



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2024 – 01:23 PM EST

PDB ID : 3IYL
EMDB ID : EMD-5160
Title : Atomic CryoEM Structure of a Nonenveloped Virus Suggests How Membrane Penetration Protein is Primed for Cell Entry
Authors : Zhang, X.; Jin, L.; Fang, Q.; Hui, W.; Zhou, Z.H.
Deposited on : 2010-02-02
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

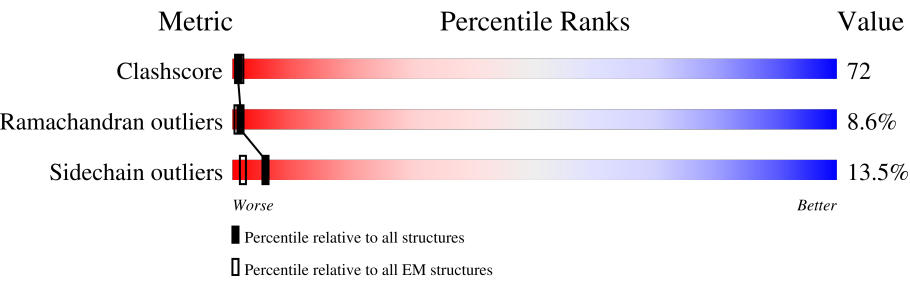
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



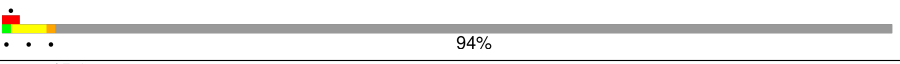
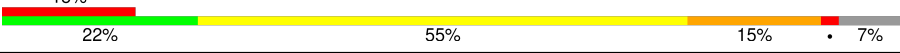
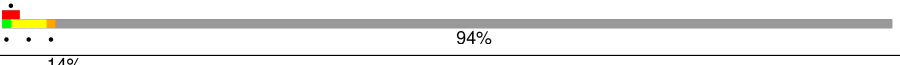
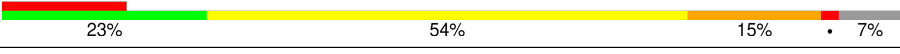
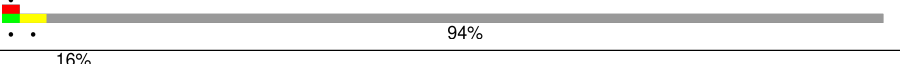
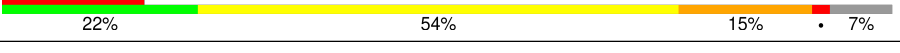
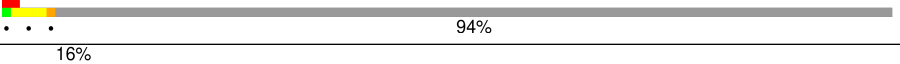
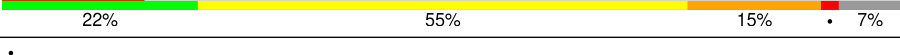
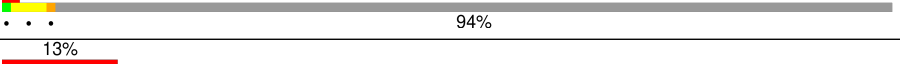
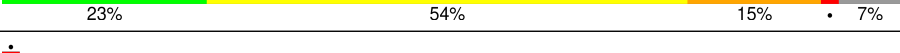
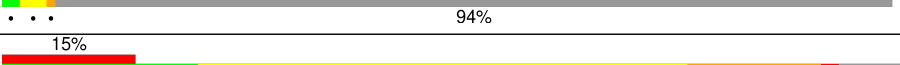
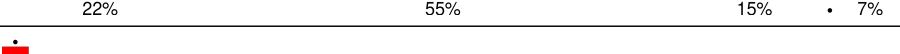


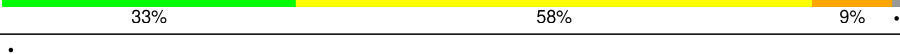
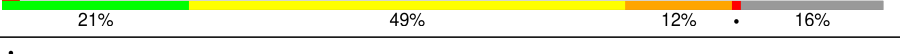
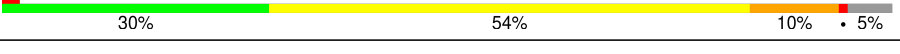
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	648	<div><div></div><div>14%</div><div>27%</div><div>51%</div><div>14%</div><div>7%</div><div>94%</div></div>
1	B	648	<div><div></div><div>13%</div><div>22%</div><div>55%</div><div>14%</div><div>7%</div><div>94%</div></div>
1	C	648	<div><div></div><div>14%</div><div>22%</div><div>54%</div><div>15%</div><div>7%</div><div>94%</div></div>
1	D	648	<div><div></div><div>14%</div><div>22%</div><div>55%</div><div>15%</div><div>7%</div><div>94%</div></div>
1	E	648	<div><div></div><div>14%</div><div>22%</div><div>55%</div><div>15%</div><div>7%</div><div>94%</div></div>
1	F	648	<div><div></div><div>14%</div><div>22%</div><div>55%</div><div>15%</div><div>7%</div><div>94%</div></div>
1	G	648	<div><div></div><div>14%</div><div>22%</div><div>55%</div><div>15%</div><div>7%</div><div>94%</div></div>
1	H	648	<div><div></div><div>14%</div><div>22%</div><div>55%</div><div>15%</div><div>7%</div><div>94%</div></div>

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Mol	Chain	Length	Quality of chain
1	I	648	
1	J	648	
1	K	648	
1	L	648	
1	M	648	
1	N	648	
1	O	648	
1	P	648	
1	Q	648	
1	R	648	
1	S	648	
1	T	648	
2	U	412	
2	V	412	
3	W	1299	
4	X	1214	
4	Y	1214	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MYR	A	649	-	-	X	-
5	MYR	C	649	-	-	X	-
5	MYR	E	649	-	-	X	-
5	MYR	G	649	-	-	X	-
5	MYR	I	649	-	-	X	-
5	MYR	K	649	-	-	X	-
5	MYR	M	649	-	-	X	-
5	MYR	O	649	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MYR	Q	649	-	-	X	-
5	MYR	S	649	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 80985 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 Outer capsid VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
1	B	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	C	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
1	D	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	E	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
1	F	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	G	41	Total	C	N	O	S	0	0
			284	174	46	63	1		
1	H	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	I	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
1	J	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	K	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
1	L	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	M	41	Total	C	N	O	S	0	0
			284	174	46	63	1		
1	N	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	O	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
1	P	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	Q	41	Total	C	N	O	S	0	0
			291	177	48	65	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	S	41	Total	C	N	O	S	0	0
			284	174	46	63	1		
1	T	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		

- Molecule 2 is a protein called Core protein VP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	411	Total	C	N	O	S	0	0
			3138	2008	544	571	15		
2	V	411	Total	C	N	O	S	0	0
			3138	2008	544	571	15		

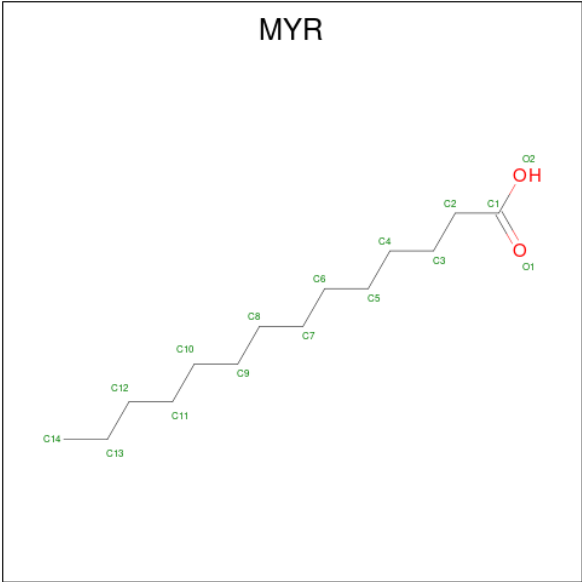
- Molecule 3 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	1284	Total	C	N	O	S	0	0
			9882	6335	1681	1839	27		

- Molecule 4 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	1018	Total	C	N	O	S	0	0
			7873	5033	1347	1447	46		
4	Y	1154	Total	C	N	O	S	0	0
			8835	5604	1525	1656	50		

- Molecule 5 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).

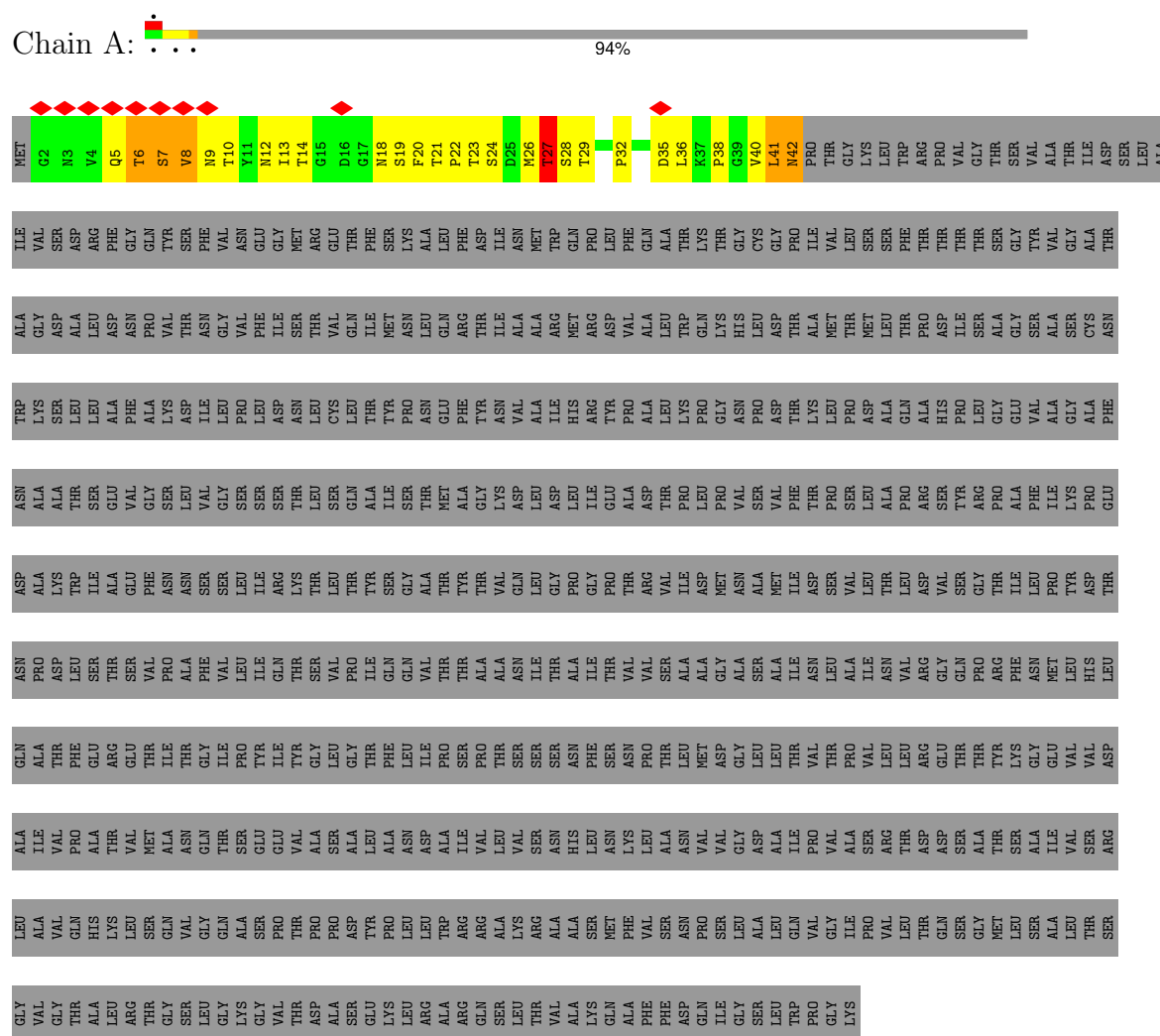


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			15	14	1	
5	C	1	Total	C	O	0
			15	14	1	
5	E	1	Total	C	O	0
			15	14	1	
5	G	1	Total	C	O	0
			15	14	1	
5	I	1	Total	C	O	0
			15	14	1	
5	K	1	Total	C	O	0
			15	14	1	
5	M	1	Total	C	O	0
			15	14	1	
5	O	1	Total	C	O	0
			15	14	1	
5	Q	1	Total	C	O	0
			15	14	1	
5	S	1	Total	C	O	0
			15	14	1	

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: Outer capsid VP4



• Molecule 1: Outer capsid VP4



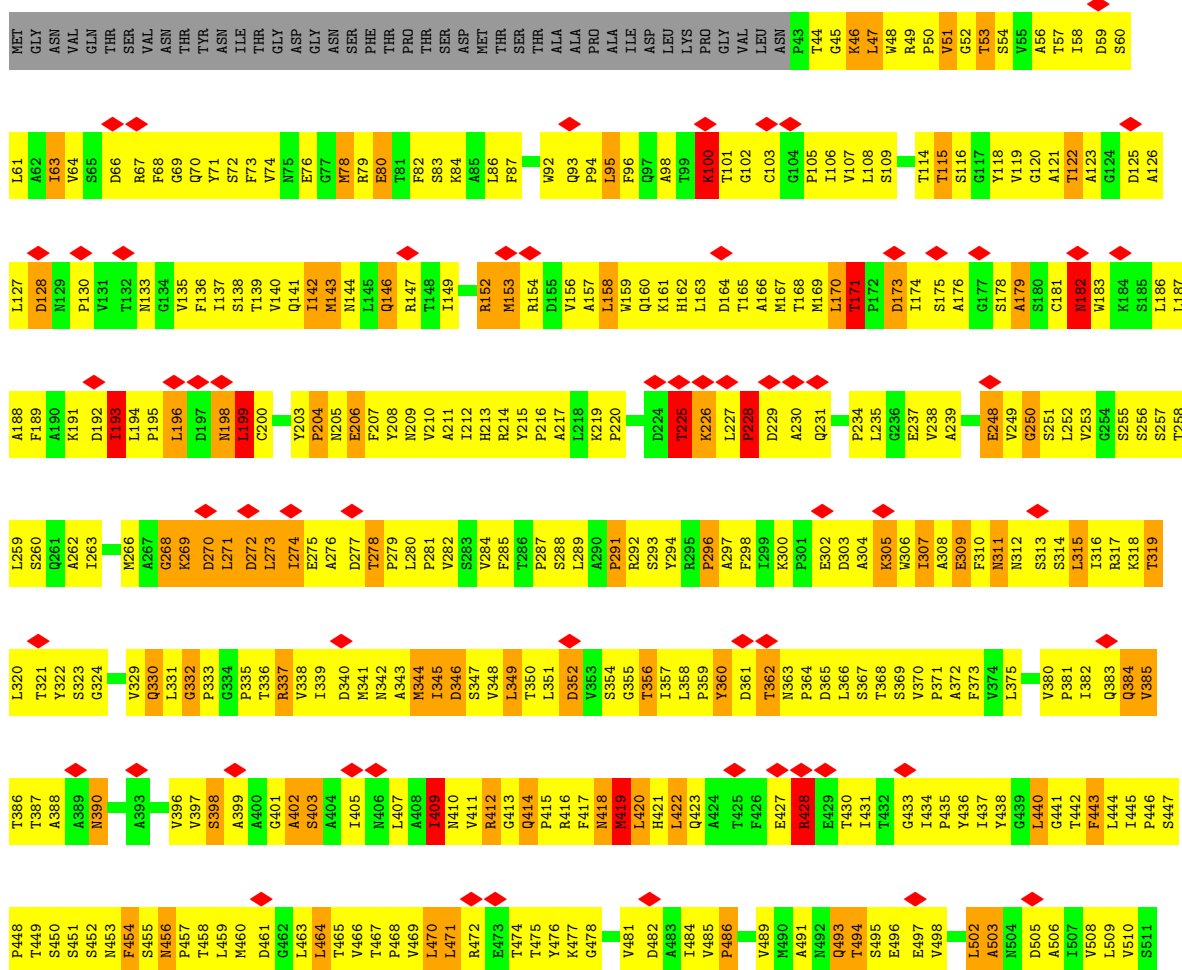


94%



ser	arg	asp	leu	thr	glu	phe
gly	leu	ala	gln	asn	asp	asn
val	ala	ile	ala	pro	ala	ala
thr	val	gln	thr	thr	lys	thr
ala	his	ala	glu	ser	ile	ser
leu	lys	thr	arg	thr	ala	glu
arg	thr	val	glu	glu	ser	val
thr	ser	met	thr	thr	phe	gly
gly	gln	ala	ile	pro	asn	ser
leu	val	asn	thr	ala	asn	leu
ser	gln	gln	gly	phe	ser	val
gly	gln	thr	ile	val	ser	gly
lys	ser	ser	pro	leu	leu	ser
val	pro	glu	tyr	ile	ile	thr
thr	thr	val	tyr	gln	arg	thr
asp	pro	ala	gly	ser	thr	leu
ala	pro	ser	leu	val	leu	ser
ser	asp	ala	gly	pro	thr	thr
glu	tyr	leu	thr	ile	tyr	ala
lys	pro	ala	phe	gln	ser	ile
leu	leu	asn	leu	gln	gly	ser
arg	leu	asp	ile	val	ala	thr
ala	trp	ala	pro	thr	thr	met
gln	arg	ile	ser	thr	thr	gly
ser	ala	leu	thr	ala	val	lys
thr	arg	ser	ser	asn	gln	asp
val	ala	asn	ser	thr	leu	leu
ala	ala	his	asn	thr	gly	asp
lys	ser	leu	phe	ile	gly	ile
gln	met	asn	ser	thr	pro	glu
thr	phe	lys	asn	val	thr	ala
phe	val	leu	pro	asn	arg	asp
phe	ser	ala	thr	ser	val	thr
asn	asn	asn	leu	ser	thr	pro
gln	pro	val	met	ala	asp	leu
ile	ser	val	asp	gly	met	pro
gly	leu	gly	gly	ala	asn	val
ser	ala	asp	leu	ser	ala	ser
leu	leu	ala	leu	ala	met	val
trp	gln	ile	thr	ile	ile	phe
pro	val	pro	val	asn	asp	thr
gly	gly	val	thr	leu	ser	pro
lys	ile	ala	pro	ala	val	leu
	pro	ser	val	ile	leu	ala
	val	arg	leu	asn	thr	leu
	thr	thr	leu	val	leu	pro
	thr	asp	arg	arg	asp	arg
	gln	asn	glu	gly	val	thr
	ser	ser	thr	gln	ser	tyr
	gly	ala	thr	pro	gly	arg
	met	thr	tyr	arg	thr	pro
	leu	ser	lys	phe	ile	ala
	ala	ala	gly	asn	phe	ser
	ser	ile	glu	thr	ile	thr
	ala	ile	glu	met	pro	lys
	thr	val	val	thr	thr	pro

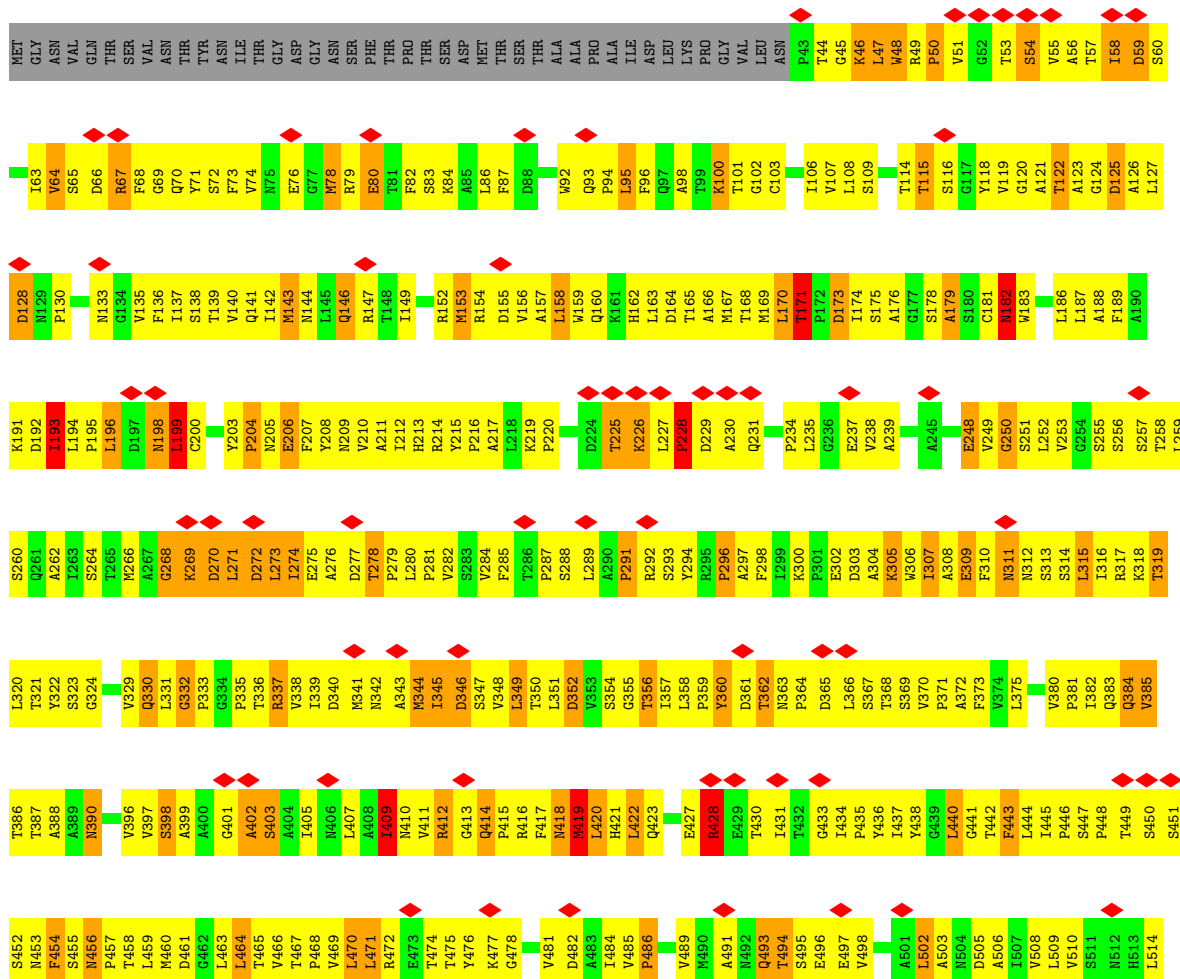
- Molecule 1: Outer capsid VP4

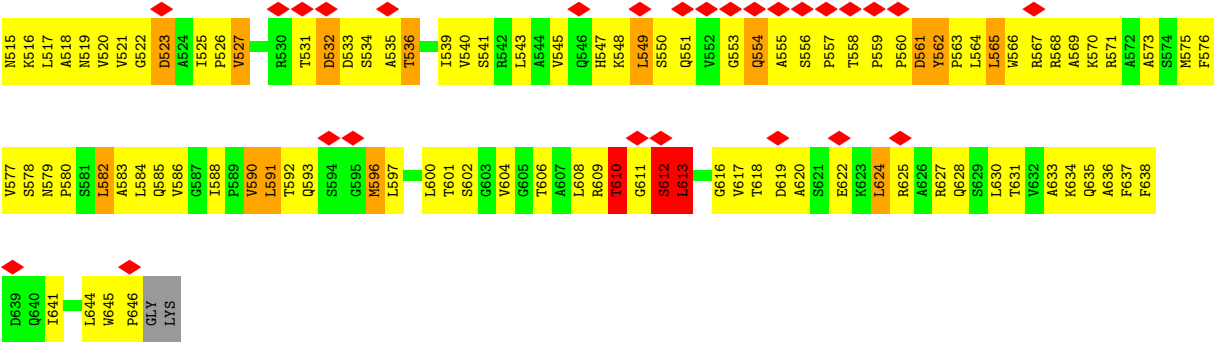




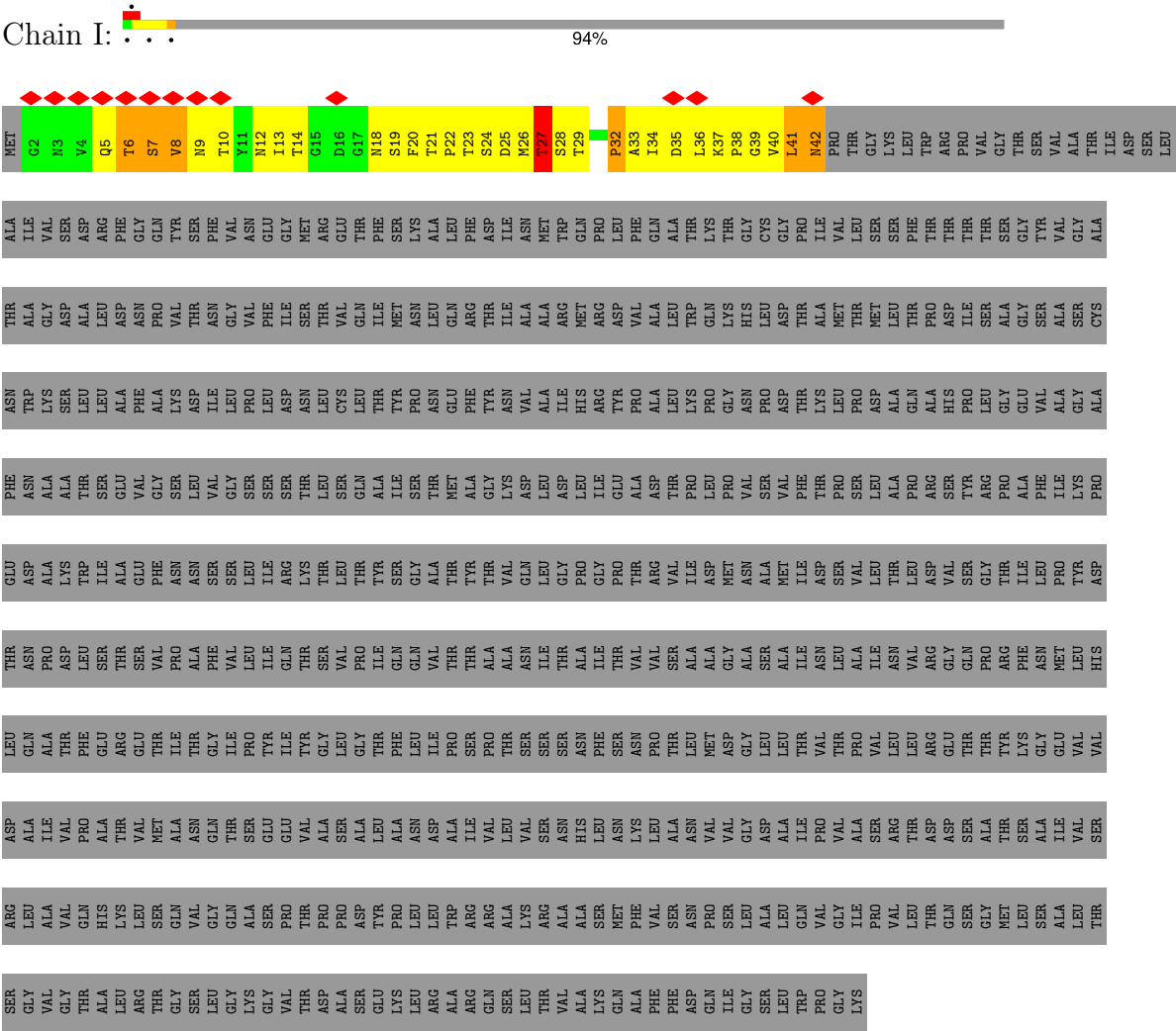
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THR	GLN	PRO	PRO	PHE	LEU	TRP	SER
ALA	HIS	ALA	ALA	GLU	THR	ILE	THR
LEU	LYS	THR	THR	ARG	THR	ALA	VAL
ARG	LEU	VAL	VAL	GLU	THR	GLU	GLY
THR	SER	MET	MET	THR	VAL	PHE	GLY
GLY	GLN	ALA	ALA	THR	PRO	ASN	SER
SER	VAL	ASN	ASN	ILE	ALA	ASN	LEU
LEU	GLY	GLN	GLN	GLY	PHE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

- Molecule 1: Outer capsid VP4

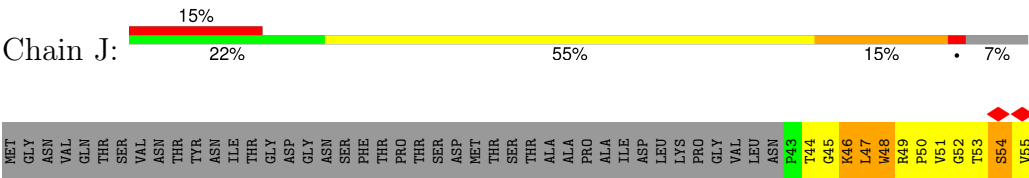


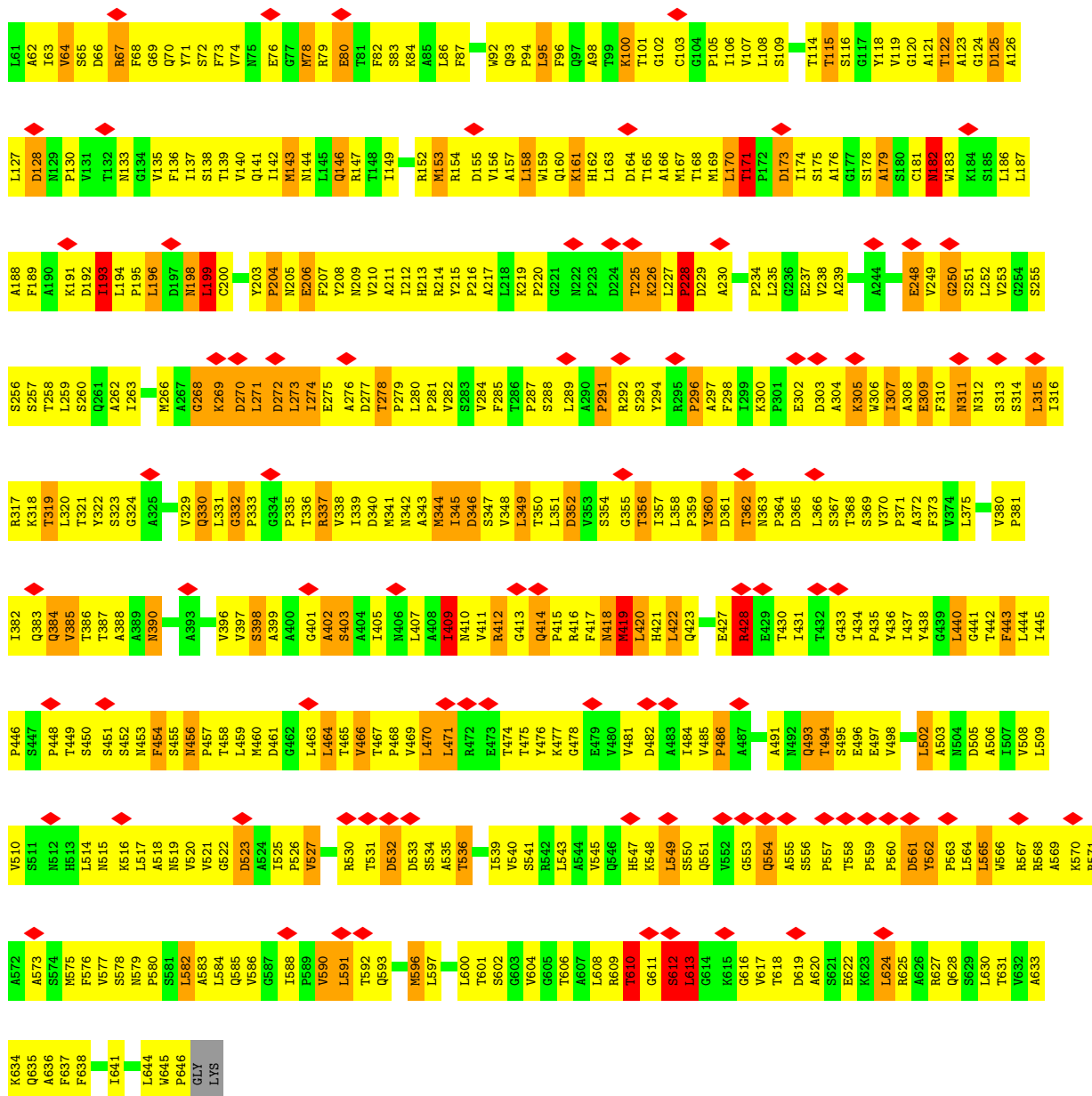


• Molecule 1: Outer capsid VP4



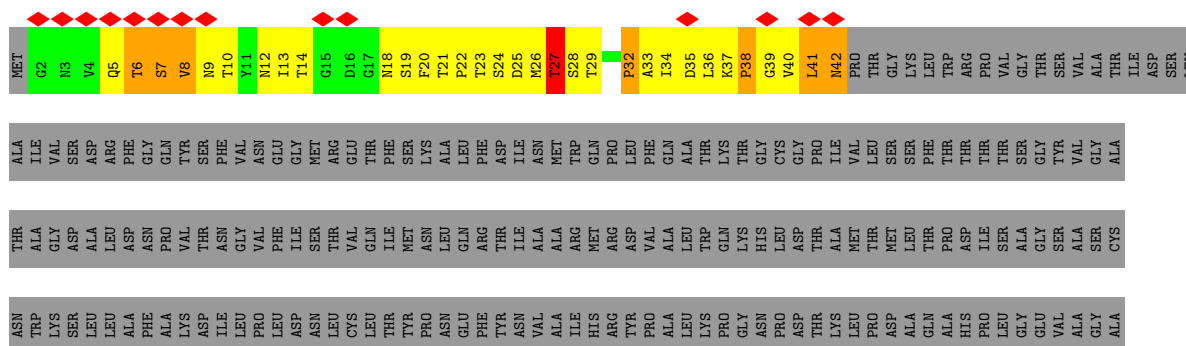
• Molecule 1: Outer capsid VP4





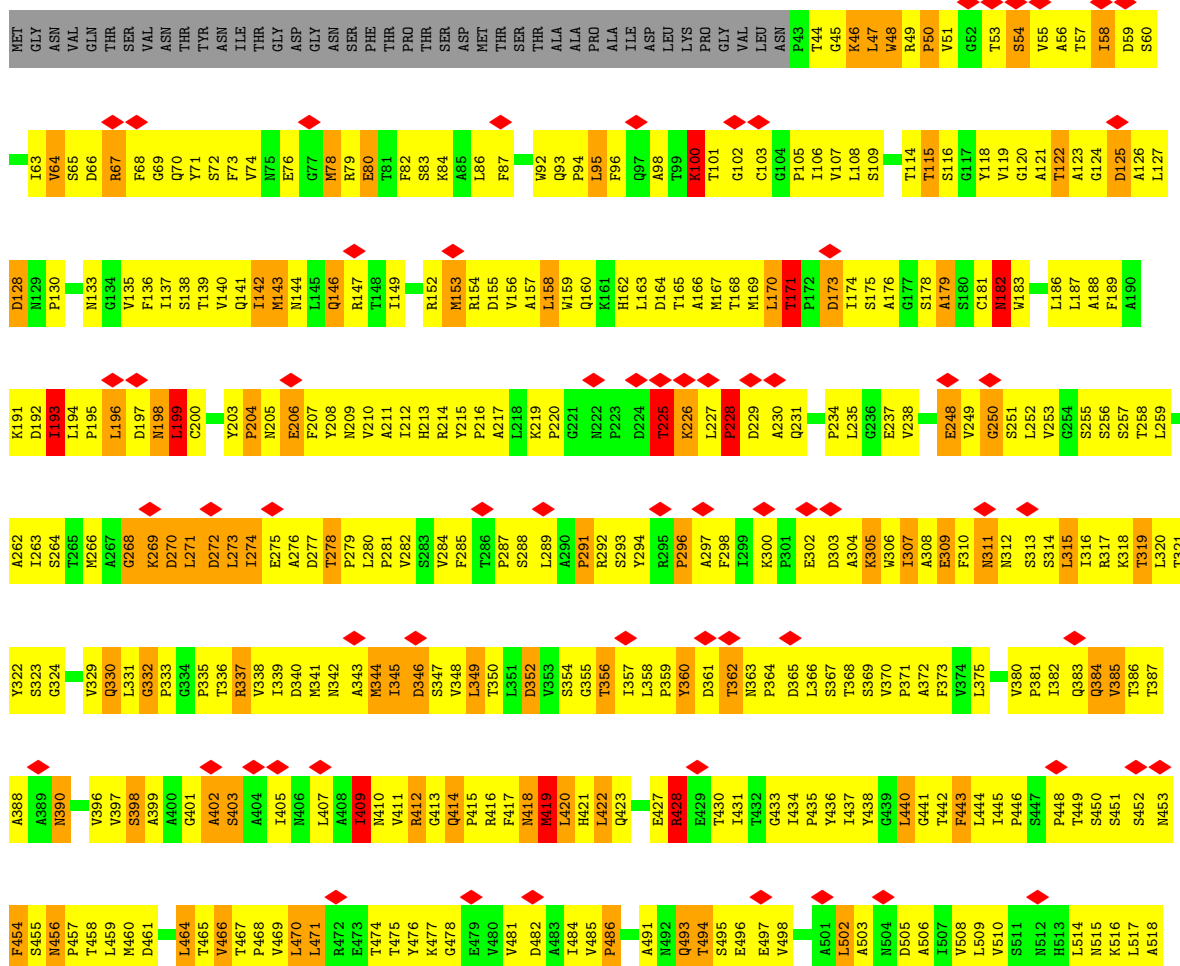
● Molecule 1: Outer capsid VP4

Chain K: 94%



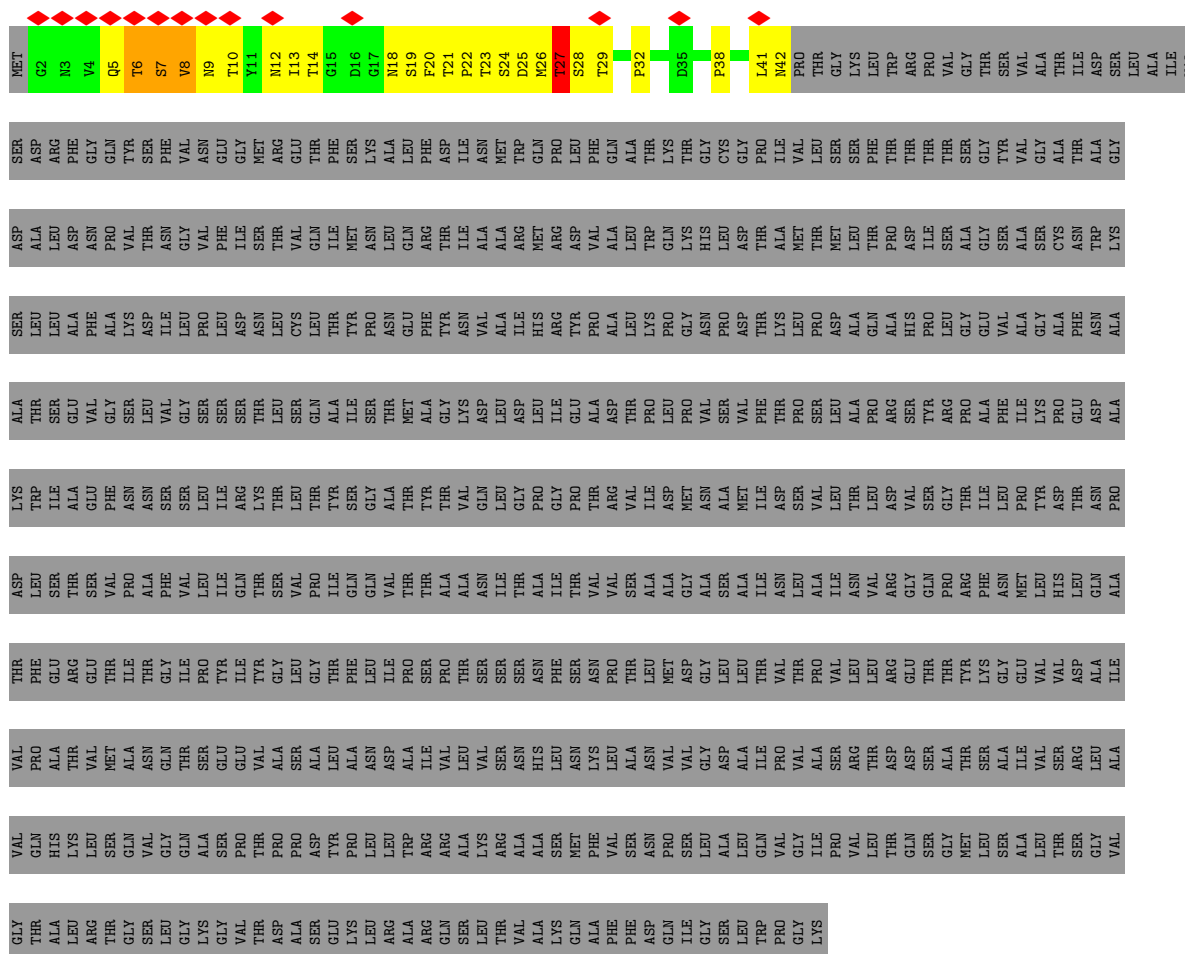
ser	arg	asp	leu	thr	glu	phe
gly	leu	ala	gln	asn	asp	asn
val	ala	ile	ala	pro	ala	ala
thr	val	gln	thr	thr	lys	thr
ala	his	ala	glu	ser	ile	ser
leu	lys	thr	arg	thr	ala	glu
arg	thr	val	glu	glu	thr	val
thr	ser	met	thr	thr	phe	gly
gly	gln	ala	ile	pro	asn	ser
leu	val	asn	thr	ala	asn	leu
ser	gly	gln	gly	phe	ser	val
gly	gln	thr	ile	val	ser	gly
lys	ser	ser	pro	leu	leu	ser
val	pro	glu	tyr	ile	ile	thr
thr	thr	val	tyr	gln	arg	thr
asp	pro	ala	gly	ser	thr	leu
ala	pro	ser	leu	val	leu	ser
ser	asp	ala	gly	pro	thr	thr
glu	tyr	leu	thr	ile	tyr	ala
lys	pro	ala	phe	gln	ser	ile
leu	leu	asn	leu	gln	gly	ser
arg	leu	asp	ile	val	ala	thr
ala	trp	ala	pro	thr	thr	met
gln	arg	ile	ser	thr	thr	gly
ser	ala	leu	thr	ala	lys	thr
thr	arg	ser	ser	asn	gln	asp
val	ala	asn	ser	thr	leu	leu
ala	ala	his	asn	thr	gly	asp
lys	ser	leu	phe	ile	gly	ile
gln	met	asn	ser	thr	pro	glu
thr	phe	lys	asn	val	thr	ala
phe	val	leu	pro	asn	arg	asp
phe	ser	ala	thr	ser	val	thr
asp	asn	asn	leu	ala	thr	pro
gln	pro	val	met	ala	ile	leu
ile	ser	val	asp	gly	met	pro
gly	leu	gly	gly	ala	asn	val
ser	ala	asp	leu	ser	ala	ser
leu	leu	ala	leu	ala	met	val
trp	gln	ile	thr	ile	ile	val
pro	val	pro	val	asn	asp	thr
gly	gly	val	thr	leu	ser	ser
lys	ile	ala	pro	ala	val	leu
	pro	ser	val	ile	thr	ala
	val	arg	leu	asn	thr	leu
	val	thr	leu	arg	asp	pro
	val	gln	arg	thr	val	arg
	thr	asn	glu	gln	ser	tyr
	gly	ala	thr	pro	gly	arg
	met	thr	tyr	arg	thr	pro
	leu	ser	lys	phe	ile	ala
	ala	ala	gly	asn	phe	thr
	ile	ile	glu	ser	leu	ile
	ala	thr	glu	met	pro	lys
	thr	val	val	thr	thr	thr
	thr	ser	val	his	asp	pro

- Molecule 1: Outer capsid VP4



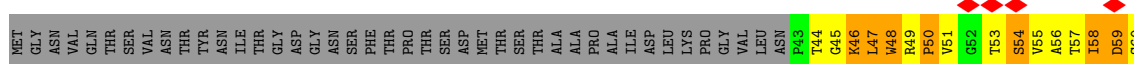
- Molecule 1: Outer capsid VP4

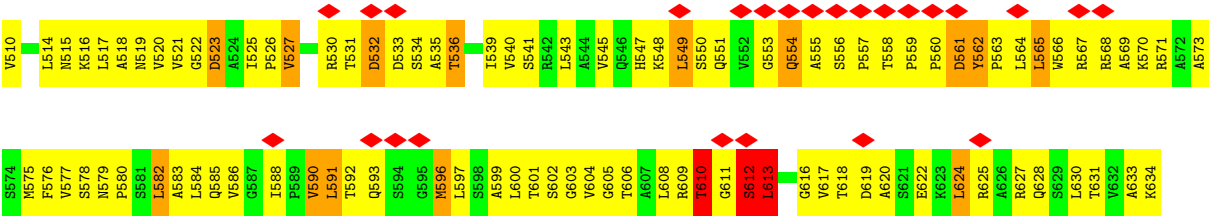
Chain M:  94%



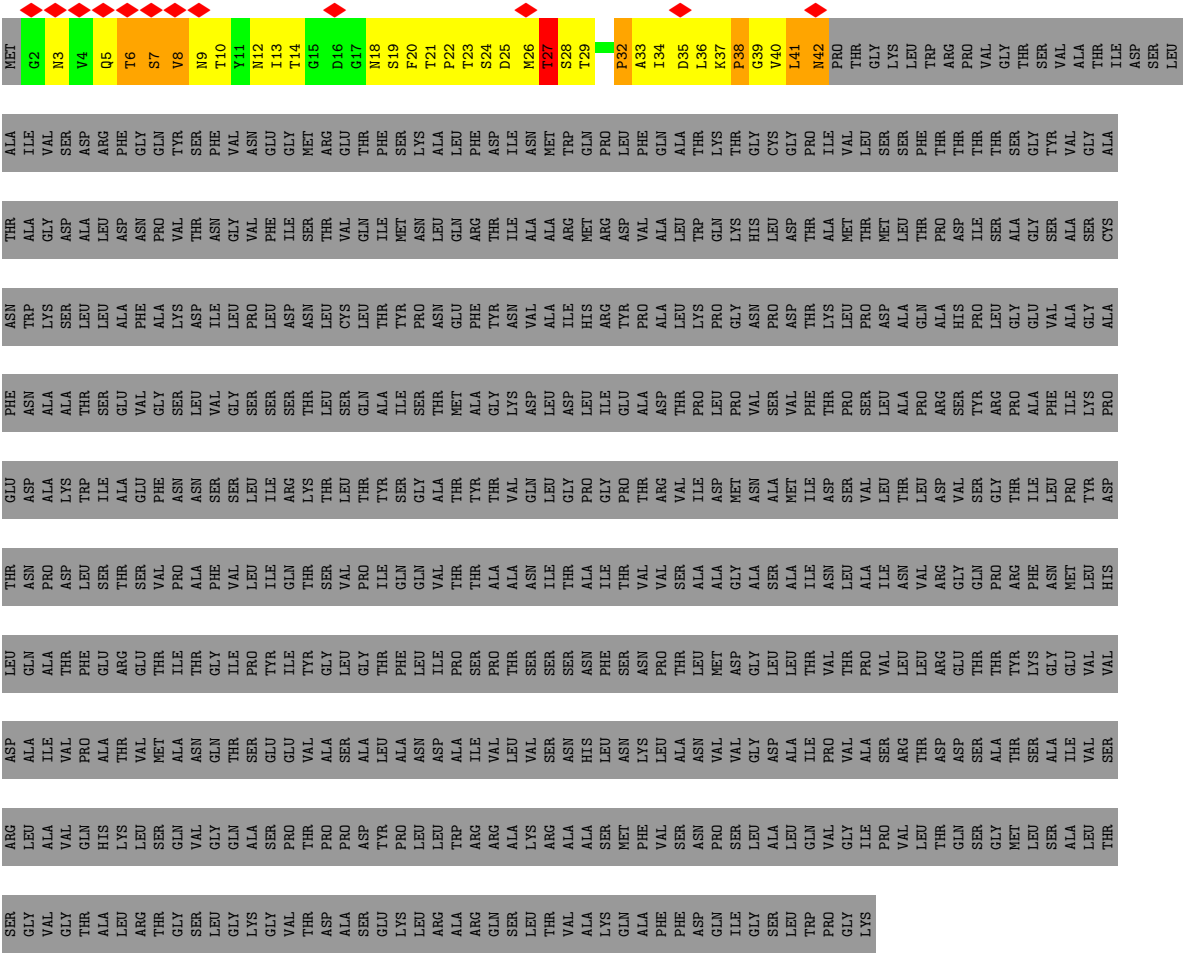
- Molecule 1: Outer capsid VP4

Chain N: 

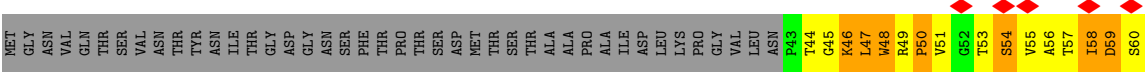




• Molecule 1: Outer capsid VP4



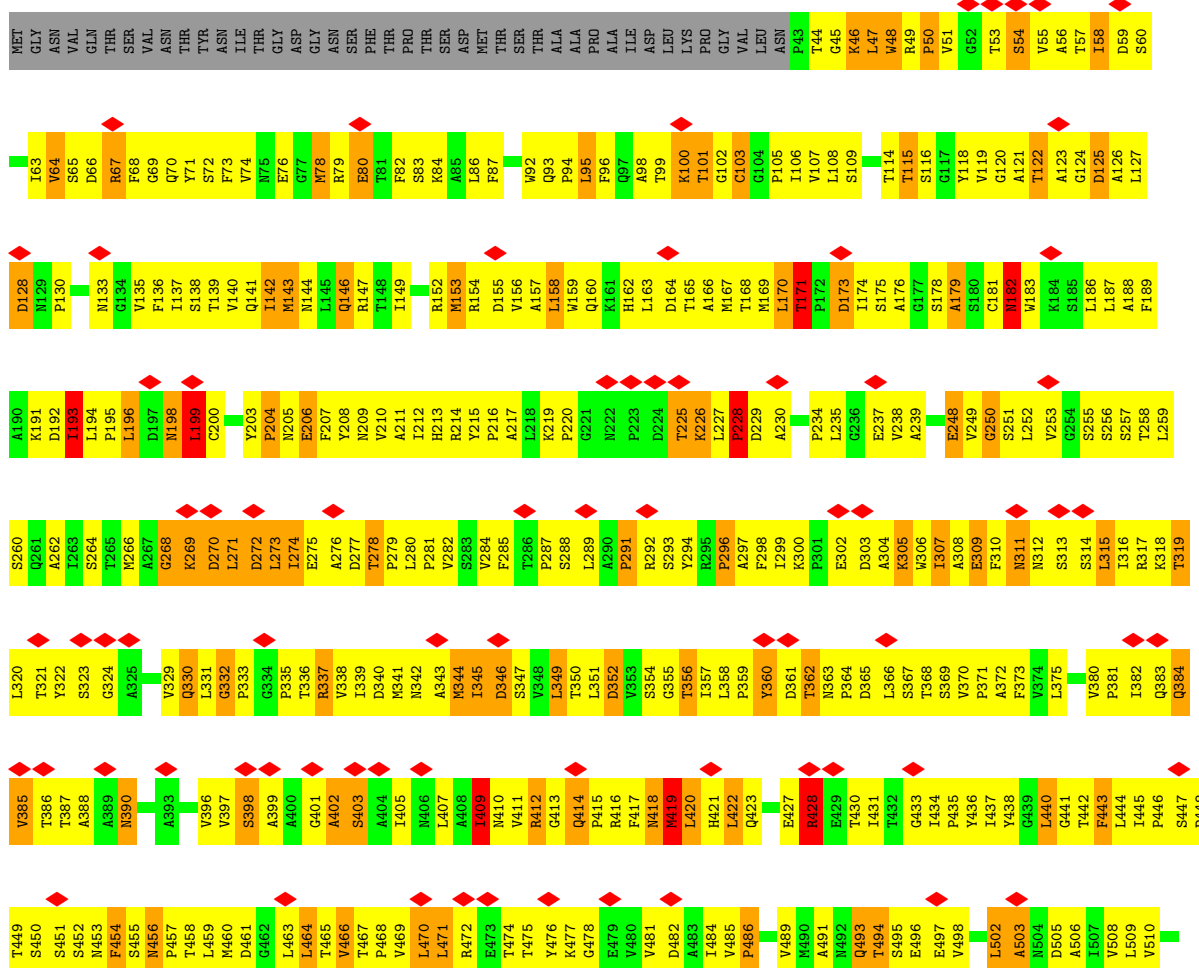
• Molecule 1: Outer capsid VP4

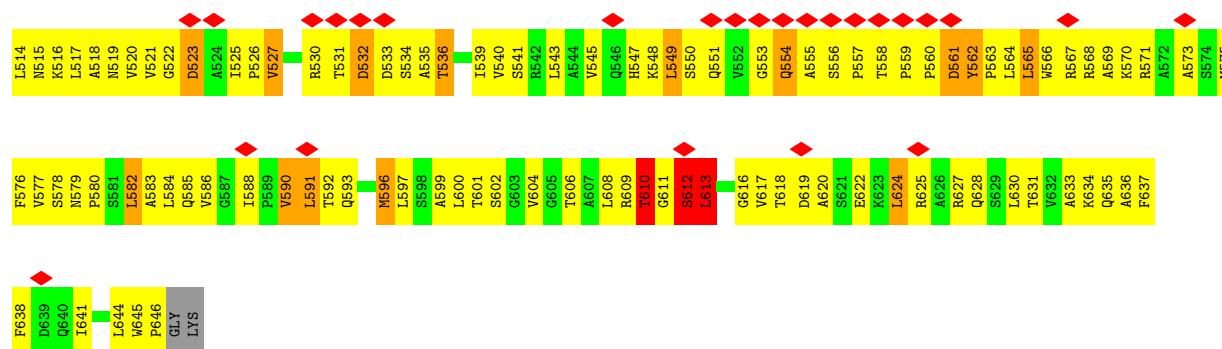




[illegible]

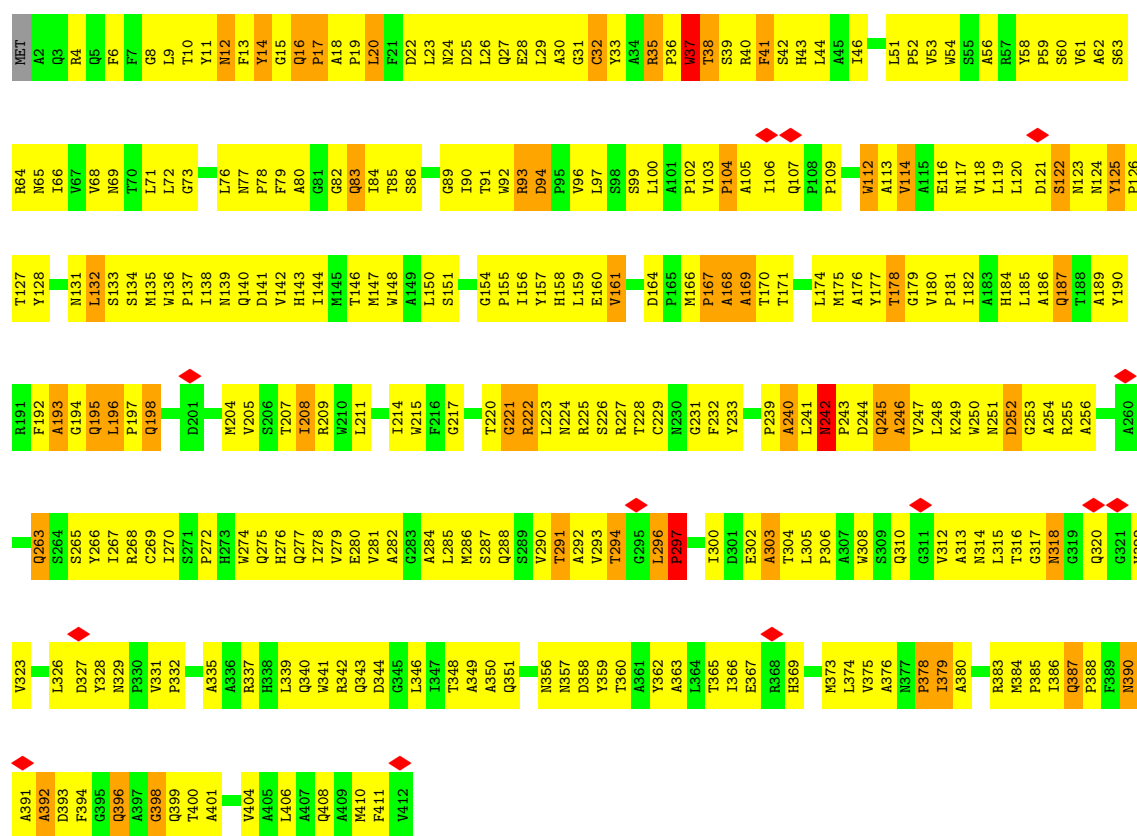
- Molecule 1: Outer capsid VP4





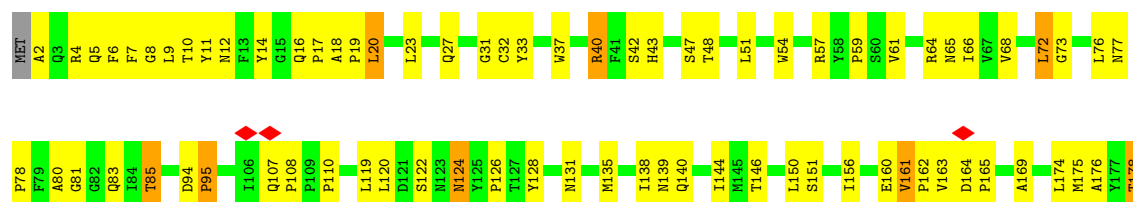
• Molecule 2: Core protein VP6

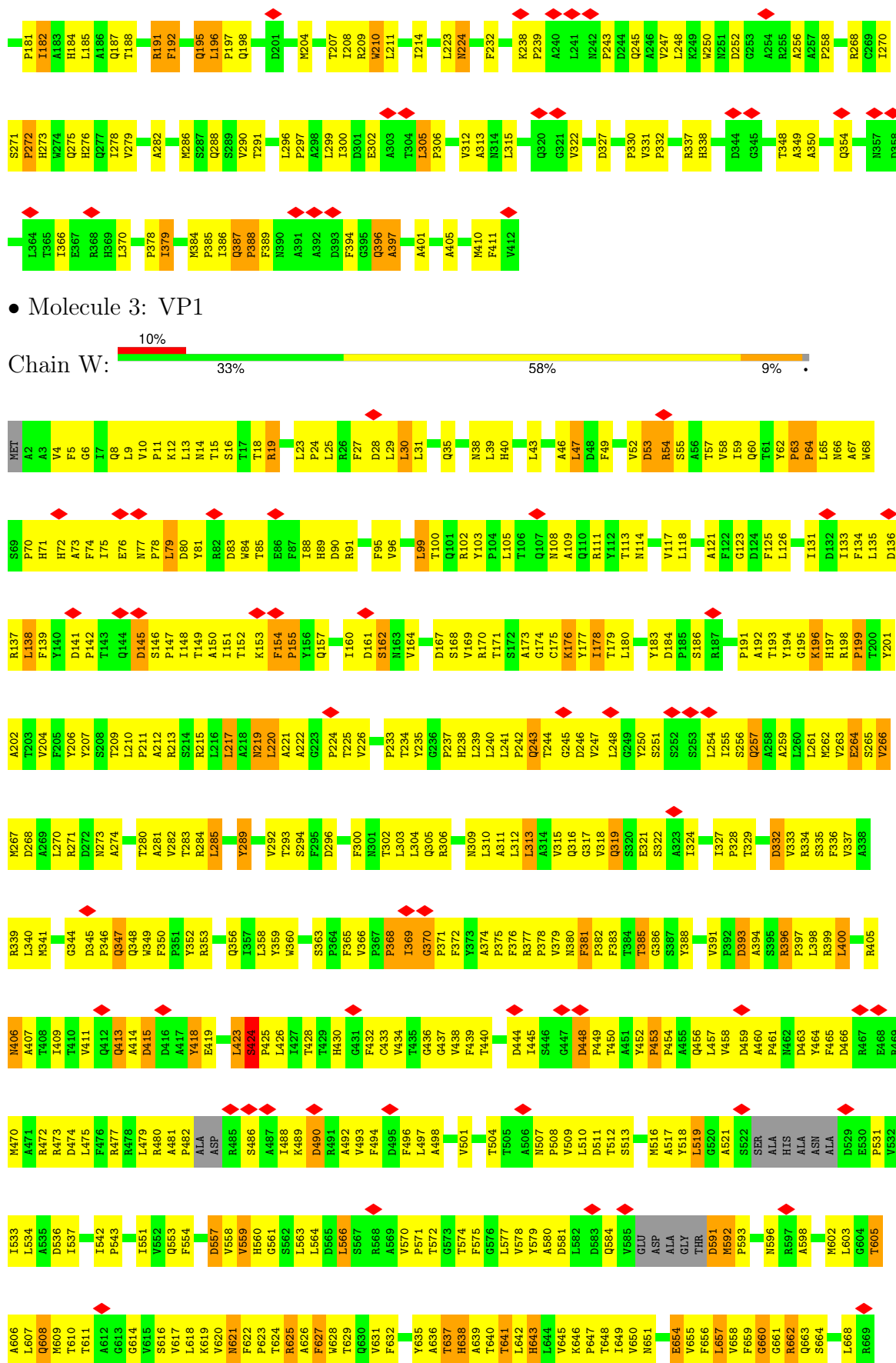
Chain U: 27% 61% 12%



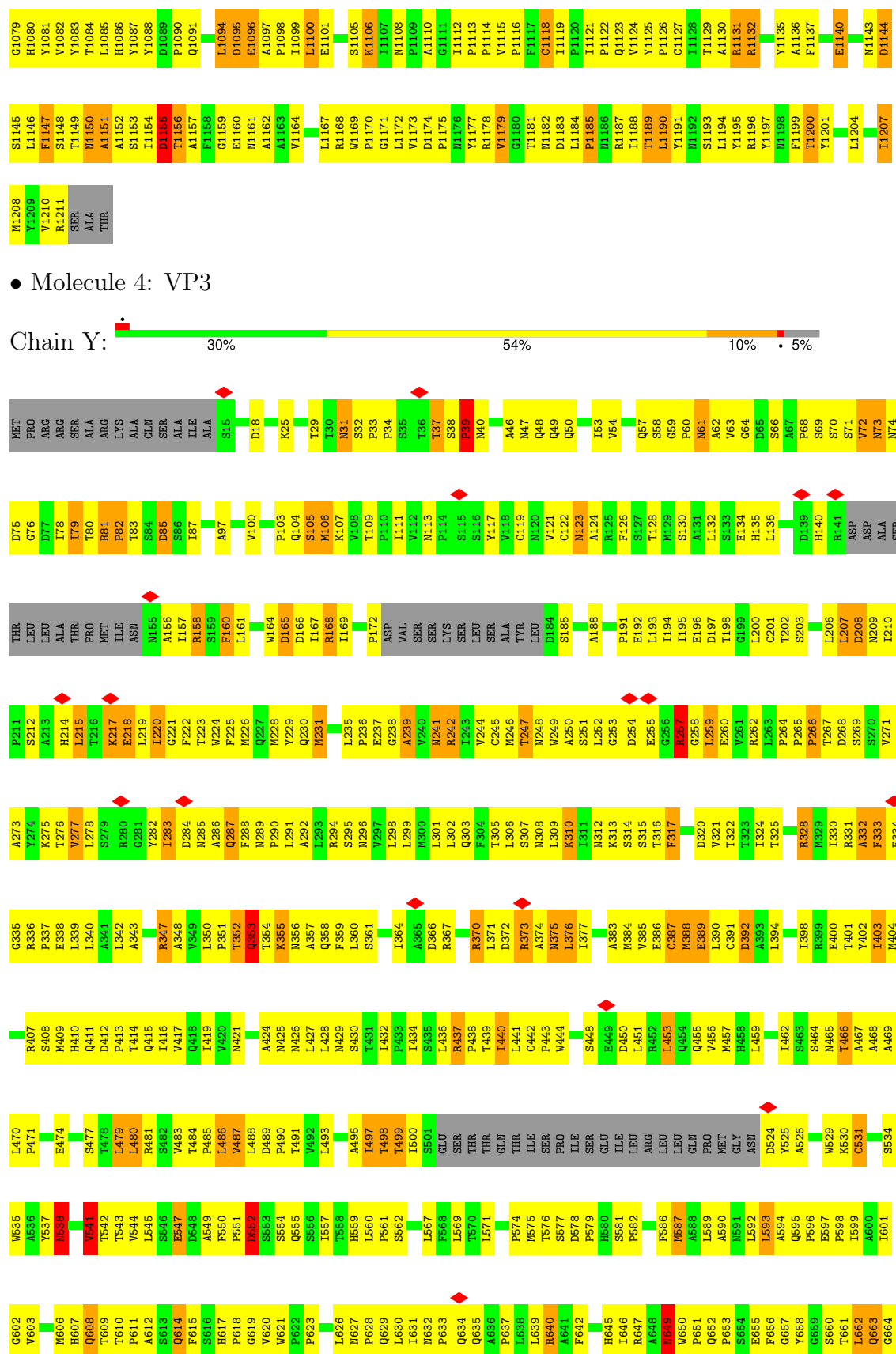
• Molecule 2: Core protein VP6

Chain V: 6% 61% 34% 5%



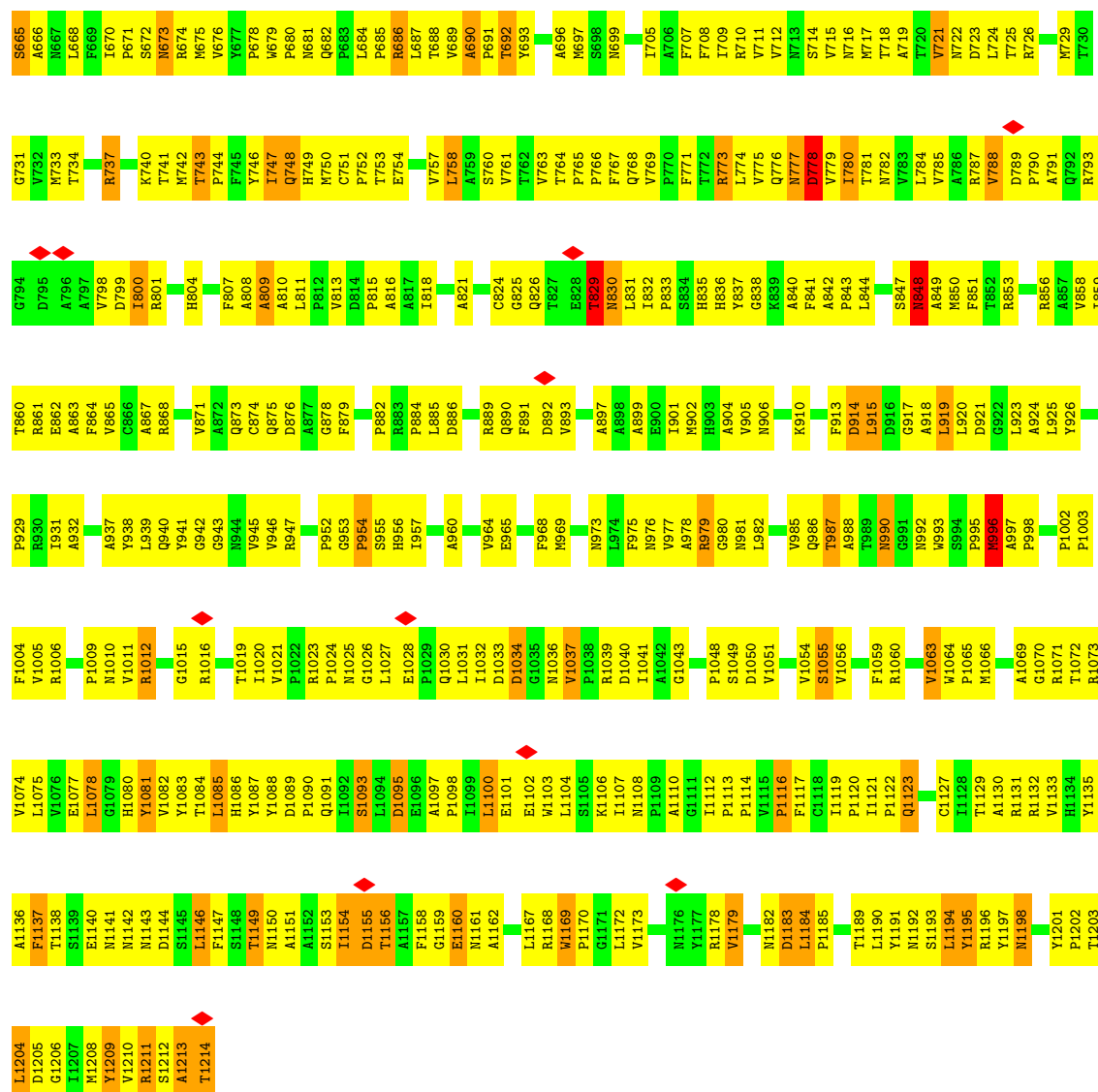






• Molecule 4: VP3

Chain Y: 30% 54% 10% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	18464	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	57700	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.305	Depositor
Minimum map value	-0.193	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	814.0, 814.0, 814.0	wwPDB
Map dimensions	740, 740, 740	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	0/295	1.00	0/405
1	B	0.52	0/4601	0.80	0/6295
1	C	0.60	0/295	1.00	0/405
1	D	0.51	0/4601	0.80	1/6295 (0.0%)
1	E	0.60	0/295	0.99	0/405
1	F	0.52	0/4601	0.80	0/6295
1	G	0.60	0/286	0.95	0/391
1	H	0.52	0/4601	0.80	0/6295
1	I	0.60	0/295	1.00	0/405
1	J	0.51	0/4601	0.80	0/6295
1	K	0.60	0/295	0.99	0/405
1	L	0.52	0/4601	0.80	0/6295
1	M	0.60	0/286	0.95	0/391
1	N	0.52	0/4601	0.80	0/6295
1	O	0.60	0/295	0.99	0/405
1	P	0.51	0/4601	0.80	0/6295
1	Q	0.60	0/295	0.99	0/405
1	R	0.52	0/4601	0.80	0/6295
1	S	0.60	0/286	0.95	0/391
1	T	0.52	0/4601	0.80	0/6295
2	U	0.33	0/3233	0.55	0/4443
2	V	0.31	0/3233	0.49	0/4443
3	W	0.32	0/10148	0.60	0/13935
4	X	0.53	0/8078	0.75	2/11071 (0.0%)
4	Y	0.38	0/9056	0.66	2/12412 (0.0%)
All	All	0.47	0/82681	0.75	5/113262 (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	B	0	1
1	D	0	1
1	F	0	1
1	H	0	1
1	J	0	1
1	L	0	1
1	N	0	1
1	P	0	1
1	R	0	1
1	T	0	1
4	X	0	3
4	Y	0	2
All	All	0	15

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	934	LEU	CA-CB-CG	-5.76	102.06	115.30
1	D	51	VAL	N-CA-C	5.75	126.53	111.00
4	Y	1002	PRO	N-CA-CB	5.60	110.02	103.30
4	Y	1003	PRO	N-CA-CB	5.52	109.93	103.30
4	X	428	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	337	ARG	Sidechain
1	D	337	ARG	Sidechain
1	F	337	ARG	Sidechain
1	H	337	ARG	Sidechain
1	J	337	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	291	0	277	54	0
1	B	4508	0	4555	643	0
1	C	291	0	277	78	0
1	D	4508	0	4555	904	0
1	E	291	0	277	77	0
1	F	4508	0	4555	874	0
1	G	284	0	267	56	0
1	H	4508	0	4555	864	0
1	I	291	0	277	81	0
1	J	4508	0	4555	891	0
1	K	291	0	277	78	0
1	L	4508	0	4555	872	0
1	M	284	0	267	57	0
1	N	4508	0	4555	882	0
1	O	291	0	277	76	0
1	P	4508	0	4555	898	0
1	Q	291	0	277	85	0
1	R	4508	0	4555	883	0
1	S	284	0	267	58	0
1	T	4508	0	4555	879	0
2	U	3138	0	3061	444	0
2	V	3138	0	3061	174	0
3	W	9882	0	9821	1051	0
4	X	7873	0	7851	1242	0
4	Y	8835	0	8748	1054	0
5	A	15	0	27	27	0
5	C	15	0	27	33	0
5	E	15	0	27	27	0
5	G	15	0	27	29	0
5	I	15	0	27	29	0
5	K	15	0	27	27	0
5	M	15	0	27	26	0
5	O	15	0	27	28	0
5	Q	15	0	27	27	0
5	S	15	0	27	30	0
All	All	80985	0	81102	11617	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 72.

The worst 5 of 11617 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:U:32:CYS:HB3	4:X:958:HIS:CE1	1.55	1.38
4:X:464:SER:HB2	4:Y:500:ILE:CG2	1.52	1.38
1:R:628:GLN:NE2	3:W:870:ALA:HA	1.41	1.35
1:D:469:VAL:HG21	1:F:575:MET:CE	1.59	1.33
1:F:469:VAL:HG21	1:H:575:MET:CE	1.59	1.33

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	B	602/648 (93%)	407 (68%)	134 (22%)	61 (10%)	0	3
1	C	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	D	602/648 (93%)	416 (69%)	129 (21%)	57 (10%)	0	3
1	E	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	F	602/648 (93%)	408 (68%)	133 (22%)	61 (10%)	0	3
1	G	37/648 (6%)	24 (65%)	8 (22%)	5 (14%)	0	1
1	H	602/648 (93%)	409 (68%)	132 (22%)	61 (10%)	0	3
1	I	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	J	602/648 (93%)	411 (68%)	132 (22%)	59 (10%)	0	3
1	K	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	L	602/648 (93%)	409 (68%)	132 (22%)	61 (10%)	0	3
1	M	37/648 (6%)	24 (65%)	8 (22%)	5 (14%)	0	1
1	N	602/648 (93%)	408 (68%)	133 (22%)	61 (10%)	0	3
1	O	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	P	602/648 (93%)	410 (68%)	132 (22%)	60 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	R	602/648 (93%)	406 (67%)	135 (22%)	61 (10%)	0	3
1	S	37/648 (6%)	24 (65%)	8 (22%)	5 (14%)	0	1
1	T	602/648 (93%)	406 (67%)	135 (22%)	61 (10%)	0	3
2	U	409/412 (99%)	283 (69%)	81 (20%)	45 (11%)	0	2
2	V	409/412 (99%)	330 (81%)	60 (15%)	19 (5%)	2	13
3	W	1276/1299 (98%)	1063 (83%)	173 (14%)	40 (3%)	3	21
4	X	1012/1214 (83%)	714 (71%)	219 (22%)	79 (8%)	1	5
4	Y	1146/1214 (94%)	860 (75%)	204 (18%)	82 (7%)	1	6
All	All	10656/17511 (61%)	7587 (71%)	2151 (20%)	918 (9%)	1	4

5 of 918 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	ASP
1	B	103	CYS
1	B	179	ALA
1	B	225	THR
1	B	228	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	34/536 (6%)	27 (79%)	7 (21%)	1	4
1	B	499/536 (93%)	426 (85%)	73 (15%)	2	12
1	C	34/536 (6%)	27 (79%)	7 (21%)	1	4
1	D	499/536 (93%)	425 (85%)	74 (15%)	2	11
1	E	34/536 (6%)	27 (79%)	7 (21%)	1	4
1	F	499/536 (93%)	426 (85%)	73 (15%)	2	12
1	G	32/536 (6%)	25 (78%)	7 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	499/536 (93%)	426 (85%)	73 (15%)	2	12
1	I	34/536 (6%)	27 (79%)	7 (21%)	1	4
1	J	499/536 (93%)	425 (85%)	74 (15%)	2	11
1	K	34/536 (6%)	27 (79%)	7 (21%)	1	4
1	L	499/536 (93%)	425 (85%)	74 (15%)	2	11
1	M	32/536 (6%)	25 (78%)	7 (22%)	1	3
1	N	499/536 (93%)	424 (85%)	75 (15%)	2	11
1	O	34/536 (6%)	27 (79%)	7 (21%)	1	4
1	P	499/536 (93%)	423 (85%)	76 (15%)	2	10
1	Q	34/536 (6%)	27 (79%)	7 (21%)	1	4
1	R	499/536 (93%)	425 (85%)	74 (15%)	2	11
1	S	32/536 (6%)	25 (78%)	7 (22%)	1	3
1	T	499/536 (93%)	424 (85%)	75 (15%)	2	11
2	U	325/326 (100%)	305 (94%)	20 (6%)	15	41
2	V	325/326 (100%)	305 (94%)	20 (6%)	15	41
3	W	1082/1092 (99%)	977 (90%)	105 (10%)	6	25
4	X	869/1030 (84%)	736 (85%)	133 (15%)	2	10
4	Y	976/1030 (95%)	864 (88%)	112 (12%)	4	18
All	All	8901/14524 (61%)	7700 (86%)	1201 (14%)	5	14

5 of 1201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	W	832	LEU
4	Y	649	ASN
3	W	1235	THR
3	W	824	ARG
4	X	880	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 351 such sidechains are listed below:

Mol	Chain	Res	Type
2	U	387	GLN
4	X	425	ASN
2	V	140	GLN

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Mol	Chain	Res	Type
3	W	347	GLN
4	X	854	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	MYR	E	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	A	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	I	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	O	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	Q	649	1	13,14,15	0.45	0	12,13,15	0.49	0
5	MYR	K	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	S	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	M	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	C	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	G	649	1	13,14,15	0.44	0	12,13,15	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MYR	E	649	1	-	8/12/12/13	-
5	MYR	A	649	1	-	8/12/12/13	-
5	MYR	I	649	1	-	8/12/12/13	-
5	MYR	O	649	1	-	8/12/12/13	-
5	MYR	Q	649	1	-	8/12/12/13	-
5	MYR	K	649	1	-	8/12/12/13	-
5	MYR	S	649	1	-	8/12/12/13	-
5	MYR	M	649	1	-	8/12/12/13	-
5	MYR	C	649	1	-	8/12/12/13	-
5	MYR	G	649	1	-	8/12/12/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	649	MYR	C3-C4-C5-C6
5	K	649	MYR	C3-C4-C5-C6
5	Q	649	MYR	C3-C4-C5-C6
5	A	649	MYR	C3-C4-C5-C6
5	C	649	MYR	C3-C4-C5-C6

There are no ring outliers.

10 monomers are involved in 283 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	649	MYR	27	0
5	A	649	MYR	27	0
5	I	649	MYR	29	0
5	O	649	MYR	28	0
5	Q	649	MYR	27	0
5	K	649	MYR	27	0
5	S	649	MYR	30	0
5	M	649	MYR	26	0
5	C	649	MYR	33	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	649	MYR	29	0

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.

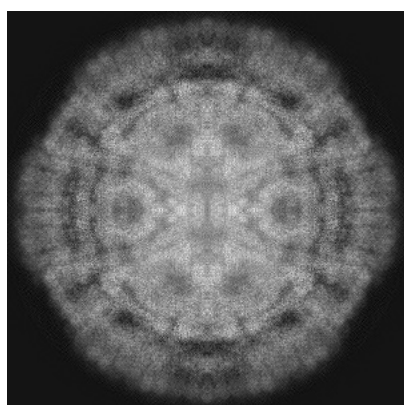
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5160. These allow visual inspection of the internal detail of the map and identification of artifacts.

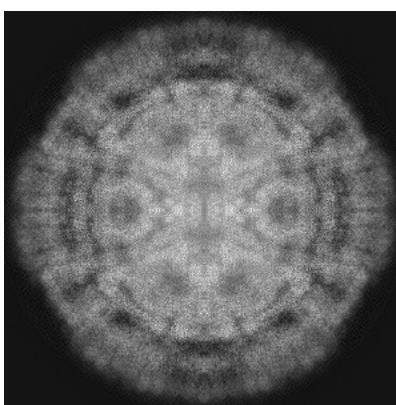
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

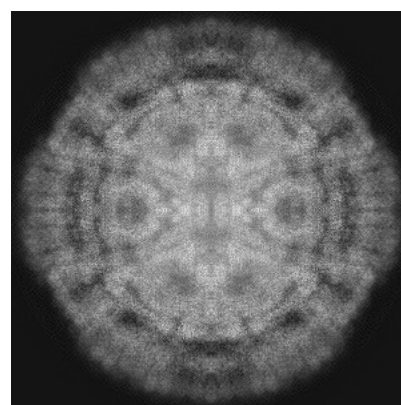
6.1.1 Primary map



X



Y

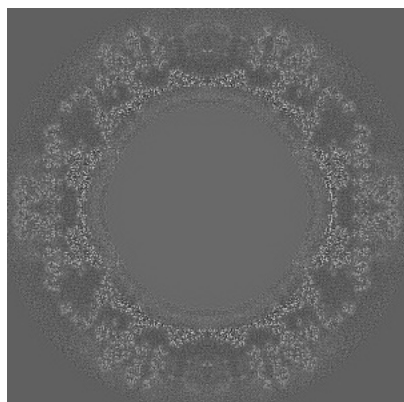


Z

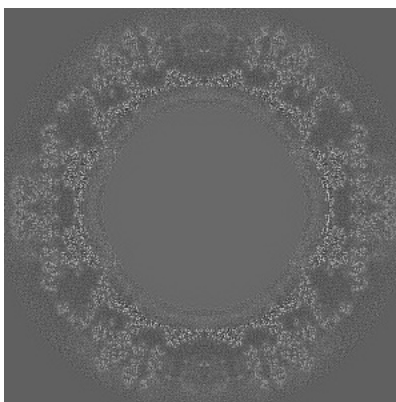
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

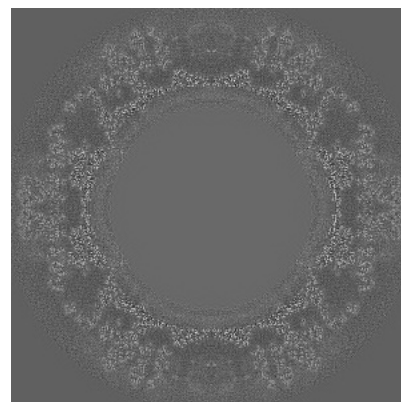
6.2.1 Primary map



X Index: 370



Y Index: 370

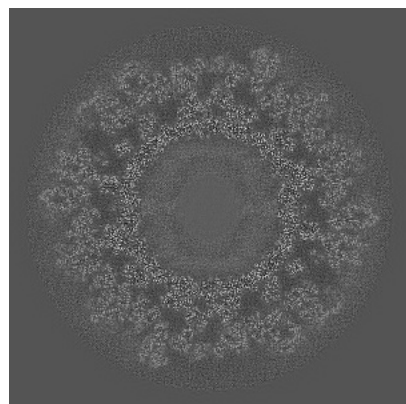


Z Index: 370

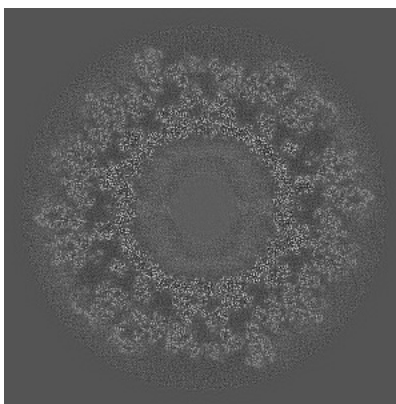
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

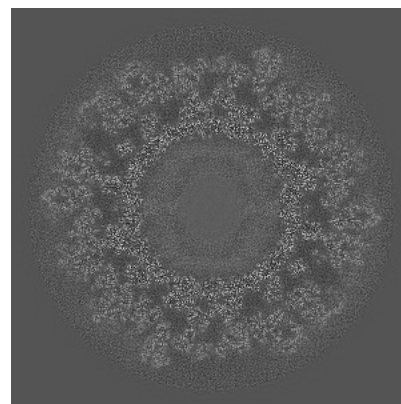
6.3.1 Primary map



X Index: 194



Y Index: 546

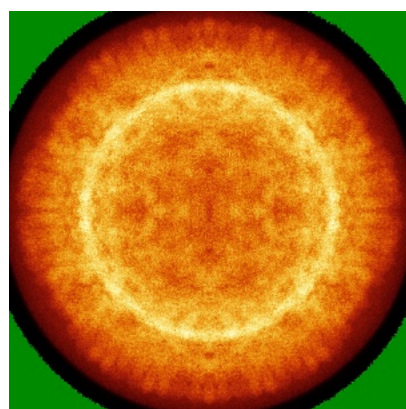


Z Index: 194

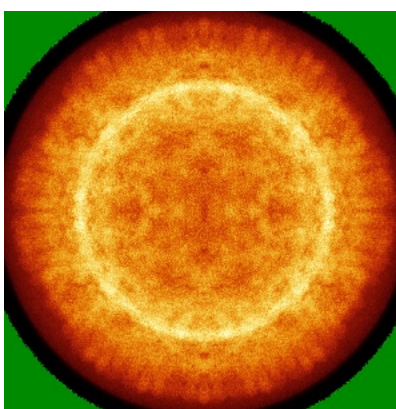
The images above show the largest variance slices of the map in three orthogonal directions.

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

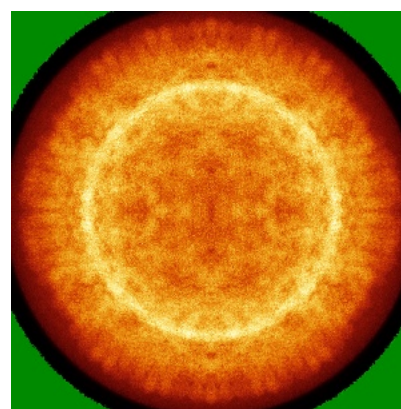
6.4.1 Primary map



X



Y

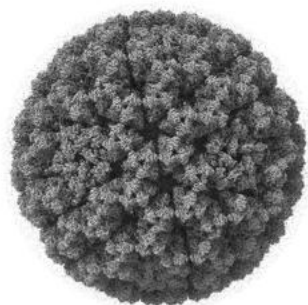


Z

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](#)

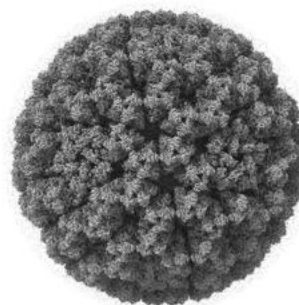
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. 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 shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

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

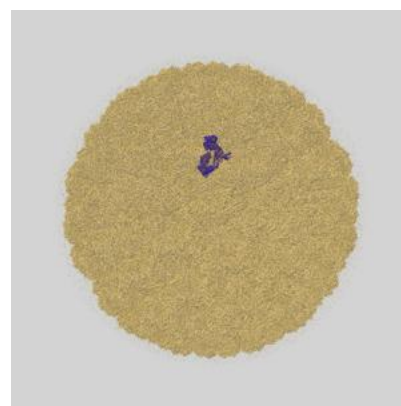
6.6.1 emd_5160_msk_1.map [i](#)



X



Y

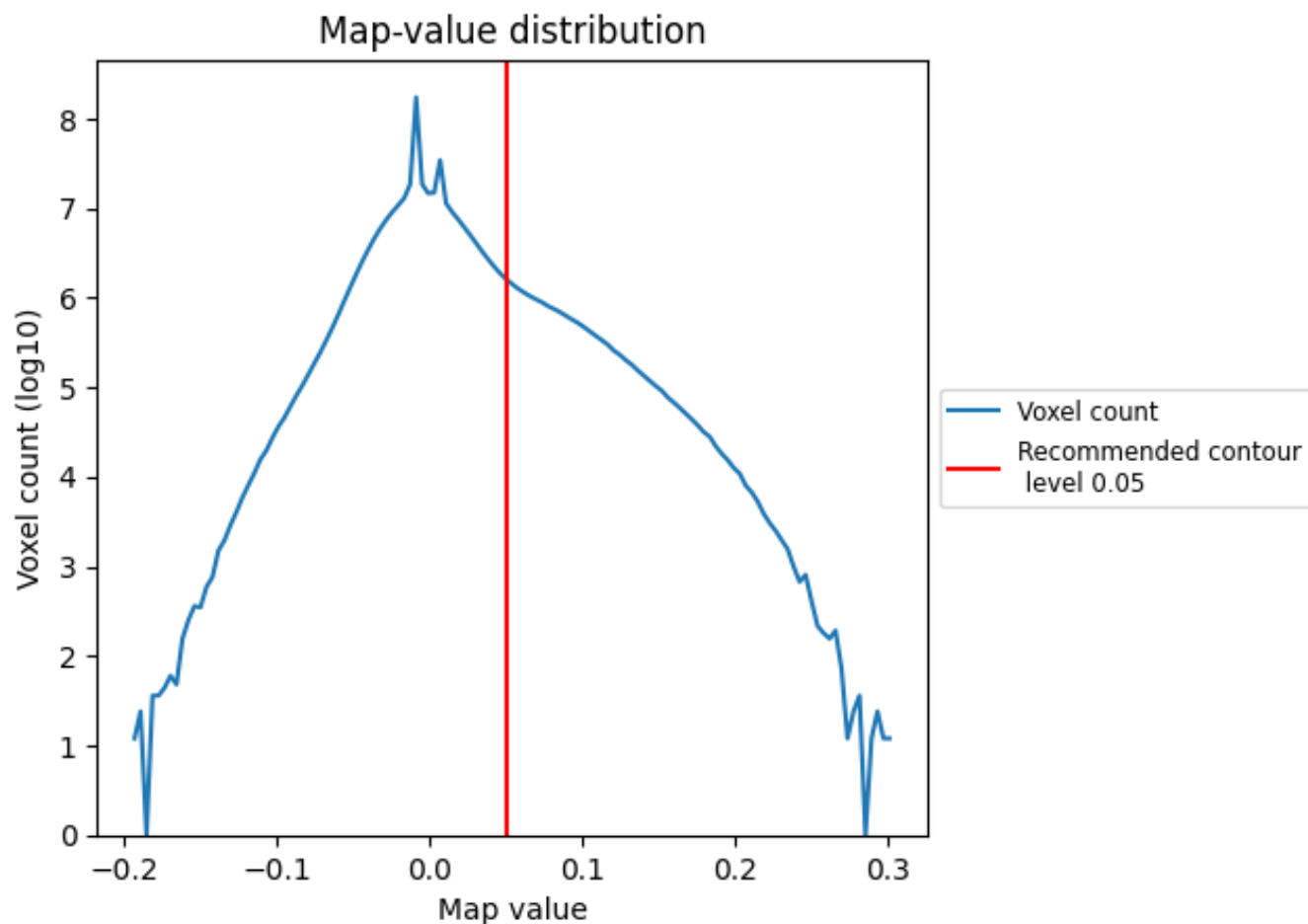


Z

7 Map analysis [i](#)

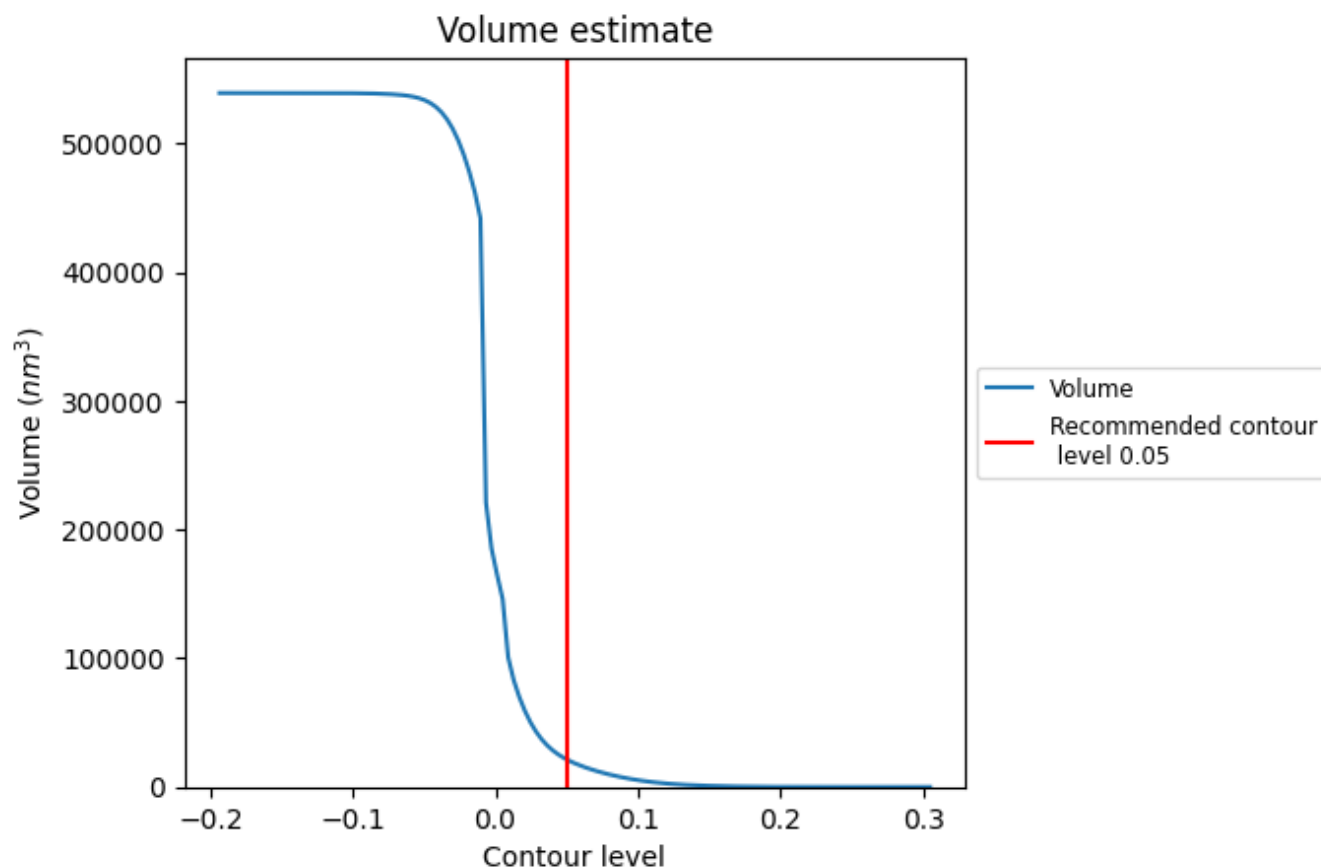
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

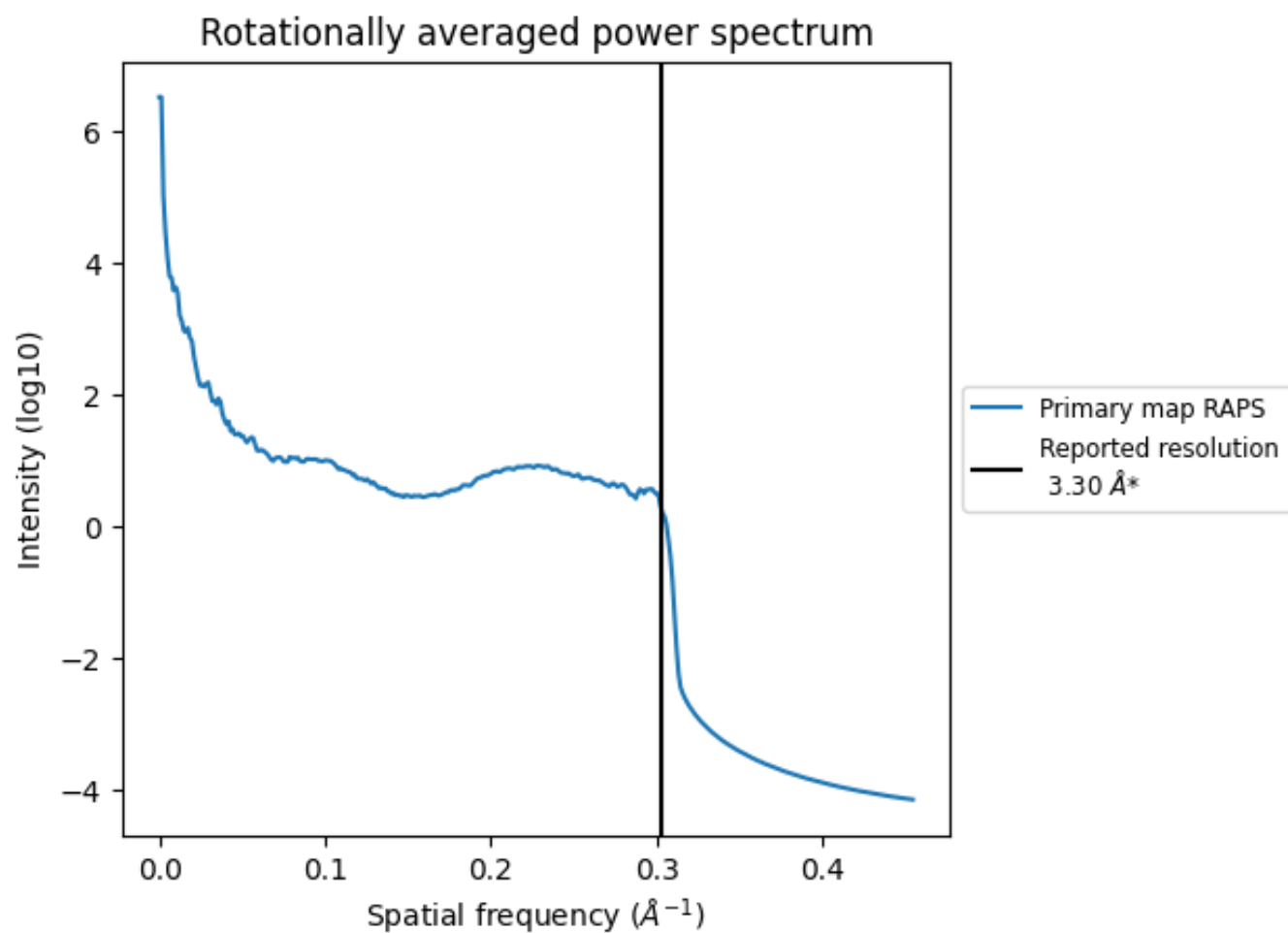
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 21462 nm^3 ; this corresponds to an approximate mass of 19387 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 0.303 Å⁻¹

8 Fourier-Shell correlation

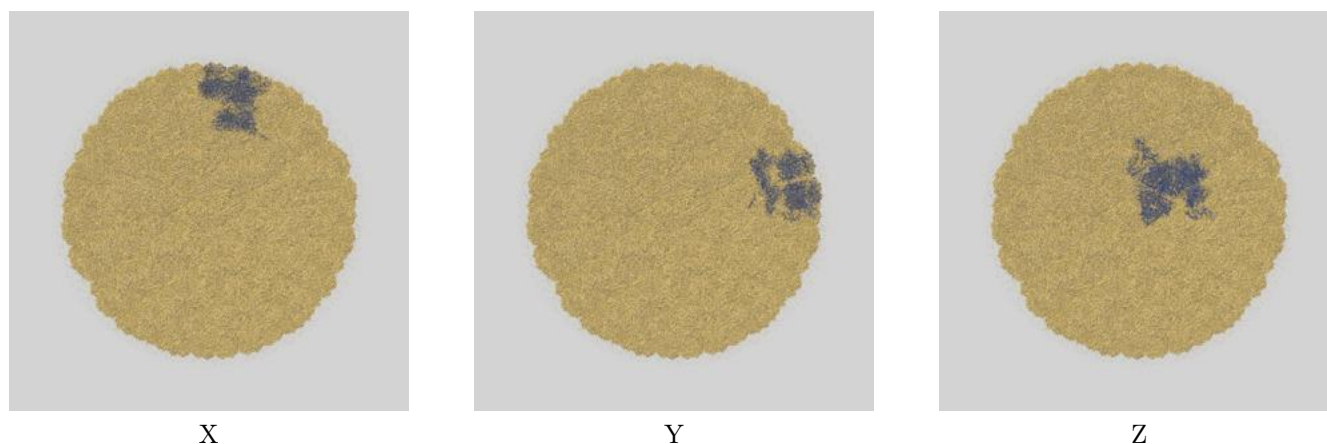
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

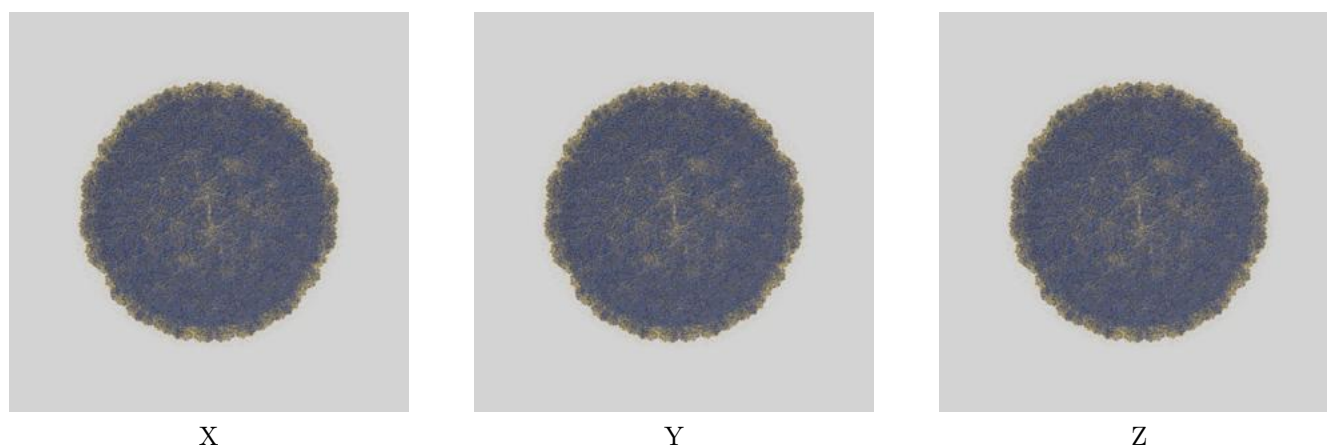
This section contains information regarding the fit between EMDB map EMD-5160 and PDB model 3IYL. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

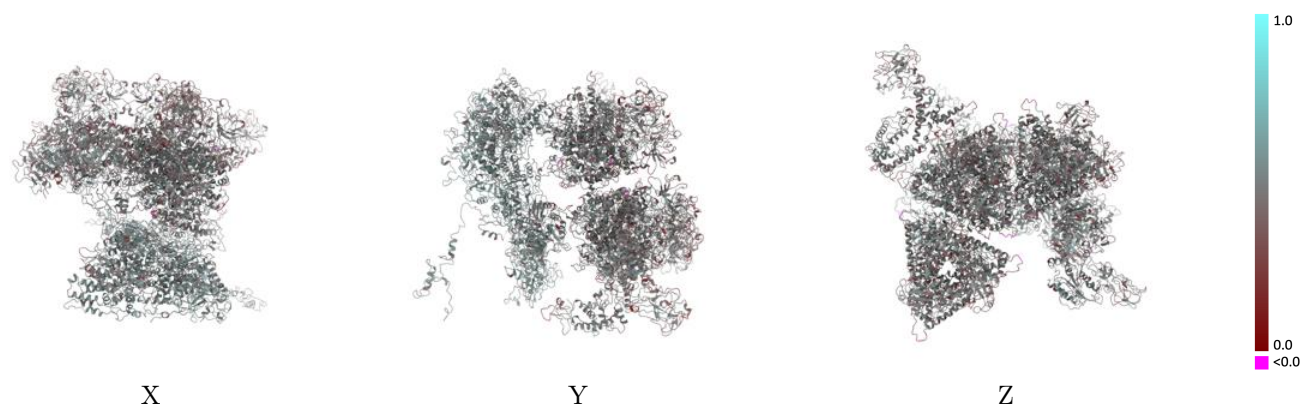


9.1.2 Map-model assembly overlay [i](#)



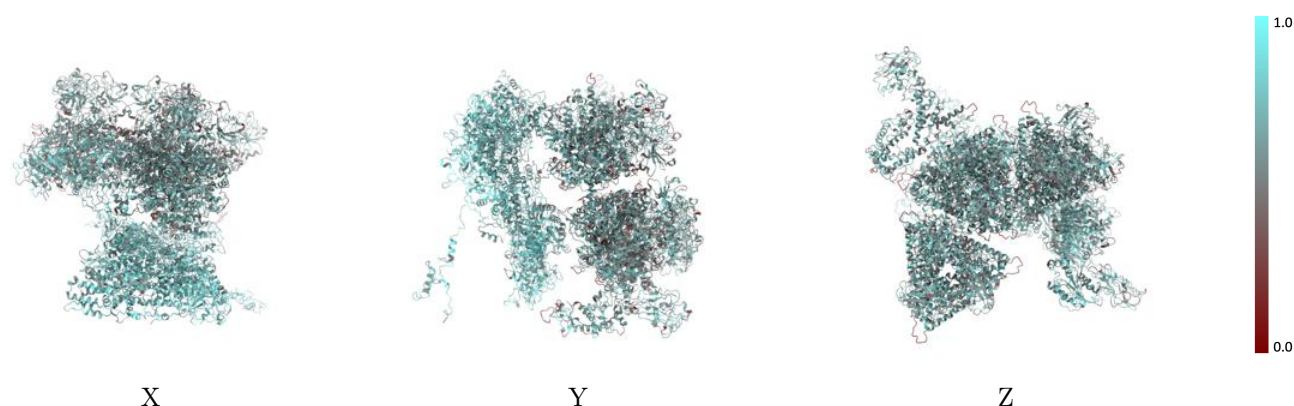
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



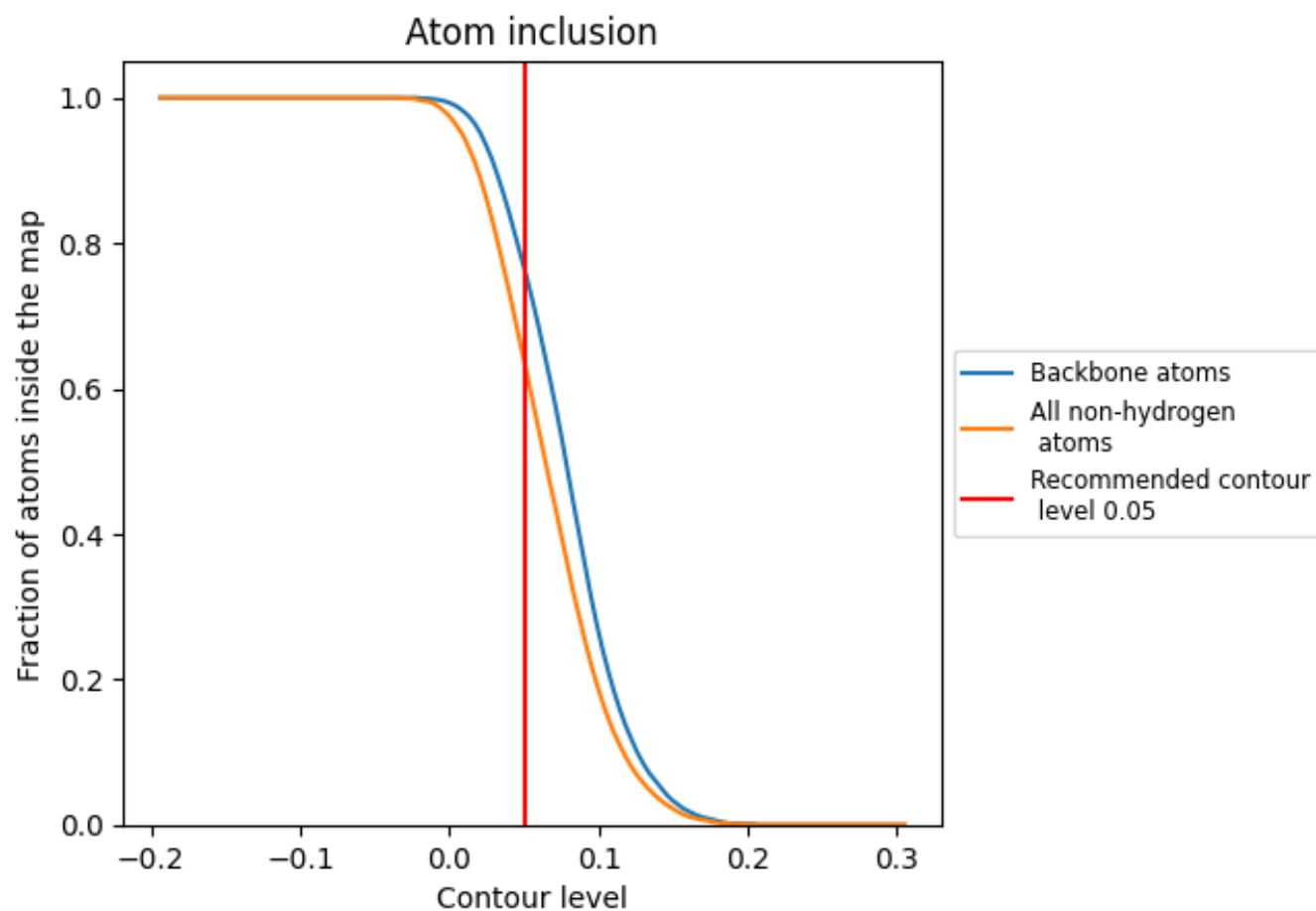
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6400	 0.4680
A	 0.4850	 0.4200
B	 0.5820	 0.4440
C	 0.5180	 0.4100
D	 0.5980	 0.4510
E	 0.4980	 0.4050
F	 0.5930	 0.4470
G	 0.5000	 0.4020
H	 0.5930	 0.4490
I	 0.4980	 0.4310
J	 0.5920	 0.4490
K	 0.4850	 0.3870
L	 0.5890	 0.4460
M	 0.5100	 0.4070
N	 0.5900	 0.4550
O	 0.5210	 0.3990
P	 0.5880	 0.4440
Q	 0.4880	 0.4090
R	 0.5920	 0.4530
S	 0.4660	 0.3980
T	 0.5860	 0.4460
U	 0.7550	 0.5140
V	 0.7040	 0.4740
W	 0.6610	 0.4690
X	 0.7580	 0.5230
Y	 0.7530	 0.5230

