



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 05:27 PM JST

PDB ID : 7BR7
EMDB ID : EMD-30158
Title : Epstein-Barr virus, C1 portal-proximal penton vertex, CATC binding
Authors : Li, Z.; Yu, X.
Deposited on : 2020-03-26
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

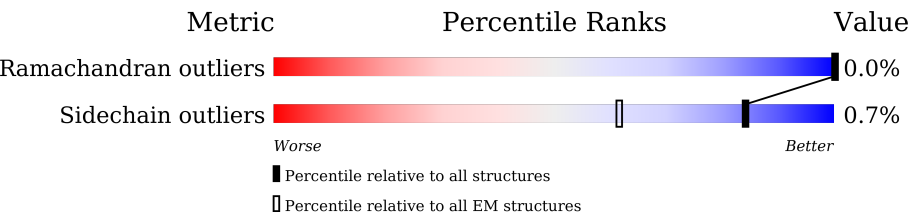
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 4.30 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	154571	4023
Sidechain outliers	154315	3826

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	G	570	<div><div>9% 14% 85%</div></div>
1	K	570	<div><div>7% 12% 88%</div></div>
2	C	507	<div><div>33% 66% 32%</div></div>
3	B	3149	<div><div> 99%</div></div>
3	O	3149	<div><div> 99%</div></div>
4	2	176	<div><div>32% 40% 58%</div></div>
4	Y	176	<div><div>25% 41% 58%</div></div>
4	Z	176	<div><div>27% 41% 58%</div></div>
4	m	176	<div><div>38% 38% 60%</div></div>

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Mol	Chain	Length	Quality of chain
4	y	176	
5	S	1381	
5	T	1381	
5	W	1381	
5	l	1381	
5	x	1381	
6	5	364	
6	e	364	
7	6	301	
7	7	301	
7	f	301	
7	g	301	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 73138 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	68	Total	C	N	O	S	0	0
			563	343	113	104	3		
1	G	84	Total	C	N	O	S	0	0
			675	412	135	125	3		

- Molecule 2 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	346	Total	C	N	O	S	0	0
			2705	1733	482	478	12		

- Molecule 3 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	35	Total	C	N	O	0	0
			301	192	61	48		
3	O	29	Total	C	N	O	0	0
			252	163	49	40		

- Molecule 4 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	m	71	Total	C	N	O	S	0	0
			600	381	111	107	1		
4	Y	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
4	Z	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
4	2	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
4	y	74	Total	C	N	O	S	0	0
			621	394	114	112	1		

- Molecule 5 is a protein called Major capsid protein.

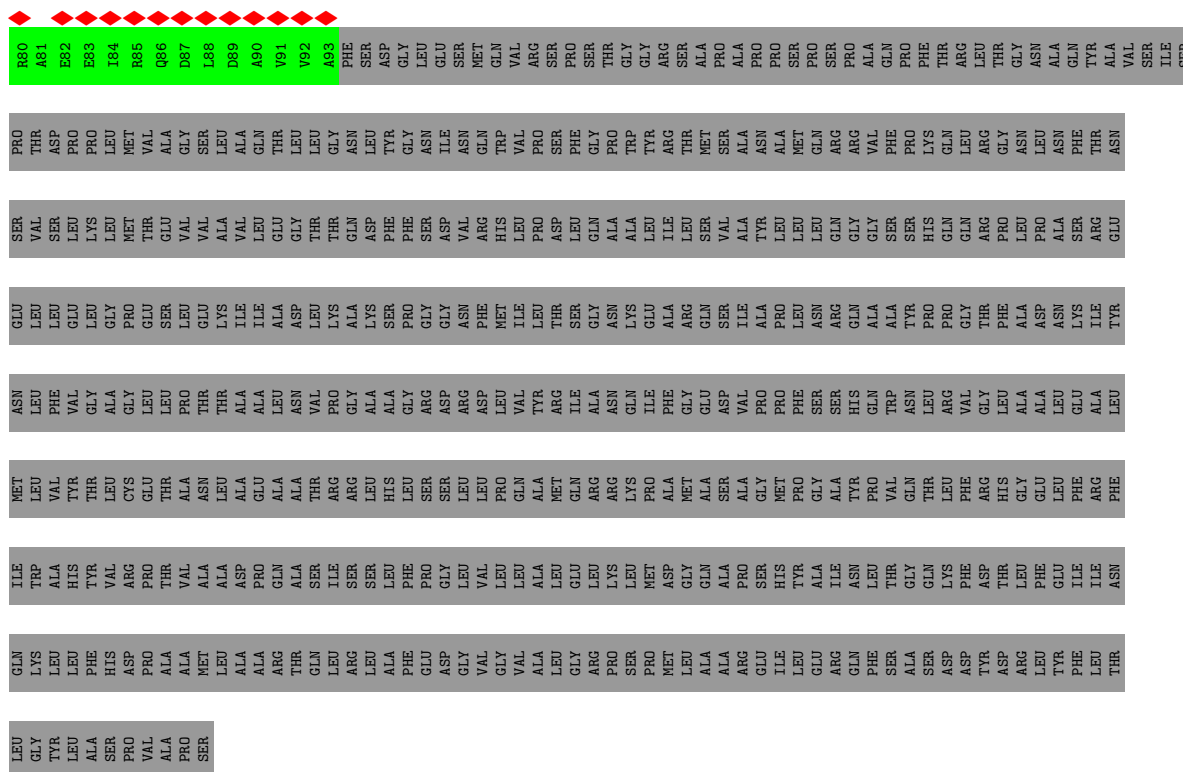
Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	1327	Total	C	N	O	S	0	0
			10455	6644	1812	1940	59		
5	T	1305	Total	C	N	O	S	0	0
			10257	6513	1780	1905	59		
5	W	1331	Total	C	N	O	S	0	0
			10463	6650	1810	1944	59		
5	x	1325	Total	C	N	O	S	0	0
			10404	6607	1803	1935	59		
5	l	1250	Total	C	N	O	S	0	0
			9872	6274	1716	1823	59		

- Molecule 6 is a protein called Triplex capsid protein 1.

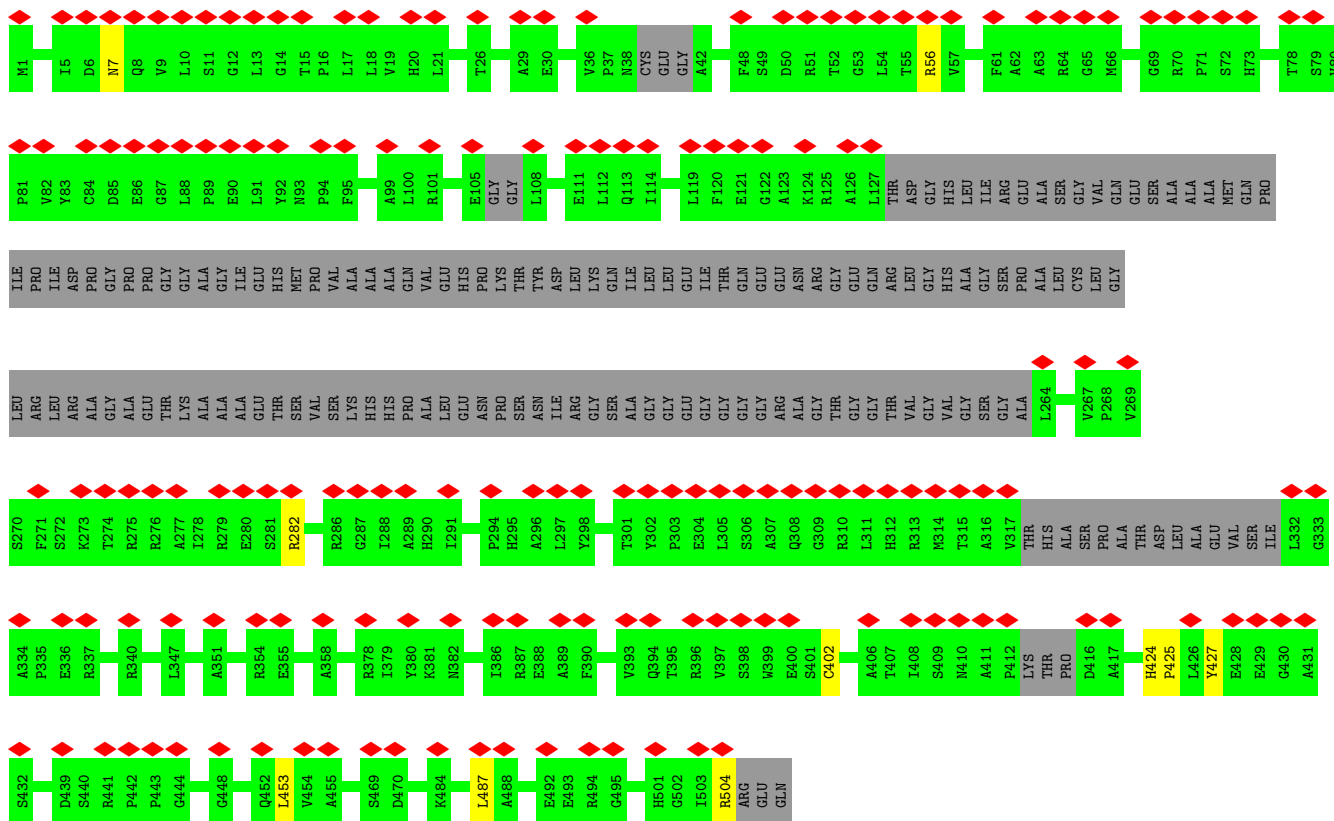
Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	319	Total	C	N	O	S	0	0
			2505	1608	444	446	7		
6	5	313	Total	C	N	O	S	0	0
			2460	1576	438	440	6		

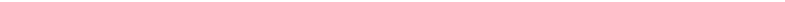
- Molecule 7 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	290	Total	C	N	O	S	0	0
			2279	1466	378	419	16		
7	g	290	Total	C	N	O	S	0	0
			2272	1464	376	414	18		
7	6	297	Total	C	N	O	S	0	0
			2329	1496	385	430	18		
7	7	287	Total	C	N	O	S	0	0
			2262	1452	375	417	18		



- Molecule 2: Capsid vertex component 1



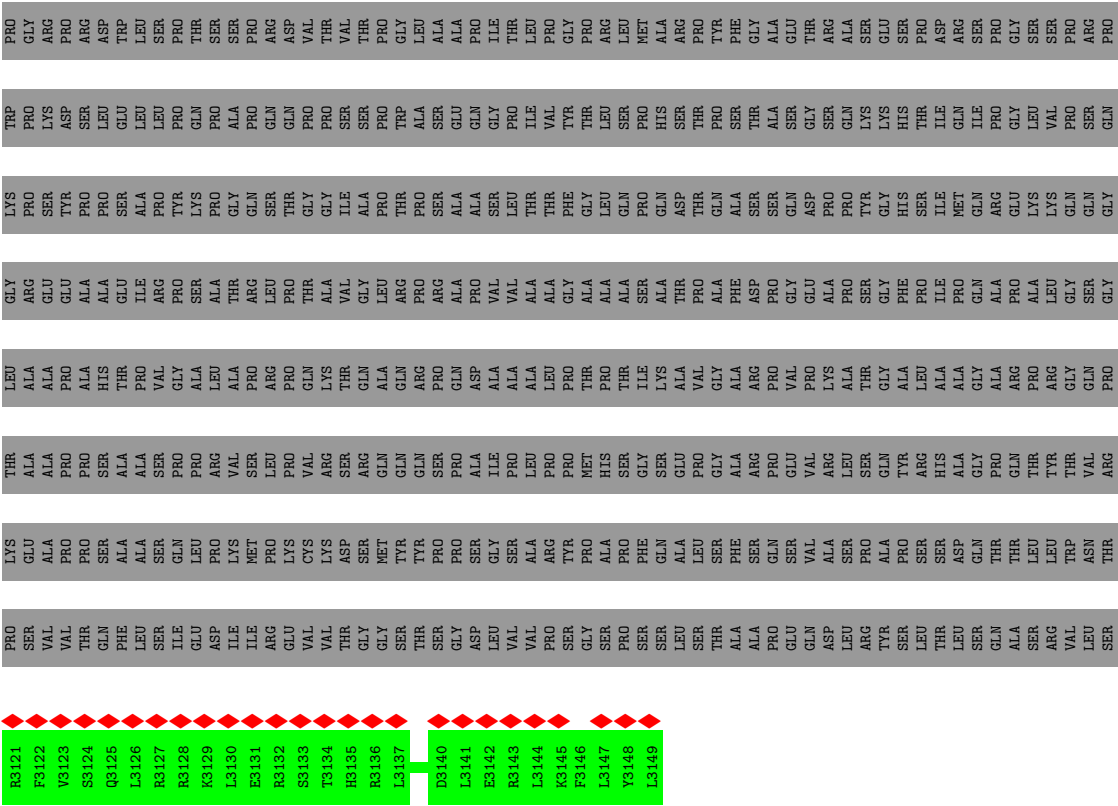
Chain B:  99%



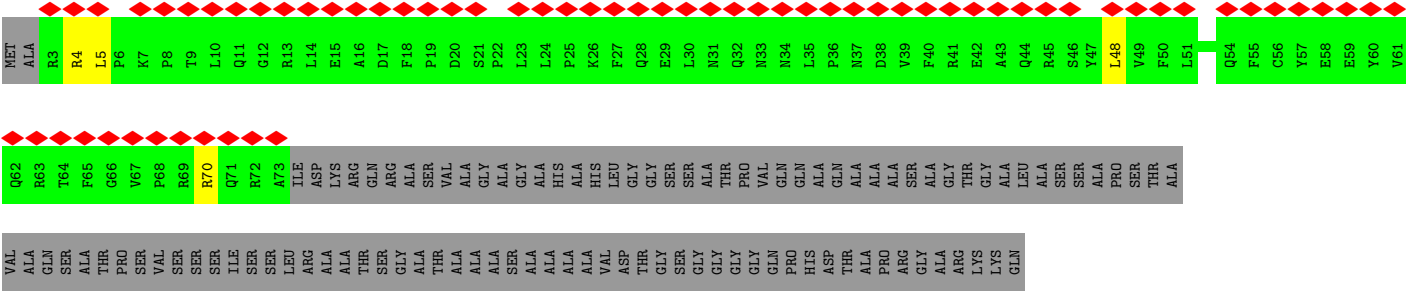




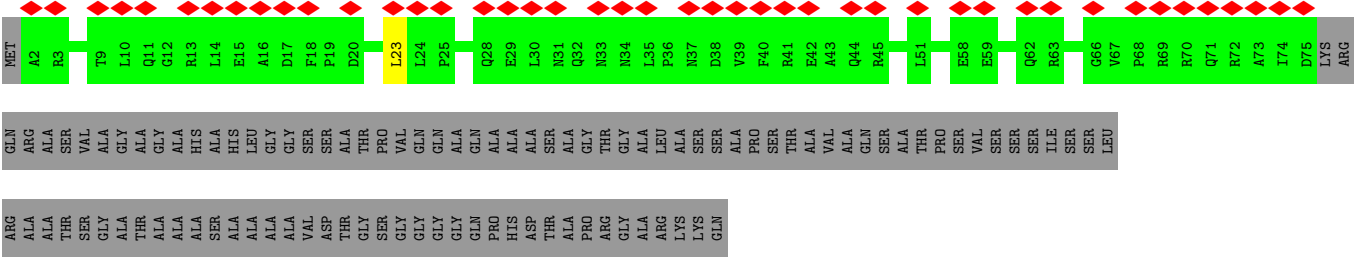




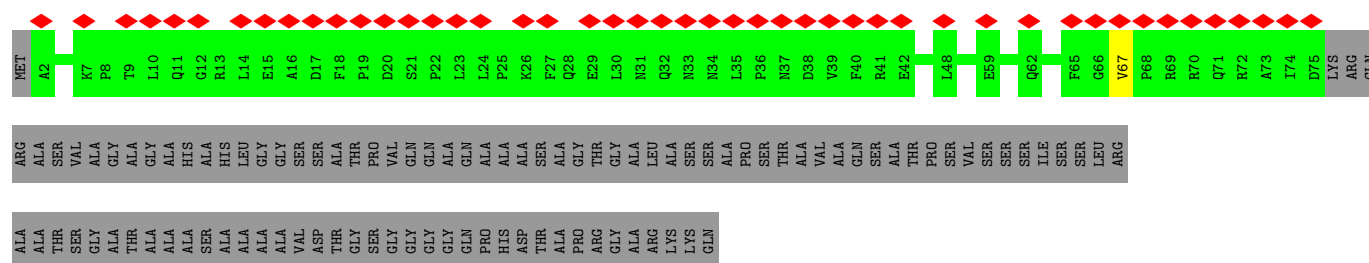
• Molecule 4: Small capsomere-interacting protein

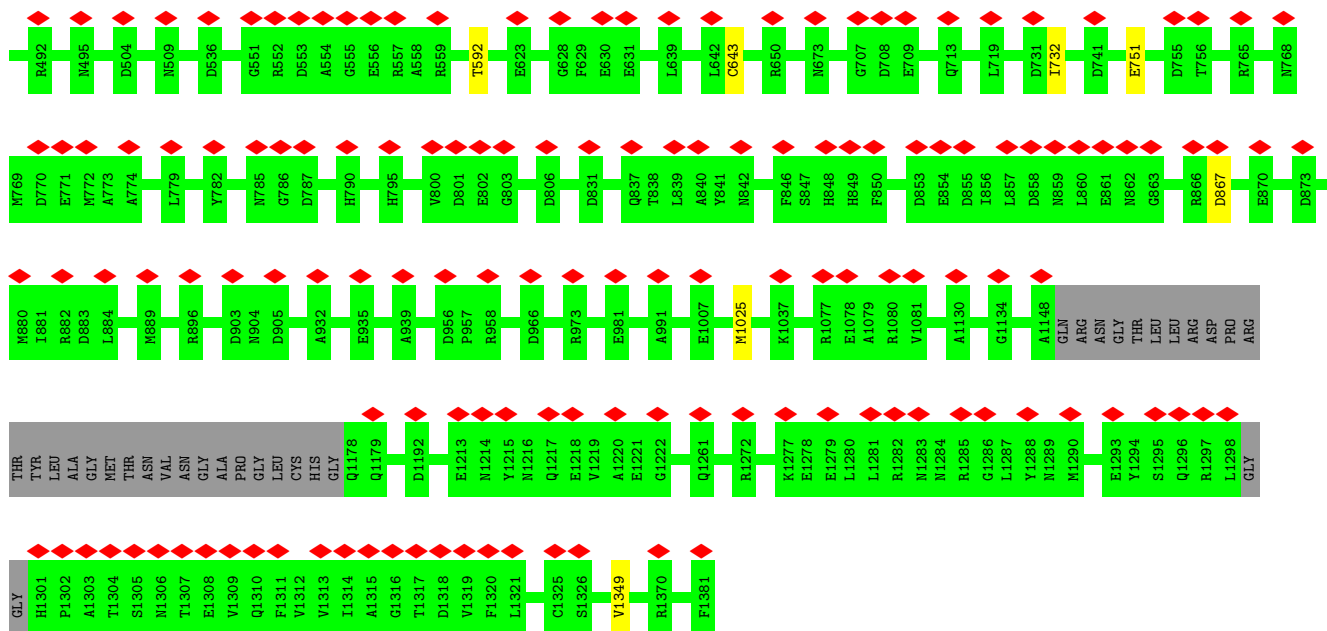


• Molecule 4: Small capsomere-interacting protein

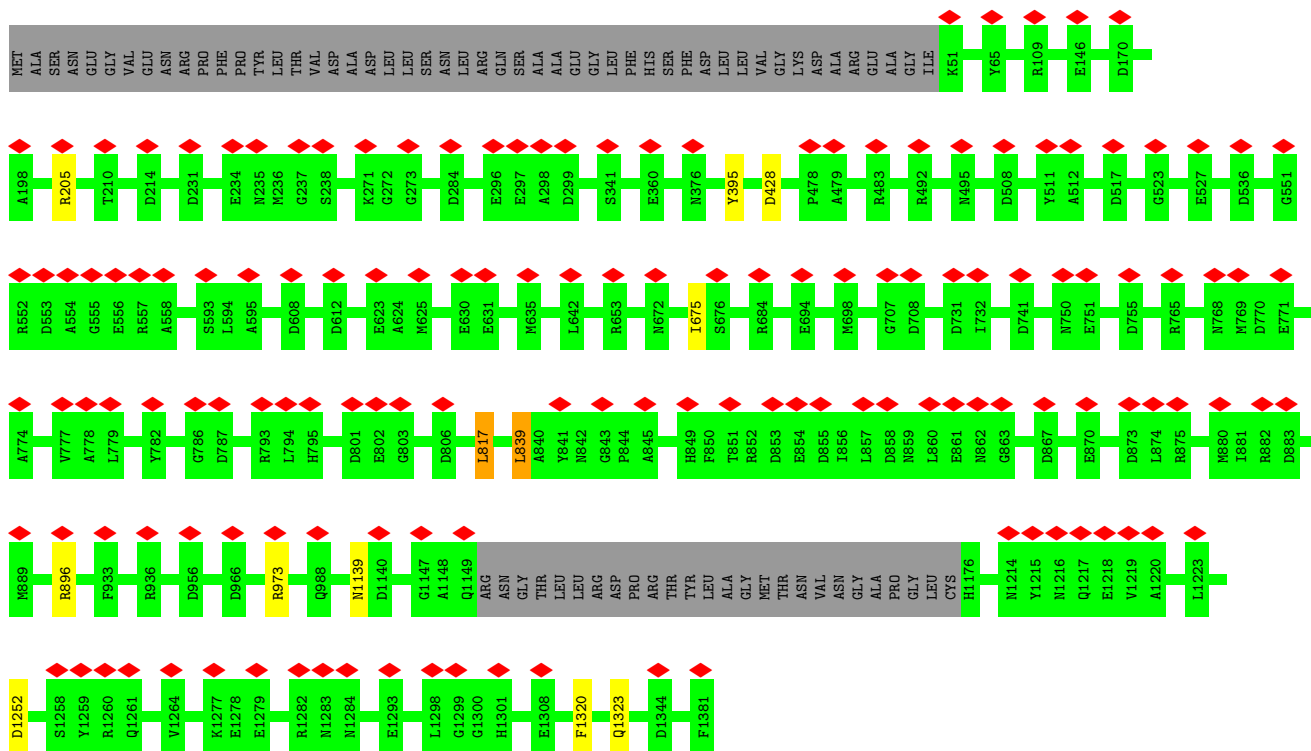


• Molecule 4: Small capsomere-interacting protein



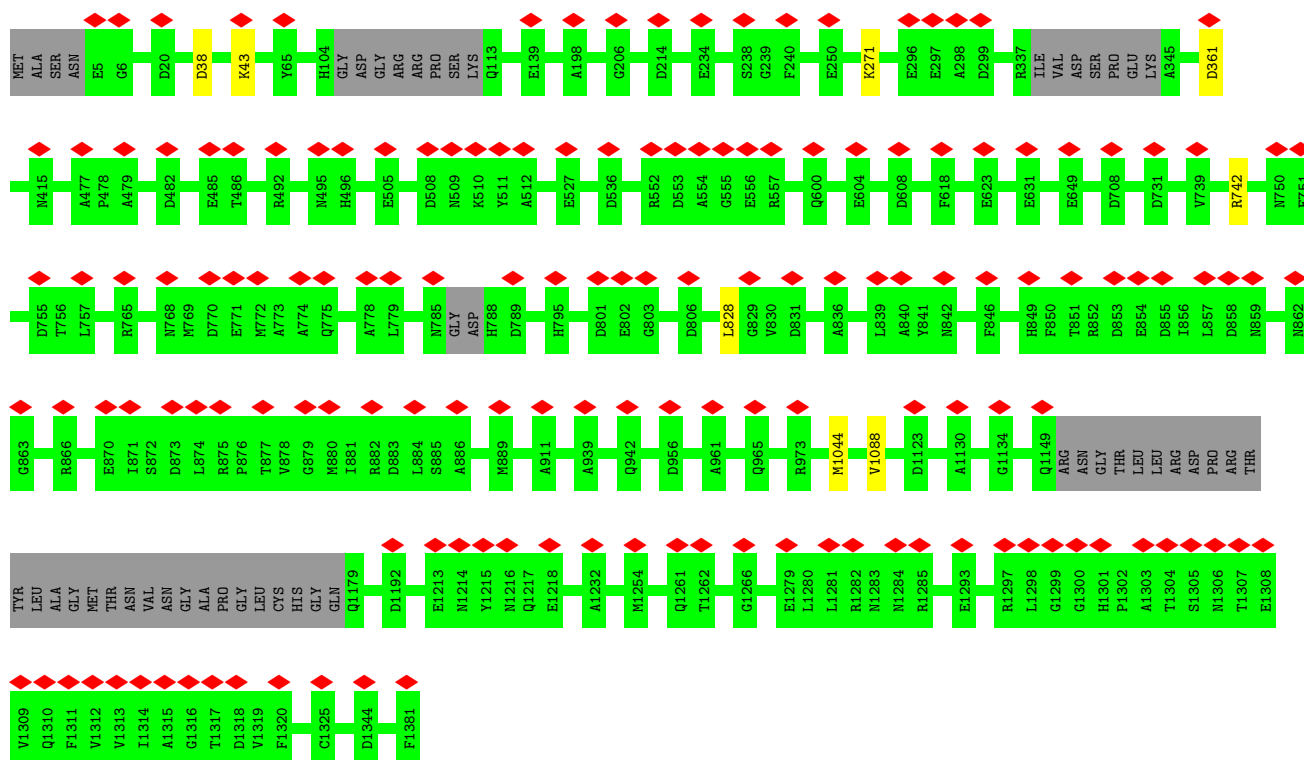


• Molecule 5: Major capsid protein

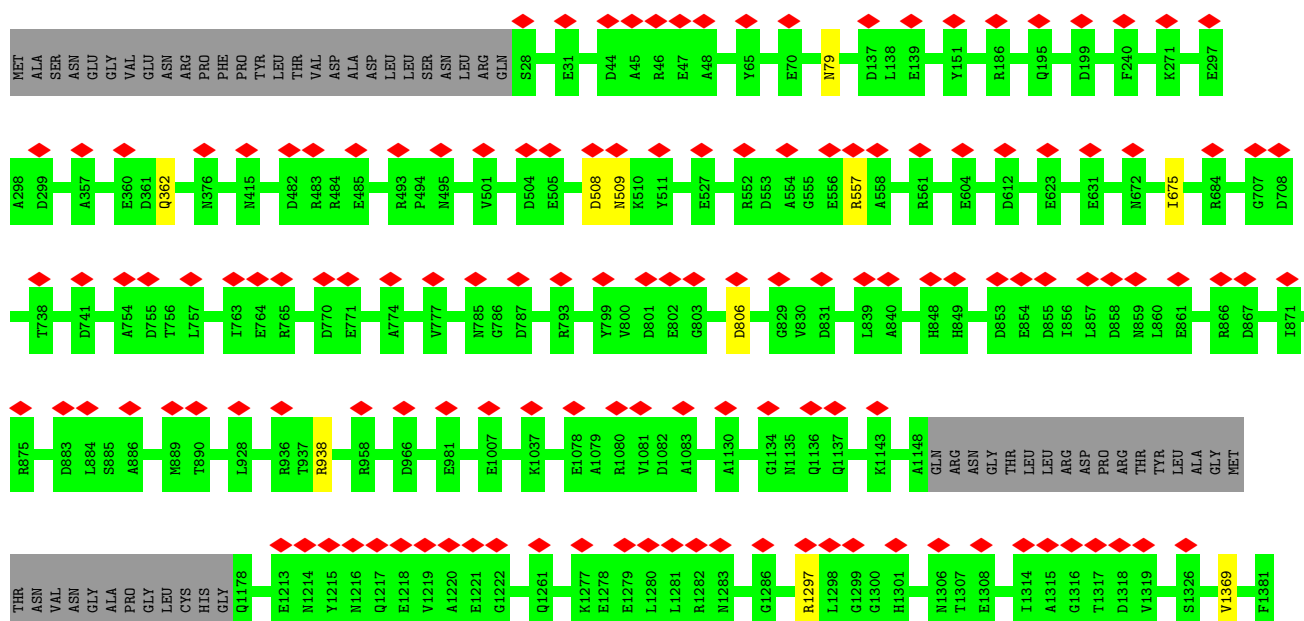


• Molecule 5: Major capsid protein

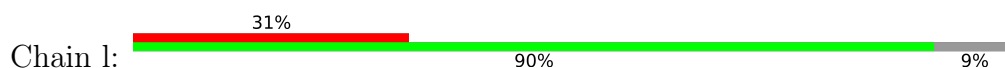


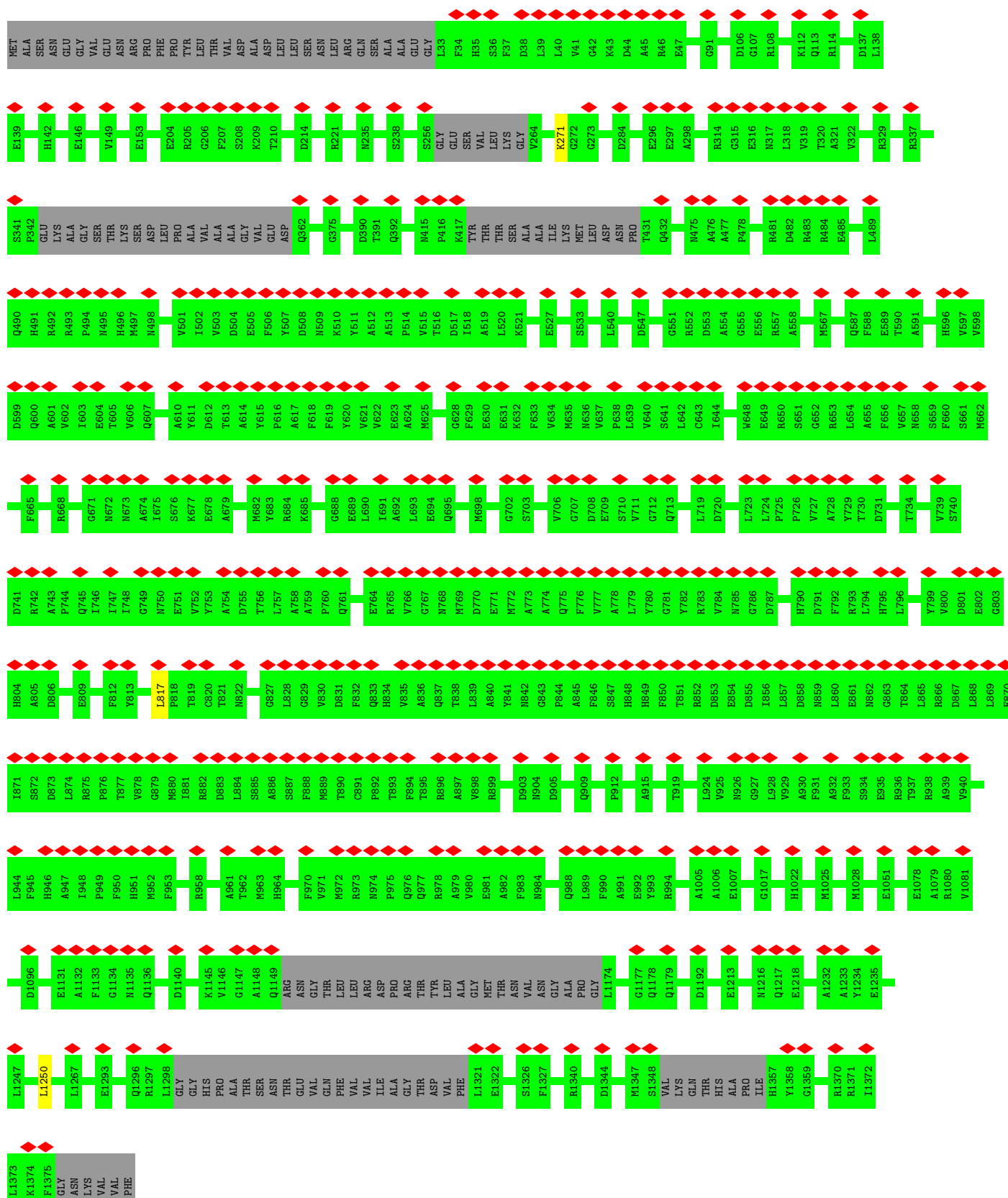


• Molecule 5: Major capsid protein




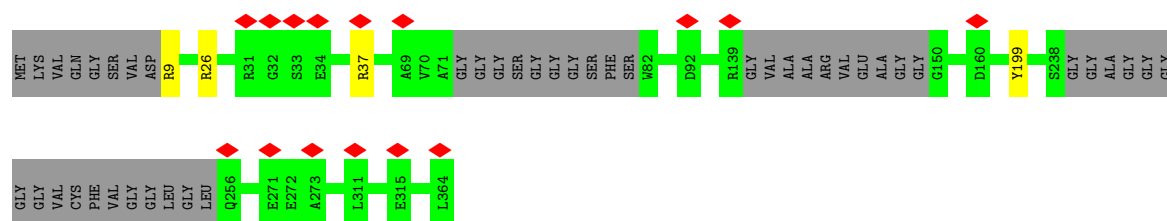
• Molecule 5: Major capsid protein






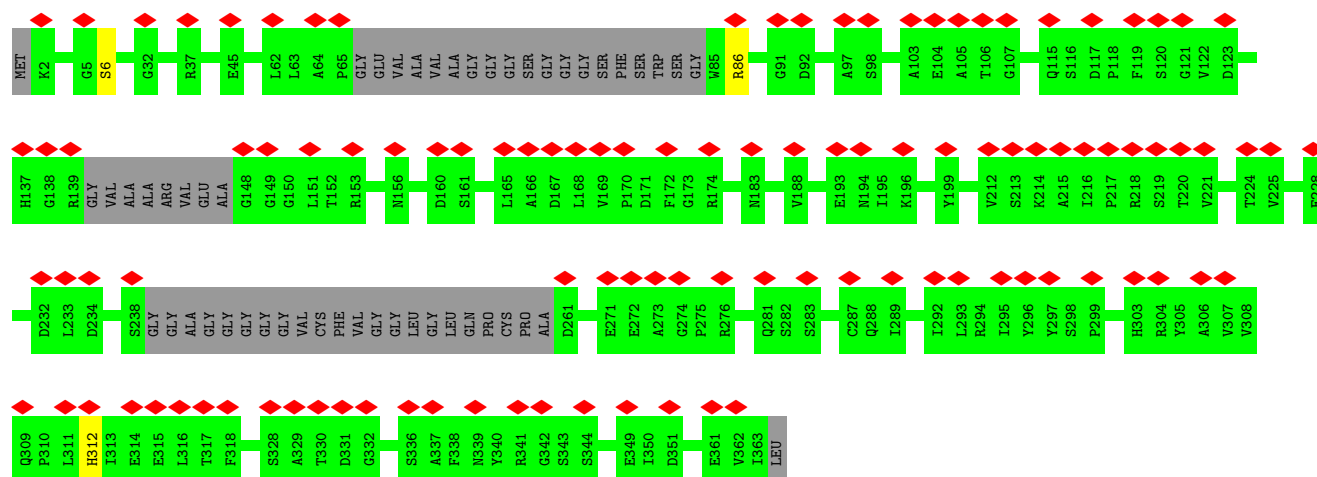
- Molecule 6: Triplex capsid protein 1

Chain e:  87% 12%



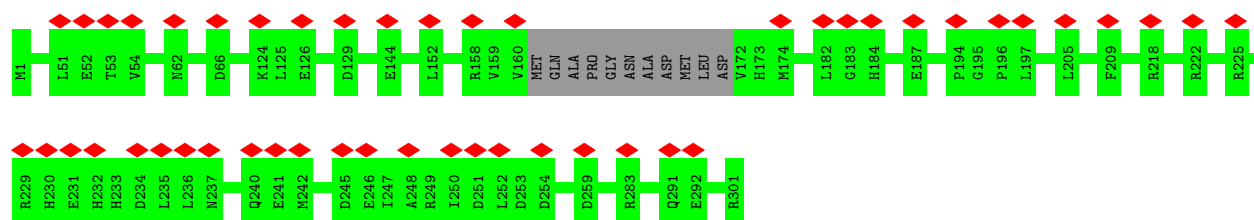
• Molecule 6: Triplex capsid protein 1

Chain 5:  30% 85% 14%



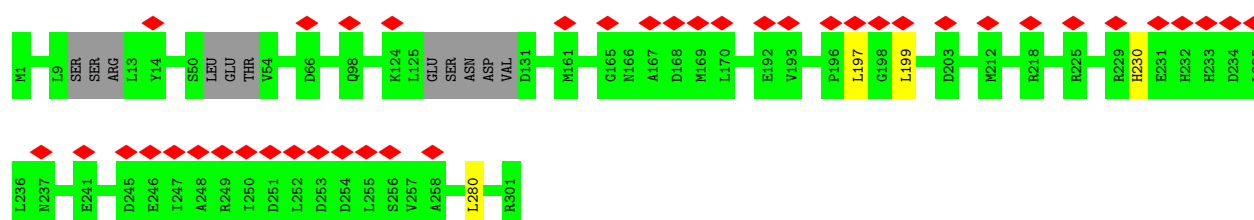
• Molecule 7: Triplex capsid protein 2

Chain f:  16% 96%



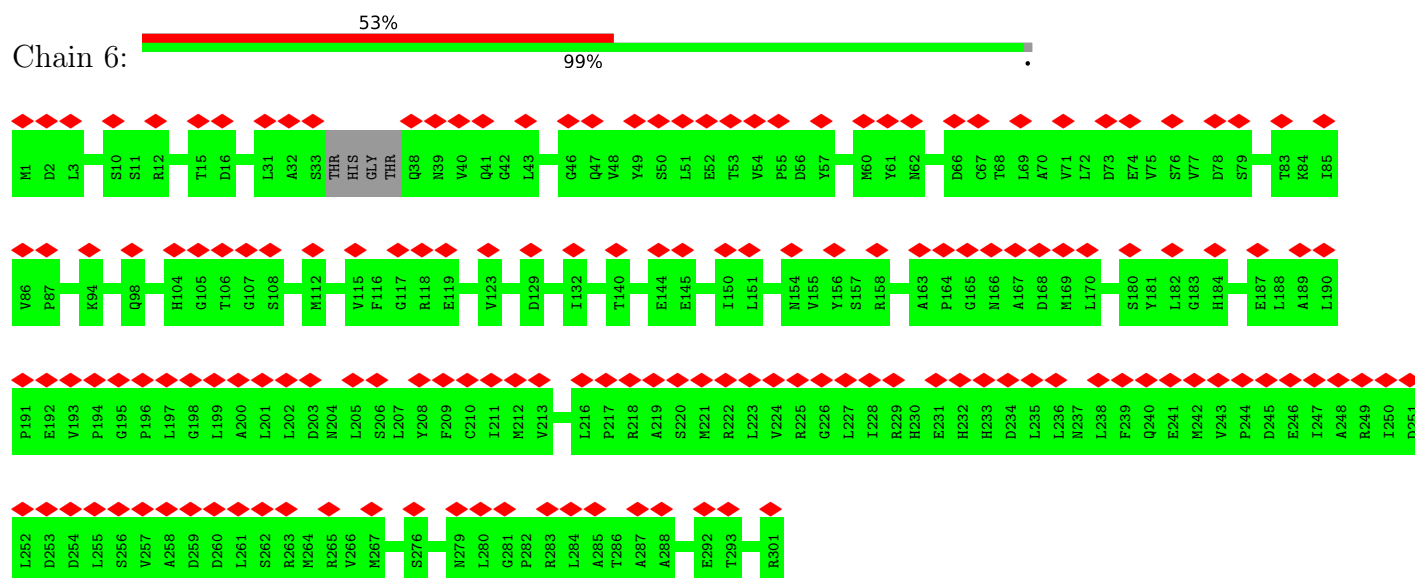
• Molecule 7: Triplex capsid protein 2

Chain g:  14% 95%



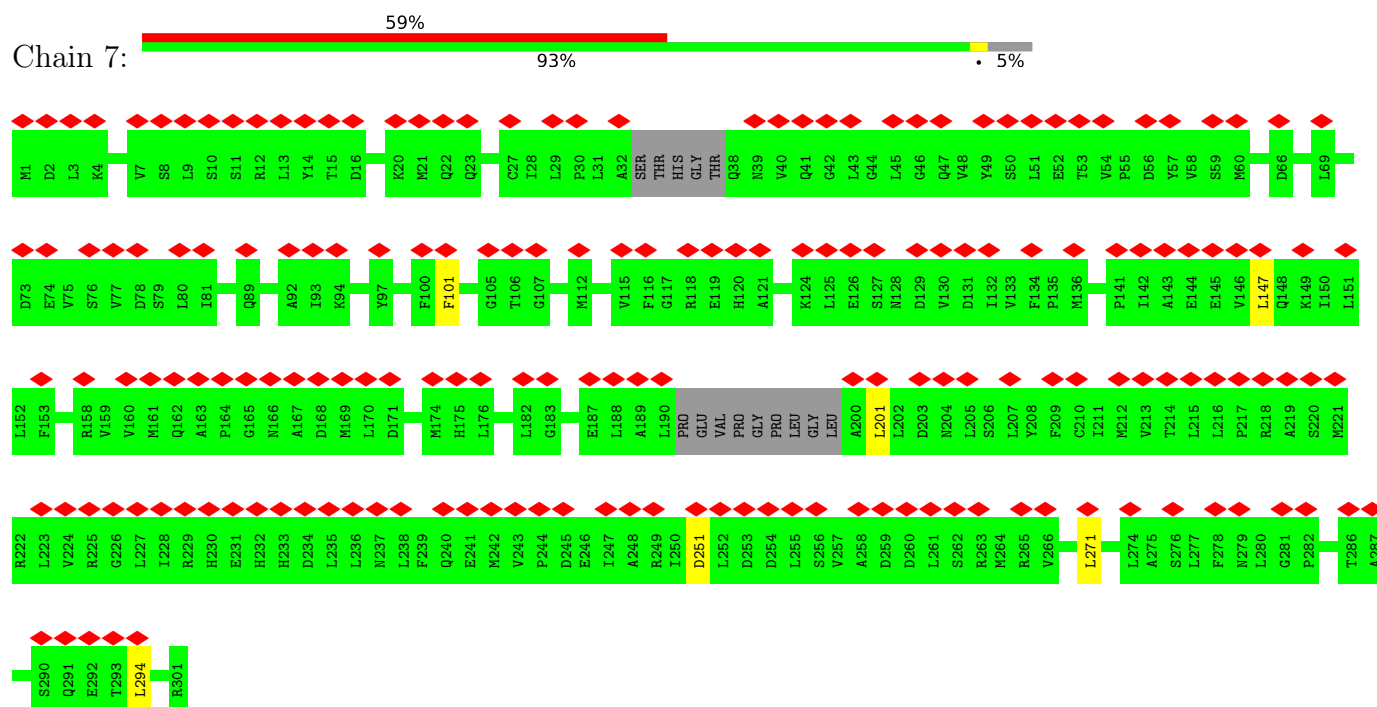
- Molecule 7: Triplex capsid protein 2

Chain 6:



- Molecule 7: Triplex capsid protein 2

Chain 7:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93334	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	392.99997, 392.99997, 392.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	G	0.37	0/684	0.59	0/924
1	K	0.27	0/570	0.59	0/765
2	C	0.46	2/2770 (0.1%)	0.61	2/3763 (0.1%)
3	B	0.25	0/304	0.46	0/404
3	O	0.28	0/255	0.66	0/339
4	2	0.34	0/636	0.67	2/861 (0.2%)
4	Y	0.31	0/636	0.61	1/861 (0.1%)
4	Z	0.31	0/636	0.54	0/861
4	m	0.34	0/615	0.59	1/832 (0.1%)
4	y	0.34	0/636	0.60	0/861
5	S	0.37	1/10699 (0.0%)	0.54	1/14537 (0.0%)
5	T	0.38	1/10499 (0.0%)	0.55	4/14270 (0.0%)
5	W	0.37	0/10706	0.54	3/14549 (0.0%)
5	l	0.34	0/10102	0.54	1/13718 (0.0%)
5	x	0.40	1/10648 (0.0%)	0.55	1/14471 (0.0%)
6	5	0.32	0/2523	0.53	0/3431
6	e	0.36	0/2572	0.53	0/3503
7	6	0.32	0/2377	0.58	0/3236
7	7	0.31	0/2306	0.65	4/3135 (0.1%)
7	f	0.33	0/2327	0.54	0/3169
7	g	0.33	0/2319	0.60	1/3155 (0.0%)
All	All	0.37	5/74820 (0.0%)	0.56	21/101645 (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
4	2	0	1
5	T	0	1
6	5	0	1
7	g	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	425	PRO	N-CA	13.35	1.70	1.47
5	x	362	GLN	C-N	8.97	1.51	1.34
5	T	1323	GLN	C-N	8.89	1.51	1.34
2	C	424	HIS	C-N	5.91	1.45	1.34
5	S	1025	MET	C-N	-5.24	1.22	1.34

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	361	ASP	CB-CG-OD1	8.72	126.15	118.30
5	T	817	LEU	CA-CB-CG	8.15	134.05	115.30
2	C	425	PRO	CA-N-CD	-7.99	100.32	111.50
7	7	271	LEU	CA-CB-CG	7.04	131.48	115.30
5	x	806	ASP	CB-CG-OD1	6.88	124.49	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	2	66	GLY	Peptide
6	5	312	HIS	Peptide
5	T	817	LEU	Peptide
7	g	230	HIS	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	82/570 (14%)	74 (90%)	8 (10%)	0	100	100
1	K	66/570 (12%)	65 (98%)	1 (2%)	0	100	100
2	C	334/507 (66%)	318 (95%)	16 (5%)	0	100	100
3	B	33/3149 (1%)	33 (100%)	0	0	100	100
3	O	27/3149 (1%)	26 (96%)	1 (4%)	0	100	100
4	2	72/176 (41%)	61 (85%)	11 (15%)	0	100	100
4	Y	72/176 (41%)	66 (92%)	6 (8%)	0	100	100
4	Z	72/176 (41%)	67 (93%)	5 (7%)	0	100	100
4	m	69/176 (39%)	66 (96%)	3 (4%)	0	100	100
4	y	72/176 (41%)	62 (86%)	10 (14%)	0	100	100
5	S	1319/1381 (96%)	1236 (94%)	83 (6%)	0	100	100
5	T	1301/1381 (94%)	1201 (92%)	100 (8%)	0	100	100
5	W	1321/1381 (96%)	1226 (93%)	95 (7%)	0	100	100
5	l	1236/1381 (90%)	1162 (94%)	74 (6%)	0	100	100
5	x	1321/1381 (96%)	1227 (93%)	94 (7%)	0	100	100
6	5	305/364 (84%)	288 (94%)	17 (6%)	0	100	100
6	e	311/364 (85%)	291 (94%)	20 (6%)	0	100	100
7	6	293/301 (97%)	280 (96%)	13 (4%)	0	100	100
7	7	281/301 (93%)	254 (90%)	26 (9%)	1 (0%)	34	72
7	f	286/301 (95%)	272 (95%)	14 (5%)	0	100	100
7	g	282/301 (94%)	259 (92%)	23 (8%)	0	100	100
All	All	9155/17662 (52%)	8534 (93%)	620 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	7	101	PHE

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	G	70/465 (15%)	68 (97%)	2 (3%)	42	64
1	K	59/465 (13%)	59 (100%)	0	100	100
2	C	288/400 (72%)	281 (98%)	7 (2%)	49	69
3	B	33/2539 (1%)	33 (100%)	0	100	100
3	O	27/2539 (1%)	27 (100%)	0	100	100
4	2	68/128 (53%)	67 (98%)	1 (2%)	65	80
4	Y	68/128 (53%)	68 (100%)	0	100	100
4	Z	68/128 (53%)	67 (98%)	1 (2%)	65	80
4	m	66/128 (52%)	63 (96%)	3 (4%)	27	54
4	y	68/128 (53%)	67 (98%)	1 (2%)	65	80
5	S	1133/1171 (97%)	1128 (100%)	5 (0%)	91	94
5	T	1111/1171 (95%)	1103 (99%)	8 (1%)	84	90
5	W	1132/1171 (97%)	1127 (100%)	5 (0%)	91	94
5	l	1069/1171 (91%)	1067 (100%)	2 (0%)	93	96
5	x	1125/1171 (96%)	1117 (99%)	8 (1%)	84	90
6	5	264/289 (91%)	262 (99%)	2 (1%)	81	89
6	e	268/289 (93%)	264 (98%)	4 (2%)	65	80
7	6	264/267 (99%)	264 (100%)	0	100	100
7	7	256/267 (96%)	255 (100%)	1 (0%)	91	94
7	f	259/267 (97%)	259 (100%)	0	100	100
7	g	256/267 (96%)	254 (99%)	2 (1%)	81	89
All	All	7952/14549 (55%)	7900 (99%)	52 (1%)	84	90

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	W	271	LYS
5	x	557	ARG
6	5	6	SER
5	W	742	ARG
5	x	79	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123

such sidechains are listed below:

Mol	Chain	Res	Type
5	W	964	HIS
5	l	997	HIS
5	x	581	GLN
5	l	926	ASN
6	5	356	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

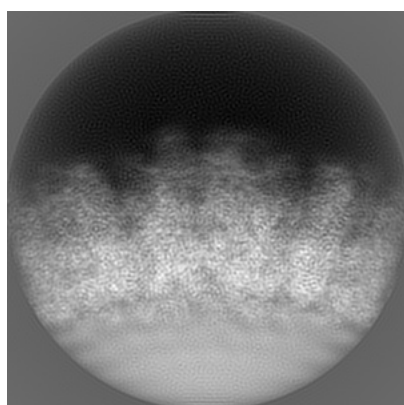
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30158. These allow visual inspection of the internal detail of the map and identification of artifacts.

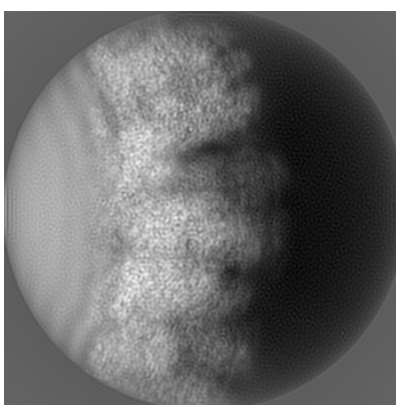
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

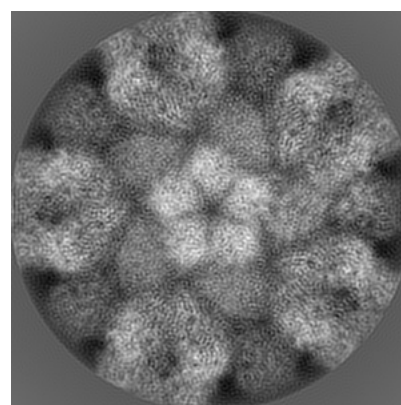
6.1.1 Primary map



X



Y

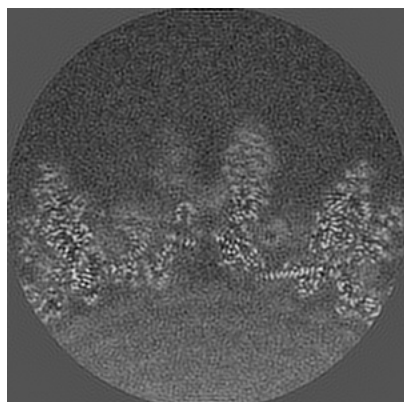


Z

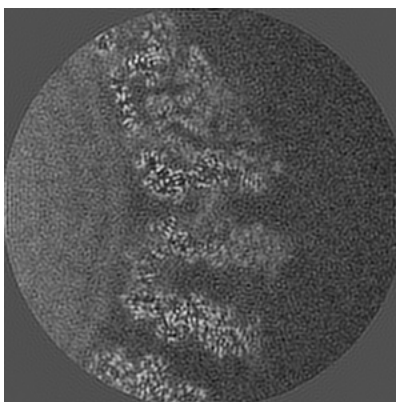
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

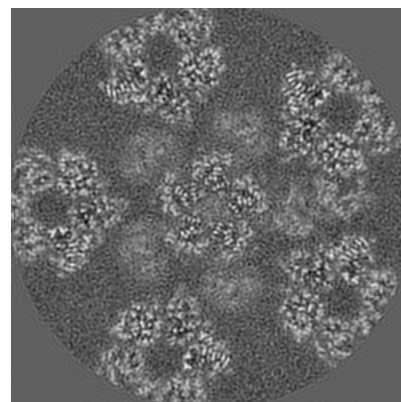
6.2.1 Primary map



X Index: 150



Y Index: 150

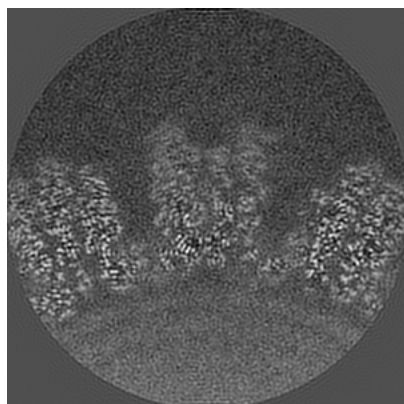


Z Index: 150

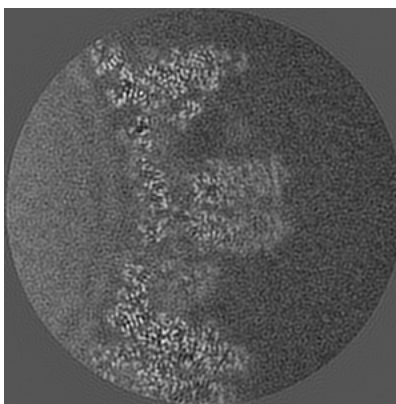
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

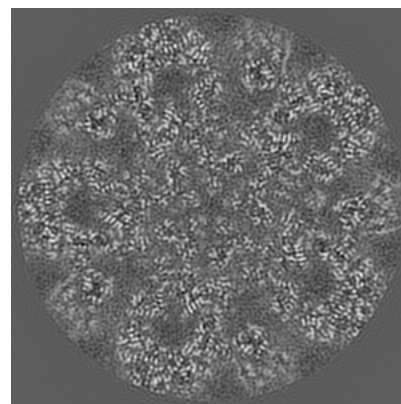
6.3.1 Primary map



X Index: 137



Y Index: 122



Z Index: 107

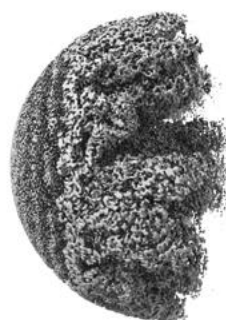
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

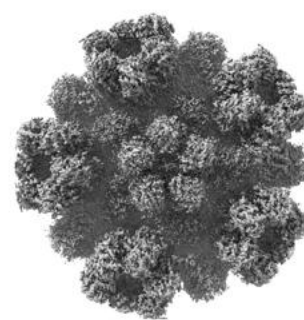
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

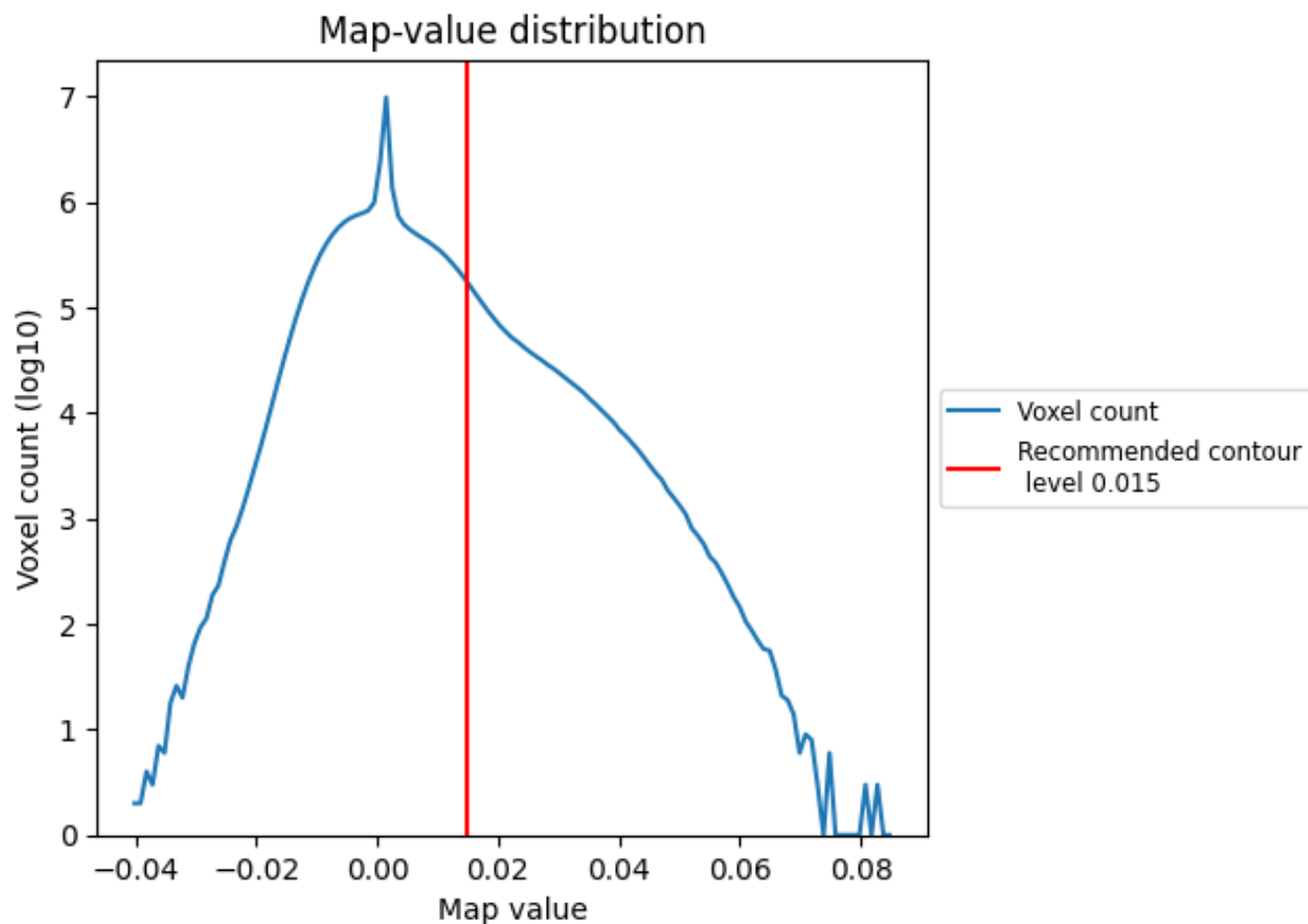
6.5 Mask visualisation

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

7 Map analysis [i](#)

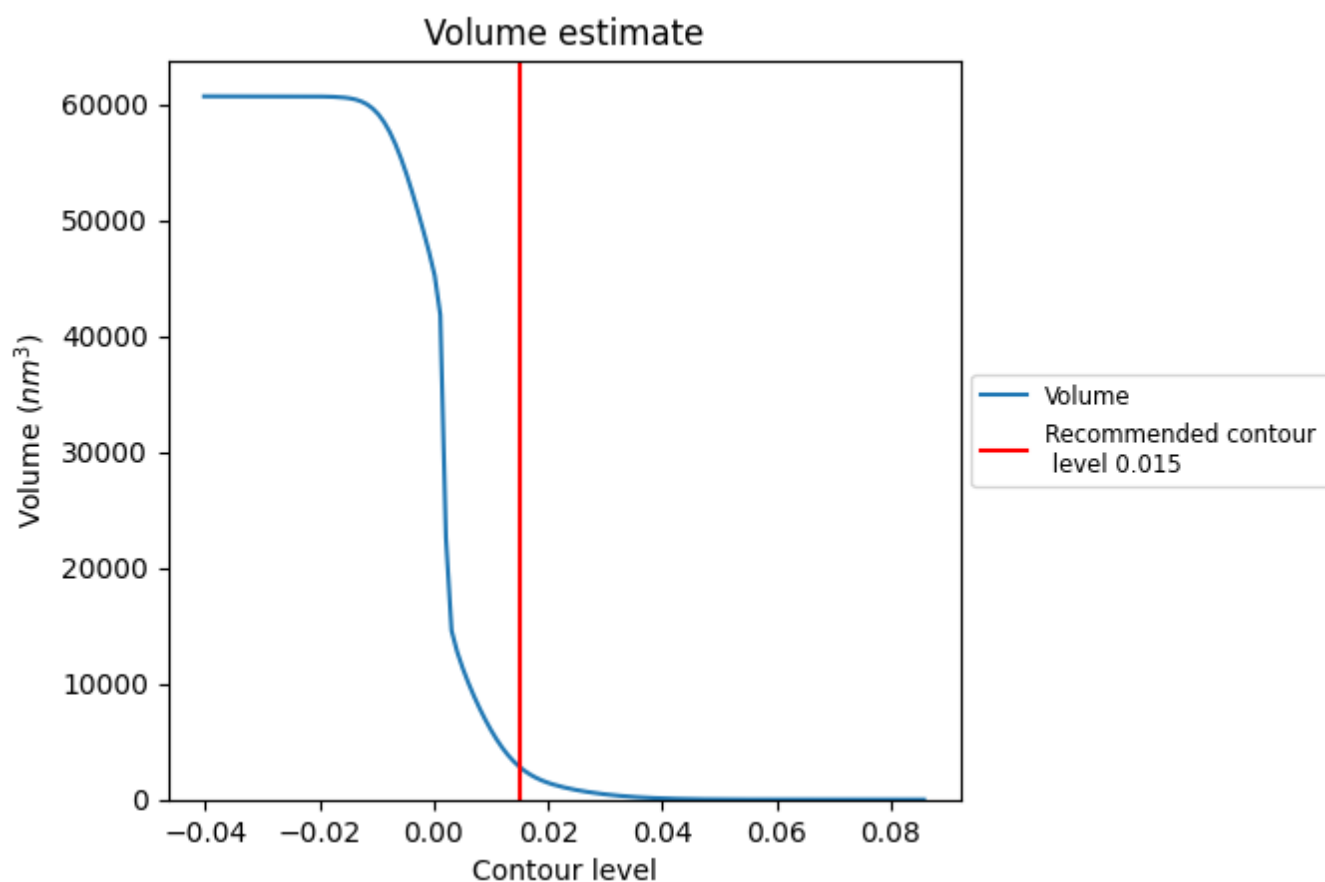
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

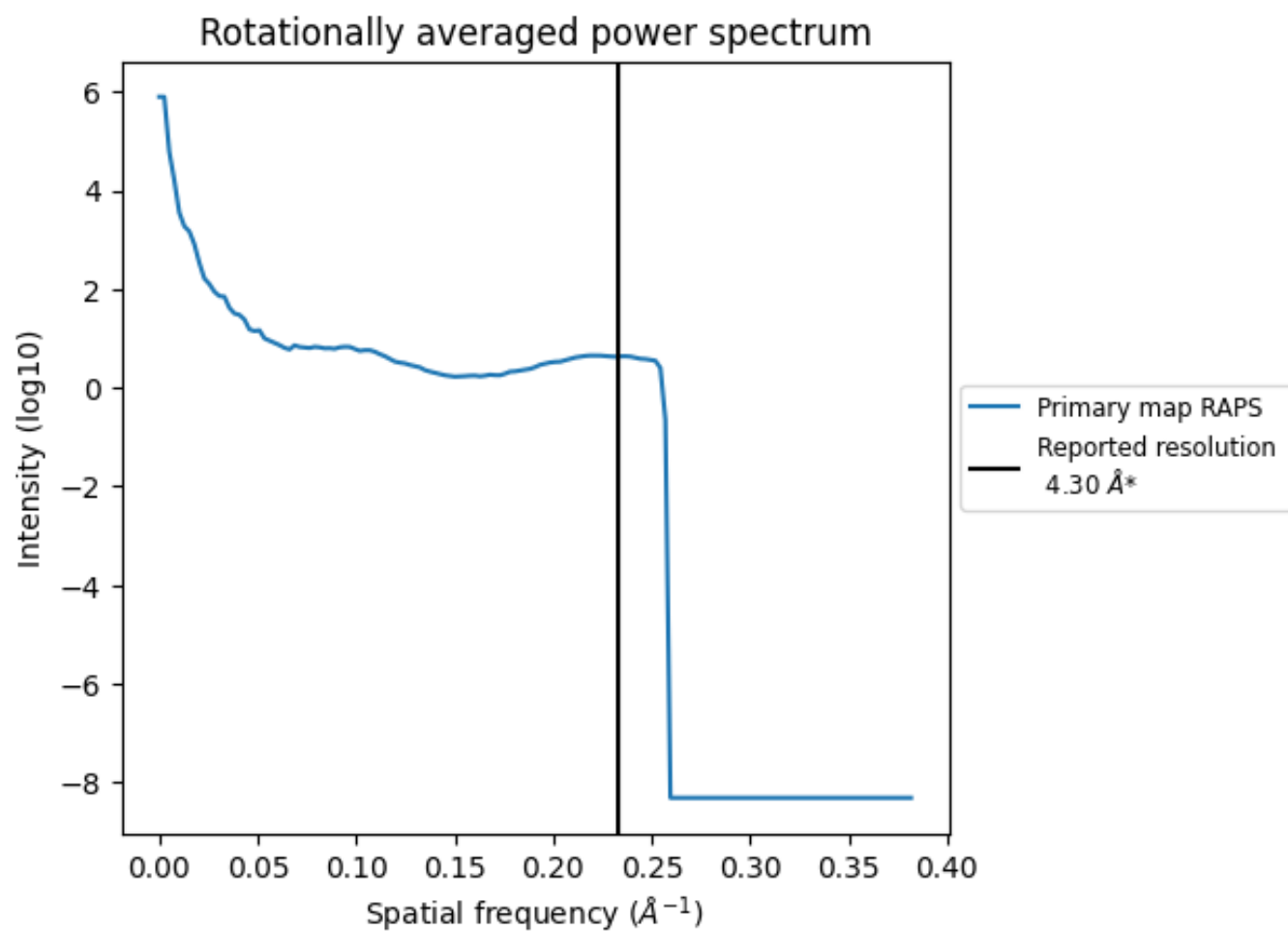
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2834 nm³; this corresponds to an approximate mass of 2560 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 0.233 Å⁻¹

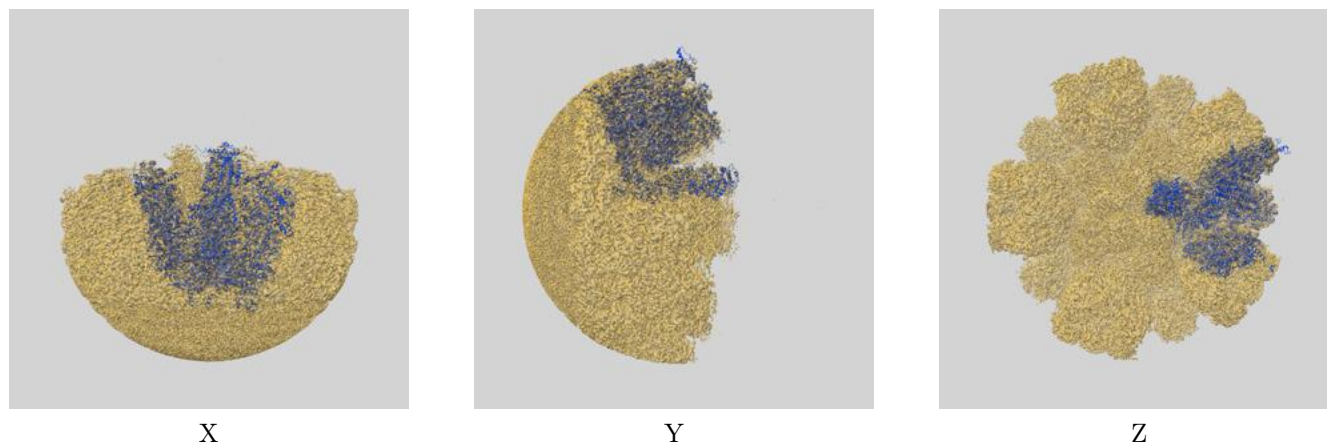
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

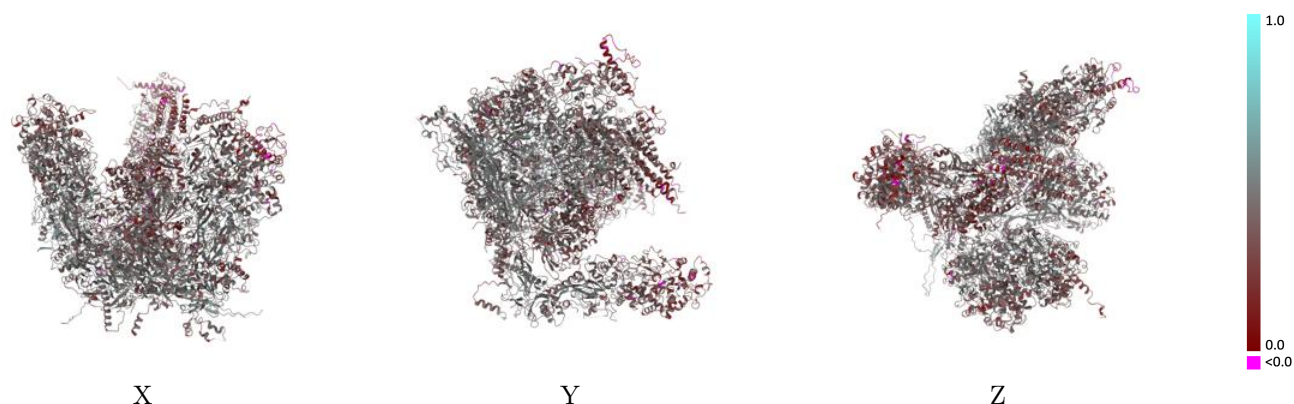
This section contains information regarding the fit between EMDB map EMD-30158 and PDB model 7BR7. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



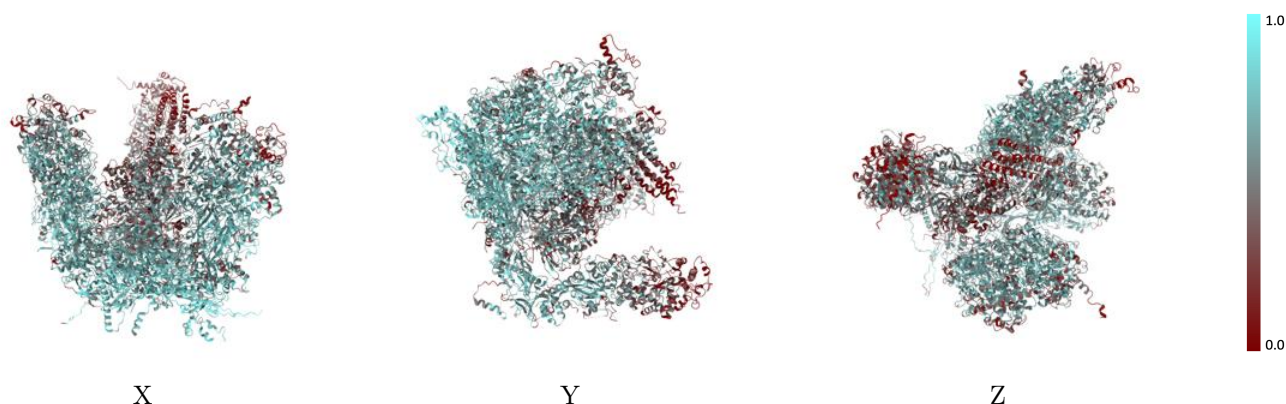
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



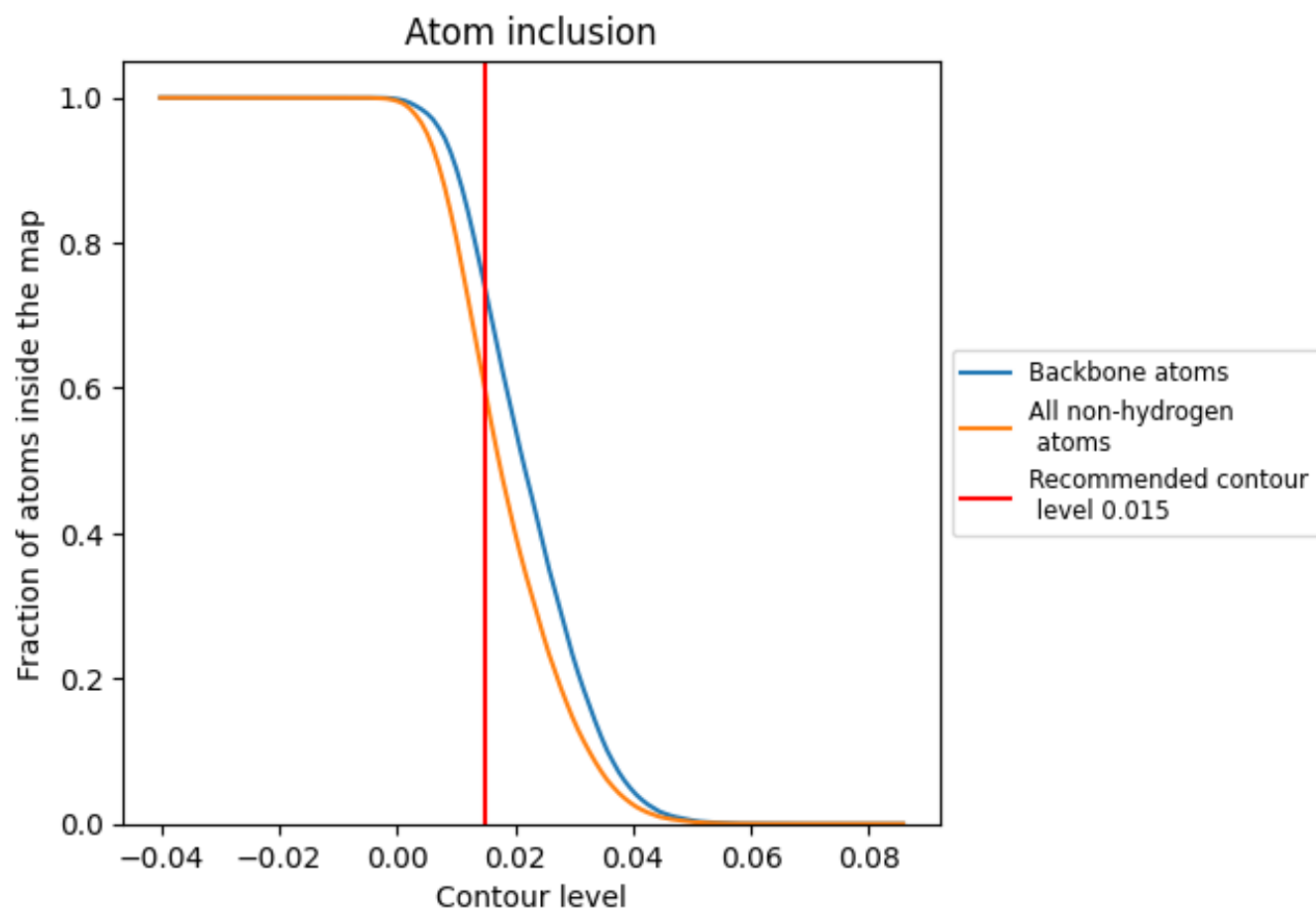
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 59% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5914	 0.4010
2	 0.2017	 0.1920
5	 0.5117	 0.3760
6	 0.3894	 0.3170
7	 0.3489	 0.2900
B	 0.1189	 0.2240
C	 0.4187	 0.3250
G	 0.3318	 0.3020
K	 0.3780	 0.3370
O	 0.1660	 0.2240
S	 0.6400	 0.4260
T	 0.6866	 0.4350
W	 0.6847	 0.4260
Y	 0.3533	 0.3450
Z	 0.3433	 0.3240
e	 0.7252	 0.4360
f	 0.6327	 0.3990
g	 0.6471	 0.4090
l	 0.5112	 0.3890
m	 0.1140	 0.2250
x	 0.6798	 0.4410
y	 0.4083	 0.3350

