wwPDB EM Validation Summary Report (i)

May 6, 2025 – 02:49 AM EDT

PDB ID	:	5URF / pdb_00005urf
EMDB ID	:	EMD-8598
Title	:	The structure of human bocavirus 1
Authors	:	Mietzsch, M.; Kailasan, S.; Garrison, J.; Ilyas, M.; Chipman, P.; Kandola, K.; Jansen, M.; Spear, J.; Sousa, D.; McKenna, R.; Soderlund-Venermo, M.; Baker, T.; Agbandje-McKenna, M.
Deposited on	:	2017-02-10
Resolution	:	2.90 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:

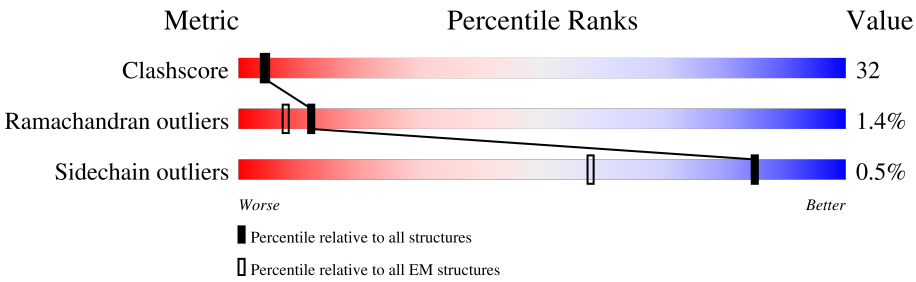
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (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 2.90 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	542	44% 46% • • 6%
1	2	542	44% 45% • • 6%
1	3	542	44% 46% • • 6%
1	4	542	45% 45% • • 6%
1	5	542	45% 45% • • 6%
1	6	542	46% 44% • • 6%
1	7	542	44% 45% • • 6%
1	8	542	46% 44% • • 6%

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Mol	Chain	Length	Quality of chain
1	A	542	43% 46% 6%
1	B	542	45% 45% 6%
1	C	542	44% 46% 6%
1	D	542	44% 46% 6%
1	E	542	44% 46% 6%
1	F	542	44% 46% 6%
1	G	542	45% 45% 6%
1	H	542	44% 46% 6%
1	I	542	45% 45% 6%
1	J	542	44% 45% 6%
1	K	542	45% 45% 6%
1	L	542	45% 45% 6%
1	M	542	45% 45% 6%
1	N	542	45% 45% 6%
1	O	542	44% 45% 6%
1	P	542	44% 46% 6%
1	Q	542	45% 45% 6%
1	R	542	45% 45% 6%
1	S	542	44% 46% 6%
1	T	542	44% 46% 6%
1	U	542	44% 45% 6%
1	V	542	44% 45% 6%
1	W	542	45% 45% 6%
1	X	542	44% 46% 6%
1	Y	542	44% 46% 6%

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Mol	Chain	Length	Quality of chain
1	Z	542	45% 44% 6%
1	a	542	44% 46% 6%
1	b	542	45% 45% 6%
1	c	542	45% 45% 6%
1	d	542	45% 45% 6%
1	e	542	44% 45% 6%
1	f	542	44% 46% 6%
1	g	542	44% 46% 6%
1	h	542	44% 46% 6%
1	i	542	45% 45% 6%
1	j	542	44% 46% 6%
1	k	542	44% 46% 6%
1	l	542	43% 46% 6%
1	m	542	45% 45% 6%
1	n	542	45% 45% 6%
1	o	542	44% 46% 6%
1	p	542	43% 46% 6%
1	q	542	44% 46% 6%
1	r	542	44% 46% 6%
1	s	542	45% 45% 6%
1	t	542	44% 46% 6%
1	u	542	46% 44% 6%
1	v	542	44% 45% 6%
1	w	542	44% 46% 6%
1	x	542	45% 45% 6%

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Mol	Chain	Length	Quality of chain
1	y	542	44% 46% 6%
1	z	542	44% 45% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 243720 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 viral protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	510	4062	2575	695	769	23	2	0
1	B	510	4062	2575	695	769	23	2	0
1	C	510	4062	2575	695	769	23	2	0
1	D	510	4062	2575	695	769	23	2	0
1	E	510	4062	2575	695	769	23	2	0
1	F	510	4062	2575	695	769	23	2	0
1	G	510	4062	2575	695	769	23	2	0
1	H	510	4062	2575	695	769	23	2	0
1	I	510	4062	2575	695	769	23	2	0
1	J	510	4062	2575	695	769	23	2	0
1	K	510	4062	2575	695	769	23	2	0
1	L	510	4062	2575	695	769	23	2	0
1	M	510	4062	2575	695	769	23	2	0
1	N	510	4062	2575	695	769	23	2	0
1	O	510	4062	2575	695	769	23	2	0
1	P	510	4062	2575	695	769	23	2	0
1	Q	510	4062	2575	695	769	23	2	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	510	4062	2575	695	769	23	2	0
1	S	510	4062	2575	695	769	23	2	0
1	T	510	4062	2575	695	769	23	2	0
1	U	510	4062	2575	695	769	23	2	0
1	V	510	4062	2575	695	769	23	2	0
1	W	510	4062	2575	695	769	23	2	0
1	X	510	4062	2575	695	769	23	2	0
1	Y	510	4062	2575	695	769	23	2	0
1	Z	510	4062	2575	695	769	23	2	0
1	1	510	4062	2575	695	769	23	2	0
1	2	510	4062	2575	695	769	23	2	0
1	3	510	4062	2575	695	769	23	2	0
1	4	510	4062	2575	695	769	23	2	0
1	5	510	4062	2575	695	769	23	2	0
1	6	510	4062	2575	695	769	23	2	0
1	a	510	4062	2575	695	769	23	2	0
1	b	510	4062	2575	695	769	23	2	0
1	c	510	4062	2575	695	769	23	2	0
1	d	510	4062	2575	695	769	23	2	0
1	e	510	4062	2575	695	769	23	2	0
1	f	510	4062	2575	695	769	23	2	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	g	510	4062	2575	695	769	23	2	0
1	h	510	4062	2575	695	769	23	2	0
1	i	510	4062	2575	695	769	23	2	0
1	j	510	4062	2575	695	769	23	2	0
1	k	510	4062	2575	695	769	23	2	0
1	l	510	4062	2575	695	769	23	2	0
1	m	510	4062	2575	695	769	23	2	0
1	n	510	4062	2575	695	769	23	2	0
1	o	510	4062	2575	695	769	23	2	0
1	p	510	4062	2575	695	769	23	2	0
1	q	510	4062	2575	695	769	23	2	0
1	r	510	4062	2575	695	769	23	2	0
1	s	510	4062	2575	695	769	23	2	0
1	t	510	4062	2575	695	769	23	2	0
1	u	510	4062	2575	695	769	23	2	0
1	v	510	4062	2575	695	769	23	2	0
1	w	510	4062	2575	695	769	23	2	0
1	x	510	4062	2575	695	769	23	2	0
1	y	510	4062	2575	695	769	23	2	0
1	z	510	4062	2575	695	769	23	2	0
1	7	510	4062	2575	695	769	23	2	0

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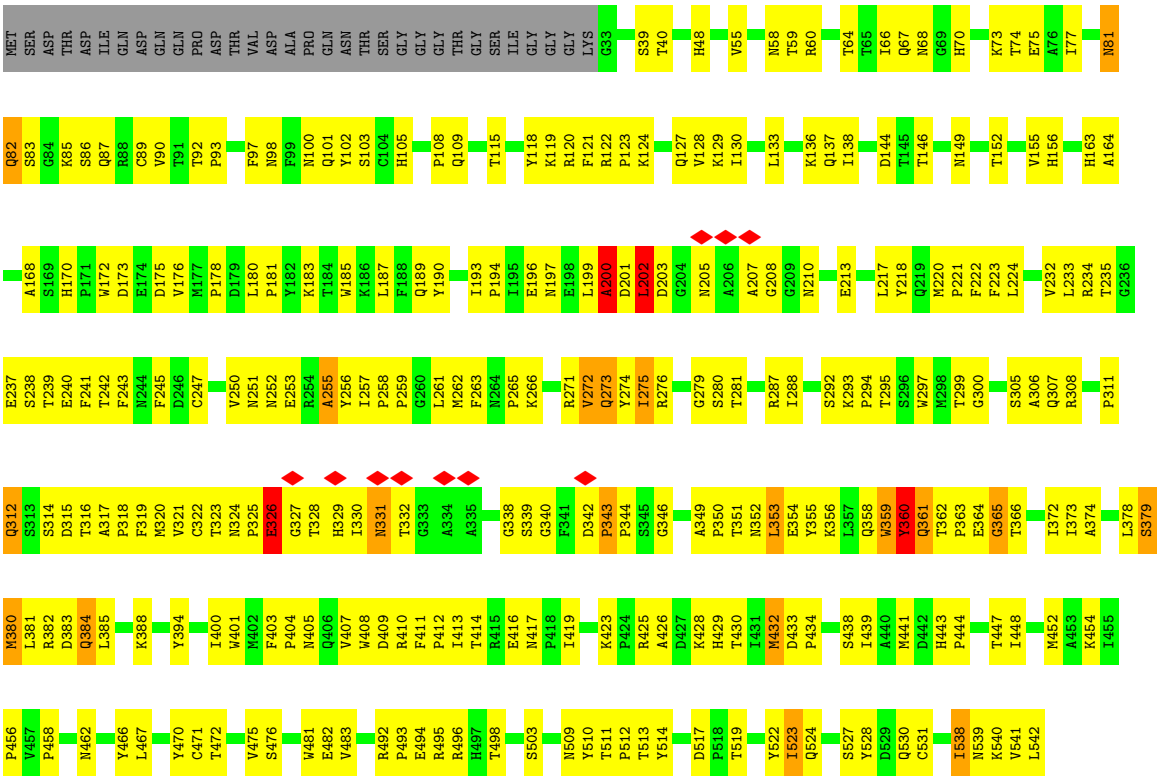
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8	510	4062	2575	695	769	23	2	0

3 Residue-property plots (i)

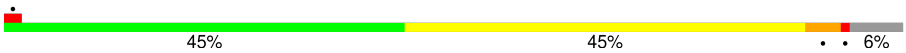
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

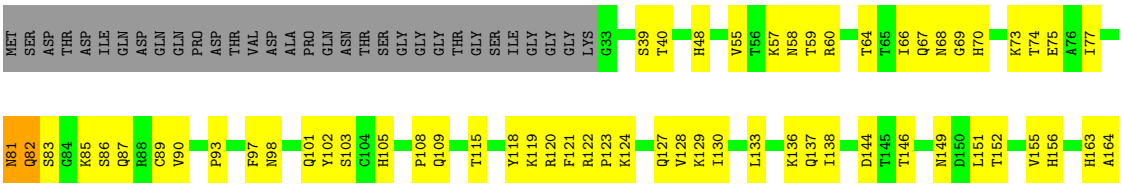
• Molecule 1: viral protein 3

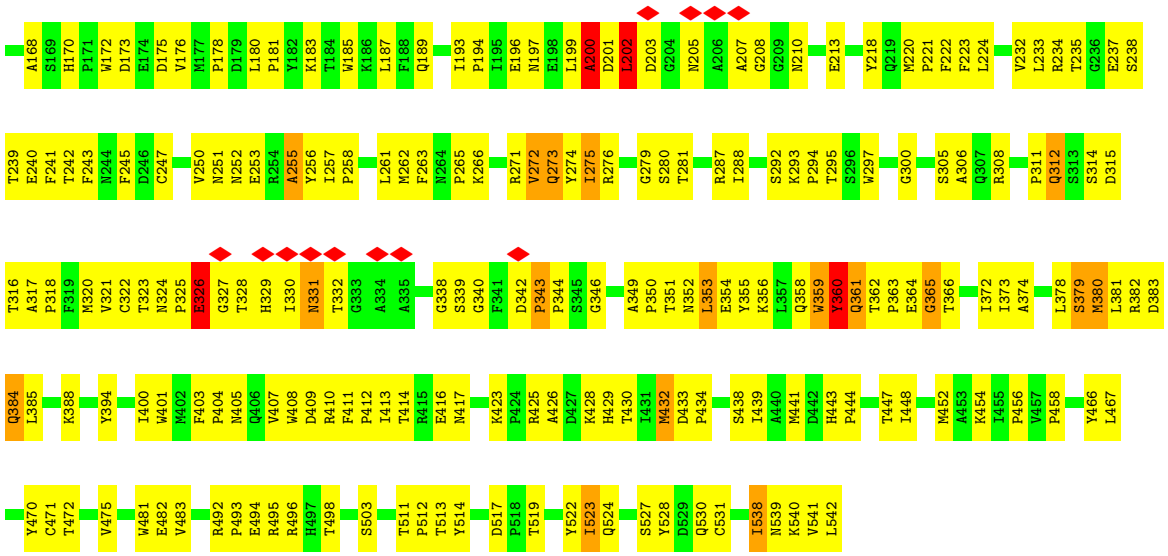
Chain A:



• Molecule 1: viral protein 3

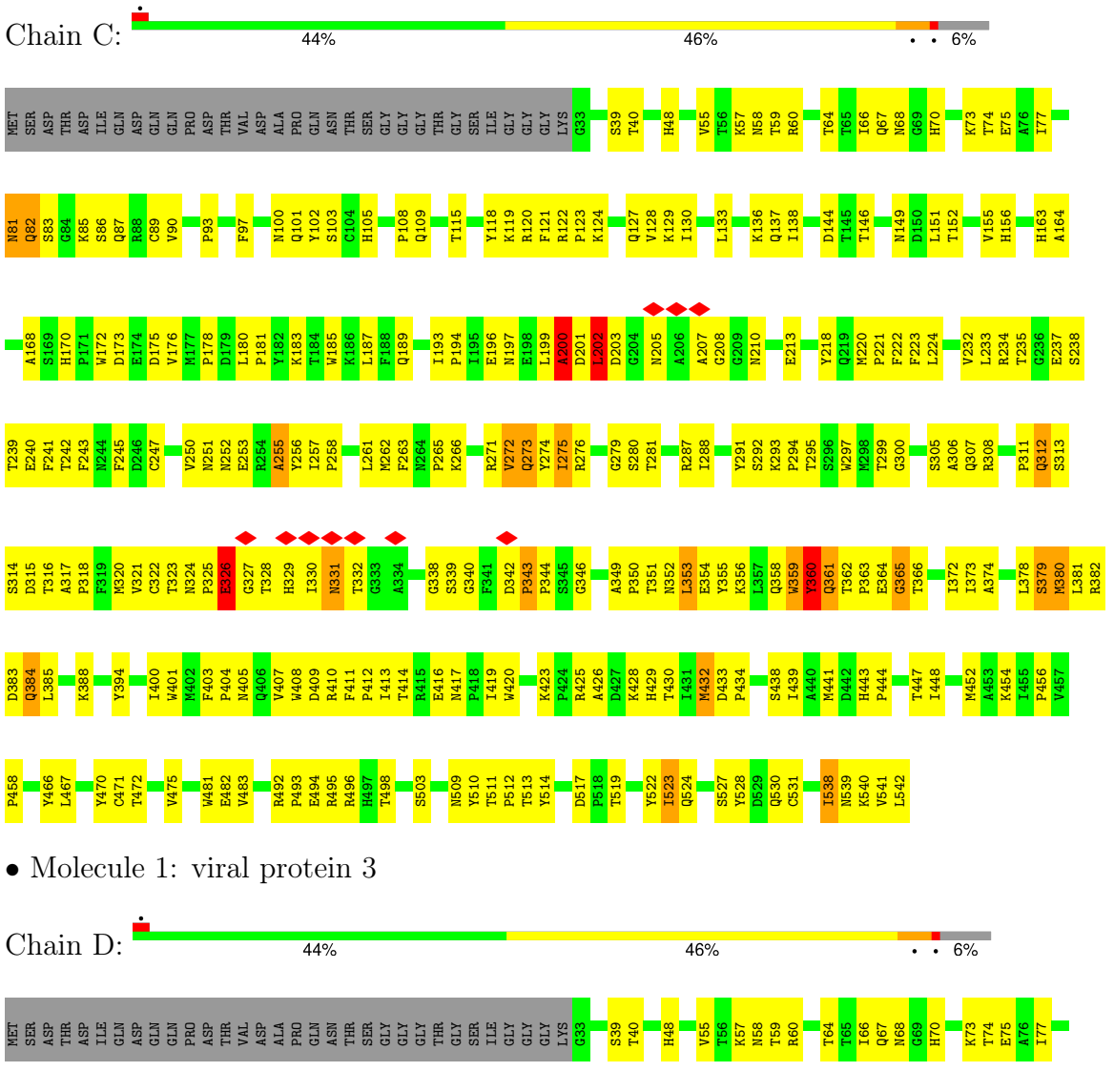
Chain B: 





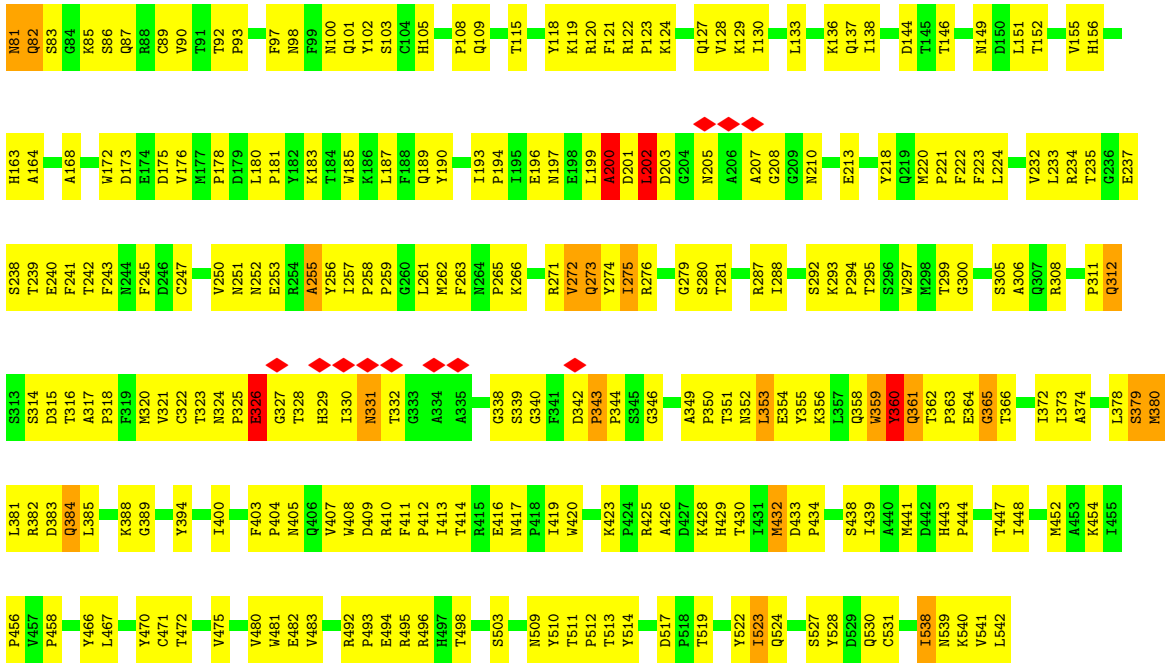
- Molecule 1: viral protein 3

Chain C:



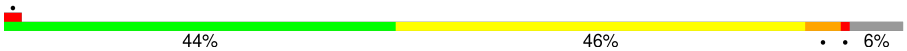
- Molecule 1: viral protein 3

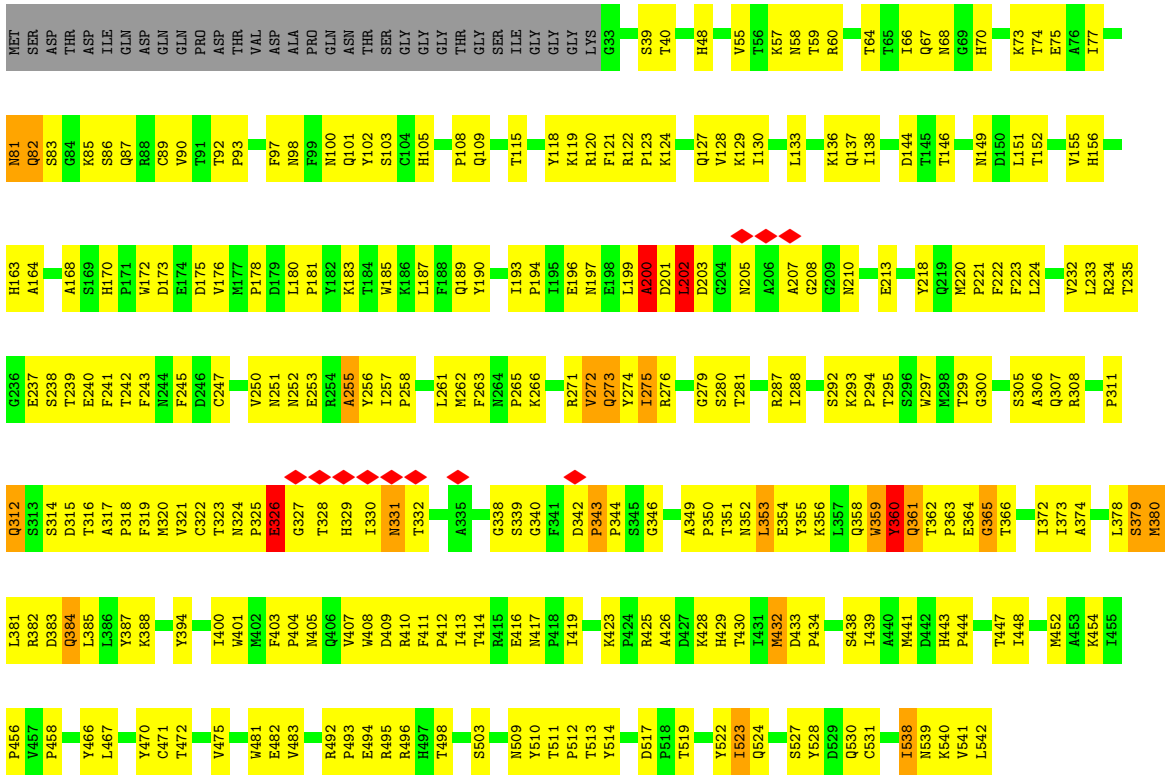
Chain D:



• Molecule 1: viral protein 3

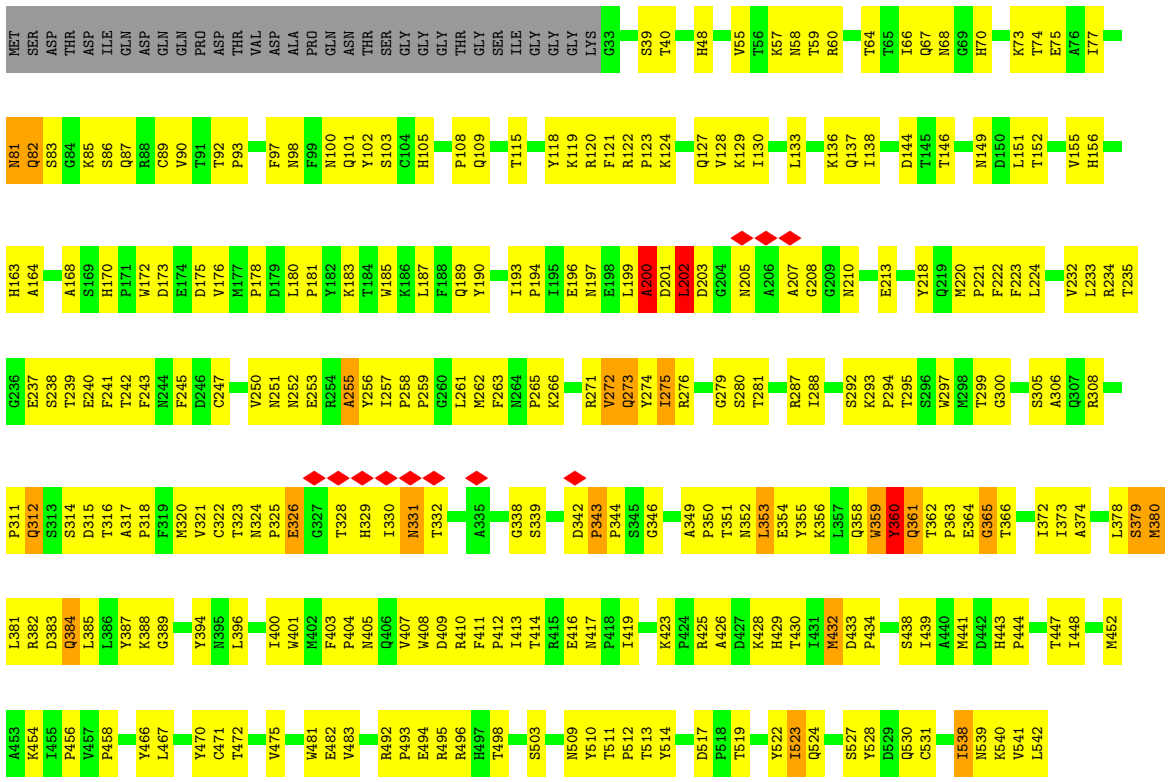
Chain E:





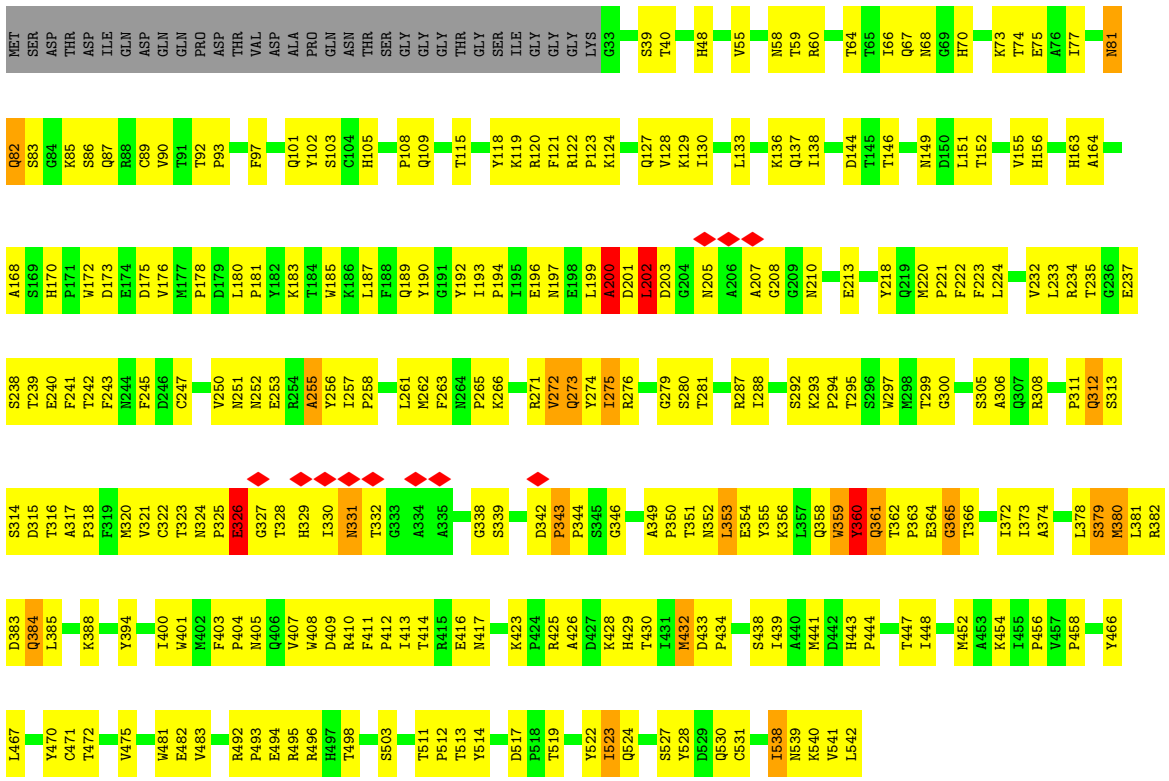
• Molecule 1: viral protein 3

Chain F:



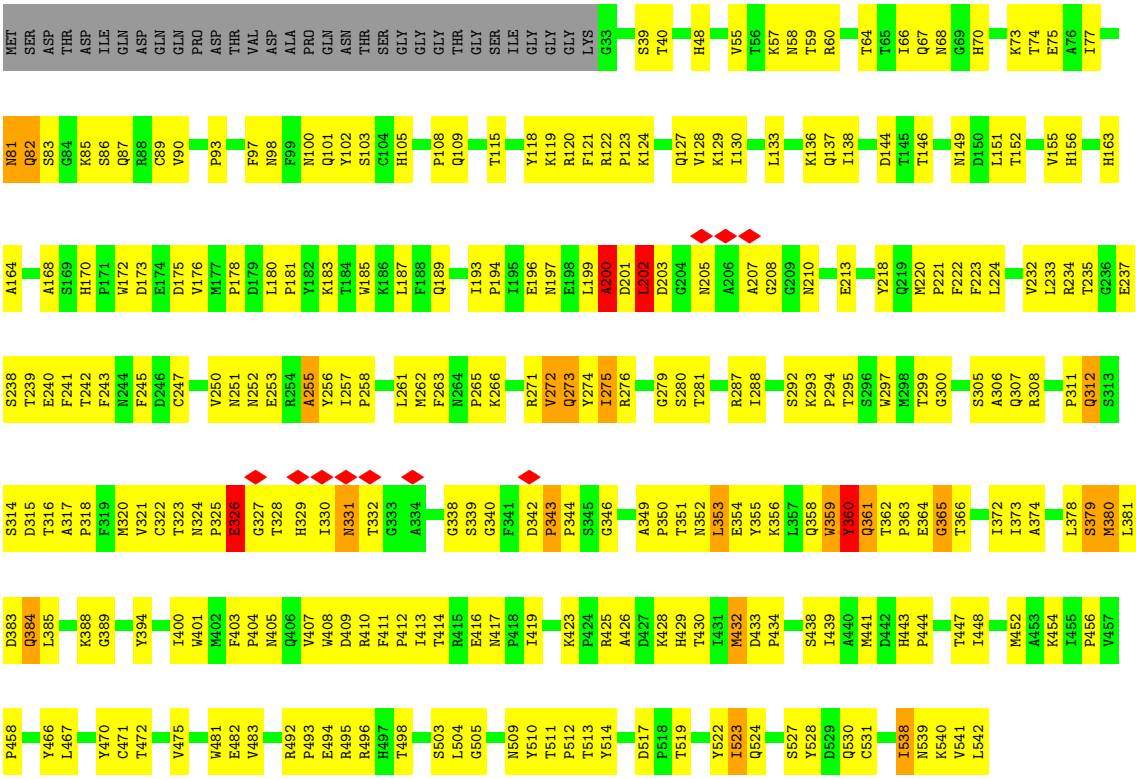
- Molecule 1: viral protein 3

Chain G: 45% 45% 6%



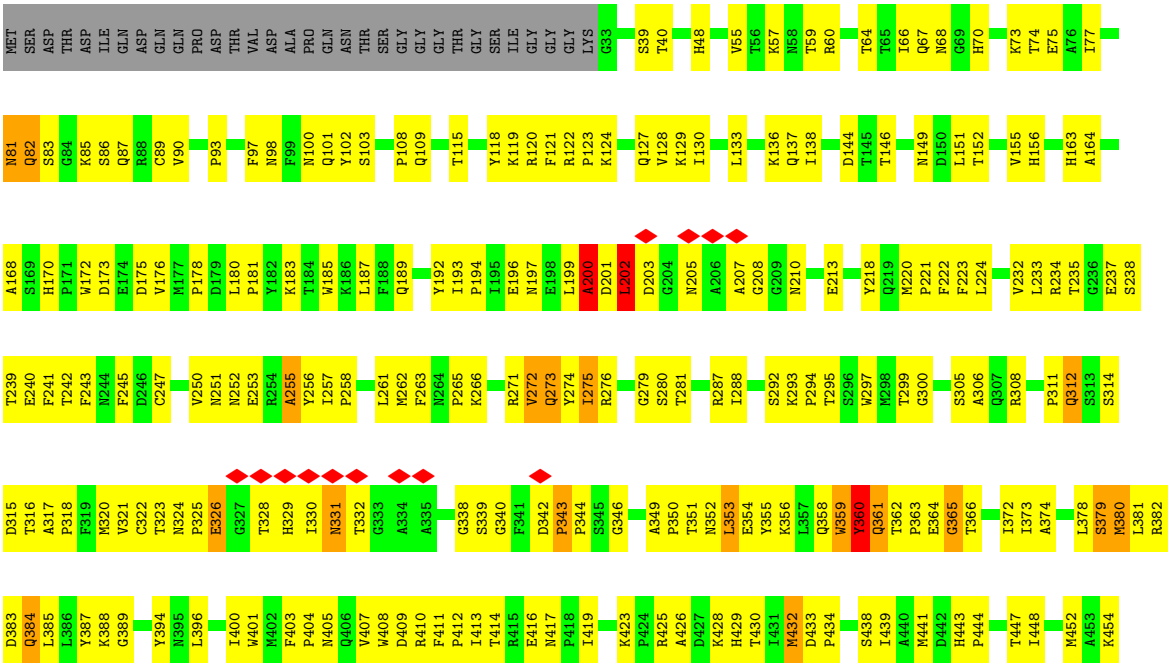
- Molecule 1: viral protein 3

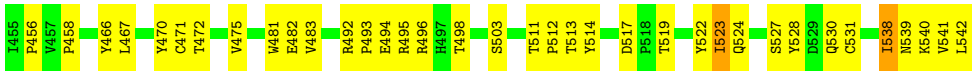
Chain H:



- Molecule 1: viral protein 3

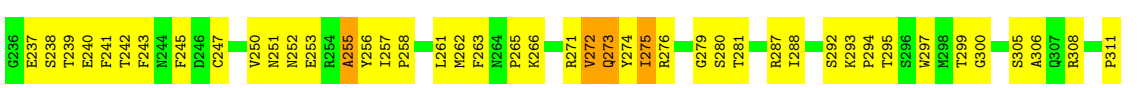
Chain I:

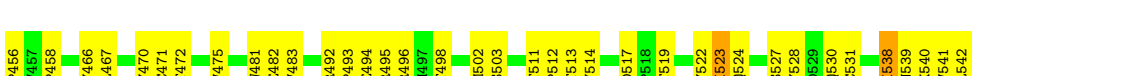




• Molecule 1: viral protein 3

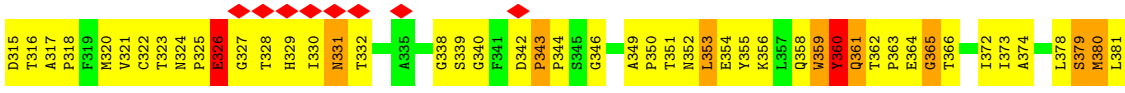
Chain J:

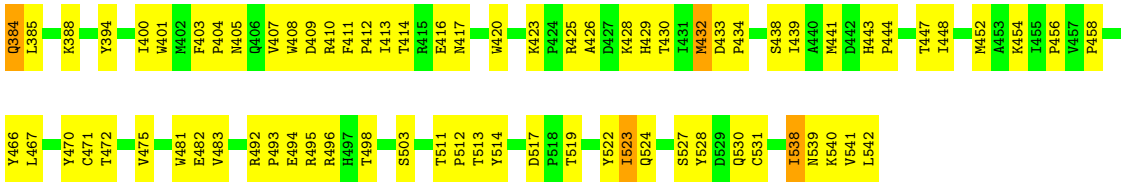




• Molecule 1: viral protein 3

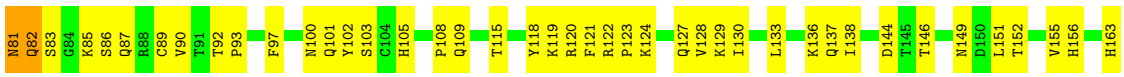
Chain K:

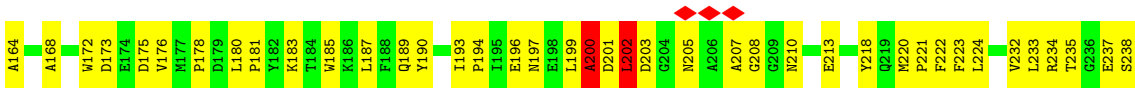


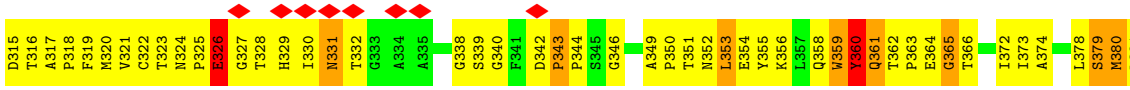


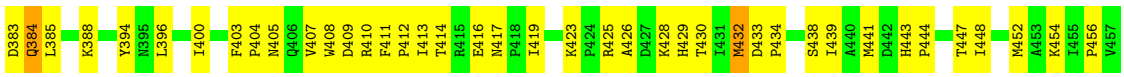
• Molecule 1: viral protein 3

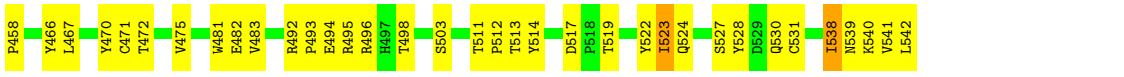
Chain L:





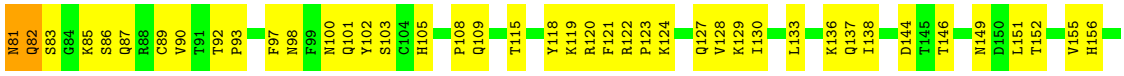


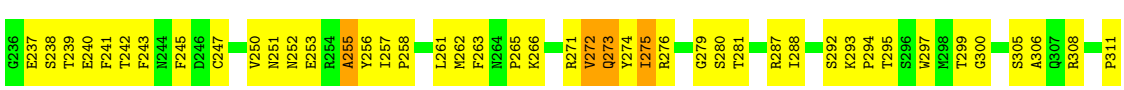


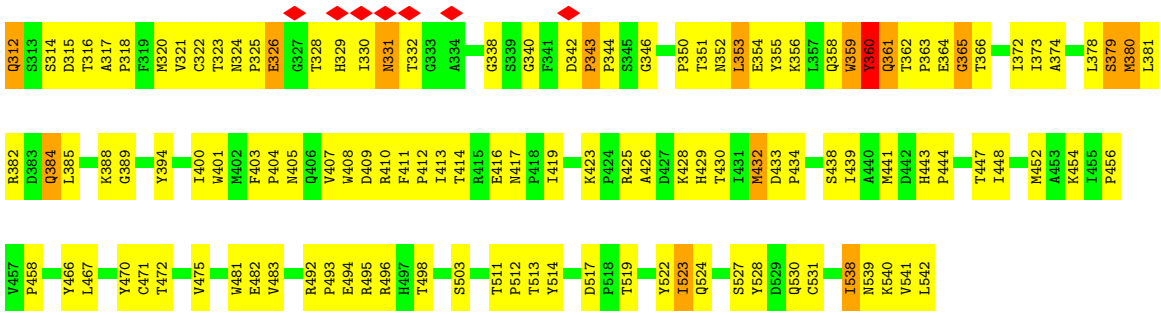


• Molecule 1: viral protein 3

Chain M:

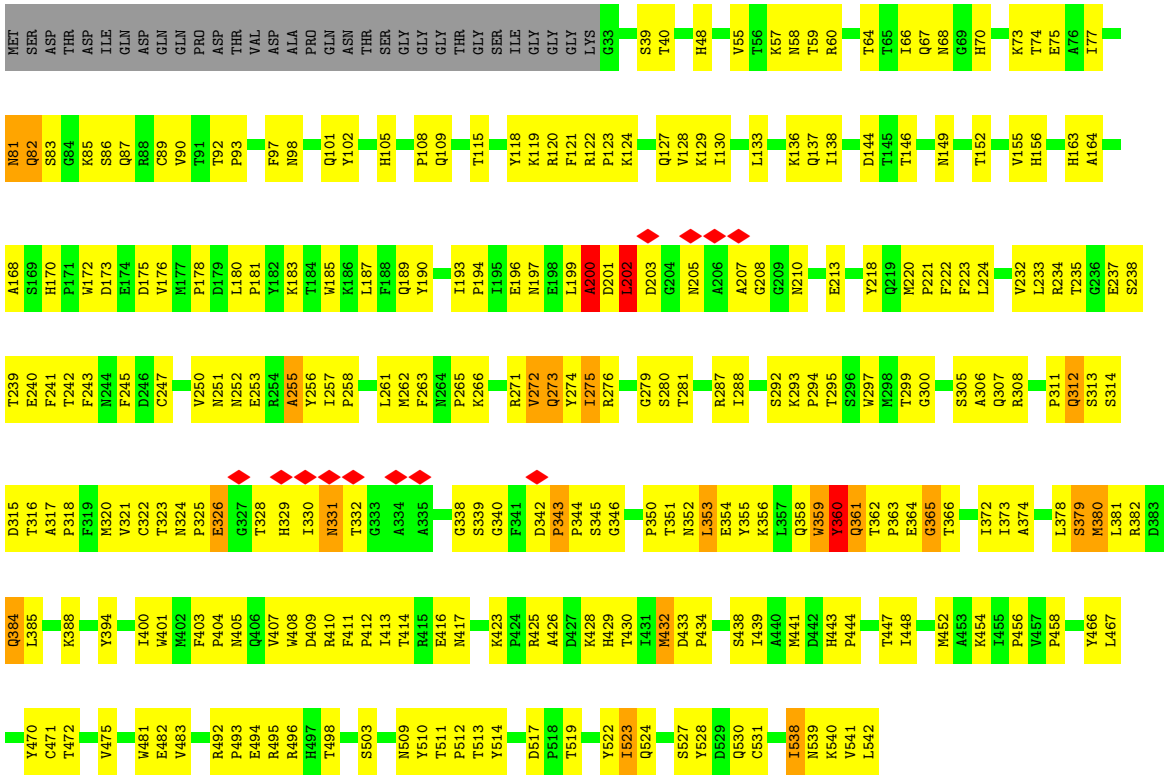






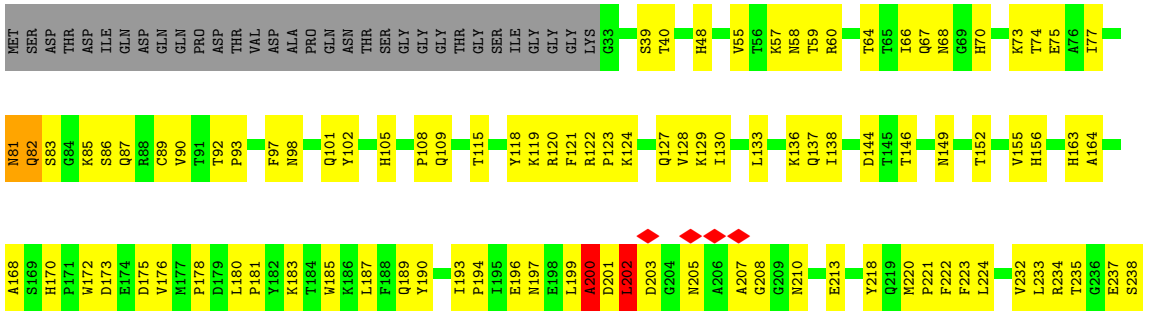
- Molecule 1: viral protein 3

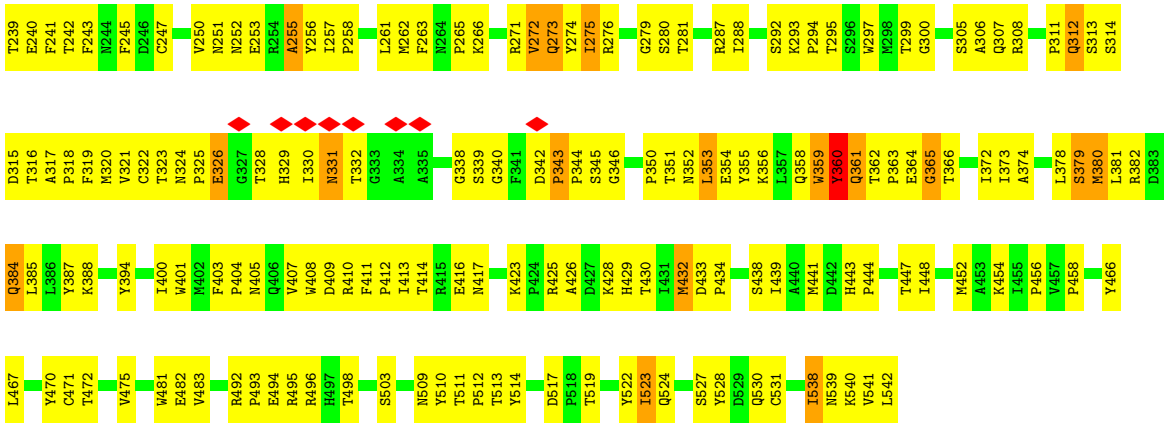
Chain N:



- Molecule 1: viral protein 3

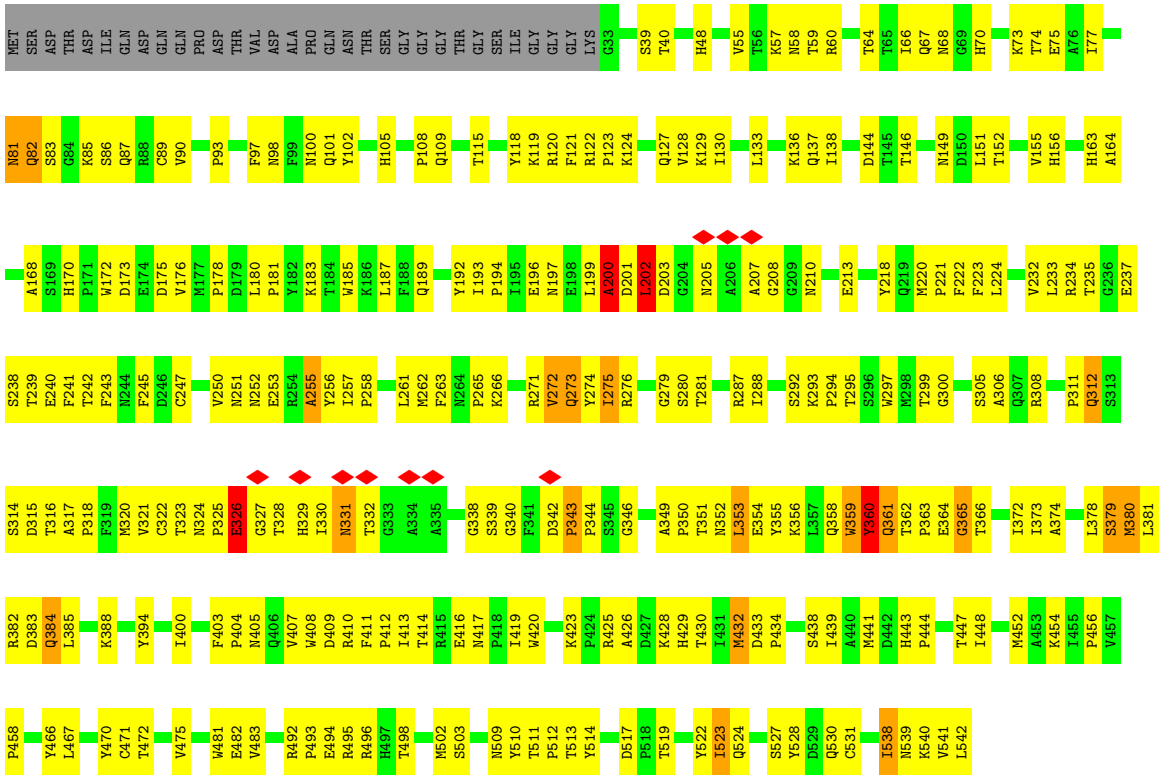
Chain O:





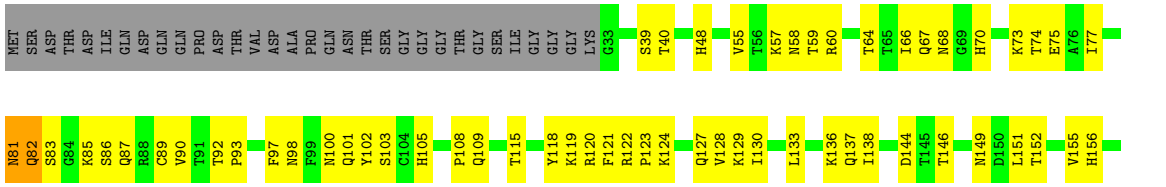
- Molecule 1: viral protein 3

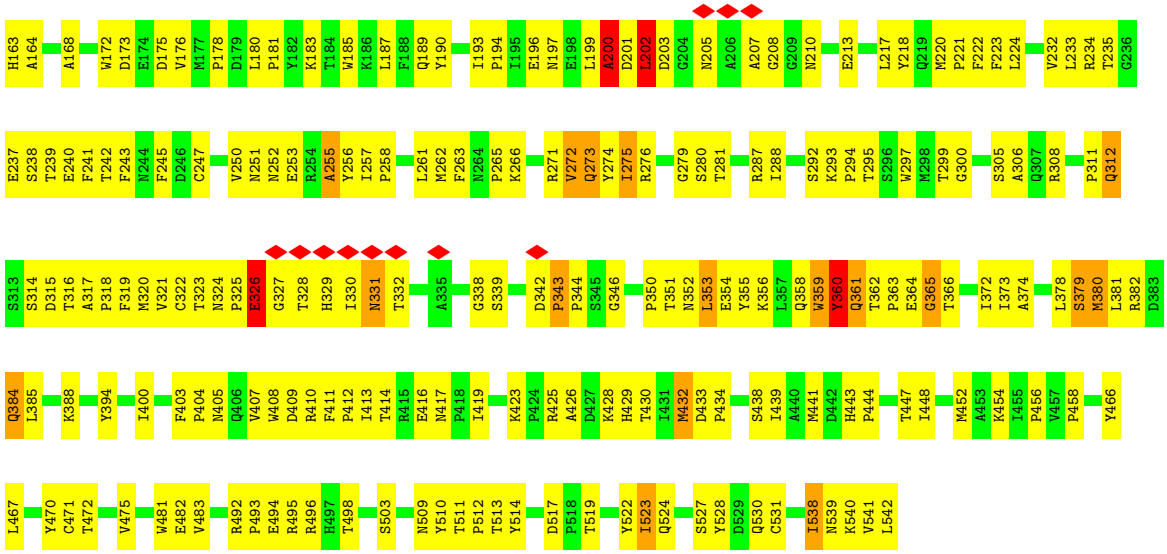
Chain P:



- Molecule 1: viral protein 3

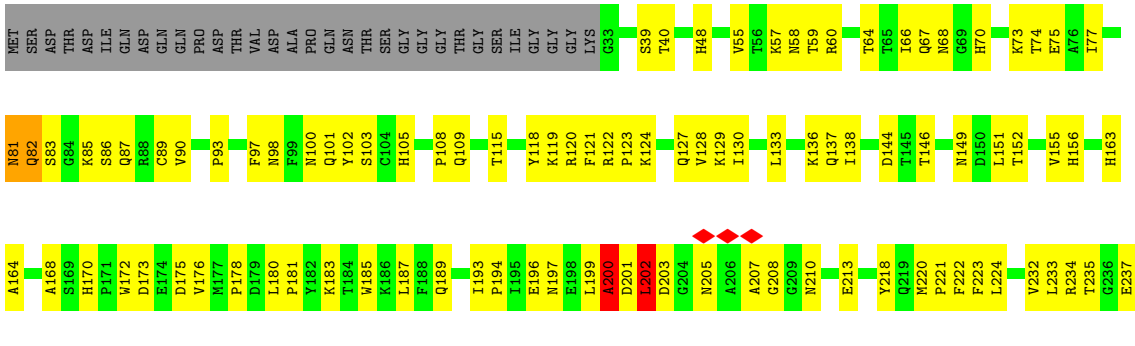
Chain Q:





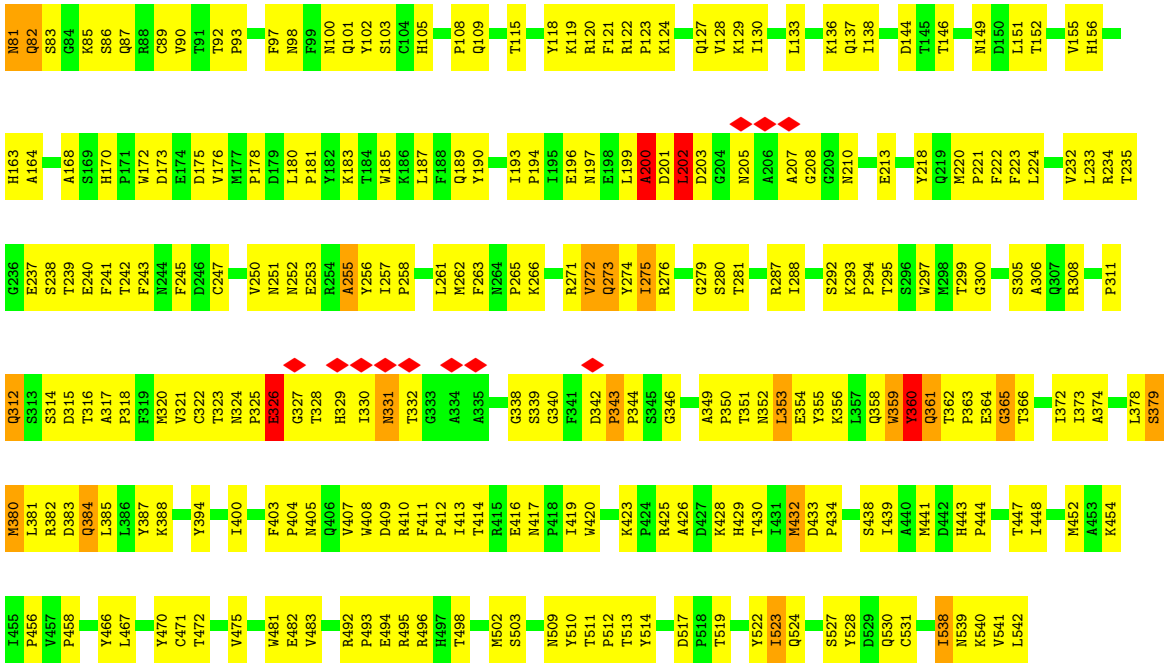
- Molecule 1: viral protein 3

Chain R:



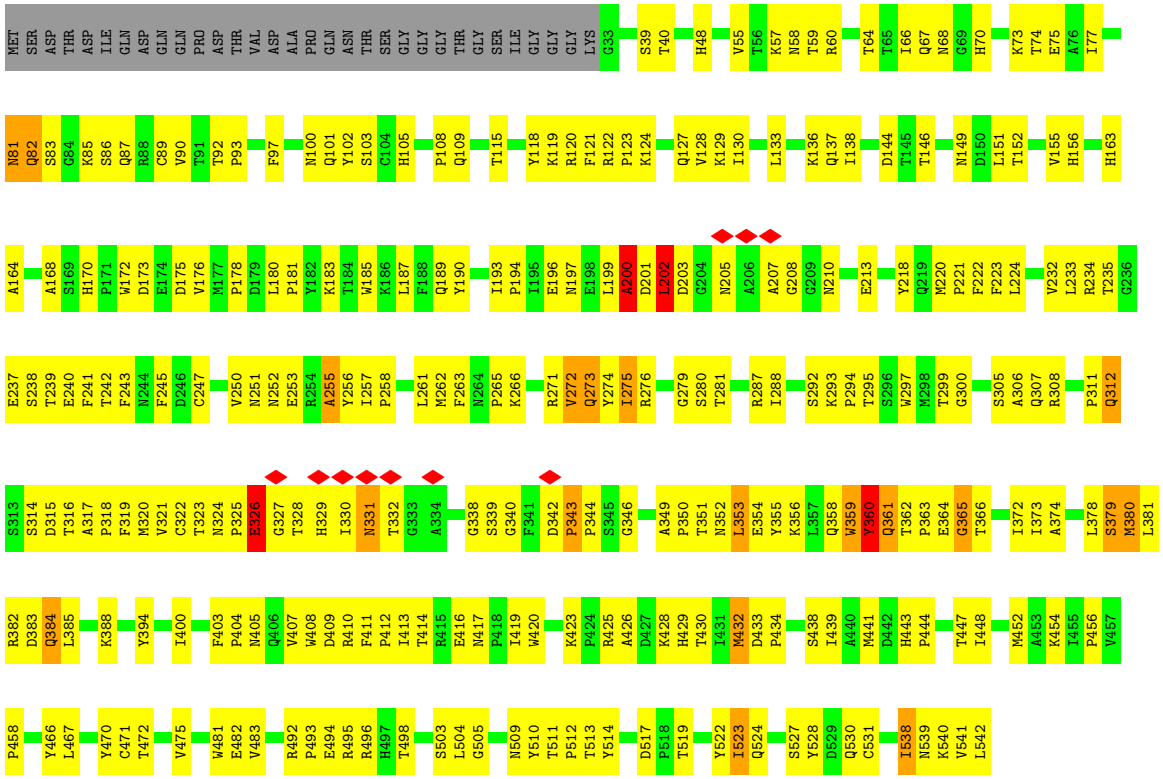
- Molecule 1: viral protein 3

Chain S:



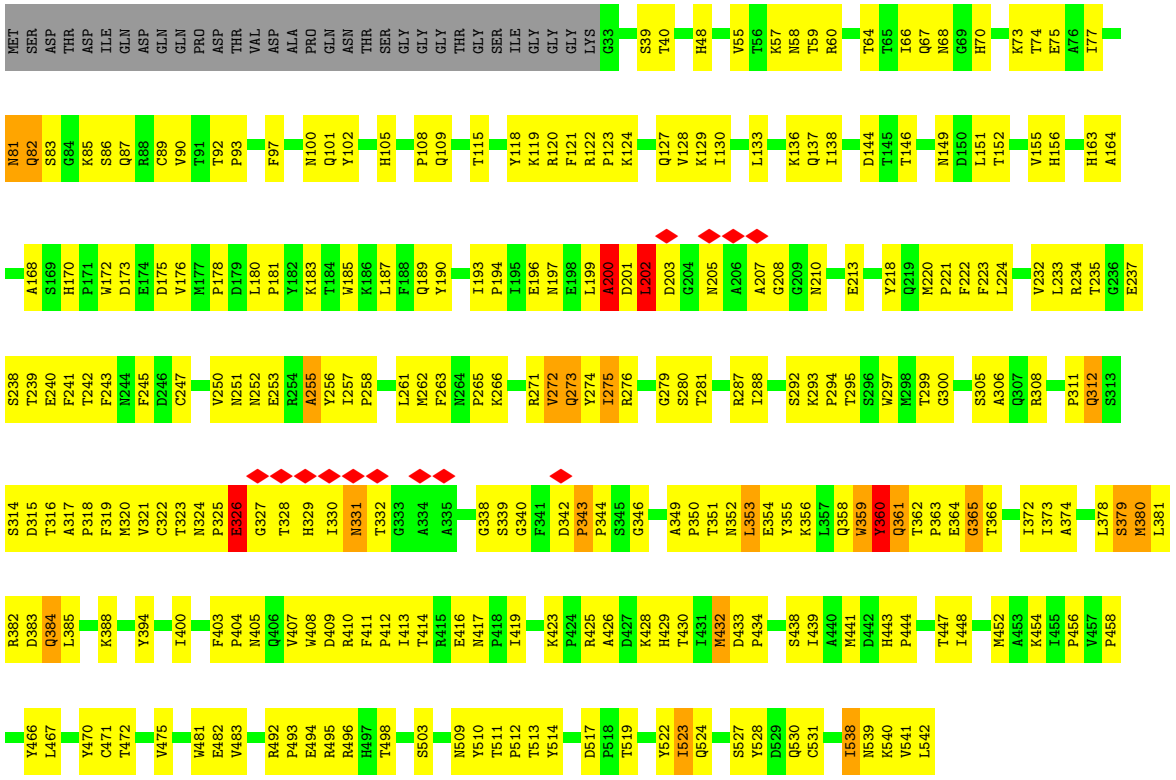
• Molecule 1: viral protein 3

Chain T:



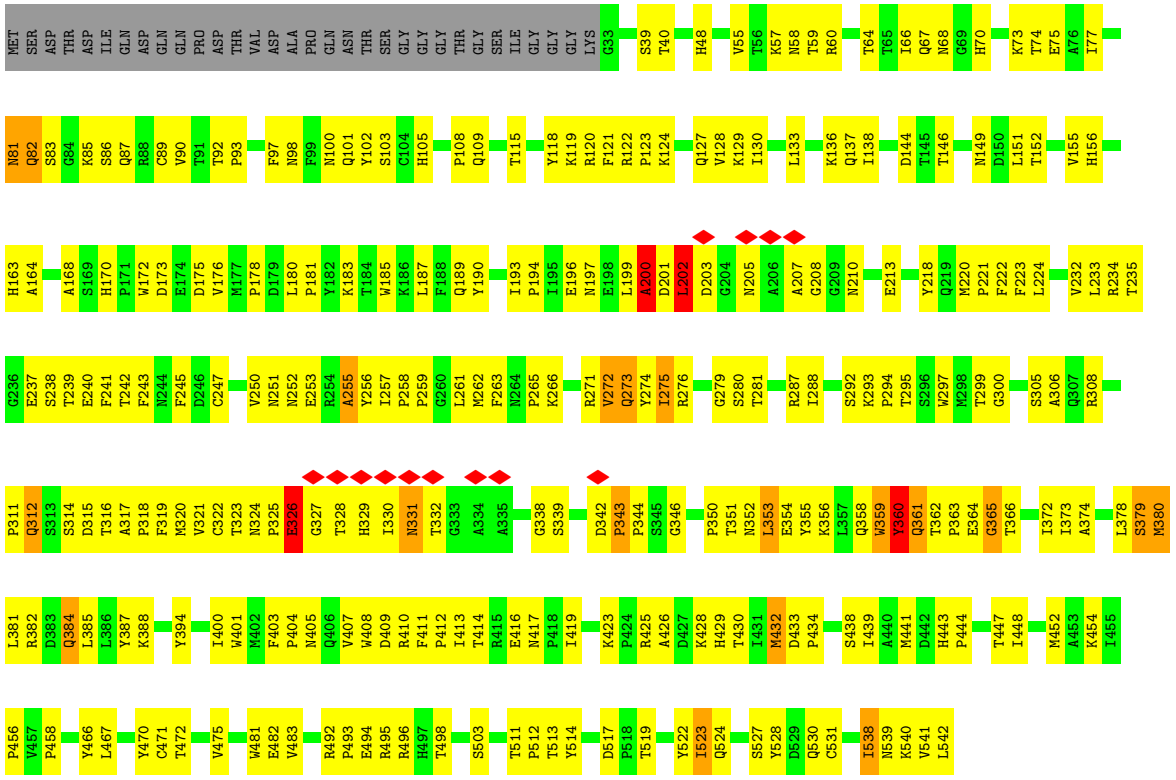
• Molecule 1: viral protein 3

Chain U:



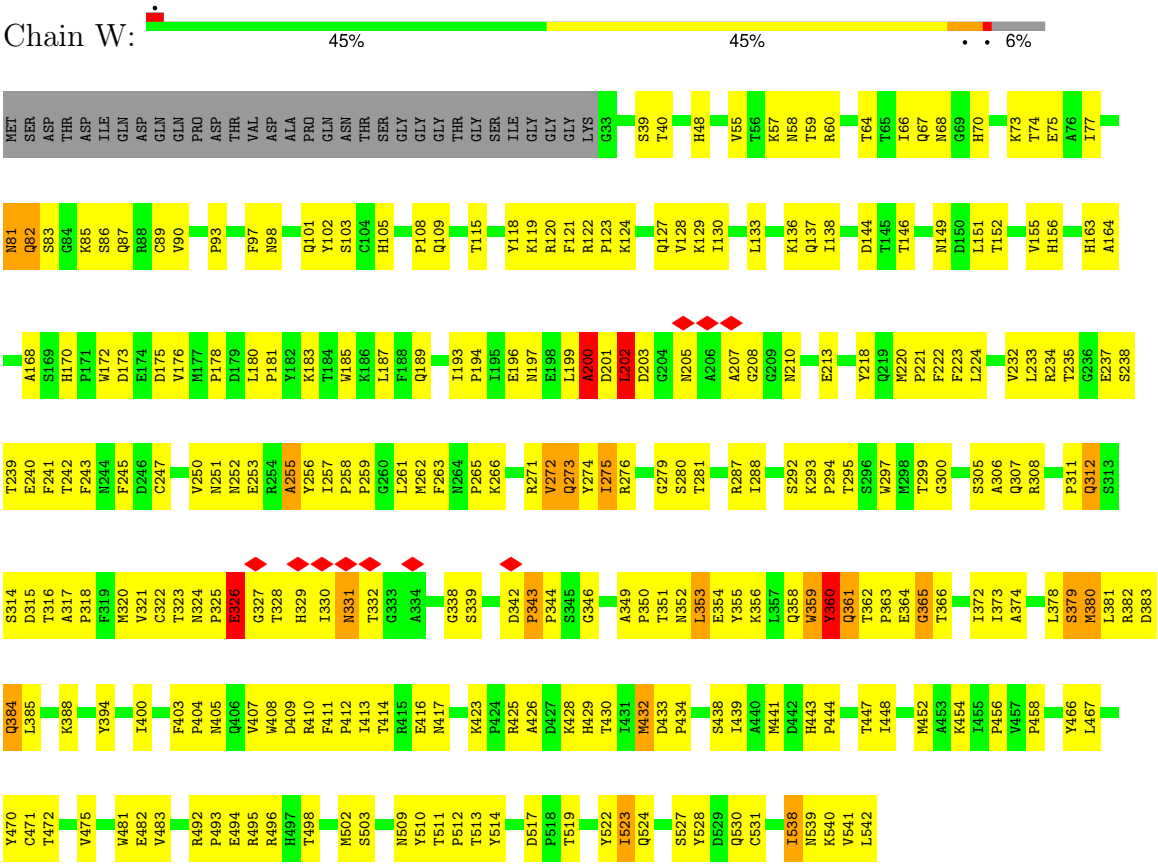
- Molecule 1: viral protein 3

Chain V:



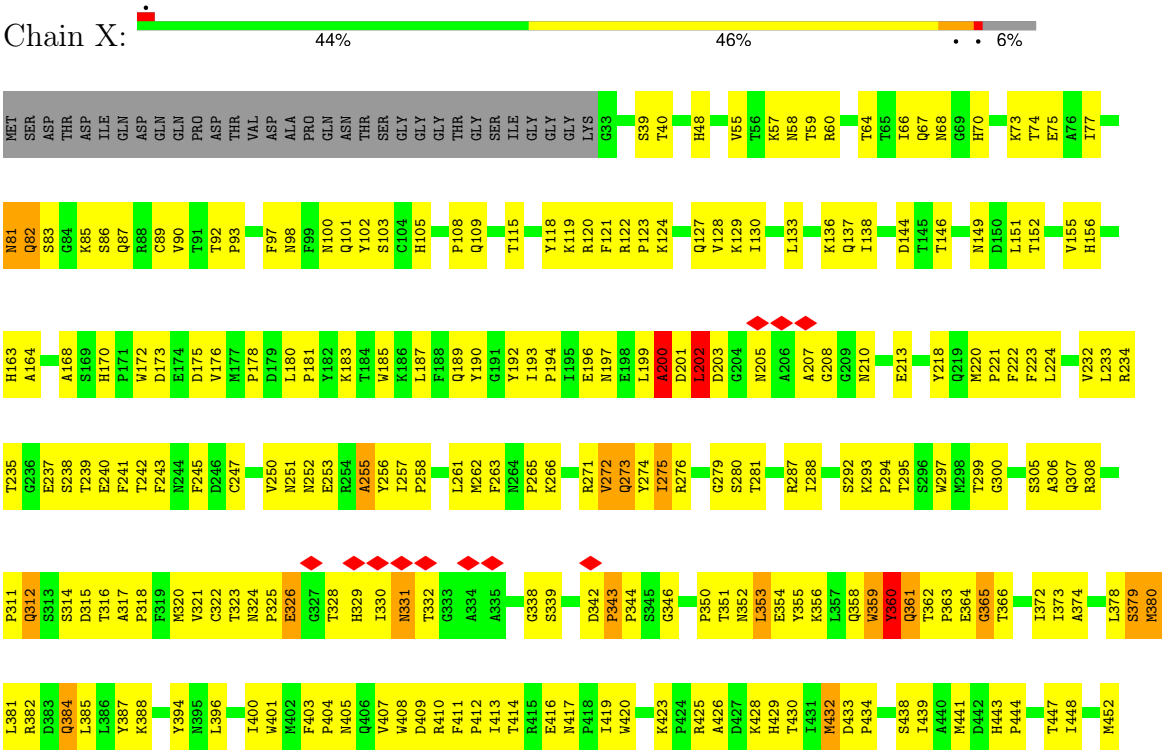
- Molecule 1: viral protein 3

Chain W:



- Molecule 1: viral protein 3

Chain X:



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- Molecule 1: viral protein 3

Chain Y:

MET SER ASP THR ASP ILE GLN ASP GLN GLN PRO ASP THR VAL ASP ALA PRO GLN ASN THR SER GLY GLY GLY THR GLY SER ILE GLY GLY GLY LYS G33 S39 T40 H48 V55 T56 K57 N58 T59 R60 T64 T65 I66 Q67 N68 G69 H70 K73 T74 E75 A76 I77

N81 Q82 S83 G84 K85 S86 Q87 R88 C89 V90 T91 T92 P93 F97 N100 Q101 Y102 S103 C104 H105 P108 Q109 T115 Y118 K119 R120 F121 R122 P123 K124 Q127 V128 K129 I130 L133 K136 Q137 I138 D144 T145 T146 N149 D150 L151 T152 V155 H156 H163

A164 A168 S169 H170 P171 W172 D173 E174 D175 V176 M177 P178 D179 L180 P181 Y182 K183 T184 W185 K186 L187 F188 Q189 Y190 I193 P194 I195 E196 N197 E198 L199 A200 D201 L202 D203 G204 N205 A206 A207 G208 G209 N210 E213 Y218 Q219 M220 P221 F222 F223 L224 V232 L233 R234 T235 G236

E237 S238 T239 E240 F241 T242 F243 N244 F245 D246 C247 V250 N251 N252 E253 R254 A255 Y256 I257 P258 L261 M262 F263 N264 P265 K266 R271 V272 Q273 Y274 I275 R276 G279 S280 T281 R287 I288 S292 K293 P294 T295 S296 W297 M298 T299 G300 S305 A306 Q307 R308 P311 Q312

S313 S314 D315 T316 A317 P318 F319 M320 V321 C322 T323 N324 P325 E326 G327 T328 H329 I330 N331 T332 G333 A334 G338 S339 G340 F341 D342 P343 P344 S345 G346 A349 P350 T351 N352 L353 E354 Y355 K356 L357 Q358 W359 Y360 Q361 T362 P363 E364 G365 T366 I372 I373 A374 L378 S379 M380 L381

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I455 P456 V457 P458 Y466 L467 Y470 C471 T472 V475 W481 E482 V483 R492 P493 E494 R495 R496 H497 T498 S503 N509 Y510 T511 P512 T513 Y514 D517 P518 T519 Y522 I523 Q524 S527 Y528 D529 Q530 C531 I538 N539 K540 V541 L542

- Molecule 1: viral protein 3

Chain Z:

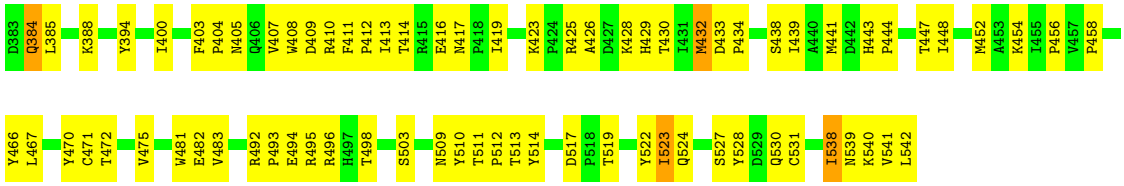
MET SER ASP THR ASP ILE GLN ASP GLN GLN PRO ASP THR VAL ASP ALA PRO GLN ASN THR SER GLY GLY GLY THR GLY SER ILE GLY GLY GLY LYS G33 S39 T40 H48 V55 T56 K57 N58 T59 R60 T64 T65 I66 Q67 N68 G69 H70 K73 T74 E75 A76 I77

N81 Q82 S83 G84 K85 S86 Q87 R88 C89 V90 T91 T92 P93 F97 N100 Q101 Y102 S103 C104 H105 P108 Q109 T115 Y118 K119 R120 F121 R122 P123 K124 Q127 V128 K129 I130 L133 K136 Q137 I138 D144 T145 T146 N149 D150 L151 T152 V155 H156 H163

A164 A168 S169 H170 P171 W172 D173 E174 D175 V176 M177 P178 D179 L180 P181 Y182 K183 T184 W185 K186 L187 F188 Q189 Y190 I193 P194 I195 E196 N197 E198 L199 A200 D201 L202 D203 G204 N205 A206 A207 G208 G209 N210 E213 Y218 Q219 M220 P221 F222 F223 L224 V232 L233 R234 T235 G236

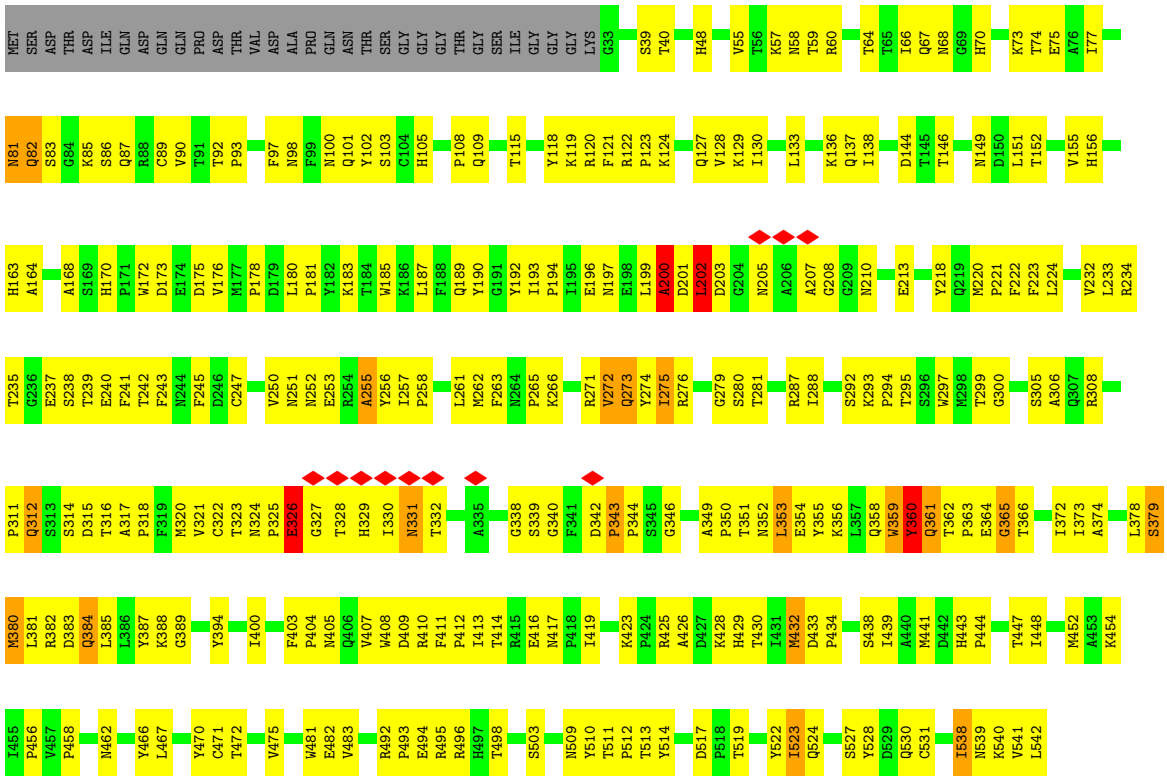
E237 S238 T239 E240 F241 T242 F243 N244 F245 D246 C247 N251 N252 E253 R254 A255 Y256 I257 P258 L261 M262 F263 N264 P265 K266 R271 V272 Q273 Y274 I275 R276 G279 S280 T281 R287 I288 S292 K293 P294 T295 S296 W297 M298 T299 G300 S305 A306 Q307 R308 P311 Q312 S313

S314 D315 T316 A317 P318 F319 M320 V321 C322 T323 N324 P325 E326 G327 T328 H329 I330 N331 T332 G333 A334 A335 G338 S339 G340 F341 D342 P343 P344 S345 G346 P350 T351 N352 L353 E354 Y355 K356 L357 Q358 W359 Y360 Q361 T362 P363 E364 G365 T366 I372 I373 A374 L378 S379 M380 L381 R382



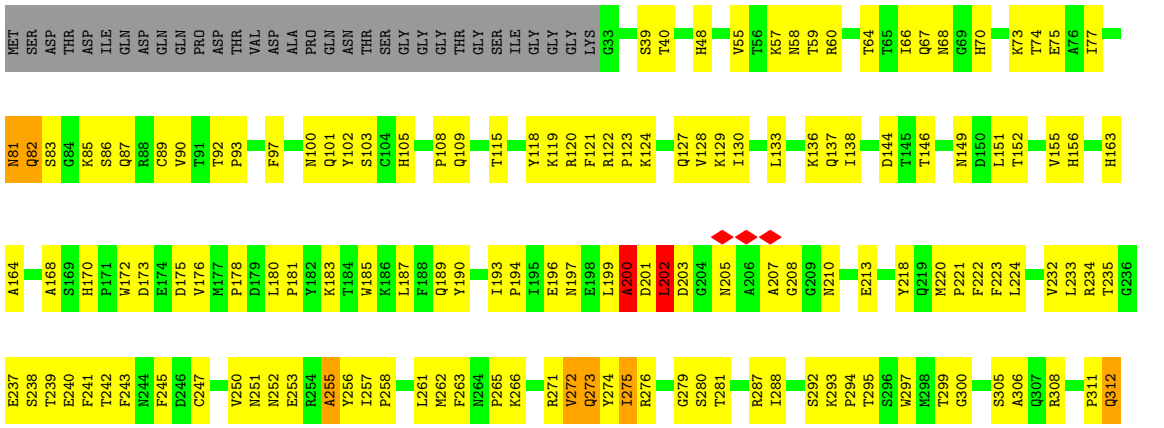
• Molecule 1: viral protein 3

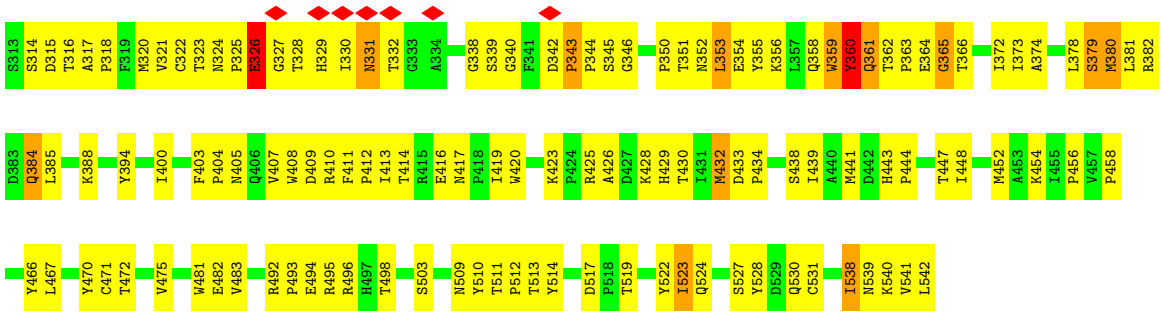
Chain 1:



• Molecule 1: viral protein 3

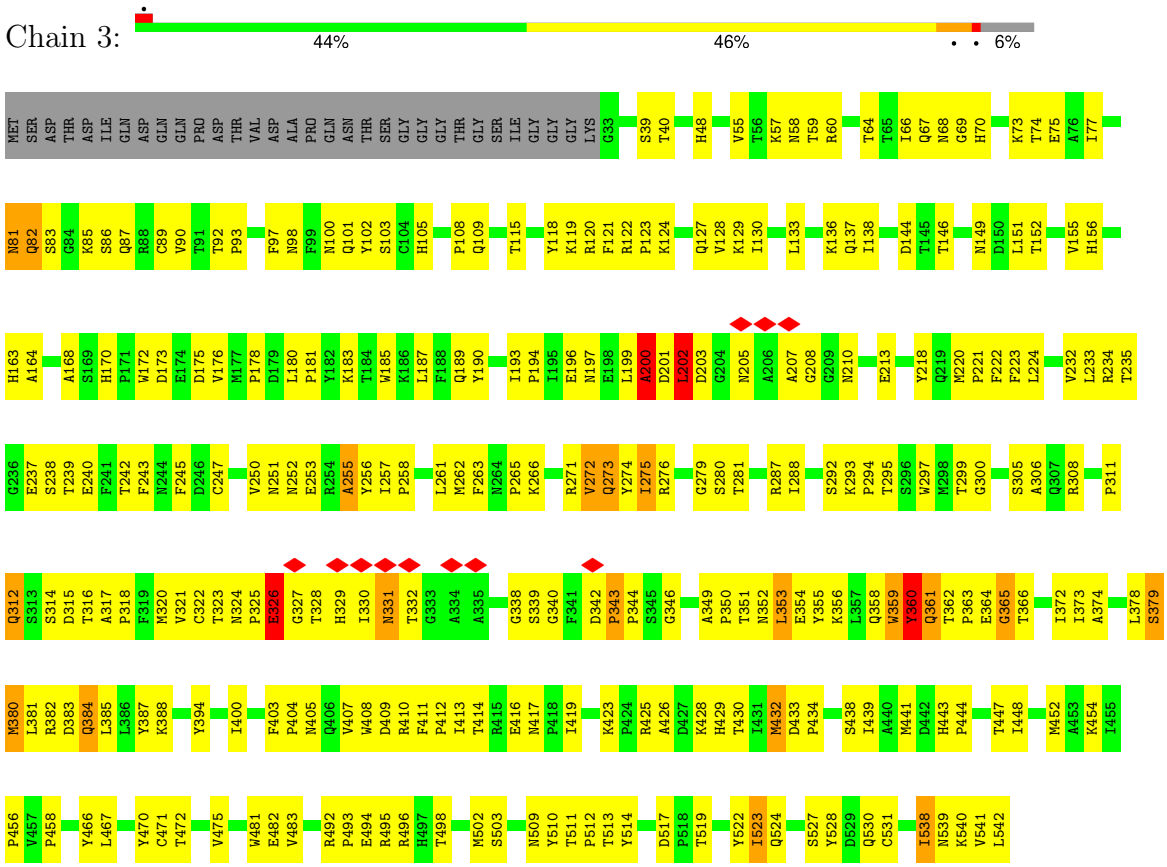
Chain 2:





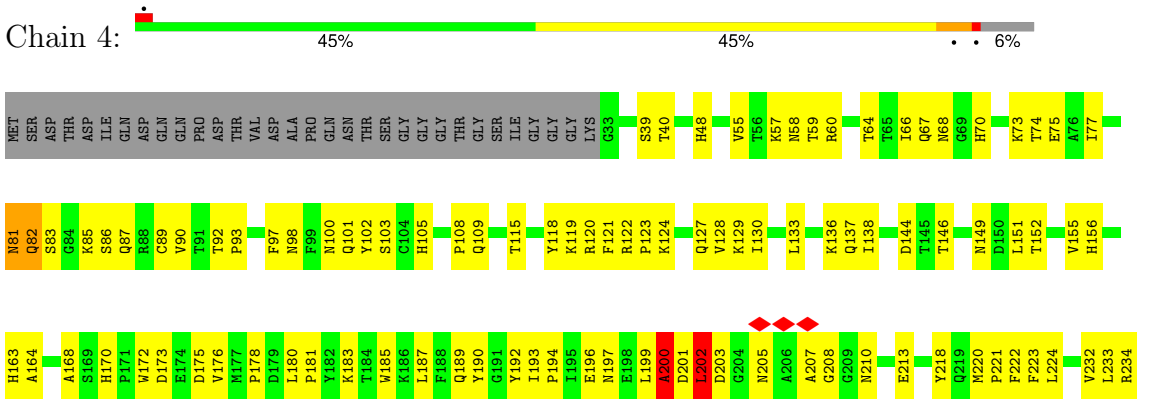
- Molecule 1: viral protein 3

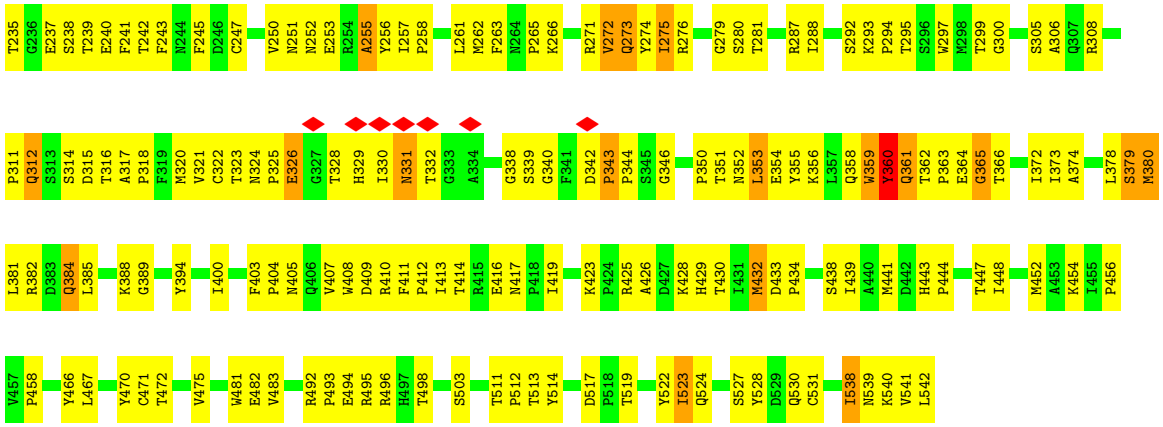
Chain 3:



- Molecule 1: viral protein 3

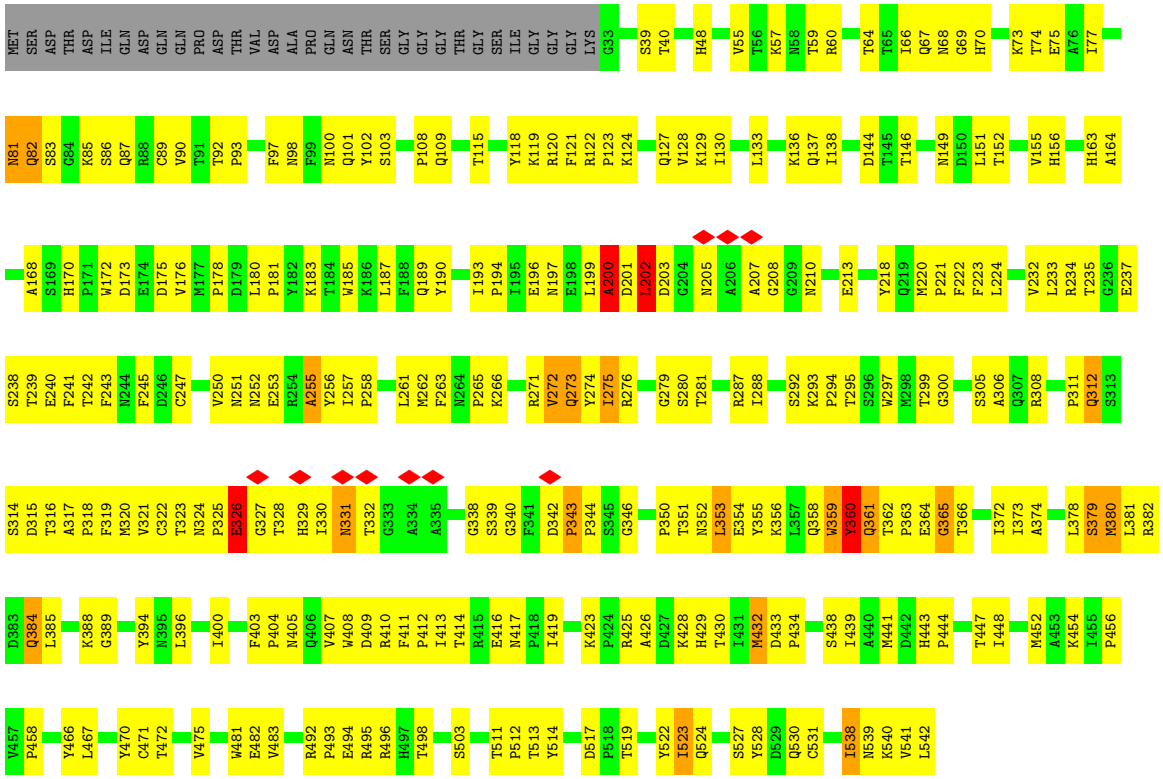
Chain 4:





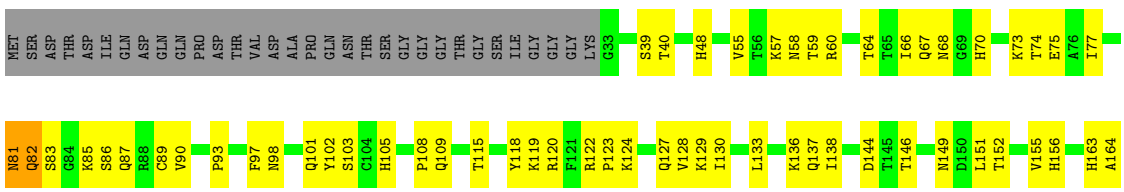
- Molecule 1: viral protein 3

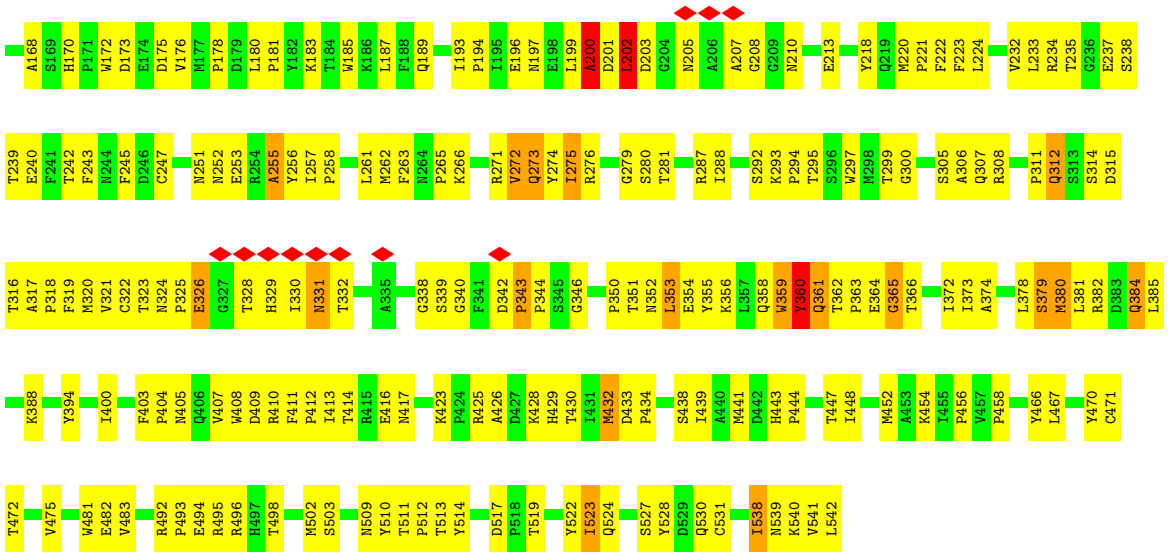
Chain 5:



- Molecule 1: viral protein 3

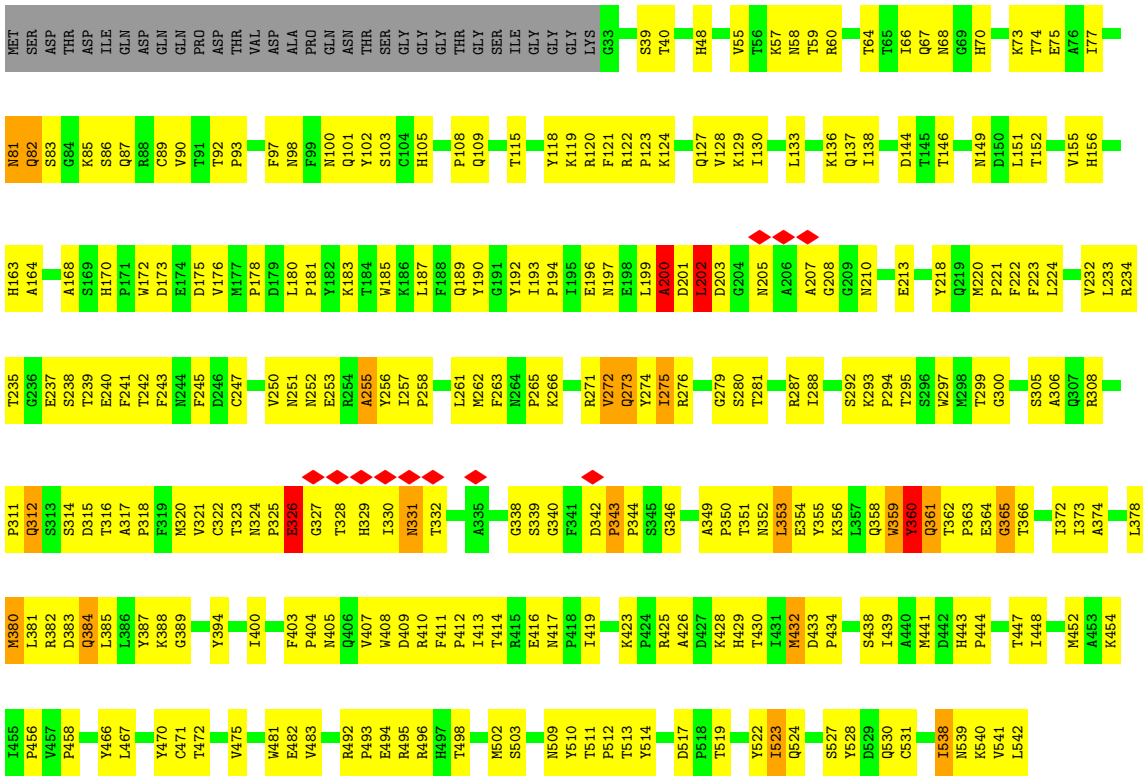
Chain 6:





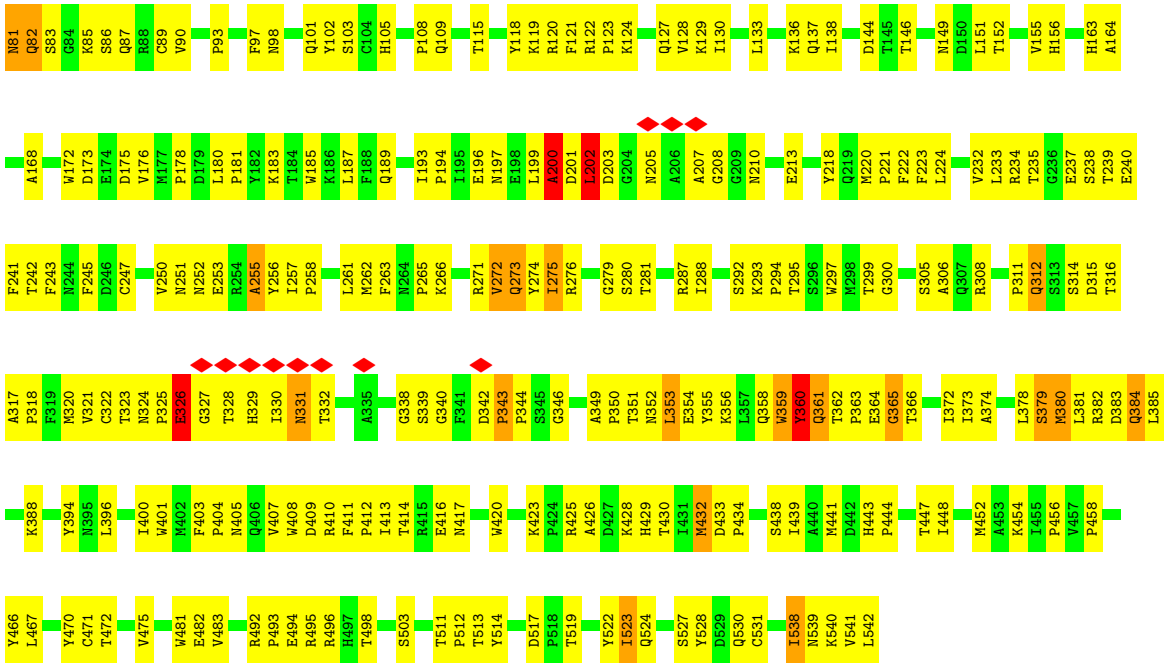
- Molecule 1: viral protein 3

Chain a:



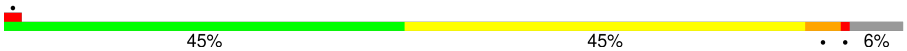
- Molecule 1: viral protein 3

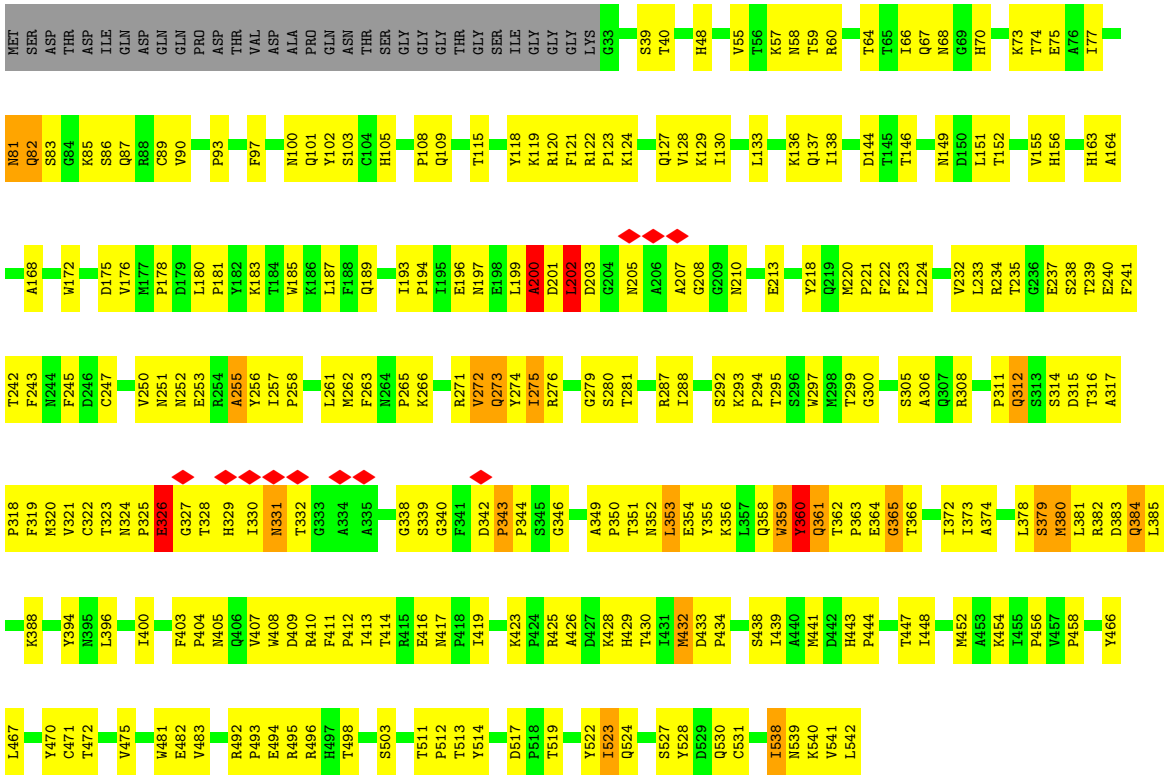
Chain b:



- Molecule 1: viral protein 3

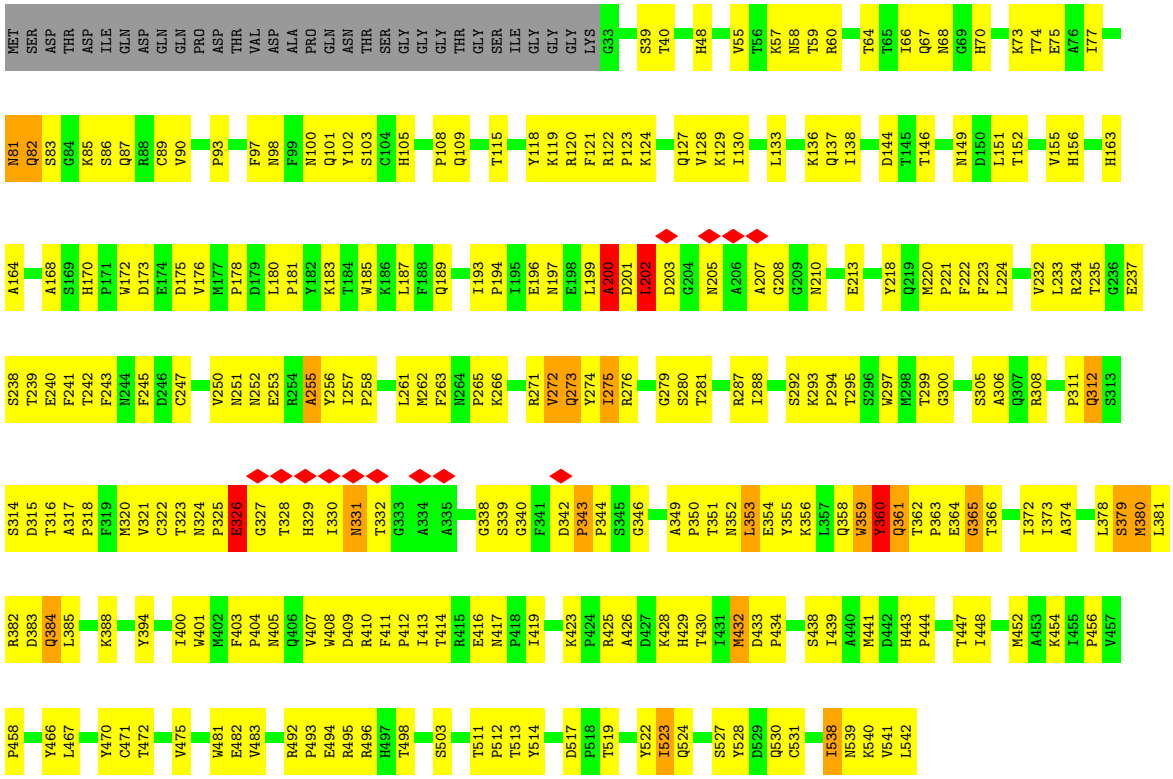
Chain c:





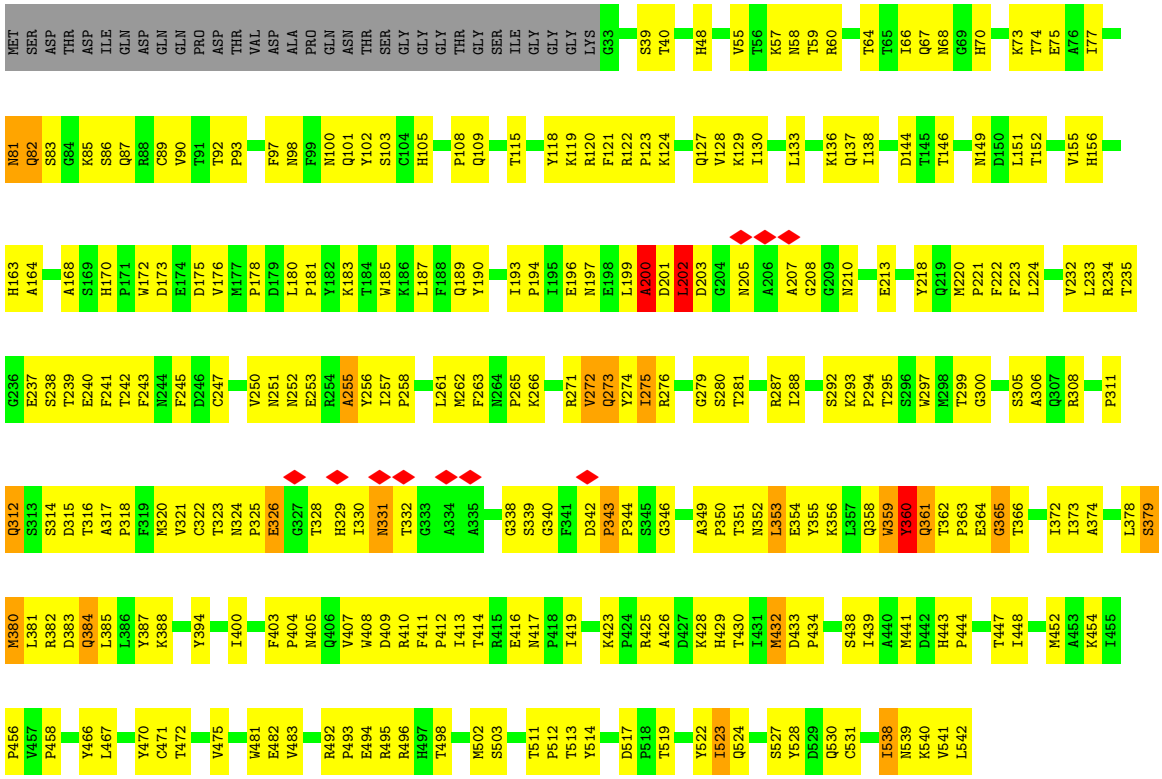
- Molecule 1: viral protein 3

Chain d:



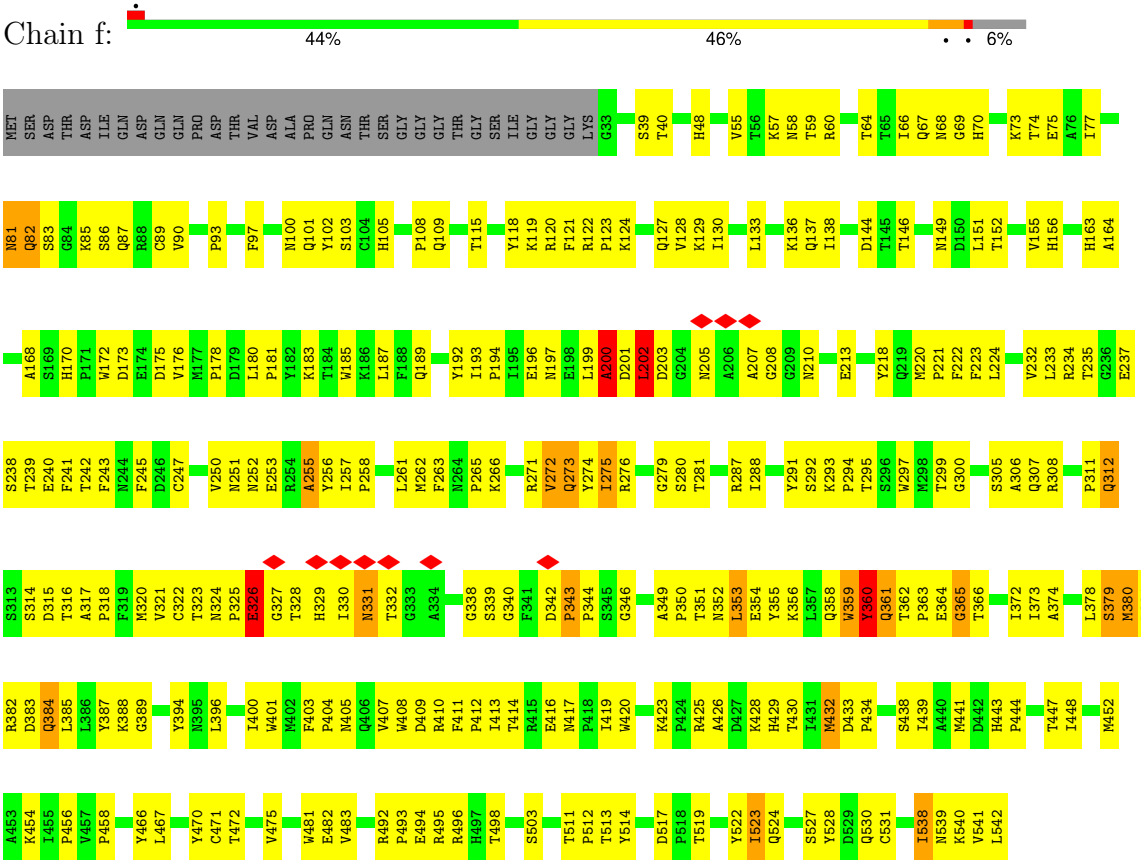
- Molecule 1: viral protein 3

Chain e:



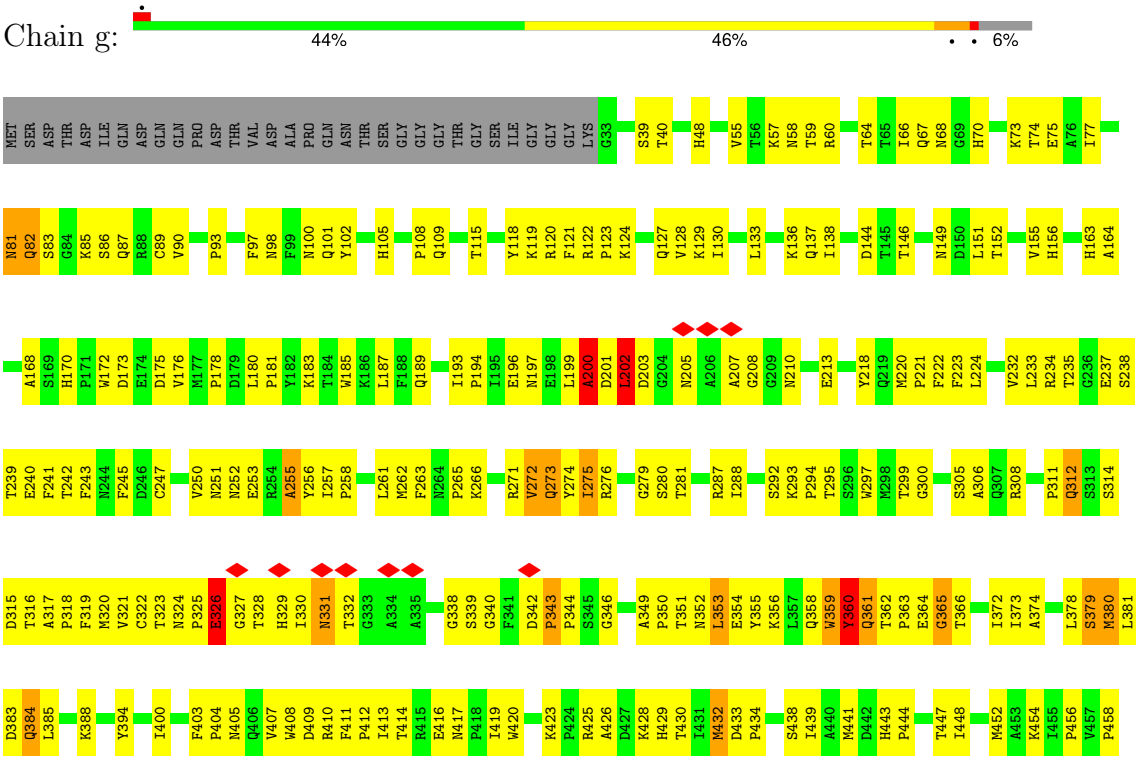
- Molecule 1: viral protein 3

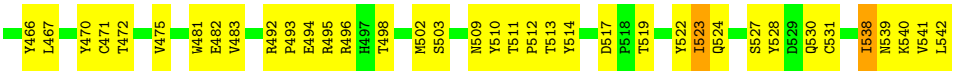
Chain f:



- Molecule 1: viral protein 3

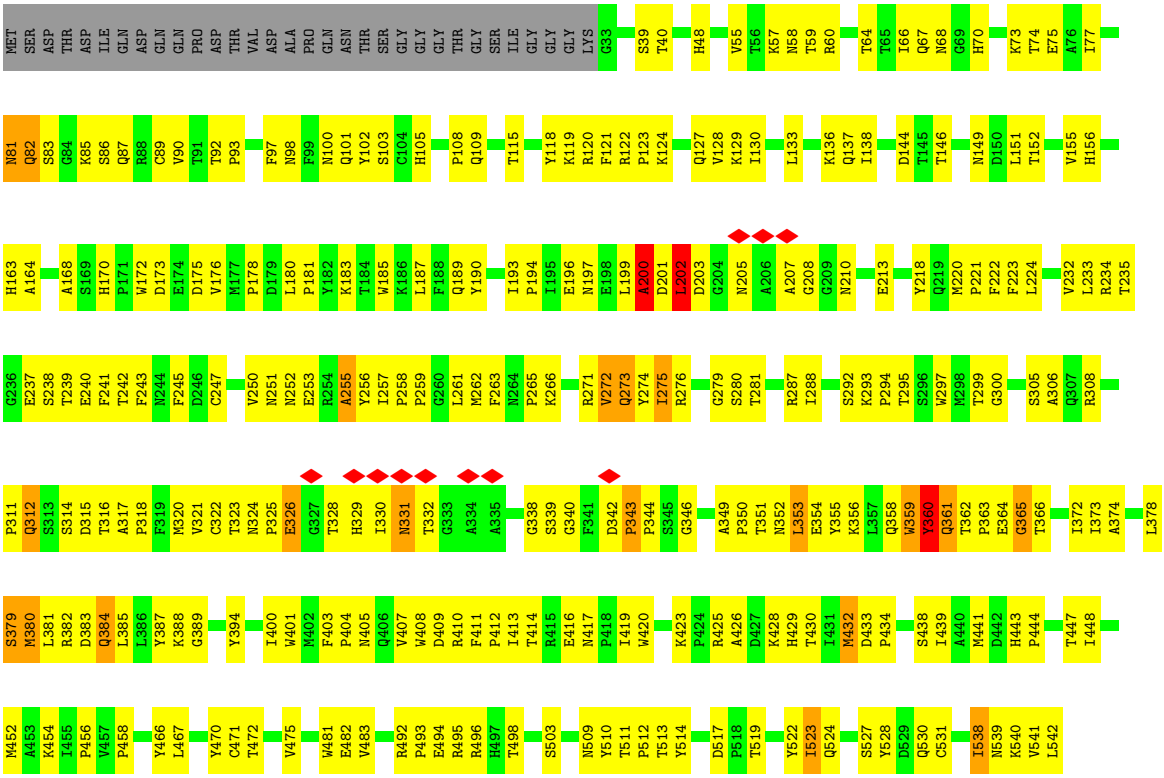
Chain g:





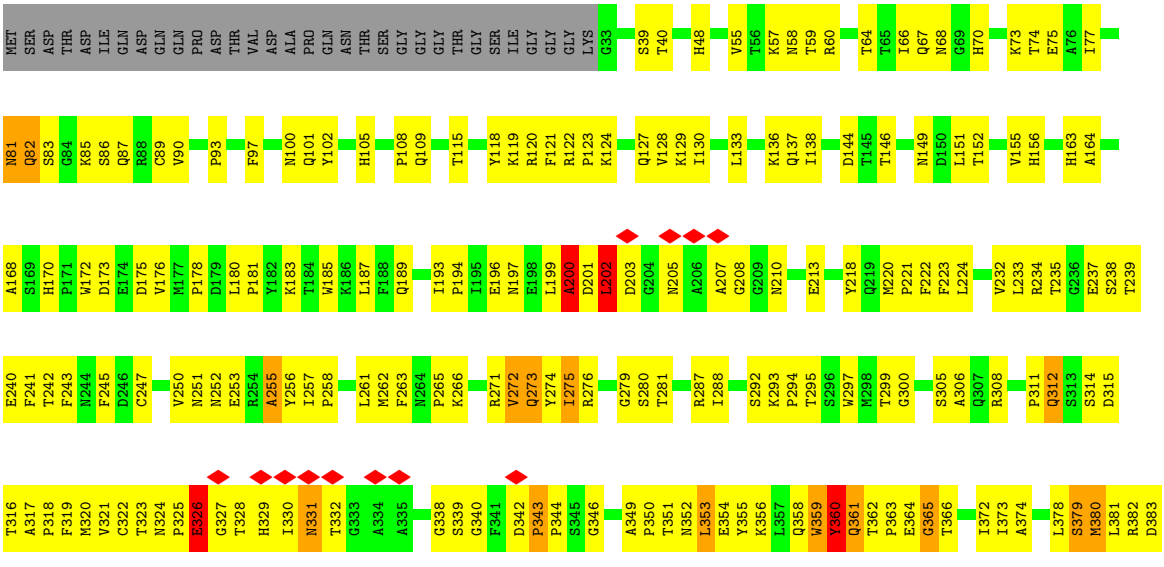
- Molecule 1: viral protein 3

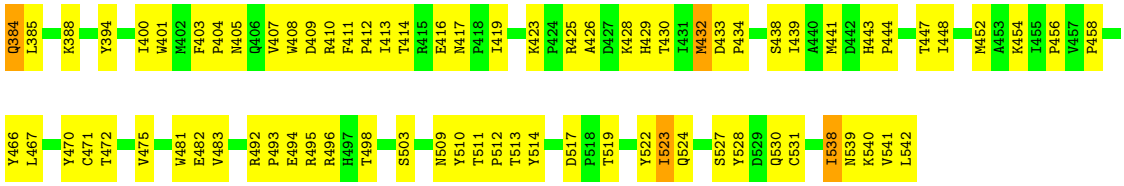
Chain h:



- Molecule 1: viral protein 3

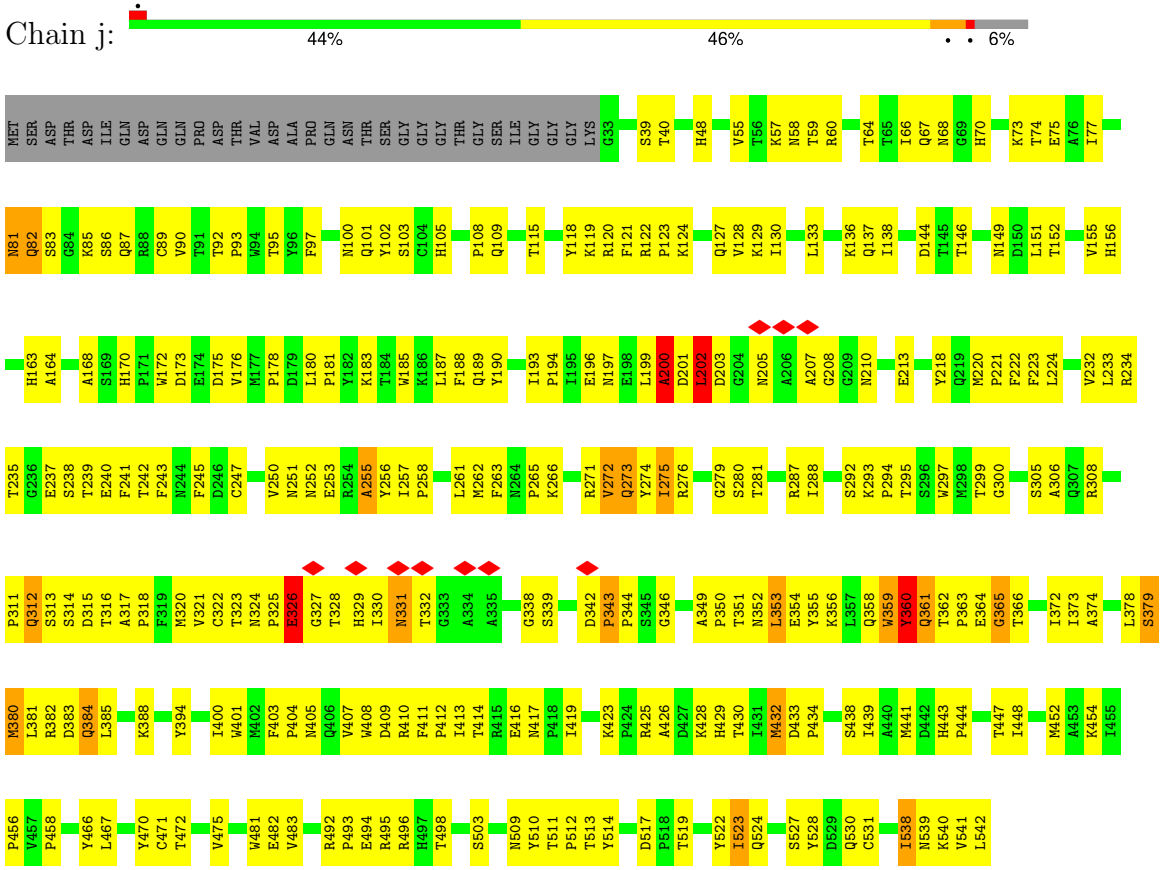
Chain i:





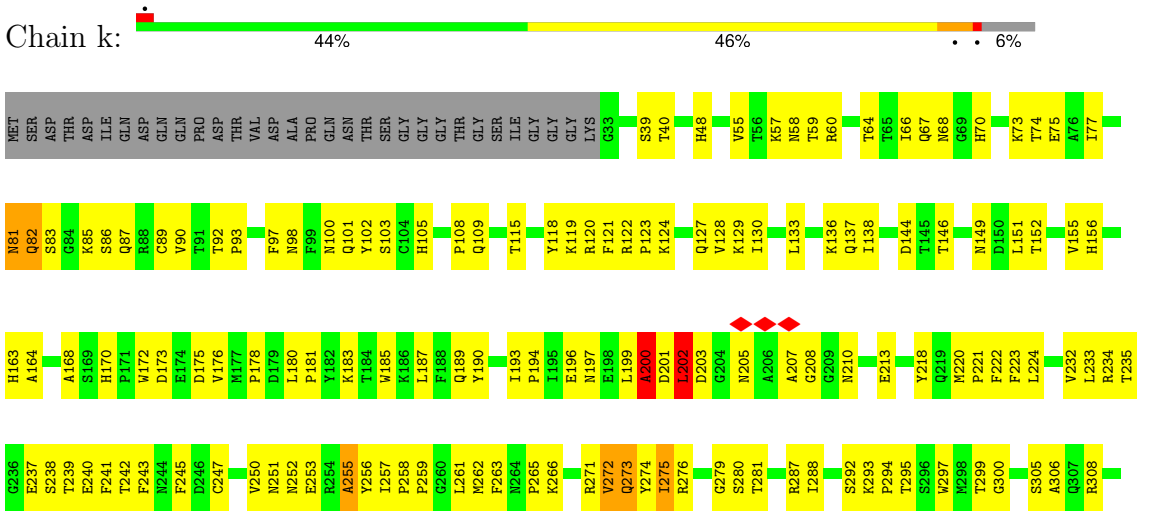
• Molecule 1: viral protein 3

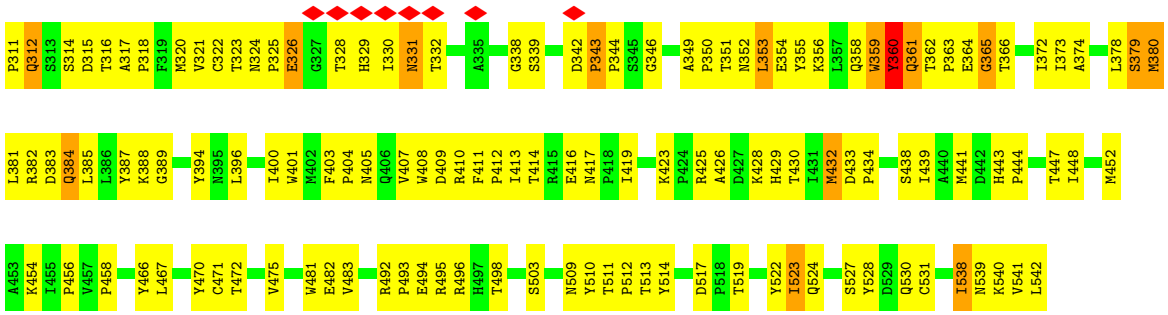
Chain j:



• Molecule 1: viral protein 3

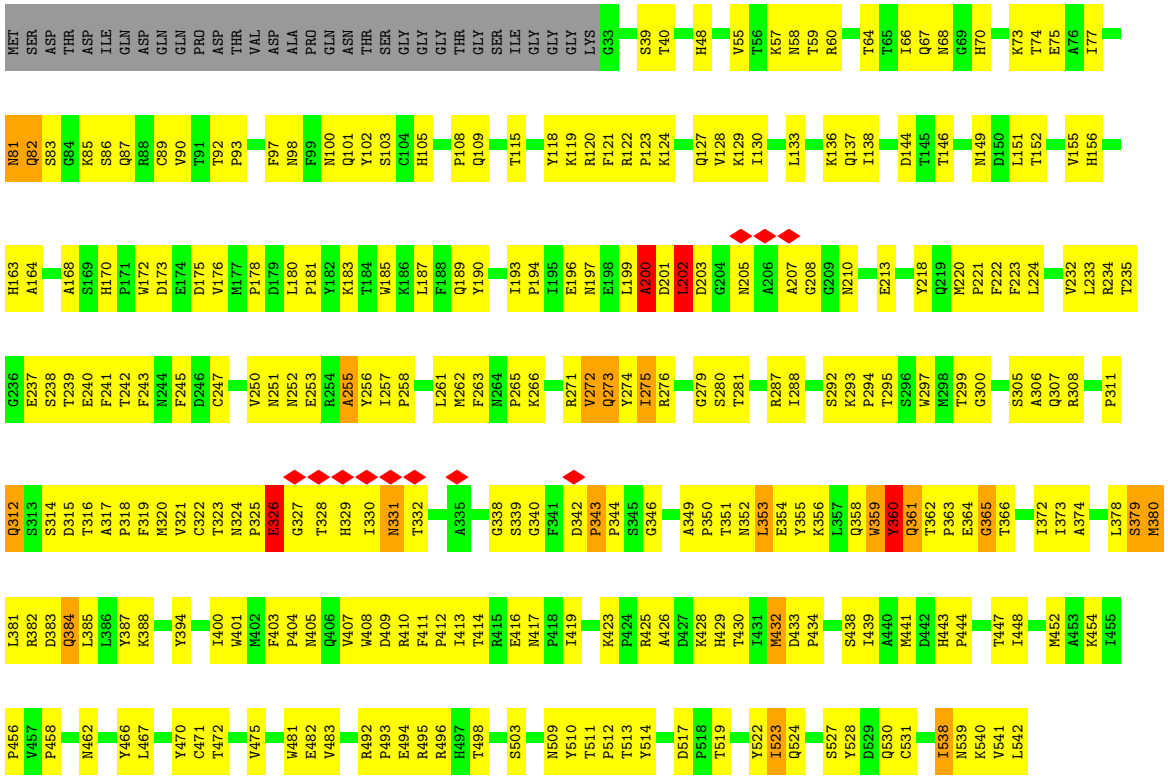
Chain k:





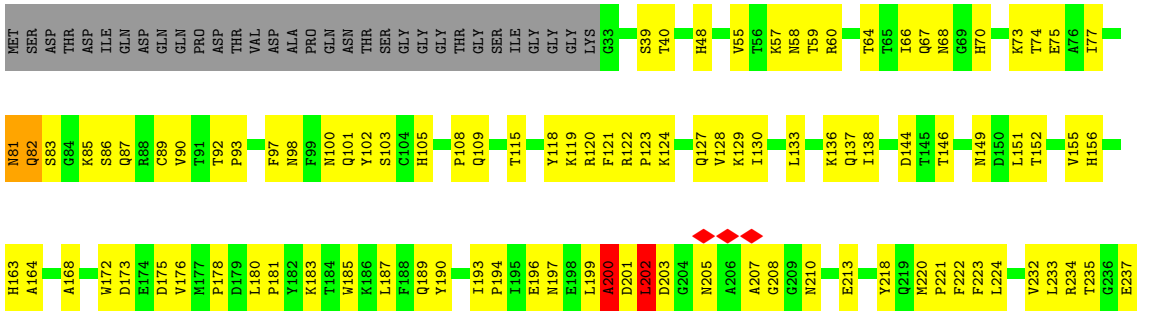
- Molecule 1: viral protein 3

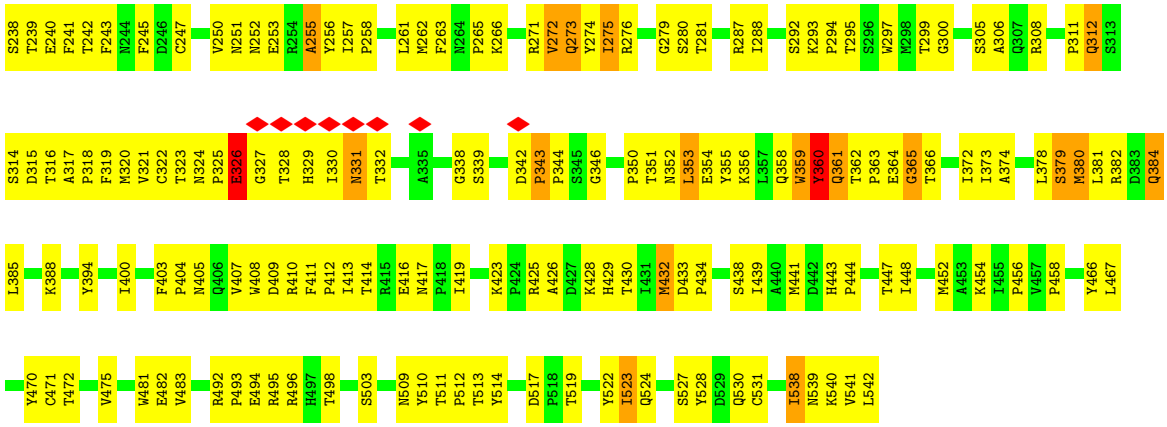
Chain l:



- Molecule 1: viral protein 3

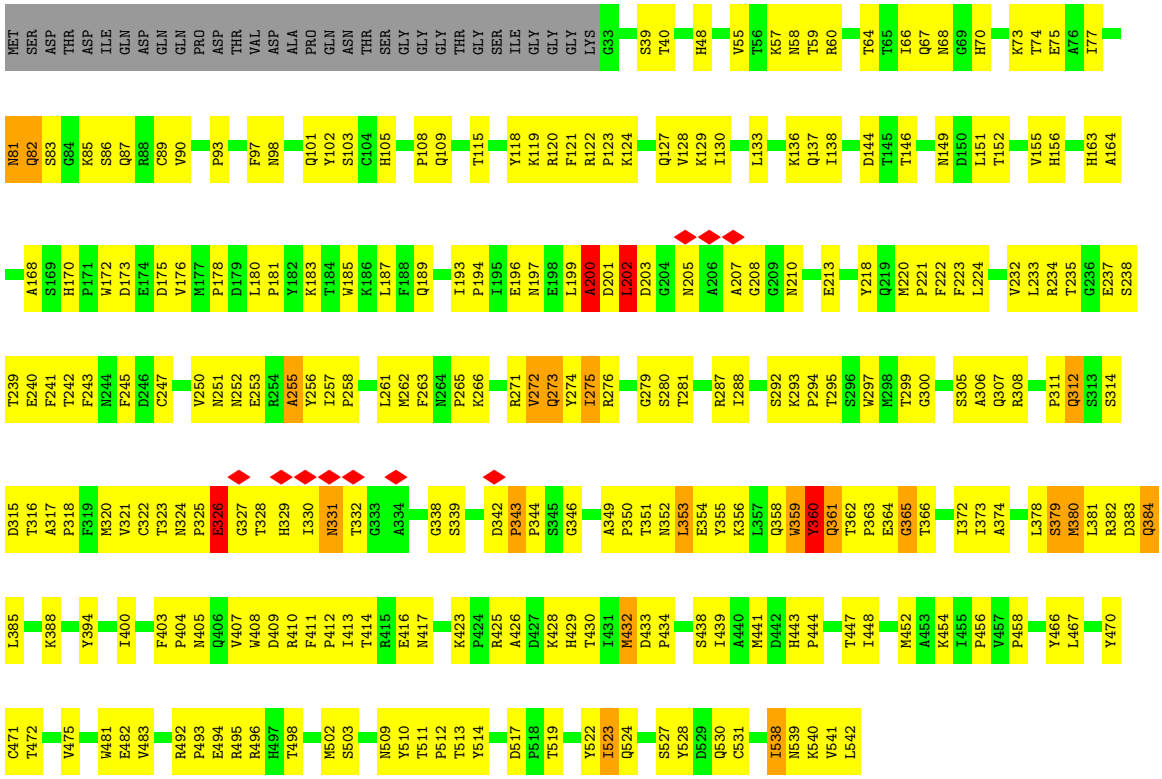
Chain m:





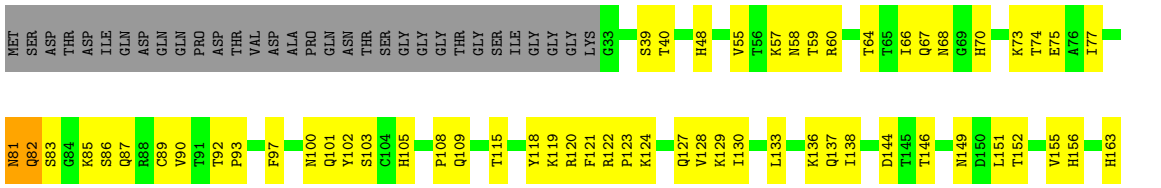
- Molecule 1: viral protein 3

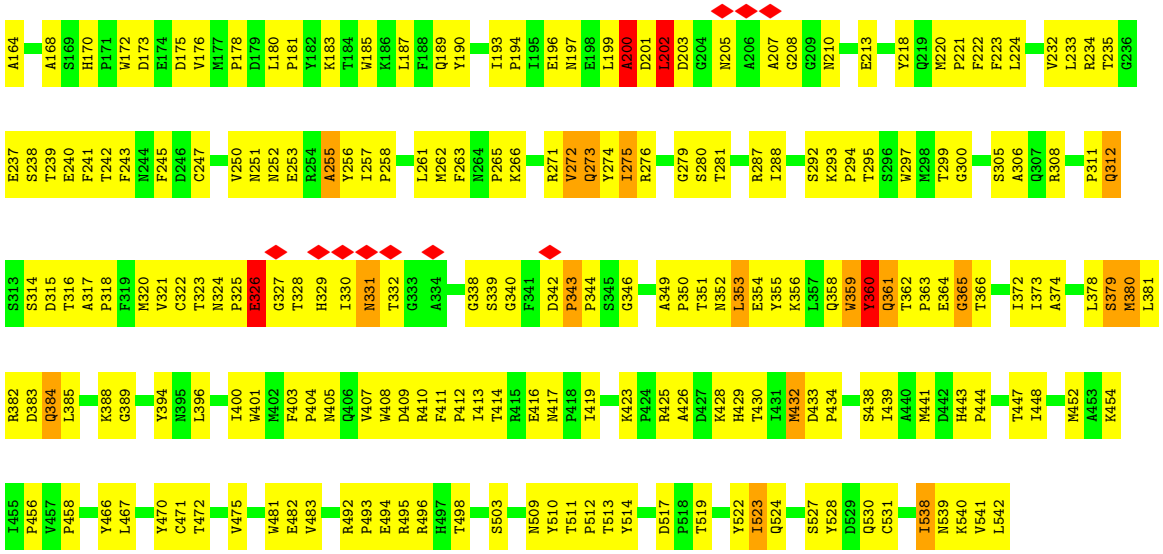
Chain n:



- Molecule 1: viral protein 3

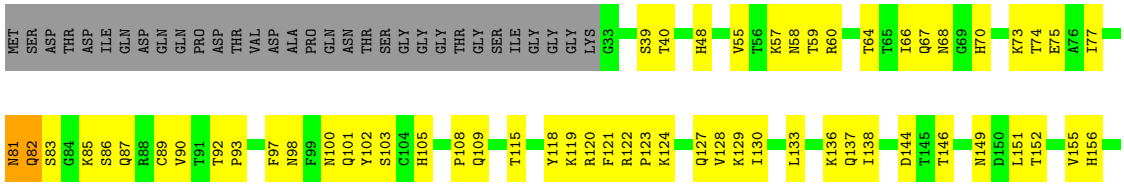
Chain o:

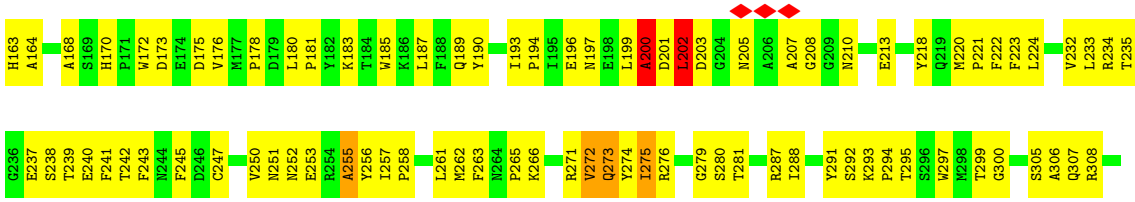


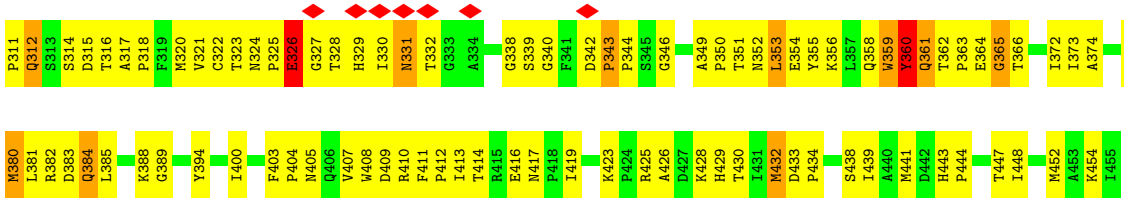


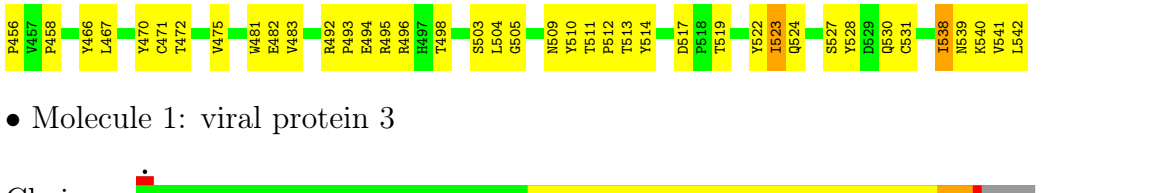
• Molecule 1: viral protein 3

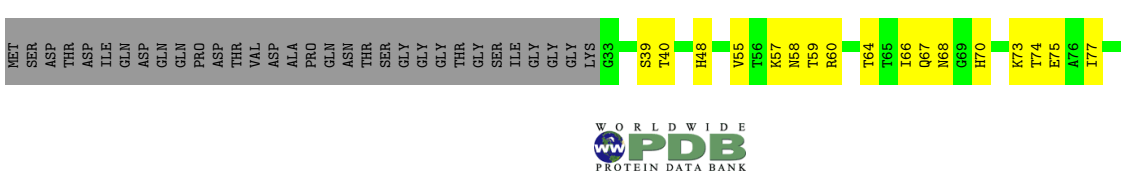
Chain p:





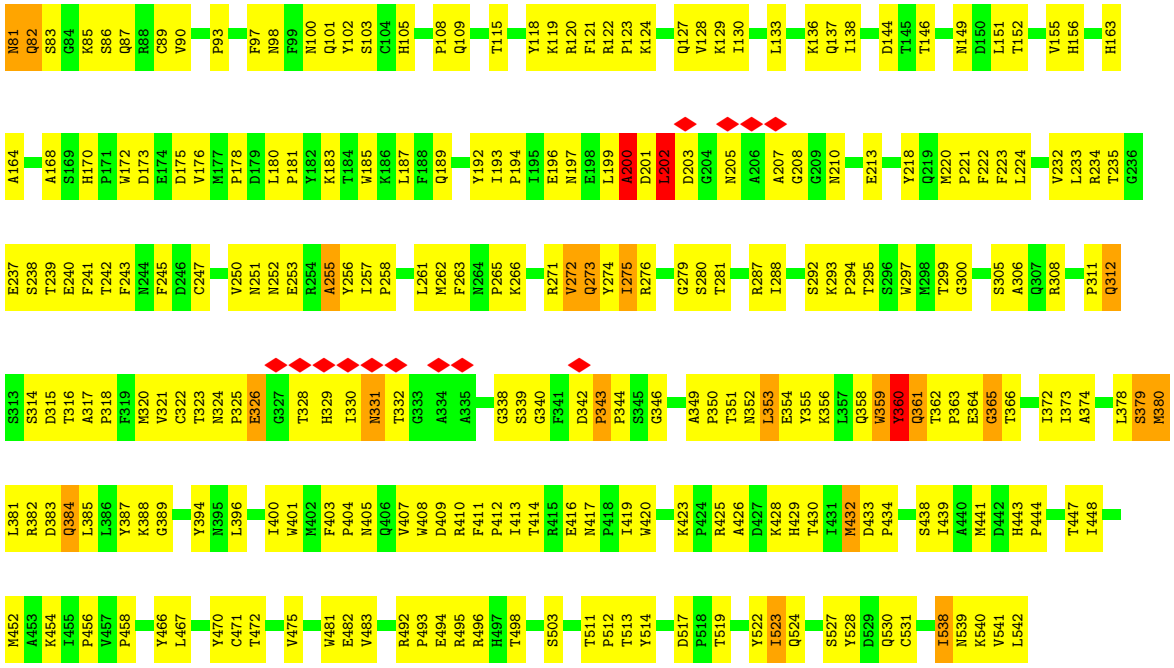






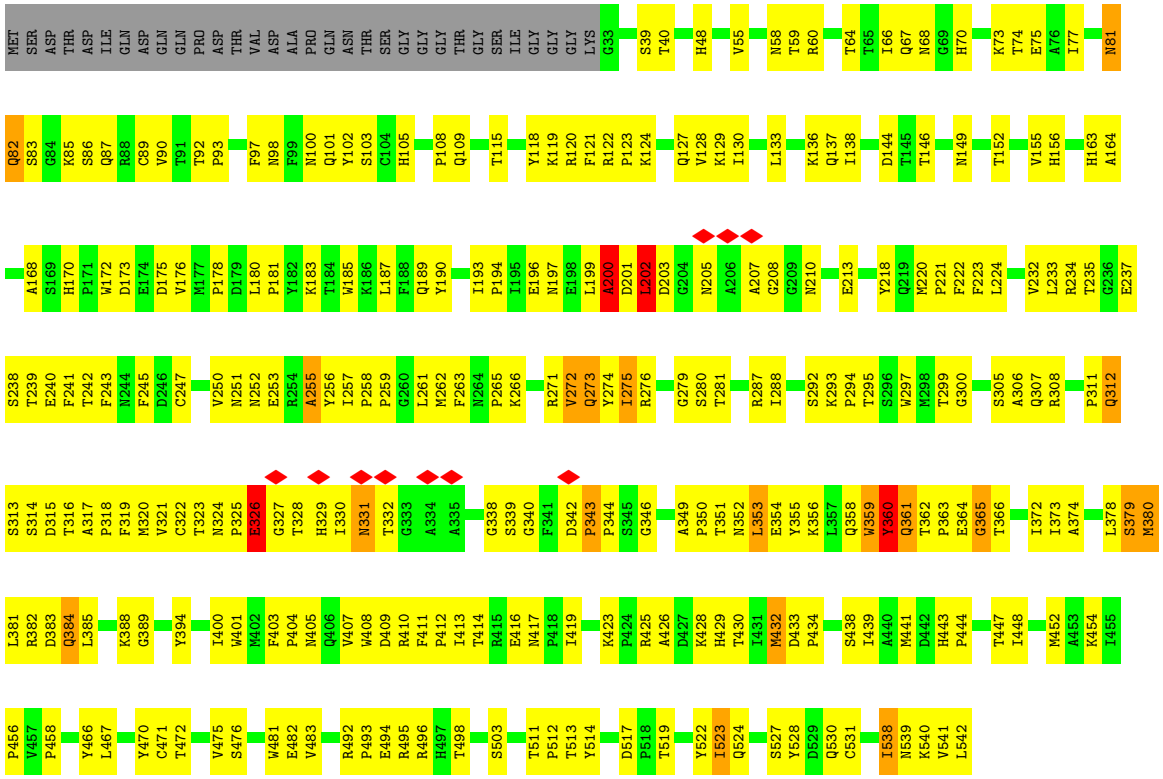
• Molecule 1: viral protein 3

Chain q:



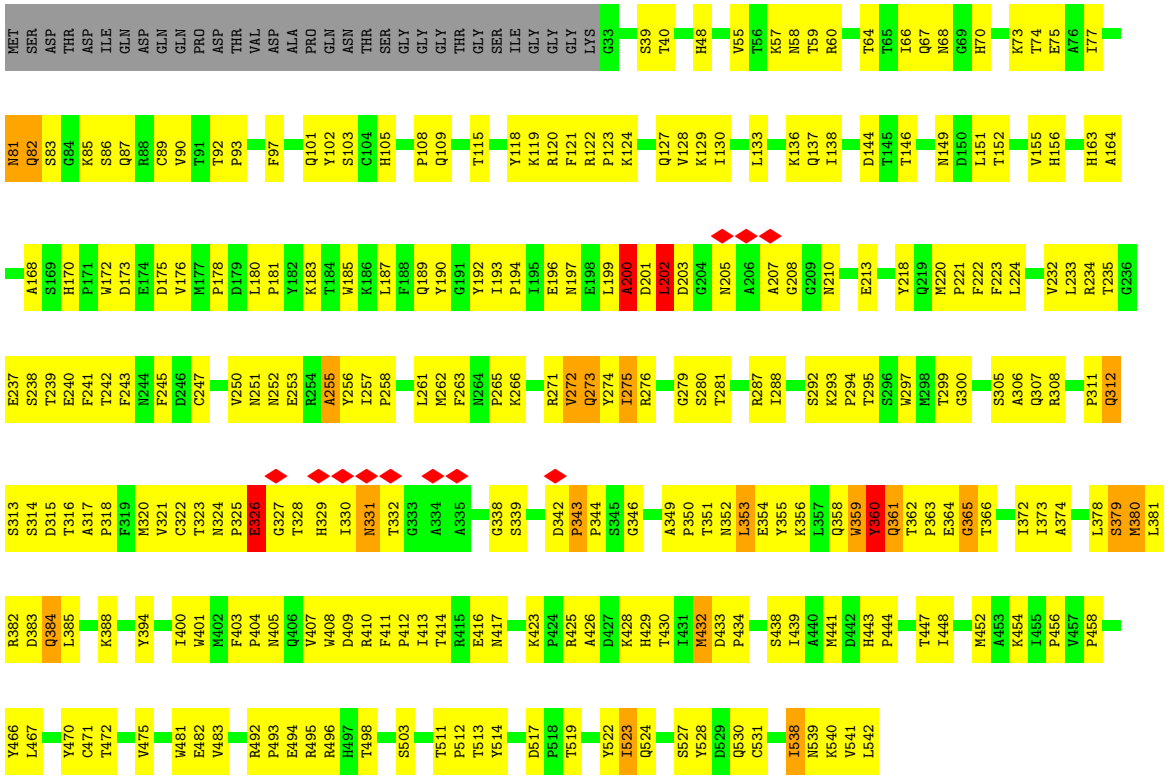
- Molecule 1: viral protein 3

Chain r:



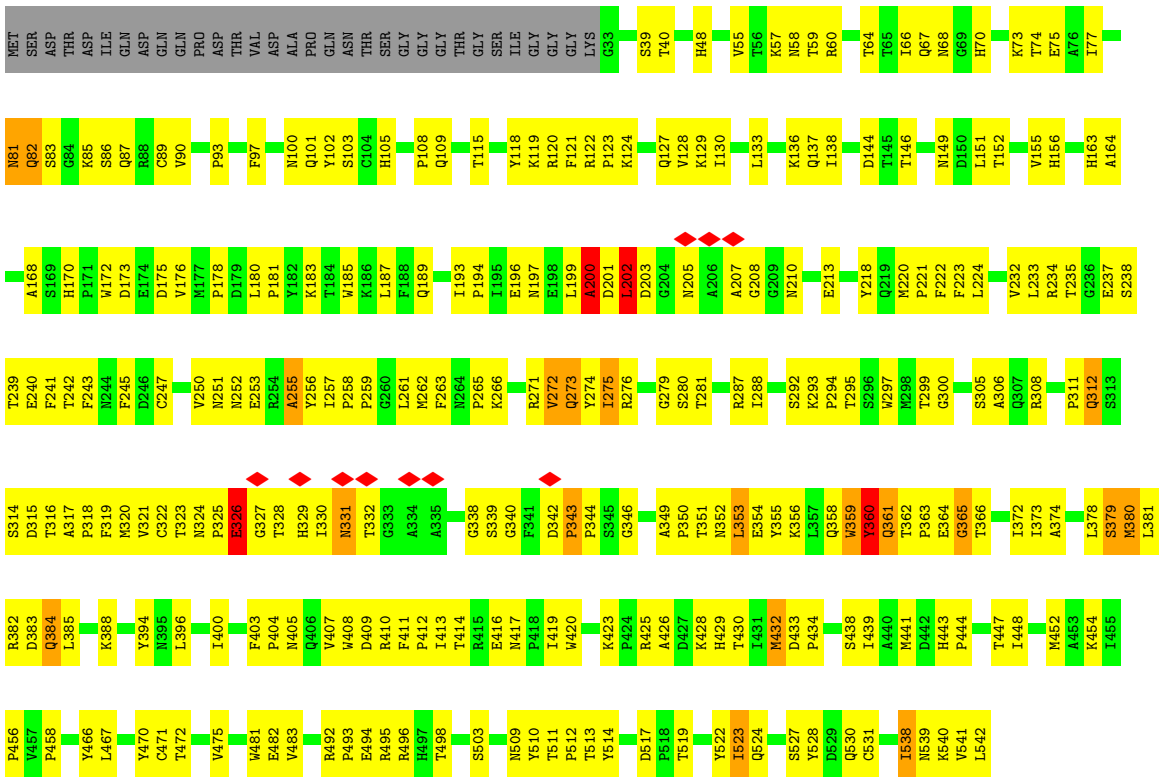
- Molecule 1: viral protein 3

Chain s:



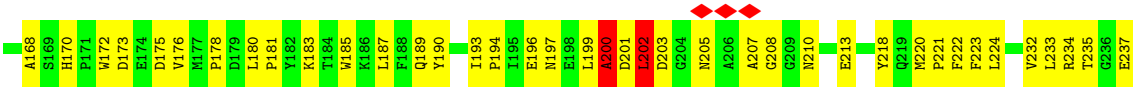
- Molecule 1: viral protein 3

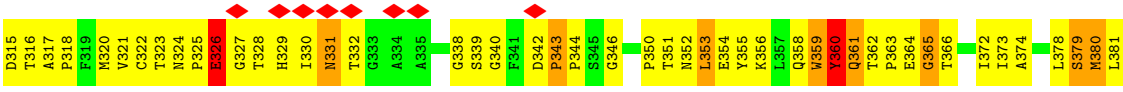
Chain t:

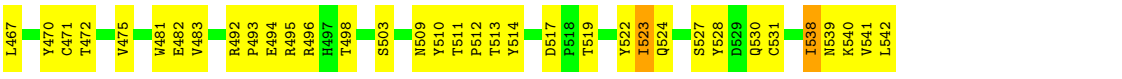


- Molecule 1: viral protein 3

Chain u:

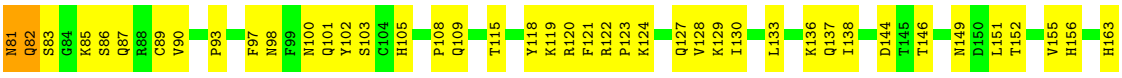


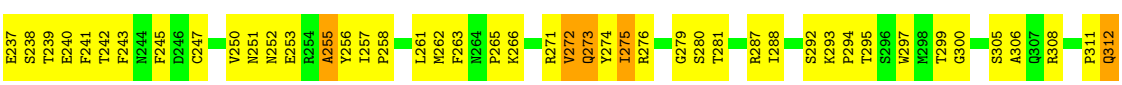


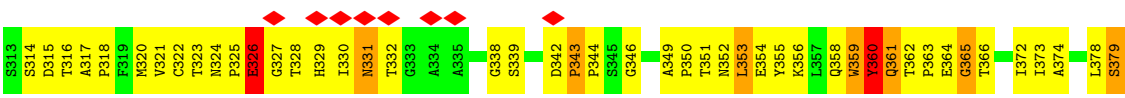


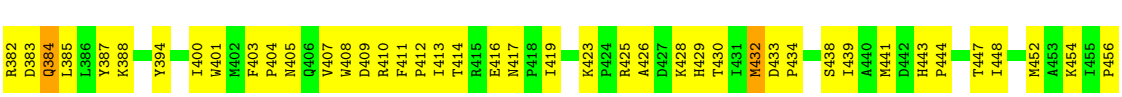
- Molecule 1: viral protein 3

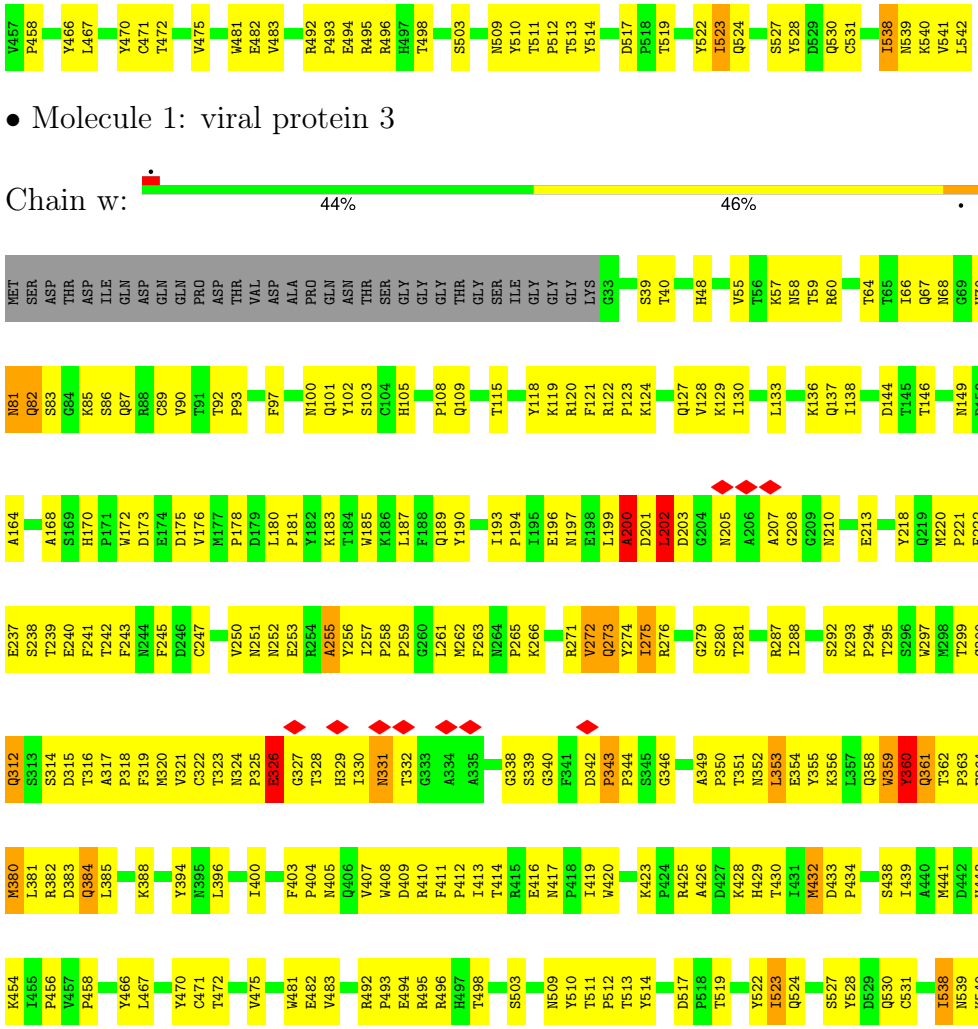
Chain v:

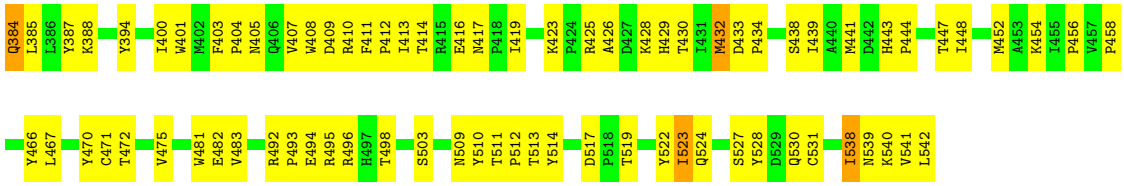






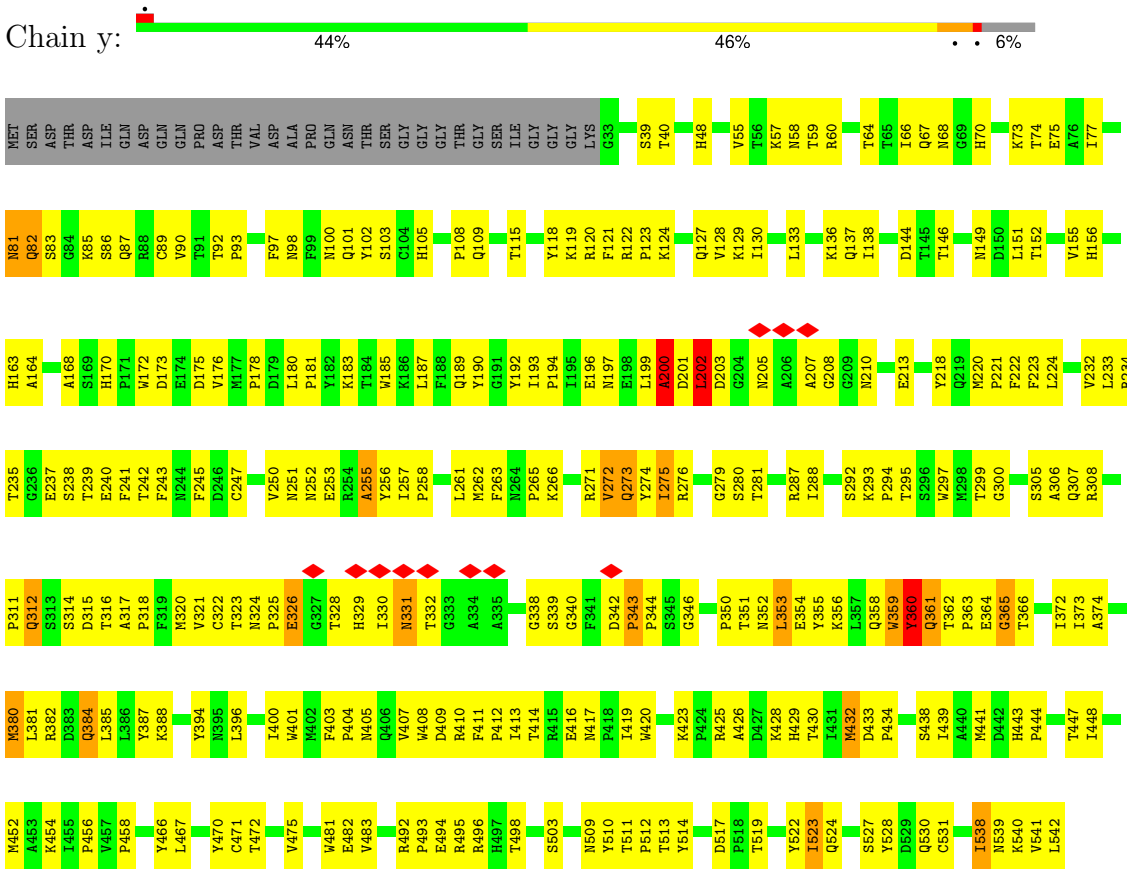



V457 P458 Y466 L467 Y470 C471 T472 V475 W481 E482 V483 R492 P493 E494 R495 R496 H497 T498 S503 N509 Y510 T511 P512 T513 Y514 D517 P518 T519 Y522 I523 Q524 S527 Y528 D529 Q530 C531 I538 N539 K540 V541 L542
• Molecule 1: viral protein 3
Chain w:
44%
46%
6%
MET SER ASP THR ASP ILE GLN ASP GLN GLN PRO ASP THR VAL ASP ALA PRO GLN ASN THR SER GLY GLY GLY THR GLY SER ILE GLY GLY GLY LYS G33 S39 T40 H48 V55 T56 K57 N58 T59 R60 T64 T65 I66 Q67 N68 G69 H70 K73 T74 E75 A76 I77
N81 Q82 S83 G84 K85 S86 Q87 R88 C89 V90 T91 T92 P93 F97 N100 Q101 Y102 S103 C104 H105 P108 Q109 T115 Y118 K119 R120 F121 R122 P123 K124 Q127 V128 K129 I130 L133 K136 Q137 I138 D144 T145 T146 N149 D150 L151 T152 V155 H156 H163
A164 A168 S169 H170 P171 W172 D173 E174 D175 V176 M177 P178 D179 L180 P181 Y182 K183 T184 W185 K186 L187 F188 Q189 Y190 I193 P194 I195 E196 N197 E198 L199 A200 D201 L202 D203 G204 N205 A206 A207 G208 G209 N210 E213 Y218 Q219 M220 P221 F222 F223 L224 V232 L233 R234 T235 G236
E237 S238 T239 E240 F241 T242 F243 N244 F245 D246 C247 V250 N251 N252 E253 R254 A255 Y256 I257 P258 P259 G260 L261 M262 F263 N264 P265 K266 R271 V272 Q273 Y274 I275 R276 G279 S280 T281 R287 I288 S292 K293 P294 T295 S296 W297 M298 T299 G300 S305 A306 Q307 R308 P311
Q312 S313 S314 D315 T316 A317 P318 F319 M320 V321 C322 T323 N324 P325 E326 G327 T328 H329 I330 N331 T332 G333 A334 A335 G338 S339 G340 F341 D342 P343 P344 S345 G346 A349 P350 T351 N352 L353 E354 Y355 K356 L357 Q358 W359 Y360 Q361 T362 P363 E364 G365 T366 I372 I373 A374 L378 S379
M380 L381 R382 D383 Q384 L385 K388 Y394 N395 L396 I400 F403 P404 N405 Q406 V407 W408 D409 R410 F411 P412 I413 T414 R415 E416 N417 P418 I419 W420 K423 P424 R425 A426 D427 K428 H429 T430 I431 M432 D433 P434 S438 I439 A440 M441 D442 H443 P444 T447 I448 M452 A453
K454 I455 P456 V457 P458 Y466 L467 Y470 C471 T472 V475 W481 E482 V483 R492 P493 E494 R495 R496 H497 T498 S503 N509 Y510 T511 P512 T513 Y514 D517 P518 T519 Y522 I523 Q524 S527 Y528 D529 Q530 C531 I538 N539 K540 V541 L542
• Molecule 1: viral protein 3
Chain x:
45%
45%
6%
MET SER ASP THR ASP ILE GLN ASP GLN GLN PRO ASP THR VAL ASP ALA PRO GLN ASN THR SER GLY GLY GLY THR GLY SER ILE GLY GLY GLY LYS G33 S39 T40 H48 V55 T56 K57 N58 T59 R60 T64 T65 I66 Q67 N68 G69 H70 K73 T74 E75 A76 I77
N81 Q82 S83 G84 K85 S86 Q87 R88 C89 V90 P93 F97 N100 Q101 Y102 S103 C104 H105 P108 Q109 T115 Y118 K119 R120 F121 R122 P123 K124 Q127 V128 K129 I130 L133 K136 Q137 I138 D144 T145 T146 N149 D150 L151 T152 V155 H156 H163 A164
A168 S169 H170 P171 W172 D173 E174 D175 V176 M177 P178 D179 L180 P181 Y182 K183 T184 W185 K186 L187 F188 Q189 Y192 I193 P194 I195 E196 N197 E198 L199 A200 D201 L202 D203 G204 N205 A206 A207 G208 G209 N210 E213 Y218 Q219 M220 P221 F222 F223 L224 V232 L233 R234 T235 G236 E237
S238 T239 E240 F241 T242 F243 N244 F245 D246 C247 N251 N252 E253 R254 A255 Y256 I257 P258 L261 M262 F263 N264 P265 K266 R271 V272 Q273 Y274 I275 R276 G279 S280 T281 R287 I288 S292 K293 P294 T295 S296 W297 M298 T299 G300 S305 A306 Q307 R308 P311 Q312 S313 S314
D315 T316 A317 P318 F319 M320 V321 C322 T323 N324 P325 E326 G327 T328 H329 I330 N331 T332 G333 A334 A335 G338 S339 D342 P343 P344 S345 G346 A349 P350 T351 N352 L353 E354 Y355 K356 L357 Q358 W359 Y360 Q361 T362 P363 E364 G365 T366 I372 I373 A374 L378 S379 M380 L381 R382 D383



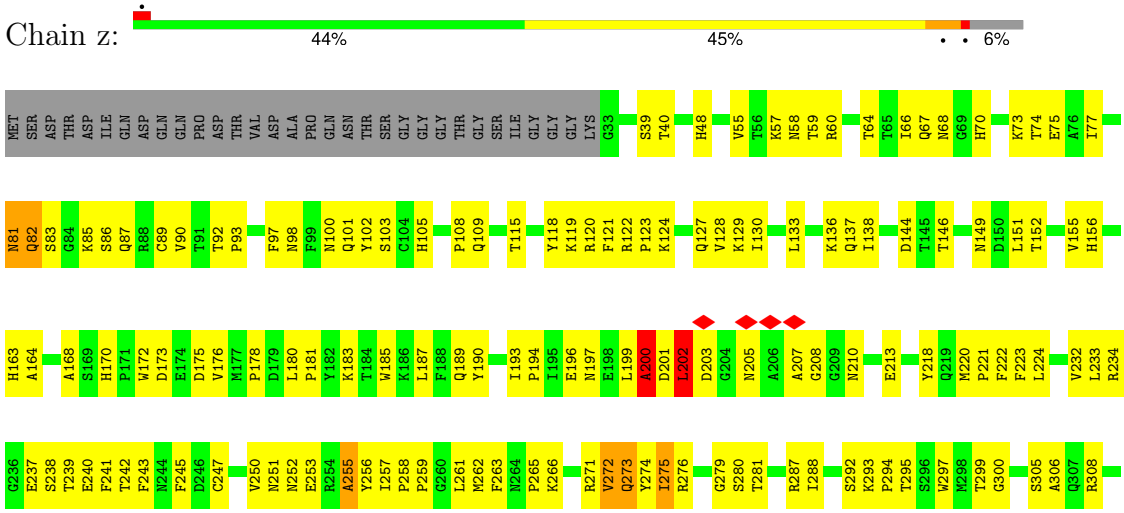
- Molecule 1: viral protein 3

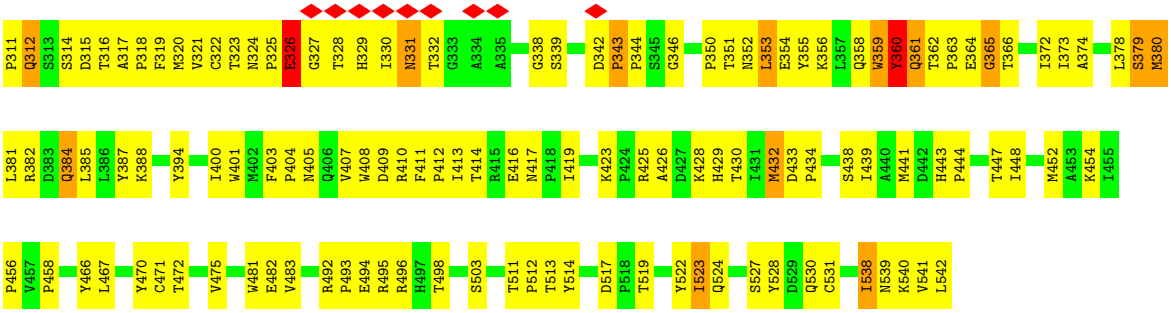
Chain y:



- Molecule 1: viral protein 3

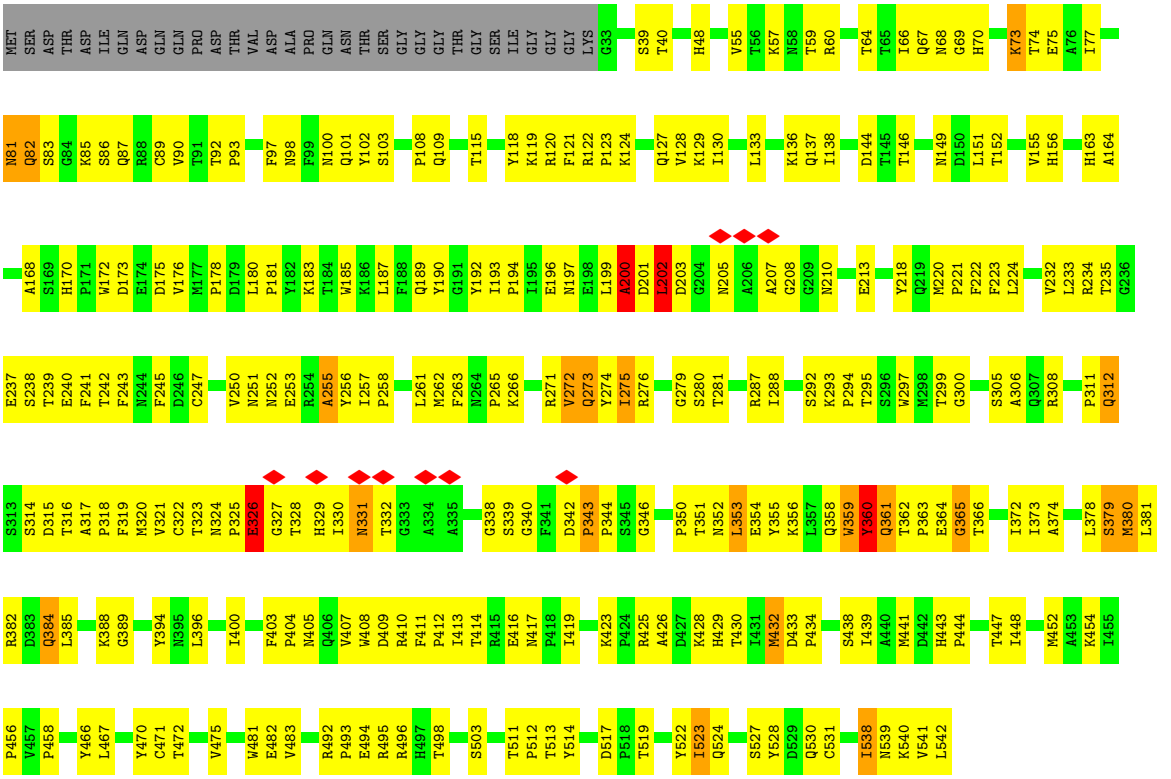
Chain z:





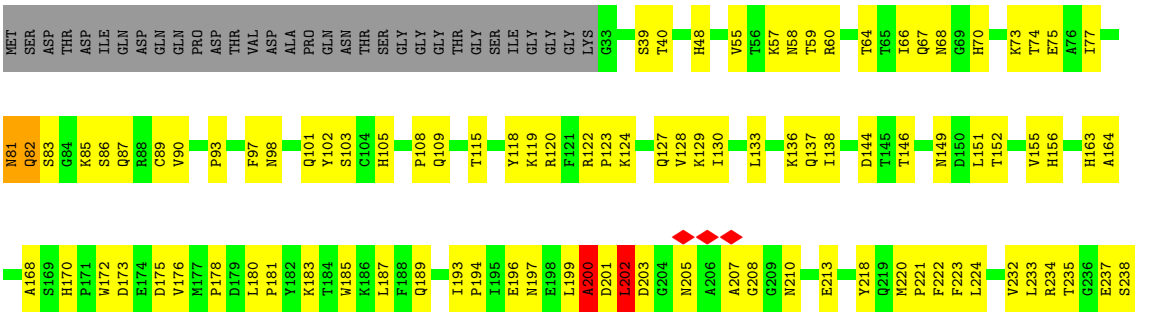
- Molecule 1: viral protein 3

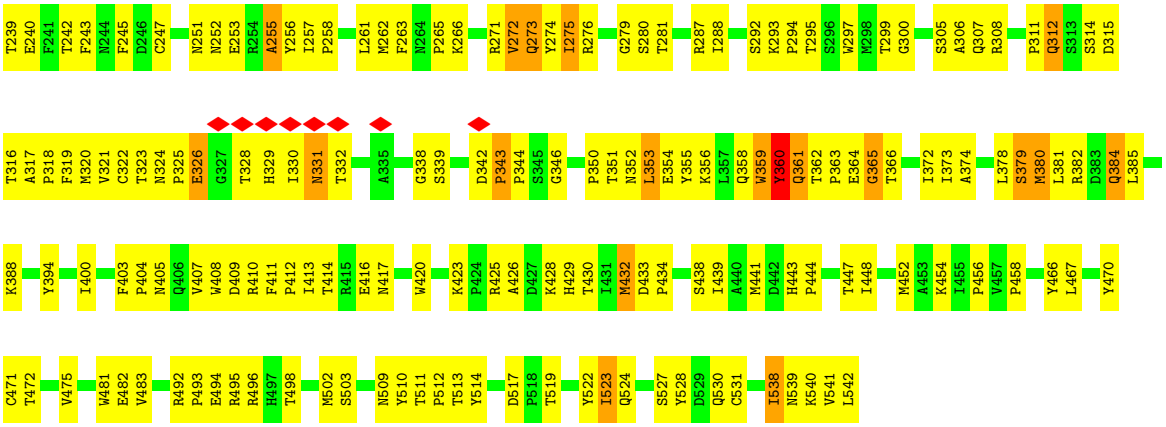
Chain 7:



- Molecule 1: viral protein 3

Chain 8:




T239 E240 F241 T242 F243 N244 F245 D246 C247
N251 N252 E253 R254 A255 Y256 I257 P258
L261 M262 F263 N264 P265 K266
R271 V272 Q273 Y274 I275 R276
G279 S280 T281
R287 I288
S292 K293 P294 T295 S296 W297 M298 T299 G300
S305 A306 Q307 R308
P311 Q312 S313 S314 D315
T316 A317 P318 F319 M320 V321 C322 T323 N324 P325 E326 G327 T328 H329 I330 N331 T332 A335 G338 S339 D342 P343 P344 S345 G346 P350 T351 N352 L353 E354 Y355 K356 L357 Q358 W359 Y360 Q361 T362 P363 E364 G365 T366 I372 I373 A374 L378 S379 M380 L381 R382 D383 Q384 L385
K388 Y394 I400 F403 P404 N405 Q406 V407 W408 D409 R410 F411 P412 I413 T414 R415 E416 N417 W420 K423 P424 R425 A426 D427 K428 H429 T430 I431 M432 D433 P434 S438 I439 A440 M441 D442 H443 P444 T447 I448 M452 A453 K454 I455 P456 V457 P458 Y466 L467 Y470
C471 T472 V475 W481 E482 V483 R492 P493 E494 R495 R496 H497 T498 M502 S503 N509 Y510 T511 P512 T513 Y514 D517 P518 T519 Y522 I523 Q524 S527 Y528 D529 Q530 C531 I538 N539 K540 V541 L542

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31064	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 ($e^-/Å^2$)	63	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	17.985	Depositor
Minimum map value	-8.903	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	379.05, 379.05, 379.05	wwPDB
Map dimensions	399, 399, 399	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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	0.50	0/4192	0.92	27/5717 (0.5%)
1	2	0.50	0/4192	0.92	26/5717 (0.5%)
1	3	0.50	0/4192	0.92	26/5717 (0.5%)
1	4	0.50	0/4192	0.92	26/5717 (0.5%)
1	5	0.50	0/4192	0.92	26/5717 (0.5%)
1	6	0.50	0/4192	0.92	26/5717 (0.5%)
1	7	0.50	0/4192	0.92	26/5717 (0.5%)
1	8	0.50	0/4192	0.92	26/5717 (0.5%)
1	A	0.50	0/4192	0.92	27/5717 (0.5%)
1	B	0.50	0/4192	0.92	26/5717 (0.5%)
1	C	0.50	0/4192	0.92	26/5717 (0.5%)
1	D	0.50	0/4192	0.92	26/5717 (0.5%)
1	E	0.50	0/4192	0.92	26/5717 (0.5%)
1	F	0.50	0/4192	0.92	26/5717 (0.5%)
1	G	0.50	0/4192	0.92	26/5717 (0.5%)
1	H	0.50	0/4192	0.92	26/5717 (0.5%)
1	I	0.50	0/4192	0.92	26/5717 (0.5%)
1	J	0.50	0/4192	0.92	26/5717 (0.5%)
1	K	0.50	0/4192	0.92	26/5717 (0.5%)
1	L	0.50	0/4192	0.92	26/5717 (0.5%)
1	M	0.50	0/4192	0.92	26/5717 (0.5%)
1	N	0.50	0/4192	0.92	26/5717 (0.5%)
1	O	0.50	0/4192	0.92	26/5717 (0.5%)
1	P	0.50	0/4192	0.92	26/5717 (0.5%)
1	Q	0.50	0/4192	0.92	26/5717 (0.5%)
1	R	0.50	0/4192	0.92	26/5717 (0.5%)
1	S	0.50	0/4192	0.92	26/5717 (0.5%)
1	T	0.50	0/4192	0.92	26/5717 (0.5%)
1	U	0.50	0/4192	0.92	26/5717 (0.5%)
1	V	0.50	0/4192	0.92	26/5717 (0.5%)
1	W	0.50	0/4192	0.92	26/5717 (0.5%)
1	X	0.50	0/4192	0.92	26/5717 (0.5%)
1	Y	0.50	0/4192	0.92	26/5717 (0.5%)
1	Z	0.50	0/4192	0.92	26/5717 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	a	0.50	0/4192	0.92	26/5717 (0.5%)
1	b	0.50	0/4192	0.92	26/5717 (0.5%)
1	c	0.50	0/4192	0.92	26/5717 (0.5%)
1	d	0.50	0/4192	0.92	26/5717 (0.5%)
1	e	0.50	0/4192	0.92	26/5717 (0.5%)
1	f	0.50	0/4192	0.92	26/5717 (0.5%)
1	g	0.50	0/4192	0.92	26/5717 (0.5%)
1	h	0.50	0/4192	0.92	26/5717 (0.5%)
1	i	0.50	0/4192	0.92	26/5717 (0.5%)
1	j	0.50	0/4192	0.92	26/5717 (0.5%)
1	k	0.50	0/4192	0.92	26/5717 (0.5%)
1	l	0.50	0/4192	0.92	27/5717 (0.5%)
1	m	0.50	0/4192	0.92	26/5717 (0.5%)
1	n	0.50	0/4192	0.92	26/5717 (0.5%)
1	o	0.50	0/4192	0.92	26/5717 (0.5%)
1	p	0.50	0/4192	0.92	26/5717 (0.5%)
1	q	0.50	0/4192	0.92	26/5717 (0.5%)
1	r	0.50	0/4192	0.92	26/5717 (0.5%)
1	s	0.50	0/4192	0.92	26/5717 (0.5%)
1	t	0.50	0/4192	0.92	26/5717 (0.5%)
1	u	0.50	0/4192	0.92	26/5717 (0.5%)
1	v	0.50	0/4192	0.92	26/5717 (0.5%)
1	w	0.50	0/4192	0.92	26/5717 (0.5%)
1	x	0.50	0/4192	0.92	26/5717 (0.5%)
1	y	0.50	0/4192	0.92	26/5717 (0.5%)
1	z	0.50	0/4192	0.92	26/5717 (0.5%)
All	All	0.50	0/251520	0.92	1563/343020 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	7
1	2	0	7
1	3	0	7
1	4	0	7
1	5	0	7
1	6	0	7
1	7	0	7
1	8	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	7
1	D	0	7
1	E	0	7
1	F	0	7
1	G	0	7
1	H	0	7
1	I	0	7
1	J	0	7
1	K	0	7
1	L	0	7
1	M	0	7
1	N	0	7
1	O	0	7
1	P	0	7
1	Q	0	7
1	R	0	7
1	S	0	7
1	T	0	7
1	U	0	7
1	V	0	7
1	W	0	7
1	X	0	7
1	Y	0	7
1	Z	0	7
1	a	0	7
1	b	0	7
1	c	0	7
1	d	0	7
1	e	0	7
1	f	0	7
1	g	0	7
1	h	0	7
1	i	0	7
1	j	0	7
1	k	0	7
1	l	0	7
1	m	0	7
1	n	0	7
1	o	0	7
1	p	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	q	0	7
1	r	0	7
1	s	0	7
1	t	0	7
1	u	0	7
1	v	0	7
1	w	0	7
1	x	0	7
1	y	0	7
1	z	0	7
All	All	0	420

There are no bond length outliers.

The worst 5 of 1563 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	379	SER	CA-C-N	8.41	136.84	121.70
1	B	379	SER	C-N-CA	8.41	136.84	121.70
1	N	379	SER	CA-C-N	8.41	136.84	121.70
1	N	379	SER	C-N-CA	8.41	136.84	121.70
1	F	379	SER	CA-C-N	8.41	136.83	121.70

There are no chirality outliers.

5 of 420 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	ALA	Peptide
1	A	273	GLN	Peptide
1	A	311	PRO	Peptide
1	A	82	GLN	Peptide
1	A	83	SER	Peptide

5.2 Too-close contacts (i)

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4062	0	3871	305	0
1	2	4062	0	3871	294	0
1	3	4062	0	3871	303	0
1	4	4062	0	3871	300	0
1	5	4062	0	3871	302	0
1	6	4062	0	3871	298	0
1	7	4062	0	3871	304	0
1	8	4062	0	3871	299	0
1	A	4062	0	3871	309	0
1	B	4062	0	3871	299	0
1	C	4062	0	3871	301	0
1	D	4062	0	3871	307	0
1	E	4062	0	3871	304	0
1	F	4062	0	3871	305	0
1	G	4062	0	3871	301	0
1	H	4062	0	3871	309	0
1	I	4062	0	3871	305	0
1	J	4062	0	3871	308	0
1	K	4062	0	3871	299	0
1	L	4062	0	3871	301	0
1	M	4062	0	3871	301	0
1	N	4062	0	3871	297	0
1	O	4062	0	3871	300	0
1	P	4062	0	3871	304	0
1	Q	4062	0	3871	299	0
1	R	4062	0	3871	298	0
1	S	4062	0	3871	305	0
1	T	4062	0	3871	298	0
1	U	4062	0	3871	304	0
1	V	4062	0	3871	306	0
1	W	4062	0	3871	305	0
1	X	4062	0	3871	310	0
1	Y	4062	0	3871	306	0
1	Z	4062	0	3871	298	0
1	a	4062	0	3871	305	0
1	b	4062	0	3871	300	0
1	c	4062	0	3871	300	0
1	d	4062	0	3871	299	0
1	e	4062	0	3871	305	0
1	f	4062	0	3871	304	0
1	g	4062	0	3871	304	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	h	4062	0	3871	307	0
1	i	4062	0	3871	303	0
1	j	4062	0	3871	302	0
1	k	4062	0	3871	304	0
1	l	4062	0	3871	304	0
1	m	4062	0	3871	297	0
1	n	4062	0	3871	306	0
1	o	4062	0	3871	308	0
1	p	4062	0	3871	308	0
1	q	4062	0	3871	307	0
1	r	4062	0	3871	309	0
1	s	4062	0	3871	304	0
1	t	4062	0	3871	307	0
1	u	4062	0	3871	296	0
1	v	4062	0	3871	302	0
1	w	4062	0	3871	307	0
1	x	4062	0	3871	297	0
1	y	4062	0	3871	311	0
1	z	4062	0	3871	303	0
All	All	243720	0	232260	15214	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 32.

The worst 5 of 15214 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:A:382:ARG:HH12	1:A:412:PRO:HD3	1.34	0.93
1:b:382:ARG:HH12	1:b:412:PRO:HD3	1.34	0.93
1:r:382:ARG:HH12	1:r:412:PRO:HD3	1.34	0.93
1:H:382:ARG:HH12	1:H:412:PRO:HD3	1.34	0.93
1:K:382:ARG:HH12	1:K:412:PRO:HD3	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	510/542 (94%)	438 (86%)	65 (13%)	7 (1%)	9	31
1	2	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	3	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	4	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	5	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	6	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	7	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	8	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	A	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	B	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	C	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	D	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	E	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	F	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	G	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	H	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	I	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	J	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	K	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	L	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	M	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	N	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	O	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	P	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	Q	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	S	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	T	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	U	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	V	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	W	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	X	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	Y	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	Z	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	a	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	b	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	c	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	d	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	e	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	f	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	g	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	h	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	i	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	j	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	k	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	l	510/542 (94%)	438 (86%)	65 (13%)	7 (1%)	9	31
1	m	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	n	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	o	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	p	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	q	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	r	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	s	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	t	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	u	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	v	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	x	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	y	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
1	z	510/542 (94%)	437 (86%)	66 (13%)	7 (1%)	9	31
All	All	30600/32520 (94%)	26222 (86%)	3958 (13%)	420 (1%)	12	31

5 of 420 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	VAL
1	A	275	ILE
1	A	538	ILE
1	B	272	VAL
1	B	275	ILE

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	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	2	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	3	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	4	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	5	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	6	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	7	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	8	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	A	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	B	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	C	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	D	443/465 (95%)	441 (100%)	2 (0%)	86	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	F	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	G	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	H	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	I	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	J	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	K	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	L	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	M	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	N	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	O	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	P	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	Q	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	R	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	S	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	T	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	U	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	V	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	W	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	X	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	Y	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	Z	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	a	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	b	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	c	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	d	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	e	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	f	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	g	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	h	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	i	443/465 (95%)	441 (100%)	2 (0%)	86	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	j	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	k	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	l	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	m	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	n	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	o	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	p	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	q	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	r	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	s	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	t	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	u	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	v	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	w	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	x	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	y	443/465 (95%)	441 (100%)	2 (0%)	86	96
1	z	443/465 (95%)	441 (100%)	2 (0%)	86	96
All	All	26580/27900 (95%)	26460 (100%)	120 (0%)	85	96

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

Mol	Chain	Res	Type
1	3	353	LEU
1	x	202	LEU
1	d	353	LEU
1	w	353	LEU
1	8	202	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1216 such sidechains are listed below:

Mol	Chain	Res	Type
1	n	369	ASN
1	y	251	ASN
1	p	58	ASN
1	n	324	ASN

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Mol	Chain	Res	Type
1	t	137	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.

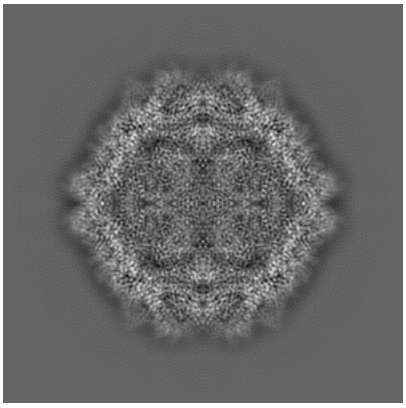
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8598. These allow visual inspection of the internal detail of the map and identification of artifacts.

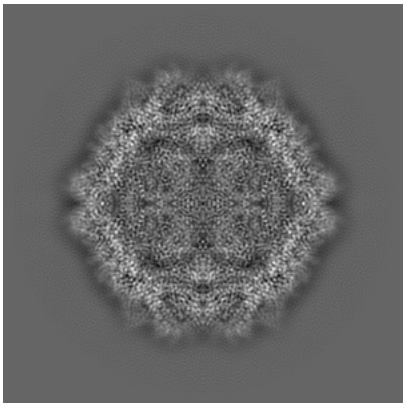
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

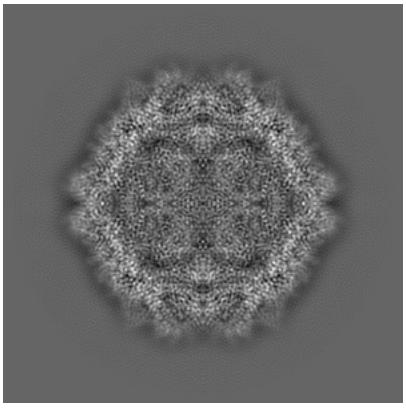
6.1.1 Primary map



X



Y

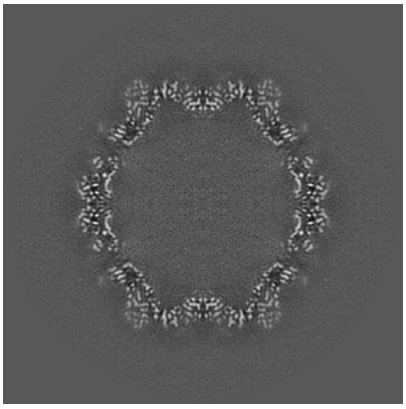


Z

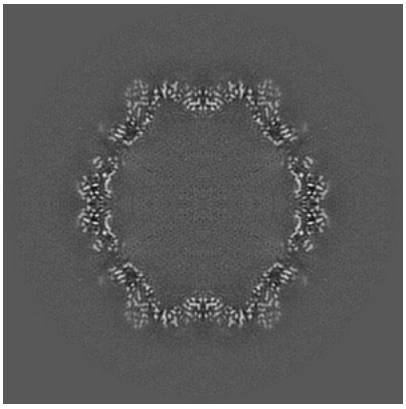
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

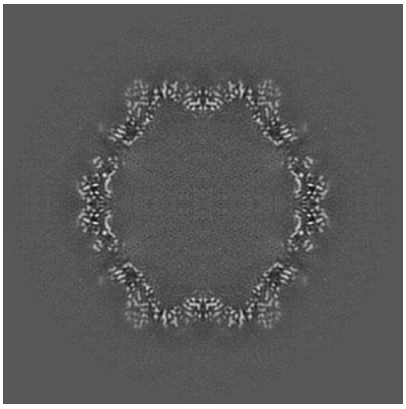
6.2.1 Primary map



X Index: 199



Y Index: 199

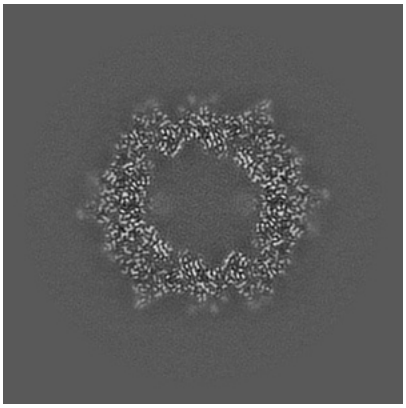


Z Index: 199

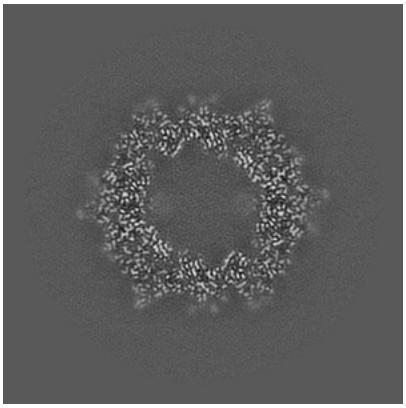
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

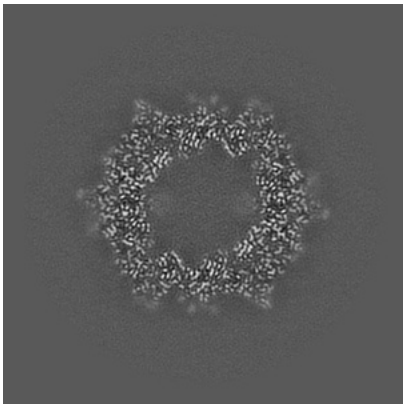
6.3.1 Primary map



X Index: 127



Y Index: 127

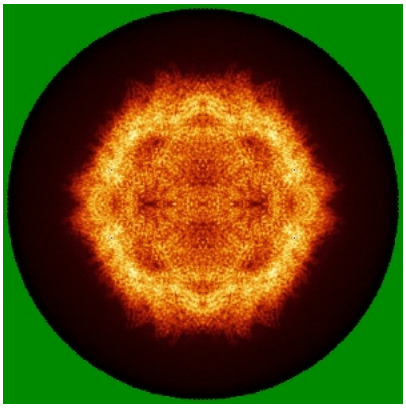


Z Index: 271

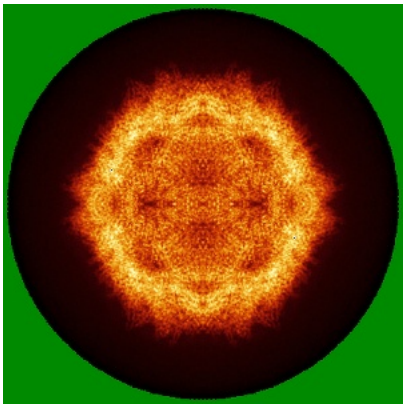
The images above show the largest variance slices of the map in three orthogonal directions.

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

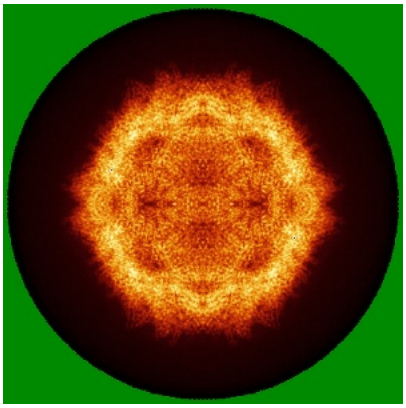
6.4.1 Primary map



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.

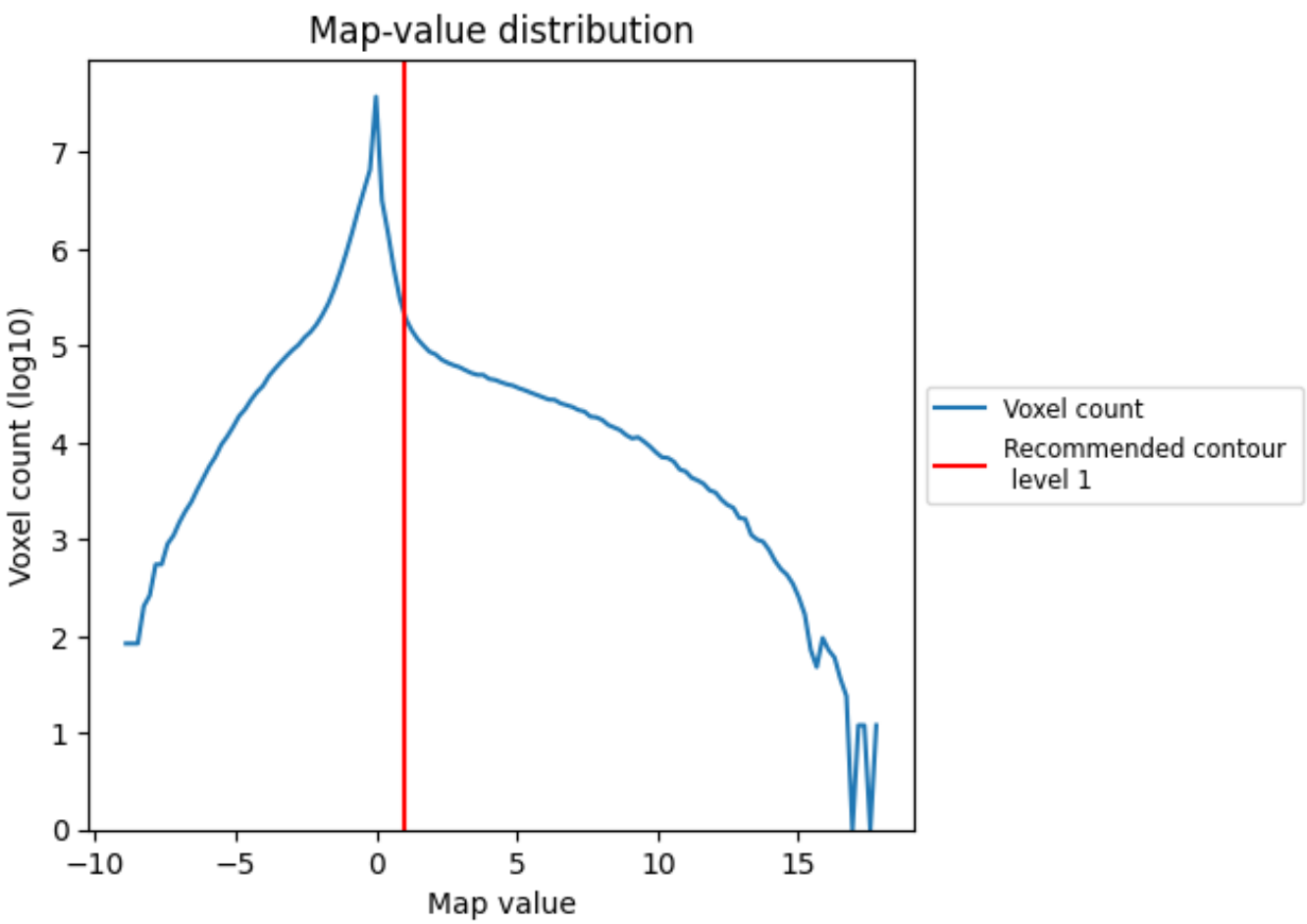
6.6 Mask visualisation (i)

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

7 Map analysis (i)

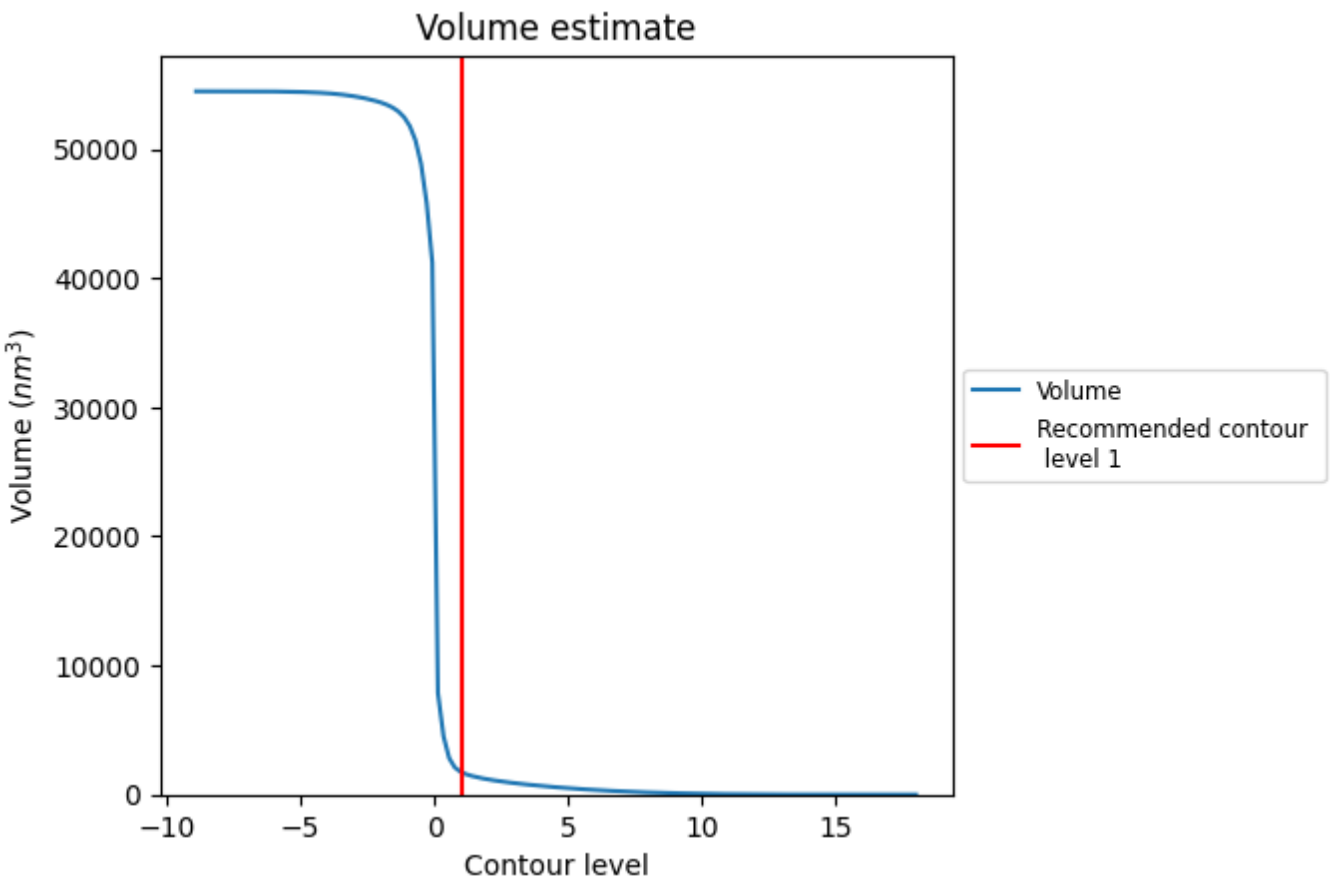
This section contains the results of statistical analysis of the map.

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.

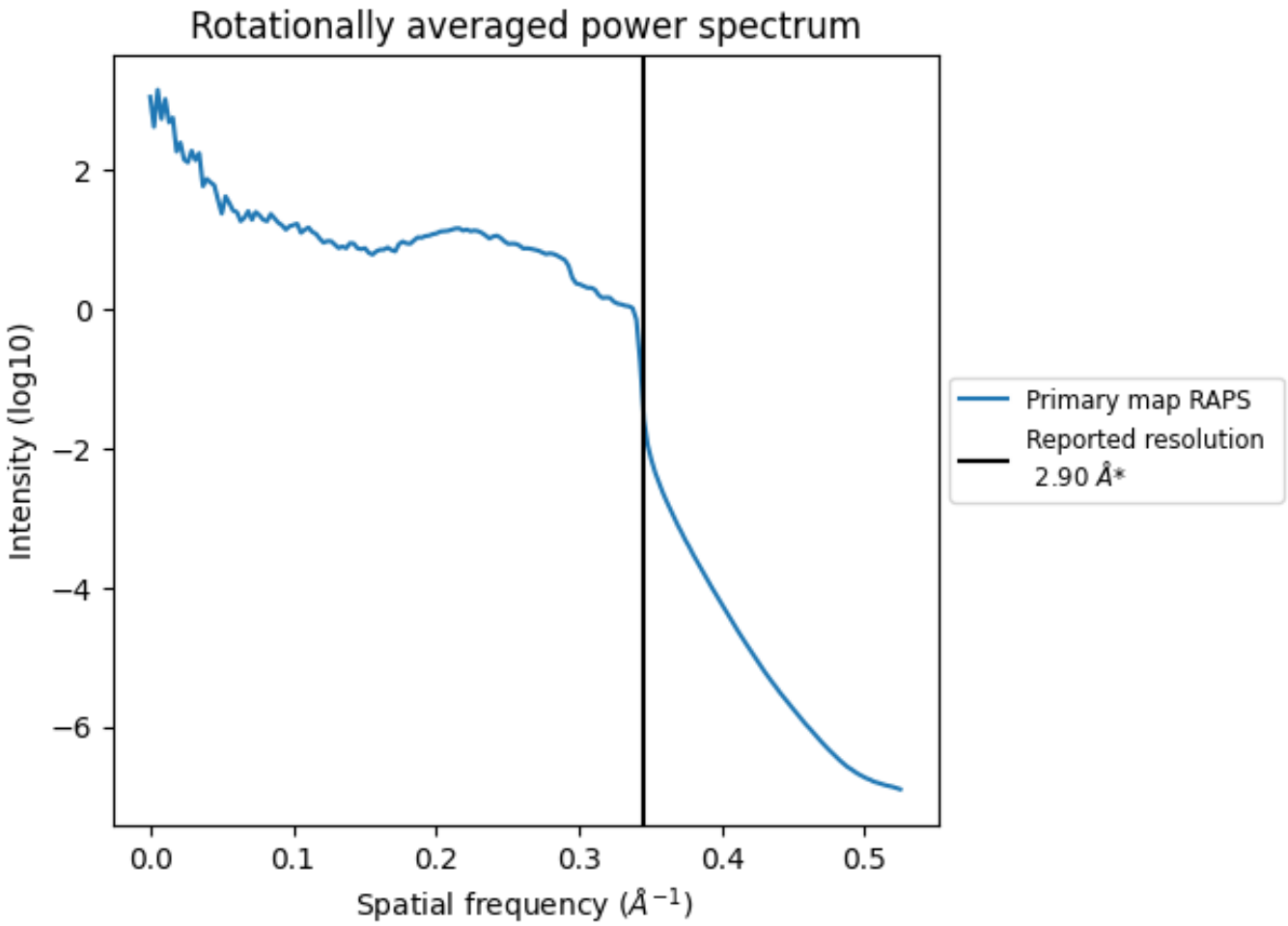
7.2 Volume estimate (i)



The volume at the recommended contour level is 1740 nm^3; this corresponds to an approximate mass of 1572 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)

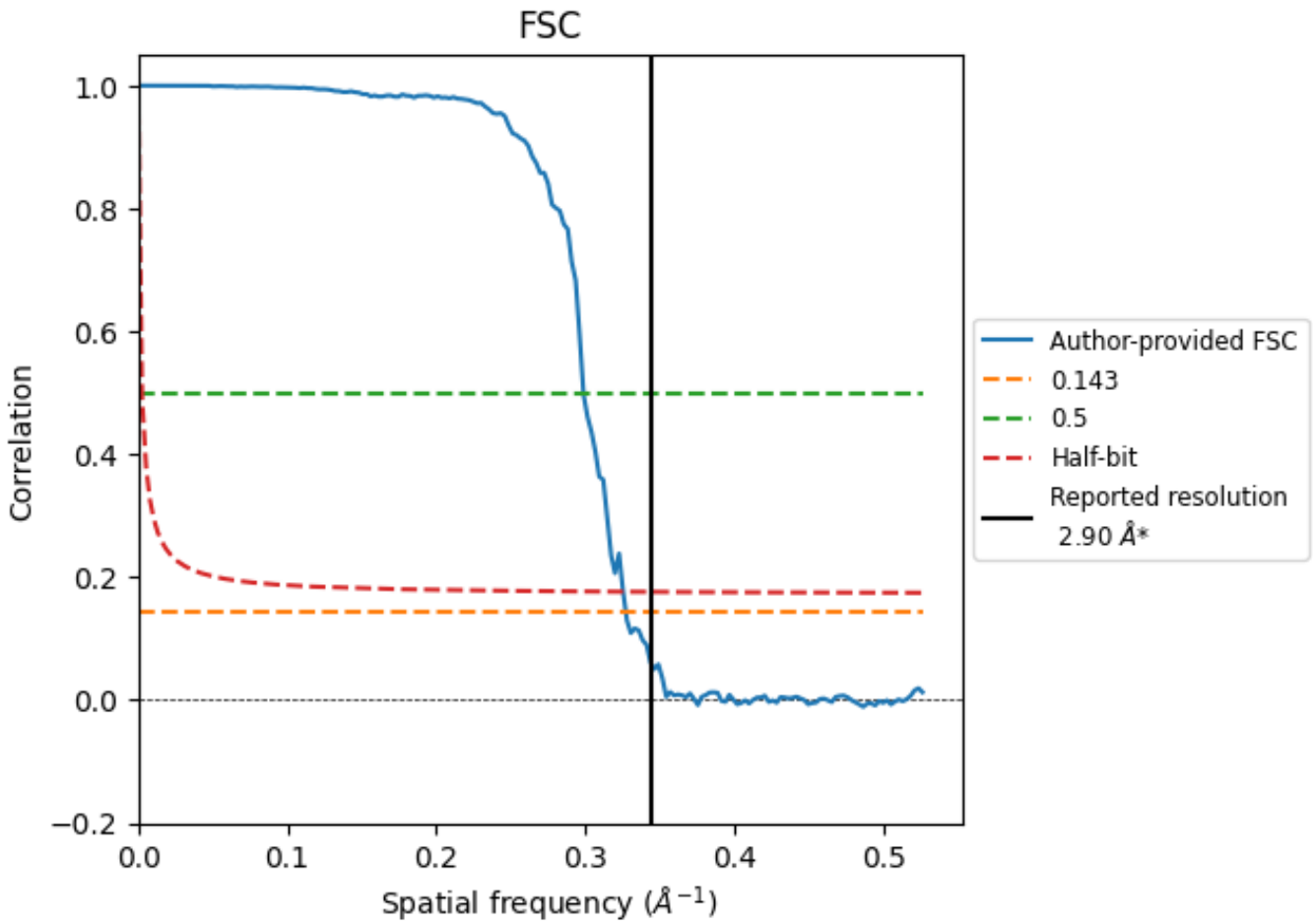


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

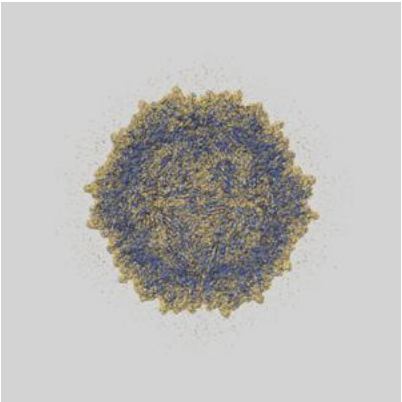
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	3.06	3.35	3.07
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

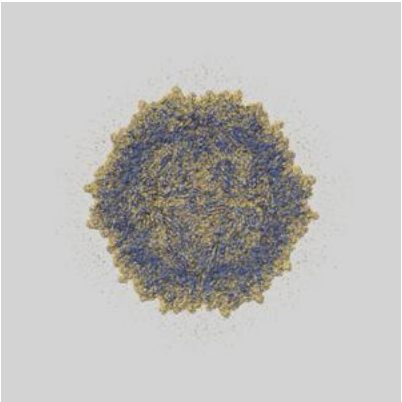
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8598 and PDB model 5URF. Per-residue inclusion information can be found in section 3 on page 10.

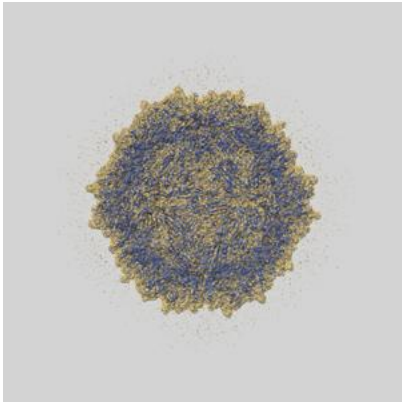
9.1 Map-model overlay (i)



X



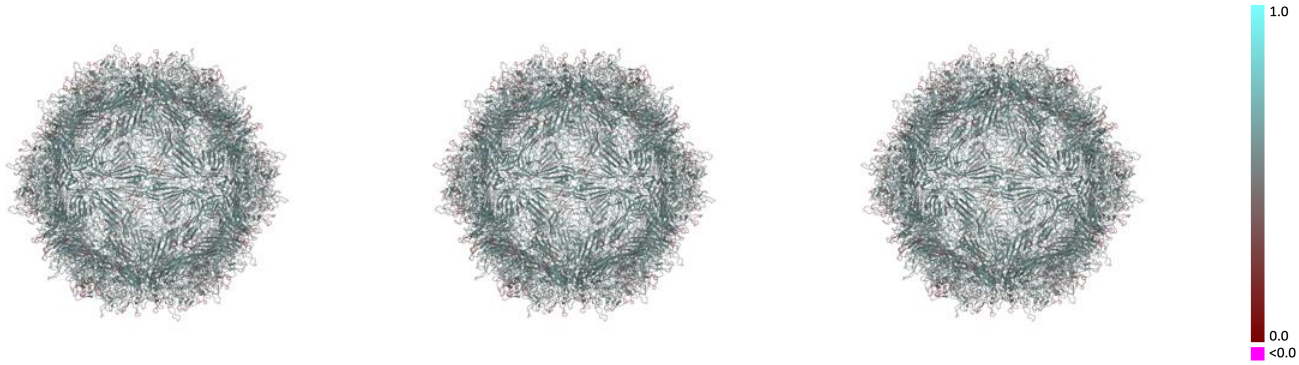
Y



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.

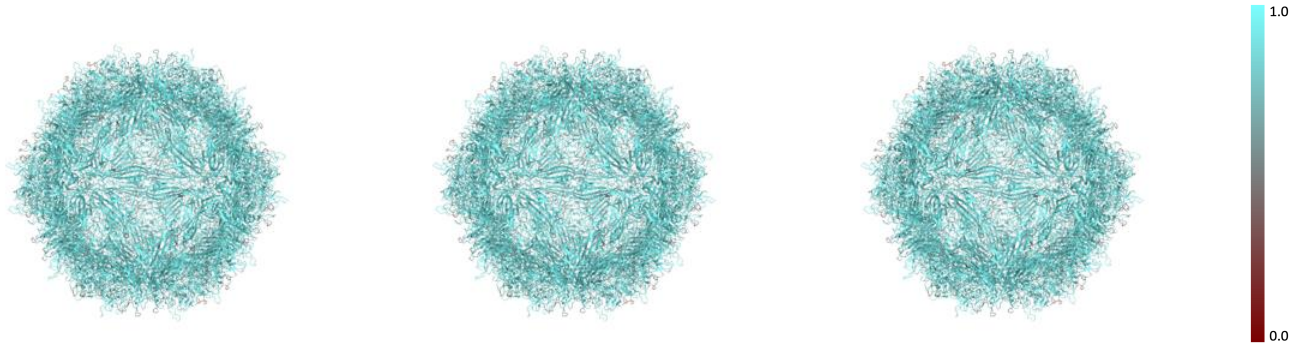
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

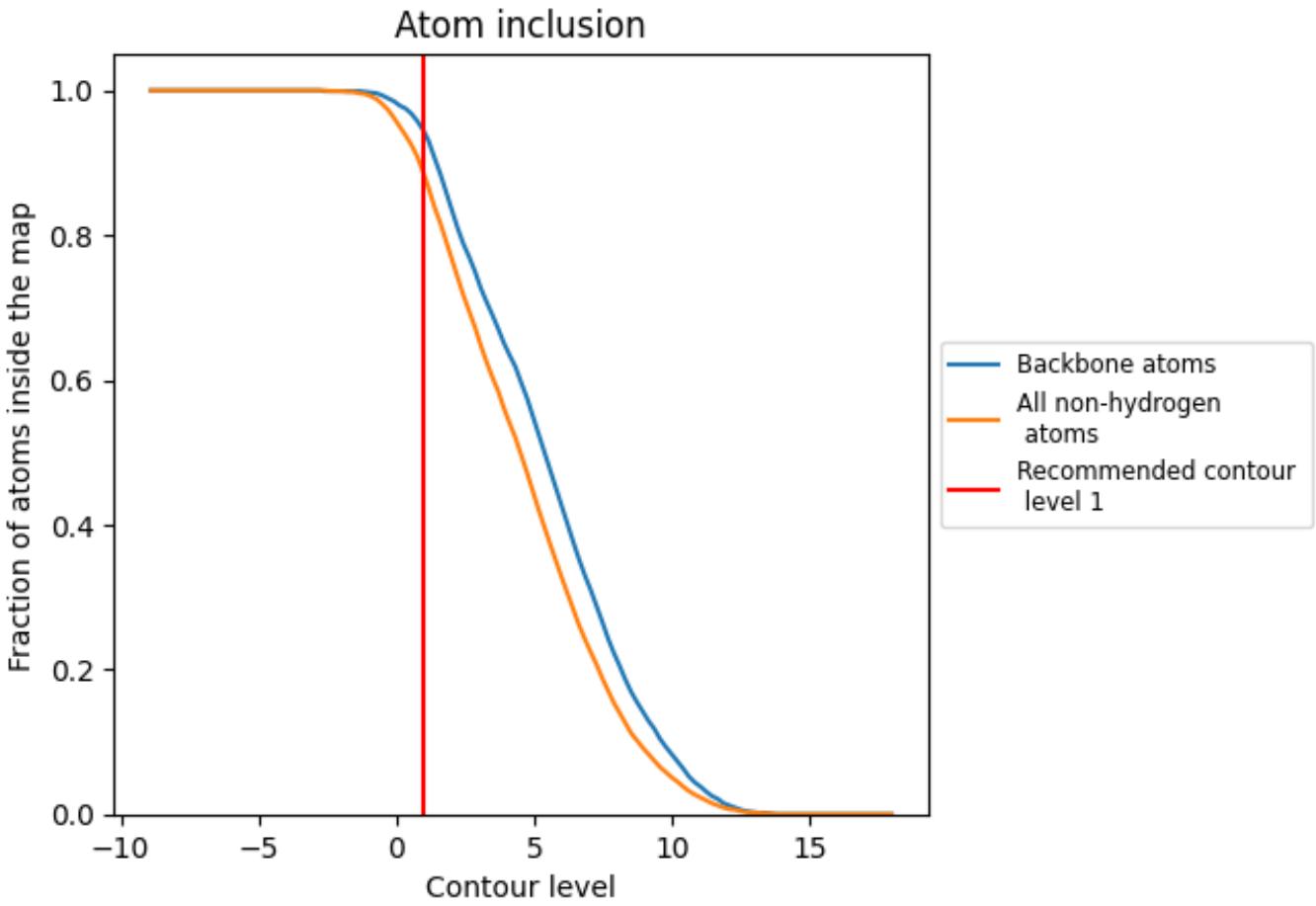
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 88% 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	0.8850	0.5290
1	0.8850	0.5280
2	0.8860	0.5300
3	0.8840	0.5280
4	0.8850	0.5290
5	0.8870	0.5290
6	0.8850	0.5290
7	0.8870	0.5300
8	0.8850	0.5290
A	0.8860	0.5300
B	0.8850	0.5280
C	0.8850	0.5310
D	0.8850	0.5290
E	0.8860	0.5300
F	0.8860	0.5300
G	0.8850	0.5280
H	0.8860	0.5290
I	0.8850	0.5280
J	0.8860	0.5290
K	0.8850	0.5280
L	0.8850	0.5290
M	0.8850	0.5300
N	0.8850	0.5300
O	0.8850	0.5290
P	0.8860	0.5300
Q	0.8850	0.5310
R	0.8870	0.5290
S	0.8850	0.5290
T	0.8850	0.5300
U	0.8850	0.5290
V	0.8840	0.5280
W	0.8850	0.5300
X	0.8860	0.5280
Y	0.8850	0.5290
Z	0.8850	0.5280

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Chain	Atom inclusion	Q-score
a	0.8860	0.5280
b	0.8850	0.5290
c	0.8850	0.5280
d	0.8850	0.5270
e	0.8870	0.5280
f	0.8860	0.5290
g	0.8860	0.5310
h	0.8850	0.5280
i	0.8850	0.5290
j	0.8870	0.5300
k	0.8850	0.5290
l	0.8850	0.5290
m	0.8850	0.5290
n	0.8850	0.5300
o	0.8860	0.5290
p	0.8850	0.5290
q	0.8840	0.5280
r	0.8870	0.5270
s	0.8850	0.5280
t	0.8860	0.5290
u	0.8850	0.5280
v	0.8850	0.5290
w	0.8860	0.5300
x	0.8840	0.5290
y	0.8850	0.5290
z	0.8840	0.5280