wwPDB EM Validation Summary Report (i)

Apr 29, 2024 – 12:09 PM EDT

PDB ID	:	8W1I
EMDB ID	:	EMD-43726
Title	:	Cryo-EM structure of BTV subcore
Authors	:	Xia, X.; Sung, P.Y.; Martynowycz, M.W.; Gonen, T.; Roy, P.; Zhou, Z.H.
Deposited on	:	2024-02-16
Resolution	:	6.50 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 (i) 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 (i)) were used in the production of this report:

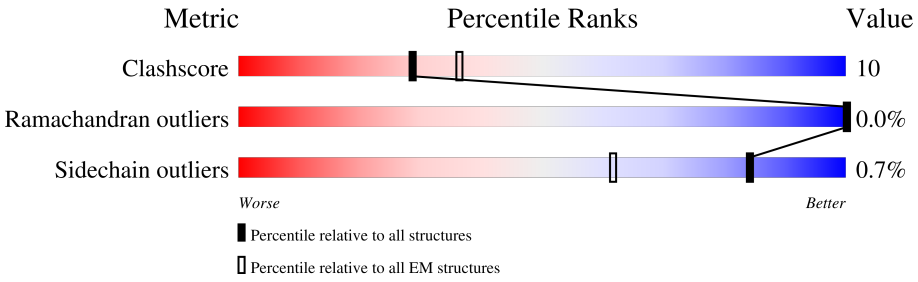
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 6.50 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	158937	4297
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 <=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	901	51% 68% 25% 6%
1	B	901	63% 72% 26% •
1	D	901	51% 71% 22% 6%
1	E	901	50% 71% 23% 6%
1	F	901	50% 72% 21% 6%
1	G	901	51% 70% 24% 6%
1	H	901	63% 74% 24% •
1	I	901	64% 72% 25% •

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Mol	Chain	Length	Quality of chain
1	J	901	
1	K	901	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 69810 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 Core protein VP3.

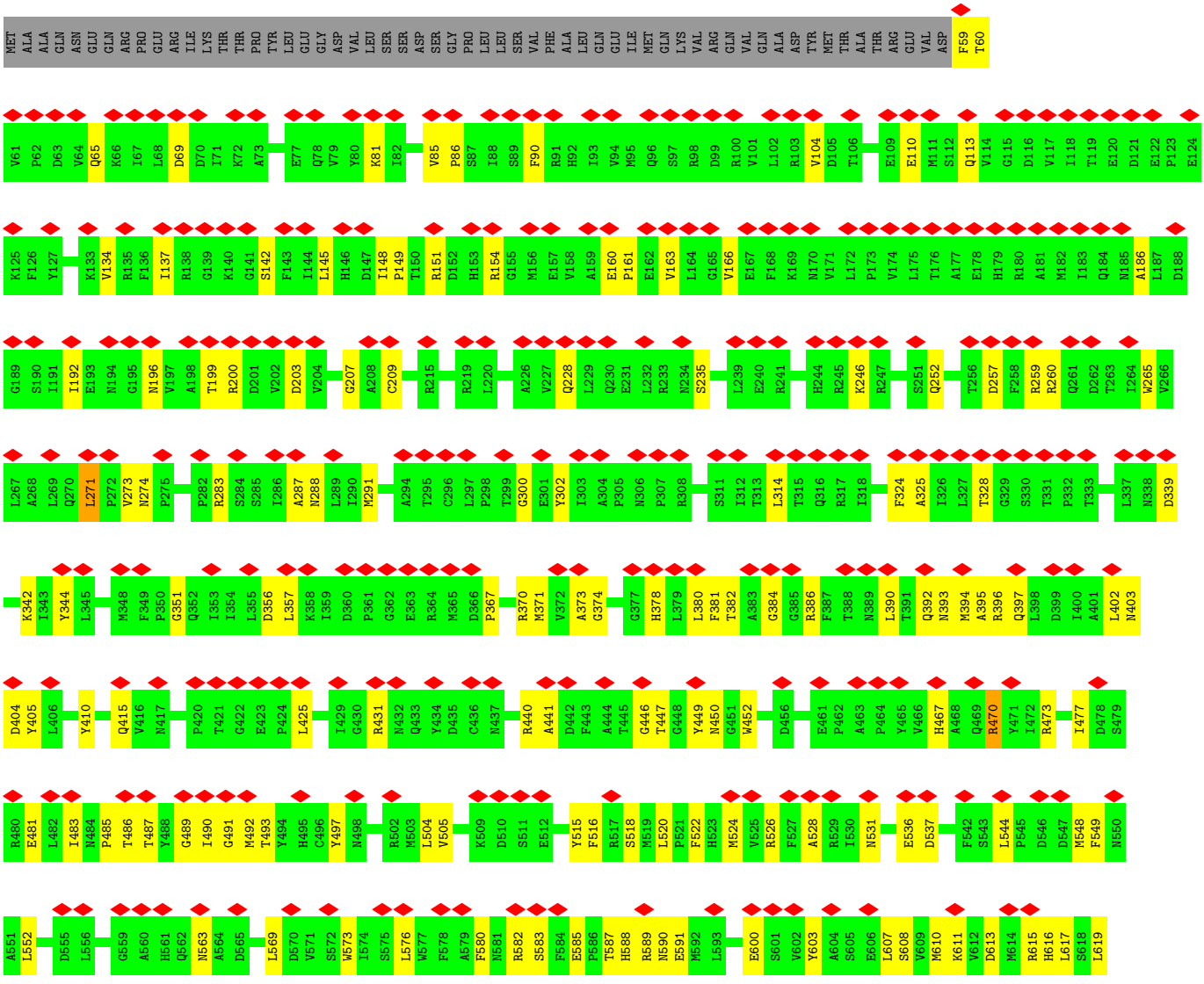
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	843	Total	C	N	O	S	0	0
			6811	4348	1182	1242	39		
1	B	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
1	D	843	Total	C	N	O	S	0	0
			6811	4348	1182	1242	39		
1	E	843	Total	C	N	O	S	0	0
			6811	4348	1182	1242	39		
1	F	843	Total	C	N	O	S	0	0
			6811	4348	1182	1242	39		
1	G	843	Total	C	N	O	S	0	0
			6811	4348	1182	1242	39		
1	H	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
1	I	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
1	J	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
1	K	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		

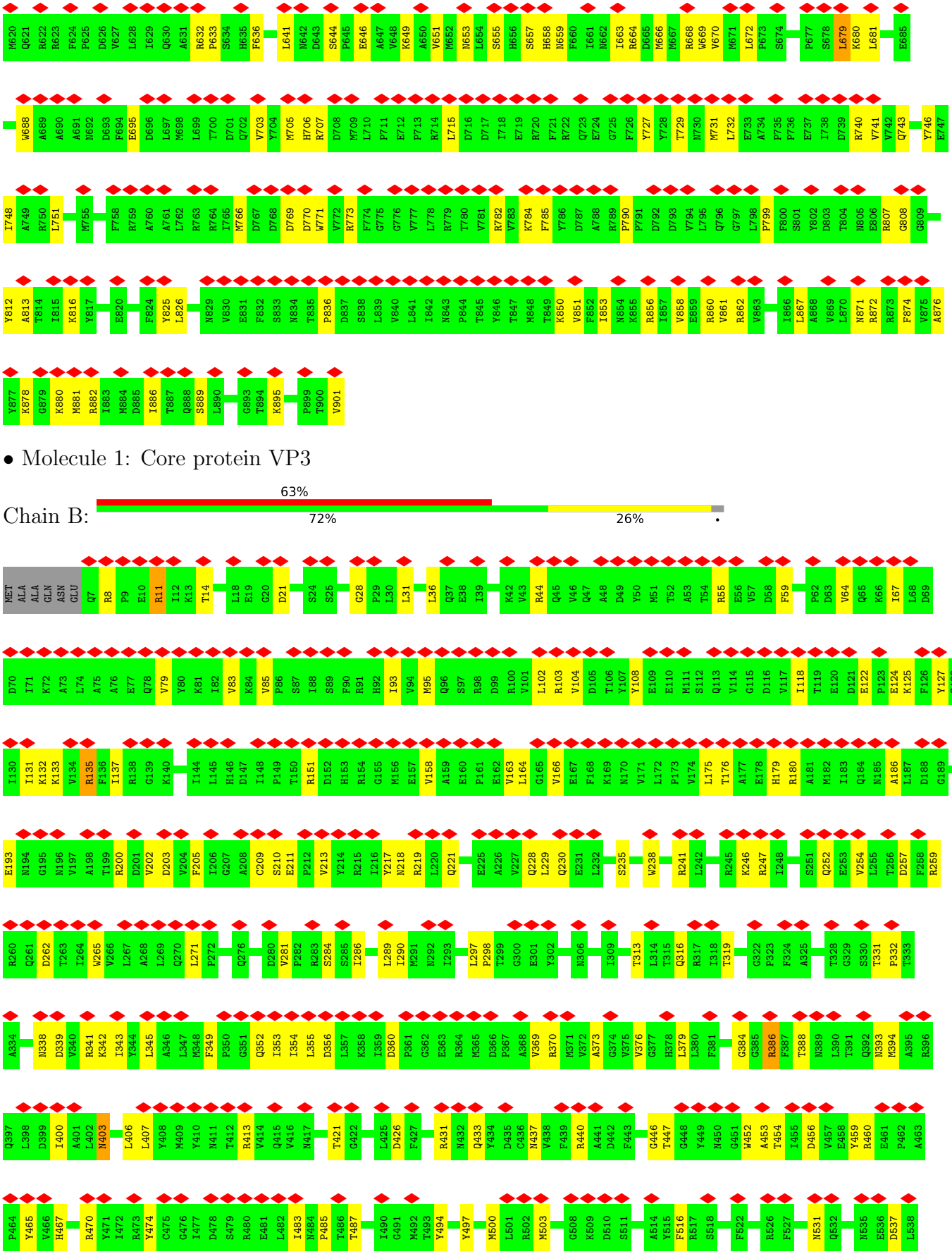
3 Residue-property plots (i)

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: Core protein VP3

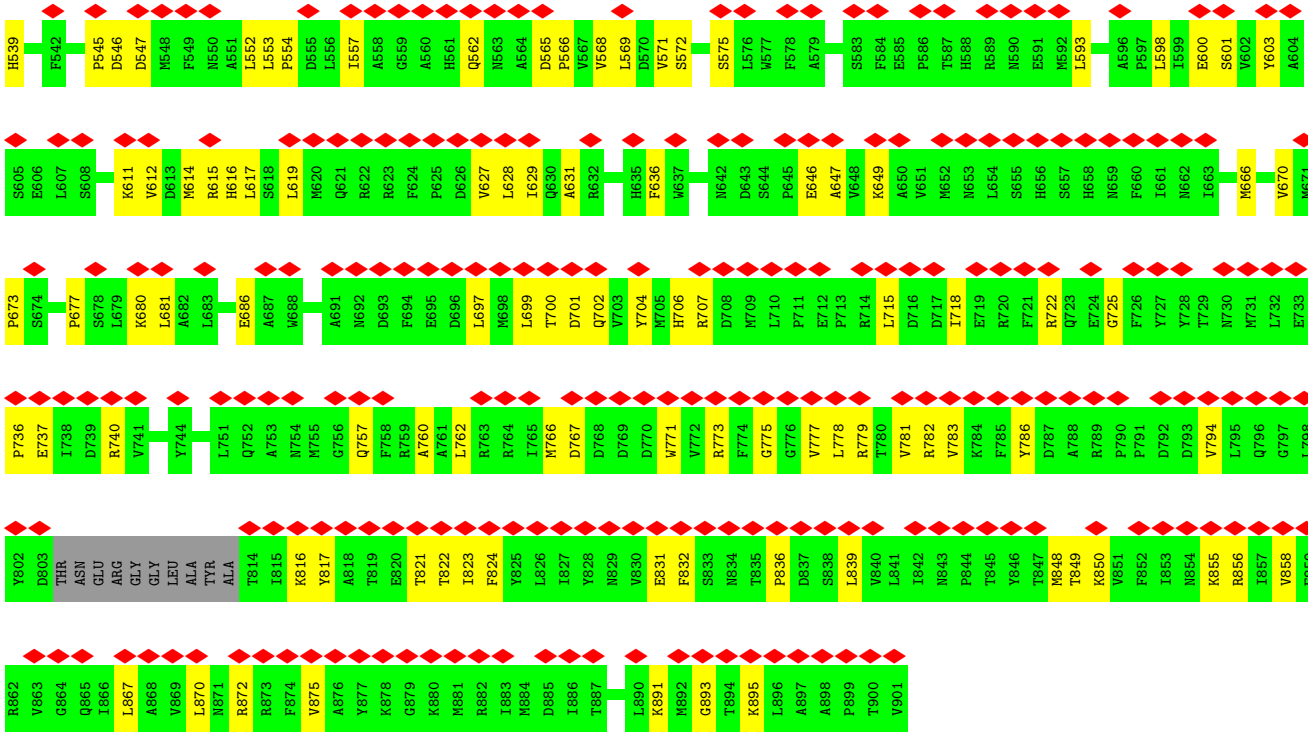
Chain A:





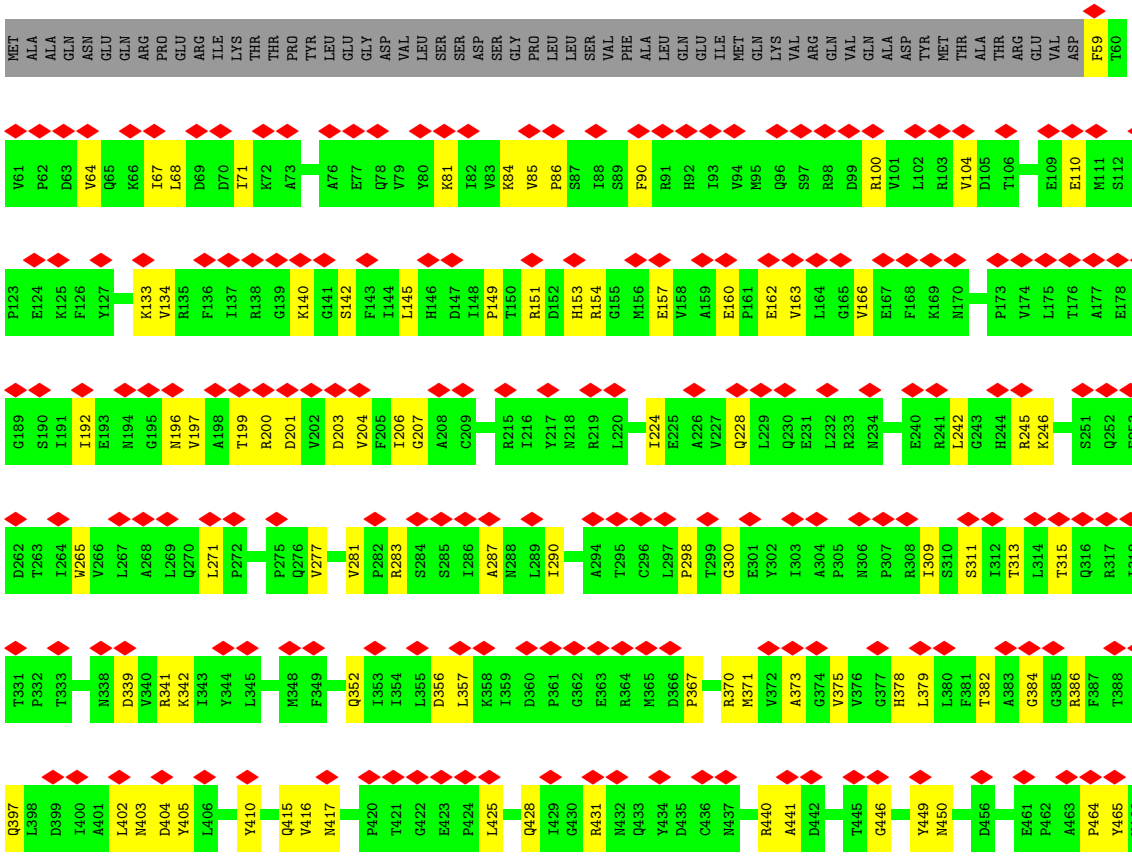
• Molecule 1: Core protein VP3

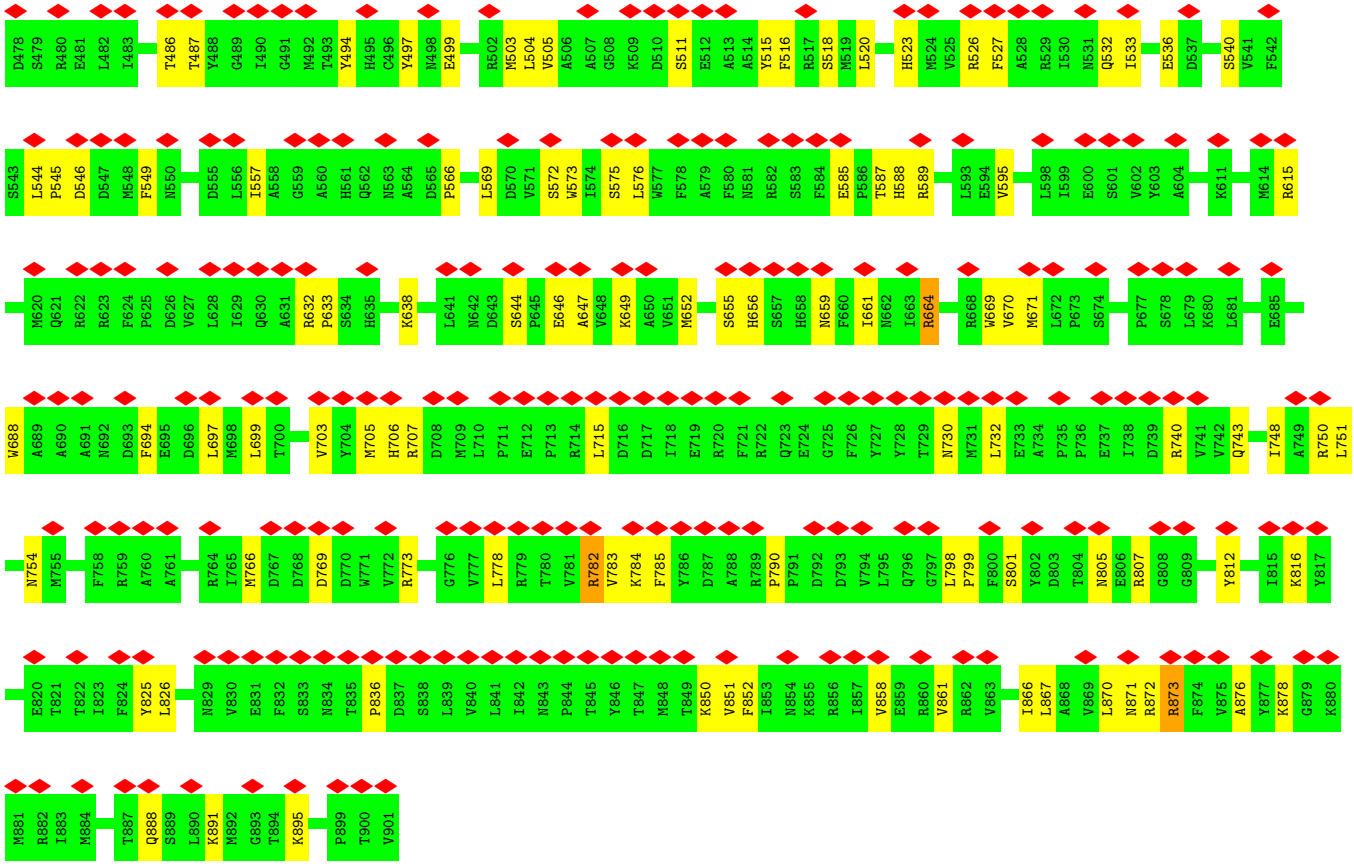
Chain B:



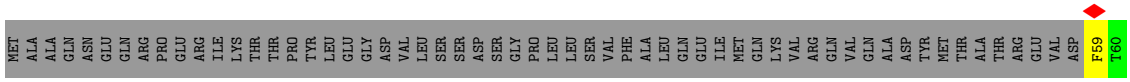
• Molecule 1: Core protein VP3

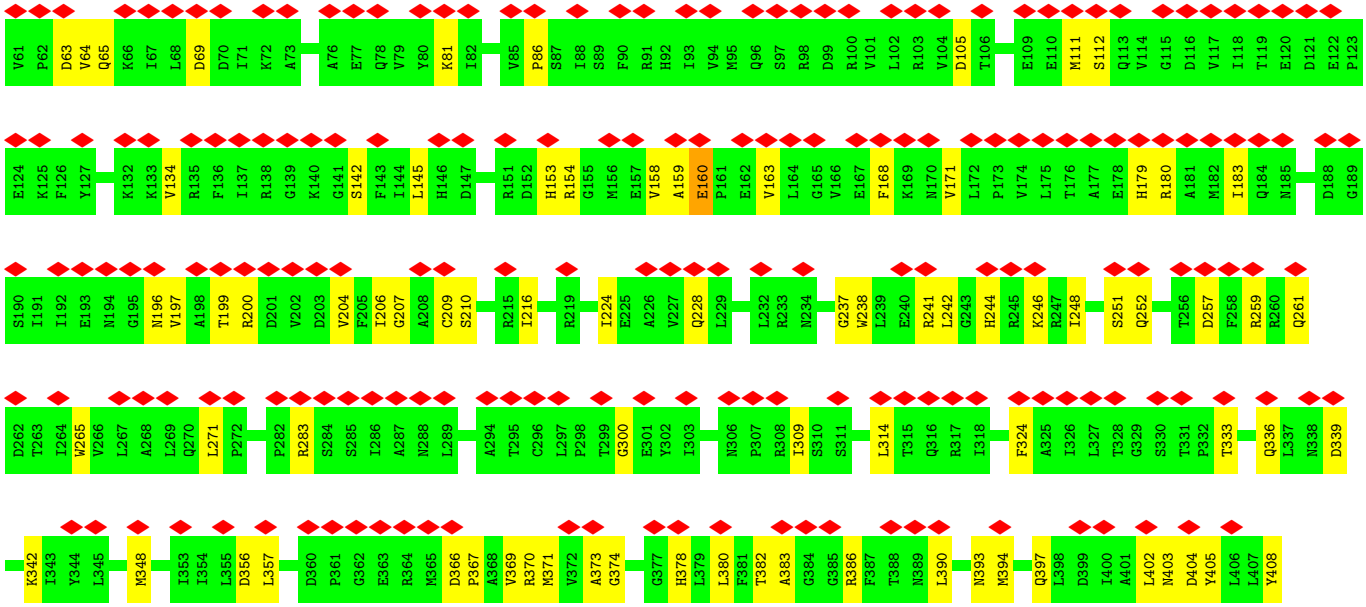
Chain D:

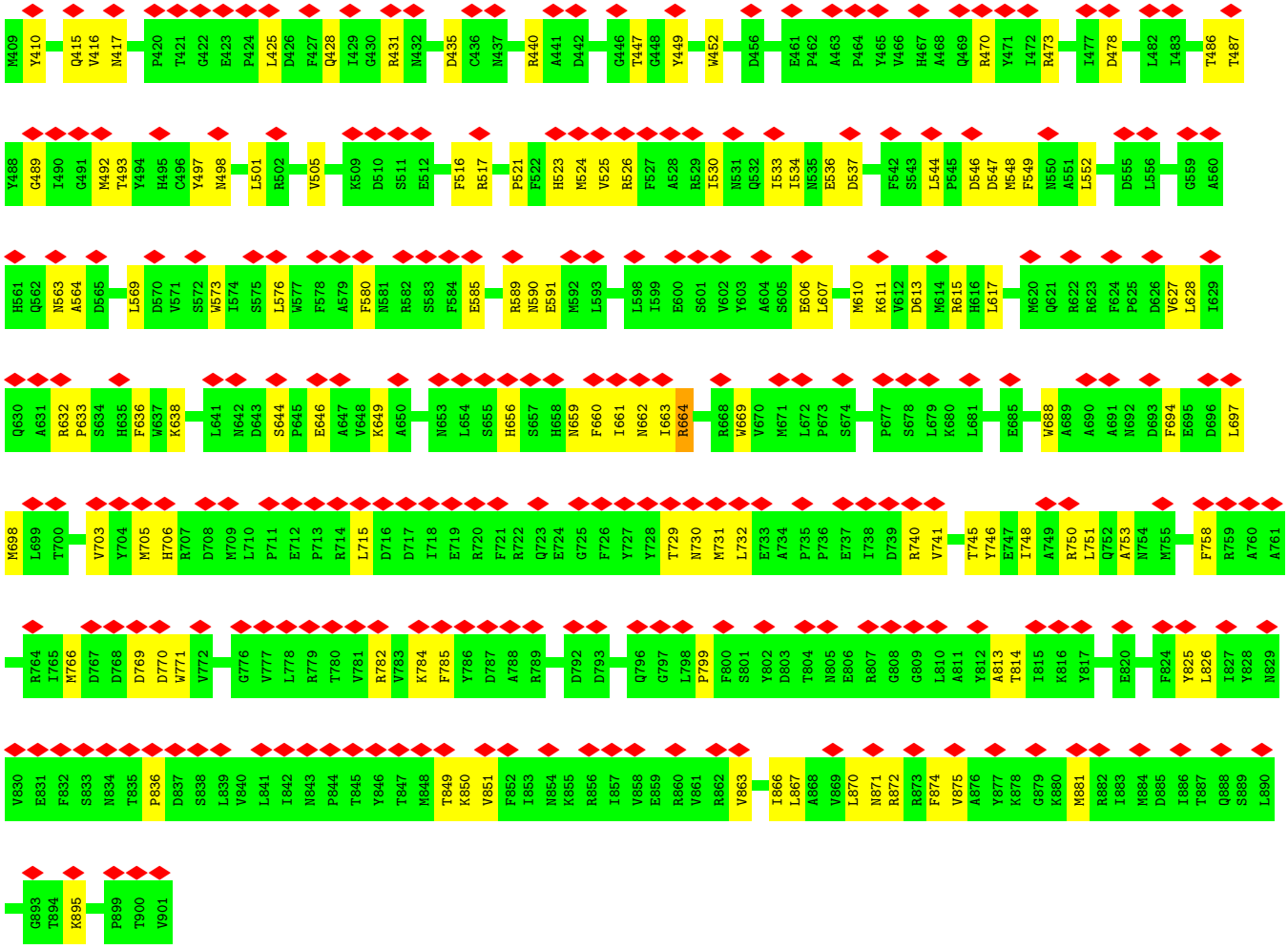




- Molecule 1: Core protein VP3

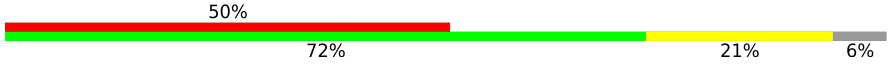


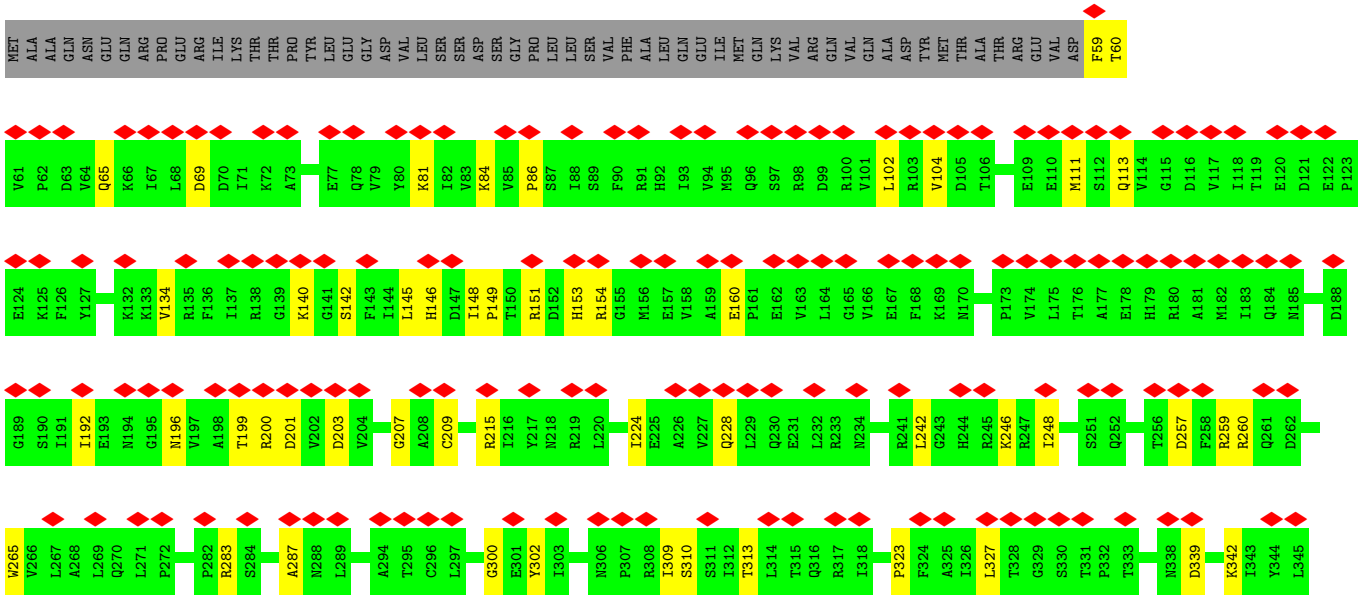


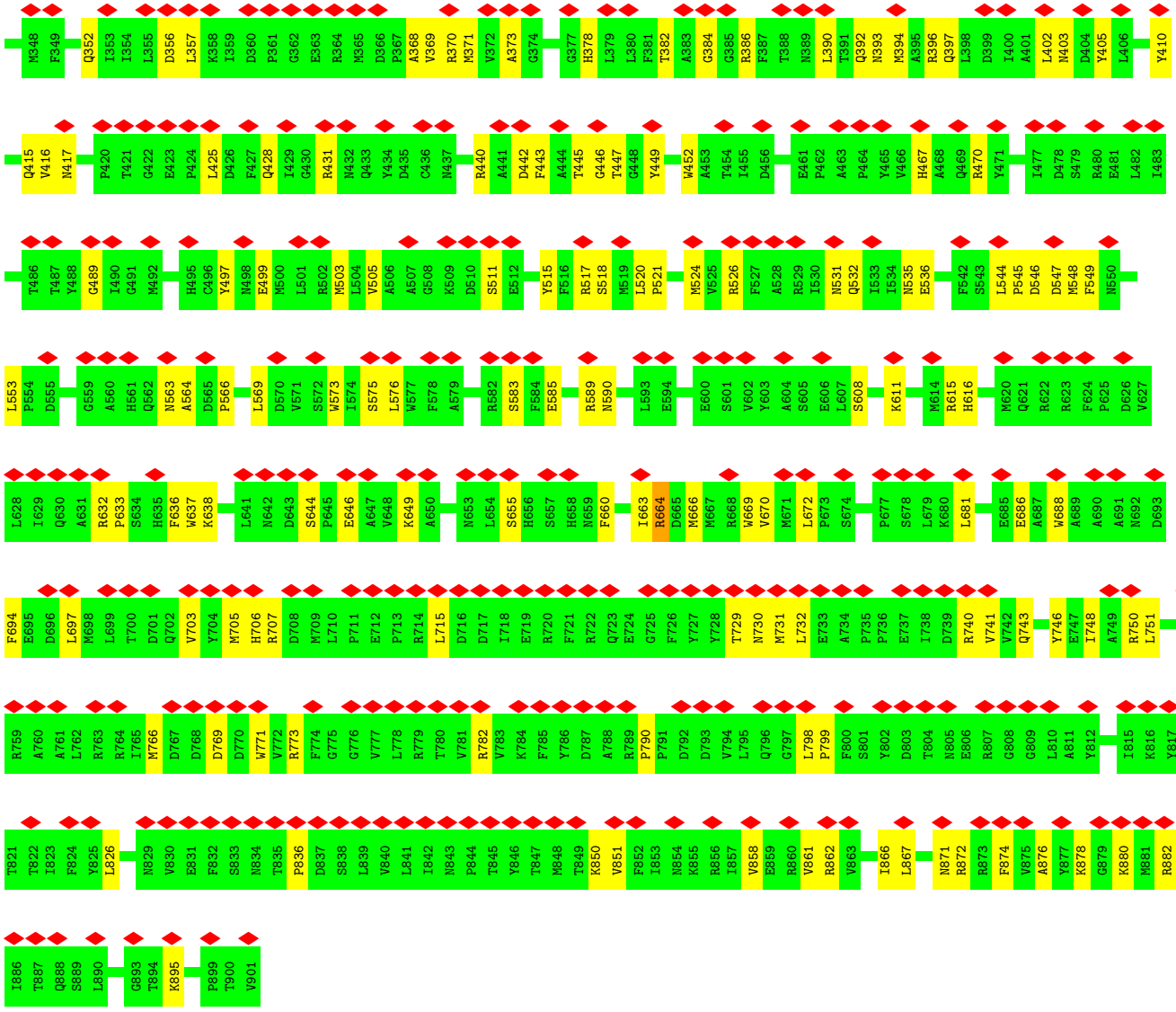


• Molecule 1: Core protein VP3

Chain F:

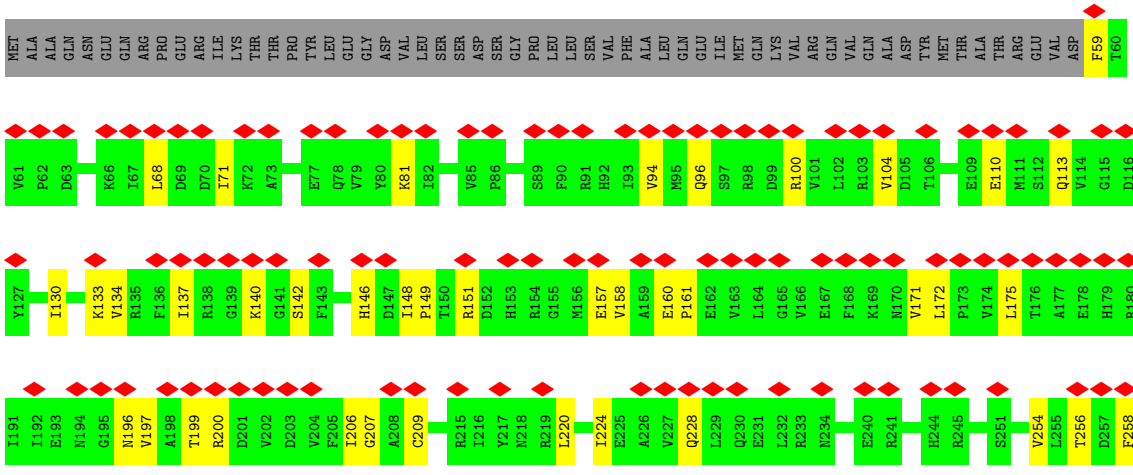


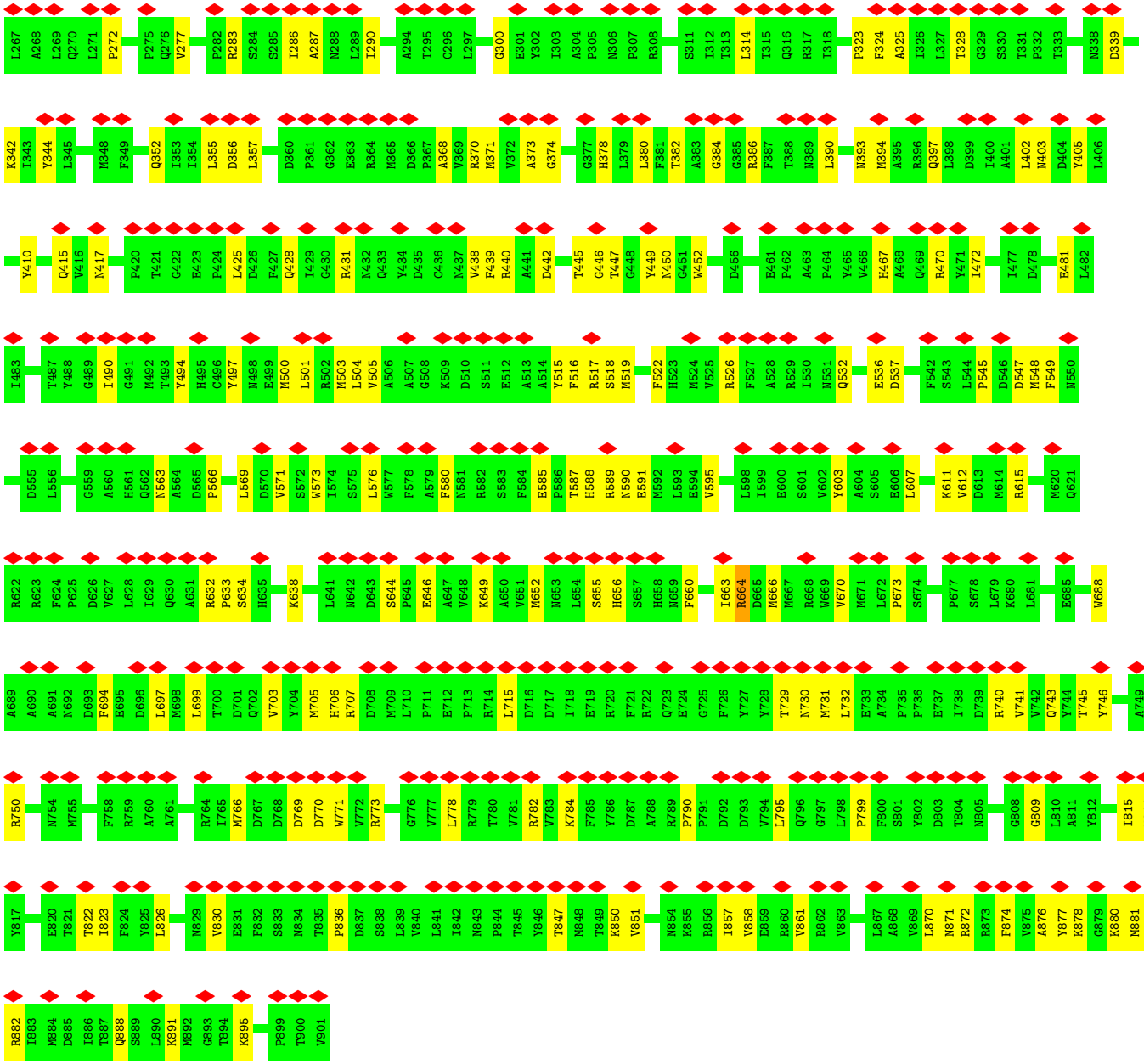




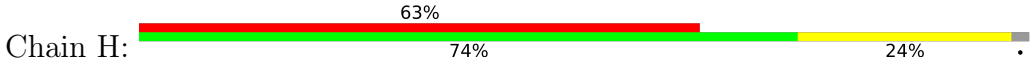
• Molecule 1: Core protein VP3

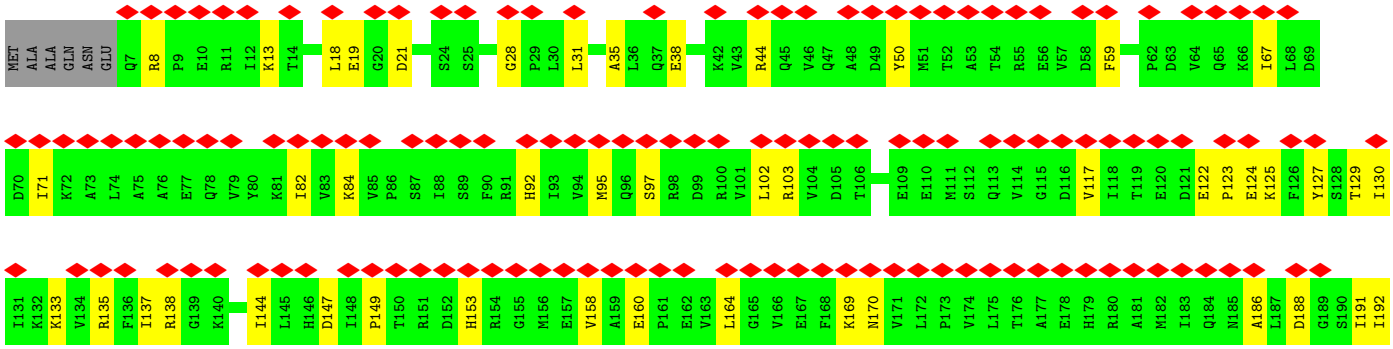
Chain G:

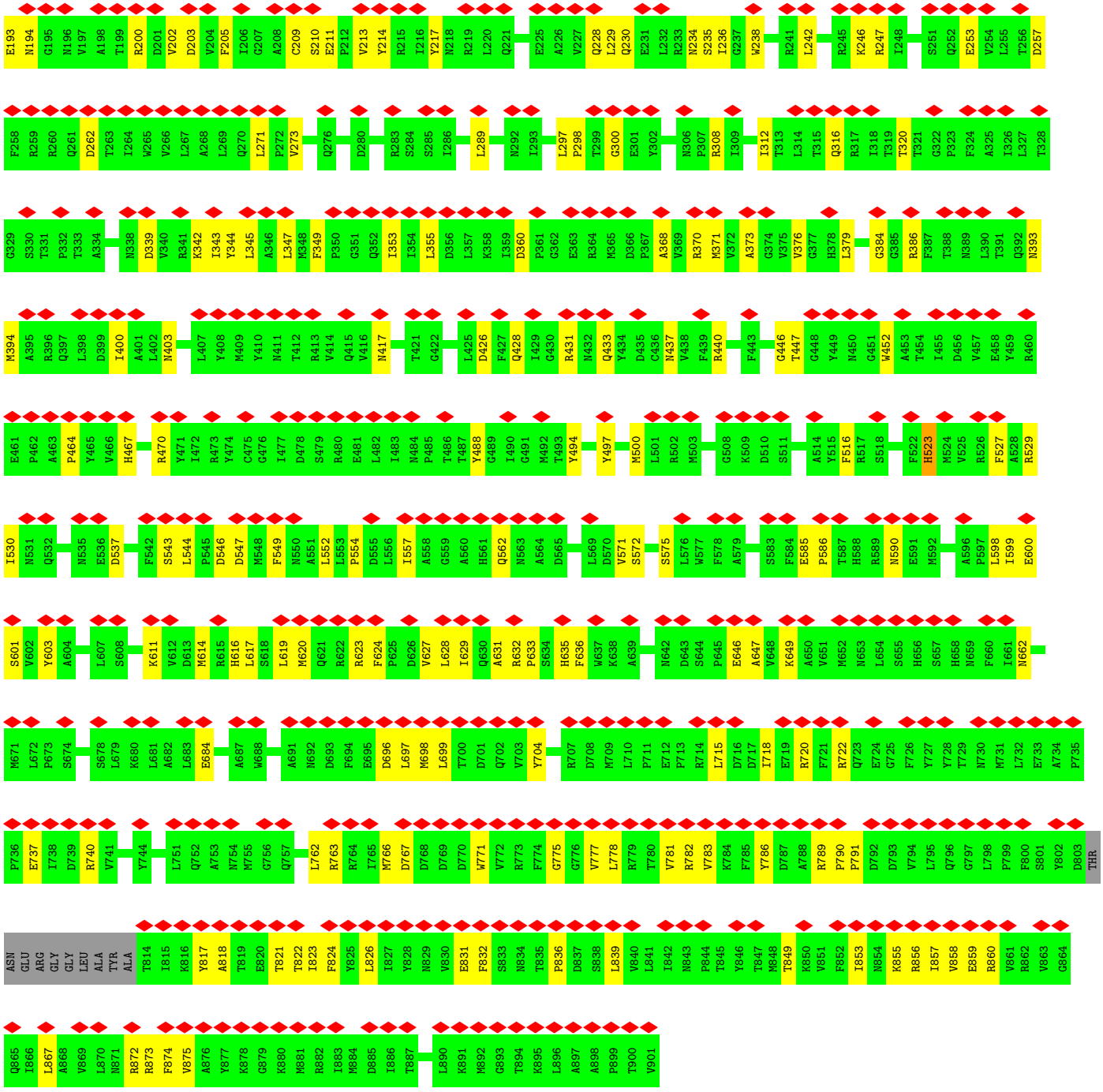




• Molecule 1: Core protein VP3

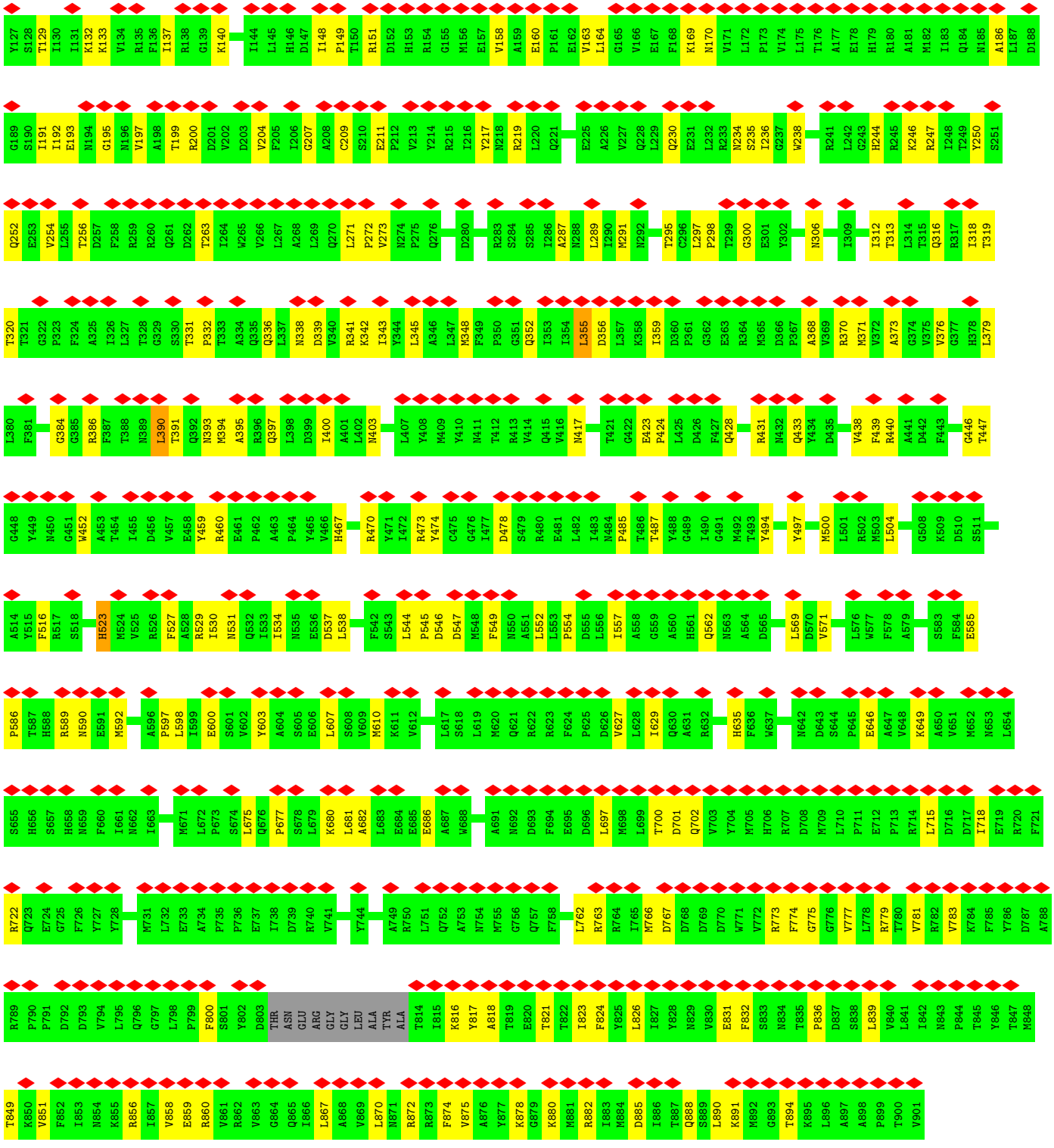






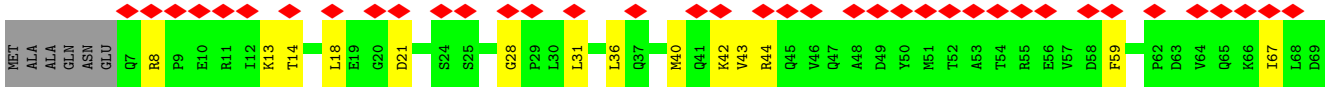
• Molecule 1: Core protein VP3

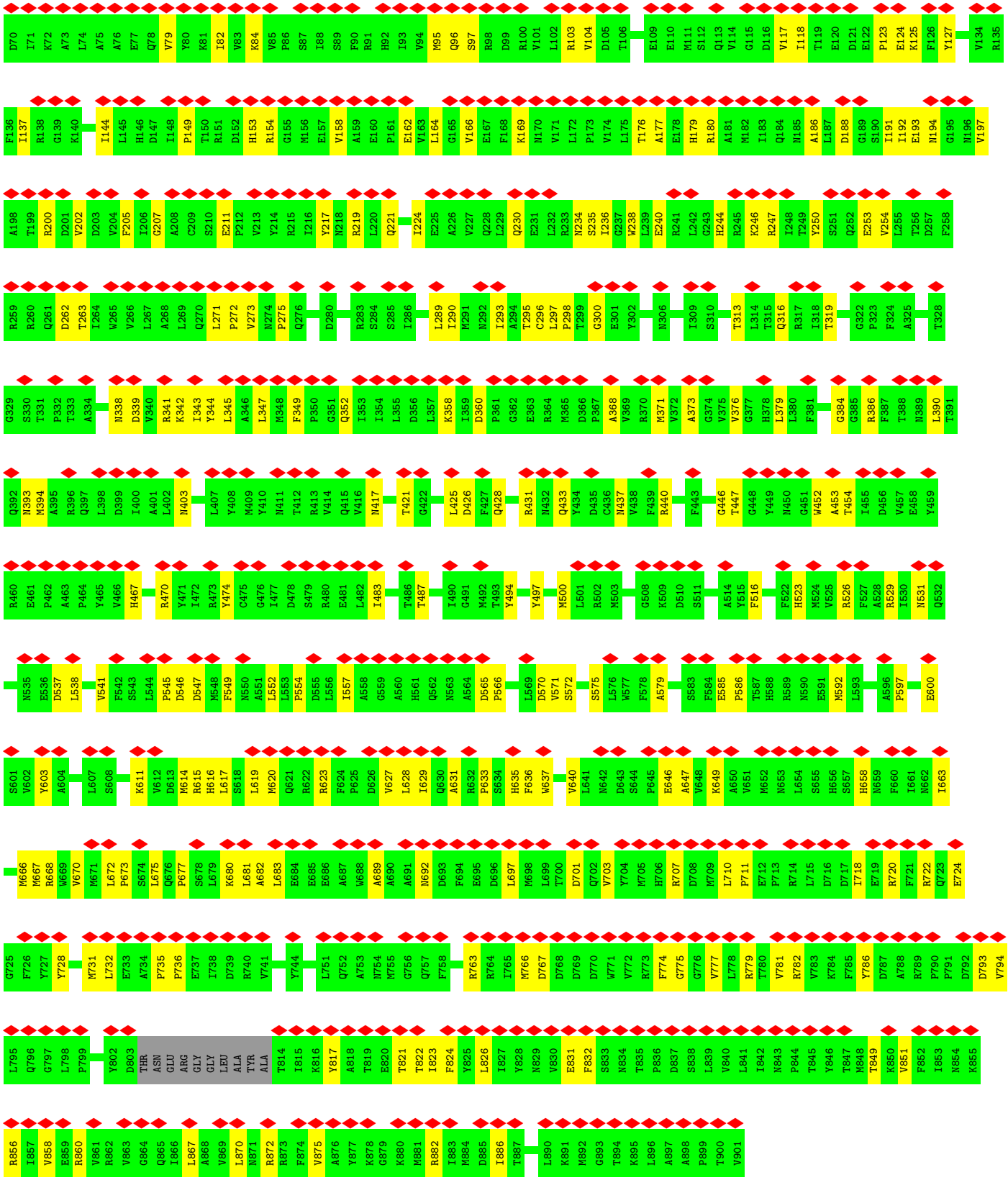
Chain I:



• Molecule 1: Core protein VP3

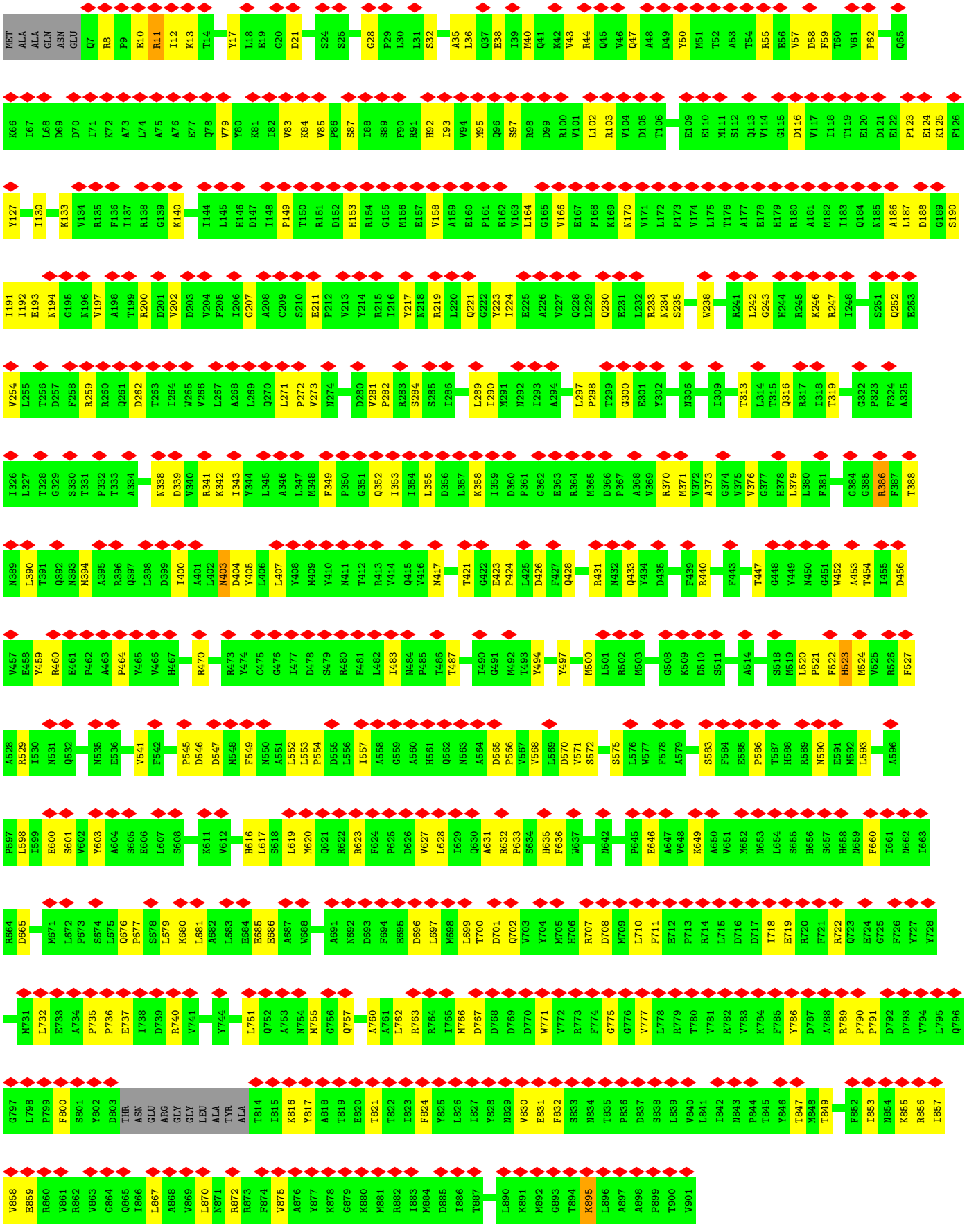
Chain J:





• Molecule 1: Core protein VP3

Chain K:


MET ALA ALA GLN ASN GLU Q7 R8 P9 E10 R11 I12 K13 T14 Y17 L18 E19 G20 D21 S24 S25 G28 P29 L30 L31 S32 A35 L36 Q37 E38 I39 M40 Q41 K42 V43 R44 Q45 V46 Q47 A48 D49 Y50 M51 T52 A53 T54 R55 E56 V57 D58 F59 T60 V61 P62 Q65
K66 I67 L68 D69 D70 I71 K72 A73 L74 A75 A76 E77 Q78 V79 Y80 K81 I82 V83 K84 V85 P86 S87 I88 S89 F90 R91 H92 I93 Y94 M95 Q96 S97 R98 D99 R100 V101 L102 R103 V104 D105 T106 E109 E110 M111 S112 Q113 V114 G115 D116 V117 I118 T119 E120 D121 E122 P123 E124 K125 F126
Y127 I130 K133 V134 R135 F136 I137 R138 G139 K140 I144 L145 H146 D147 I148 P149 T150 R151 D152 H153 R154 G155 M156 E157 V158 A159 E160 P161 E162 V163 L164 G165 V166 E167 F168 K169 N170 V171 L172 P173 V174 L175 T176 A177 E178 H179 R180 A181 M182 I183 Q184 N185 A186 L187 D188 G189 S190
I191 I192 E193 N194 G195 N196 V197 A198 T199 R200 D201 V202 D203 V204 F205 I206 G207 A208 C209 S210 E211 P212 V213 Y214 R215 I216 Y217 N218 R219 L220 Q221 G222 Y223 I224 E225 A226 V227 Q228 L229 Q230 E231 L232 R233 N234 S235 W238 R241 L242 G243 H244 R245 K246 R247 I248 S251 Q252 E253
V254 L255 T256 D257 F258 R259 R260 Q261 D262 T263 I264 W265 V266 L267 A268 L269 Q270 L271 P272 V273 N274 D280 V281 P282 R283 S284 S285 I286 L289 I290 M291 N292 I293 A294 L297 P298 T299 G300 E301 Y302 N306 I309 T313 L314 T315 Q316 R317 I318 T319 G322 P323 F324 A325
I326 L327 T328 G329 S330 T331 P332 T333 A334 N338 D339 Y340 R341 K342 I343 Y344 L345 A346 L347 M348 F349 P350 G351 Q352 I353 I354 L355 D356 L357 K358 I359 D360 P361 G362 E363 R364 M365 D366 P367 A368 V369 R370 M371 V372 A373 G374 V375 V376 G377 H378 L379 L380 F381 G384 G385 R386 F387 T388
N389 L390 T391 Q392 N393 M394 A395 R396 Q397 L398 D399 I400 A401 L402 N403 D404 Y405 L406 L407 Y408 M409 Y410 N411 T412 R413 Y414 Q415 V416 N417 T421 G422 E423 P424 L425 D426 F427 Q428 R431 N432 Q433 Y434 D435 F439 R440 F443 T447 G448 Y449 N450 G451 W452 A453 T454 I455 D456
V457 E458 Y459 R460 E461 P462 A463 P464 Y465 V466 H467 R470 R473 Y474 C475 G476 I477 D478 S479 R480 E481 L482 I483 N484 P485 T486 T487 I490 G491 M492 T493 Y494 Y497 M500 L501 R502 M503 G508 K509 D510 S511 A514 S518 M519 L520 P521 F522 H523 M524 V525 R526 F527
A528 R529 I530 N531 Q532 N535 E536 V541 F542 P545 D546 D547 M548 F549 N550 A551 L552 L553 P554 D555 L556 I557 A558 G559 A560 H561 Q562 N563 A564 D565 P566 V567 V568 L569 D570 V571 S572 S575 L576 W577 F578 A579 S583 F584 E585 P586 T587 H588 R589 N590 E591 M592 L593 A596
P597 L598 I599 E600 S601 V602 Y603 A604 S605 E606 L607 S608 K611 V612 H616 L617 S618 L619 M620 Q621 R622 R623 F624 P625 D626 V627 L628 I629 Q630 A631 R632 P633 S634 H635 F636 W637 N642 P645 E646 A647 V648 K649 A650 V651 M652 N653 L654 S655 H656 S657 H658 N659 F660 I661 N662 I663
R664 D665 M671 L672 P673 S674 L675 Q676 P677 S678 L679 K680 L681 A682 L683 E684 E685 E686 A687 W688 A691 N692 D693 F694 E695 D696 L697 M698 L699 T700 D701 Q702 V703 Y704 M705 H706 R707 D708 M709 L710 P711 E712 P713 R714 L715 D716 D717 I718 E719 R720 F721 R722 Q723 E724 G725 F726 Y727 Y728
M731 L732 E733 A734 P735 P736 E737 I738 D739 R740 V741 Y744 L751 Q752 A753 N754 M755 G756 Q757 A760 A761 L762 R763 R764 R765 M766 D767 D768 D769 D770 W771 V772 R773 F774 G775 G776 V777 L778 R779 T780 V781 R782 V783 K784 F785 Y786 D787 A788 R789 P790 P791 D792 D793 V794 L795 Q796
G797 L798 P799 F800 S801 Y802 D803 THR ASN GLU ARG GLY GLY LEU ALA TYR ALA T814 I815 K816 Y817 A818 T819 G820 T821 T822 I823 F824 Y825 L826 I827 Y828 N829 V830 E831 F832 S833 N834 T835 P836 D837 S838 L839 V840 L841 I842 N843 P844 T845 Y846 T847 M848 T849 F852 I853 N854 K855 R856 I857
V858 E859 R860 V861 R862 V863 G864 Q865 I866 L867 A868 V869 L870 N871 R872 R873 F874 V875 A876 Y877 K878 G879 K880 M881 R882 I883 M884 D885 I886 T887 L890 K891 M892 G893 T894 K895 L896 A897 A898 P899 T900 V901

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	2124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.33	0/6966	0.61	0/9462
1	B	0.28	0/7310	0.58	0/9927
1	D	0.31	0/6966	0.61	0/9462
1	E	0.30	0/6966	0.60	0/9462
1	F	0.31	0/6966	0.60	0/9462
1	G	0.30	0/6966	0.60	0/9462
1	H	0.28	0/7310	0.57	0/9927
1	I	0.31	0/7310	0.60	0/9927
1	J	0.28	0/7310	0.57	0/9927
1	K	0.28	0/7310	0.60	0/9927
All	All	0.30	0/71380	0.59	0/96945

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	6811	0	6791	152	0
1	B	7151	0	7137	162	0
1	D	6811	0	6791	150	0
1	E	6811	0	6791	137	0
1	F	6811	0	6791	140	0
1	G	6811	0	6791	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	7151	0	7137	148	0
1	I	7151	0	7137	172	0
1	J	7151	0	7137	158	0
1	K	7151	0	7137	166	0
All	All	69810	0	69640	1449	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 10.

The worst 5 of 1449 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)
1:F:300:GLY:HA3	1:F:585:GLU:O	1.56	1.03
1:E:300:GLY:HA3	1:E:585:GLU:O	1.59	1.02
1:A:300:GLY:HA3	1:A:585:GLU:O	1.60	1.00
1:D:300:GLY:HA3	1:D:585:GLU:O	1.66	0.95
1:G:300:GLY:HA3	1:G:585:GLU:O	1.67	0.94

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	841/901 (93%)	813 (97%)	28 (3%)	0	100	100
1	B	881/901 (98%)	845 (96%)	36 (4%)	0	100	100
1	D	841/901 (93%)	811 (96%)	30 (4%)	0	100	100
1	E	841/901 (93%)	819 (97%)	22 (3%)	0	100	100
1	F	841/901 (93%)	822 (98%)	19 (2%)	0	100	100
1	G	841/901 (93%)	816 (97%)	24 (3%)	1 (0%)	51	85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	881/901 (98%)	849 (96%)	32 (4%)	0	100	100
1	I	881/901 (98%)	842 (96%)	39 (4%)	0	100	100
1	J	881/901 (98%)	844 (96%)	37 (4%)	0	100	100
1	K	881/901 (98%)	845 (96%)	36 (4%)	0	100	100
All	All	8610/9010 (96%)	8306 (96%)	303 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	272	PRO

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	741/792 (94%)	733 (99%)	8 (1%)	73	84
1	B	782/792 (99%)	775 (99%)	7 (1%)	78	88
1	D	741/792 (94%)	733 (99%)	8 (1%)	73	84
1	E	741/792 (94%)	736 (99%)	5 (1%)	84	90
1	F	741/792 (94%)	737 (100%)	4 (0%)	88	93
1	G	741/792 (94%)	737 (100%)	4 (0%)	88	93
1	H	782/792 (99%)	779 (100%)	3 (0%)	91	94
1	I	782/792 (99%)	776 (99%)	6 (1%)	81	89
1	J	782/792 (99%)	780 (100%)	2 (0%)	92	95
1	K	782/792 (99%)	776 (99%)	6 (1%)	81	89
All	All	7615/7920 (96%)	7562 (99%)	53 (1%)	84	90

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	386	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	664	ARG
1	K	386	ARG
1	F	467	HIS
1	G	277	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	523	HIS
1	I	523	HIS
1	H	562	GLN
1	I	888	GLN
1	D	252	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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.

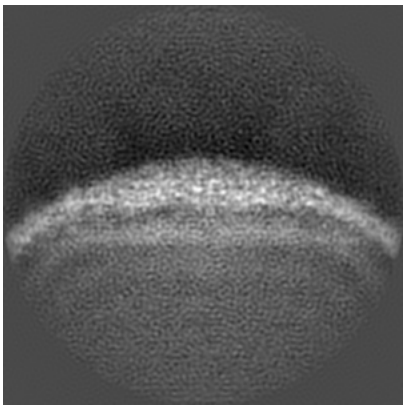
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43726. These allow visual inspection of the internal detail of the map and identification of artifacts.

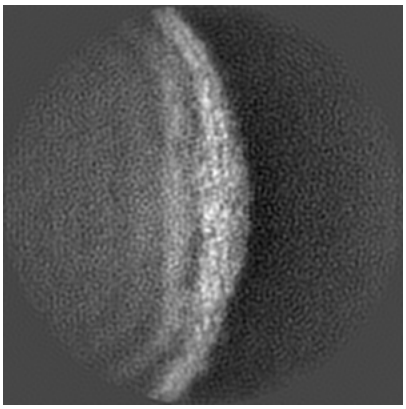
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

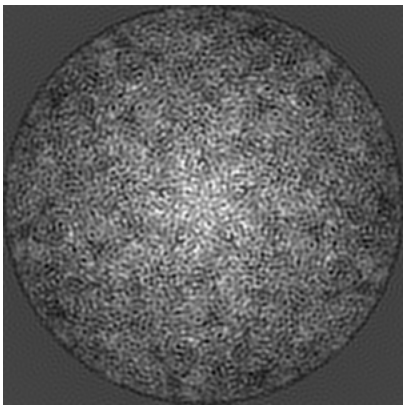
6.1.1 Primary map



X

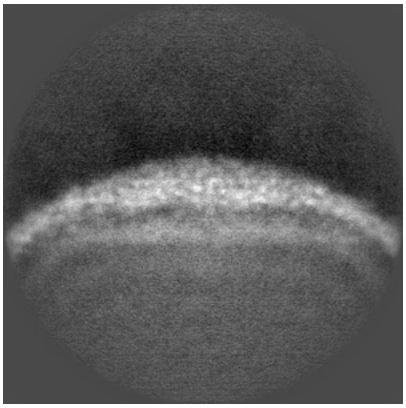


Y

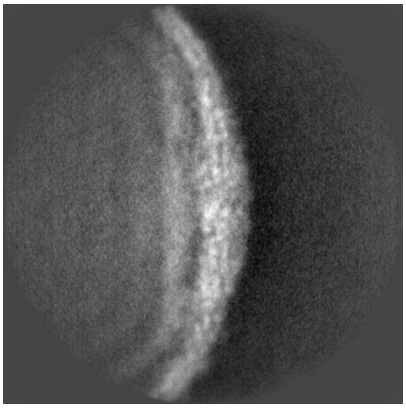


Z

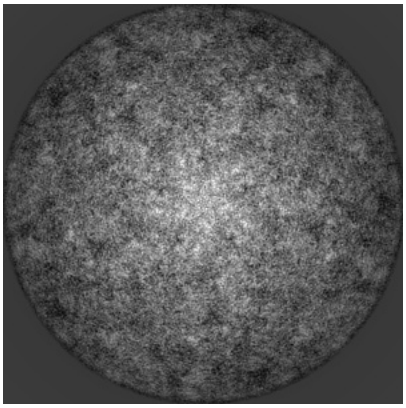
6.1.2 Raw map



X



Y

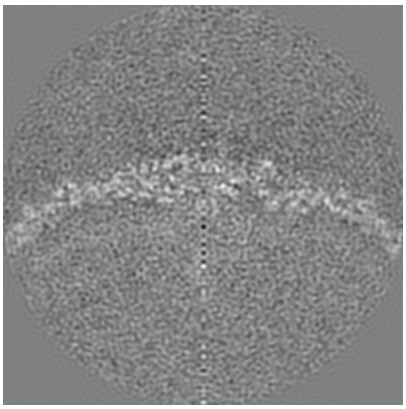


Z

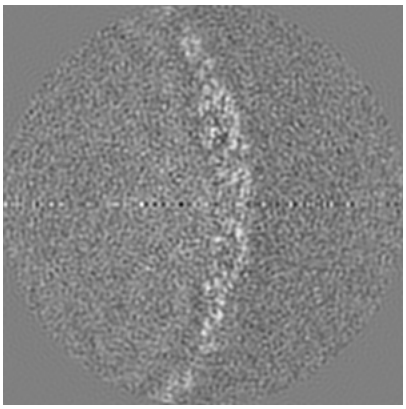
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

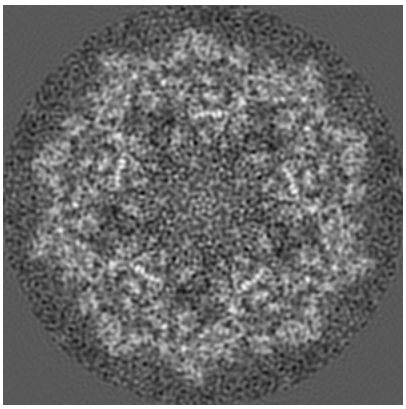
6.2.1 Primary map



X Index: 160

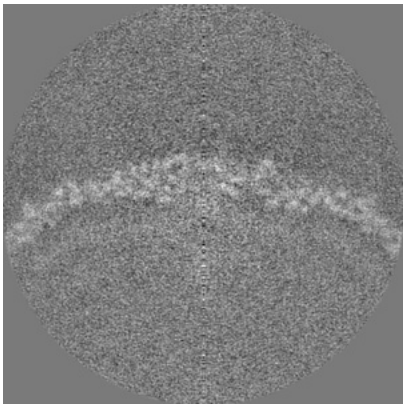


Y Index: 160

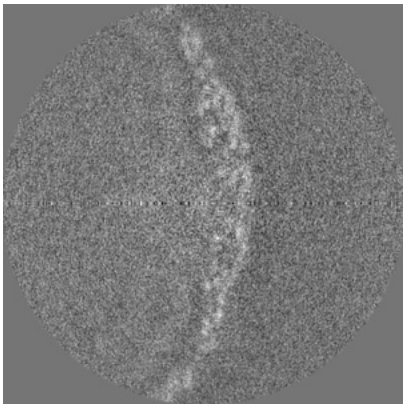


Z Index: 160

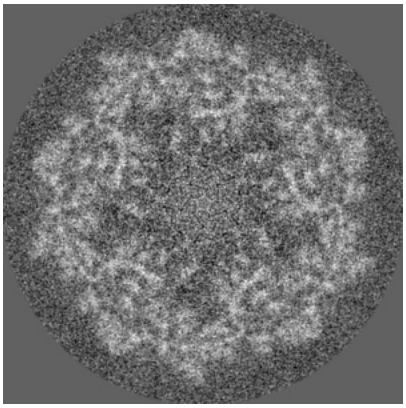
6.2.2 Raw map



X Index: 160



Y Index: 160

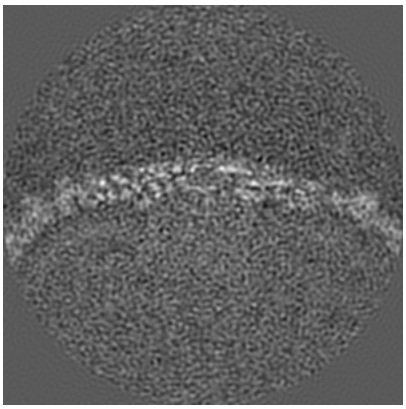


Z Index: 160

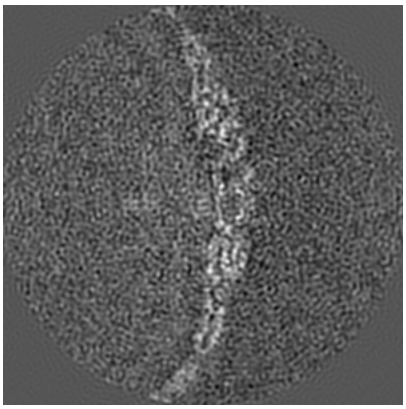
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

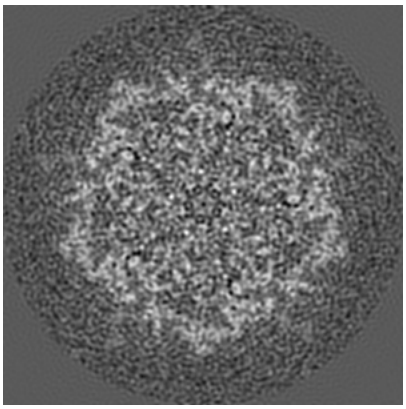
6.3.1 Primary map



X Index: 153

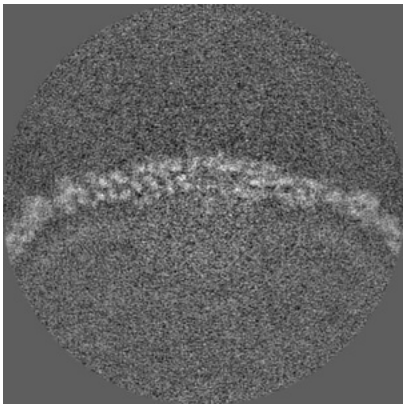


Y Index: 164

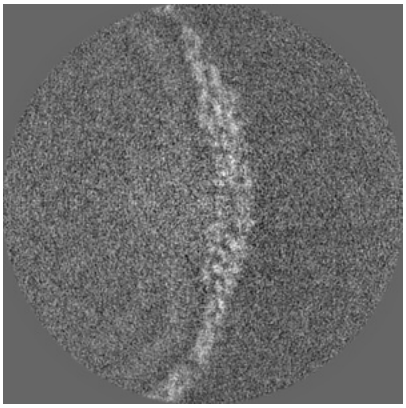


Z Index: 170

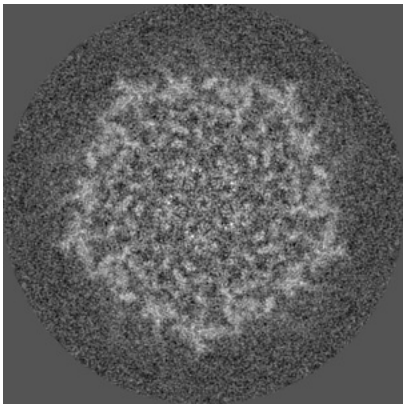
6.3.2 Raw map



X Index: 152



Y Index: 156

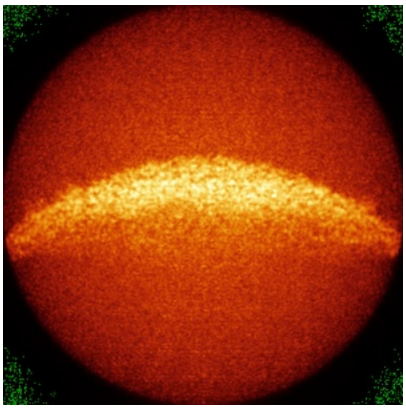


Z Index: 171

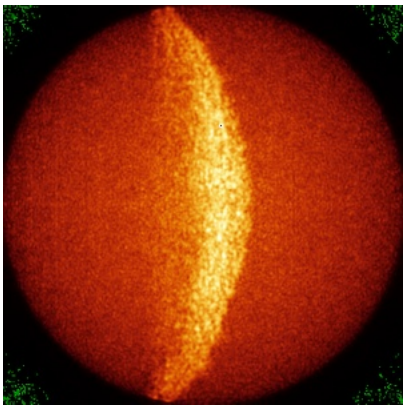
The images above show the largest variance slices of the map in three orthogonal directions.

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

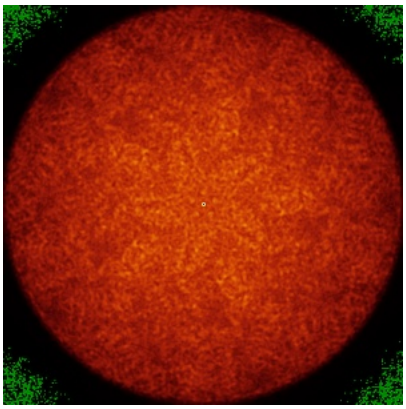
6.4.1 Primary map



X

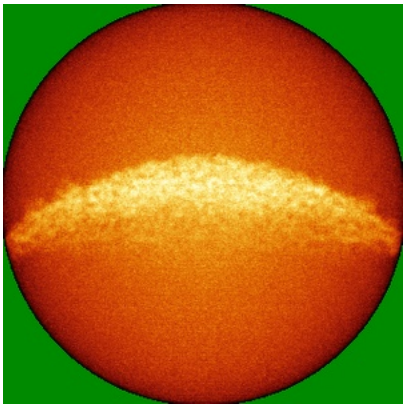


Y

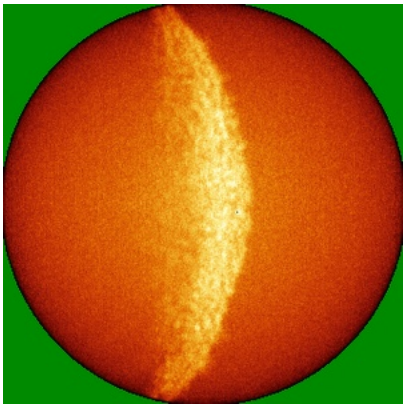


Z

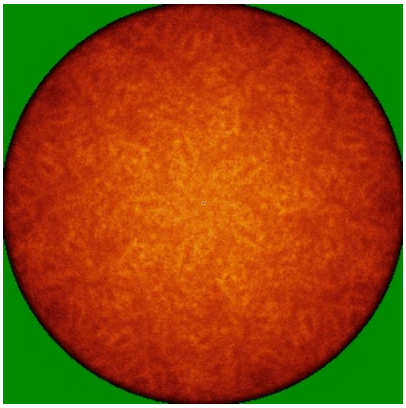
6.4.2 Raw map



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 0.015. 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.

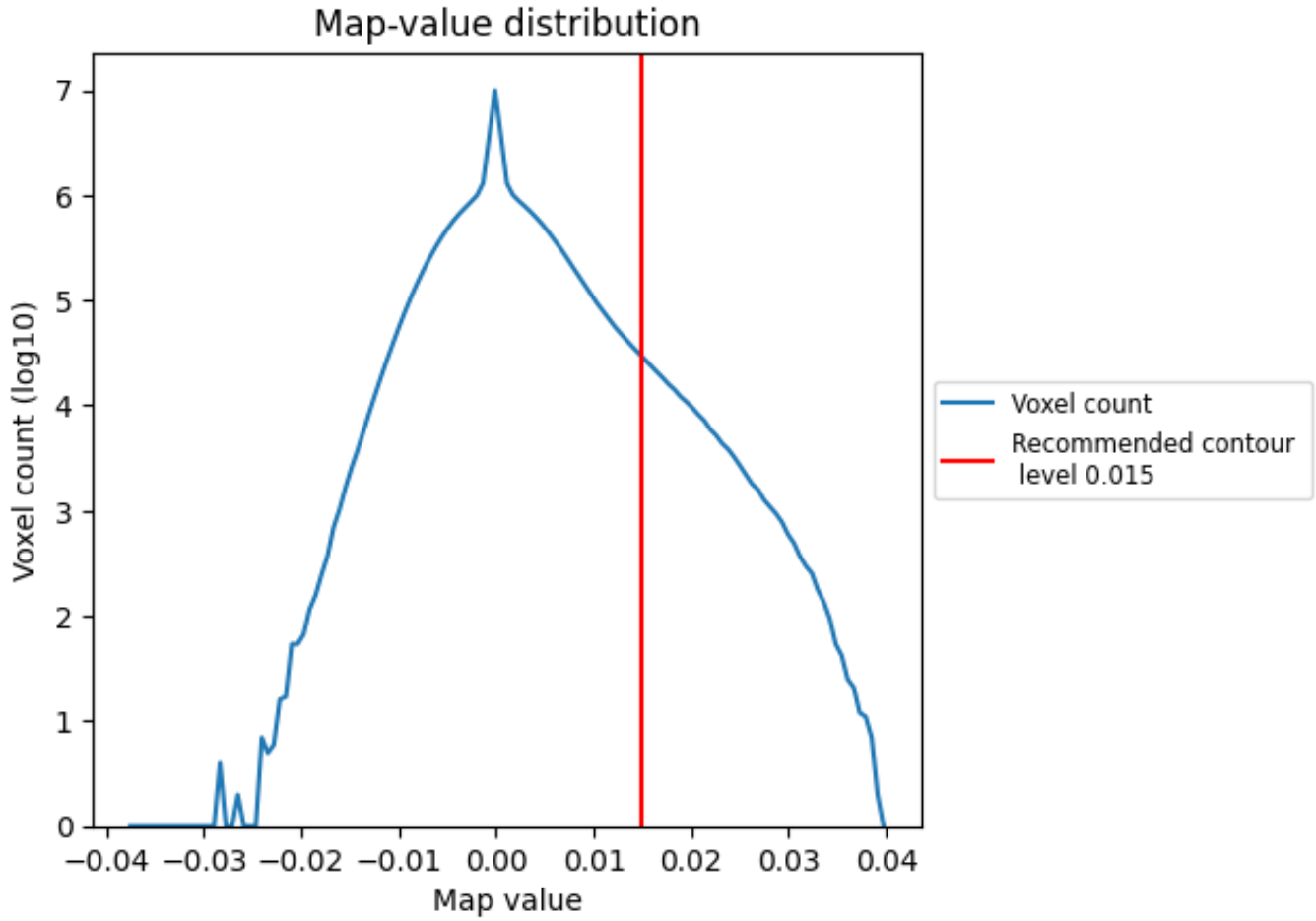
6.6 Mask visualisation (i)

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

7 Map analysis

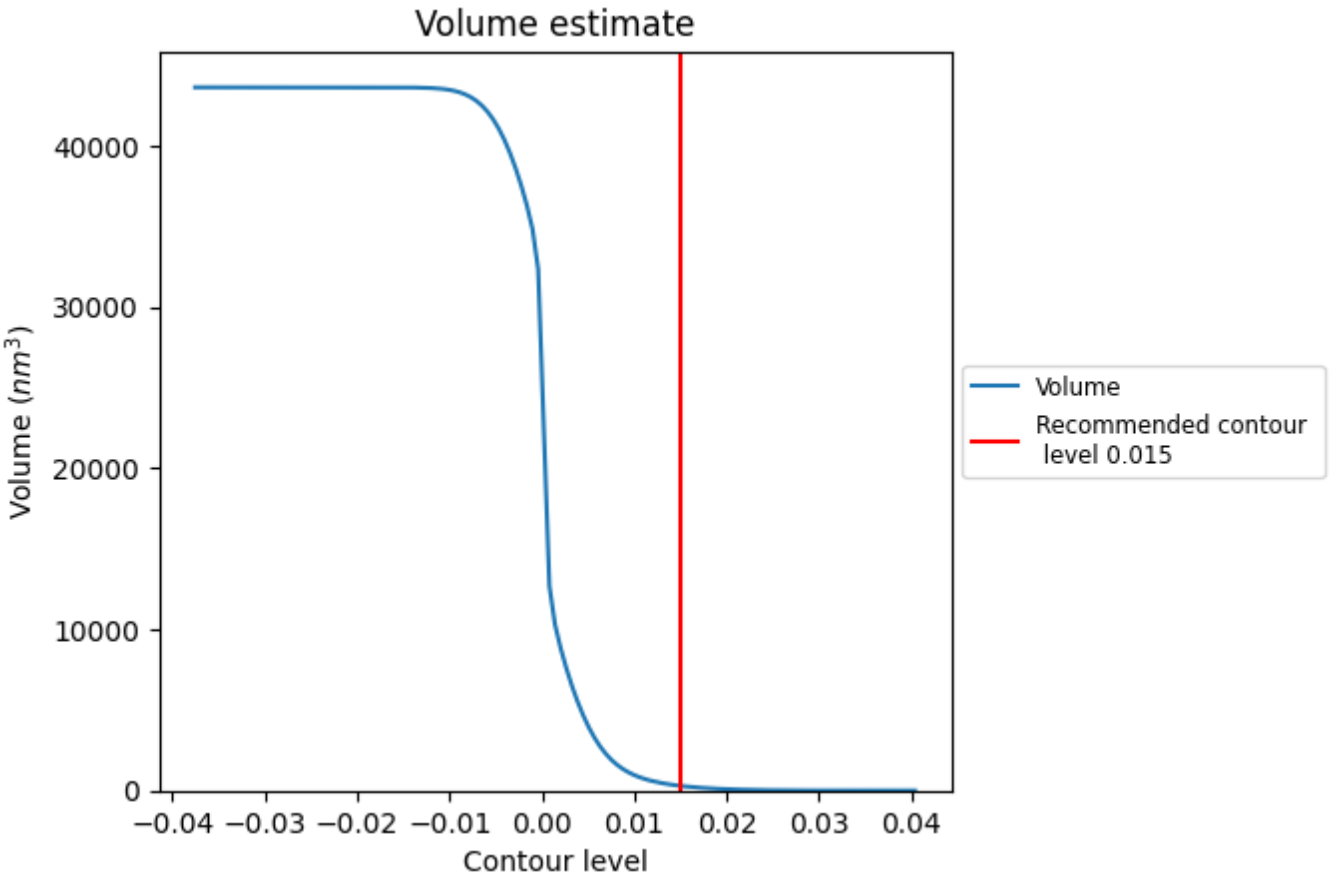
This section contains the results of statistical analysis of the map.

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.

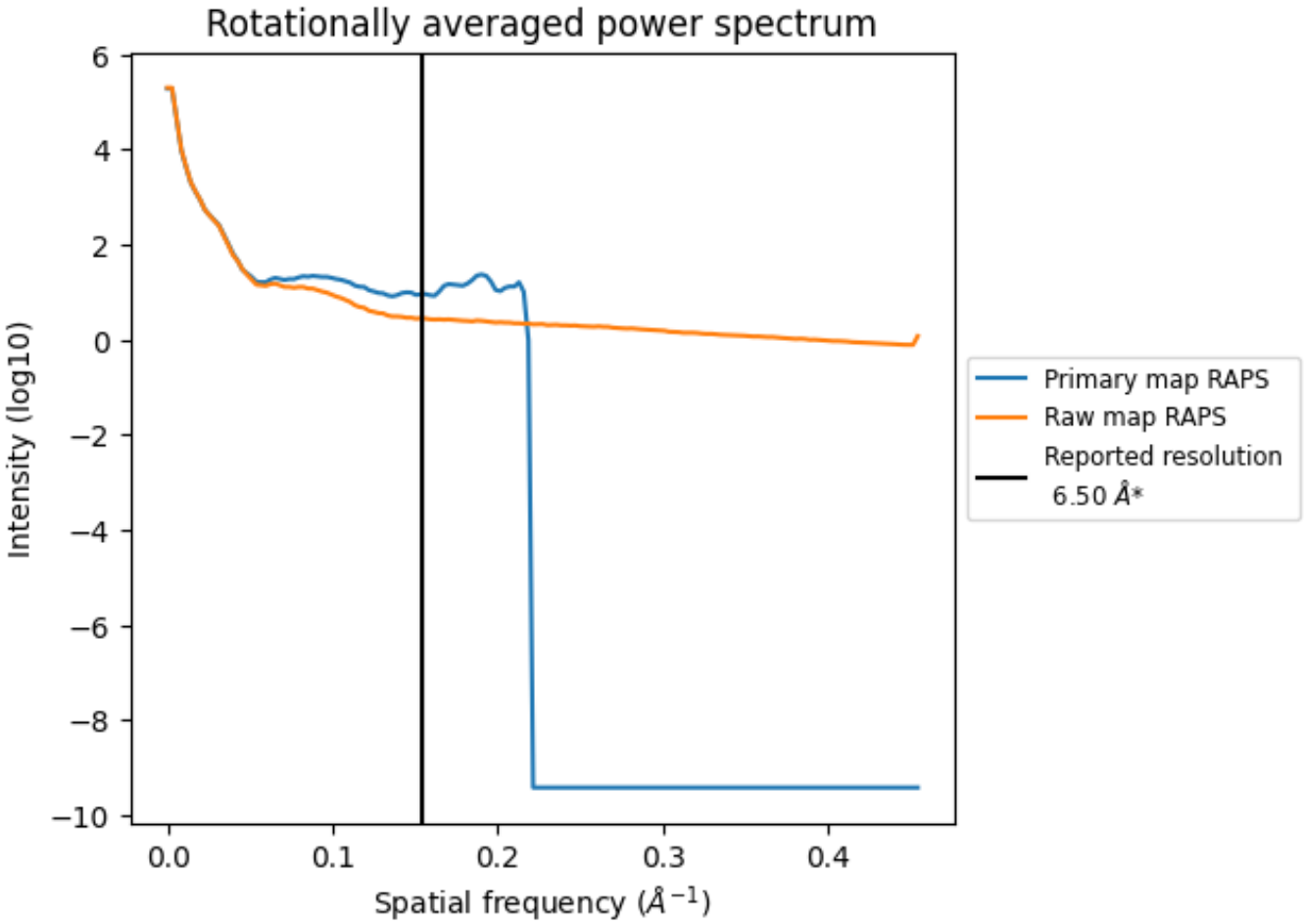
7.2 Volume estimate (i)



The volume at the recommended contour level is 290 nm^3; this corresponds to an approximate mass of 262 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)

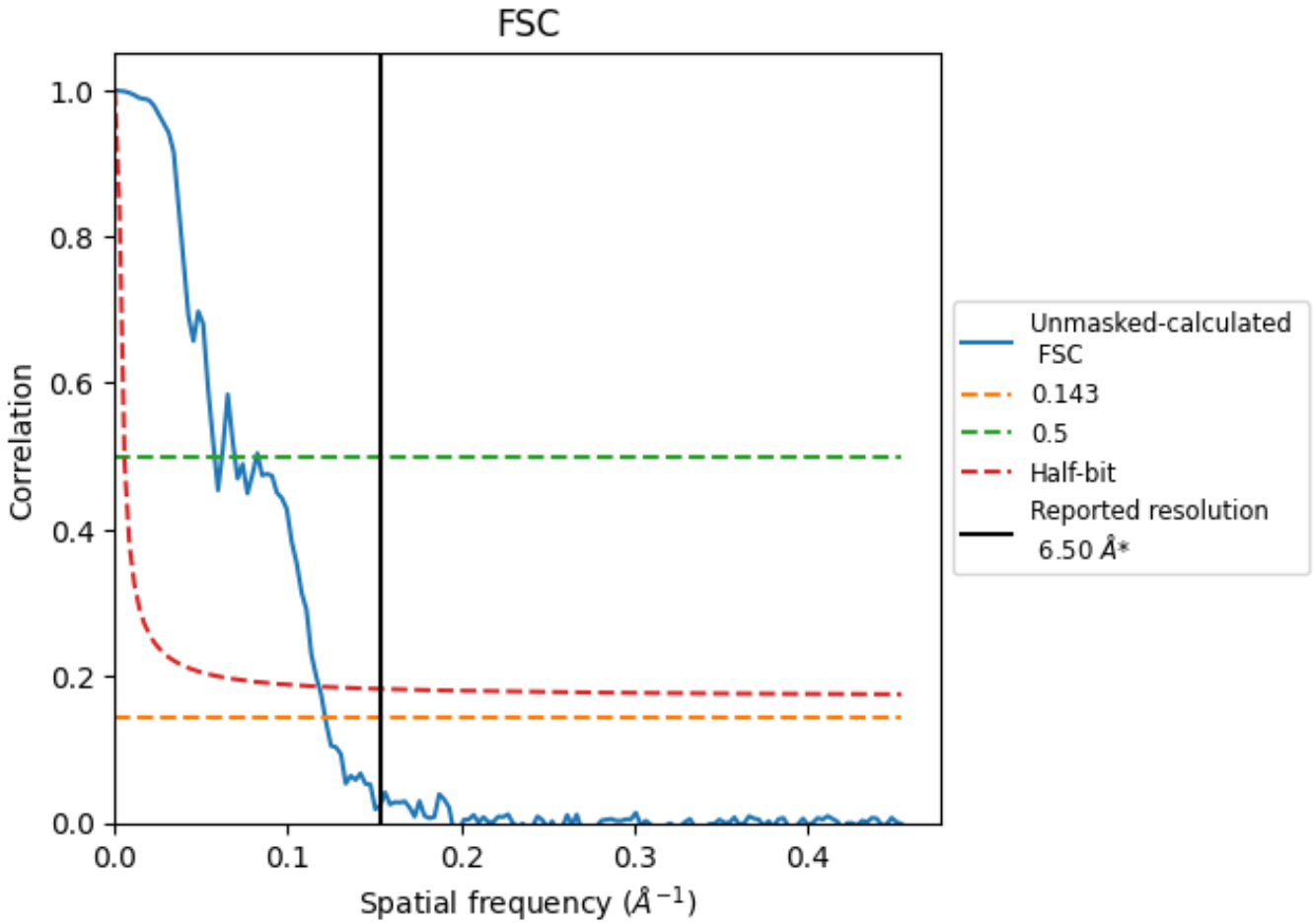


*Reported resolution corresponds to spatial frequency of 0.154 Å^{-1}

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 0.154 Å^{-1}

8.2 Resolution estimates (i)

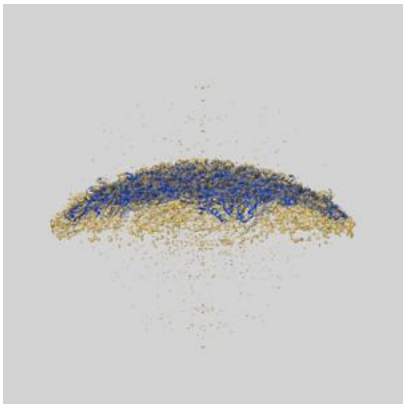
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.22	17.33	8.47

*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 8.22 differs from the reported value 6.5 by more than 10 %

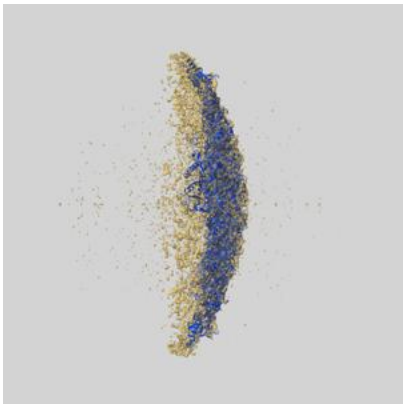
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43726 and PDB model 8W1I. Per-residue inclusion information can be found in section 3 on page 5.

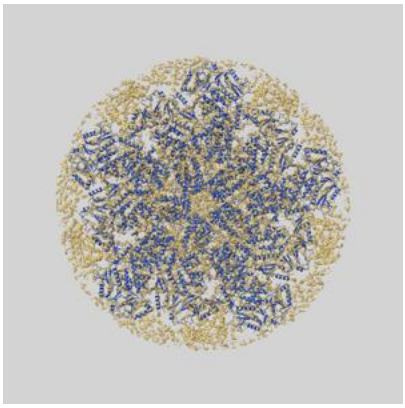
9.1 Map-model overlay



X



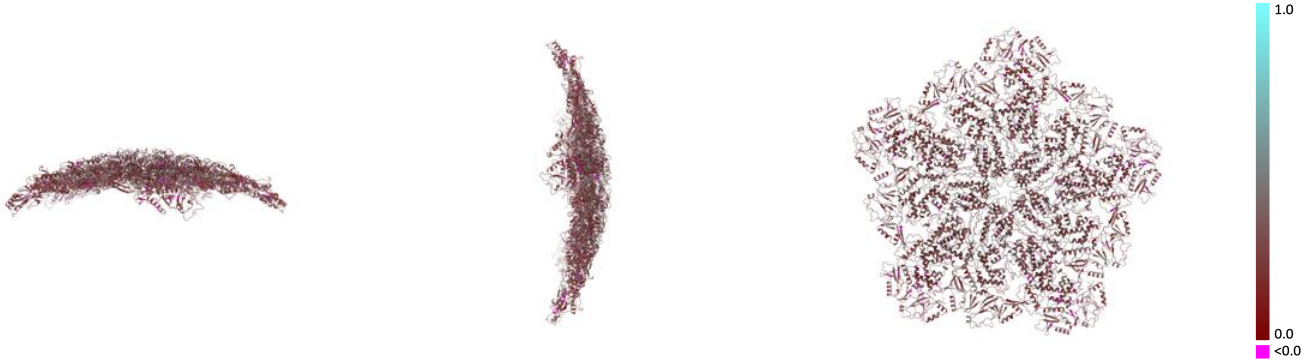
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

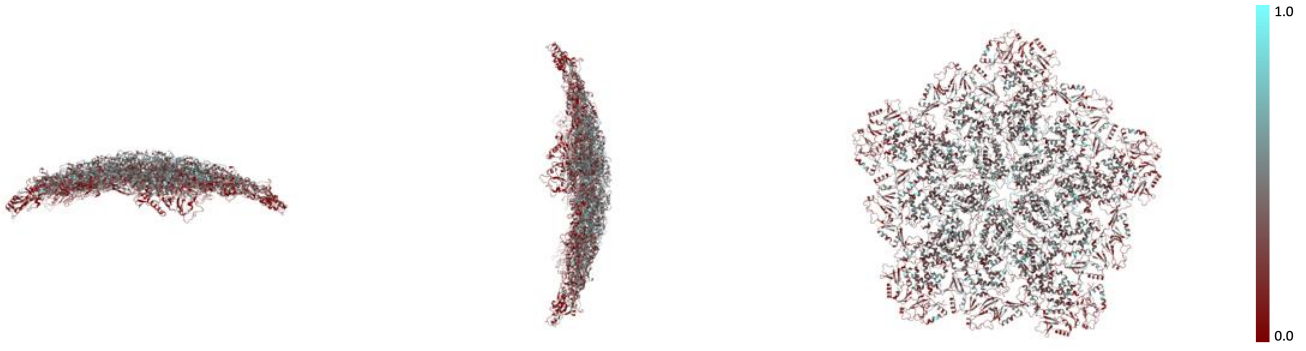
9.2 Q-score mapped to coordinate model



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.

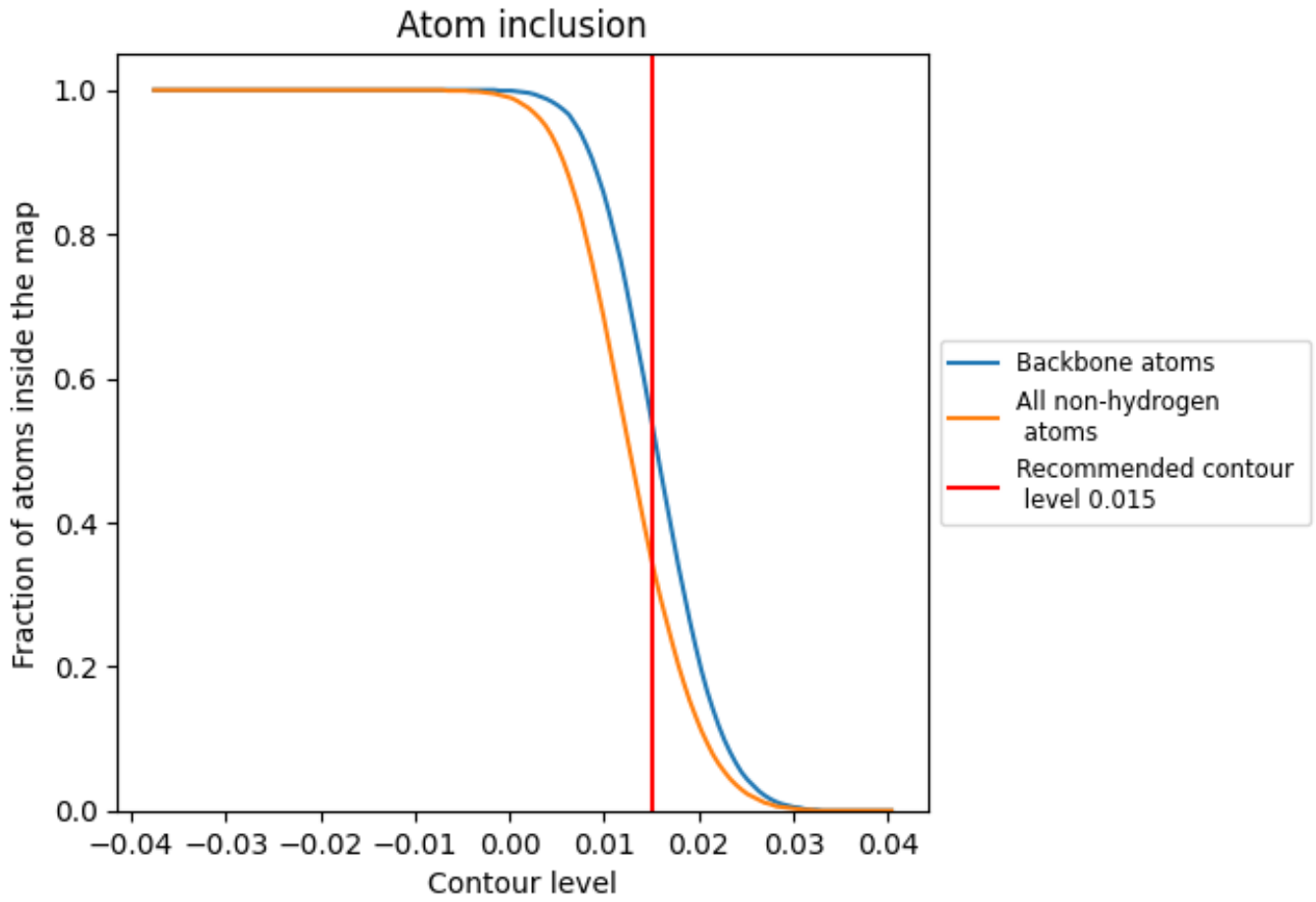
9.3 Atom inclusion mapped to coordinate model



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 35% 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	0.3490	0.3000
A	0.3760	0.3080
B	0.3220	0.2950
D	0.3770	0.3090
E	0.3780	0.3070
F	0.3800	0.3070
G	0.3780	0.3080
H	0.3220	0.2930
I	0.3210	0.2910
J	0.3210	0.2920
K	0.3210	0.2940