wwPDB EM Validation Summary Report (i)

May 13, 2025 – 10:40 PM EDT

PDB ID	:	6B9Q / pdb_00006b9q
EMDB ID	:	EMD-7071
Title	:	Single particle cryo-EM structure determination of the LuIII capsid protein
Authors	:	Pittman, N.C.; Agbandje-McKenna, M.
Deposited on	:	2017-10-11
Resolution	:	3.17 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

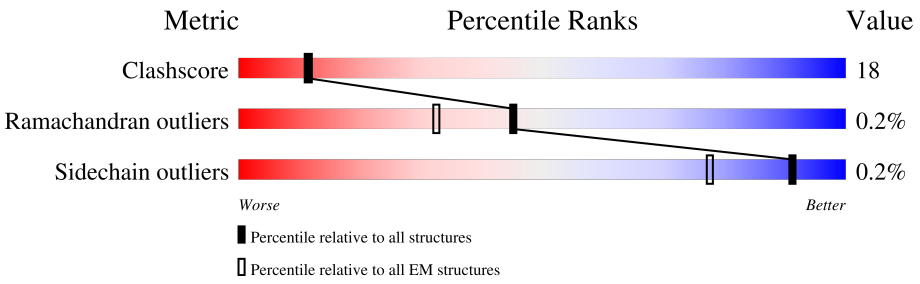
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.17 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 <=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	587	59% 35% 6%
1	2	587	58% 36% 6%
1	3	587	58% 36% 6%
1	4	587	59% 35% 6%
1	5	587	58% 36% 6%
1	6	587	58% 35% 6%
1	7	587	58% 35% 6%
1	8	587	58% 35% 6%

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Mol	Chain	Length	Quality of chain
1	A	587	58% 36% 6%
1	B	587	59% 35% 6%
1	C	587	58% 35% 6%
1	D	587	58% 35% 6%
1	E	587	59% 35% 6%
1	F	587	58% 35% 6%
1	G	587	58% 35% 6%
1	H	587	58% 35% 6%
1	I	587	59% 35% 6%
1	J	587	59% 35% 6%
1	K	587	58% 35% 6%
1	L	587	59% 35% 6%
1	M	587	58% 36% 6%
1	N	587	58% 35% 6%
1	O	587	58% 35% 6%
1	P	587	59% 35% 6%
1	Q	587	58% 35% 6%
1	R	587	58% 36% 6%
1	S	587	59% 35% 6%
1	T	587	59% 34% 6%
1	U	587	58% 35% 6%
1	V	587	58% 36% 6%
1	W	587	58% 35% 6%
1	X	587	59% 35% 6%
1	Y	587	58% 36% 6%

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Mol	Chain	Length	Quality of chain
1	Z	587	59% 35% 6%
1	a	587	59% 35% 6%
1	b	587	59% 35% 6%
1	c	587	58% 35% 6%
1	d	587	58% 36% 6%
1	e	587	58% 35% 6%
1	f	587	59% 35% 6%
1	g	587	58% 36% 6%
1	h	587	59% 35% 6%
1	i	587	58% 35% 6%
1	j	587	59% 35% 6%
1	k	587	59% 35% 6%
1	l	587	59% 35% 6%
1	m	587	59% 35% 6%
1	n	587	59% 35% 6%
1	o	587	58% 36% 6%
1	p	587	58% 35% 6%
1	q	587	58% 36% 6%
1	r	587	59% 35% 6%
1	s	587	58% 36% 6%
1	t	587	58% 35% 6%
1	u	587	58% 35% 6%
1	v	587	59% 35% 6%
1	w	587	59% 35% 6%
1	x	587	59% 35% 6%

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Mol	Chain	Length	Quality of chain
1	y	587	59% 35% 6%
1	z	587	58% 35% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 263940 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	551	4399	2766	773	845	15	1	0
1	B	551	4399	2766	773	845	15	1	0
1	C	551	4399	2766	773	845	15	1	0
1	D	551	4399	2766	773	845	15	1	0
1	E	551	4399	2766	773	845	15	1	0
1	F	551	4399	2766	773	845	15	1	0
1	G	551	4399	2766	773	845	15	1	0
1	H	551	4399	2766	773	845	15	1	0
1	I	551	4399	2766	773	845	15	1	0
1	J	551	4399	2766	773	845	15	1	0
1	K	551	4399	2766	773	845	15	1	0
1	L	551	4399	2766	773	845	15	1	0
1	M	551	4399	2766	773	845	15	1	0
1	N	551	4399	2766	773	845	15	1	0
1	O	551	4399	2766	773	845	15	1	0
1	P	551	4399	2766	773	845	15	1	0
1	Q	551	4399	2766	773	845	15	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	551	4399	2766	773	845	15	1	0
1	S	551	4399	2766	773	845	15	1	0
1	T	551	4399	2766	773	845	15	1	0
1	U	551	4399	2766	773	845	15	1	0
1	V	551	4399	2766	773	845	15	1	0
1	W	551	4399	2766	773	845	15	1	0
1	X	551	4399	2766	773	845	15	1	0
1	Y	551	4399	2766	773	845	15	1	0
1	Z	551	4399	2766	773	845	15	1	0
1	1	551	4399	2766	773	845	15	1	0
1	2	551	4399	2766	773	845	15	1	0
1	3	551	4399	2766	773	845	15	1	0
1	4	551	4399	2766	773	845	15	1	0
1	5	551	4399	2766	773	845	15	1	0
1	6	551	4399	2766	773	845	15	1	0
1	a	551	4399	2766	773	845	15	1	0
1	b	551	4399	2766	773	845	15	1	0
1	c	551	4399	2766	773	845	15	1	0
1	d	551	4399	2766	773	845	15	1	0
1	e	551	4399	2766	773	845	15	1	0
1	f	551	4399	2766	773	845	15	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	g	551	4399	2766	773	845	15	1	0
1	h	551	4399	2766	773	845	15	1	0
1	i	551	4399	2766	773	845	15	1	0
1	j	551	4399	2766	773	845	15	1	0
1	k	551	4399	2766	773	845	15	1	0
1	l	551	4399	2766	773	845	15	1	0
1	m	551	4399	2766	773	845	15	1	0
1	n	551	4399	2766	773	845	15	1	0
1	o	551	4399	2766	773	845	15	1	0
1	p	551	4399	2766	773	845	15	1	0
1	q	551	4399	2766	773	845	15	1	0
1	r	551	4399	2766	773	845	15	1	0
1	s	551	4399	2766	773	845	15	1	0
1	t	551	4399	2766	773	845	15	1	0
1	u	551	4399	2766	773	845	15	1	0
1	v	551	4399	2766	773	845	15	1	0
1	w	551	4399	2766	773	845	15	1	0
1	x	551	4399	2766	773	845	15	1	0
1	y	551	4399	2766	773	845	15	1	0
1	z	551	4399	2766	773	845	15	1	0
1	7	551	4399	2766	773	845	15	1	0

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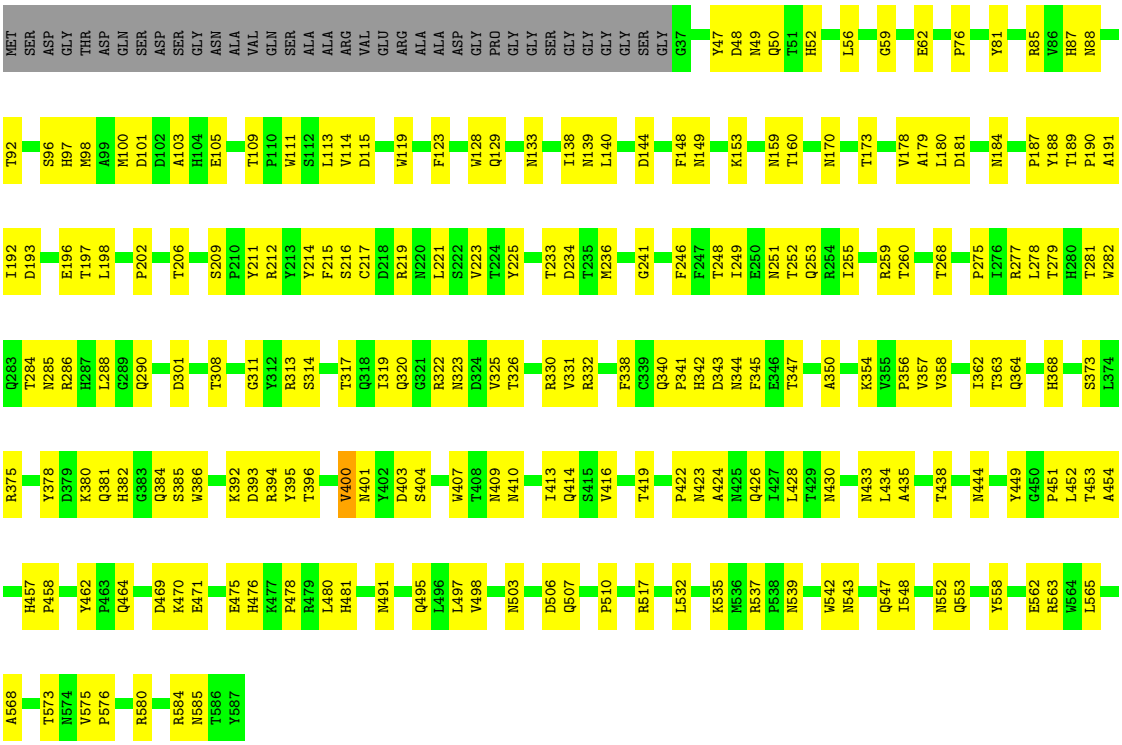
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8	551	4399	2766	773	845	15	1	0

3 Residue-property plots (i)

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

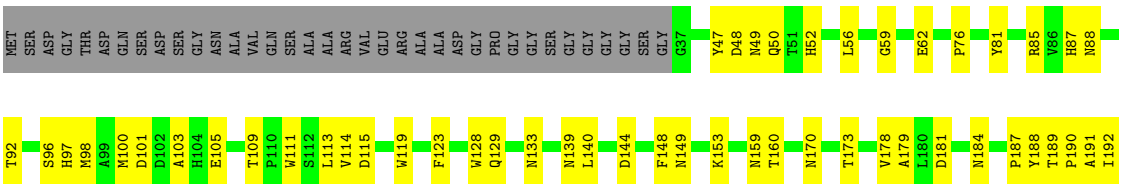
• Molecule 1: Capsid protein VP2

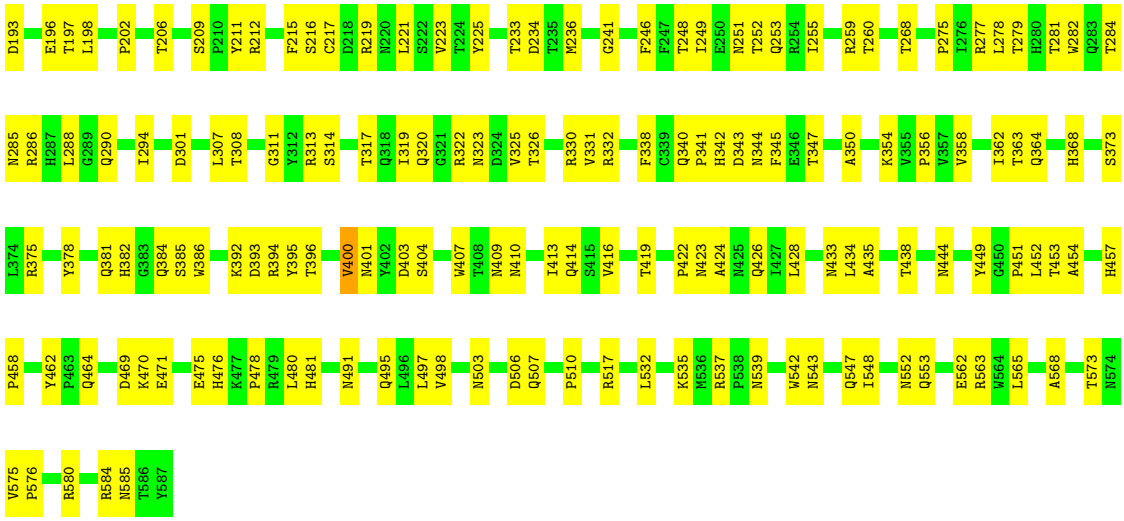
Chain A: 58% 36% 6%



• Molecule 1: Capsid protein VP2

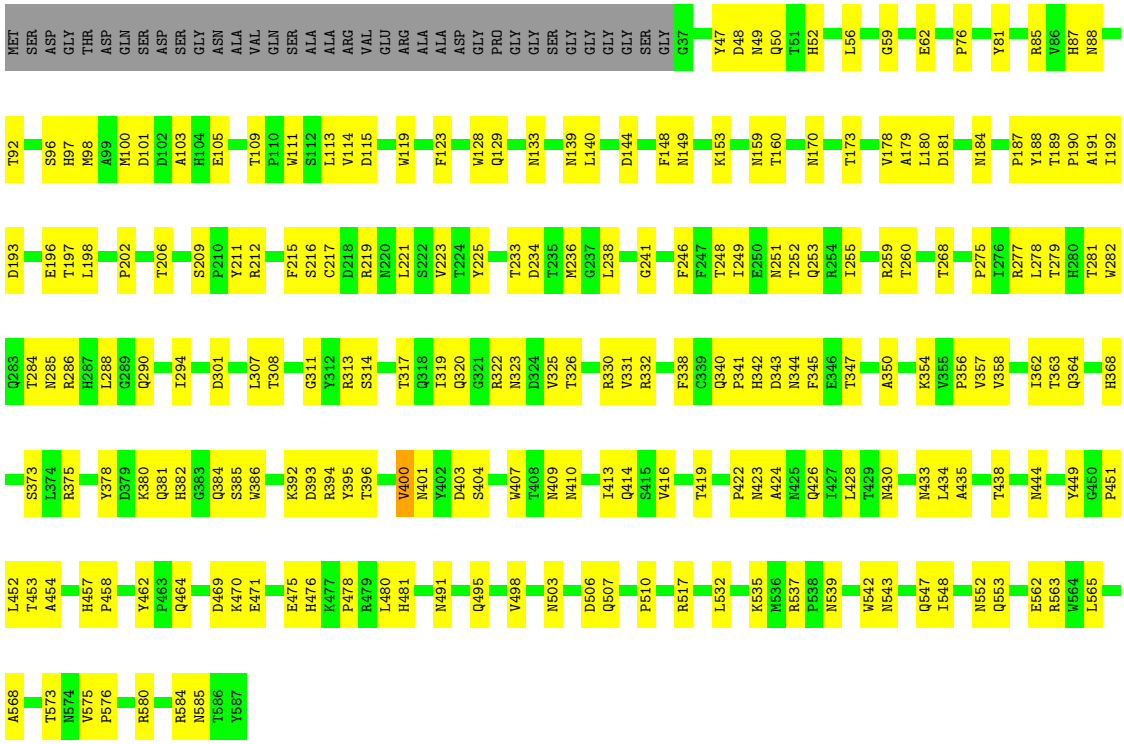
Chain B: 59% 35% 6%





- Molecule 1: Capsid protein VP2

Chain C:



- Molecule 1: Capsid protein VP2

Chain D:

T92 S96 H97 M98 A99 M100 D101 D102 A103 H104 E105 T109 P110 W111 S112 L113 V114 D115 W119 F123 W128 Q129 N133 I138 N139 L140 D144 F148 N149 K153 N159 T160 N170 T173 V178 A179 L180 D181 N184 P187 Y188 T189 P190 A191

I192 D193 E196 T197 L198 P202 T206 S209 P210 Y211 R212 Y213 Y214 F215 S216 C217 D218 R219 N220 L221 S222 V223 T224 Y225 T233 D234 T235 M236 G241 F246 F247 T248 I249 E250 N251 T252 Q253 R254 I255 R259 T260 T268 P275 I276 R277 L278 T279 H280 T281 W282

Q283 T284 N285 R286 H287 L288 G289 Q290 I294 D301 L307 T308 G311 Y312 R313 S314 T317 Q320 G321 R322 N323 D324 V325 T326 E327 R330 V331 R332 F338 C339 Q340 P341 H342 D343 N344 F345 E346 T347 A350 K354 V355 P356 V357 V358 I362 T363 Q364 H368

S373 L374 R375 Y378 Q381 H382 G383 Q384 S385 W386 K392 D393 R394 Y395 T396 V400 N401 Y402 D403 S404 W407 T408 N409 N410 I413 Q414 S415 V416 T419 N423 A424 N425 Q426 I427 L428 T429 N430 N433 L434 A435 T438 N444 Y449 G450 P451 L452 T453

A454 H457 P458 Y462 P463 Q464 D469 K470 E471 E475 H476 K477 P478 R479 L480 H481 N491 Q495 L496 L497 V498 N503 D506 Q507 P510 R517 L532 K535 M536 R537 P538 N539 W542 N543 Q547 I548 N552 Q553 Y558 E562 R563 W564 L565

A568 T573 N574 V575 P576 R580 R584 N585 T586 Y587

- Molecule 1: Capsid protein VP2

Chain E: 59% 35% 6%

MET SER ASP GLY THR ASP GLN SER ASP SER GLY ASN ALA VAL GLN SER ALA ALA ARG VAL GLU ARG ALA ALA ASP GLY PRO GLY GLY SER GLY GLY GLY GLY GLY SER GLY G37 Y47 D48 N49 Q50 T51 H52 L56 G59 E62 P76 Y81 R85 V86 H87 N88

T92 S96 H97 M98 A99 M100 D101 D102 A103 H104 E105 T109 P110 W111 S112 L113 V114 D115 W119 F123 W128 Q129 N133 N139 L140 D144 F148 N149 K153 N159 T160 N170 T173 V178 A179 L180 N184 P187 Y188 T189 P190 A191 I192 D193

E196 T197 L198 P202 T206 S209 P210 Y211 R212 Y213 Y214 F215 S216 C217 D218 R219 N220 L221 S222 V223 T224 Y225 T233 D234 T235 M236 G241 F246 F247 T248 I249 E250 N251 T252 Q253 R254 I255 R259 T260 T268 P275 I276 R277 L278 T279 H280 T281 W282 Q283 T284

N285 R286 H287 L288 G289 Q290 D301 T308 G311 Y312 R313 S314 T317 Q318 I319 Q320 G321 R322 N323 D324 V325 T326 E327 R330 V331 R332 F338 C339 Q340 P341 H342 D343 N344 F345 E346 T347 A350 K354 V355 P356 V357 V358 I362 T363 Q364 H368 S373 L374 R375

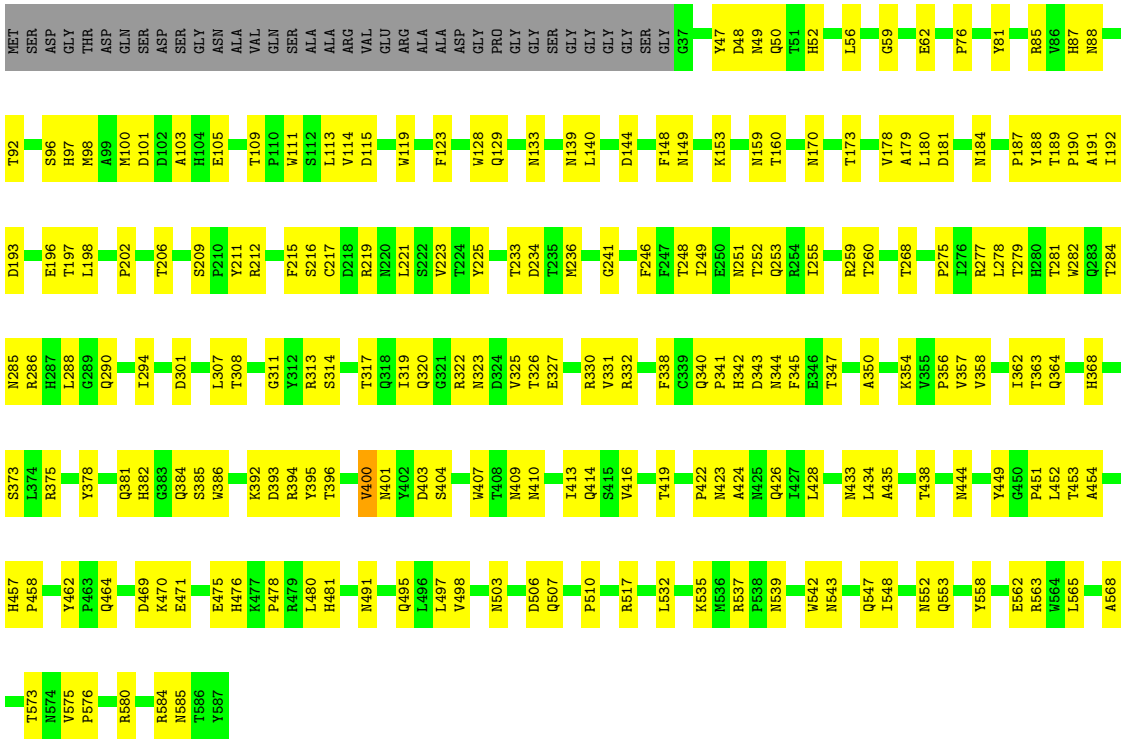
Y378 Q381 H382 G383 Q384 S385 W386 K392 D393 R394 Y395 T396 V400 N401 Y402 D403 S404 W407 T408 N409 N410 I413 Q414 S415 V416 T419 P422 N423 A424 N425 Q426 I427 L428 N433 L434 A435 T438 N444 Y449 G450 P451 L452 T453 A454 H457 P458

Y462 P463 Q464 D469 K470 E471 E475 H476 K477 P478 R479 L480 H481 N491 Q495 V498 N503 D506 Q507 P510 R517 L532 K535 M536 R537 P538 N539 W542 N543 Q547 I548 N552 Q553 Y558 E562 R563 W564 L565 A568 T573 N574 V575

P576 R580 R584 N585 T586 Y587

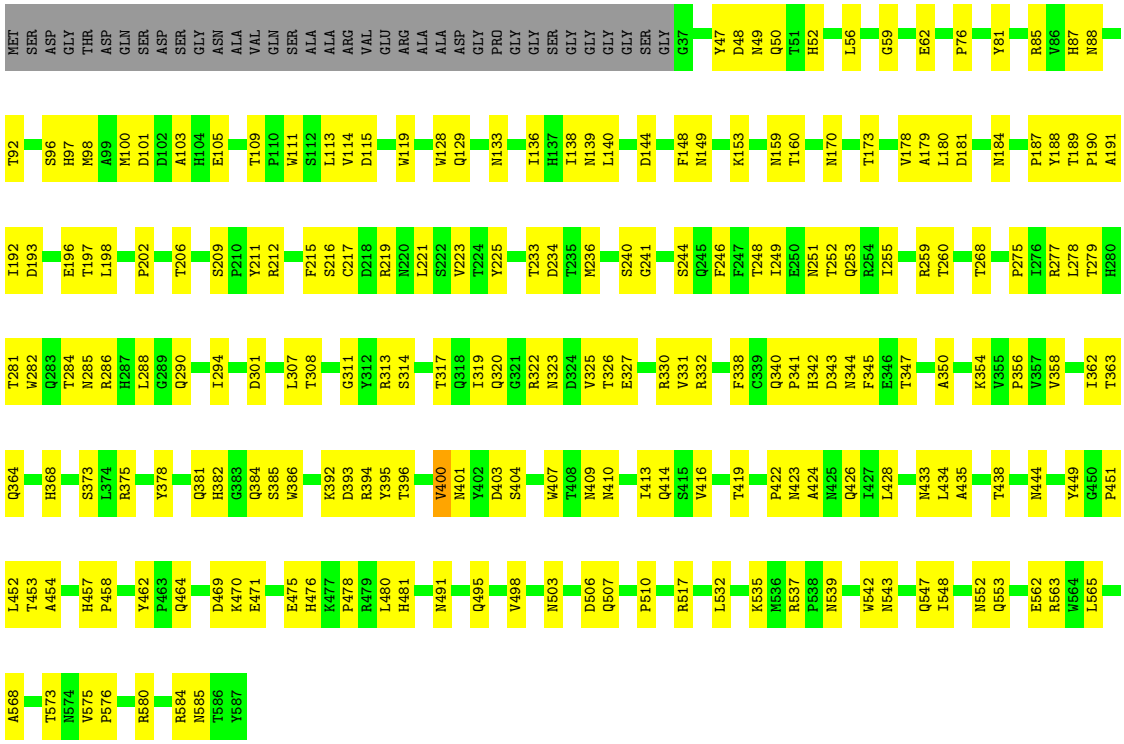
- Molecule 1: Capsid protein VP2

Chain F: 58% 35% 6%



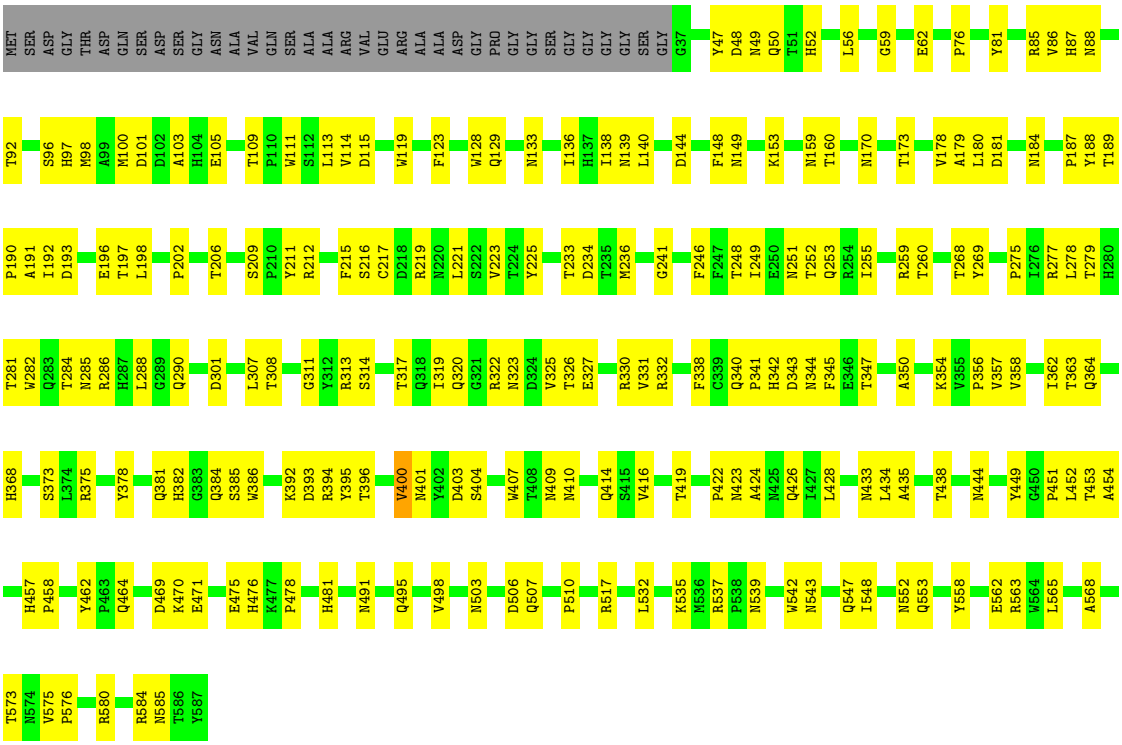
• Molecule 1: Capsid protein VP2

Chain G:



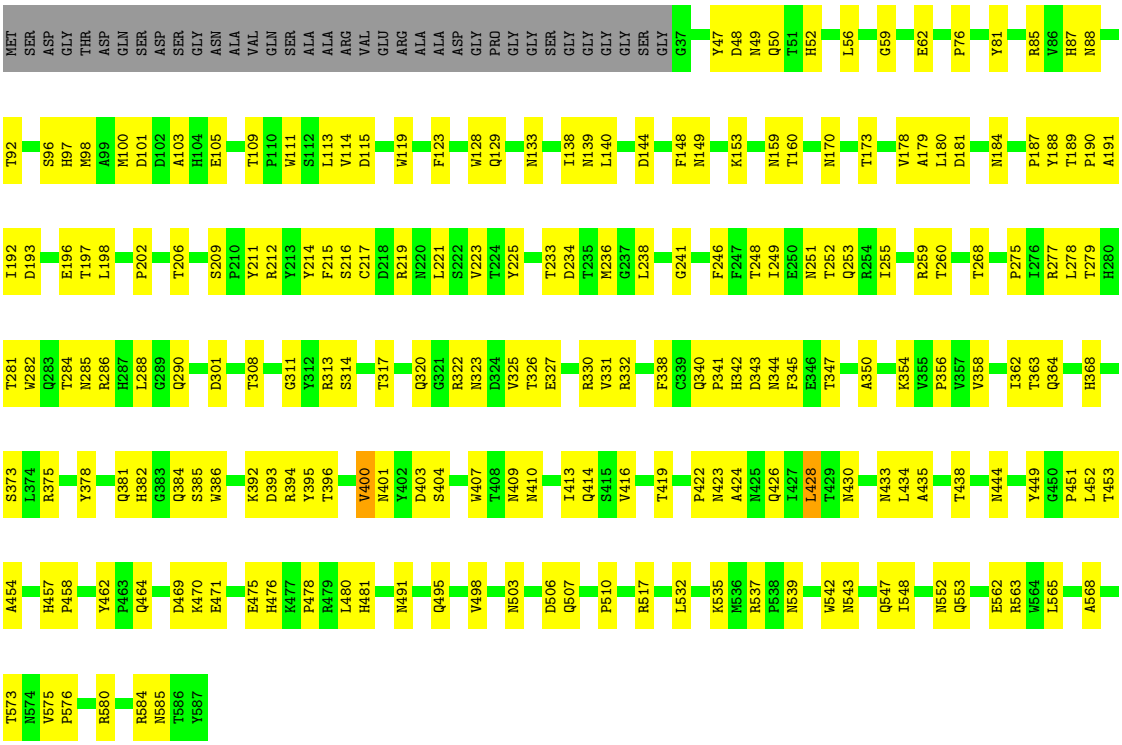
• Molecule 1: Capsid protein VP2

Chain H: 58% 35% 6%



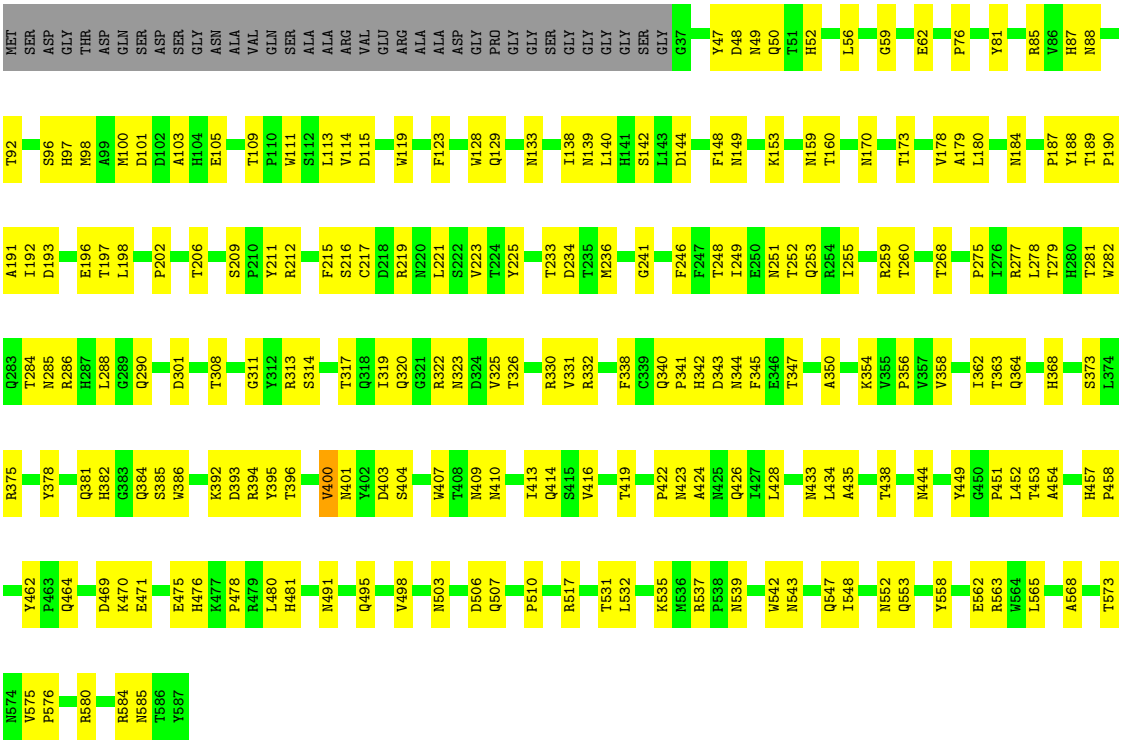
- Molecule 1: Capsid protein VP2

Chain I: 59% 35% 6%



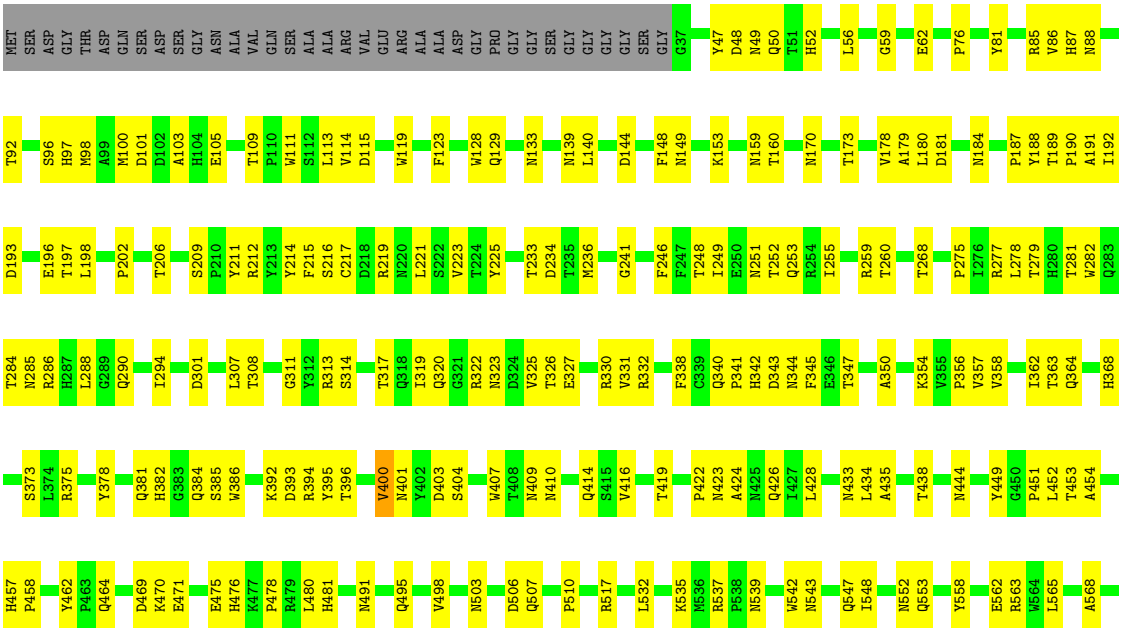
- Molecule 1: Capsid protein VP2

Chain J: 59% 35% 6%



- Molecule 1: Capsid protein VP2

Chain K: 58% 35% 6%



T573 N574 V575 P576 R580 R584 N585 T586 Y587

• Molecule 1: Capsid protein VP2

Chain L: 59% 35% 6%

MET SER ASP GLY THR ASP GLN SER ASP SER GLY ASN ALA VAL GLN SER ALA ALA ARG VAL GLU ARG ALA ALA ASP GLY PRO GLY GLY SER GLY GLY GLY GLY SER GLY G37 Y47 D48 N49 Q50 T51 H52 L56 G59 E62 P76 R85 V86 H87 N88 T92

S96 H97 M98 A99 M100 D101 D102 A103 H104 E105 T109 P110 W111 S112 L113 V114 D115 W119 F123 W128 Q129 N133 I138 N139 L140 D144 F148 N149 K153 N159 T160 N170 T173 V178 A179 L180 D181 N184 P187 Y188 T189 P190 A191 I192 D193

E196 T197 L198 P202 T206 S209 P210 Y211 R212 F215 S216 C217 D218 R219 N220 L221 S222 V223 T224 Y225 T233 D234 T235 M236 G237 L238 G241 F246 I249 E250 N251 T252 Q253 R254 I255 R259 T260 T268 P275 I276 R277 L278 T279 H280 T281 W282 Q283 T284

N285 R286 H287 L288 G289 Q290 D301 T308 G311 Y312 R313 S314 T317 Q318 I319 Q320 G321 R322 N323 D324 V325 T326 R330 V331 R332 F338 C339 Q340 P341 H342 D343 N344 F345 E346 T347 A350 K354 V355 P356 V357 V358 I362 T363 Q364 H368 S373 L374 R375

Y378 Q381 H382 G383 Q384 S385 W386 K392 D393 R394 Y395 T396 V400 N401 Y402 D403 S404 W407 T408 N409 N410 I413 Q414 S415 V416 T419 P422 N423 A424 N425 Q426 I427 L428 N433 L434 A435 T438 N444 Y449 G450 P451 L452 T453 A454 H457 P458 Y462

P463 Q464 D469 K470 E471 E475 H476 K477 P478 R479 L480 H481 N491 Q495 L496 L497 V498 N503 D506 Q507 P510 R517 L532 K535 M536 R537 P538 N539 W542 N543 Q547 I548 N552 Q553 Y558 E562 R563 W564 L565 A568 T573 N574 V575

P576 R580 R584 N585 T586 Y587

• Molecule 1: Capsid protein VP2

Chain M: 58% 36% 6%

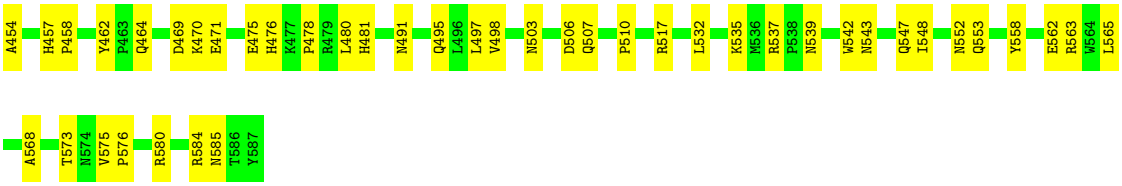
MET SER ASP GLY THR ASP GLN SER ASP SER GLY ASN ALA VAL GLN SER ALA ALA ARG VAL GLU ARG ALA ALA ASP GLY PRO GLY GLY SER GLY GLY GLY GLY SER GLY G37 Y47 D48 N49 Q50 T51 H52 L56 G59 E62 P76 Y81 R85 V86 H87 N88

T92 S96 H97 M98 A99 M100 D101 D102 A103 H104 E105 T109 P110 W111 S112 L113 V114 D115 W119 F123 W128 Q129 N133 N139 L140 D144 F148 N149 K153 N159 T160 N170 T173 V178 A179 L180 D181 N184 P187 Y188 T189 P190 A191 I192

D193 E196 T197 L198 P202 T206 S209 P210 Y211 R212 Y213 Y214 F215 S216 C217 D218 R219 N220 L221 S222 V223 T224 Y225 T233 D234 T235 M236 S240 G241 S244 Q245 F246 F247 T248 I249 E250 N251 T252 Q253 R254 I255 R259 T260 T268 P275 I276 R277 L278 T279 H280

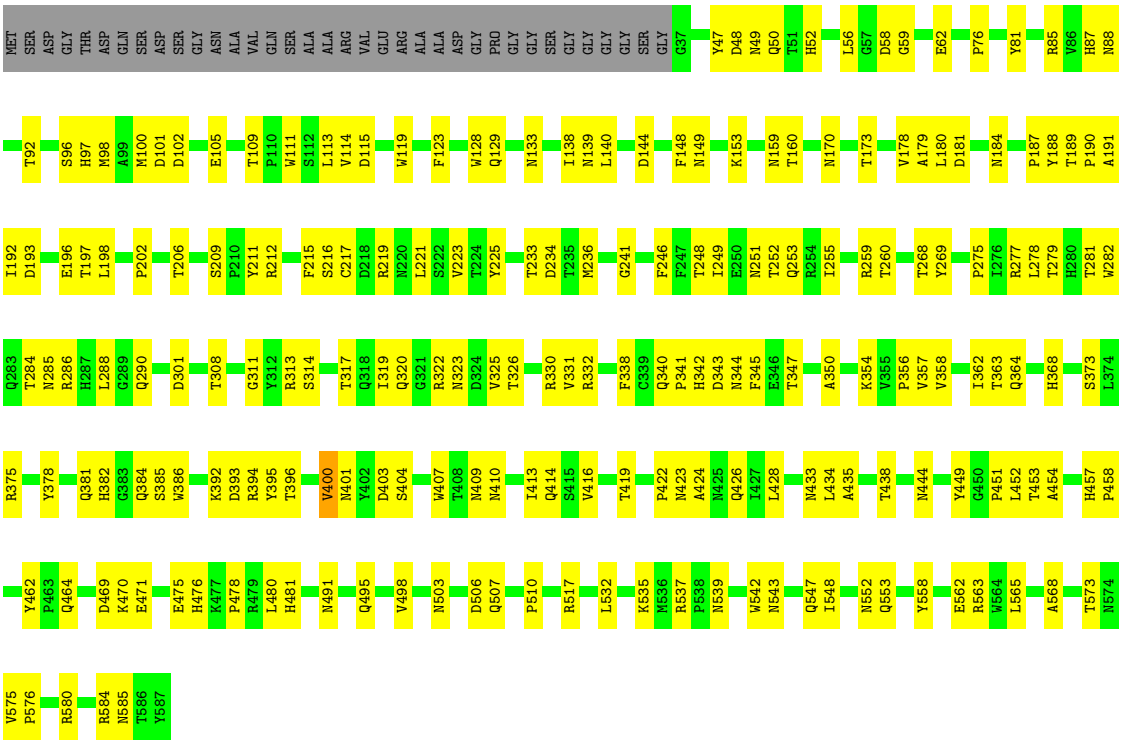
T281 W282 Q283 T284 N285 R286 H287 L288 G289 Q290 D301 T308 G311 Y312 R313 S314 T317 Q318 I319 Q320 G321 R322 N323 D324 V325 T326 R330 V331 R332 F338 C339 Q340 P341 H342 D343 N344 F345 E346 T347 A350 K354 V355 P356 V357 V358 I362 T363 Q364 H368

S373 L374 R375 Y378 Q381 H382 G383 Q384 S385 W386 K392 D393 R394 Y395 T396 V400 N401 Y402 D403 S404 W407 T408 N409 N410 I413 Q414 S415 V416 T419 P422 N423 A424 N425 Q426 I427 L428 T429 N430 N433 L434 A435 T438 N444 Y449 G450 P451 L452 T453



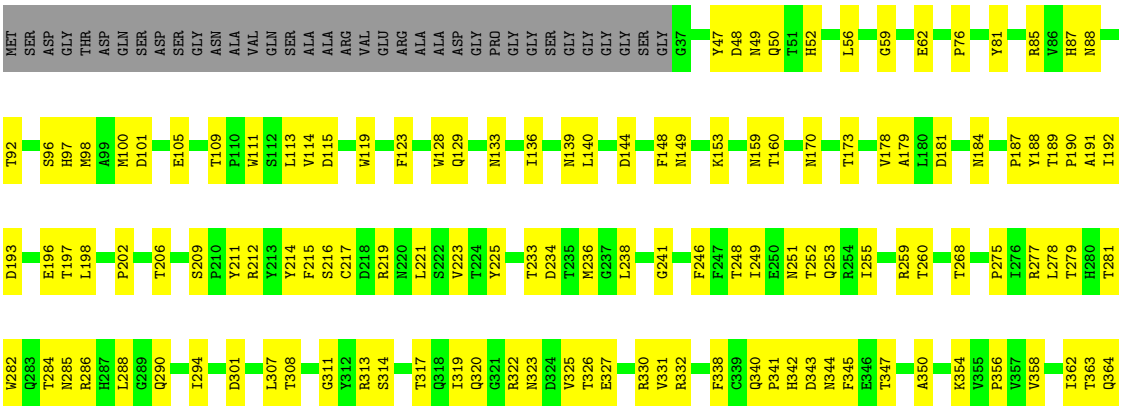
• Molecule 1: Capsid protein VP2

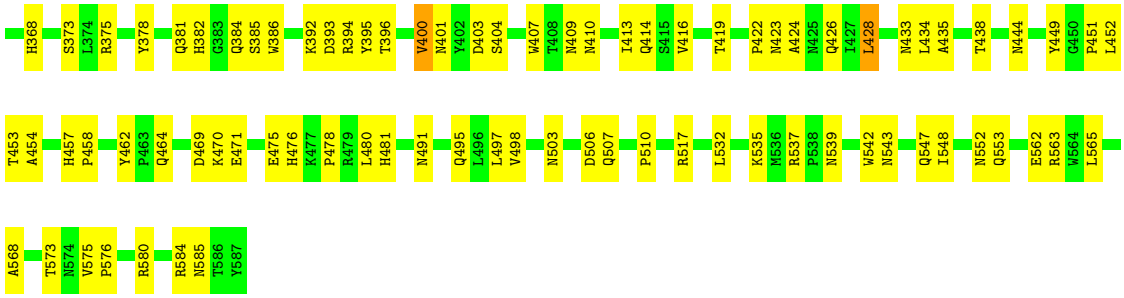
Chain N:



• Molecule 1: Capsid protein VP2

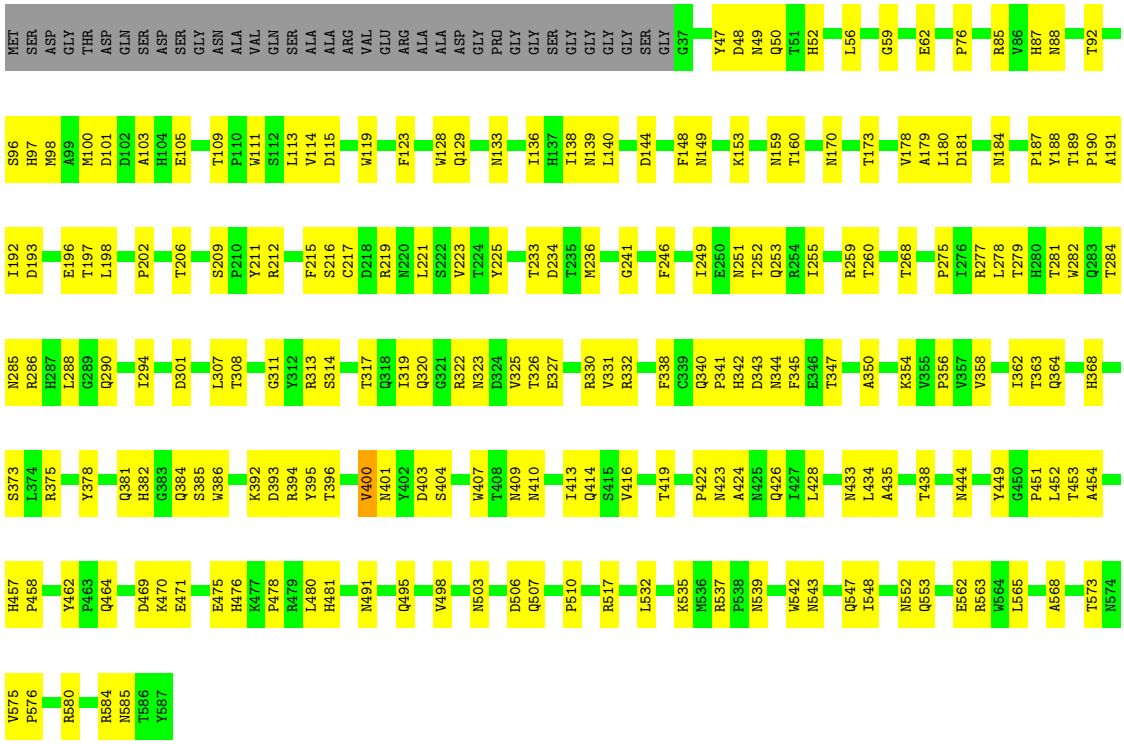
Chain O:





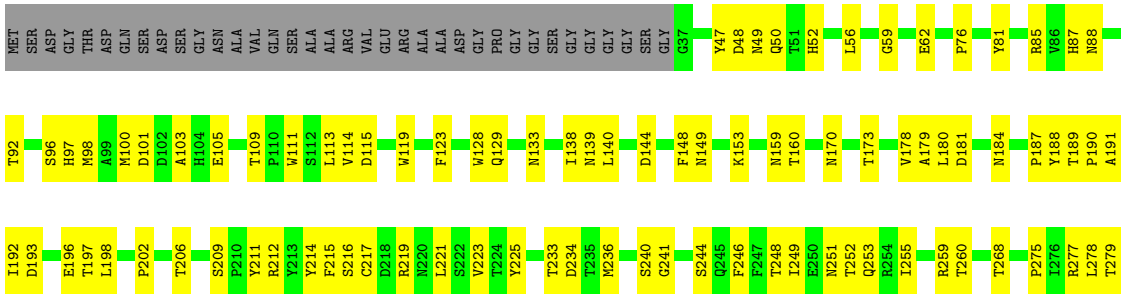
- Molecule 1: Capsid protein VP2

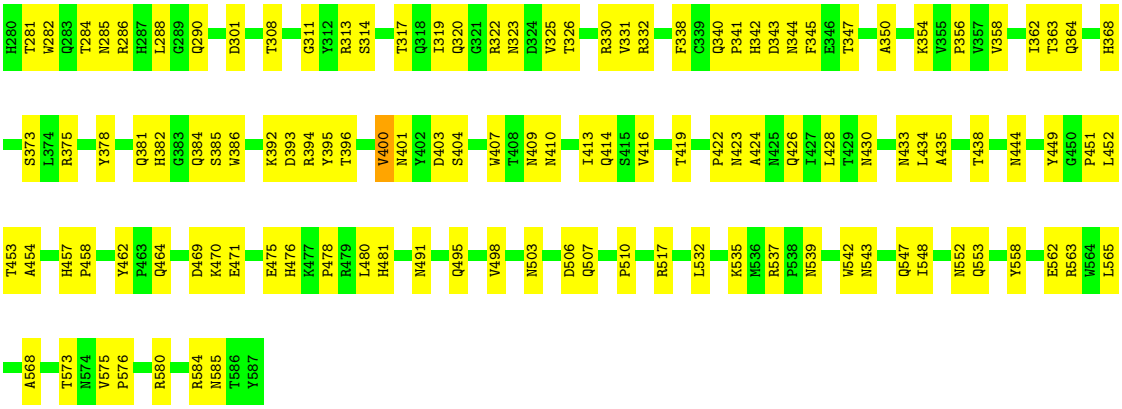
Chain P:



- Molecule 1: Capsid protein VP2

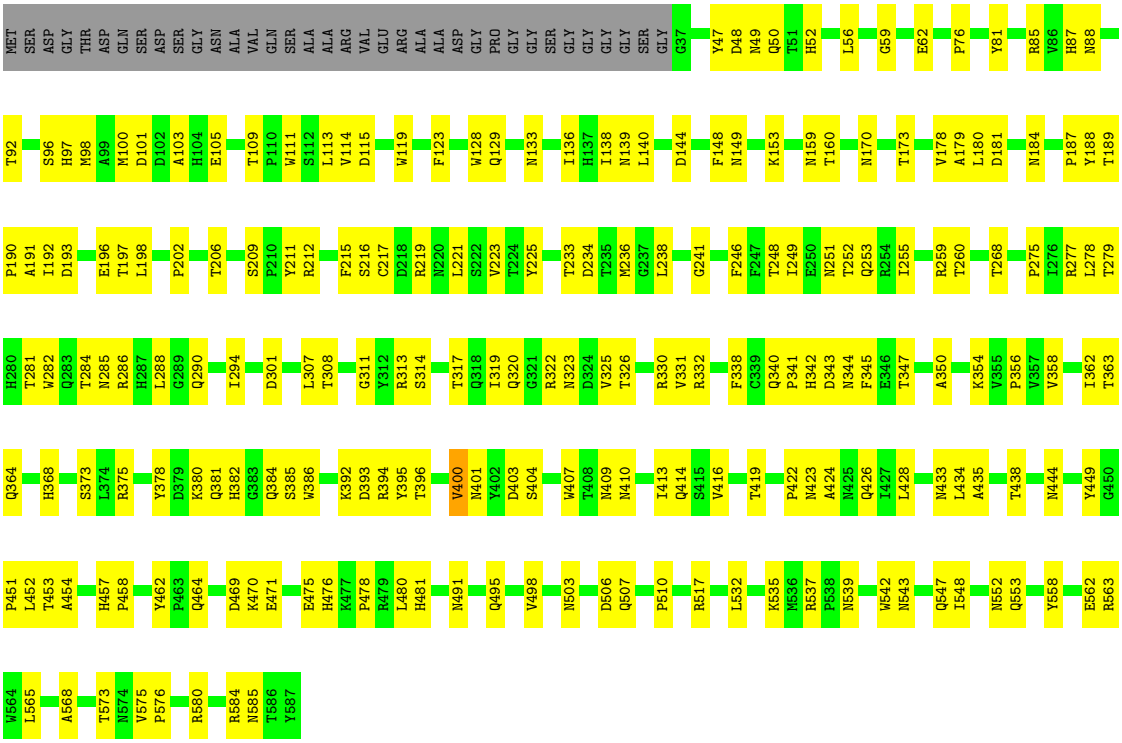
Chain Q:





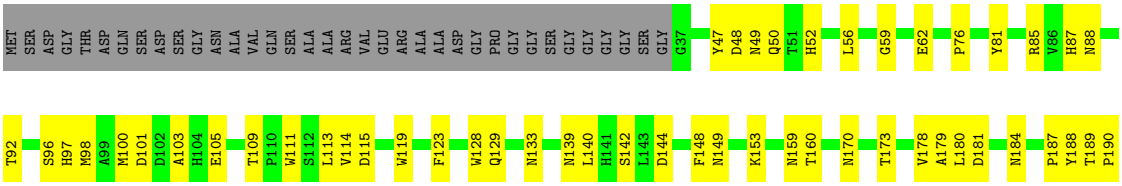
- Molecule 1: Capsid protein VP2

Chain R:



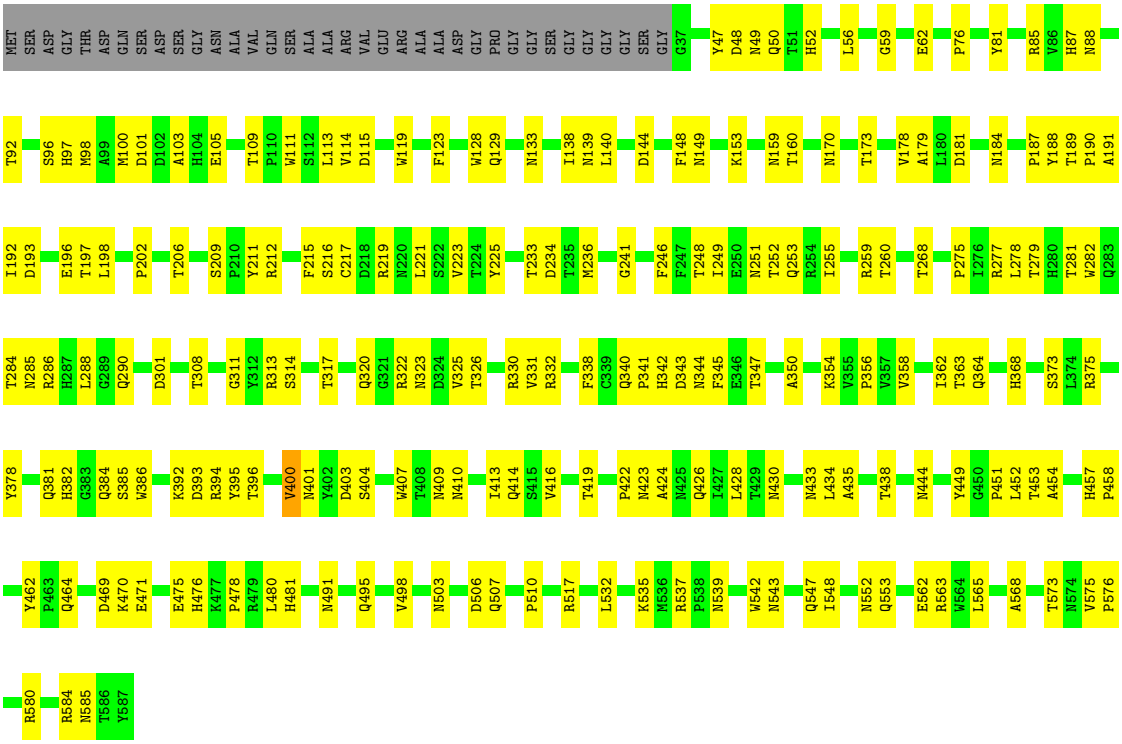
- Molecule 1: Capsid protein VP2

Chain S:



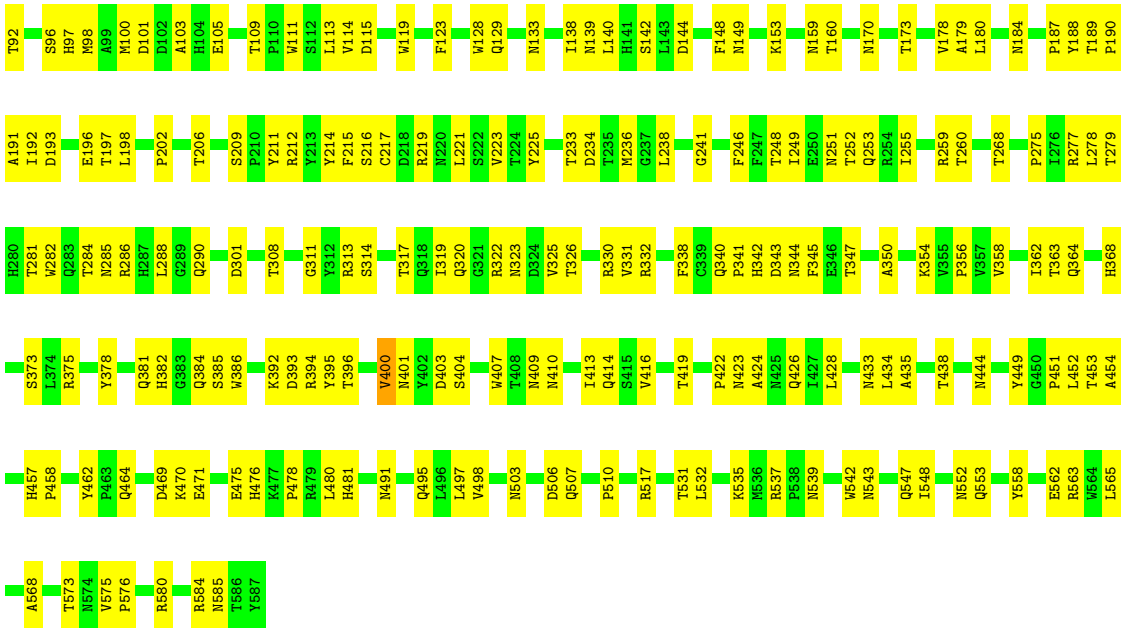
- Molecule 1: Capsid protein VP2

Chain T:



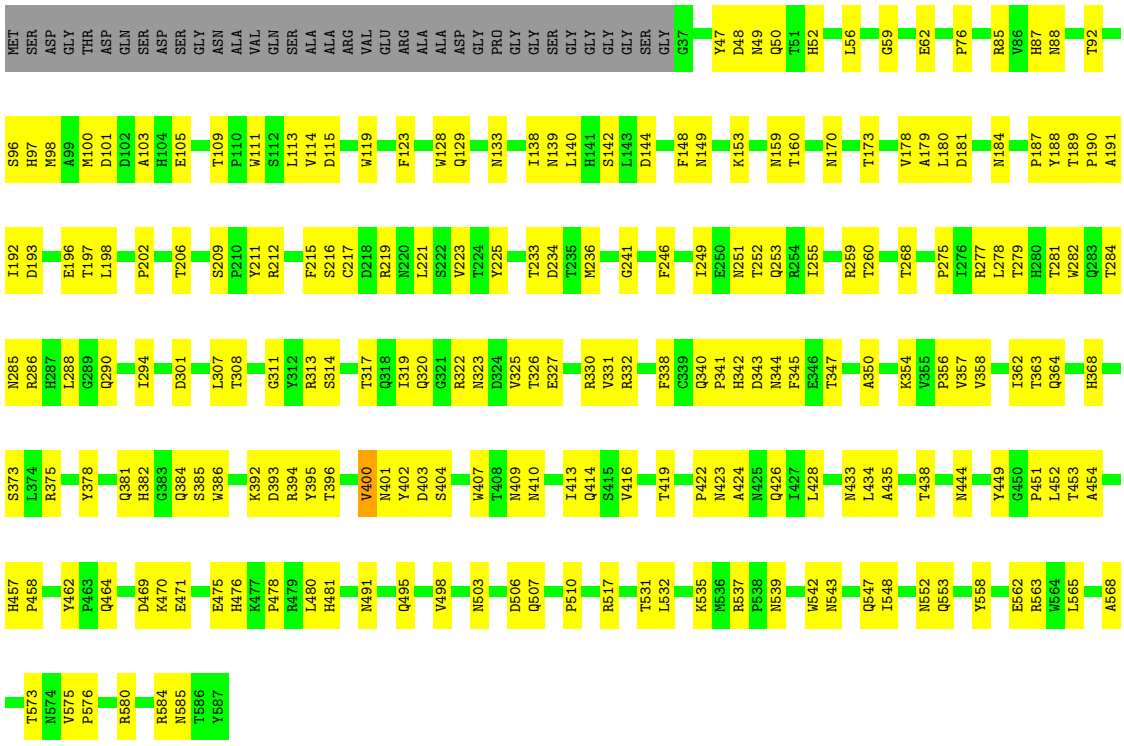
- Molecule 1: Capsid protein VP2

Chain U:



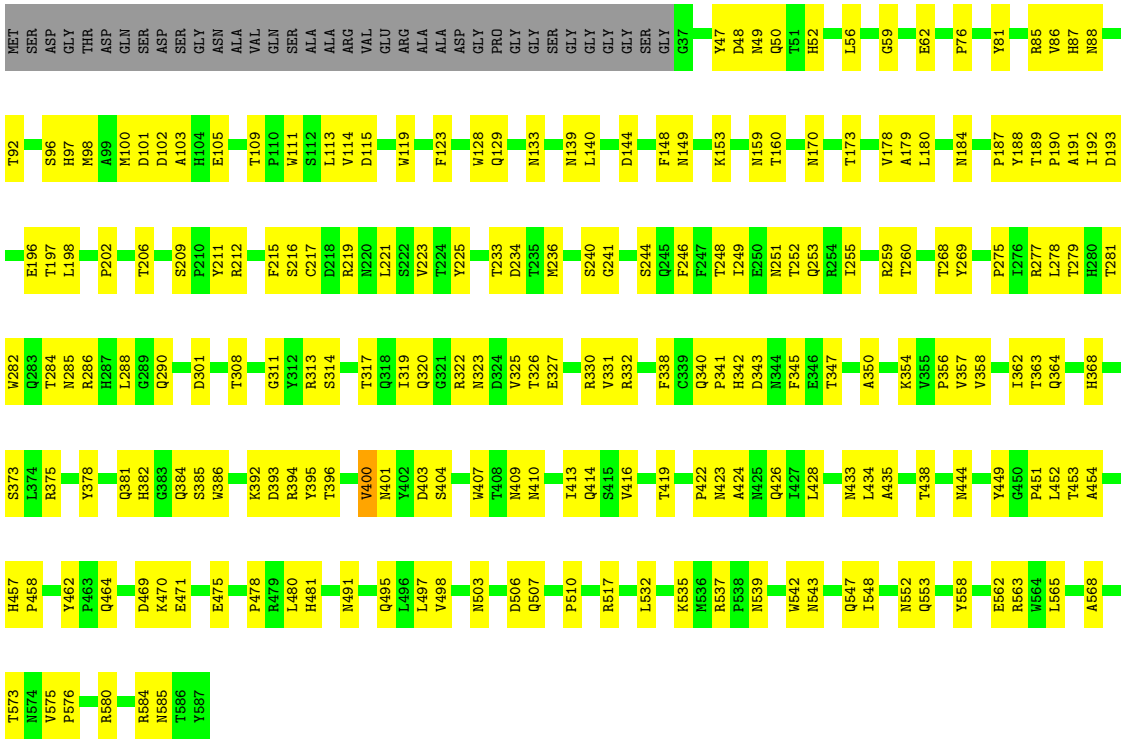
- Molecule 1: Capsid protein VP2

Chain V:



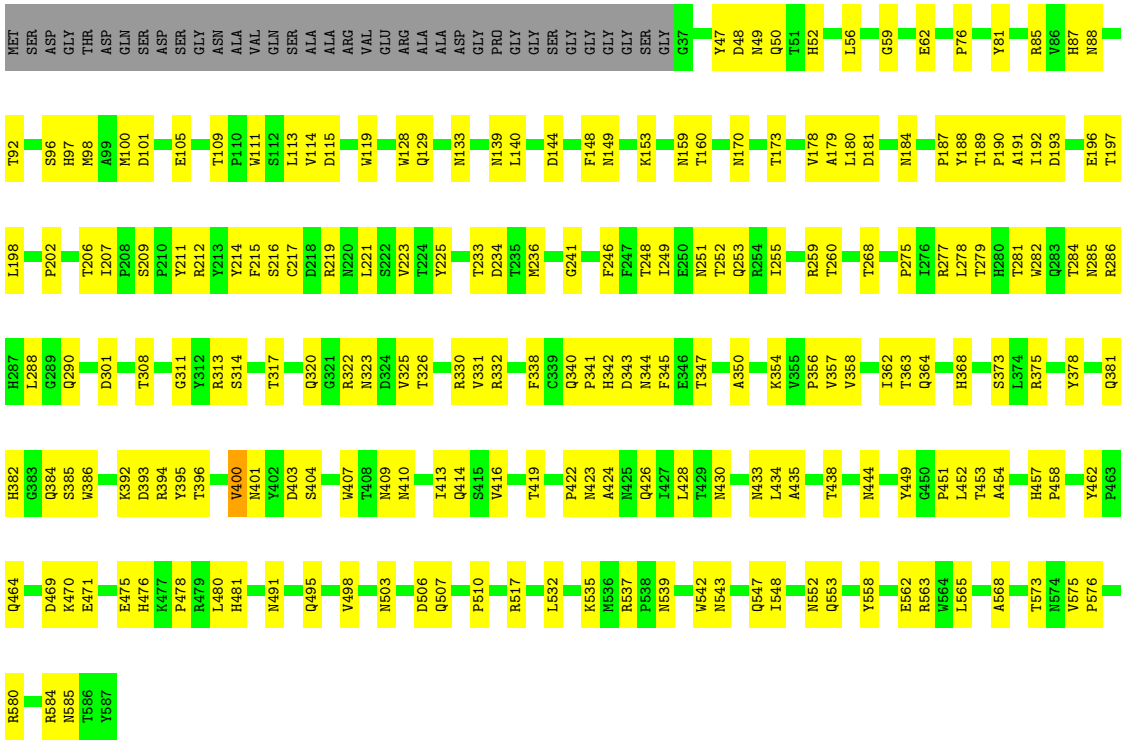
- Molecule 1: Capsid protein VP2

Chain W:



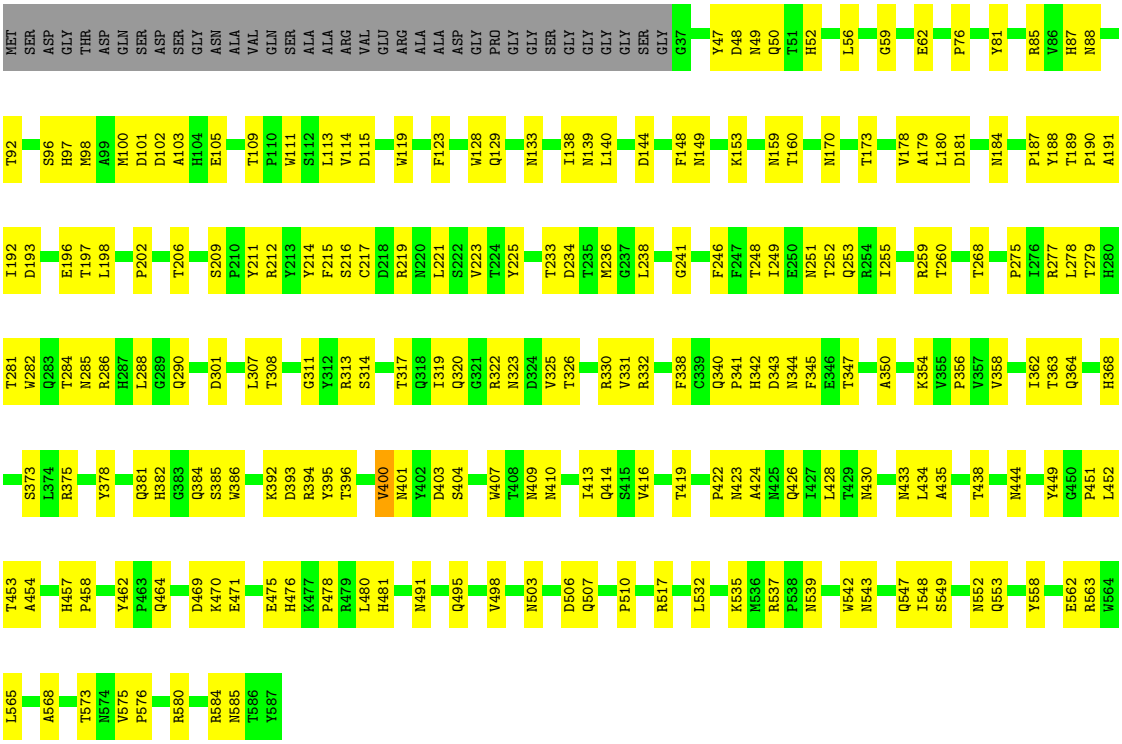
- Molecule 1: Capsid protein VP2

Chain X:



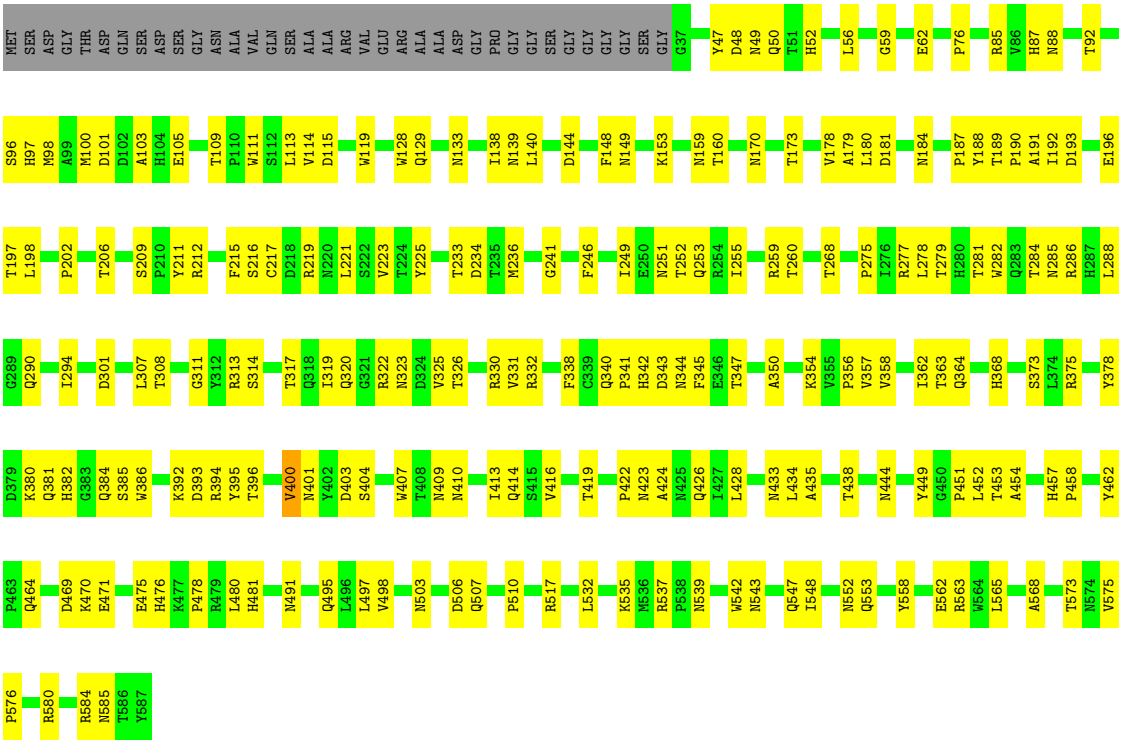
- Molecule 1: Capsid protein VP2

Chain Y: 58% 36% 6%



- Molecule 1: Capsid protein VP2

Chain Z: 59% 35% 6%



• Molecule 1: Capsid protein VP2

Chain 1: 59% 35% 6%

MET SER ASP GLY THR ASP GLN SER ASP SER GLY ASN ALA VAL GLN SER ALA ALA ARG VAL GLU ARG ALA ALA ASP GLY PRO GLY GLY SER GLY GLY GLY GLY SER GLY G37 Y47 D48 N49 Q50 T51 H52 L56 G59 E62 P76 Y81 R85 V86 H87 N88

T92 S96 H97 M98 A99 M100 D101 D102 E105 T109 P110 W111 S112 L113 V114 D115 W119 F123 W128 Q129 N133 N139 L140 D144 F148 N149 K153 N159 T160 N170 T173 V178 A179 L180 N184 P187 Y188 T189 P190 A191 I192 D193

E196 T197 L198 P202 T206 S209 P210 Y211 R212 F215 S216 C217 D218 R219 N220 L221 S222 V223 T224 Y225 T233 D234 T235 M236 G237 L238 G241 F246 F247 T248 I249 E250 N251 T252 Q253 R254 I255 R259 T260 T268 P275 I276 R277 L278 T279 H280 T281 W282 Q283 T284

N285 R286 H287 L288 G289 Q290 D301 T308 G311 Y312 R313 S314 T317 Q318 I319 Q320 G321 R322 N323 D324 V325 T326 E327 R330 V331 R332 F338 C339 Q340 P341 H342 D343 N344 F345 E346 T347 A350 K354 V355 P356 V357 V358 I362 T363 Q364 H368 S373 L374 R375

Y378 Q381 H382 G383 Q384 S385 W386 K392 D393 R394 Y395 T396 V400 N401 Y402 D403 S404 W407 T408 N409 N410 I413 Q414 S415 V416 T419 P422 N423 A424 N425 Q426 I427 L428 T429 N430 N433 L434 A435 T438 N444 Y449 G450 P451 L452 T453 A454 H457

P458 Y462 P463 Q464 D469 K470 E471 E475 H476 K477 P478 R479 L480 H481 N491 Q495 V498 N503 D506 Q507 P510 R517 L532 K535 M536 R537 P538 N539 W542 N543 Q547 I548 N552 Q553 Y558 E562 R563 W564 L565 A568 T573

N574 V575 P576 R580 R584 N585 T586 Y587

• Molecule 1: Capsid protein VP2

Chain 2: 58% 36% 6%

MET SER ASP GLY THR ASP GLN SER ASP SER GLY ASN ALA VAL GLN SER ALA ALA ARG VAL GLU ARG ALA ALA ASP GLY PRO GLY GLY SER GLY GLY GLY GLY SER GLY G37 Y47 D48 N49 Q50 T51 H52 L56 G59 E62 P76 Y81 R85 V86 H87 N88

T92 S96 H97 M98 A99 M100 D101 D102 A103 H104 E105 T109 P110 W111 S112 L113 V114 D115 W119 F123 W128 Q129 N133 I136 N139 L140 D144 F148 N149 K153 N159 T160 N170 T173 V178 A179 L180 D181 N184 P187 Y188 T189 P190

A191 I192 D193 E196 T197 L198 P202 T206 S209 P210 Y211 R212 F215 S216 C217 D218 R219 N220 L221 S222 V223 T224 Y225 T233 D234 T235 M236 G237 L238 G241 F246 F247 T248 I249 E250 N251 T252 Q253 R254 I255 R259 T260 T268 P275 I276 R277 L278 T279 H280

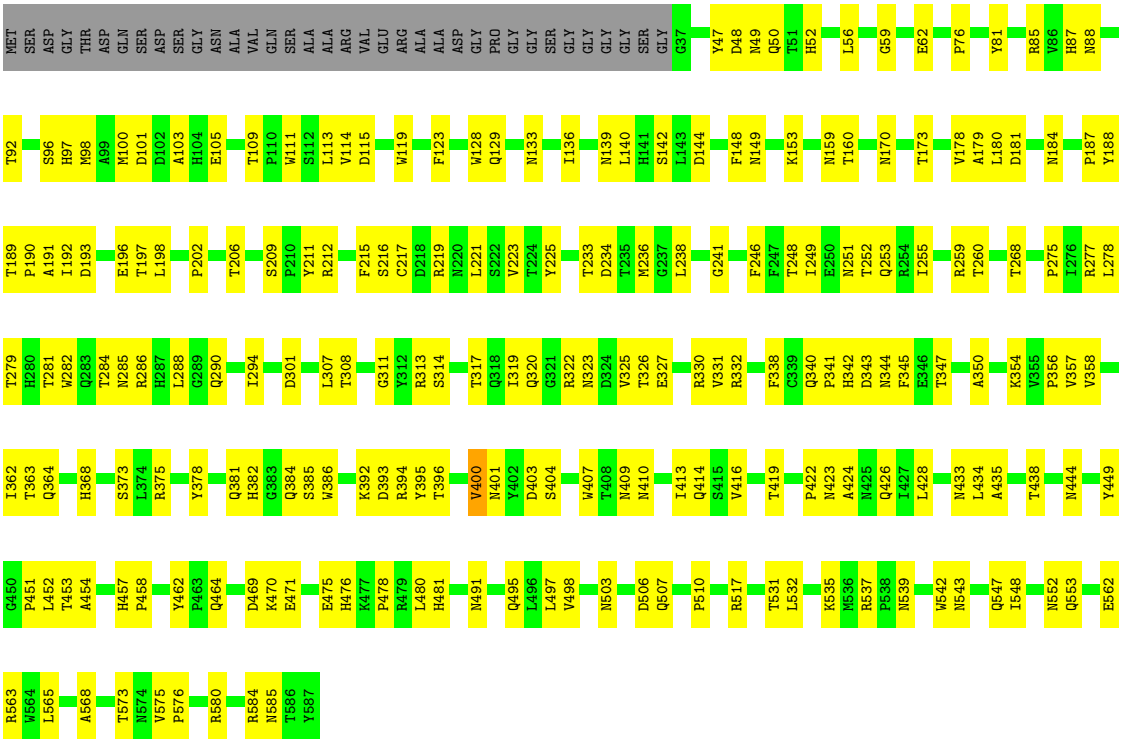
T281 W282 Q283 T284 N285 R286 H287 L288 G289 Q290 I294 D301 L307 T308 G311 Y312 R313 S314 T317 Q318 I319 Q320 G321 R322 N323 D324 V325 T326 E327 R330 V331 R332 F338 C339 Q340 P341 H342 D343 N344 F345 E346 T347 A350 K354 V355 P356 V357 V358 I362 T363

Q364 H368 S373 L374 R375 Y378 Q381 H382 G383 Q384 S385 W386 K392 D393 R394 Y395 T396 V400 N401 Y402 D403 S404 W407 T408 N409 N410 I413 Q414 S415 V416 T419 P422 N423 A424 N425 Q426 I427 L428 N433 L434 A435 T438 N444 Y449 G450 P451

L452 T453 A454 H457 P458 Y462 P463 Q464 D469 K470 E471 E475 H476 K477 P478 R479 L480 H481 N491 Q495 L496 L497 V498 N503 D506 Q507 P510 R517 L532 K535 M536 R537 P538 N539 W542 N543 Q547 I548 N552 Q553 E562 R563 W564 L565

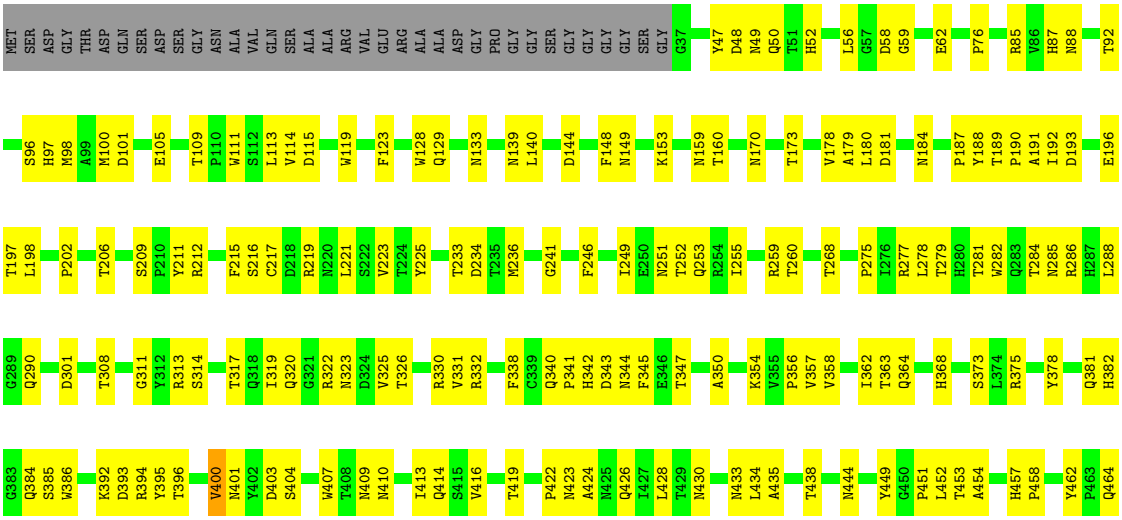
• Molecule 1: Capsid protein VP2

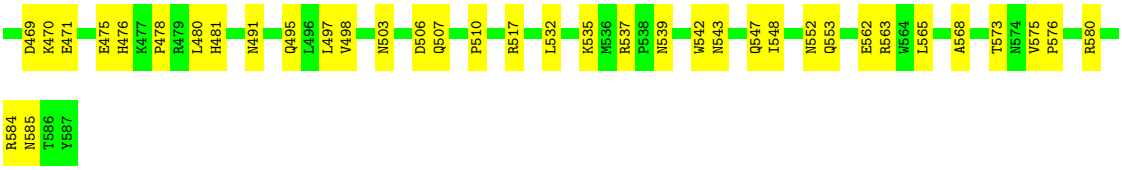
Chain 3:



• Molecule 1: Capsid protein VP2

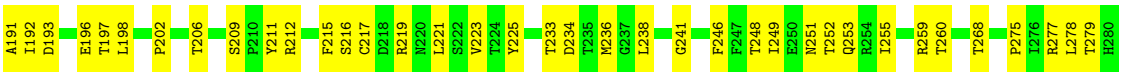
Chain 4:

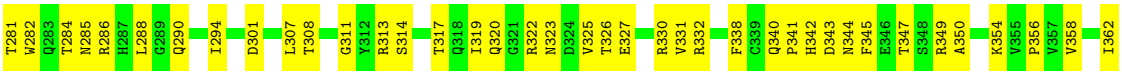




• Molecule 1: Capsid protein VP2

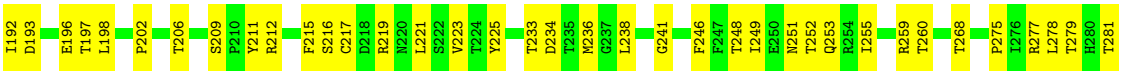
Chain 5:

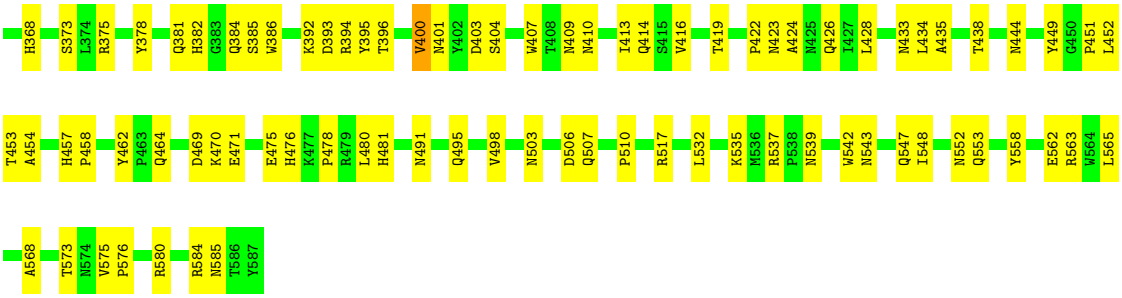




• Molecule 1: Capsid protein VP2

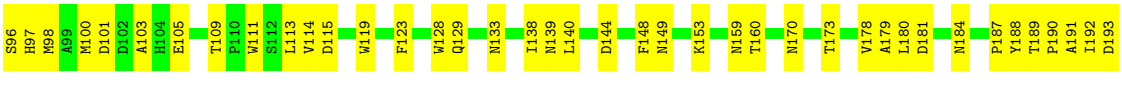
Chain 6:

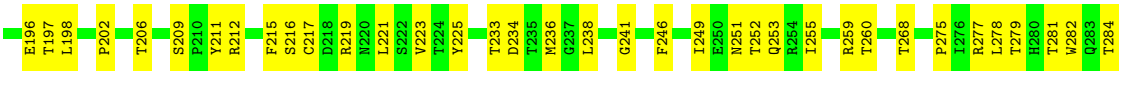


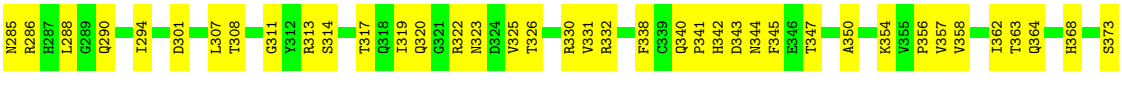


• Molecule 1: Capsid protein VP2

Chain a:

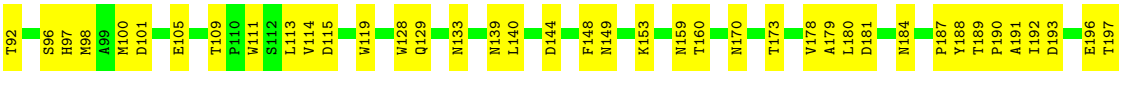


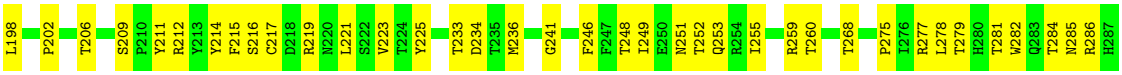




• Molecule 1: Capsid protein VP2

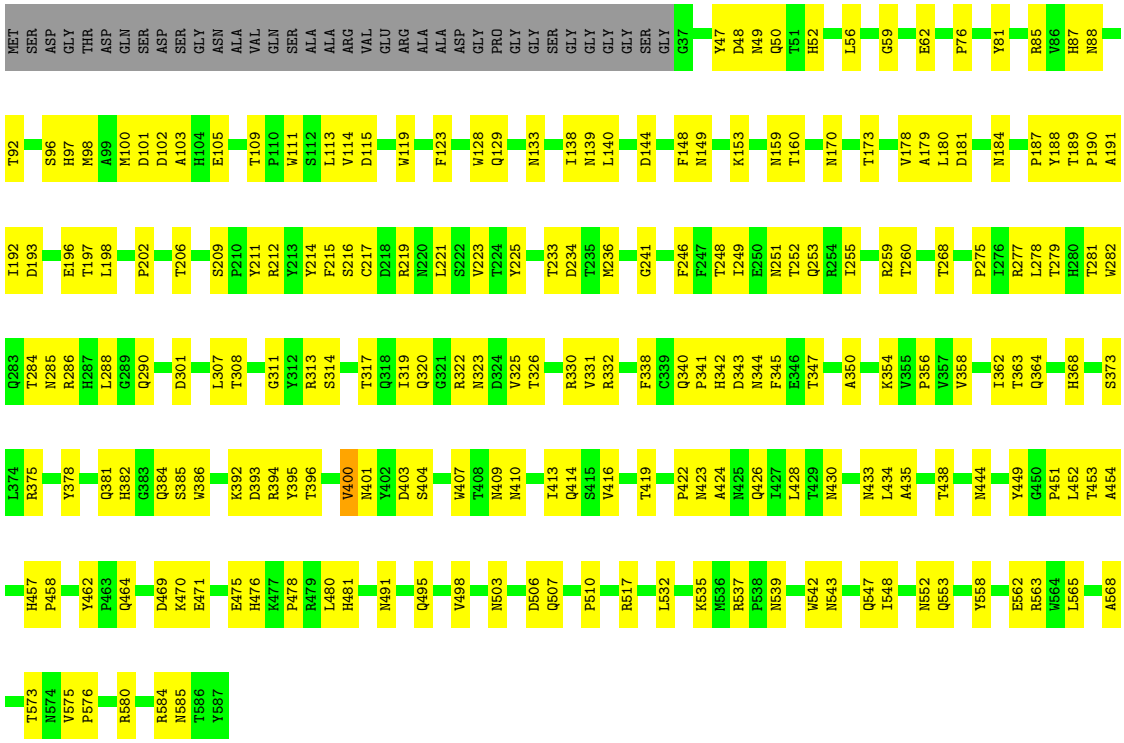
Chain b:





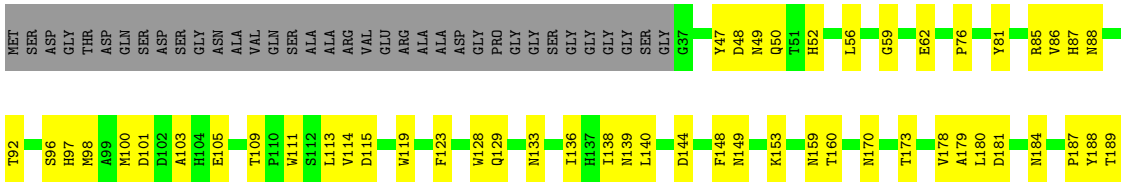
- Molecule 1: Capsid protein VP2

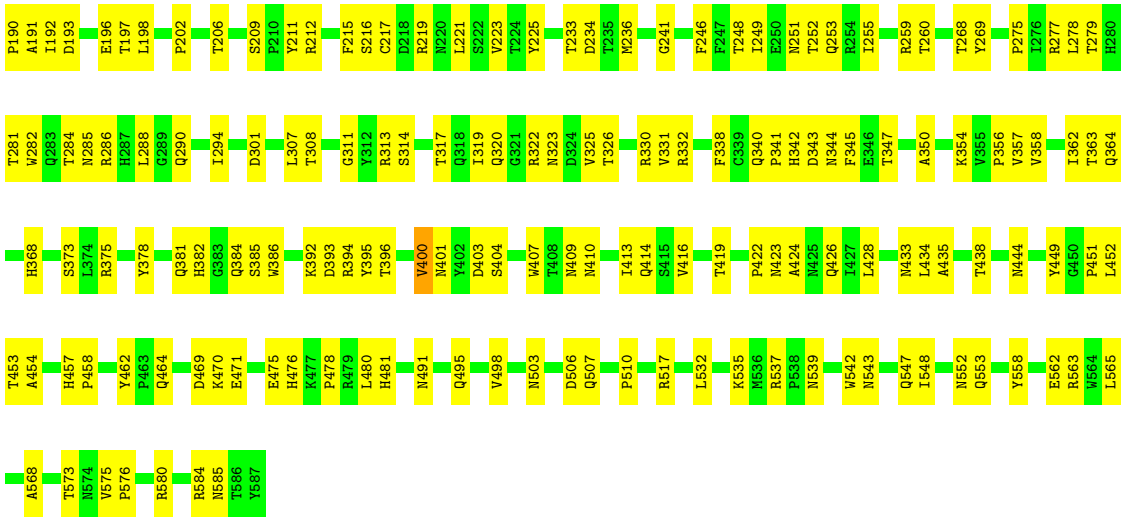
Chain c:



- Molecule 1: Capsid protein VP2

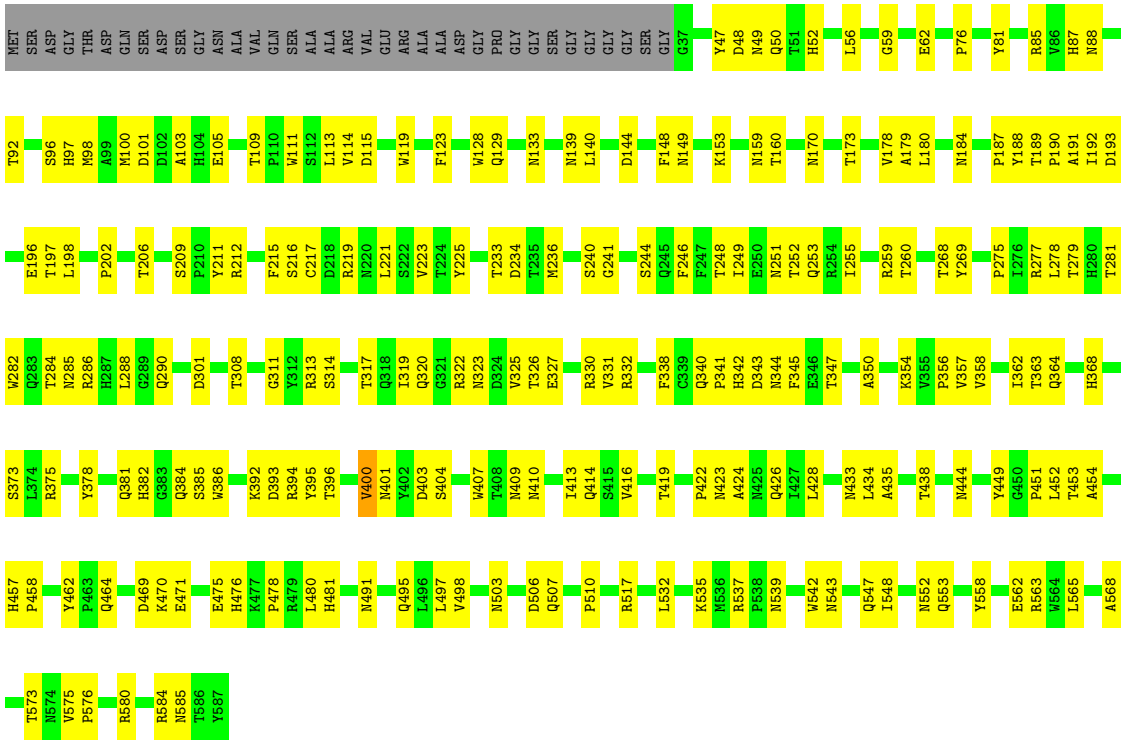
Chain d:





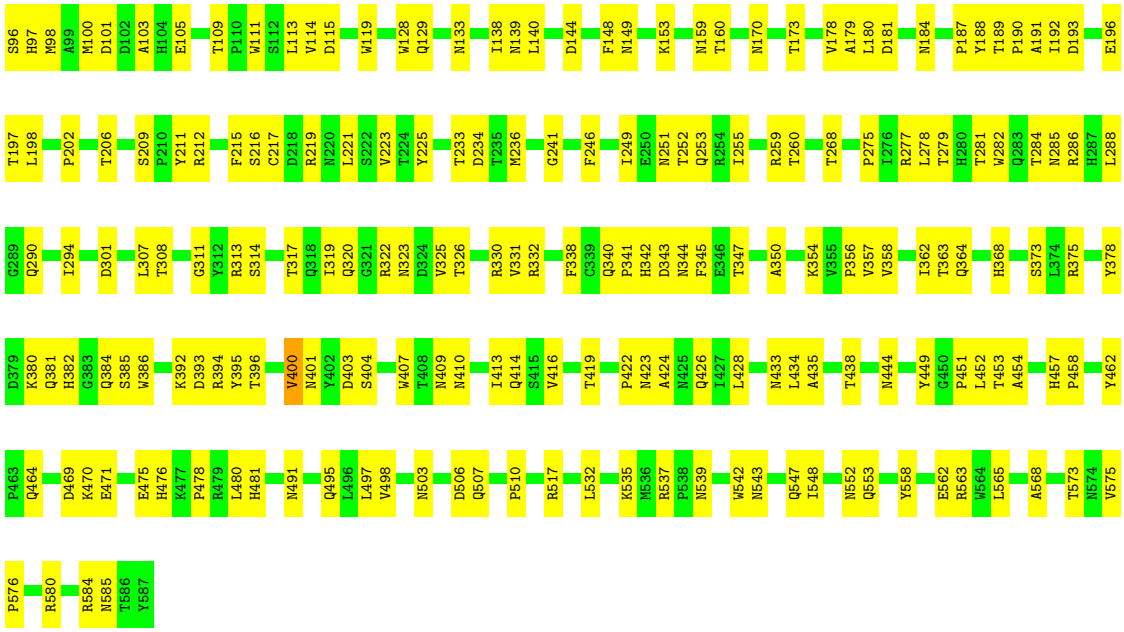
- Molecule 1: Capsid protein VP2

Chain e:



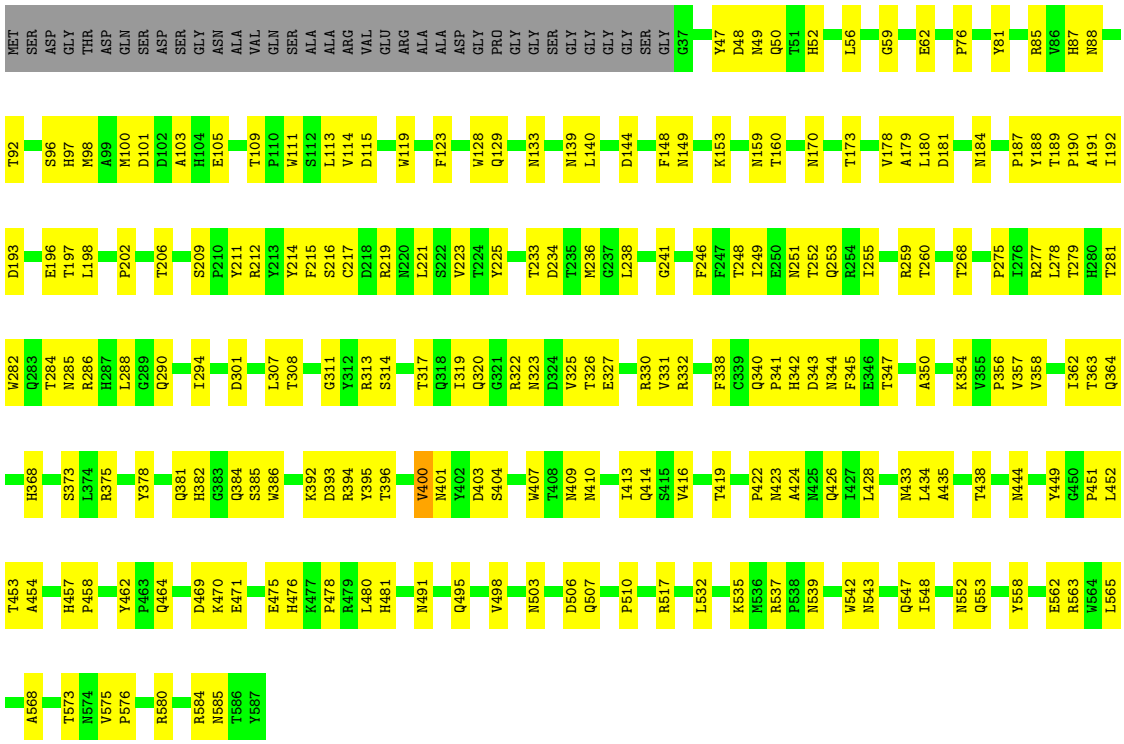
- Molecule 1: Capsid protein VP2

Chain f:



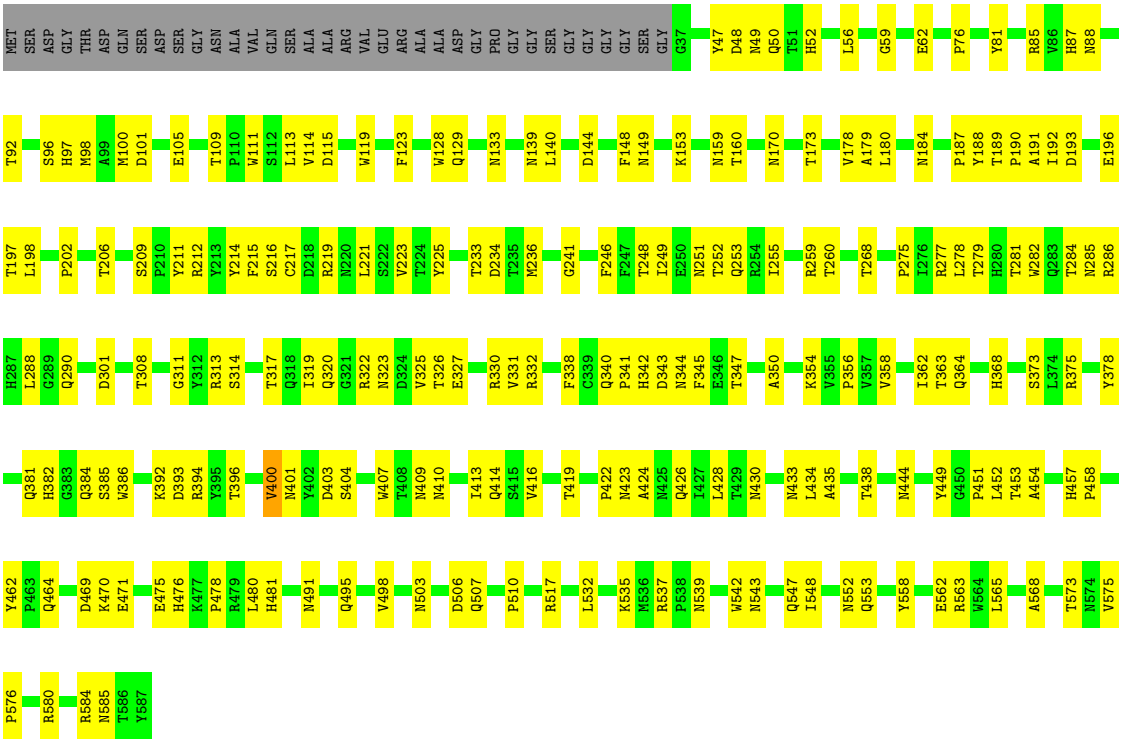
- Molecule 1: Capsid protein VP2

Chain g:



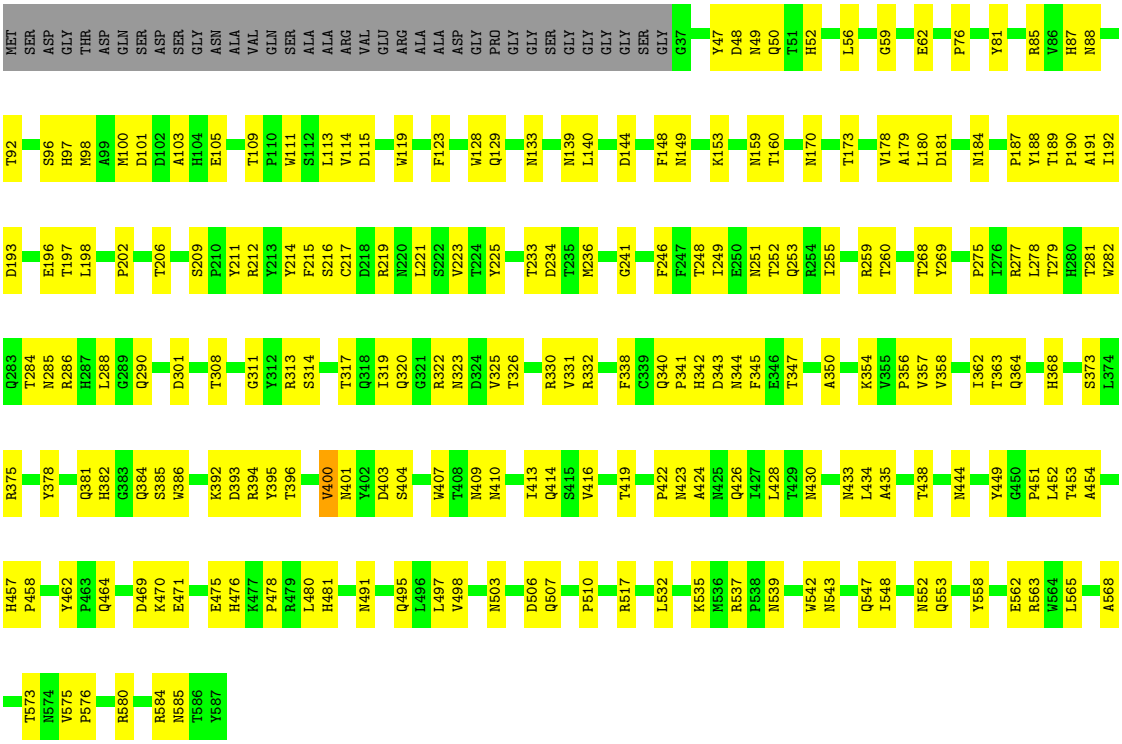
- Molecule 1: Capsid protein VP2

Chain h:



• Molecule 1: Capsid protein VP2

Chain i:



• Molecule 1: Capsid protein VP2

Chain j: 59% 35% 6%

MET SER ASP GLY THR ASP GLN SER ASP SER GLY ASN ALA VAL GLN SER ALA ALA ARG VAL GLU ARG ALA ALA ASP GLY PRO GLY GLY SER GLY GLY GLY GLY SER GLY G37 Y47 D48 N49 Q50 T51 H52 L56 G59 E62 P76 Y81 R85 V86 H87 N88

T92 S96 H97 M98 A99 M100 D101 D102 A103 H104 E105 T109 P110 W111 S112 L113 V114 D115 W119 W128 Q129 N133 N139 L140 D144 F148 N149 K153 N159 T160 N170 T173 V178 A179 L180 D181 N184 P187 Y188 T189 P190 A191 I192 D193

E196 T197 L198 P202 T206 S209 P210 Y211 R212 F215 S216 C217 D218 R219 N220 L221 S222 V223 T224 Y225 T233 D234 T235 M236 G237 L238 G241 F246 F247 T248 I249 E250 N251 T252 Q253 R254 I255 R259 T260 T268 P275 I276 R277 L278 T279 H280 T281 W282 Q283 T284

N285 R286 H287 L288 G289 Q290 I294 D301 L307 T308 G311 Y312 R313 S314 T317 Q318 I319 Q320 G321 R322 N323 D324 V325 T326 R330 V331 R332 F338 C339 Q340 P341 H342 D343 N344 F345 E346 T347 A350 K354 V355 P356 V357 V358 I362 T363 Q364 H368 S373

L374 R375 Y378 Q381 H382 G383 Q384 S385 W386 K392 D393 R394 Y395 T396 V400 N401 Y402 D403 S404 W407 T408 N409 N410 I413 Q414 S415 V416 T419 P422 N423 A424 N425 Q426 I427 L428 N433 L434 A435 T438 N444 Y449 G450 P451 L452 T453 A454 H457

P458 Y462 P463 Q464 D469 K470 E471 E475 H476 K477 P478 R479 L480 H481 N491 Q495 V498 N503 D506 Q507 P510 R517 L532 K535 M536 R537 P538 N539 W542 N543 Q547 I548 N552 Q553 E562 R563 W564 L565 A568 T573 N574 V575

P576 R580 R584 N585 T586 Y587

- Molecule 1: Capsid protein VP2

Chain k: 59% 35% 6%

MET SER ASP GLY THR ASP GLN SER ASP SER GLY ASN ALA VAL GLN SER ALA ALA ARG VAL GLU ARG ALA ALA ASP GLY PRO GLY GLY SER GLY GLY GLY GLY SER GLY G37 Y47 D48 N49 Q50 T51 H52 L56 G59 E62 P76 Y81 R85 V86 H87 N88

T92 S96 H97 M98 A99 M100 D101 D102 A103 H104 E105 T109 P110 W111 S112 L113 V114 D115 W119 F123 W128 Q129 N133 I136 N139 L140 D144 F148 N149 K153 N159 T160 N170 T173 V178 A179 L180 D181 N184 P187 Y188 T189 P190

A191 I192 D193 E196 T197 L198 P202 T206 S209 P210 Y211 R212 F215 S216 C217 D218 R219 N220 L221 S222 V223 T224 Y225 T233 D234 T235 M236 G241 F246 F247 T248 I249 E250 N251 T252 Q253 R254 I255 R259 T260 T268 P275 I276 R277 L278 T279 H280 T281 W282

Q283 T284 N285 R286 H287 L288 G289 Q290 I294 D301 L307 T308 G311 Y312 R313 S314 T317 Q318 I319 Q320 G321 R322 N323 D324 V325 T326 R330 V331 R332 F338 C339 Q340 P341 H342 D343 N344 F345 E346 T347 A350 K354 Y355 P356 V357 V358 I362 T363 Q364 H368

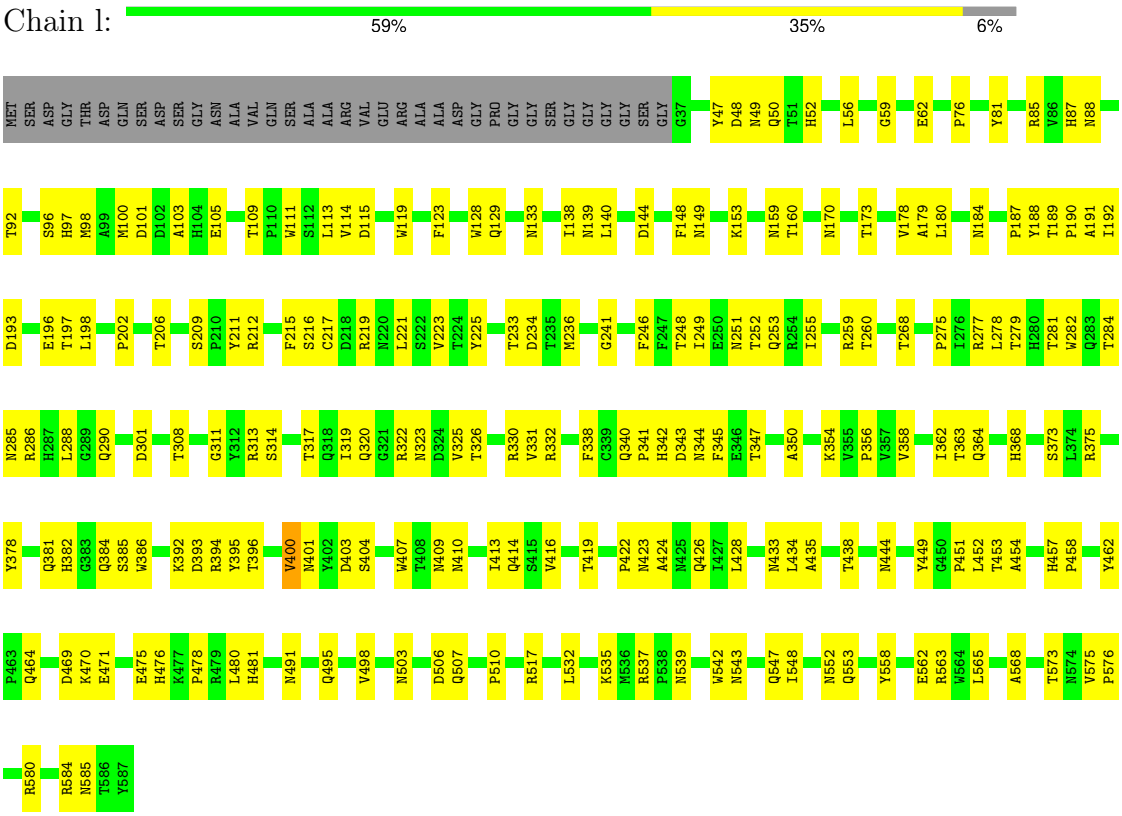
S373 L374 R375 Y378 Q381 H382 G383 Q384 S385 W386 K392 D393 R394 Y395 T396 V400 N401 Y402 D403 S404 W407 T408 N409 N410 I413 Q414 S415 V416 T419 P422 N423 A424 N425 Q426 I427 L428 N433 L434 A435 T438 N444 Y449 G450 P451 L452 T453 A454

H457 P458 Y462 P463 Q464 D469 K470 E471 E475 H476 K477 P478 R479 L480 H481 N491 Q495 L496 L497 V498 N503 D506 Q507 P510 R517 L532 K535 M536 R537 P538 N539 W542 N543 Q547 I548 N552 Q553 E562 R563 W564 L565 A568

T573 N574 V575 P576 R580 R584 N585 T586 Y587

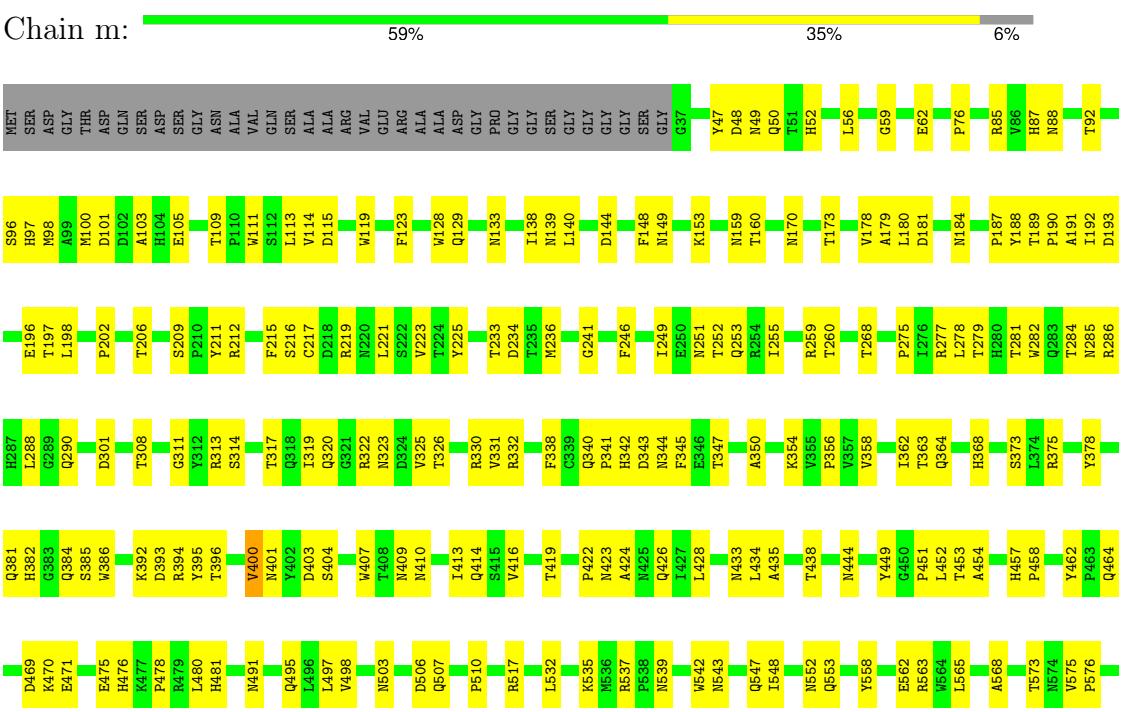
- Molecule 1: Capsid protein VP2

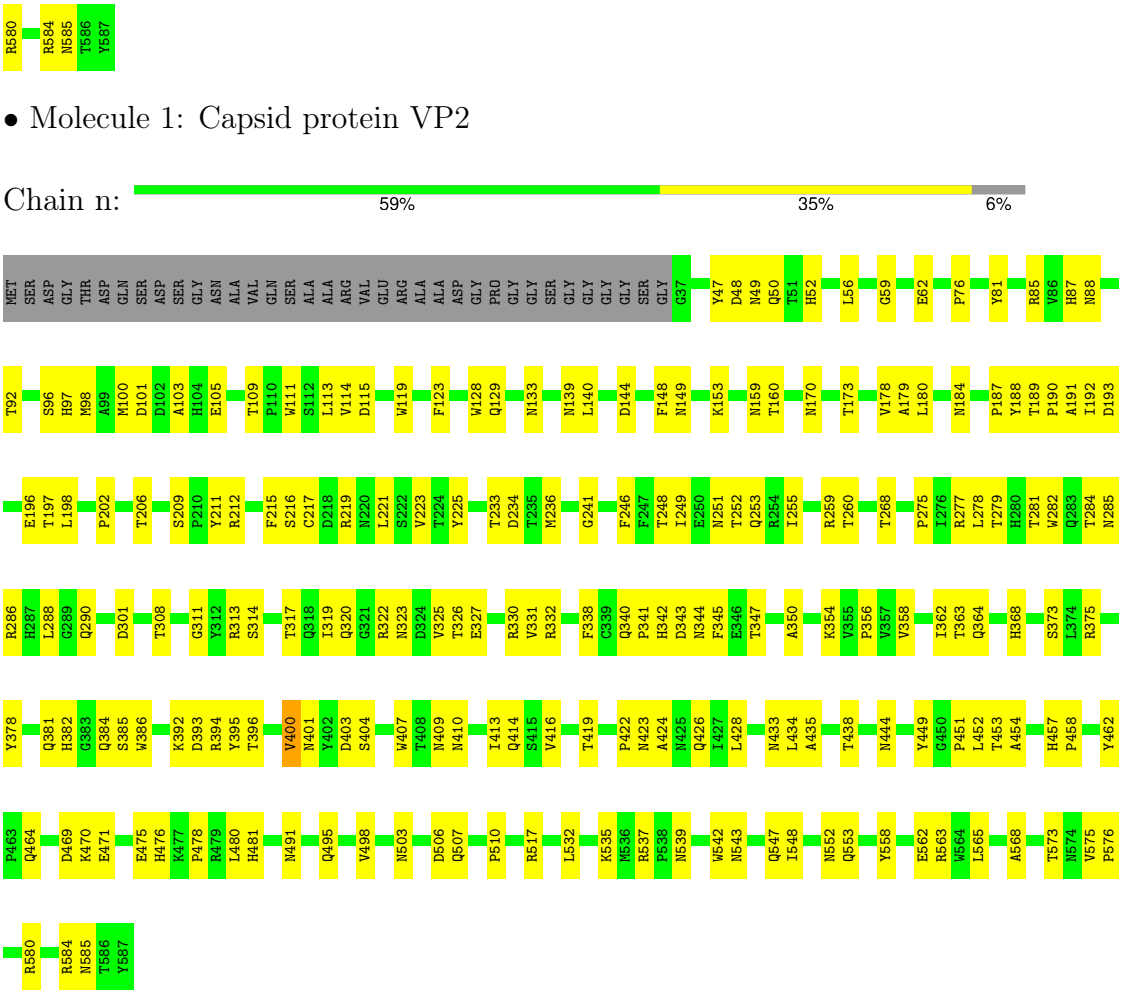
Chain l:

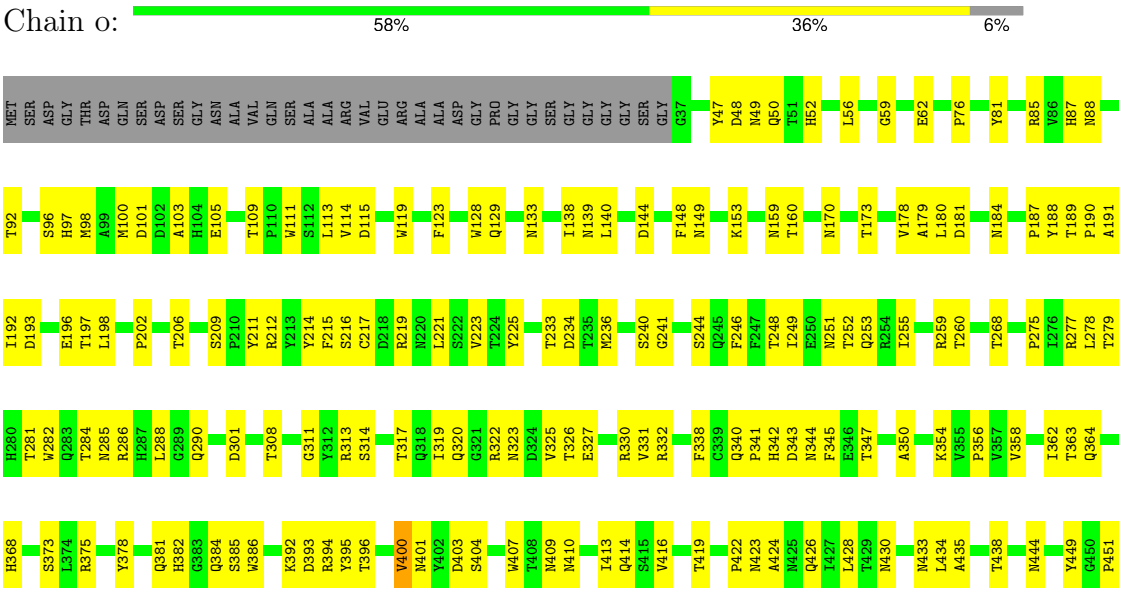


- Molecule 1: Capsid protein VP2

Chain m:




R580 R584 N585 T586 Y587
• Molecule 1: Capsid protein VP2
Chain n:
59%
35%
6%
MET SER ASP GLY THR ASP GLN SER ASP SER GLY ASN ALA VAL GLN SER ALA ALA ARG VAL GLU ARG ALA ALA ASP GLY PRO GLY GLY SER GLY GLY GLY GLY SER GLY G37 Y47 D48 N49 Q50 T51 H52 L56 G59 E62 P76 Y81 R85 V86 H87 N88
T92 S96 H97 M98 A99 M100 D101 D102 A103 H104 E105 T109 P110 W111 S112 L113 V114 D115 W119 F123 W128 Q129 N133 N139 L140 D144 F148 N149 K153 N159 T160 N170 T173 V178 A179 L180 N184 P187 Y188 T189 P190 A191 I192 D193
E196 T197 L198 P202 T206 S209 P210 Y211 R212 F215 S216 C217 D218 R219 N220 L221 S222 V223 T224 Y225 T233 D234 T235 M236 G241 F246 F247 T248 I249 E250 N251 T252 Q253 R254 I255 R259 T260 T268 P275 I276 R277 L278 T279 H280 T281 W282 Q283 T284 N285
R286 H287 L288 G289 Q290 D301 T308 G311 Y312 R313 S314 T317 Q318 I319 Q320 G321 R322 N323 D324 V325 T326 E327 R330 V331 R332 F338 C339 Q340 P341 H342 D343 N344 F345 E346 T347 A350 K354 V355 P356 V357 V358 I362 T363 Q364 H368 S373 L374 R375
Y378 Q381 H382 G383 Q384 S385 W386 K392 D393 R394 Y395 T396 V400 N401 Y402 D403 S404 W407 T408 N409 N410 I413 Q414 S415 V416 T419 P422 N423 A424 N425 Q426 I427 L428 N433 L434 A435 T438 N444 Y449 G450 P451 L452 T453 A454 H457 P458 Y462
P463 Q464 D469 K470 E471 E475 H476 K477 P478 R479 L480 H481 N491 Q495 V498 N503 D506 Q507 P510 R517 L532 K535 M536 R537 P538 N539 W542 N543 Q547 I548 N552 Q553 Y558 E562 R563 W564 L565 A568 T573 N574 V575 P576
R580 R584 N585 T586 Y587


• Molecule 1: Capsid protein VP2
Chain o:
58%
36%
6%
MET SER ASP GLY THR ASP GLN SER ASP SER GLY ASN ALA VAL GLN SER ALA ALA ARG VAL GLU ARG ALA ALA ASP GLY PRO GLY GLY SER GLY GLY GLY GLY SER GLY G37 Y47 D48 N49 Q50 T51 H52 L56 G59 E62 P76 Y81 R85 V86 H87 N88
T92 S96 H97 M98 A99 M100 D101 D102 A103 H104 E105 T109 P110 W111 S112 L113 V114 D115 W119 F123 W128 Q129 N133 I138 N139 L140 D144 F148 N149 K153 N159 T160 N170 T173 V178 A179 L180 D181 N184 P187 Y188 T189 P190 A191
I192 D193 E196 T197 L198 P202 T206 S209 P210 Y211 R212 Y213 Y214 F215 S216 C217 D218 R219 N220 L221 S222 V223 T224 Y225 T233 D234 T235 M236 S240 G241 S244 Q245 F246 F247 T248 I249 E250 N251 T252 Q253 R254 I255 R259 T260 T268 P275 I276 R277 L278 T279
H280 T281 W282 Q283 T284 N285 R286 H287 L288 G289 Q290 D301 T308 G311 Y312 R313 S314 T317 Q318 I319 Q320 G321 R322 N323 D324 V325 T326 E327 R330 V331 R332 F338 C339 Q340 P341 H342 D343 N344 F345 E346 T347 A350 K354 V355 P356 V357 V358 I362 T363 Q364
H368 S373 L374 R375 Y378 Q381 H382 G383 Q384 S385 W386 K392 D393 R394 Y395 T396 V400 N401 Y402 D403 S404 W407 T408 N409 N410 I413 Q414 S415 V416 T419 P422 N423 A424 N425 Q426 I427 L428 T429 N430 N433 L434 A435 T438 N444 Y449 G450 P451

L452 T453 A454 H457 P458 Y462 P463 Q464 D469 K470 E471 E475 H476 K477 P478 R479 L480 H481 N491 Q495 V498 N503 D506 Q507 P510 R517 L532 K535 M536 R537 P538 N539 W542 N543 Q547 I548 N552 Q553 Y558 E562 R563 W564

L565 A568 T573 N574 V575 P576 R580 R584 N585 T586 Y587

• Molecule 1: Capsid protein VP2

Chain p: 58% 35% 6%

MET SER ASP GLY THR ASP GLN SER ASP SER GLY ASN ALA VAL GLN SER ALA ALA ARG VAL GLU ARG ALA ALA ASP GLY PRO GLY GLY SER GLY GLY GLY GLY SER GLY G37 Y47 D48 N49 Q50 T51 H52 L56 G59 E62 P76 Y81 R85 V86 H87 N88

T92 S96 H97 N98 A99 M100 D101 D102 A103 H104 E105 T109 P110 W111 S112 L113 V114 D115 W119 F123 W128 Q129 N133 N139 L140 D144 F148 N149 K153 N159 T160 N170 T173 V178 A179 L180 D181 N184 P187 Y188 T189 P190 A191 I192

D193 E196 T197 L198 P202 T206 S209 P210 Y211 R212 Y213 Y214 F215 S216 C217 D218 R219 N220 L221 S222 V223 T224 Y225 T233 D234 T235 M236 G241 F246 F247 T248 I249 E250 N251 T252 Q253 R254 I255 R259 T260 T268 P275 I276 R277 L278 T279 H280 T281 W282 Q283

T284 N285 R286 H287 L288 G289 Q290 I294 D301 L307 T308 G311 Y312 R313 S314 T317 Q318 I319 Q320 G321 R322 N323 D324 V325 T326 R330 V331 R332 F338 C339 Q340 P341 H342 D343 N344 F345 E346 T347 A350 K354 V355 P356 V357 V358 I362 T363 Q364 H368

S373 L374 R375 Y378 Q381 H382 G383 Q384 S385 W386 K392 D393 R394 Y395 T396 V400 N401 Y402 D403 S404 W407 T408 N409 N410 I413 Q414 S415 V416 T419 P422 N423 A424 N425 Q426 I427 L428 N433 L434 A435 T438 N444 Y449 G450 P451 L452 T453 A454

H457 P458 Y462 P463 Q464 D469 K470 E471 E475 H476 K477 P478 R479 L480 H481 N491 Q495 L496 L497 V498 N503 D506 Q507 P510 R517 L532 K535 M536 R537 P538 N539 W542 N543 Q547 I548 N552 Q553 Y558 E562 R563 W564 L565 A568

T573 N574 V575 P576 R580 R584 N585 T586 Y587

• Molecule 1: Capsid protein VP2

Chain q: 58% 36% 6%

MET SER ASP GLY THR ASP GLN SER ASP SER GLY ASN ALA VAL GLN SER ALA ALA ARG VAL GLU ARG ALA ALA ASP GLY PRO GLY GLY SER GLY GLY GLY GLY SER GLY G37 Y47 D48 N49 Q50 T51 H52 L56 G57 D58 G59 E62 P76 Y81 R85 V86 H87 N88

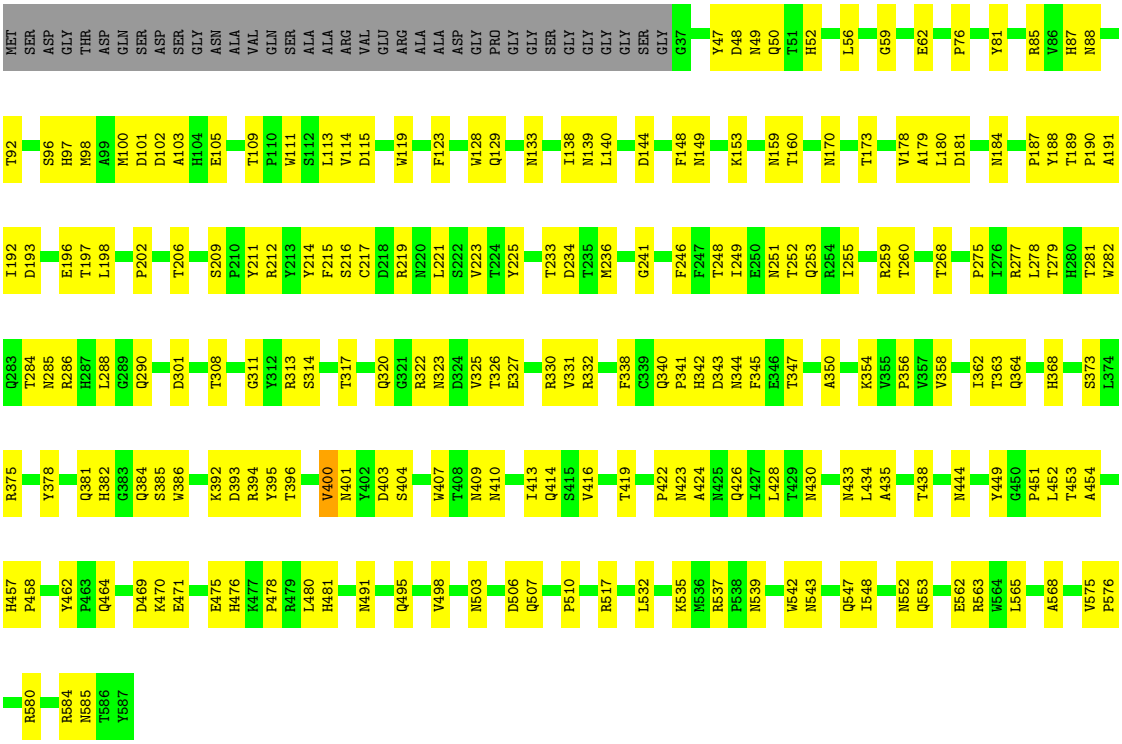
T92 S96 H97 N98 A99 M100 D101 D102 A103 H104 E105 T109 P110 W111 S112 L113 V114 D115 W119 F123 W128 Q129 N133 I136 H137 I138 N139 L140 D144 F148 N149 K153 N159 T160 N170 T173 V178 A179 L180 D181 N184 P187 Y188

T189 P190 A191 I192 D193 E196 T197 L198 P202 T206 S209 P210 Y211 R212 F215 S216 C217 D218 R219 N220 L221 S222 V223 T224 Y225 T233 D234 T235 M236 S240 G241 S244 Q245 F246 F247 T248 I249 E250 N251 T252 Q253 R254 I255 R259 T260 T268 P275 I276 R277

L278 T279 H280 T281 W282 Q283 T284 N285 R286 H287 L288 G289 Q290 I294 D301 L307 T308 G311 Y312 R313 S314 T317 Q318 I319 Q320 G321 R322 N323 D324 V325 T326 E327 R330 V331 R332 F338 C339 Q340 P341 H342 D343 N344 F345 E346 T347 A350 K354 V355 P356 V357 V358

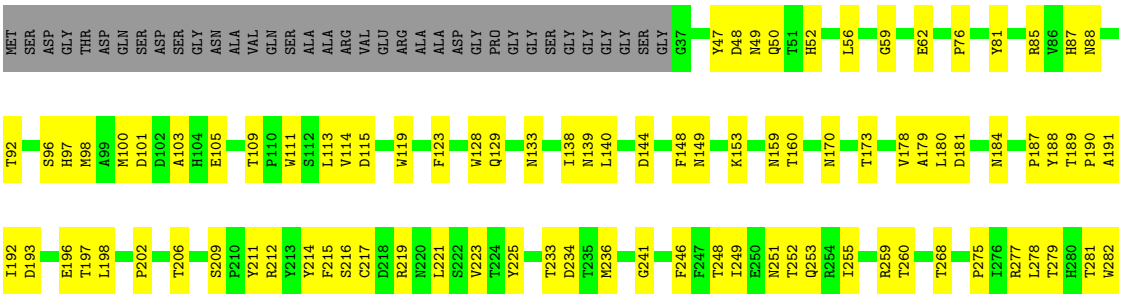
- Molecule 1: Capsid protein VP2

Chain r:



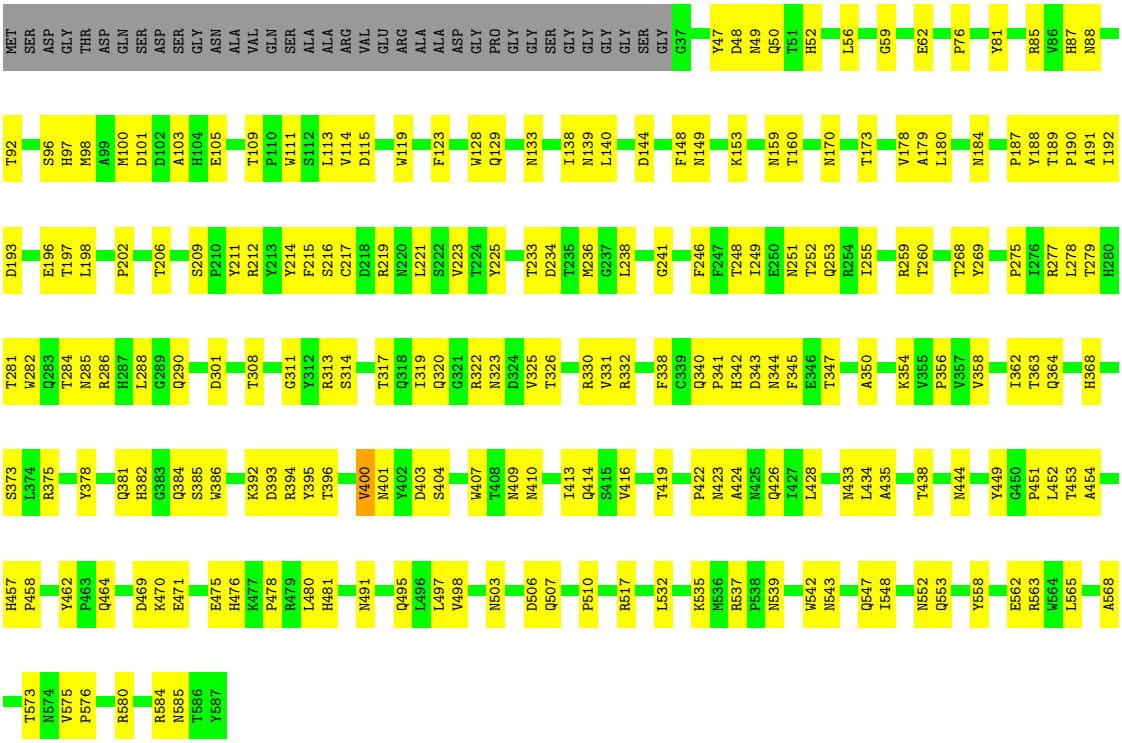
- Molecule 1: Capsid protein VP2

Chain s:



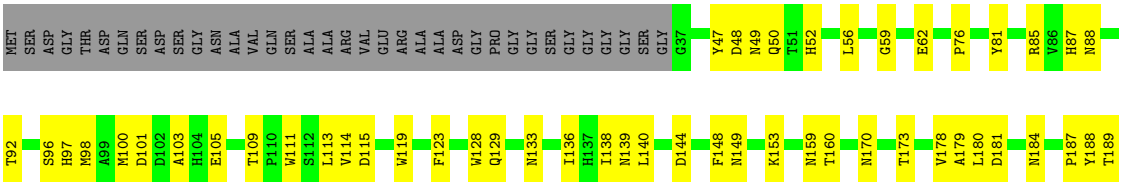
- Molecule 1: Capsid protein VP2

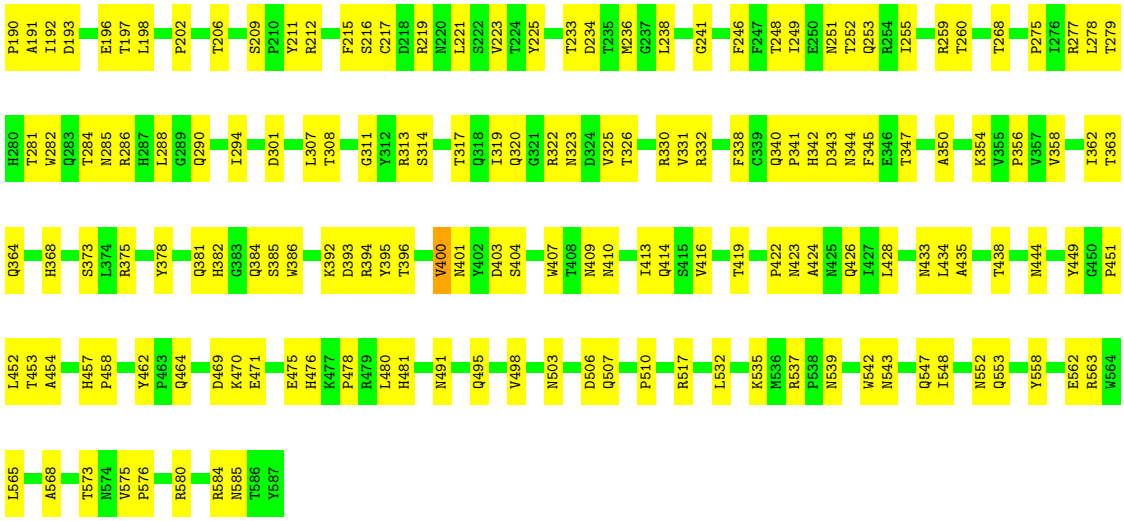
Chain t:



- Molecule 1: Capsid protein VP2

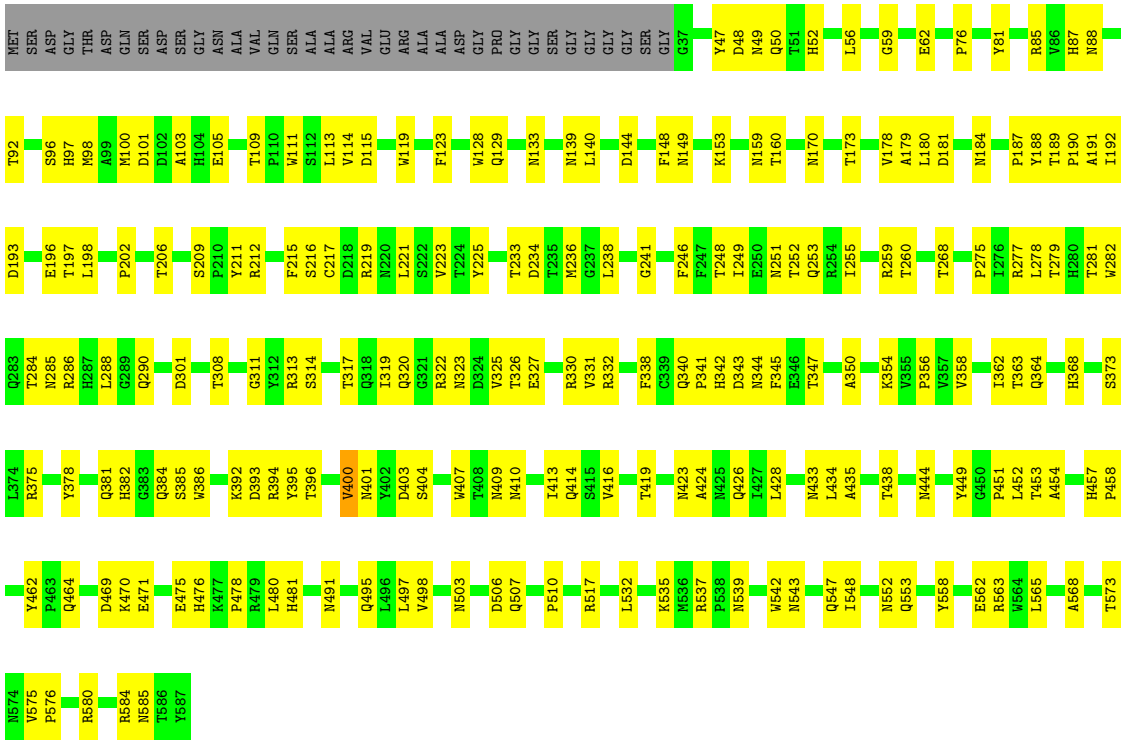
Chain u:





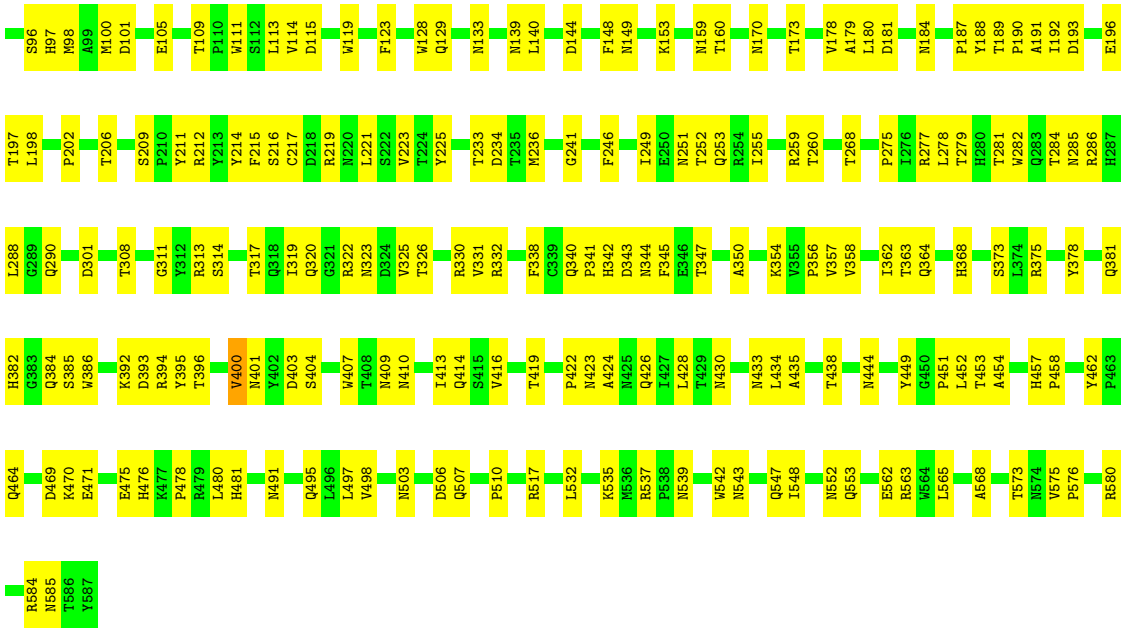
- Molecule 1: Capsid protein VP2

Chain v: 59% 35% 6%



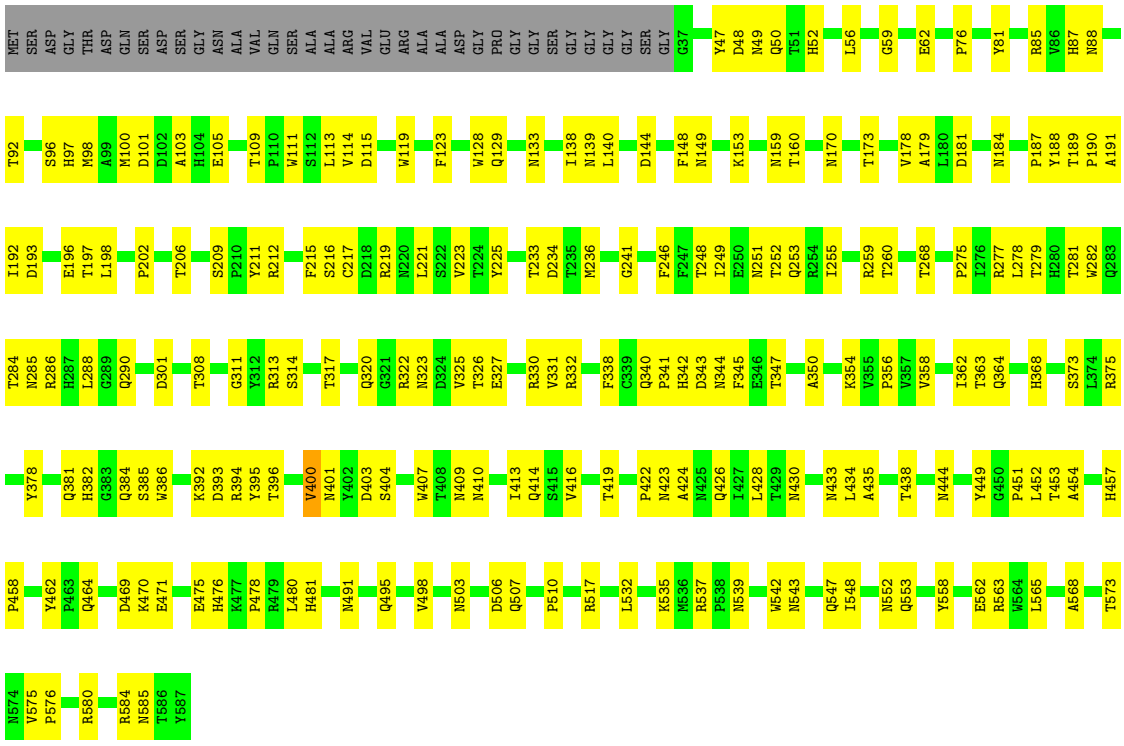
- Molecule 1: Capsid protein VP2

Chain w: 59% 35% 6%



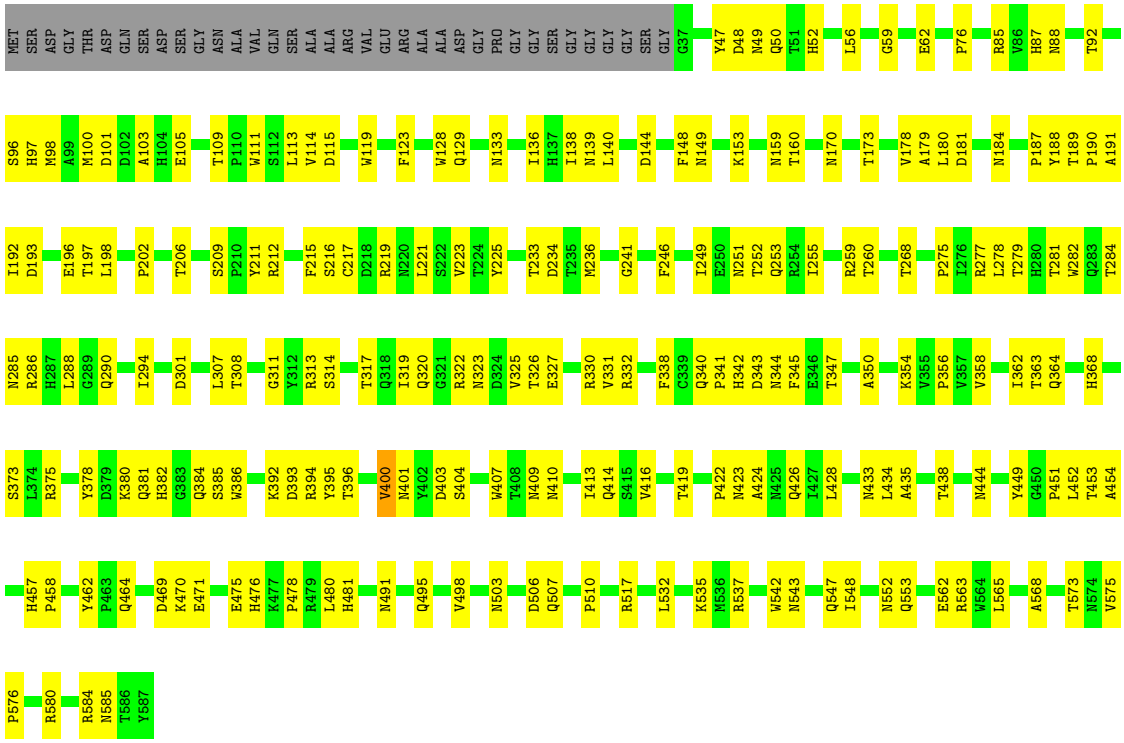
- Molecule 1: Capsid protein VP2

Chain x: 59% 35% 6%



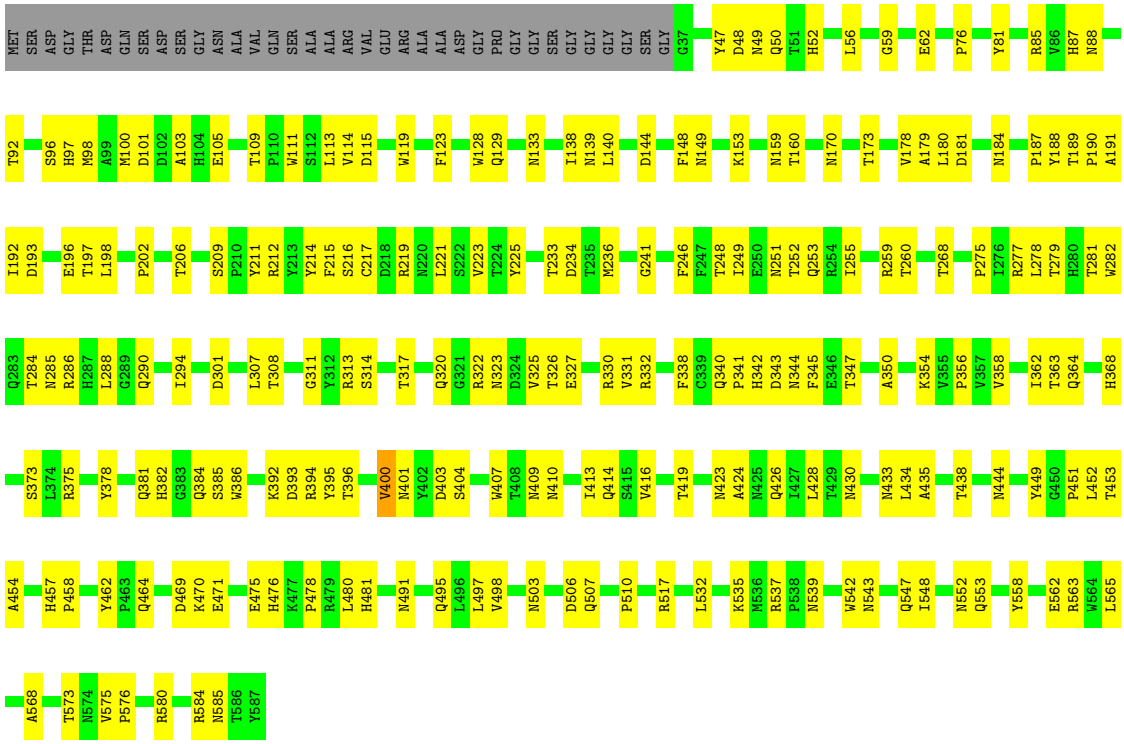
- Molecule 1: Capsid protein VP2

Chain y: 59% 35% 6%



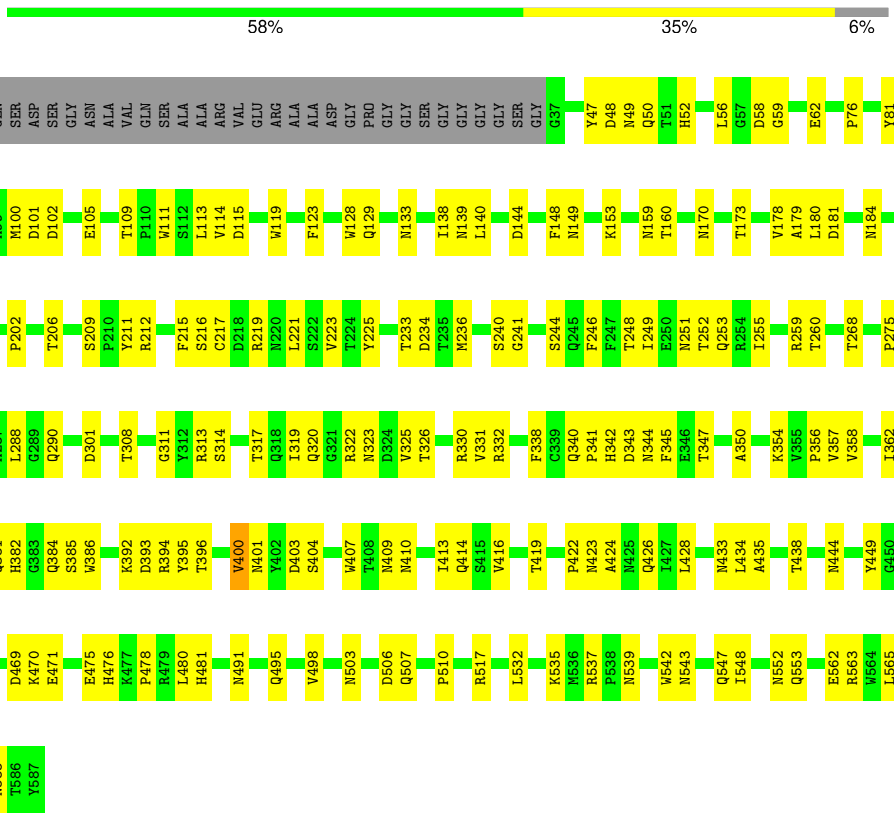
- Molecule 1: Capsid protein VP2

Chain z:



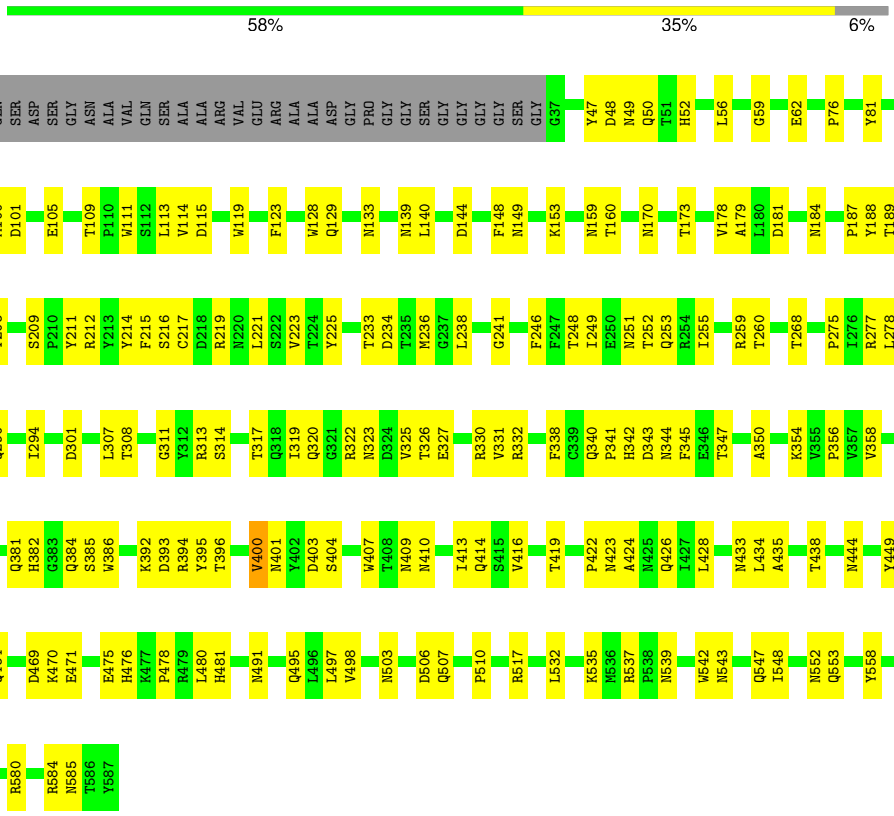
- Molecule 1: Capsid protein VP2

Chain 7:



- Molecule 1: Capsid protein VP2

Chain 8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18134	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	14.712	Depositor
Minimum map value	-7.755	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	381.976, 381.976, 381.976	wwPDB
Map dimensions	359, 359, 359	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.41	0/4528	0.49	0/6193
1	2	0.41	0/4528	0.49	0/6193
1	3	0.41	0/4528	0.49	0/6193
1	4	0.41	0/4528	0.49	0/6193
1	5	0.41	0/4528	0.49	0/6193
1	6	0.41	0/4528	0.49	0/6193
1	7	0.41	0/4528	0.49	0/6193
1	8	0.41	0/4528	0.49	0/6193
1	A	0.41	0/4528	0.49	0/6193
1	B	0.41	0/4528	0.49	0/6193
1	C	0.41	0/4528	0.49	0/6193
1	D	0.41	0/4528	0.49	0/6193
1	E	0.41	0/4528	0.49	0/6193
1	F	0.41	0/4528	0.49	0/6193
1	G	0.41	0/4528	0.49	0/6193
1	H	0.41	0/4528	0.49	0/6193
1	I	0.41	0/4528	0.49	0/6193
1	J	0.41	0/4528	0.49	0/6193
1	K	0.41	0/4528	0.49	0/6193
1	L	0.41	0/4528	0.49	0/6193
1	M	0.41	0/4528	0.49	0/6193
1	N	0.41	0/4528	0.49	0/6193
1	O	0.41	0/4528	0.49	0/6193
1	P	0.41	0/4528	0.49	0/6193
1	Q	0.41	0/4528	0.49	0/6193
1	R	0.41	0/4528	0.49	0/6193
1	S	0.41	0/4528	0.49	0/6193
1	T	0.41	0/4528	0.49	0/6193
1	U	0.41	0/4528	0.49	0/6193
1	V	0.41	0/4528	0.49	0/6193
1	W	0.41	0/4528	0.49	0/6193
1	X	0.41	0/4528	0.49	0/6193
1	Y	0.41	0/4528	0.49	0/6193
1	Z	0.41	0/4528	0.49	0/6193

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	a	0.41	0/4528	0.49	0/6193
1	b	0.41	0/4528	0.49	0/6193
1	c	0.41	0/4528	0.49	0/6193
1	d	0.41	0/4528	0.49	0/6193
1	e	0.41	0/4528	0.49	0/6193
1	f	0.41	0/4528	0.49	0/6193
1	g	0.41	0/4528	0.49	0/6193
1	h	0.41	0/4528	0.49	0/6193
1	i	0.41	0/4528	0.49	0/6193
1	j	0.41	0/4528	0.49	0/6193
1	k	0.41	0/4528	0.49	0/6193
1	l	0.41	0/4528	0.49	0/6193
1	m	0.41	0/4528	0.49	0/6193
1	n	0.41	0/4528	0.49	0/6193
1	o	0.41	0/4528	0.49	0/6193
1	p	0.41	0/4528	0.49	0/6193
1	q	0.41	0/4528	0.49	0/6193
1	r	0.41	0/4528	0.49	0/6193
1	s	0.41	0/4528	0.49	0/6193
1	t	0.41	0/4528	0.49	0/6193
1	u	0.41	0/4528	0.49	0/6193
1	v	0.41	0/4528	0.49	0/6193
1	w	0.41	0/4528	0.49	0/6193
1	x	0.41	0/4528	0.49	0/6193
1	y	0.41	0/4528	0.49	0/6193
1	z	0.41	0/4528	0.49	0/6193
All	All	0.41	0/271680	0.49	0/371580

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	4399	0	4169	181	0
1	2	4399	0	4169	190	0
1	3	4399	0	4169	192	0
1	4	4399	0	4169	185	0
1	5	4399	0	4169	192	0
1	6	4399	0	4169	190	0
1	7	4399	0	4169	186	0
1	8	4399	0	4169	185	0
1	A	4399	0	4169	189	0
1	B	4399	0	4169	184	0
1	C	4399	0	4169	189	0
1	D	4399	0	4169	189	0
1	E	4399	0	4169	183	0
1	F	4399	0	4169	186	0
1	G	4399	0	4169	185	0
1	H	4399	0	4169	190	0
1	I	4399	0	4169	188	0
1	J	4399	0	4169	186	0
1	K	4399	0	4169	188	0
1	L	4399	0	4169	189	0
1	M	4399	0	4169	189	0
1	N	4399	0	4169	188	0
1	O	4399	0	4169	184	0
1	P	4399	0	4169	184	0
1	Q	4399	0	4169	188	0
1	R	4399	0	4169	187	0
1	S	4399	0	4169	185	0
1	T	4399	0	4169	184	0
1	U	4399	0	4169	188	0
1	V	4399	0	4169	189	0
1	W	4399	0	4169	187	0
1	X	4399	0	4169	187	0
1	Y	4399	0	4169	193	0
1	Z	4399	0	4169	187	0
1	a	4399	0	4169	187	0
1	b	4399	0	4169	185	0
1	c	4399	0	4169	190	0
1	d	4399	0	4169	191	0
1	e	4399	0	4169	190	0
1	f	4399	0	4169	186	0
1	g	4399	0	4169	189	0
1	h	4399	0	4169	182	0
1	i	4399	0	4169	188	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	4399	0	4169	186	0
1	k	4399	0	4169	185	0
1	l	4399	0	4169	185	0
1	m	4399	0	4169	188	0
1	n	4399	0	4169	183	0
1	o	4399	0	4169	187	0
1	p	4399	0	4169	186	0
1	q	4399	0	4169	191	0
1	r	4399	0	4169	185	0
1	s	4399	0	4169	191	0
1	t	4399	0	4169	188	0
1	u	4399	0	4169	188	0
1	v	4399	0	4169	187	0
1	w	4399	0	4169	185	0
1	x	4399	0	4169	186	0
1	y	4399	0	4169	184	0
1	z	4399	0	4169	189	0
All	All	263940	0	250140	9055	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 18.

The worst 5 of 9055 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:340:GLN:HE22	1:S:358:VAL:HG22	1.34	0.93
1:v:340:GLN:HE22	1:v:358:VAL:HG22	1.34	0.93
1:t:340:GLN:HE22	1:t:358:VAL:HG22	1.34	0.93
1:G:340:GLN:HE22	1:G:358:VAL:HG22	1.34	0.93
1:U:340:GLN:HE22	1:U:358:VAL:HG22	1.34	0.93

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	2	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	3	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	4	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	5	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	6	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	7	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	8	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	A	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	B	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	C	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	D	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	E	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	F	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	G	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	H	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	I	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	J	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	K	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	L	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	M	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	N	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	O	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	P	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	Q	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	R	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	S	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	T	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	U	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	V	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	X	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	Y	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	Z	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	a	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	b	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	c	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	d	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	e	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	f	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	g	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	h	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	i	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	j	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	k	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	l	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	m	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	n	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	o	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	p	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	q	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	r	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	s	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	t	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	u	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	v	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	w	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	x	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	y	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
1	z	550/587 (94%)	538 (98%)	11 (2%)	1 (0%)	44	73
All	All	33000/35220 (94%)	32280 (98%)	660 (2%)	60 (0%)	45	73

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	VAL
1	B	400	VAL
1	C	400	VAL
1	D	400	VAL
1	E	400	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	2	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	3	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	4	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	5	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	6	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	7	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	8	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	A	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	B	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	C	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	D	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	E	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	F	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	G	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	H	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	I	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	J	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	K	479/500 (96%)	478 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	M	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	N	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	O	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	P	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	Q	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	R	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	S	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	T	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	U	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	V	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	W	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	X	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	Y	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	Z	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	a	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	b	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	c	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	d	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	e	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	f	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	g	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	h	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	i	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	j	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	k	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	l	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	m	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	n	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	o	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	p	479/500 (96%)	478 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	q	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	r	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	s	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	t	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	u	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	v	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	w	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	x	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	y	479/500 (96%)	478 (100%)	1 (0%)	92	97
1	z	479/500 (96%)	478 (100%)	1 (0%)	92	97
All	All	28740/30000 (96%)	28680 (100%)	60 (0%)	91	97

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	428	LEU
1	x	428	LEU
1	d	428	LEU
1	w	428	LEU
1	8	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1575 such sidechains are listed below:

Mol	Chain	Res	Type
1	d	149	ASN
1	l	457	HIS
1	e	323	ASN
1	d	141	HIS
1	h	381	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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)

There are no chain breaks in this entry.

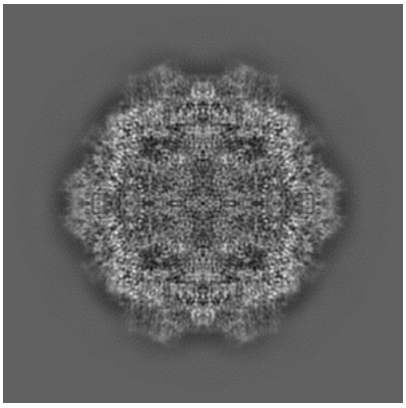
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7071. These allow visual inspection of the internal detail of the map and identification of artifacts.

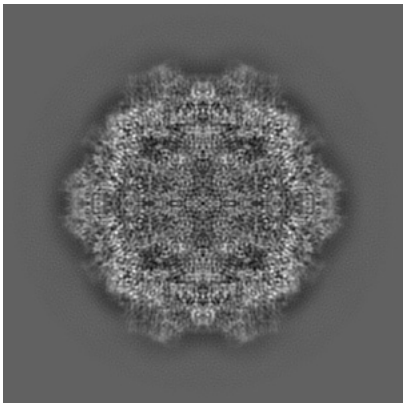
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

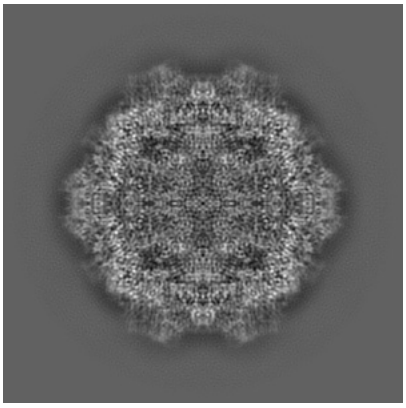
6.1.1 Primary map



X



Y

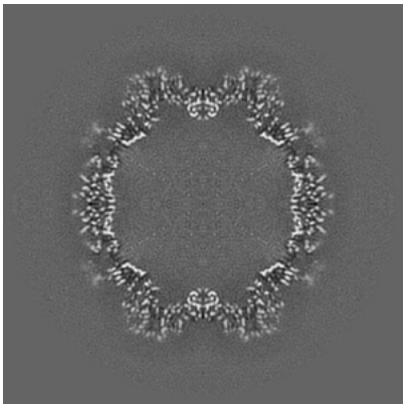


Z

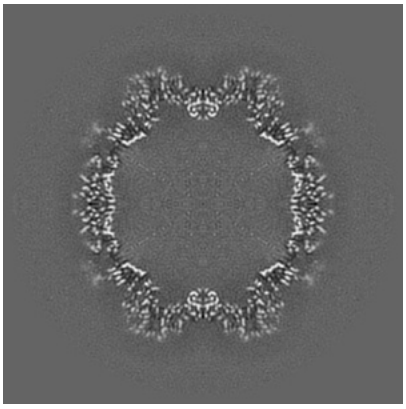
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

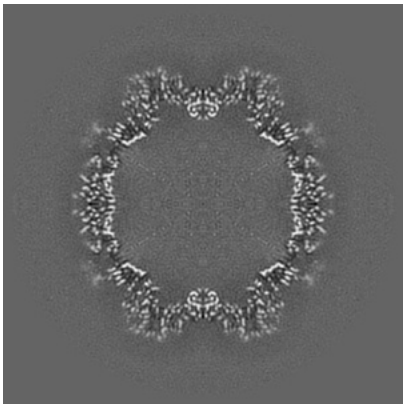
6.2.1 Primary map



X Index: 179



Y Index: 179

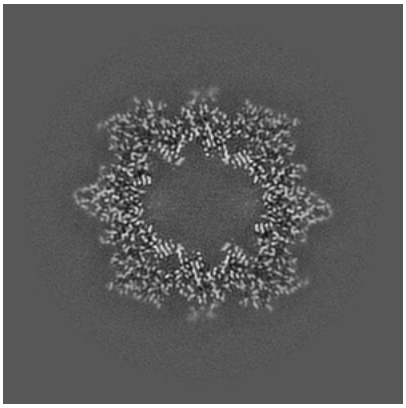


Z Index: 179

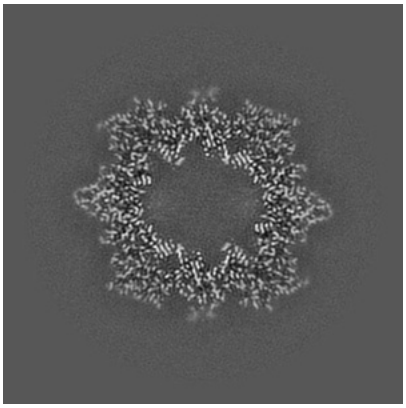
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

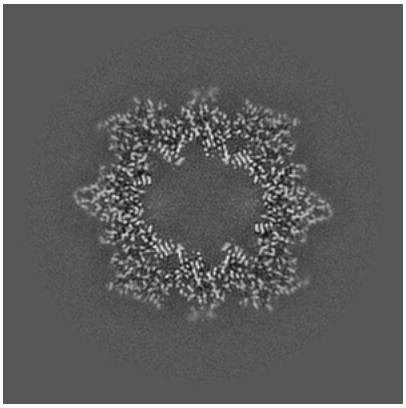
6.3.1 Primary map



X Index: 115



Y Index: 115

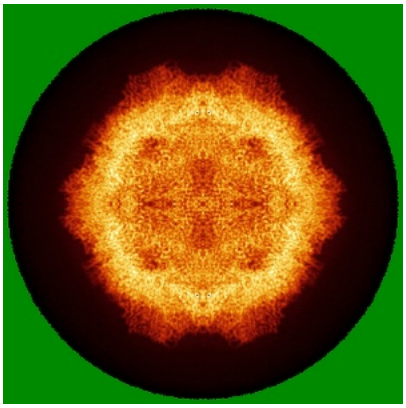


Z Index: 115

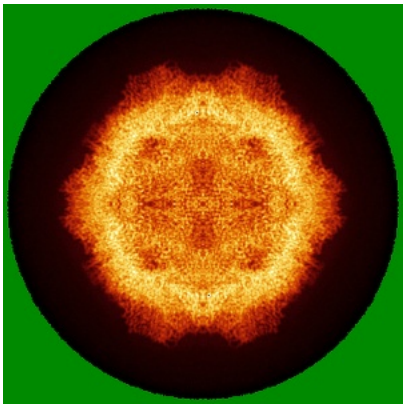
The images above show the largest variance slices of the map in three orthogonal directions.

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

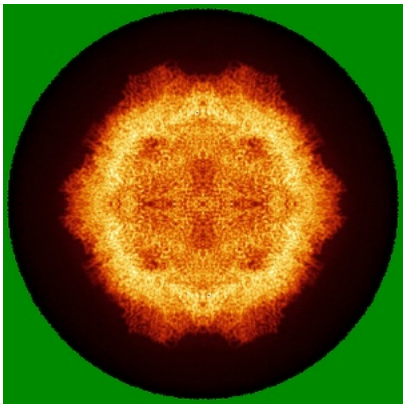
6.4.1 Primary map



X



Y

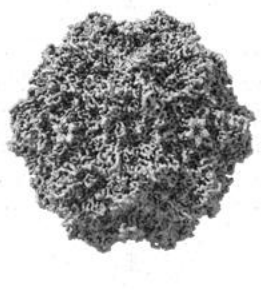


Z

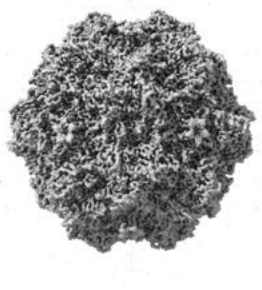
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

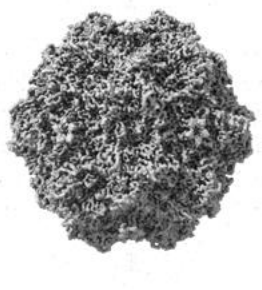
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

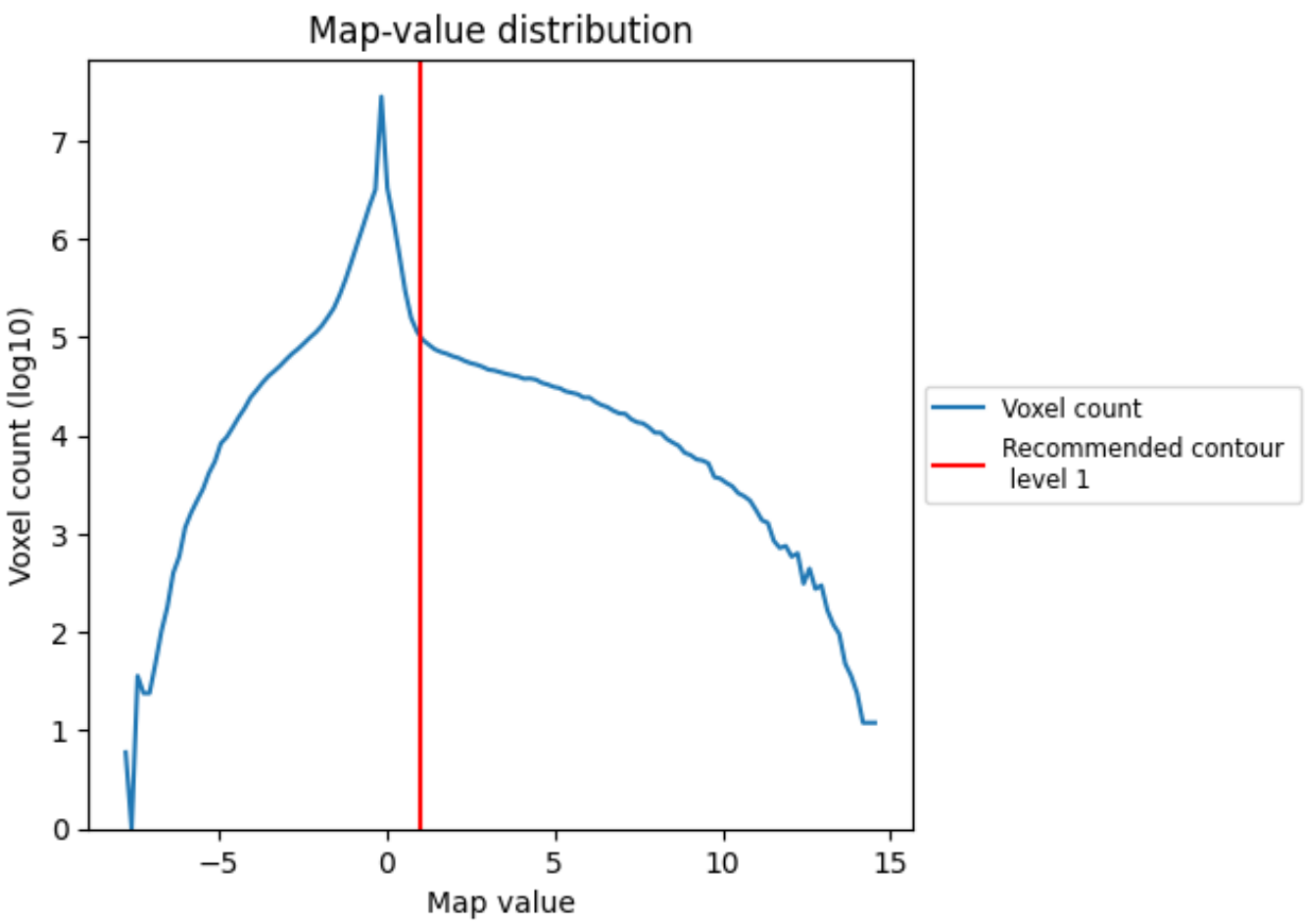
6.6 Mask visualisation (i)

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

7 Map analysis (i)

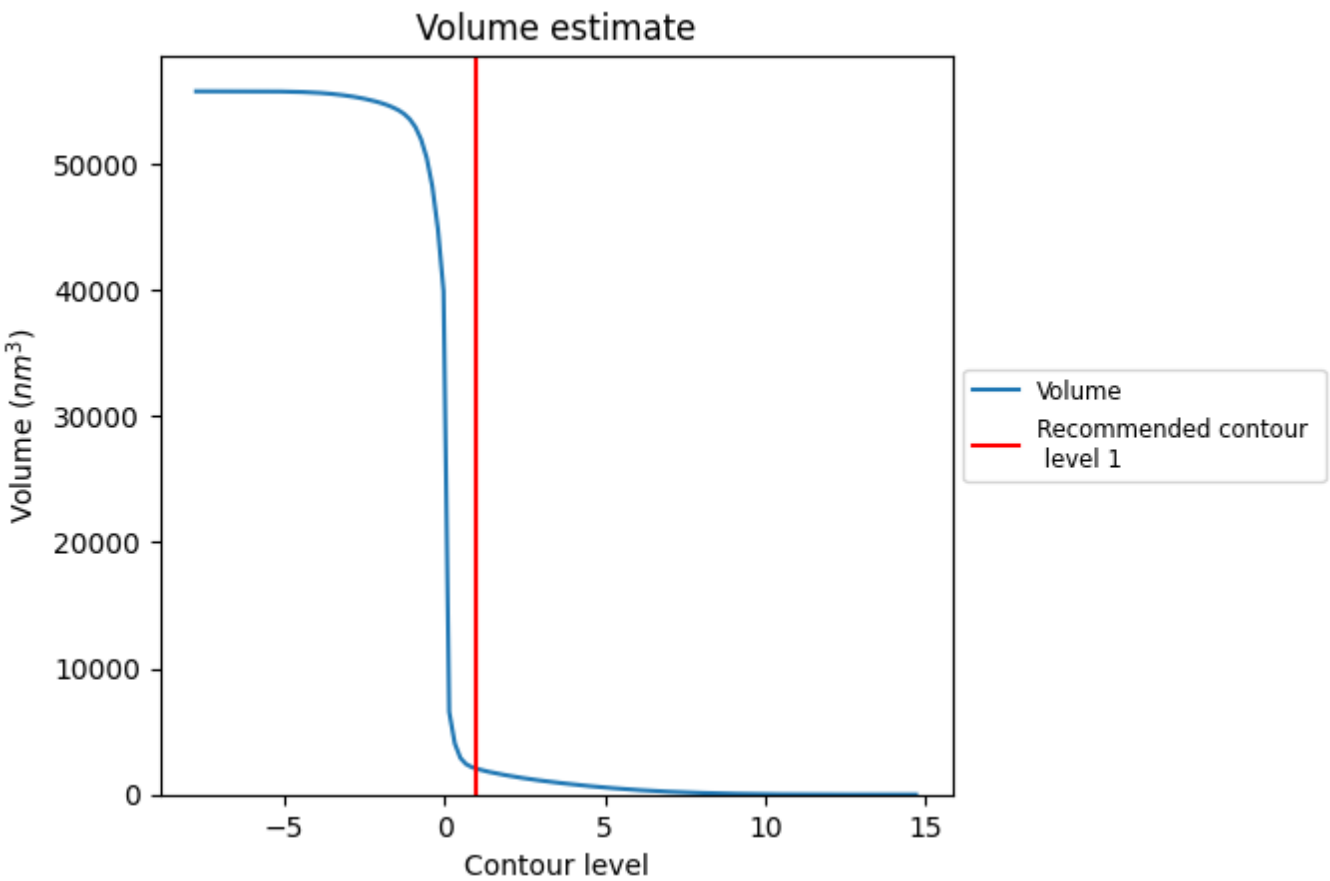
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

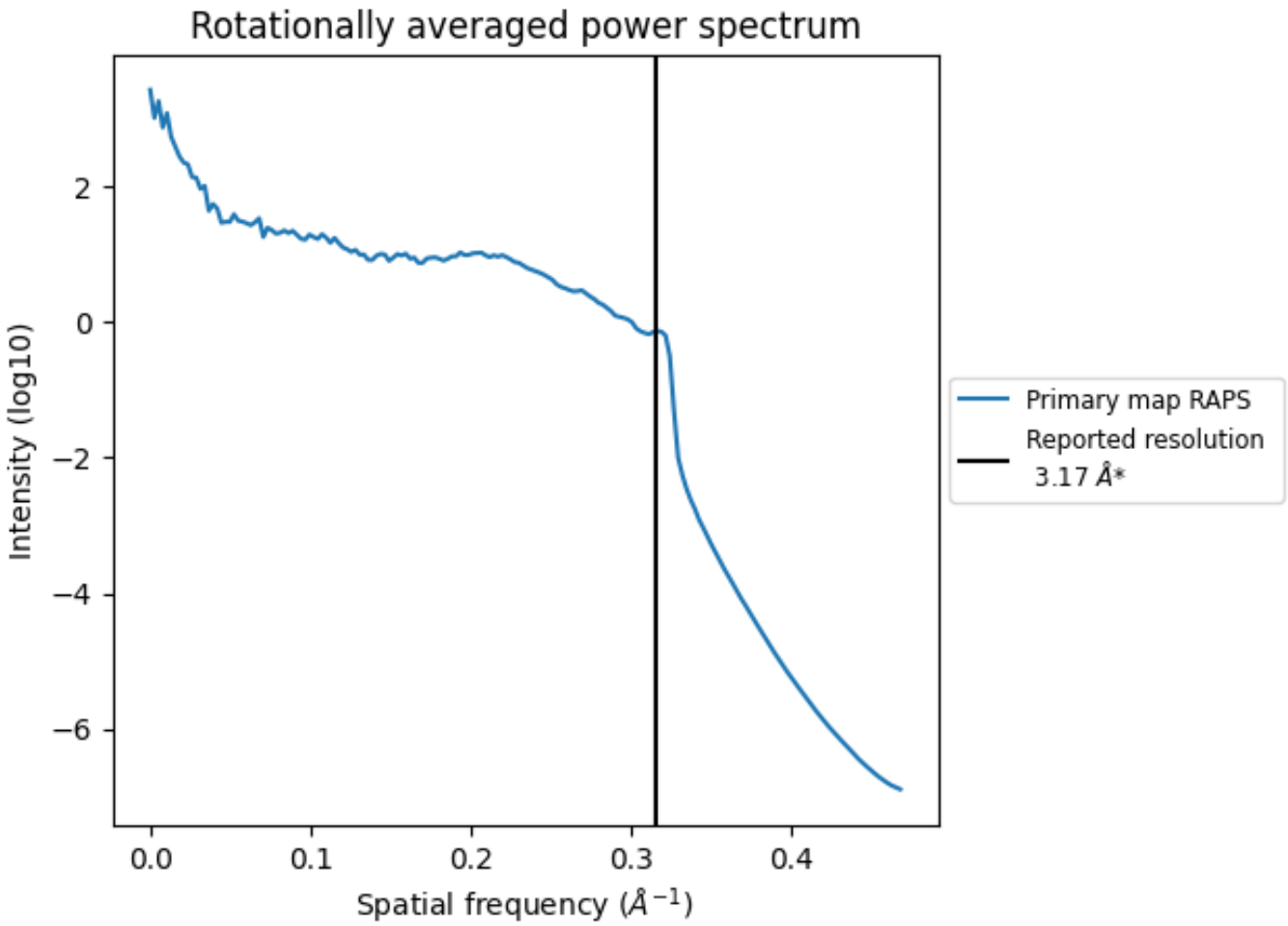
7.2 Volume estimate (i)



The volume at the recommended contour level is 2048 nm^3; this corresponds to an approximate mass of 1850 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.315 Å^{-1}

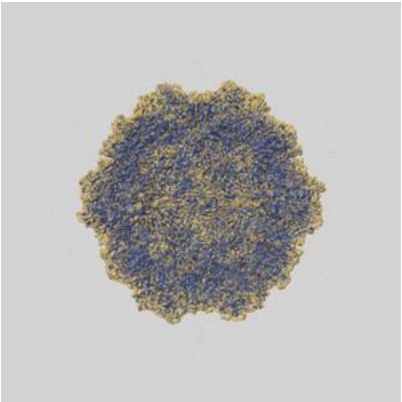
8 Fourier-Shell correlation (i)

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

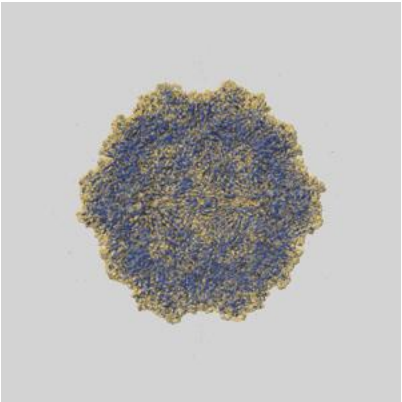
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7071 and PDB model 6B9Q. Per-residue inclusion information can be found in section 3 on page 10.

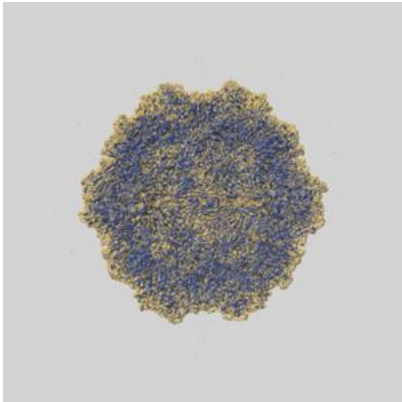
9.1 Map-model overlay (i)



X



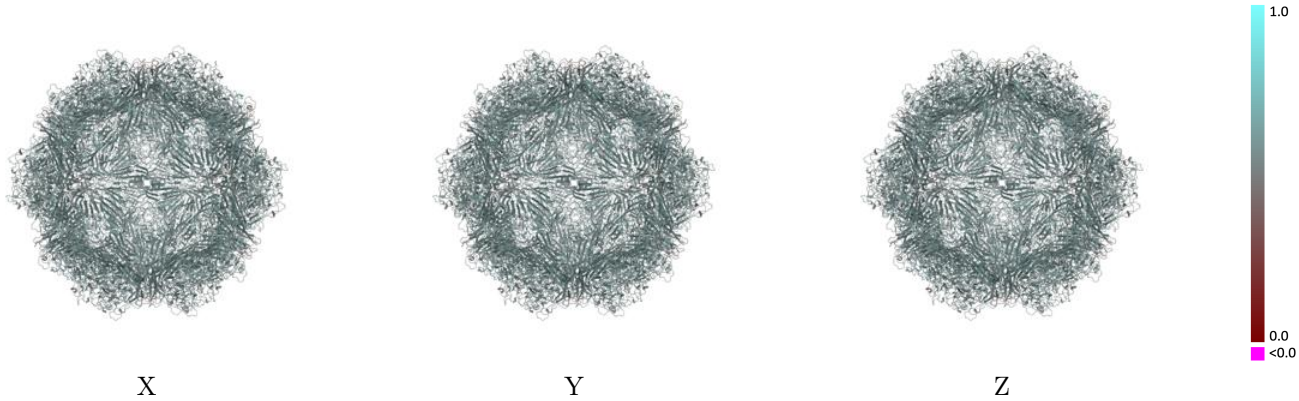
Y



Z

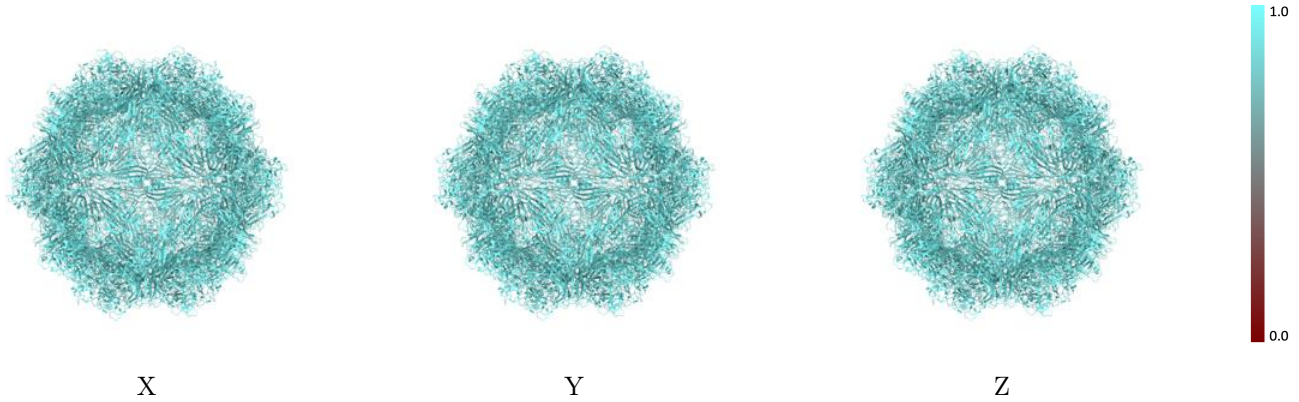
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



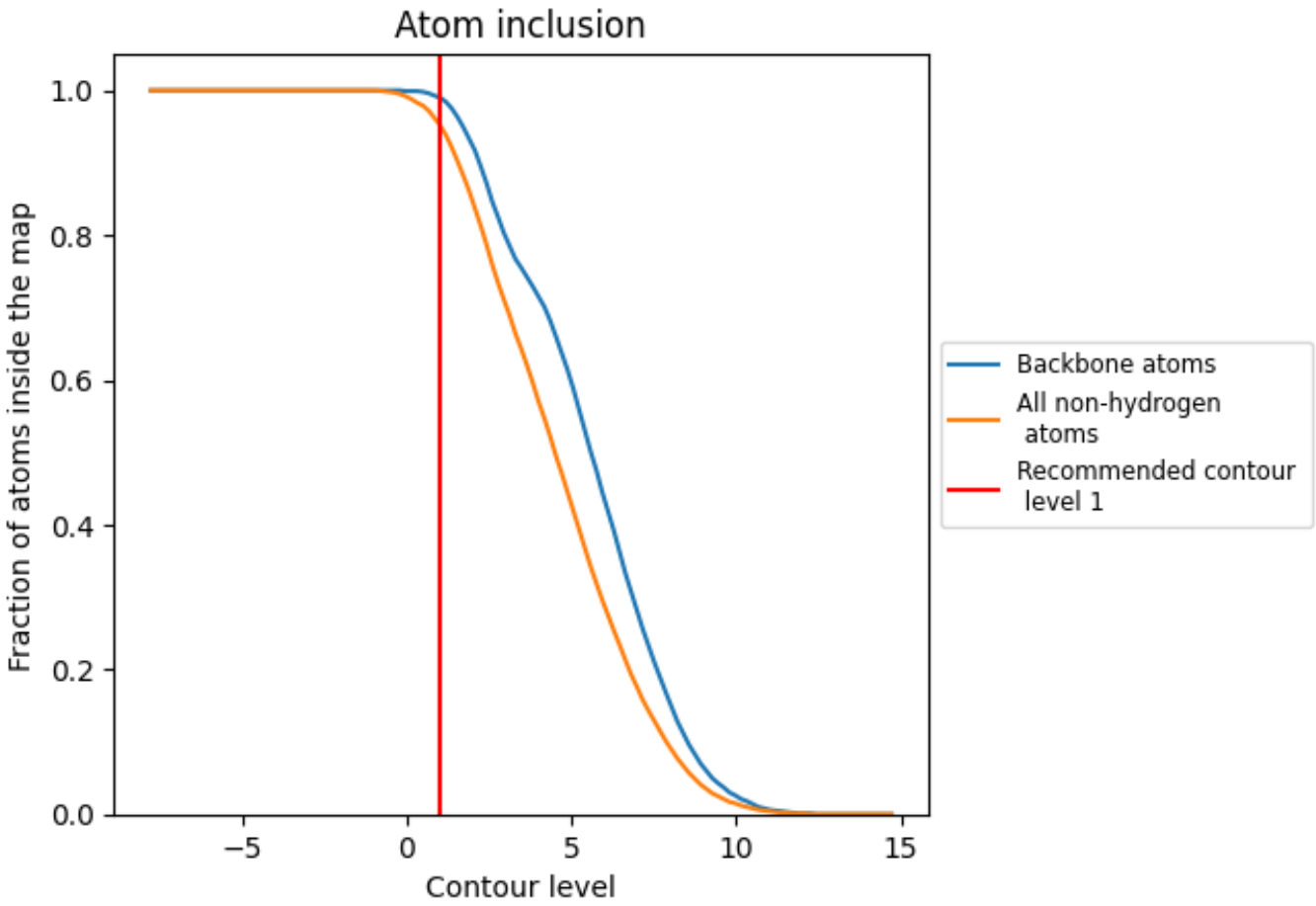
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 99% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.9530	0.5620
1	0.9540	0.5640
2	0.9540	0.5640
3	0.9540	0.5640
4	0.9540	0.5630
5	0.9540	0.5630
6	0.9540	0.5630
7	0.9520	0.5630
8	0.9520	0.5620
A	0.9540	0.5630
B	0.9540	0.5620
C	0.9510	0.5620
D	0.9530	0.5620
E	0.9520	0.5620
F	0.9540	0.5610
G	0.9520	0.5620
H	0.9520	0.5620
I	0.9510	0.5610
J	0.9540	0.5620
K	0.9520	0.5620
L	0.9550	0.5620
M	0.9520	0.5640
N	0.9520	0.5630
O	0.9520	0.5630
P	0.9520	0.5620
Q	0.9510	0.5610
R	0.9540	0.5610
S	0.9540	0.5630
T	0.9510	0.5620
U	0.9540	0.5620
V	0.9520	0.5600
W	0.9520	0.5610
X	0.9520	0.5620
Y	0.9500	0.5630
Z	0.9520	0.5630

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Chain	Atom inclusion	Q-score
a	0.9510	0.5620
b	0.9520	0.5630
c	0.9520	0.5630
d	0.9520	0.5620
e	0.9530	0.5630
f	0.9520	0.5630
g	0.9520	0.5620
h	0.9540	0.5640
i	0.9520	0.5630
j	0.9520	0.5600
k	0.9540	0.5610
l	0.9540	0.5620
m	0.9540	0.5630
n	0.9520	0.5620
o	0.9510	0.5610
p	0.9540	0.5620
q	0.9520	0.5630
r	0.9510	0.5600
s	0.9540	0.5610
t	0.9540	0.5620
u	0.9550	0.5620
v	0.9540	0.5620
w	0.9540	0.5620
x	0.9520	0.5620
y	0.9520	0.5610
z	0.9530	0.5620