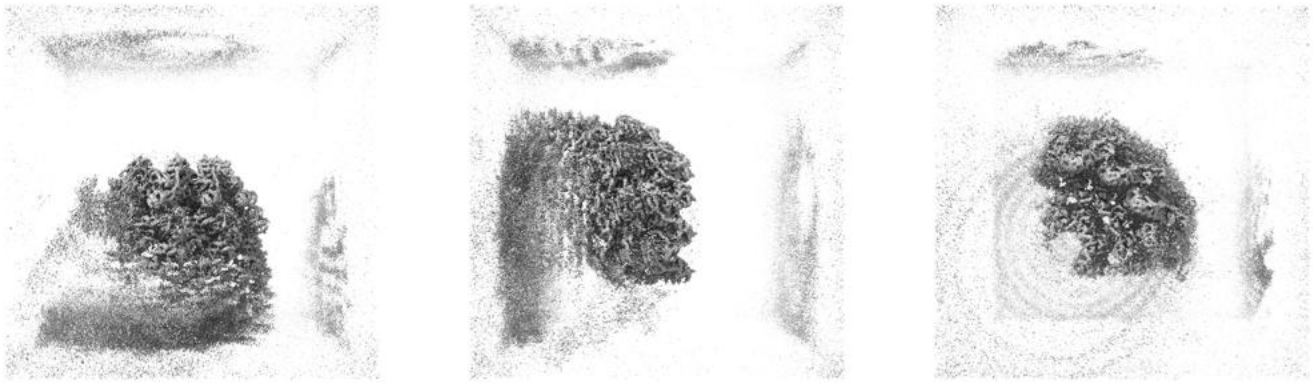
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.298. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

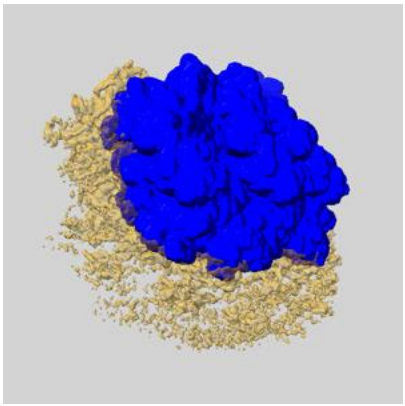
6.6 Mask visualisation (i)

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

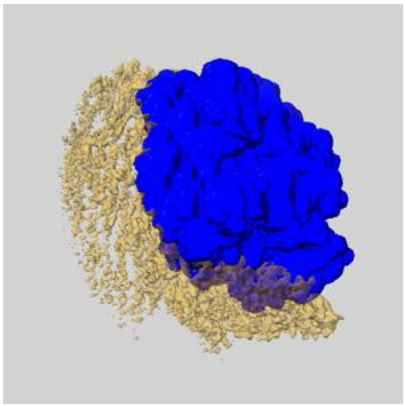
A mask typically either:

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

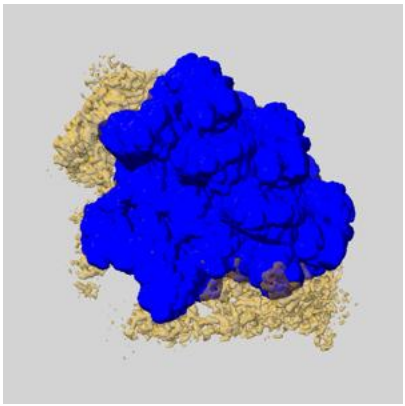
6.6.1 emd_43588_msk_1.map (i)



X



Y

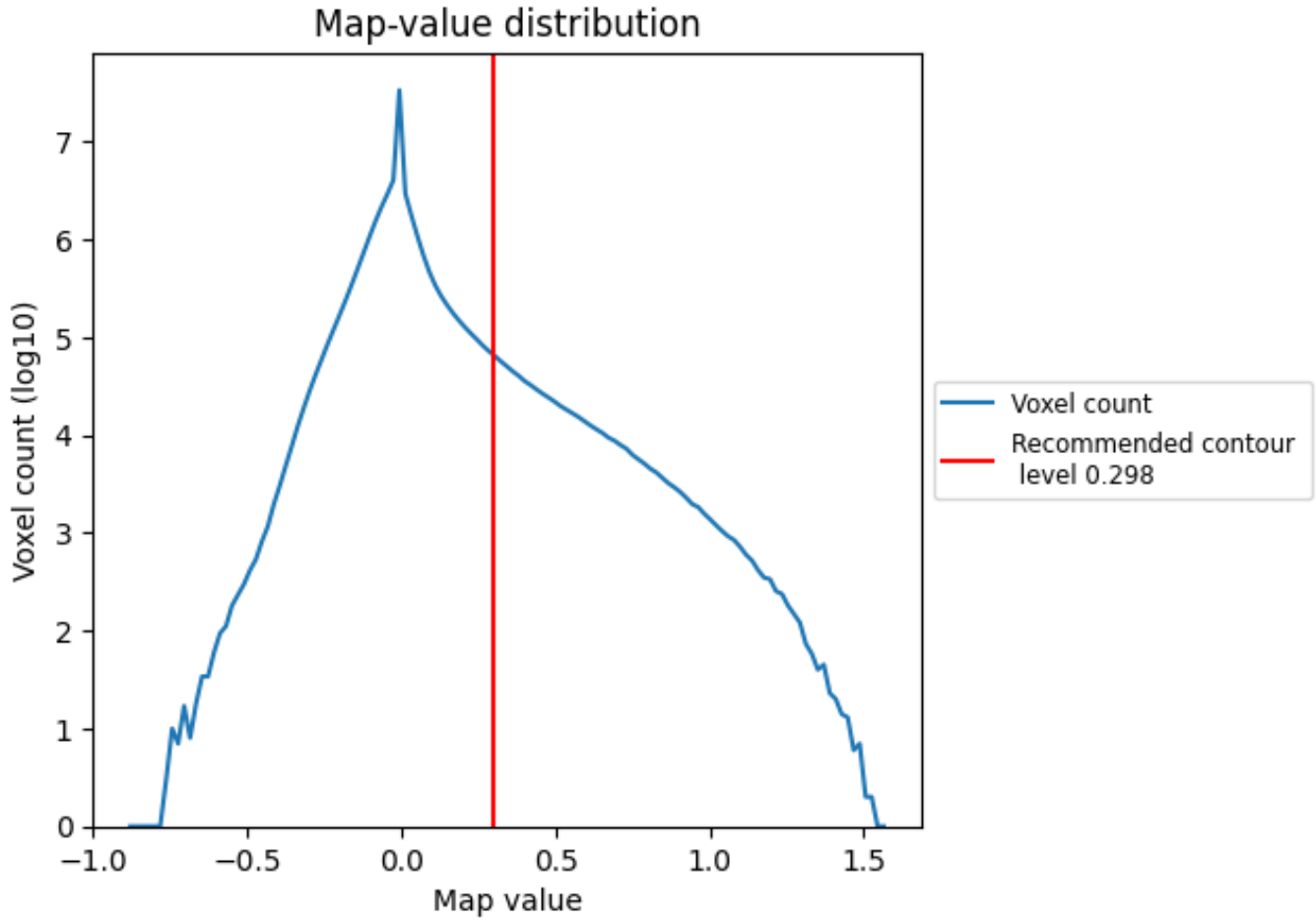


Z

7 Map analysis

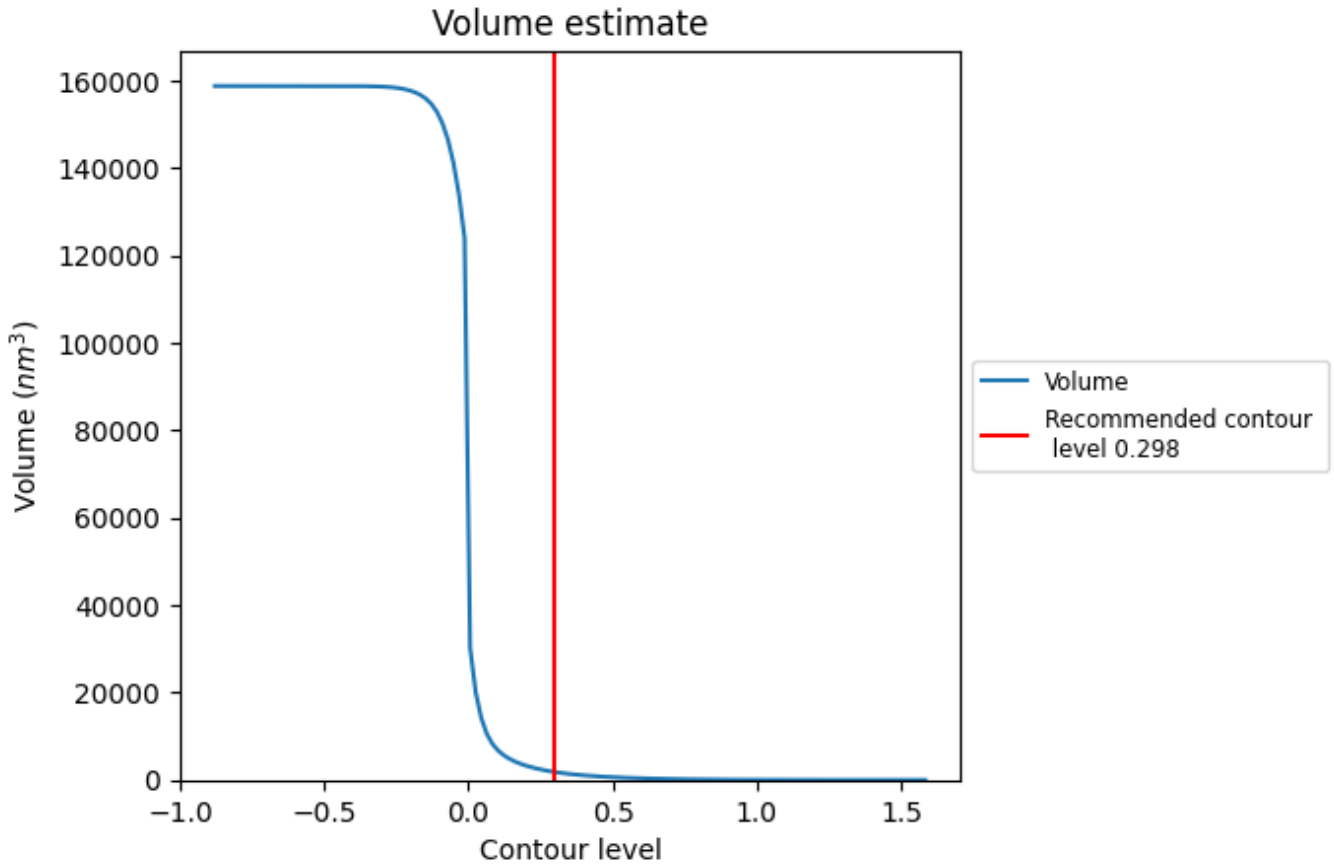
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

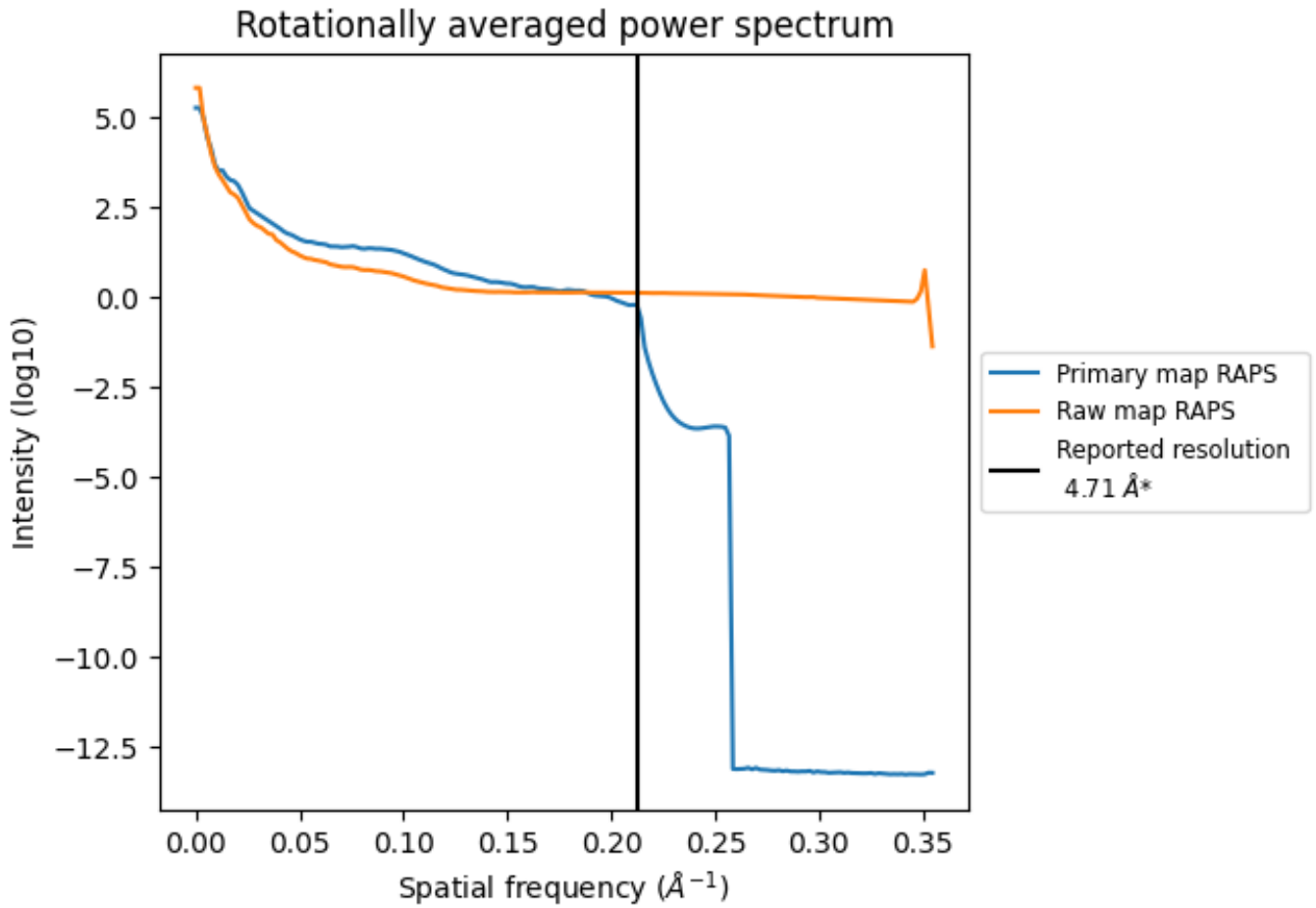
7.2 Volume estimate



The volume at the recommended contour level is 1824 nm^3; this corresponds to an approximate mass of 1648 kDa.

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

7.3 Rotationally averaged power spectrum (i)

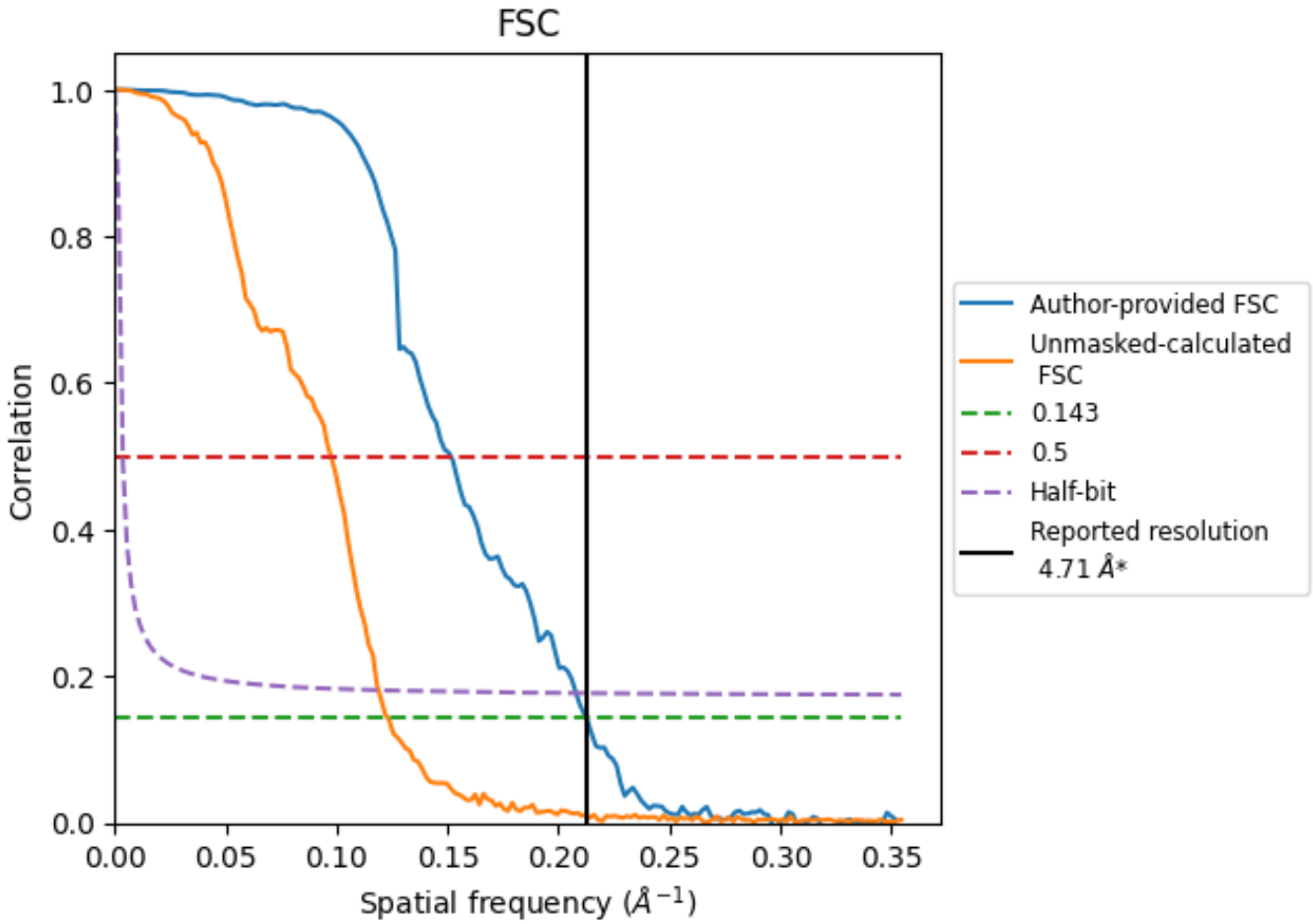


*Reported resolution corresponds to spatial frequency of 0.212 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.212 Å^{-1}

8.2 Resolution estimates (i)

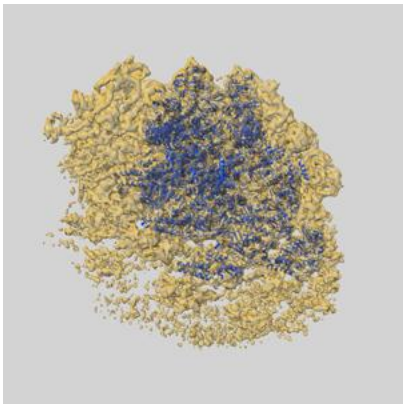
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.71	-	-
Author-provided FSC curve	4.71	6.61	4.81
Unmasked-calculated*	8.12	10.26	8.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.12 differs from the reported value 4.71 by more than 10 %

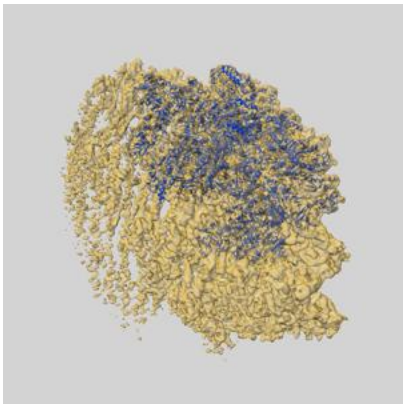
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43588 and PDB model 8VWI. Per-residue inclusion information can be found in section 3 on page 9.

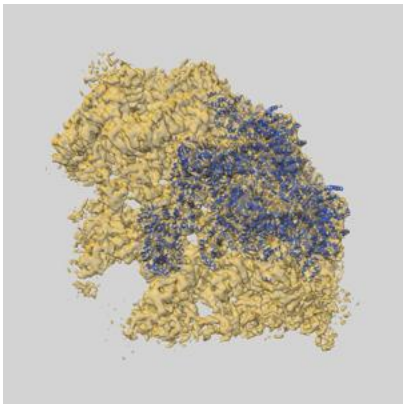
9.1 Map-model overlay



X



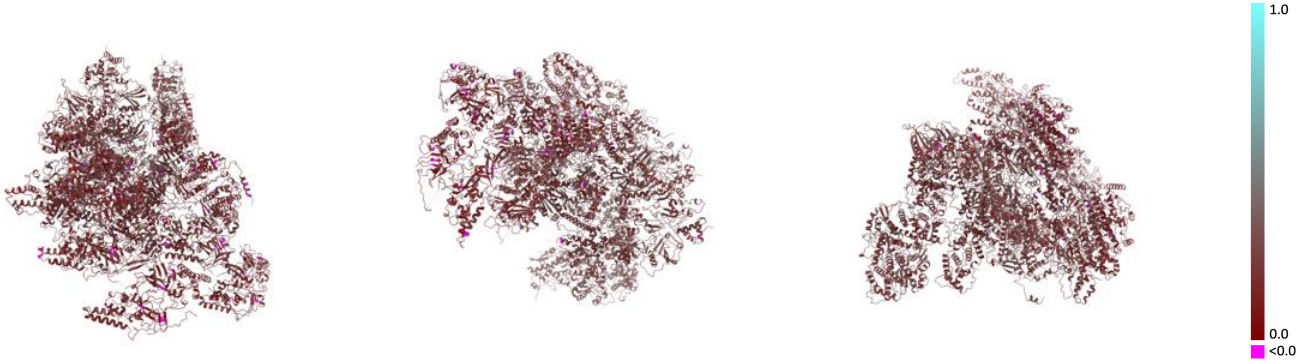
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.298 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

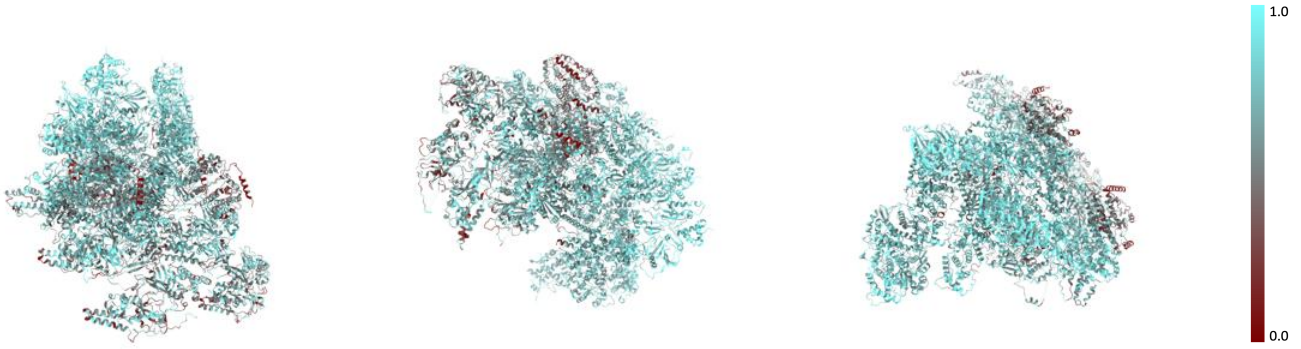
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

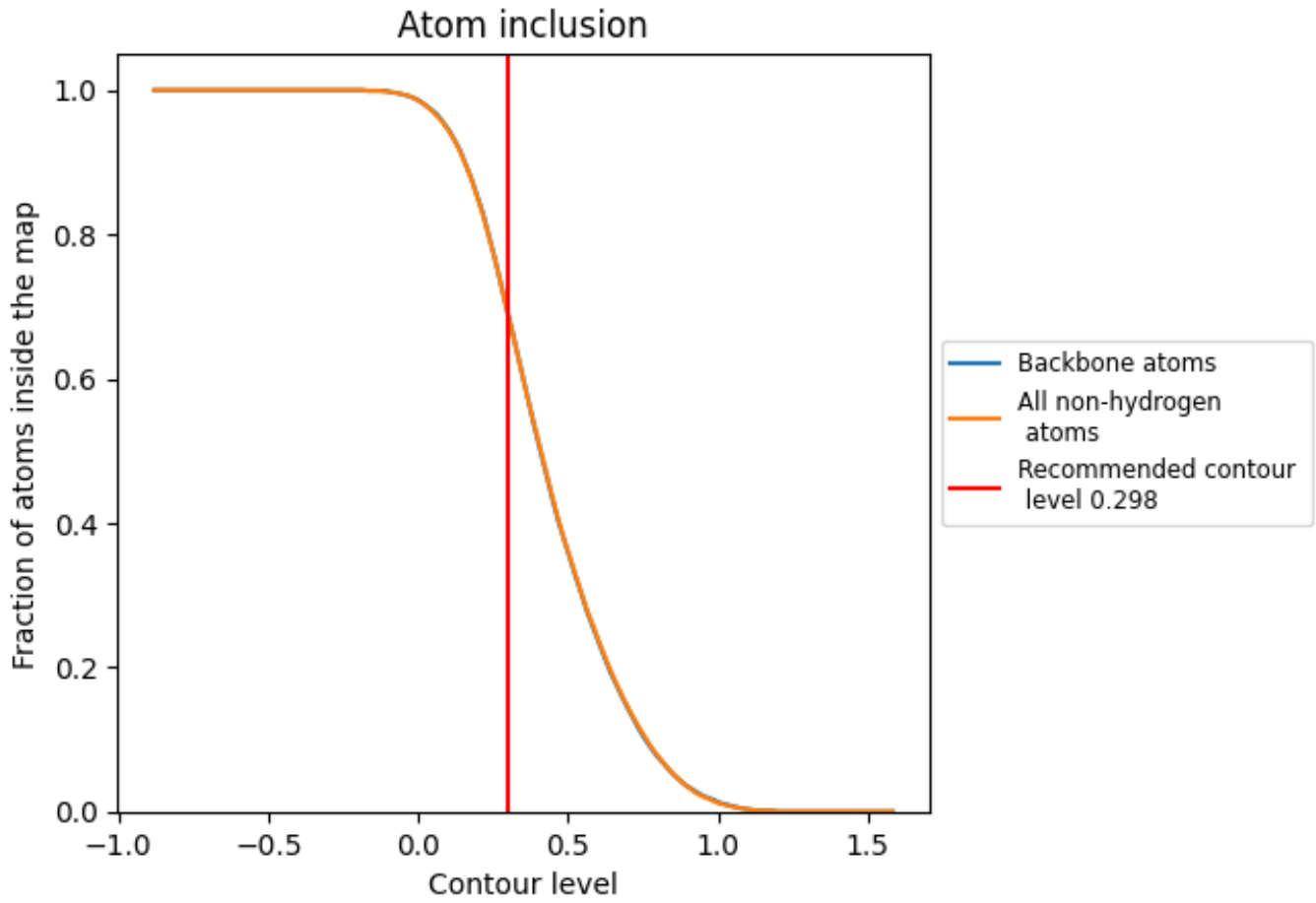
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.298).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 69% 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 (0.298) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6930	0.2520
A	0.6130	0.2180
B	0.5590	0.2110
C	0.6850	0.2290
D	0.7360	0.2550
E	0.7770	0.2670
F	0.7330	0.2550
G	0.4240	0.2300
H	0.5010	0.2160
I	0.7470	0.2330
J	0.6670	0.2520
K	0.6970	0.2510
L	0.7270	0.2530
M	0.7440	0.2820
N	0.8220	0.2910
O	0.8410	0.2880
P	0.5800	0.2460
Q	0.7610	0.2790
R	0.8130	0.2580
S	0.7370	0.2880
T	0.7850	0.2700
V	0.5910	0.2020
W	0.5820	0.2110
X	0.6820	0.2240
Y	0.7280	0.2370
Z	0.7820	0.2480
a	0.6960	0.2430
b	0.4350	0.2170
c	0.5280	0.2070
d	0.7960	0.2410
e	0.6610	0.2540
f	0.7260	0.2680
g	0.7470	0.2620
h	0.7510	0.2840
i	0.8350	0.2810

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Chain	Atom inclusion	Q-score
j	0.8640	0.2880
k	0.5970	0.2500