



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 01:58 PM UTC

PDB ID : 6WH3 / pdb_00006wh3
EMDB ID : EMD-21667
Title : Capsid structure of Penaeus monodon metallodensovirus at pH 8.2
Authors : Penzes, J.J.; Pham, H.T.; Chipman, P.; Bhattacharya, N.; McKenna, R.;
Agbandje-McKenna, M.; Tijssen, P.
Deposited on : 2020-04-07
Resolution : 2.96 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

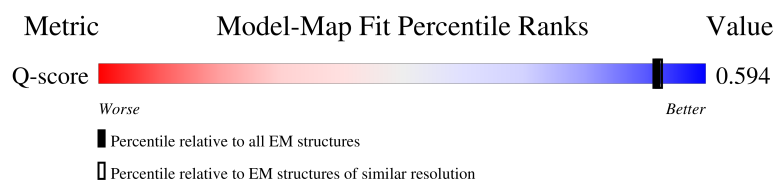
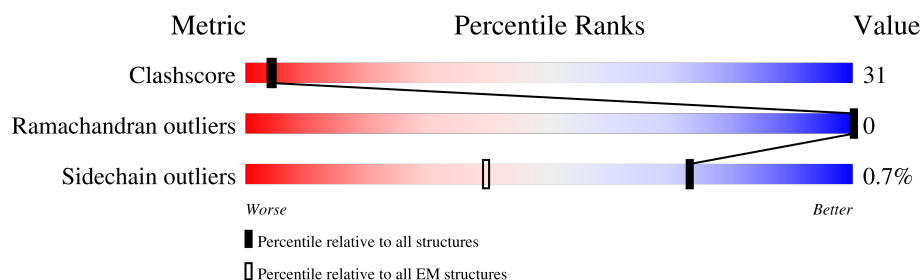
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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.



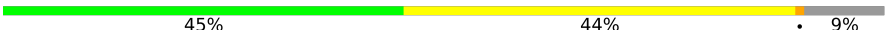
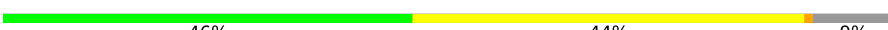
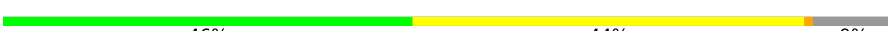
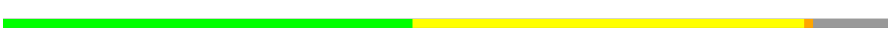
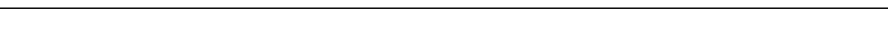
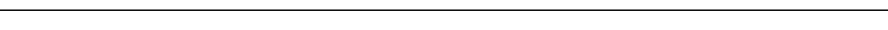
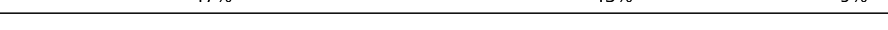
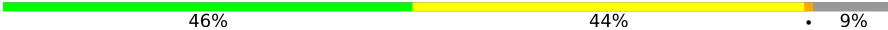
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	1	369	46% 44% 9%
1	2	369	45% 44% 9%
1	3	369	46% 44% 9%
1	4	369	45% 44% 9%

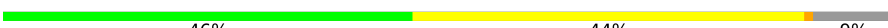
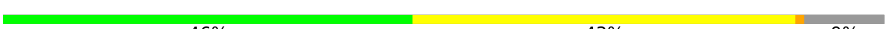
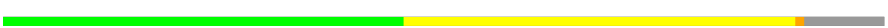
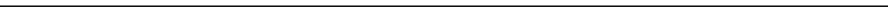
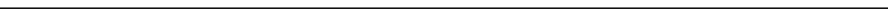
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Mol	Chain	Length	Quality of chain
1	5	369	 45% 44% 9%
1	6	369	 46% 43% 9%
1	7	369	 46% 43% 9%
1	8	369	 46% 44% 9%
1	A	369	 46% 44% 9%
1	B	369	 46% 44% 9%
1	C	369	 46% 43% 9%
1	D	369	 46% 44% 9%
1	E	369	 46% 43% 9%
1	F	369	 46% 43% 9%
1	G	369	 46% 43% 9%
1	H	369	 46% 44% 9%
1	I	369	 46% 44% 9%
1	J	369	 47% 43% 9%
1	K	369	 46% 43% 9%
1	L	369	 45% 44% 9%
1	M	369	 46% 44% 9%
1	N	369	 46% 44% 9%
1	O	369	 46% 44% 9%
1	P	369	 46% 44% 9%
1	Q	369	 46% 44% 9%
1	R	369	 46% 43% 9%
1	S	369	 46% 44% 9%
1	T	369	 46% 44% 9%
1	U	369	 46% 44% 9%

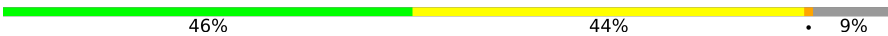
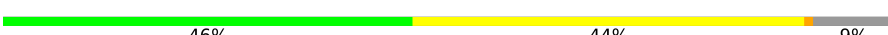
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Mol	Chain	Length	Quality of chain		
1	V	369		45%	44% 9%
1	W	369		46%	44% 9%
1	X	369		46%	44% 9%
1	Y	369		46%	44% 9%
1	Z	369		46%	43% 9%
1	a	369		45%	44% 9%
1	b	369		46%	44% 9%
1	c	369		46%	44% 9%
1	d	369		46%	44% 9%
1	e	369		46%	44% 9%
1	f	369		46%	43% 9%
1	g	369		46%	43% 9%
1	h	369		46%	44% 9%
1	i	369		46%	44% 9%
1	j	369		47%	43% 9%
1	k	369		46%	44% 9%
1	l	369		46%	43% 9%
1	m	369		45%	44% 9%
1	n	369		46%	43% 9%
1	o	369		45%	44% 9%
1	p	369		46%	44% 9%
1	q	369		46%	43% 9%
1	r	369		46%	44% 9%
1	s	369		46%	44% 9%
1	t	369		46%	44% 9%

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Mol	Chain	Length	Quality of chain
1	u	369	
1	v	369	
1	w	369	
1	x	369	
1	y	369	
1	z	369	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 157740 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 Penaeus monodon metallogenovirus major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	B	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	C	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	D	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	E	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	F	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	G	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	H	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	I	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	J	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	K	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	L	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	M	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	N	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	O	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	P	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	Q	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	S	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	T	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	U	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	V	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	W	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	X	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	Y	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	Z	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	8	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	7	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	6	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	5	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	4	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	3	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	a	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	b	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	c	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	d	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	e	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	f	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	h	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	i	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	j	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	k	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	l	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	m	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	n	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	o	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	p	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	q	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	r	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	s	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	t	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	u	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	v	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	w	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	x	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	y	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	z	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		
1	1	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	334	Total	C	N	O	S	0	0
			2628	1659	453	502	14		

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Ca	0
			1	1	
2	B	1	Total	Ca	0
			1	1	
2	C	1	Total	Ca	0
			1	1	
2	D	1	Total	Ca	0
			1	1	
2	E	1	Total	Ca	0
			1	1	
2	F	1	Total	Ca	0
			1	1	
2	G	1	Total	Ca	0
			1	1	
2	H	1	Total	Ca	0
			1	1	
2	I	1	Total	Ca	0
			1	1	
2	J	1	Total	Ca	0
			1	1	
2	K	1	Total	Ca	0
			1	1	
2	L	1	Total	Ca	0
			1	1	
2	M	1	Total	Ca	0
			1	1	
2	N	1	Total	Ca	0
			1	1	
2	O	1	Total	Ca	0
			1	1	
2	P	1	Total	Ca	0
			1	1	
2	Q	1	Total	Ca	0
			1	1	
2	R	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
2	S	1	Total 1	Ca 1	0
2	T	1	Total 1	Ca 1	0
2	U	1	Total 1	Ca 1	0
2	V	1	Total 1	Ca 1	0
2	W	1	Total 1	Ca 1	0
2	X	1	Total 1	Ca 1	0
2	Y	1	Total 1	Ca 1	0
2	Z	1	Total 1	Ca 1	0
2	8	1	Total 1	Ca 1	0
2	7	1	Total 1	Ca 1	0
2	6	1	Total 1	Ca 1	0
2	5	1	Total 1	Ca 1	0
2	4	1	Total 1	Ca 1	0
2	3	1	Total 1	Ca 1	0
2	a	1	Total 1	Ca 1	0
2	b	1	Total 1	Ca 1	0
2	c	1	Total 1	Ca 1	0
2	d	1	Total 1	Ca 1	0
2	e	1	Total 1	Ca 1	0
2	f	1	Total 1	Ca 1	0
2	g	1	Total 1	Ca 1	0

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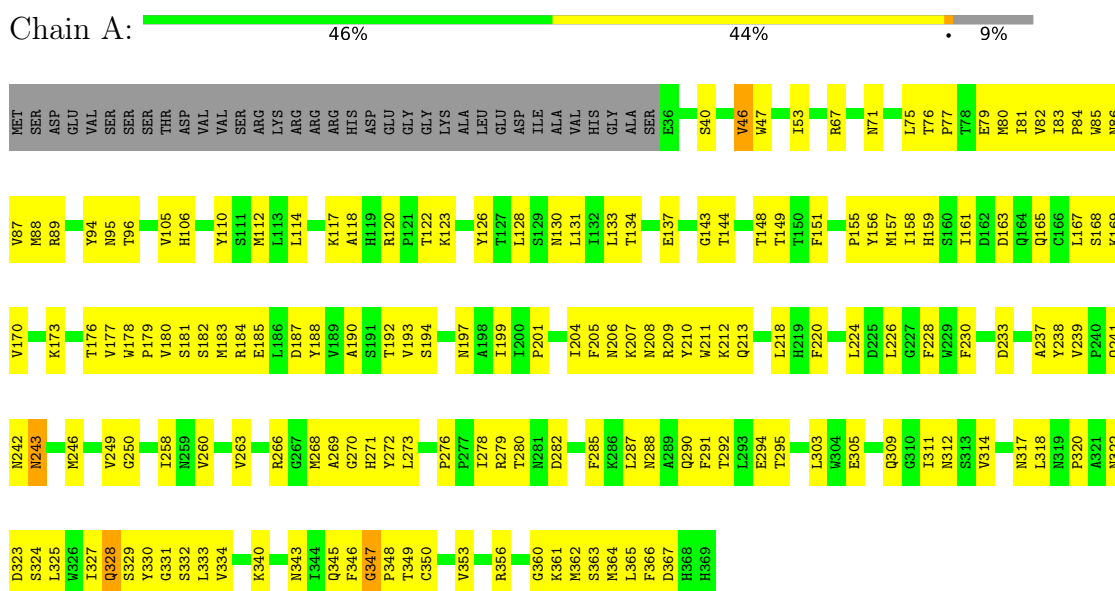
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Mol	Chain	Residues	Atoms		AltConf
2	h	1	Total 1	Ca 1	0
2	i	1	Total 1	Ca 1	0
2	j	1	Total 1	Ca 1	0
2	k	1	Total 1	Ca 1	0
2	l	1	Total 1	Ca 1	0
2	m	1	Total 1	Ca 1	0
2	n	1	Total 1	Ca 1	0
2	o	1	Total 1	Ca 1	0
2	p	1	Total 1	Ca 1	0
2	q	1	Total 1	Ca 1	0
2	r	1	Total 1	Ca 1	0
2	s	1	Total 1	Ca 1	0
2	t	1	Total 1	Ca 1	0
2	u	1	Total 1	Ca 1	0
2	v	1	Total 1	Ca 1	0
2	w	1	Total 1	Ca 1	0
2	x	1	Total 1	Ca 1	0
2	y	1	Total 1	Ca 1	0
2	z	1	Total 1	Ca 1	0
2	1	1	Total 1	Ca 1	0
2	2	1	Total 1	Ca 1	0

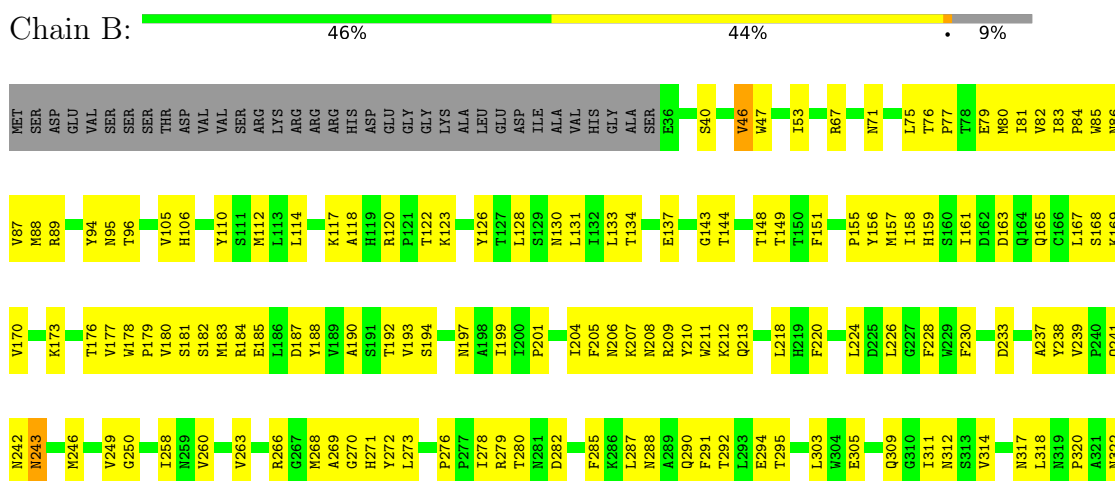
3 Residue-property plots [i](#)

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

- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein



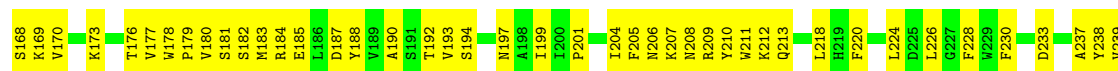
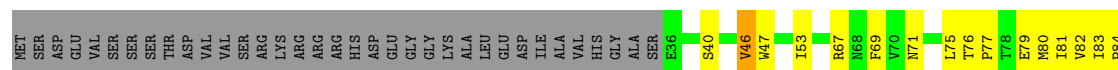
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein





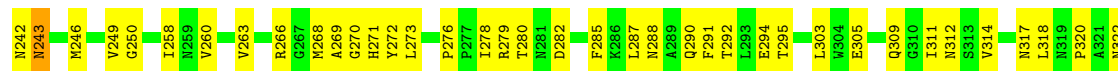
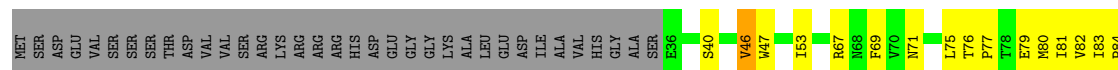
- Molecule 1: *Penaeus monodon* metalloidenovirus major capsid protein

Chain C: 46% 43% 9%



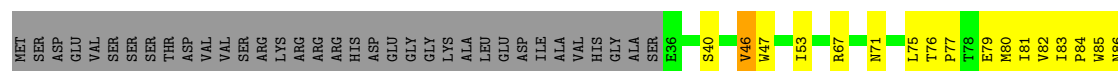
- Molecule 1: *Penaeus monodon* metalloidenovirus major capsid protein

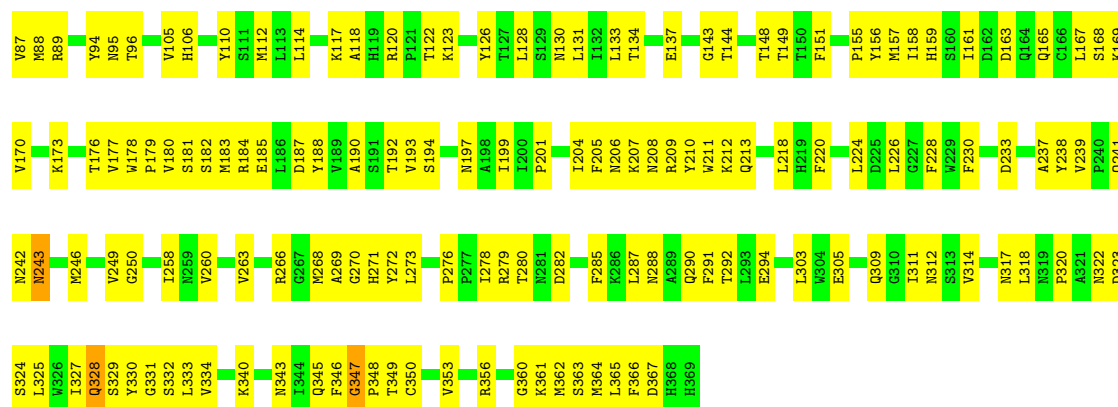
Chain D: 46% 44% 9%



- Molecule 1: *Penaeus monodon* metalloidenovirus major capsid protein

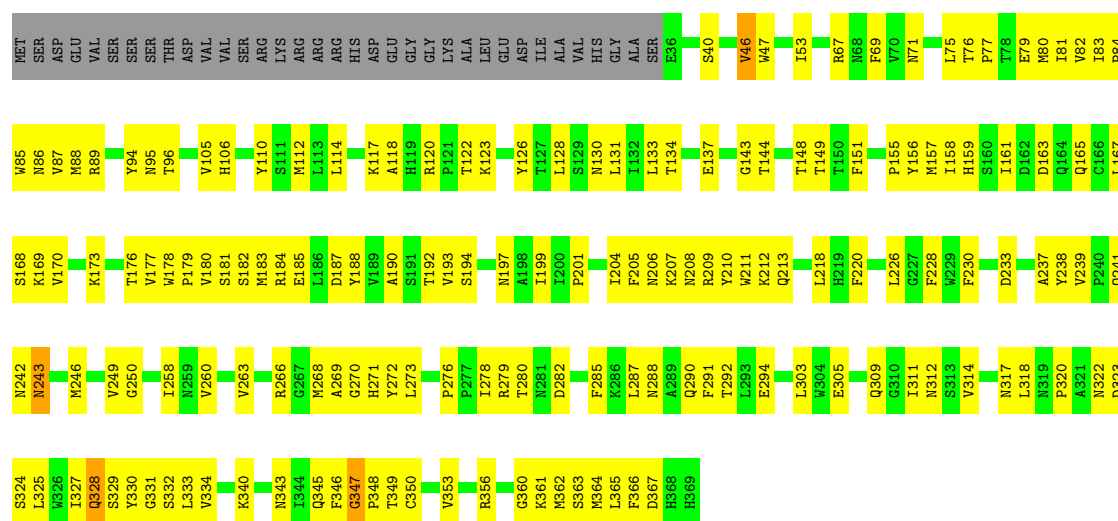
Chain E: 46% 43% 9%





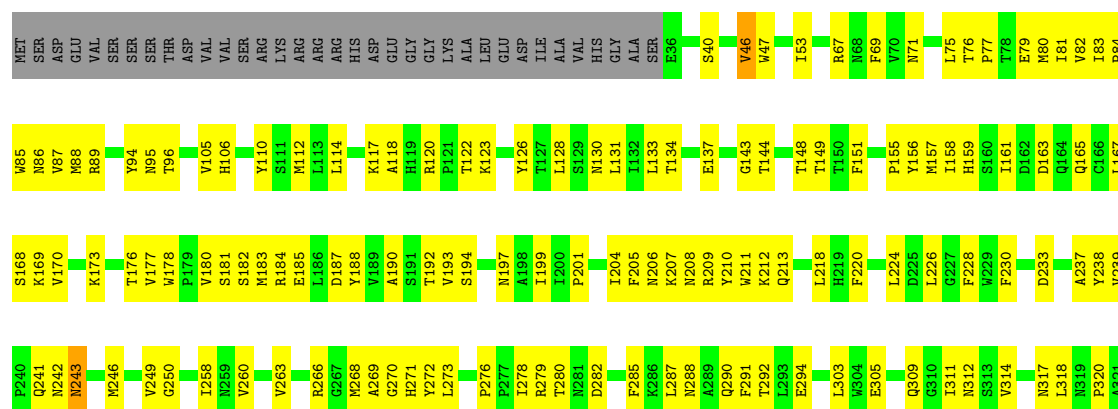
• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain F: 46% 43% 9%



• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

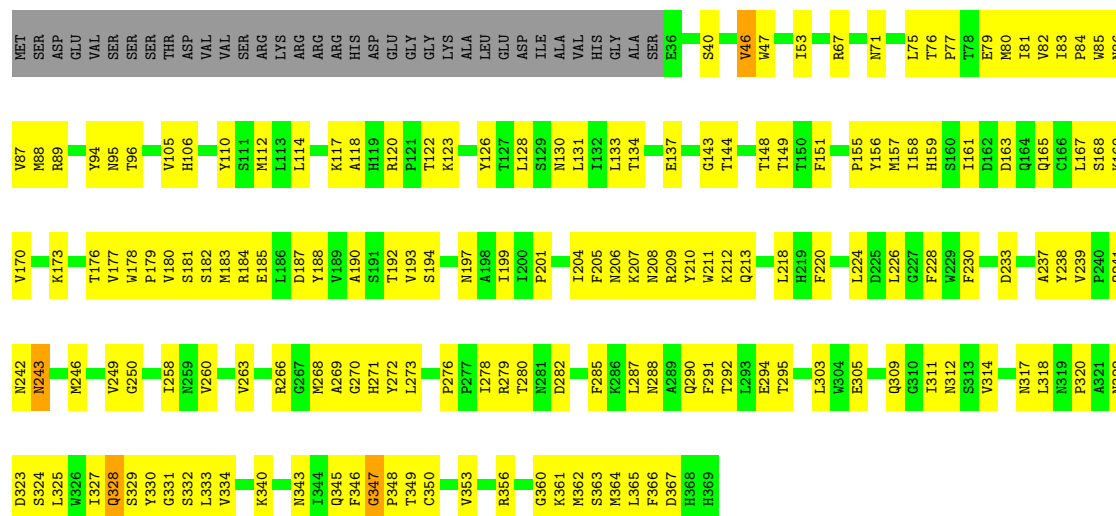
Chain G: 46% 43% 9%





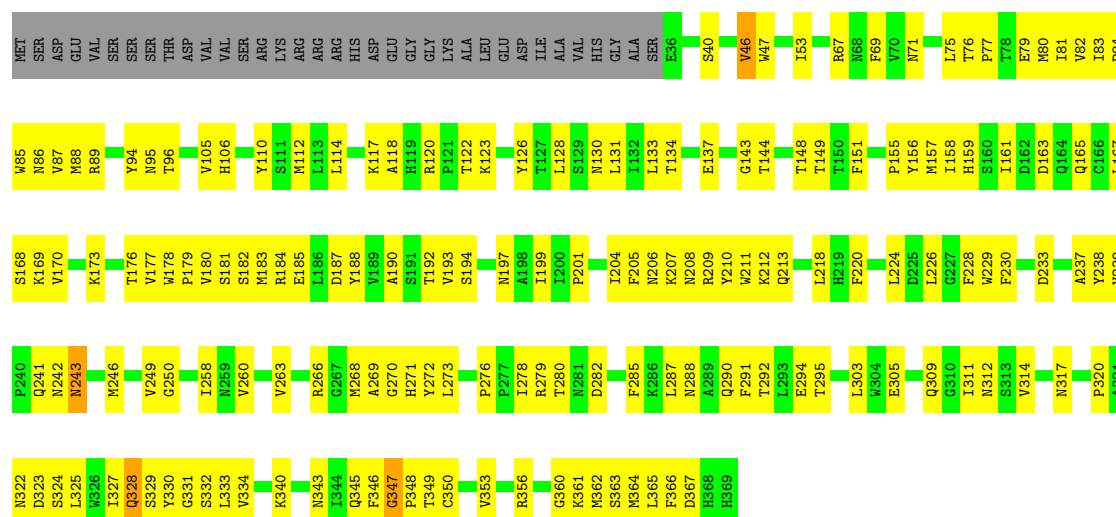
- Molecule 1: *Penaeus monodon* metalloidenovirus major capsid protein

Chain H: 46% 44% 9%



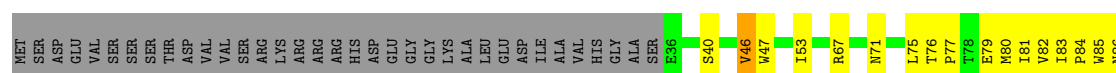
- Molecule 1: *Penaeus monodon* metalloidenovirus major capsid protein

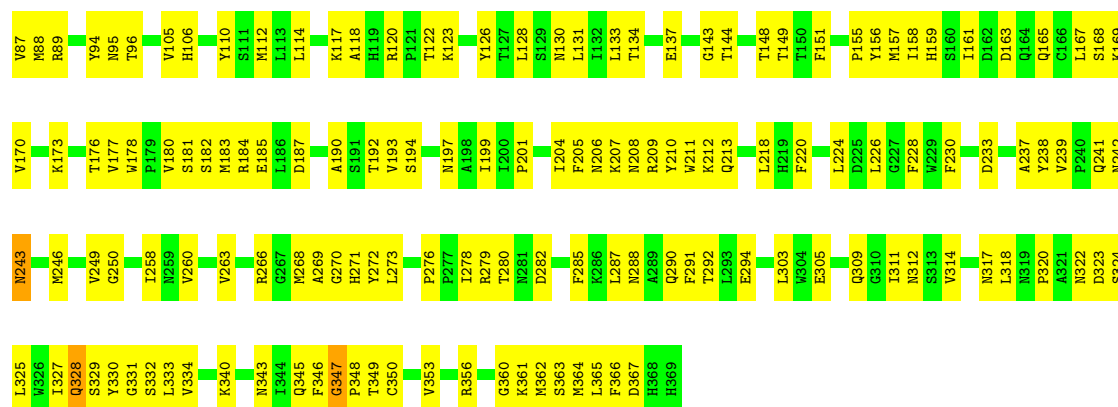
Chain I: 46% 44% 9%



- Molecule 1: *Penaeus monodon* metalloidenovirus major capsid protein

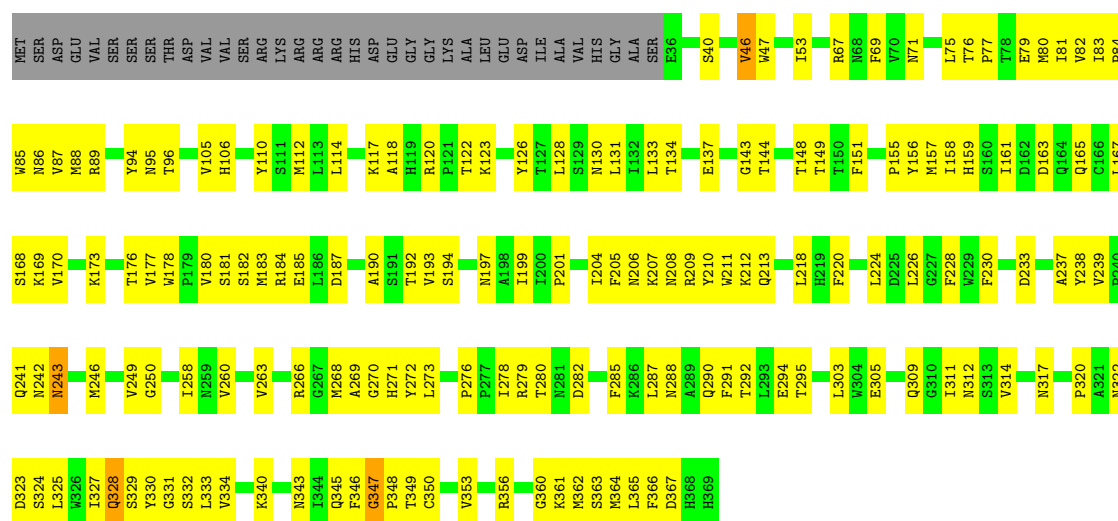
Chain J: 47% 43% 9%





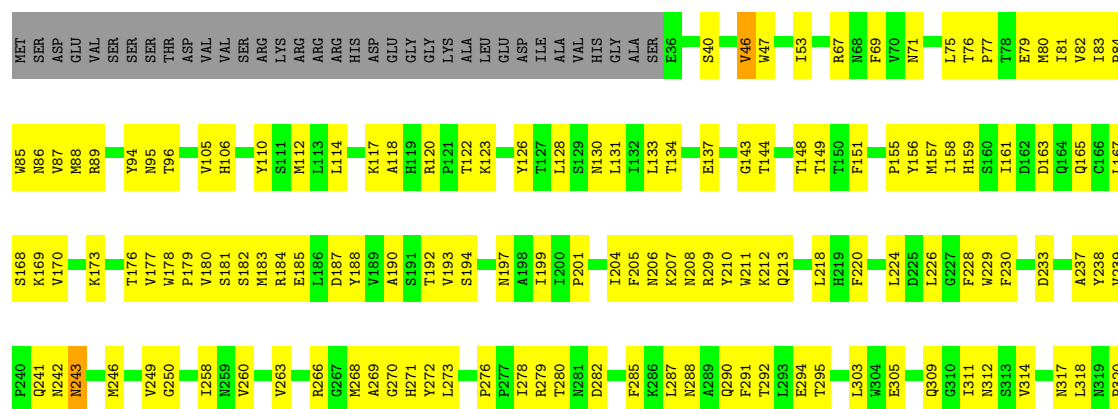
• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain K: 46% 43% 9%



• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

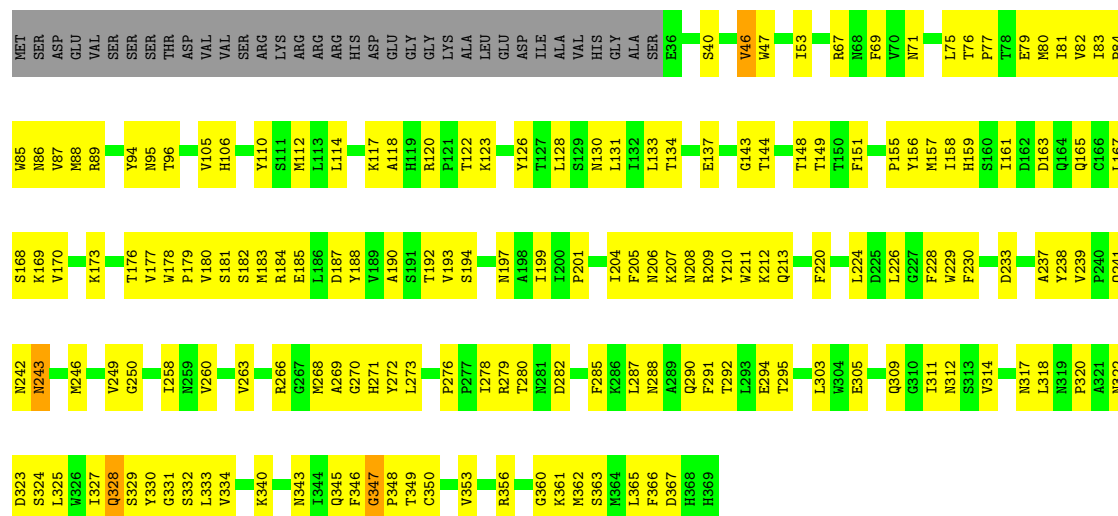
Chain L: 45% 44% 9%





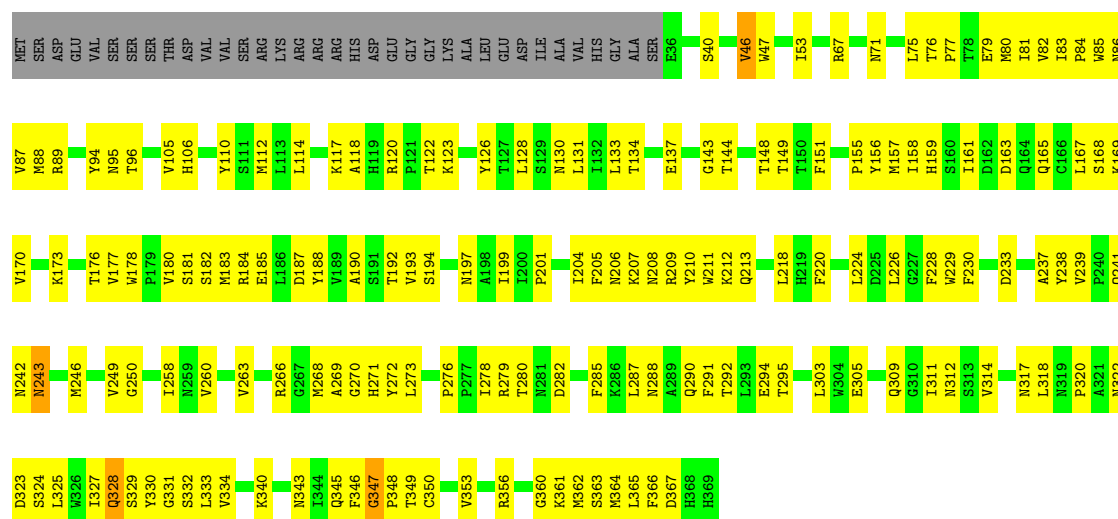
- Molecule 1: Penaeus monodon metallodensovirus major capsid protein

Chain M: 46% 44% 9%



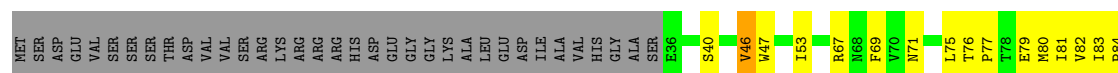
- Molecule 1: Penaeus monodon metallodensovirus major capsid protein

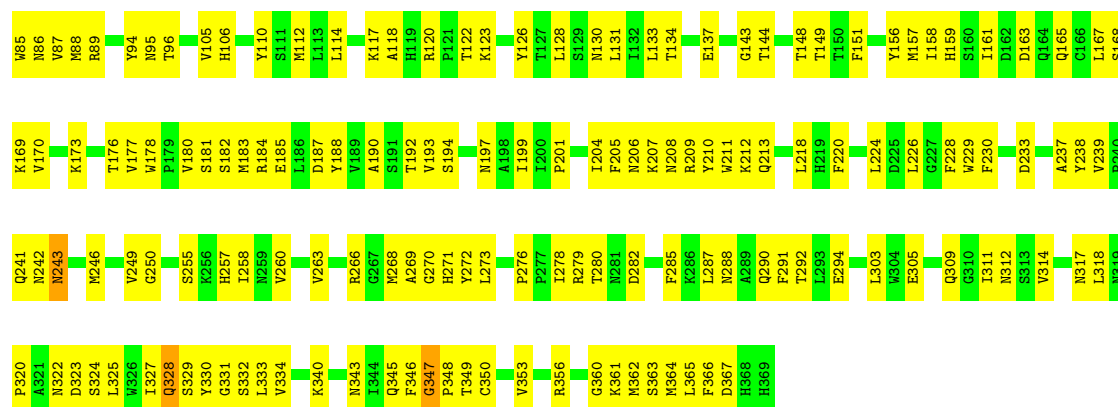
Chain N: 46% 44% 9%



- Molecule 1: Penaeus monodon metallodensovirus major capsid protein

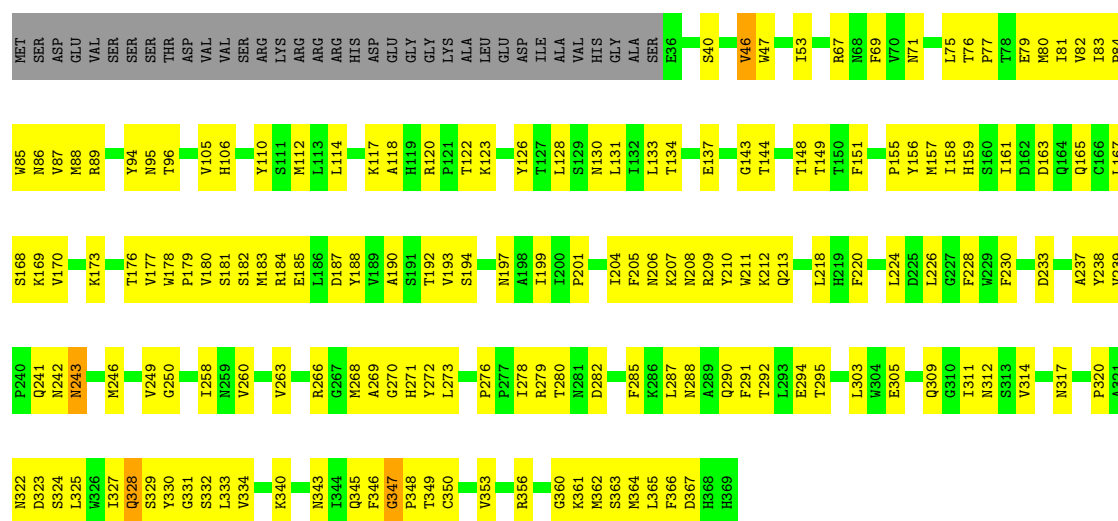
Chain O: 46% 44% 9%





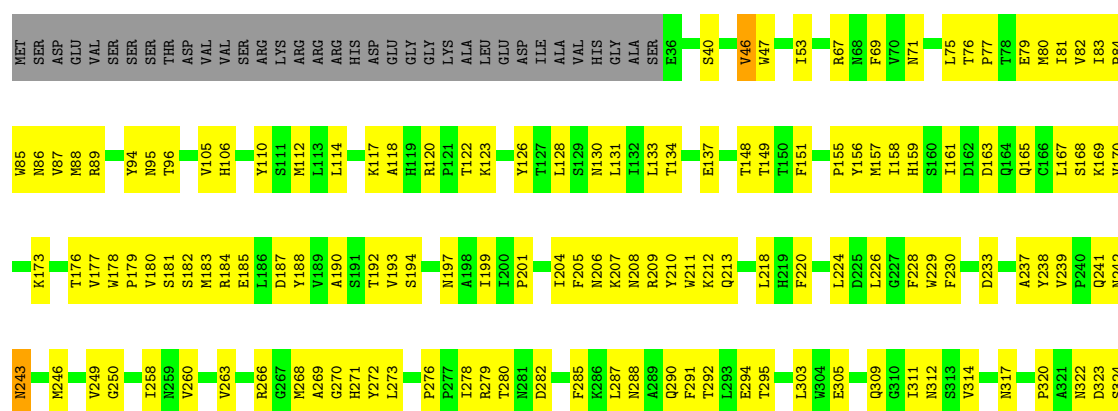
• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain P: 46% 44% 9%



• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

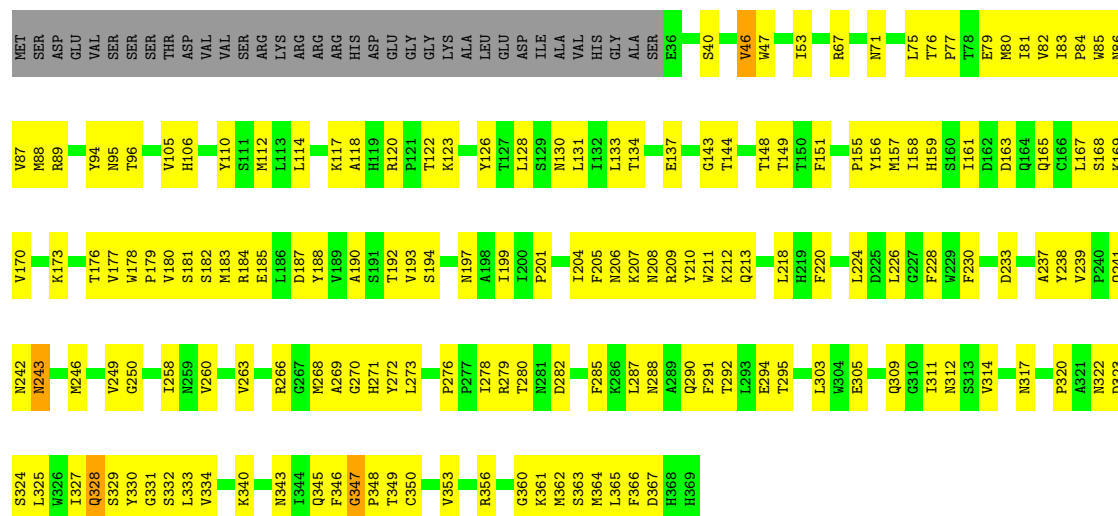
Chain Q: 46% 44% 9%





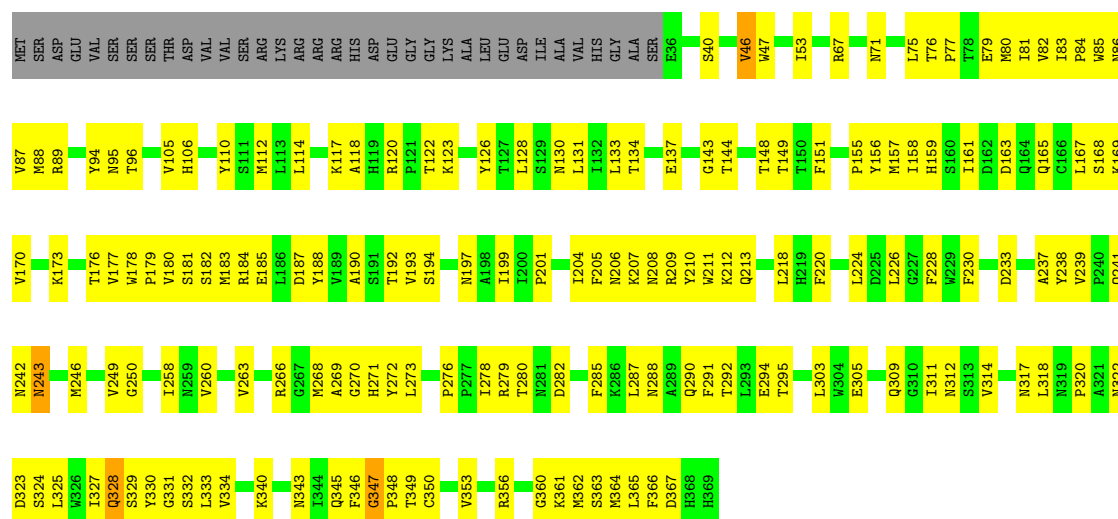
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain R: 46% 43% 9%



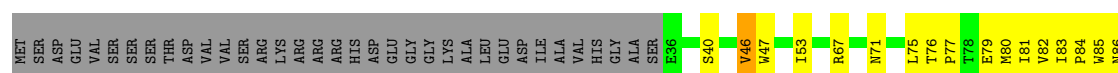
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

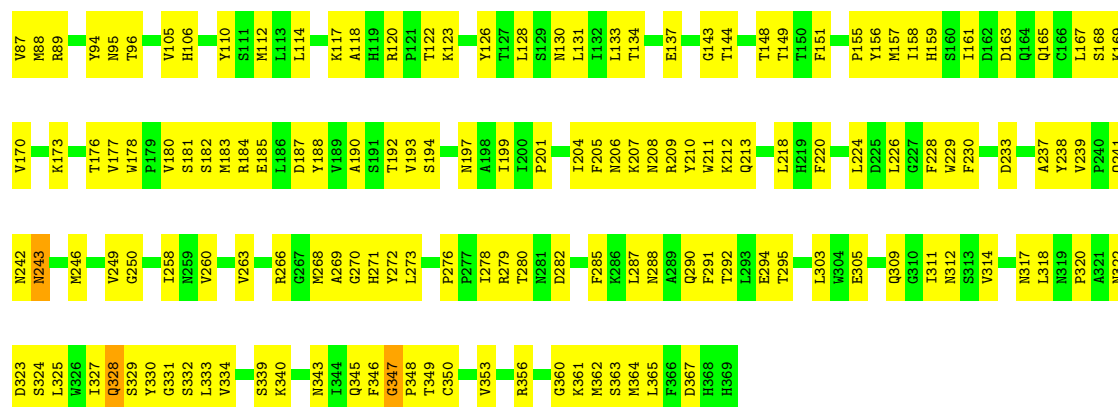
Chain S: 46% 44% 9%



- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

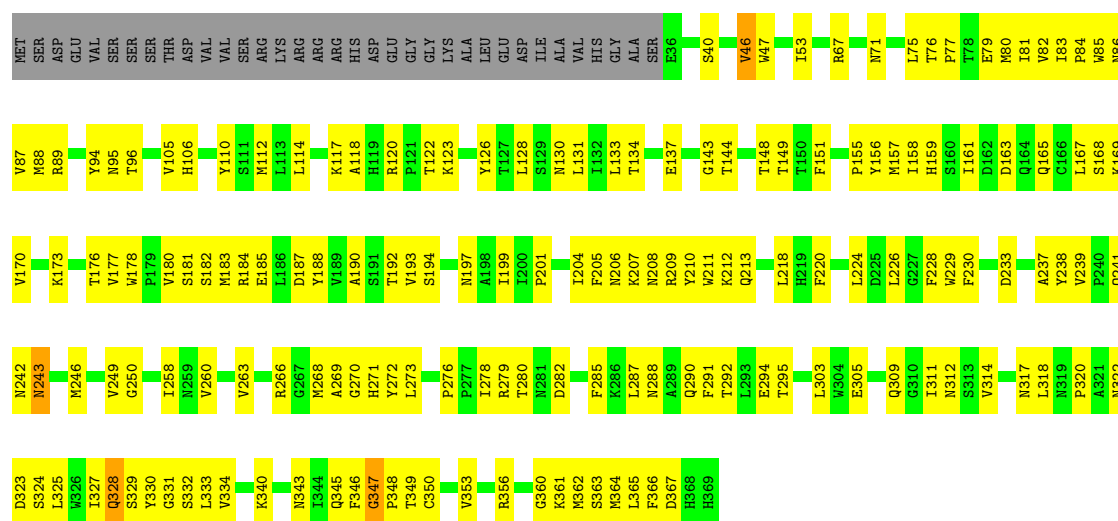
Chain T: 46% 44% 9%





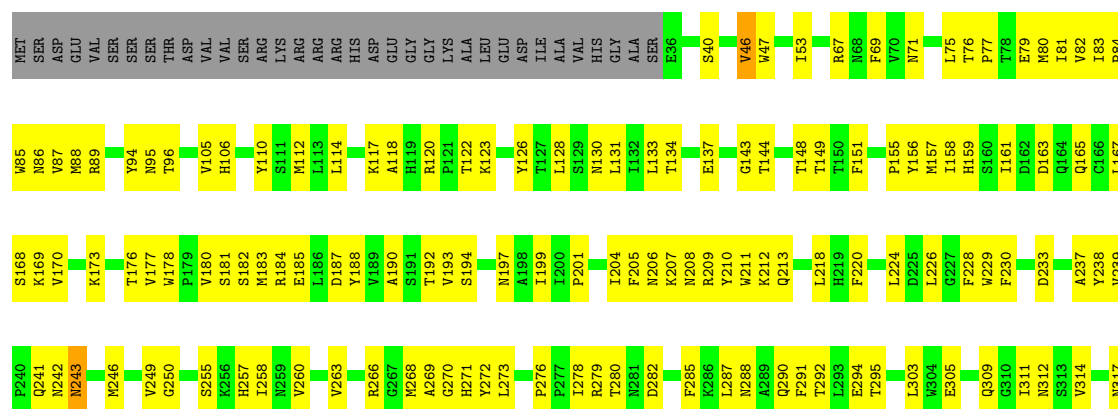
• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

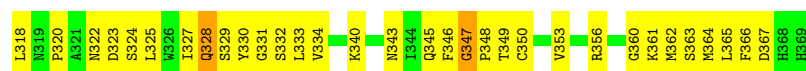
Chain U: 46% 44% 9%



• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

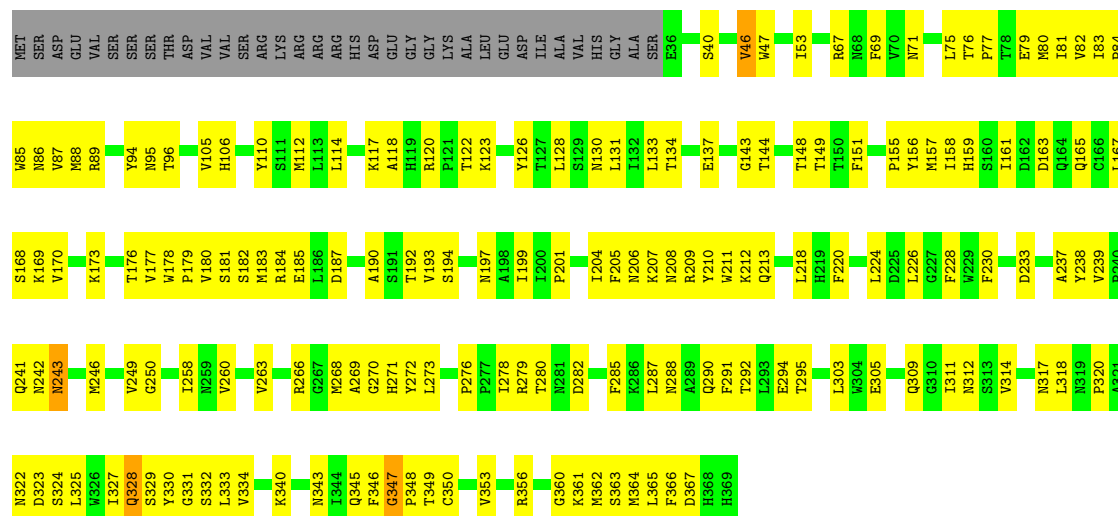
Chain V: 45% 44% 9%





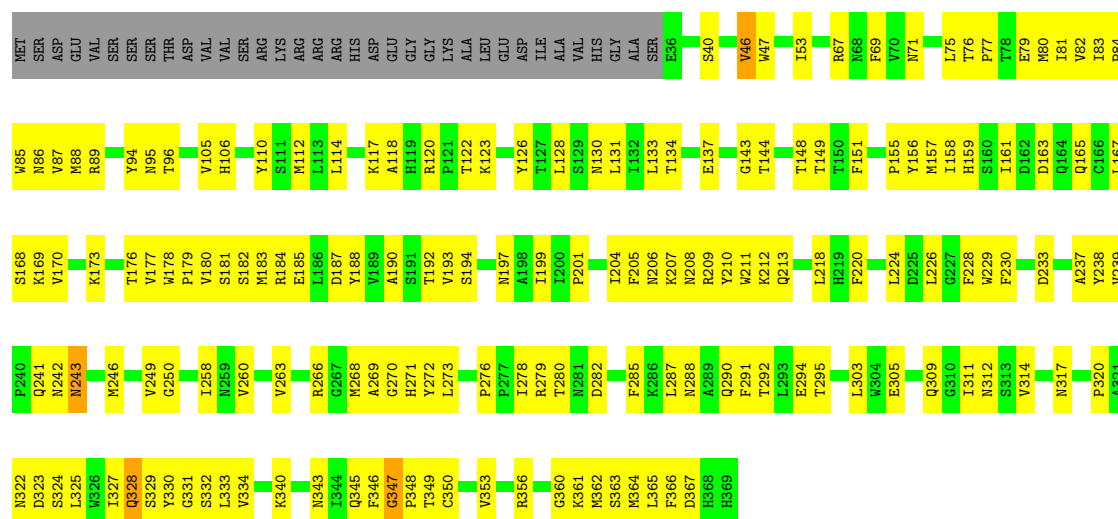
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain W: 46% 44% 9%



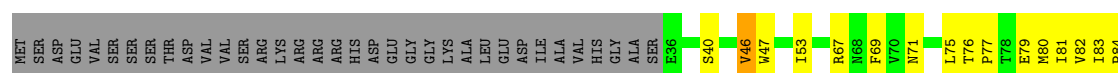
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

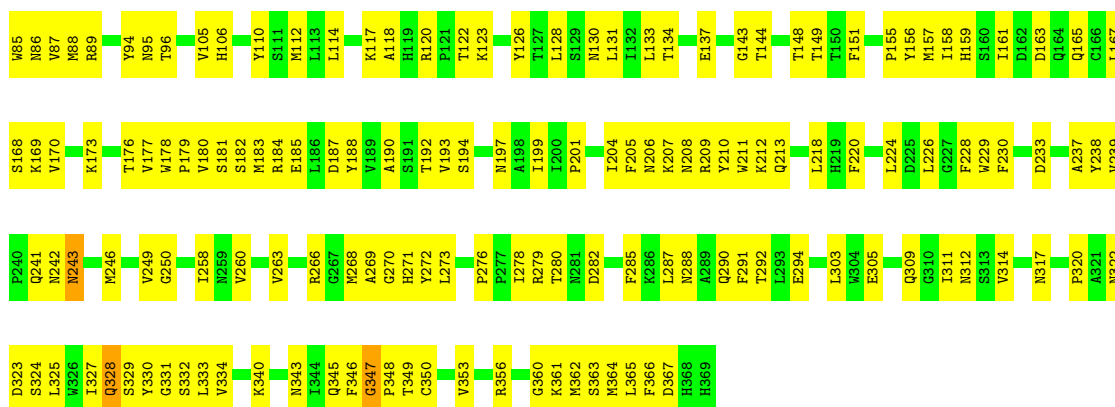
Chain X: 46% 44% 9%



- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

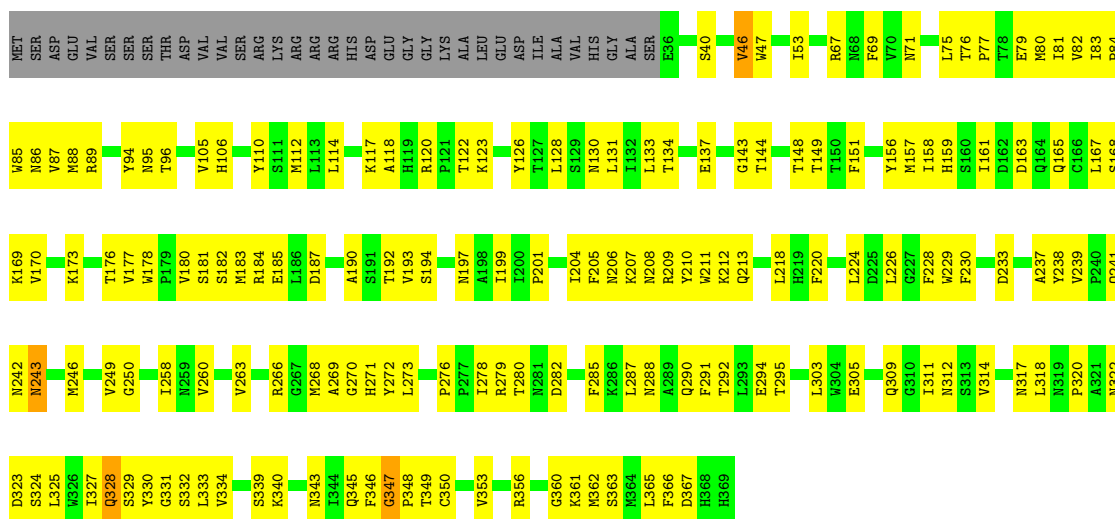
Chain Y: 46% 44% 9%





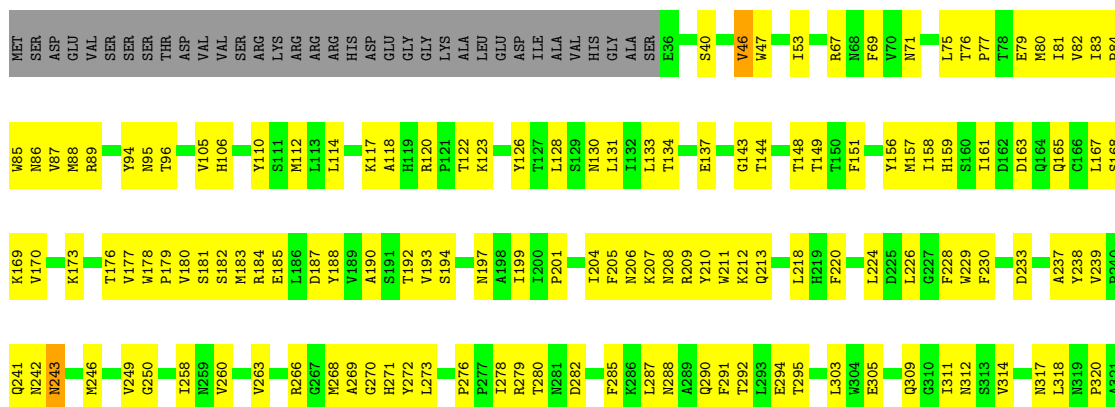
• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain Z: 46% 43% 9%



• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

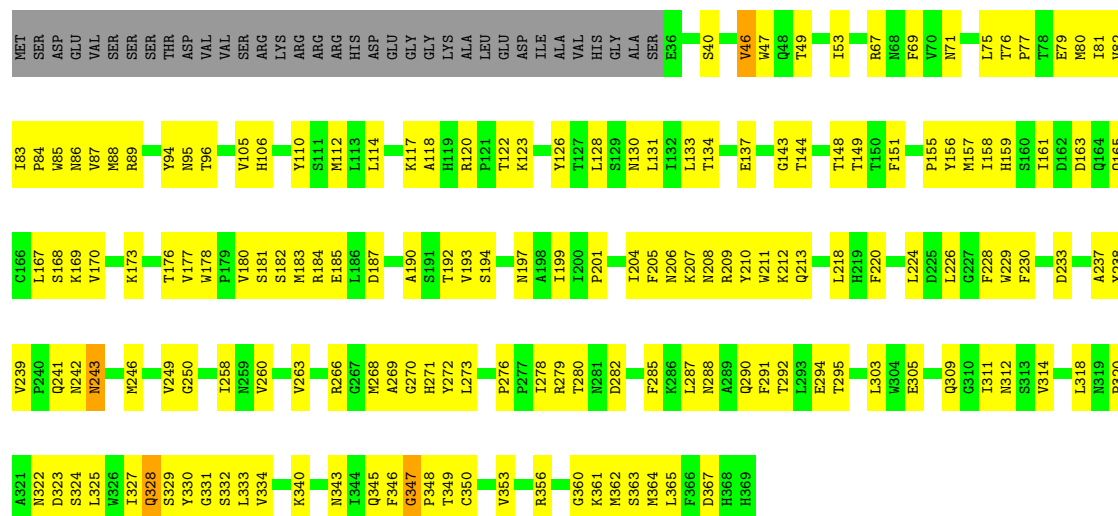
Chain 8: 46% 44% 9%





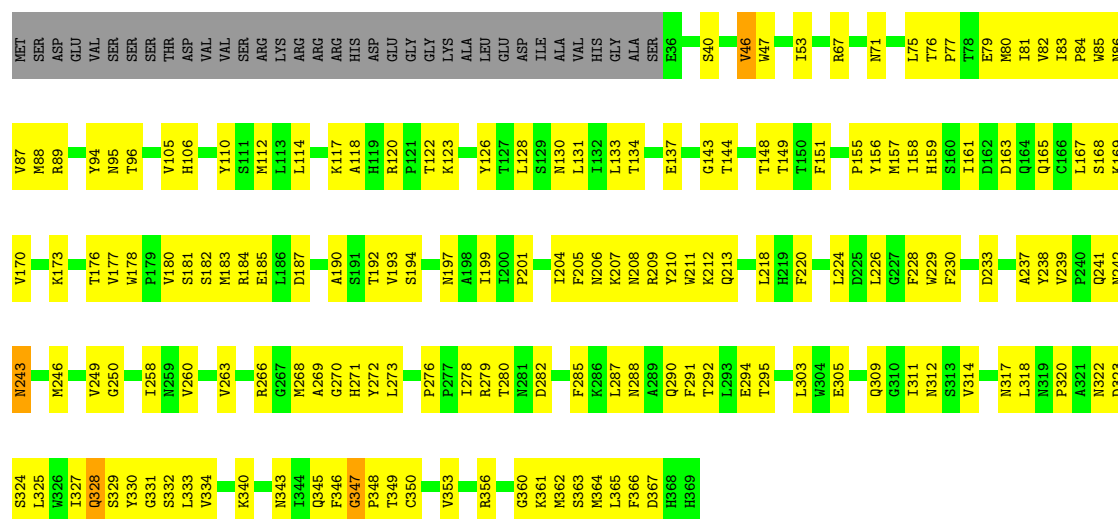
- Molecule 1: *Penaeus monodon* metalloidenovirus major capsid protein

Chain 7: 46% 43% 9%



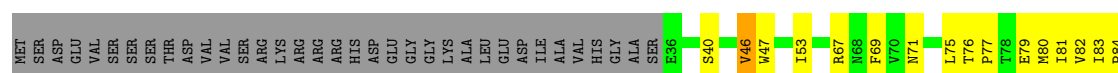
- Molecule 1: *Penaeus monodon* metalloidenovirus major capsid protein

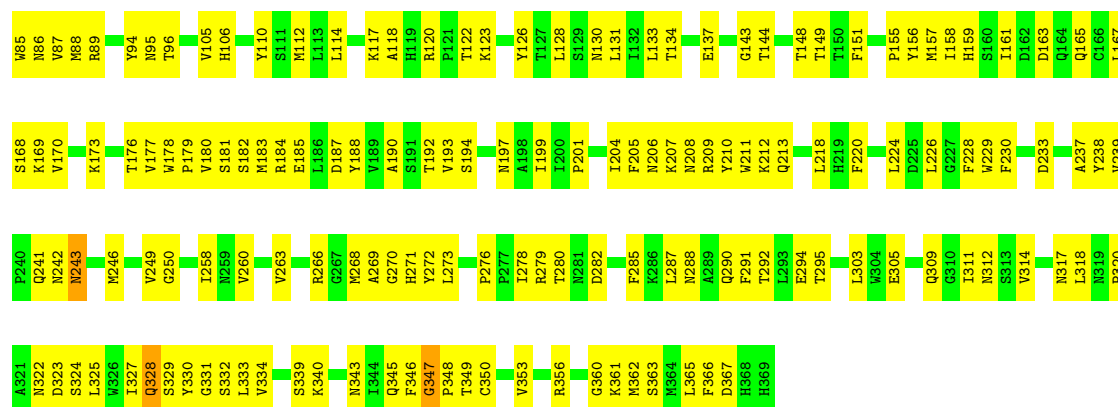
Chain 6: 46% 43% 9%



- Molecule 1: *Penaeus monodon* metalloidenovirus major capsid protein

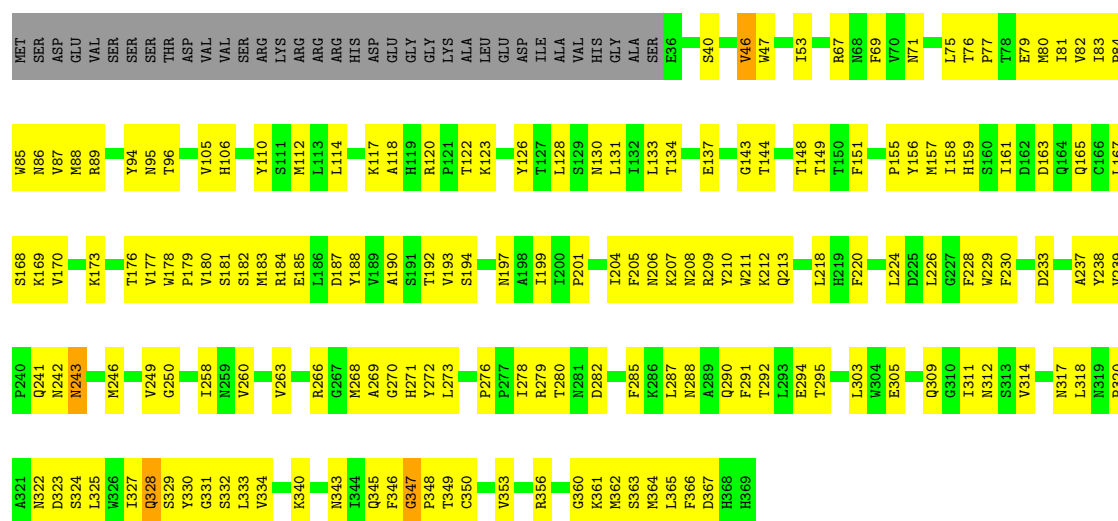
Chain 5: 45% 44% 9%





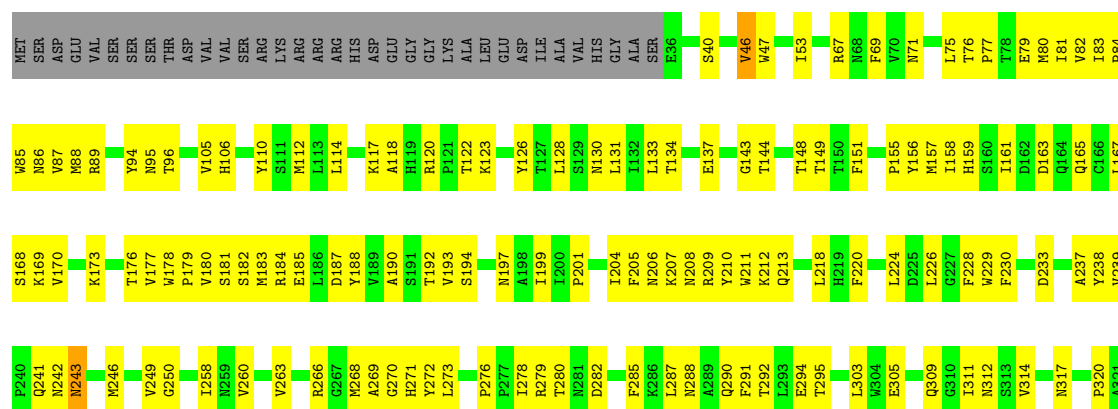
• Molecule 1: Penaeus monodon metallodensovirus major capsid protein

Chain 4: 45% 44% 9%



• Molecule 1: Penaeus monodon metallodensovirus major capsid protein

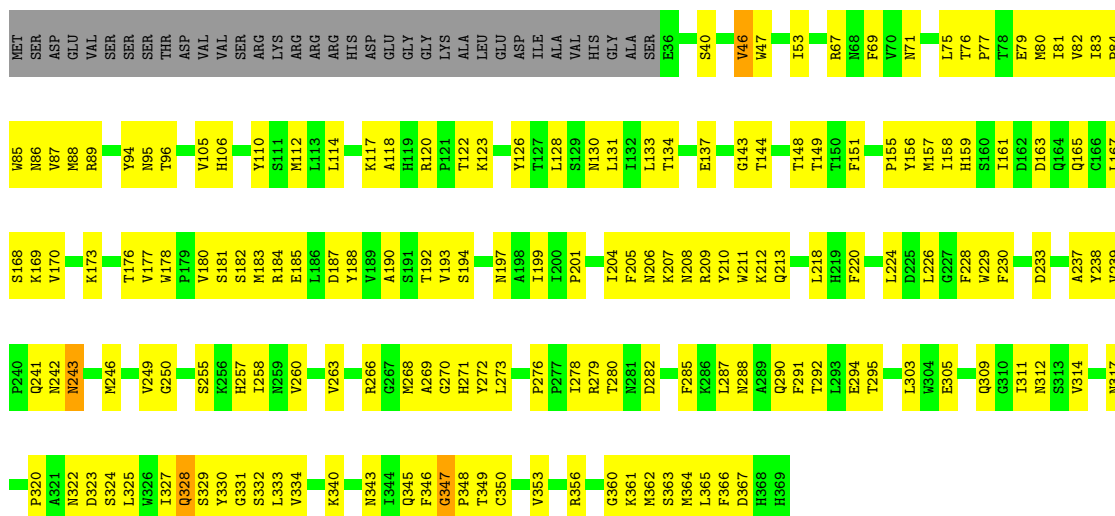
Chain 3: 46% 44% 9%





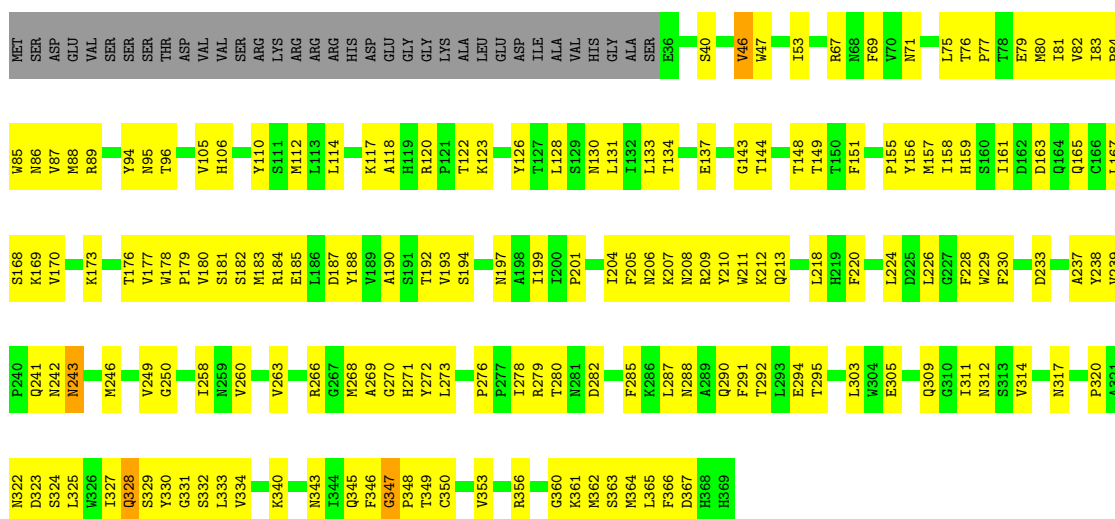
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain a: 45% 44% 9%



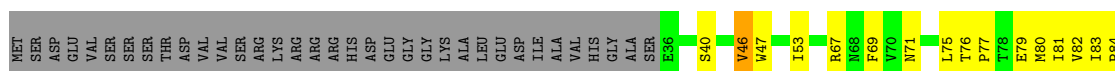
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

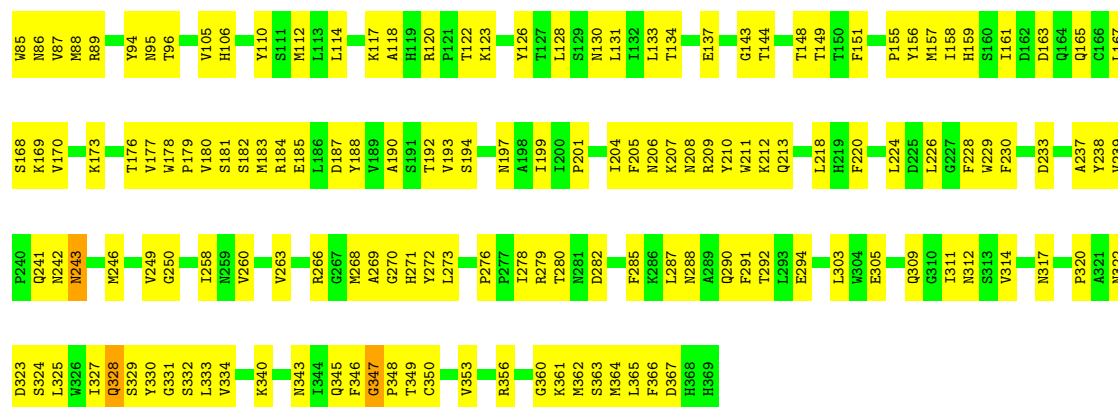
Chain b: 46% 44% 9%



- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

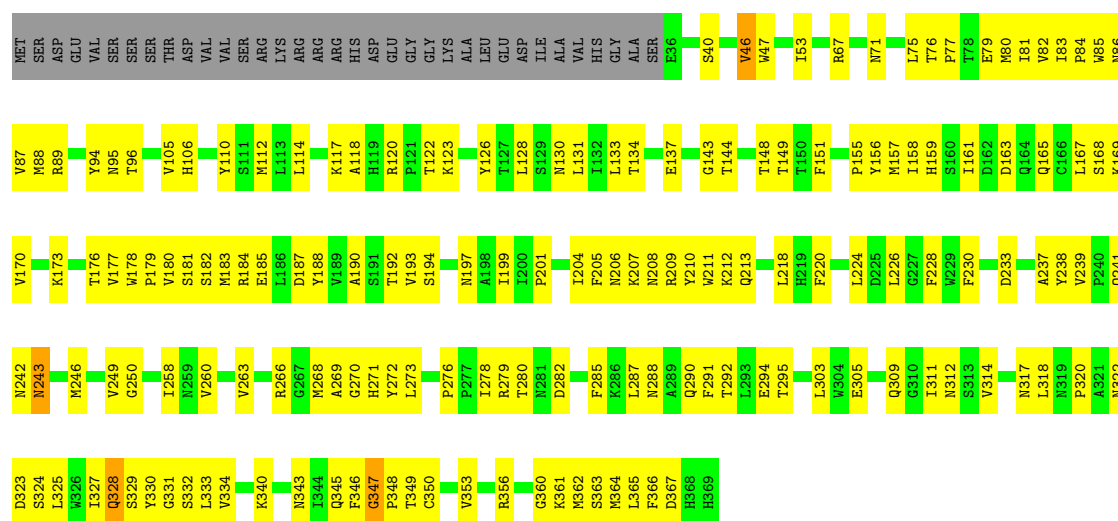
Chain c: 46% 44% 9%





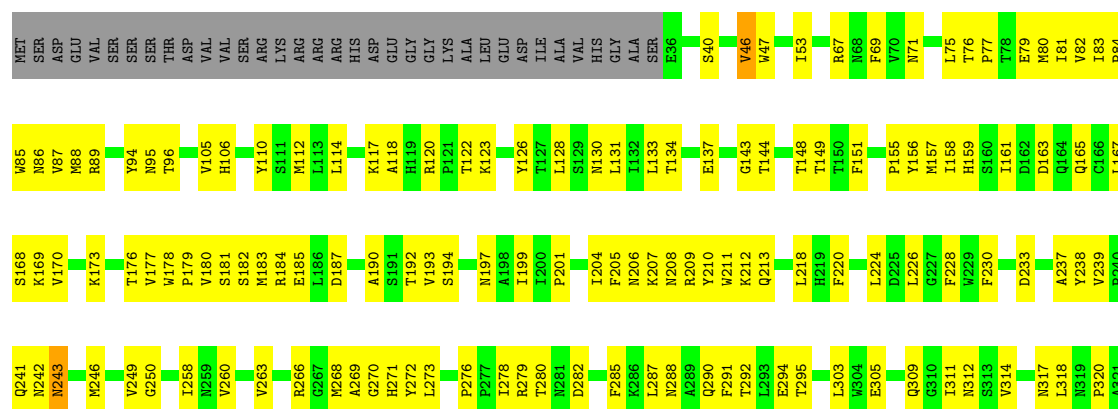
• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain d: 46% 44% 9%



• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

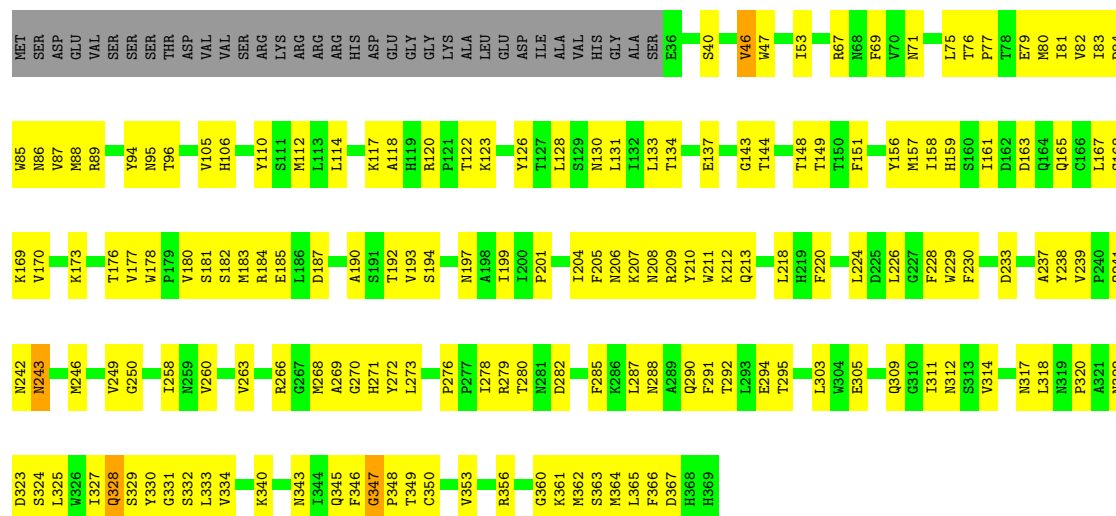
Chain e: 46% 44% 9%





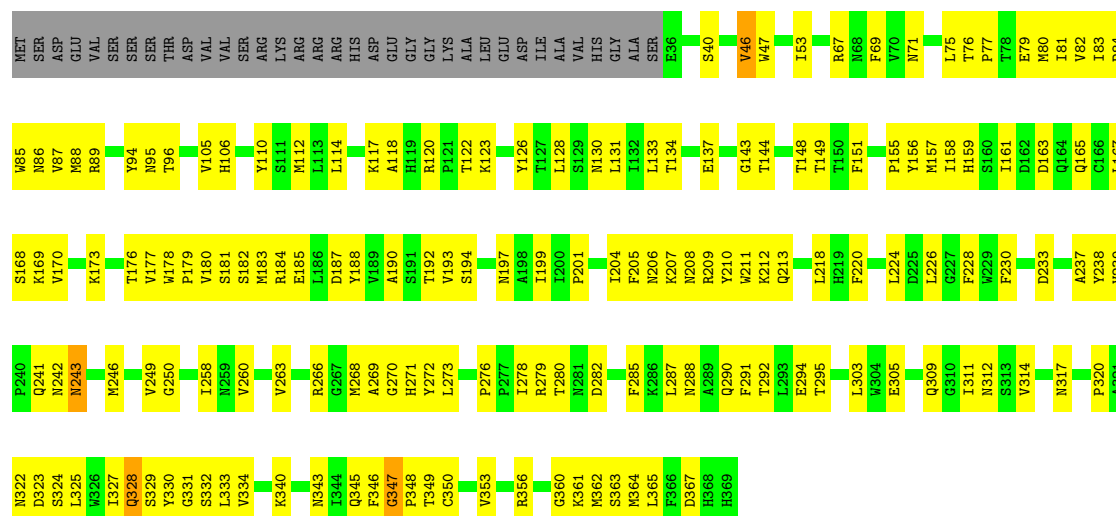
- Molecule 1: *Penaeus monodon* metalloidensovirus major capsid protein

Chain f: 46% 43% 9%



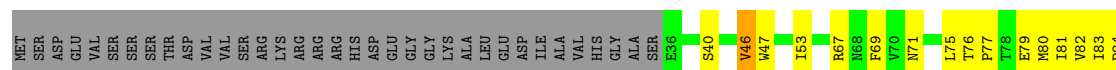
- Molecule 1: *Penaeus monodon* metalloidensovirus major capsid protein

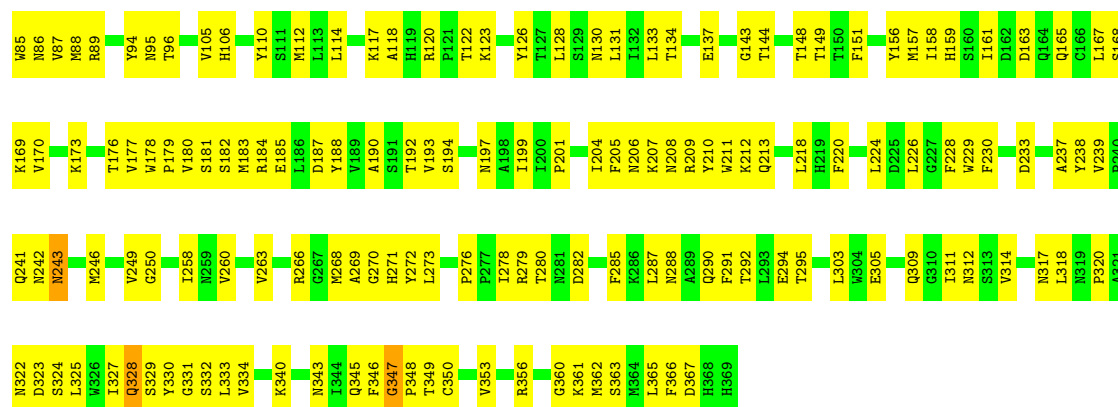
Chain g: 46% 43% 9%



- Molecule 1: *Penaeus monodon* metalloidensovirus major capsid protein

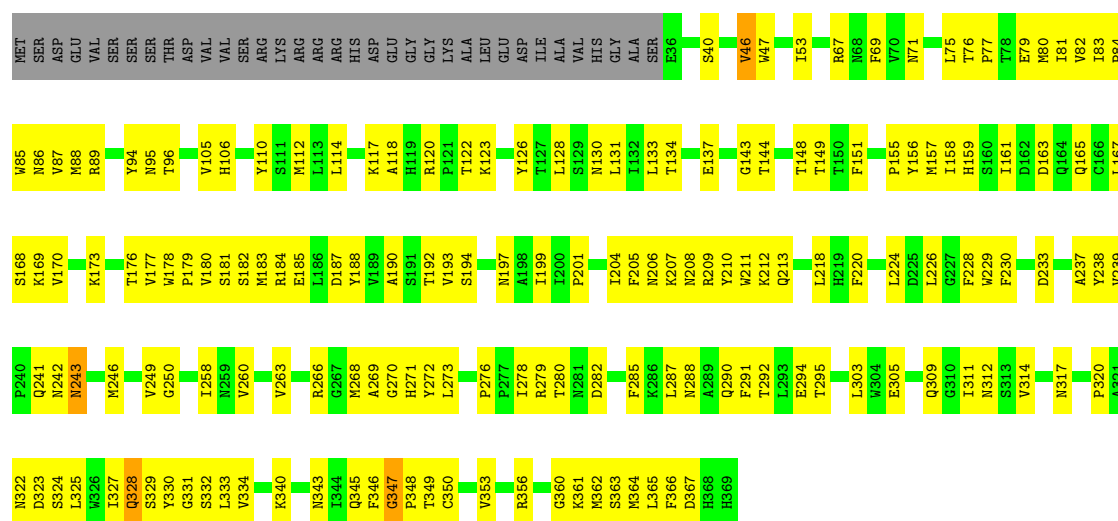
Chain h: 46% 44% 9%





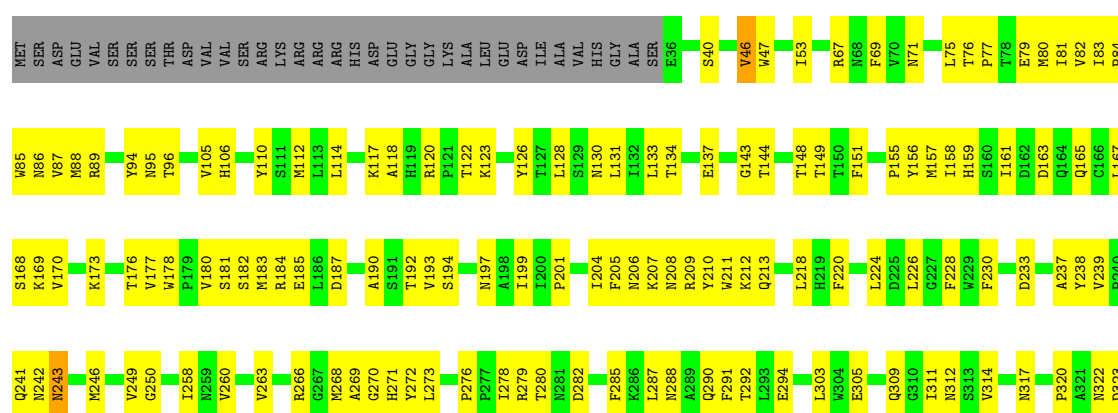
• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain i: 46% 44% 9%



• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

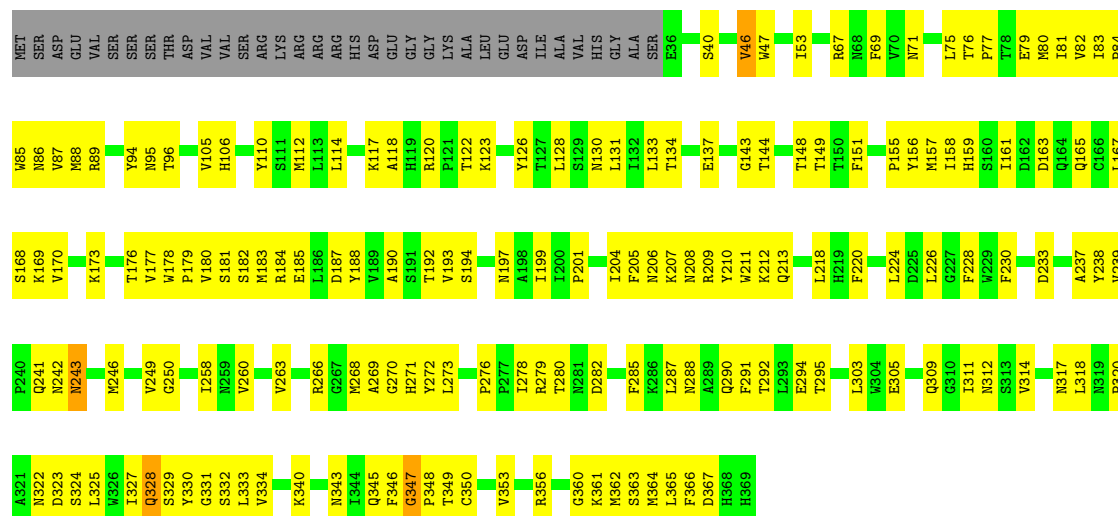
Chain j: 47% 43% 9%





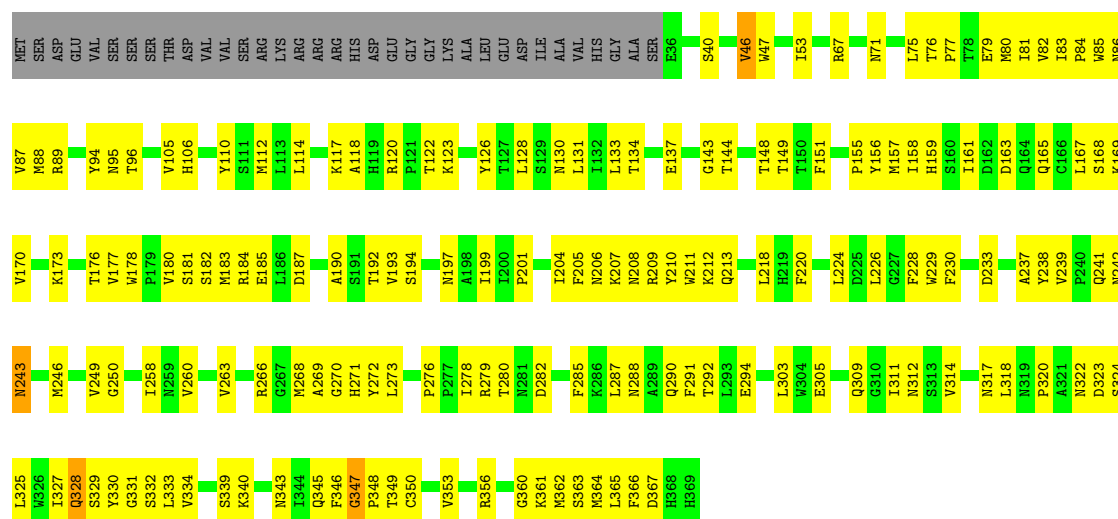
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain k: 46% 44% 9%



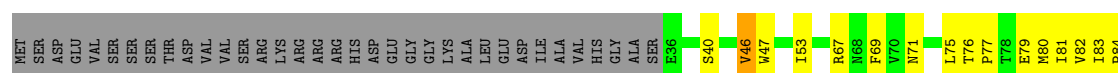
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

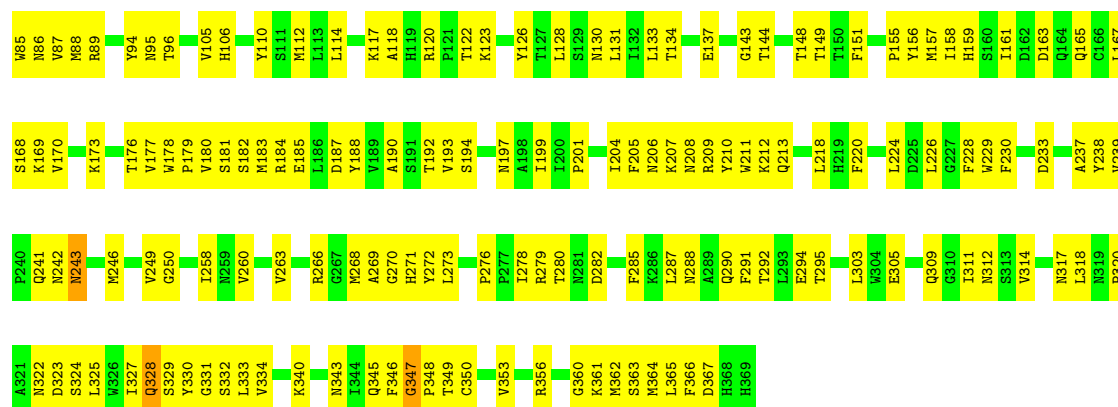
Chain l: 46% 43% 9%



- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

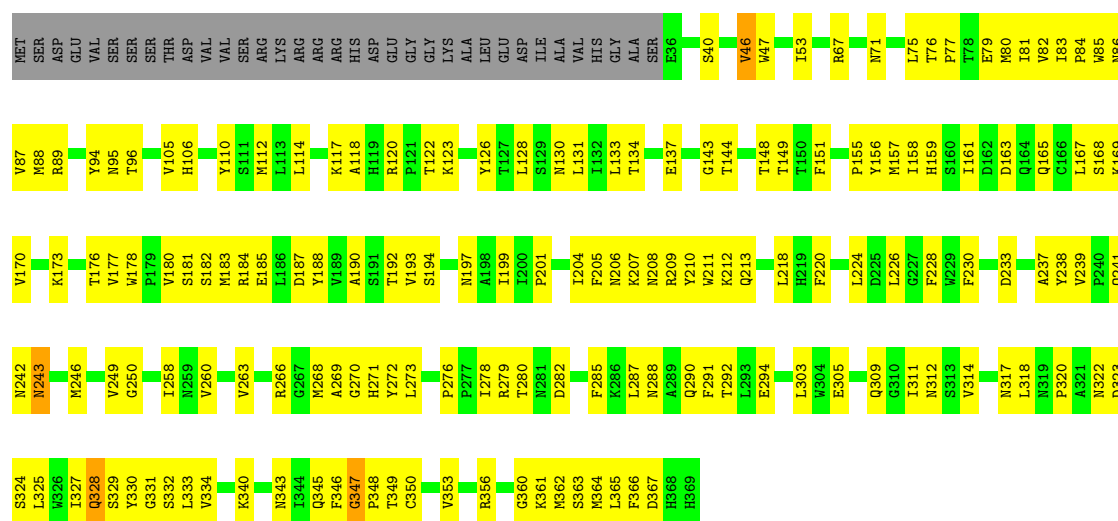
Chain m: 45% 44% 9%





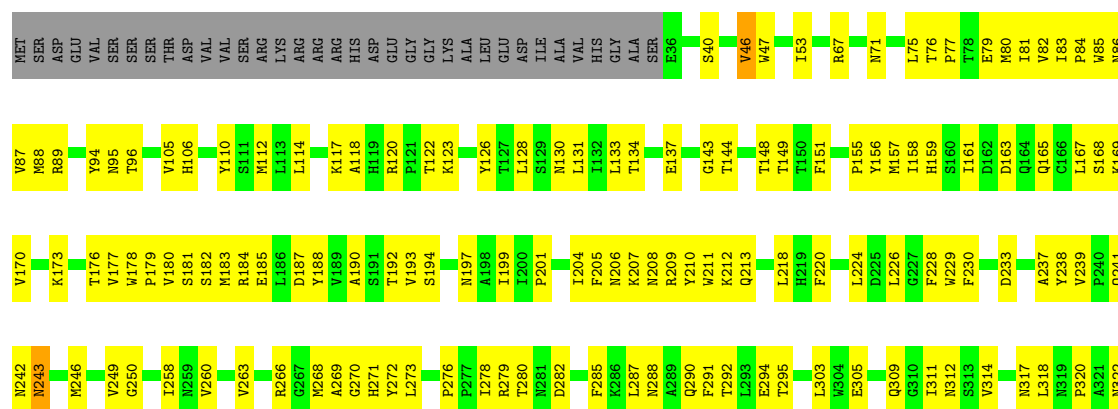
• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain n: 46% 43% 9%



• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

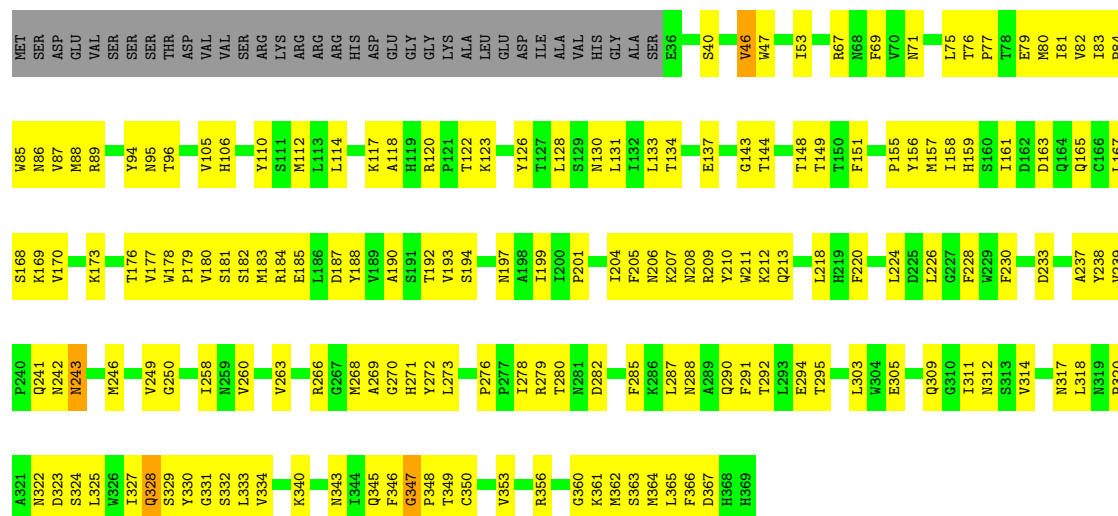
Chain o: 45% 44% 9%





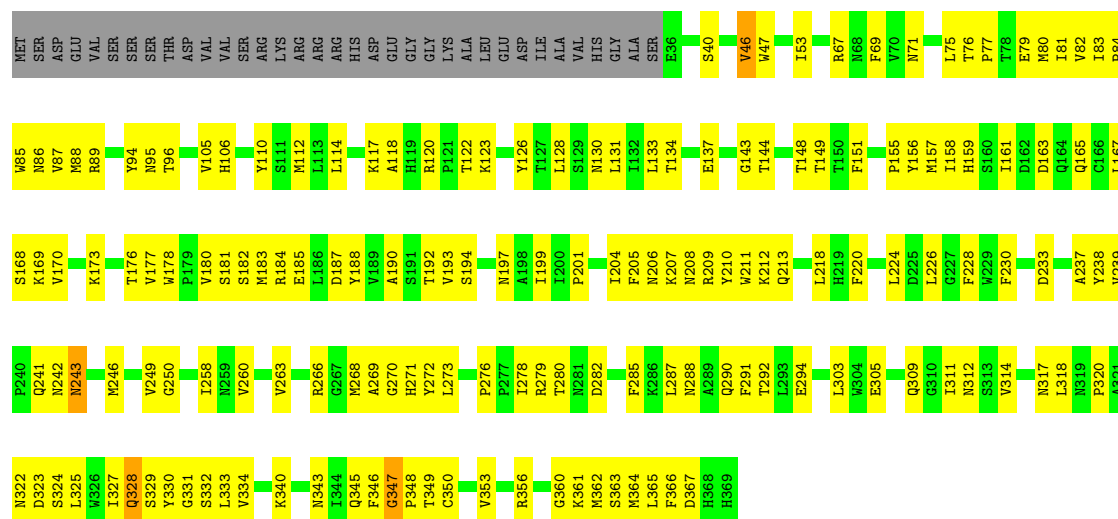
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain p: 46% 44% 9%



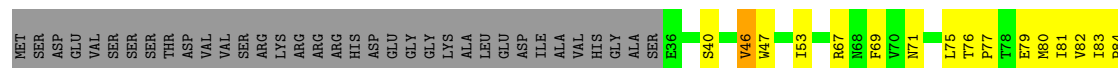
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

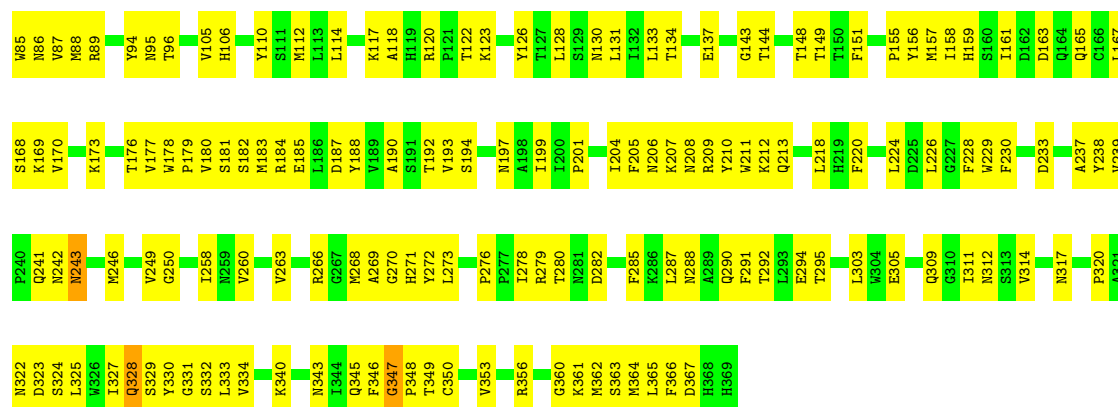
Chain q: 46% 43% 9%



- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

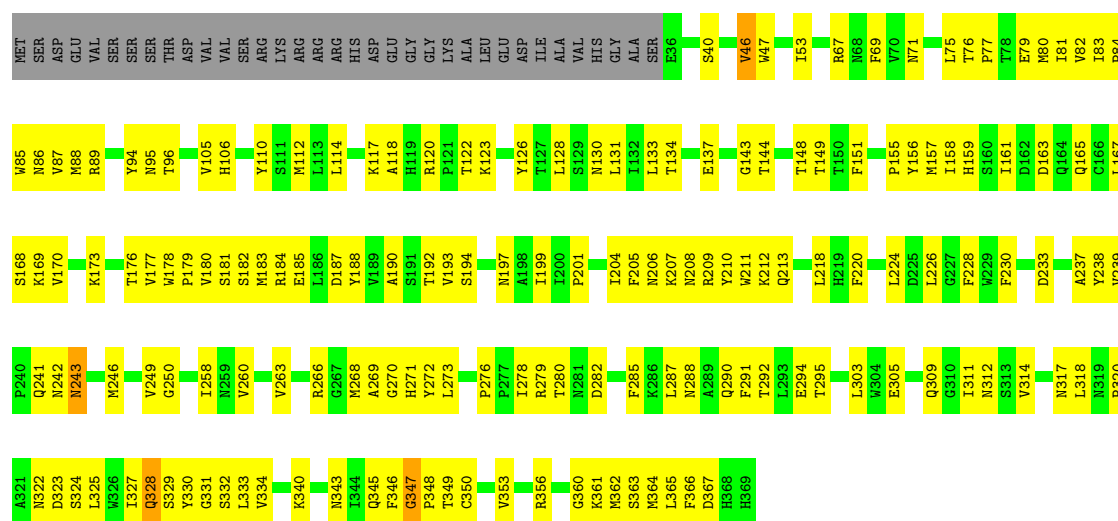
Chain r: 46% 44% 9%





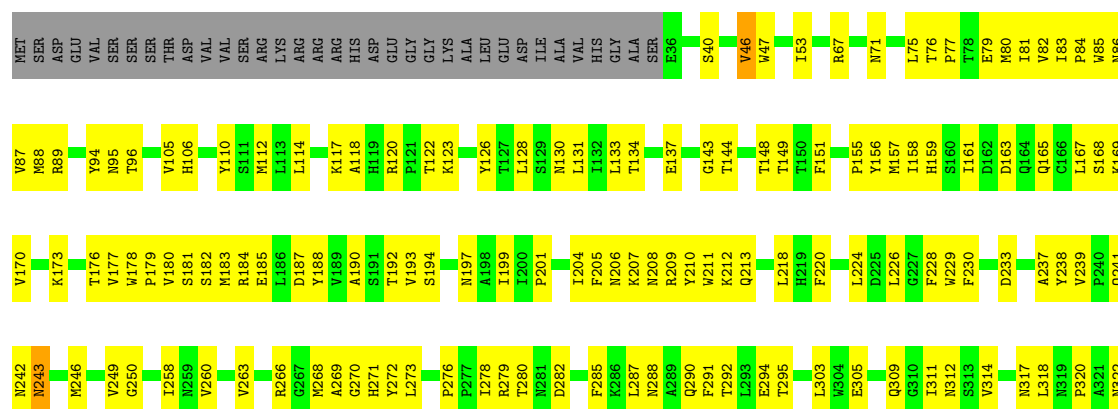
• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain s: 46% 44% 9%



• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

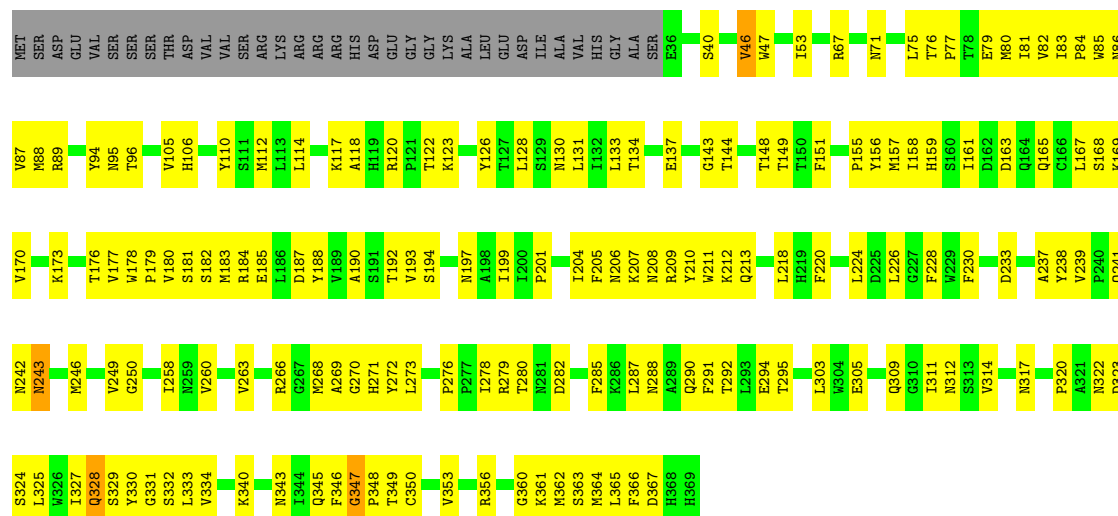
Chain t: 46% 44% 9%





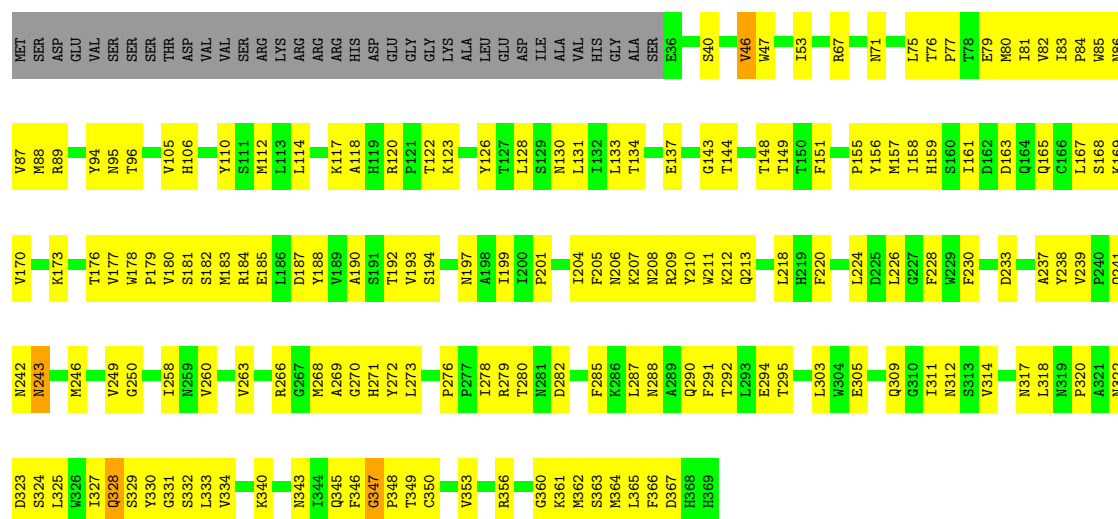
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain u: 46% 43% 9%



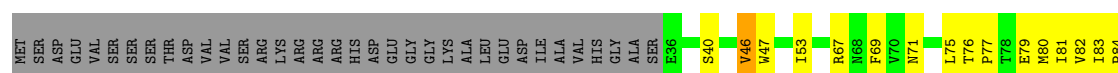
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

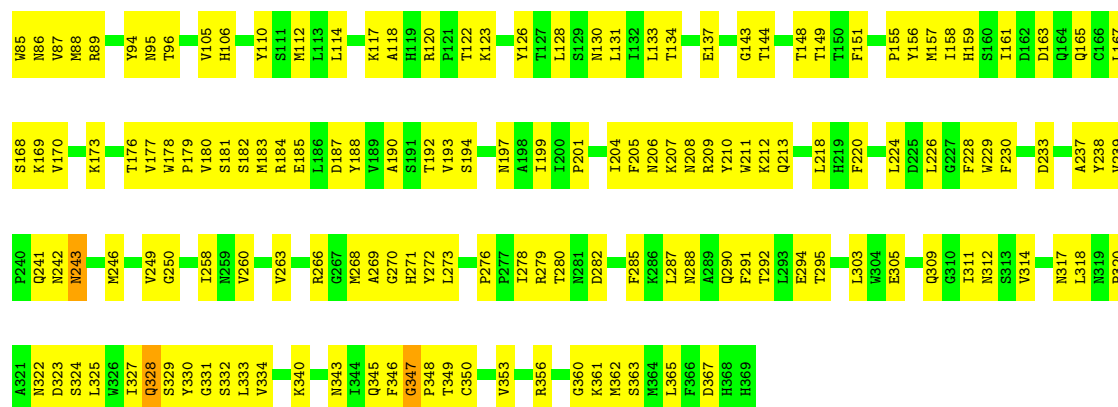
Chain v: 46% 44% 9%



- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

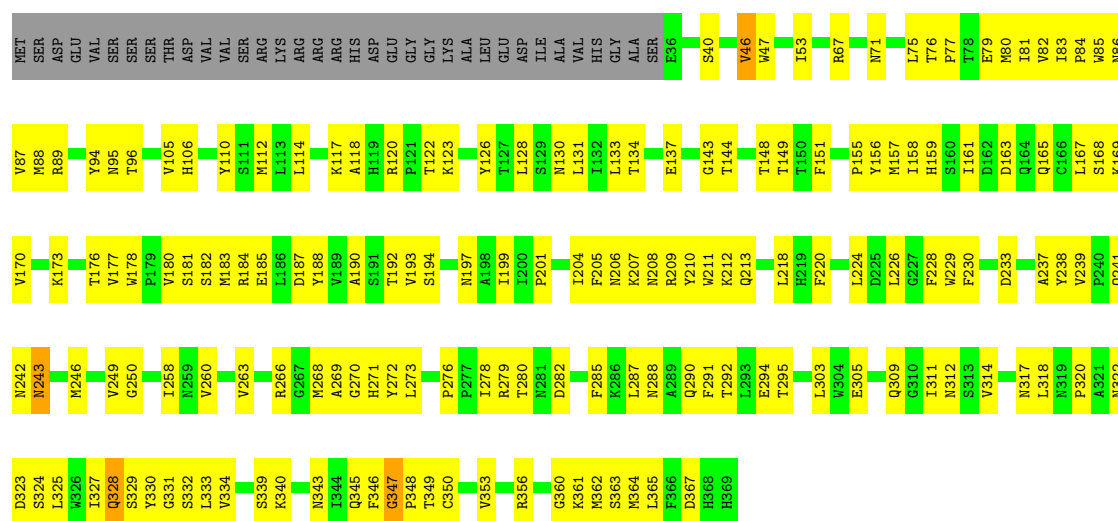
Chain w: 46% 44% 9%





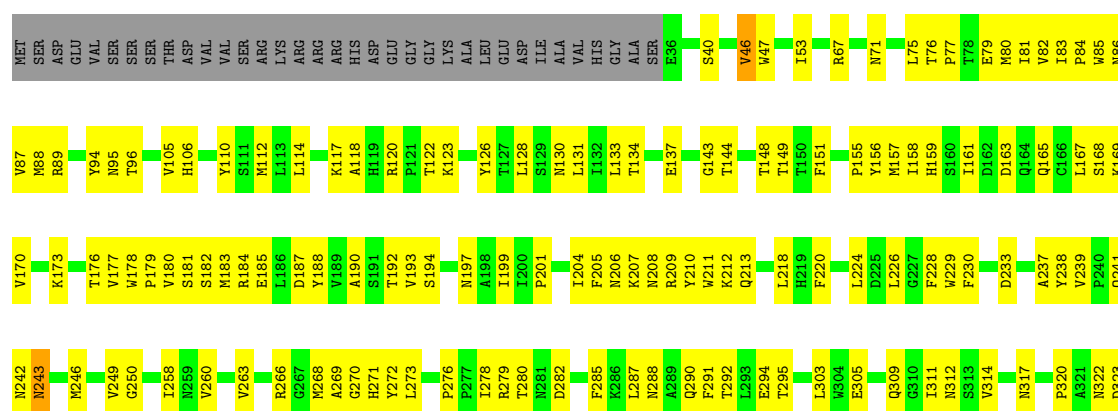
• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain x: 46% 44% 9%



• Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

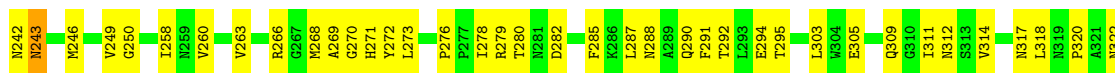
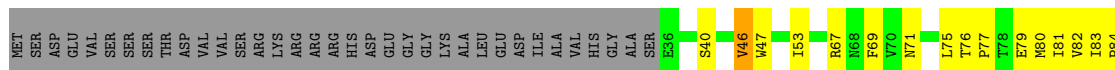
Chain y: 46% 44% 9%





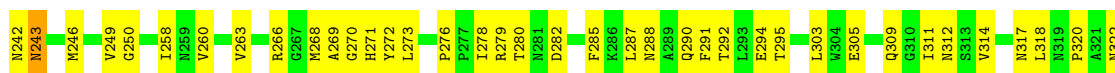
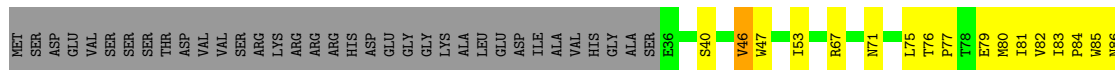
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain z: 46% 44% 9%



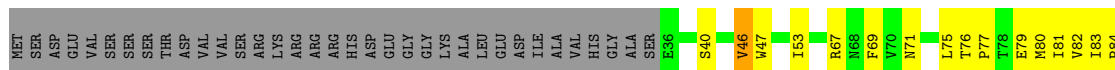
- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain 1: 46% 44% 9%



- Molecule 1: *Penaeus monodon* metallodensovirus major capsid protein

Chain 2: 45% 44% 9%



A	R319	Q241	K169	W85
	P320	M242	V170	N86
	A321	M243		V87
	N322	M246	K173	M88
	D323			R89
	S324			
	L325	V249	T176	Y94
	V326	C250	W177	N95
	I327		P179	T96
	Q328	S255	V180	V105
S329	V256	S181	H106	
Y330	H257	S182		
G331	T258	M183	Y110	
S332	C259	K184	S111	
L333	M260	E185	M112	
V334		L186	L113	
	V263	D187	L114	
		Y188		
K340		V189	K117	
N343	C267	A190	A118	
L344	M268	S191	H119	
Q345	A269	T192		
F346	C270	V193	P121	
G347	H271	S194	T122	
P348	V272		K123	
T349	L273	M197		
C350		A198	Y126	
	P276	I199	T127	
V353	P277	T200	L128	
	L278	P201	S129	
R356	T279		N130	
G360	M281	T204	F205	
K361	D282	N206	L131	
M362		K207	L132	
S363	F285	N208	L133	
M364	C286	R209	T134	
L365	L287	V210		
F366	N288	W211	E137	
D367	A289	K212	G143	
H368	Q290	Q213	T144	
	F291			
	T292	L218	T148	
	E294	H219	T149	
	T295	F220	T150	
			F151	
	L303	L224		
	W304	D225	Y156	
E305		L226	M157	
		G227	I158	
		F228	H159	
Q309	Q309	W229	S160	
G310	G310	F230	L161	
	T311		D162	
S312	N313	D233	L163	
S313	S313		Q164	
V314	V314	A237	Q165	
		Y238	C166	
N317	N317	V239	L167	
L318	L318	F240	S169	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	12873	Depositor
Resolution determination method	FSC 3 SIGMA CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	21.777	Depositor
Minimum map value	-12.179	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size ($\text{\AA}$)	415.436, 415.436, 415.436	wwPDB
Map dimensions	401, 401, 401	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.036, 1.036, 1.036	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1	0.49	0/2696	0.67	4/3669 (0.1%)
1	2	0.49	0/2696	0.67	4/3669 (0.1%)
1	3	0.49	0/2696	0.67	4/3669 (0.1%)
1	4	0.49	0/2696	0.67	4/3669 (0.1%)
1	5	0.49	0/2696	0.67	4/3669 (0.1%)
1	6	0.49	0/2696	0.67	4/3669 (0.1%)
1	7	0.49	0/2696	0.67	4/3669 (0.1%)
1	8	0.48	0/2696	0.67	4/3669 (0.1%)
1	A	0.48	0/2696	0.67	4/3669 (0.1%)
1	B	0.49	0/2696	0.67	4/3669 (0.1%)
1	C	0.49	0/2696	0.67	4/3669 (0.1%)
1	D	0.49	0/2696	0.67	4/3669 (0.1%)
1	E	0.49	0/2696	0.67	4/3669 (0.1%)
1	F	0.49	0/2696	0.67	4/3669 (0.1%)
1	G	0.49	0/2696	0.67	4/3669 (0.1%)
1	H	0.49	0/2696	0.67	4/3669 (0.1%)
1	I	0.49	0/2696	0.67	4/3669 (0.1%)
1	J	0.49	0/2696	0.67	4/3669 (0.1%)
1	K	0.49	0/2696	0.67	4/3669 (0.1%)
1	L	0.49	0/2696	0.67	4/3669 (0.1%)
1	M	0.49	0/2696	0.67	4/3669 (0.1%)
1	N	0.49	0/2696	0.67	4/3669 (0.1%)
1	O	0.49	0/2696	0.67	4/3669 (0.1%)
1	P	0.49	0/2696	0.67	4/3669 (0.1%)
1	Q	0.49	0/2696	0.67	4/3669 (0.1%)
1	R	0.49	0/2696	0.67	4/3669 (0.1%)
1	S	0.49	0/2696	0.67	4/3669 (0.1%)
1	T	0.49	0/2696	0.67	4/3669 (0.1%)
1	U	0.49	0/2696	0.67	4/3669 (0.1%)
1	V	0.49	0/2696	0.67	4/3669 (0.1%)
1	W	0.49	0/2696	0.67	4/3669 (0.1%)
1	X	0.48	0/2696	0.67	4/3669 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.49	0/2696	0.67	4/3669 (0.1%)
1	Z	0.49	0/2696	0.67	4/3669 (0.1%)
1	a	0.49	0/2696	0.67	4/3669 (0.1%)
1	b	0.49	0/2696	0.67	4/3669 (0.1%)
1	c	0.49	0/2696	0.67	4/3669 (0.1%)
1	d	0.49	0/2696	0.67	4/3669 (0.1%)
1	e	0.49	0/2696	0.67	4/3669 (0.1%)
1	f	0.49	0/2696	0.67	4/3669 (0.1%)
1	g	0.49	0/2696	0.67	4/3669 (0.1%)
1	h	0.49	0/2696	0.67	4/3669 (0.1%)
1	i	0.49	0/2696	0.67	4/3669 (0.1%)
1	j	0.49	0/2696	0.67	4/3669 (0.1%)
1	k	0.49	0/2696	0.67	4/3669 (0.1%)
1	l	0.49	0/2696	0.67	4/3669 (0.1%)
1	m	0.49	0/2696	0.67	4/3669 (0.1%)
1	n	0.49	0/2696	0.67	4/3669 (0.1%)
1	o	0.49	0/2696	0.67	4/3669 (0.1%)
1	p	0.49	0/2696	0.67	4/3669 (0.1%)
1	q	0.49	0/2696	0.67	4/3669 (0.1%)
1	r	0.49	0/2696	0.67	4/3669 (0.1%)
1	s	0.49	0/2696	0.67	4/3669 (0.1%)
1	t	0.49	0/2696	0.67	4/3669 (0.1%)
1	u	0.49	0/2696	0.67	4/3669 (0.1%)
1	v	0.49	0/2696	0.67	4/3669 (0.1%)
1	w	0.49	0/2696	0.67	4/3669 (0.1%)
1	x	0.49	0/2696	0.67	4/3669 (0.1%)
1	y	0.49	0/2696	0.67	4/3669 (0.1%)
1	z	0.49	0/2696	0.67	4/3669 (0.1%)
All	All	0.49	0/161760	0.67	240/220140 (0.1%)

There are no bond length outliers.

The worst 5 of 240 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	347	GLY	CA-C-N	7.02	126.95	120.21
1	Z	347	GLY	C-N-CA	7.02	126.95	120.21
1	2	347	GLY	CA-C-N	7.02	126.95	120.21
1	2	347	GLY	C-N-CA	7.02	126.95	120.21
1	i	347	GLY	CA-C-N	7.01	126.94	120.21

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	1	2628	0	2527	189	0
1	2	2628	0	2527	188	0
1	3	2628	0	2527	188	0
1	4	2628	0	2527	189	0
1	5	2628	0	2527	186	0
1	6	2628	0	2527	188	0
1	7	2628	0	2527	194	0
1	8	2628	0	2527	189	0
1	A	2628	0	2527	188	0
1	B	2628	0	2527	187	0
1	C	2628	0	2527	191	0
1	D	2628	0	2527	187	0
1	E	2628	0	2527	190	0
1	F	2628	0	2527	186	0
1	G	2628	0	2527	187	0
1	H	2628	0	2527	190	0
1	I	2628	0	2527	188	0
1	J	2628	0	2527	185	0
1	K	2628	0	2527	187	0
1	L	2628	0	2527	191	0
1	M	2628	0	2527	189	0
1	N	2628	0	2527	187	0
1	O	2628	0	2527	187	0
1	P	2628	0	2527	191	0
1	Q	2628	0	2527	188	0
1	R	2628	0	2527	185	0
1	S	2628	0	2527	189	0
1	T	2628	0	2527	187	0
1	U	2628	0	2527	188	0
1	V	2628	0	2527	190	0
1	W	2628	0	2527	191	0
1	X	2628	0	2527	188	0
1	Y	2628	0	2527	188	0
1	Z	2628	0	2527	187	0
1	a	2628	0	2527	187	0
1	b	2628	0	2527	187	0
1	c	2628	0	2527	187	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	2628	0	2527	190	0
1	e	2628	0	2527	191	0
1	f	2628	0	2527	187	0
1	g	2628	0	2527	188	0
1	h	2628	0	2527	188	0
1	i	2628	0	2527	187	0
1	j	2628	0	2527	186	0
1	k	2628	0	2527	188	0
1	l	2628	0	2527	186	0
1	m	2628	0	2527	189	0
1	n	2628	0	2527	189	0
1	o	2628	0	2527	189	0
1	p	2628	0	2527	190	0
1	q	2628	0	2527	187	0
1	r	2628	0	2527	188	0
1	s	2628	0	2527	190	0
1	t	2628	0	2527	189	0
1	u	2628	0	2527	185	0
1	v	2628	0	2527	189	0
1	w	2628	0	2527	183	0
1	x	2628	0	2527	188	0
1	y	2628	0	2527	189	0
1	z	2628	0	2527	185	0
2	1	1	0	0	0	0
2	2	1	0	0	0	0
2	3	1	0	0	0	0
2	4	1	0	0	0	0
2	5	1	0	0	0	0
2	6	1	0	0	0	0
2	7	1	0	0	0	0
2	8	1	0	0	0	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
2	Y	1	0	0	0	0
2	Z	1	0	0	0	0
2	a	1	0	0	0	0
2	b	1	0	0	0	0
2	c	1	0	0	0	0
2	d	1	0	0	0	0
2	e	1	0	0	0	0
2	f	1	0	0	0	0
2	g	1	0	0	0	0
2	h	1	0	0	0	0
2	i	1	0	0	0	0
2	j	1	0	0	0	0
2	k	1	0	0	0	0
2	l	1	0	0	0	0
2	m	1	0	0	0	0
2	n	1	0	0	0	0
2	o	1	0	0	0	0
2	p	1	0	0	0	0
2	q	1	0	0	0	0
2	r	1	0	0	0	0
2	s	1	0	0	0	0
2	t	1	0	0	0	0
2	u	1	0	0	0	0
2	v	1	0	0	0	0
2	w	1	0	0	0	0
2	x	1	0	0	0	0
2	y	1	0	0	0	0
2	z	1	0	0	0	0
All	All	157740	0	151620	9696	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 31.

The worst 5 of 9696 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:B:209:ARG:HB3	1:L:46:VAL:HG11	1.20	1.20
1:f:260:VAL:HG11	1:f:328:GLN:HG3	1.20	1.20
1:Z:260:VAL:HG11	1:Z:328:GLN:HG3	1.20	1.20
1:6:260:VAL:HG11	1:6:328:GLN:HG3	1.20	1.19
1:k:209:ARG:HB3	1:m:46:VAL:HG11	1.21	1.19

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	1	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	2	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	3	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	4	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	5	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	6	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	7	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	8	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	A	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	B	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	C	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	D	332/369 (90%)	319 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	F	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	G	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	H	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	I	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	J	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	K	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	L	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	M	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	N	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	O	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	P	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	Q	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	R	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	S	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	T	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	U	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	V	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	W	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	X	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	Y	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	Z	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	a	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	b	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	c	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	d	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	e	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	f	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	g	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	h	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	i	332/369 (90%)	319 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	j	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	k	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	l	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	m	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	n	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	o	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	p	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	q	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	r	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	s	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	t	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	u	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	v	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	w	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	x	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	y	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
1	z	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
All	All	19920/22140 (90%)	19140 (96%)	780 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	2	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	3	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	4	292/321 (91%)	290 (99%)	2 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	6	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	7	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	8	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	A	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	B	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	C	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	D	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	E	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	F	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	G	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	H	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	I	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	J	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	K	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	L	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	M	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	N	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	O	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	P	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	Q	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	R	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	S	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	T	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	U	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	V	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	W	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	X	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	Y	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	Z	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	a	292/321 (91%)	290 (99%)	2 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	c	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	d	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	e	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	f	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	g	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	h	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	i	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	j	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	k	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	l	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	m	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	n	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	o	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	p	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	q	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	r	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	s	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	t	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	u	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	v	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	w	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	x	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	y	292/321 (91%)	290 (99%)	2 (1%)	76	87
1	z	292/321 (91%)	290 (99%)	2 (1%)	76	87
All	All	17520/19260 (91%)	17400 (99%)	120 (1%)	73	87

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	6	243	ASN
1	x	46	VAL
1	d	243	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	w	243	ASN
1	2	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 719 such sidechains are listed below:

Mol	Chain	Res	Type
1	g	271	HIS
1	p	290	GLN
1	h	271	HIS
1	g	259	ASN
1	l	206	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 60 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.

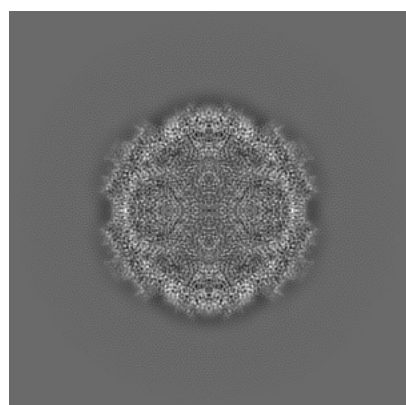
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21667. These allow visual inspection of the internal detail of the map and identification of artifacts.

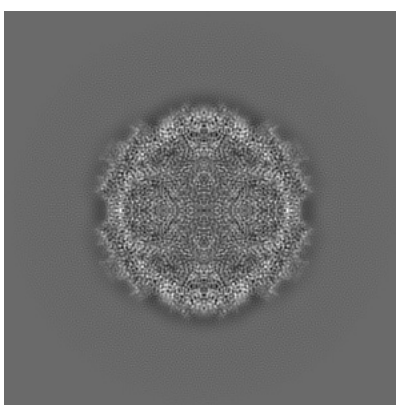
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

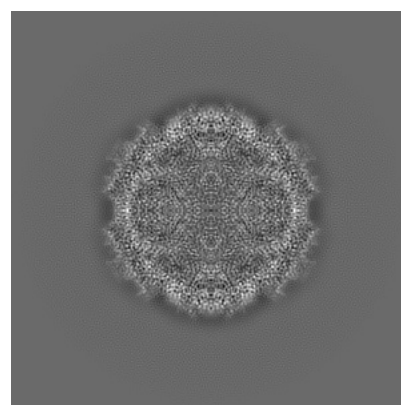
6.1.1 Primary map



X



Y

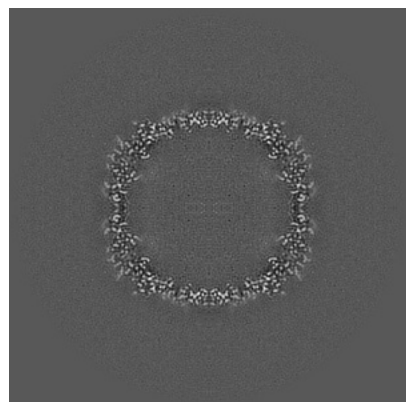


Z

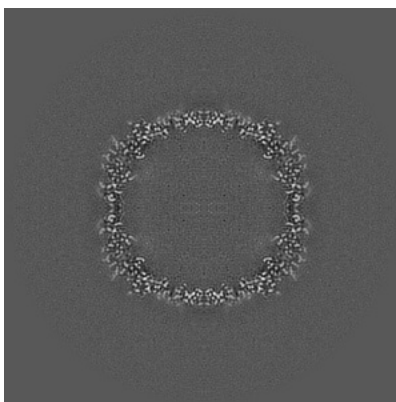
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

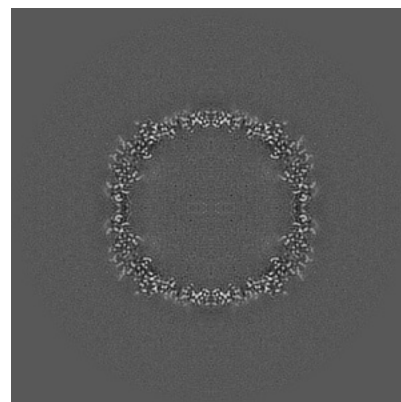
6.2.1 Primary map



X Index: 200



Y Index: 200

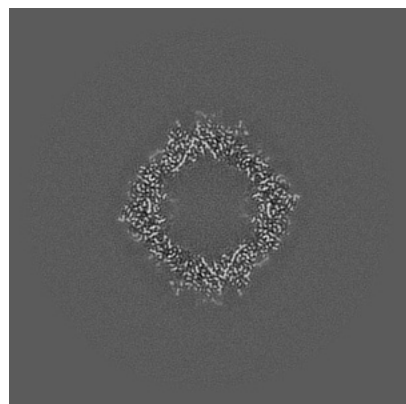


Z Index: 200

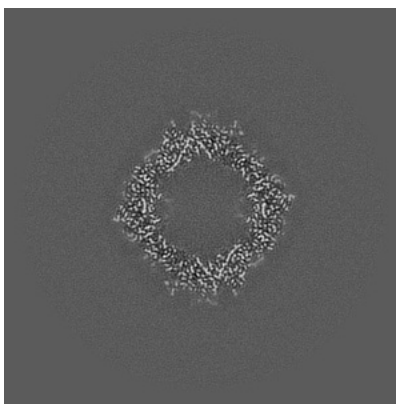
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

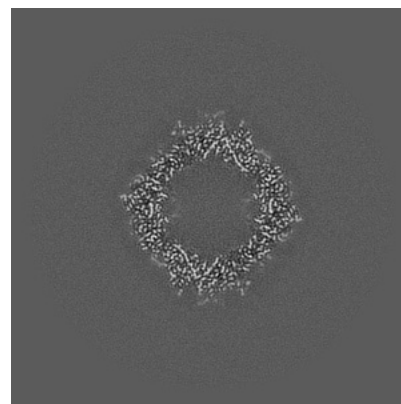
6.3.1 Primary map



X Index: 135



Y Index: 135

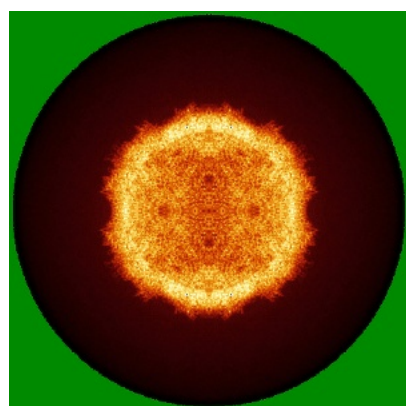


Z Index: 265

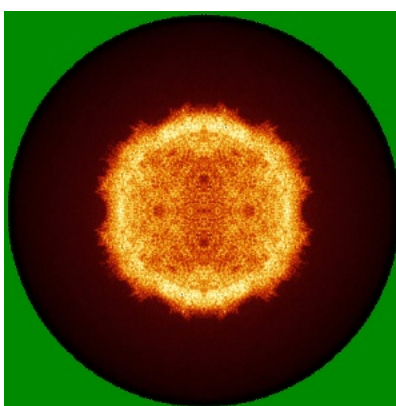
The images above show the largest variance slices of the map in three orthogonal directions.

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

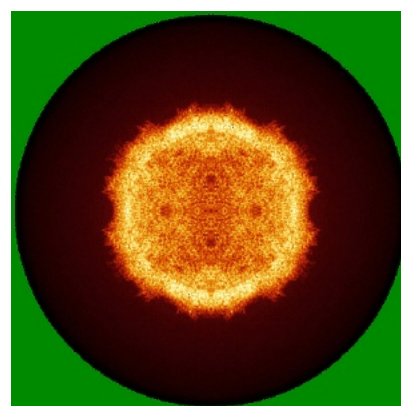
6.4.1 Primary map



X



Y

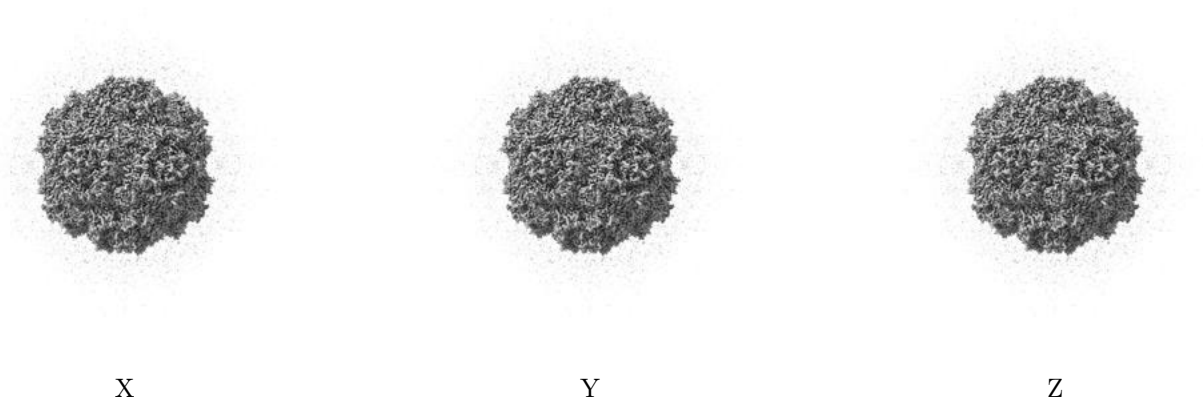


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

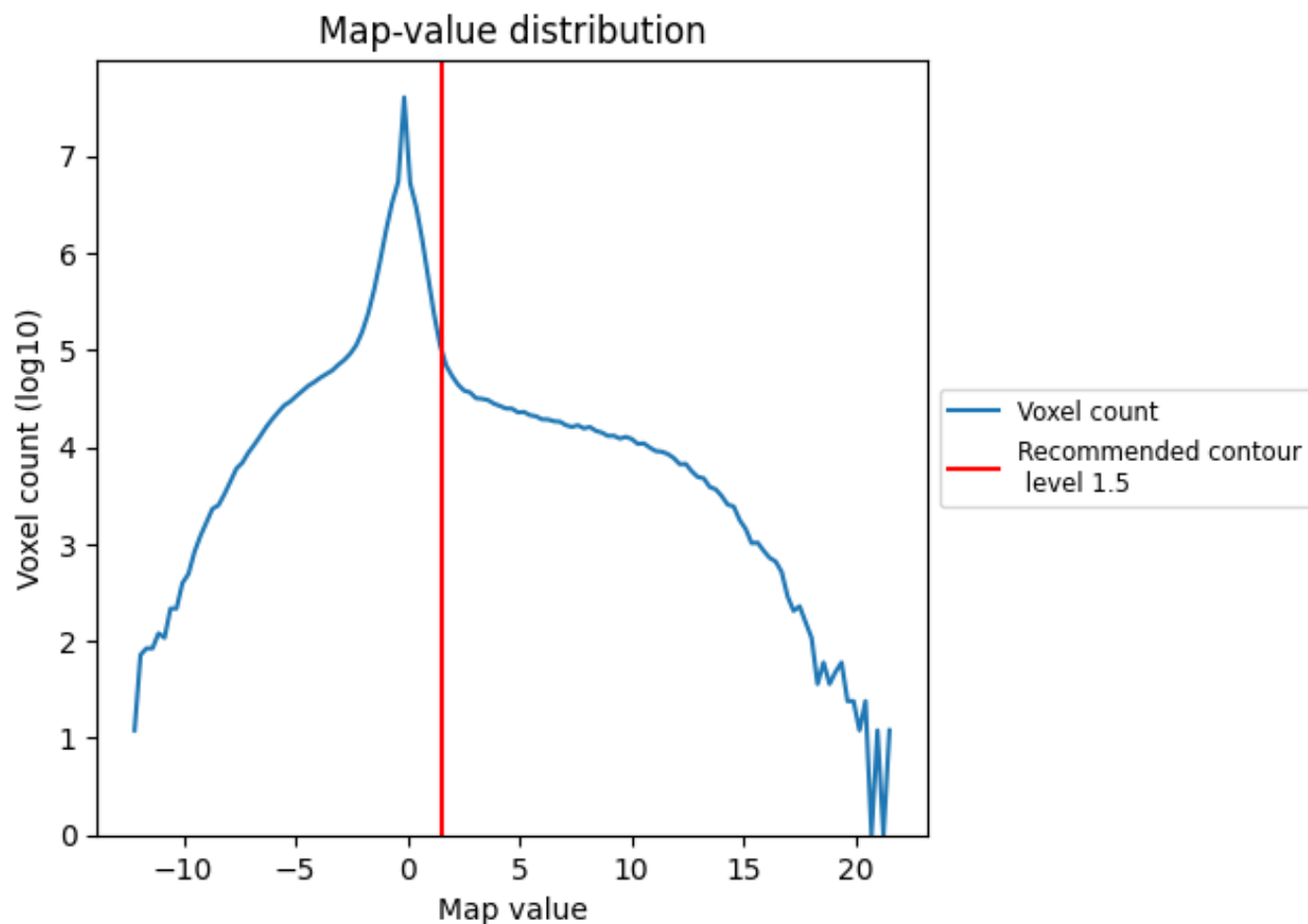
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

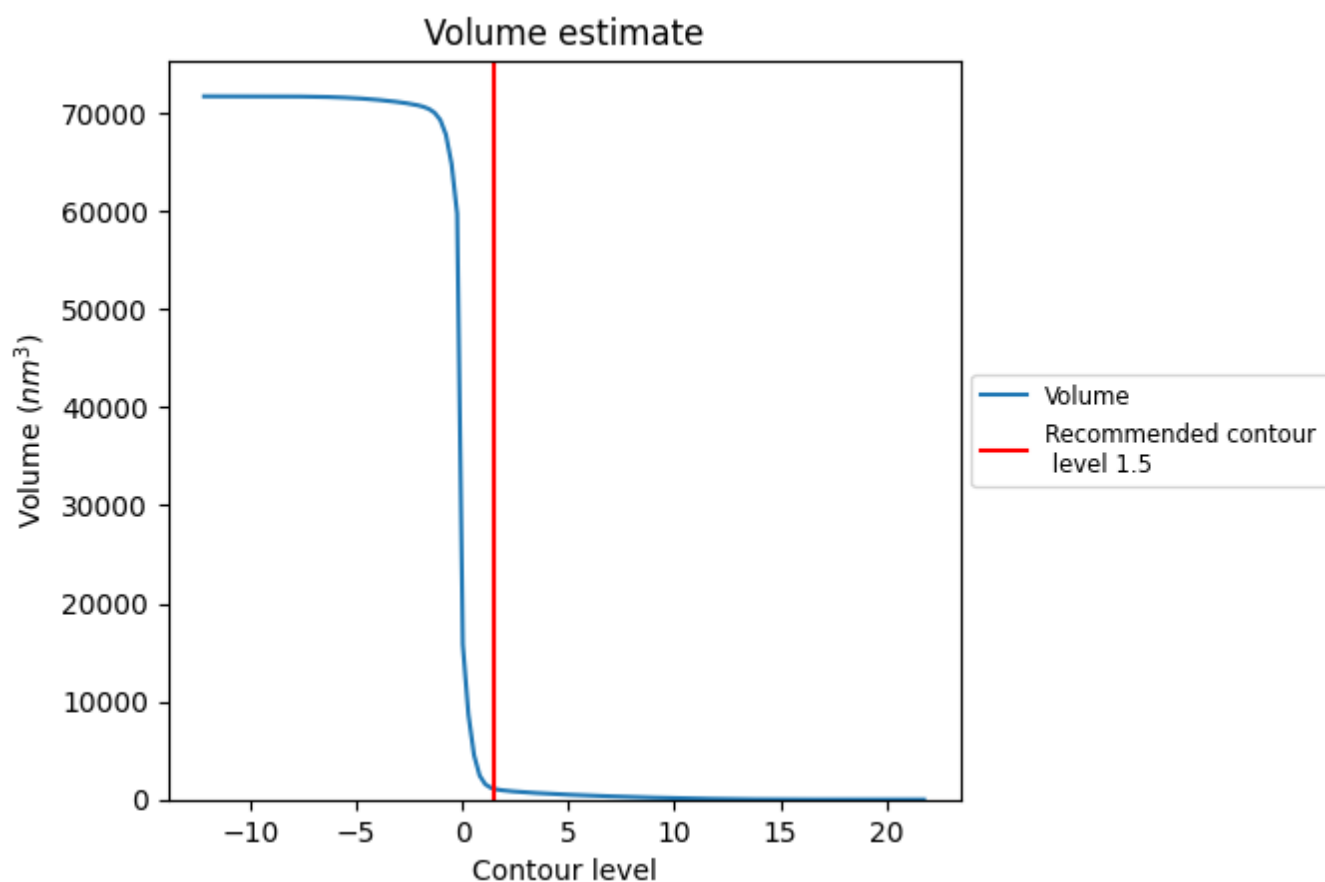
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

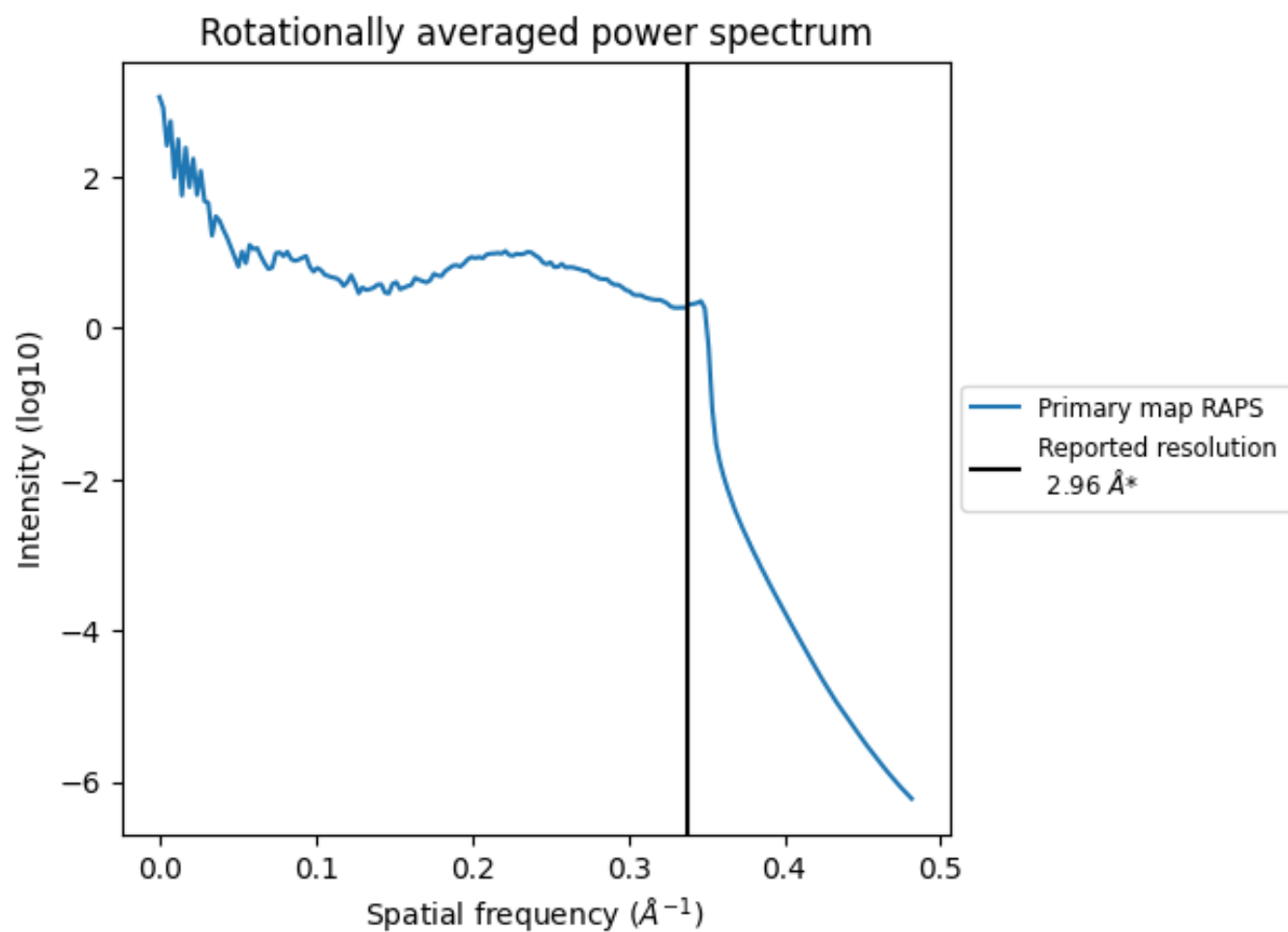
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1106 nm³; this corresponds to an approximate mass of 999 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 0.338 Å⁻¹

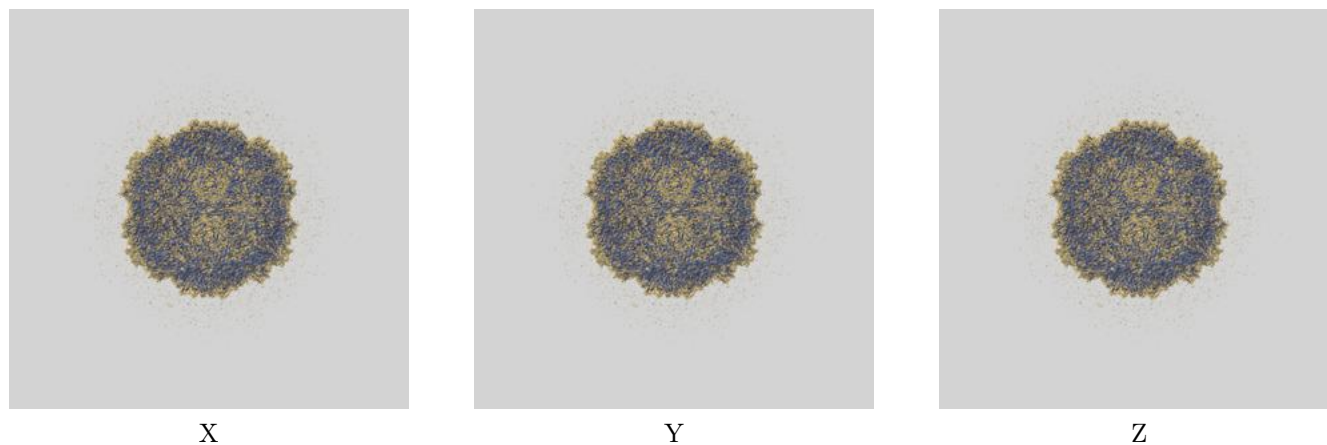
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

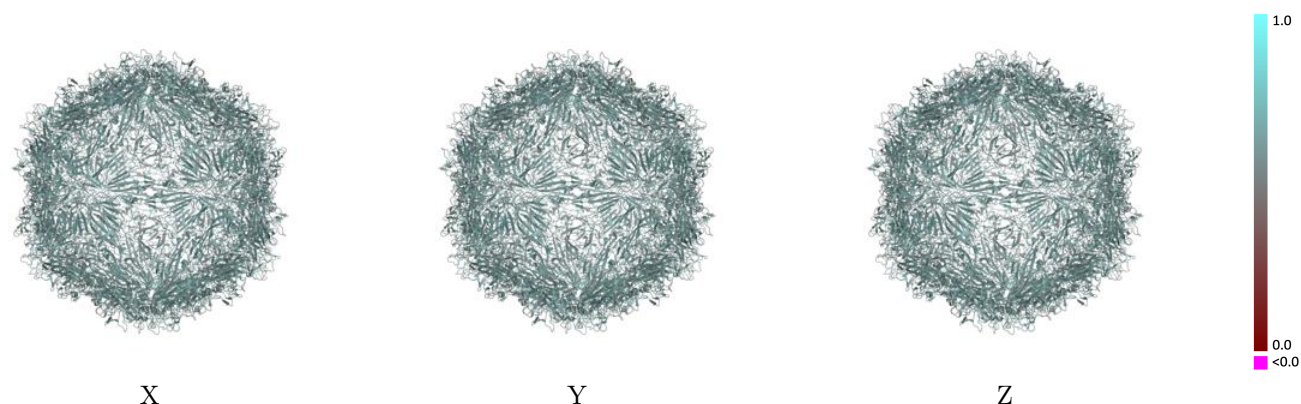
This section contains information regarding the fit between EMDB map EMD-21667 and PDB model 6WH3. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



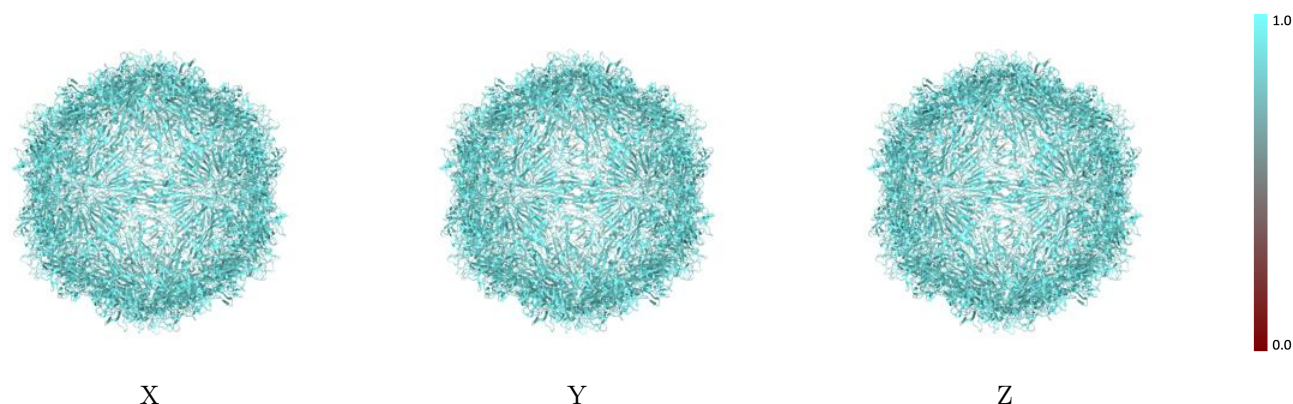
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



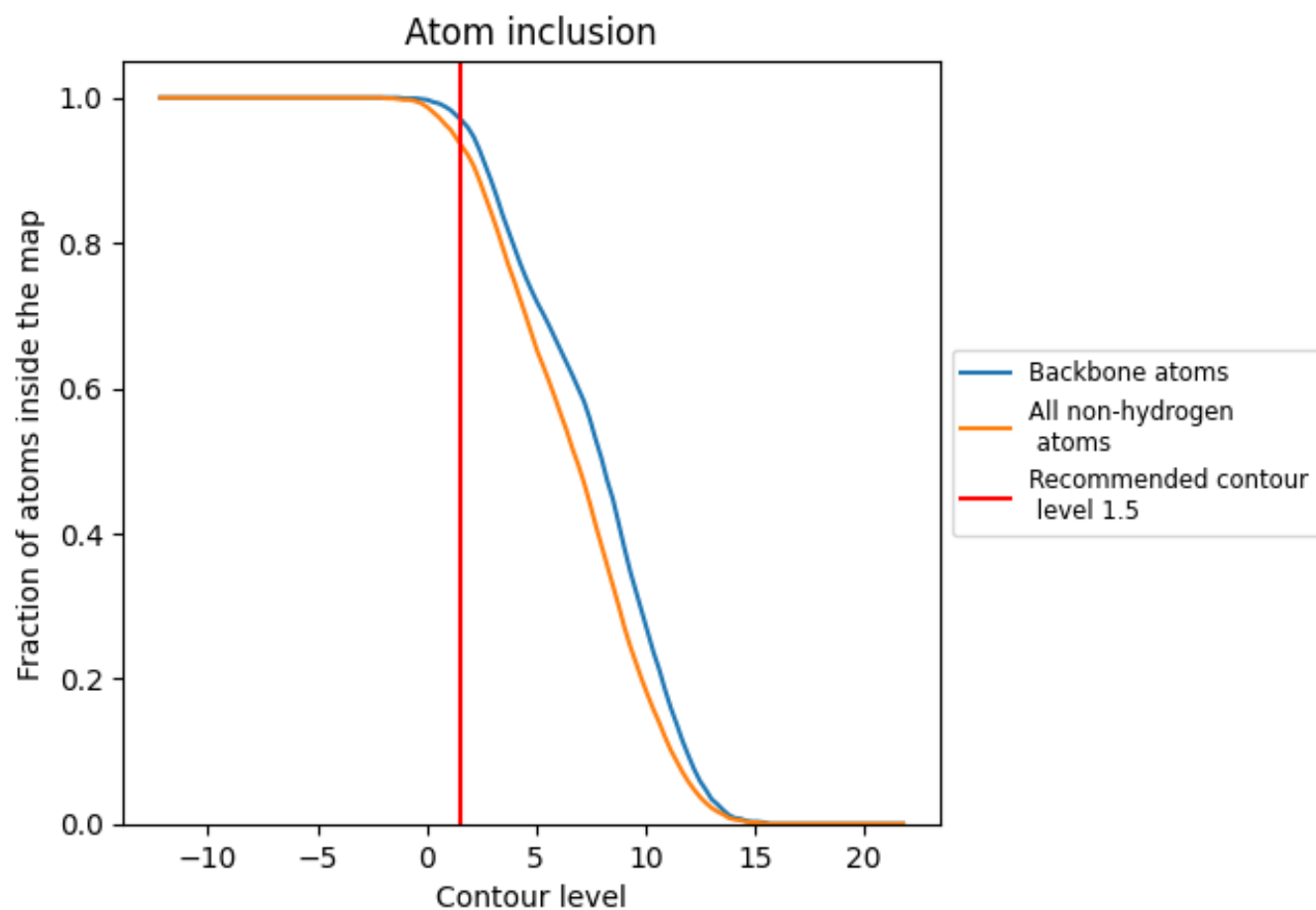
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9380	 0.5940
1	 0.9390	 0.5930
2	 0.9370	 0.5930
3	 0.9400	 0.5930
4	 0.9390	 0.5930
5	 0.9390	 0.5940
6	 0.9390	 0.5940
7	 0.9380	 0.5950
8	 0.9390	 0.5930
A	 0.9400	 0.5930
B	 0.9380	 0.5940
C	 0.9350	 0.5940
D	 0.9390	 0.5940
E	 0.9370	 0.5940
F	 0.9400	 0.5940
G	 0.9370	 0.5930
H	 0.9380	 0.5970
I	 0.9360	 0.5940
J	 0.9380	 0.5950
K	 0.9360	 0.5940
L	 0.9380	 0.5940
M	 0.9370	 0.5940
N	 0.9390	 0.5940
O	 0.9370	 0.5940
P	 0.9380	 0.5940
Q	 0.9360	 0.5950
R	 0.9380	 0.5960
S	 0.9380	 0.5940
T	 0.9360	 0.5940
U	 0.9380	 0.5940
V	 0.9360	 0.5950
W	 0.9390	 0.5940
X	 0.9370	 0.5950
Y	 0.9390	 0.5940
Z	 0.9370	 0.5940



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Chain	Atom inclusion	Q-score
a	 0.9360	 0.5930
b	 0.9370	 0.5950
c	 0.9390	 0.5950
d	 0.9380	 0.5960
e	 0.9390	 0.5930
f	 0.9370	 0.5940
g	 0.9360	 0.5950
h	 0.9380	 0.5920
i	 0.9370	 0.5940
j	 0.9360	 0.5950
k	 0.9380	 0.5950
l	 0.9380	 0.5950
m	 0.9380	 0.5940
n	 0.9370	 0.5930
o	 0.9360	 0.5950
p	 0.9390	 0.5930
q	 0.9370	 0.5920
r	 0.9360	 0.5930
s	 0.9400	 0.5930
t	 0.9380	 0.5940
u	 0.9380	 0.5950
v	 0.9380	 0.5950
w	 0.9390	 0.5950
x	 0.9360	 0.5940
y	 0.9380	 0.5950
z	 0.9390	 0.5930