wwPDB EM Validation Summary Report ⓘ

Nov 9, 2022 – 03:24 AM JST

PDB ID	:	6ID1
EMDB ID	:	EMD-9647
Title	:	Cryo-EM structure of a human intron lariat spliceosome after Prp43 loaded (ILS2 complex) at 2.9 angstrom resolution
Authors	:	Zhang, X.; Zhan, X.; Yan, C.; Shi, Y.
Deposited on	:	2018-09-07
Resolution	:	2.86 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:

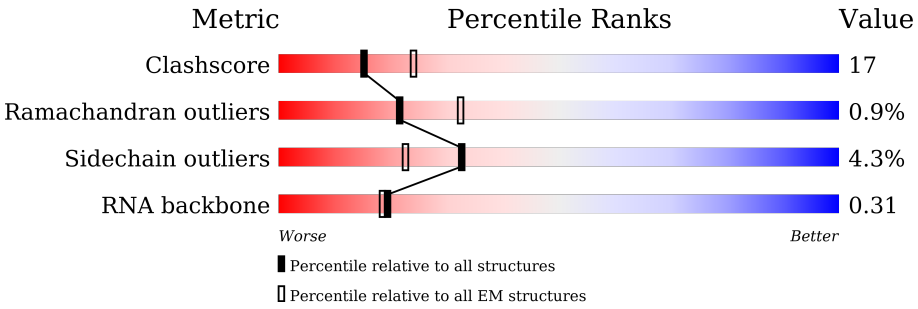
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.86 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
RNA backbone	4643	859

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	2335	70% 14% • 15%
2	B	117	• 24% 28% 32% 16%
3	C	972	• 70% 20% • 9%
4	E	357	34% 36% 14% • 15%
5	F	107	• 36% 31% 15% 8% 9%
6	J	848	30% 60% 7% 33%
7	L	802	23% 48% 9% • 41%

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Mol	Chain	Length	Quality of chain
8	M	243	44% 9% 47%
9	N	144	82% 17%
10	O	420	5% 43% 23% 31%
11	P	229	47% 5% 48%
12	R	536	39% 10% 49%
13	S	166	5% 70% 25%
14	T	514	47% 14% 38%
15	W	579	21% 5% 73%
16	G	272	7% 9% 7% 75%
17	H	188	49% 12% 34% 24% 28%
18	U	894	28% 9% 61%
19	a	126	5% 64% 36%
19	h	126	63% 63% 37%
20	b	231	6% 37% 63%
20	i	231	36% 37% 63%
21	c	119	69% 31%
21	j	119	68% 69% 31%
22	d	118	10% 81% 18%
22	k	118	72% 71% 28%
23	f	86	9% 86% 14%
23	m	86	86% 86% 14%
24	e	92	11% 86% 14%
24	l	92	86% 86% 14%
25	g	76	14% 97%
25	n	76	87% 88% 12%

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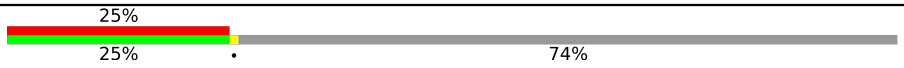
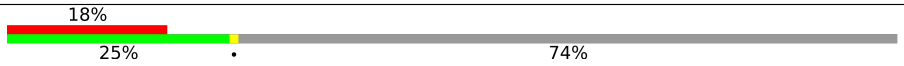
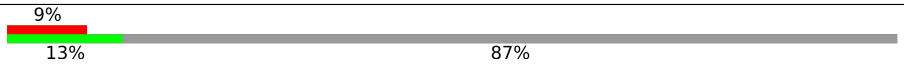
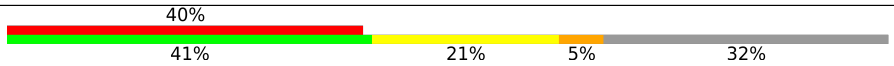
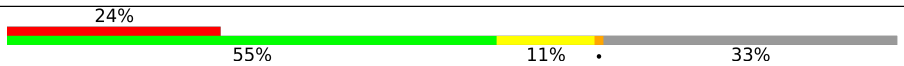
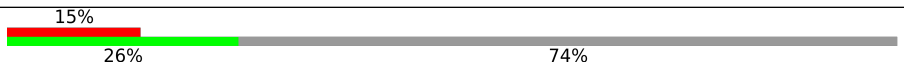
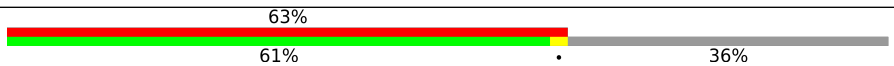
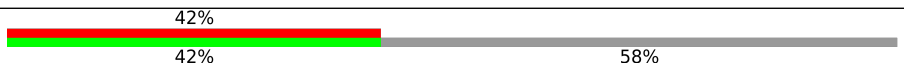
Mol	Chain	Length	Quality of chain
26	q	504	
26	r	504	
26	s	504	
26	t	504	
27	K	225	
28	I	855	
29	Q	1485	
30	y	301	
31	o	255	
32	p	225	
33	V	795	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	GTP	C	1500	-	-	X	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 79882 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 Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1981	16477	10621	2883	2902	71	0	0

- Molecule 2 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	98	2060	923	341	698	98	0	0

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	888	7022	4494	1172	1322	34	0	0

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	303	2366	1487	415	451	13	0	0

- Molecule 5 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	F	97	2075	928	381	669	97	0	0

- Molecule 6 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	568	3817	2379	717	715	6	0	0

- Molecule 7 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	475	Total	C	N	O	S	0	0
			3369	2094	634	635	6		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	130	Total	C	N	O	S	0	0
			1098	684	204	208	2		

- Molecule 9 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 10 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	290	Total	C	N	O	S	0	0
			2340	1469	415	436	20		

- Molecule 11 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	118	Total	C	N	O	S	0	0
			985	601	194	188	2		

- Molecule 12 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	R	272	Total	C	N	O	P	S	0	0
			2165	1357	393	401	2	12		

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 14 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	317	Total	C	N	O	S	0	0
			2496	1574	453	461	8		

- Molecule 15 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	158	Total	C	N	O	S	0	0
			1276	803	217	252	4		

- Molecule 16 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	68	Total	C	N	O	P	0	0
			1201	529	148	456	68		

- Molecule 17 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	136	Total	C	N	O	P	0	0
			2884	1289	496	963	136		

- Molecule 18 is a protein called CWF19-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	347	Total	C	N	O	S	0	0
			2864	1817	496	529	22		

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	a	81	Total	C	N	O	0	0
			399	237	81	81		
19	h	80	Total	C	N	O	0	0
			393	233	80	80		

- Molecule 20 is a protein called Small nuclear ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	b	86	Total	C	N	O	0	0
			424	252	86	86		
20	i	86	Total	C	N	O	0	0
			424	252	86	86		

- Molecule 21 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	c	82	Total 406	C 242	N 82	O 82	0	0
21	j	82	Total 406	C 242	N 82	O 82	0	0

- Molecule 22 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	d	97	Total 480	C 286	N 97	O 97	0	0
22	k	85	Total 422	C 252	N 85	O 85	0	0

- Molecule 23 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	f	74	Total 361	C 213	N 74	O 74	0	0
23	m	74	Total 361	C 213	N 74	O 74	0	0

- Molecule 24 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	e	79	Total 391	C 233	N 79	O 79	0	0
24	l	79	Total 391	C 233	N 79	O 79	0	0

- Molecule 25 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	g	74	Total 363	C 215	N 74	O 74	0	0
25	n	67	Total 329	C 195	N 67	O 67	0	0

- Molecule 26 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	q	132	Total	C	N	O	0	0
			659	395	132	132		
26	r	131	Total	C	N	O	0	0
			654	392	131	131		
26	s	67	Total	C	N	O	0	0
			335	201	67	67		
26	t	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 27 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	K	152	Total	C	N	O	S	0	0
			980	612	177	189	2		

- Molecule 28 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	I	576	Total	C	N	O	S	0	0
			2875	1716	579	579	1		

- Molecule 29 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Q	1322	Total	C	N	O	0	0
			6554	3910	1322	1322		

- Molecule 30 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	y	79	Total	C	N	O	0	0
			390	232	79	79		

- Molecule 31 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	o	162	Total	C	N	O	0	0
			804	480	162	162		

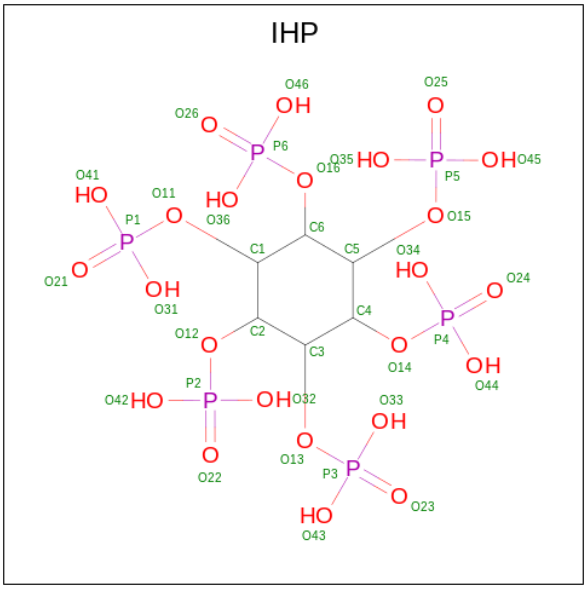
- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
32	p	94	Total	C	N	O	0	0
			464	276	94	94		

- Molecule 33 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX15.

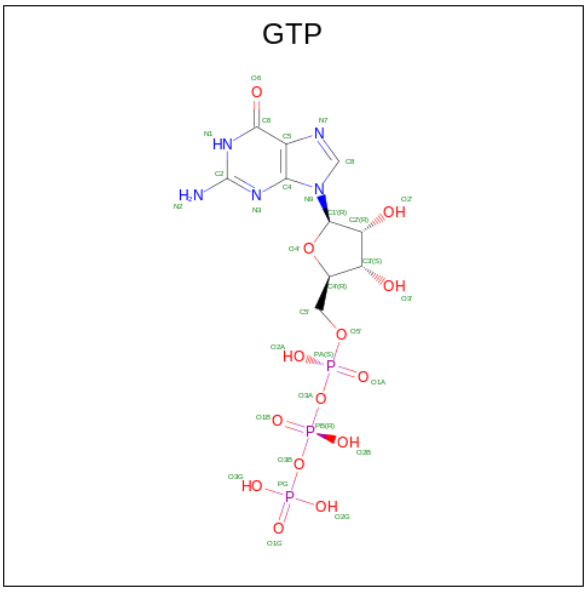
Mol	Chain	Residues	Atoms				AltConf	Trace
33	V	663	Total	C	N	O	0	0
			3285	1959	663	663		

- Molecule 34 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 35 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
35	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	C	1	Total	Mg	0
			1	1	
36	F	6	Total	Mg	0
			6	6	

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

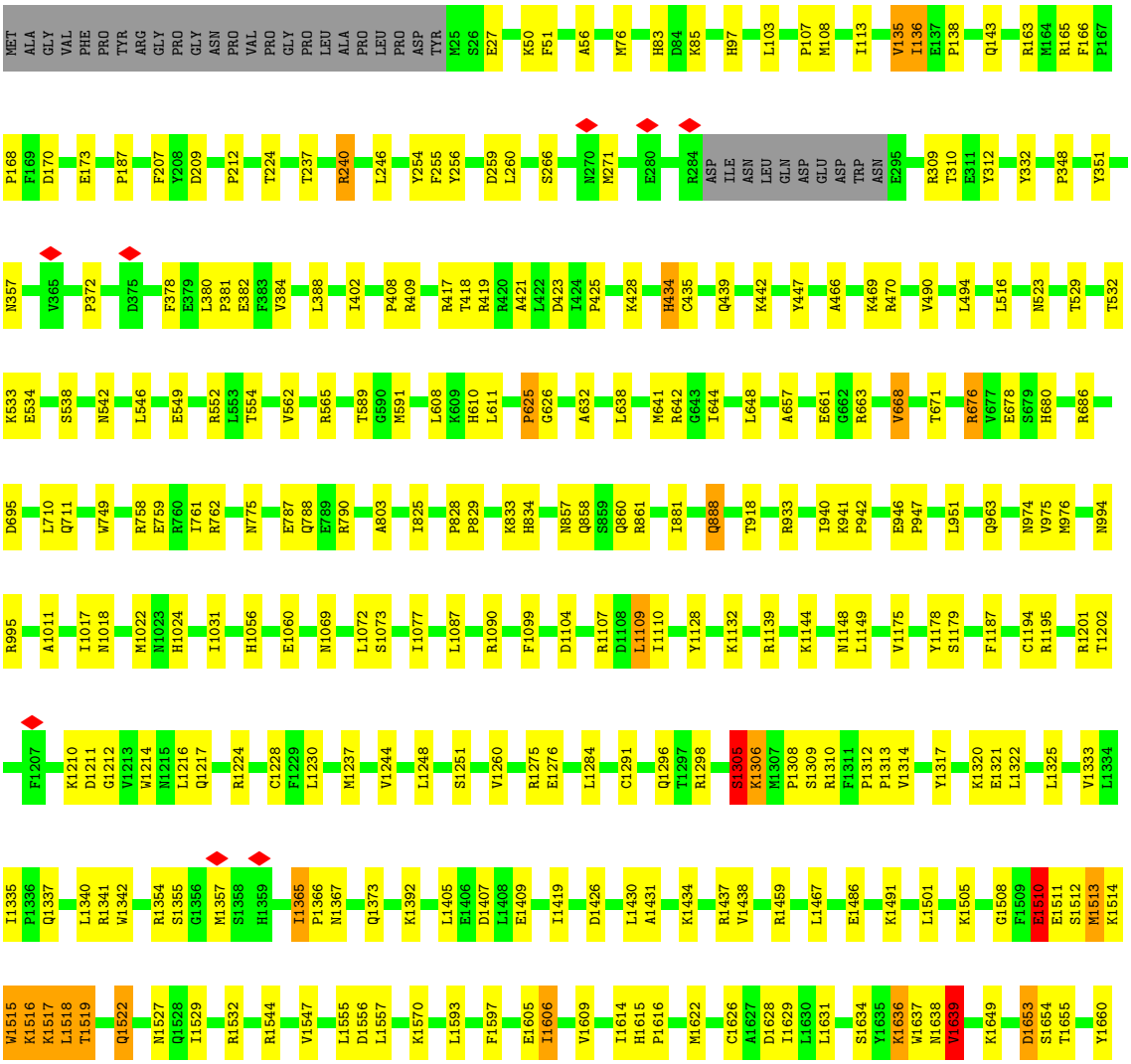
Mol	Chain	Residues	Atoms		AltConf
37	N	3	Total	Zn	0
			3	3	
37	O	3	Total	Zn	0
			3	3	
37	U	1	Total	Zn	0
			1	1	

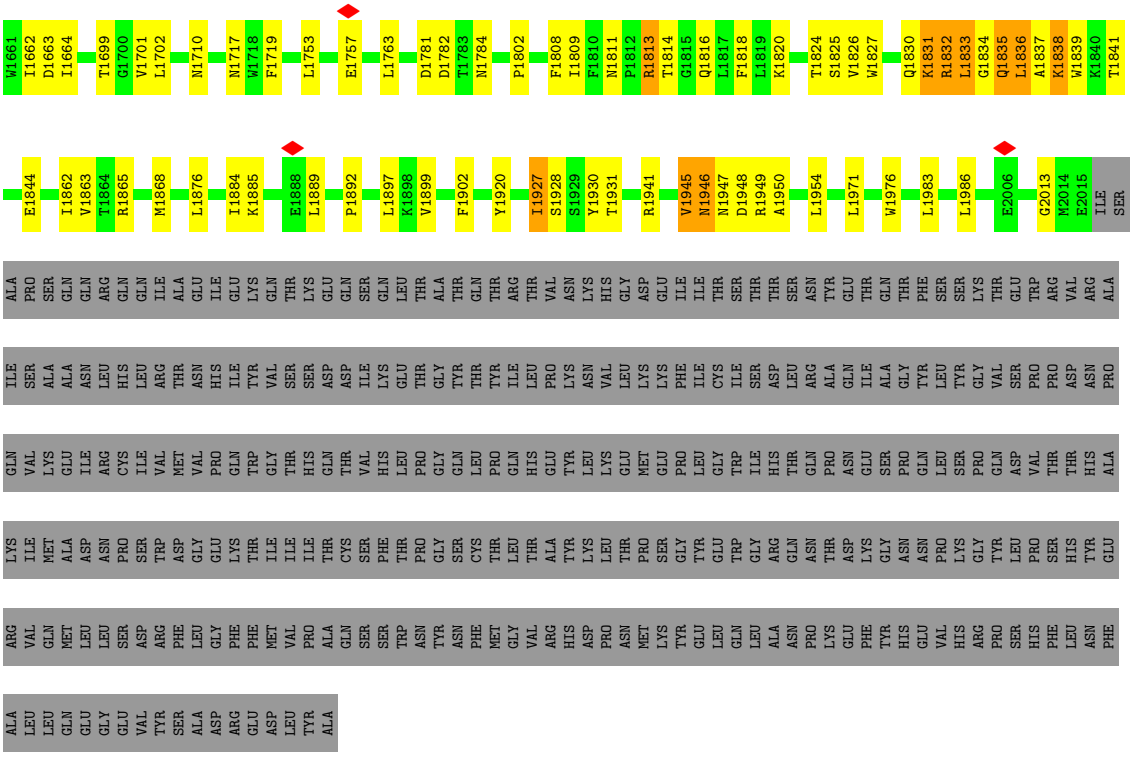
3 Residue-property plots (i)

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: Pre-mRNA-processing-splicing factor 8

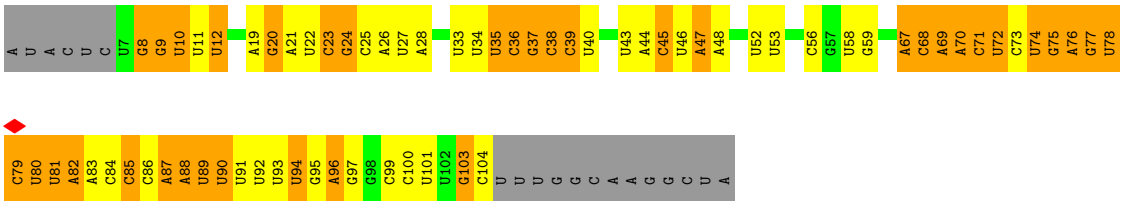
Chain A:





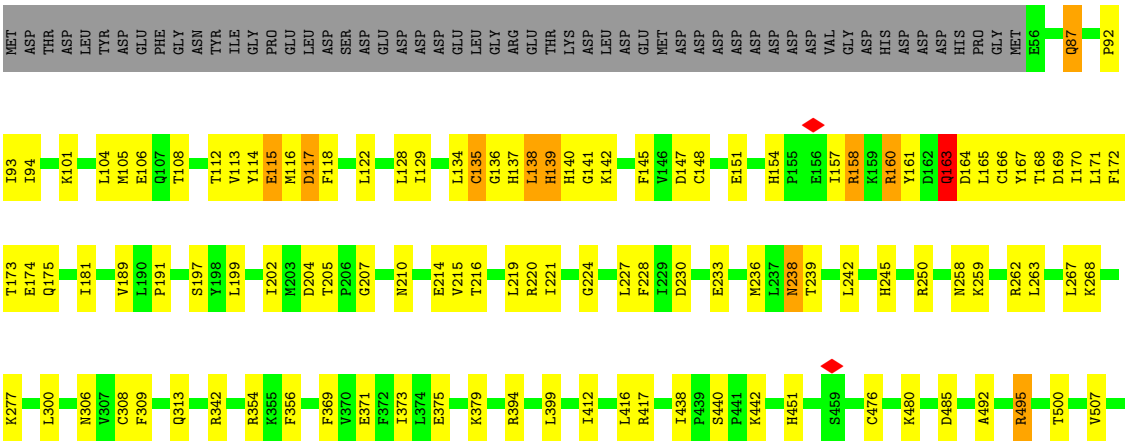
• Molecule 2: U5snRNA

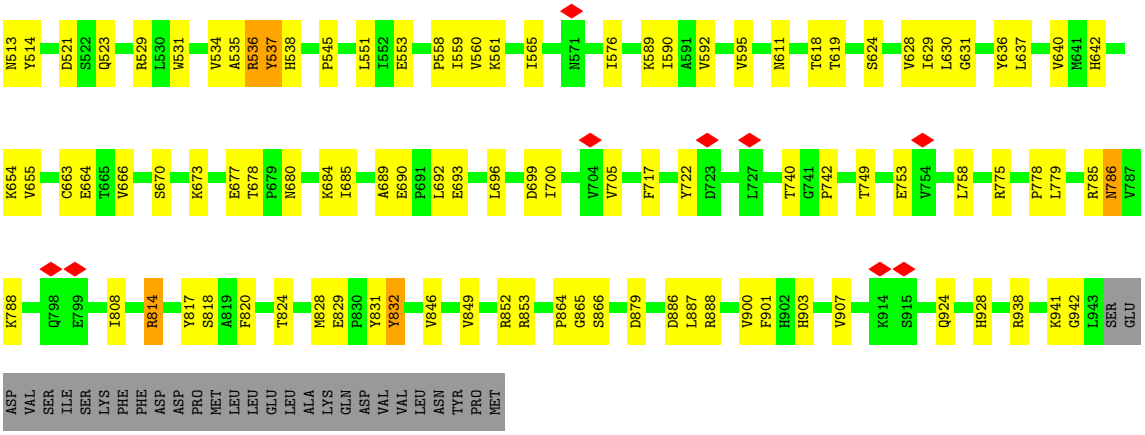
Chain B:



• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

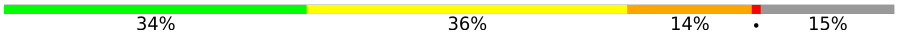
Chain C:

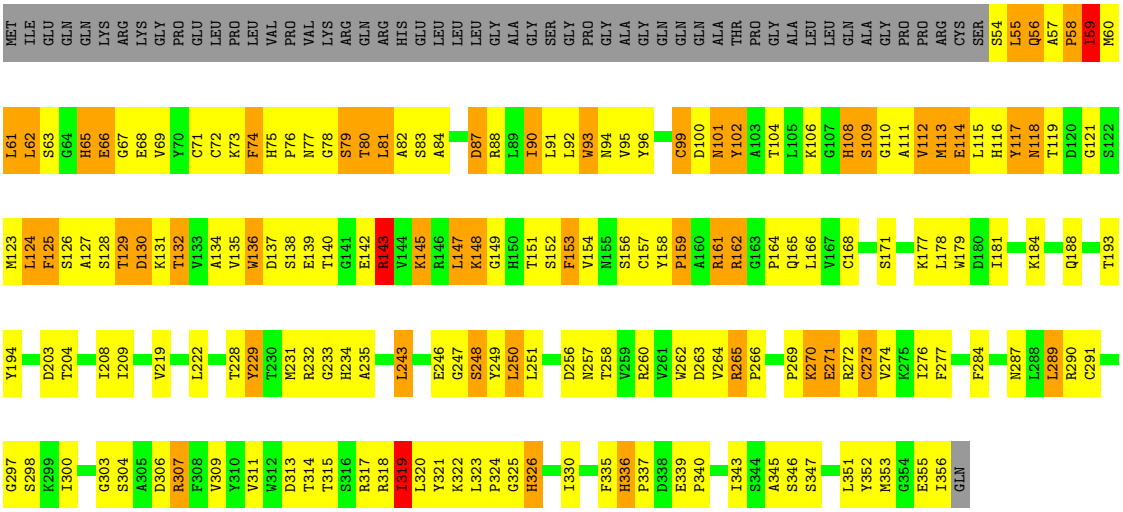




• Molecule 4: U5 small nuclear ribonucleoprotein 40 kDa protein

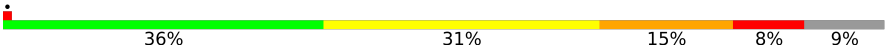
Chain E:

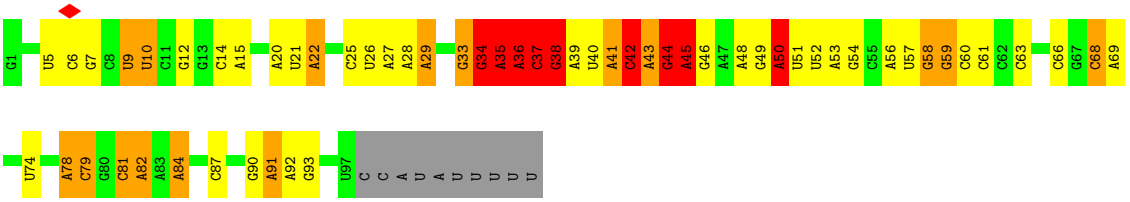




• Molecule 5: U6snRNA

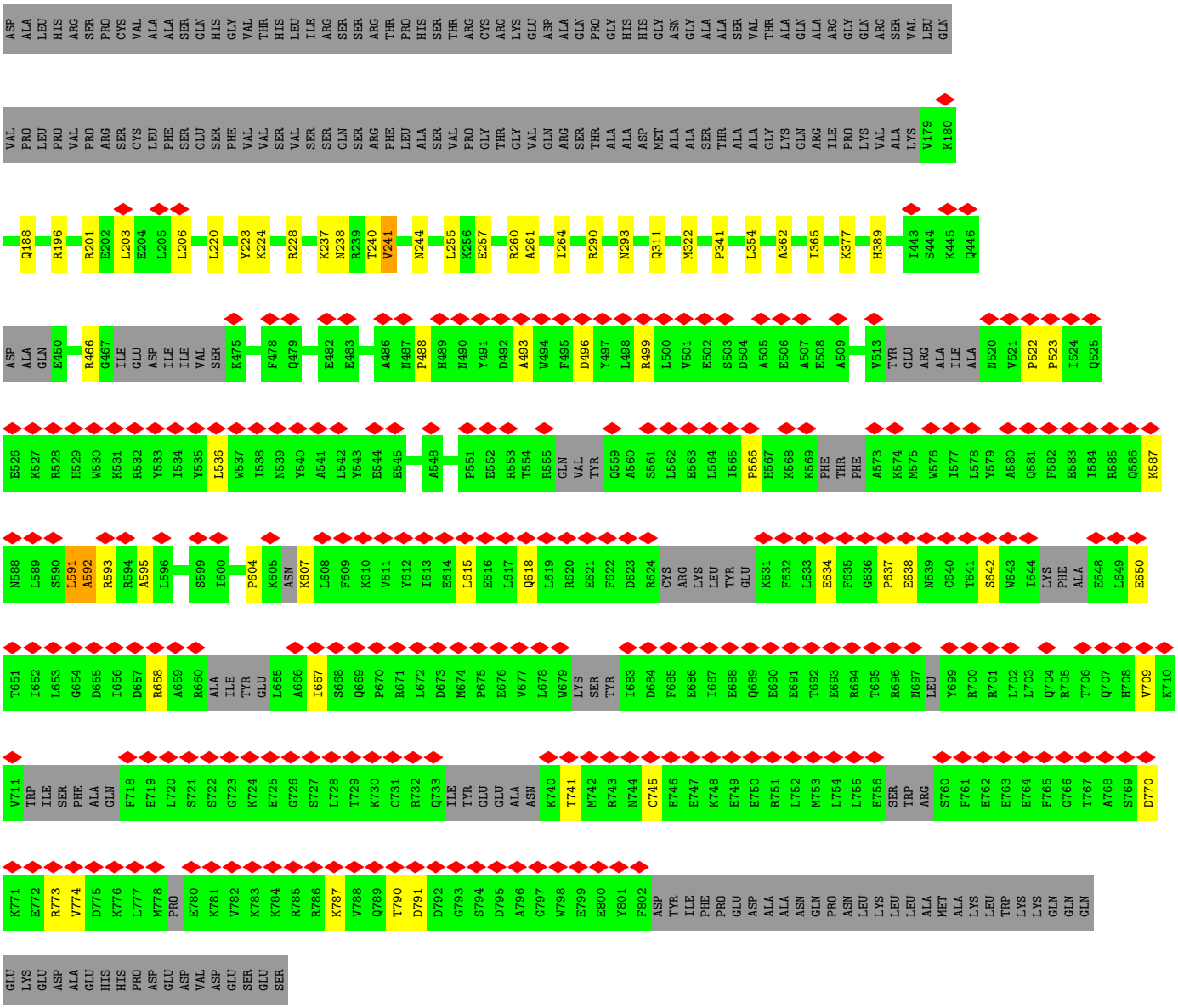
Chain F:





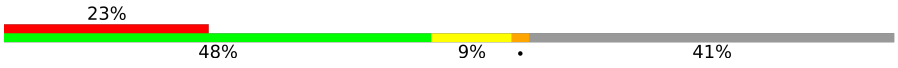
• Molecule 6: Crooked neck-like protein 1

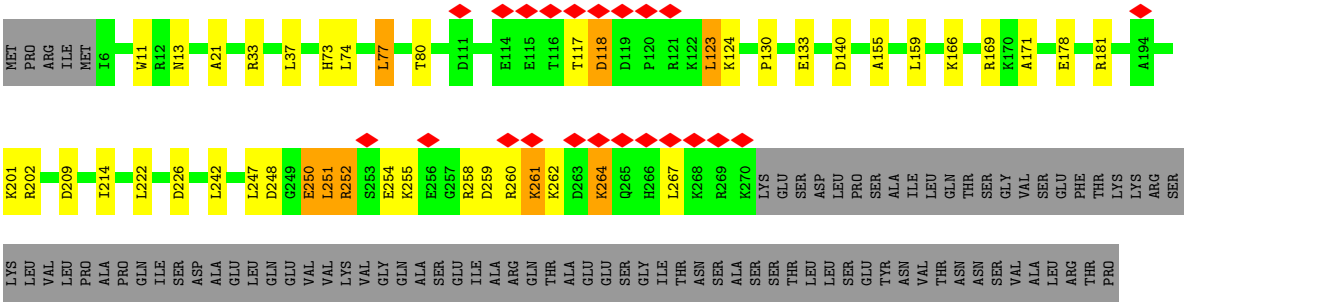
Chain J:

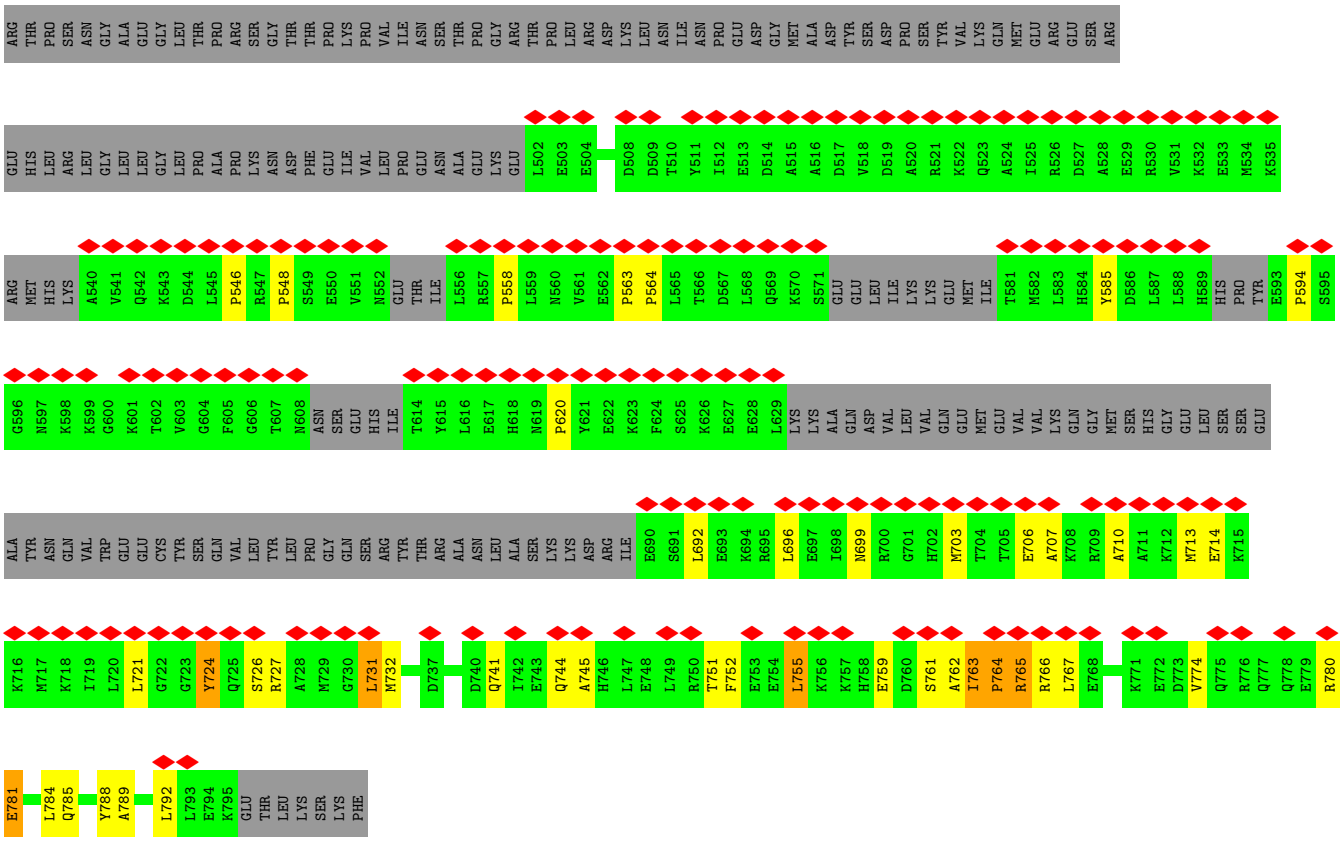


• Molecule 7: Cell division cycle 5-like protein

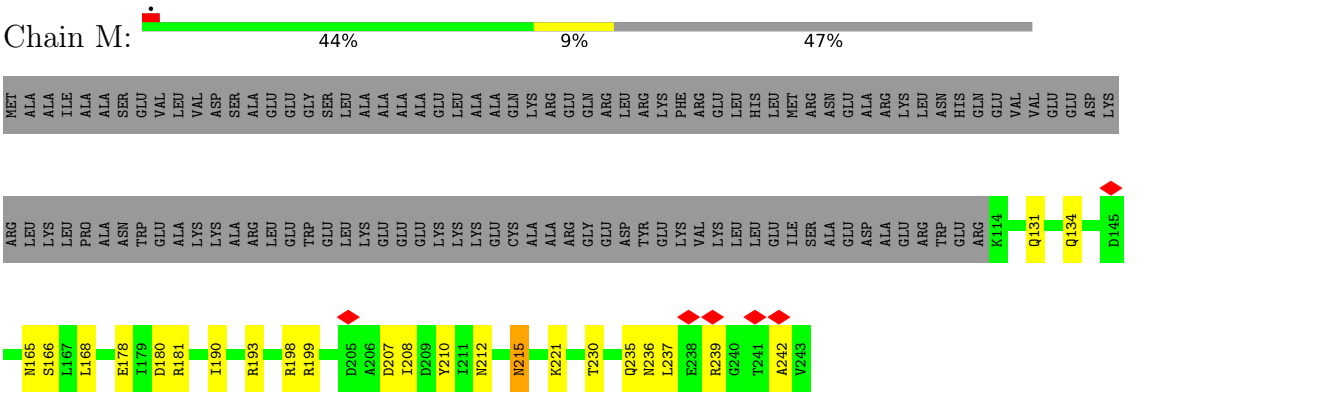
Chain L:





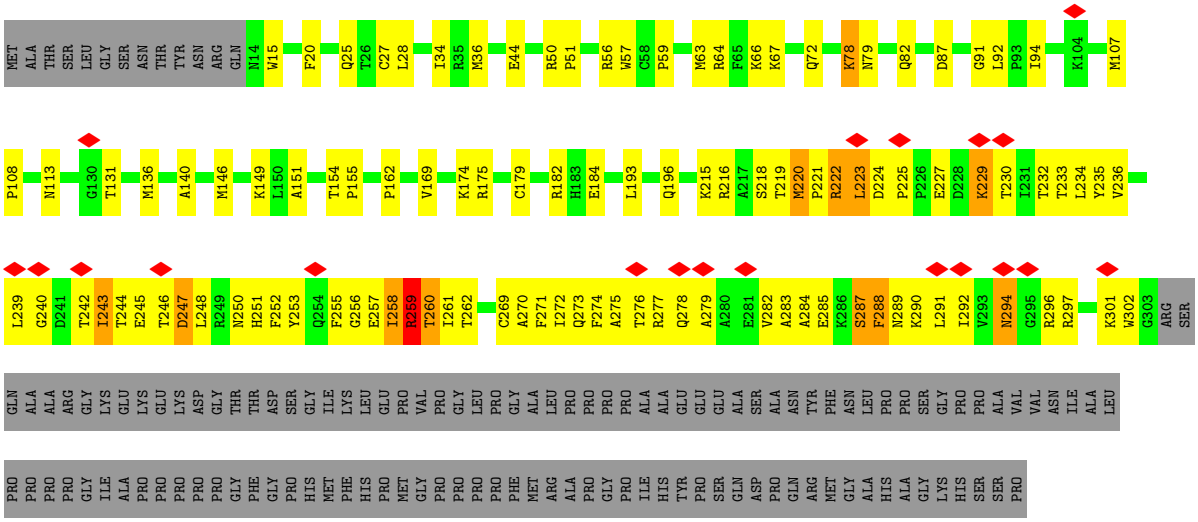


• Molecule 8: Pre-mRNA-splicing factor SYF2



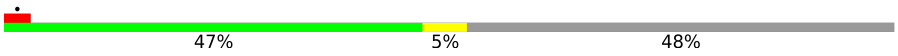
• Molecule 9: Protein BUD31 homolog

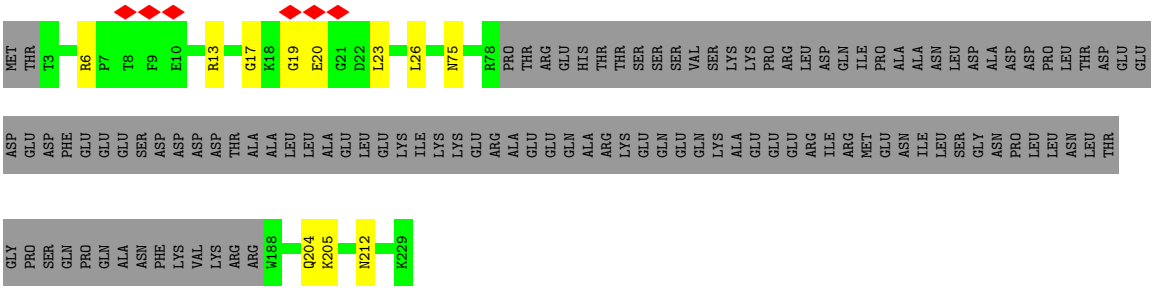
• Molecule 10: Pre-mRNA-splicing factor RBM22



• Molecule 11: Spliceosome-associated protein CWC15 homolog

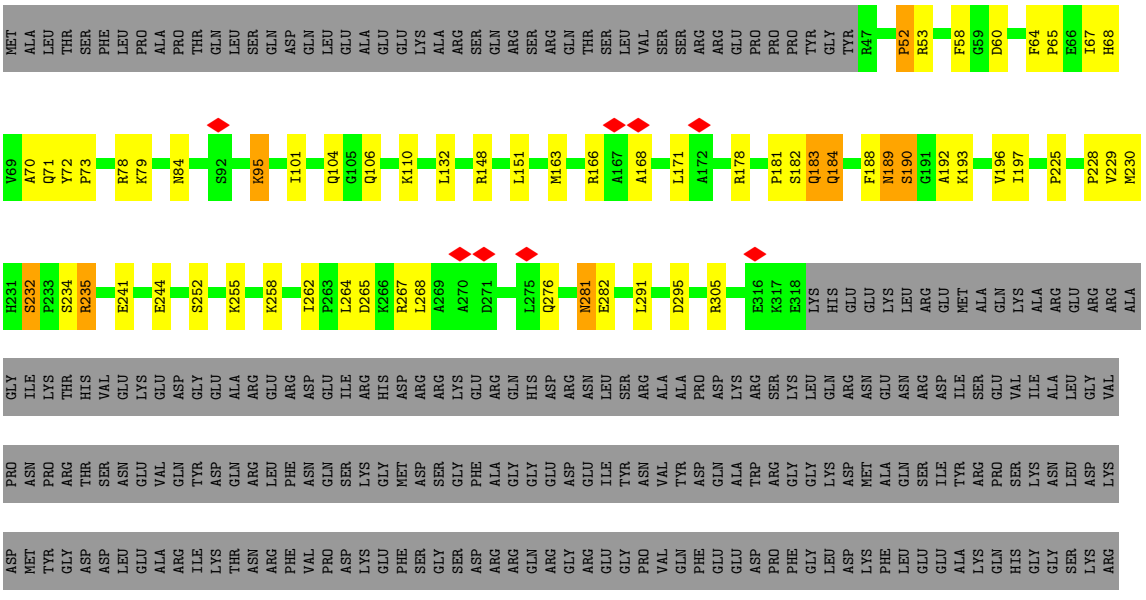
Chain P:





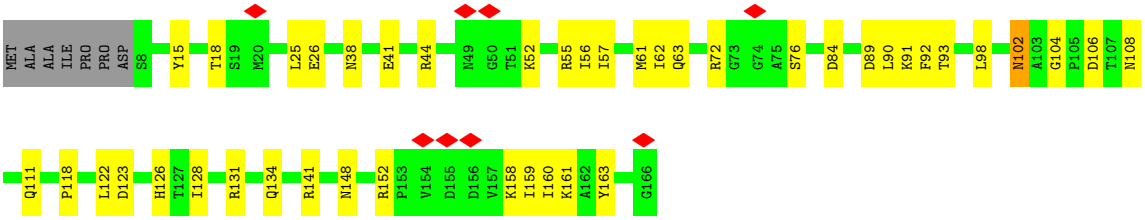
• Molecule 12: SNW domain-containing protein 1

Chain R:



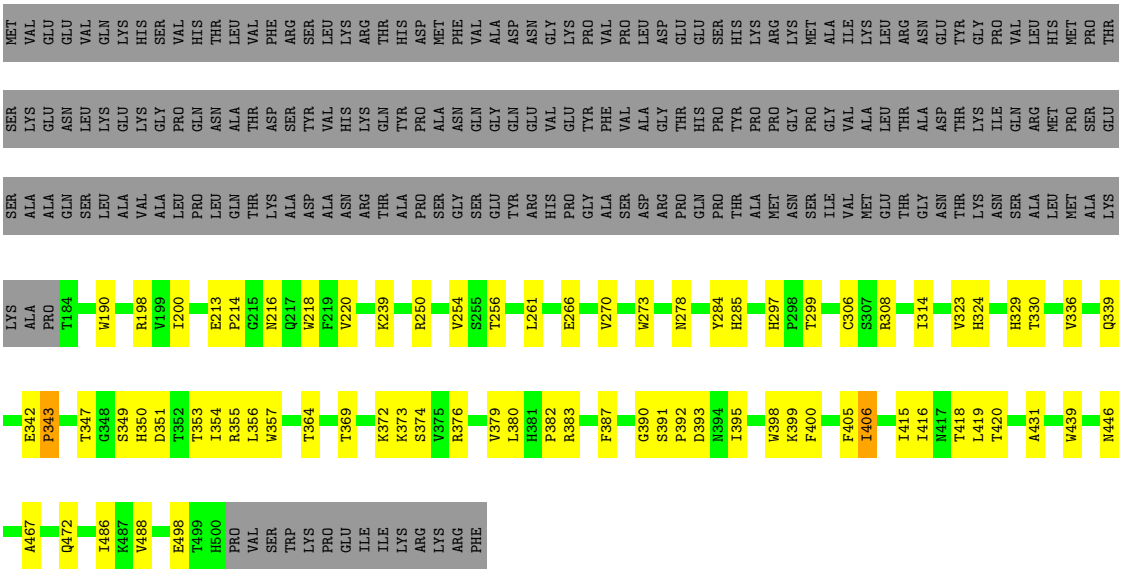
• Molecule 13: Peptidyl-prolyl cis-trans isomerase-like 1

Chain S:



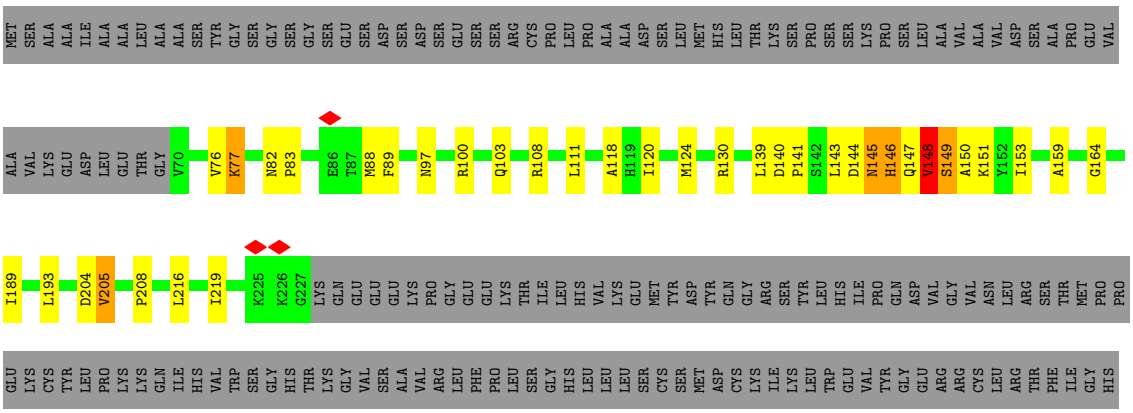
• Molecule 14: Pleiotropic regulator 1

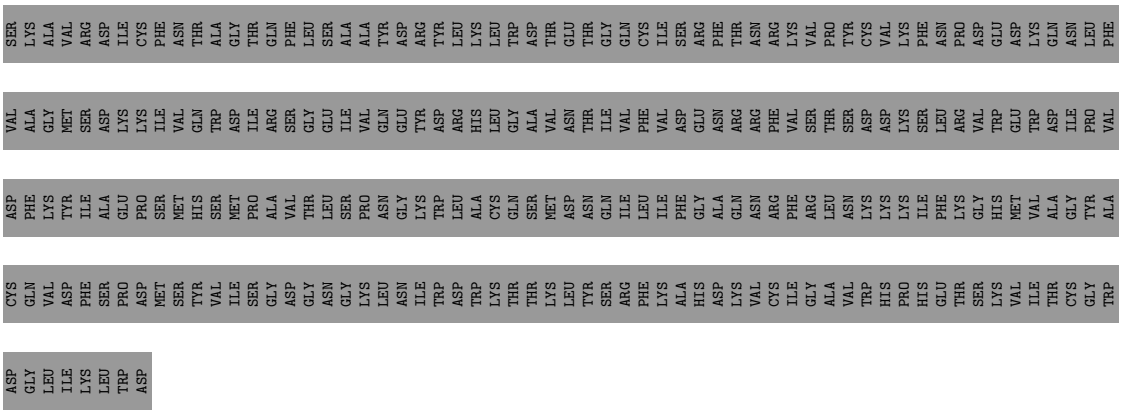
Chain T:



• Molecule 15: Pre-mRNA-processing factor 17

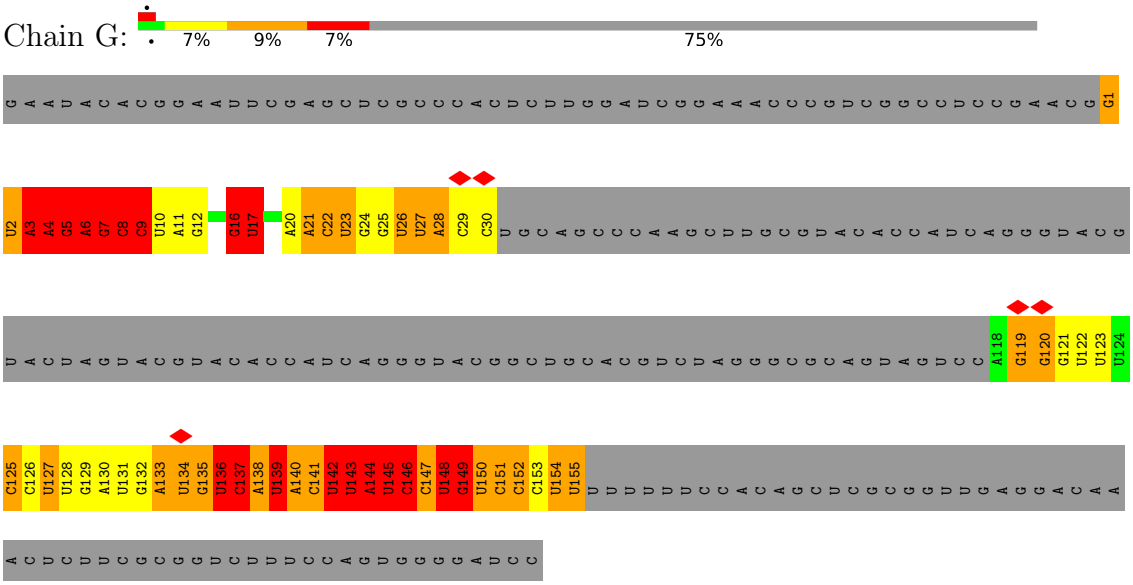
Chain W:





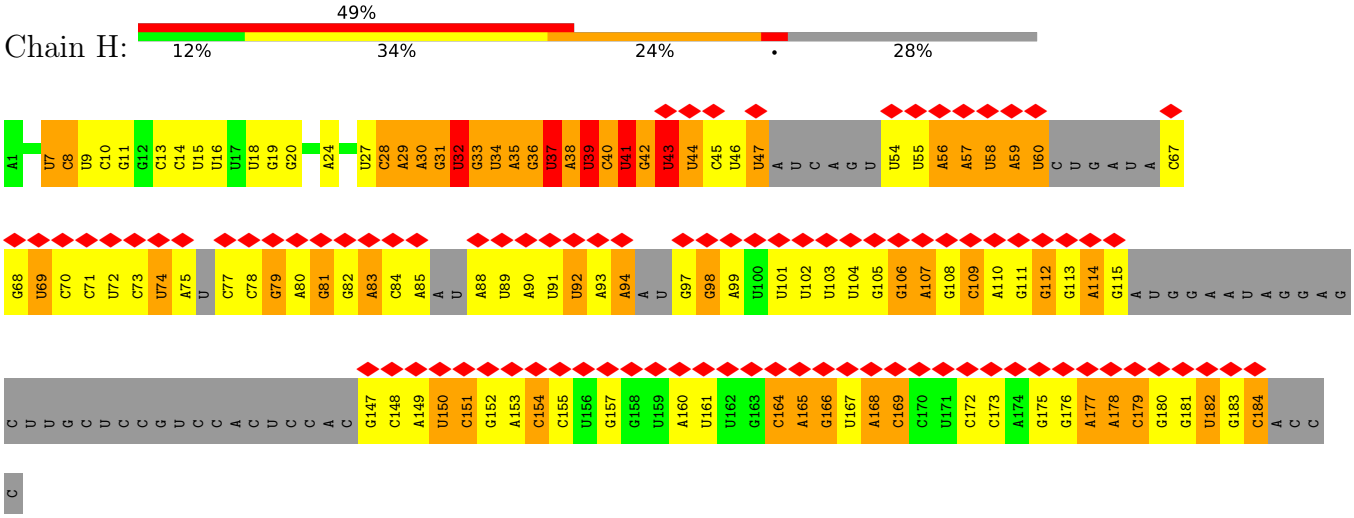
• Molecule 16: pre-mRNA

Chain G:



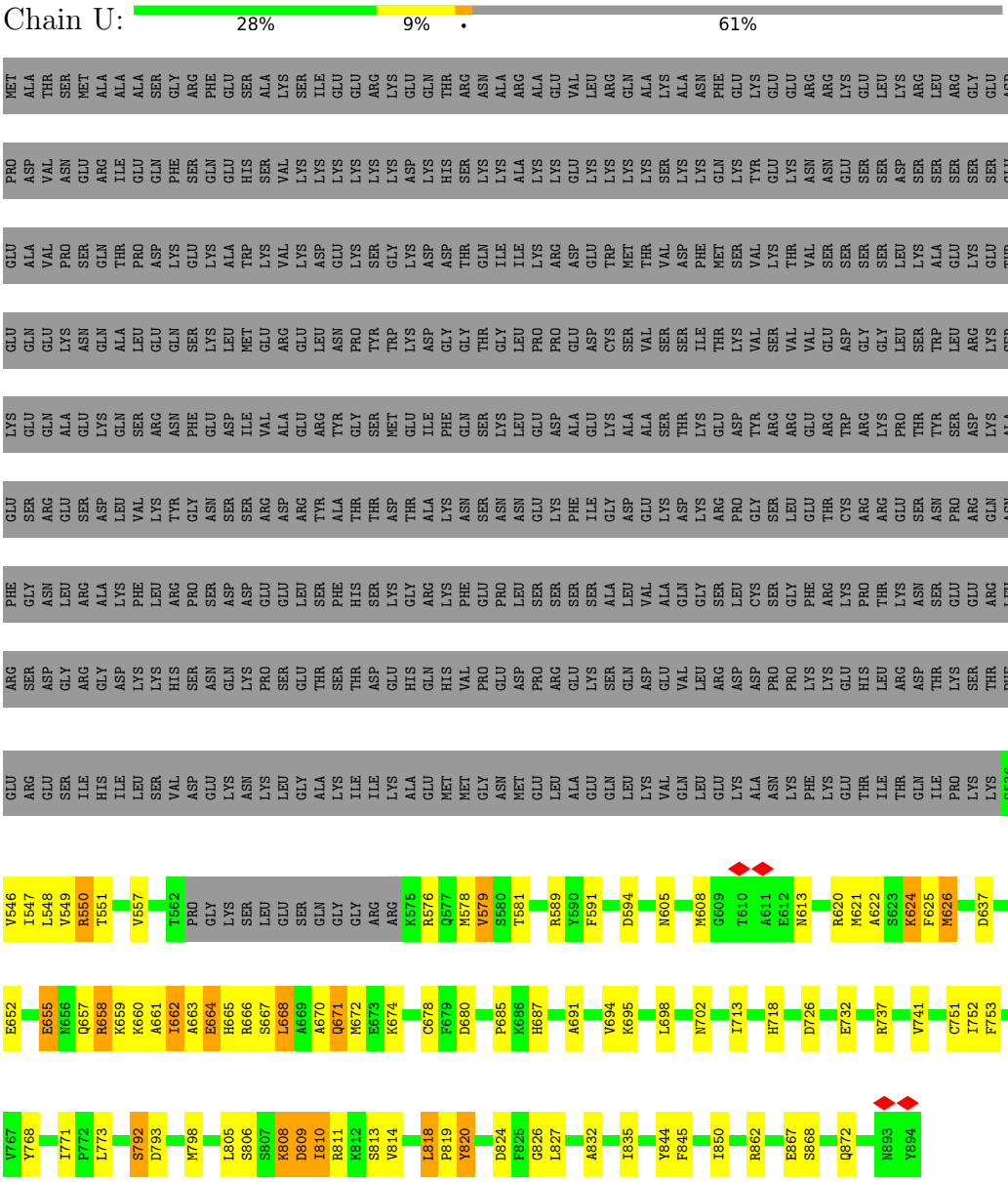
• Molecule 17: U2snRNA

Chain H:



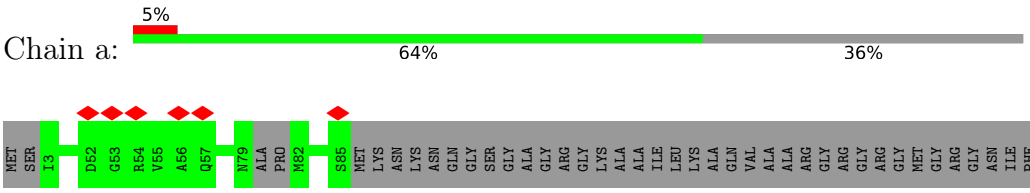
• Molecule 18: CWF19-like protein 2

Chain U:



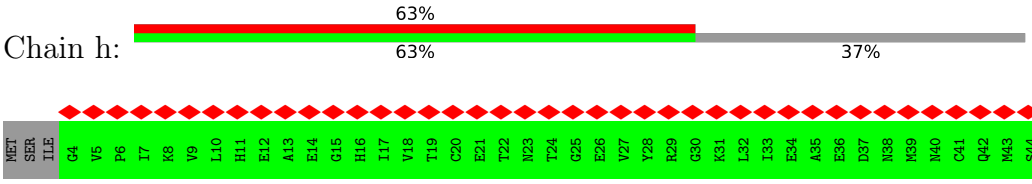
• Molecule 19: Small nuclear ribonucleoprotein Sm D3

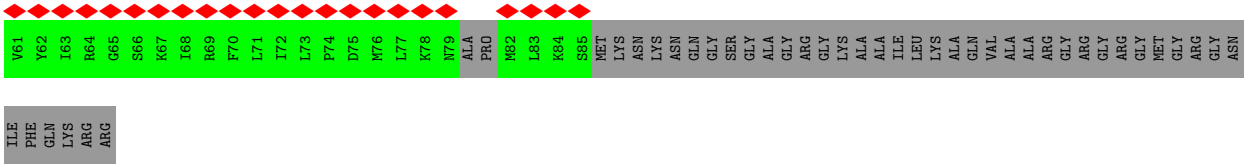
Chain a:



• Molecule 19: Small nuclear ribonucleoprotein Sm D3

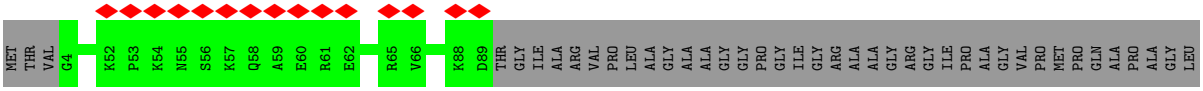
Chain h:





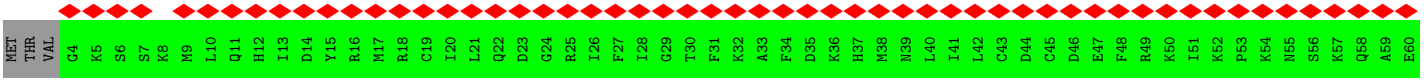
• Molecule 20: Small nuclear ribonucleoprotein-associated protein

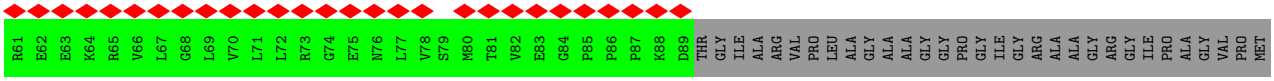
Chain b:

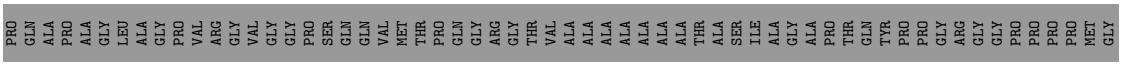


• Molecule 20: Small nuclear ribonucleoprotein-associated protein

Chain i:

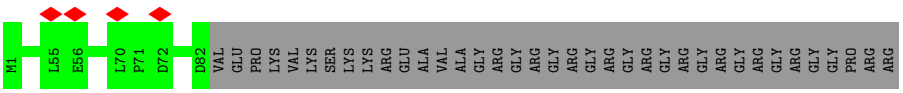






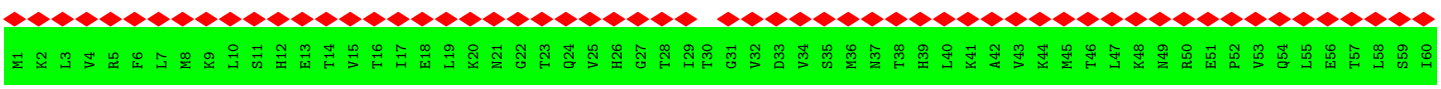
• Molecule 21: Small nuclear ribonucleoprotein Sm D1

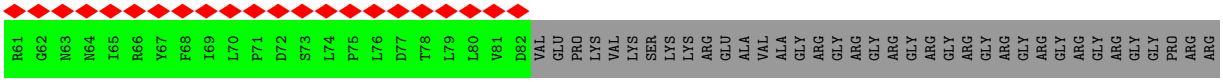
Chain c:



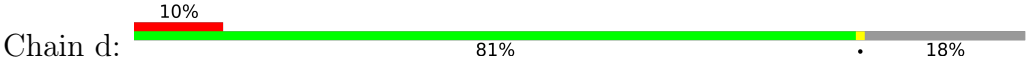
• Molecule 21: Small nuclear ribonucleoprotein Sm D1

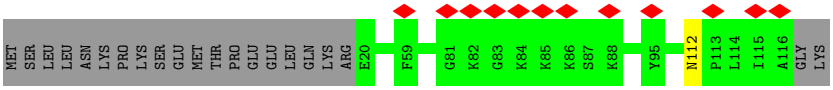
Chain j:



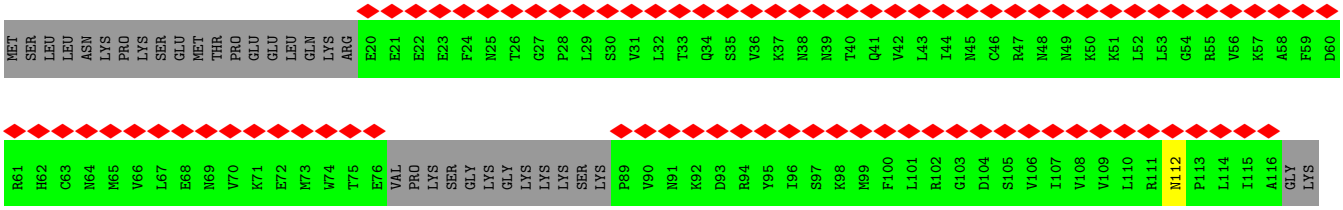


• Molecule 22: Small nuclear ribonucleoprotein Sm D2

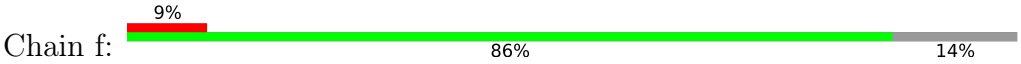


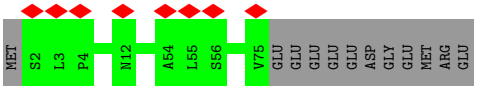


• Molecule 22: Small nuclear ribonucleoprotein Sm D2

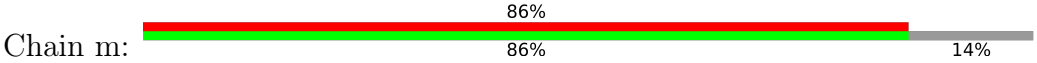


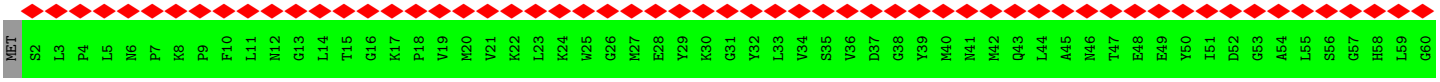
• Molecule 23: Small nuclear ribonucleoprotein F

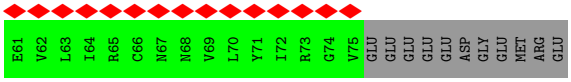




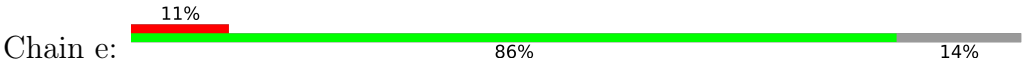
• Molecule 23: Small nuclear ribonucleoprotein F

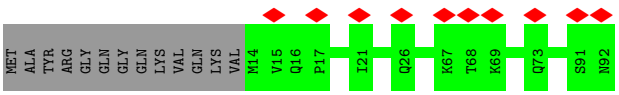






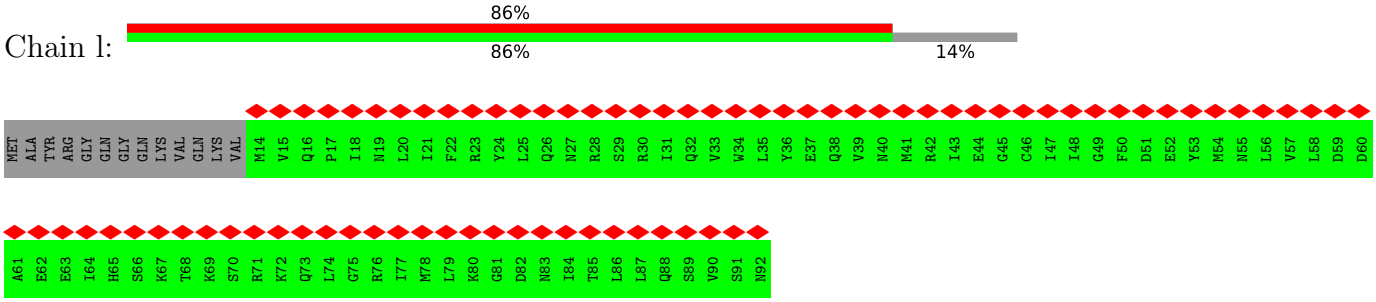
• Molecule 24: Small nuclear ribonucleoprotein E





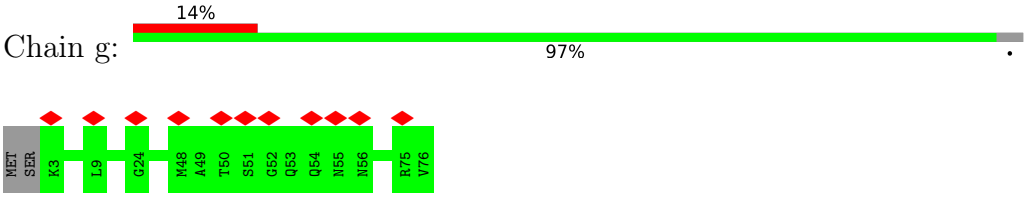
• Molecule 24: Small nuclear ribonucleoprotein E

Chain l:



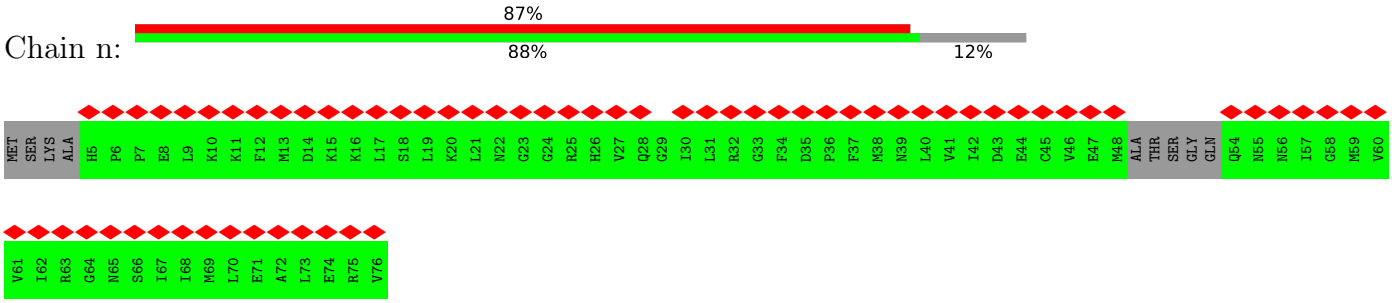
• Molecule 25: Small nuclear ribonucleoprotein G

Chain g:



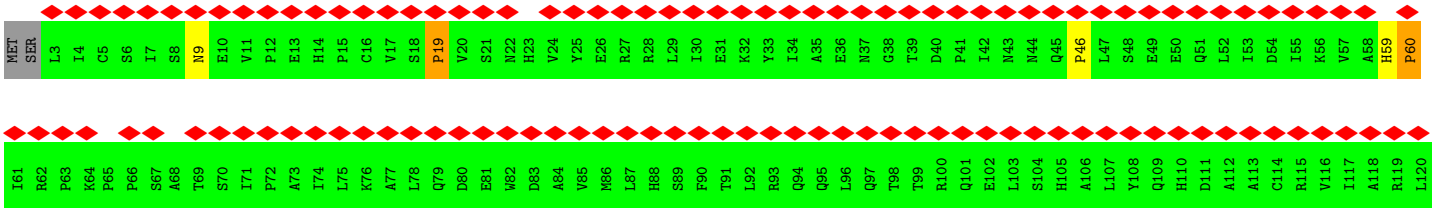
• Molecule 25: Small nuclear ribonucleoprotein G

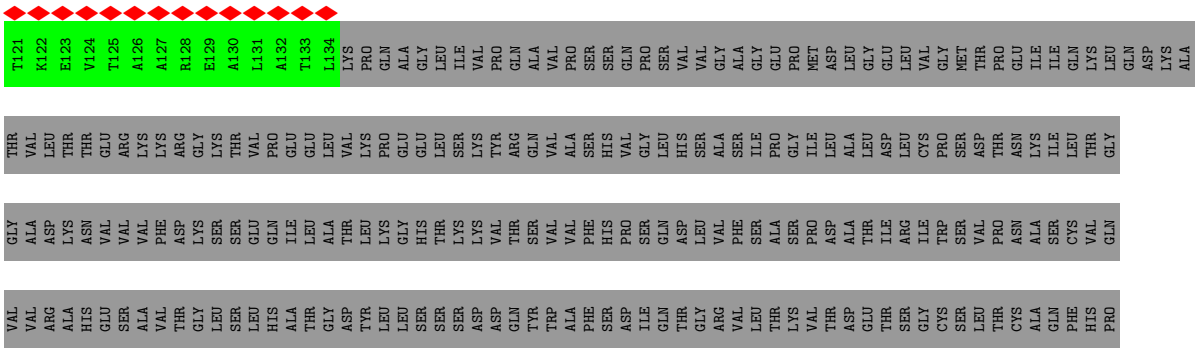
Chain n:

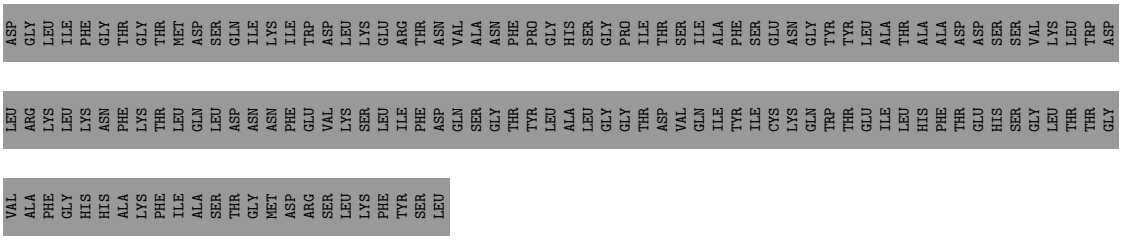


• Molecule 26: Pre-mRNA-processing factor 19

Chain q:

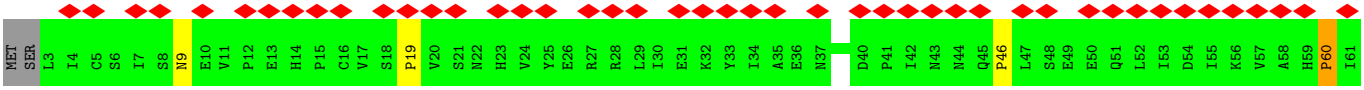


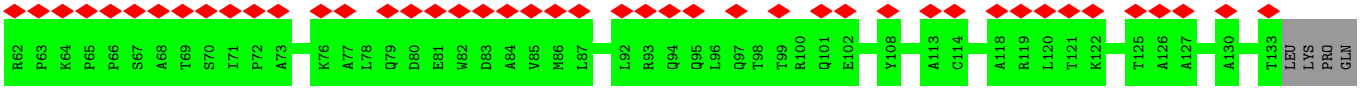




• Molecule 26: Pre-mRNA-processing factor 19

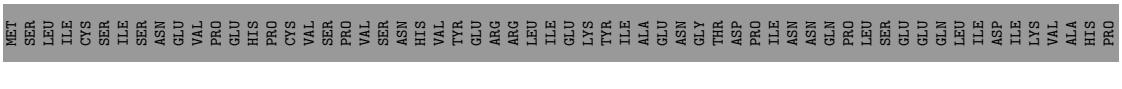
Chain r:

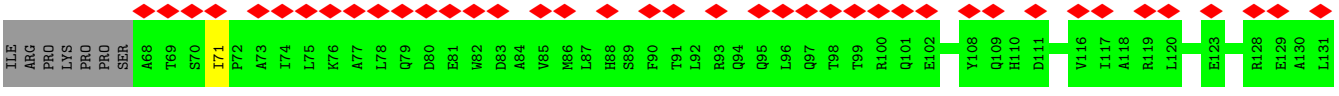


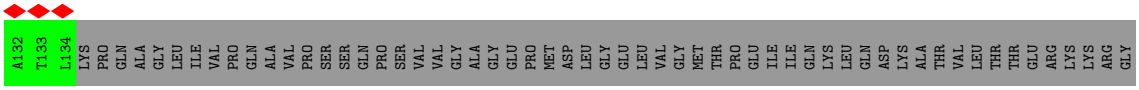


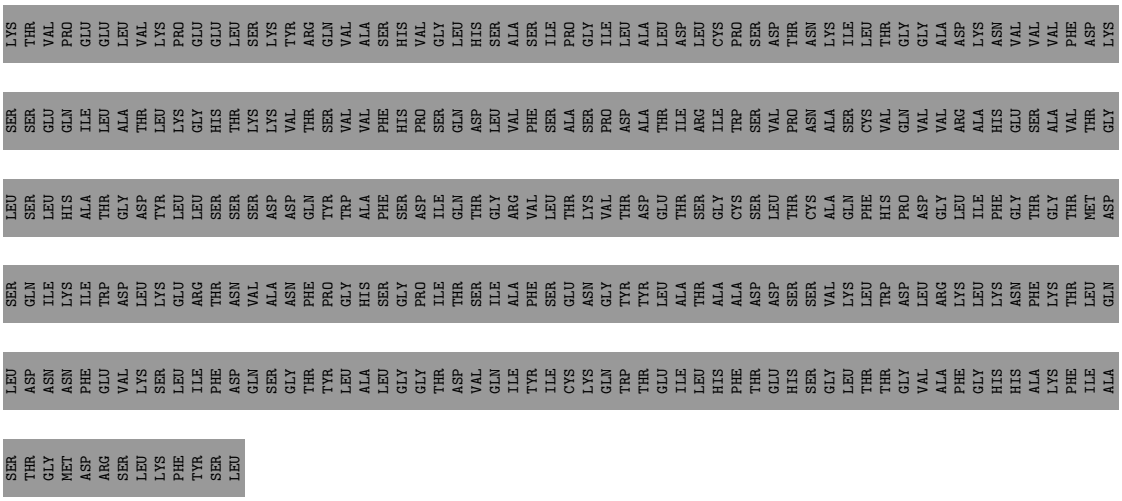
• Molecule 26: Pre-mRNA-processing factor 19

Chain s:



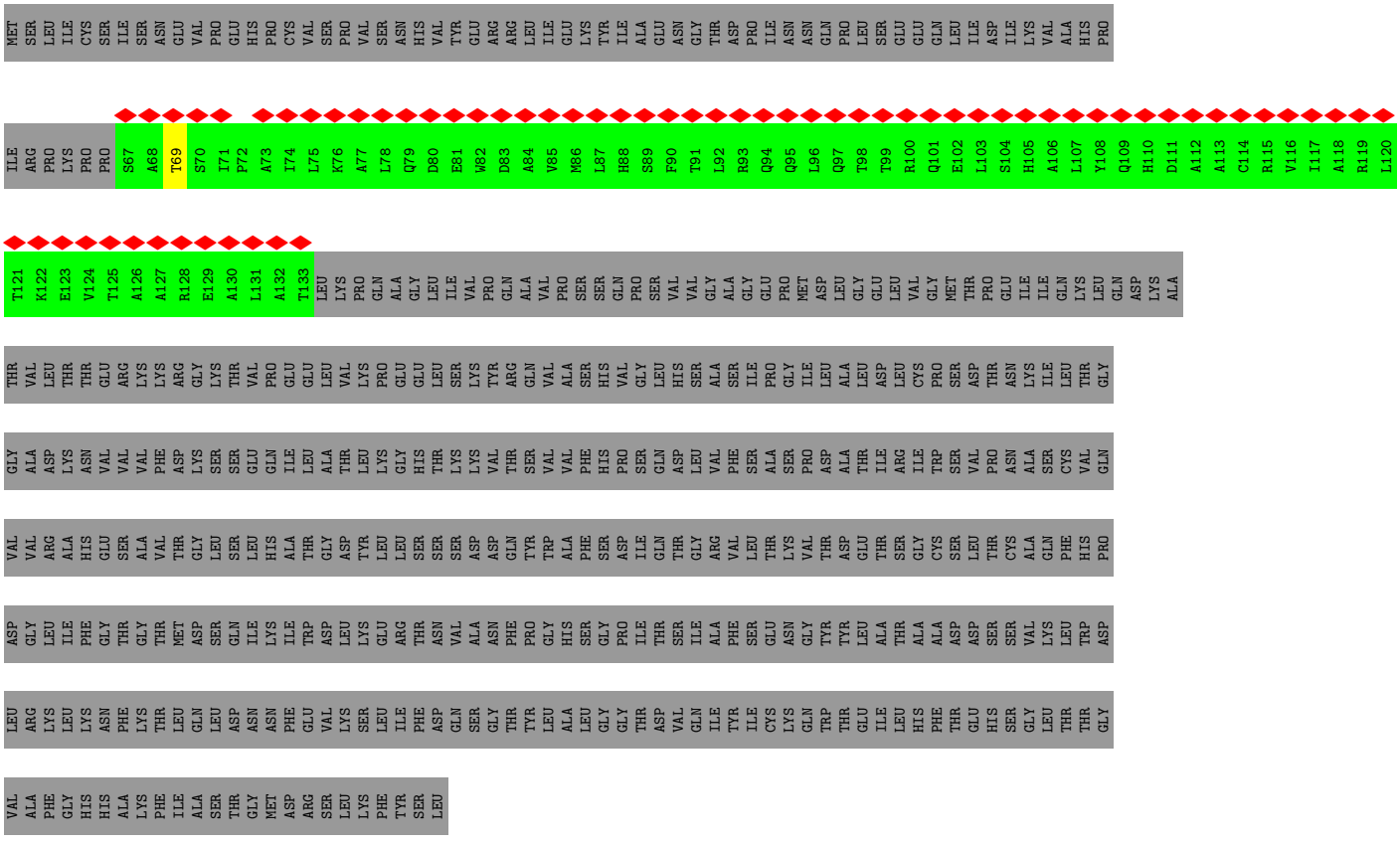






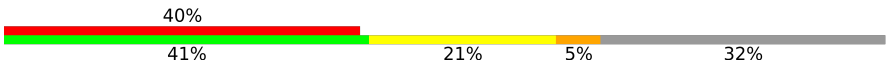
• Molecule 26: Pre-mRNA-processing factor 19

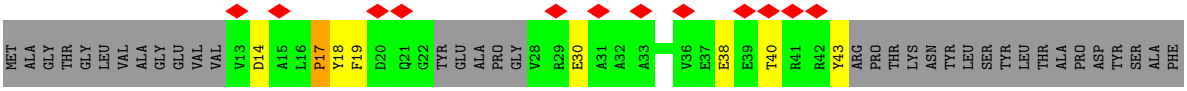
Chain t:

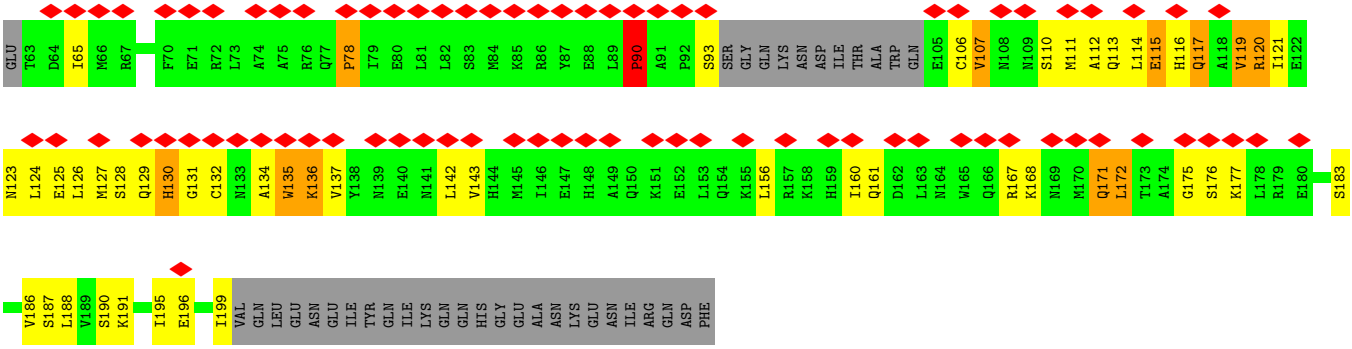


• Molecule 27: Pre-mRNA-splicing factor SPF27

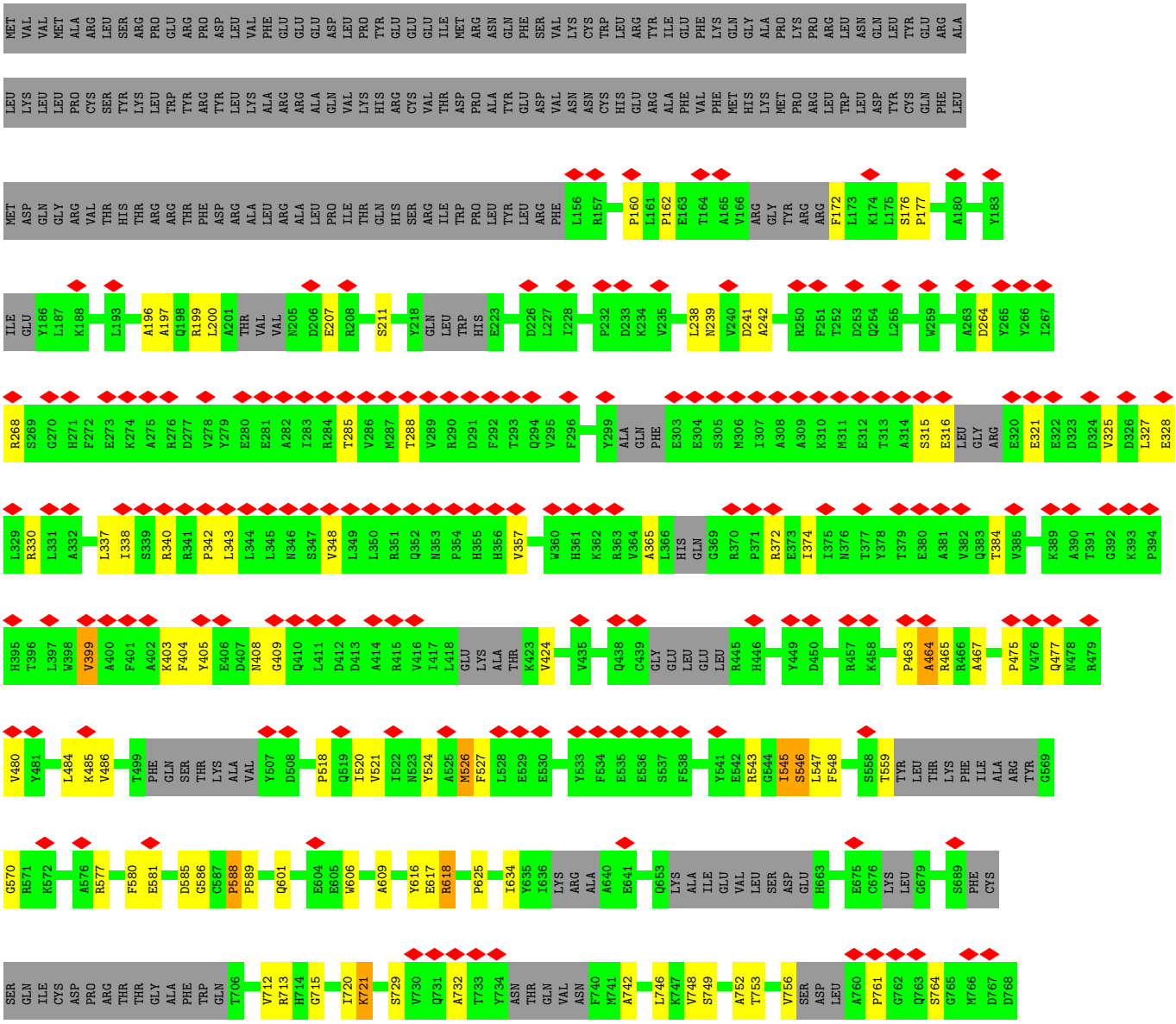
Chain K:

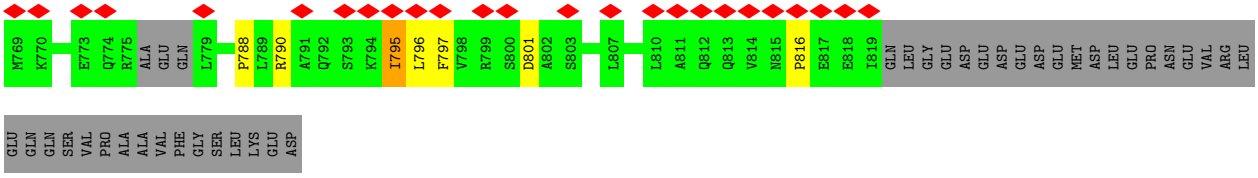






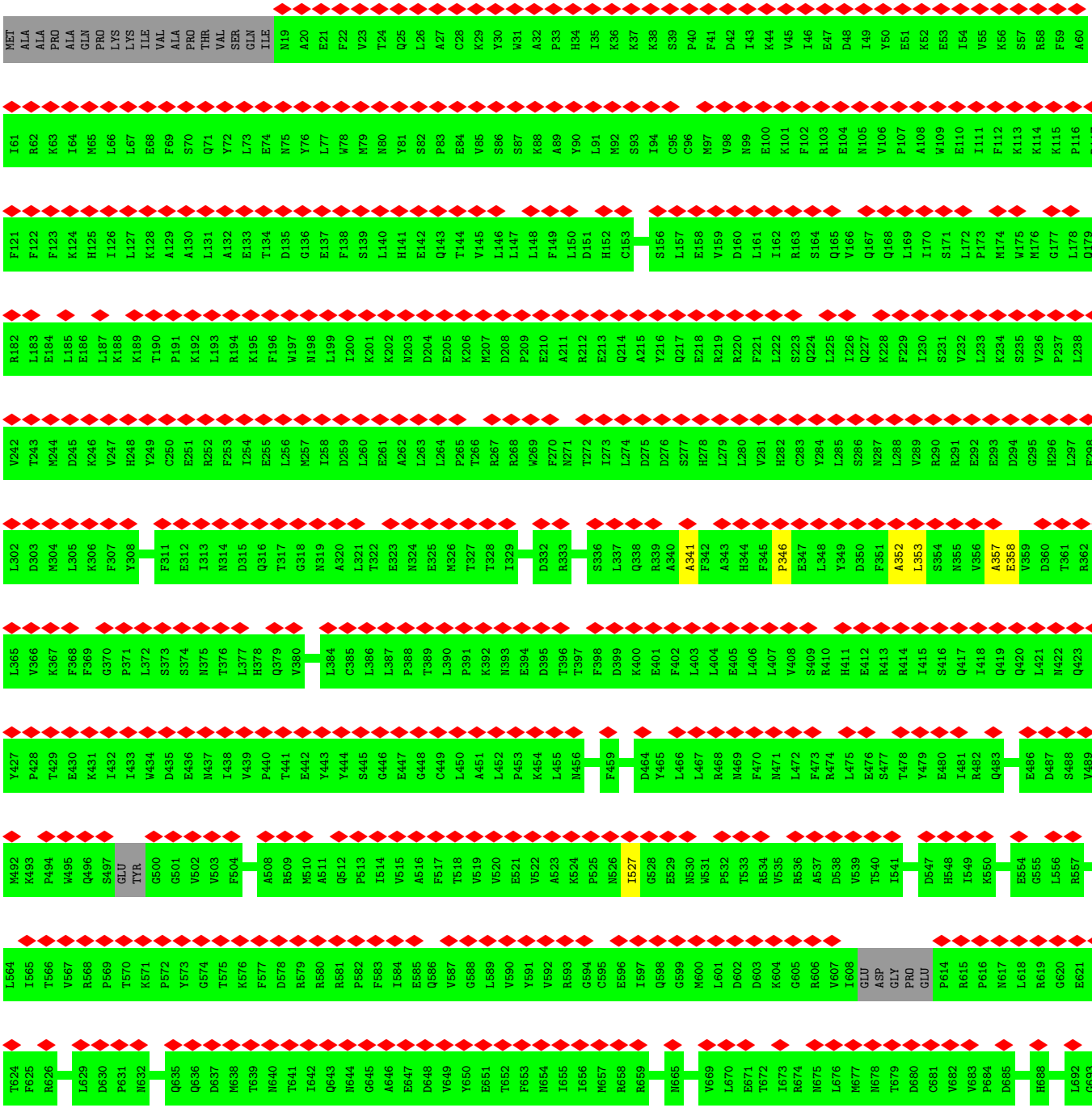
• Molecule 28: Pre-mRNA-splicing factor SYF1

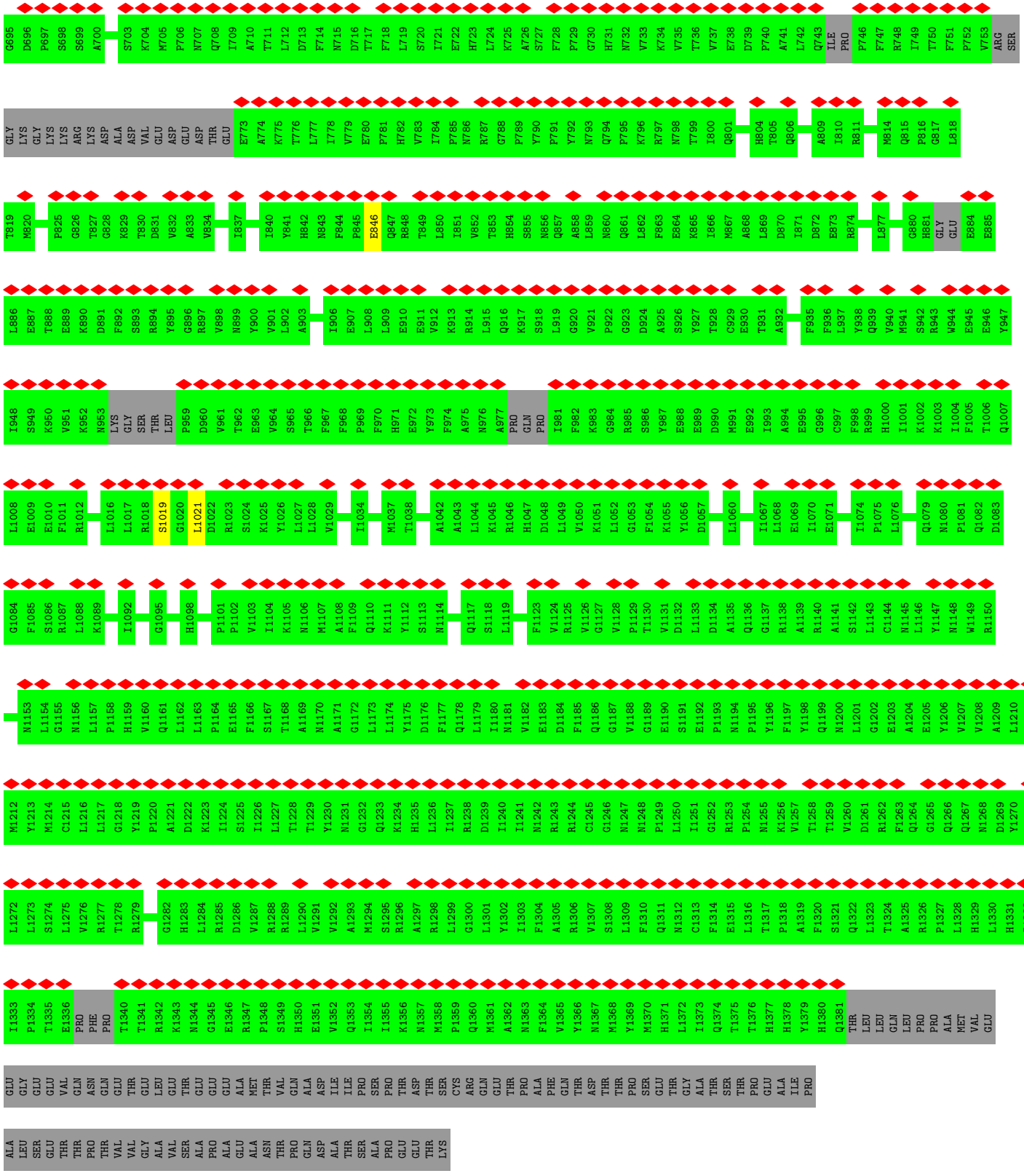




• Molecule 29: RNA helicase aquarius

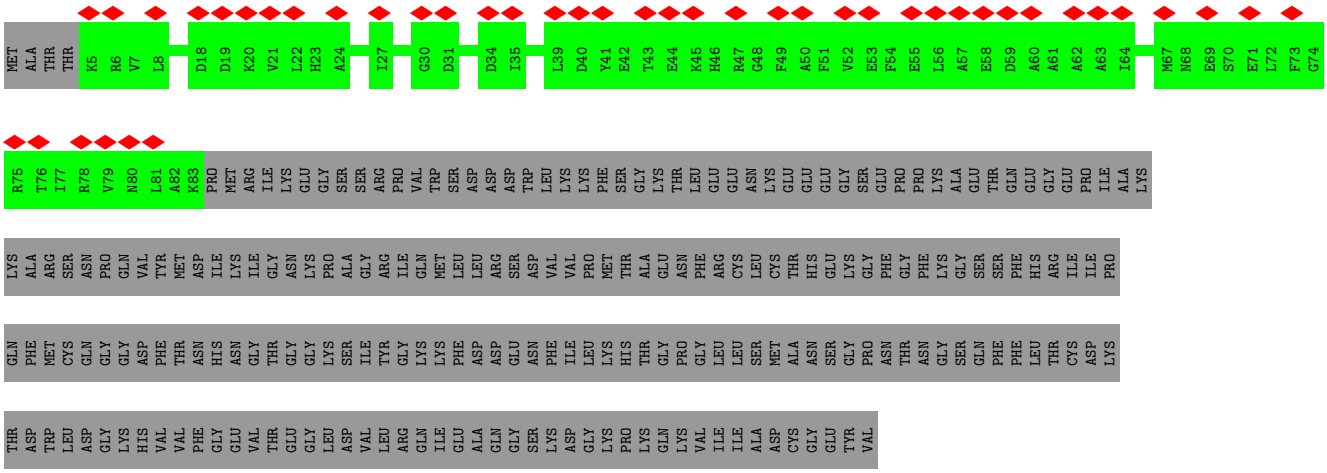
Chain Q:





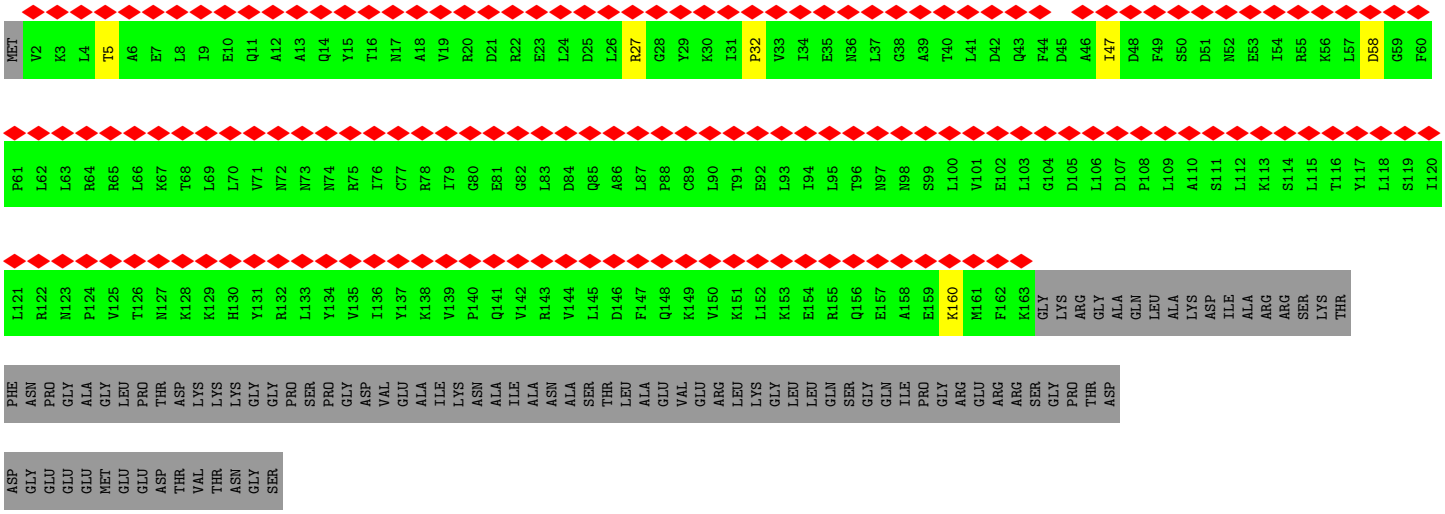
• Molecule 30: Peptidyl-prolyl cis-trans isomerase E

Chain y:



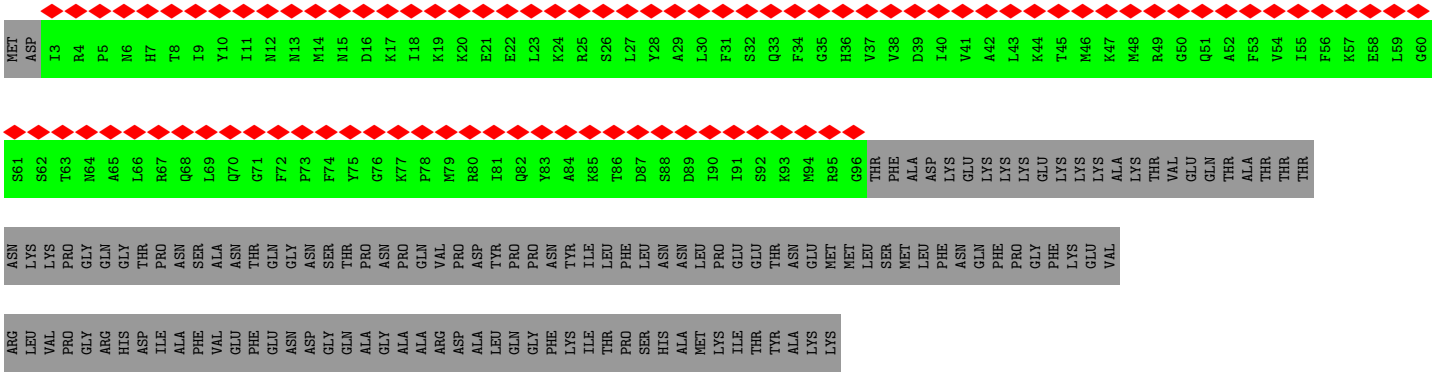
• Molecule 31: U2 small nuclear ribonucleoprotein A'

Chain o:



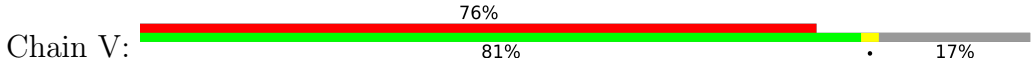
• Molecule 32: U2 small nuclear ribonucleoprotein B"

Chain p:



• Molecule 33: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX15

Chain V:



MET SER LYS ARG HIS ARG LEU ASP LEU GLY GLU ASP TYR PRO SER GLY LYS LYS ARG ALA GLY THR ASP GLY LYS ASP ARG ASP ARG ASP ARG ASP ARG GLU ASP ARG SER LYS ASP ARG ASP ARG GLY ASP ARG GLU ARG GLU ARG GLU LYS GLU LYS GLU

LEU ARG ALA SER THR ASN ALA MET LEU ILE SER ALA GLY LEU PRO PRO LEU LYS ALA SER HIS SER ALA HIS SER THR HIS SER ALA HIS SER THR HIS SER ALA HIS SER THR HIS SER ALA HIS SER THR HIS ALA GLY HIS ALA GLY HIS THR SER LEU PRO GLN C114 I115 N116 P117 F118 T119 N120

L121 P122 H123 T124 P125 R126 Y127 Y128 D129 I130 L131 K132 K133 R134 L135 Q136 L137 P138 V139 W140 E141 Y142 K143 D144 R145 F146 T147 D148 I149 L150 V151 R152 H153 Q154 S155 F156 V157 L158 V159 G160 E161 T162 G163 S164 G165 K166 T167 T168 Q169 I170 P171 Q172 W173 C174 V175 E176 Y177 M178 R179 S180

L181 P182 G183 P184 K185 R186 G187 V188 A189 C190 T191 Q192 P193 R194 R195 V196 A197 A198 M199 S200 V201 A202 Q203 R204 V205 A206 D207 E208 M209 D210 V211 M212 L213 G214 Q215 E216 V217 G218 Y219 S220 I221 R222 F223 E224 D225 C226 S227 S228 A229 K230 T231 I232 L233 K234 Y235 M236 T237 D238 G239 M240

L241 E244 A245 M246 N247 D248 P249 L250 L251 E252 R253 Y254 G255 V256 I257 I258 L259 A262 H263 E264 R265 T266 L267 A268 T269 D270 I271 L272 M273 G274 V275 L276 K277 E278 V279 V280 R281 Q282 R283 S284 D285 L286 K287 V288 I289 V290 M291 S292 A293 T294 L295 D296 A297 G298 K299 F300 Q301 I302

Y303 F304 D305 N306 C307 P308 L309 L310 T311 I312 P313 G314 R315 T316 H317 P318 V319 E320 I321 F322 Y323 T324 P325 E326 P327 E328 R329 D330 Y331 L332 E333 A334 A335 I336 R337 T338 V339 I340 Q341 I342 H343 M344 C345 E346 E347 E348 E349 G350 D351 L352 L353 L354 F355 L356 T357 G358 Q359 E360 E361 I362

D363 E364 A365 C366 K367 R368 I369 K370 R371 E372 V373 D374 D375 L376 G377 P378 E379 V380 G381 K384 I385 I386 P387 L388 Y389 S390 T391 L392 P393 P394 Q395 Q396 R399 I400 P401 E402 P403 P404 P405 P406 K407 K408 Q409 N410 G411 A412 I413 G414 R415 K416 V417 V418 V419 S420 T421 N422 I423 A424

E425 T426 S427 L428 T429 I430 D431 G432 V433 V434 F435 V436 I437 D438 P439 G440 F441 A442 K443 Q444 K445 V446 Y447 N448 P449 R450 I451 R452 V453 E454 S455 L456 L457 V458 T459 A460 I461 S462 K463 A464 S465 A466 Q467 Q468 R469 A470 G471 R472 A473 G474 R475 T476 R477 P478 G479 K480 C481 F482 R483 L484

Y485 T486 E487 K488 A489 Y490 K491 T492 E493 M494 Q495 D496 N497 T498 Y499 P500 E501 I502 L503 R504 S505 G508 S509 V510 V511 L512 Q513 L514 K515 K516 L517 G518 I519 D520 D521 L522 V523 H524 F525 D526 F527 M528 D529 P530 P531 A532 P533 E534 T535 L536 M537 R538 A539 L540 E541 L542 L543 N544 Y545

L546 A547 A548 L549 N550 D551 D552 G553 D554 L555 T556 E557 L558 G559 S560 M561 M562 A563 E564 F565 P566 P569 V575 I576 A577 S578 C579 D580 Y581 N582 C583 S584 N585 E586 V587 L588 S589 I590 T591 A592 M593 L594 S595 V596 P597 Q598 C599 F600 V601 P602 T604 E605 A606 K607 K608 A609

E612 A613 K614 M615 R616 F617 A618 H619 I620 D621 G622 D623 H624 L625 T626 L627 L628 N629 E564 V630 Y631 H632 A633 F634 K635 Q636 N637 H638 E639 S640 V641 Q642 W643 C644 Y645 D646 N647 F648 I649 N650 Y651 R652 S653 L654 M655 S656 A657 D658 N659 V660 R661 Q662 Q663 L664 S665 R666 I667 M668 D669 R670 F671

N672 L673 P674 R675 R676 S677 T678 D679 F680 T681 S682 R683 D684 Y685 Y686 I687 N688 I689 R690 K691 A692 L693 V694 T695 G696 Y697 F698 M699 Q700 V701 A702 H703 L704 E705 R706 T707 G708 H709 Y710 L711 T712 V713 K714 D715 N716 Q717 V718 V719 Q720 L721 H722 P723 S724 T725 V726 L727 D728 H729 K730 P731

E732 W733 V734 L735 Y736 N737 E738 F739 V740 L741 T742 T743 K744 N745 Y746 I747 R748 T749 C750 T751 D752 I753 K754 P755 E756 W757 L758 V759 K760 I761 A762 P763 Q764 Y765 Y766 D767 M768 S769 N770 F771 P772 Q773 C774 E775 A776 LYS ARG GLN LEU ASP ARG ILE ILE ALA LYS LEU GLN SER LYS GLU

TYR SER GLN TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	499840	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	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	0.577	Depositor
Minimum map value	-0.264	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, SEP, IHP, 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	0.33	0/16926	0.61	7/22947 (0.0%)
2	B	0.43	1/2296 (0.0%)	0.88	0/3569
3	C	0.30	0/7181	0.62	3/9758 (0.0%)
4	E	0.42	0/2420	0.69	0/3281
5	F	0.56	4/2323 (0.2%)	1.11	13/3619 (0.4%)
6	J	0.33	0/3863	0.55	6/5250 (0.1%)
7	L	0.39	2/3401 (0.1%)	0.59	10/4570 (0.2%)
8	M	0.27	0/1119	0.55	1/1497 (0.1%)
9	N	1.19	7/1210 (0.6%)	0.76	0/1622
10	O	0.38	0/2390	0.62	1/3227 (0.0%)
11	P	0.30	0/1000	0.54	0/1330
12	R	0.32	0/2186	0.69	3/2937 (0.1%)
13	S	0.29	0/1268	0.57	1/1714 (0.1%)
14	T	0.42	1/2562 (0.0%)	0.69	0/3492
15	W	0.30	0/1306	0.60	1/1760 (0.1%)
16	G	0.89	10/1327 (0.8%)	1.60	40/2053 (1.9%)
17	H	0.58	9/3214 (0.3%)	0.99	9/4989 (0.2%)
18	U	0.33	0/2928	0.68	3/3928 (0.1%)
19	a	0.47	0/397	0.61	0/549
19	h	0.47	0/391	0.61	0/540
20	b	0.51	0/423	0.72	0/587
20	i	0.50	0/423	0.73	0/587
21	c	0.58	0/405	0.73	0/563
21	j	0.57	0/405	0.73	0/563
22	d	0.69	0/479	0.85	0/666
22	k	0.70	0/420	0.85	0/583
23	f	0.75	0/360	0.82	0/497
23	m	0.75	0/360	0.81	0/497
24	e	0.66	0/390	0.80	0/542
24	l	0.64	0/390	0.80	0/542
25	g	0.54	0/362	0.71	0/501
25	n	0.53	0/327	0.72	0/451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	q	0.35	0/658	0.58	3/919 (0.3%)
26	r	0.33	0/653	0.59	3/912 (0.3%)
26	s	0.27	0/334	0.37	0/466
26	t	0.31	0/334	0.38	0/466
27	K	1.05	9/982 (0.9%)	0.69	5/1318 (0.4%)
28	I	0.35	0/2858	0.61	11/3948 (0.3%)
29	Q	0.22	0/6545	0.43	0/9115
30	y	0.29	0/389	0.73	0/540
31	o	0.64	0/803	1.49	4/1119 (0.4%)
32	p	0.62	0/463	1.26	0/643
33	V	0.66	0/3284	0.75	0/4578
All	All	0.45	43/81755 (0.1%)	0.72	124/113235 (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	A	0	10
3	C	0	3
5	F	0	1
6	J	0	1
7	L	0	2
11	P	0	1
12	R	0	1
14	T	0	2
15	W	0	2
16	G	0	8
18	U	0	2
22	d	0	1
22	k	0	1
29	Q	0	1
33	V	0	1
All	All	0	37

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K	106	CYS	CB-SG	-23.11	1.43	1.82
9	N	101	CYS	CB-SG	-16.04	1.54	1.82
9	N	137	CYS	CB-SG	-12.01	1.61	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	119	CYS	CB-SG	-10.98	1.63	1.82
9	N	142	CYS	CB-SG	-9.64	1.65	1.82

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	4	A	O4'-C1'-N9	18.63	123.10	108.20
16	G	3	A	N9-C1'-C2'	13.62	131.71	114.00
16	G	8	C	N1-C1'-C2'	10.36	127.47	114.00
5	F	35	A	C4'-C3'-O3'	10.21	133.43	113.00
16	G	143	U	N1-C1'-C2'	9.61	126.49	114.00

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	PRO	Peptide
1	A	1305	SER	Peptide
1	A	135	VAL	Peptide
1	A	1555	LEU	Peptide
1	A	166	PHE	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	16477	0	16462	280	0
2	B	2060	0	1044	98	0
3	C	7022	0	7046	168	0
4	E	2366	0	2303	421	0
5	F	2075	0	1048	127	0
6	J	3817	0	2912	46	0
7	L	3369	0	2929	157	0
8	M	1098	0	1082	19	0
9	N	1184	0	1189	15	0
10	O	2340	0	2316	193	0
11	P	985	0	965	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	R	2165	0	2214	74	0
13	S	1236	0	1210	31	0
14	T	2496	0	2446	47	0
15	W	1276	0	1221	66	0
16	G	1201	0	609	232	0
17	H	2884	0	1461	279	0
18	U	2864	0	2814	146	0
19	a	399	0	173	0	0
19	h	393	0	170	0	0
20	b	424	0	179	0	0
20	i	424	0	179	0	0
21	c	406	0	170	0	0
21	j	406	0	170	0	0
22	d	480	0	200	0	0
22	k	422	0	175	0	0
23	f	361	0	158	0	0
23	m	361	0	158	0	0
24	e	391	0	163	0	0
24	l	391	0	163	0	0
25	g	363	0	160	0	0
25	n	329	0	138	0	0
26	q	659	0	296	0	0
26	r	654	0	294	0	0
26	s	335	0	168	0	0
26	t	335	0	168	0	0
27	K	980	0	741	158	0
28	I	2875	0	1374	82	0
29	Q	6554	0	2828	23	0
30	y	390	0	190	0	0
31	o	804	0	350	0	0
32	p	464	0	205	0	0
33	V	3285	0	1442	5	0
34	A	36	0	6	2	0
35	C	32	0	12	9	0
36	C	1	0	0	0	0
36	F	6	0	0	0	0
37	N	3	0	0	0	0
37	O	3	0	0	0	0
37	U	1	0	0	0	0
All	All	79882	0	61701	2254	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 17.

The worst 5 of 2254 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)
10:O:155:PRO:HG3	12:R:188:PHE:CD1	1.21	1.62
16:G:120:G:H2'	29:Q:1019:SER:CB	1.24	1.60
6:J:658:ARG:HA	6:J:667:ILE:CB	1.39	1.53
6:J:496:ASP:CB	6:J:536:LEU:H	1.23	1.51
10:O:260:THR:HG23	10:O:273:GLN:CB	1.32	1.50

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	1977/2335 (85%)	1799 (91%)	160 (8%)	18 (1%)	17	43
3	C	886/972 (91%)	799 (90%)	84 (10%)	3 (0%)	41	68
4	E	301/357 (84%)	268 (89%)	22 (7%)	11 (4%)	3	11
6	J	536/848 (63%)	495 (92%)	37 (7%)	4 (1%)	22	50
7	L	459/802 (57%)	421 (92%)	33 (7%)	5 (1%)	14	38
8	M	128/243 (53%)	115 (90%)	13 (10%)	0	100	100
9	N	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
10	O	288/420 (69%)	262 (91%)	24 (8%)	2 (1%)	22	50
11	P	114/229 (50%)	96 (84%)	17 (15%)	1 (1%)	17	43
12	R	268/536 (50%)	234 (87%)	30 (11%)	4 (2%)	10	30
13	S	157/166 (95%)	141 (90%)	16 (10%)	0	100	100
14	T	315/514 (61%)	297 (94%)	16 (5%)	2 (1%)	25	53
15	W	156/579 (27%)	134 (86%)	18 (12%)	4 (3%)	5	17
18	U	343/894 (38%)	289 (84%)	49 (14%)	5 (2%)	10	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
19	h	76/126 (60%)	75 (99%)	1 (1%)	0	100	100
20	b	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
20	i	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
21	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
21	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
22	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
22	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
23	f	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
23	m	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
24	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
24	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
25	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
25	n	63/76 (83%)	61 (97%)	2 (3%)	0	100	100
26	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	4	14
26	r	129/504 (26%)	119 (92%)	8 (6%)	2 (2%)	9	28
26	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	10	30
26	t	65/504 (13%)	64 (98%)	0	1 (2%)	10	30
27	K	144/225 (64%)	130 (90%)	7 (5%)	7 (5%)	2	6
28	I	538/855 (63%)	501 (93%)	25 (5%)	12 (2%)	6	21
29	Q	1304/1485 (88%)	1278 (98%)	25 (2%)	1 (0%)	51	79
30	y	77/301 (26%)	74 (96%)	3 (4%)	0	100	100
31	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	12	33
32	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
33	V	661/795 (83%)	614 (93%)	40 (6%)	7 (1%)	14	38
All	All	10524/16892 (62%)	9733 (92%)	695 (7%)	96 (1%)	21	43

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1306	LYS
1	A	1519	THR
1	A	1639	VAL

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Mol	Chain	Res	Type
1	A	1653	ASP
1	A	1948	ASP

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	1792/2108 (85%)	1754 (98%)	38 (2%)	53 79
3	C	787/866 (91%)	762 (97%)	25 (3%)	39 69
4	E	259/300 (86%)	203 (78%)	56 (22%)	1 2
6	J	242/751 (32%)	241 (100%)	1 (0%)	91 96
7	L	248/709 (35%)	233 (94%)	15 (6%)	19 45
8	M	117/209 (56%)	114 (97%)	3 (3%)	46 75
9	N	130/130 (100%)	130 (100%)	0	100 100
10	O	259/361 (72%)	237 (92%)	22 (8%)	10 28
11	P	104/203 (51%)	102 (98%)	2 (2%)	57 81
12	R	227/457 (50%)	217 (96%)	10 (4%)	28 58
13	S	129/134 (96%)	127 (98%)	2 (2%)	62 84
14	T	273/441 (62%)	272 (100%)	1 (0%)	91 96
15	W	135/502 (27%)	131 (97%)	4 (3%)	41 72
18	U	313/806 (39%)	292 (93%)	21 (7%)	16 39
27	K	54/196 (28%)	44 (82%)	10 (18%)	1 4
28	I	12/749 (2%)	6 (50%)	6 (50%)	0 0
All	All	5081/8922 (57%)	4865 (96%)	216 (4%)	33 59

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	318	ARG
10	O	220	MET
18	U	810	ILE

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Mol	Chain	Res	Type
6	J	591	LEU
7	L	731	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
10	O	254	GLN
15	W	184	ASN
11	P	75	ASN
12	R	281	ASN
1	A	1784	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	G	67/272 (24%)	55 (82%)	14 (20%)
17	H	129/188 (68%)	53 (41%)	2 (1%)
2	B	97/117 (82%)	57 (58%)	4 (4%)
5	F	96/107 (89%)	42 (43%)	7 (7%)
All	All	389/684 (56%)	207 (53%)	27 (6%)

5 of 207 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	8	G
2	B	9	G
2	B	10	U
2	B	11	U
2	B	12	U

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	G	7	G
16	G	21	A
16	G	150	U
16	G	16	G
16	G	22	C

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	SEP	R	232	12	8,9,10	0.98	0	8,12,14	2.08	2 (25%)
12	SEP	R	224	12	8,9,10	0.83	0	8,12,14	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	SEP	R	232	12	-	1/5/8/10	-
12	SEP	R	224	12	-	0/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	R	232	SEP	OG-CB-CA	4.44	112.47	108.14
12	R	232	SEP	P-OG-CB	-2.36	111.81	118.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	R	232	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	R	232	SEP	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
34	IHP	A	3000	-	36,36,36	0.71	0	54,60,60	0.96	0
35	GTP	C	1500	36	26,34,34	0.98	1 (3%)	32,54,54	1.49	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	IHP	A	3000	-	-	5/30/54/54	0/1/1/1
35	GTP	C	1500	36	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	1500	GTP	C6-N1	-2.98	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	C	1500	GTP	PA-O3A-PB	-3.99	119.15	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	C	1500	GTP	PB-O3B-PG	-3.76	119.91	132.83
35	C	1500	GTP	C5-C6-N1	2.66	118.65	113.95
35	C	1500	GTP	O6-C6-C5	-2.35	119.78	124.37
35	C	1500	GTP	C8-N7-C5	2.27	107.32	102.99

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	C	1500	GTP	C5'-O5'-PA-O3A
35	C	1500	GTP	C5'-O5'-PA-O1A
35	C	1500	GTP	C5'-O5'-PA-O2A
34	A	3000	IHP	C1-O11-P1-O21
34	A	3000	IHP	C3-O13-P3-O23

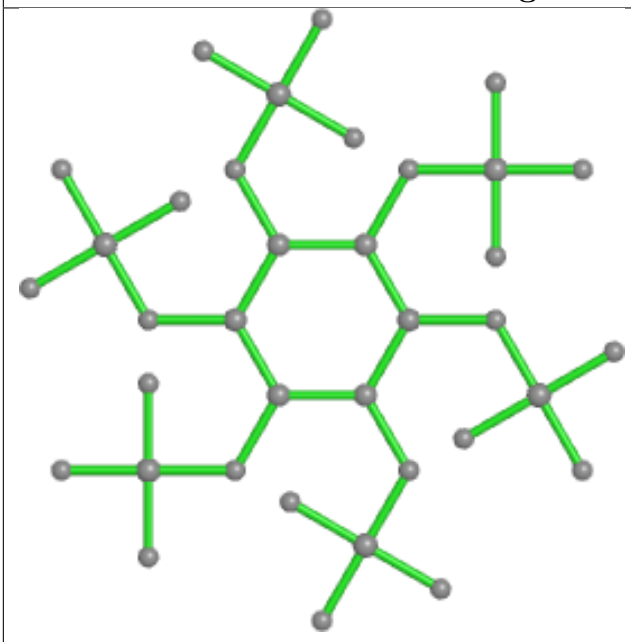
There are no ring outliers.

2 monomers are involved in 11 short contacts:

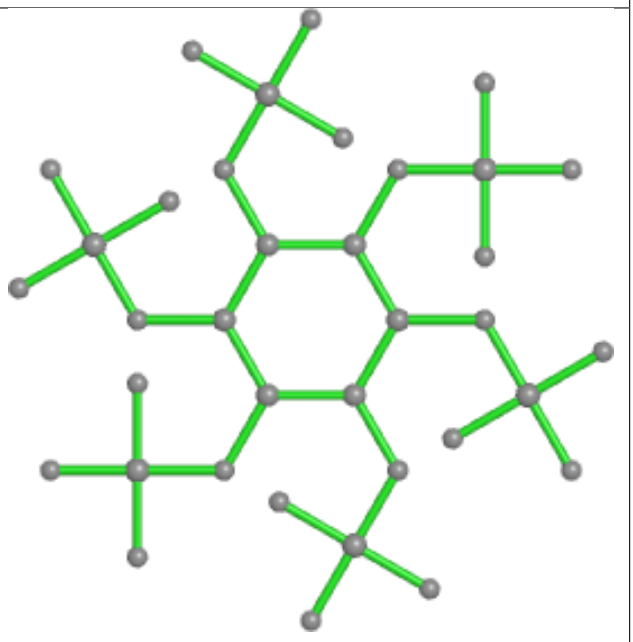
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	3000	IHP	2	0
35	C	1500	GTP	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

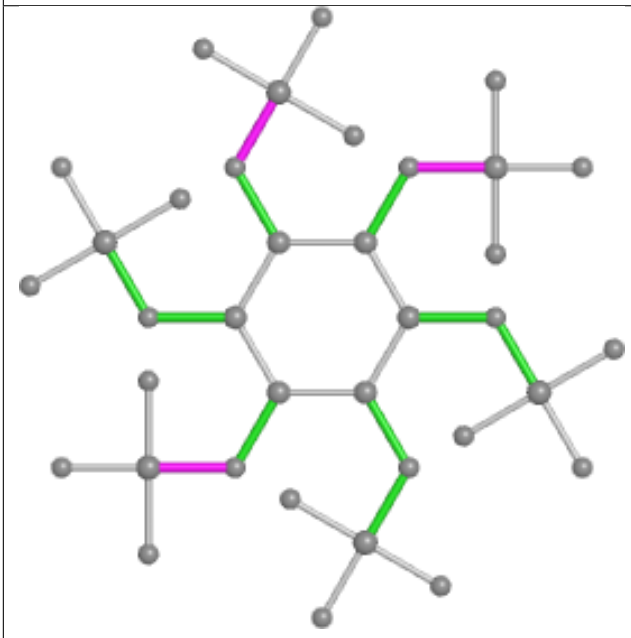
Ligand IHP A 3000



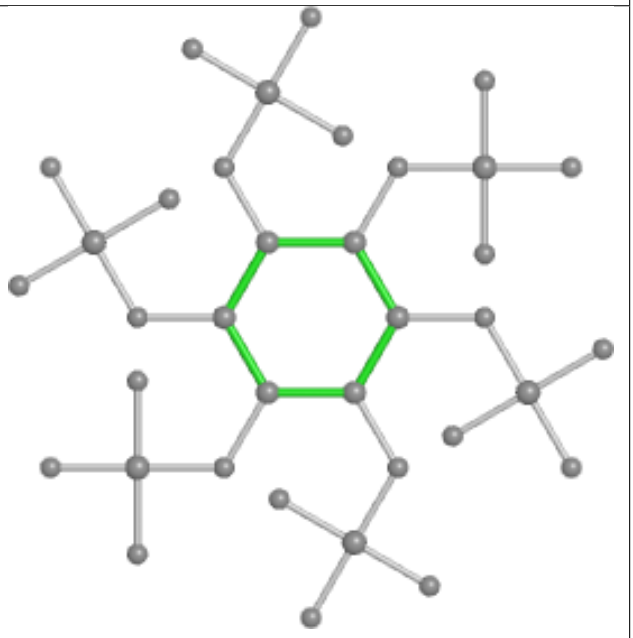
Bond lengths



Bond angles

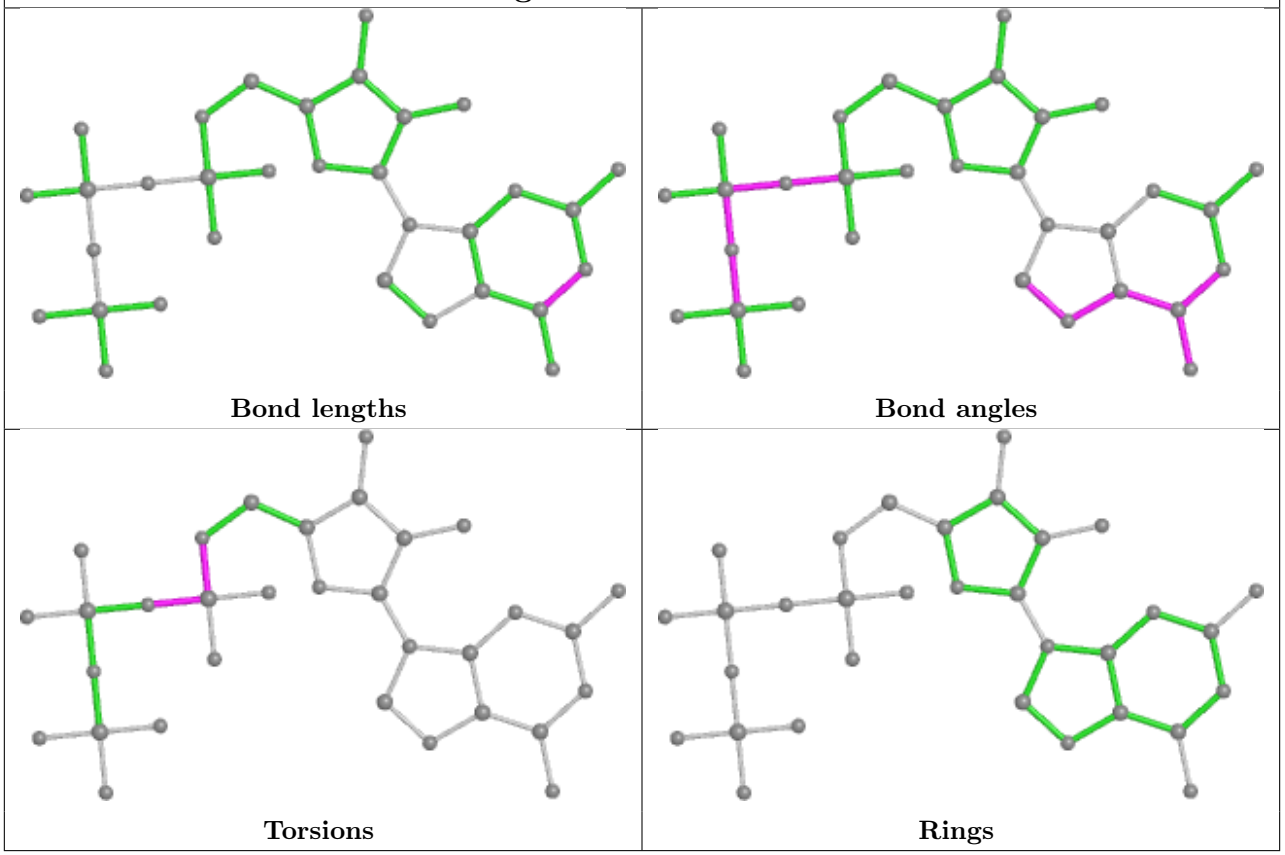


Torsions



Rings

Ligand GTP C 1500



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.

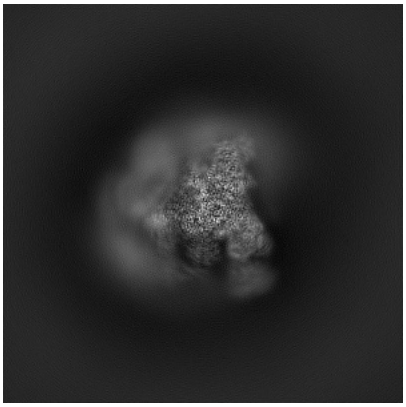
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9647. These allow visual inspection of the internal detail of the map and identification of artifacts.

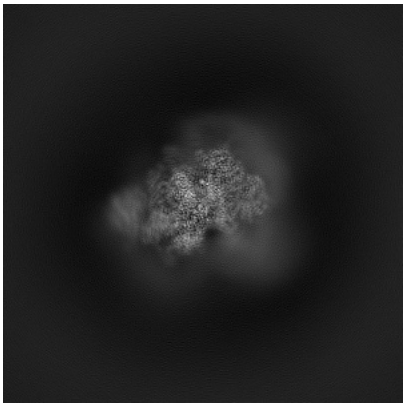
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

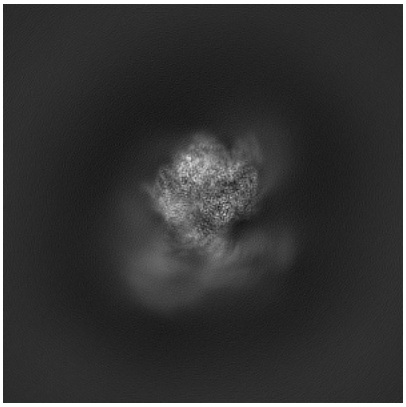
6.1.1 Primary map



X



Y

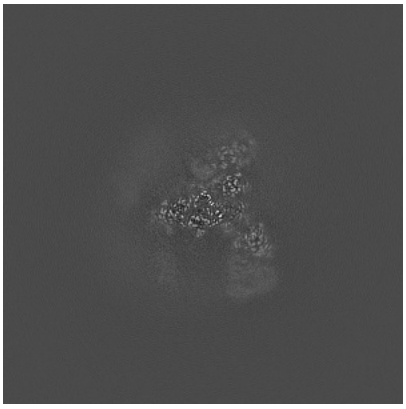


Z

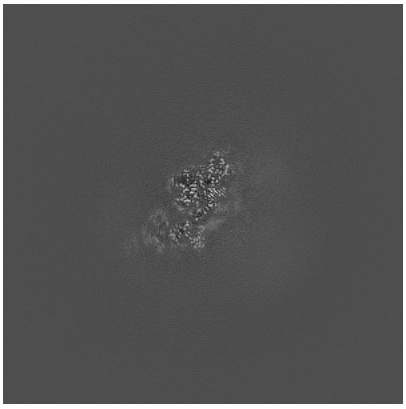
The images above show the map projected in three orthogonal directions.

6.2 Central slices

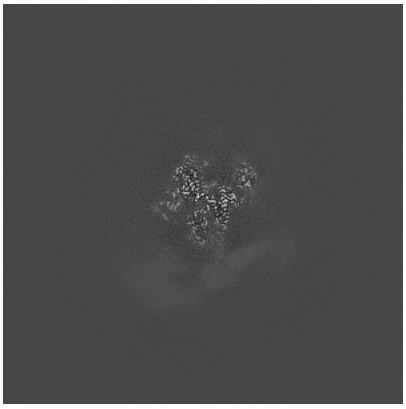
6.2.1 Primary map



X Index: 200



Y Index: 200

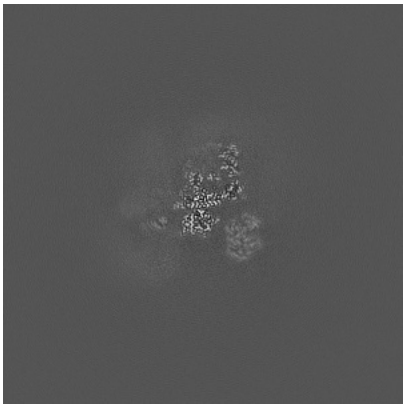


Z Index: 200

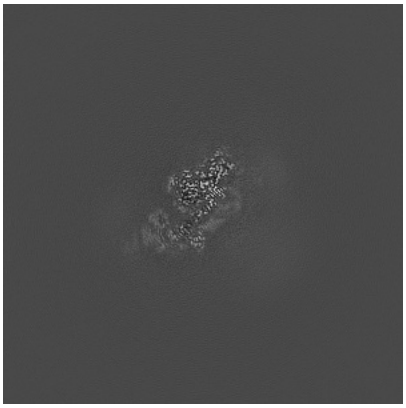
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

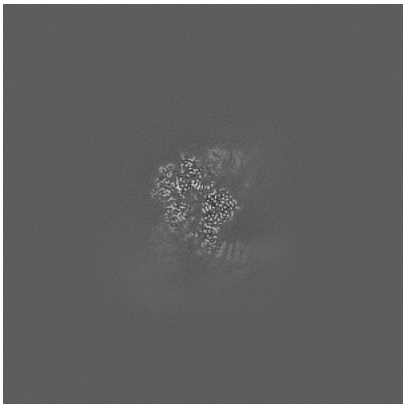
6.3.1 Primary map



X Index: 221



Y Index: 201



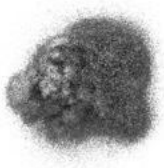
Z Index: 185

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

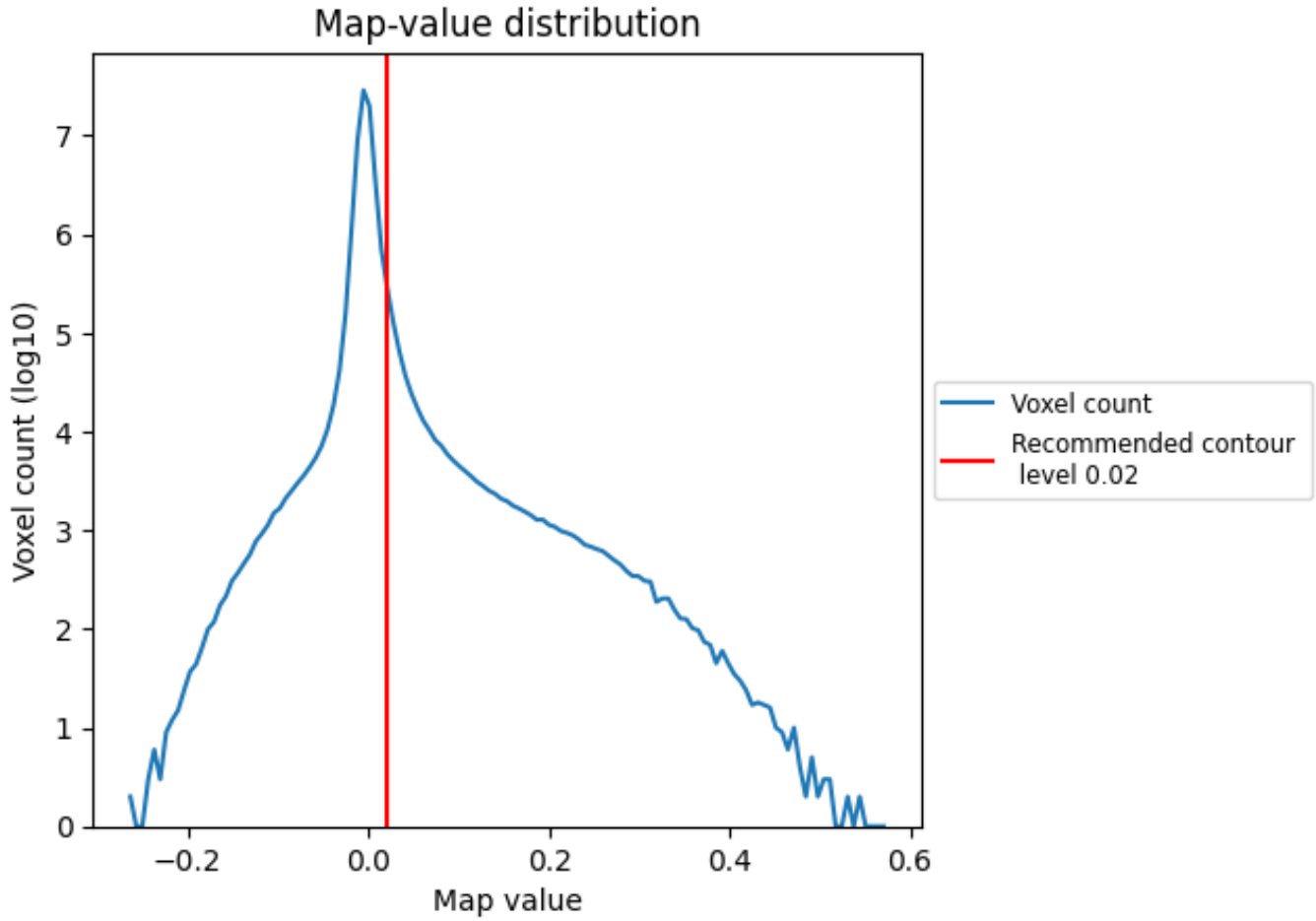
6.5 Mask visualisation (i)

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

7 Map analysis

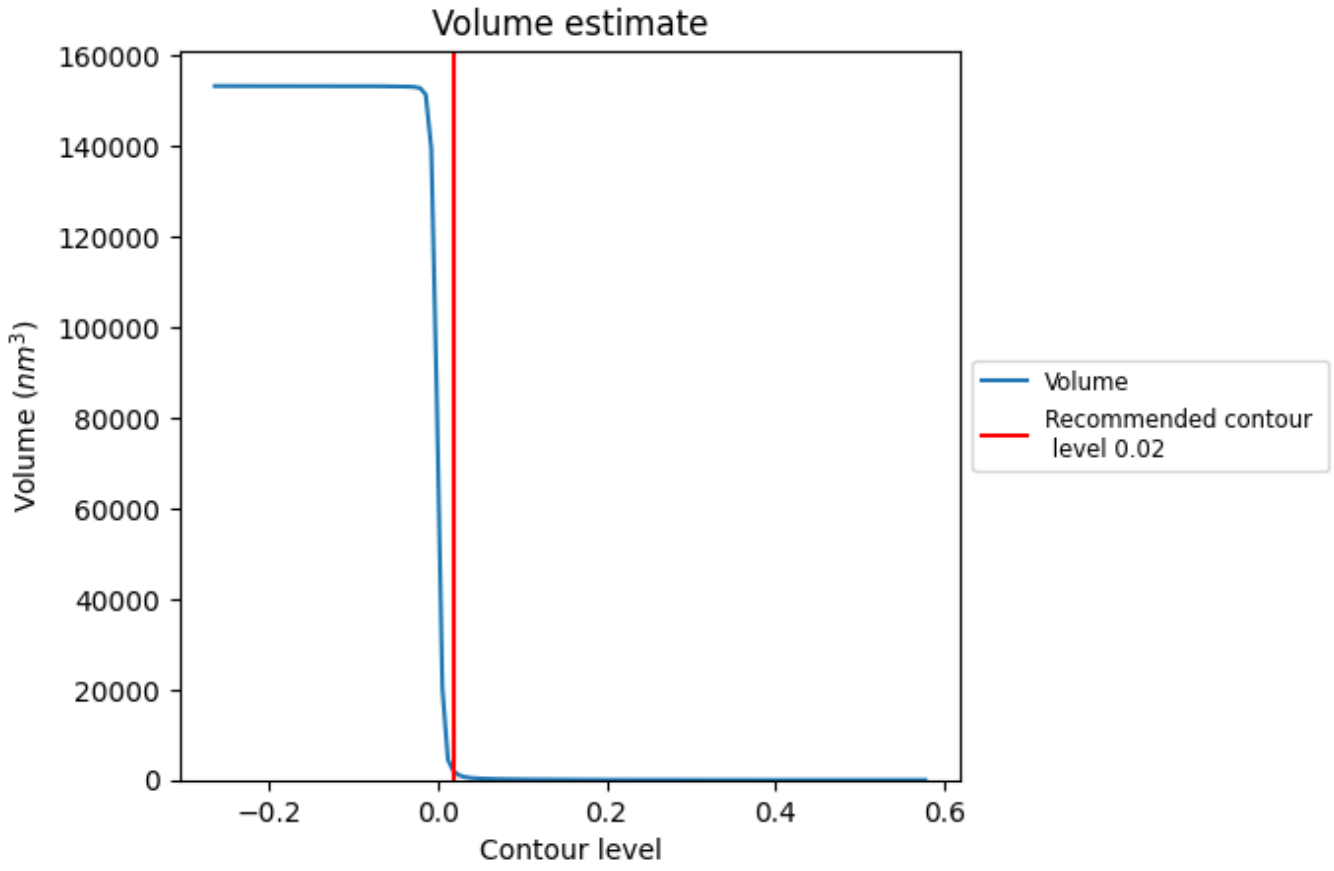
This section contains the results of statistical analysis of the map.

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.

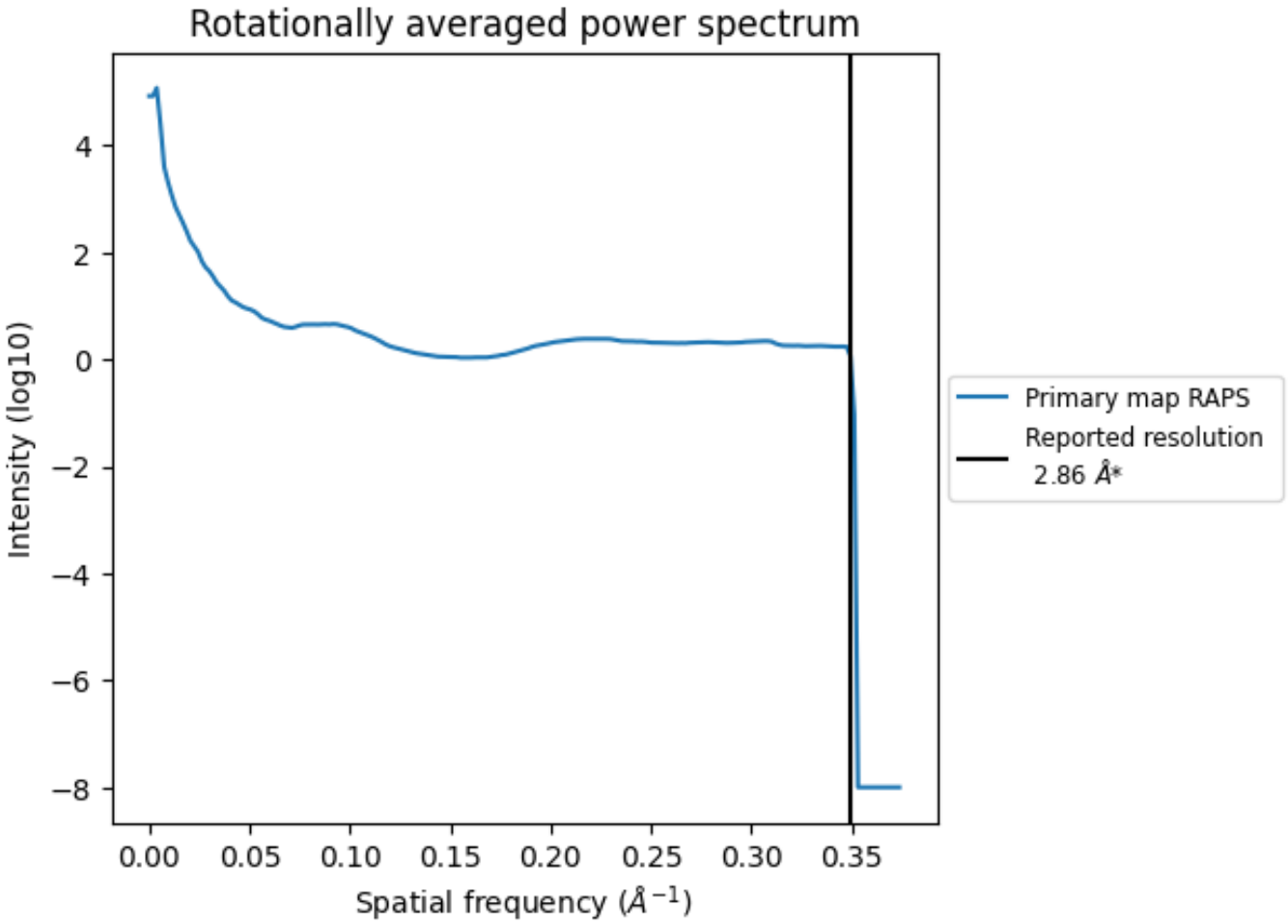
7.2 Volume estimate (i)



The volume at the recommended contour level is 1797 nm^3; this corresponds to an approximate mass of 1623 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 0.350 Å^{-1}

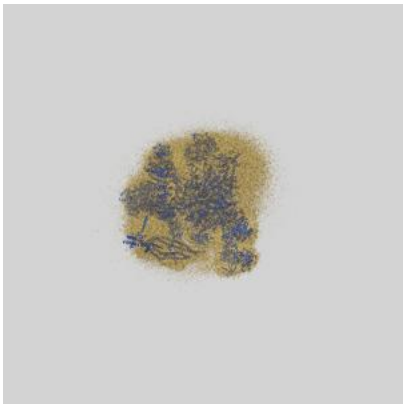
8 Fourier-Shell correlation (i)

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

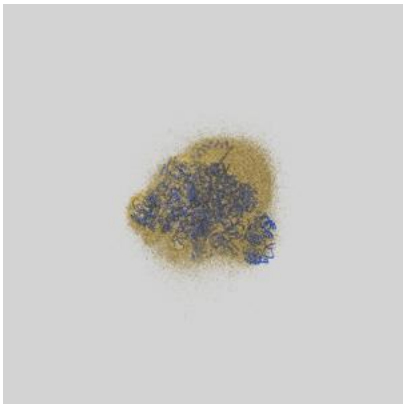
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9647 and PDB model 6ID1. Per-residue inclusion information can be found in section 3 on page 12.

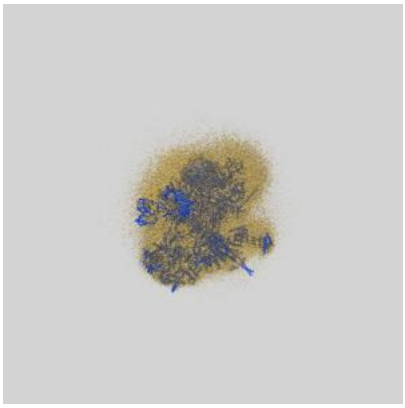
9.1 Map-model overlay



X



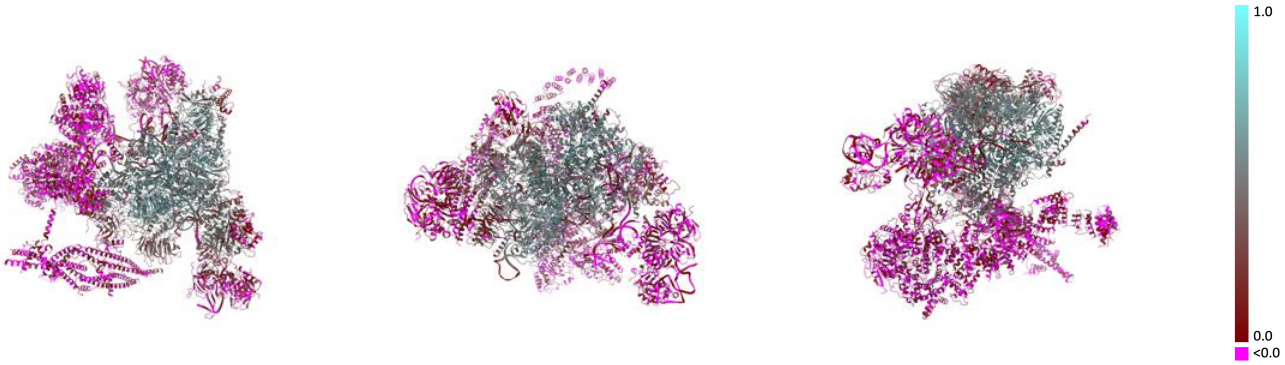
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

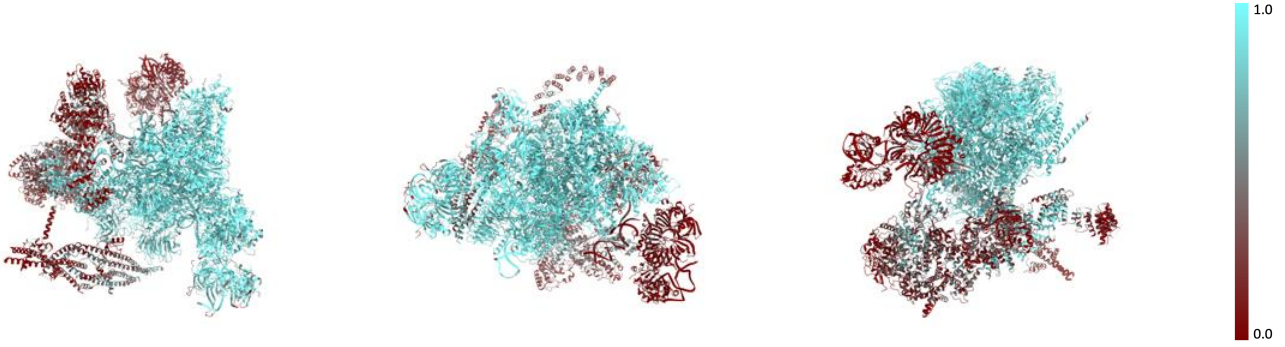
9.2 Q-score mapped to coordinate model



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.

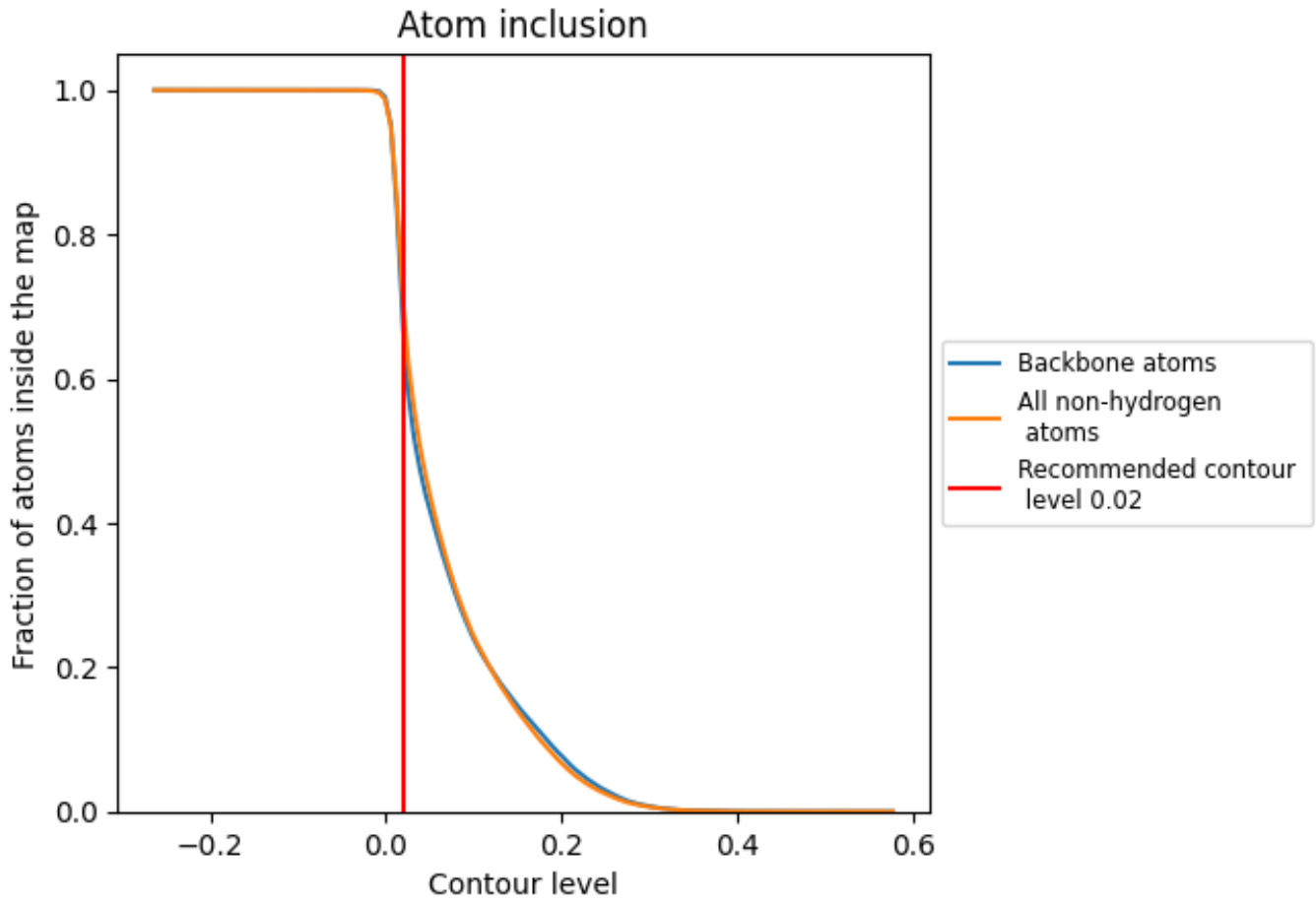
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7005	0.2910
A	0.9464	0.5070
B	0.9160	0.3290
C	0.9184	0.3560
E	0.9003	0.2990
F	0.9433	0.4390
G	0.7810	0.1720
H	0.3200	0.0900
I	0.6001	0.0420
J	0.6427	0.2780
K	0.3967	0.0550
L	0.6340	0.2560
M	0.8280	0.4070
N	0.9670	0.5630
O	0.8546	0.3890
P	0.8588	0.4360
Q	0.2360	0.0140
R	0.8908	0.4260
S	0.8483	0.2520
T	0.9799	0.5940
U	0.9238	0.4780
V	0.1903	0.0130
W	0.8400	0.3760
a	0.8897	0.2050
b	0.7925	0.1000
c	0.9064	0.1090
d	0.8458	0.0450
e	0.7801	0.0620
f	0.7950	-0.0090
g	0.7576	0.0680
h	0.1094	0.0110
i	0.1179	0.0280
j	0.0887	0.0510
k	0.0166	-0.0070
l	0.0281	0.0100

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Chain	Atom inclusion	Q-score
m	0.0166	-0.0010
n	0.0942	0.0070
o	0.0585	0.0290
p	0.0603	0.0360
q	0.1214	-0.0070
r	0.3716	0.0170
s	0.4000	-0.0250
t	0.1642	0.0090
y	0.4692	0.0440