wwPDB EM Validation Summary Report (i)

Nov 15, 2022 – 01:42 AM JST

PDB ID	:	6JPU
EMDB ID	:	EMD-9871
Title	:	CryoEM structure of Abo1 hexamer - apo complex
Authors	:	Cho, C.; Jang, J.; Song, J.J.
Deposited on	:	2019-03-28
Resolution	:	4.27 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:

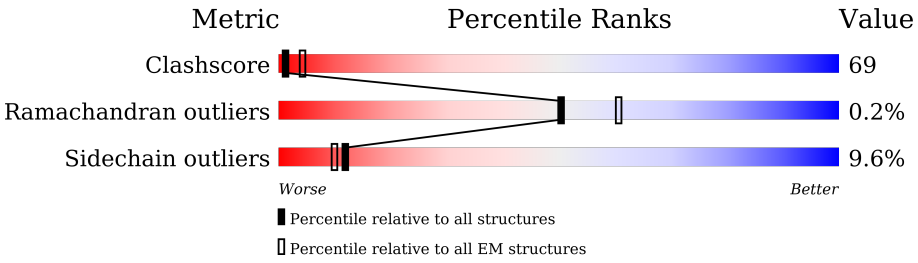
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.27 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1198	15% 10% 35% • 52%
1	B	1198	17% 10% 35% • 52%
1	C	1198	15% 11% 34% • 52%
1	D	1198	14% 10% 35% • 52%
1	E	1198	17% 11% 35% • 52%
1	F	1198	14% 10% 35% • 52%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 30378 atoms, of which 2610 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 Uncharacterized AAA domain-containing protein C31G5.19.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	577	Total	C	H	N	O	S	0	0
			5063	2963	435	789	854	22		
1	B	577	Total	C	H	N	O	S	0	0
			5063	2963	435	789	854	22		
1	C	577	Total	C	H	N	O	S	0	0
			5063	2963	435	789	854	22		
1	D	577	Total	C	H	N	O	S	0	0
			5063	2963	435	789	854	22		
1	E	577	Total	C	H	N	O	S	0	0
			5063	2963	435	789	854	22		
1	F	577	Total	C	H	N	O	S	0	0
			5063	2963	435	789	854	22		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP O14114
A	-6	ALA	-	expression tag	UNP O14114
A	-5	MET	-	expression tag	UNP O14114
A	-4	GLY	-	expression tag	UNP O14114
A	-3	SER	-	expression tag	UNP O14114
A	-2	GLY	-	expression tag	UNP O14114
A	-1	ILE	-	expression tag	UNP O14114
A	0	GLN	-	expression tag	UNP O14114
B	-7	GLY	-	expression tag	UNP O14114
B	-6	ALA	-	expression tag	UNP O14114
B	-5	MET	-	expression tag	UNP O14114
B	-4	GLY	-	expression tag	UNP O14114
B	-3	SER	-	expression tag	UNP O14114
B	-2	GLY	-	expression tag	UNP O14114
B	-1	ILE	-	expression tag	UNP O14114
B	0	GLN	-	expression tag	UNP O14114
C	-7	GLY	-	expression tag	UNP O14114
C	-6	ALA	-	expression tag	UNP O14114

Continued on next page...

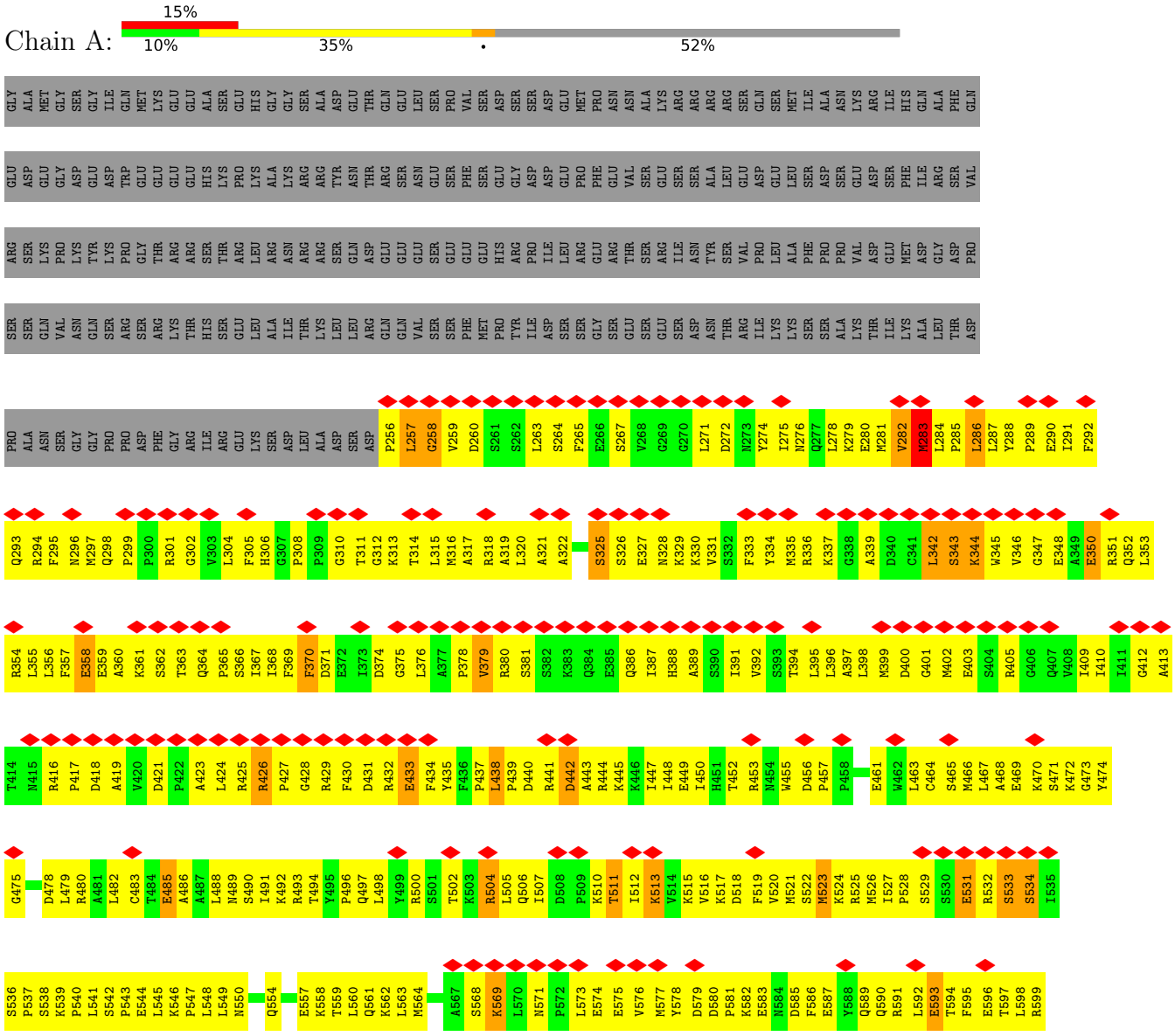
Continued from previous page...

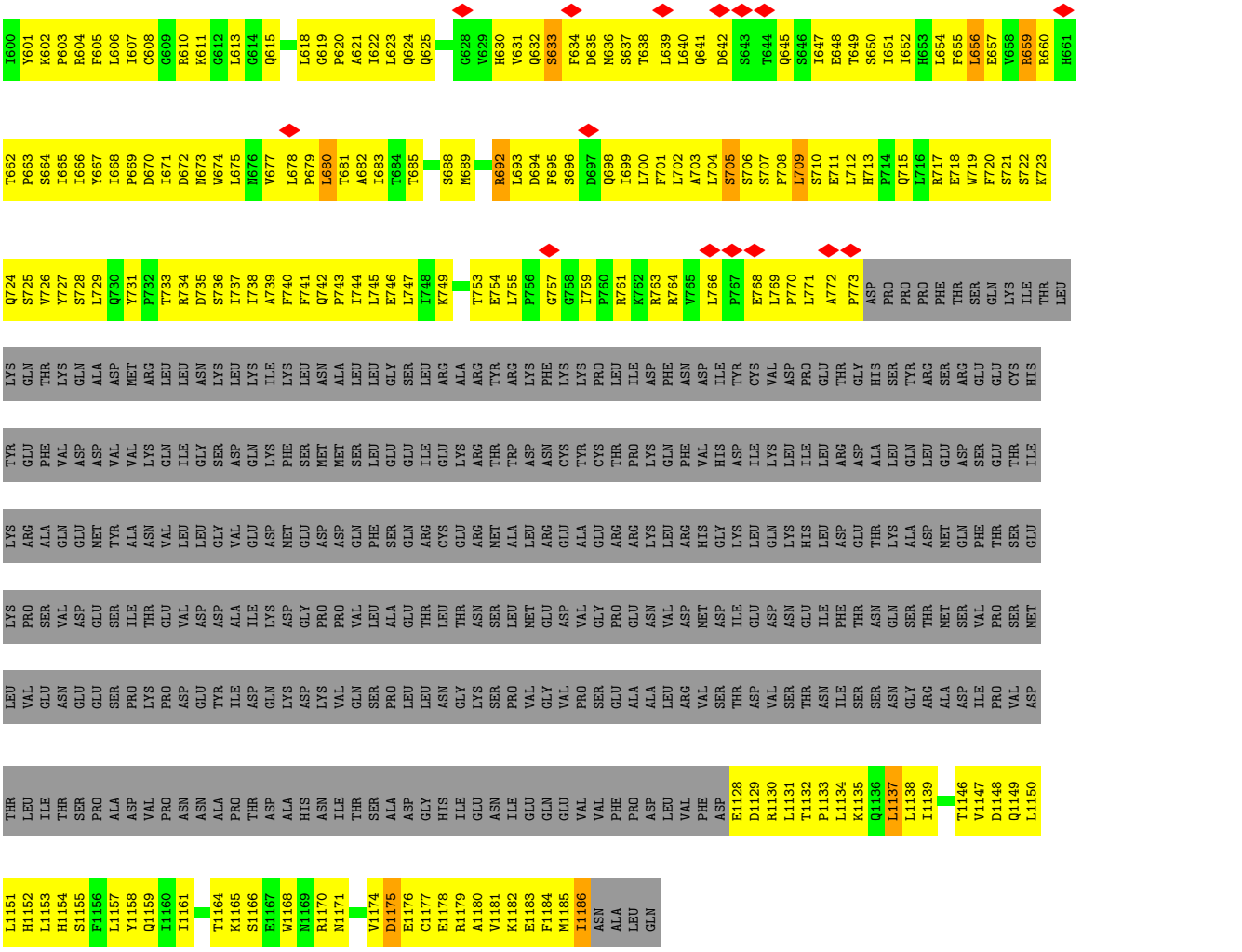
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	MET	-	expression tag	UNP O14114
C	-4	GLY	-	expression tag	UNP O14114
C	-3	SER	-	expression tag	UNP O14114
C	-2	GLY	-	expression tag	UNP O14114
C	-1	ILE	-	expression tag	UNP O14114
C	0	GLN	-	expression tag	UNP O14114
D	-7	GLY	-	expression tag	UNP O14114
D	-6	ALA	-	expression tag	UNP O14114
D	-5	MET	-	expression tag	UNP O14114
D	-4	GLY	-	expression tag	UNP O14114
D	-3	SER	-	expression tag	UNP O14114
D	-2	GLY	-	expression tag	UNP O14114
D	-1	ILE	-	expression tag	UNP O14114
D	0	GLN	-	expression tag	UNP O14114
E	-7	GLY	-	expression tag	UNP O14114
E	-6	ALA	-	expression tag	UNP O14114
E	-5	MET	-	expression tag	UNP O14114
E	-4	GLY	-	expression tag	UNP O14114
E	-3	SER	-	expression tag	UNP O14114
E	-2	GLY	-	expression tag	UNP O14114
E	-1	ILE	-	expression tag	UNP O14114
E	0	GLN	-	expression tag	UNP O14114
F	-7	GLY	-	expression tag	UNP O14114
F	-6	ALA	-	expression tag	UNP O14114
F	-5	MET	-	expression tag	UNP O14114
F	-4	GLY	-	expression tag	UNP O14114
F	-3	SER	-	expression tag	UNP O14114
F	-2	GLY	-	expression tag	UNP O14114
F	-1	ILE	-	expression tag	UNP O14114
F	0	GLN	-	expression tag	UNP O14114

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.

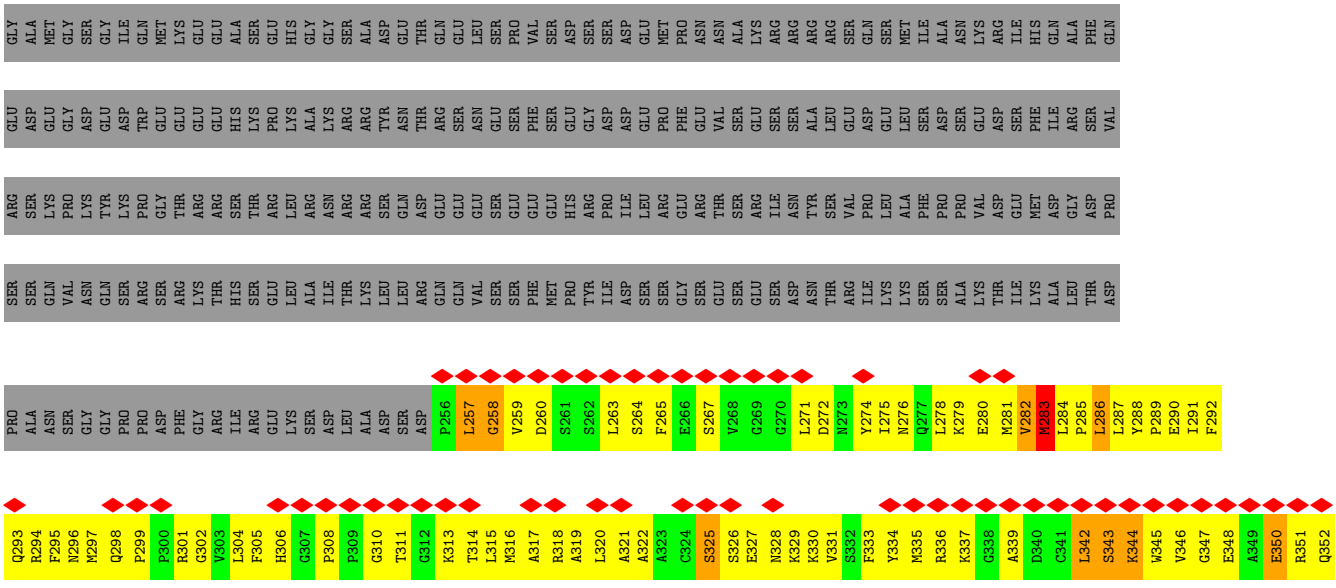
- Molecule 1: Uncharacterized AAA domain-containing protein C31G5.19

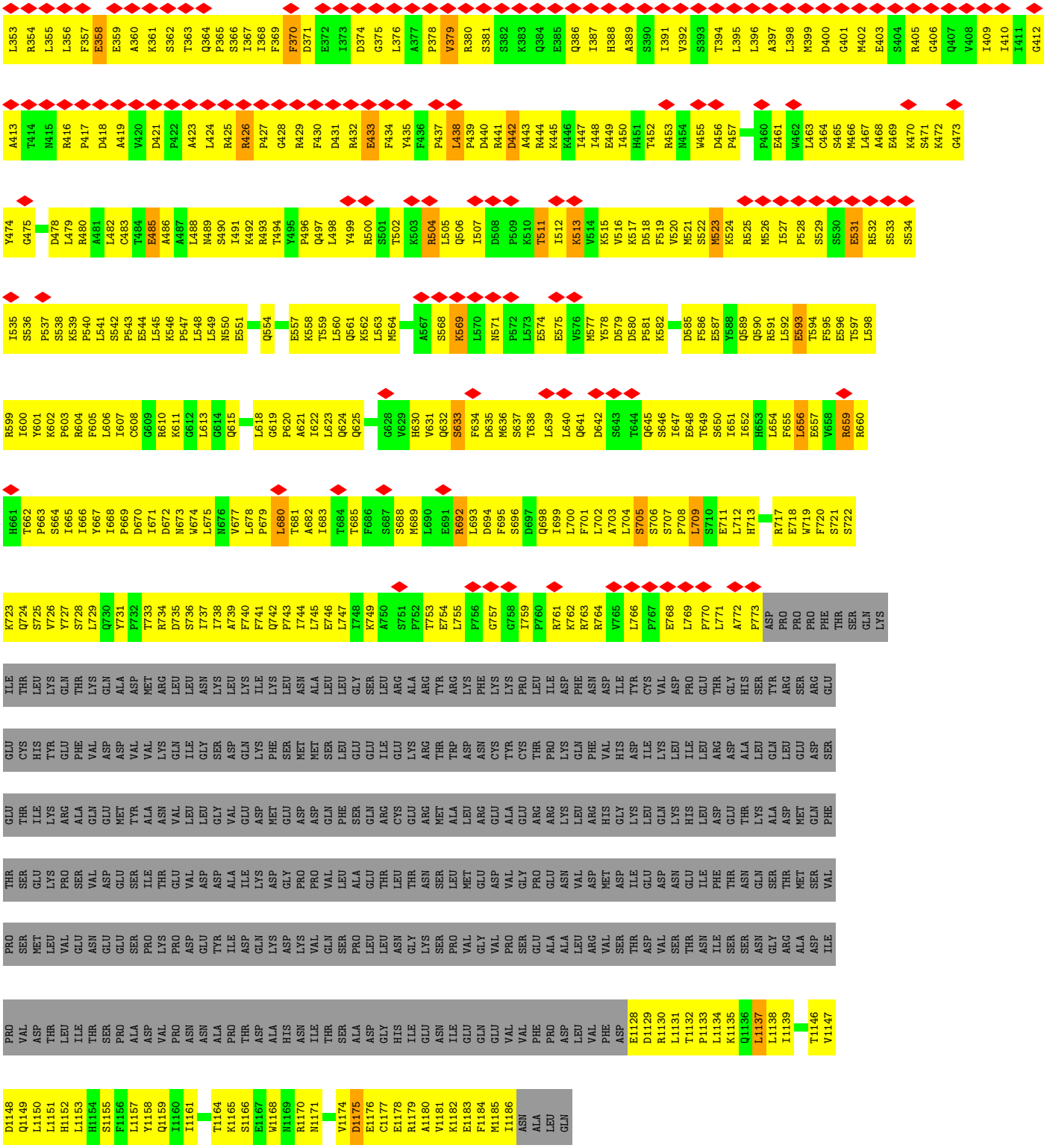




• Molecule 1: Uncharacterized AAA domain-containing protein C31G5.19

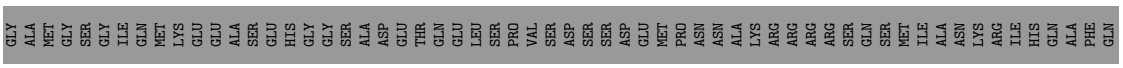
Chain B:

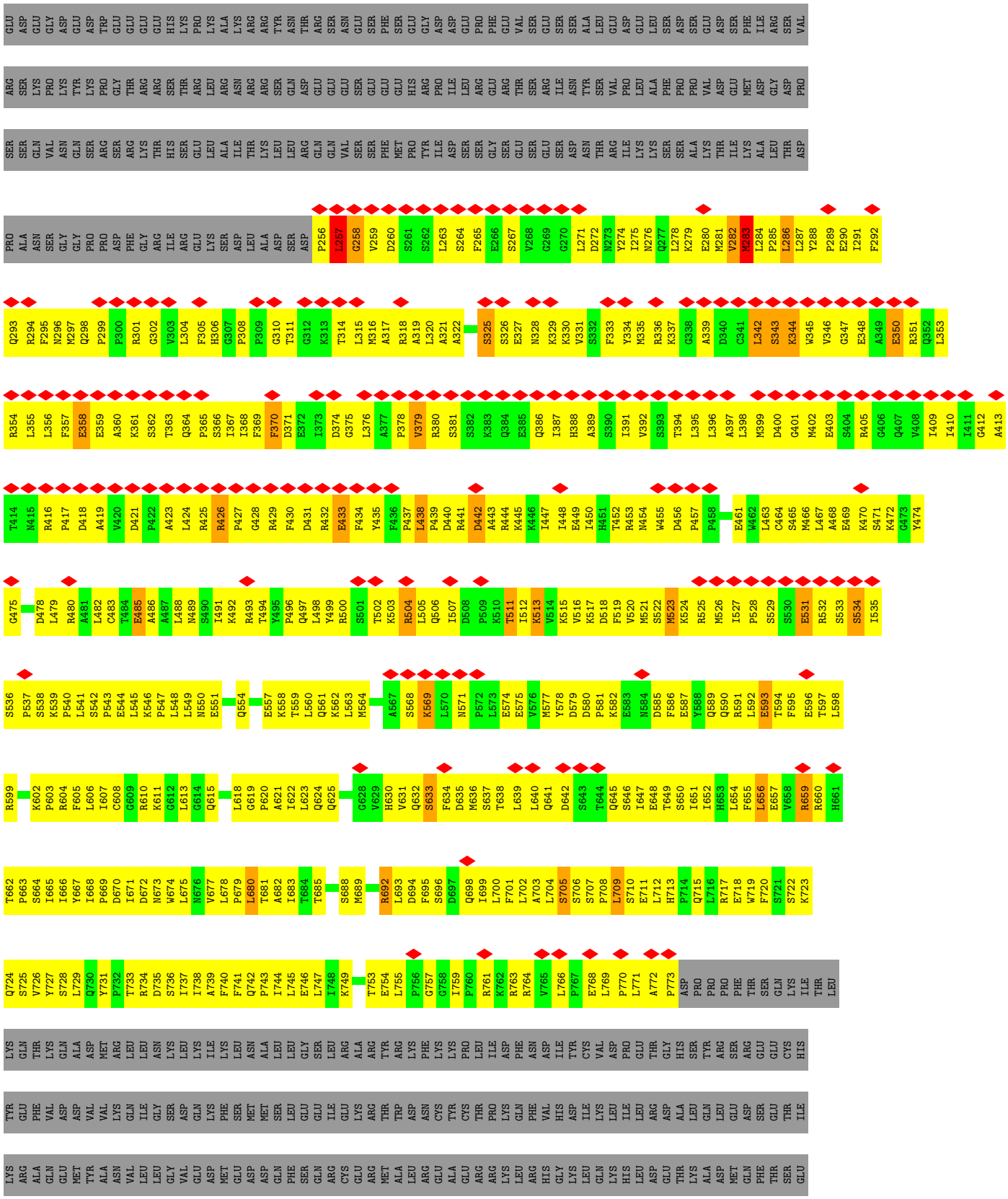


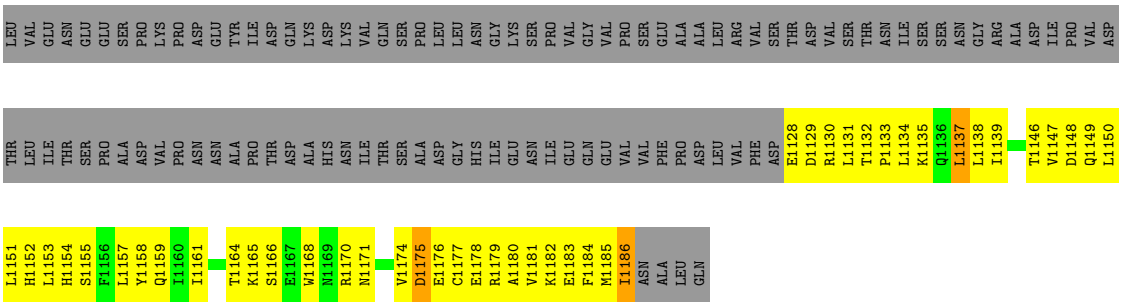


• Molecule 1: Uncharacterized AAA domain-containing protein C31G5.19

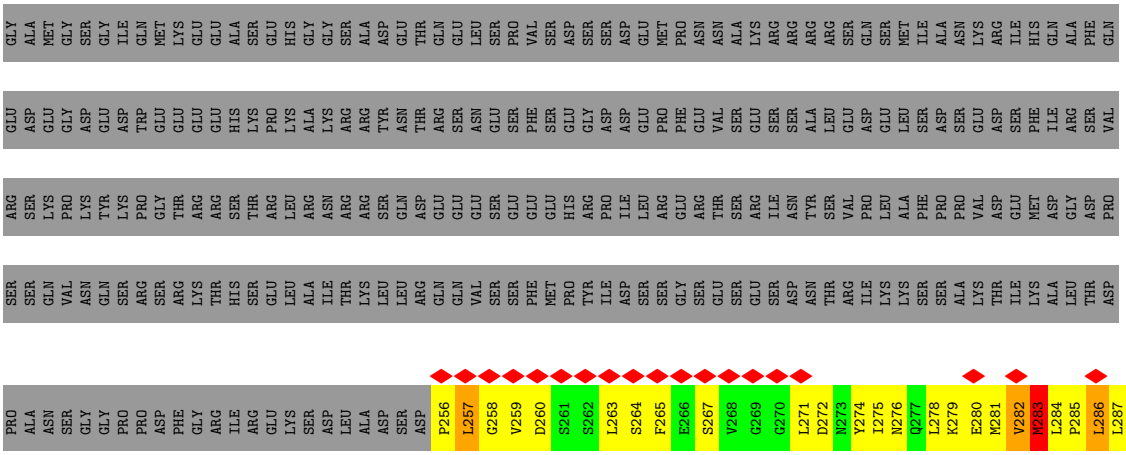
Chain C:

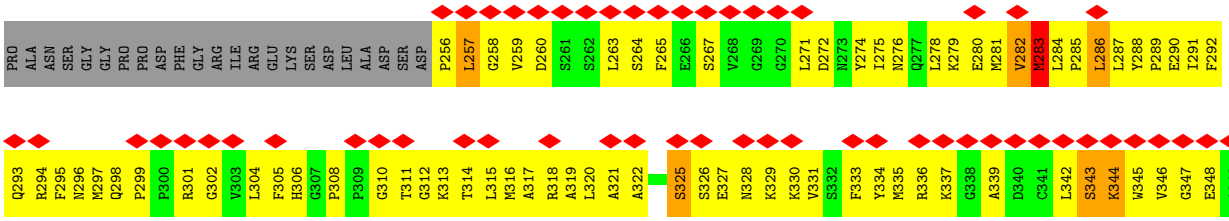


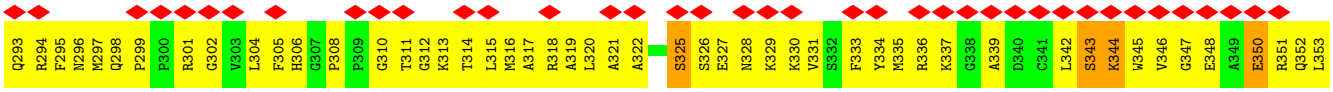

GLU ASP GLU GLY ASP GLU ASP TRP GLU GLU GLU GLU HIS LYS PRO LYS ALA LYS ARG ARG TYR ASN THR ARG SER ASN GLU SER PHE SER GLU GLY ASP ASP GLU PRO PHE GLU VAL SER GLU SER SER ALA LEU GLU ASP GLU LEU SER ASP SER GLU ASP SER PHE ILE ARG SER VAL
ARG SER LYS PRO LYS TYR LYS PRO GLY THR ARG ARG ARG SER THR ARG LEU ARG ASN ARG ARG SER GLN ASP GLU GLU GLU SER GLU GLU GLU HIS ARG PRO ILE LEU ARG GLU ARG THR SER ARG ILE ASN TYR SER VAL PRO LEU ALA PHE PRO PRO VAL ASP GLU MET ASP GLY ASP PRO
SER SER GLN VAL ASN GLN SER ARG SER ARG LYS THR HIS SER GLU LEU ALA ILE THR LYS LEU LEU ARG GLN GLN VAL SER SER PHE MET PRO TYR ILE ASP SER SER GLY SER GLU SER GLU GLU SER ASP ASN THR ARG ILE LYS LYS THR ILE LYS ALA LEU THR ASP
PRO ALA ASN SER GLY GLY PRO PRO ASP PHE GLY ARG ILE ARG GLU LYS SER ASP LEU ALA ASP SER ASP P256 L257 G258 V259 D260 S261 S262 L263 S264 F265 E266 S267 V268 G269 G270 L271 D272 N273 Y274 I275 N276 Q277 L278 K279 E280 M281 V282 M283 L284 P285 L286 L287 Y288 P289 E290 I291 F292
Q293 R294 F295 N296 M297 Q298 P299 P300 R301 G302 V303 L304 F305 H306 G307 P308 P309 G310 T311 G312 K313 T314 L315 M316 A317 R318 A319 L320 A321 A322 S325 S326 E327 N328 K329 K330 V331 S332 F333 Y334 M335 R336 K337 G338 A339 D340 C341 L342 S343 K344 W345 V346 G347 E348 A349 E350 R351 Q352 L353
R354 L355 L356 F357 E358 E359 A360 K361 S362 T363 Q364 P365 S366 I367 I368 F369 F370 D371 E372 I373 D374 G375 L376 A377 P378 V379 R380 S381 S382 K383 Q384 E385 Q386 I387 H388 A389 S390 I391 V392 S393 T394 L395 L396 A397 L398 M399 D400 G401 M402 E403 S404 R405 G406 Q407 V408 I409 I410 I411 G412 A413
T414 N415 R416 P417 D418 A419 V420 D421 P422 A423 L424 R425 R426 P427 G428 R429 F430 D431 R432 E433 F434 Y435 F436 P437 L438 P439 D440 R441 D442 A443 R444 K445 K446 I447 I448 E449 I450 H451 T452 R453 N454 W455 D456 P457 P458 E461 W462 L463 C464 S465 M466 L467 A468 E469 K470 S471 K472 C473 Y474
G475 D478 L479 R480 A481 L482 C483 T484 E485 A486 A487 L488 N489 S490 I491 K492 R493 T494 Y495 P496 Q497 L498 Y499 R500 S501 T502 K503 R504 L505 Q506 I507 D508 P509 K510 T511 I512 K513 V514 K515 V516 K517 D518 F519 V520 M521 S522 M523 K524 R525 M526 I527 P528 S529 S530 E531 R532 S533 S534 I535
S536 P537 S538 K539 P540 L541 S542 P543 E544 L545 K546 P547 L548 L549 N550 E551 Q554 E557 K558 T559 L560 Q561 K562 L563 M564 A567 S568 K569 L570 N571 P572 L573 E574 E575 V576 M577 Y578 D579 D580 P581 K582 E583 N584 D585 F586 E587 Y588 Q589 Q590 R591 L592 E593 T594 F595 E596 T597 L598
R599 K602 P603 R604 F605 L606 I607 C608 G609 R610 K611 G612 L613 G614 Q615 L618 G619 P620 A621 I622 L623 Q624 Q625 G628 V629 H630 V631 Q632 S633 F634 D635 M636 S637 T638 L639 L640 Q641 D642 S643 T644 Q645 S646 I647 E648 T649 S650 I651 I652 H653 L654 F655 L656 E657 V658 R659 R660 H661
T662 P663 S664 I665 I666 Y667 I668 P669 D670 I671 D672 N673 W674 L675 N676 V677 L678 P679 L680 T681 A682 I683 T684 T685 S688 M689 R692 L693 D694 F695 S696 D697 Q698 I699 L700 F701 L702 A703 L704 S705 S706 S707 P708 L709 S710 E711 L712 H713 P714 Q715 L716 R717 E718 W719 F720 S721 S722 K723
Q724 S725 V726 Y727 S728 L729 Q730 Y731 P732 T733 R734 D735 S736 I737 I738 A739 F740 F741 Q742 P743 I744 L745 E746 L747 I748 K749 T753 E754 L755 P756 G757 G758 I759 P760 R761 K762 R763 R764 V765 L766 P767 E768 L769 P770 L771 A772 P773 ASP PRO PRO PRO PHE THR SER GLN LYS ILE THR LEU
LYS GLN THR LYS GLN ALA ASP MET ARG LEU LEU ASN LYS LEU LYS ILE LYS LEU ASN ALA LEU LEU GLY SER LEU ARG ALA ARG TYR ARG LYS PHE LYS LYS PRO LEU ILE ASP PHE ASN ASP ILE TYR CYS VAL ASP PRO GLU THR GLY HIS SER TYR ARG SER ARG GLU GLU CYS HIS
TYR GLU PHE VAL ASP ASP VAL VAL LYS GLN ILE GLY SER ASP GLN LYS PHE SER MET MET SER LEU GLU GLU ILE GLU LYS ARG THR TRP ASP ASN CYS TYR CYS THR PRO LYS GLN PHE VAL HIS ASP ILE LYS LEU ILE LEU ARG ASP ALA LEU GLN LEU GLU ASP SER GLU THR ILE
LYS ARG ALA GLN GLU MET TYR ALA ASN VAL LEU LEU GLY VAL GLU ASP MET GLU ASP ASP GLN PHE SER GLN ARG CYS GLU ARG MET ALA LEU ARG ARG LYS LEU LEU ARG HIS GLY LYS LEU GLN LYS HIS LEU ASP GLU THR LYS ALA ASP MET GLN PHE THR SER GLU
LYS PRO SER VAL ASP GLU SER ILE THR GLU VAL ASP ASP ALA ILE LYS ASP GLY PRO PRO VAL LEU ALA GLU THR LEU THR ASN SER LEU MET GLU ASP VAL GLY PRO GLU ASN VAL ASP MET ASP ILE GLU ASP ASN GLU ILE PHE THR ASN GLN SER THR MET SER VAL PRO SER MET

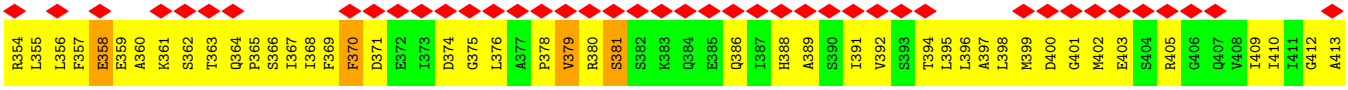


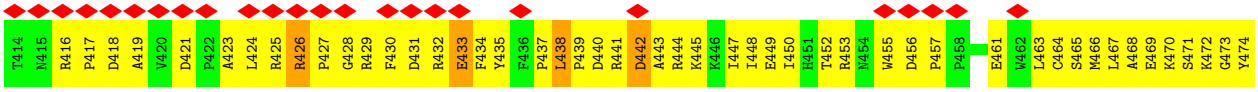
• Molecule 1: Uncharacterized AAA domain-containing protein C31G5.19

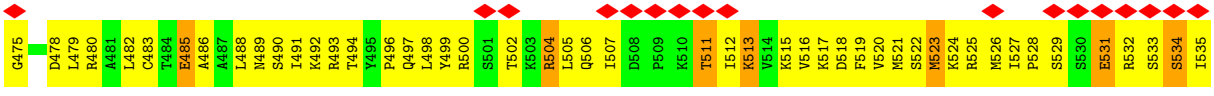


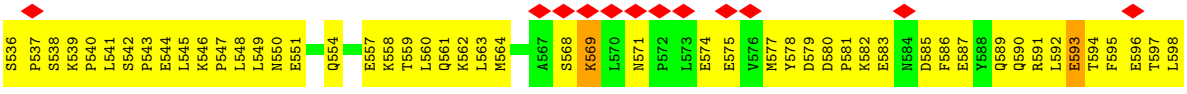


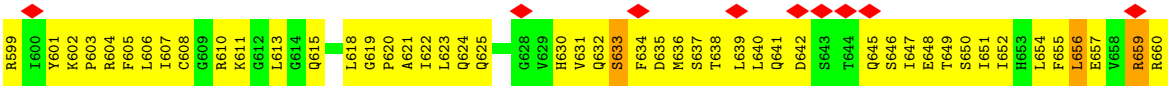


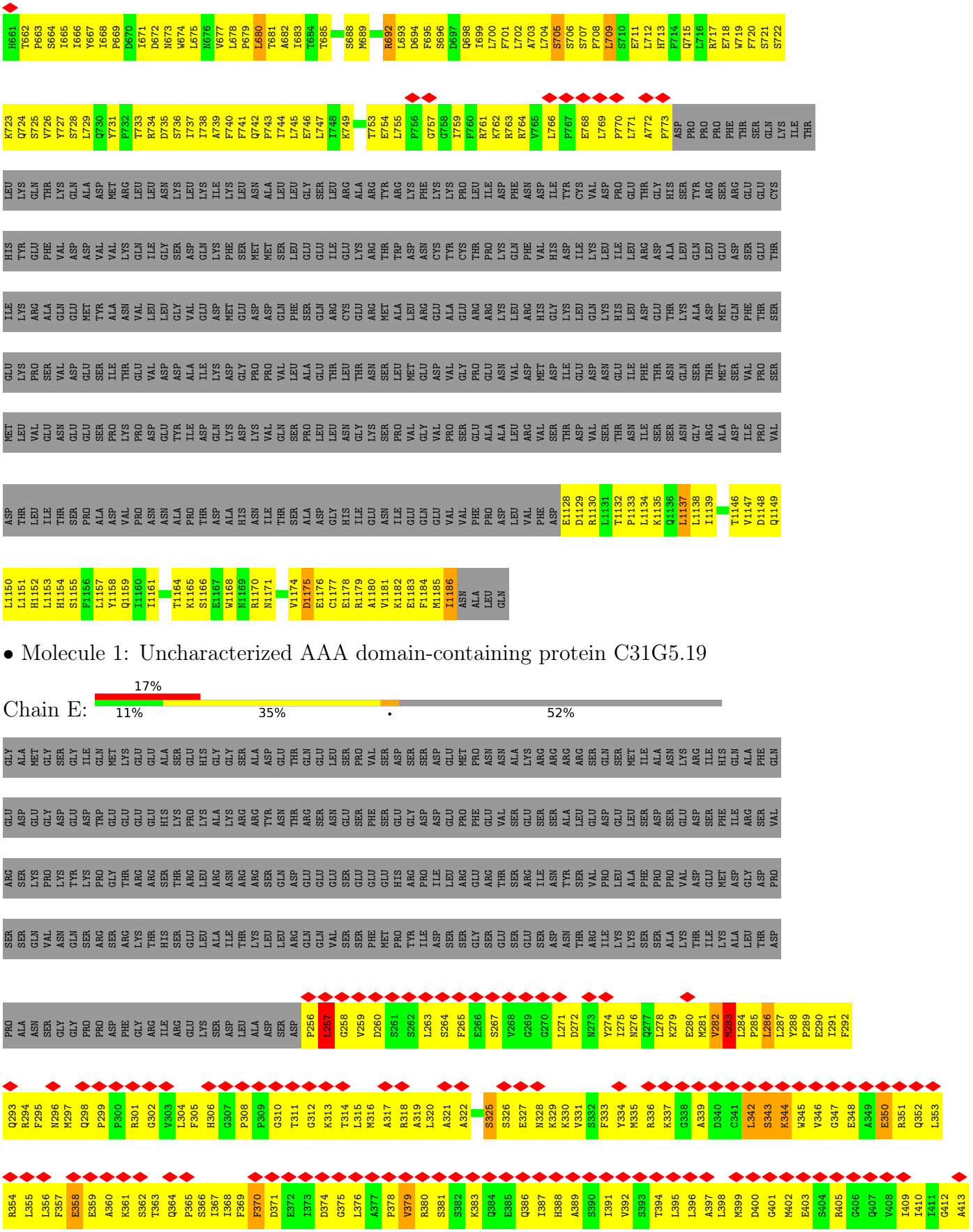






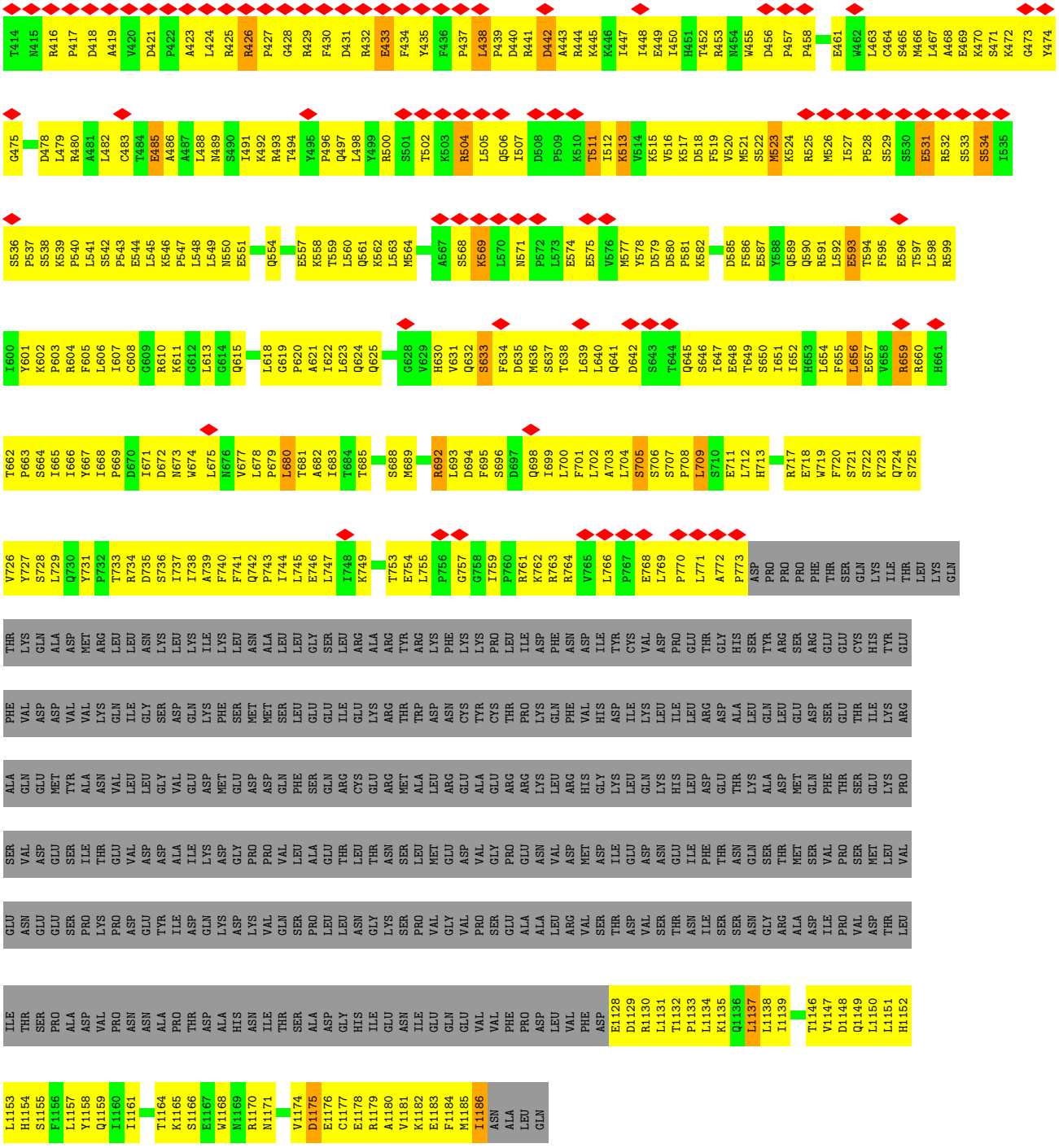






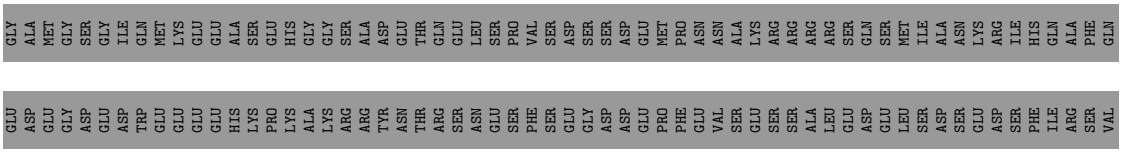
• Molecule 1: Uncharacterized AAA domain-containing protein C31G5.19

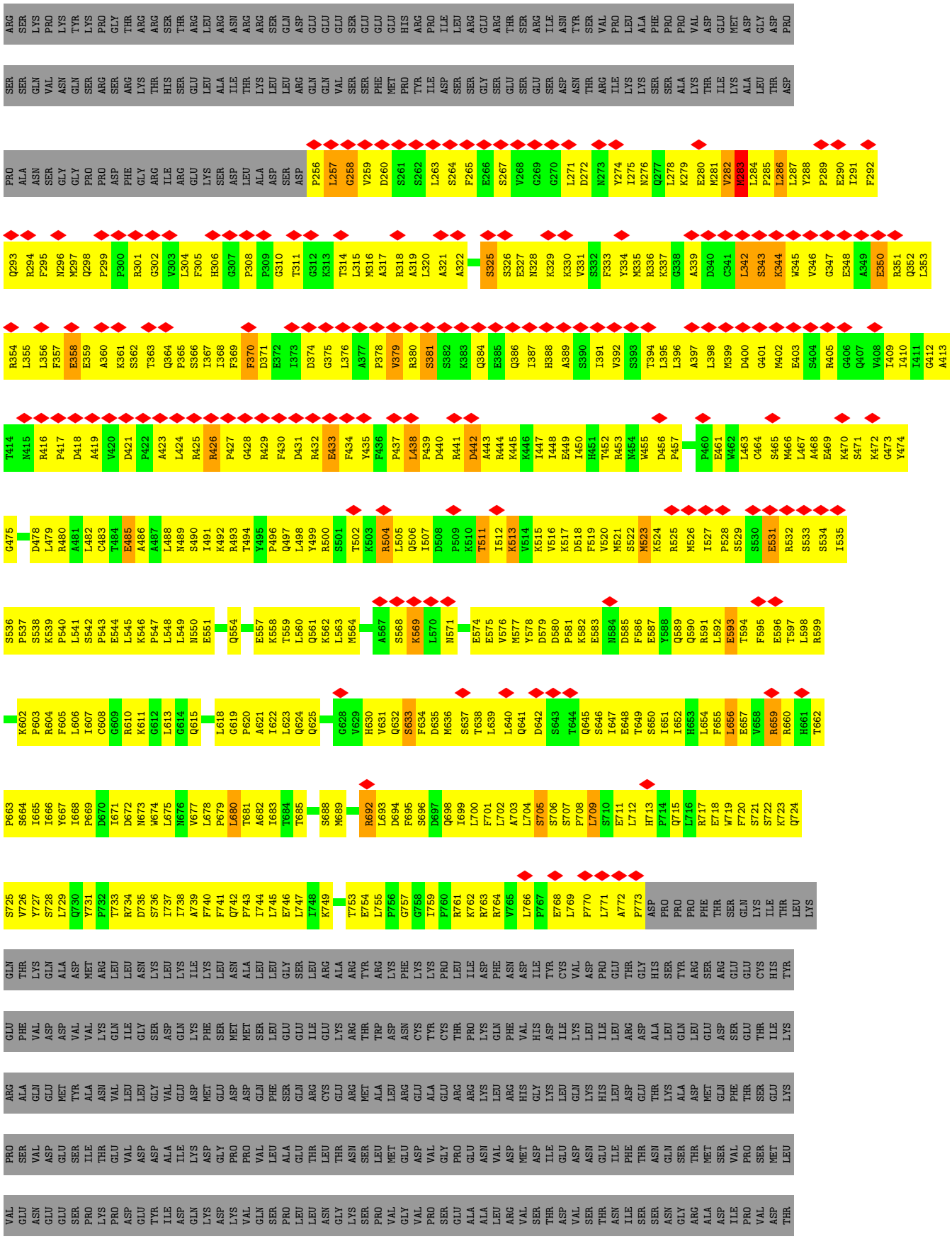
Chain E:

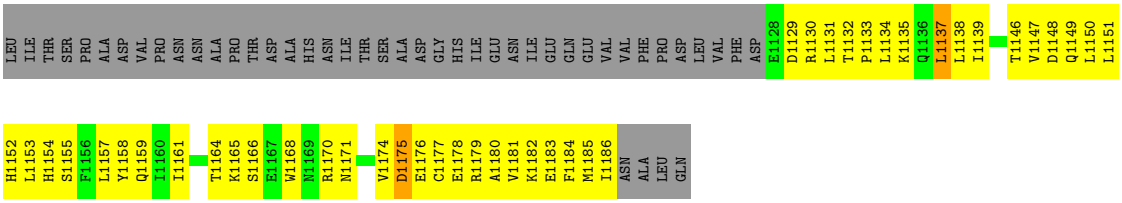


• Molecule 1: Uncharacterized AAA domain-containing protein C31G5.19

Chain F:




ARG SER LYS PRO LYS TYR LYS PRO GLY THR ARG ARG SER THR ARG LEU ARG ASN ARG ARG SER GLN GLU GLU GLU SER GLU GLU GLU HIS ARG PRO TYR ILE LEU ARG GLU ARG THR SER ARG ILE ASN TYR SER VAL PRO LEU ALA PHE PRO PRO VAL ASP GLU MET ASP GLY ASP PRO
SER SER GLN VAL ASN GLN SER ARG SER ARG LYS THR HIS SER GLU LEU ALA ILE THR LYS LEU LEU GLN GLN VAL SER SER PHE MET PRO TYR ILE ASP SER SER GLY SER GLU SER GLU SER ASP ASN THR ARG ILE LYS LYS SER ALA LYS THR ILE LYS ALA LEU THR ASP
PRO ALA ASN SER GLY GLY PRO PRO ASP PHE GLY ARG ILE ARG GLU LYS SER ASP LEU ALA ALA ASP SER ASP P256 L257 G258 V259 D260 S261 S262 L263 S264 F265 E266 S267 Y268 G269 G270 L271 D272 M273 Y274 I275 N276 Q277 L278 K279 E280 M281 V282 M283 L284 P285 L286 L287 Y288 P289 E290 I291 F292
Q293 R294 F295 N296 M297 Q298 P299 P300 R301 G302 V303 L304 F305 H306 G307 P308 P309 G310 T311 G312 K313 T314 L315 M316 A317 R318 A319 L320 A321 A322 S325 S326 E327 N328 K329 K330 V331 S332 F333 Y334 M335 R336 K337 G338 A339 D340 C341 L342 S343 K344 W345 V346 G347 E348 A349 E350 R351 Q352 L353
R354 L355 L356 F357 E358 E359 A360 K361 S362 T363 Q364 P365 S366 I367 I368 F369 F370 D371 E372 I373 D374 G375 L376 A377 P378 V379 R380 S381 S382 K383 Q384 E385 Q386 I387 H388 A389 S390 I391 V392 S393 T394 L395 L396 A397 L398 M399 D400 G401 M402 E403 S404 R405 G406 Q407 V408 I409 I410 I411 G412 A413
T414 N415 R416 P417 D418 A419 V420 D421 P422 A423 L424 R425 R426 P427 G428 R429 F430 D431 R432 E433 F434 Y435 F436 P437 L438 P439 D440 R441 D442 A443 R444 K445 K446 I447 I448 E449 I450 H451 T452 R453 N454 W455 D456 P457 P460 E461 W462 L463 C464 S465 M466 L467 A468 E469 K470 S471 K472 G473 Y474
G475 D478 L479 R480 A481 L482 C483 T484 E485 A486 A487 L488 N489 S490 I491 K492 R493 T494 Y495 P496 Q497 L498 Y499 R500 S501 T502 K503 R504 L505 Q506 I507 D508 P509 K510 T511 I512 K513 V514 K515 V516 K517 D518 F519 V520 M521 S522 M523 K524 R525 M526 I527 P528 S529 S530 E531 R532 S533 S534 I535
S536 P537 S538 K539 P540 L541 S542 P543 E544 L545 K546 P547 L548 L549 N550 E551 Q554 E557 K558 T559 L560 Q561 K562 L563 M564 A567 S568 K569 L570 N571 E574 E575 V576 M577 Y578 D579 D580 P581 K582 E583 N584 D585 F586 E587 Y588 Q589 Q590 R591 L592 E593 T594 F595 E596 T597 L598 R599
K602 P603 R604 F605 L606 I607 C608 G609 R610 K611 G612 L613 G614 Q615 L618 G619 P620 A621 I622 L623 Q624 Q625 G628 V629 H630 V631 Q632 S633 F634 D635 M636 S637 T638 L639 L640 Q641 D642 S643 T644 Q645 S646 I647 E648 T649 S650 I651 I652 H653 L654 F655 L656 E657 V658 R659 R660 H661 T662
P663 S664 I665 I666 Y667 I668 P669 D670 I671 D672 N673 W674 L675 N676 V677 L678 P679 L680 T681 A682 I683 T684 T685 S688 M689 R692 L693 D694 F695 S696 D697 Q698 I699 L700 F701 L702 A703 L704 S705 S706 S707 P708 L709 S710 E711 L712 H713 P714 Q715 L716 R717 E718 W719 F720 S721 S722 K723 Q724
S725 V726 Y727 S728 L729 Q730 V731 P732 T733 R734 D735 S736 I737 I738 A739 F740 F741 Q742 P743 I744 L745 E746 L747 I748 K749 T753 E754 L755 P756 G757 G758 I759 P760 R761 K762 R763 R764 V765 L766 P767 E768 L769 P770 L771 A772 P773 ASP PRO PRO PRO PHE THR SER GLN LYS ILE THR LEU LYS
GLN THR LYS GLN ALA ASP MET ARG LEU LEU ASN LYS LEU LYS ILE LYS LEU ASN ALA LEU LEU GLY SER LEU ARG ALA ARG TYR ARG LYS PHE LYS LYS PRO LEU ILE ASP PHE ASN ASP ILE TYR CYS VAL ASP PRO GLU THR GLY HIS SER TYR ARG SER ARG GLU GLU CYS HIS TYR
GLU PHE VAL ASP ASP VAL VAL LYS GLN ILE GLY SER ASP GLN LYS PHE SER MET MET SER LEU GLU GLU ILE GLU LYS ARG THR TRP ASP ASN CYS TYR CYS THR PRO LYS GLN PHE VAL HIS ASP ILE LYS LEU ILE LEU ARG ASP ALA LEU GLN LEU GLU ASP SER GLU THR ILE LYS
ARG ALA GLN GLU MET TYR ALA ASN VAL LEU LEU GLY VAL GLU ASP MET GLU GLU ASP ASP GLN PHE SER GLN ARG CYS GLU ARG MET ALA LEU ARG GLU ALA GLU ARG ARG LYS LEU LEU ARG HIS GLY LYS LEU GLN LYS HIS LEU ASP GLU THR LYS ALA ASP MET GLN PHE THR SER GLU LYS
PRO SER VAL ASP GLU SER ILE THR GLU VAL ASP ASP ALA ILE LYS ASP GLY PRO PRO VAL LEU ALA GLU LEU THR LEU THR ASN SER LEU MET GLU GLY ASP VAL ASP GLY PRO GLU ASN VAL LEU ASP MET ASP ILE GLU ASP ASN GLU ILE PHE THR ASN GLN SER THR MET SER VAL PRO SER MET LEU
VAL GLU ASN GLU GLU SER PRO LYS PRO ASP GLU TYR ILE ASP GLN LYS ASP LYS VAL GLN SER PRO LEU LEU ASN GLY LYS SER PRO VAL GLY VAL PRO SER GLU GLY ALA ALA LEU ARG VAL SER THR ASP VAL SER THR ASN ILE SER SER ASN GLY ARG ALA ASP ILE PRO VAL ASP THR


LEU ILE THR SER PRO ALA ASP VAL PRO ASN ASN ALA PRO THR ASP ALA HIS ASN ILE THR SER ALA ASP GLY HIS ILE GLU ASN ILE GLU GLN GLU VAL VAL PHE PRO ASP LEU VAL PHE ASP
E1128 D1129 R1130 L1131 T1132 P1133 L1134 K1135 Q1136 L1137 L1138 I1139
T1146 V1147 D1148 Q1149 L1150 L1151
H1152 L1153 H1154 S1155 F1156 L1157 Y1158 Q1159 I1160 I1161
T1164 K1165 S1166 E1167 W1168 N1169 R1170 N1171
V1174 D1175 E1176 C1177 E1178 R1179 A1180 V1181 K1182 E1183 F1184 M1185 I1186
ASN ALA LEU GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	125874	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	8.458	Depositor
Minimum map value	-3.915	Depositor
Average map value	-0.011	Depositor
Map value standard deviation	0.371	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	A	0.37	1/4734 (0.0%)	0.57	2/6411 (0.0%)
1	B	0.37	1/4734 (0.0%)	0.57	2/6411 (0.0%)
1	C	0.37	1/4734 (0.0%)	0.57	2/6411 (0.0%)
1	D	0.37	1/4734 (0.0%)	0.57	2/6411 (0.0%)
1	E	0.37	1/4734 (0.0%)	0.57	2/6411 (0.0%)
1	F	0.37	1/4734 (0.0%)	0.57	2/6411 (0.0%)
All	All	0.37	6/28404 (0.0%)	0.57	12/38466 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	12

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	379	VAL	CB-CG2	6.42	1.66	1.52
1	F	379	VAL	CB-CG2	6.42	1.66	1.52
1	B	379	VAL	CB-CG2	6.42	1.66	1.52
1	A	379	VAL	CB-CG2	6.42	1.66	1.52
1	C	379	VAL	CB-CG2	6.40	1.66	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	442	ASP	CB-CG-OD2	6.70	124.33	118.30
1	F	442	ASP	CB-CG-OD2	6.67	124.30	118.30
1	C	442	ASP	CB-CG-OD2	6.64	124.28	118.30
1	B	442	ASP	CB-CG-OD2	6.63	124.27	118.30
1	E	442	ASP	CB-CG-OD2	6.61	124.25	118.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	LEU	Peptide
1	A	511	THR	Peptide
1	B	257	LEU	Peptide
1	B	511	THR	Peptide
1	C	257	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4628	435	4700	670	0
1	B	4628	435	4700	700	0
1	C	4628	435	4700	690	0
1	D	4628	435	4700	655	0
1	E	4628	435	4700	661	0
1	F	4628	435	4700	656	0
All	All	27768	2610	28200	3877	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 69.

The worst 5 of 3877 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:E:440:ASP:HA	1:E:472:LYS:HE2	1.40	1.04
1:F:440:ASP:HA	1:F:472:LYS:HE2	1.40	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:ASP:HA	1:B:472:LYS:HE2	1.40	1.04
1:C:440:ASP:HA	1:C:472:LYS:HE2	1.40	1.03
1:F:646:SER:HG	1:F:649:THR:HG1	1.04	1.03

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	573/1198 (48%)	516 (90%)	56 (10%)	1 (0%)	47	81
1	B	573/1198 (48%)	516 (90%)	56 (10%)	1 (0%)	47	81
1	C	573/1198 (48%)	516 (90%)	56 (10%)	1 (0%)	47	81
1	D	573/1198 (48%)	516 (90%)	56 (10%)	1 (0%)	47	81
1	E	573/1198 (48%)	516 (90%)	56 (10%)	1 (0%)	47	81
1	F	573/1198 (48%)	516 (90%)	56 (10%)	1 (0%)	47	81
All	All	3438/7188 (48%)	3096 (90%)	336 (10%)	6 (0%)	50	81

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	GLY
1	B	258	GLY
1	C	258	GLY
1	D	258	GLY
1	E	258	GLY

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	A	522/1086 (48%)	472 (90%)	50 (10%)	8 30
1	B	522/1086 (48%)	472 (90%)	50 (10%)	8 30
1	C	522/1086 (48%)	472 (90%)	50 (10%)	8 30
1	D	522/1086 (48%)	472 (90%)	50 (10%)	8 30
1	E	522/1086 (48%)	472 (90%)	50 (10%)	8 30
1	F	522/1086 (48%)	472 (90%)	50 (10%)	8 30
All	All	3132/6516 (48%)	2832 (90%)	300 (10%)	12 30

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	523	MET
1	F	575	GLU
1	E	633	SER
1	F	343	SER
1	B	1166	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	624	GLN
1	E	615	GLN
1	D	1149	GLN
1	E	489	ASN
1	E	1149	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 monosaccharides 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.

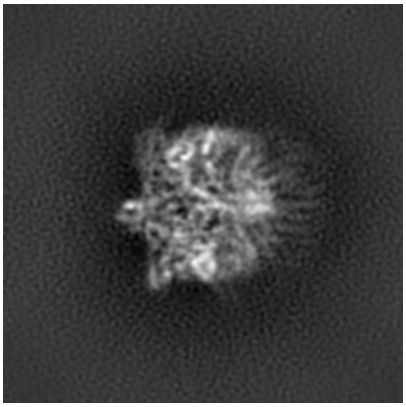
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9871. These allow visual inspection of the internal detail of the map and identification of artifacts.

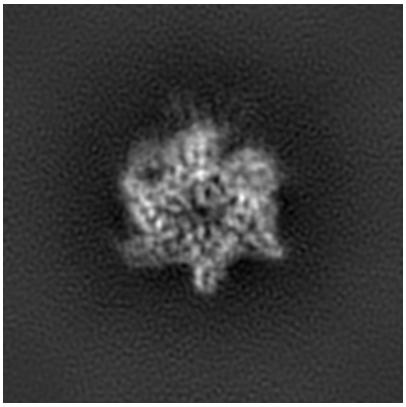
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

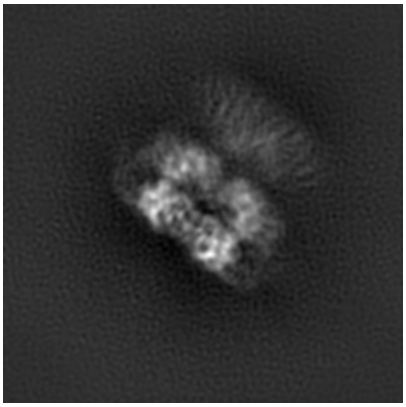
6.1.1 Primary map



X



Y

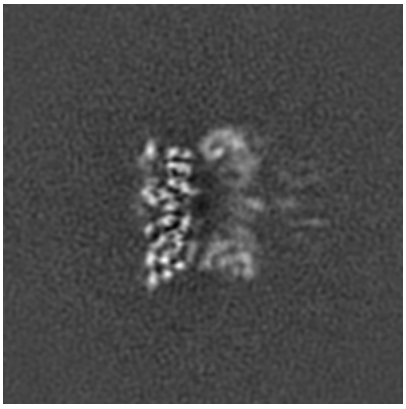


Z

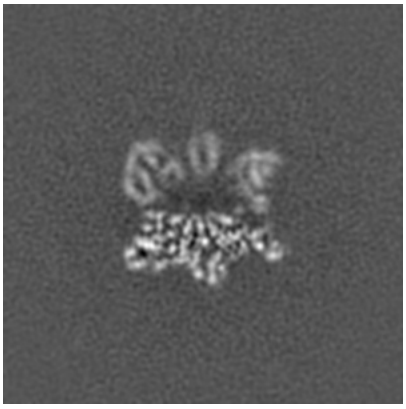
The images above show the map projected in three orthogonal directions.

6.2 Central slices

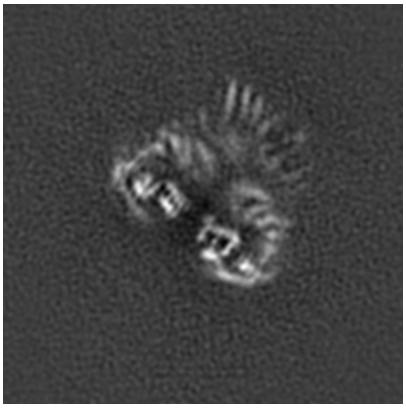
6.2.1 Primary map



X Index: 150



Y Index: 150

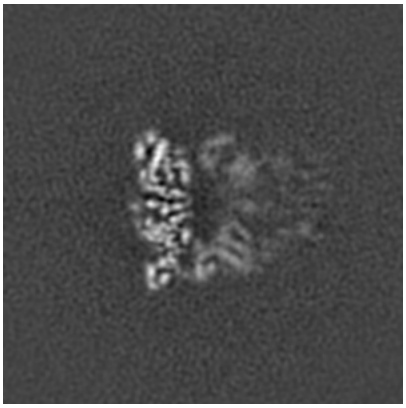


Z Index: 150

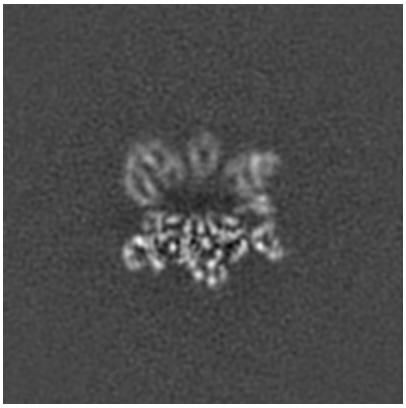
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

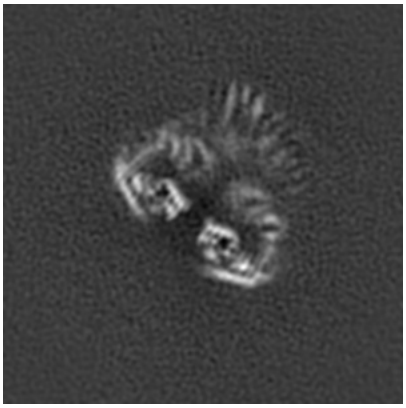
6.3.1 Primary map



X Index: 157



Y Index: 152

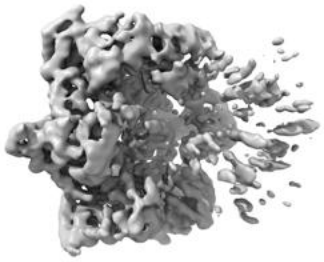


Z Index: 148

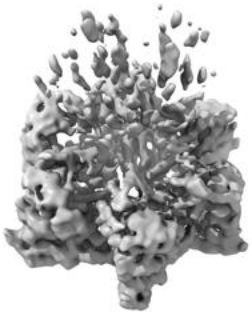
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

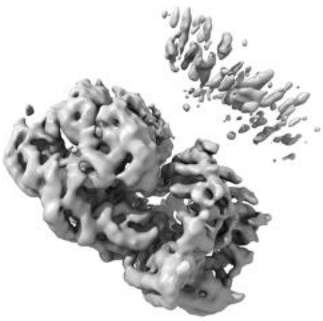
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

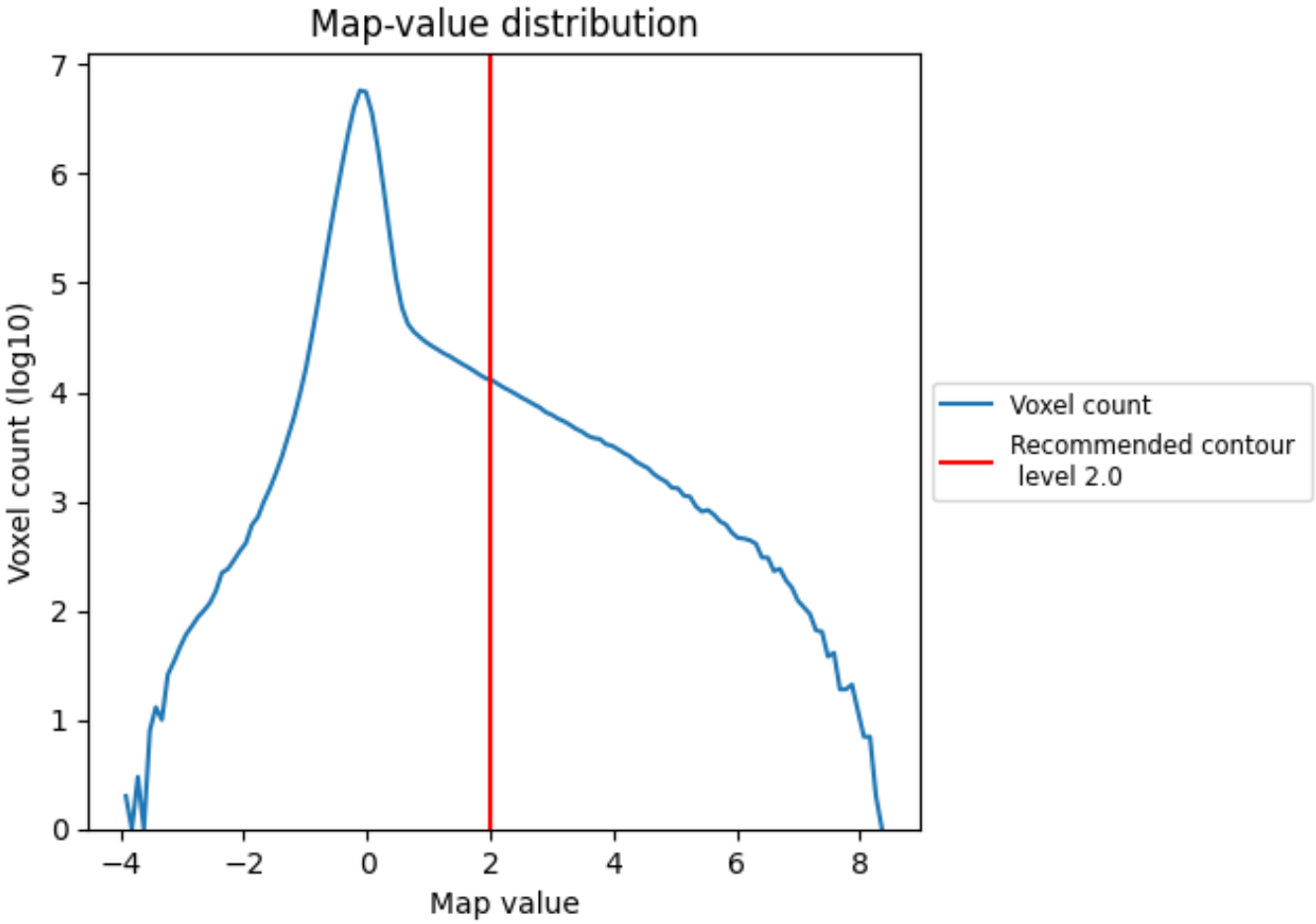
6.5 Mask visualisation (i)

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

7 Map analysis

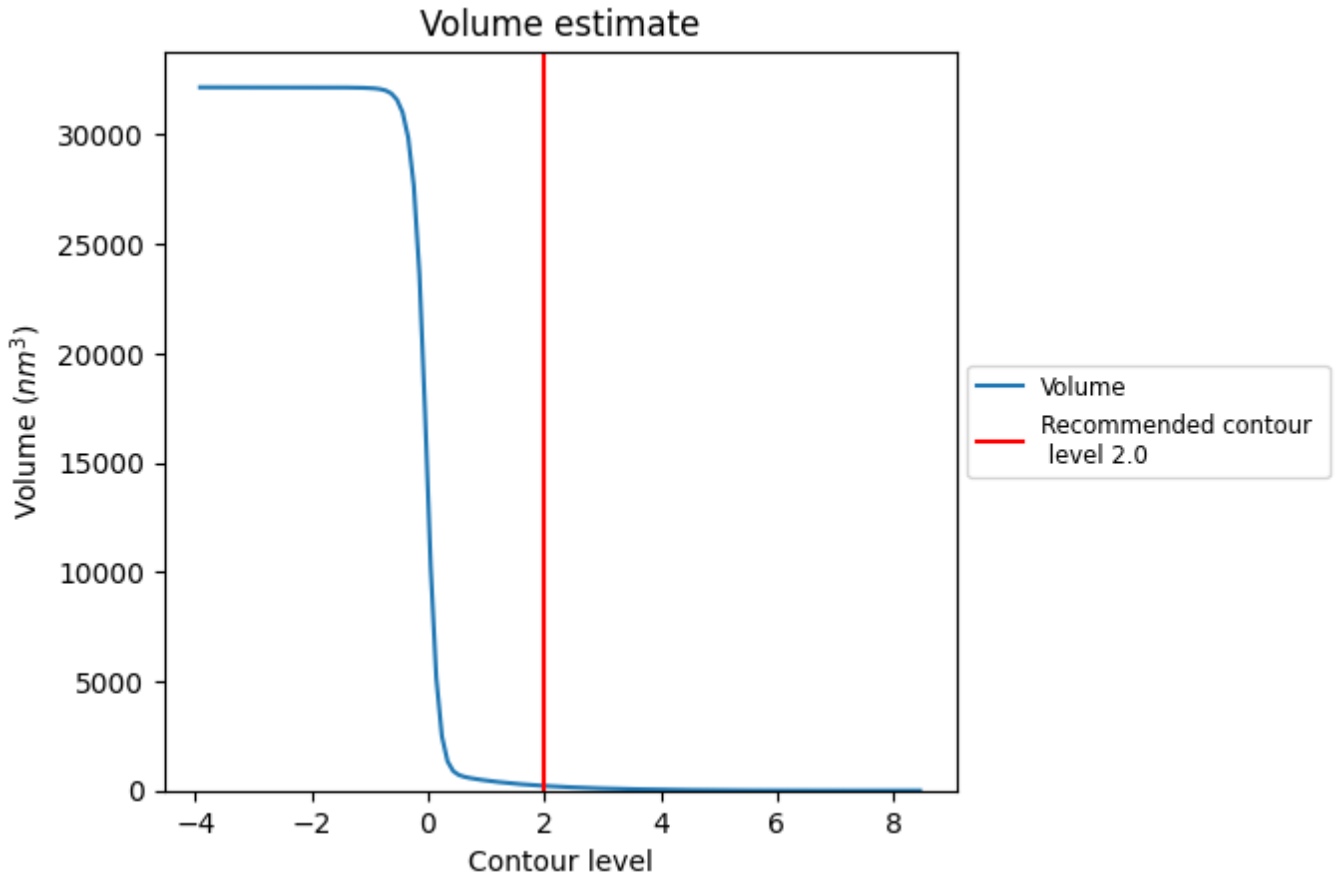
This section contains the results of statistical analysis of the map.

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.

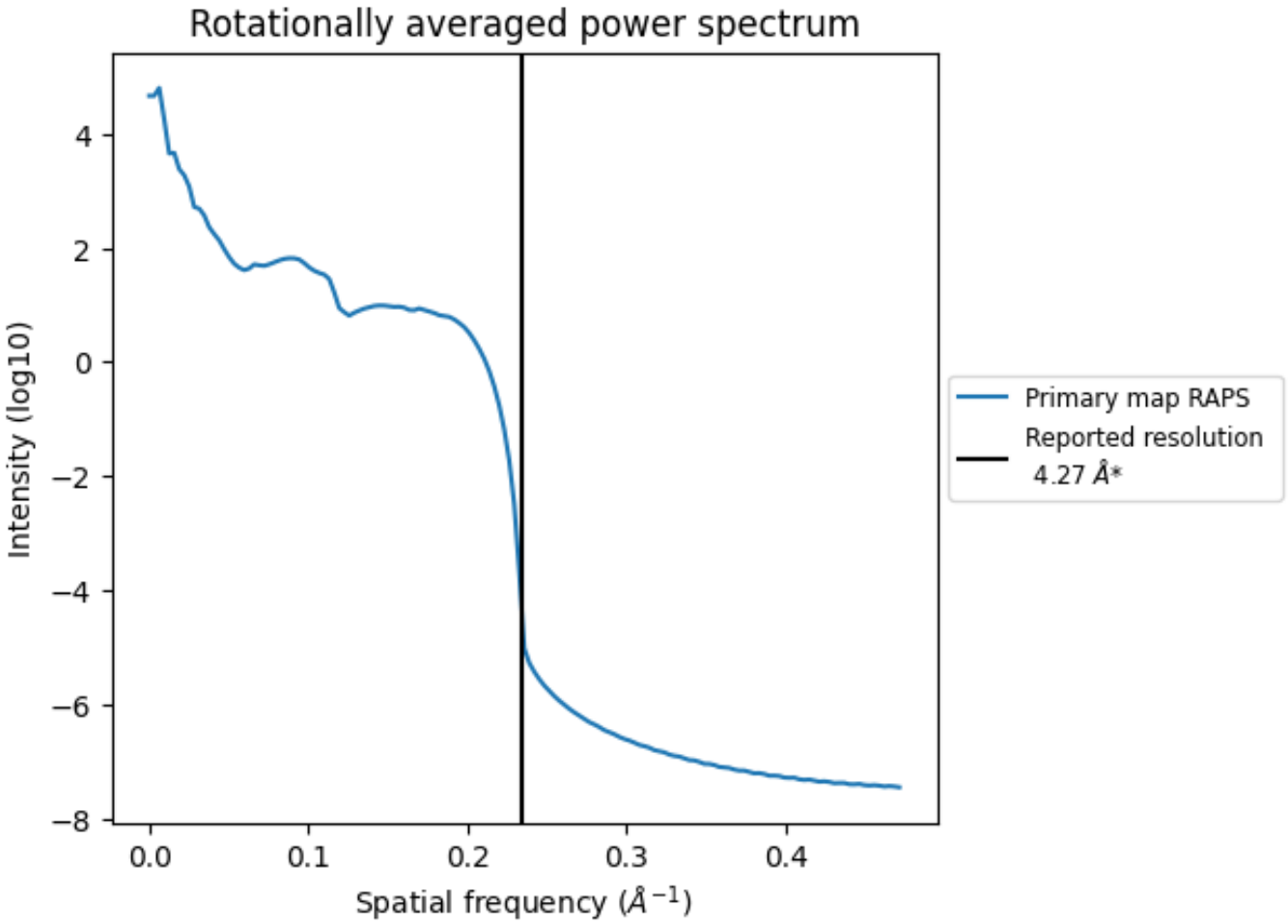
7.2 Volume estimate (i)



The volume at the recommended contour level is 215 nm^3; this corresponds to an approximate mass of 195 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 0.234 Å^{-1}

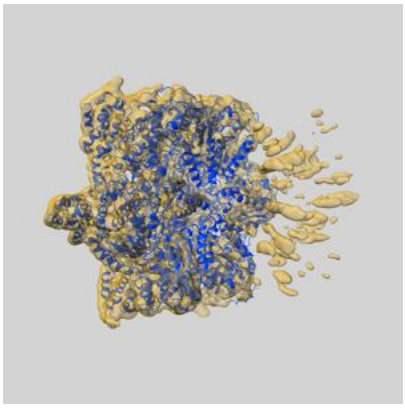
8 Fourier-Shell correlation

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

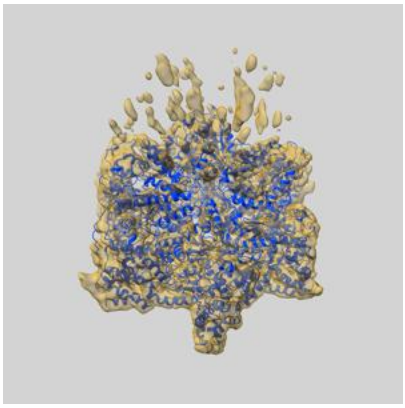
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9871 and PDB model 6JPU. Per-residue inclusion information can be found in section 3 on page 5.

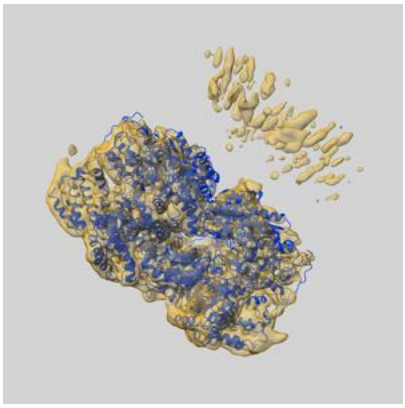
9.1 Map-model overlay



X



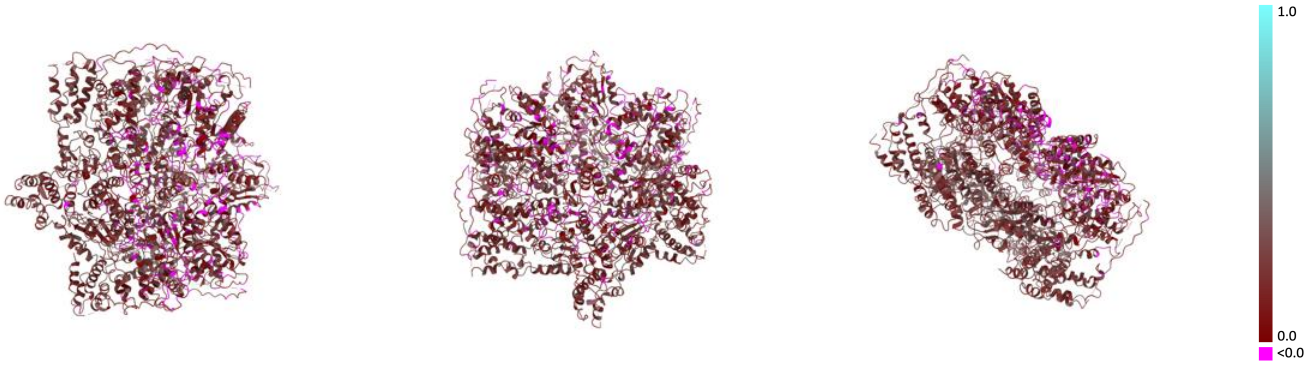
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 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.

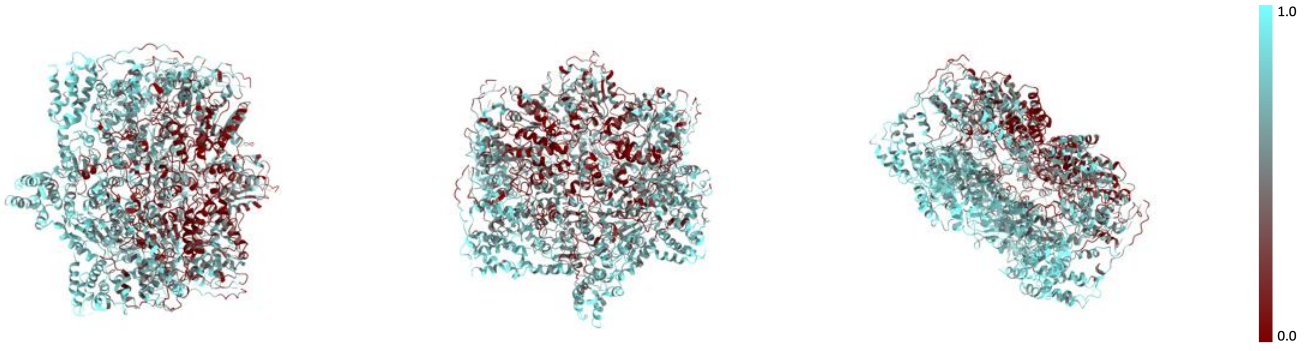
9.2 Q-score mapped to coordinate model (i)



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.

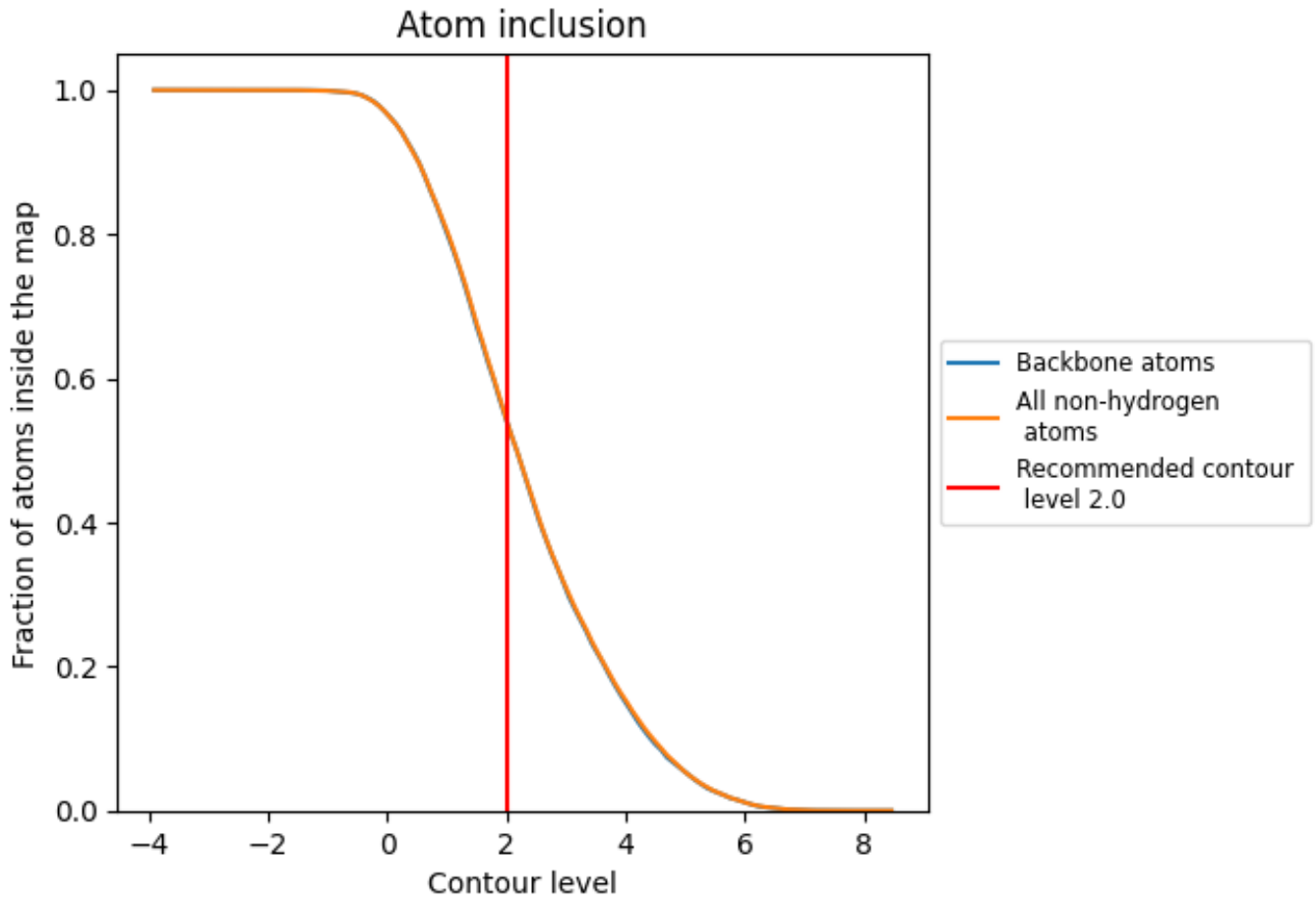
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 54% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5412	0.1810
A	0.5671	0.1860
B	0.5163	0.1740
C	0.5450	0.1850
D	0.5649	0.1800
E	0.5280	0.1800
F	0.5735	0.1830