wwPDB EM Validation Summary Report

Mar 9, 2026 – 09:45 AM UTC

PDB ID	:	8FNW / pdb_00008fnw
EMDB ID	:	EMD-29328
Title	:	Structure of RdrA-RdrB complex from Escherichia coli RADAR defense system
Authors	:	Duncan-Lowey, B.; Johnson, A.G.; Rawson, S.; Mayer, M.L.; Kranzusch, P.J.
Deposited on	:	2022-12-28
Resolution	:	6.73 Å(reported)

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

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

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

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

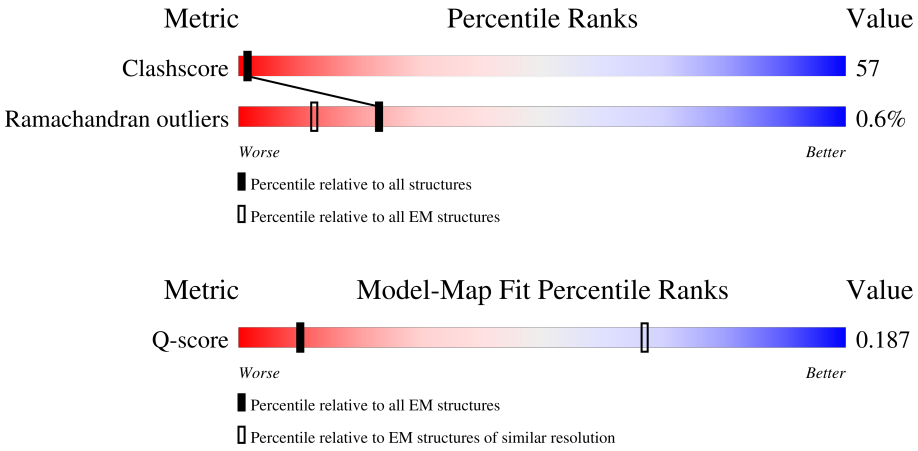
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.73 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	481 (6.23 - 7.23)

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	A	799	62% 56% 40%
1	B	799	58% 54% 41%
1	C	799	21% 52% 44%
1	D	799	22% 46% 49%
1	E	799	48% 51% 45%

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Mol	Chain	Length	Quality of chain
1	F	799	44% 55% 41%
1	G	799	45% 52% 43%
1	H	799	37% 54% 41%
1	I	799	34% 49% 47%
1	J	799	42% 52% 43%
1	K	799	34% 50% 45%
1	L	799	59% 52% 44%
2	M	947	42% 13% 70% 17%
2	N	947	41% 13% 69% 17%
2	O	947	48% 13% 70% 17%
2	P	947	45% 13% 69% 17%
2	Q	947	42% 12% 70% 17%
2	R	947	47% 13% 70% 17%
2	S	947	44% 13% 70% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 118867 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 Adenosine deaminase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	B	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	C	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	D	767	Total	C	N	O	S	0	0
			6221	3989	1078	1120	34		
1	E	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	F	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	G	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	H	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	I	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	J	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	K	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	L	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	THR	ILE	conflict	UNP A0A8E2SFD7
B	274	THR	ILE	conflict	UNP A0A8E2SFD7
C	274	THR	ILE	conflict	UNP A0A8E2SFD7
D	274	THR	ILE	conflict	UNP A0A8E2SFD7
E	274	THR	ILE	conflict	UNP A0A8E2SFD7
F	274	THR	ILE	conflict	UNP A0A8E2SFD7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	274	THR	ILE	conflict	UNP A0A8E2SFD7
H	274	THR	ILE	conflict	UNP A0A8E2SFD7
I	274	THR	ILE	conflict	UNP A0A8E2SFD7
J	274	THR	ILE	conflict	UNP A0A8E2SFD7
K	274	THR	ILE	conflict	UNP A0A8E2SFD7
L	274	THR	ILE	conflict	UNP A0A8E2SFD7

- Molecule 2 is a protein called Archaeal ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		
2	N	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		
2	O	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		
2	P	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		
2	Q	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		
2	R	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		
2	S	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	11	LYS	GLU	conflict	UNP A0A8H9B1T2
M	24	SER	PRO	conflict	UNP A0A8H9B1T2
M	67	PRO	SER	conflict	UNP A0A8H9B1T2
M	335	SER	GLY	conflict	UNP A0A8H9B1T2
M	409	ASP	ASN	conflict	UNP A0A8H9B1T2
M	428	ASN	SER	conflict	UNP A0A8H9B1T2
M	583	ASN	HIS	conflict	UNP A0A8H9B1T2
M	586	GLU	GLY	conflict	UNP A0A8H9B1T2
M	636	ARG	LEU	conflict	UNP A0A8H9B1T2
M	858	ILE	VAL	conflict	UNP A0A8H9B1T2
N	11	LYS	GLU	conflict	UNP A0A8H9B1T2
N	24	SER	PRO	conflict	UNP A0A8H9B1T2
N	67	PRO	SER	conflict	UNP A0A8H9B1T2
N	335	SER	GLY	conflict	UNP A0A8H9B1T2

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Chain	Residue	Modelled	Actual	Comment	Reference
N	409	ASP	ASN	conflict	UNP A0A8H9B1T2
N	428	ASN	SER	conflict	UNP A0A8H9B1T2
N	583	ASN	HIS	conflict	UNP A0A8H9B1T2
N	586	GLU	GLY	conflict	UNP A0A8H9B1T2
N	636	ARG	LEU	conflict	UNP A0A8H9B1T2
N	858	ILE	VAL	conflict	UNP A0A8H9B1T2
O	11	LYS	GLU	conflict	UNP A0A8H9B1T2
O	24	SER	PRO	conflict	UNP A0A8H9B1T2
O	67	PRO	SER	conflict	UNP A0A8H9B1T2
O	335	SER	GLY	conflict	UNP A0A8H9B1T2
O	409	ASP	ASN	conflict	UNP A0A8H9B1T2
O	428	ASN	SER	conflict	UNP A0A8H9B1T2
O	583	ASN	HIS	conflict	UNP A0A8H9B1T2
O	586	GLU	GLY	conflict	UNP A0A8H9B1T2
O	636	ARG	LEU	conflict	UNP A0A8H9B1T2
O	858	ILE	VAL	conflict	UNP A0A8H9B1T2
P	11	LYS	GLU	conflict	UNP A0A8H9B1T2
P	24	SER	PRO	conflict	UNP A0A8H9B1T2
P	67	PRO	SER	conflict	UNP A0A8H9B1T2
P	335	SER	GLY	conflict	UNP A0A8H9B1T2
P	409	ASP	ASN	conflict	UNP A0A8H9B1T2
P	428	ASN	SER	conflict	UNP A0A8H9B1T2
P	583	ASN	HIS	conflict	UNP A0A8H9B1T2
P	586	GLU	GLY	conflict	UNP A0A8H9B1T2
P	636	ARG	LEU	conflict	UNP A0A8H9B1T2
P	858	ILE	VAL	conflict	UNP A0A8H9B1T2
Q	11	LYS	GLU	conflict	UNP A0A8H9B1T2
Q	24	SER	PRO	conflict	UNP A0A8H9B1T2
Q	67	PRO	SER	conflict	UNP A0A8H9B1T2
Q	335	SER	GLY	conflict	UNP A0A8H9B1T2
Q	409	ASP	ASN	conflict	UNP A0A8H9B1T2
Q	428	ASN	SER	conflict	UNP A0A8H9B1T2
Q	583	ASN	HIS	conflict	UNP A0A8H9B1T2
Q	586	GLU	GLY	conflict	UNP A0A8H9B1T2
Q	636	ARG	LEU	conflict	UNP A0A8H9B1T2
Q	858	ILE	VAL	conflict	UNP A0A8H9B1T2
R	11	LYS	GLU	conflict	UNP A0A8H9B1T2
R	24	SER	PRO	conflict	UNP A0A8H9B1T2
R	67	PRO	SER	conflict	UNP A0A8H9B1T2
R	335	SER	GLY	conflict	UNP A0A8H9B1T2
R	409	ASP	ASN	conflict	UNP A0A8H9B1T2
R	428	ASN	SER	conflict	UNP A0A8H9B1T2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	583	ASN	HIS	conflict	UNP A0A8H9B1T2
R	586	GLU	GLY	conflict	UNP A0A8H9B1T2
R	636	ARG	LEU	conflict	UNP A0A8H9B1T2
R	858	ILE	VAL	conflict	UNP A0A8H9B1T2
S	11	LYS	GLU	conflict	UNP A0A8H9B1T2
S	24	SER	PRO	conflict	UNP A0A8H9B1T2
S	67	PRO	SER	conflict	UNP A0A8H9B1T2
S	335	SER	GLY	conflict	UNP A0A8H9B1T2
S	409	ASP	ASN	conflict	UNP A0A8H9B1T2
S	428	ASN	SER	conflict	UNP A0A8H9B1T2
S	583	ASN	HIS	conflict	UNP A0A8H9B1T2
S	586	GLU	GLY	conflict	UNP A0A8H9B1T2
S	636	ARG	LEU	conflict	UNP A0A8H9B1T2
S	858	ILE	VAL	conflict	UNP A0A8H9B1T2

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0
3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0
3	E	1	Total Zn 1 1	0
3	F	1	Total Zn 1 1	0
3	G	1	Total Zn 1 1	0
3	H	1	Total Zn 1 1	0
3	I	1	Total Zn 1 1	0
3	J	1	Total Zn 1 1	0
3	K	1	Total Zn 1 1	0
3	L	1	Total Zn 1 1	0

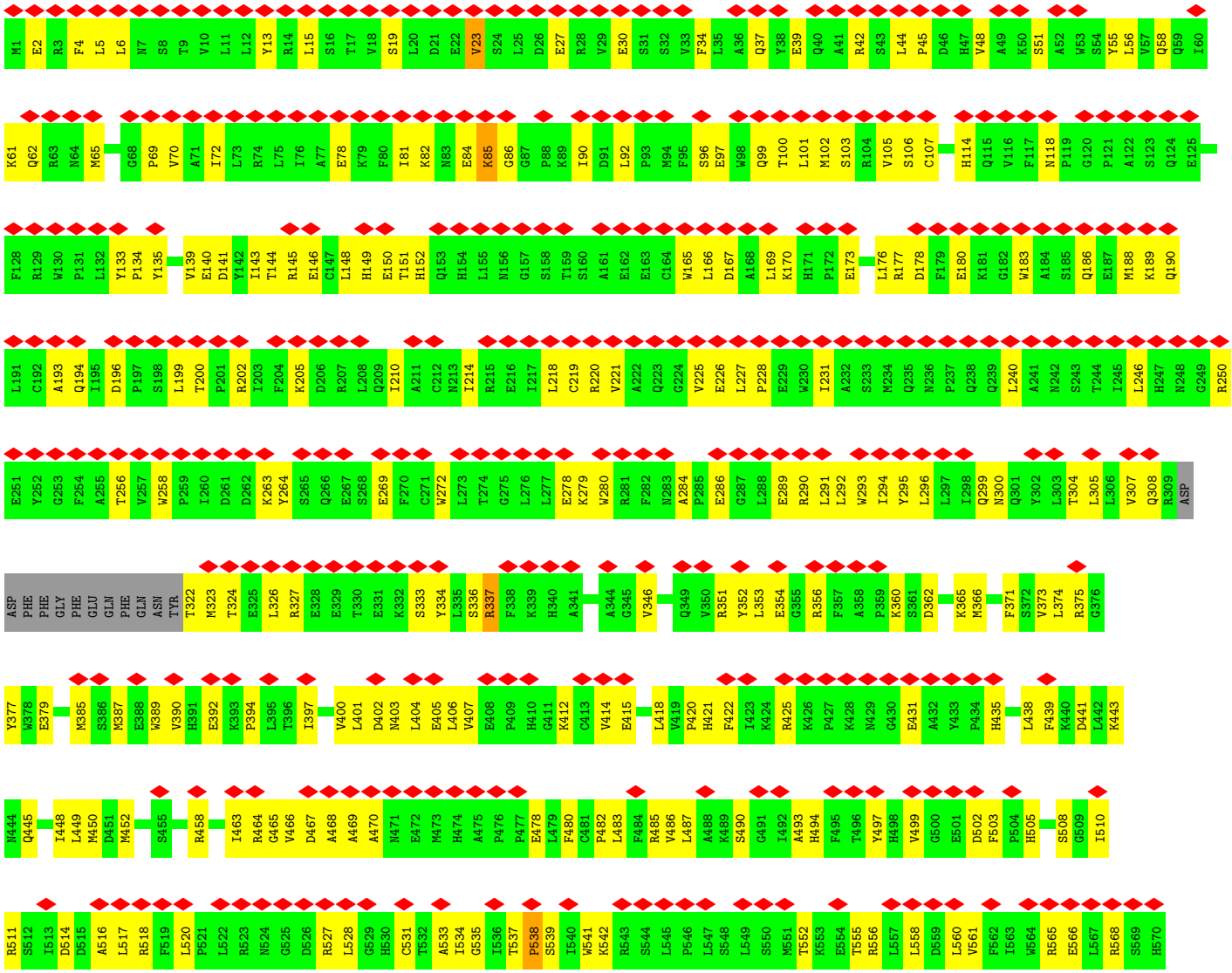
3 Residue-property plots (i)

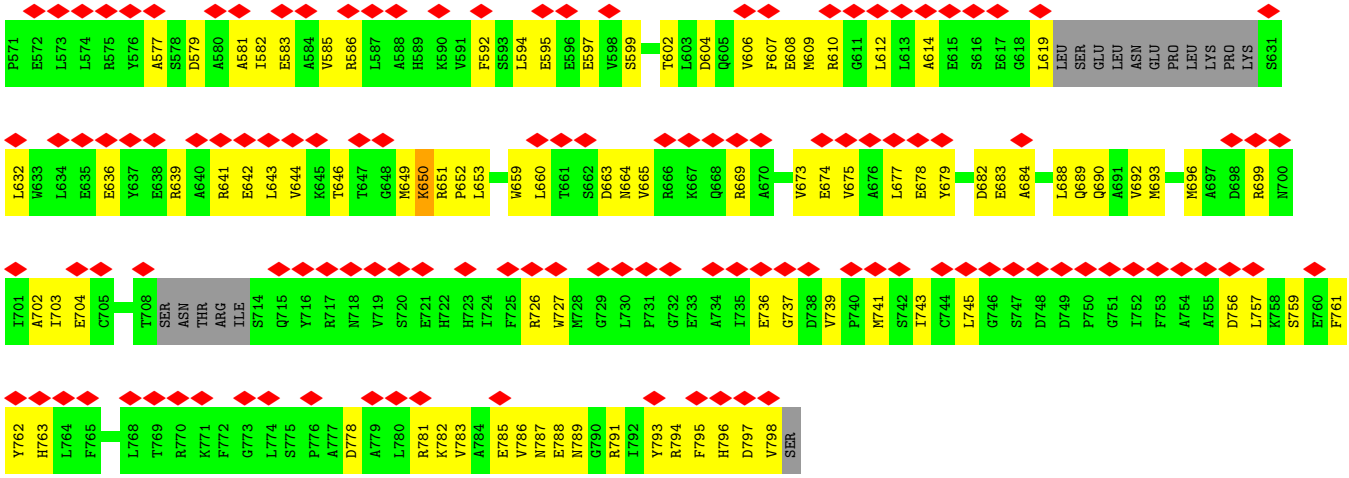
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:



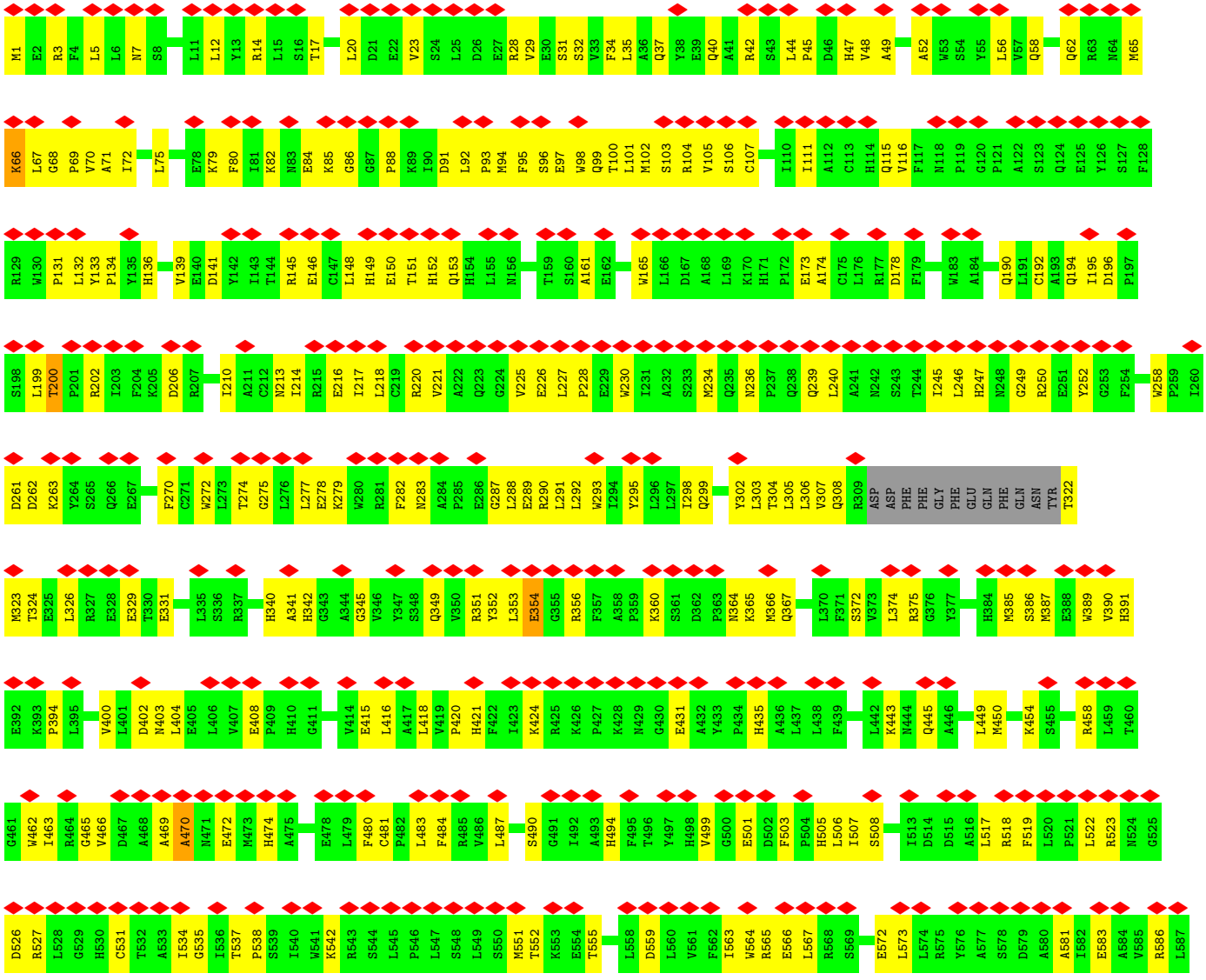




• Molecule 1: Adenosine deaminase

Chain B:



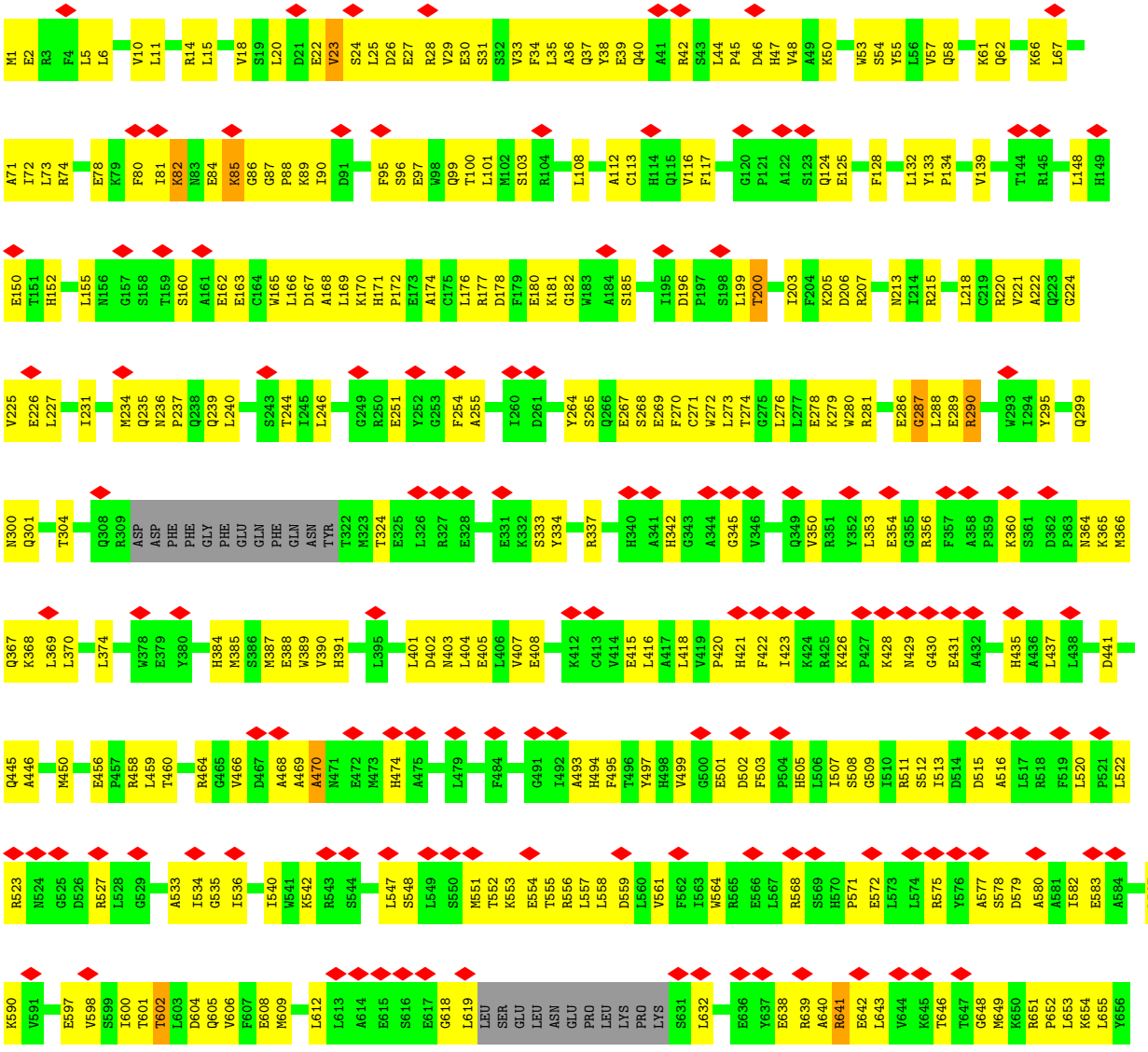


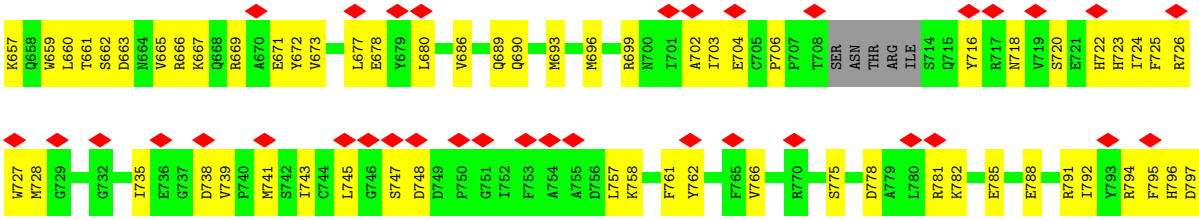


• Molecule 1: Adenosine deaminase

Chain C:



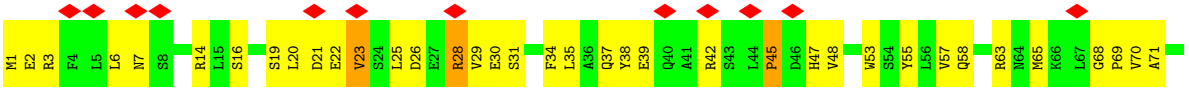


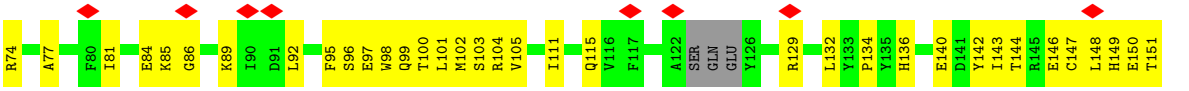


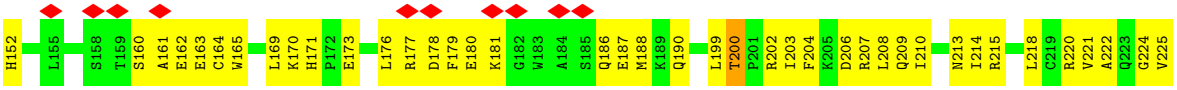
• Molecule 1: Adenosine deaminase

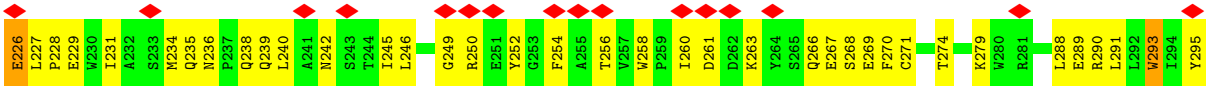
Chain D:

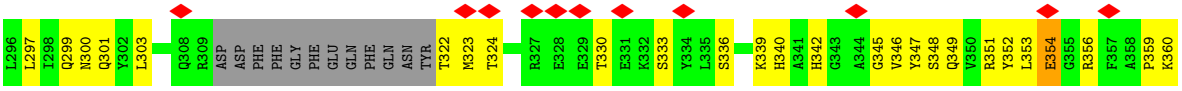


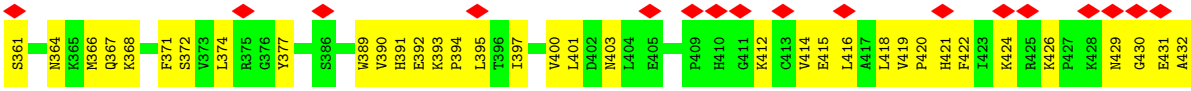


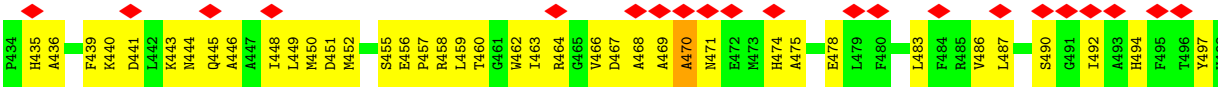


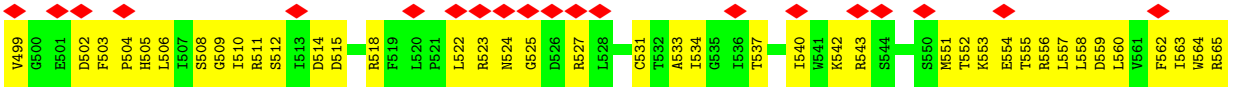


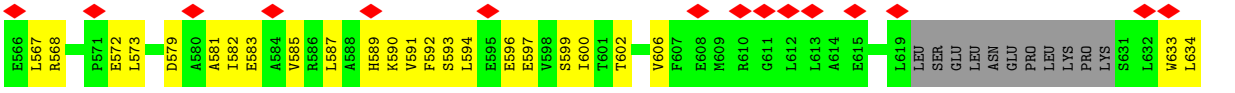


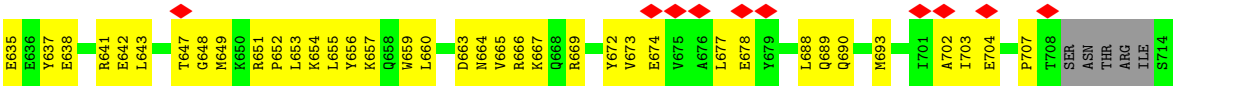


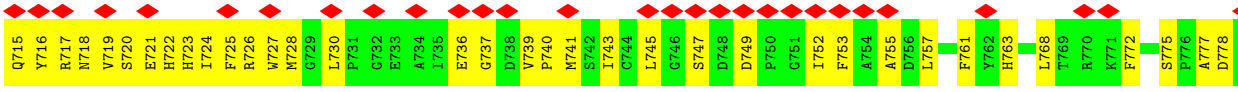




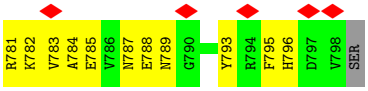








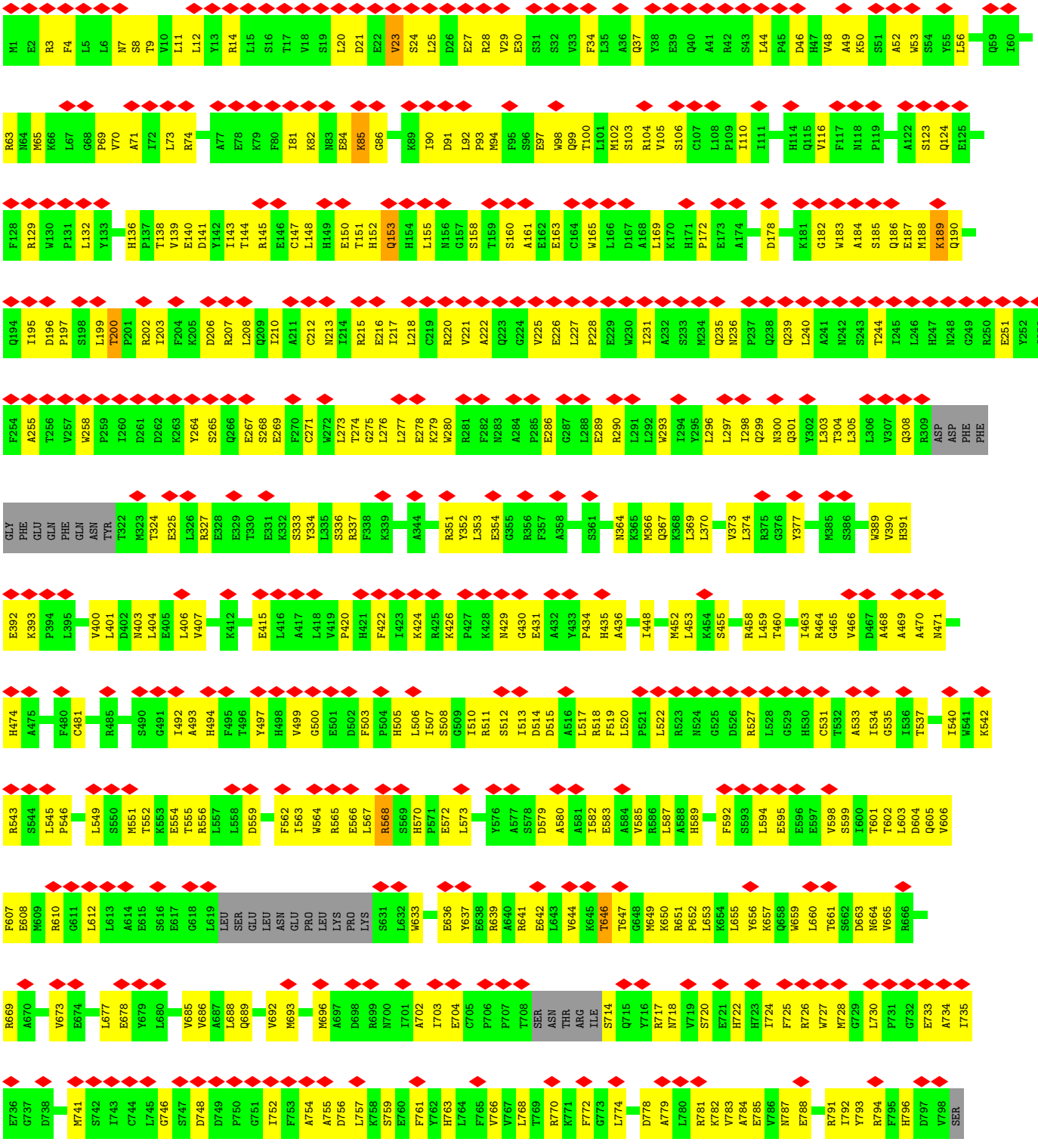




• Molecule 1: Adenosine deaminase

Chain E:

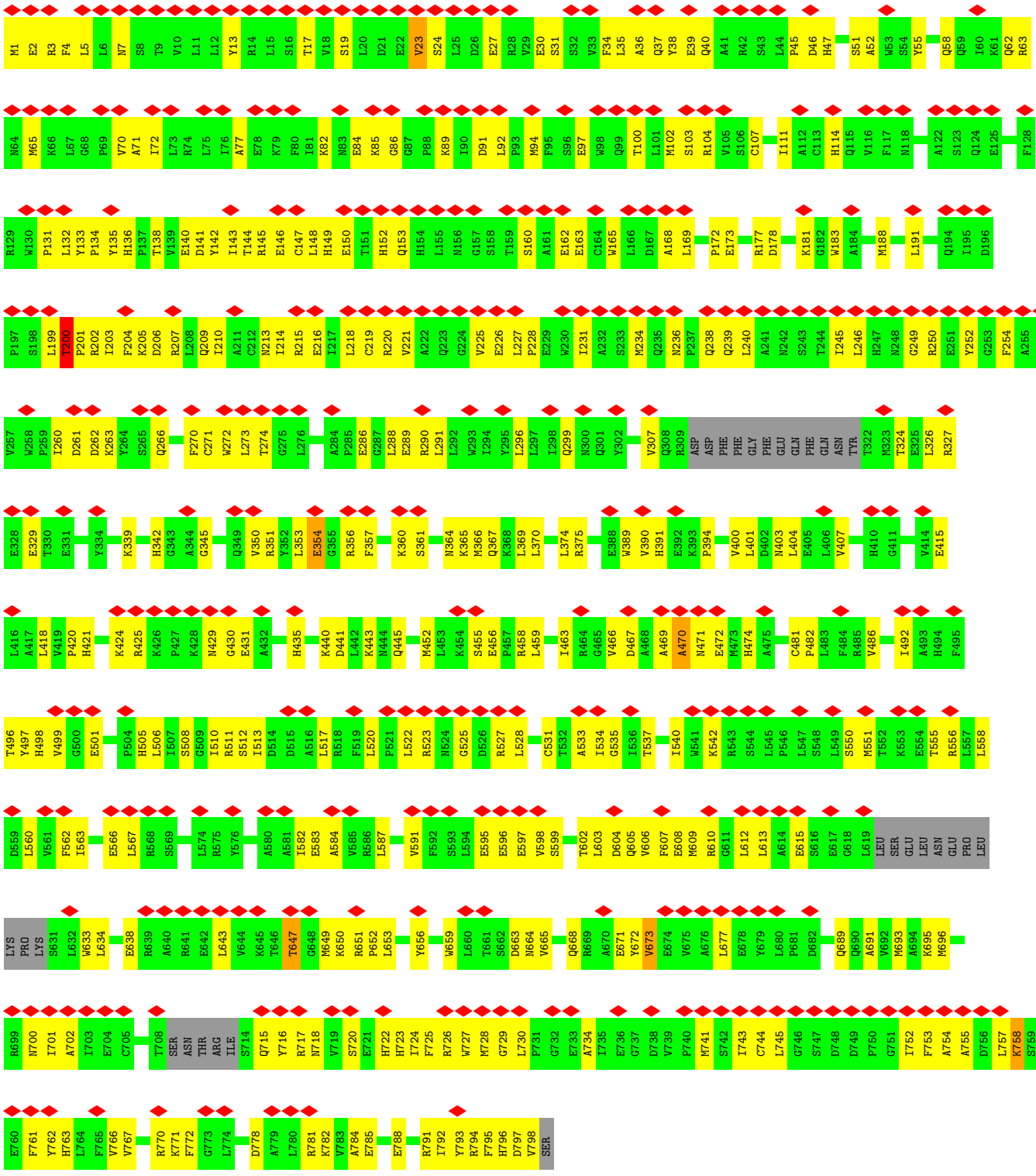




• Molecule 1: Adenosine deaminase

Chain F:

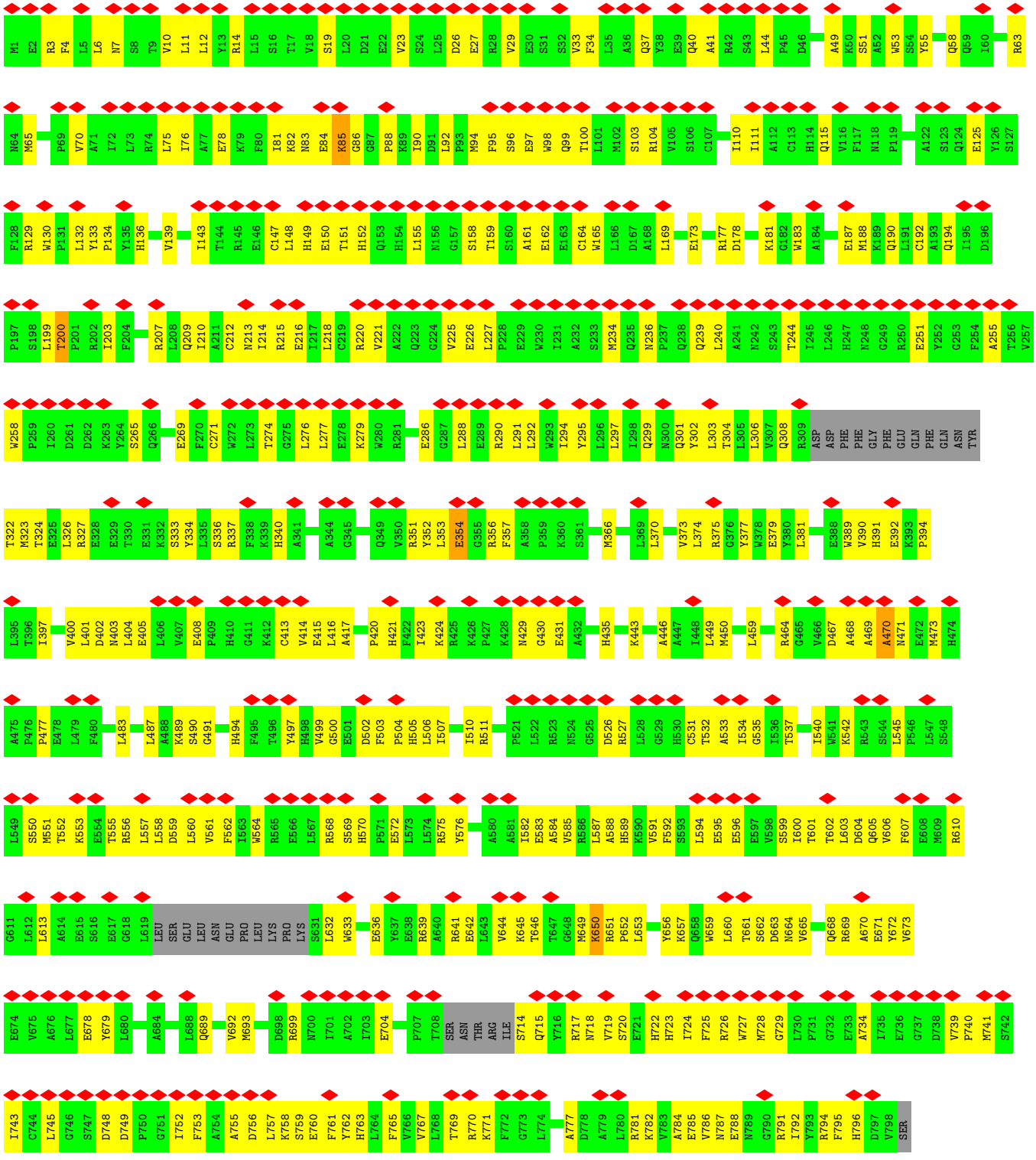




• Molecule 1: Adenosine deaminase

Chain G:

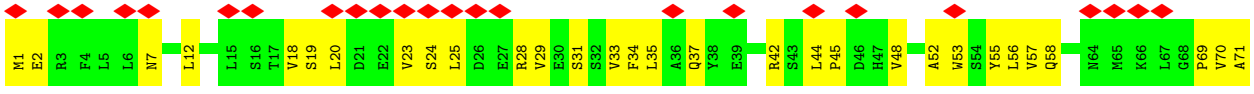


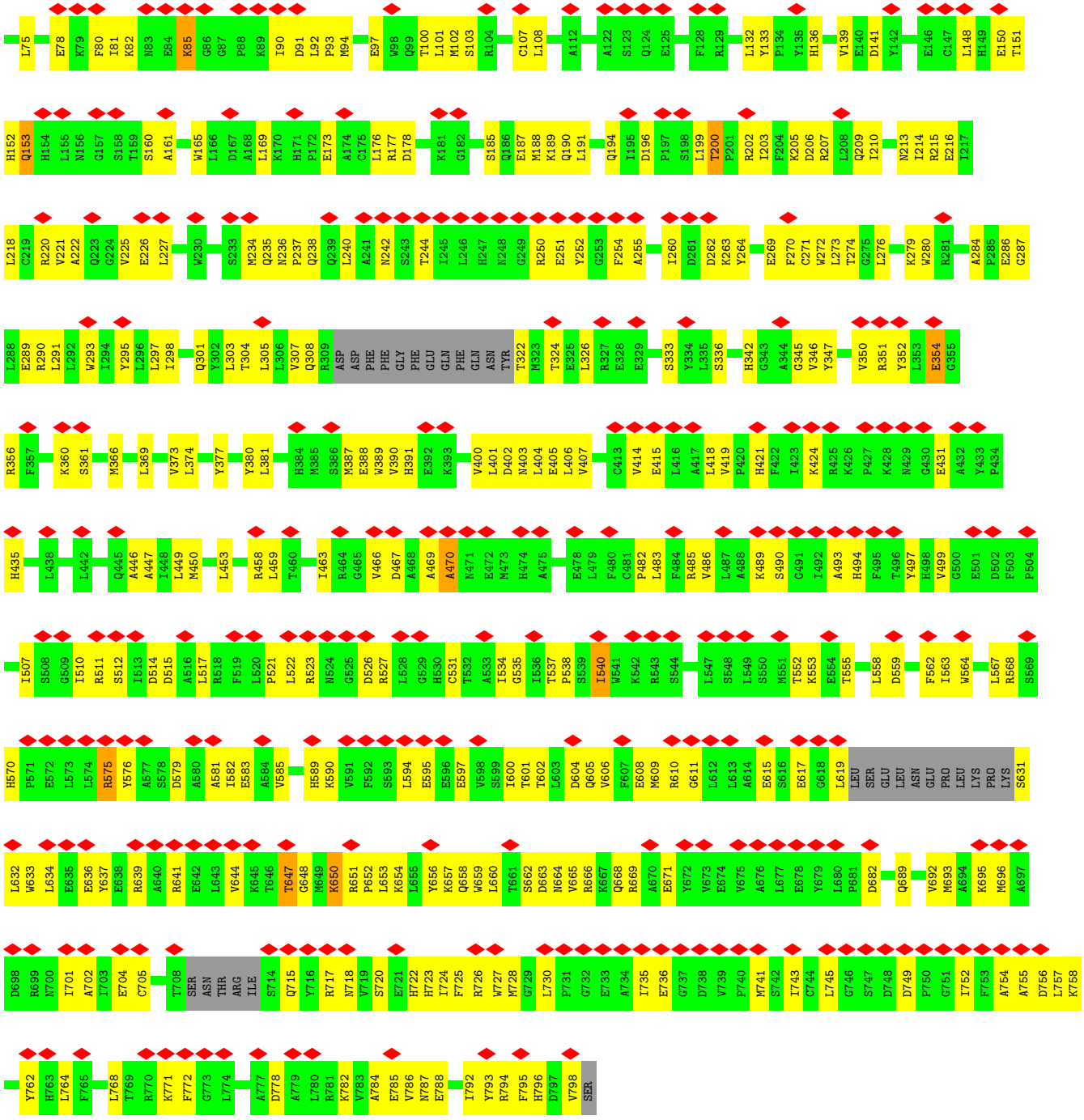


• Molecule 1: Adenosine deaminase

Chain H:



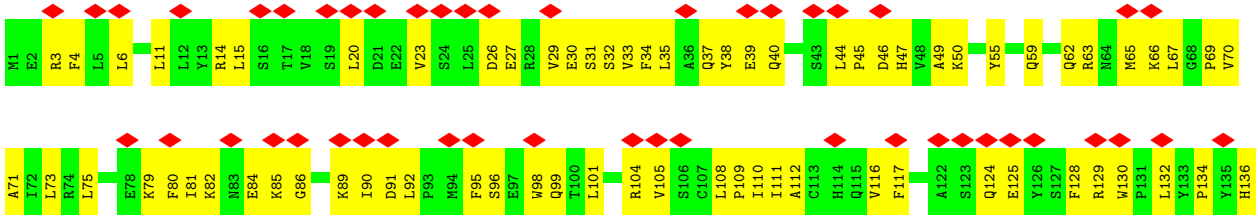


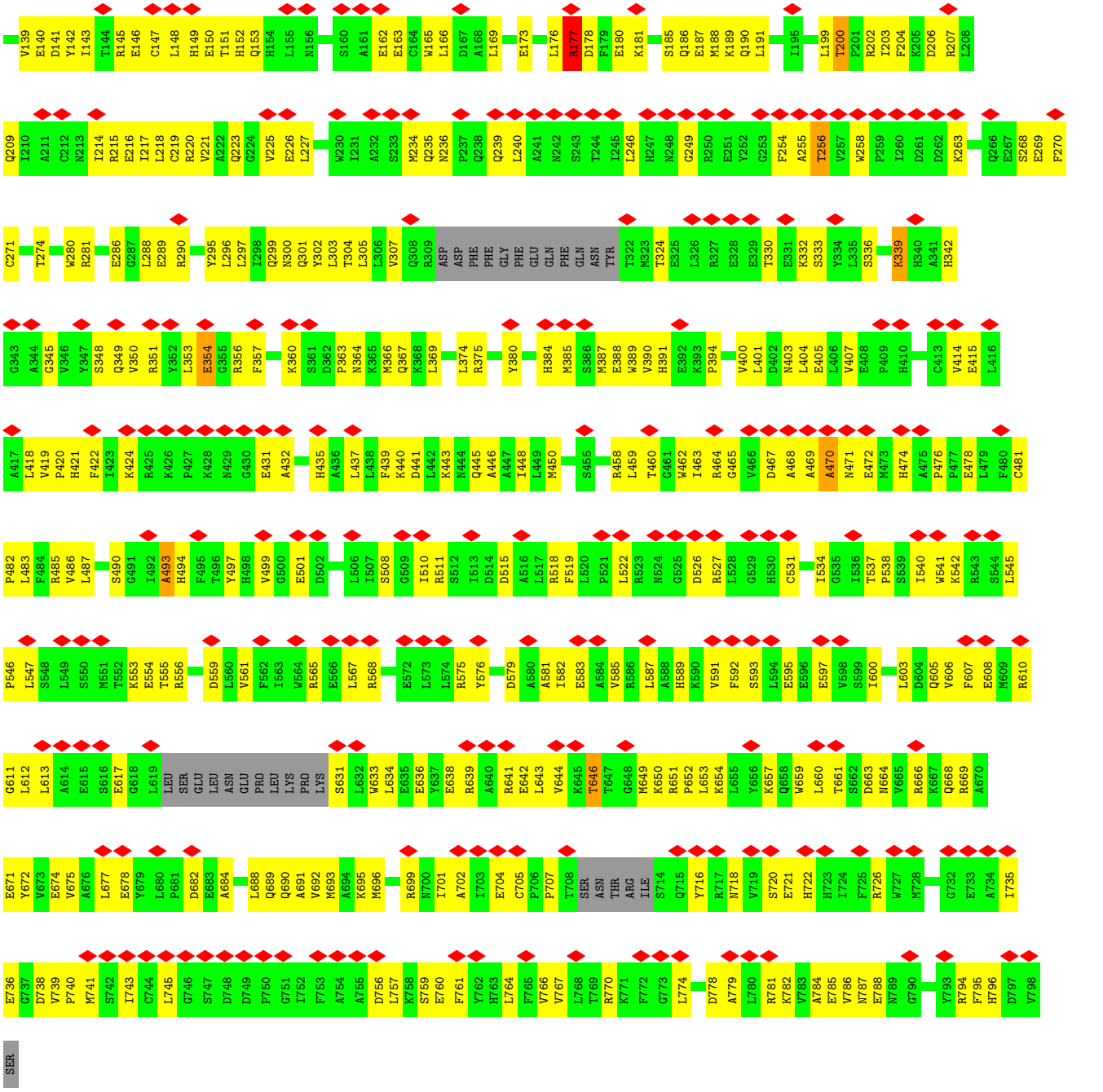


• Molecule 1: Adenosine deaminase

Chain I:



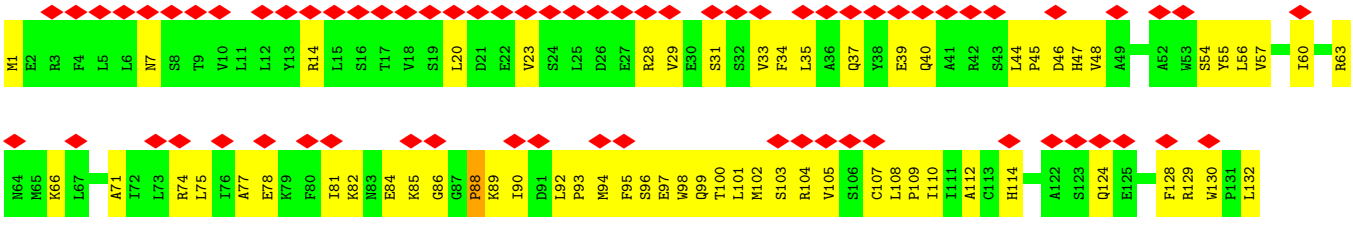


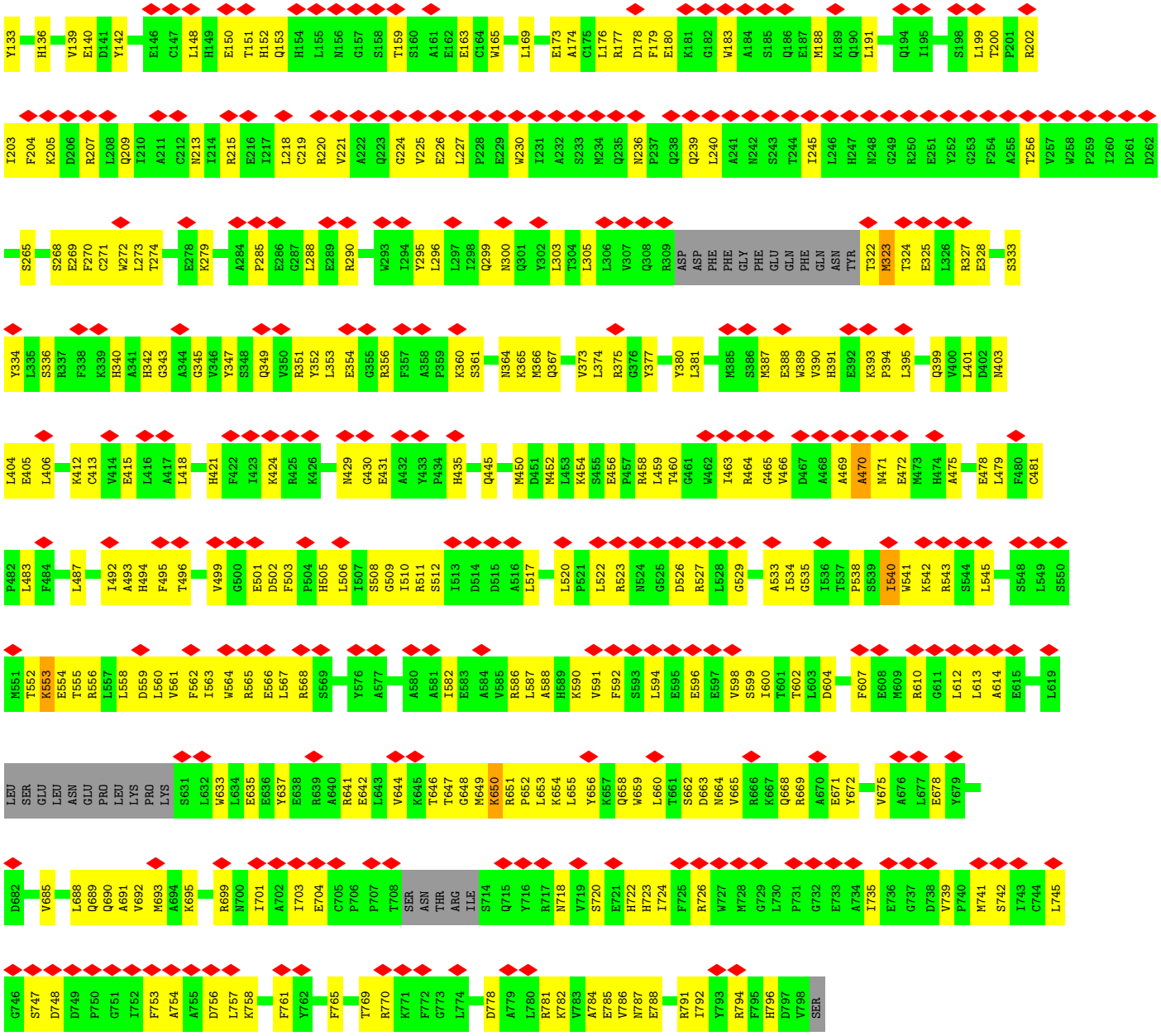


• Molecule 1: Adenosine deaminase

Chain J:



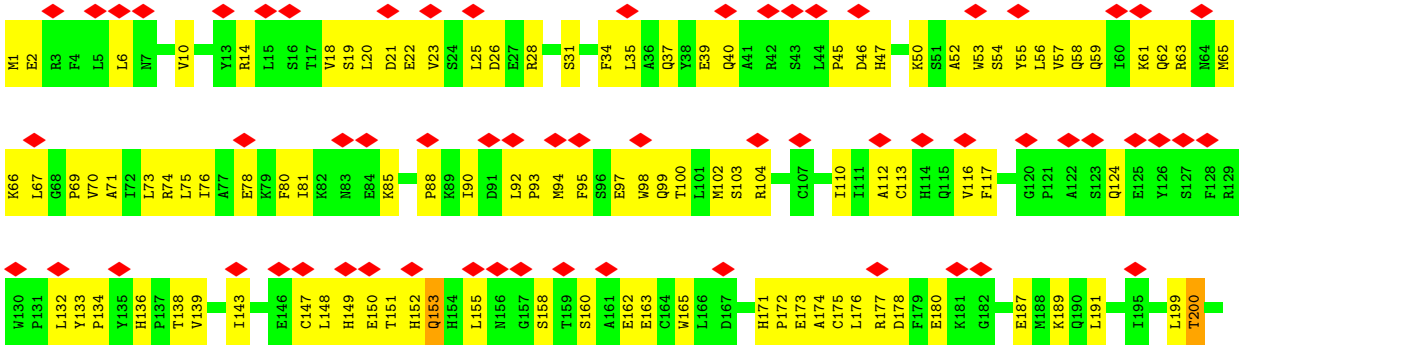


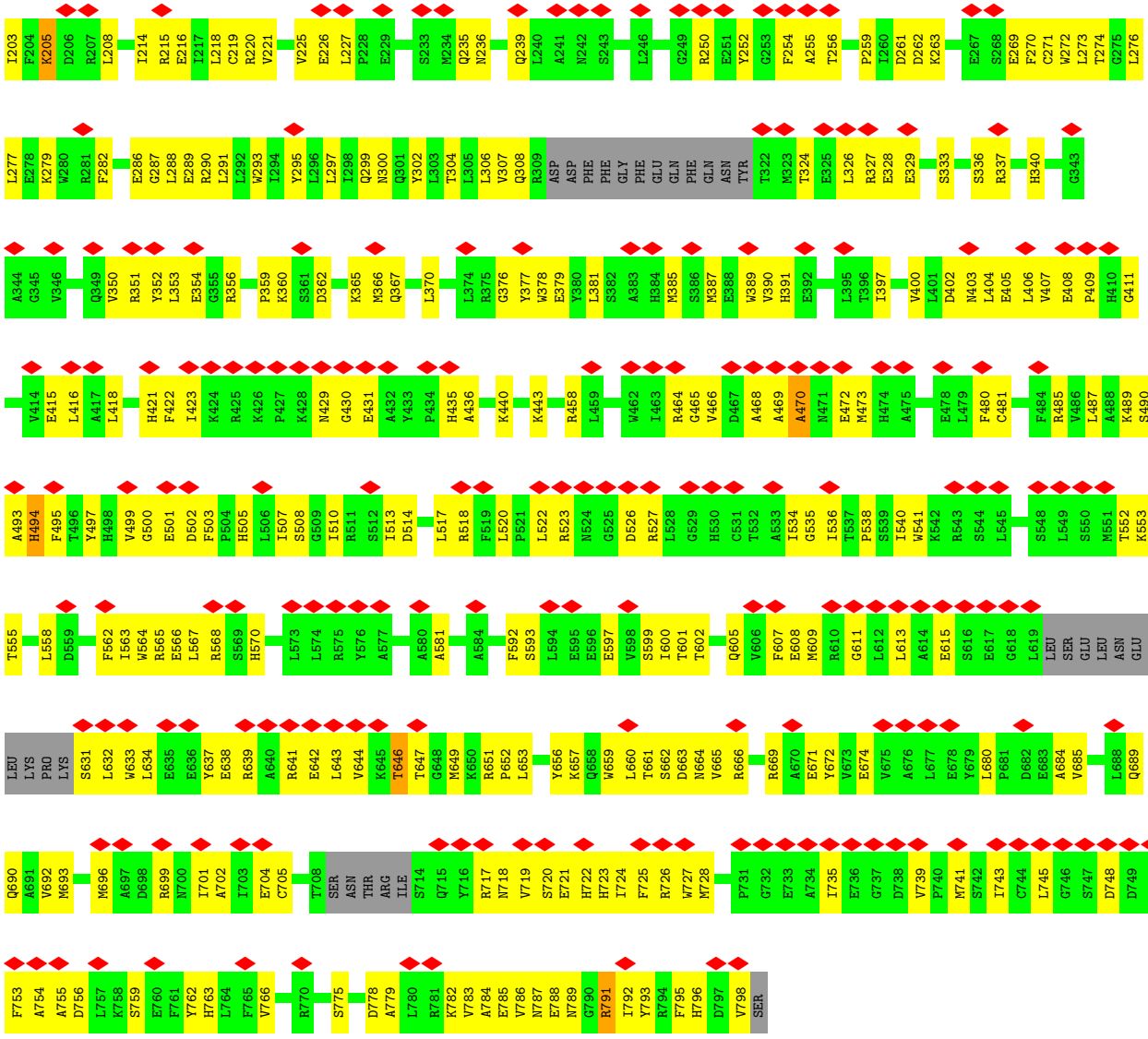


• Molecule 1: Adenosine deaminase

Chain K:



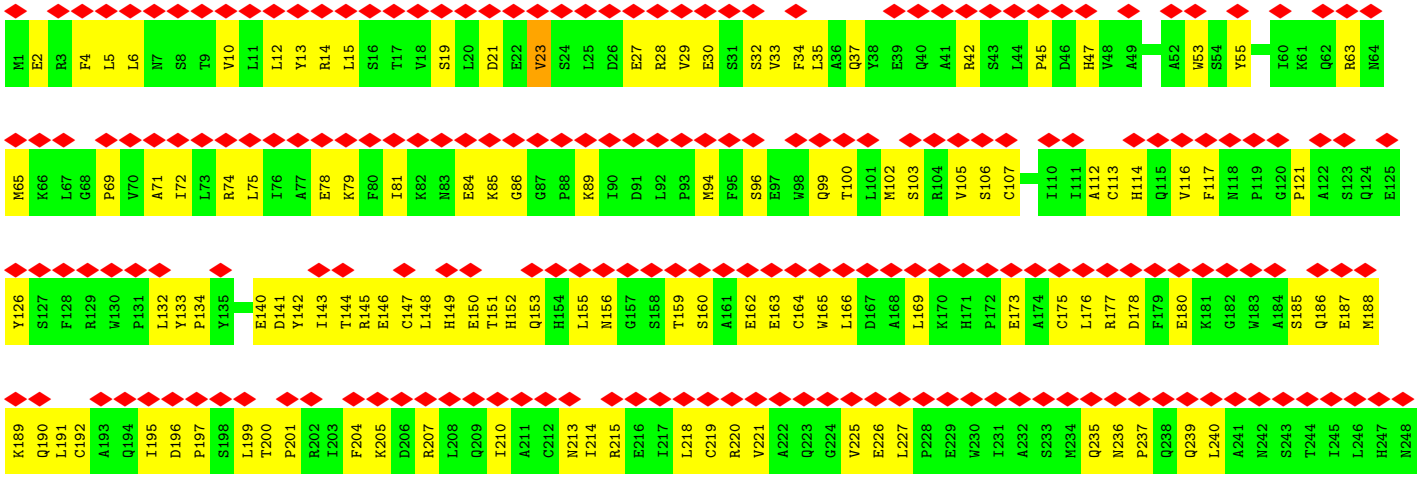


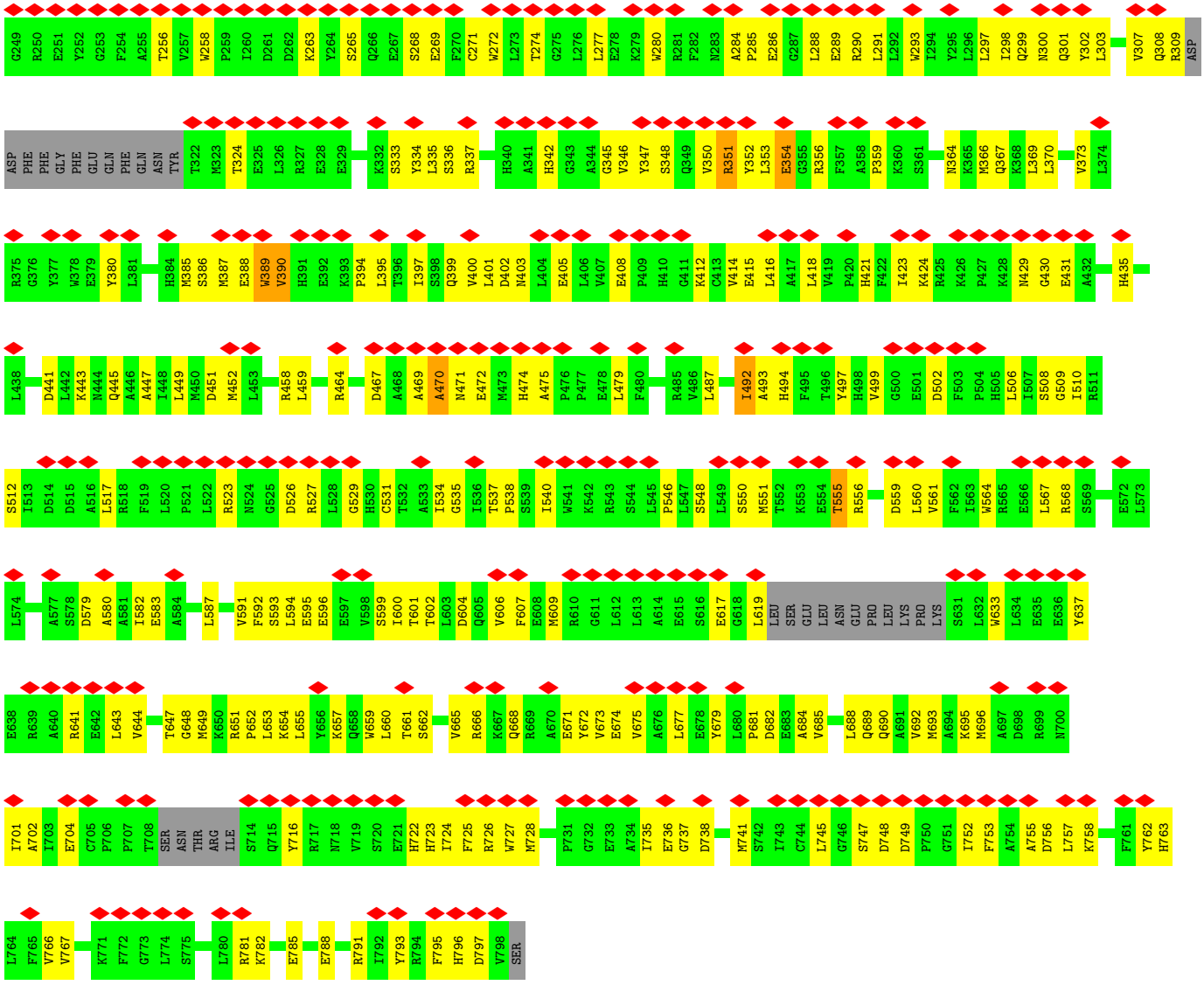


• Molecule 1: Adenosine deaminase

Chain L:

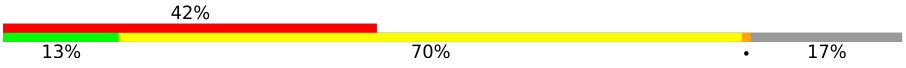


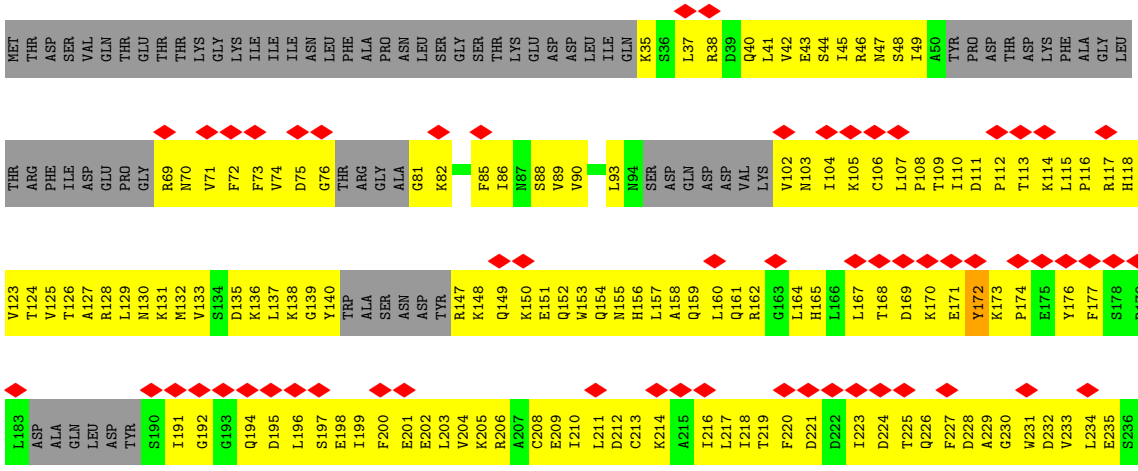


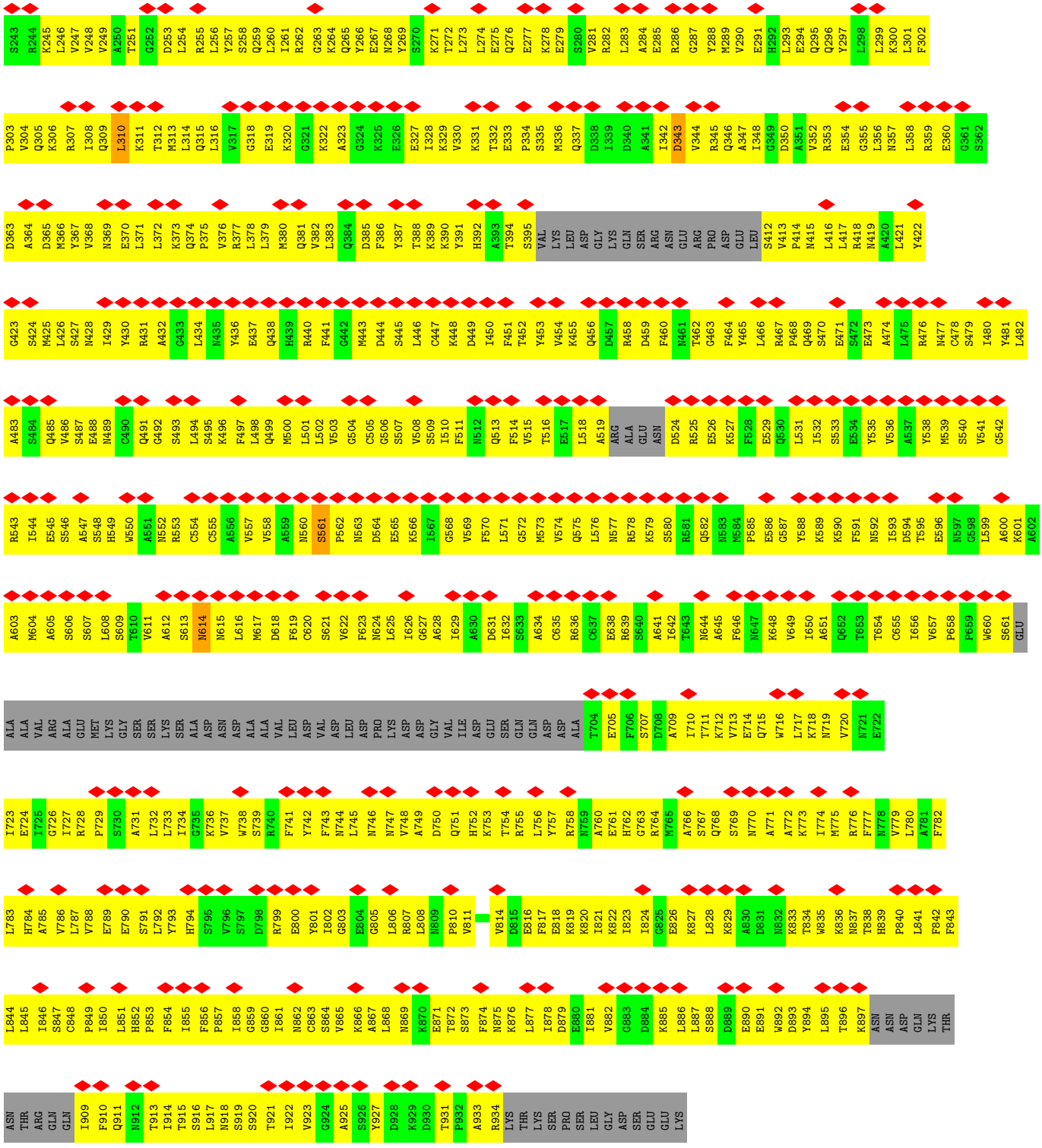


• Molecule 2: Archaeal ATPase

Chain M:

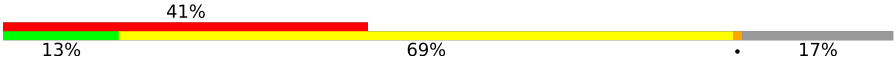


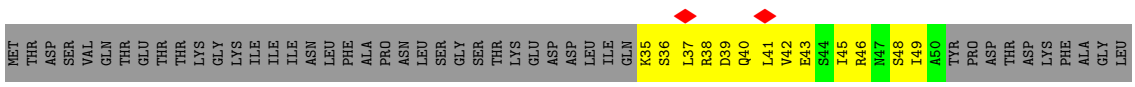


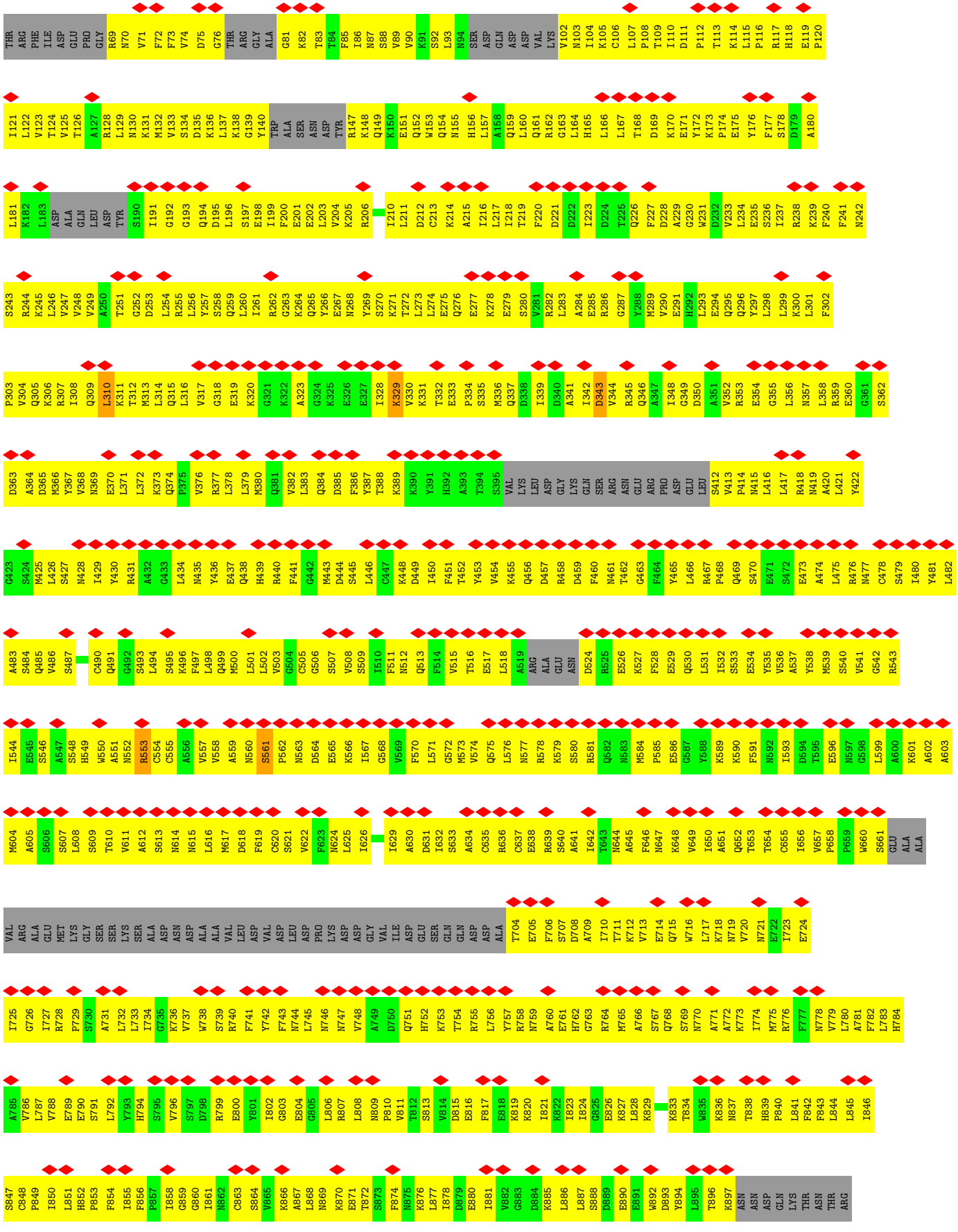


- Molecule 2: Archaeal ATPase

Chain N:



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I121 L122 V123 T124 V125 T126 A127 R128 L129 N130 K131 M132 V133 S134 D135 K136 L137 K138 G139 Y140 TRP ALA SER ASN ASP TYR R147 K148 Q149 K150 E151 Q152 W153 Q154 N155 H156 L157 A158 Q159 L160 Q161 R162 G163 L164 H165 L166 L167 T168 D169 K170 E171 Y172 K173 P174 E175 Y176 F177 S178 D179 A180
L181 K182 L183 ASP ALA GLN LEU ASP TYR S190 I191 G192 G193 Q194 D195 L196 S197 E198 I199 F200 E201 E202 L203 V204 K205 R206 I210 L211 D212 C213 K214 A215 I216 L217 I218 T219 F220 D221 D222 I223 D224 T225 Q226 F227 D228 A229 G230 W231 D232 V233 L234 E235 S236 I237 R238 K239 F240 F241 N242
S243 R244 K245 L246 V247 V248 V249 A250 T251 G252 D253 L254 R255 L256 Y257 S258 Q259 L260 I261 R262 G263 K264 Q265 Y266 E267 N268 Y269 S270 K271 T272 L273 L274 E275 Q276 E277 K278 E279 S280 V281 R282 L283 A284 E285 R286 G287 Y288 M289 V290 E291 H292 L293 E294 Q295 Q296 Y297 L298 L299 K300 L301 F302
P303 V304 Q305 K306 R307 I308 Q309 L310 K311 T312 M313 L314 Q315 L316 V317 G318 E319 K320 G321 K322 A323 G324 K325 E326 E327 I328 K329 V330 K331 T332 E333 P334 S335 M336 Q337 D338 I339 D340 A341 I342 D343 V344 R345 Q346 A347 I348 G349 D350 A351 V352 R353 E354 G355 L356 N357 L358 R359 E360 G361 S362
D363 A364 D365 M366 Y367 V368 N369 E370 L371 L372 K373 Q374 P375 V376 R377 L378 L379 M380 Q381 V382 L383 Q384 D385 F386 Y387 T388 K389 K390 Y391 H392 A393 T394 S395 VAL LYS LEU ASP GLY LYS GLN SER ARG ASN GLU ARG PRO ASP GLU LEU S412 V413 P414 N415 L416 L417 R418 N419 A420 L421 Y422
G423 S424 M425 L426 S427 N428 I429 Y430 R431 A432 G433 L434 N435 Y436 E437 Q438 H439 R440 F441 G442 M443 D444 S445 L446 C447 K448 D449 I450 F451 T452 Y453 V454 K455 Q456 D457 R458 D459 F460 N461 T462 G463 F464 Y465 L466 R467 P468 Q469 S470 E471 S472 E473 A474 L475 R476 N477 C478 S479 I480 Y481 L482
A483 S484 Q485 V486 S487 C490 Q491 G492 S493 L494 S495 K496 F497 L498 Q499 M500 L501 L502 V503 G504 C505 G506 S507 V508 S509 I510 F511 N512 Q513 F514 V515 T516 E517 L518 A519 ARG ALA GLU ASN D524 R525 E526 K527 F528 E529 Q530 L531 I532 S533 E534 Y535 V536 A537 Y538 M539 S540 V541 G542 R543
I544 E545 S546 A547 S548 H549 W550 A551 N552 R553 C554 C555 A556 V557 V558 A559 N560 S561 P562 N563 D564 E565 K566 I567 G568 V569 F570 L571 G572 M573 V574 Q575 L576 N577 R578 K579 S580 R581 Q582 N583 M584 P585 E586 G587 Y588 K589 K590 F591 N592 I593 D594 T595 E596 N597 G598 L599 A600 K601 A602 A603
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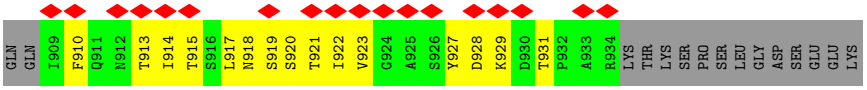
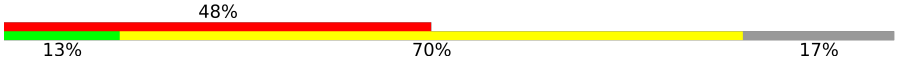
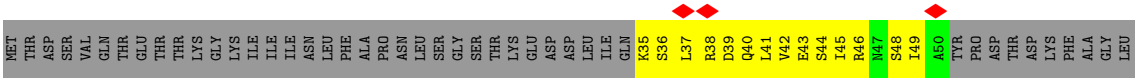
VAL ARG ALA GLU MET LYS GLY SER SER LYS SER ALA ASP ASN ASP ALA ALA VAL LEU ASP VAL ASP LEU ASP PRO LYS ASP ASP GLY VAL ILE ASP GLU SER GLN GLN ASP ASP ALA T704 E705 F706 S707 D708 A709 I710 T711 K712 V713 E714 Q715 W716 L717 K718 N719 V720 N721 E722 I723 E724
I725 G726 I727 R728 P729 S730 A731 L732 L733 I734 G735 K736 V737 W738 S739 R740 F741 Y742 F743 N744 L745 N746 N747 V748 A749 D750 Q751 H752 K753 T754 R755 L756 Y757 R758 N759 A760 E761 H762 G763 R764 M765 A766 S767 Q768 S769 N770 A771 A772 K773 I774 M775 R776 F777 N778 V779 L780 A781 F782 L783 H784
A785 V786 L787 V788 E789 E790 S791 L792 Y793 H794 S795 V796 S797 D798 R799 E800 Y801 I802 G803 E804 G805 L806 R807 L808 N809 P810 V811 T812 S813 V814 D815 E816 F817 E818 K819 K820 I821 K822 I823 I824 G825 E826 K827 L828 K829 K833 T834 W835 K836 N837 T838 H839 P840 L841 F842 F843 L844 L845 I846
S847 C848 P849 I850 L851 H852 P853 F854 I855 F856 P857 I858 G859 G860 I861 N862 C863 S864 V865 K866 A867 L868 N869 K870 E871 T872 S873 F874 N875 K876 L877 I878 D879 E880 I881 V882 G883 D884 K885 L886 L887 S888 D889 E890 E891 W892 D893 Y894 L895 T896 K897 ASN ASN ASP GLN LYS THR ASN THR ARG

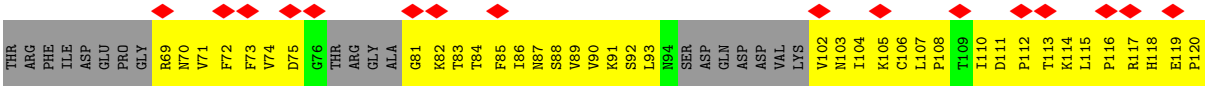


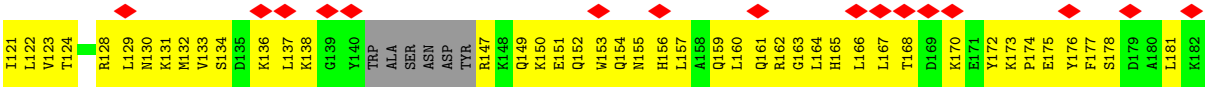
• Molecule 2: Archaeal ATPase

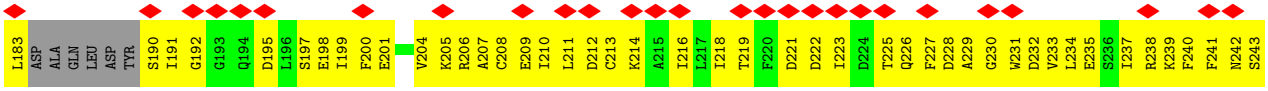
Chain O:

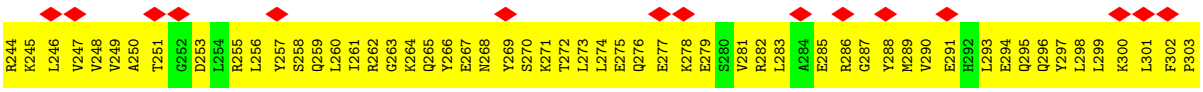


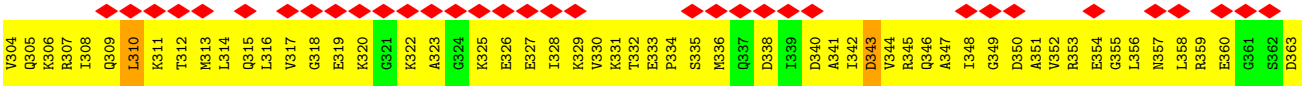


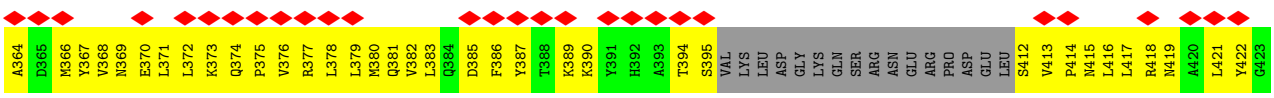








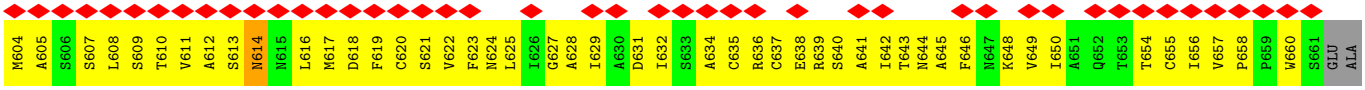


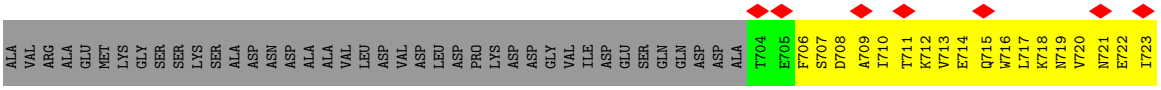


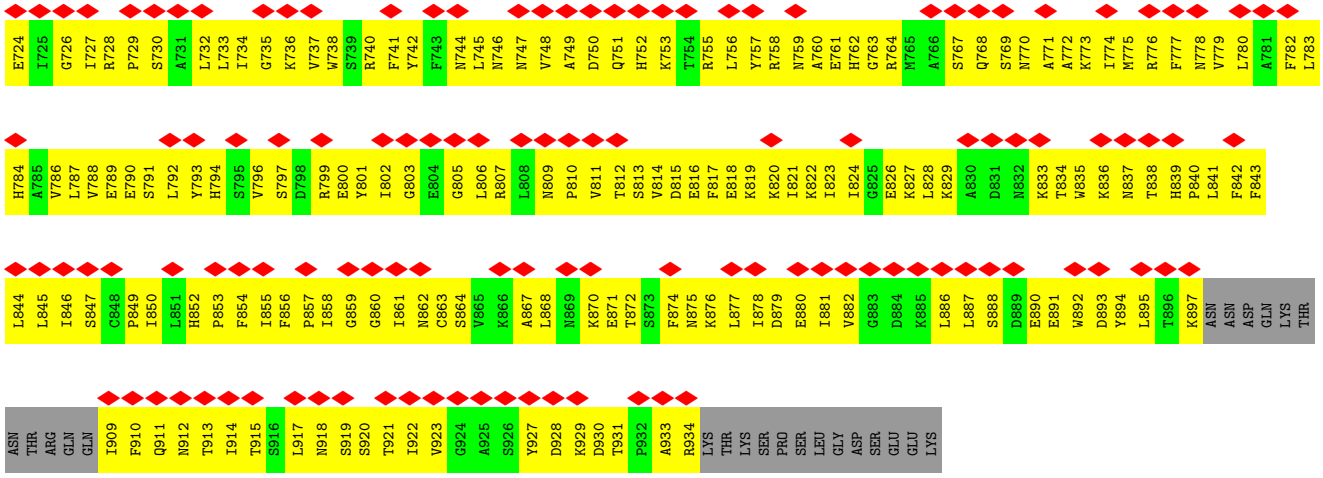






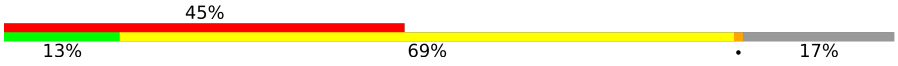


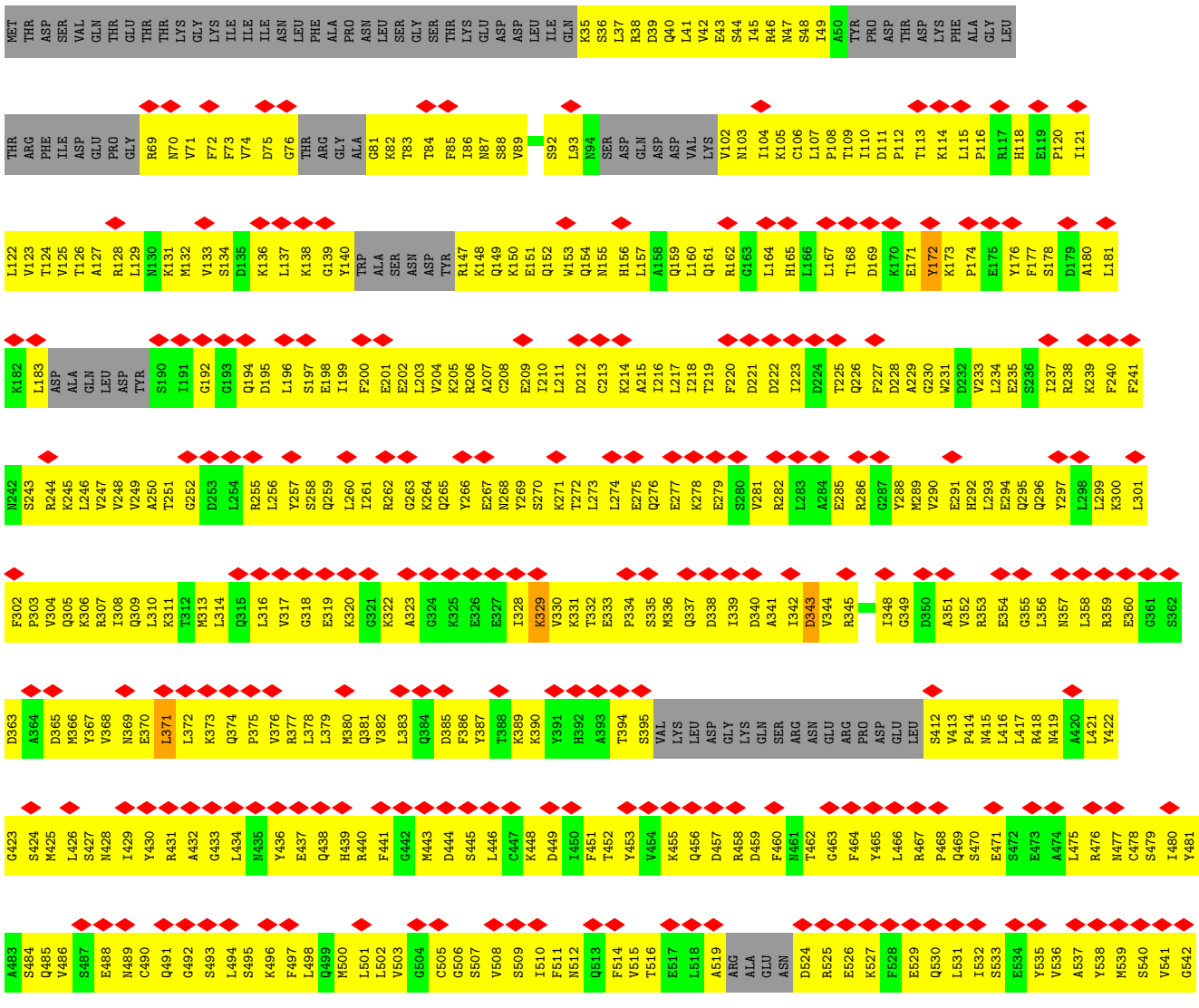


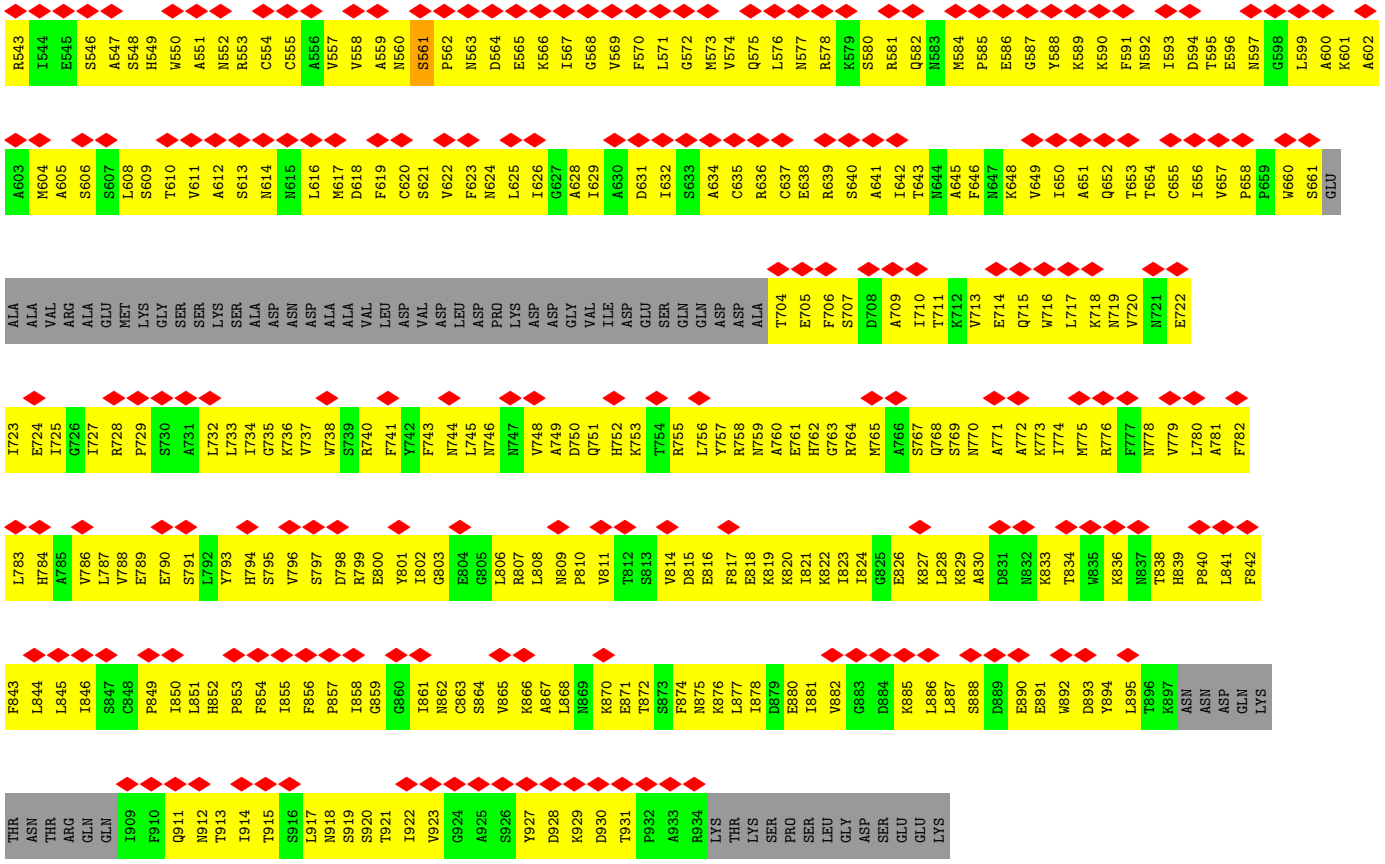


• Molecule 2: Archaeal ATPase

Chain P:

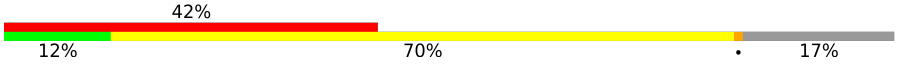


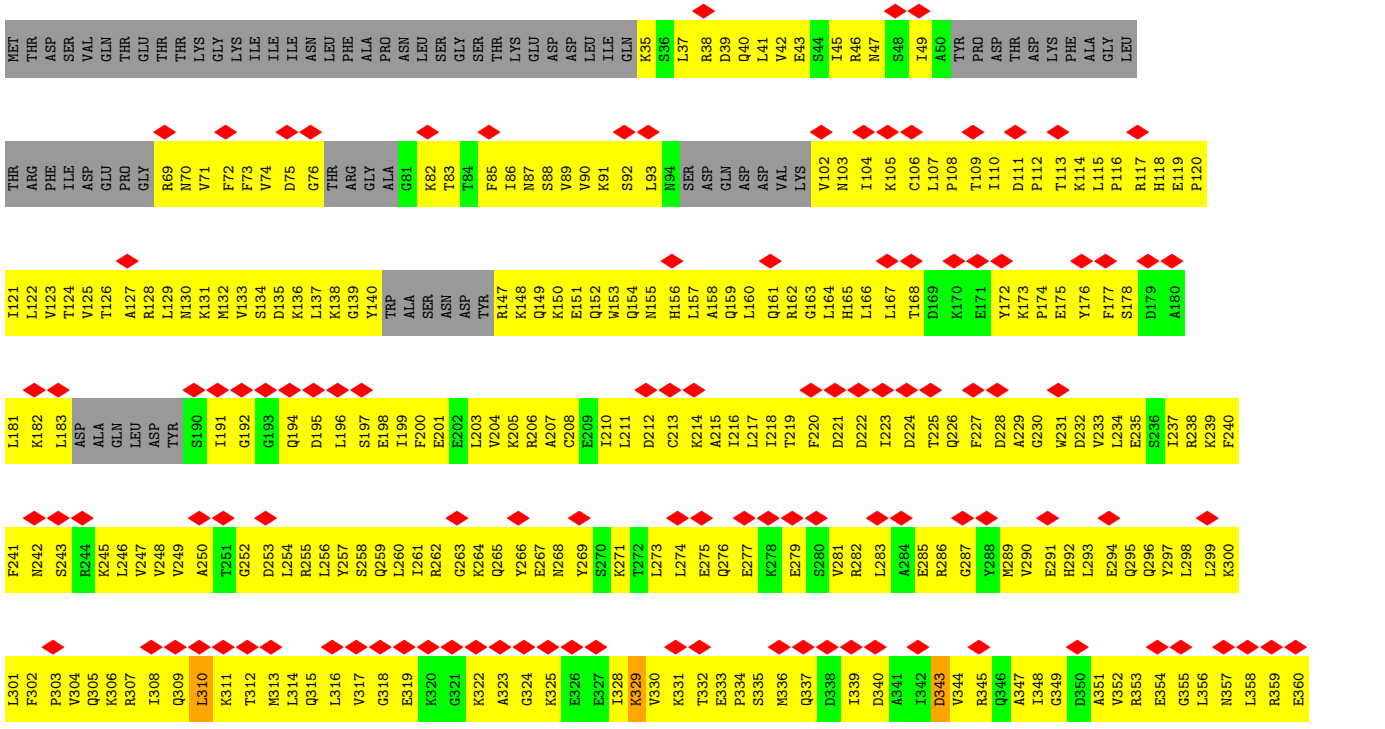


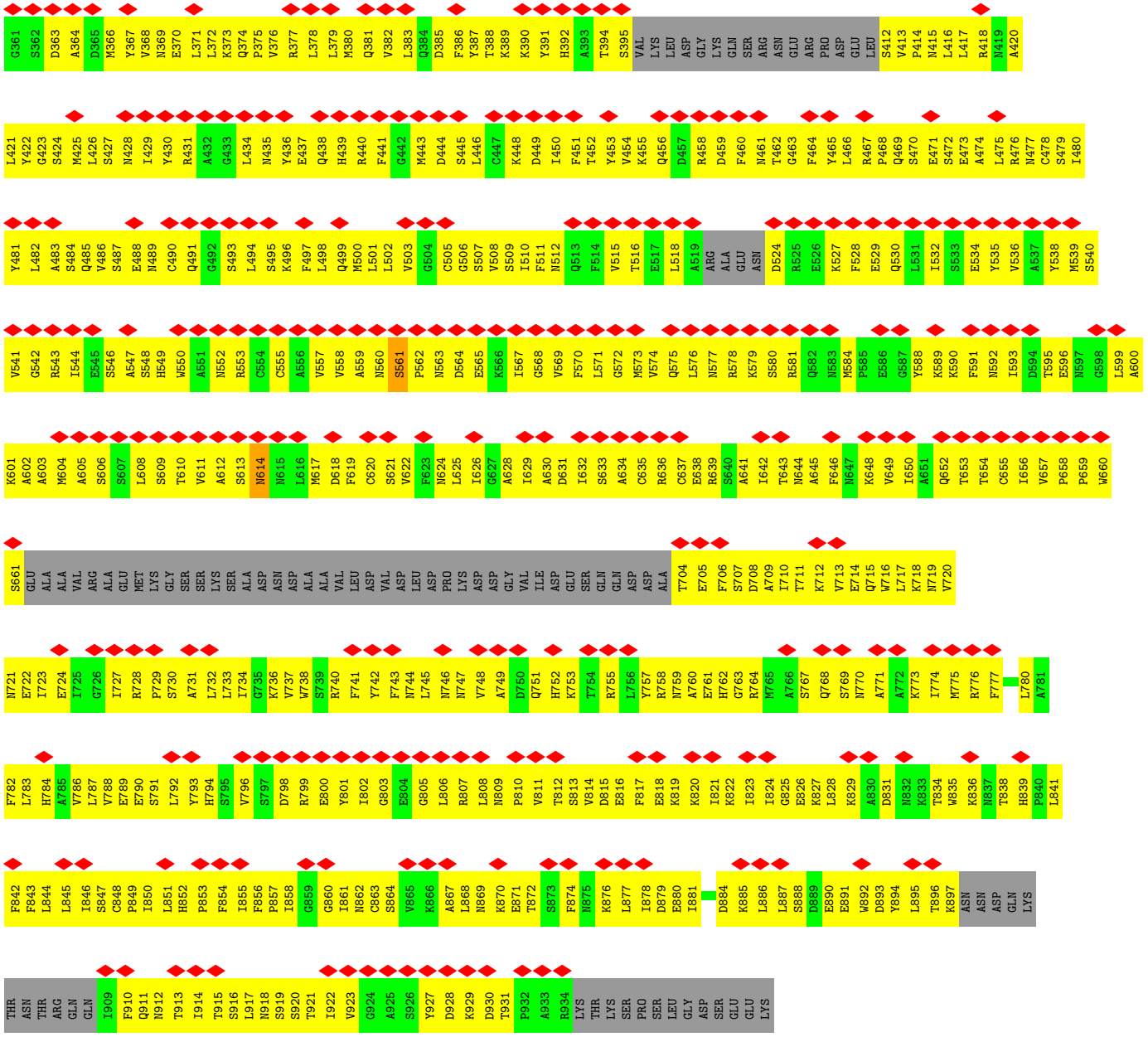


• Molecule 2: Archaeal ATPase

Chain Q:



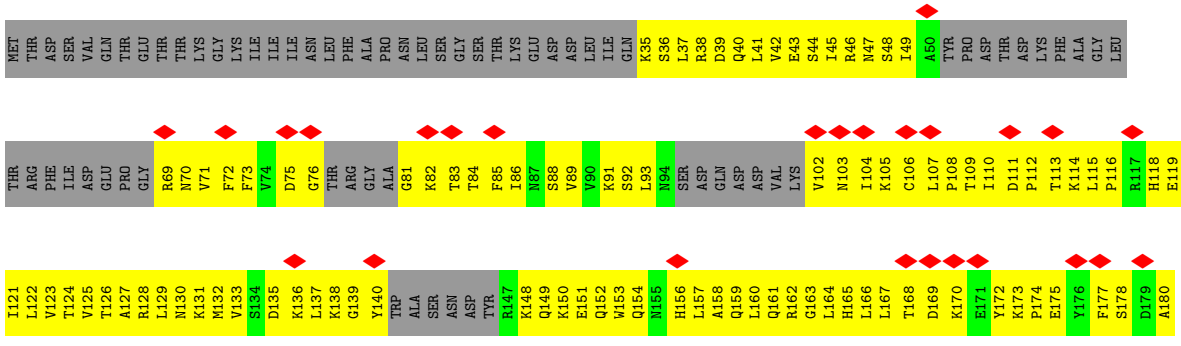


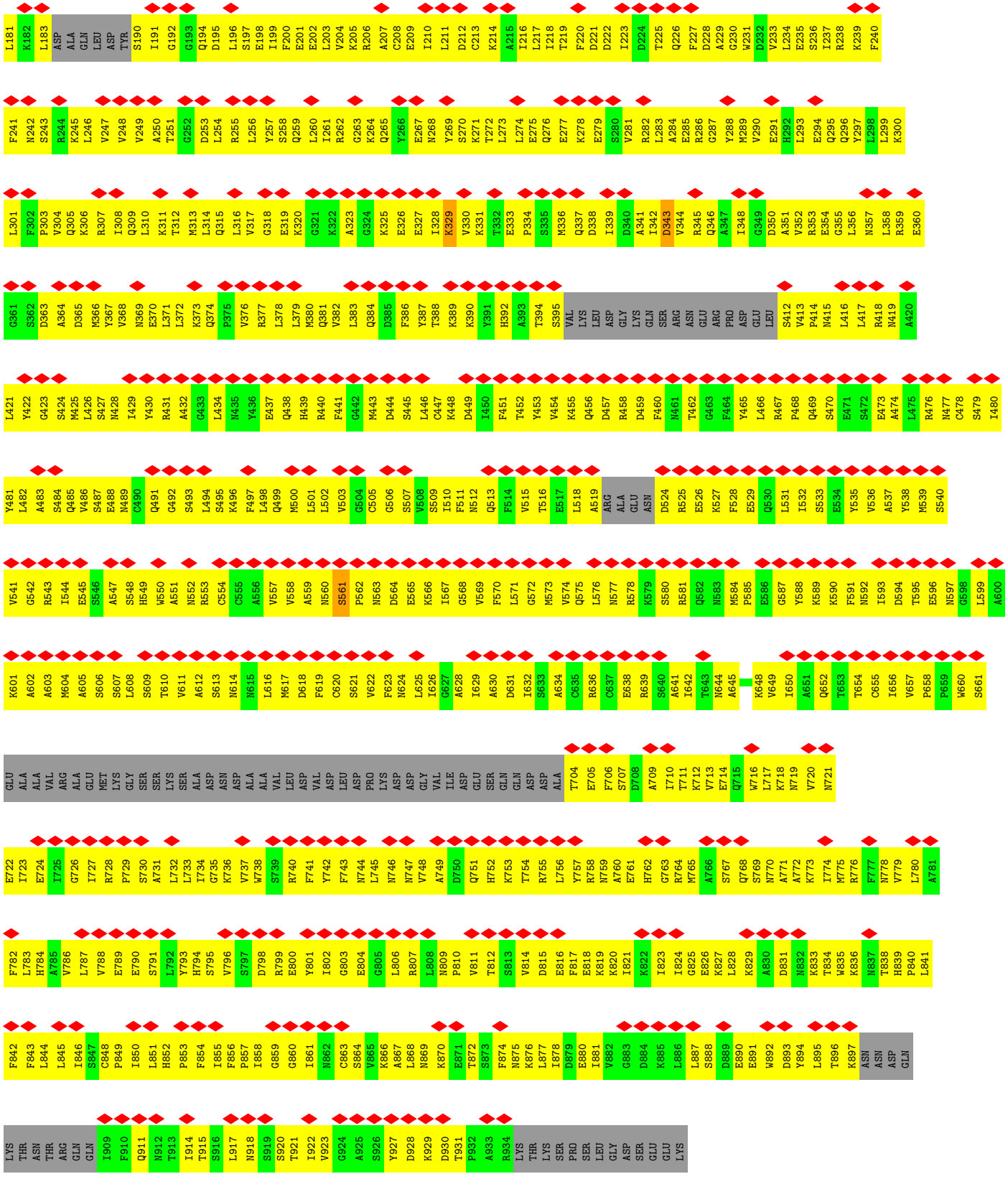


• Molecule 2: Archaeal ATPase

Chain R:

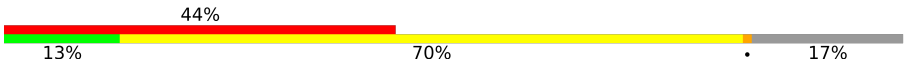


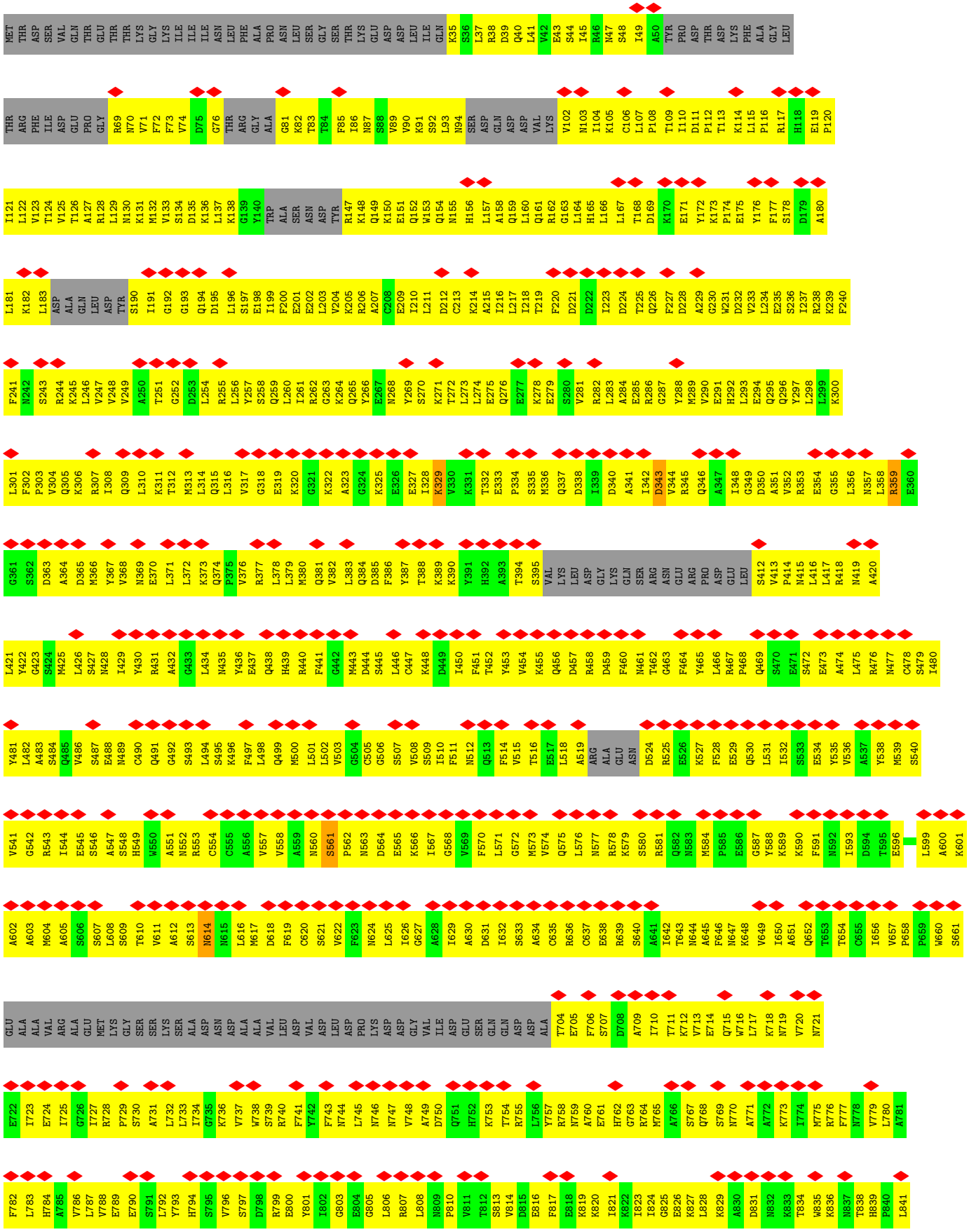




• Molecule 2: Archaeal ATPase

Chain S:

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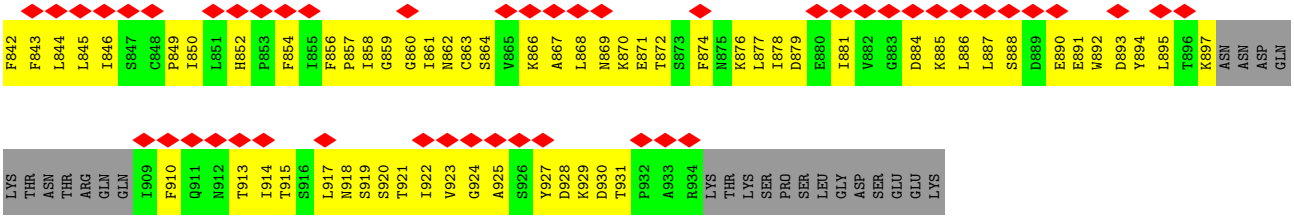
THR ARG PHE ILE ASP GLU PRO GLY R69 N70 V71 F72 F73 V74 D75 G76 THR ARG GLY ALA G81 K82 T83 T84 F85 I86 N87 S88 V89 V90 K91 S92 L93 N94 SER ASP GLN ASP ASP VAL LYS V102 N103 I104 K105 C106 L107 P108 T109 I110 D111 P112 T113 K114 L115 P116 R117 H118 E119 P120
I121 L122 V123 T124 V125 T126 A127 R128 L129 N130 K131 M132 V133 S134 D135 K136 L137 K138 G139 Y140 TRP ALA SER ASN ASP TYR R147 K148 Q149 K150 E151 Q152 W153 Q154 N155 H156 L157 A158 Q159 L160 Q161 R162 G163 L164 H165 L166 L167 T168 D169 K170 E171 Y172 K173 P174 E175 Y176 F177 S178 D179 A180
L181 K182 L183 ASP ALA GLN LEU ASP TYR S190 I191 G192 G193 Q194 D195 L196 S197 E198 I199 F200 E201 E202 L203 V204 K205 R206 A207 C208 E209 I210 L211 D212 C213 K214 A215 I216 L217 I218 T219 F220 D221 D222 I223 D224 T225 Q226 F227 D228 A229 G230 W231 D232 V233 L234 E235 S236 I237 R238 K239 F240
F241 W242 S243 R244 K245 L246 V247 V248 Y249 A250 T251 G252 D253 L254 R255 L256 Y257 S258 Q259 L260 I261 R262 G263 K264 Q265 Y266 E267 N268 Y269 S270 K271 T272 L273 L274 E275 Q276 E277 K278 E279 S280 V281 R282 L283 A284 E285 R286 G287 Y288 M289 V290 E291 H292 L293 E294 Q295 Q296 Y297 L298 L299 K300
L301 F302 P303 V304 Q305 K306 R307 I308 Q309 L310 K311 T312 M313 L314 Q315 L316 V317 G318 E319 K320 G321 K322 A323 G324 K325 E326 E327 I328 K329 V330 K331 T332 E333 P334 S335 M336 Q337 D338 I339 D340 A341 I342 D343 V344 R345 Q346 A347 I348 G349 D350 A351 V352 R353 E354 G355 L356 N357 L358 R359 E360
G361 S362 D363 A364 D365 M366 Y367 V368 N369 E370 L371 L372 K373 Q374 P375 V376 R377 L378 L379 M380 Q381 V382 L383 Q384 D385 F386 Y387 T388 K389 K390 Y391 H392 A393 T394 S395 VAL LYS LEU ASP GLY LYS GLN SER ARG ASN GLU ARG PRO ASP GLU LEU S412 V413 P414 N415 L416 L417 R418 N419 A420
L421 Y422 G423 S424 M425 L426 S427 N428 I429 Y430 R431 A432 G433 L434 N435 Y436 E437 Q438 H439 M440 F441 G442 M443 D444 S445 L446 C447 K448 D449 I450 F451 T452 Y453 V454 K455 Q456 D457 R458 D459 F460 N461 T462 G463 F464 Y465 L466 R467 P468 Q469 S470 E471 S472 E473 A474 L475 R476 N477 C478 S479 I480
Y481 L482 A483 S484 Q485 V486 S487 E488 N489 C490 Q491 G492 S493 L494 S495 K496 F497 L498 Q499 M500 L501 L502 V503 G504 C505 G506 S507 V508 S509 I510 F511 N512 Q513 F514 V515 T516 E517 L518 A519 ARG ALA GLU ASN D524 R525 E526 K527 F528 E529 Q530 L531 I532 S533 E534 Y535 V536 A537 Y538 M539 S540
V541 G542 R543 I544 E545 S546 A547 S548 H549 W550 A551 N552 R553 C554 C555 A556 V557 V558 A559 N560 S561 P562 N563 D564 E565 K566 I567 G568 V569 F570 L571 G572 M573 V574 Q575 L576 N577 R578 K579 S580 R581 Q582 N583 M584 P585 E586 G587 Y588 K589 K590 F591 N592 I593 D594 T595 E596 L599 A600 K601
A602 A603 M604 A605 S606 S607 L608 S609 T610 V611 A612 S613 N614 N615 L616 M617 D618 F619 C620 S621 V622 F623 N624 L625 I626 G627 A628 I629 A630 D631 I632 S633 A634 C635 R636 C637 E638 R639 S640 A641 I642 T643 N644 A645 F646 N647 K648 V649 I650 A651 Q652 T653 T654 C655 I656 V657 P658 P659 W660 S661
GLU ALA ALA VAL ARG ALA GLU MET LYS GLY SER SER LYS SER ALA ASP ASN ASP ALA ALA VAL LEU ASP VAL ASP LEU ASP PRO LYS ASP ASP GLY VAL ILE ASP GLU SER GLN GLN ASP ASP ALA T704 E705 F706 S707 D708 A709 I710 T711 K712 V713 E714 Q715 W716 L717 K718 N719 V720 N721
E722 I723 E724 I725 G726 I727 R728 P729 S730 A731 L732 L733 I734 G735 K736 V737 W738 S739 R740 F741 Y742 F743 N744 L745 N746 N747 V748 A749 D750 Q751 H752 K753 T754 R755 L756 Y757 R758 N759 A760 E761 H762 G763 R764 M765 A766 S767 Q768 S769 N770 A771 A772 K773 I774 M775 R776 F777 N778 V779 L780 A781
F782 L783 H784 A785 V786 L787 V788 E789 E790 S791 L792 Y793 H794 S795 V796 S797 D798 R799 E800 Y801 I802 G803 E804 G805 L806 R807 L808 N809 P810 V811 T812 S813 V814 D815 E816 F817 E818 K819 K820 I821 K822 I823 I824 G825 E826 K827 L828 K829 A830 D831 N832 K833 T834 W835 K836 N837 T838 H839 P840 L841


F842 F843 L844 L845 I846 S847 C848 P849 I850 L851 H852 P853 F854 I855 F856 P857 I858 G859 G860 I861 N862 C863 S864 V865 K866 A867 L868 N869 K870 E871 T872 S873 F874 N875 K876 L877 I878 D879 E880 I881 V882 G883 D884 K885 L886 L887 S888 D889 E890 E891 W892 D893 Y894 L895 T896 K897 ASN ASN ASP GLN
LYS THR ASN THR ARG GLN GLN I909 F910 Q911 N912 T913 I914 T915 S916 L917 N918 S919 S920 T921 I922 V923 G924 A925 S926 Y927 D928 K929 D930 T931 P932 A933 R934 LYS THR LYS SER PRO SER LEU GLY ASP SER GLU GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.256	Depositor
Minimum map value	-3.896	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.303	Depositor
Recommended contour level	1.9	Depositor
Map size (Å)	659.9987, 659.9987, 659.9987	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.57812, 2.57812, 2.57812	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.22	0/6400	0.57	12/8672 (0.1%)
1	B	0.22	0/6400	0.51	8/8672 (0.1%)
1	C	0.26	0/6400	0.59	12/8672 (0.1%)
1	D	0.29	1/6375 (0.0%)	0.58	12/8637 (0.1%)
1	E	0.24	0/6400	0.56	8/8672 (0.1%)
1	F	0.23	0/6400	0.56	11/8672 (0.1%)
1	G	0.23	0/6400	0.51	4/8672 (0.0%)
1	H	0.24	0/6400	0.63	15/8672 (0.2%)
1	I	0.25	0/6400	0.57	9/8672 (0.1%)
1	J	0.24	0/6400	0.52	7/8672 (0.1%)
1	K	0.26	0/6400	0.59	10/8672 (0.1%)
1	L	0.23	0/6400	0.63	16/8672 (0.2%)
2	M	0.22	0/6379	0.52	2/8592 (0.0%)
2	N	0.23	0/6379	0.55	0/8592
2	O	0.21	0/6379	0.51	0/8592
2	P	0.22	0/6379	0.52	3/8592 (0.0%)
2	Q	0.22	0/6379	0.52	0/8592
2	R	0.22	0/6379	0.51	0/8592
2	S	0.23	0/6379	0.52	0/8592
All	All	0.23	1/121428 (0.0%)	0.55	129/164173 (0.1%)

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	C	0	1
1	E	0	1
1	H	0	2
1	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
1	K	0	1
1	L	0	1
2	N	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	45	PRO	CG-CD	-5.27	1.32	1.50

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	647	THR	CA-C-N	15.00	152.82	121.17
1	H	647	THR	C-N-CA	15.00	152.82	121.17
1	L	492	ILE	CA-C-N	12.14	138.85	121.50
1	L	492	ILE	C-N-CA	12.14	138.85	121.50
1	B	354	GLU	CA-C-N	10.86	142.69	121.41

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	290	ARG	Sidechain
1	E	568	ARG	Sidechain
1	H	540	ILE	Peptide
1	H	575	ARG	Sidechain
1	I	177	ARG	Sidechain

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	A	6245	0	6229	277	0
1	B	6245	0	6229	281	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6245	0	6229	334	0
1	D	6221	0	6209	361	0
1	E	6245	0	6229	356	0
1	F	6245	0	6229	299	0
1	G	6245	0	6229	329	0
1	H	6245	0	6229	294	0
1	I	6245	0	6229	345	0
1	J	6245	0	6229	296	0
1	K	6245	0	6229	349	0
1	L	6245	0	6229	329	0
2	M	6277	0	6328	1447	0
2	N	6277	0	6328	1555	0
2	O	6277	0	6328	1453	0
2	P	6277	0	6328	1458	0
2	Q	6277	0	6328	1471	0
2	R	6277	0	6328	1489	0
2	S	6277	0	6328	1478	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
All	All	118867	0	119024	13670	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 57.

The worst 5 of 13670 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:173:LYS:NZ	2:S:175:GLU:HG3	1.07	1.40
2:P:751:GLN:OE1	2:P:811:VAL:CG1	1.70	1.38
2:M:751:GLN:OE1	2:M:811:VAL:CG1	1.69	1.38
2:R:751:GLN:OE1	2:R:811:VAL:CG1	1.76	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:751:GLN:OE1	2:O:811:VAL:CG1	1.73	1.33

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	A	762/799 (95%)	697 (92%)	61 (8%)	4 (0%)	24	63
1	B	762/799 (95%)	706 (93%)	51 (7%)	5 (1%)	18	56
1	C	762/799 (95%)	697 (92%)	60 (8%)	5 (1%)	18	56
1	D	757/799 (95%)	688 (91%)	64 (8%)	5 (1%)	18	56
1	E	762/799 (95%)	693 (91%)	65 (8%)	4 (0%)	24	63
1	F	762/799 (95%)	693 (91%)	64 (8%)	5 (1%)	18	56
1	G	762/799 (95%)	690 (91%)	67 (9%)	5 (1%)	18	56
1	H	762/799 (95%)	692 (91%)	65 (8%)	5 (1%)	18	56
1	I	762/799 (95%)	704 (92%)	53 (7%)	5 (1%)	18	56
1	J	762/799 (95%)	696 (91%)	61 (8%)	5 (1%)	18	56
1	K	762/799 (95%)	690 (91%)	66 (9%)	6 (1%)	16	54
1	L	762/799 (95%)	697 (92%)	60 (8%)	5 (1%)	18	56
2	M	766/947 (81%)	704 (92%)	58 (8%)	4 (0%)	24	63
2	N	766/947 (81%)	695 (91%)	66 (9%)	5 (1%)	18	56
2	O	766/947 (81%)	704 (92%)	58 (8%)	4 (0%)	24	63
2	P	766/947 (81%)	680 (89%)	82 (11%)	4 (0%)	24	63
2	Q	766/947 (81%)	698 (91%)	63 (8%)	5 (1%)	18	56
2	R	766/947 (81%)	706 (92%)	56 (7%)	4 (0%)	24	63
2	S	766/947 (81%)	700 (91%)	61 (8%)	5 (1%)	18	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	14501/16217 (89%)	13230 (91%)	1181 (8%)	90 (1%)	23 59

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	B	23	VAL
1	C	23	VAL
1	D	23	VAL
1	E	23	VAL

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

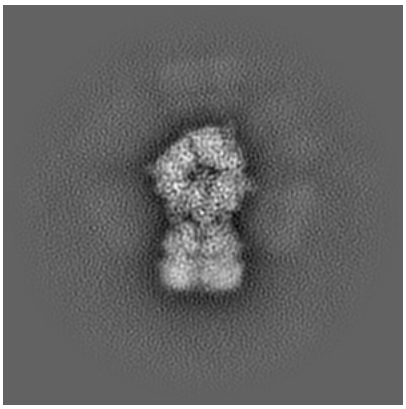
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29328. These allow visual inspection of the internal detail of the map and identification of artifacts.

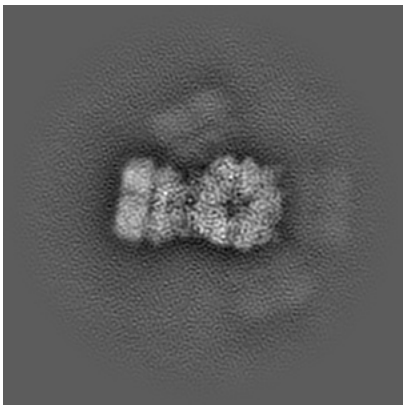
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

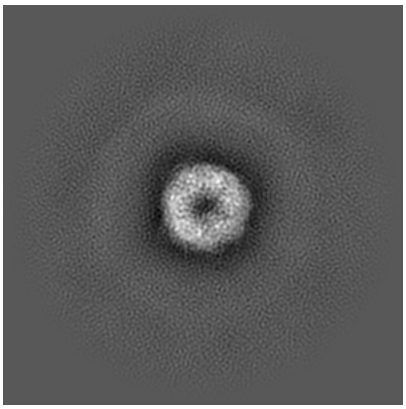
6.1.1 Primary map



X

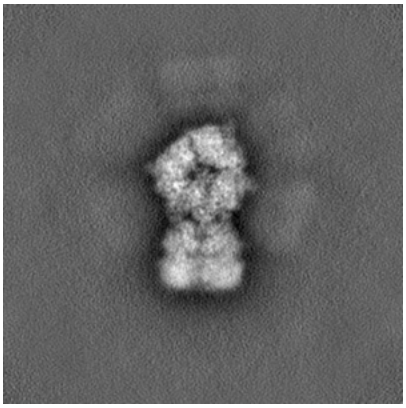


Y

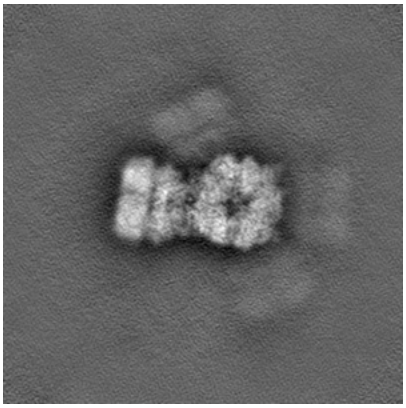


Z

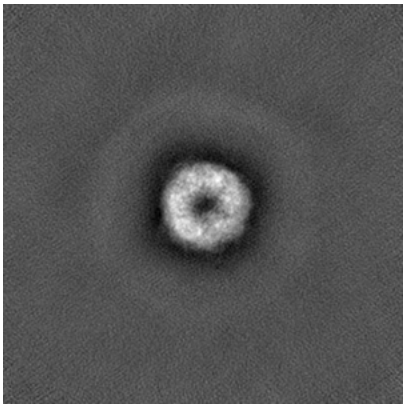
6.1.2 Raw map



X



Y

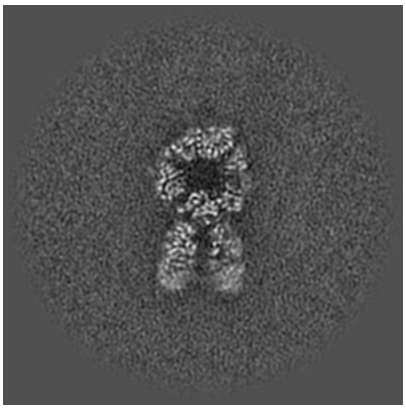


Z

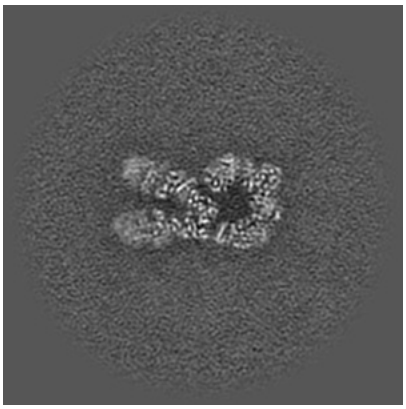
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

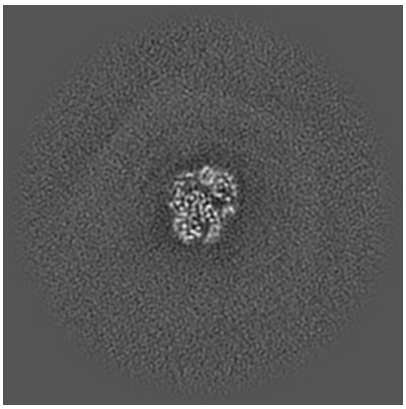
6.2.1 Primary map



X Index: 128

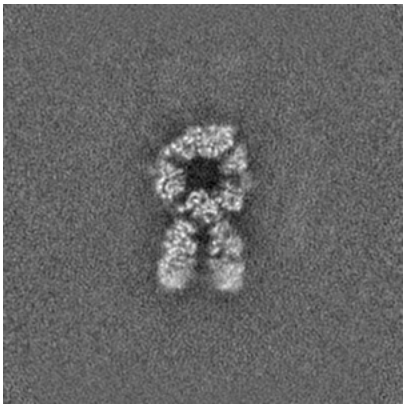


Y Index: 128

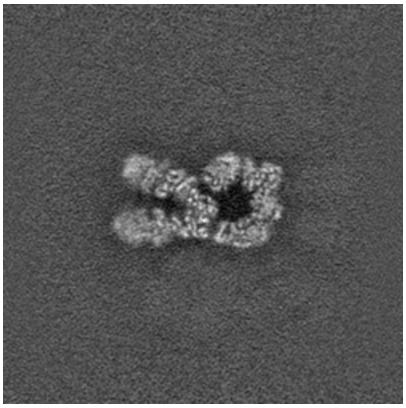


Z Index: 128

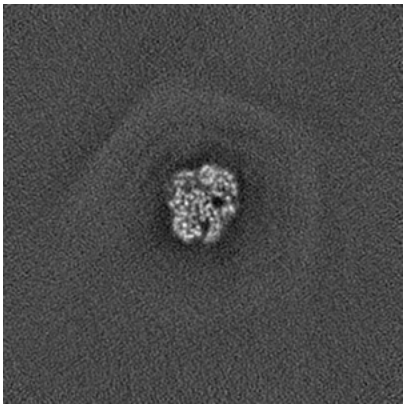
6.2.2 Raw map



X Index: 128



Y Index: 128

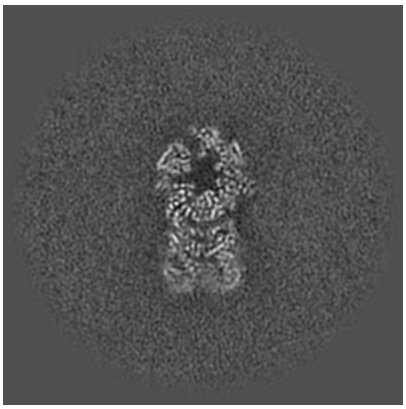


Z Index: 128

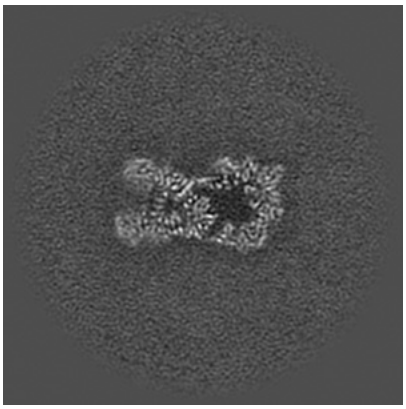
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

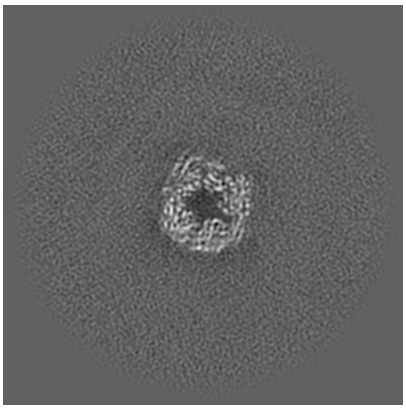
6.3.1 Primary map



X Index: 121

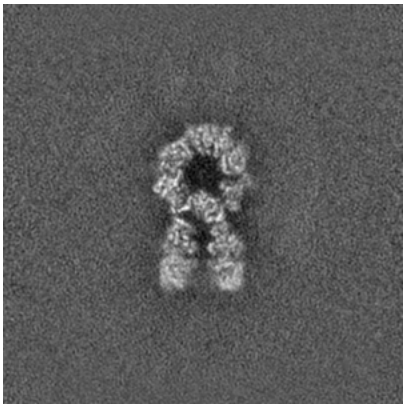


Y Index: 131

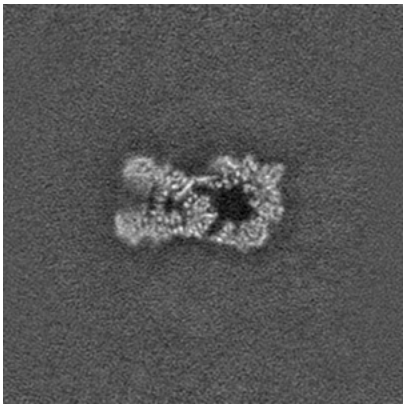


Z Index: 141

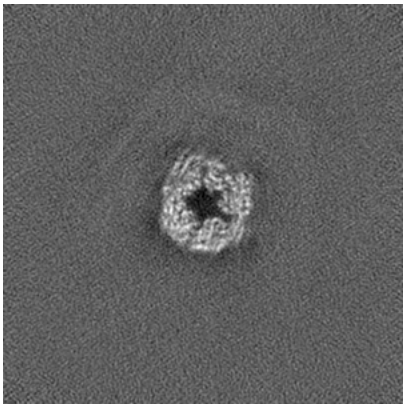
6.3.2 Raw map



X Index: 126



Y Index: 131

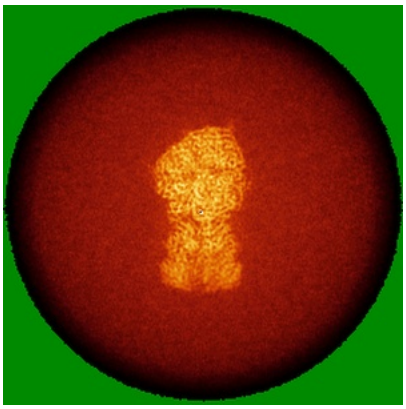


Z Index: 141

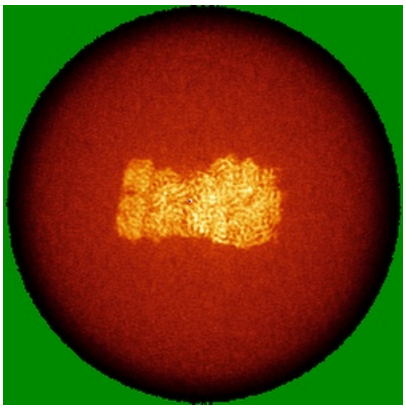
The images above show the largest variance slices of the map in three orthogonal directions.

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

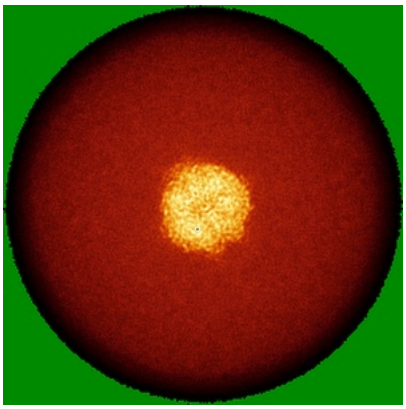
6.4.1 Primary map



X

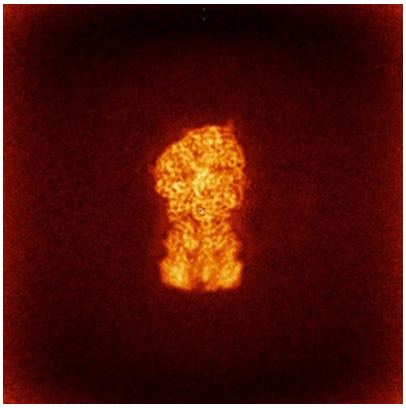


Y

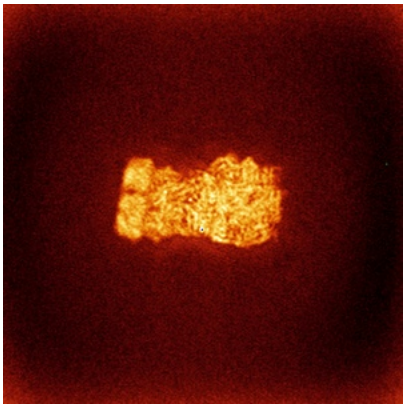


Z

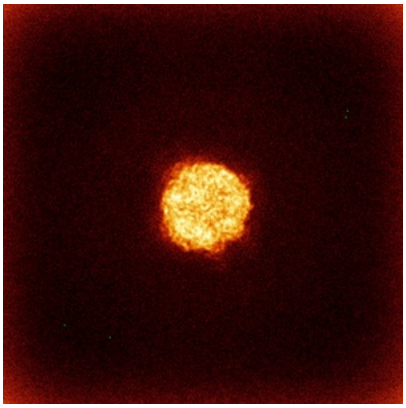
6.4.2 Raw map



X



Y



Z

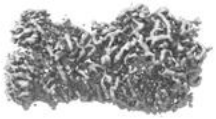
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 1.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

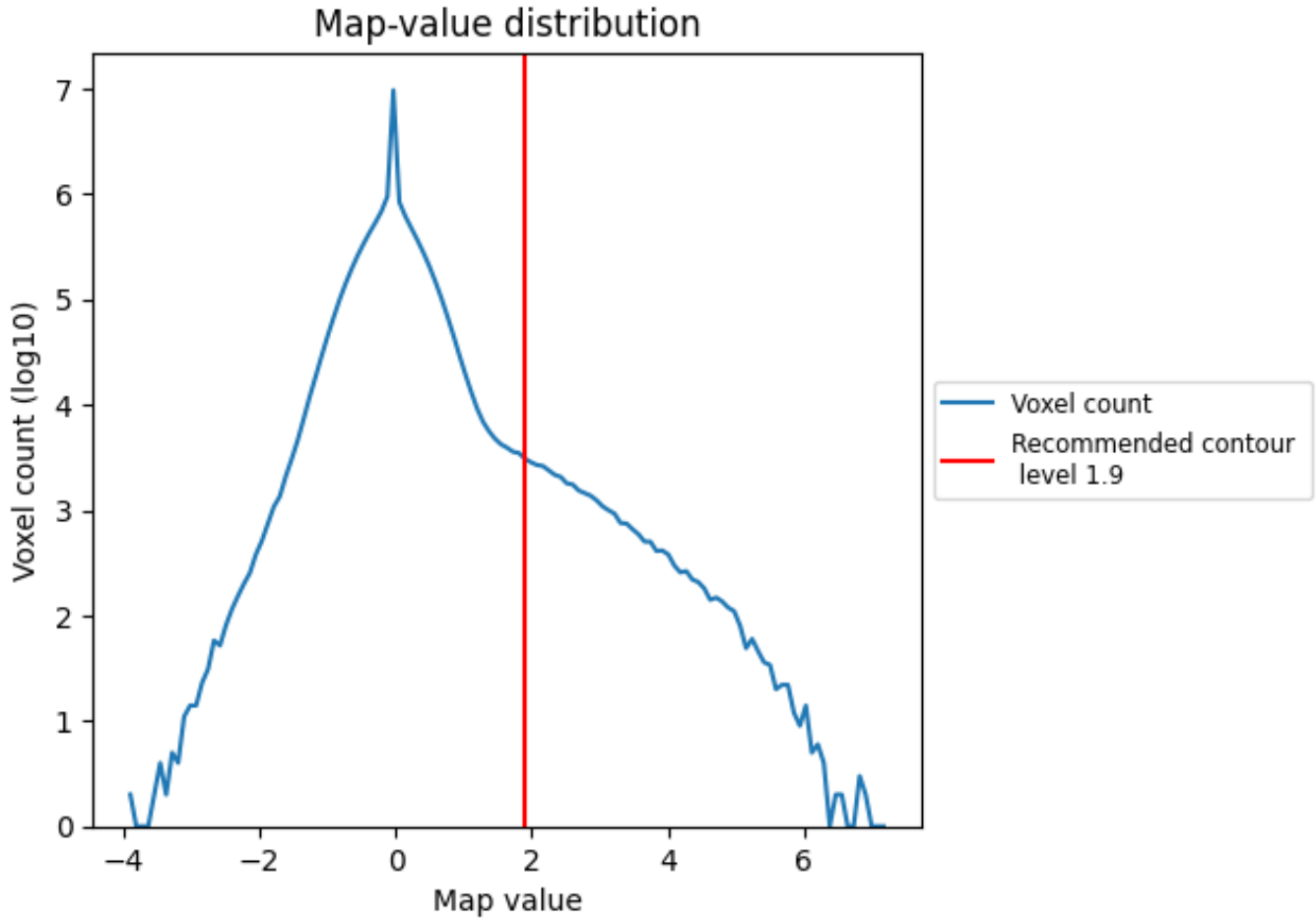
6.6 Mask visualisation (i)

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

7 Map analysis

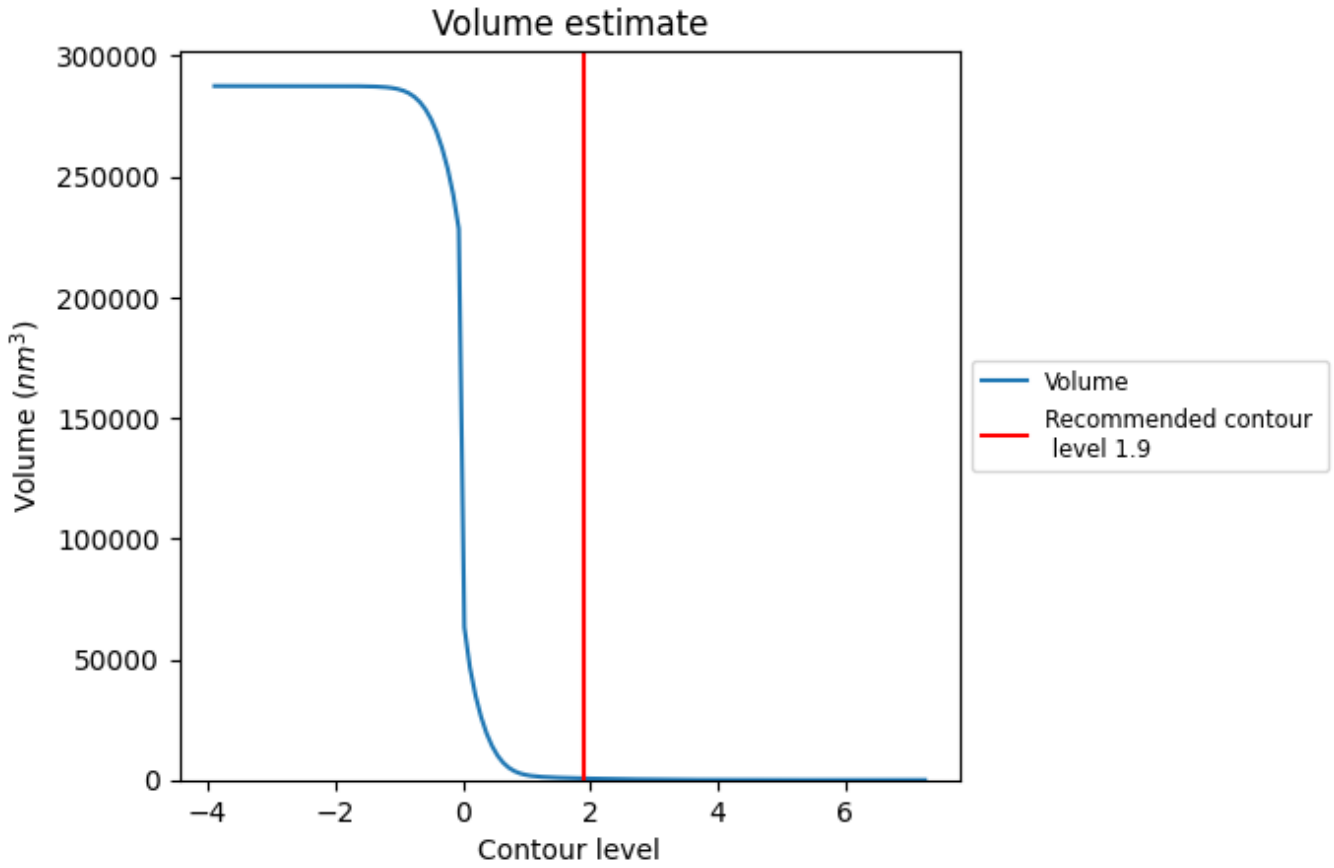
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

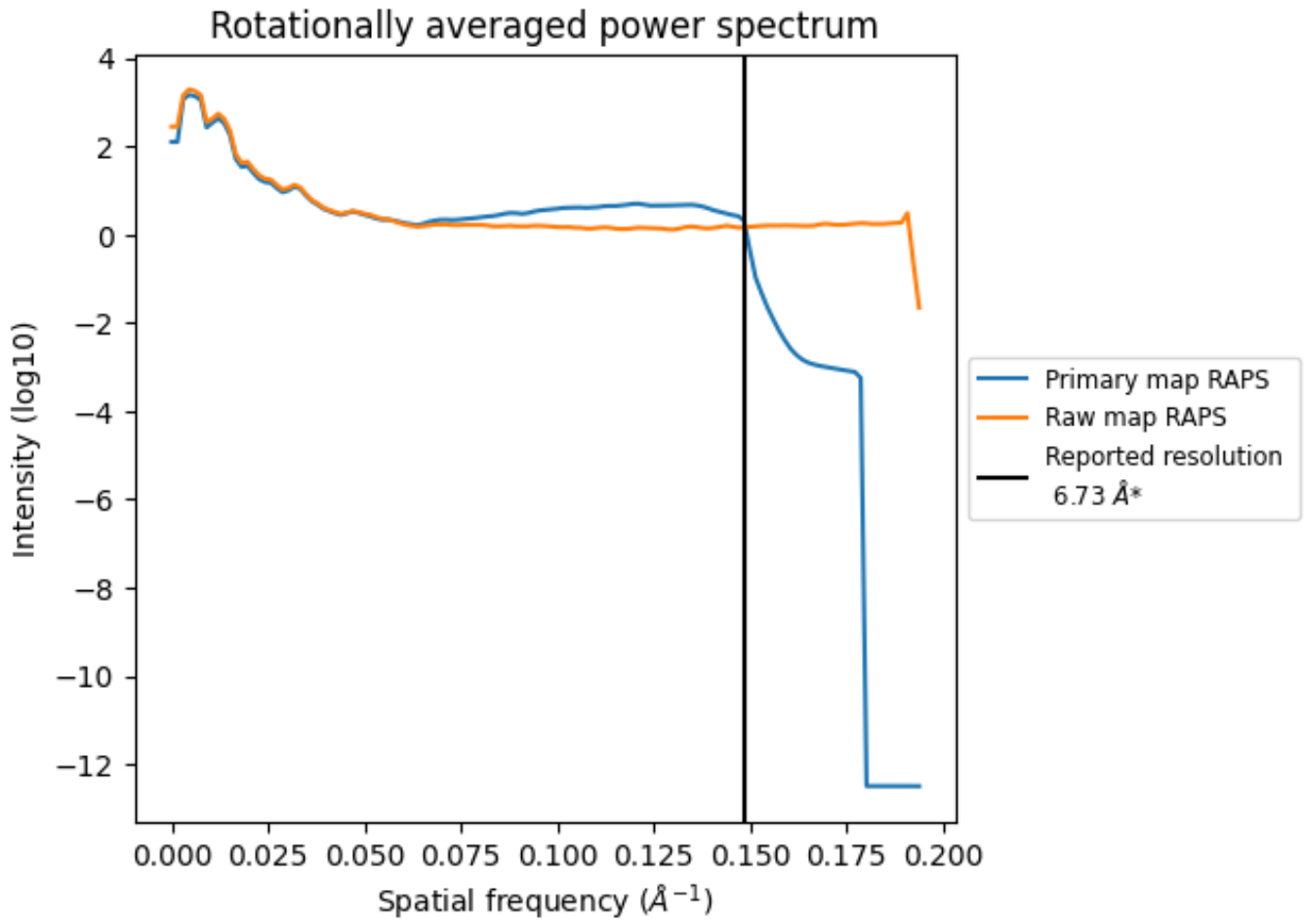
7.2 Volume estimate (i)



The volume at the recommended contour level is 643 nm^3; this corresponds to an approximate mass of 581 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)

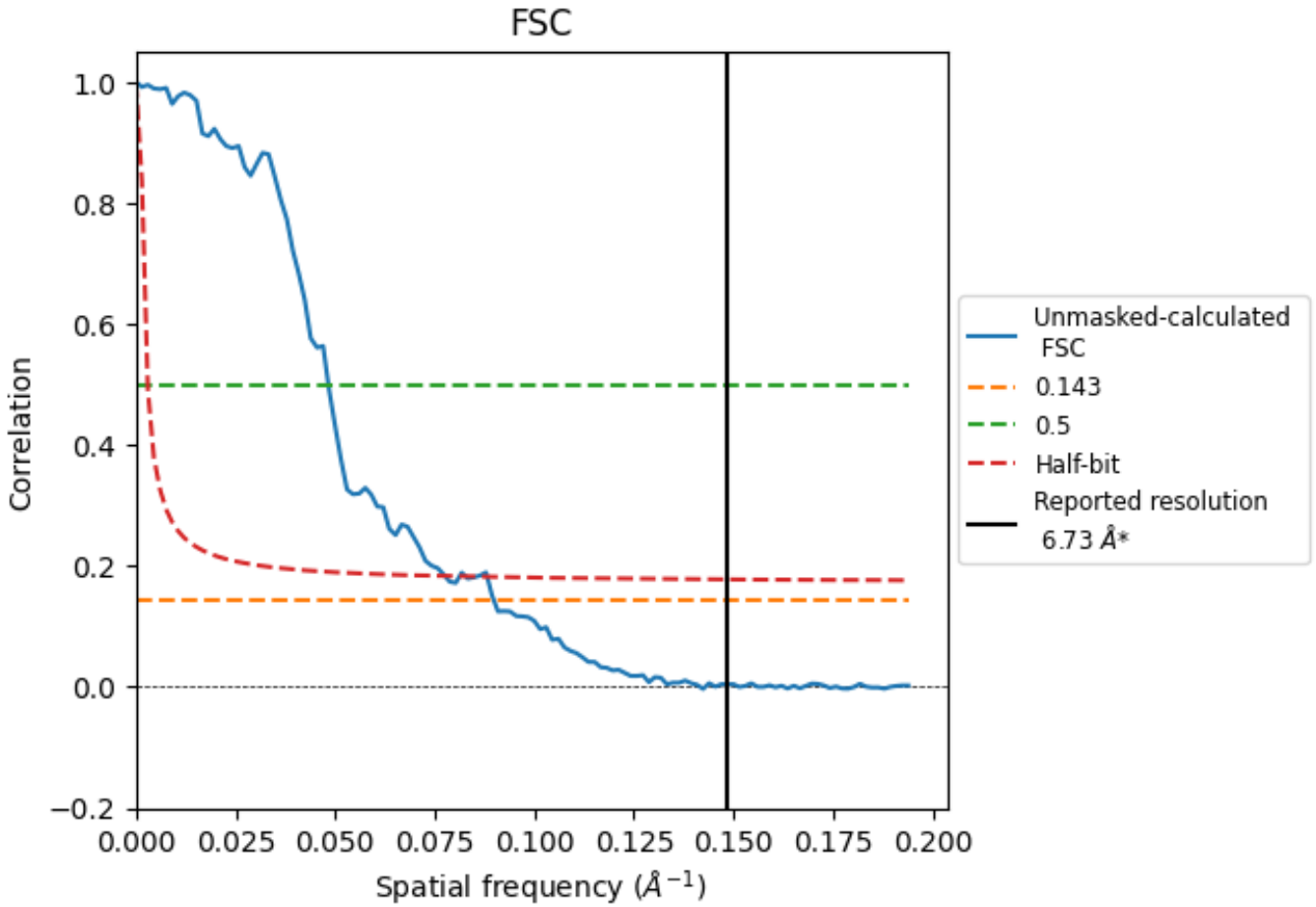


*Reported resolution corresponds to spatial frequency of 0.149 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.149 Å^{-1}

8.2 Resolution estimates (i)

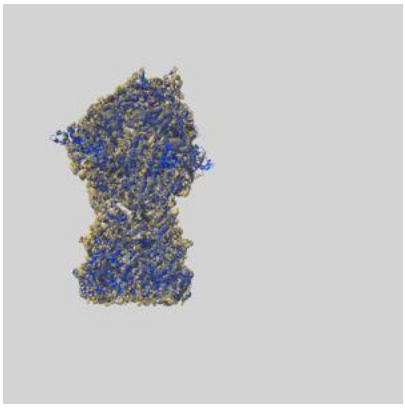
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	11.12	20.70	12.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 11.12 differs from the reported value 6.73 by more than 10 %

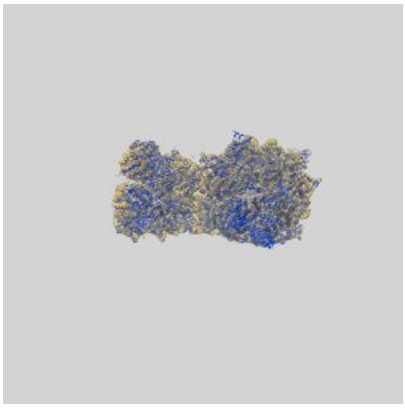
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29328 and PDB model 8FNW. Per-residue inclusion information can be found in section 3 on page 8.

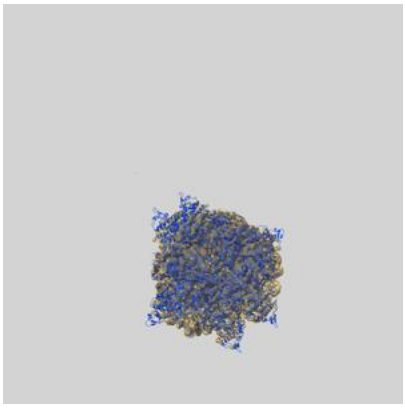
9.1 Map-model overlay



X



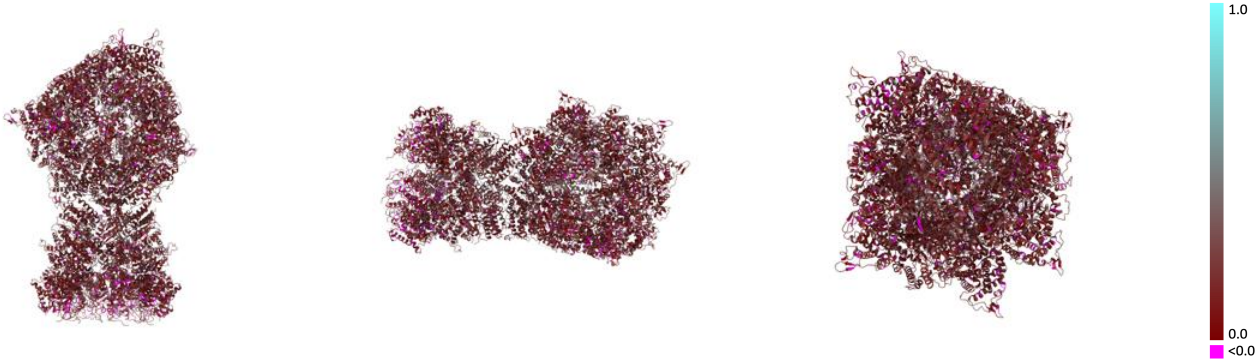
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.9 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.

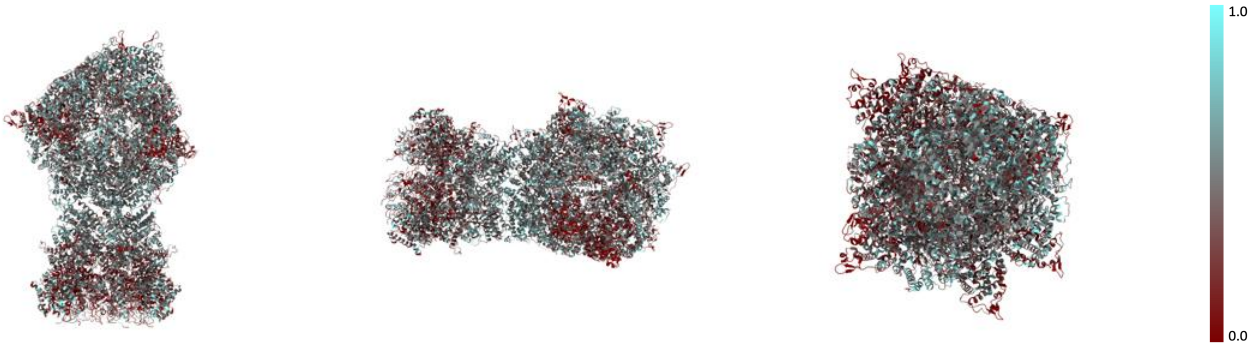
9.2 Q-score mapped to coordinate model



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.

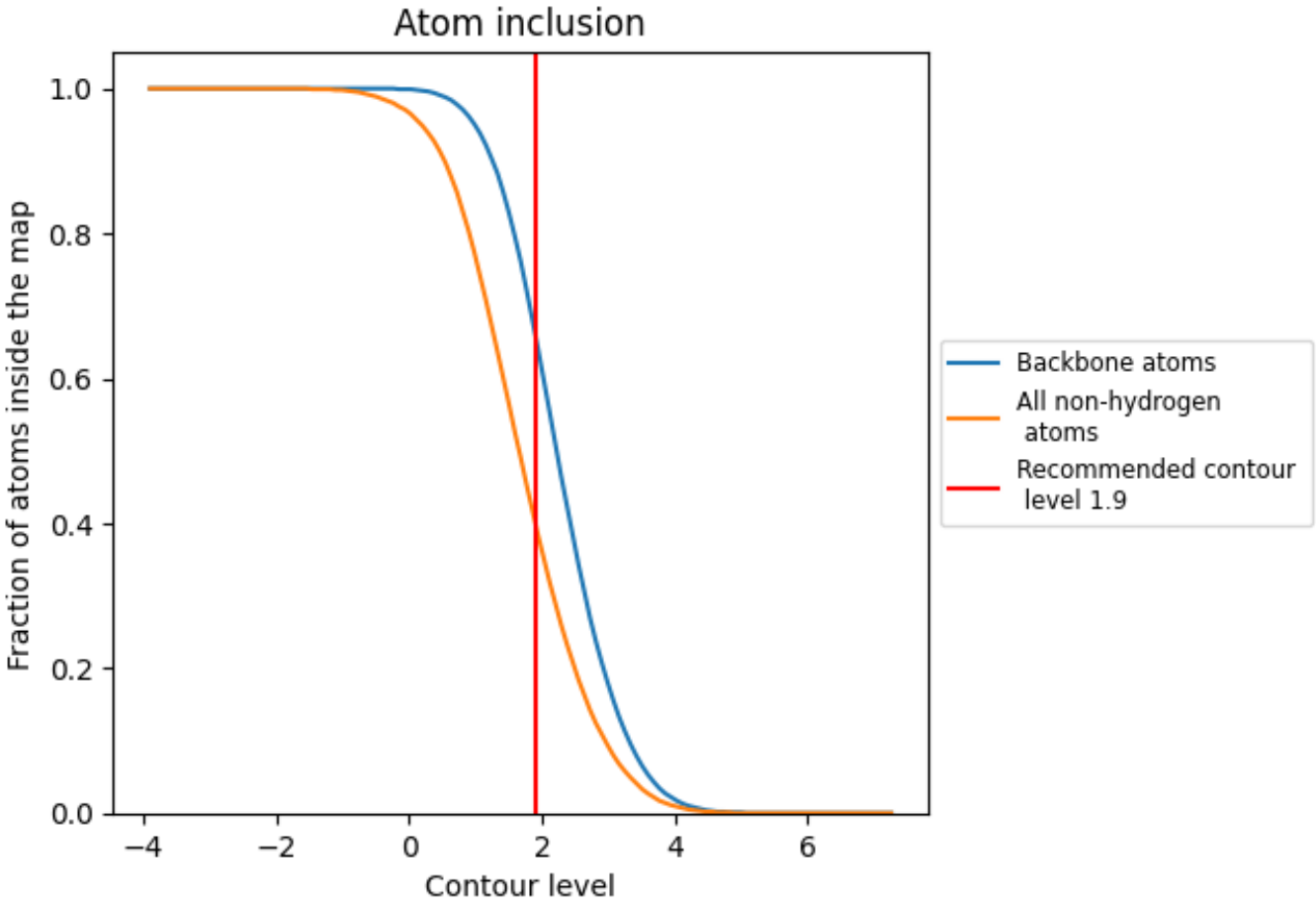
9.3 Atom inclusion mapped to coordinate model



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).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4000	0.1870
A	0.3030	0.1790
B	0.3440	0.1840
C	0.5370	0.1950
D	0.5220	0.2000
E	0.3900	0.1880
F	0.4130	0.1900
G	0.4080	0.1880
H	0.4500	0.1930
I	0.4540	0.1920
J	0.4250	0.1920
K	0.4540	0.1920
L	0.3170	0.1890
M	0.3820	0.1870
N	0.3940	0.1850
O	0.3420	0.1760
P	0.3700	0.1820
Q	0.3830	0.1820
R	0.3470	0.1820
S	0.3680	0.1830

