



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 04:38 AM UTC

PDB ID : 5ZZ8 / pdb_00005zz8
EMDB ID : EMD-6976
Title : Structure of the Herpes simplex virus type 2 C-capsid with capsid-vertex-specific component
Authors : Wang, J.L.; Yuan, S.; Zhu, D.J.; Tang, H.; Wang, N.; Chen, W.Y.; Gao, Q.; Li, Y.H.; Wang, J.Z.; Liu, H.R.; Zhang, X.Z.; Rao, Z.H.; Wang, X.X.
Deposited on : 2018-05-31
Resolution : 3.75 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

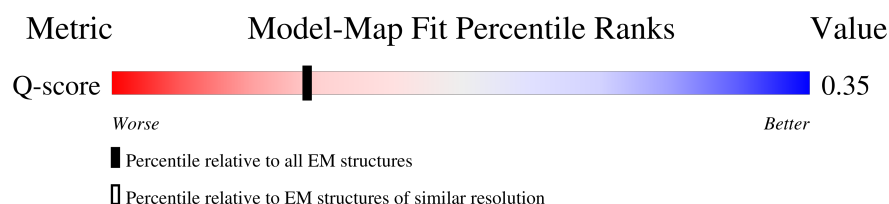
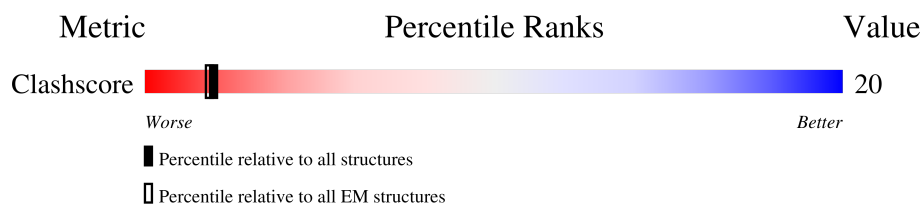
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

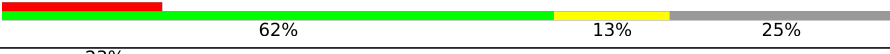
The reported resolution of this entry is 3.75 Å.

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	-
Q-score	-	25397	10301 (3.25 - 4.25)

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	466	
1	Q	466	
1	T	466	
1	W	466	
1	w	466	
2	2	318	

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Mol	Chain	Length	Quality of chain
2	3	318	
2	R	318	
2	S	318	
2	U	318	
2	V	318	
2	X	318	
2	Y	318	
2	x	318	
2	y	318	
3	A	1374	
3	B	1374	
3	C	1374	
3	D	1374	
3	E	1374	
3	F	1374	
3	G	1374	
3	H	1374	
3	I	1374	
3	J	1374	
3	K	1374	
3	L	1374	
3	M	1374	
3	N	1374	
3	O	1374	
3	P	1374	

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Mol	Chain	Length	Quality of chain
4	b	112	79%
4	c	112	79%
4	d	112	78%
4	e	112	79%
4	f	112	79%
4	g	112	78%
4	h	112	79%
4	i	112	71%
4	j	112	67%
4	k	112	71%
4	l	112	59%
4	m	112	70%
4	n	112	56%
4	o	112	70%
4	p	112	63%
4	q	112	72%
4	r	112	58%
4	s	112	71%
4	t	112	79%
4	u	112	58%
4	v	112	77%
4	w	112	59%
4	x	112	74%
4	y	112	69%
5	q	702	15%
6	r	585	48%
6	s	585	10%
6	t	585	10%
7	t	3122	98%
7	u	3122	98%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 218714 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 VP19C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	350	Total	C	N	O	S	0	0
			2589	1620	493	461	15		
1	T	350	Total	C	N	O	S	0	0
			2595	1623	496	461	15		
1	W	350	Total	C	N	O	S	0	0
			2577	1613	490	459	15		
1	1	350	Total	C	N	O	S	0	0
			2589	1620	493	461	15		
1	w	350	Total	C	N	O	S	0	0
			2595	1623	496	461	15		

- Molecule 2 is a protein called VP23.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	286	Total	C	N	O	S	0	0
			2102	1343	374	379	6		
2	S	308	Total	C	N	O	S	0	0
			2337	1484	413	429	11		
2	U	286	Total	C	N	O	S	0	0
			2102	1343	374	379	6		
2	V	308	Total	C	N	O	S	0	0
			2337	1484	413	429	11		
2	X	286	Total	C	N	O	S	0	0
			2102	1343	374	379	6		
2	Y	308	Total	C	N	O	S	0	0
			2337	1484	413	429	11		
2	3	286	Total	C	N	O	S	0	0
			2102	1343	374	379	6		
2	2	308	Total	C	N	O	S	0	0
			2334	1481	413	429	11		
2	x	286	Total	C	N	O	S	0	0
			2102	1343	374	379	6		
2	y	308	Total	C	N	O	S	0	0
			2328	1478	410	429	11		

- Molecule 3 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	1362	Total	C	N	O	S	0	0
			10418	6584	1873	1905	56		
3	J	1364	Total	C	N	O	S	0	0
			10408	6582	1863	1907	56		
3	K	1364	Total	C	N	O	S	0	0
			10414	6585	1866	1907	56		
3	L	1362	Total	C	N	O	S	0	0
			10422	6586	1873	1907	56		
3	M	1366	Total	C	N	O	S	0	0
			10449	6603	1877	1913	56		
3	A	1259	Total	C	N	O	S	0	0
			9646	6107	1725	1762	52		
3	H	1362	Total	C	N	O	S	0	0
			10416	6583	1873	1905	55		
3	N	1362	Total	C	N	O	S	0	0
			10397	6574	1868	1899	56		
3	O	1366	Total	C	N	O	S	0	0
			10417	6585	1877	1899	56		
3	P	1364	Total	C	N	O	S	0	0
			10407	6582	1866	1903	56		
3	B	1357	Total	C	N	O	S	0	0
			10349	6542	1854	1897	56		
3	C	1356	Total	C	N	O	S	0	0
			10355	6545	1857	1897	56		
3	D	1364	Total	C	N	O	S	0	0
			10413	6583	1872	1902	56		
3	E	1362	Total	C	N	O	S	0	0
			10405	6578	1870	1901	56		
3	F	1362	Total	C	N	O	S	0	0
			10392	6571	1862	1903	56		
3	G	1346	Total	C	N	O	S	0	0
			10261	6487	1845	1874	55		

- Molecule 4 is a protein called VP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	h	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	i	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	j	101	Total	C	N	O	S	0	0
			773	489	143	138	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	k	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	l	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	m	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	n	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	o	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	p	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	b	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	c	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	d	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	e	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	f	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	g	101	Total	C	N	O	S	0	0
			773	489	143	138	3		

- Molecule 5 is a protein called UL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	q	554	Total	C	N	O	S	0	0
			4241	2700	774	749	18		

- Molecule 6 is a protein called UL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	r	94	Total	C	N	O	S	0	0
			764	490	136	136	2		
6	s	80	Total	C	N	O	S	0	0
			651	413	123	114	1		

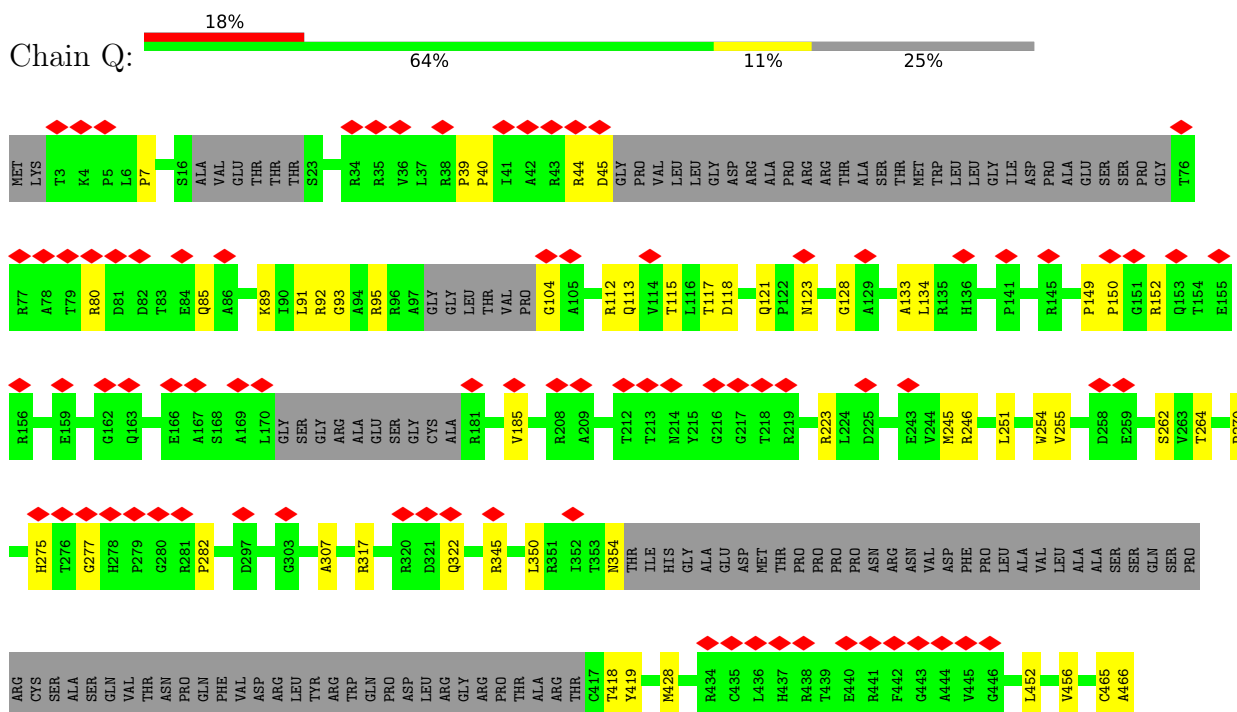
- Molecule 7 is a protein called UL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	t	47	Total 383	C 234	N 87	O 60	S 2	0	0
7	u	47	Total 383	C 234	N 87	O 60	S 2	0	0

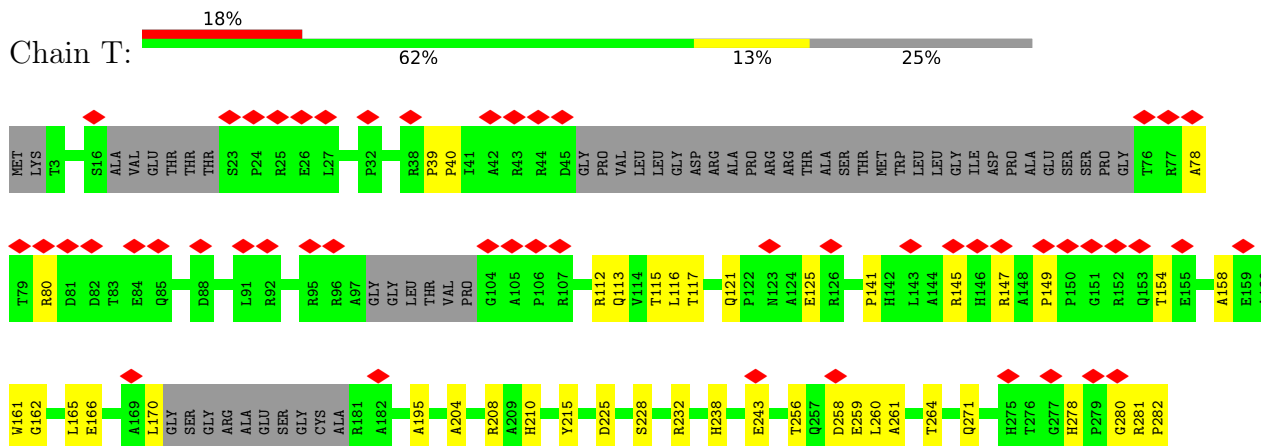
3 Residue-property plots

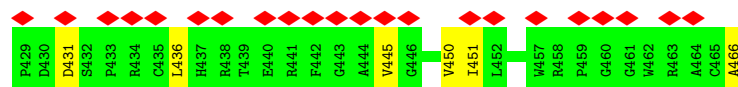
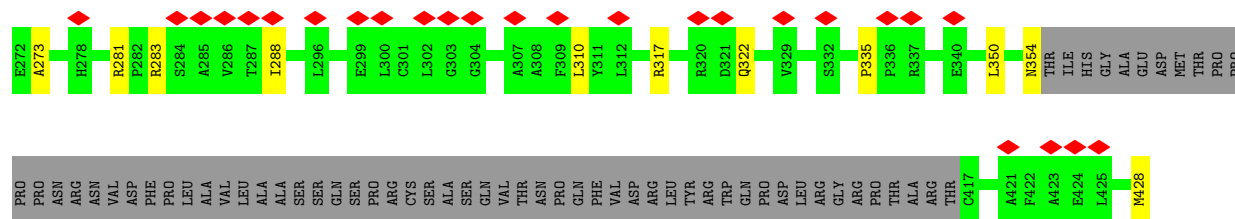
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: VP19C

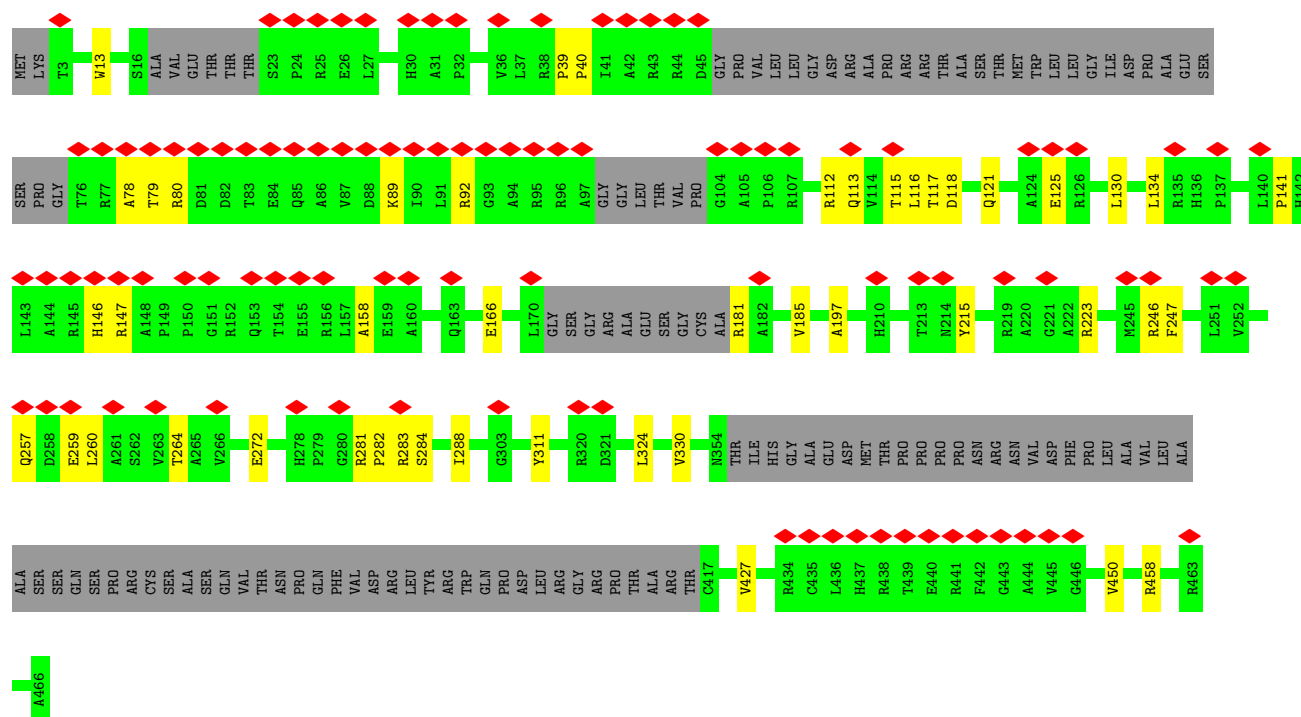


• Molecule 1: VP19C

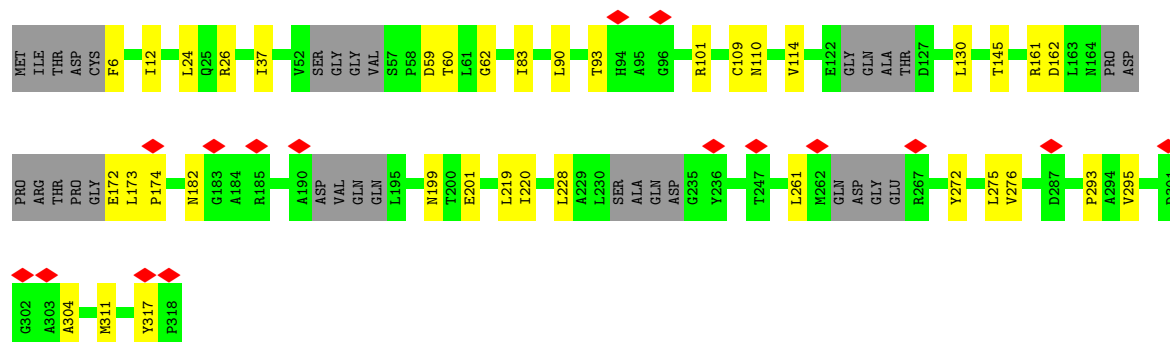
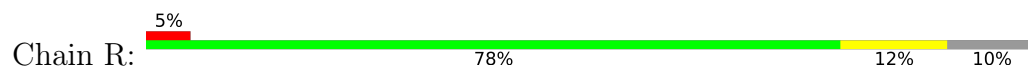




• Molecule 1: VP19C

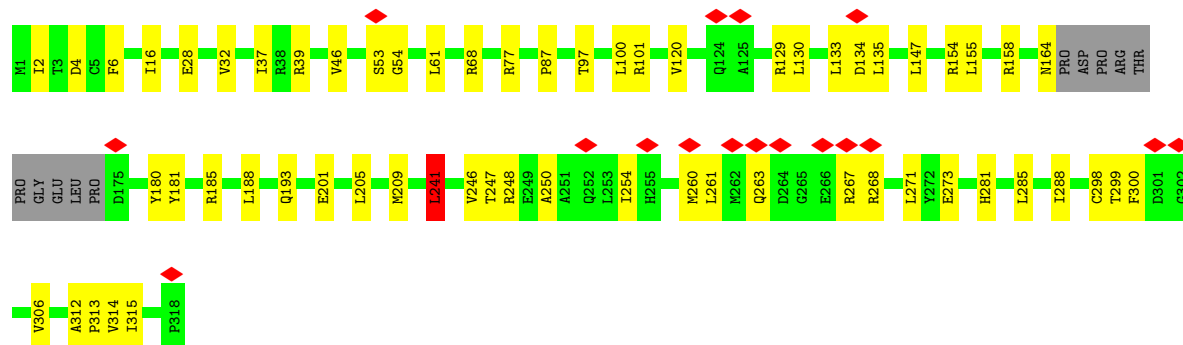


• Molecule 2: VP23



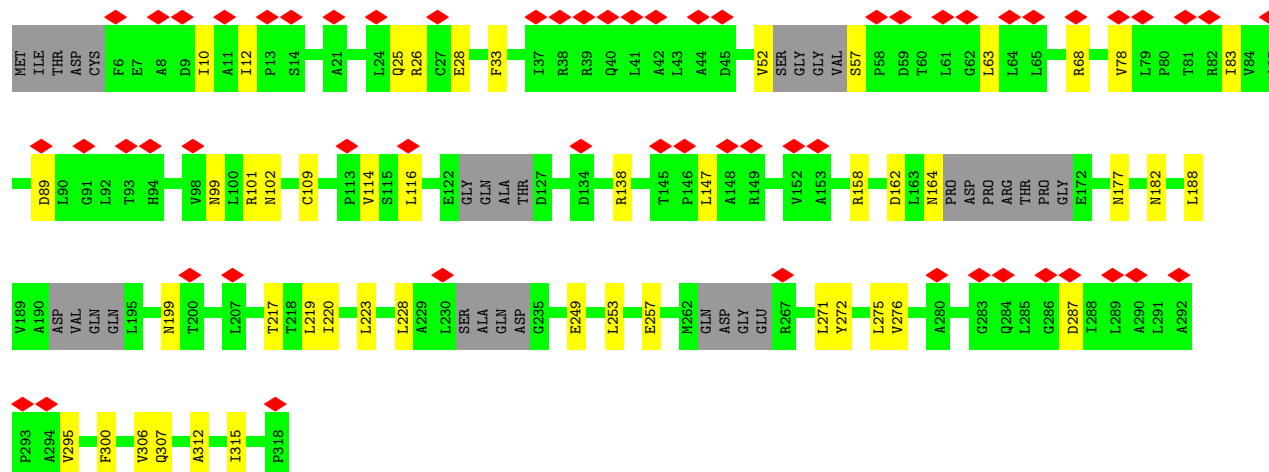
- Molecule 2: VP23

Chain S: 



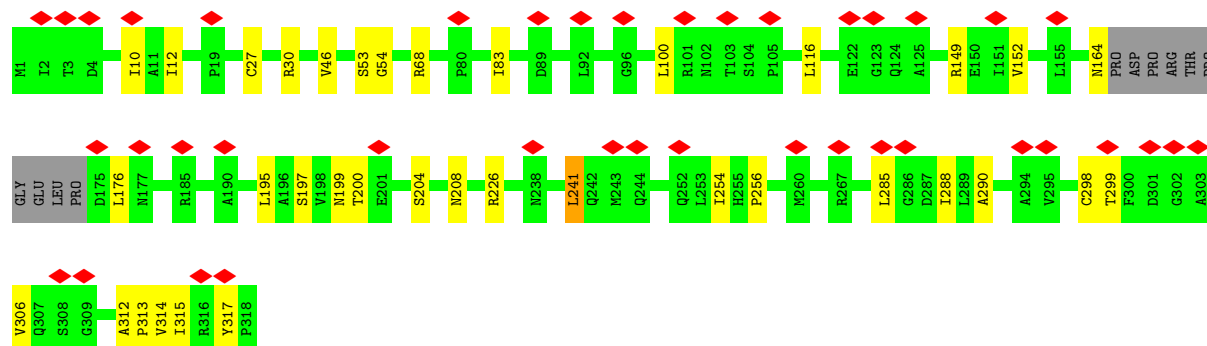
- Molecule 2: VP23

Chain U: 



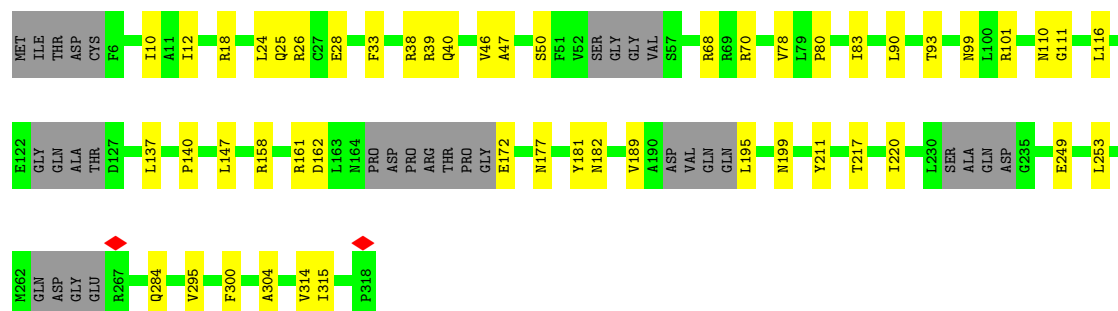
- Molecule 2: VP23

Chain V: 

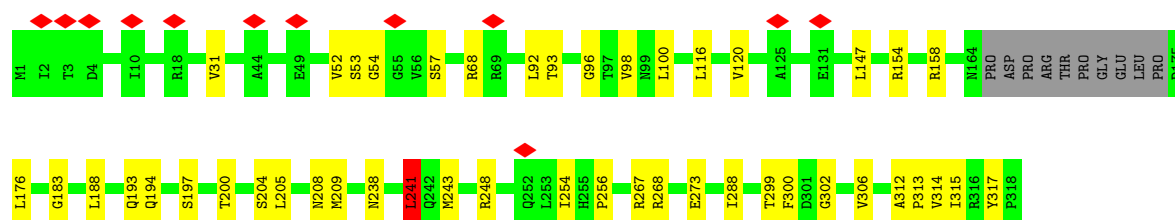
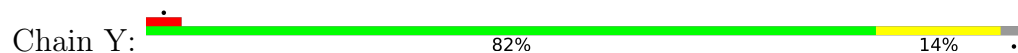


- Molecule 2: VP23

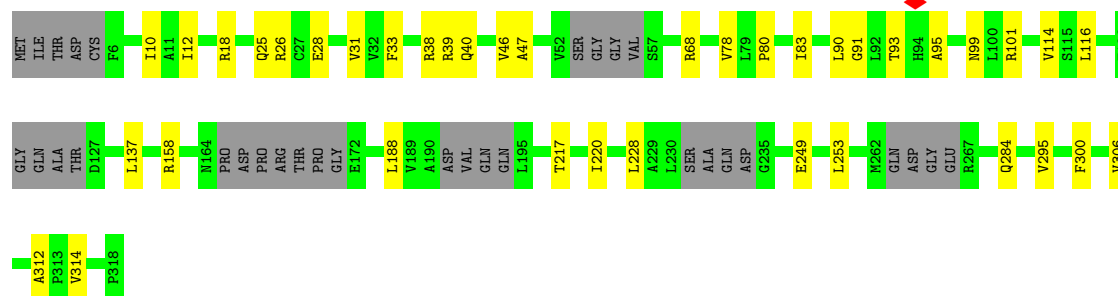
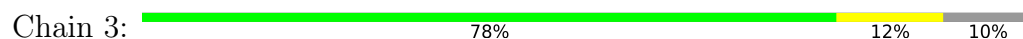
Chain X: 



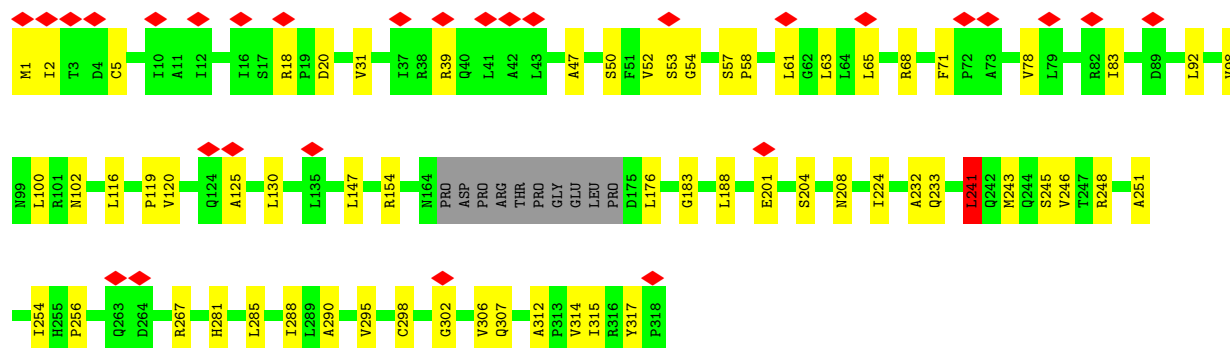
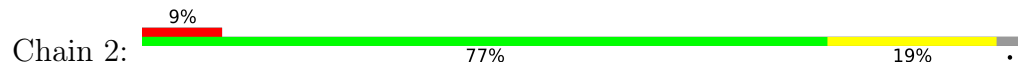
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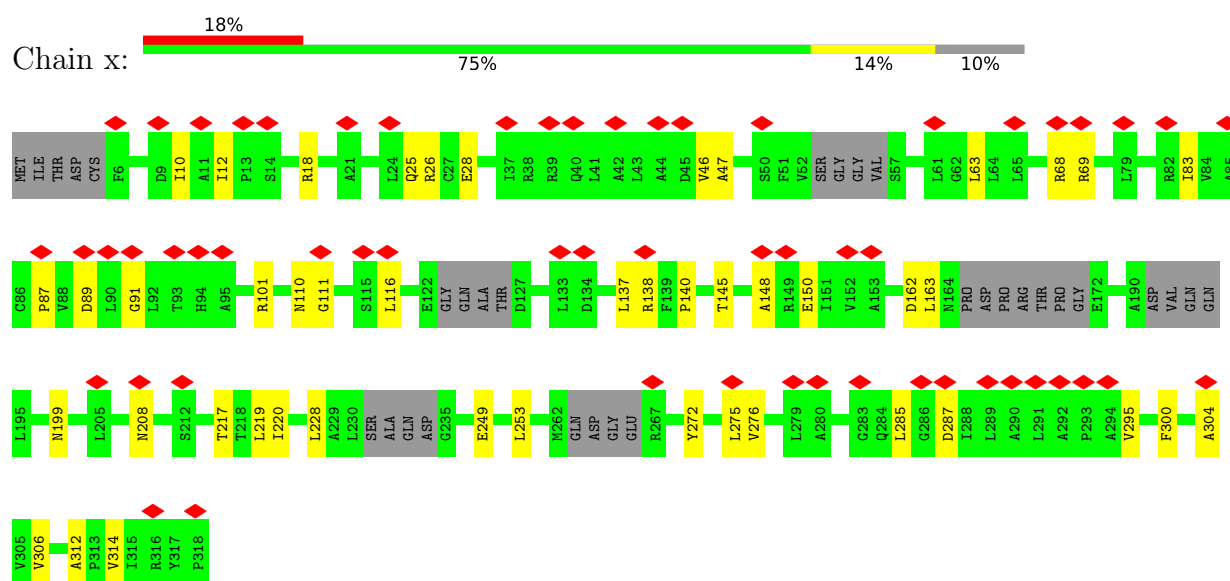
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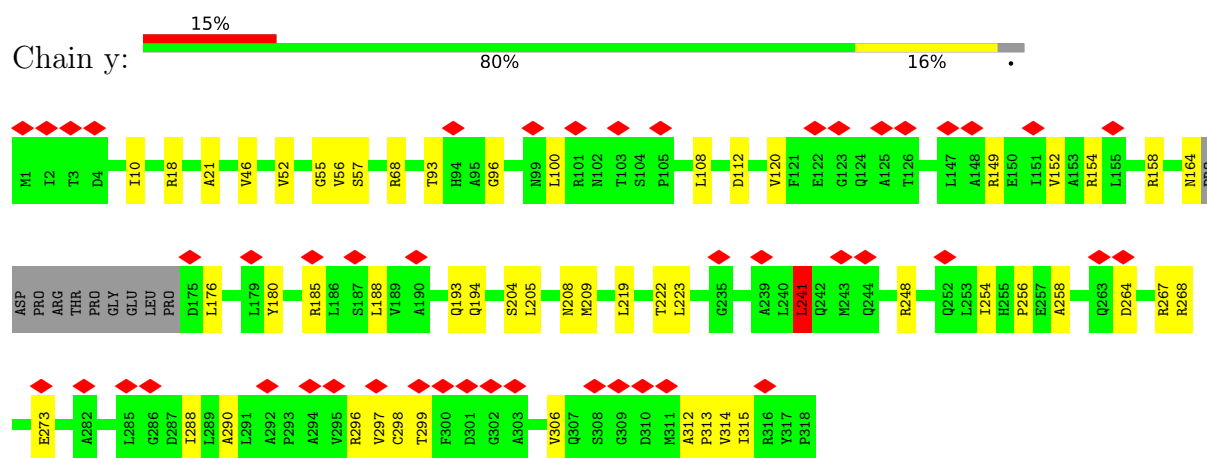
- Molecule 2: VP23



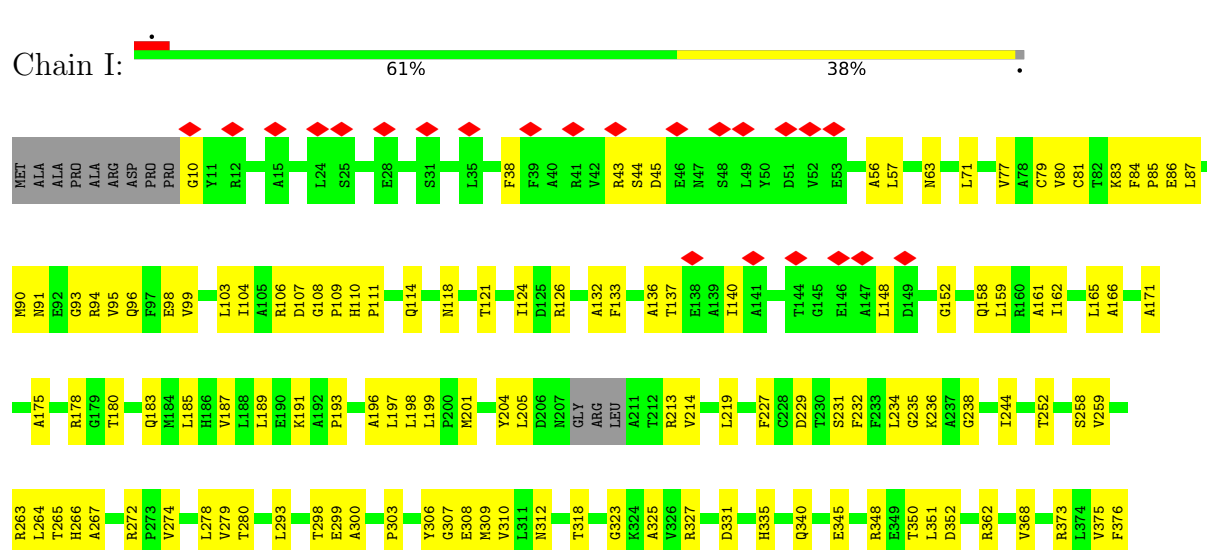
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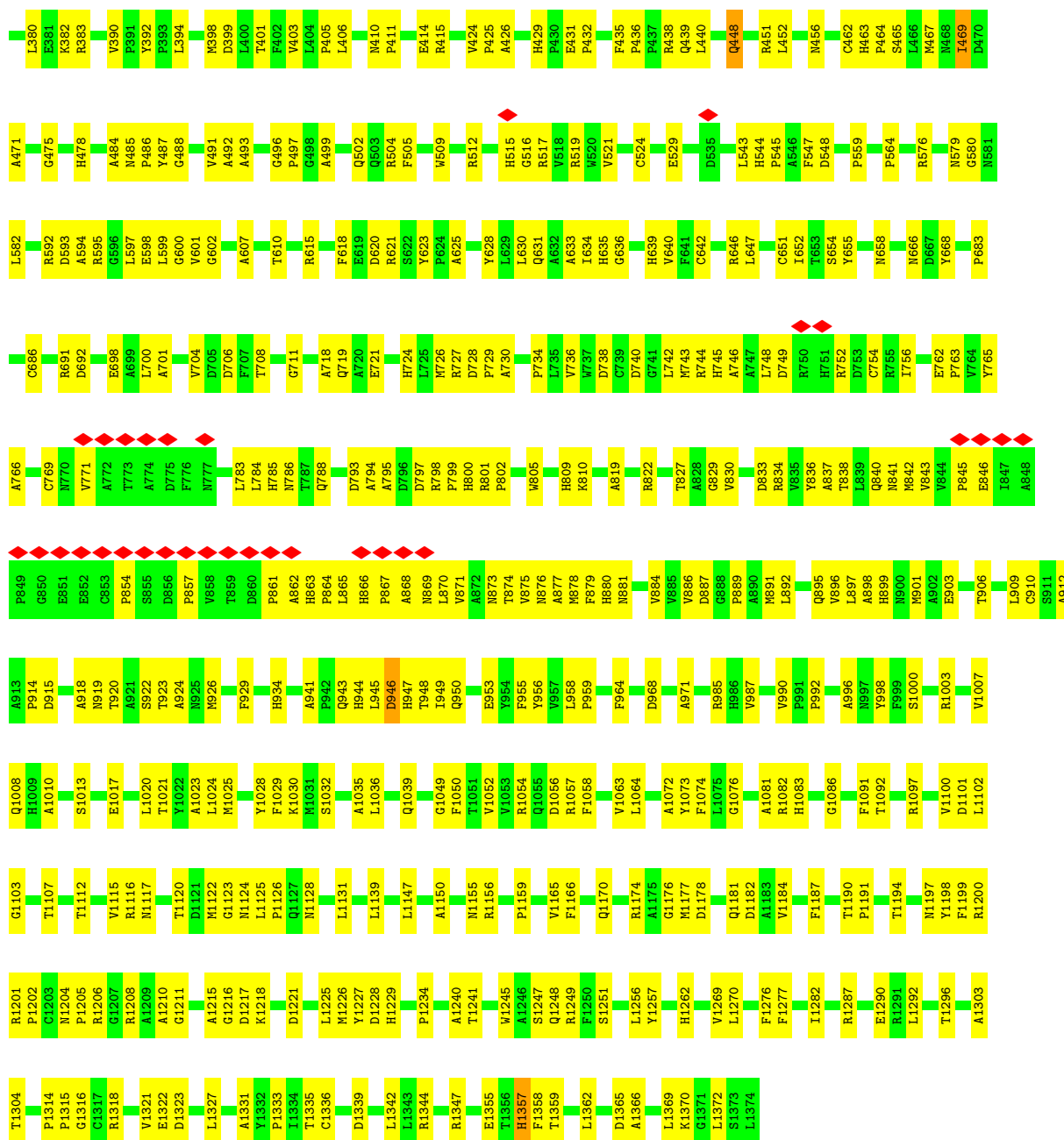


• Molecule 2: VP23



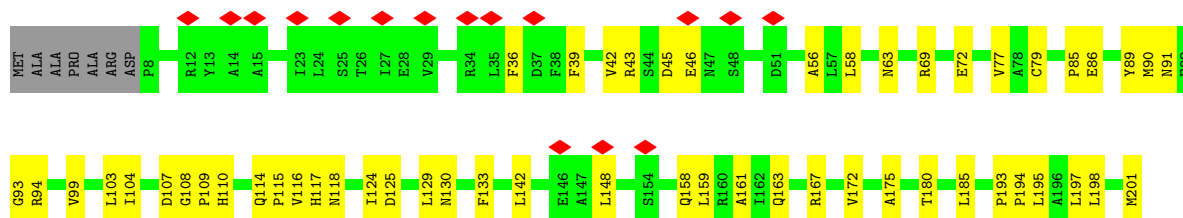
• Molecule 3: Major capsid protein



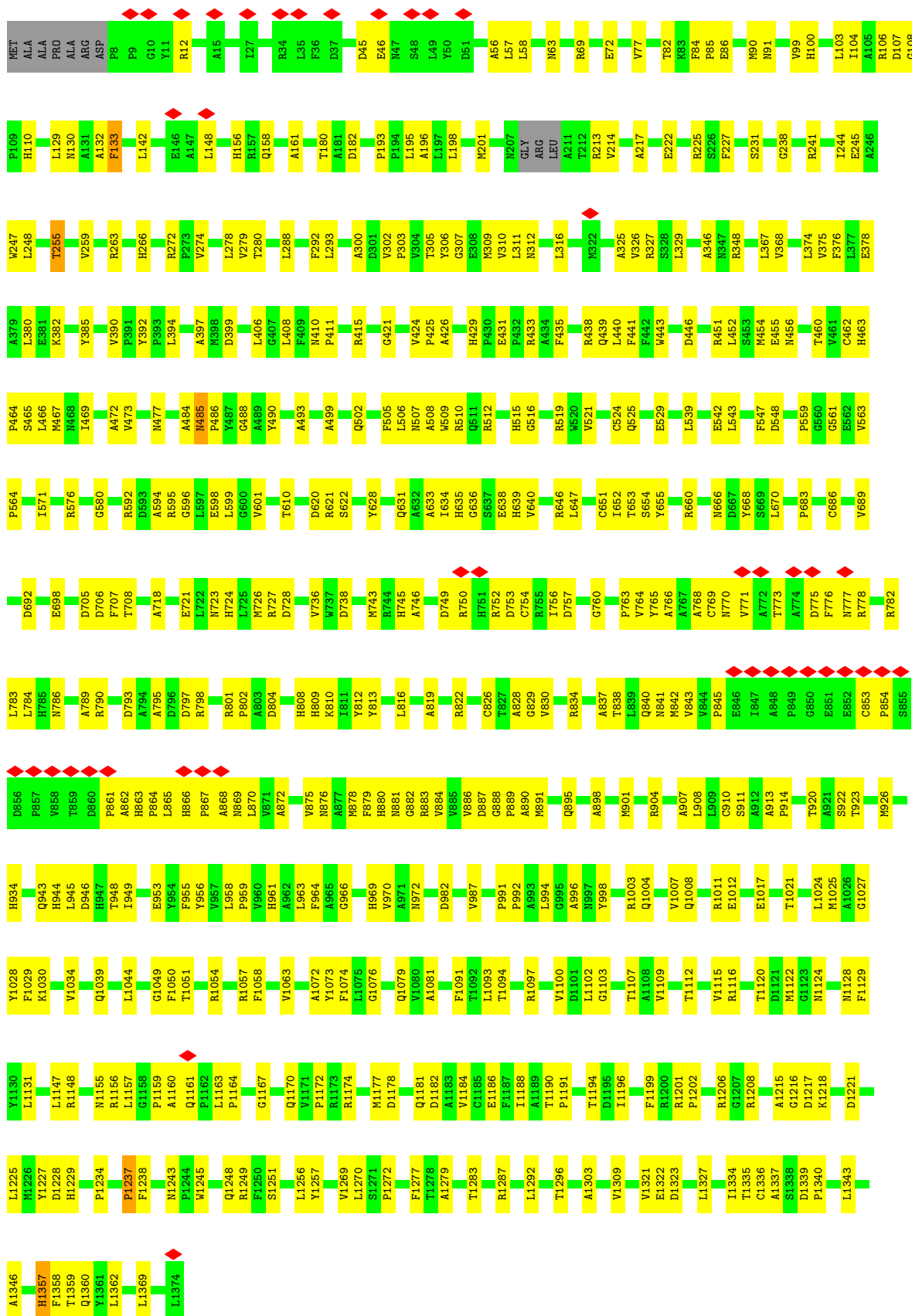


• Molecule 3: Major capsid protein

Chain J: 63% 36%

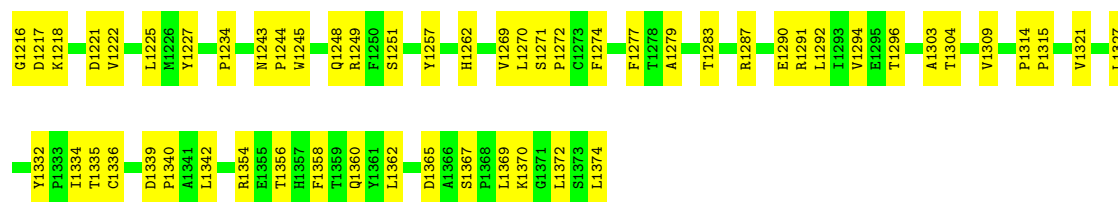




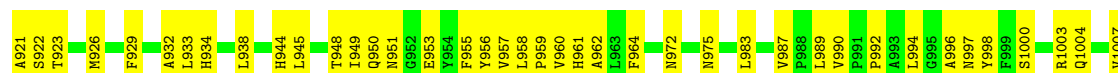
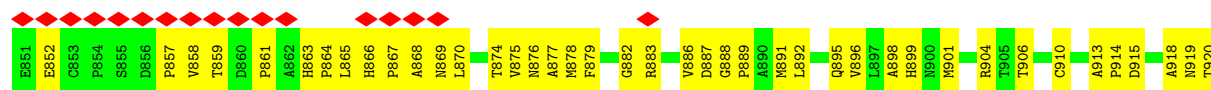
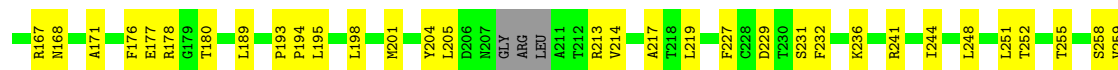
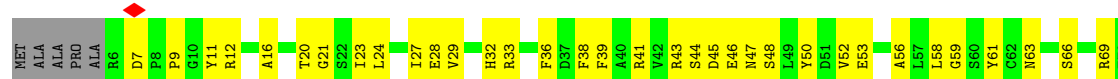


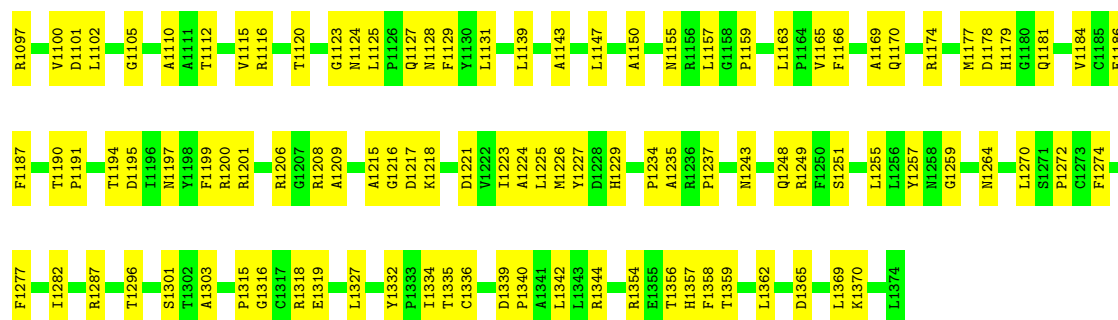
• Molecule 3: Major capsid protein



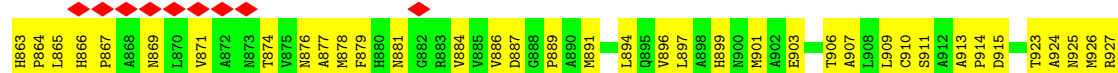
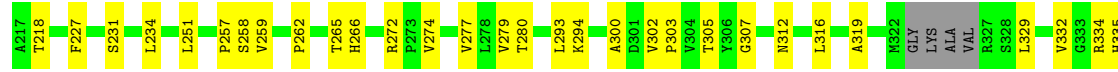
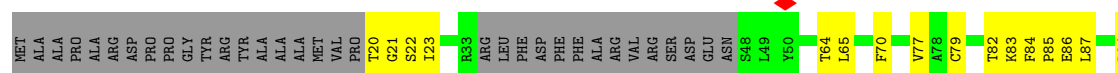


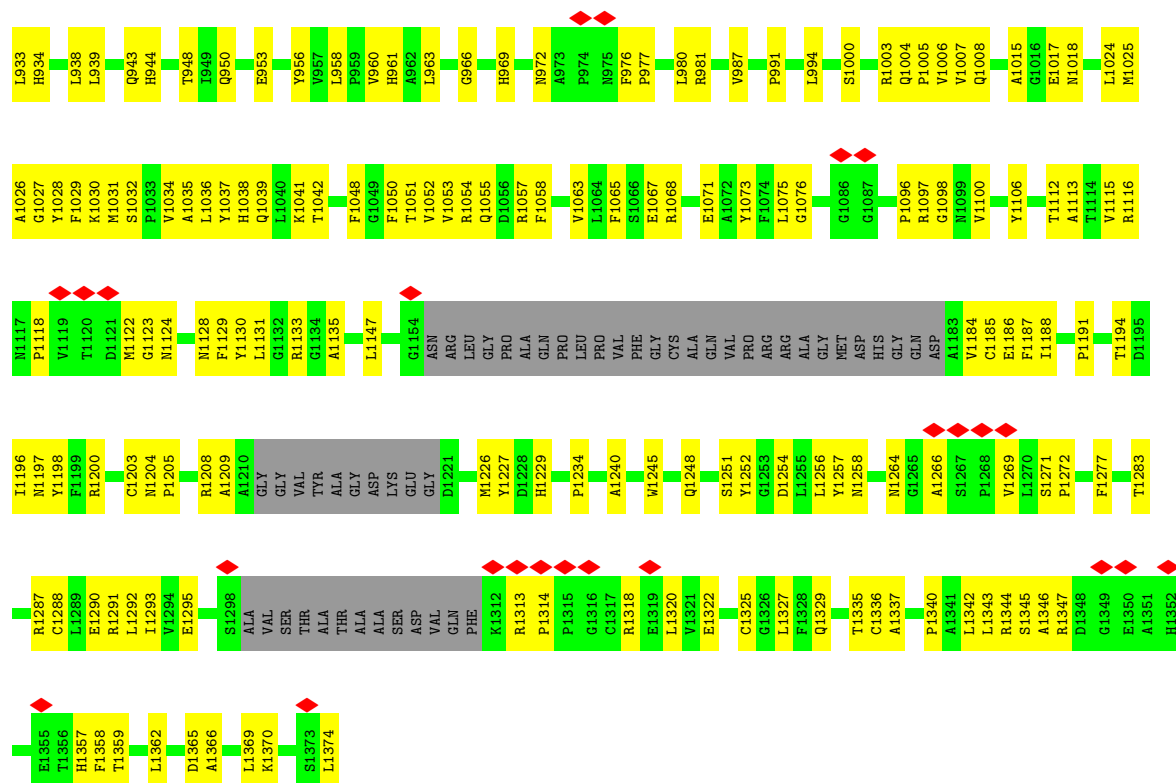
• Molecule 3: Major capsid protein



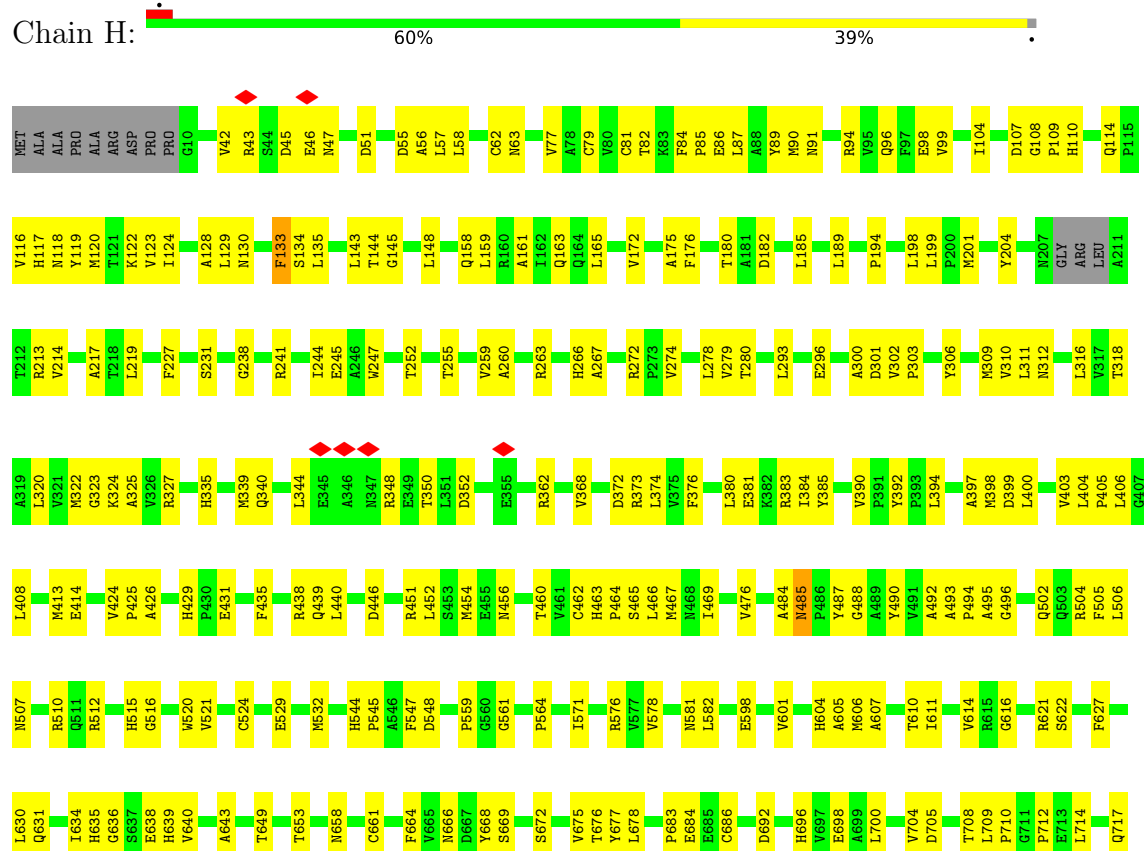


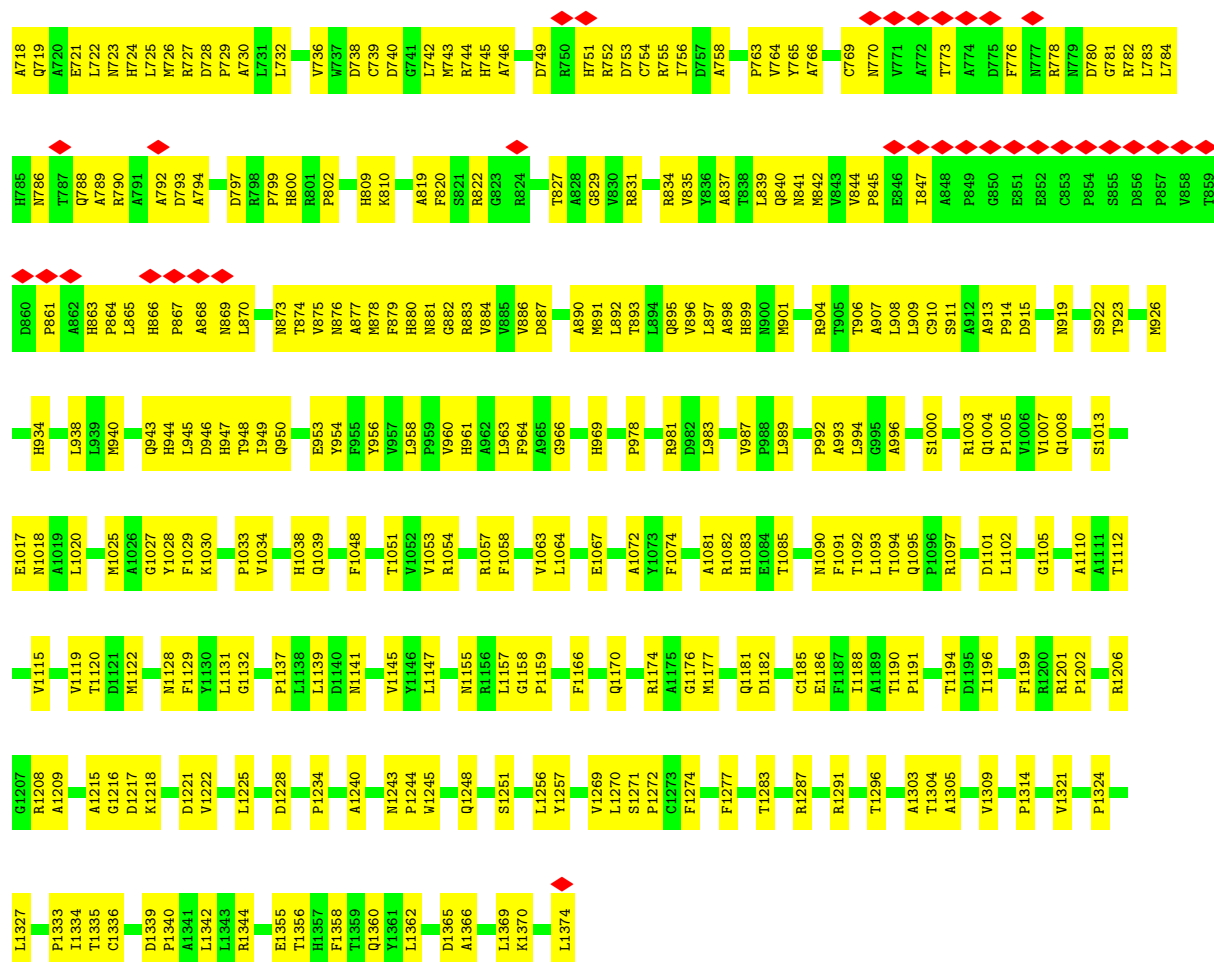
• Molecule 3: Major capsid protein



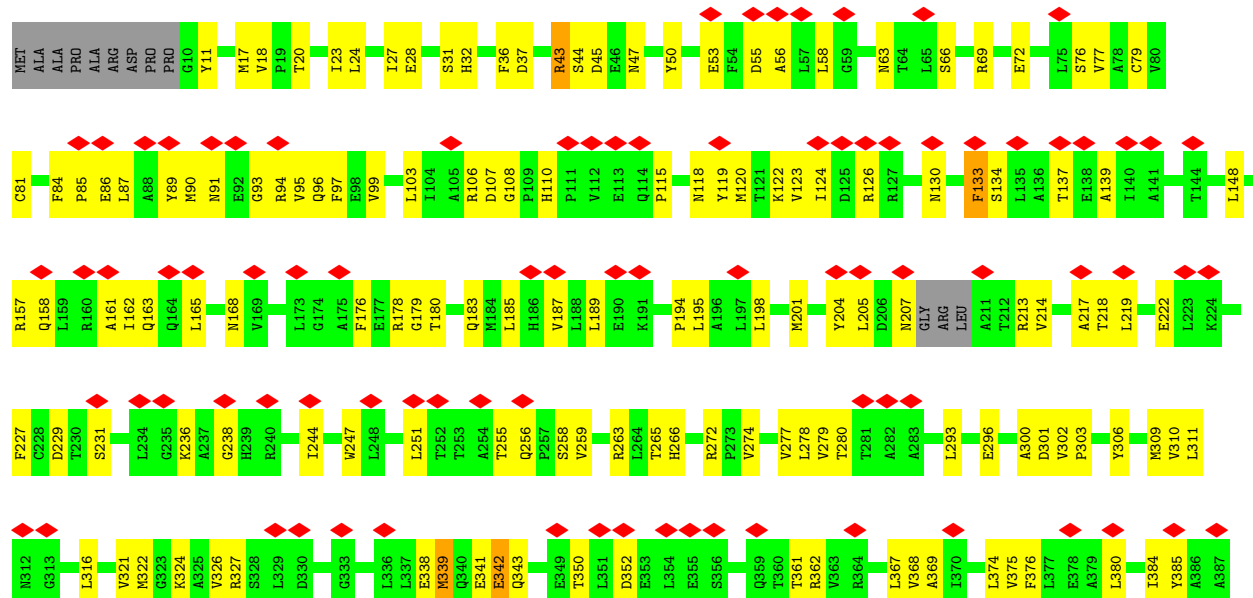


• Molecule 3: Major capsid protein





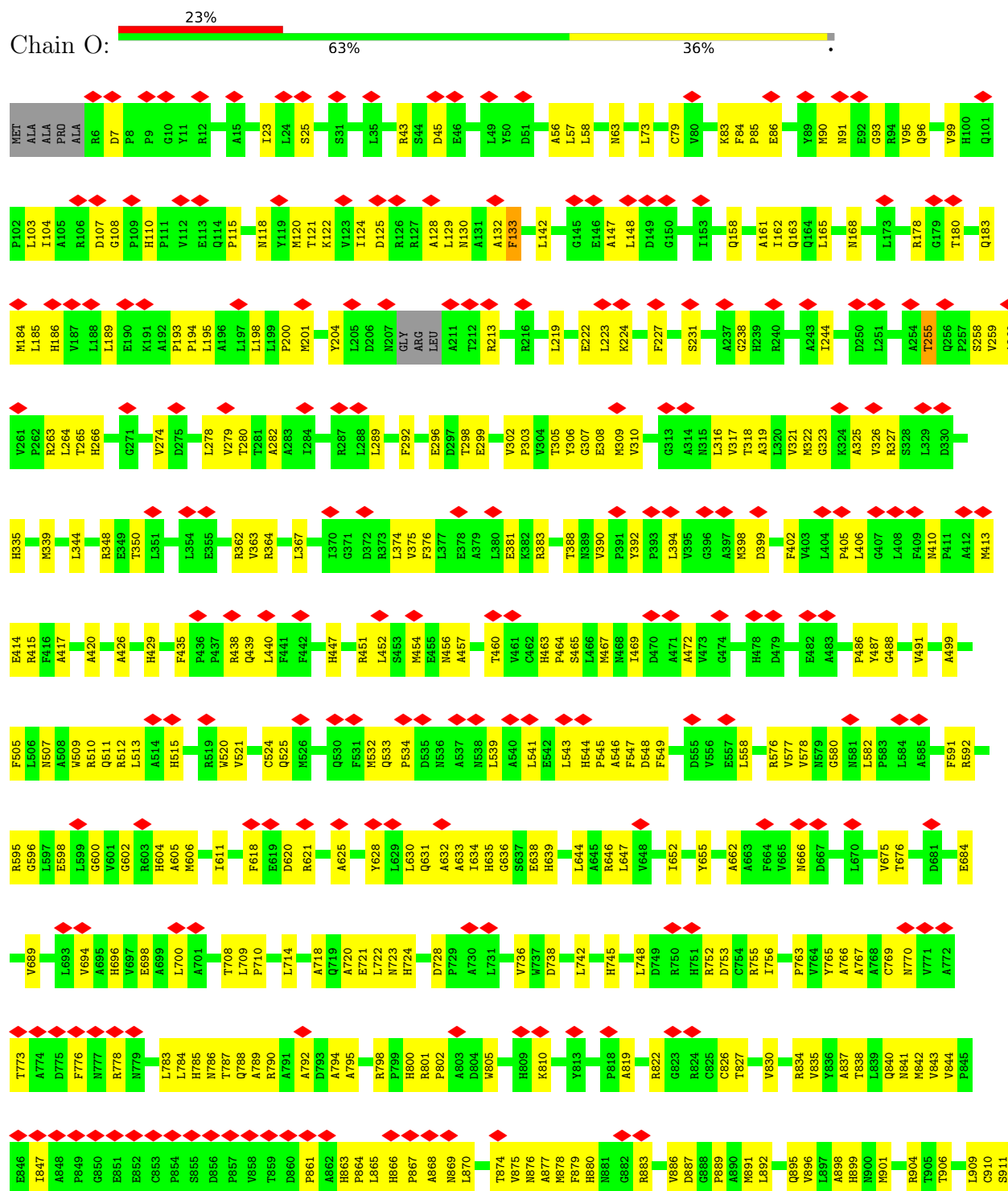
• Molecule 3: Major capsid protein

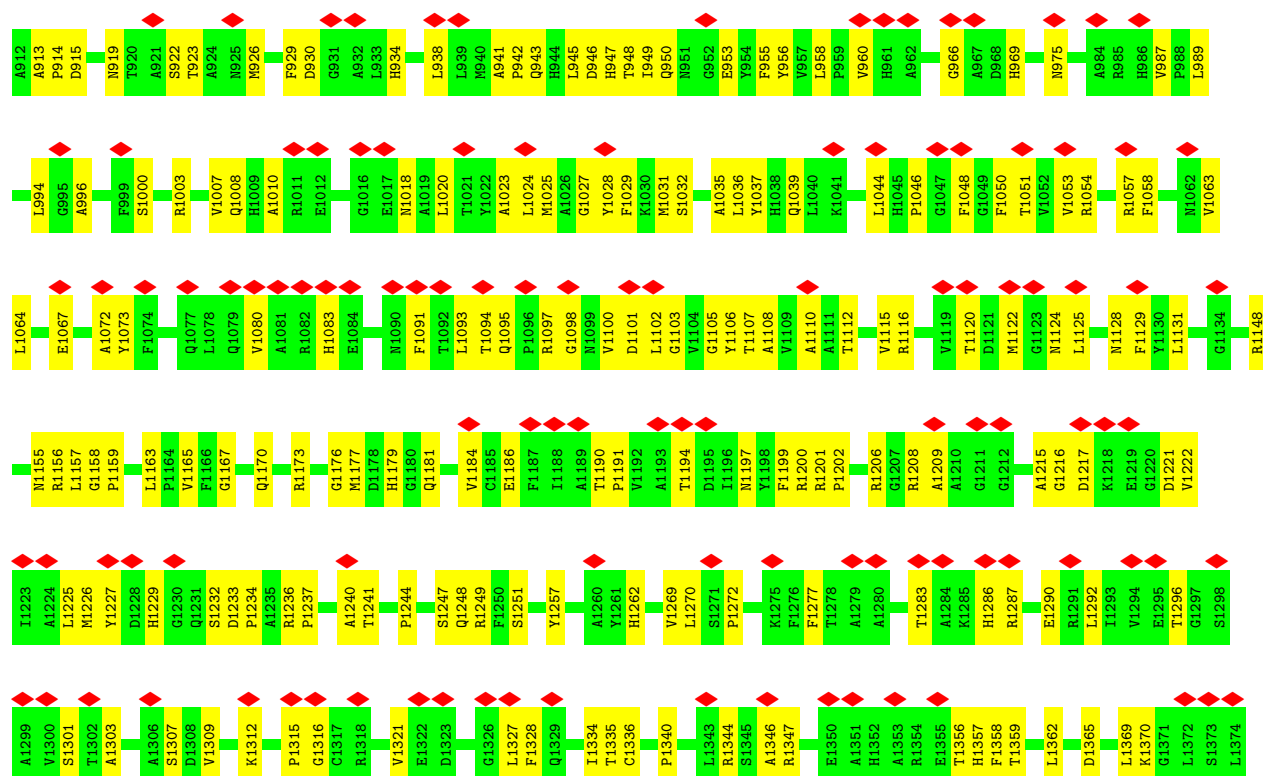




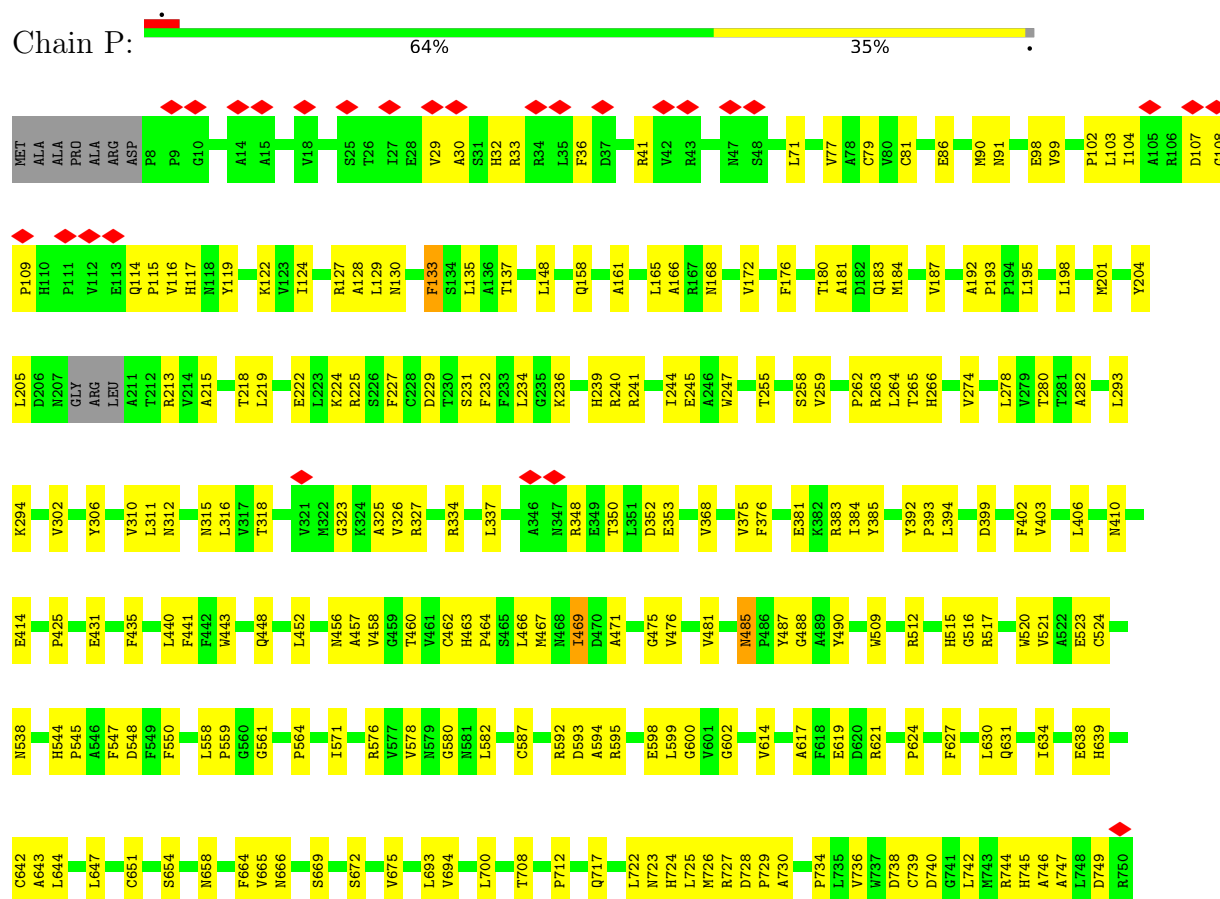


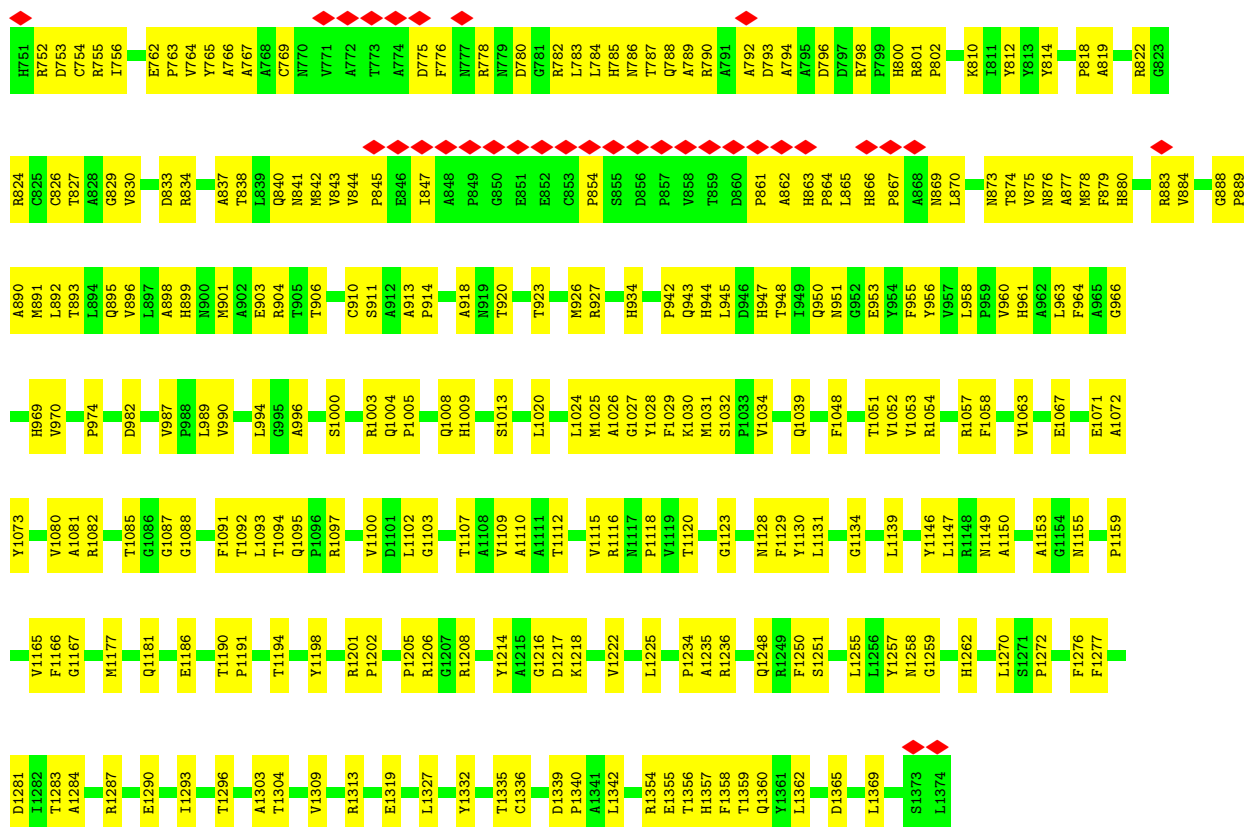
• Molecule 3: Major capsid protein





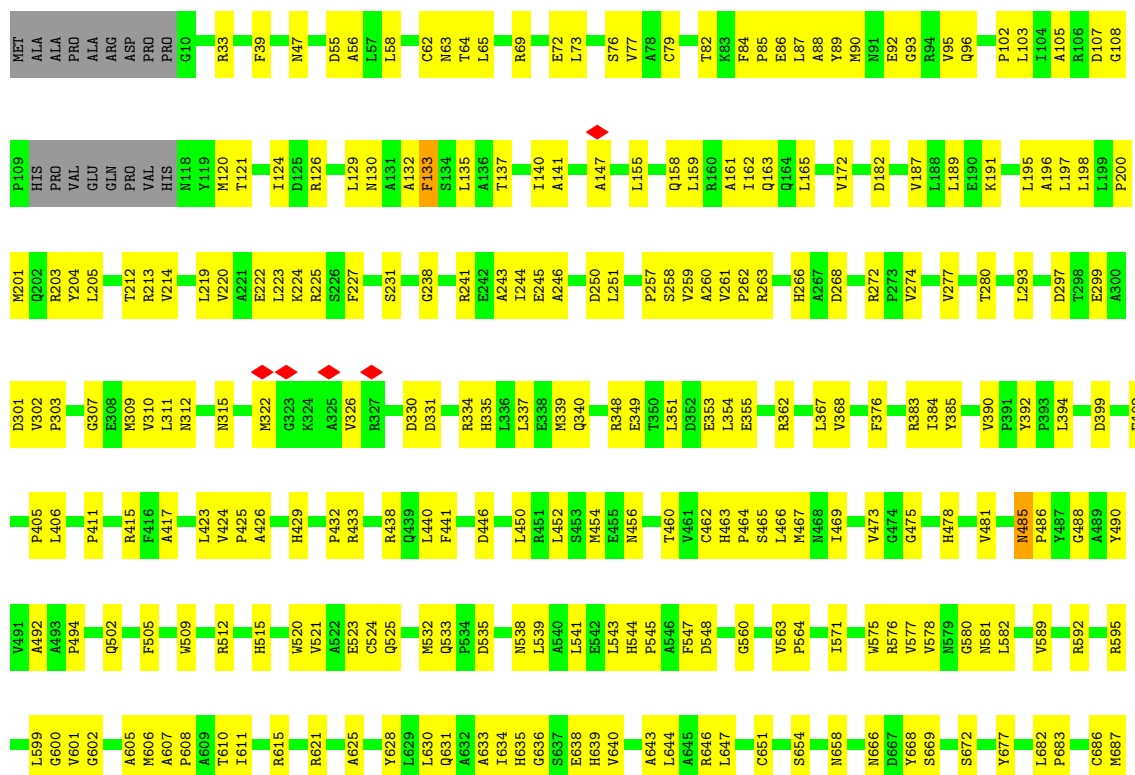
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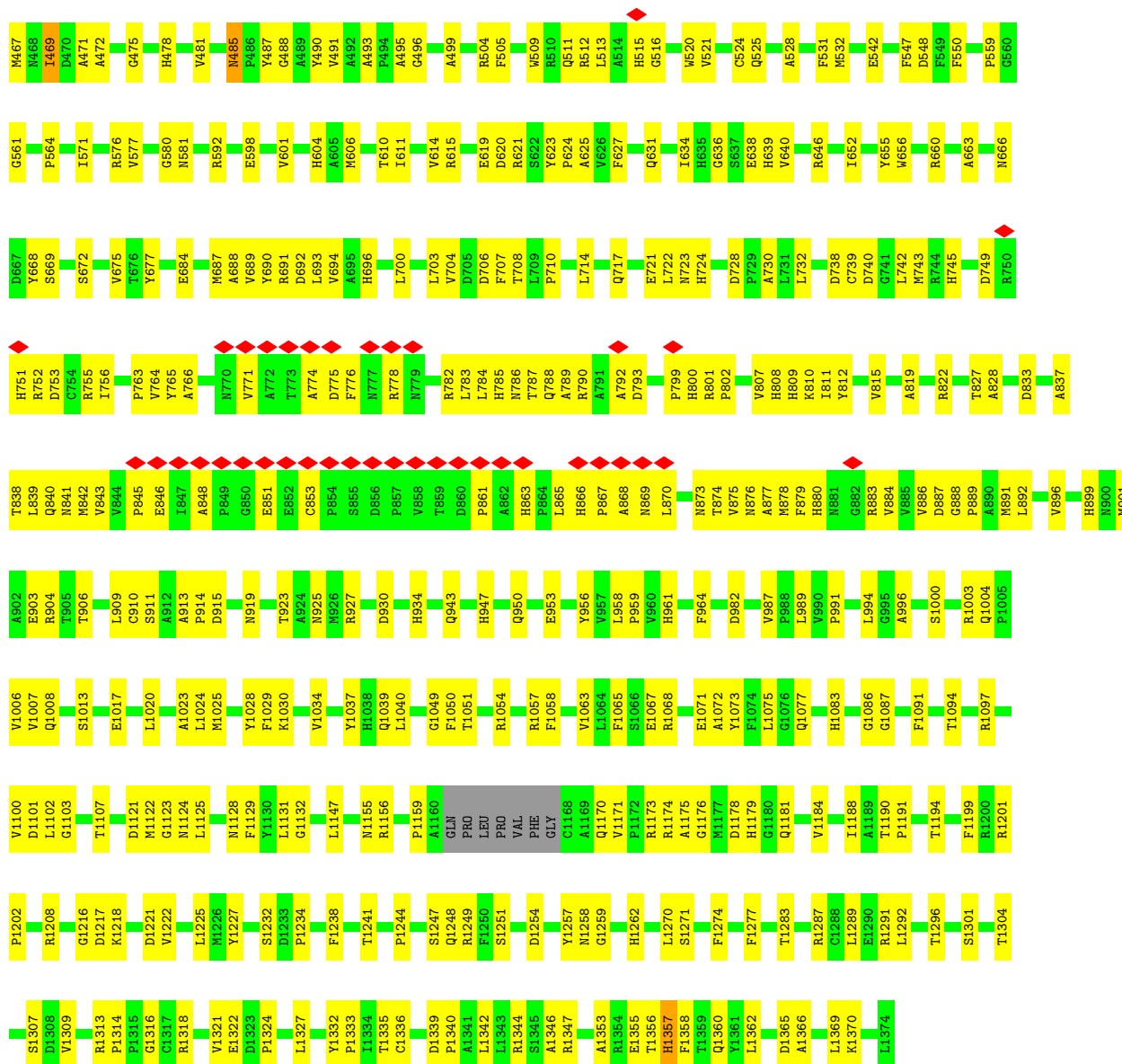




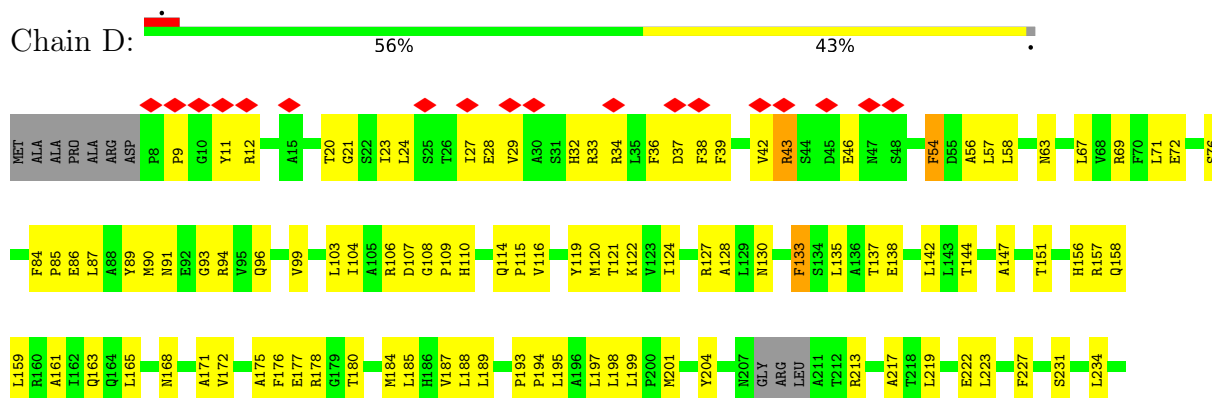
• Molecule 3: Major capsid protein

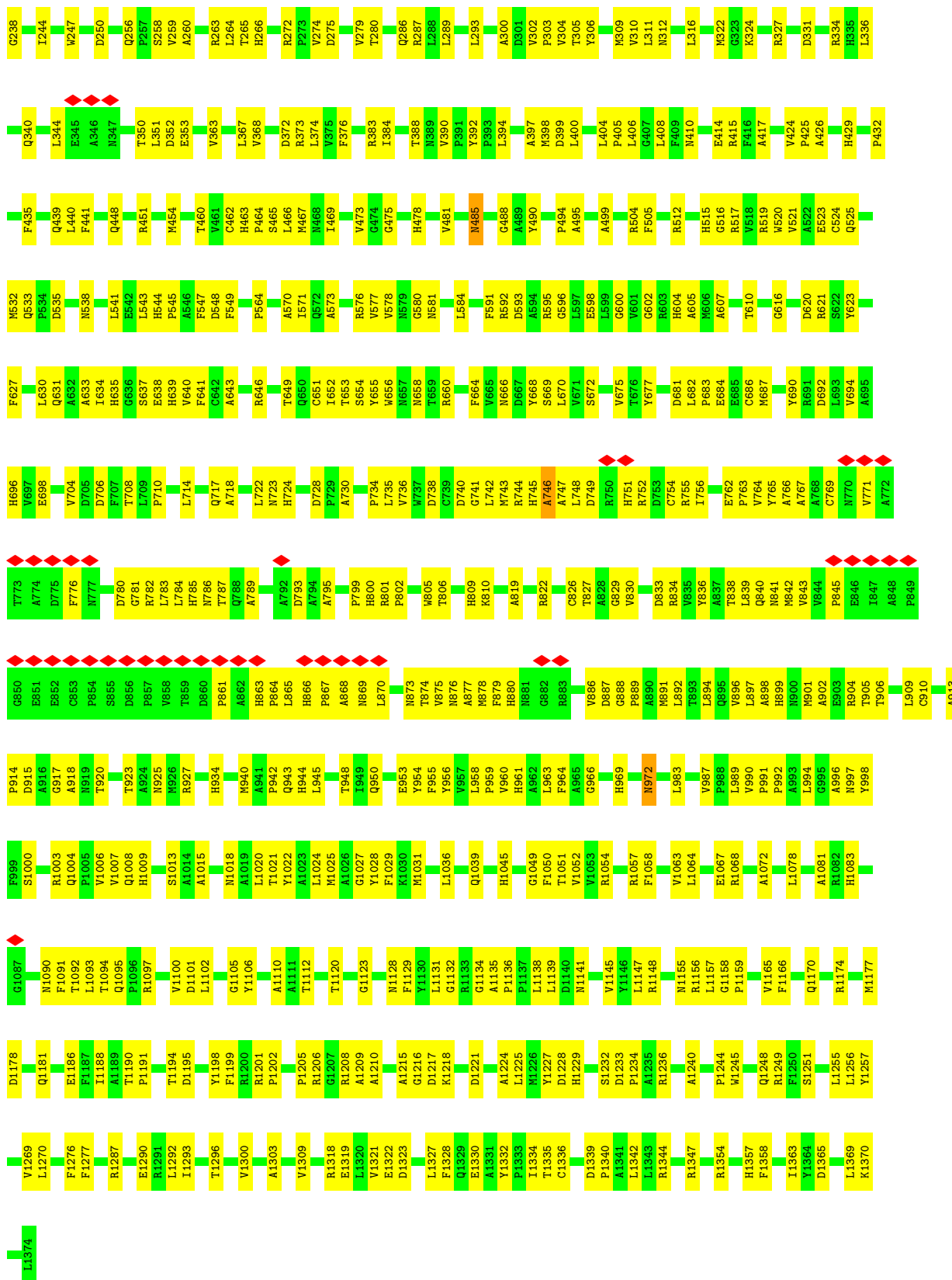
Chain B: 60% 38%





• Molecule 3: Major capsid protein

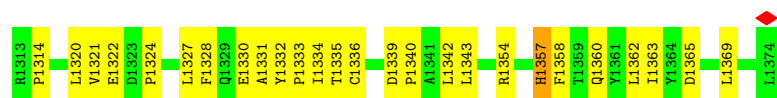




• Molecule 3: Major capsid protein

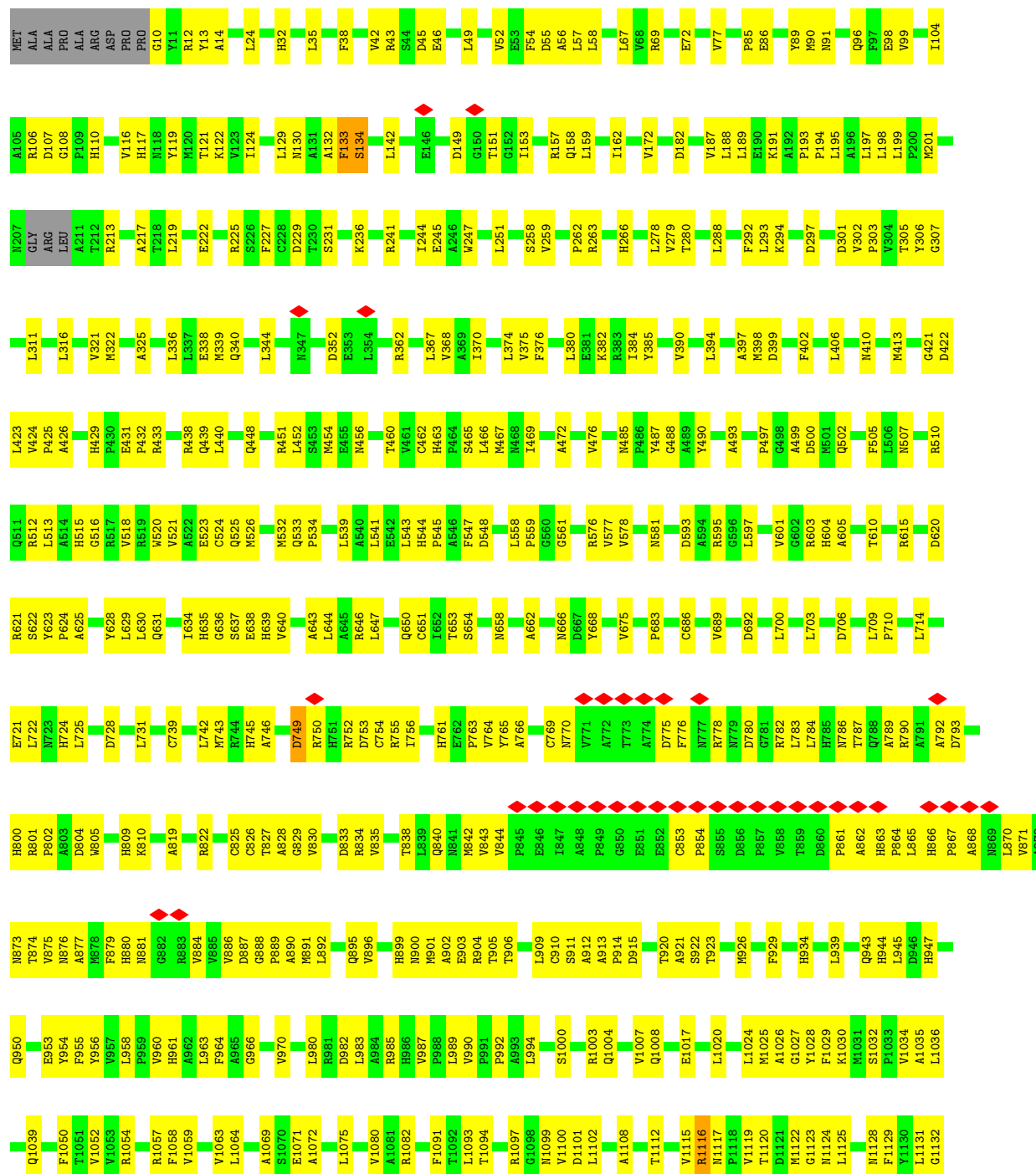
Chain E:  59% 39% ..

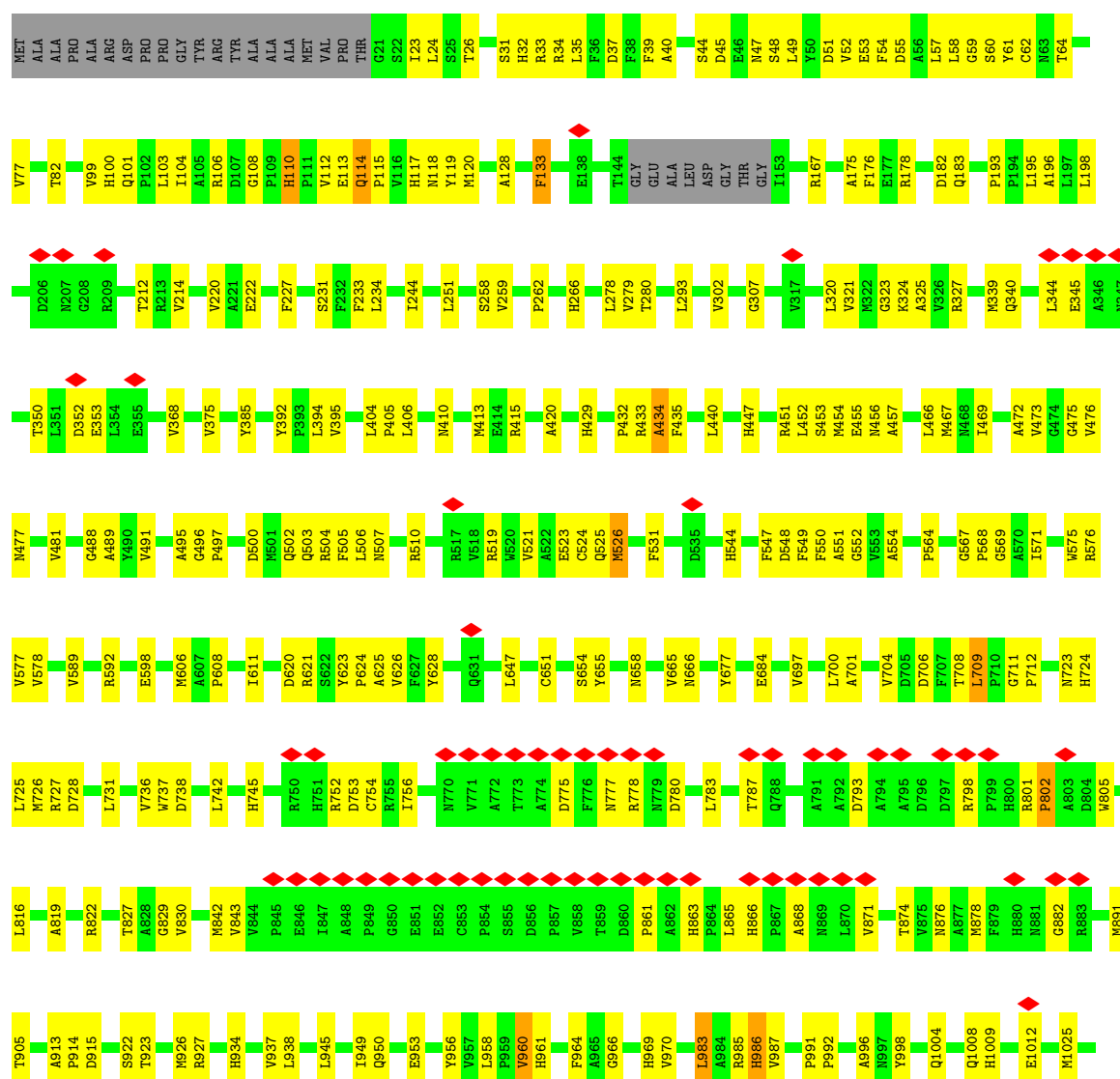
MET	ALA	ALA	PRO	ALA	ARG	ASP	PRO	G10	Y11	R12	R33	R34	L35	F38	V42	R43	S44	D51	V52	D55	L57	L58	G59	N63	T64	L65	S66	R69	F70	L71	E72	L73	C79	F80	C81	T82	R83	F84	P85	E86	L87	A88	M90	N91	Q96	V99		
P200	M201	Y204	N207	GLY	ARG	LEU	L311	A211	T212	R213	V214	A217	L218	T219	E222	L223	F227	S231	F232	F233	L234	G238	L244	T255	S258	V259	R263	L264	T265	H266	A267	D268	T269	R270	P273	V274	L278	V279	L280	L289	F292	L293	D301	V302				
P303	V304	T305	Y306	G307	E308	M309	V310	L311	N312	N315	L316	A319	L320	V321	M322	G323	K324	A325	V326	R327	Q340	E341	E342	R348	R362	L367	V368	V375	F376	R383	L384	Y385	V390	P391	Y392	P393	L394	M398	D399	L400	F402	V403	L404	P405	L408	F409	N410	

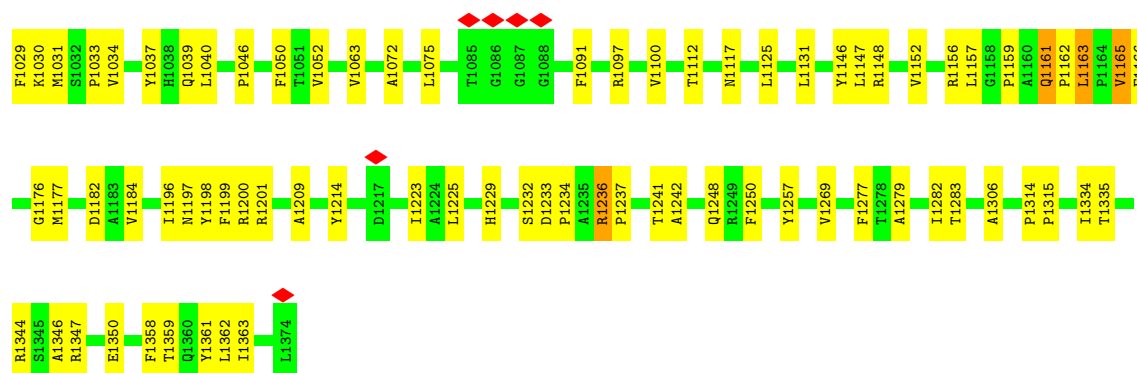


• Molecule 3: Major capsid protein

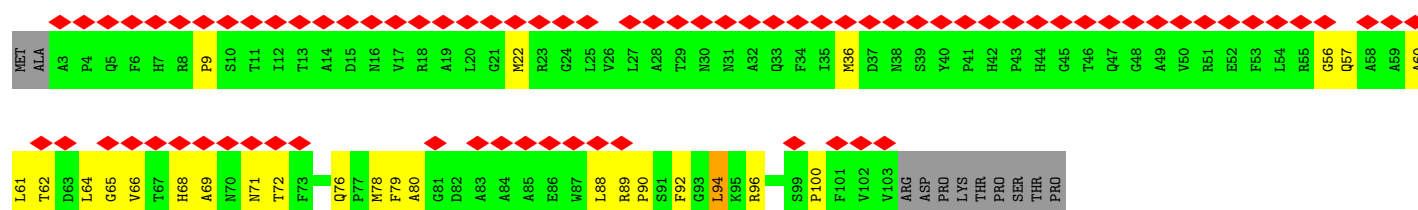
Chain F: 60% 38%



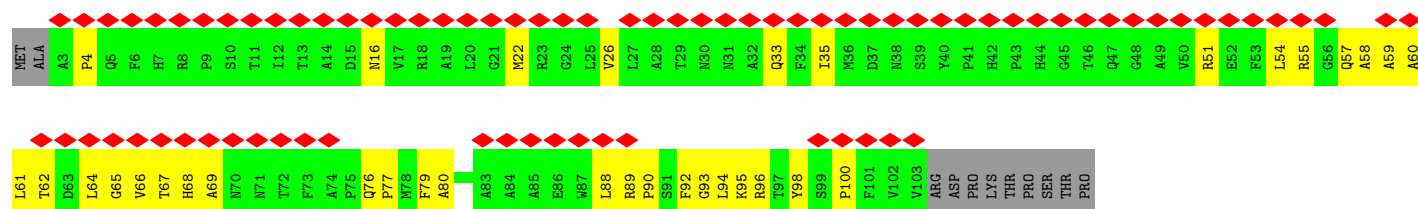




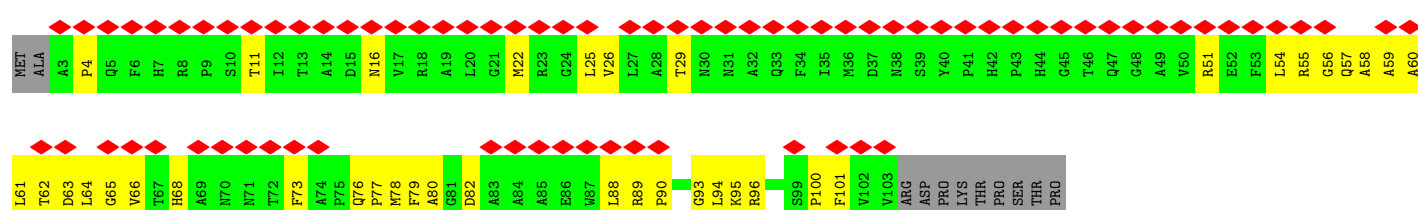
• Molecule 4: VP26



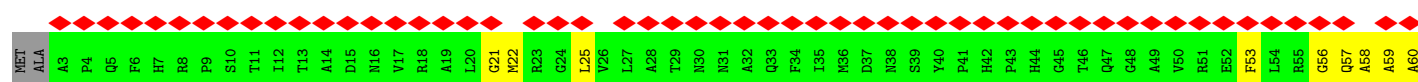
• Molecule 4: VP26



• Molecule 4: VP26



• Molecule 4: VP26

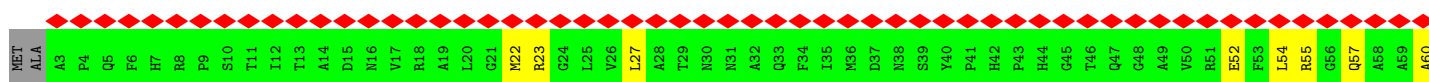




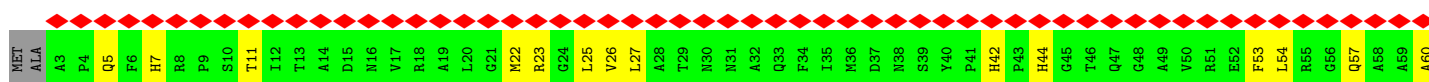
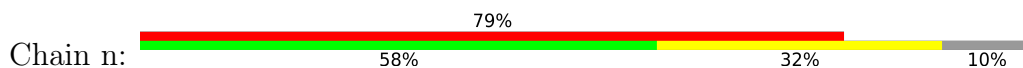
• Molecule 4: VP26



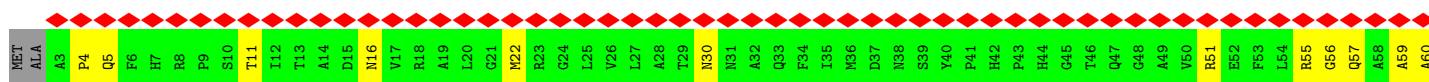
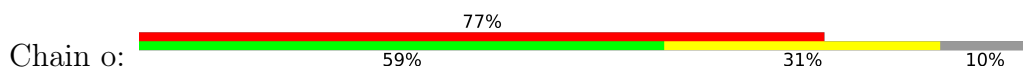
• Molecule 4: VP26



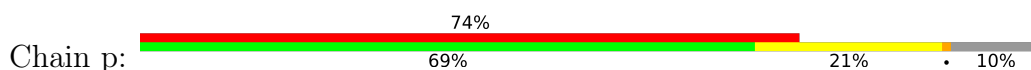
• Molecule 4: VP26

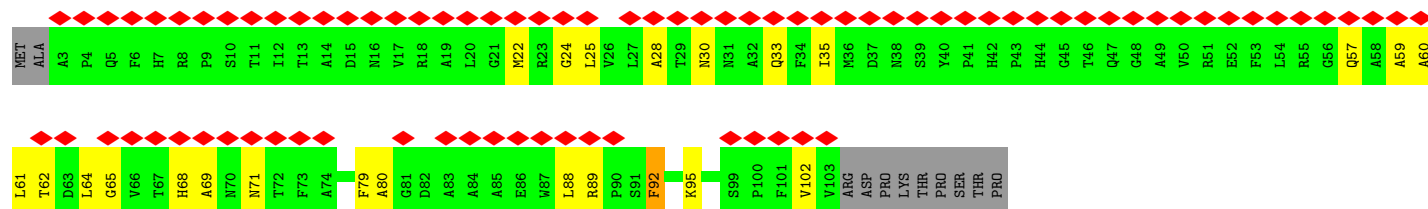


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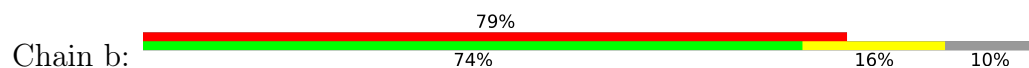


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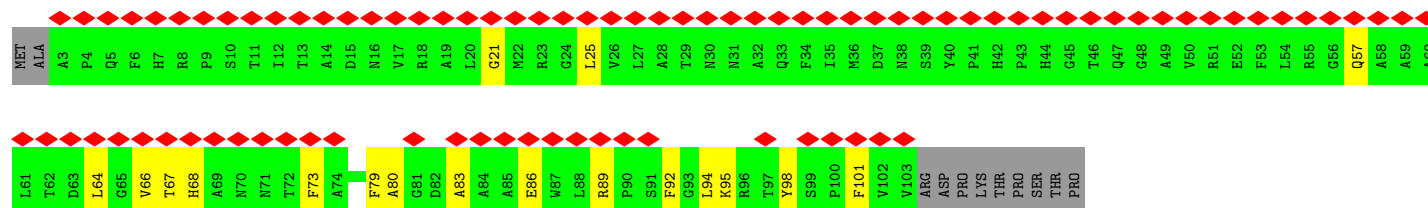
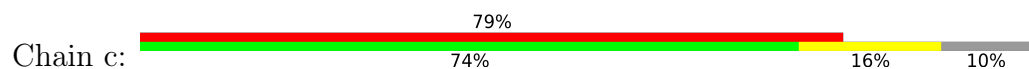




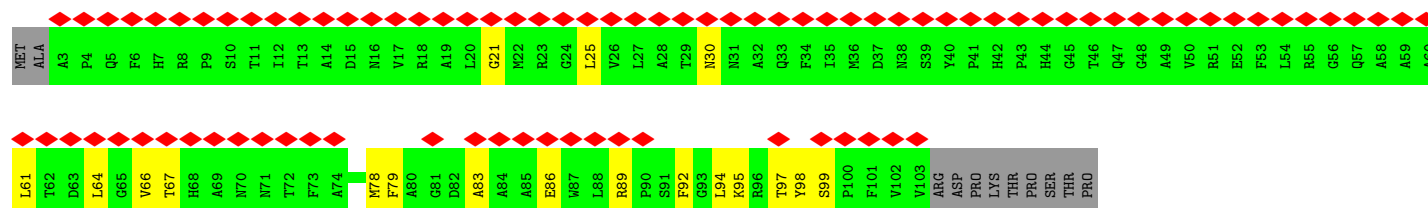
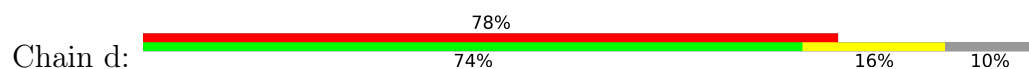
● Molecule 4: VP26



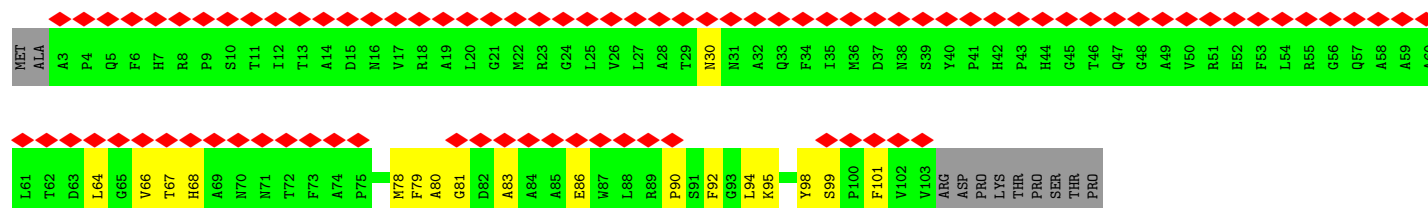
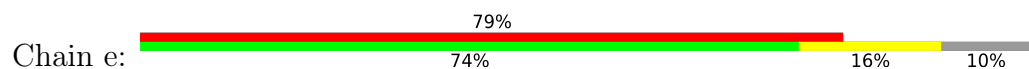
● Molecule 4: VP26



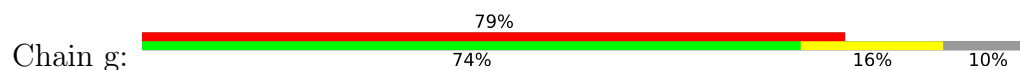
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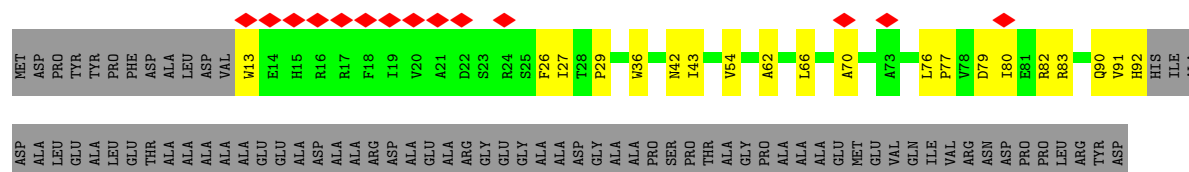


● Molecule 4: VP26



Chain f:





GLY	ARG	LEU	LEU	GLY	LEU	GLY	LEU	ALA	THR
PHE	ASN	TYR	LEU	ASP	ALA	VAL	ASN	LEU	ASN
ILE	THR	GLN	ALA	VAL	ALA	VAL	ALA	ARG	LEU
PRO	THR	ALA	ASN	PRO	LEU	PRO	LEU	LEU	PRO
GLN	THR	ASP	GLY	ARG	ASP	ASP	ALA	SER	LEU
TYR	PRO	THR	ASN	ASP	ASN	THR	VAL	LEU	ASP
LEU	VAL	PRO	VAL	THR	VAL	ILE	ARG	GLN	LEU
LEU	GLY	VAL	TYR	SER	ILE	THR	GLY	SER	LEU
SER	GLY	GLU	ALA	THR	GLY	THR	ASP	CYS	HIS
VAL	ILE	ILE	THR	ARG	VAL	VAL	ASP	GLY	MET
ALA	ASN	GLN	LEU	ASN	SER	LEU	SER	ARG	TYR
	ALA	LEU	ASP	PRO	GLY	ARG	THR	TYR	ALA
	HIS	PHE	ASN	ASP	ASN	ASP	ARG	VAL	ALA
	ASP	PRO	PRO	VAL	PRO	VAL	ASP	GLY	GLY
	ALA	LEU	LEU	VAL	GLN	ALA	TYR	ARG	VAL
	LEU	GLY	ALA	ALA	ALA	TYR	ARG	HIS	ALA
	GLY	ALA	GLY	HIS	LEU	TYR	THR	ALA	GLY
	ILE	ALA	MET	ARG	GLY	ARG	THR	THR	GLY
	GLN	LEU	LEU	ASP	ALA	ALA	ARG	SER	SER
	TYR	CYS	ILE	VAL	LEU	ALA	ASP	ALA	GLY
	GLU	LEU	ILE	VAL	ASP	ALA	ASP	PHE	GLY
	GLN	ASP	PRO	ASN	LYS	LEU	LYS	GLY	VAL
	GLY	ALA	GLY	ARG	LEU	PRO	PRO	CYS	VAL
	LEU	GLN	ALA	ALA	PRO	ALA	ALA	ALA	PHE
	GLY	ALA	VAL	ALA	LYS	VAL	VAL	GLY	GLY
	LEU	GLY	GLY	ALA	ALA	ALA	LEU	LEU	THR
	LEU	GLY	PRO	ALA	ALA	ALA	LEU	LEU	THR
	LEU	ARG	ALA	ALA	ALA	ALA	TYR	TYR	TRP
	LEU	PRO	GLY	PHE	PHE	PHE	LEU	LEU	ARG
	ALA	LEU	ALA	LEU	ALA	ALA	ALA	LEU	THR
	GLN	LEU	ILE	ALA	ILE	ALA	ALA	ILE	THR
	GLN	ALA	ALA	GLY	GLY	GLY	GLY	ARG	GLU
	GLY	ARG	ALA	ASN	TYR	TYR	THR	THR	THR
	LEU	VAL	VAL	LEU	GLY	PHE	GLU	HIS	ILE
	ALA	VAL	ASP	LEU	LEU	LEU	ASP	LEU	ALA
	ASN	ASP	SER	GLU	ALA	GLY	SER	PRO	PHE
	LYS	SER	SER	ASP	LEU	ASP	LEU	ASP	LEU
	ARG	GLY	GLY	GLN	ALA	GLN	ALA	ASP	LEU
	PHE	ALA	ILE	THR	ILE	THR	ARG	ARG	THR
	ALA	ARG	GLN	LEU	HIS	THR	ASP	THR	THR
	THR	GLN	SER	LEU	VAL	VAL	ARG	SER	ARG
	PHE	ALA	GLY	ARG	ALA	ALA	ALA	ALA	ALA
	ASN	LEU	ASN	THR	ALA	ILE	THR	VAL	VAL
	VAL	LEU	VAL	ALA	ASN	ALA	ALA	GLY	GLY
	GLY	VAL	ASN	THR	ALA	THR	ALA	ASP	ASP
	SER	ARG	ASN	ASN	THR	THR	THR	ASP	GLY
	THR	LEU	LEU	GLN	ALA	VAL	VAL	LEU	THR
	THR	GLU	GLY	VAL	CYS	GLY	VAL	LEU	MET
	TYR	LEU	LEU	LEU	VAL	VAL	VAL	ALA	SER
	PHE	LEU	ASN	ALA	LEU	VAL	ALA	ARG	LYS
	LEU	GLU	ASN	LEU	VAL	VAL	ARG	ALA	THR
	THR	ILE	TYR	THR	THR	THR	THR	PRO	PHE
	ASN	ASN	ASN	VAL	TYR	VAL	PRO	ALA	THR
	LEU	THR	PRO	ARG	ALA	ALA	PRO	ARG	THR

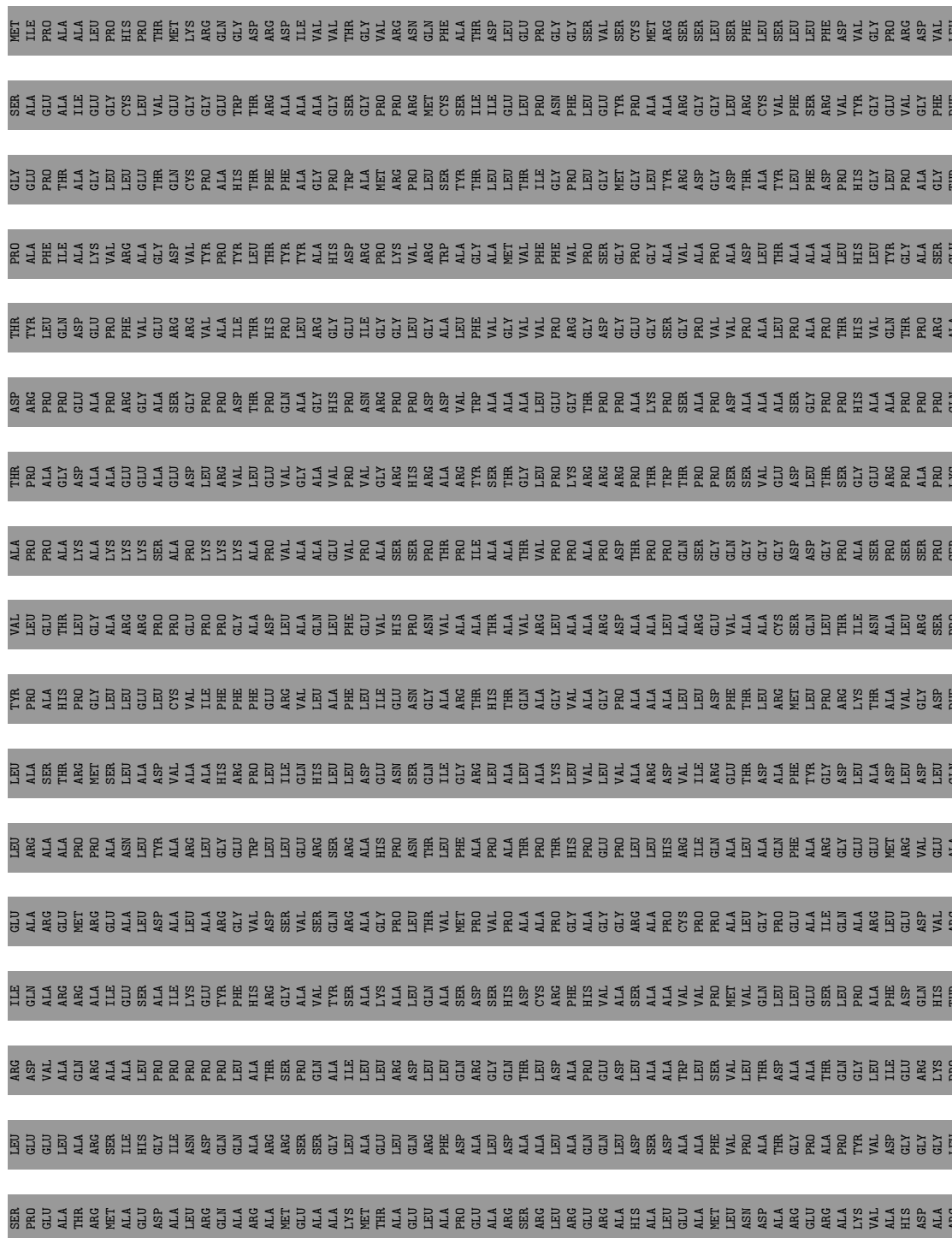
- Molecule 7: UL36

Chain t: 98%

LEU	ALA	PRO	PRO	VAL	ALA	THR	ASP	THR	PRO	GLY	SER	MET
ALA	SER	PRO	PRO	LEU	PRO	ALA	ARG	ARG	ALA	GLU	ALA	ILE
THR	HIS	ALA	THR	THR	GLY	ASP	PRO	GLN	ILE	THR	GLU	PRO
ARG	PRO	LYS	LEU	GLY	PRO	GLY	GLU	ASP	ALA	ILE	ALA	ALA
MET	GLY	ALA	ALA	ALA	ALA	ALA	ALA	GLU	LYS	GLY	GLU	PRO
SER	LEU	LYS	ALA	GLY	GLU	GLU	PRO	PHE	VAL	LEU	GLY	LEU
LEU	ALA	LYS	GLY	ARG	GLY	ALA	ARG	PHE	ARG	CYS	CYS	HIS
ALA	GLY	LYS	ARG	PRO	PRO	GLY	GLY	VAL	VAL	GLN	GLY	THR
ALA	LEU	LYS	GLY	LEU	PRO	LEU	PRO	VAL	TYR	PRO	GLY	ARG
HIS	ARG	LYS	VAL	VAL	ASP	ILE	ASP	ALA	PRO	ALA	GLU	GLN
ARG	PHE	LYS	VAL	VAL	THR	ALA	THR	THR	THR	LEU	THR	THR
PRO	PHE	ALA	ALA	ALA	LEU	ALA	PRO	HIS	THR	ARG	THR	ASP
LEU	GLY	PRO	GLY	VAL	GLY	GLY	ASN	ILE	ARG	PHE	ALA	ASP
ILE	ARG	VAL	LEU	ALA	GLY	ALA	GLN	PRO	TYR	PHE	ALA	ASP
GLN	LEU	ALA	ALA	GLN	ALA	ALA	GLY	ARG	TYR	ALA	ALA	ILE
HIS	LEU	ALA	ALA	GLY	GLU	GLY	HIS	GLY	ARG	ALA	ALA	VAL
LEU	LEU	ALA	LEU	LEU	VAL	PHE	PHE	GLY	GLU	GLY	GLY	VAL
LEU	ASP	VAL	GLY	GLY	VAL	VAL	VAL	ILE	ARG	ALA	GLY	GLY
ASN	GLY	ALA	ALA	HIS	SER	GLY	ARG	PRO	GLY	PRO	PRO	VAL
SER	ASN	PRO	PRO	PRO	SER	ASN	PRO	THR	VAL	PRO	ARG	ASN
GLN	GLY	ASN	PRO	HIS	PRO	ASN	ASP	GLY	VAL	LEU	MET	GLN
GLY	GLY	ALA	VAL	ALA	THR	ALA	ALA	ASP	TRP	ALA	CYS	PHE
ARG	THR	ILE	ALA	THR	ILE	THR	TRP	ALA	GLY	THR	ILE	THR
LEU	HIS	ALA	ALA	THR	SER	SER	ALA	ALA	ALA	LEU	ILE	ASP
ALA	THR	ALA	ALA	ALA	ALA	ALA	ALA	VAL	MET	LEU	ILE	LEU
LEU	GLN	VAL	VAL	VAL	THR	GLY	ALA	VAL	VAL	THR	LEU	GLU
ALA	ALA	VAL	VAL	ARG	VAL	LEU	LEU	VAL	PHE	ILE	PRO	PRO
LYS	GLY	PRO	LEU	LEU	PRO	PRO	GLY	PRO	GLY	GLY	ASN	GLY
LEU	VAL	ALA	ALA	ALA	PRO	ALA	GLY	VAL	VAL	PRO	PHE	GLY
VAL	ALA	ALA	ALA	ALA	ALA	ALA	THR	ARG	PRO	LEU	SER	SER
VAL	ALA	GLN	ALA	ALA	GLN	ALA	PRO	GLY	ALA	TYR	ALA	ARG
LEU	LEU	ARG	SER	ALA	SER	THR	SER	GLY	VAL	ARG	ARG	SER
ILE	LEU	GLY	GLY	GLY	ASP	GLY	PRO	GLY	ALA	ASP	GLY	GLY
ARG	ASP	GLY	GLY	VAL	VAL	VAL	PRO	GLY	PRO	GLY	LEU	LEU
THR	THR	ALA	ALA	ALA	SER	SER	ALA	GLY	ASP	THR	ARG	PHE
ASP	LEU	GLY	GLY	ALA	GLY	VAL	ALA	ALA	LEU	ALA	CYS	LEU
ALA	ARG	ASP	CYS	CYS	GLY	GLY	ALA	LEU	THR	VAL	VAL	SER
PHE	THR	ASN	ASP	ASP	ASP	ASP	SER	PRO	ALA	LEU	PHE	LEU
GLY	LEU	GLN	GLY	GLY	GLY	GLY	GLY	GLY	ALA	PHE	SER	LEU
GLY	PRO	GLY	THR	THR	THR	THR	PRO	GLY	PRO	ASP	ARG	PHE
LEU	LYS	ALA	ILE	ILE	ALA	GLY	HIS	HIS	HIS	PRO	VAL	VAL
ALA	THR	ASN	ASN	ASN	PRO	GLY	ALA	VAL	LEU	GLY	GLY	PRO
ASP	ALA	PRO	SER	ARG	THR	ARG	ALA	THR	LEU	TYR	GLY	ARG
ASP	GLY	VAL	SER	LEU	LEU	GLN	PRO	THR	GLY	GLY	VAL	ARG
LEU	THR	PRO	SER	PRO	PRO	ALA	PRO	PRO	GLY	ALA	GLY	VAL
ILE	PHE	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR









LEU	PRO	GLN	THR	PRO	ALA	GLY	ALA	THR	ALA	THR	PRO	GLY	SER	ALA	SER	ALA	GLU	LEU	GLN
PRO	VAL	PRO	HIS	THR	ARG	ASP	ALA	PRO	VAL	PRO	ALA	SER	GLU	ALA	ARG	GLU	PRO	ALA	ALA
GLN	ALA	PRO	ILE	ARG	ALA	ARG	ALA	PRO	ALA	PRO	ALA	GLY	GLU	PRO	ASP	PRO	ALA	ALA	ALA
ASN	PRO	LEU	SER	ILE	ARG	GLY	PRO	ALA	SER	ALA	LEU	GLU	VAL	ASP	CYS	HIS	PRO	ALA	VAL
A3083	VAL	PRO	ASP	ALA	ARG	ARG	PRO	ALA	ALA	ASP	PRO	ARG	PRO	ASP	ASP	VAL	SER	VAL	SER
S3076	VAL	THR	GLU	SER	VAL	THR	GLY	VAL	PRO	THR	PRO	ALA	PHE	ALA	GLY	TYR	LEU	VAL	GLY
T3077	ARG	THR	SER	PRO	VAL	THR	LEU	VAL	ASP	PRO	ALA	ALA	ARG	ALA	ALA	PRO	ARG	ARG	ARG
G3078	ARG	LEU	ASP	GLN	GLN	ALA	ALA	GLN	ASP	PRO	THR	PRO	ALA	ILE	LEU	SER	THR	THR	MET
L3082	TYR	THR	ALA	PRO	PRO	GLY	PRO	PRO	PRO	GLN	ASP	ALA	ILE	VAL	VAL	ARG	GLY	GLY	CYS
A3083	VAL	ASP	SER	PRO	PRO	SER	THR	THR	THR	ALA	TYR	VAL	GLY	VAL	VAL	PRO	GLN	LEU	PRO
V3084	THR	SER	LEU	LEU	THR	PRO	THR	PHE	VAL	VAL	SER	GLN	GLY	VAL	VAL	GLY	HIS	PRO	PRO
L3085	ARG	SER	ARG	GLN	ALA	THR	ALA	GLY	GLY	SER	THR	PRO	PRO	ILE	ASP	PRO	ALA	ALA	SER
A3088	ASP	ASP	PHE	PRO	PRO	PRO	VAL	VAL	SER	ALA	ILE	LEU	GLY	THR	THR	VAL	HIS	THR	THR
G3089	THR	SER	ALA	PRO	PRO	PRO	LEU	LEU	ALA	VAL	GLY	LEU	GLU	TRP	VAL	VAL	ARG	CYS	THR
R3090	THR	THR	ALA	THR	GLN	PRO	GLY	GLY	ARG	ALA	PRO	THR	THR	GLU	SER	PRO	THR	PRO	THR
R3091	THR	THR	PRO	PRO	PRO	PRO	PRO	VAL	ARG	VAL	ALA	ALA	ALA	PRO	ILE	ALA	ALA	ALA	PRO
I3092	ASN	THR	LEU	LEU	VAL	LEU	VAL	PRO	PRO	THR	THR	THR	GLY	GLU	GLU	ASP	ALA	ASP	ASP
Q3093	THR	THR	PRO	PRO	ALA	THR	ALA	ARG	ARG	ALA	ALA	THR	HIS	PRO	PRO	THR	VAL	THR	TYR
Q3094	THR	THR	PRO	PRO	GLN	PRO	PHE	ALA	ALA	PHE	ALA	GLY	VAL	TRP	VAL	VAL	ALA	ALA	GLY
Q3095	ASN	THR	LEU	LEU	PRO	LEU	PRO	ARG	PRO	ARG	THR	VAL	GLN	PRO	GLY	ASP	LEU	SER	SER
R3098	VAL	VAL	HIS	LEU	LEU	VAL	PRO	THR	ARG	ALA	PRO	PRO	ARG	PRO	LEU	LEU	VAL	VAL	THR
T3099	SER	SER	LEU	GLN	ALA	SER	LEU	ARG	ALA	ARG	SER	PRO	PRO	VAL	VAL	VAL	VAL	VAL	PHE
R3100	ALA	VAL	PRO	PRO	GLY	LEU	GLY	LYS	VAL	LEU	VAL	LEU	HIS	ASP	LEU	ASP	LEU	ASP	THR
F3101	THR	THR	PRO	PRO	THR	SER	ALA	SER	PRO	MET	ALA	ASP	THR	PHE	THR	ALA	ALA	ALA	GLY
A3102	ALA	ALA	ALA	LEU	VAL	ALA	PHE	ARG	VAL	TRP	ALA	GLY	ASP	VAL	VAL	ASP	ALA	ALA	ALA
F3104	ASP	SER	GLU	PRO	VAL	SER	VAL	VAL	ALA	ALA	GLN	ALA	GLU	GLY	GLY	VAL	VAL	VAL	LEU
N3108	TRP	ALA	PRO	GLN	PRO	LEU	PRO	ARG	GLN	PRO	GLN	TRP	ALA	SER	ASN	LEU	LEU	ALA	ALA
S3113	ALA	SER	GLY	SER	PRO	ASN	GLY	ALA	ARG	ASN	ILE	GLY	GLY	GLU	PRO	LEU	GLY	ARG	ARG
L3114	LEU	LEU	LEU	LEU	PRO	LEU	PRO	SER	ALA	GLY	HIS	GLY	SER	THR	ALA	ALA	ILE	GLY	ALA
H3115	ALA	ALA	ALA	ALA	VAL	PRO	VAL	ALA	ALA	ARG	VAL	LEU	ALA	GLU	ASN	PRO	GLY	GLY	GLY
H3116	ALA	SER	GLN	PRO	ALA	SER	PRO	PRO	ALA	PRO	GLY	GLU	PRO	GLU	ALA	VAL	VAL	VAL	SER
V3117	ALA	ASP	ALA	ALA	ILE	PRO	ILE	PRO	PRO	VAL	VAL	LEU	THR	LEU	VAL	VAL	VAL	VAL	GLY
F3118	ASP	VAL	VAL	VAL	ARG	ARG	ARG	THR	GLY	VAL	VAL	ALA	THR	ALA	PRO	PRO	VAL	VAL	GLY
M3119	HIS	ASP	HIS	LEU	PRO	PRO	PRO	GLY	PRO	GLY	ALA	ALA	ALA	PHE	ALA	ALA	ALA	ALA	THR
L3120	GLN	ALA	GLN	ALA	PRO	PRO	PRO	ARG	ARG	ARG	ALA	ASP	ARG	VAL	GLN	GLN	ARG	ARG	GLY
L3121	SER	PRO	SER	SER	PRO	ALA	PRO	PRO	ALA	ASP	ASP	ASP	PRO	THR	ALA	ASN	ASN	GLY	THR
GLY	PRO	PRO	HIS	PRO	PRO	HIS	SER	PRO	GLY	ASP	ALA	GLY	ASP	ALA	PRO	THR	THR	ALA	ALA
	THR	THR	THR	THR	ALA	ALA	ALA	LEU	GLY	LEU	PRO	GLY	GLY	GLY	GLY	GLY	THR	GLY	GLY
	GLN	GLN	GLN	GLN	VAL	VAL	VAL	VAL	VAL	VAL	PRO	THR	ALA	VAL	VAL	VAL	VAL	VAL	VAL
	LEU	LEU	LEU	LEU	PRO	SER	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56901	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	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	16.874	Depositor
Minimum map value	-9.664	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.739	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	1656.0, 1656.0, 1656.0	wwPDB
Map dimensions	1200, 1200, 1200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.38, 1.38, 1.38	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	1	0.36	0/2641	0.63	3/3594 (0.1%)
1	Q	0.28	0/2641	0.59	4/3594 (0.1%)
1	T	0.28	0/2647	0.60	3/3601 (0.1%)
1	W	0.29	0/2629	0.65	1/3579 (0.0%)
1	w	0.25	0/2647	0.59	3/3601 (0.1%)
2	2	0.51	0/2374	0.71	2/3247 (0.1%)
2	3	0.47	0/2134	0.69	1/2921 (0.0%)
2	R	0.30	0/2134	0.61	1/2921 (0.0%)
2	S	0.30	0/2377	0.60	2/3251 (0.1%)
2	U	0.34	0/2134	0.66	1/2921 (0.0%)
2	V	0.32	0/2377	0.60	2/3251 (0.1%)
2	X	0.39	0/2134	0.68	0/2921
2	Y	0.39	0/2377	0.64	2/3251 (0.1%)
2	x	0.31	0/2134	0.62	1/2921 (0.0%)
2	y	0.31	0/2368	0.59	2/3240 (0.1%)
3	A	0.42	0/9879	0.61	0/13481
3	B	0.69	5/10603 (0.0%)	0.74	0/14473
3	C	0.69	3/10610 (0.0%)	0.77	5/14483 (0.0%)
3	D	0.69	3/10672 (0.0%)	0.79	4/14569 (0.0%)
3	E	0.71	2/10663 (0.0%)	0.81	7/14556 (0.0%)
3	F	0.70	1/10649 (0.0%)	0.79	3/14539 (0.0%)
3	G	0.40	1/10514 (0.0%)	0.71	32/14356 (0.2%)
3	H	0.52	0/10674	0.70	2/14570 (0.0%)
3	I	0.55	1/10676 (0.0%)	0.72	6/14572 (0.0%)
3	J	0.56	1/10668 (0.0%)	0.72	1/14567 (0.0%)
3	K	0.55	1/10674 (0.0%)	0.72	4/14574 (0.0%)
3	L	0.55	2/10680 (0.0%)	0.69	0/14577
3	M	0.50	1/10709 (0.0%)	0.68	6/14619 (0.0%)
3	N	0.52	2/10654 (0.0%)	0.69	1/14544 (0.0%)
3	O	0.51	2/10676 (0.0%)	0.69	0/14577
3	P	0.57	2/10667 (0.0%)	0.71	0/14565
4	b	0.25	0/795	0.46	0/1084
4	c	0.25	0/795	0.46	0/1084
4	d	0.25	0/795	0.46	0/1084

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	e	0.25	0/795	0.46	0/1084
4	f	0.25	0/795	0.46	0/1084
4	g	0.25	0/795	0.46	0/1084
4	h	0.21	0/795	0.55	0/1084
4	i	0.22	0/795	0.55	0/1084
4	j	0.23	0/795	0.58	0/1084
4	k	0.21	0/795	0.55	0/1084
4	l	0.24	0/795	0.58	0/1084
4	m	0.23	0/795	0.56	0/1084
4	n	0.20	0/795	0.53	0/1084
4	o	0.20	0/795	0.54	0/1084
4	p	0.22	0/795	0.56	0/1084
5	q	0.26	0/4350	0.58	3/5934 (0.1%)
6	r	0.20	0/786	0.51	0/1074
6	s	0.23	0/667	0.55	0/908
7	t	0.17	0/385	0.53	0/514
7	u	0.19	0/385	0.54	0/514
All	All	0.53	27/223914 (0.0%)	0.70	102/305640 (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
1	1	0	2
1	Q	0	3
1	T	0	2
1	W	0	2
1	w	0	2
2	2	0	1
2	S	0	1
2	U	0	1
2	V	0	1
2	X	0	1
2	Y	0	1
2	y	0	1
3	A	0	1
3	B	0	3
3	C	0	3
3	D	0	2
3	E	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	4
3	G	0	1
3	H	0	1
3	I	0	4
3	J	0	3
3	K	0	3
3	L	0	2
3	M	0	2
3	N	0	5
3	O	0	1
3	P	0	2
4	h	0	1
4	p	0	1
5	q	0	2
All	All	0	62

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	485	ASN	C-N	-17.32	0.93	1.33
3	C	485	ASN	C-N	-13.26	0.97	1.34
3	P	485	ASN	C-N	-13.08	0.98	1.34
3	L	485	ASN	C-N	-12.99	0.98	1.34
3	F	1116	ARG	C-N	-11.58	1.11	1.33

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	43	ARG	N-CA-C	-17.85	86.97	110.53
1	W	199	ASP	N-CA-C	14.39	126.47	111.07
3	N	339	MET	N-CA-C	-9.66	100.75	111.28
3	E	1116	ARG	N-CA-C	-9.35	98.47	110.53
3	I	83	LYS	CA-C-N	-8.92	109.22	121.61

There are no chirality outliers.

5 of 62 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Q	40	PRO	Peptide
1	Q	7	PRO	Peptide
1	Q	80	ARG	Peptide

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Mol	Chain	Res	Type	Group
2	S	241	LEU	Peptide
1	T	40	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2589	0	2487	79	0
1	Q	2589	0	2487	59	0
1	T	2595	0	2497	120	0
1	W	2577	0	2461	145	0
1	w	2595	0	2496	79	0
2	2	2334	0	2405	55	0
2	3	2102	0	2108	65	0
2	R	2102	0	2108	52	0
2	S	2337	0	2414	82	0
2	U	2102	0	2108	38	0
2	V	2337	0	2417	22	0
2	X	2102	0	2108	70	0
2	Y	2337	0	2415	50	0
2	x	2102	0	2108	35	0
2	y	2328	0	2396	34	0
3	A	9646	0	9463	422	0
3	B	10349	0	10126	550	0
3	C	10355	0	10128	567	0
3	D	10413	0	10203	687	0
3	E	10405	0	10194	549	0
3	F	10392	0	10170	553	0
3	G	10261	0	10036	607	0
3	H	10416	0	10203	609	0
3	I	10418	0	10211	557	0
3	J	10408	0	10182	478	0
3	K	10414	0	10193	400	0
3	L	10422	0	10215	470	0
3	M	10449	0	10232	601	0
3	N	10397	0	10187	481	0
3	O	10417	0	10204	473	0
3	P	10407	0	10187	404	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	b	773	0	748	43	0
4	c	773	0	748	40	0
4	d	773	0	748	38	0
4	e	773	0	748	41	0
4	f	773	0	748	14	0
4	g	773	0	748	21	0
4	h	773	0	748	45	0
4	i	773	0	748	49	0
4	j	773	0	748	46	0
4	k	773	0	748	39	0
4	l	773	0	748	41	0
4	m	773	0	748	37	0
4	n	773	0	748	38	0
4	o	773	0	748	54	0
4	p	773	0	748	22	0
5	q	4241	0	4188	226	0
6	r	764	0	740	92	0
6	s	651	0	643	38	0
7	t	383	0	418	13	0
7	u	383	0	418	27	0
All	All	218714	0	214776	8501	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 20.

The worst 5 of 8501 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)
2:X:284:GLN:HG2	3:H:1166:PHE:CZ	1.16	1.65
1:T:170:LEU:HD11	3:I:1262:HIS:CB	1.15	1.61
3:H:339:MET:HE2	3:C:17:MET:CE	1.14	1.60
2:S:300:PHE:CE2	3:A:111:PRO:CA	1.80	1.59
2:S:300:PHE:HE2	3:A:111:PRO:CA	0.93	1.58

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	1
3	F	1
3	L	1
3	P	1

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Mol	Chain	Number of breaks
3	C	1
3	B	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	1312:LYS	C	1313:ARG	N	1.16
1	F	1116:ARG	C	1117:ASN	N	1.11
1	L	485:ASN	C	486:PRO	N	0.98
1	P	485:ASN	C	486:PRO	N	0.98
1	C	485:ASN	C	486:PRO	N	0.97

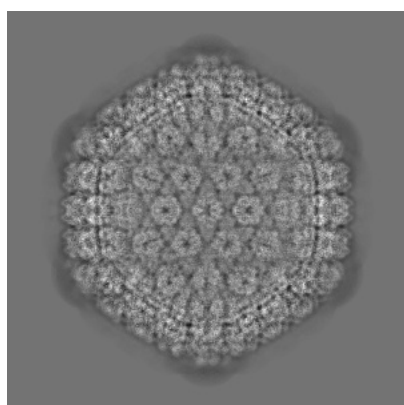
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6976. These allow visual inspection of the internal detail of the map and identification of artifacts.

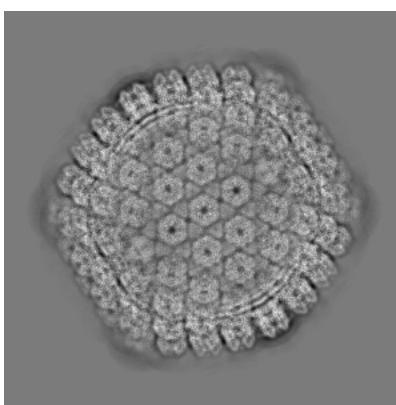
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

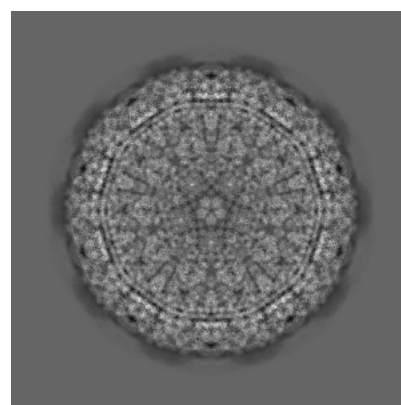
6.1.1 Primary map



X



Y



Z

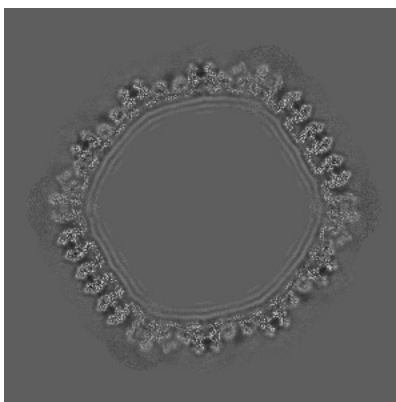
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

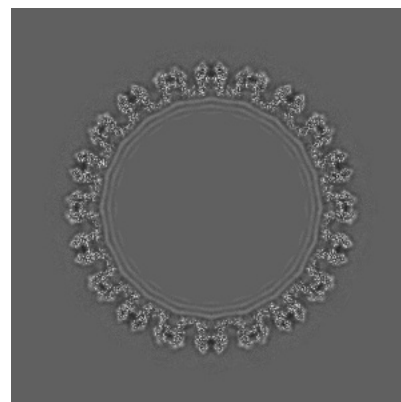
6.2.1 Primary map



X Index: 600



Y Index: 600

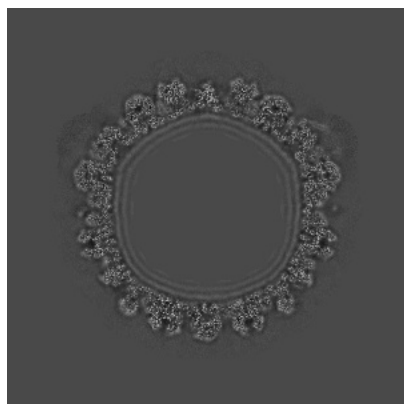


Z Index: 600

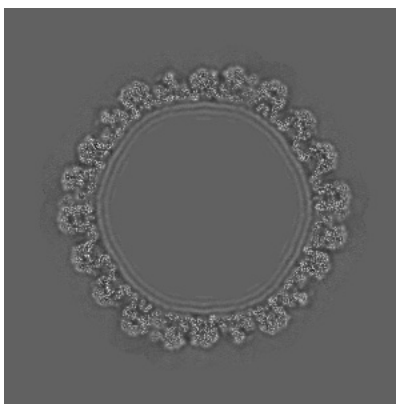
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

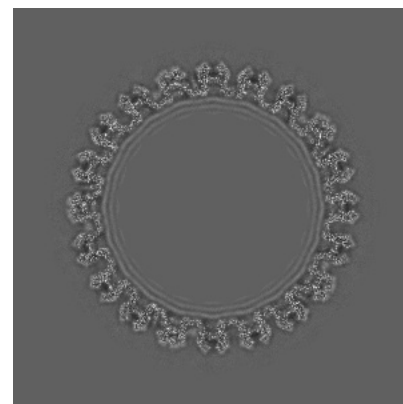
6.3.1 Primary map



X Index: 775



Y Index: 502

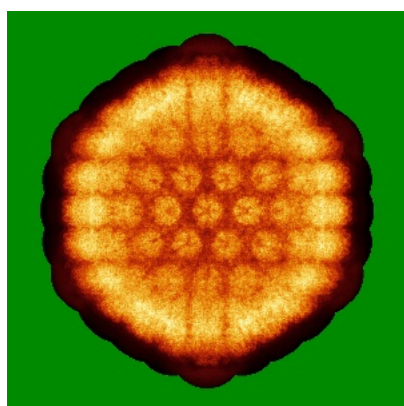


Z Index: 595

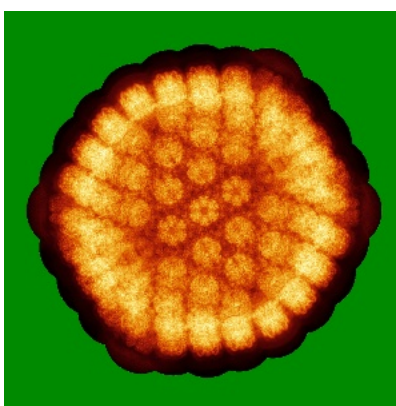
The images above show the largest variance slices of the map in three orthogonal directions.

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

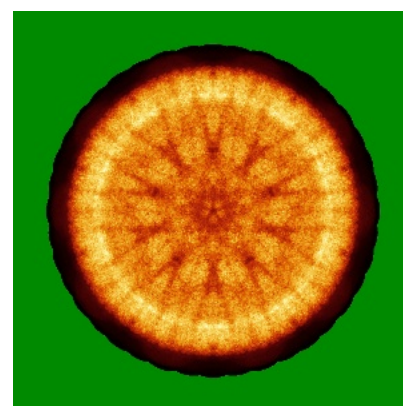
6.4.1 Primary map



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

This section was not generated.

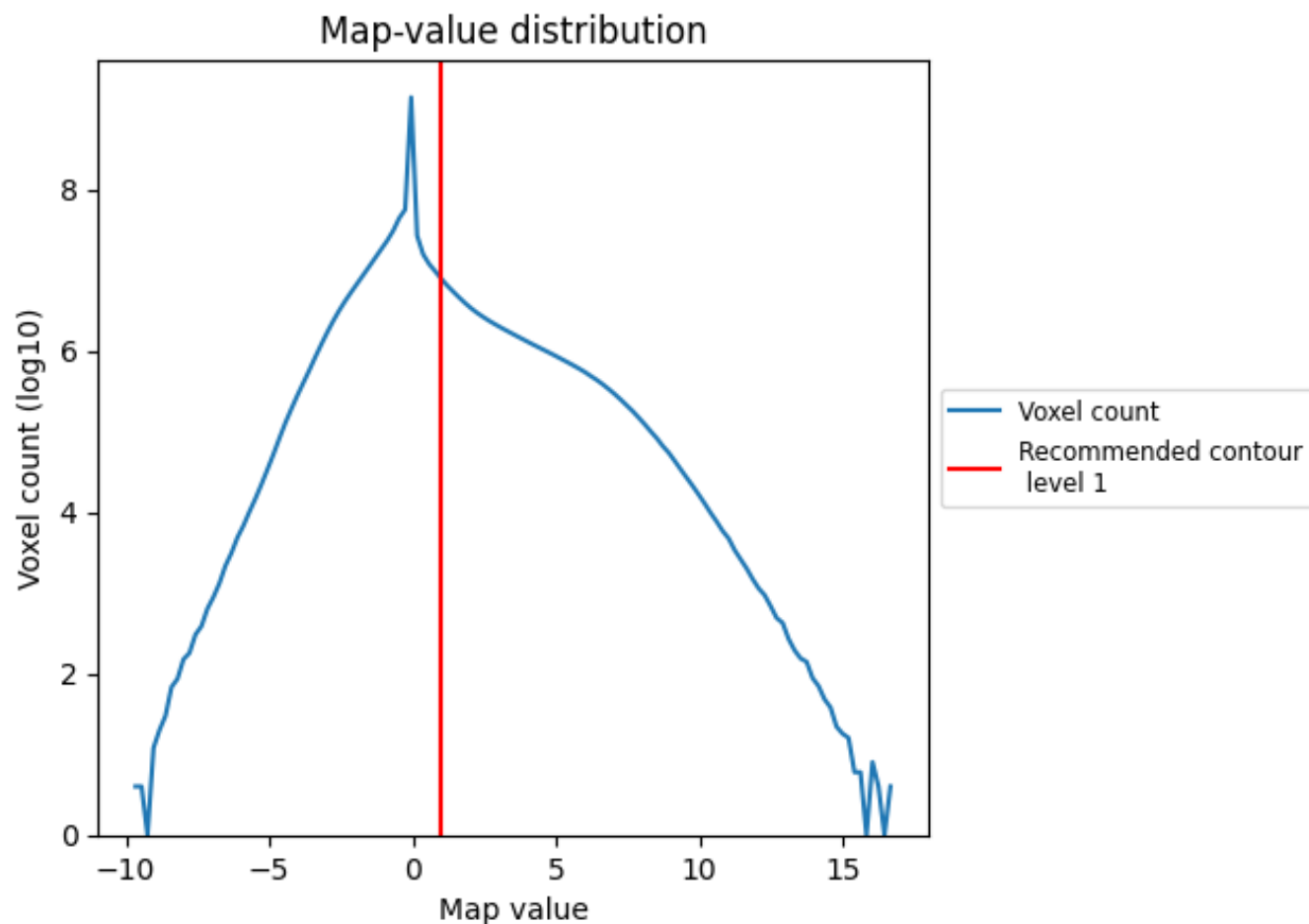
6.6 Mask visualisation

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

7 Map analysis [i](#)

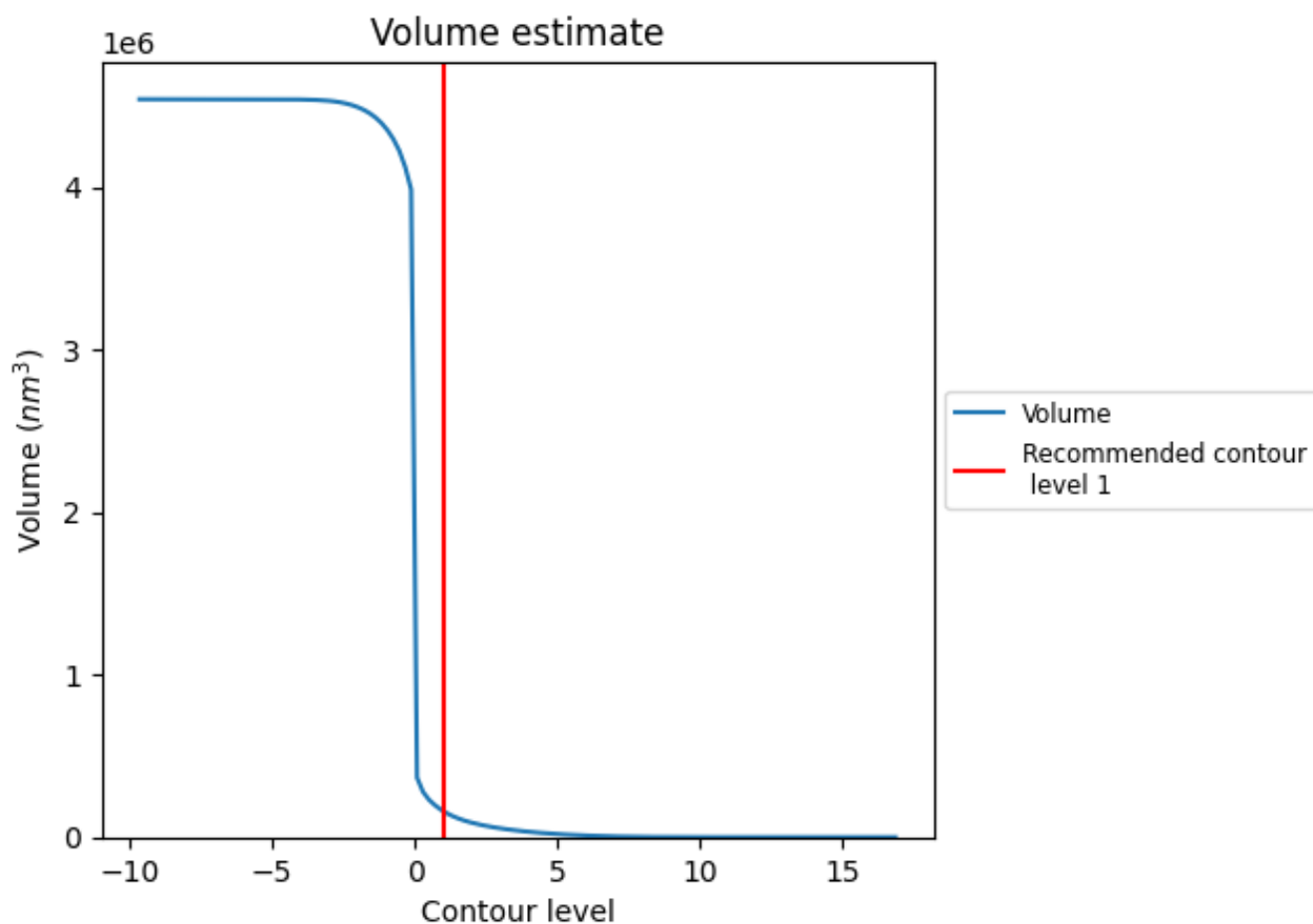
This section contains the results of statistical analysis of the map.

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.

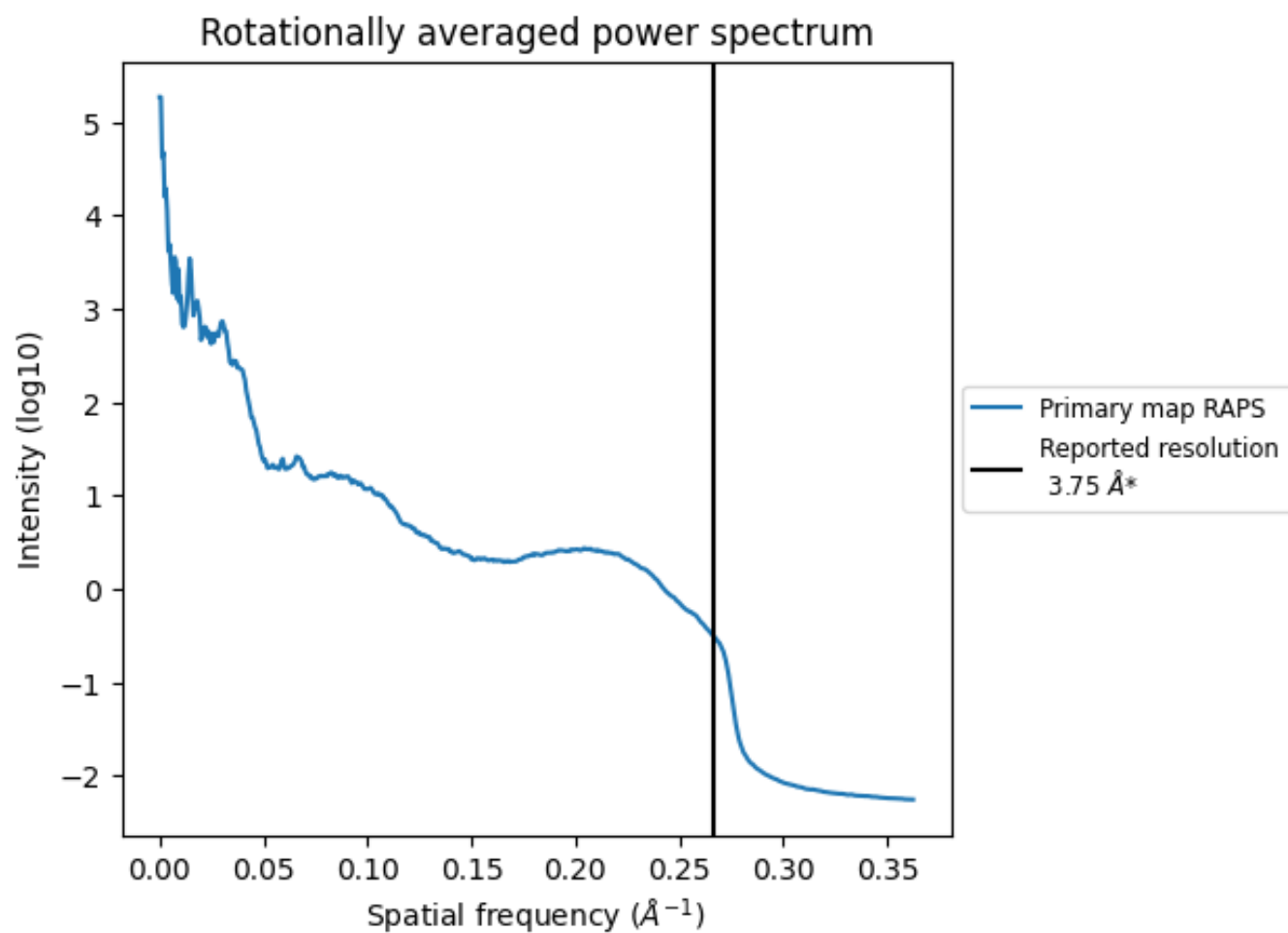
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 160951 nm^3 ; this corresponds to an approximate mass of 145391 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 0.267 Å⁻¹

8 Fourier-Shell correlation

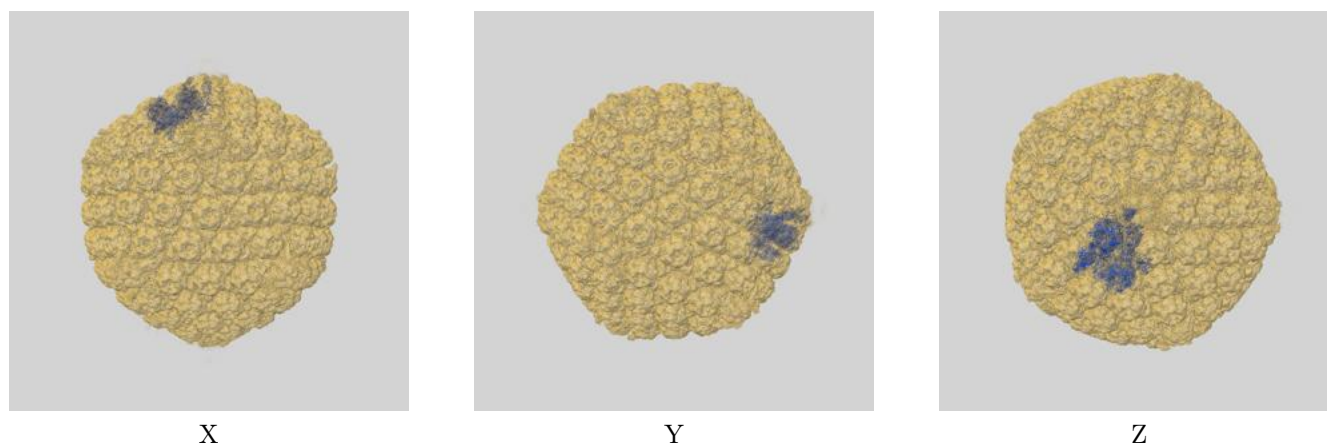
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

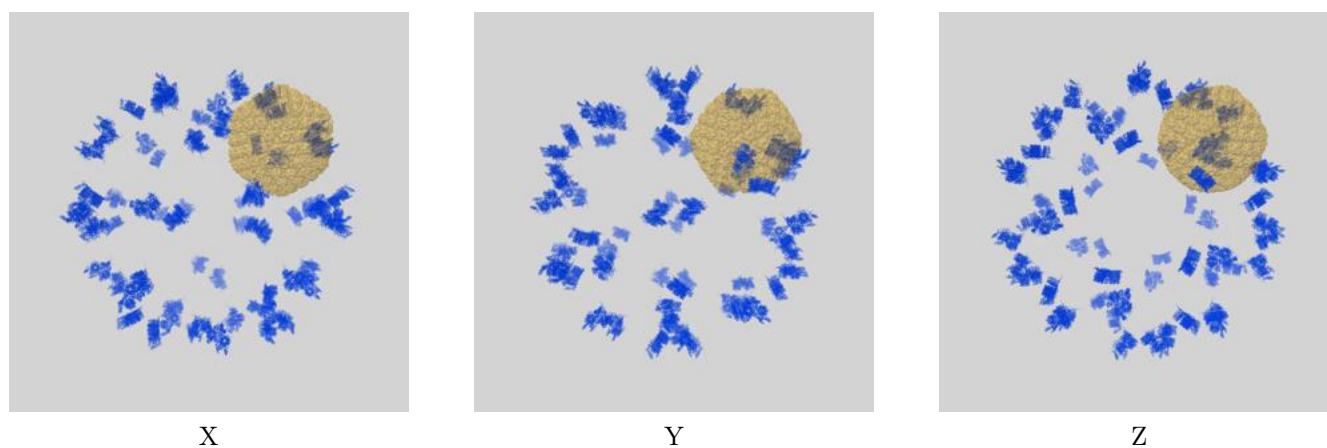
This section contains information regarding the fit between EMDB map EMD-6976 and PDB model 5ZZ8. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

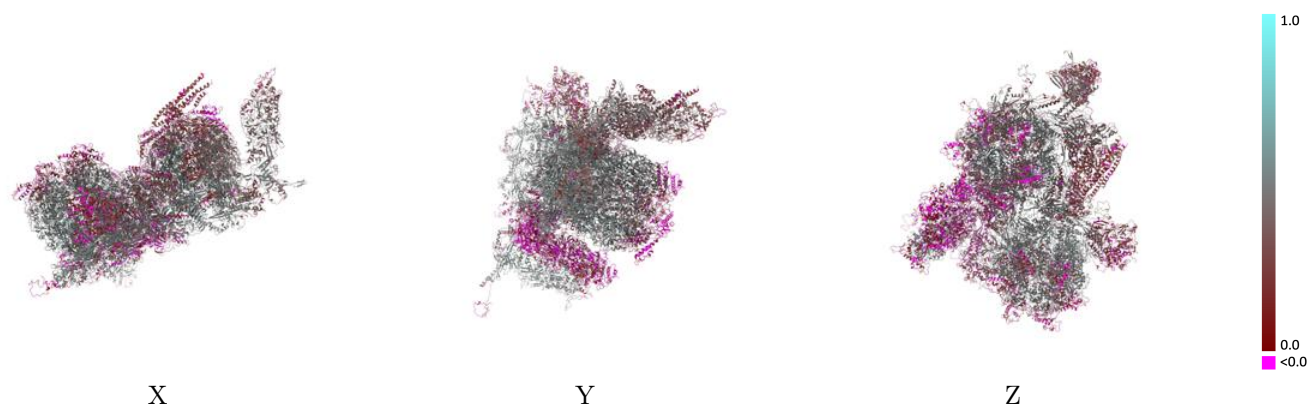


9.1.2 Map-model assembly overlay [i](#)



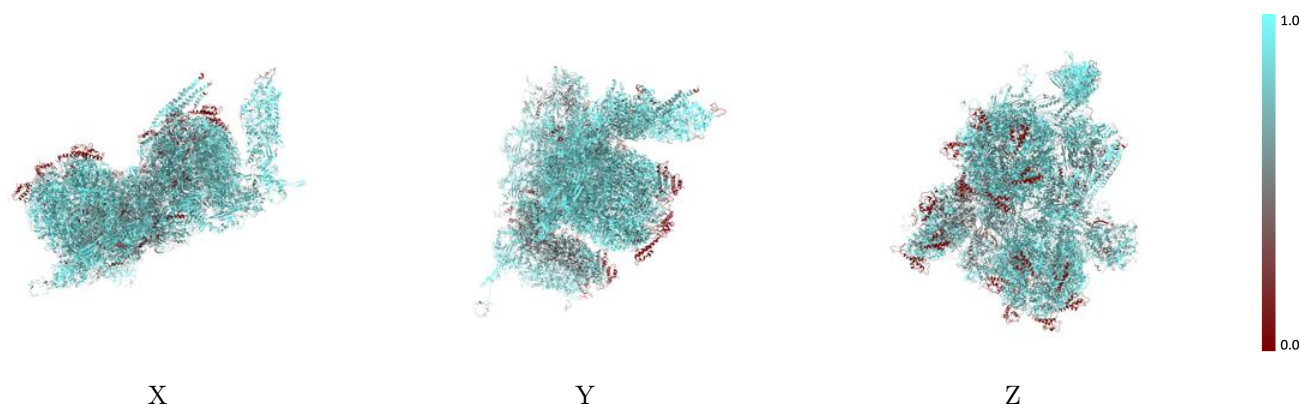
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



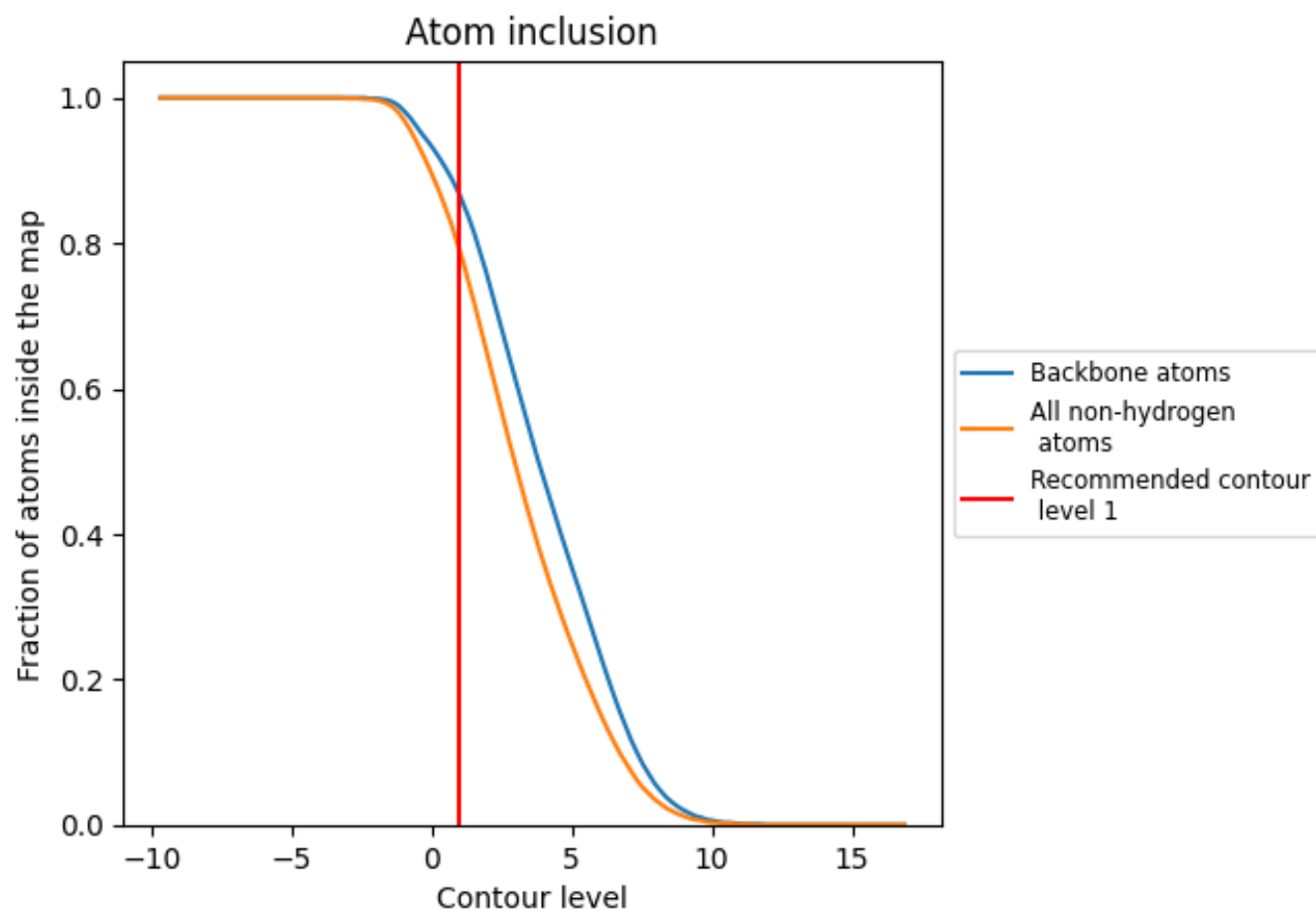
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7910	 0.3500
1	 0.6180	 0.1710
2	 0.7910	 0.3110
3	 0.8980	 0.4270
A	 0.8460	 0.3780
B	 0.8810	 0.4450
C	 0.9040	 0.4570
D	 0.8840	 0.4460
E	 0.8840	 0.4510
F	 0.8990	 0.4480
G	 0.8300	 0.3650
H	 0.8950	 0.4480
I	 0.8940	 0.4440
J	 0.8920	 0.4470
K	 0.8890	 0.4450
L	 0.8840	 0.4400
M	 0.9030	 0.4530
N	 0.6140	 0.0620
O	 0.6470	 0.0930
P	 0.8940	 0.4520
Q	 0.6400	 0.2530
R	 0.8020	 0.3460
S	 0.8050	 0.3830
T	 0.6450	 0.2260
U	 0.7140	 0.1450
V	 0.6880	 0.1630
W	 0.6000	 0.2500
X	 0.8970	 0.4290
Y	 0.8290	 0.3740
b	 0.1180	 0.0060
c	 0.1340	 -0.0140
d	 0.1380	 -0.0000
e	 0.1310	 -0.0240
f	 0.1310	 -0.0100
g	 0.1200	 0.0070



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Chain	Atom inclusion	Q-score
h	 0.1920	 0.0870
i	 0.2090	 0.0920
j	 0.2250	 0.1070
k	 0.2090	 0.0860
l	 0.1940	 0.1280
m	 0.2200	 0.1180
n	 0.1430	 -0.0060
o	 0.1570	 0.0230
p	 0.1790	 0.1130
q	 0.6840	 0.2560
r	 0.6540	 0.1910
s	 0.6770	 0.2030
t	 0.7300	 0.2140
u	 0.8600	 0.2120
w	 0.6040	 0.1840
x	 0.6980	 0.1760
y	 0.7180	 0.2490