



wwPDB EM Validation Summary Report ⓘ

May 14, 2025 – 10:41 AM EDT

PDB ID : 8VWJ / pdb_00008vwj
EMDB ID : EMD-43589
Title : The base complex of the AcMNPV baculovirus nucleocapsid (Class 2, localised reconstruction)
Authors : Johnstone, B.A.; Koszalka, P.; Ha, J.; Venugopal, H.; Coulibaly, F.
Deposited on : 2024-02-01
Resolution : 4.78 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

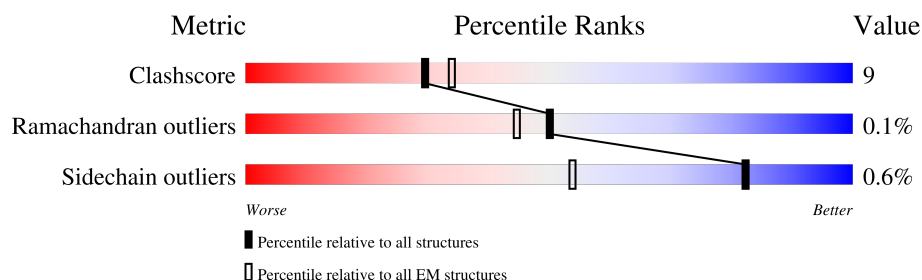
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.78 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)
Clashscore	210492	15764
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	347	
1	B	347	
1	C	347	
1	D	347	
1	E	347	
1	F	347	
1	V	347	
1	W	347	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	X	347	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	j	477	<div><div></div><div>77%</div><div>21%</div><div></div><div></div></div>
7	P	320	<div><div>17%</div><div></div><div>77%</div><div>19%</div><div></div><div></div></div>
7	k	320	<div><div>17%</div><div></div><div>75%</div><div>20%</div><div></div><div></div></div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 156295 atoms, of which 77632 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	284	Total	C	H	N	O	S	0	0
			4529	1442	2235	403	437	12		
1	E	283	Total	C	H	N	O	S	0	0
			4509	1443	2223	398	432	13		
1	F	286	Total	C	H	N	O	S	0	0
			4552	1457	2242	403	437	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
			4509	1443	2223	398	432	13		
1	a	286	Total	C	H	N	O	S	0	0
			4552	1457	2242	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
			3225	1049	1609	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	197	Total	C	H	N	O	S	0	0
			3286	1066	1644	269	295	12		
2	c	206	Total	C	H	N	O	S	0	0
			3449	1113	1730	289	304	13		
2	d	224	Total	C	H	N	O	S	0	0
			3748	1209	1870	315	340	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	186	Total	C	H	N	O	S	0	0
			3004	976	1494	238	288	8		
3	S	223	Total	C	H	N	O	S	0	0
			3628	1170	1814	286	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
			3625	1150	1807	307	345	16		
4	T	222	Total	C	H	N	O	S	0	0
			3670	1161	1834	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).

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 (CCD ID: 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	

Continued on next page...

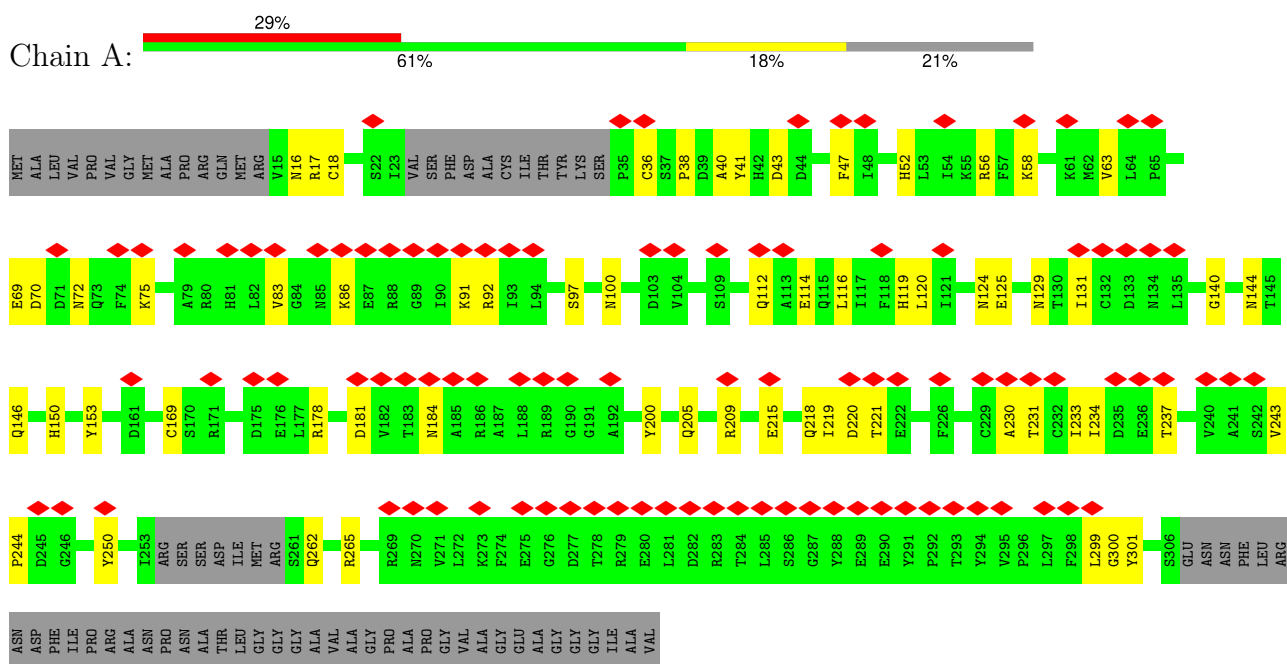
Continued from previous page...

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

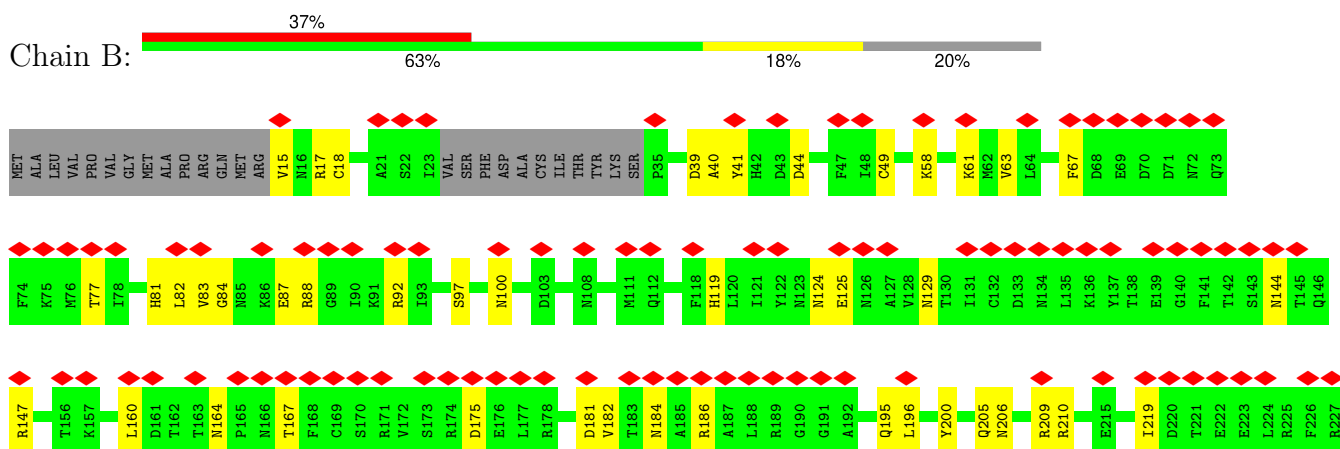
3 Residue-property plots

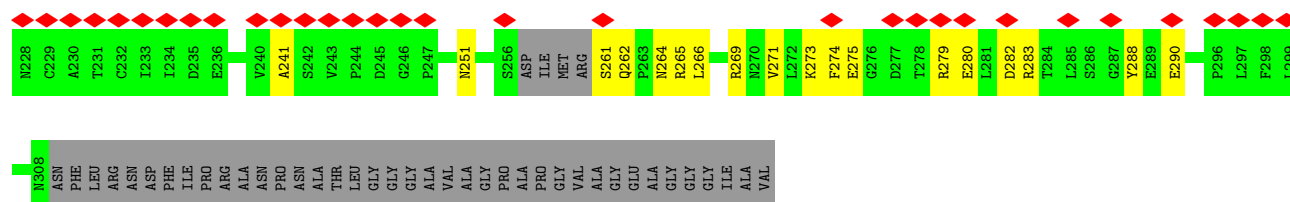
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Major capsid protein

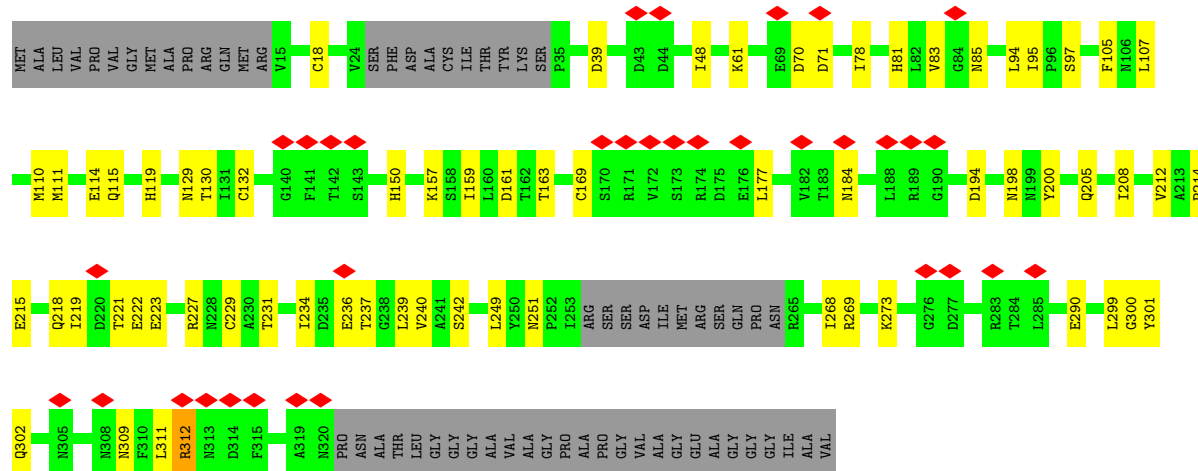


• Molecule 1: Major capsid protein

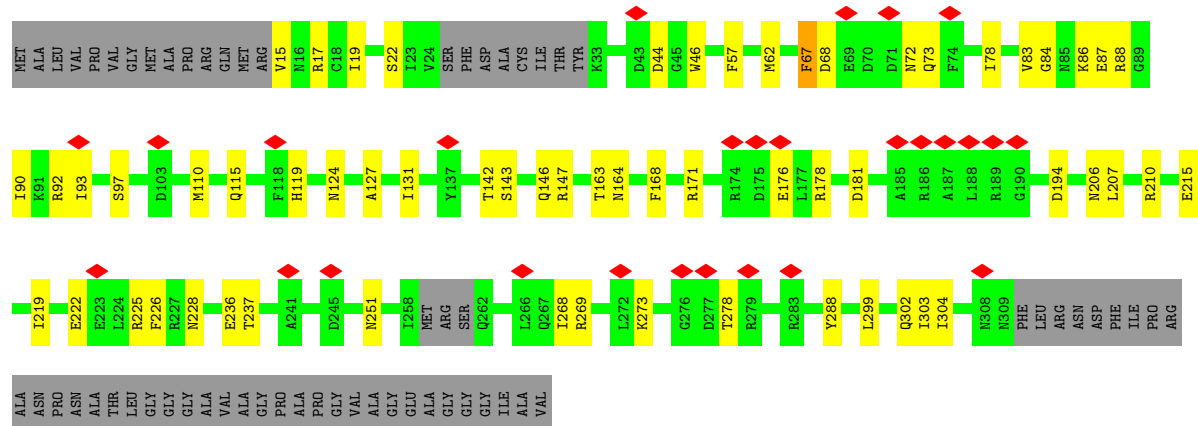




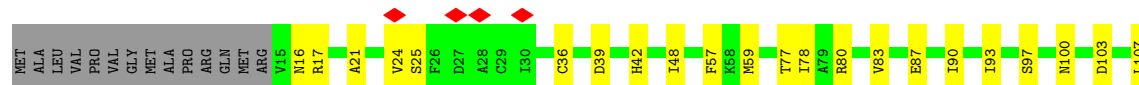
• Molecule 1: Major capsid protein

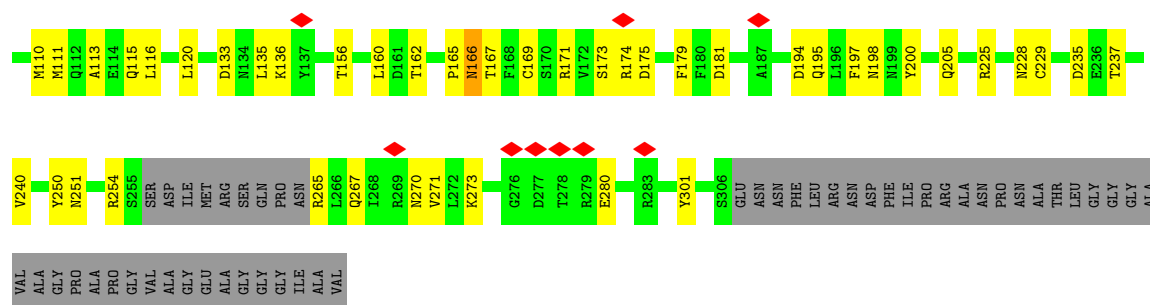


• Molecule 1: Major capsid protein

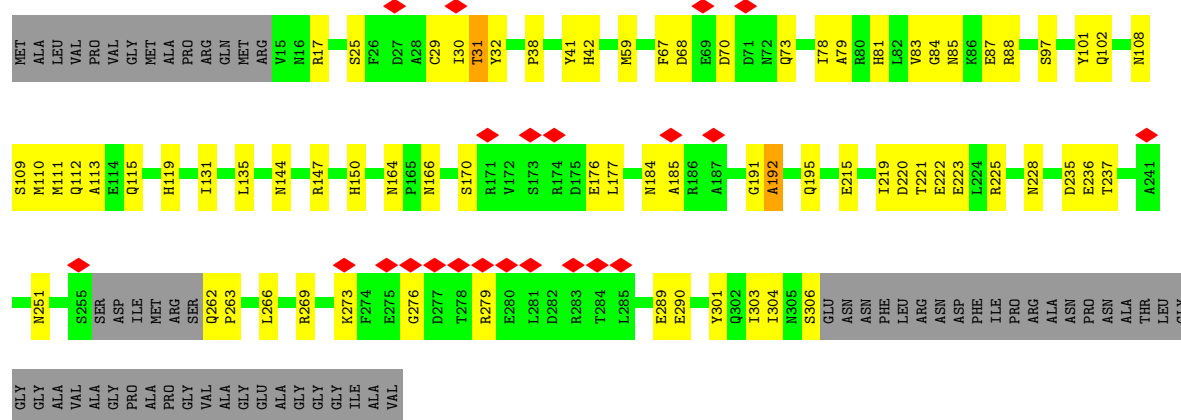


• Molecule 1: Major capsid protein

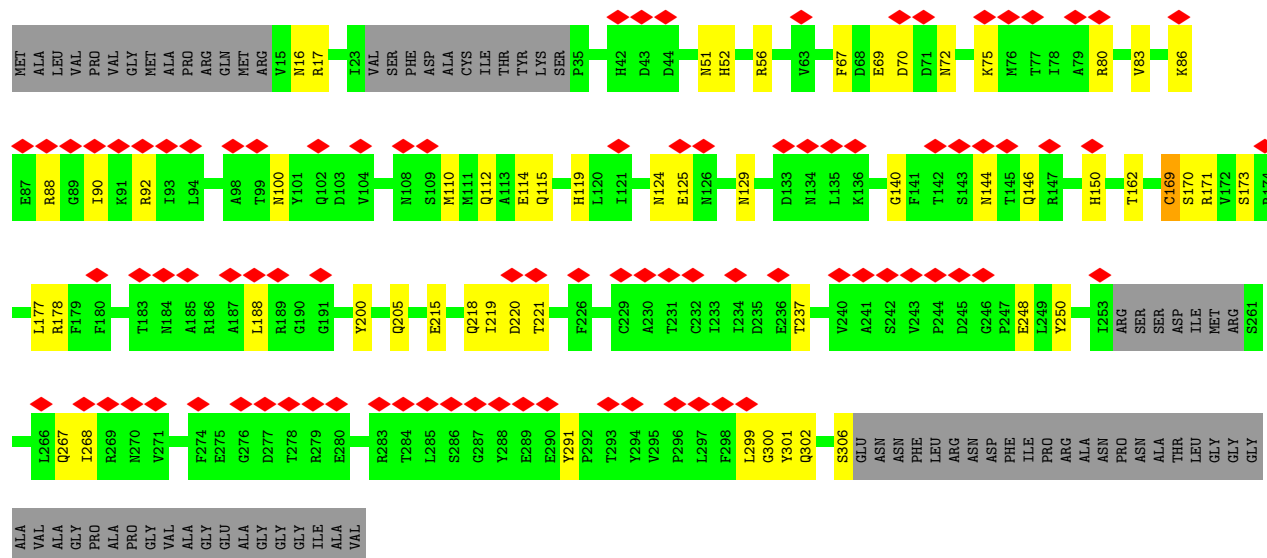




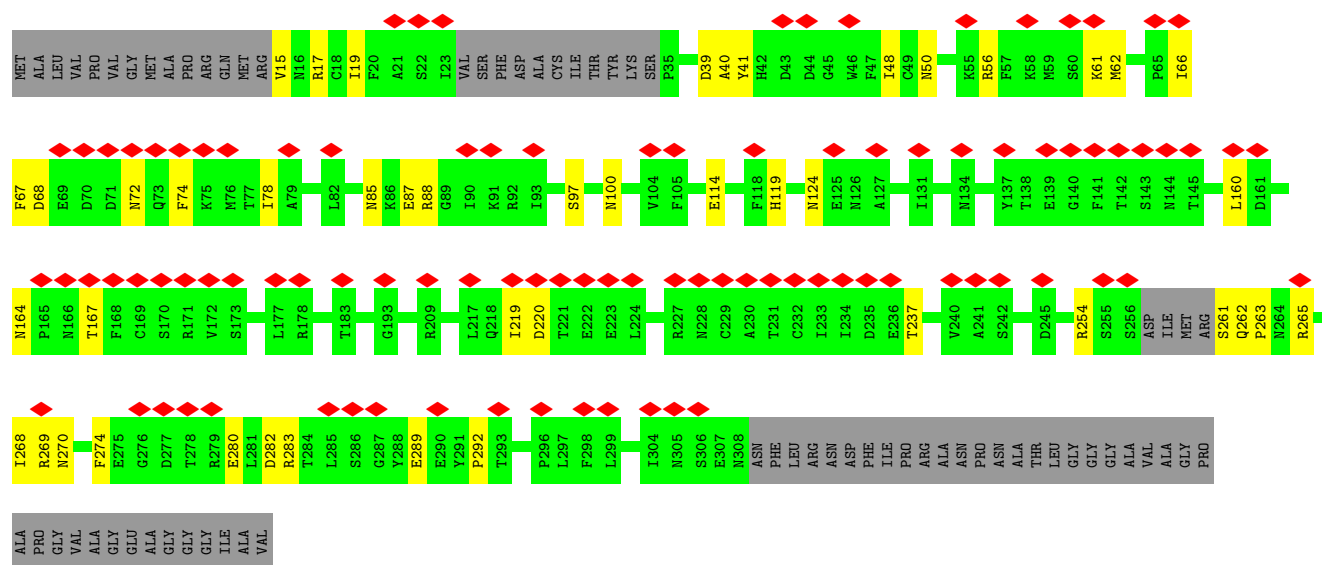
- Molecule 1: Major capsid protein



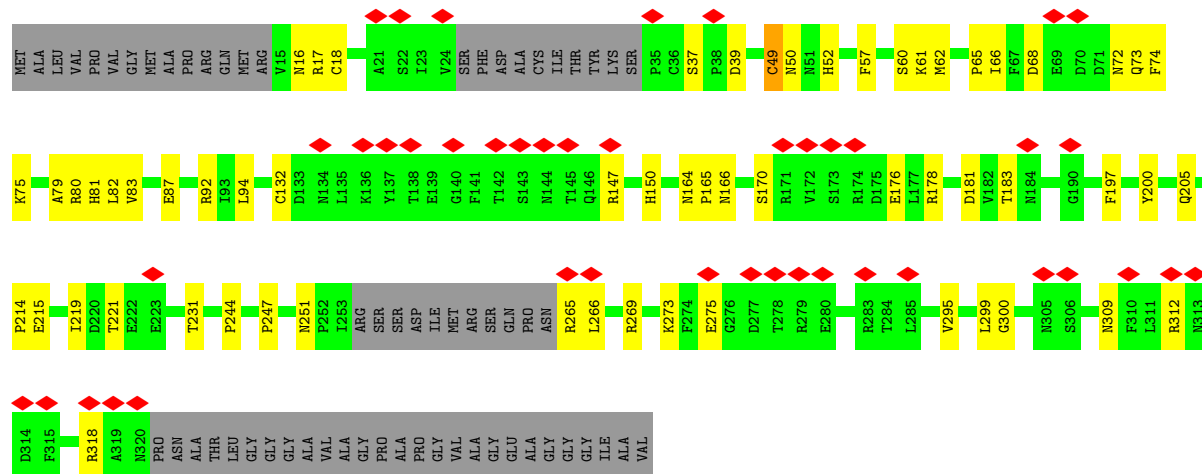
- Molecule 1: Major capsid protein



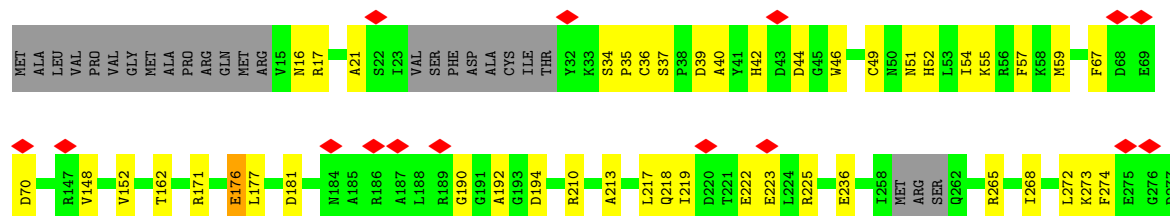
- Molecule 1: Major capsid protein

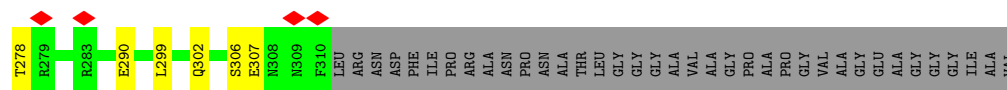


• Molecule 1: Major capsid protein

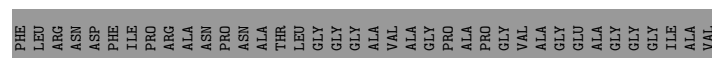
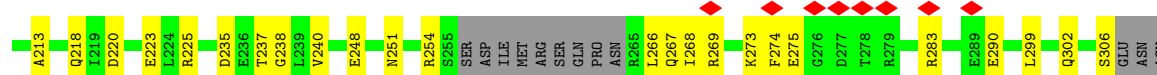
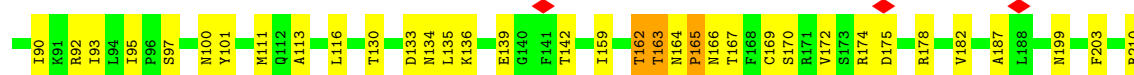


• Molecule 1: Major capsid protein

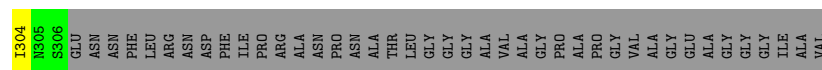
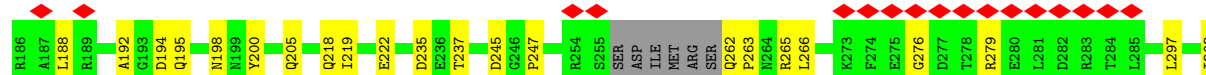
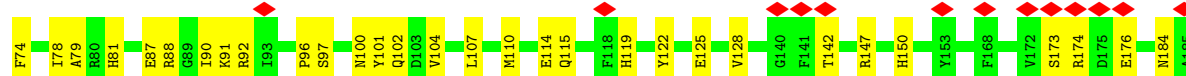




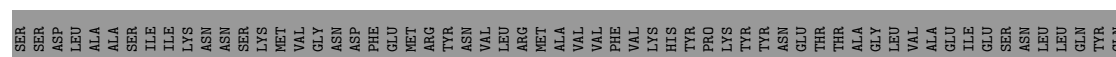
- Molecule 1: Major capsid protein

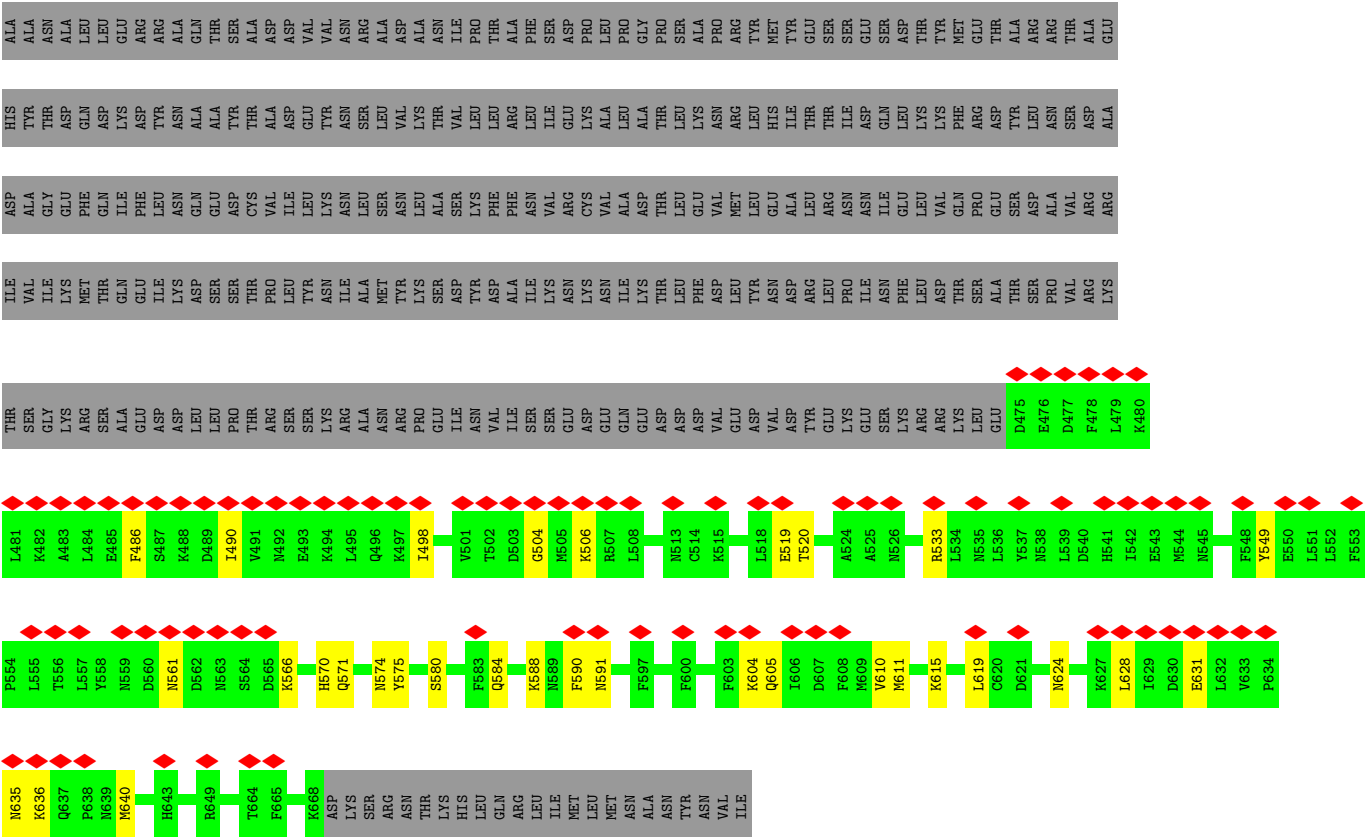


- Molecule 1: Major capsid protein

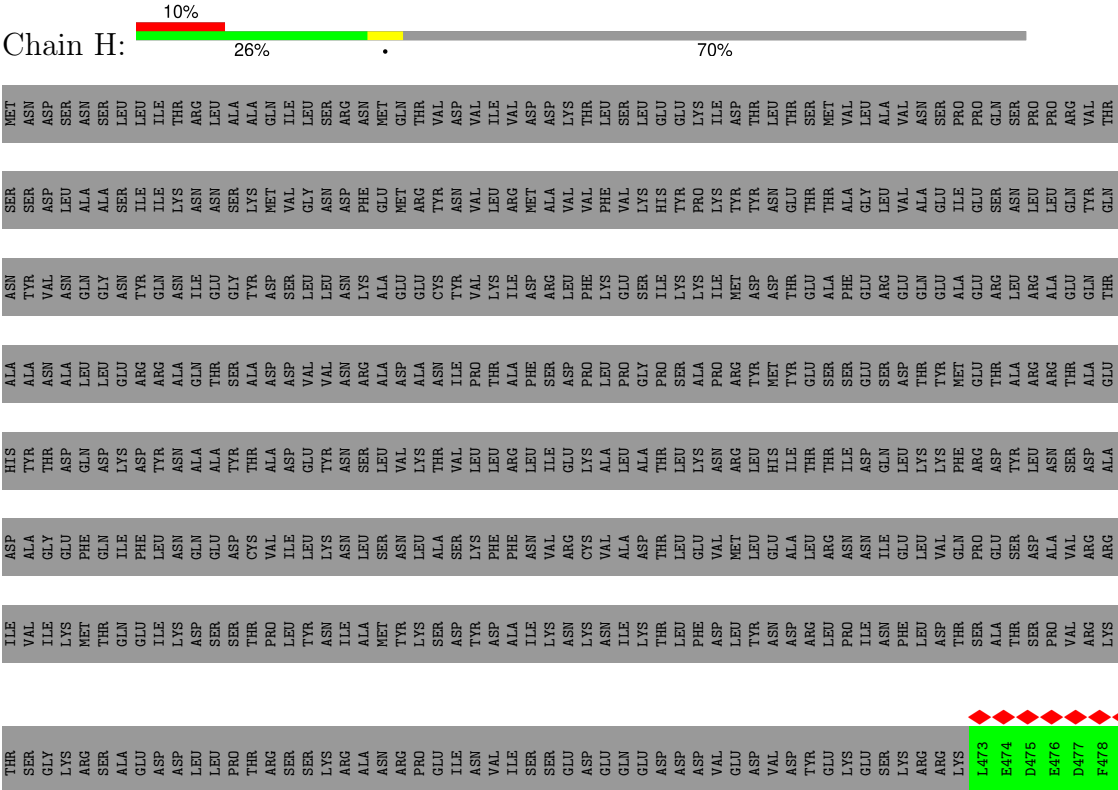


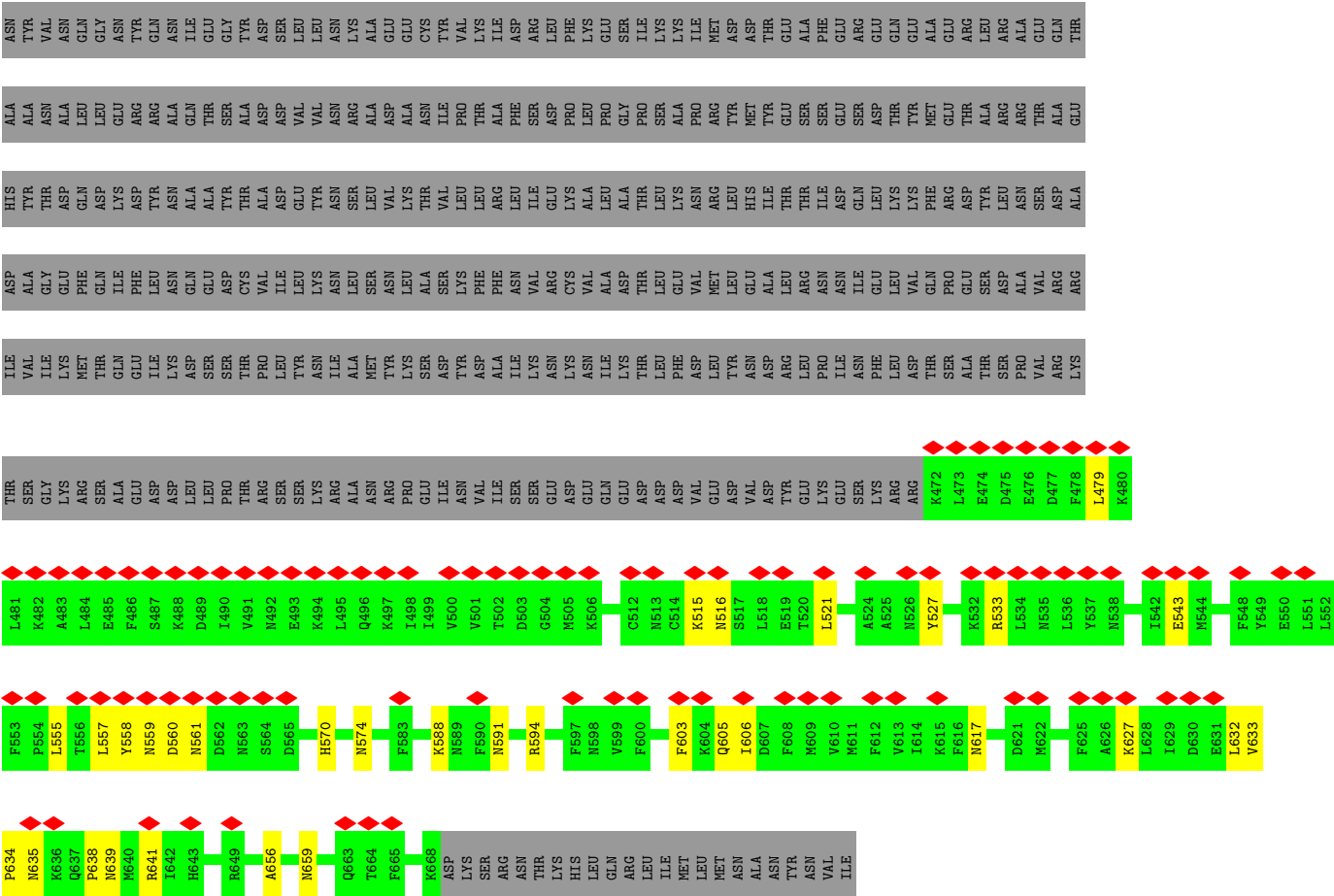
- Molecule 2: Capsid-associated protein VP80



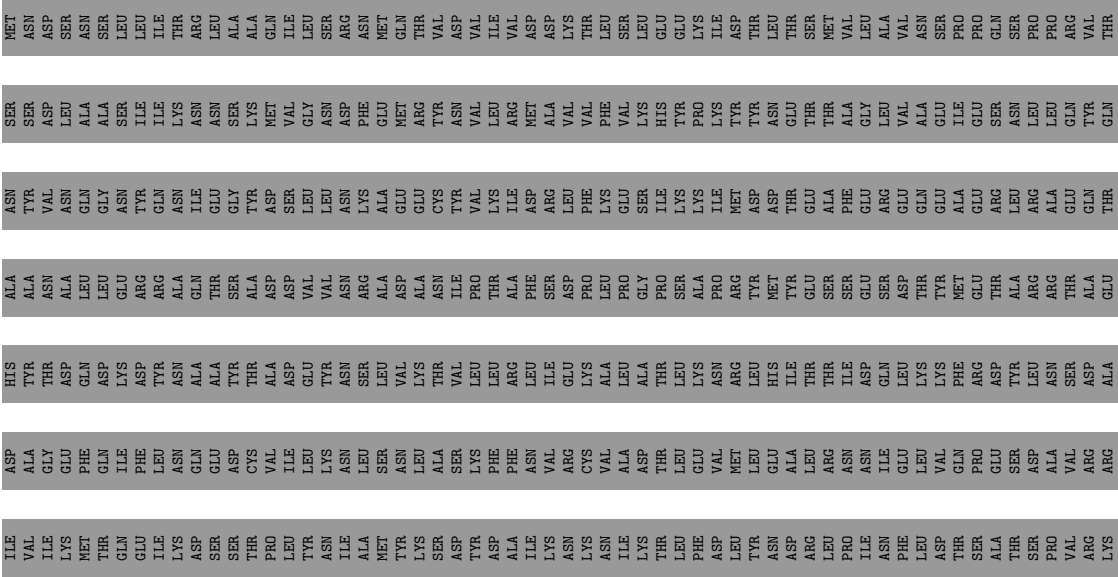


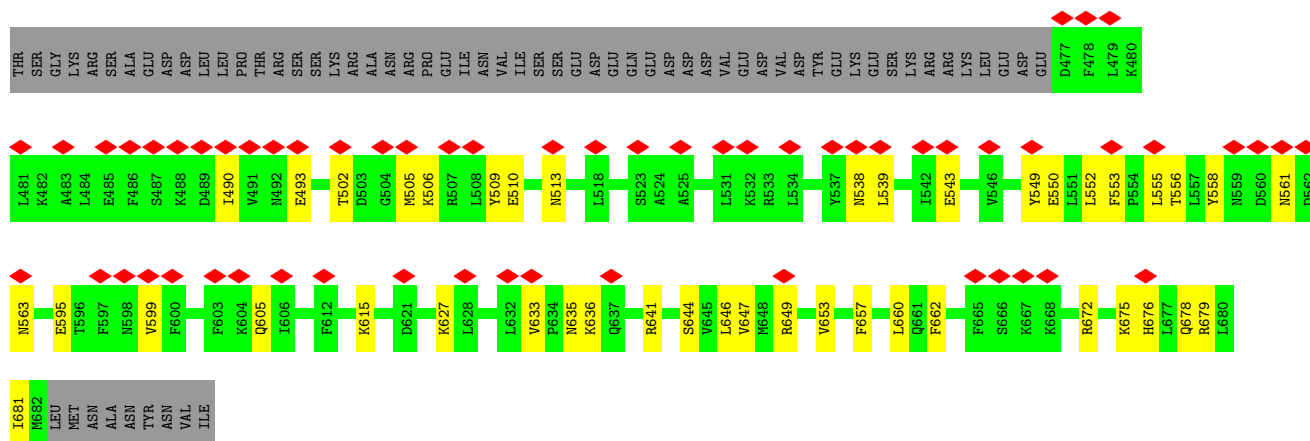
• Molecule 2: Capsid-associated protein VP80



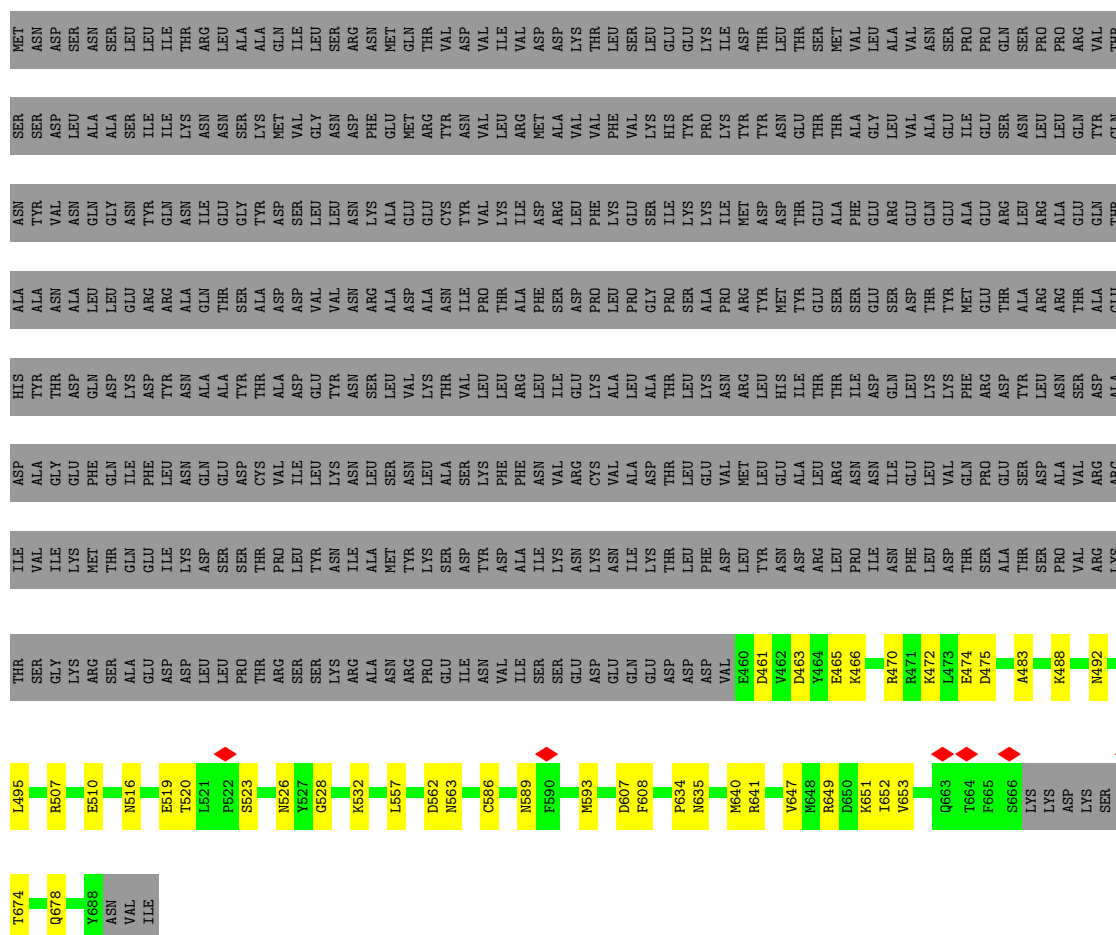


● Molecule 2: Capsid-associated protein VP80



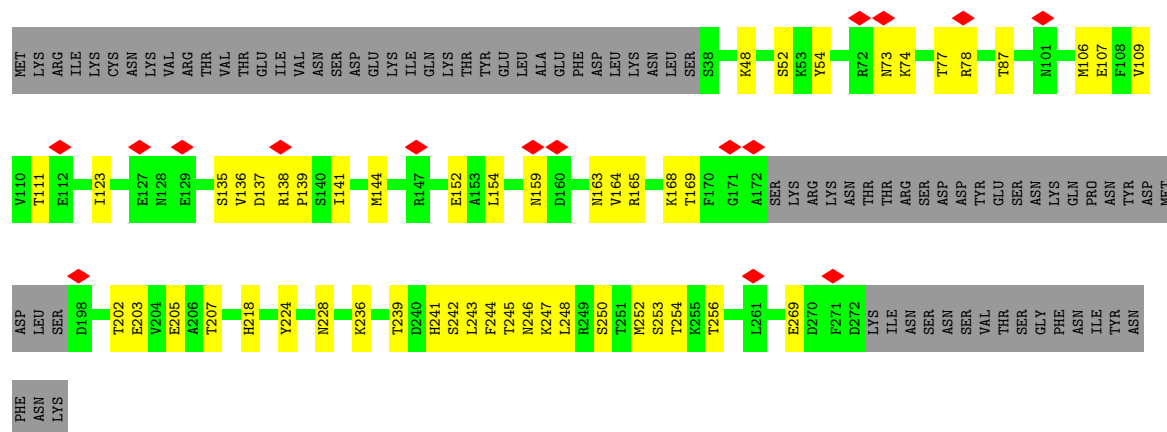


• Molecule 2: Capsid-associated protein VP80

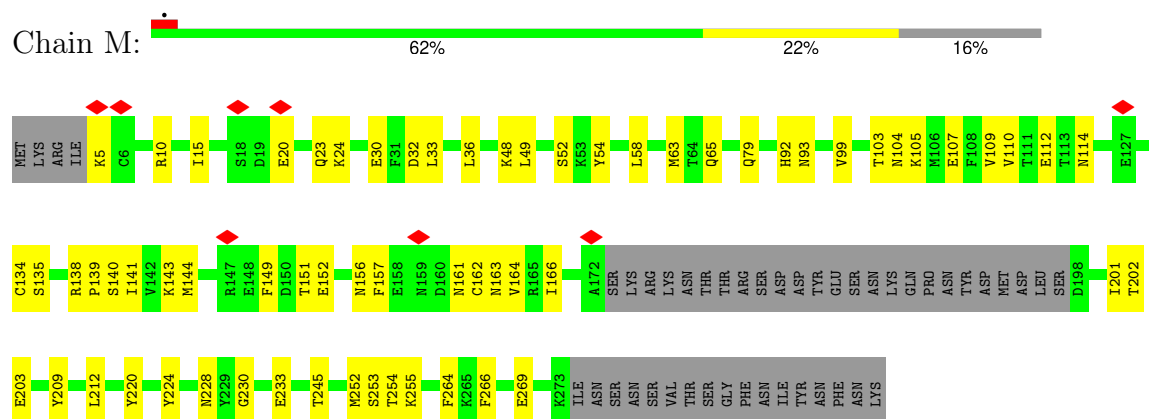


• Molecule 3: Occlusion-derived virus envelope protein E27

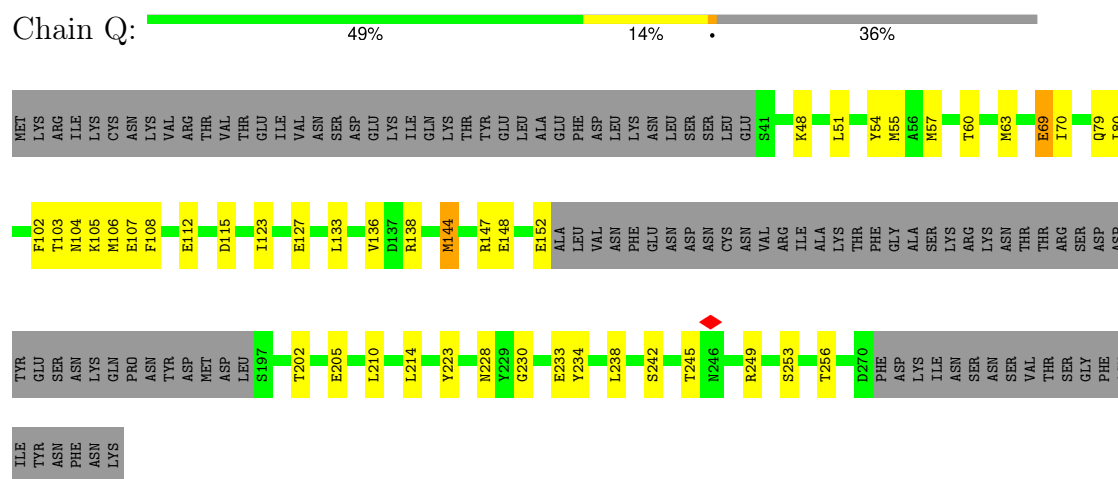




• Molecule 3: Occlusion-derived virus envelope protein E27



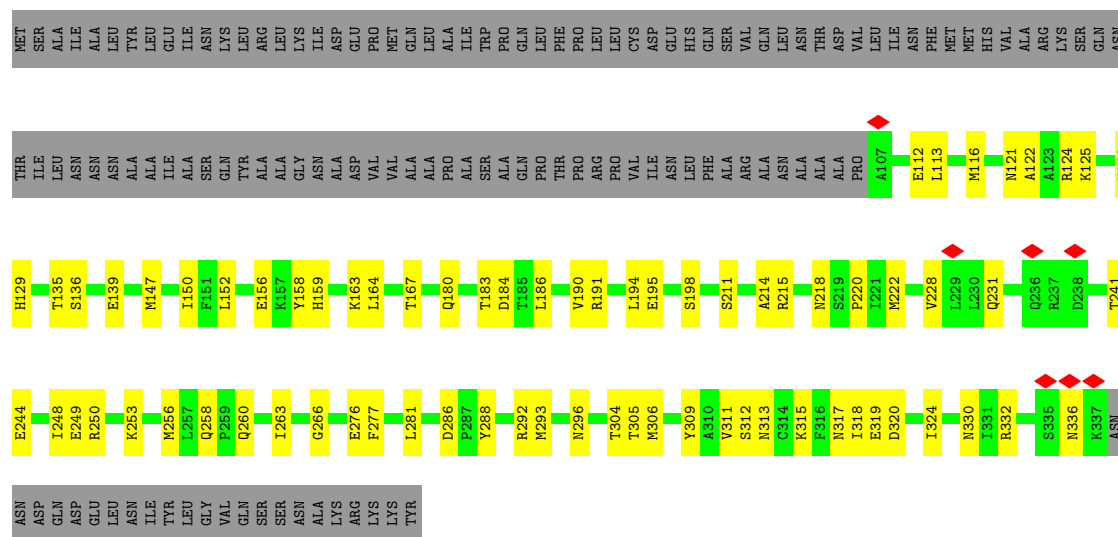
• Molecule 3: Occlusion-derived virus envelope protein E27



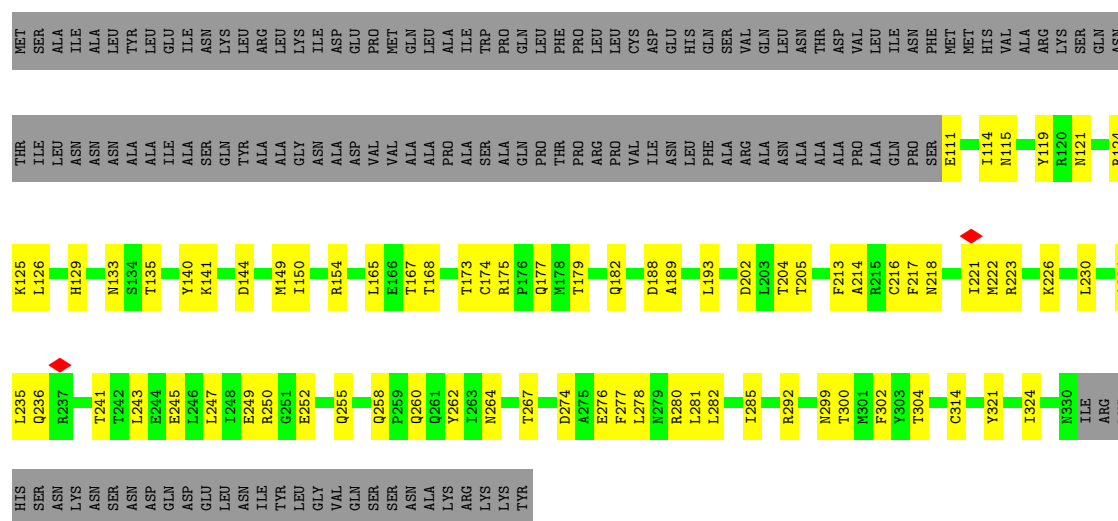
• Molecule 3: Occlusion-derived virus envelope protein E27



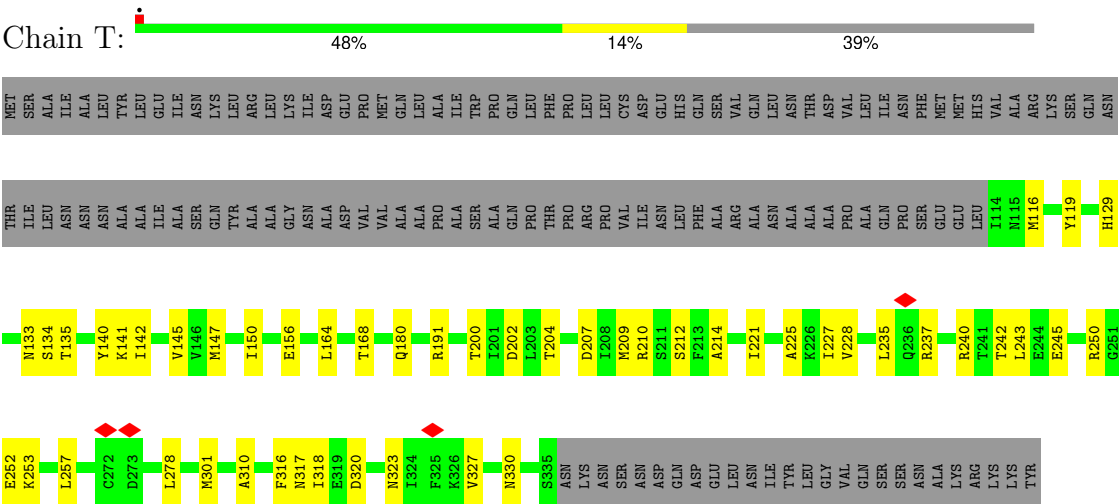
- Molecule 4: Protein C42



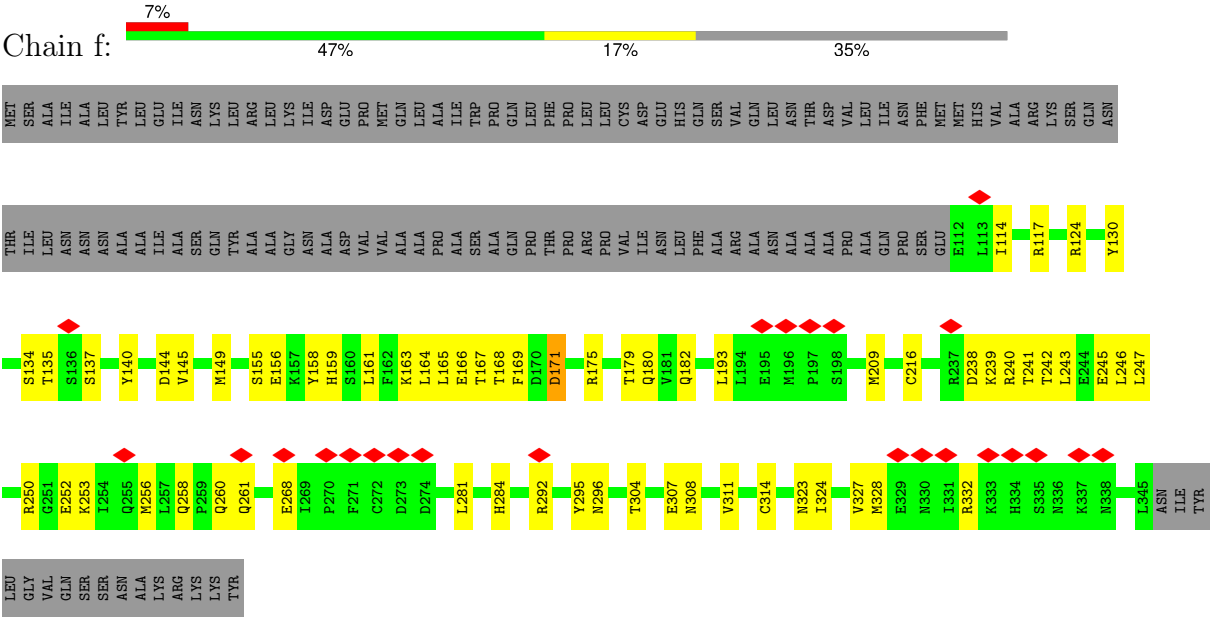
- Molecule 4: Protein C42



- Molecule 4: Protein C42



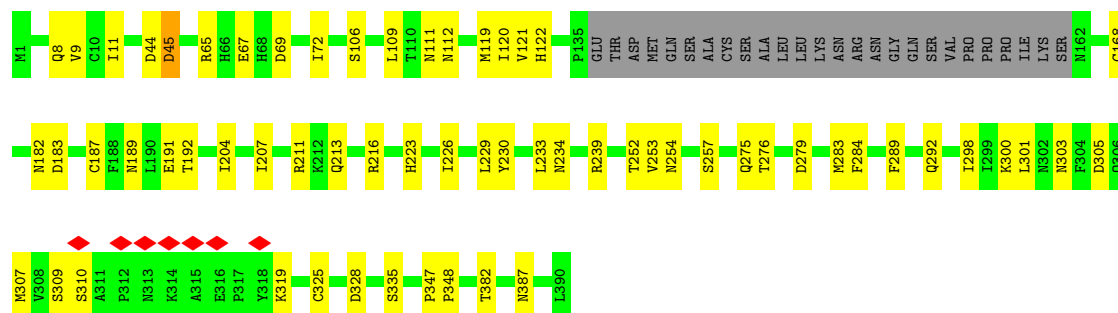
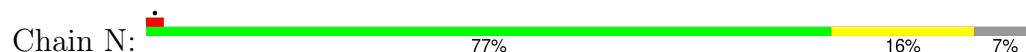
• Molecule 4: Protein C42



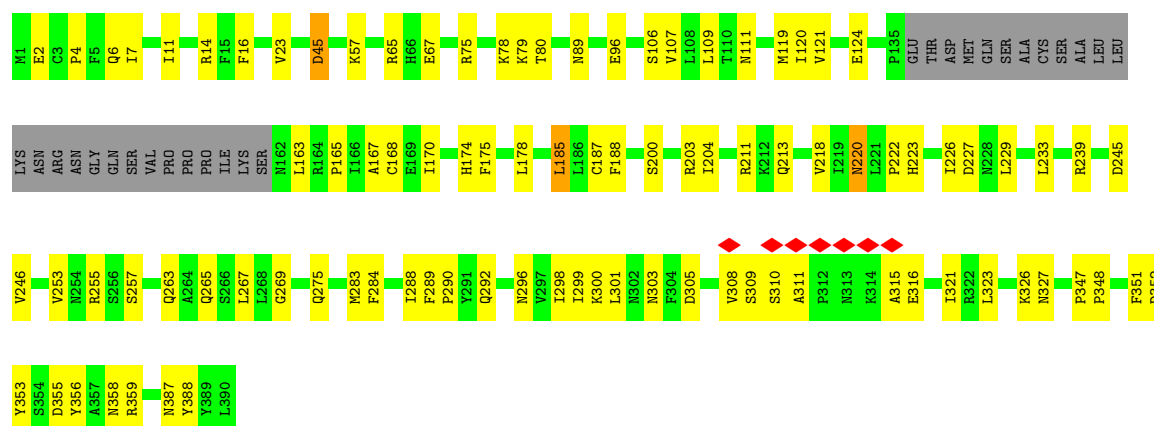
• Molecule 4: Protein C42



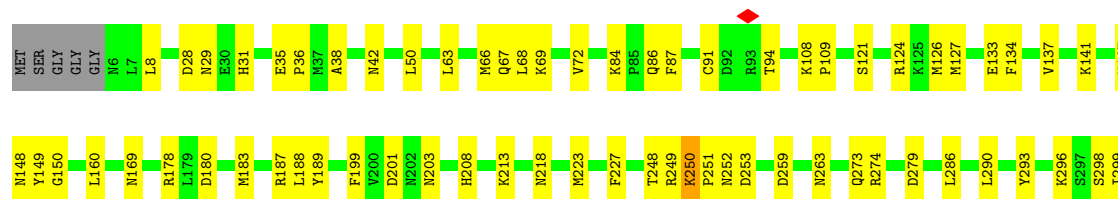
- Molecule 5: Protein AC109

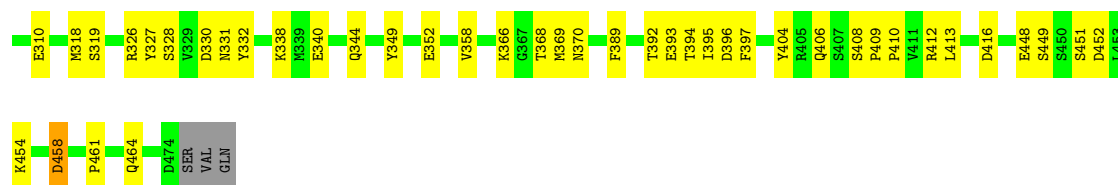


- Molecule 5: Protein AC109



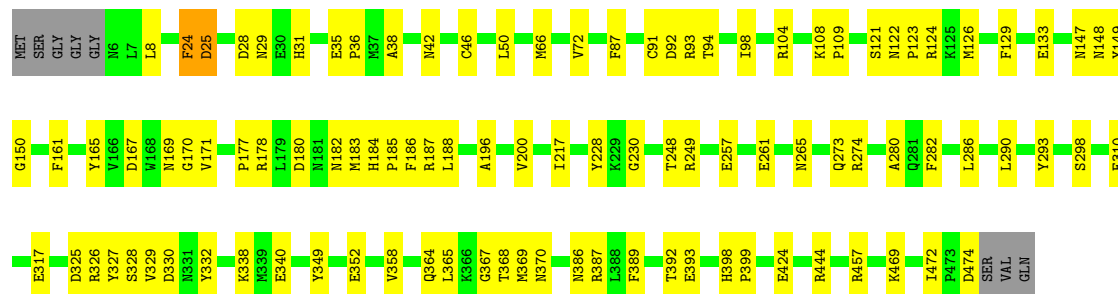
- Molecule 6: Protein AC142





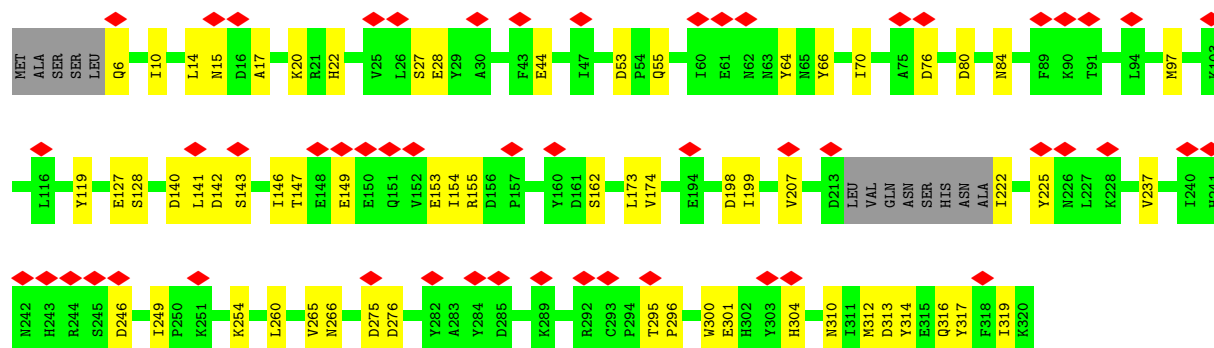
• Molecule 6: Protein AC142

Chain j: 77% 21% .



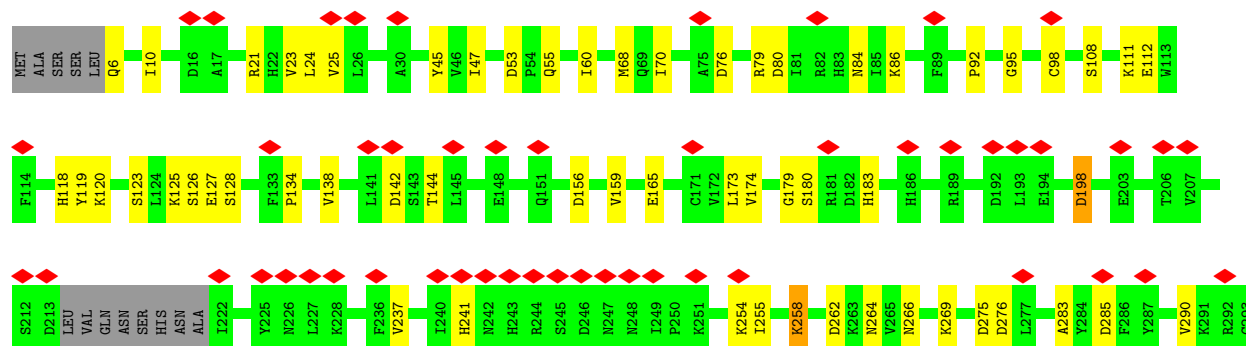
• Molecule 7: 38K (AC98)

Chain P: 17% 77% 19% .



• Molecule 7: 38K (AC98)

Chain k: 17% 75% 20% . .





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	1.615	Depositor
Minimum map value	-0.816	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.294	Depositor
Map size (\AA)	541.44, 541.44, 541.44	wwPDB
Map dimensions	384, 384, 384	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 ⓘ

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	0.12	0/2258	0.35	0/3058
1	B	0.12	0/2298	0.31	0/3111
1	C	0.15	0/2358	0.40	0/3193
1	D	0.15	0/2338	0.37	0/3166
1	E	0.16	0/2332	0.38	0/3159
1	F	0.18	0/2357	0.43	0/3194
1	V	0.14	0/2258	0.35	0/3058
1	W	0.12	0/2298	0.31	0/3111
1	X	0.14	0/2358	0.36	0/3193
1	Y	0.15	0/2356	0.39	0/3190
1	Z	0.17	0/2332	0.44	1/3159 (0.0%)
1	a	0.16	0/2357	0.42	0/3194
2	G	0.14	0/1650	0.36	0/2221
2	H	0.15	0/1788	0.36	0/2404
2	I	0.21	0/1914	0.44	1/2572 (0.0%)
2	b	0.15	0/1676	0.42	0/2255
2	c	0.15	0/1754	0.40	0/2358
2	d	0.15	0/1914	0.38	0/2572
3	J	0.17	0/1732	0.35	0/2344
3	M	0.20	0/2012	0.40	0/2719
3	Q	0.18	0/1540	0.42	0/2084
3	S	0.18	0/1847	0.39	0/2497
3	e	0.16	0/1732	0.36	0/2344
3	h	0.19	0/2003	0.44	0/2708
4	K	0.23	0/1968	0.46	0/2657
4	L	0.21	0/1941	0.44	0/2621
4	R	0.17	0/1851	0.44	0/2501
4	T	0.18	0/1870	0.41	0/2525
4	f	0.26	0/1968	0.45	0/2657
4	g	0.20	0/1927	0.44	0/2601
5	N	0.18	0/3040	0.37	0/4132
5	i	0.19	0/3040	0.42	0/4132

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	O	0.18	0/3956	0.37	0/5357
6	j	0.20	0/3956	0.41	1/5357 (0.0%)
7	P	0.15	0/2662	0.40	0/3603
7	k	0.15	0/2662	0.40	0/3603
All	All	0.17	0/80303	0.40	3/108610 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	162	THR	N-CA-C	-5.73	101.56	110.10
2	I	592	TYR	N-CA-C	-5.67	105.10	111.28
6	j	24	PHE	N-CA-C	5.04	118.20	107.67

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	594	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2214	2157	2157	40	0
1	B	2254	2195	2192	43	0
1	C	2312	2252	2250	44	0
1	D	2294	2235	2234	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2286	2223	2231	47	0
1	F	2310	2242	2250	48	0
1	V	2214	2157	2156	37	0
1	W	2254	2195	2192	33	0
1	X	2312	2252	2252	40	0
1	Y	2310	2244	2242	39	0
1	Z	2286	2223	2230	57	0
1	a	2310	2242	2253	47	0
2	G	1616	1609	1619	21	0
2	H	1753	1760	1767	17	0
2	I	1878	1862	1878	38	0
2	b	1642	1644	1651	24	0
2	c	1719	1730	1740	27	0
2	d	1878	1870	1878	27	0
3	J	1699	1690	1693	39	0
3	M	1977	1979	1983	53	0
3	Q	1510	1494	1516	37	0
3	S	1814	1814	1828	35	0
3	e	1699	1685	1693	27	0
3	h	1968	1965	1970	51	0
4	K	1934	1908	1921	62	0
4	L	1906	1903	1903	57	0
4	R	1818	1807	1810	62	0
4	T	1836	1834	1836	41	0
4	f	1934	1907	1922	47	0
4	g	1892	1890	1890	61	0
5	N	2964	2953	2956	41	0
5	i	2964	2953	2956	71	0
6	O	3857	3852	3851	67	0
6	j	3857	3852	3851	72	0
7	P	2590	2528	2526	36	0
7	k	2590	2526	2524	39	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	V	1	0	0	0	0
8	W	1	0	0	0	0
8	X	1	0	0	0	0
8	Y	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Z	1	0	0	0	0
8	a	1	0	0	0	0
All	All	78663	77632	77801	1404	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1404 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:i:356:TYR:OH	6:j:392:THR:O	1.84	0.95
4:f:256:MET:O	4:f:258:GLN:NE2	2.00	0.94
3:J:245:THR:HG23	4:K:327:VAL:HG21	1.50	0.93
4:R:126:LEU:O	4:R:129:HIS:ND1	2.05	0.90
5:i:300:LYS:NZ	6:j:474:ASP:OD2	2.05	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/347 (77%)	246 (92%)	22 (8%)	0	100	100
1	B	273/347 (79%)	255 (93%)	18 (7%)	0	100	100
1	C	279/347 (80%)	250 (90%)	28 (10%)	1 (0%)	30	68
1	D	278/347 (80%)	254 (91%)	24 (9%)	0	100	100
1	E	279/347 (80%)	256 (92%)	23 (8%)	0	100	100
1	F	282/347 (81%)	248 (88%)	33 (12%)	1 (0%)	30	68
1	V	268/347 (77%)	252 (94%)	16 (6%)	0	100	100
1	W	273/347 (79%)	262 (96%)	11 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	279/347 (80%)	257 (92%)	22 (8%)	0	100	100
1	Y	279/347 (80%)	251 (90%)	28 (10%)	0	100	100
1	Z	279/347 (80%)	246 (88%)	32 (12%)	1 (0%)	30	68
1	a	282/347 (81%)	246 (87%)	36 (13%)	0	100	100
2	G	192/691 (28%)	165 (86%)	27 (14%)	0	100	100
2	H	208/691 (30%)	178 (86%)	30 (14%)	0	100	100
2	I	220/691 (32%)	205 (93%)	15 (7%)	0	100	100
2	b	195/691 (28%)	176 (90%)	19 (10%)	0	100	100
2	c	204/691 (30%)	171 (84%)	33 (16%)	0	100	100
2	d	220/691 (32%)	203 (92%)	17 (8%)	0	100	100
3	J	206/290 (71%)	194 (94%)	12 (6%)	0	100	100
3	M	240/290 (83%)	213 (89%)	27 (11%)	0	100	100
3	Q	182/290 (63%)	163 (90%)	19 (10%)	0	100	100
3	S	219/290 (76%)	196 (90%)	22 (10%)	1 (0%)	25	64
3	e	206/290 (71%)	193 (94%)	13 (6%)	0	100	100
3	h	239/290 (82%)	207 (87%)	32 (13%)	0	100	100
4	K	232/361 (64%)	206 (89%)	25 (11%)	1 (0%)	30	68
4	L	229/361 (63%)	200 (87%)	29 (13%)	0	100	100
4	R	218/361 (60%)	201 (92%)	17 (8%)	0	100	100
4	T	220/361 (61%)	190 (86%)	30 (14%)	0	100	100
4	f	232/361 (64%)	202 (87%)	30 (13%)	0	100	100
4	g	227/361 (63%)	197 (87%)	29 (13%)	1 (0%)	30	68
5	N	360/390 (92%)	326 (91%)	34 (9%)	0	100	100
5	i	360/390 (92%)	318 (88%)	41 (11%)	1 (0%)	37	72
6	O	467/477 (98%)	434 (93%)	33 (7%)	0	100	100
6	j	467/477 (98%)	436 (93%)	30 (6%)	1 (0%)	44	78
7	P	303/320 (95%)	272 (90%)	31 (10%)	0	100	100
7	k	303/320 (95%)	272 (90%)	31 (10%)	0	100	100
All	All	9468/14590 (65%)	8541 (90%)	919 (10%)	8 (0%)	50	83

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	K	339	SER
6	j	25	ASP
1	Z	165	PRO
1	C	312	ARG
4	g	318	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	247/299 (83%)	246 (100%)	1 (0%)	89	91
1	B	252/299 (84%)	252 (100%)	0	100	100
1	C	257/299 (86%)	255 (99%)	2 (1%)	79	85
1	D	257/299 (86%)	254 (99%)	3 (1%)	67	79
1	E	255/299 (85%)	252 (99%)	3 (1%)	67	79
1	F	258/299 (86%)	257 (100%)	1 (0%)	89	91
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%)	255 (99%)	2 (1%)	79	85
1	Y	258/299 (86%)	257 (100%)	1 (0%)	89	91
1	Z	255/299 (85%)	251 (98%)	4 (2%)	58	74
1	a	258/299 (86%)	257 (100%)	1 (0%)	89	91
2	G	184/634 (29%)	184 (100%)	0	100	100
2	H	200/634 (32%)	199 (100%)	1 (0%)	86	90
2	I	213/634 (34%)	209 (98%)	4 (2%)	52	70
2	b	187/634 (30%)	187 (100%)	0	100	100
2	c	196/634 (31%)	196 (100%)	0	100	100
2	d	213/634 (34%)	213 (100%)	0	100	100
3	J	195/273 (71%)	195 (100%)	0	100	100
3	M	228/273 (84%)	228 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	175/273 (64%)	172 (98%)	3 (2%)	56	73
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%)	222 (98%)	5 (2%)	47	66
4	K	222/326 (68%)	219 (99%)	3 (1%)	62	76
4	L	218/326 (67%)	217 (100%)	1 (0%)	86	90
4	R	208/326 (64%)	208 (100%)	0	100	100
4	T	210/326 (64%)	209 (100%)	1 (0%)	86	90
4	f	222/326 (68%)	221 (100%)	1 (0%)	86	90
4	g	217/326 (67%)	215 (99%)	2 (1%)	75	83
5	N	343/366 (94%)	342 (100%)	1 (0%)	91	92
5	i	343/366 (94%)	340 (99%)	3 (1%)	75	83
6	O	435/440 (99%)	433 (100%)	2 (0%)	86	90
6	j	435/440 (99%)	435 (100%)	0	100	100
7	P	293/304 (96%)	293 (100%)	0	100	100
7	k	293/304 (96%)	289 (99%)	4 (1%)	62	76
All	All	8915/13206 (68%)	8865 (99%)	50 (1%)	82	88

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	132	CYS
4	f	171	ASP
7	k	285	ASP
1	Y	176	GLU
1	Z	164	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
1	V	144	ASN
1	Z	146	GLN
6	j	70	HIS
1	V	305	ASN
1	Y	119	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

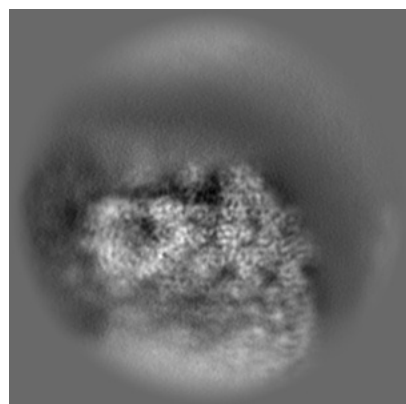
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43589. These allow visual inspection of the internal detail of the map and identification of artifacts.

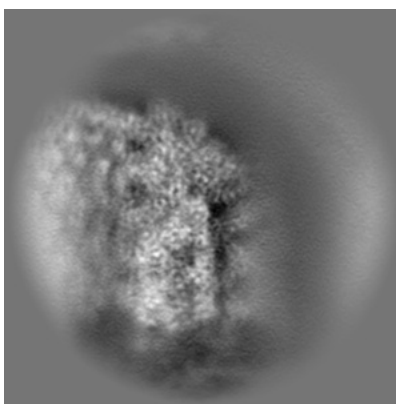
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

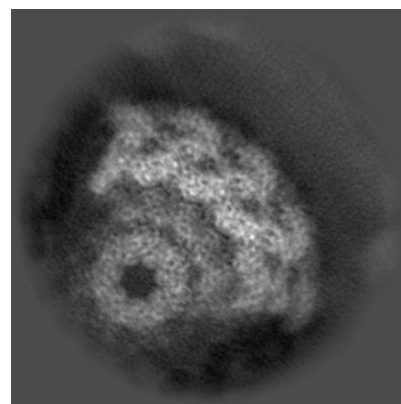
6.1.1 Primary map



X

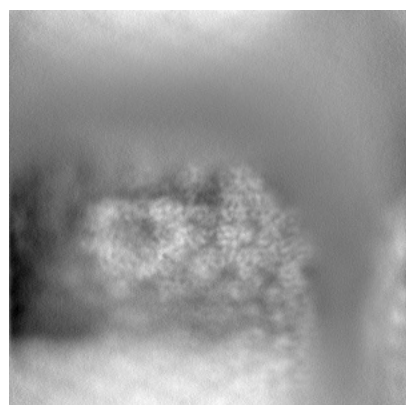


Y

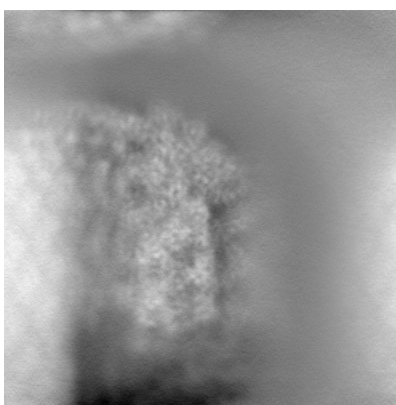


Z

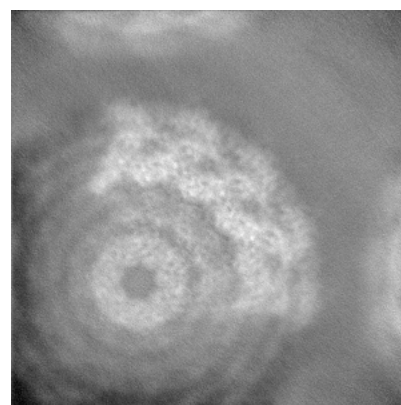
6.1.2 Raw map



X



Y

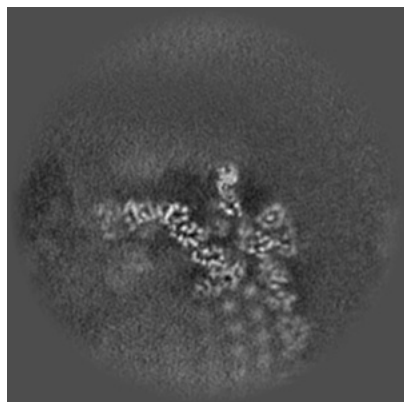


Z

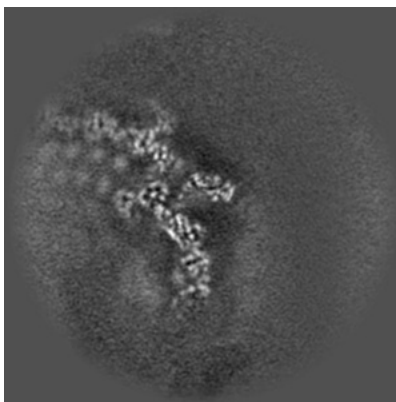
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

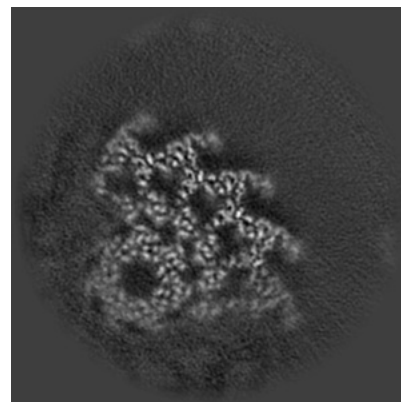
6.2.1 Primary map



X Index: 192



Y Index: 192

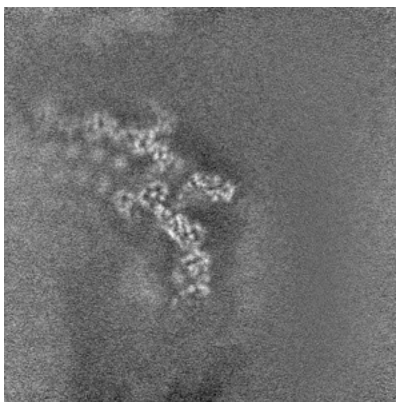


Z Index: 192

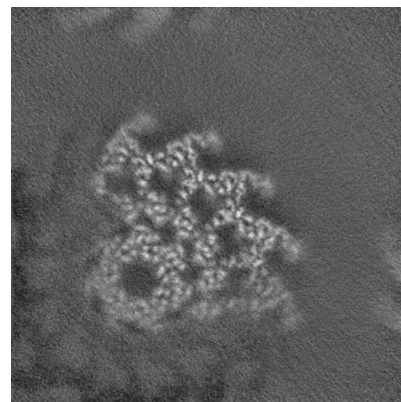
6.2.2 Raw map



X Index: 192



Y Index: 192

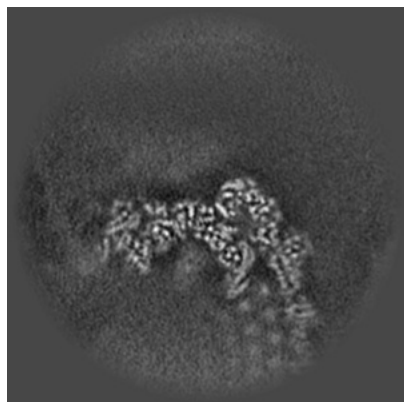


Z Index: 192

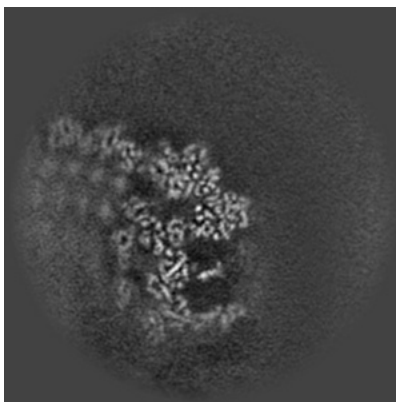
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

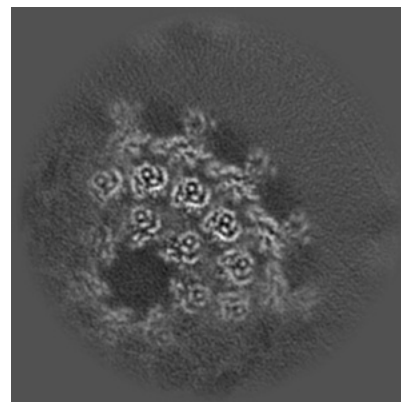
6.3.1 Primary map



X Index: 165

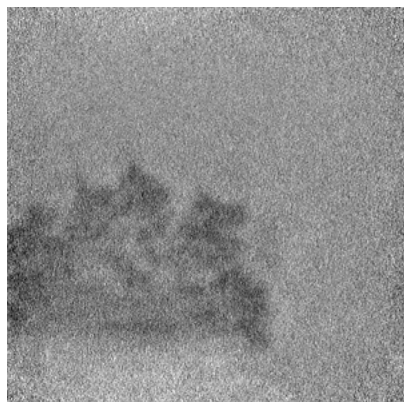


Y Index: 215

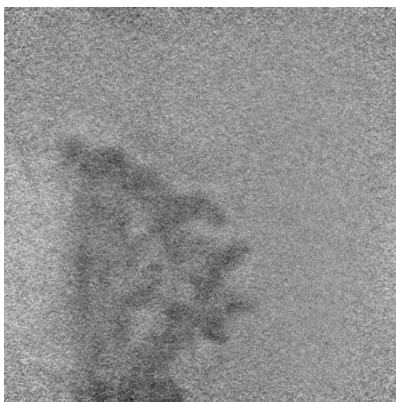


Z Index: 168

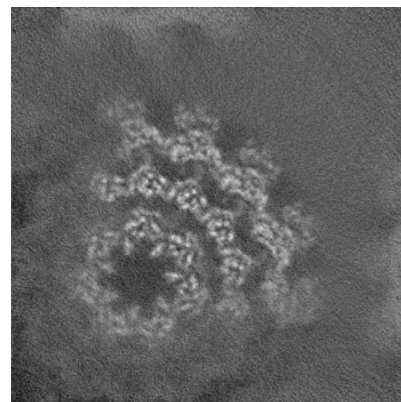
6.3.2 Raw map



X Index: 3



Y Index: 3

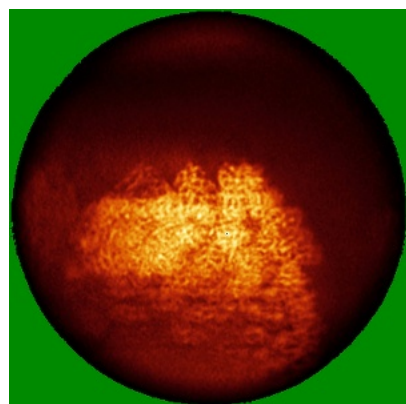


Z Index: 160

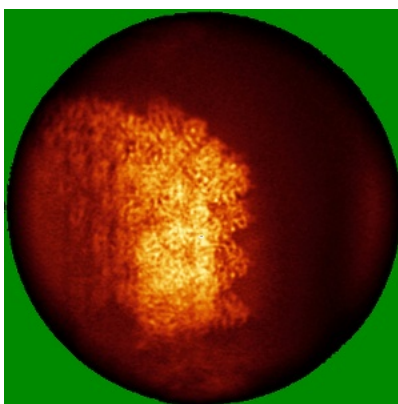
The images above show the largest variance slices of the map in three orthogonal directions.

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

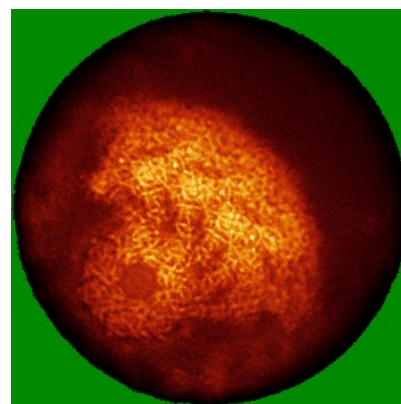
6.4.1 Primary map



X

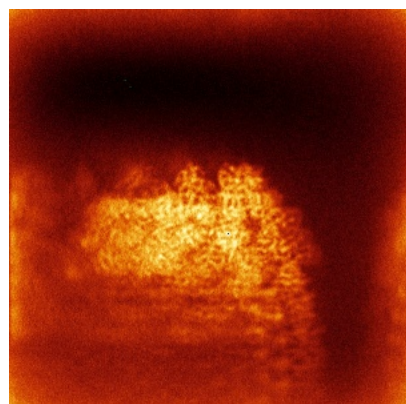


Y

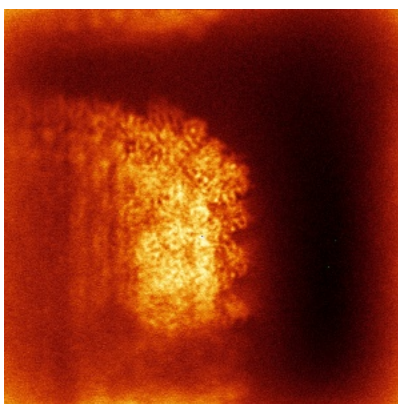


Z

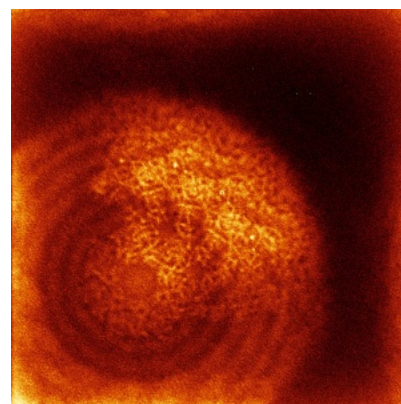
6.4.2 Raw map



X



Y

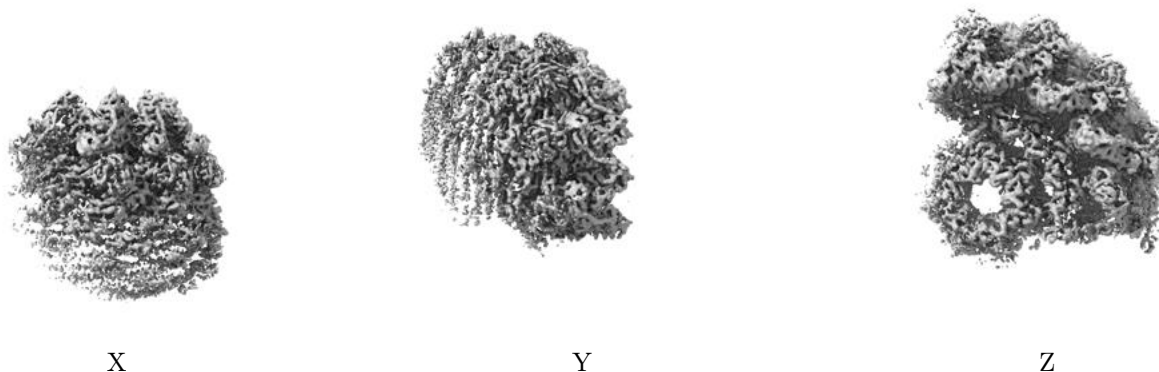


Z

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

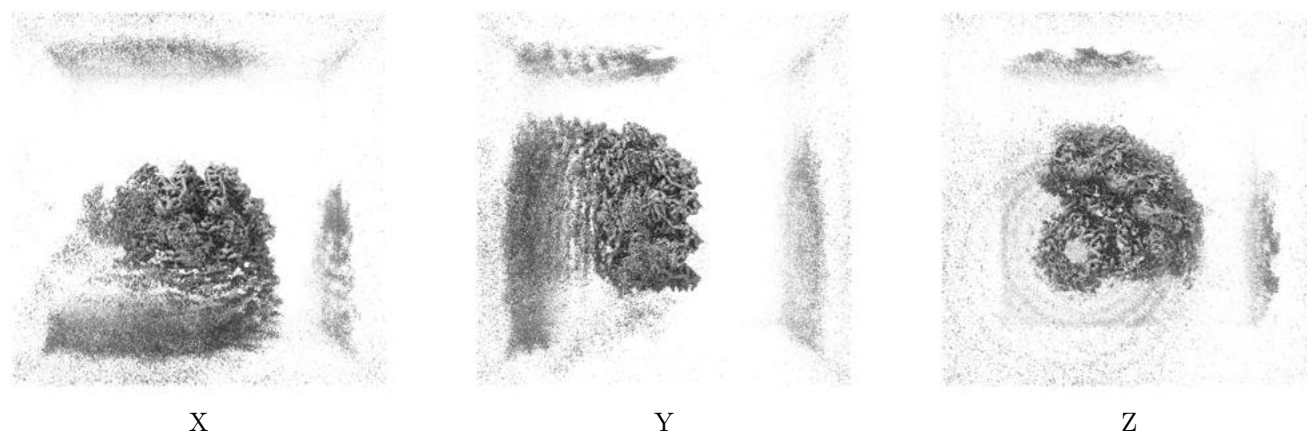
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.294. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

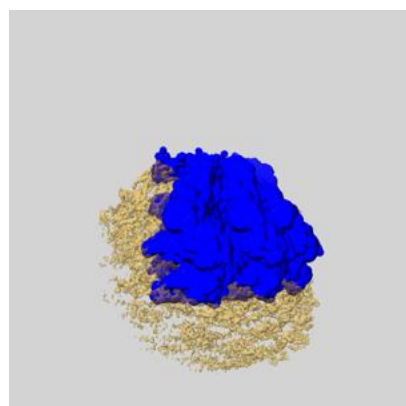
6.6 Mask visualisation [i](#)

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

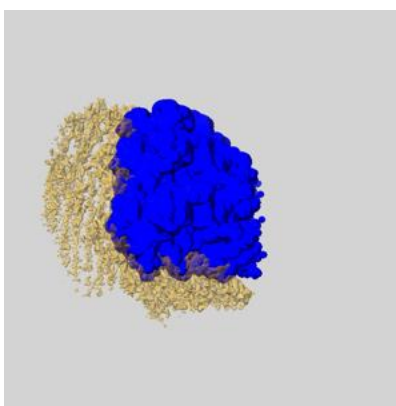
A mask typically either:

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

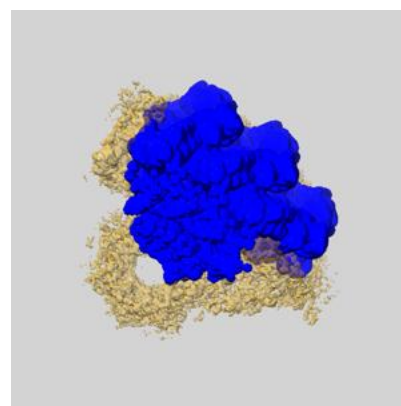
6.6.1 emd_43589_msk_1.map [i](#)



X



Y

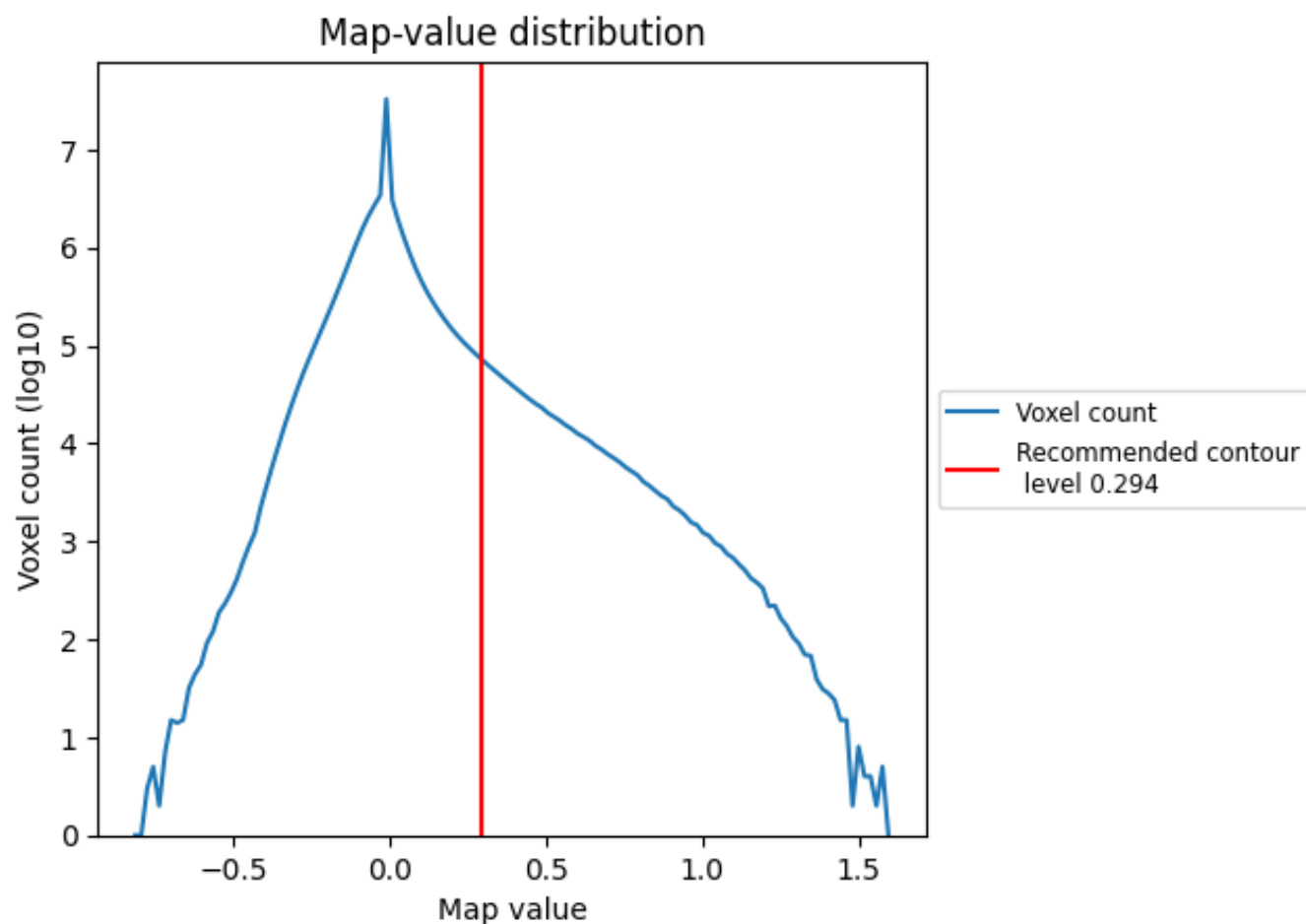


Z

7 Map analysis [i](#)

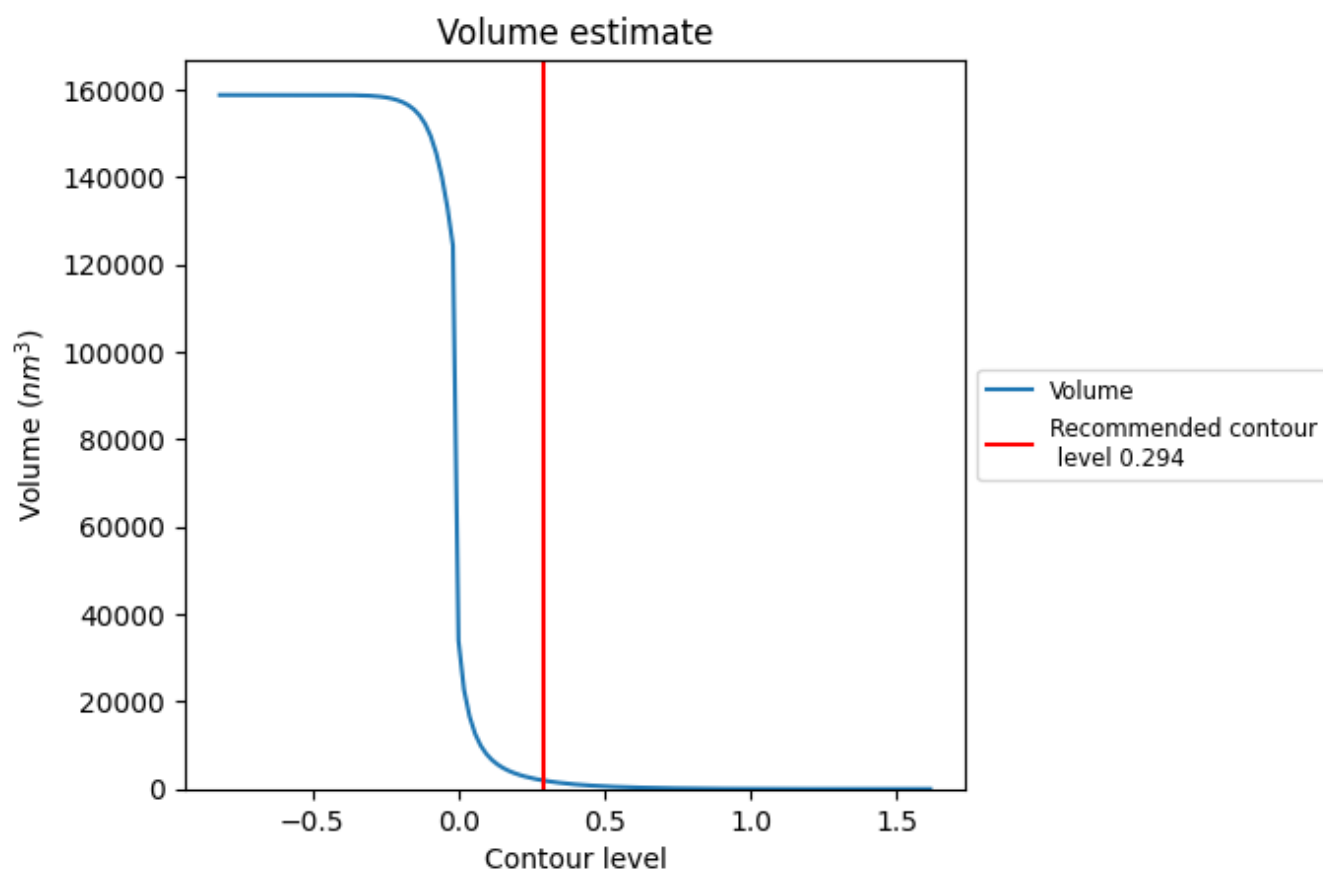
This section contains the results of statistical analysis of the map.

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.

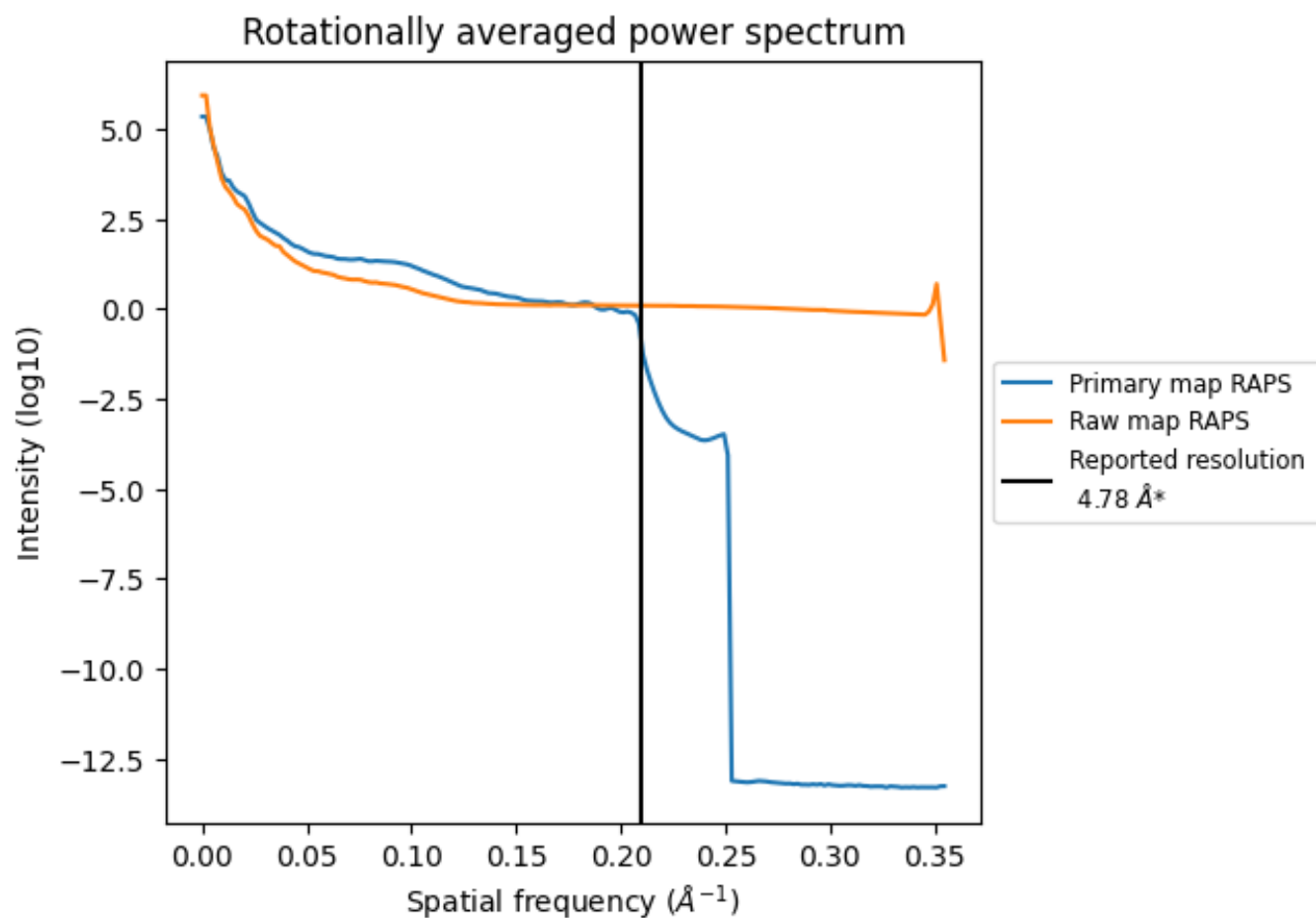
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1916 nm³; this corresponds to an approximate mass of 1731 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 ⓘ

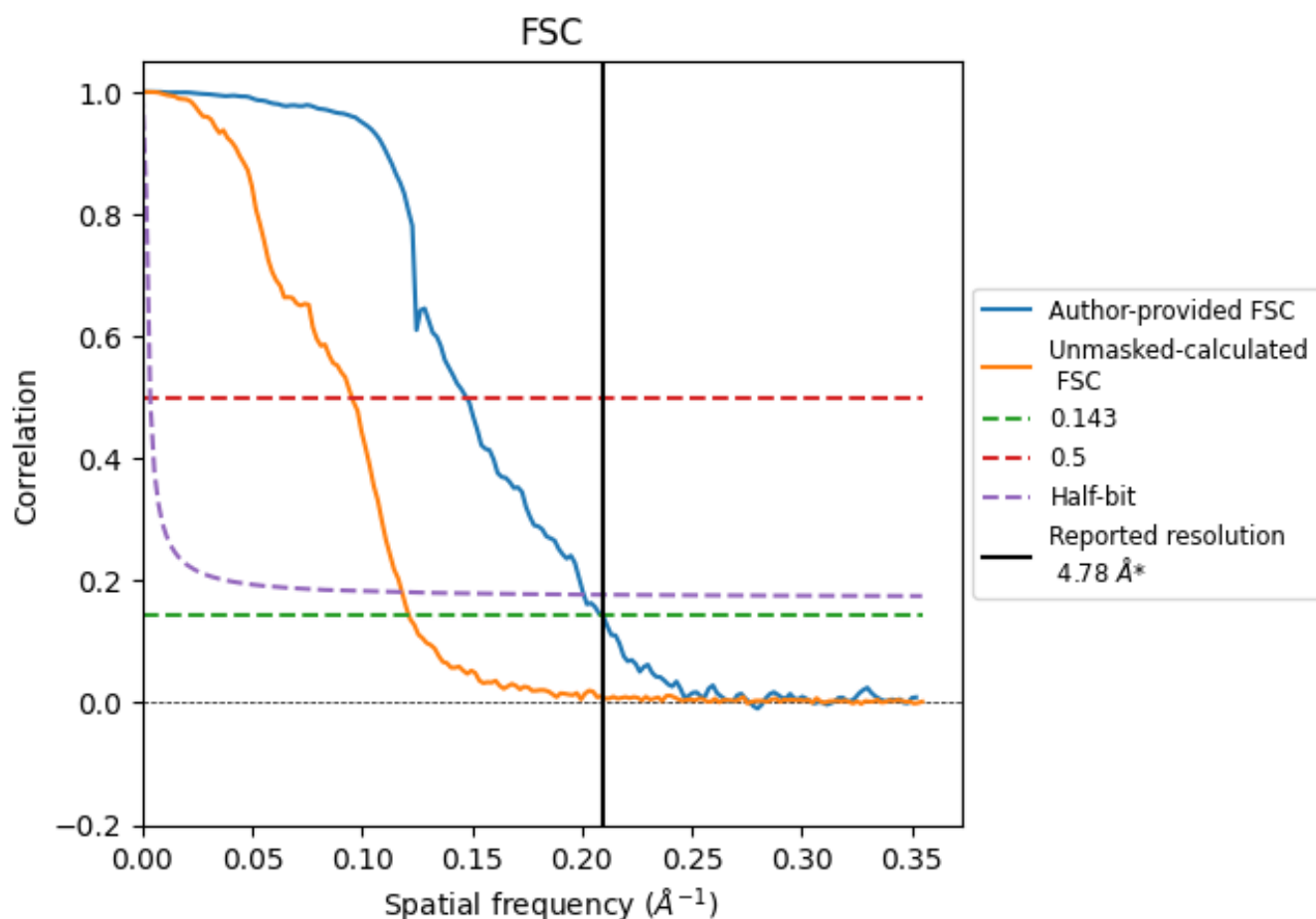


*Reported resolution corresponds to spatial frequency of 0.209 \AA^{-1}

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 0.209 \AA^{-1}

8.2 Resolution estimates [i](#)

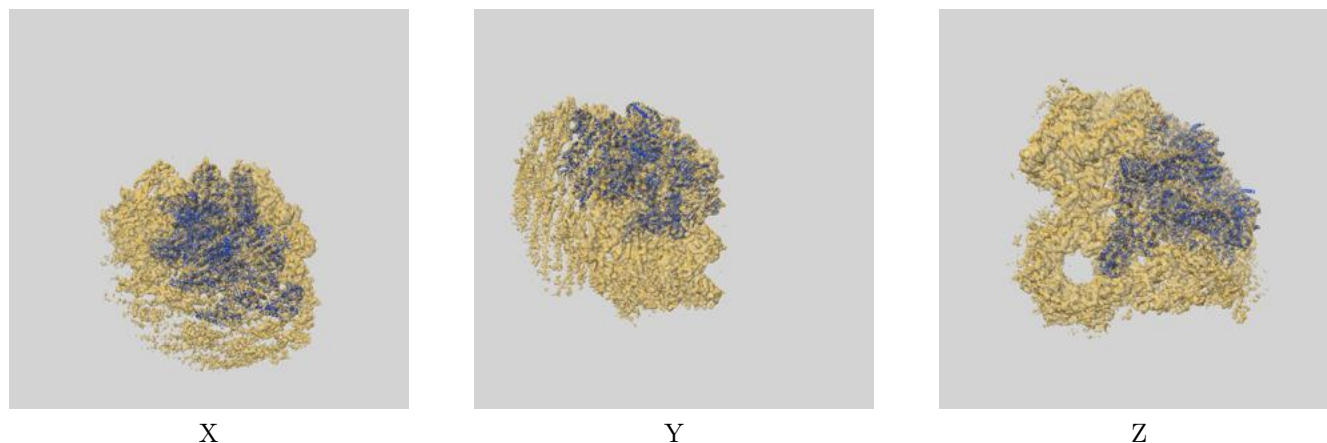
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.78	-	-
Author-provided FSC curve	4.78	6.78	4.98
Unmasked-calculated*	8.25	10.49	8.47

*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 8.25 differs from the reported value 4.78 by more than 10 %

9 Map-model fit [i](#)

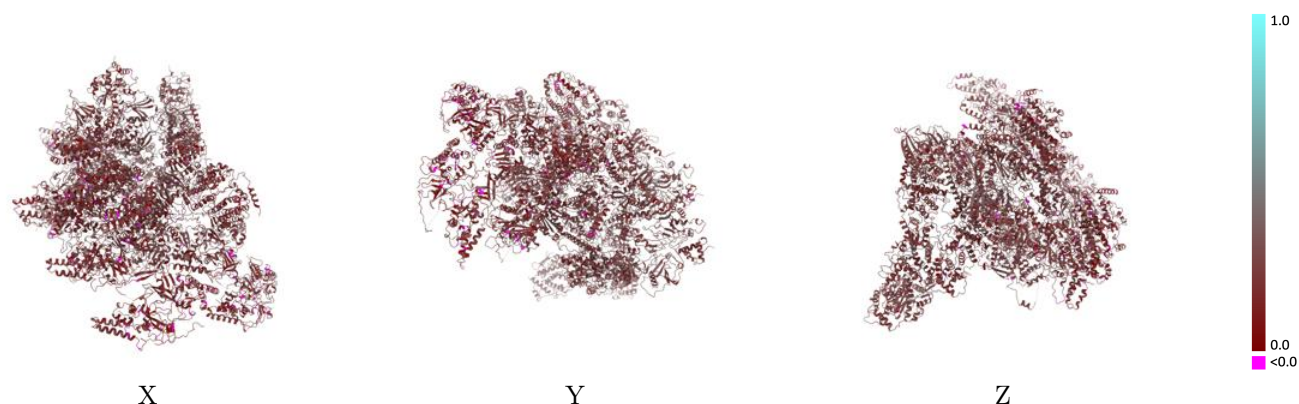
This section contains information regarding the fit between EMDB map EMD-43589 and PDB model 8VWJ. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



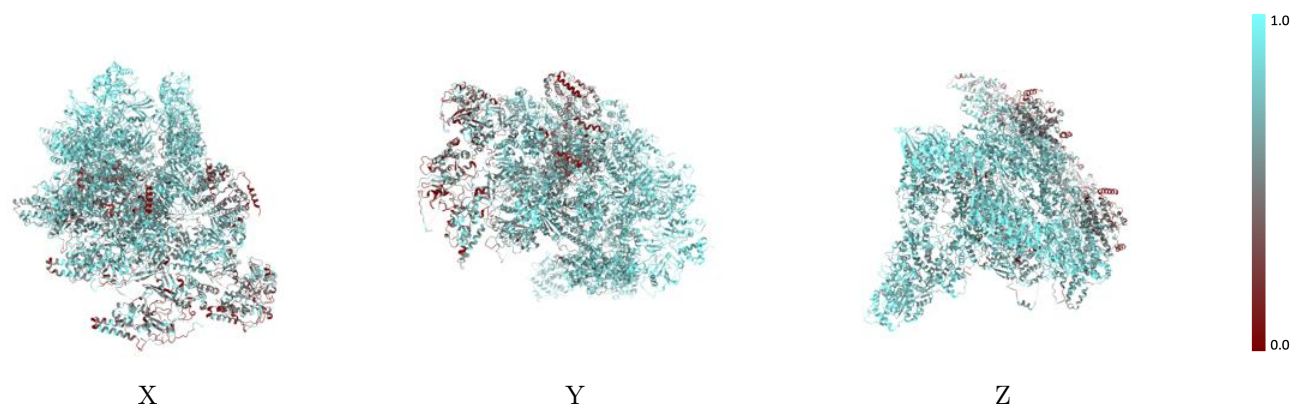
The images above show the 3D surface view of the map at the recommended contour level 0.294 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



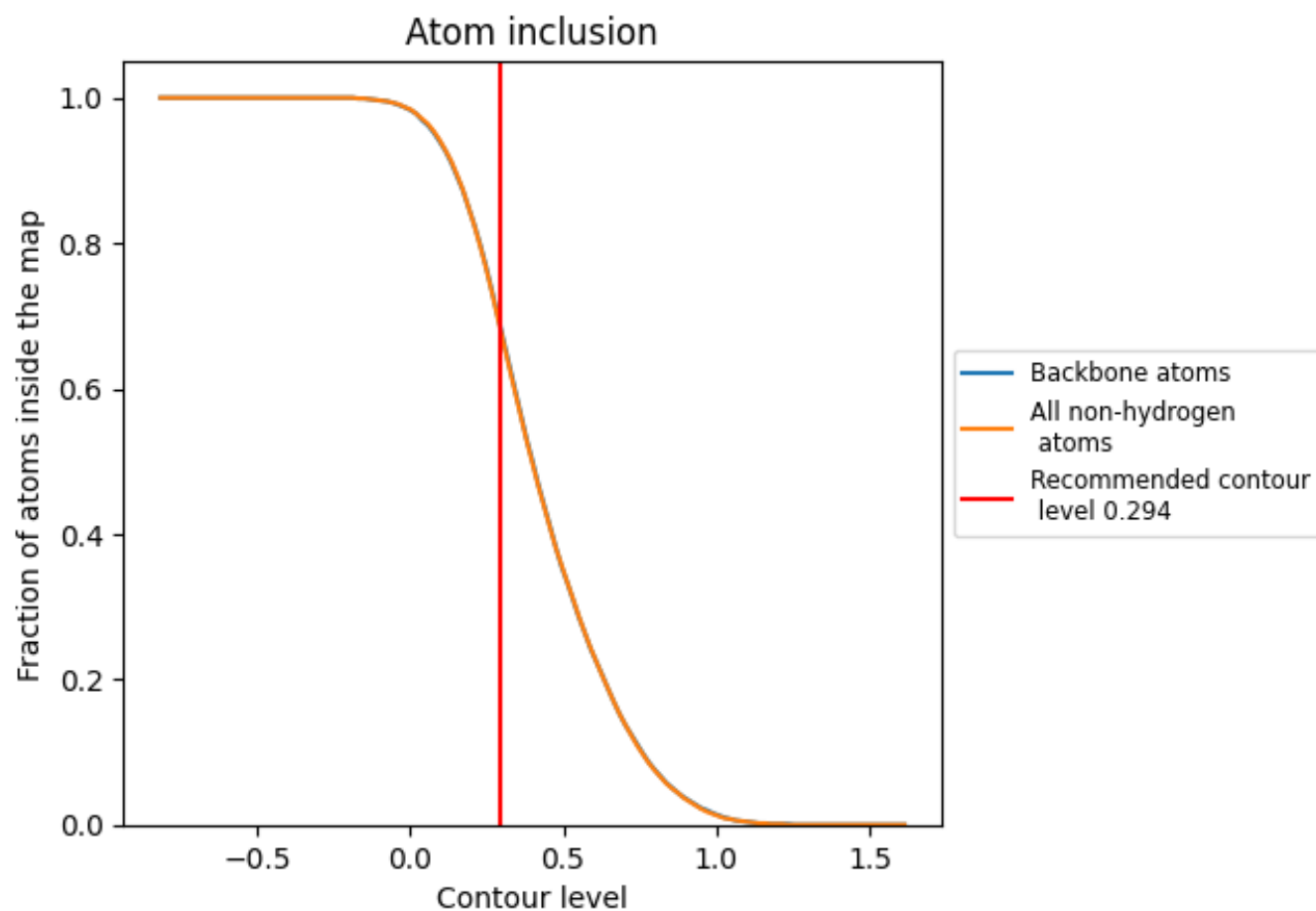
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.294).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 68% 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 (0.294) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6830	 0.2430
A	 0.4870	 0.2150
B	 0.4540	 0.2090
C	 0.6940	 0.2290
D	 0.7220	 0.2420
E	 0.7760	 0.2510
F	 0.7540	 0.2490
G	 0.4180	 0.2260
H	 0.5000	 0.2250
I	 0.7290	 0.2320
J	 0.6760	 0.2520
K	 0.7280	 0.2600
L	 0.7540	 0.2520
M	 0.7460	 0.2780
N	 0.8160	 0.2950
O	 0.8560	 0.2900
P	 0.5880	 0.2400
Q	 0.7720	 0.2690
R	 0.8260	 0.2570
S	 0.7400	 0.2780
T	 0.8020	 0.2620
V	 0.5130	 0.1940
W	 0.5030	 0.1780
X	 0.6660	 0.2190
Y	 0.7400	 0.2290
Z	 0.7740	 0.2330
a	 0.6780	 0.2270
b	 0.4070	 0.2100
c	 0.5210	 0.2020
d	 0.7930	 0.2090
e	 0.6490	 0.2340
f	 0.7100	 0.2310
g	 0.7480	 0.2430
h	 0.7460	 0.2710
i	 0.8510	 0.2690



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.8590	 0.2740
k	 0.5910	 0.2330