wwPDB EM Validation Summary Report (i)

Oct 6, 2024 – 07:38 pm BST

PDB ID	:	8RO2
EMDB ID	:	EMD-19399
Title	:	Integrative Structure of the human intron lariat Spliceosome (ILS")
Authors	:	Rothe, P.; Vorlaender, M.K.; Plaschka, C.
Deposited on	:	2024-01-11
Resolution	:	3.50 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 (1)) were used in the production of this report:

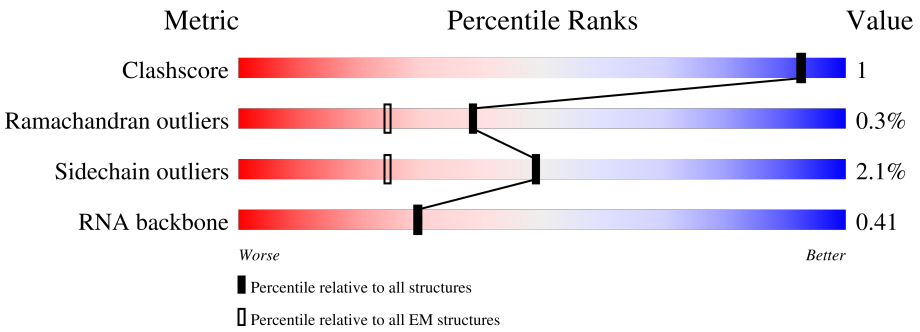
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	2	188	18%; 7%, 12%, •, 79%
2	6	106	80%; 33%, 42%, 14%, •, 8%
3	C	972	5%; 88%, 5%, 7%
4	D	285	12%; 18%, 82%
5	DX	795	56%; 81%, •, 18%
6	E	357	•; 80%, •, 16%
7	J	848	32%; 66%, 34%

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Mol	Chain	Length	Quality of chain
8	K	225	8% 83% 16%
9	L1	538	51% 51% 49%
10	N	144	10% 93% 6%
11	O	420	29% 65% 31%
12	Q	1485	80% 93% 7%
13	R	536	26% 57% 41%
14	S	166	11% 85% 10%
15	W	579	13% 24% 73%
16	Z	166	21% 55% 45%
17	a	126	63% 34%
18	c	119	14% 64% 32%
19	d	118	27% 72% 8% 19%
20	e	92	15% 82% 14%
21	f	86	16% 80% 16%
22	g	76	17% 84% 11%
23	q	504	8% 20% 80%
23	r	504	10% 23% 76%
23	s	504	26% 74%
23	t	504	8% 20% 80%
24	z	451	5% 6% 94%
25	3	476	11% 13% 87%
26	5	116	16% 41% 24% 13% 21%
27	A	2335	17% 79% 5% 15%
28	I	855	20% 88% 12%
29	IN	154	23% 24% 73%

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Mol	Chain	Length	Quality of chain
30	L	802	27% 67% 31%
31	L2	894	13% 36% 59%
32	M	243	42% 67% 32%
33	P	229	24% 46% 51%
34	PX	917	20% 32% 68%
35	T	514	64% 6% 30%
36	TF	837	25% 67% 32%
37	b	240	9% 35% 61%

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 81753 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 RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	39	823	368	137	279	39	0	0

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	6	97	2075	928	381	669	97	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	908	7184	4598	1194	1357	35	0	0

- Molecule 4 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	51	253	151	51	51	0	0

- Molecule 5 is a protein called ATP-dependent RNA helicase DHX15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	DX	650	3220	1920	650	650	0	0

- Molecule 6 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	299	2341	1470	411	447	13	0	0

- Molecule 7 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	J	561	2793	1671	561	561	0	0

- Molecule 8 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	K	189	941	563	189	189	0	0

- Molecule 9 is a protein called CWF19-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	L1	275	1353	803	275	275	0	0

- Molecule 10 is a protein called Protein BUD31 homolog.

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

- Molecule 11 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	O	288	2328	1463	412	433	20	0	0

- Molecule 12 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	Q	1384	6859	4091	1384	1384	0	0

- Molecule 13 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	R	317	1571	937	317	317	0	0

- Molecule 14 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

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

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

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

- Molecule 16 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	Z	92	459	275	92	92	0	0

- Molecule 17 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	a	83	651	408	114	122	7	0	0

- Molecule 18 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	c	81	641	409	112	116	4	0	0

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	d	96	775	485	146	139	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	e	79	653	412	116	120	5	0	0

- Molecule 21 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	f	72	564	364	93	102	5	0	0

- Molecule 22 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	g	73	568	358	102	102	6	0	0

- Molecule 23 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	s	132	659	395	132	132	0	0
23	q	103	514	308	103	103	0	0
23	r	119	594	356	119	119	0	0
23	t	103	514	308	103	103	0	0

- Molecule 24 is a protein called Splicing regulator SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	z	25	198	119	35	41	3	0	0

- Molecule 25 is a protein called Splicing factor ESS-2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	3	60	499	311	85	102	1	0	0

- Molecule 26 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	5	92	1936	867	322	655	92	0	0

- Molecule 27 is a protein called Pre-mRNA-processing-splicing factor 8.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	I	753	3739	2233	753	753	0	0

- Molecule 29 is a RNA chain called INTRON.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	O	P		
29	IN	41	492	205	246	41	0	0

- Molecule 30 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	L	555	3623	2216	695	705	7	0	0

- Molecule 31 is a protein called CWF19-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	L2	369	3049	1930	527	569	23	0	0

- Molecule 32 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	M	166	827	495	166	166	0	0

- Molecule 33 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	P	112	942	575	184	181	2	0	0

- Molecule 34 is a protein called PAX3- and PAX7-binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	PX	295	1465	875	295	295	0	0

- Molecule 35 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	T	360	2854	1800	521	523	10	0	0

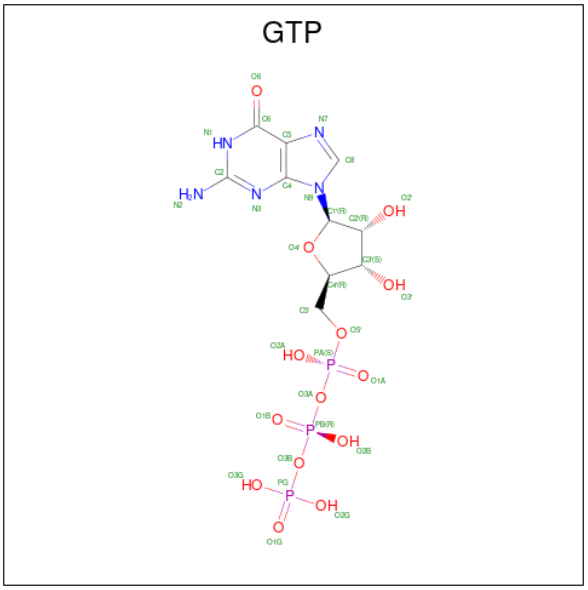
- Molecule 36 is a protein called Tuftelin-interacting protein 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	TF	572	2835	1690	572	573	0	0

- Molecule 37 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	b	94	717	449	135	126	7	0	0

- Molecule 38 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

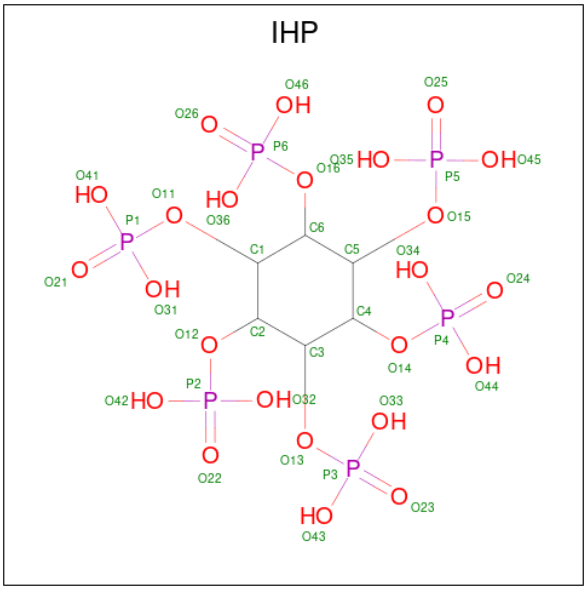


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
38	C	1	32	10	5	14	3	0

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
39	N	3	3	3	0

- Molecule 40 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



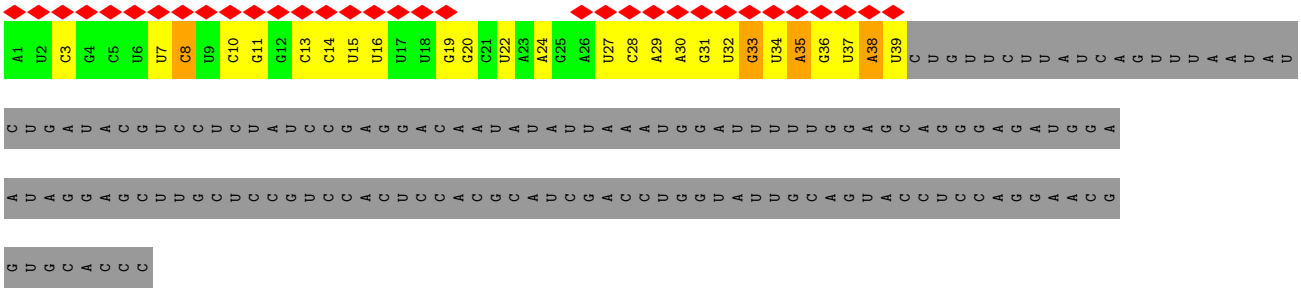
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
40	A	1	36	6	24	6	0

3 Residue-property plots (i)

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

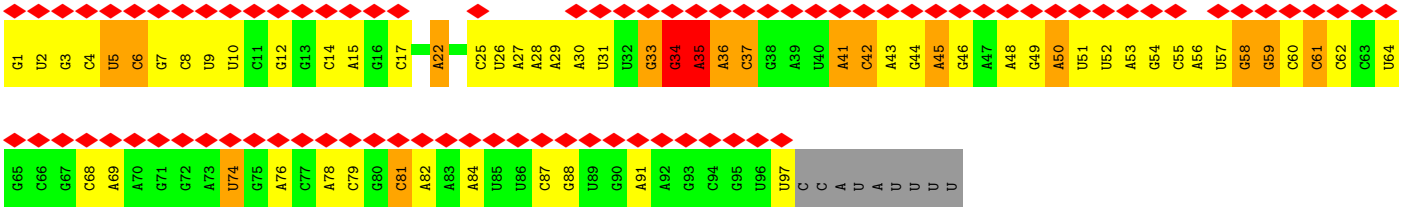
- Molecule 1: U2 snRNA

Chain 2: 18% 7% 12% • 79%



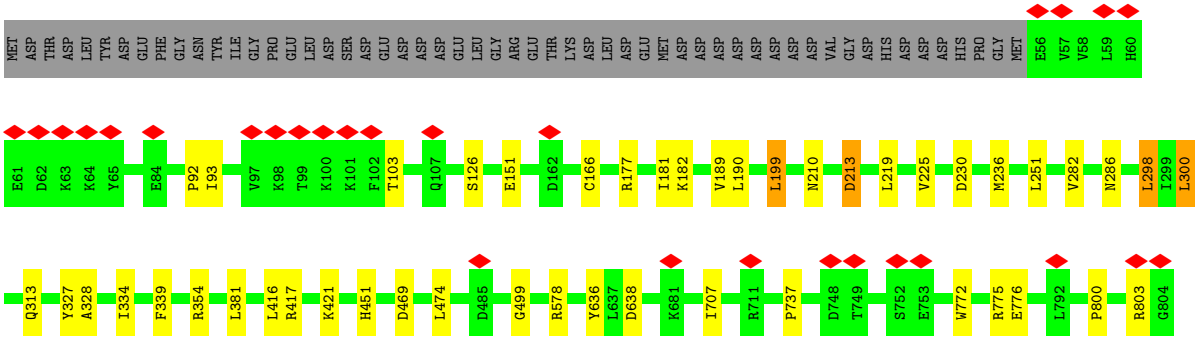
- Molecule 2: U6 snRNA

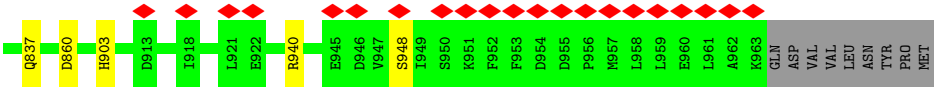
Chain 6: 80% 33% 42% 14% • 8%



- Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

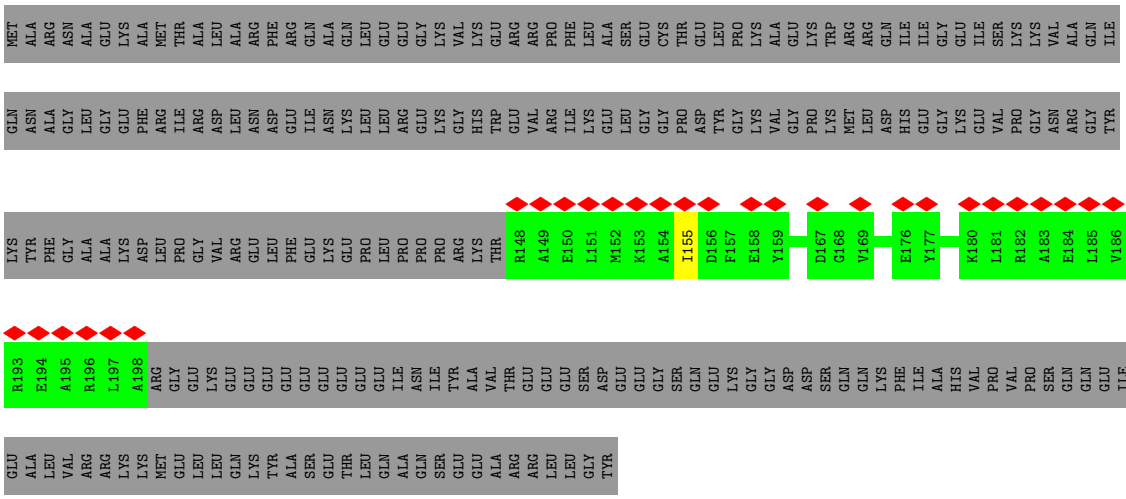
Chain C: 5% 88% 5% 7%





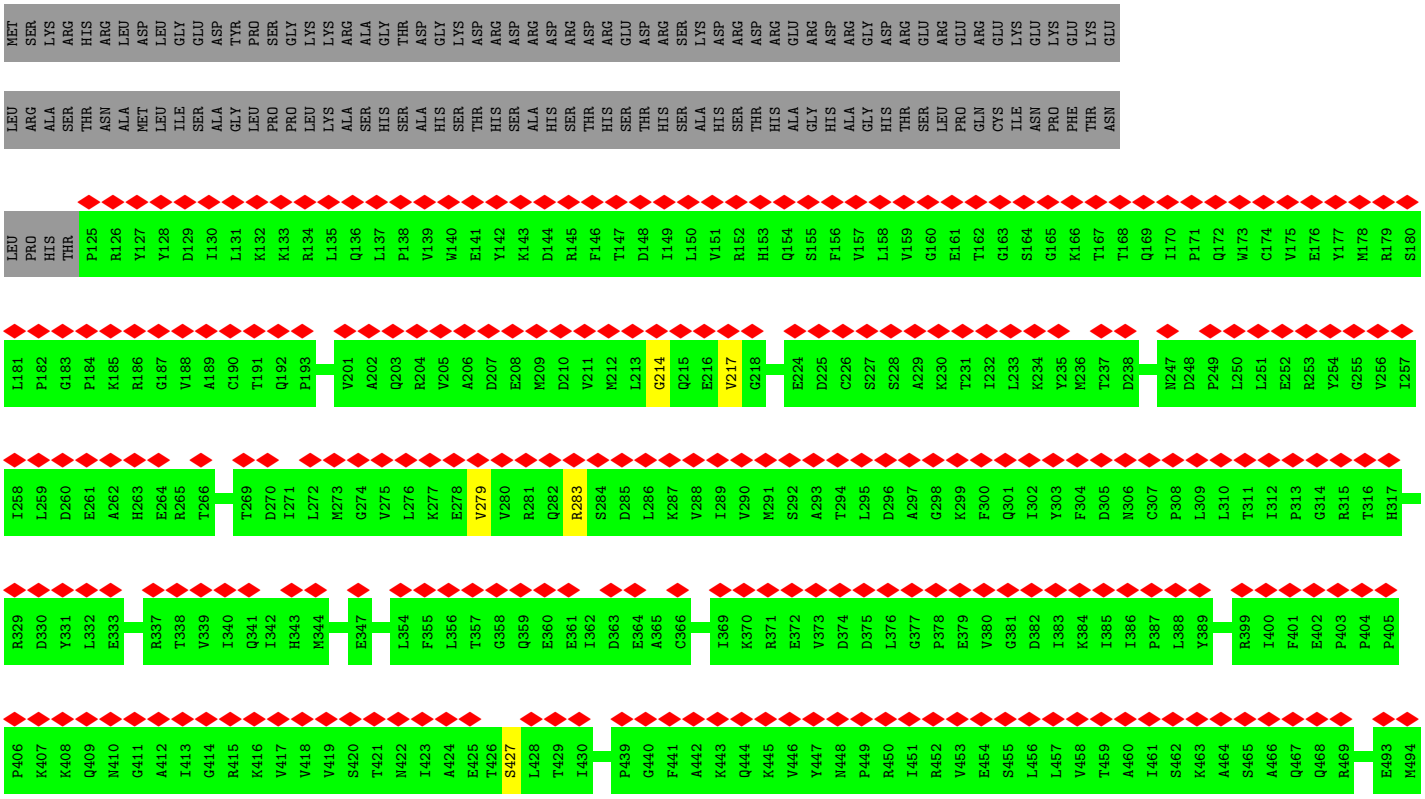
- Molecule 4: Pre-mRNA-splicing factor ISY1 homolog

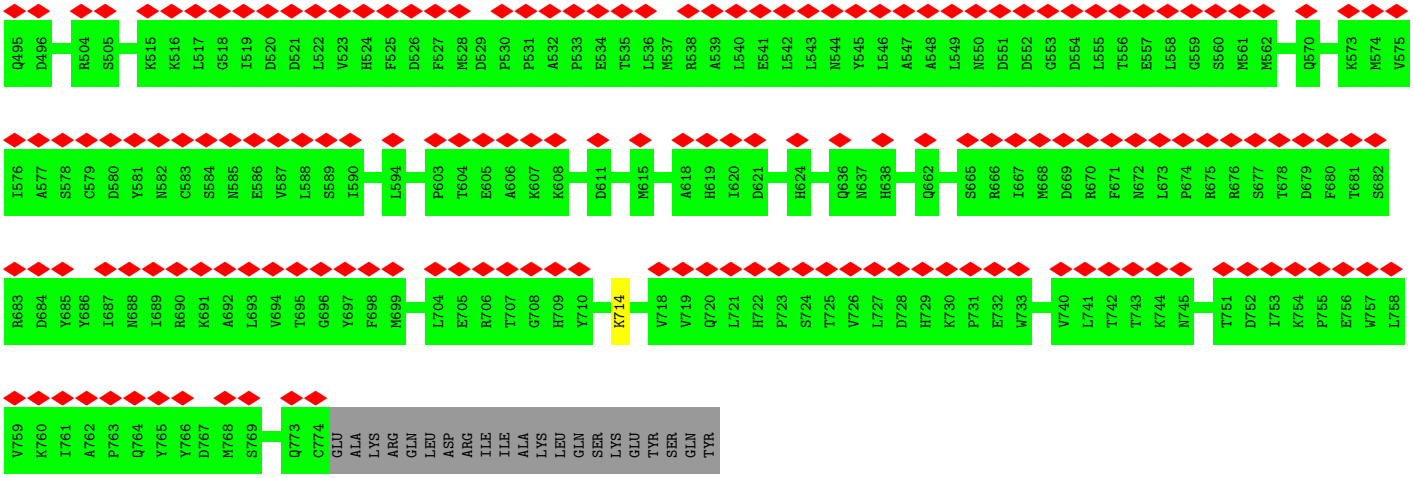
Chain D:



- Molecule 5: ATP-dependent RNA helicase DHX15

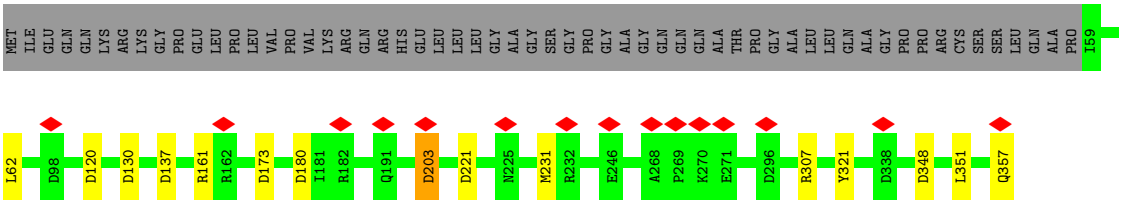
Chain DX:





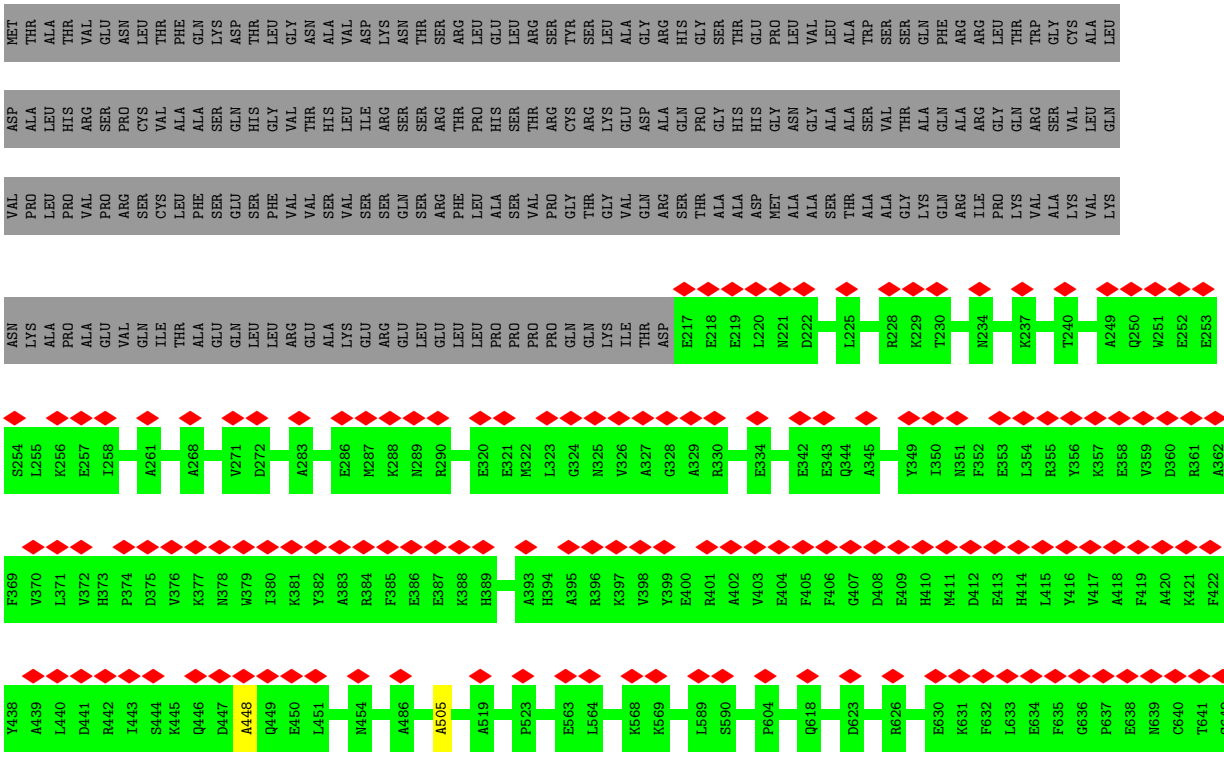
- Molecule 6: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:



- Molecule 7: Crooked neck-like protein 1

Chain J:



E648 T651 I652 L653 G654 D655 I656 D657 A661 E664 L665 A666 I667 S668 Q669 P670 R671 L672 D673 M674 P675 E676 V677 D684 F685 E686 I687 E688 Q689 E690 E691 T692 E693 R696 N697 L698 Y699 R700 R701 L702 L703 Q704 R705 T706 Q707 H708 V709 K710 V711 W712 I713 S714 F715 A716 Q717

F718 E719 L720 S721 S722 G723 K724 E725 G726 S727 L728 T729 K730 C731 R732 Q733 E736 E737 A738 N739 K740 T741 M742 R743 N744 C745 E746 E747 K748 E749 E750 R751 L752 M753 L754 L755 E756 S757 W758 R759 S760 F761 E762 E763 E764 F765 G766 T767 A768 S769 D770 K771 E772 R773 V774 D775 K776 L777 MET

PRO GLU LYS VAL LYS LYS ARG ARG LYS VAL GLN THR ASP ASP GLY SER ASP ALA GLY TRP GLU GLU TYR PHE ASP TYR ILE PHE PRO GLU ASP ALA ALA ASN GLN PRO ASN LEU LYS LEU LEU ALA MET ALA LYS LEU TRP LYS LYS GLN GLN GLN GLN GLU LYS GLU ASP ALA GLU HIS HIS

PRO ASP GLU ASP VAL ASP GLU SER GLU SER

- Molecule 8: Pre-mRNA-splicing factor SPF27

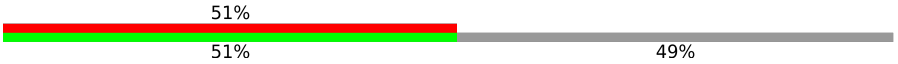
Chain K:

MET ALA GLY THR GLY LEU VAL ALA GLY GLU VAL VAL VAL ASP ALA LEU PRO TYR PHE ASP GLN GLY TYR GLU ALA PRO GLY V28 P45 A60 Q77 P78 I79 E80 L81 L82 S83 M84 K85 R86 Y87 E88 L89 P90 S93 S94 G95 Q96 K97 N98 A216 ASN LYS GLU ASN

ILE ARG GLN ASP PHE

- Molecule 9: CWF19-like protein 1

Chain L1:



M1 A2 Q3 K4 P5 L6 R7 L8 L9 A10 C11 G12 D13 V14 E15 G16 K17 F18 D19 I20 L21 F22 N23 R24 V25 Q26 A27 I28 Q29 K30 K31 S32 G33 N34 F35 D36 L37 L38 L39 C40 V41 G42 N43 F44 F45 G46 S47 T48 Q49 D50 A51 E52 W53 E54 E55 Y56 K57 T58 G59 I60

K61 K62 A63 P64 I65 Q66 T67 Y68 V69 L70 G71 A72 N73 N74 Q75 E76 T77 V78 K79 Y80 F81 Q82 D83 A84 D85 G86 C87 E88 L89 A90 E91 N92 I93 T94 Y95 L96 G97 R98 K99 G100 I101 F102 T103 G104 S105 S106 G107 L108 Q109 I110 V111 Y112 L113 S114 G115 T116 E117 S118 L119 N120

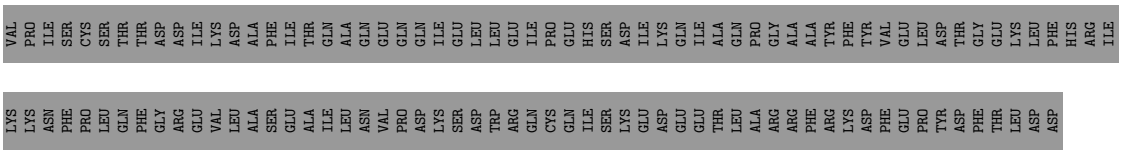
E121 P122 V123 P124 G125 Y126 S127 F128 S129 P130 K131 D132 V133 S134 S135 L136 R137 M138 M139 L140 C141 T142 T143 S144 Q145 F146 K147 G148 V149 D150 I151 L152 L153 T154 S155 P156 W157 P158 K159 C160 V161 G162 N163 F164 G165 N166 S167 S168 G169 E170 V171 D172 T173 K174 K175 C176 G177 S178 A179 L180

V181 S182 S183 L184 A185 T186 G187 L188 K189 P190 R191 Y192 H193 F194 A195 A196 L197 E198 K199 T200 Y201 Y202 E203 R204 L205 P206 Y207 R208 N209 H210 I211 Q214 E215 N216 A217 Q218 H219 A220 T221 R222 F223 I224 A225 L226 A227 N228 Y229 G230 N231 P232 E233 K234 K235 K236 Y237 L238 Y239 A240 F241

S242 I243 V244 P245 M246 K247 L248 M249 D250 A251 A252 E253 L254 V255 K256 Q257 P258 P259 D260 V261 T262 E263 N264 P265 Y266 R267 K268 S269 G270 Q271 E272 A273 S274 I275 GLY LYS GLN ILE LEU ALA PRO VAL GLU GLU SER ALA CYS GLN PHE PHE PHE ASP LEU ASN GLU LYS GLN GLY ARG LYS

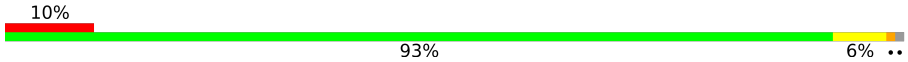
ARG SER SER THR GLY ARG ASP SER LYS SER SER PRO HIS PRO LYS GLN PRO ARG LYS PRO PRO GLN PRO PRO PRO GLY PRO CYS TRP PHE CYS LEU ALA SER PRO GLU VAL GLU LYS HIS LEU VAL VAL ASN ILE GLY THR HIS CYS TYR LEU ALA LEU ALA LYS GLY GLY LEU SER ASP ASP

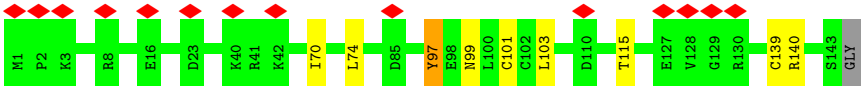
HIS VAL LEU ILE LEU PRO ILE GLY HIS TYR GLN SER VAL VAL GLU LEU SER ALA GLU VAL VAL GLU GLU VAL GLU LYS TYR LYS ALA THR LEU ARG ARG PHE PHE LYS SER ARG GLY LYS TRP CYS VAL VAL PHE GLU ARG ASN TYR LYS SER HIS HIS LEU GLN LEU GLN VAL ILE PRO



- Molecule 10: Protein BUD31 homolog

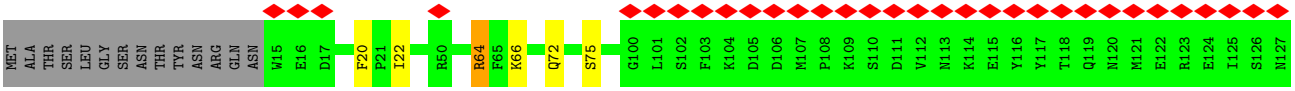
Chain N:

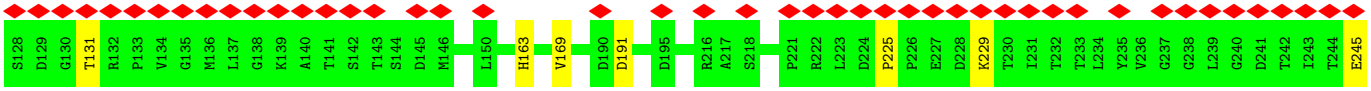




- Molecule 11: Pre-mRNA-splicing factor RBM22

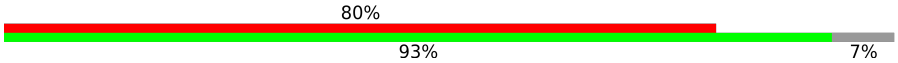
Chain O:

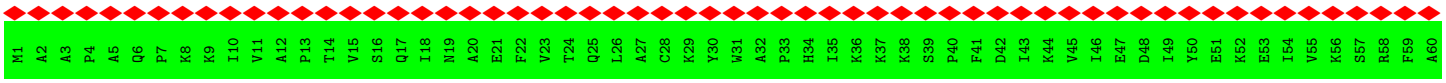


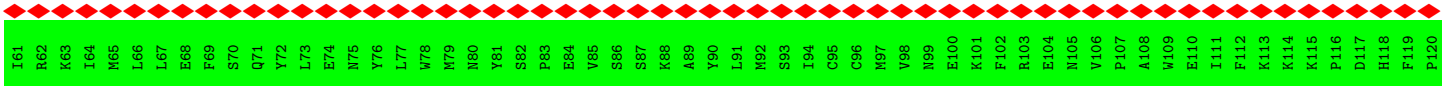


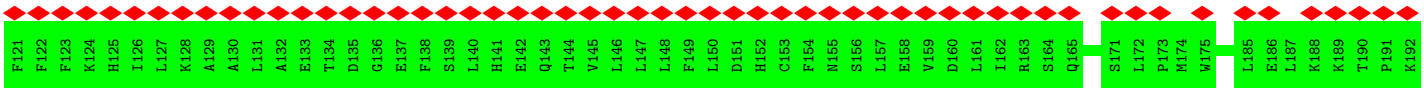
- Molecule 12: Intron-binding protein aquarius

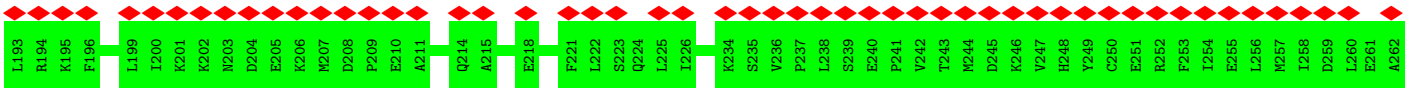
Chain Q:











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E358 V359 D360 T361 R362 E363 S364 L365 V366 K367 F368 F369 G370 P371 L372 S373 S374 N375 T376 L377 V380 A381 L384 C385 L386 L387 P388 T389 L390 P391 K392 N393 E394 D395 T396 T397 F398 D399 K400 E401 F402 L403 L404 E405 L406 L407 V408 S409 R410 H411 E412 D413 R414 I415 S416 L426 Y427

P428 T429 E430 K431 I432 I433 W434 D435 E436 M437 I438 V439 P440 T441 E442 Y443 Y444 S445 G446 E447 G448 C449 L450 A451 L452 P453 K454 L455 N456 L457 L462 Y465 L466 L467 R468 N469 F470 N471 L472 F473 R474 L475 E476 S477 T478 Y479 E480 I481 R482 Q483 D484 I485 E486 D487 S488 V489 S490 R491

M492 K493 P494 W495 Q496 S497 E498 Y499 G500 G501 V502 V503 F504 G505 G506 W507 A508 R509 M510 A511 Q512 P513 I514 V515 A516 F517 T518 V519 V520 E521 V522 A523 K524 P525 N526 I527 G528 E529 N530 W531 P532 T533 R534 V535 R536 A537 D538 V539 T540 I541 N542 L543 N544 V545 R546 D547 H548 I549 K550 D551

E552 W553 E554 G555 L556 R557 K558 H559 D560 V561 C562 F563 L564 I565 T566 V567 R568 P569 T570 K571 P572 Y573 G574 T575 K576 F577 D578 R579 R580 R581 P582 F583 I584 E585 Q586 V587 G588 L589 V590 Y591 V592 R593 G594 C595 E596 I597 Q598 G599 M600 L601 D602 D603 K604 G605 R606 V607 I608 E609 D610 G611

P612 E613 P614 R615 P616 N617 L618 R619 G620 E621 S622 R623 T624 F625 R626 V627 F628 L629 D630 Q633 Y634 Q635 Q636 D637 M638 T639 N640 T641 I642 Q643 N644 G645 A646 E647 D648 V649 Y650 E651 T652 F653 N654 I655 I656 M657 R658 R659 K660 P661 K662 N665 F666 K667 A668 V669 L670 E671 T672 I673

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E738 D739 P740 A741 L742 Q743 I744 P745 P746 F747 R748 I749 T750 F751 P752 V753 R754 S755 G756 K757 G758 K759 K760 R761 K762 D763 A764 D765 V766 E767 D768 E769 D770 T771 E772 E773 A774 K775 T776 L777 I778 V779 E780 P781 H782 V783 I784 P785 N786 R787 G788 P789 Y790 P791 Y792 N793 Q794 P795 K796 R797

N798 T799 I800 Q801 F802 T803 H804 T805 Q806 I807 E808 A809 I810 R811 A812 G813 M814 Q815 V821 V822 G823 P824 P825 G826 T827 G828 K829 T830 D831 V832 A833 V834 Q835 I836 I837 S838 T849 L850 I851 V852 S855 N856 Q857 A858 L859 N860 Q861 L862 F863 E864 K865 I866 M867 A868 L869 D870 I871

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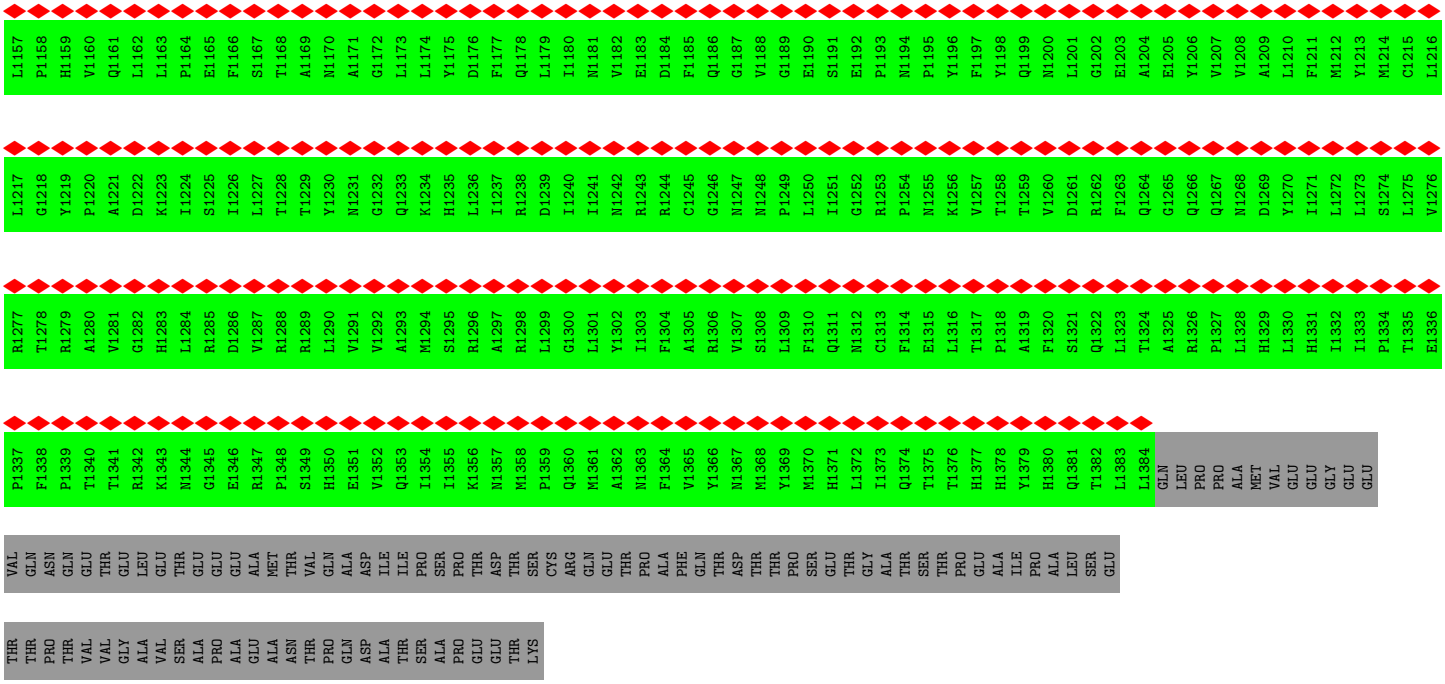
A932 G933 Y934 F935 F936 L937 Y938 Q939 K954 G955 S956 T957 L958 P959 D960 V961 T962 E963 V964 S965 T966 F967 H971 E972 Y973 F974 A975 N976 A977 P978 Q979 P980 I981 F982 K983 G984 R985 S986 Y987 E988 E989 D990 M991 E992 I993 A994 E995 G996 C997 F998 R999 H1000 T1006 Q1007 L1008 E1009 E1010

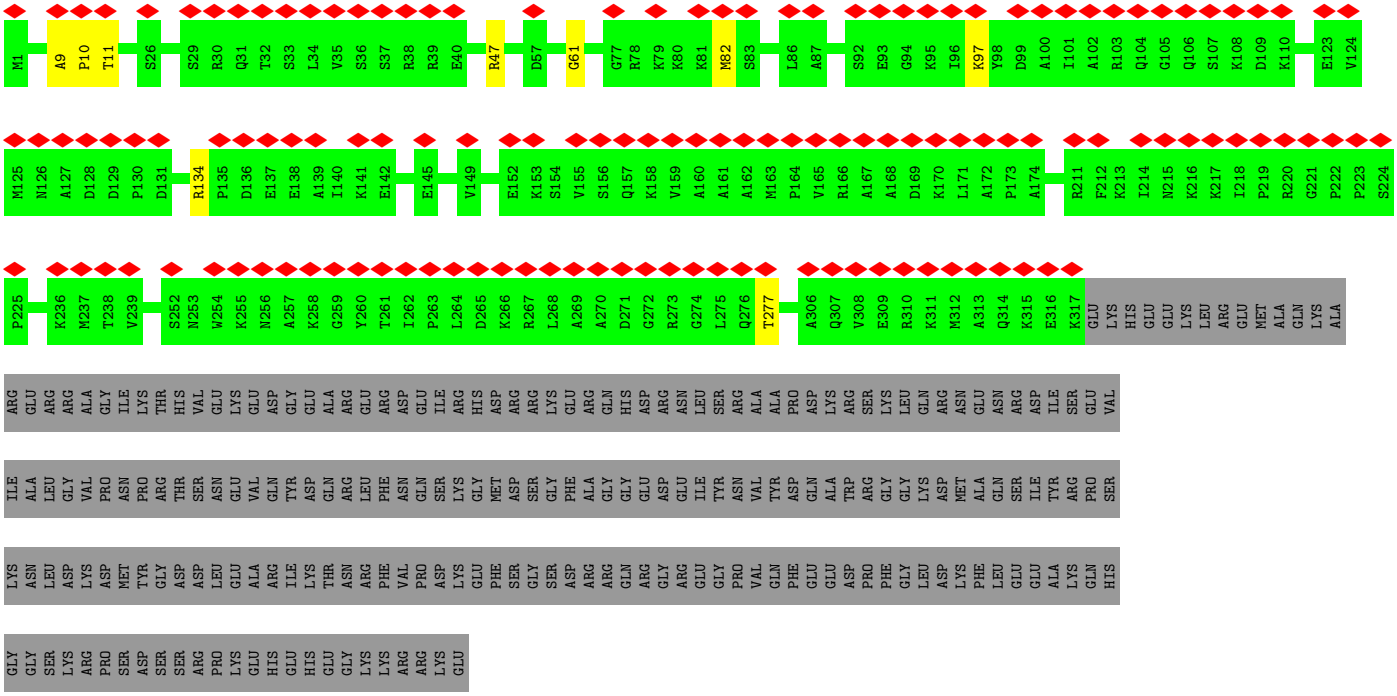
F1011 R1012 A1013 S1014 E1015 L1016 L1017 R1018 S1019 G1020 L1021 D1022 R1023 S1024 K1025 E1031 A1032 K1033 I1034 I1035 A1036 M1037 H1047 D1048 L1049 V1050 K1051 L1052 G1053 F1054 N1058 I1059 L1060 M1061 E1062 E1063 A1064 A1065 Q1066 I1067 L1068 E1069 I1070 E1071 T1072 F1073 I1074 P1075 L1076 P1081 Q1082 D1083 G1084 F1085 I1094

G1095 D1096 H1097 H1098 Q1099 L1100 P1101 P1102 V1103 I1104 K1105 N1106 M1107 A1108 F1109 Q1110 K1111 Y1112 S1113 N1114 M1115 E1116 Q1117 S1118 L1119 R1122 F1123 V1124 R1125 V1126 G1127 V1128 V1131 D1132 L1133 D1134 A1135 Q1136 G1137 R1138 A1139 R1140 A1141 S1142 L1143 C1144 N1145 L1146 Y1147 N1148 W1149 R1150 Y1151 K1152 N1153 L1154 G1155 N1156



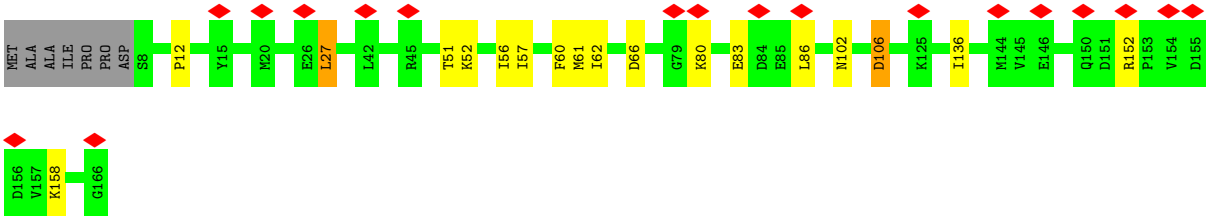
- Molecule 13: SNW domain-containing protein 1

Chain R:



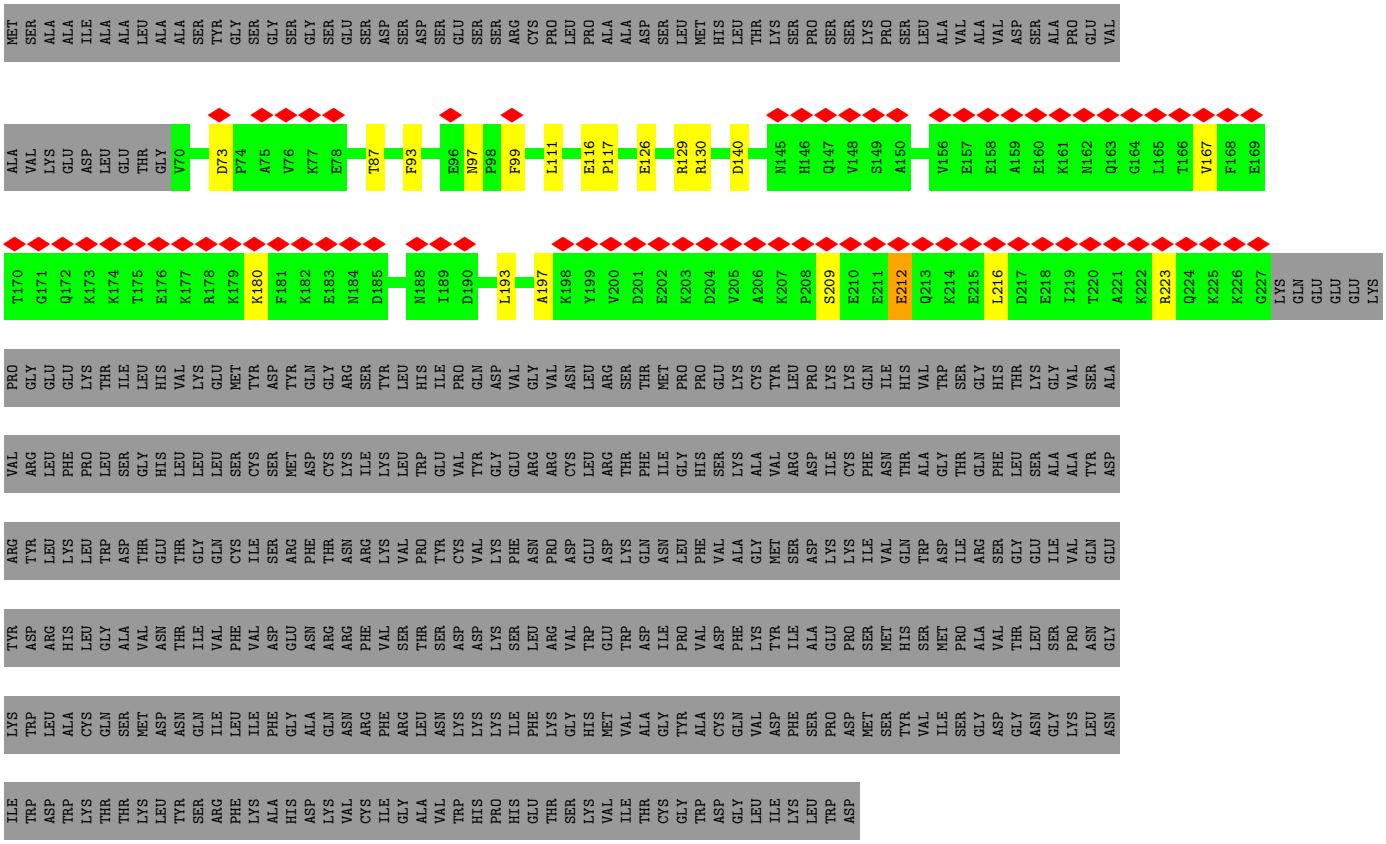
- Molecule 14: Peptidyl-prolyl cis-trans isomerase-like 1

Chain S:



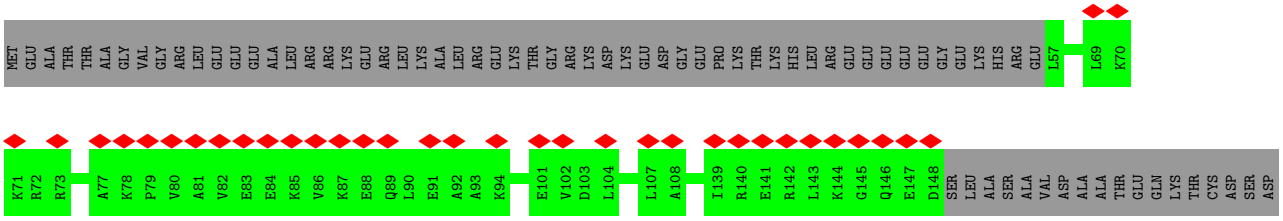
• Molecule 15: Pre-mRNA-processing factor 17

Chain W:



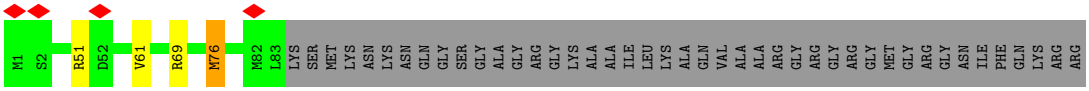
• Molecule 16: Coiled-coil domain-containing protein 12

Chain Z:



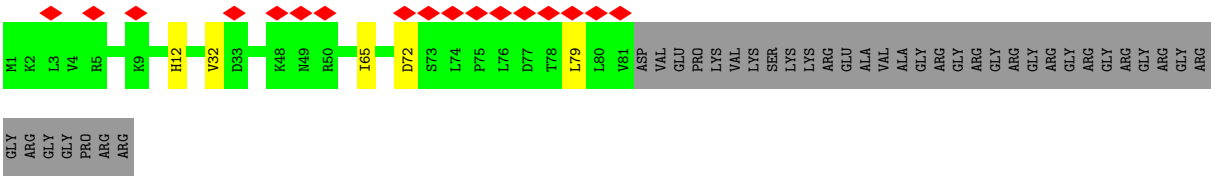
• Molecule 17: Small nuclear ribonucleoprotein Sm D3

Chain a:



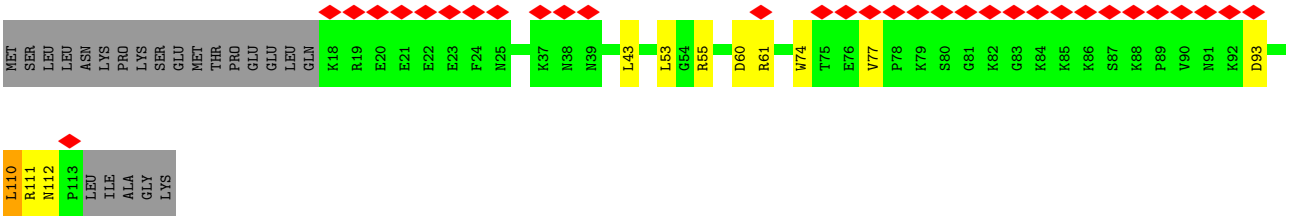
- Molecule 18: Small nuclear ribonucleoprotein Sm D1

Chain c:



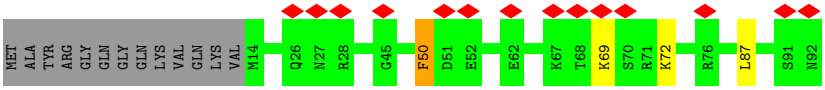
- Molecule 19: Small nuclear ribonucleoprotein Sm D2

Chain d:



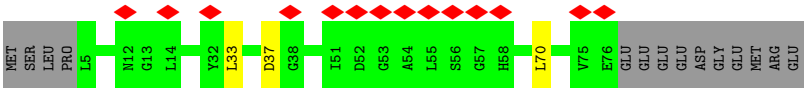
- Molecule 20: Small nuclear ribonucleoprotein E

Chain e:



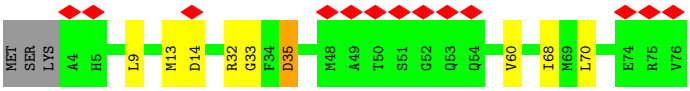
- Molecule 21: Small nuclear ribonucleoprotein F

Chain f:



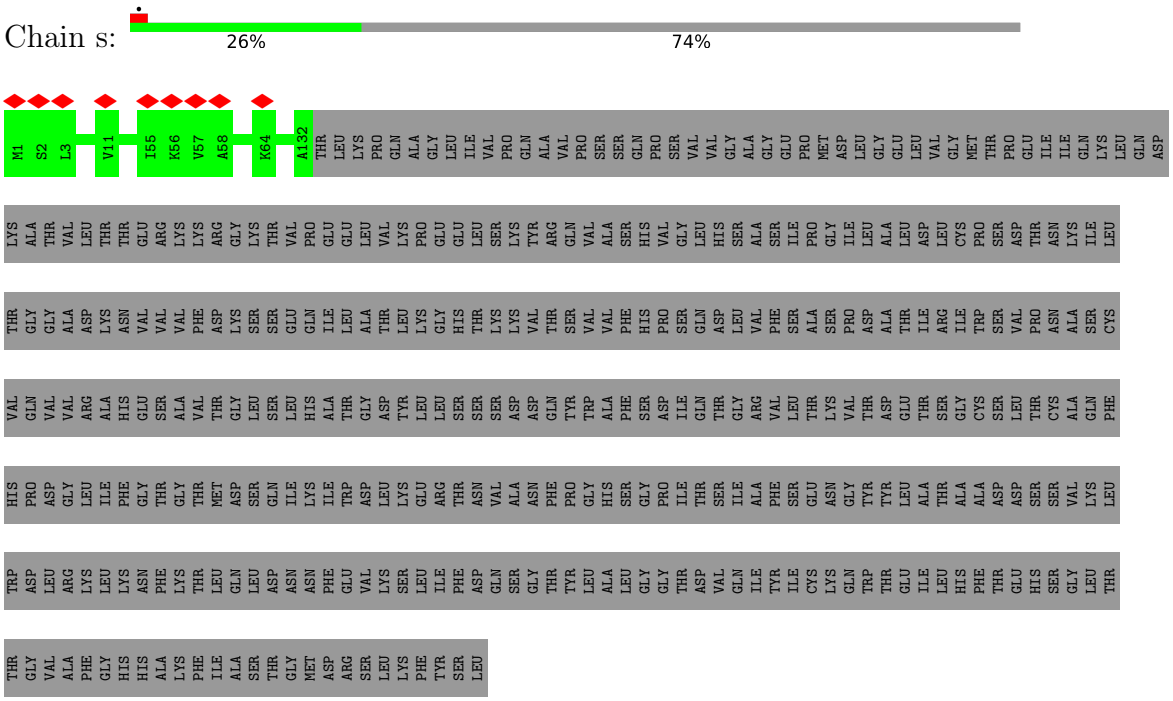
- Molecule 22: Small nuclear ribonucleoprotein G

Chain g:



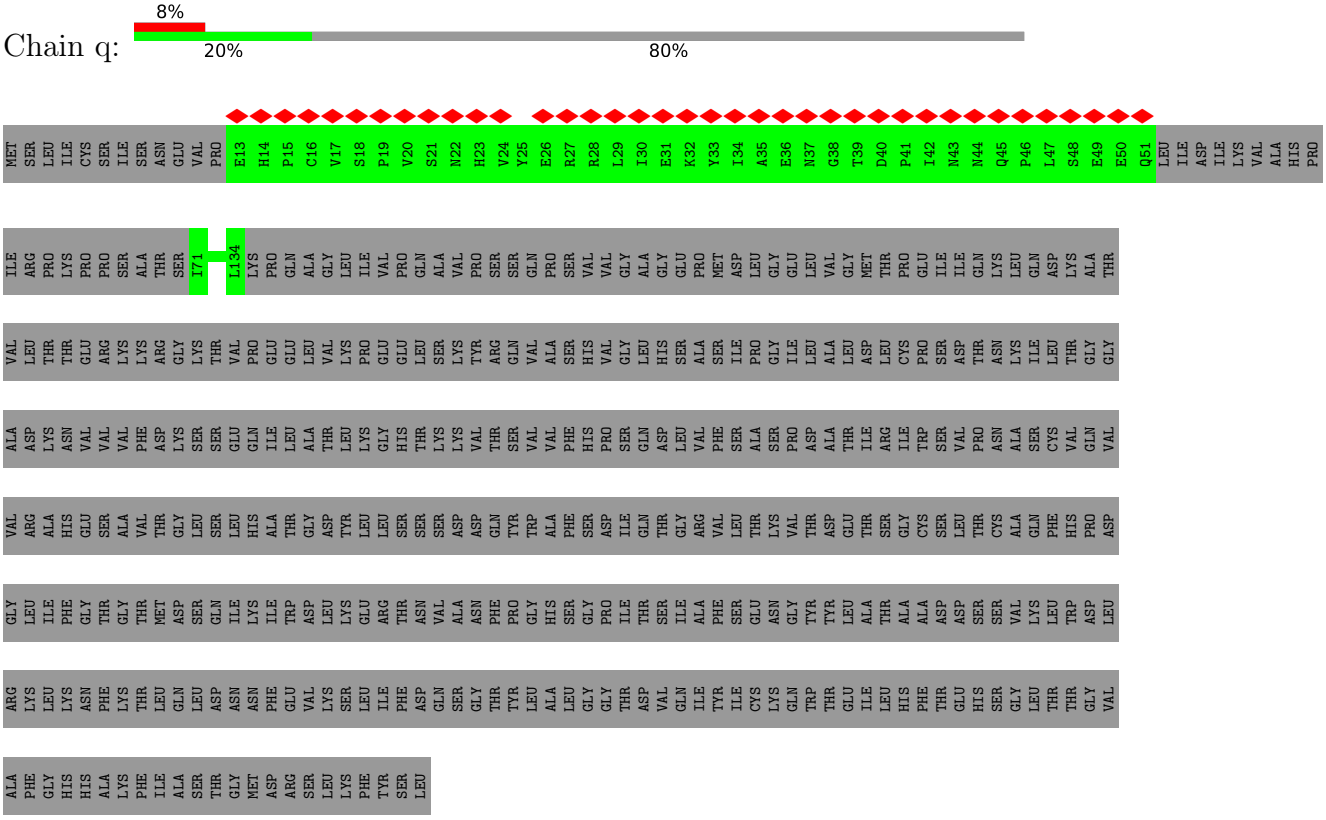
- Molecule 23: Pre-mRNA-processing factor 19

Chain s:



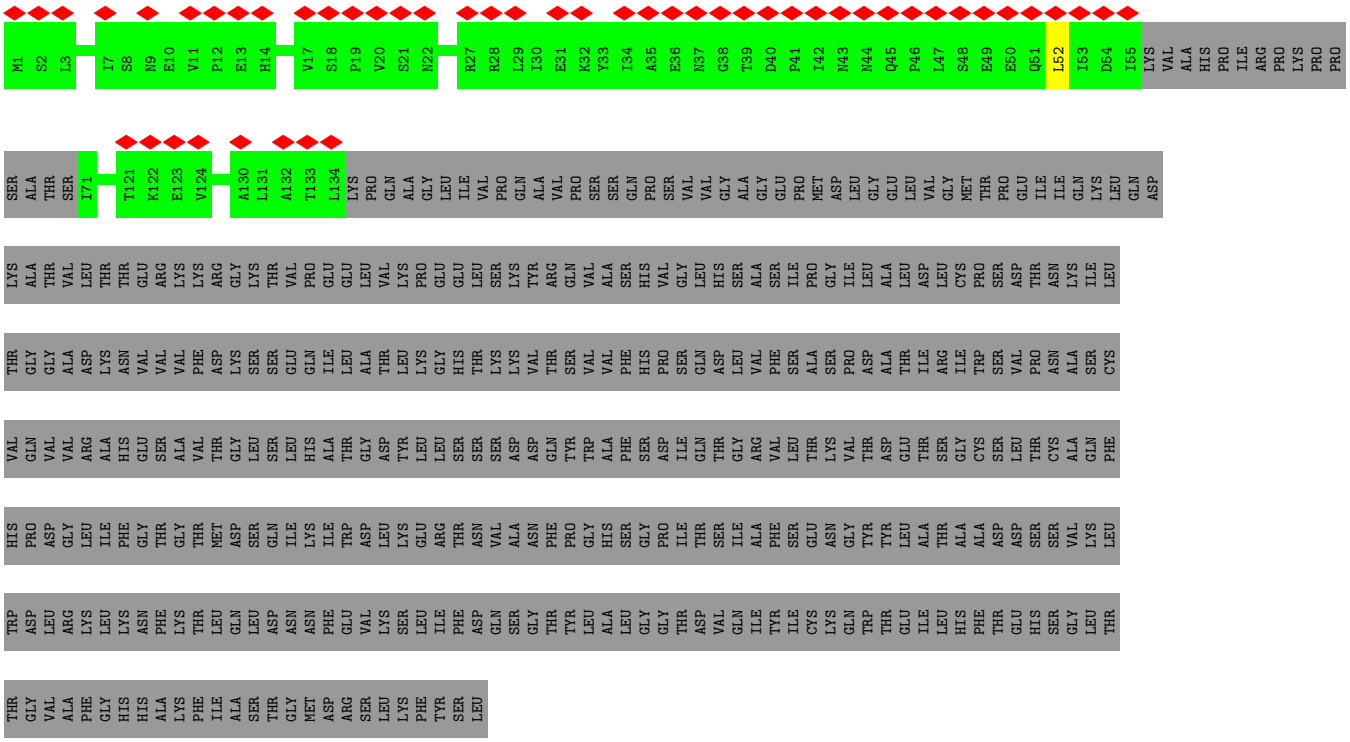
- Molecule 23: Pre-mRNA-processing factor 19

Chain q:



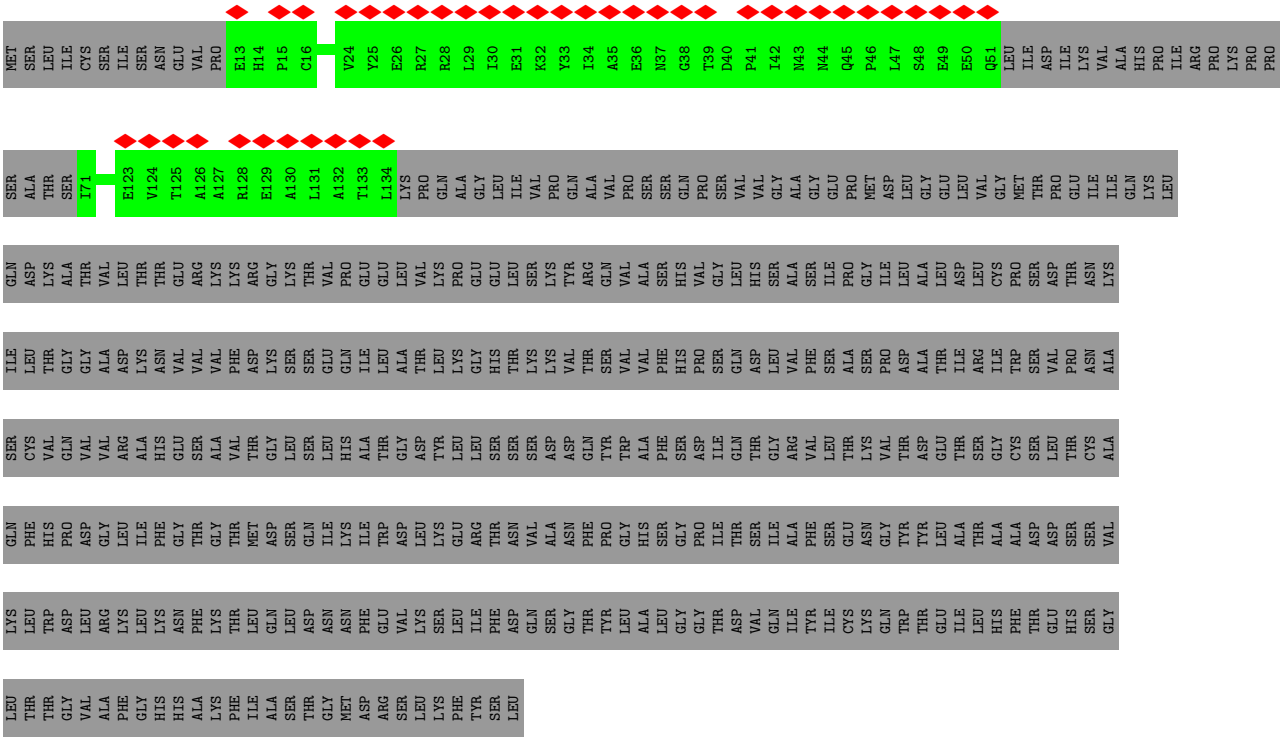
- Molecule 23: Pre-mRNA-processing factor 19

Chain r:



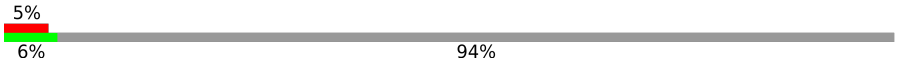
• Molecule 23: Pre-mRNA-processing factor 19

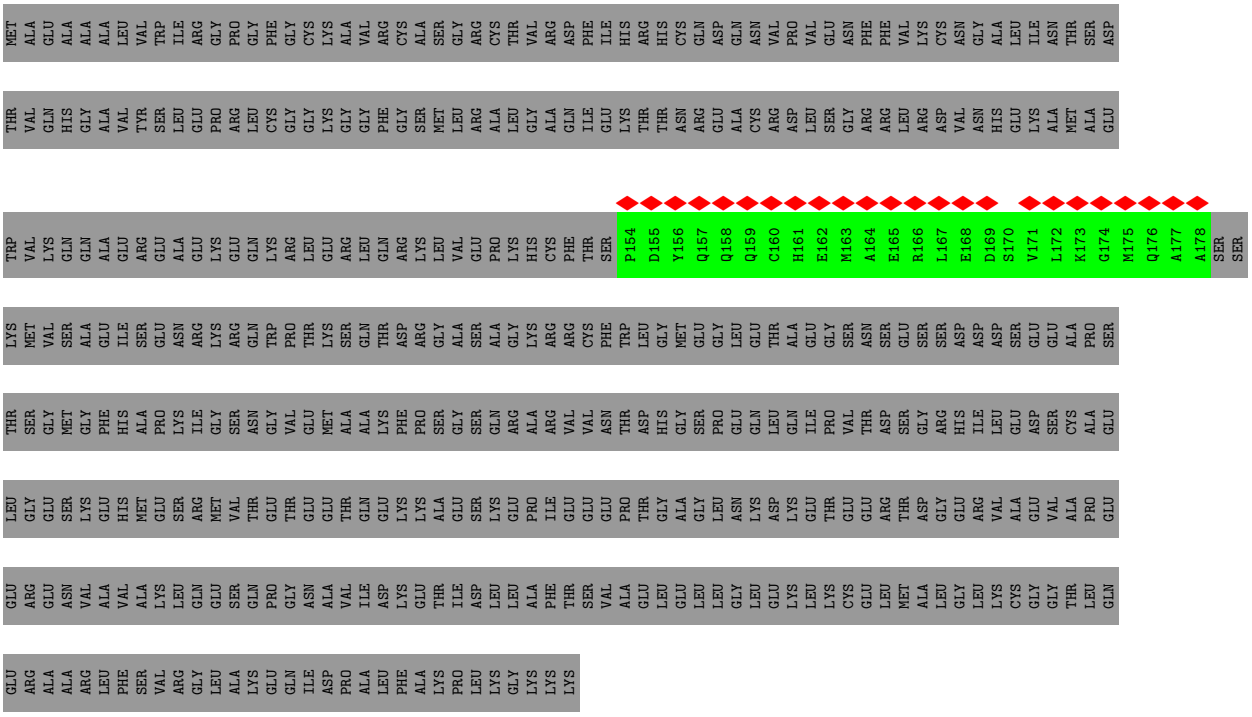
Chain t:



• Molecule 24: Splicing regulator SDE2

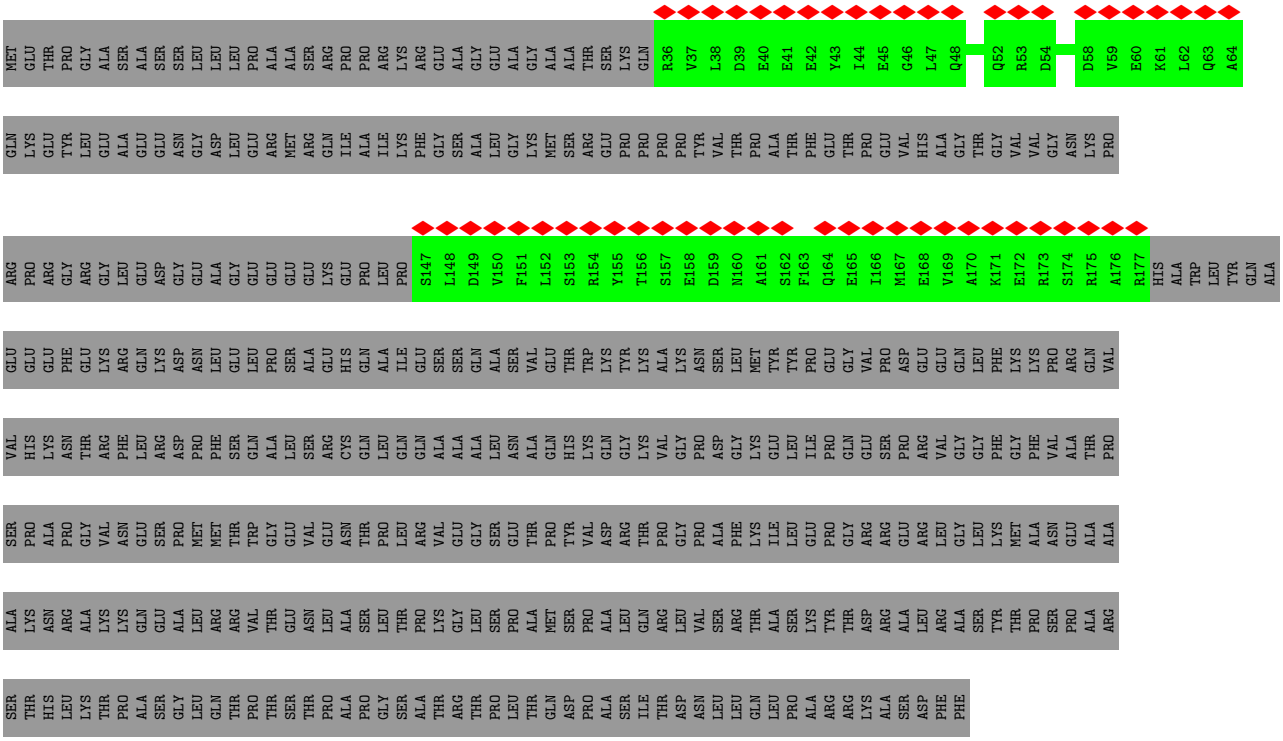
Chain z:





- Molecule 25: Splicing factor ESS-2 homolog

Chain 3:



- Molecule 26: U5 snRNA

Chain 5: 16% 41% 24% 13% • 21%

A U A C U C U G G9 U10 U11 U12 C13 U14 G20 A21 U22 C23 G24 U34 U35 G36 G37 C38 C39 U40 U41 U42 U43 A44 C45 U46 A47 U52 U53 G57 U58 G59 G65 A69 A C U C U G A G U C U U A A

C C85 C86 U89 U90 U91 U92 U93 U94 G95 A96 G97 C98 C99 U100 U101 G102 C103 C104 U105 U106 G107 G108 C109 A110 A111 G112 G113 C114 U115 A

• Molecule 27: Pre-mRNA-processing-splicing factor 8

Chain A: 17% 79% 5% 15%

MET ALA GLY VAL PHE PRO TYR ARG GLY PRO GLY ASN PRO VAL PRO GLY PRO LEU ALA PRO LEU PRO ASP TYR M25 S26 E47 K48 R49 K50 F51 G52 D55 E59 R71 R79 R82 H83 H97 P109 R156 R159 R165 F166 E172 D177

D200 Q211 R214 D215 T224 R240 D248 L249 V250 D251 D252 N253 D259 L260 K267 A268 L269 N270 G276 P277 K278 F279 E280 P281 L282 V283 R284 ASP ILE ASN LEU GLN ASP GLU ASP TRP ASN E295 F296 N297 L319 H326 V327 Y351 H363 S364 V365 K366

S367 Q368 L371 P381 D396 R409 L413 R417 P425 K428 C435 P436 A437 G438 Q439 K442 V443 R444 K460 H461 R462 K469 T479 D488 N514 D519 N523 K528 T529 K536 R539 L546 E549 R552 L578 Q579

Y580 I581 Y596 K597 K609 N617 T618 G619 P620 V621 G622 K623 W630 R642 L648 E661 G662 R663 H664 S665 K666 G667 V668 A669 K670 T671 V672 T673 K674 Q675 R676 E699 G700 I701 K702 Q703 N704 K705 A706 R707 T766 V767 D768 K769 T802 E805 L830

S851 V852 K853 S854 R855 I881 H884 T918 E929 R933 K941 D964 T991 R995 D1002 H1003 N1004 D1021 L1072 L1087 F1088 C1089 L1109 D1119 P1120 N1121 N1122 E1123 N1124 I1125 V1126 G1127 Y1128 N1129 N1130 K1131 K1132 C1133 W1134 P1135 R1136 D1137 A1138 R1139 M1140

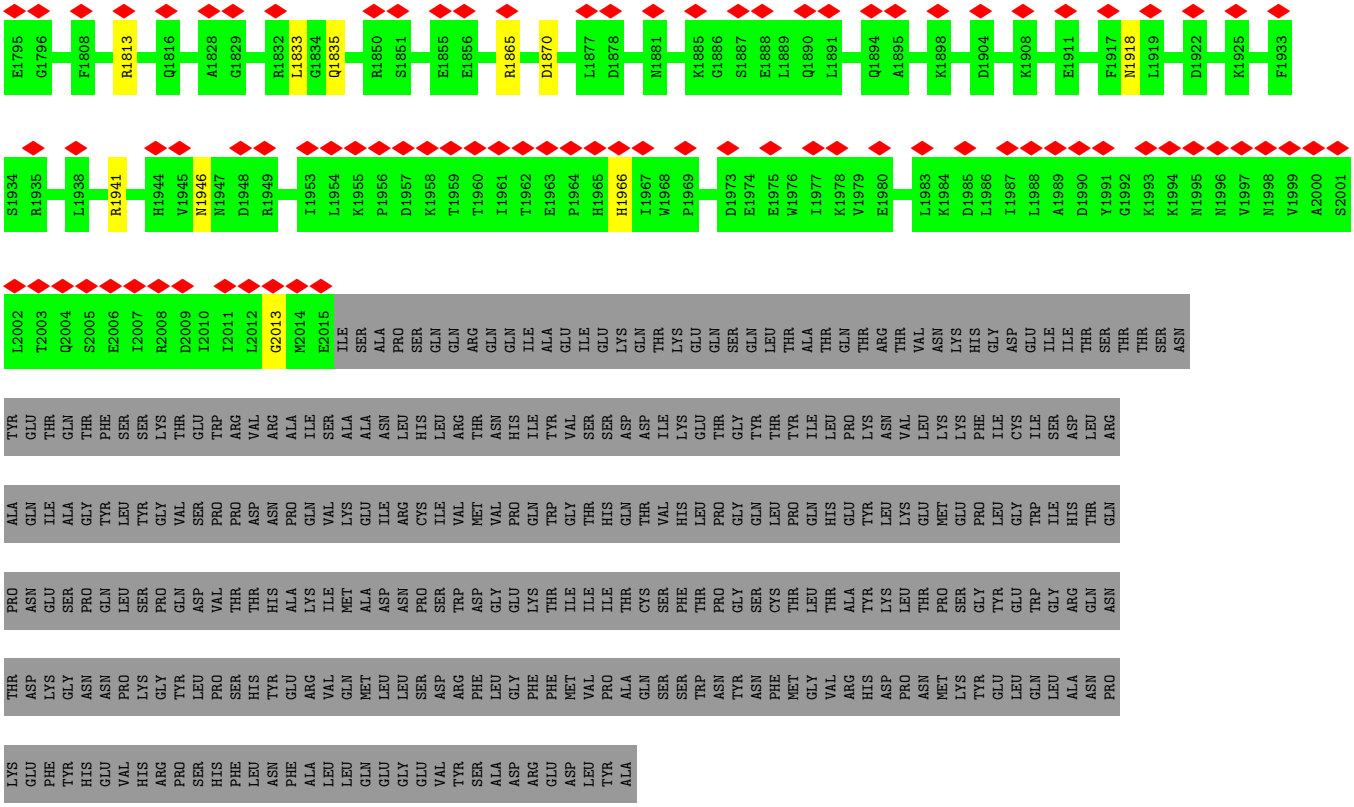
R1141 L1142 M1143 K1144 N1148 W1155 N1159 L1185 R1195 T1202 S1203 Y1204 E1205 E1206 F1207 T1208 H1209 K1210 D1211 K1222 D1233 D1234 N1242 R1243 V1244 R1245 Q1246 A1250 S1251 G1252 S1253 T1254 T1255 V1278 L1284 N1293 N1304 S1305 K1306 M1307 P1308 S1309 R1310 E1321

H1332 V1333 L1334 I1335 T1346 D1347 V1348 G1349 S1355 G1356 M1357 S1358 H1359 E1360 E1361 D1362 I1365 R1393 Q1394 E1395 A1396 I1397 A1398 Q1399 N1400 R1401 R1402 L1467 R1471 T1472 D1473 K1491 E1504 K1505 A1506 S1507 G1508 F1509 E1510 E1511 S1512 M1513 K1514 W1515 K1516 K1517 L1518 T1519 N1520 A1521 Q1522 R1523

S1524 G1525 L1526 N1527 Q1528 I1529 P1530 N1531 R1532 R1533 L1536 R1544 A1545 N1546 V1547 Y1548 Y1549 G1550 F1551 D1556 L1557 K1565 H1580 L1581 W1582 E1587 M1591 D1592 L1593 C1594 Q1595 V1596 F1597 D1598 Q1599 E1600 L1601 D1602 A1603 L1604 E1605 I1606 E1607 T1608 V1609 Q1610 K1611 E1612 T1613 I1614 H1615 P1616 R1617

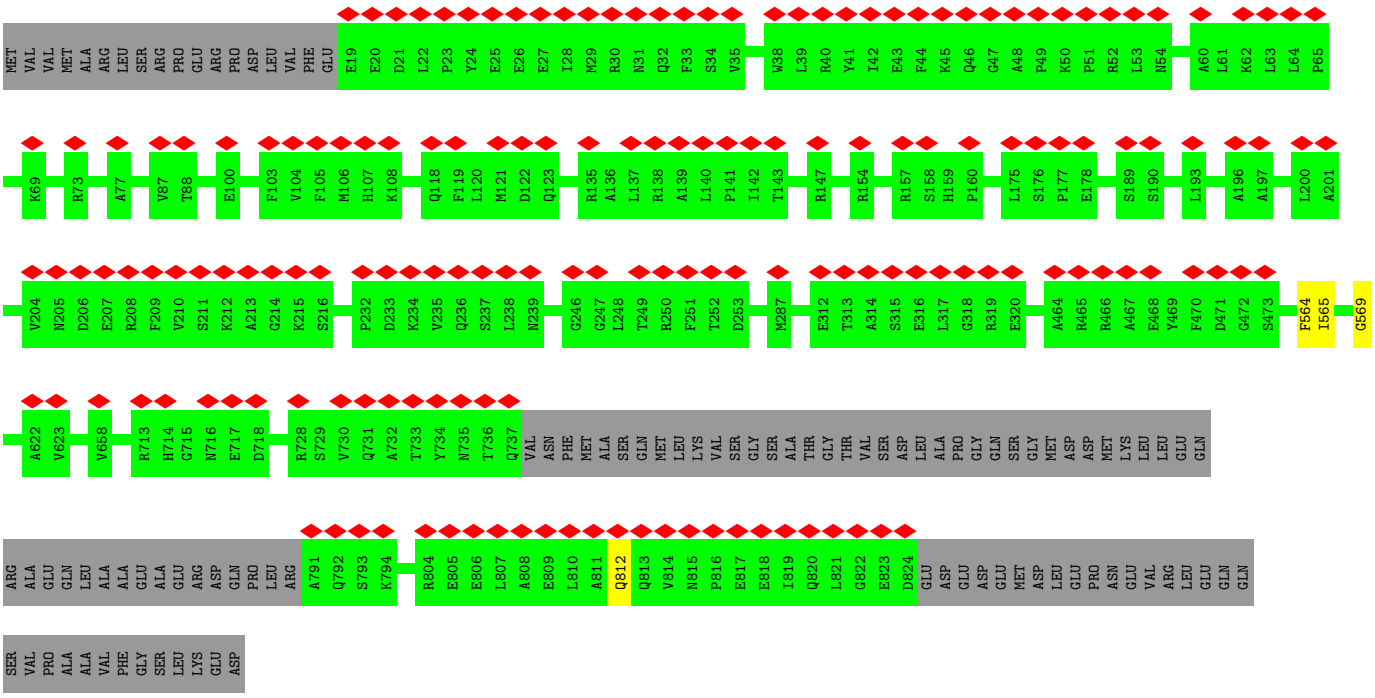
K1618 K1621 M1622 N1623 S1624 S1625 C1626 A1627 D1628 I1629 L1630 L1631 F1632 A1633 S1634 Y1635 K1636 W1637 N1638 V1639 S1640 R1641 P1642 S1643 L1644 L1645 A1646 D1647 S1648 K1649 D1650 V1651 M1652 D1653 S1654 T1655 T1656 T1657 Q1658 K1659 Y1660 W1661 I1662 D1663 D1670 R1678 R1681 A1682 K1683 F1684 L1685 D1686 Y1687 T1688 T1689 D1690

N1691 M1692 S1693 I1694 Y1695 P1696 S1697 P1698 T1699 G1700 V1701 L1702 N1710 G1716 N1717 W1718 F1719 P1720 G1721 S1722 K1723 P1724 L1725 I1726 Q1727 Q1728 A1729 K1732 L1753 P1758 T1759 E1760 P1761 Y1762 L1763 S1764 S1765 Q1766 N1767 Y1768 G1769 E1770 L1771 F1772 S1773 N1774 Q1775 I1776 D1781 D1782 V1785 F1794



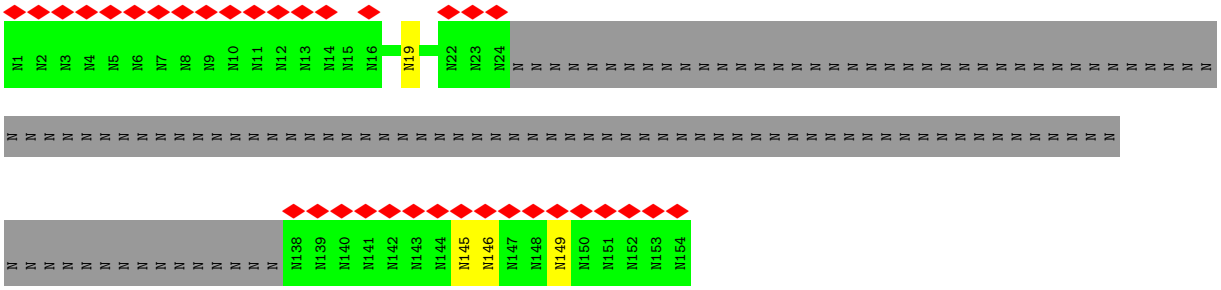
- Molecule 28: Pre-mRNA-splicing factor SYF1

Chain I:



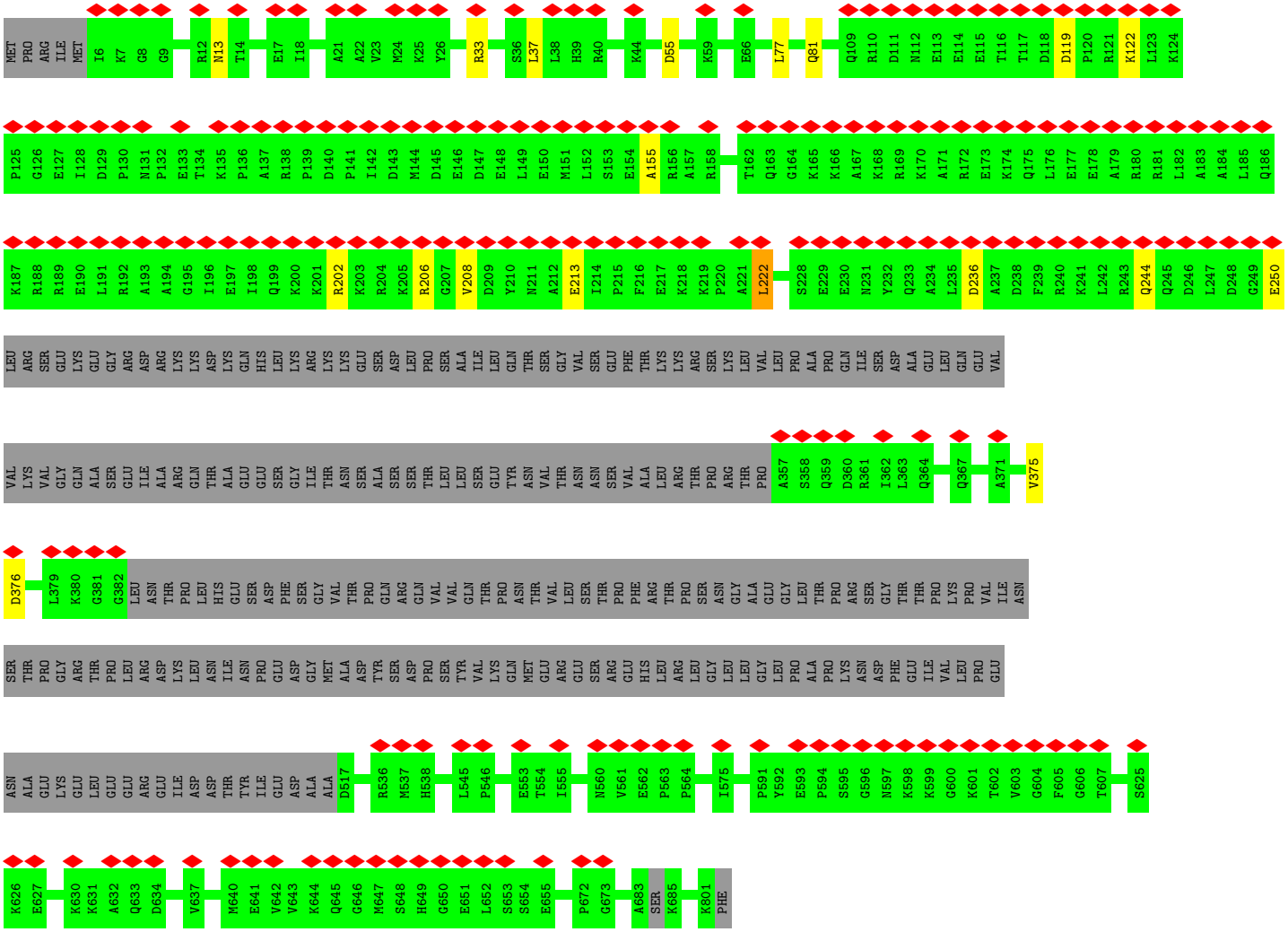
- Molecule 29: INTRON

Chain IN: 23% 24% • 73%



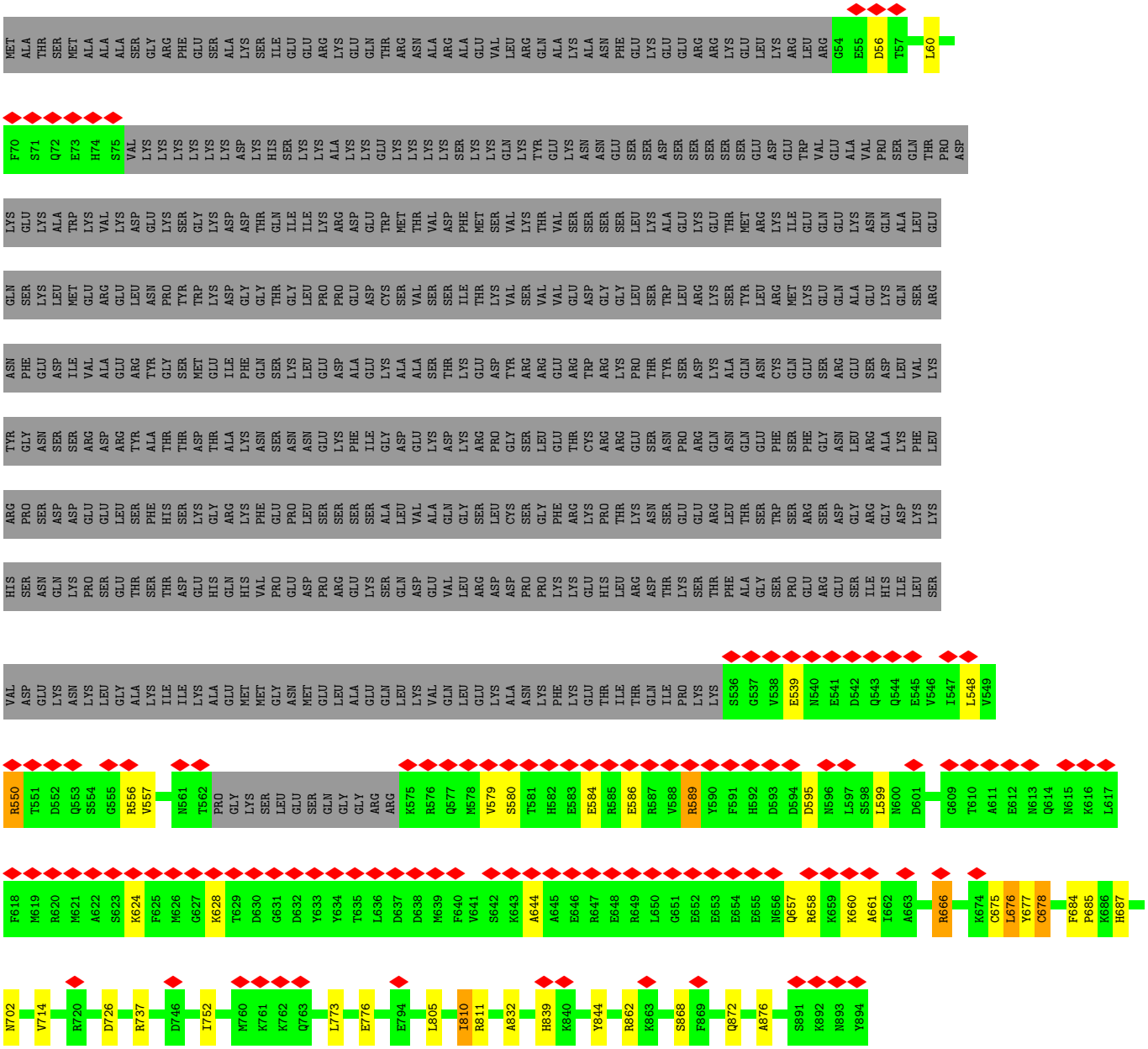
• Molecule 30: Cell division cycle 5-like protein

Chain L: 27% 67% • 31%



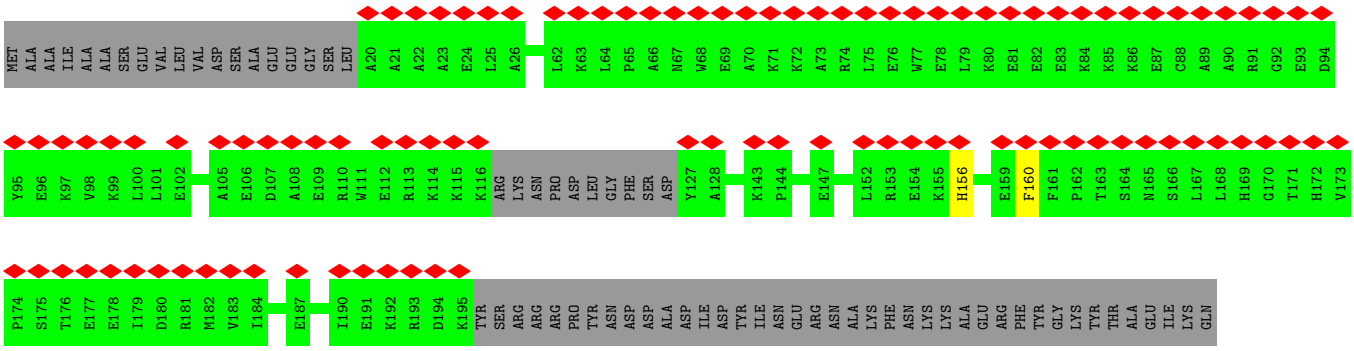
• Molecule 31: CWF19-like protein 2

Chain L2: 13% 36% • • 59%

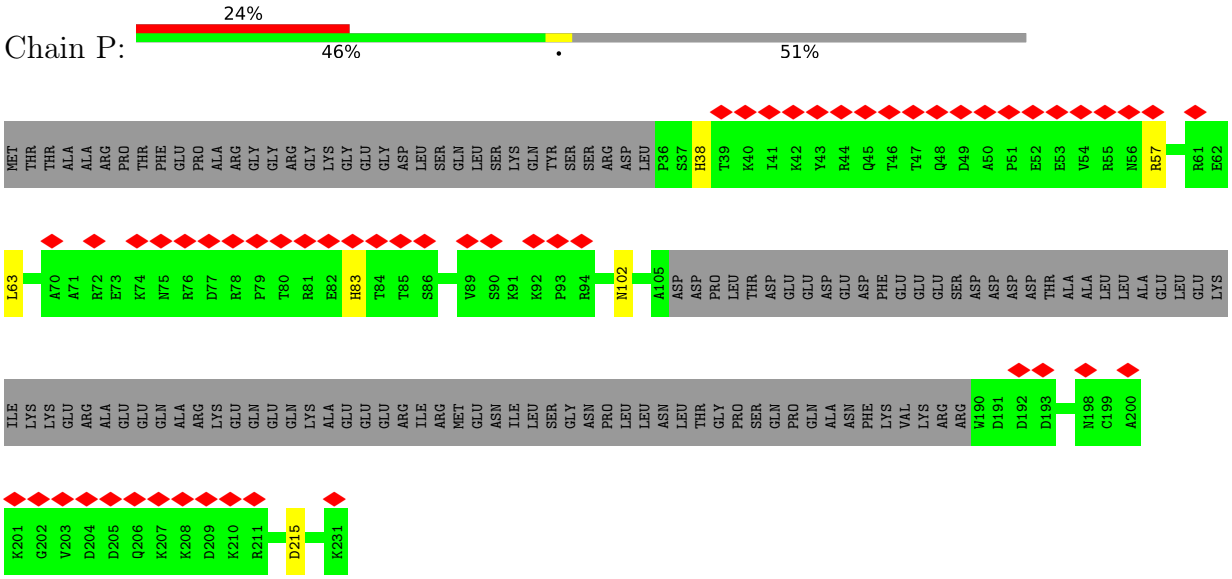


- Molecule 32: Pre-mRNA-splicing factor SYF2

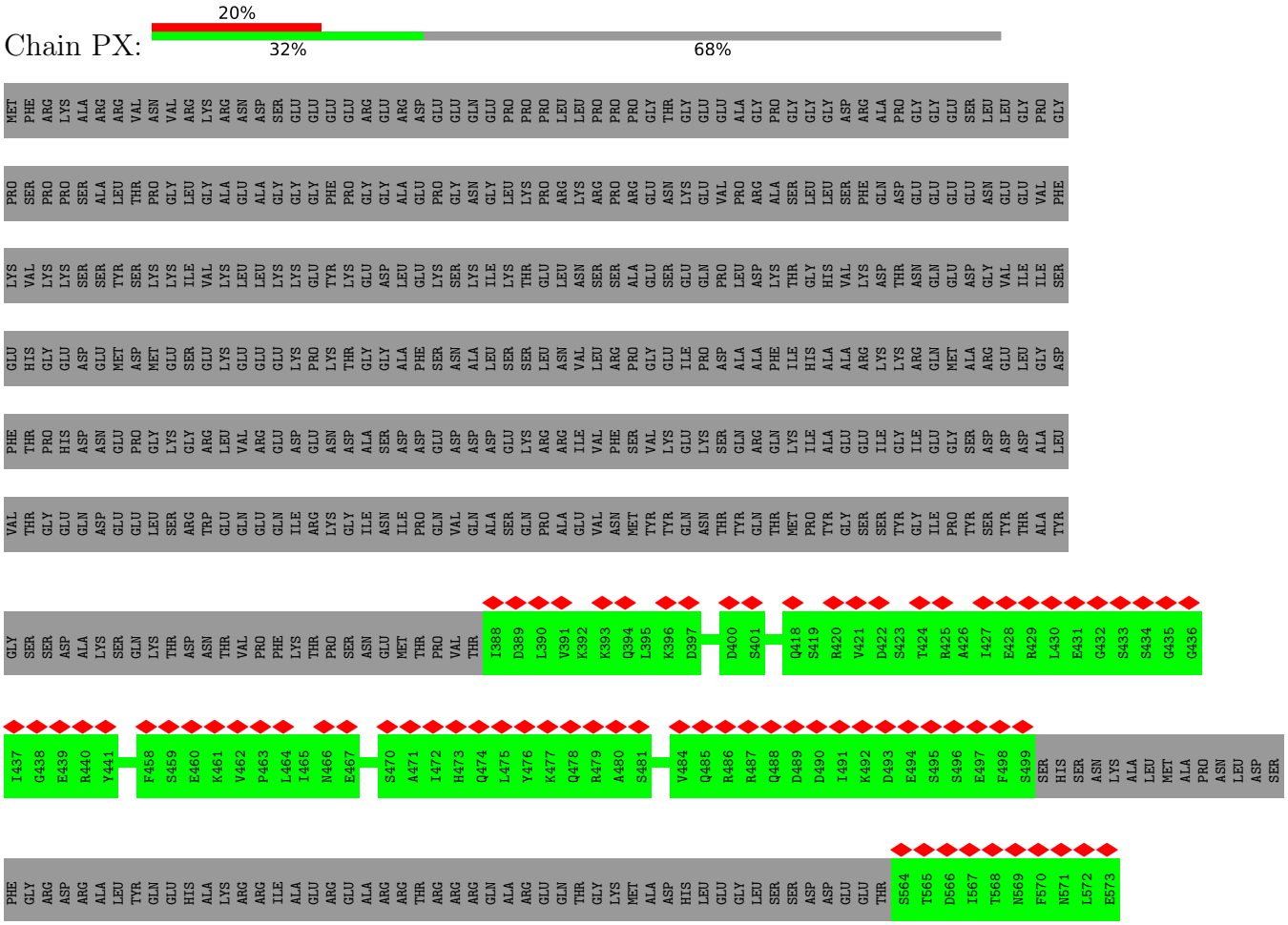
Chain M:

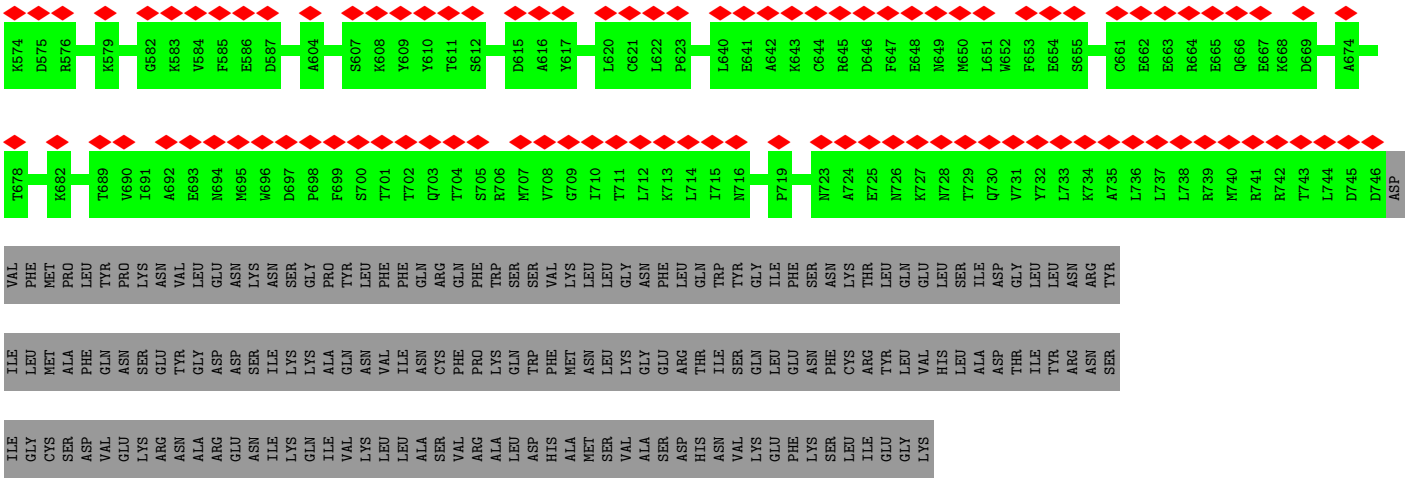


• Molecule 33: Spliceosome-associated protein CWC15 homolog



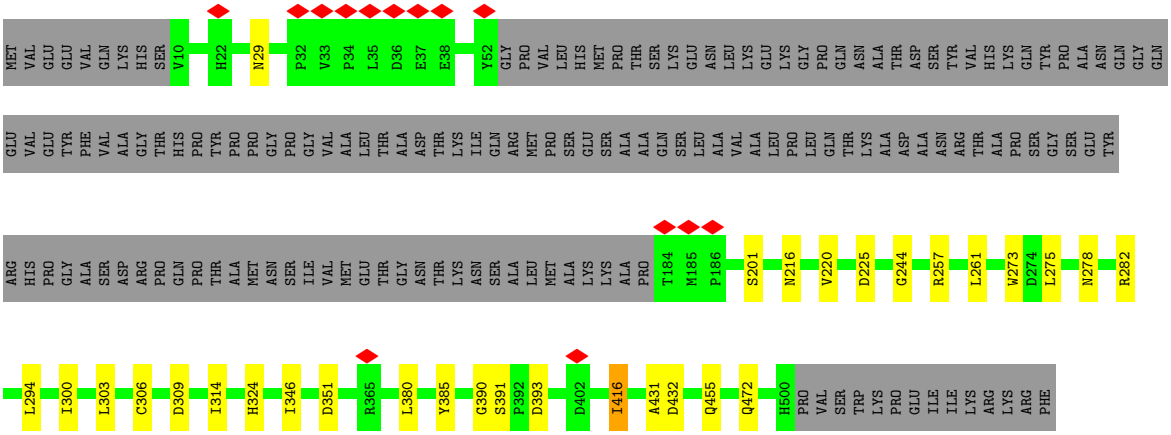
• Molecule 34: PAX3- and PAX7-binding protein 1





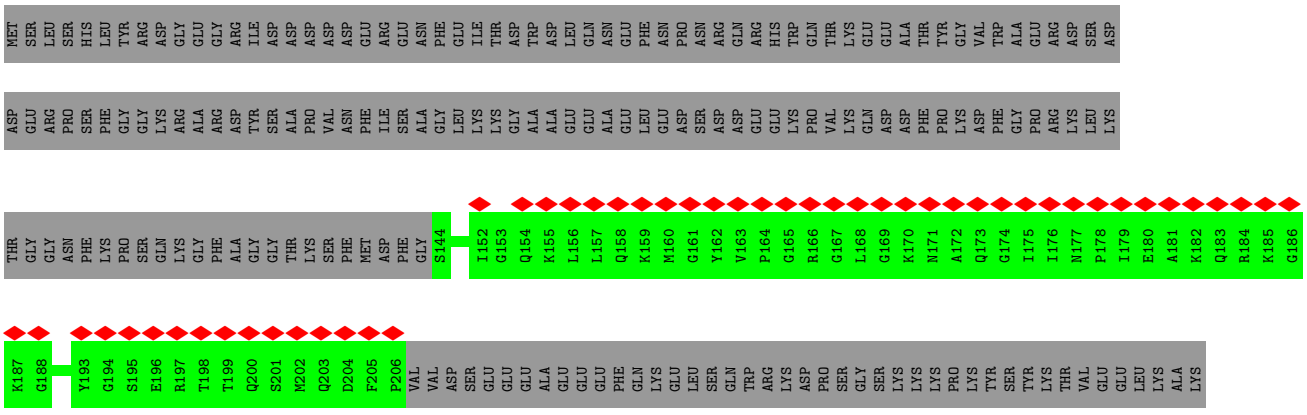
- Molecule 35: Pleiotropic regulator 1

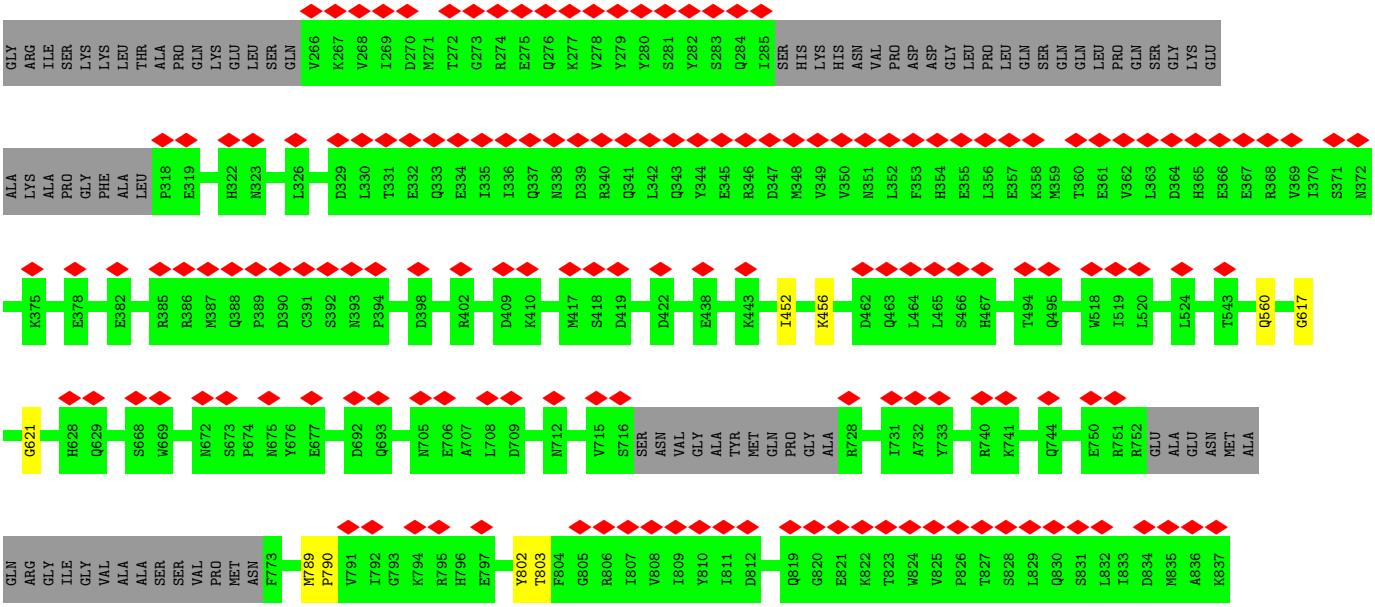
Chain T:



- Molecule 36: Tuftelin-interacting protein 11

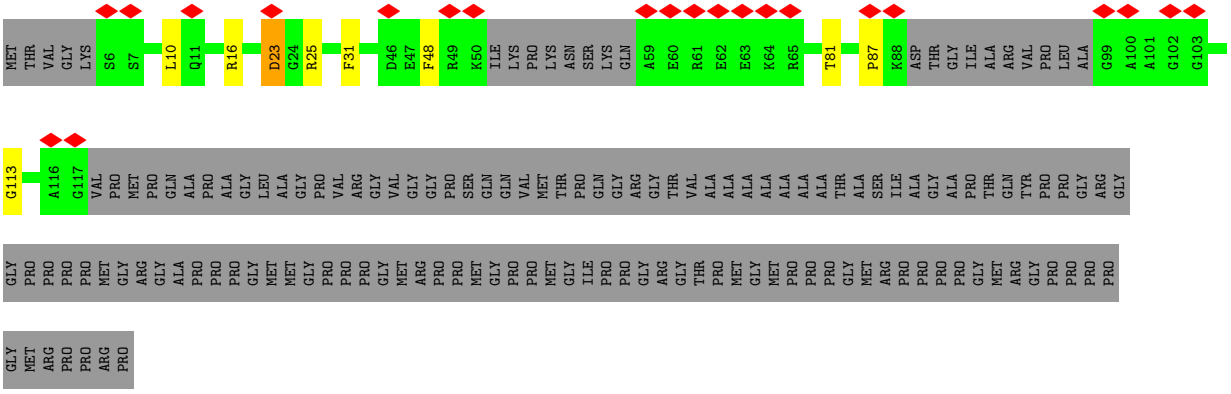
Chain TF:





- Molecule 37: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain b:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87951	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.823	Depositor
Minimum map value	0.000	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.127	Depositor
Recommended contour level	0.975	Depositor
Map size (Å)	519.75, 519.75, 519.75	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2375, 1.2375, 1.2375	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	2	0.62	1/917 (0.1%)	1.56	19/1425 (1.3%)
2	6	0.56	1/2323 (0.0%)	1.52	50/3619 (1.4%)
3	C	0.34	0/7346	0.70	6/9980 (0.1%)
4	D	0.35	0/252	0.57	0/350
5	DX	0.30	0/3219	0.59	0/4487
6	E	0.36	0/2394	0.79	7/3243 (0.2%)
7	J	0.29	0/2792	0.48	0/3900
8	K	0.33	0/940	0.49	0/1312
9	L1	0.29	0/1352	0.59	0/1878
10	N	0.38	0/1210	0.76	1/1622 (0.1%)
11	O	0.40	1/2378 (0.0%)	0.81	2/3211 (0.1%)
12	Q	0.30	0/6858	0.52	0/9563
13	R	0.34	0/1558	0.67	0/2168
14	S	0.33	0/1268	0.73	2/1714 (0.1%)
15	W	0.36	0/1306	0.75	3/1760 (0.2%)
16	Z	0.31	0/458	0.54	0/639
17	a	0.38	0/659	0.92	2/888 (0.2%)
18	c	0.37	0/649	1.00	3/877 (0.3%)
19	d	0.43	0/785	1.02	3/1049 (0.3%)
20	e	0.38	0/661	0.96	0/886
21	f	0.43	0/575	1.01	3/776 (0.4%)
22	g	0.45	0/575	1.01	4/768 (0.5%)
23	q	0.33	0/512	0.47	0/713
23	r	0.35	0/592	0.56	0/825
23	s	0.31	0/658	0.55	0/919
23	t	0.32	0/512	0.49	0/713
24	z	0.28	0/200	0.56	0/266
25	3	0.31	0/504	0.59	0/675
26	5	0.52	0/2157	1.59	58/3351 (1.7%)
27	A	0.35	1/16926 (0.0%)	0.73	21/22947 (0.1%)
28	I	0.30	0/3737	0.50	0/5213
30	L	0.31	0/3657	0.64	4/4979 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	L2	0.36	1/3117 (0.0%)	0.77	6/4183 (0.1%)
32	M	0.30	0/825	0.47	0/1150
33	P	0.34	0/957	0.75	2/1276 (0.2%)
34	PX	0.31	0/1463	0.49	0/2039
35	T	0.36	1/2927 (0.0%)	0.81	5/3980 (0.1%)
36	TF	0.31	0/2830	0.55	0/3937
37	b	0.36	0/726	0.90	2/966 (0.2%)
All	All	0.36	6/82775 (0.0%)	0.78	203/114247 (0.2%)

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
3	C	0	1
17	a	0	2
19	d	0	3
20	e	0	1
22	g	0	1
27	A	0	3
All	All	0	11

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	225	PRO	C-N	6.48	1.46	1.34
2	6	35	A	N9-C4	5.92	1.41	1.37
31	L2	678	CYS	CB-SG	-5.63	1.72	1.81
1	2	35	A	N9-C8	-5.43	1.33	1.37
35	T	306	CYS	CB-SG	-5.37	1.73	1.81

The worst 5 of 203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6	36	A	C8-N9-C4	-14.35	100.06	105.80
26	5	86	C	N1-C2-O2	13.81	127.18	118.90
2	6	36	A	N7-C8-N9	13.30	120.45	113.80
26	5	86	C	C2-N1-C1'	12.61	132.67	118.80
26	5	24	G	O4'-C1'-N9	-11.78	98.78	108.20

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	940	ARG	Sidechain
17	a	51	ARG	Sidechain
17	a	69	ARG	Sidechain
19	d	55	ARG	Sidechain
19	d	61	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	823	0	416	2	0
2	6	2075	0	1048	12	0
3	C	7184	0	7206	20	0
4	D	253	0	120	0	0
5	DX	3220	0	1416	2	0
6	E	2341	0	2275	4	0
7	J	2793	0	1241	0	0
8	K	941	0	424	0	0
9	L1	1353	0	620	0	0
10	N	1184	0	1189	5	0
11	O	2328	0	2317	8	0
12	Q	6859	0	2971	0	0
13	R	1571	0	725	3	0
14	S	1236	0	1210	7	0
15	W	1276	0	1221	11	0
16	Z	459	0	204	0	0
17	a	651	0	669	0	0
18	c	641	0	689	0	0
19	d	775	0	818	0	0
20	e	653	0	668	0	0
21	f	564	0	572	0	0
22	g	568	0	590	0	0
23	q	514	0	236	0	0
23	r	594	0	270	0	0
23	s	659	0	299	0	0
23	t	514	0	236	0	0
24	z	198	0	184	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	3	499	0	479	0	0
26	5	1936	0	982	10	0
27	A	16477	0	16462	46	0
28	I	3739	0	1699	2	0
29	IN	492	0	330	4	0
30	L	3623	0	2842	6	0
31	L2	3049	0	2973	21	0
32	M	827	0	380	1	0
33	P	942	0	929	2	0
34	PX	1465	0	620	0	0
35	T	2854	0	2812	15	0
36	TF	2835	0	1200	4	0
37	b	717	0	736	0	0
38	C	32	0	12	0	0
39	N	3	0	0	0	0
40	A	36	0	6	1	0
All	All	81753	0	62296	154	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 1.

The worst 5 of 154 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:59:G:H1	2:6:76:A:H61	1.01	0.96
2:6:59:G:H1	2:6:76:A:N6	1.75	0.84
14:S:56:ILE:HG12	14:S:62:ILE:HG23	1.78	0.65
14:S:57:ILE:HD13	15:W:97:ASN:HB3	1.80	0.63
2:6:1:G:O2'	10:N:99:ASN:ND2	2.33	0.62

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	
3	C	906/972 (93%)	868 (96%)	35 (4%)	3 (0%)	37	68
4	D	49/285 (17%)	48 (98%)	0	1 (2%)	6	33
5	DX	648/795 (82%)	631 (97%)	15 (2%)	2 (0%)	37	68
6	E	297/357 (83%)	285 (96%)	12 (4%)	0	100	100
7	J	559/848 (66%)	548 (98%)	9 (2%)	2 (0%)	30	64
8	K	187/225 (83%)	182 (97%)	3 (2%)	2 (1%)	12	45
9	L1	273/538 (51%)	264 (97%)	9 (3%)	0	100	100
10	N	141/144 (98%)	125 (89%)	16 (11%)	0	100	100
11	O	286/420 (68%)	265 (93%)	21 (7%)	0	100	100
12	Q	1382/1485 (93%)	1346 (97%)	35 (2%)	1 (0%)	48	79
13	R	313/536 (58%)	281 (90%)	27 (9%)	5 (2%)	8	38
14	S	157/166 (95%)	143 (91%)	11 (7%)	3 (2%)	6	34
15	W	156/579 (27%)	137 (88%)	19 (12%)	0	100	100
16	Z	90/166 (54%)	83 (92%)	7 (8%)	0	100	100
17	a	81/126 (64%)	71 (88%)	10 (12%)	0	100	100
18	c	79/119 (66%)	69 (87%)	10 (13%)	0	100	100
19	d	94/118 (80%)	82 (87%)	12 (13%)	0	100	100
20	e	77/92 (84%)	63 (82%)	13 (17%)	1 (1%)	10	41
21	f	70/86 (81%)	64 (91%)	6 (9%)	0	100	100
22	g	71/76 (93%)	65 (92%)	6 (8%)	0	100	100
23	q	99/504 (20%)	97 (98%)	2 (2%)	0	100	100
23	r	115/504 (23%)	112 (97%)	2 (2%)	1 (1%)	14	49
23	s	130/504 (26%)	126 (97%)	4 (3%)	0	100	100
23	t	99/504 (20%)	97 (98%)	2 (2%)	0	100	100
24	z	23/451 (5%)	23 (100%)	0	0	100	100
25	3	56/476 (12%)	56 (100%)	0	0	100	100
27	A	1977/2335 (85%)	1863 (94%)	112 (6%)	2 (0%)	48	79
28	I	749/855 (88%)	728 (97%)	20 (3%)	1 (0%)	48	79
30	L	547/802 (68%)	514 (94%)	32 (6%)	1 (0%)	44	75
31	L2	363/894 (41%)	321 (88%)	37 (10%)	5 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	M	162/243 (67%)	159 (98%)	3 (2%)	0	100	100
33	P	108/229 (47%)	103 (95%)	5 (5%)	0	100	100
34	PX	291/917 (32%)	286 (98%)	5 (2%)	0	100	100
35	T	356/514 (69%)	337 (95%)	19 (5%)	0	100	100
36	TF	562/837 (67%)	549 (98%)	12 (2%)	1 (0%)	44	75
37	b	88/240 (37%)	78 (89%)	8 (9%)	2 (2%)	5	31
All	All	11641/18942 (62%)	11069 (95%)	539 (5%)	33 (0%)	38	68

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	L2	579	VAL
3	C	166	CYS
13	R	47	ARG
13	R	277	THR
3	C	126	SER

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	
3	C	807/866 (93%)	797 (99%)	10 (1%)	67	82
6	E	256/300 (85%)	254 (99%)	2 (1%)	79	88
10	N	130/130 (100%)	128 (98%)	2 (2%)	60	77
11	O	258/361 (72%)	254 (98%)	4 (2%)	58	76
14	S	129/134 (96%)	125 (97%)	4 (3%)	35	63
15	W	135/502 (27%)	130 (96%)	5 (4%)	29	58
17	a	73/101 (72%)	72 (99%)	1 (1%)	62	79
18	c	76/101 (75%)	74 (97%)	2 (3%)	41	66
19	d	90/110 (82%)	84 (93%)	6 (7%)	13	40
20	e	74/84 (88%)	71 (96%)	3 (4%)	26	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	f	61/74 (82%)	61 (100%)	0	100	100
22	g	63/66 (96%)	58 (92%)	5 (8%)	10	34
24	z	21/371 (6%)	21 (100%)	0	100	100
25	3	55/395 (14%)	55 (100%)	0	100	100
27	A	1792/2108 (85%)	1761 (98%)	31 (2%)	56	75
30	L	231/709 (33%)	224 (97%)	7 (3%)	36	63
31	L2	334/806 (41%)	323 (97%)	11 (3%)	33	61
33	P	103/203 (51%)	101 (98%)	2 (2%)	52	73
35	T	313/441 (71%)	309 (99%)	4 (1%)	65	81
37	b	74/177 (42%)	68 (92%)	6 (8%)	9	33
All	All	5075/8039 (63%)	4970 (98%)	105 (2%)	49	71

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	A	964	ASP
27	A	1833	LEU
37	b	10	LEU
27	A	1089	CYS
27	A	1582	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
27	A	1468	ASN
35	T	455	GLN
27	A	1830	GLN
35	T	278	ASN
27	A	1531	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	38/188 (20%)	19 (50%)	1 (2%)
2	6	96/106 (90%)	42 (43%)	7 (7%)
26	5	90/116 (77%)	26 (28%)	2 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	IN	0/154	-	-
All	All	224/564 (39%)	87 (38%)	10 (4%)

5 of 87 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	8	C
1	2	14	C
1	2	15	U
1	2	16	U
1	2	19	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	6	82	A
26	5	92	U
26	5	95	G
2	6	35	A
2	6	50	A

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	$\#\|Z\| > 2$
13	SEP	R	224	13	3,4,10	0.71	0	2,4,14	1.30	0
13	SEP	R	232	13	3,4,10	0.75	0	2,4,14	1.37	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
13	SEP	R	224	13	-	0/0/2/10	-
13	SEP	R	232	13	-	0/0/2/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
40	IHP	A	3000	-	36,36,36	1.50	6 (16%)	54,60,60	0.78	3 (5%)
38	GTP	C	1500	-	26,34,34	1.22	2 (7%)	32,54,54	1.56	7 (21%)

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
40	IHP	A	3000	-	-	4/30/54/54	0/1/1/1
38	GTP	C	1500	-	-	3/18/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	C	1500	GTP	C5-C6	-4.25	1.38	1.47
40	A	3000	IHP	P1-O11	3.22	1.65	1.59
40	A	3000	IHP	P3-O13	3.21	1.65	1.59
40	A	3000	IHP	P6-O16	3.18	1.65	1.59
40	A	3000	IHP	P2-O12	3.15	1.65	1.59

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	C	1500	GTP	PA-O3A-PB	-3.90	119.43	132.83
38	C	1500	GTP	C5-C6-N1	2.96	119.18	113.95
40	A	3000	IHP	C5-C6-C1	2.86	116.68	110.41
38	C	1500	GTP	PB-O3B-PG	-2.85	123.05	132.83
38	C	1500	GTP	C2-N1-C6	-2.77	120.00	125.10

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

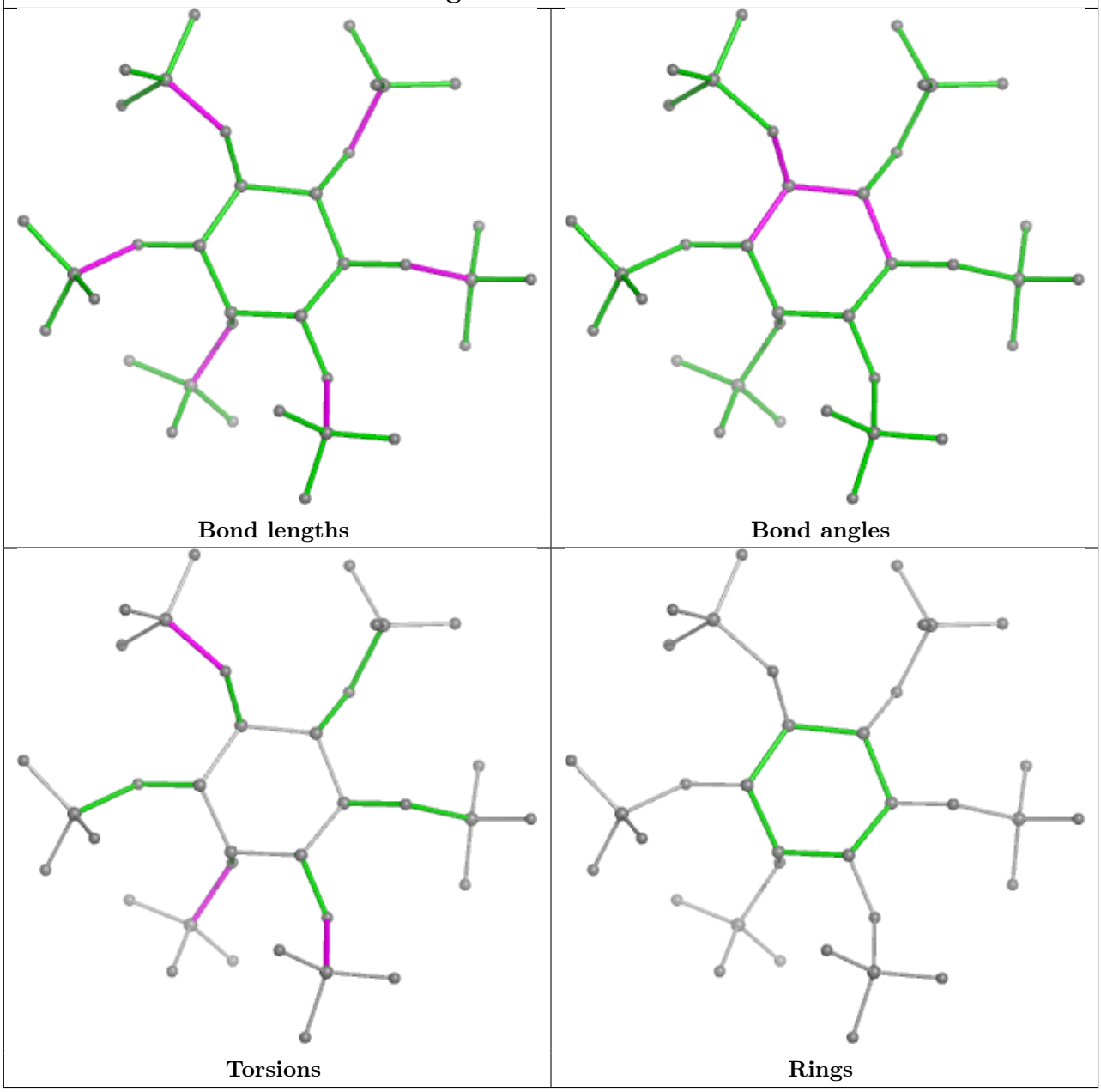
1 monomer is involved in 1 short contact:

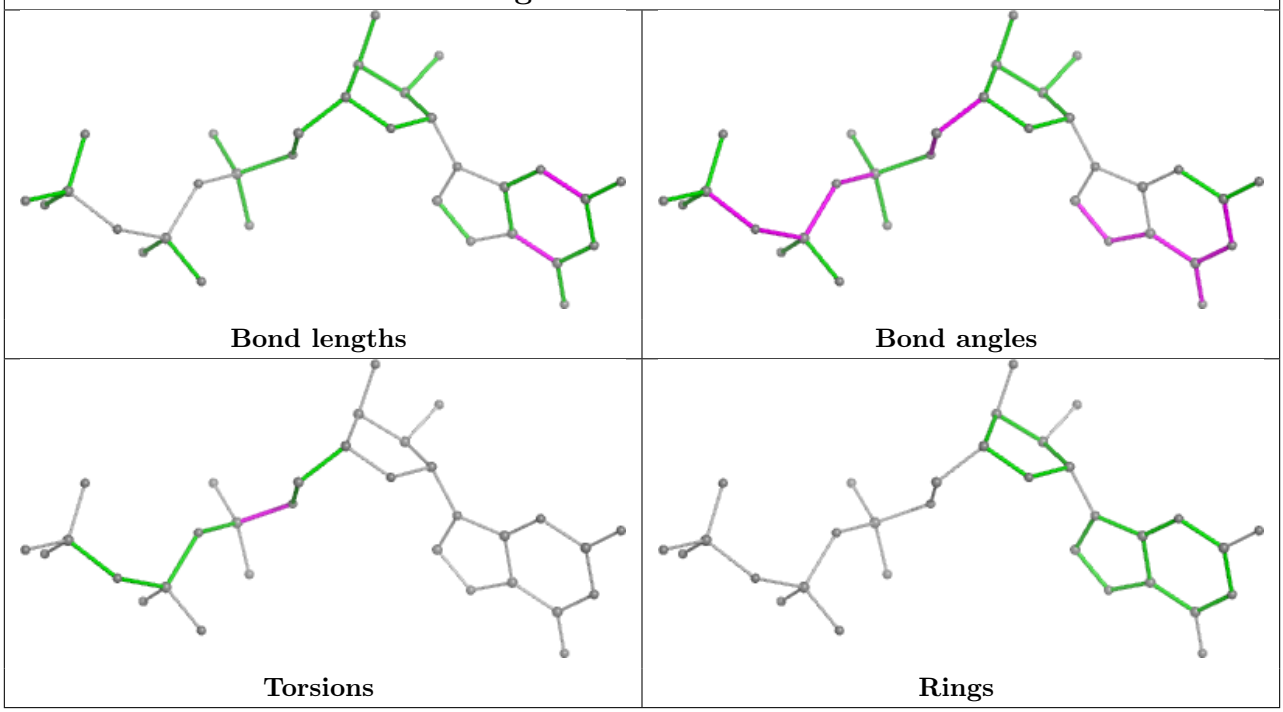
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	A	3000	IHP	1	0

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



Ligand GTP C 1500	
 Bond lengths	Bond angles
Torsions	Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

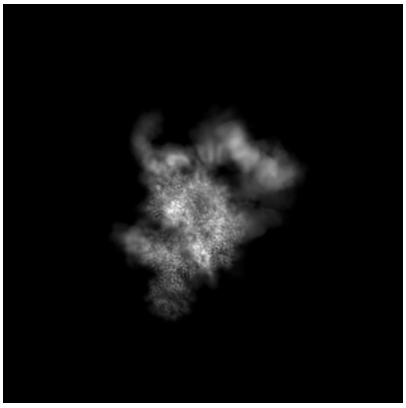
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-19399. These allow visual inspection of the internal detail of the map and identification of artifacts.

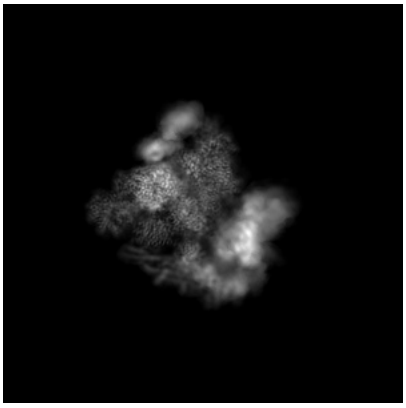
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

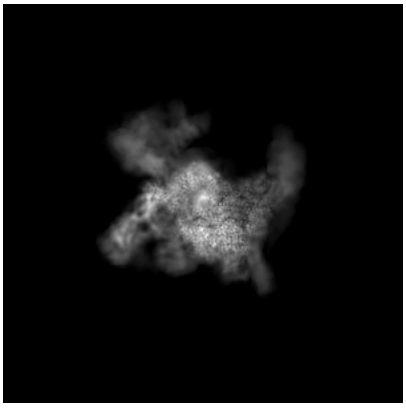
6.1.1 Primary map



X



Y

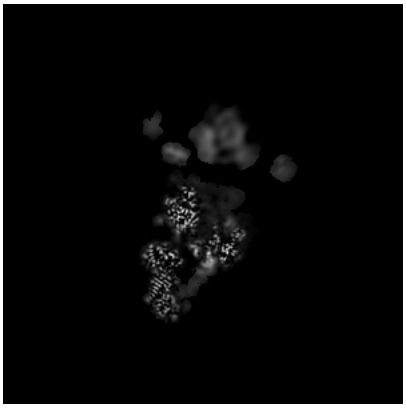


Z

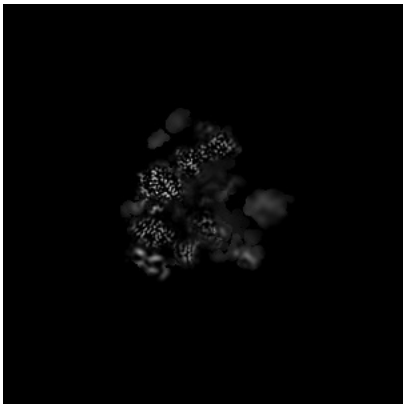
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

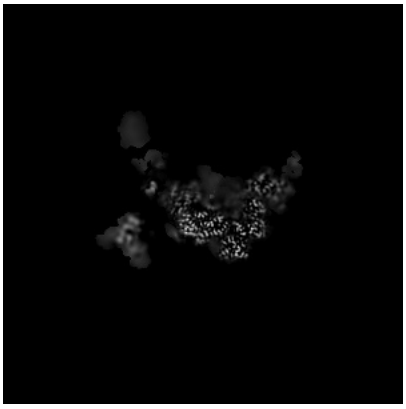
6.2.1 Primary map



X Index: 210



Y Index: 210

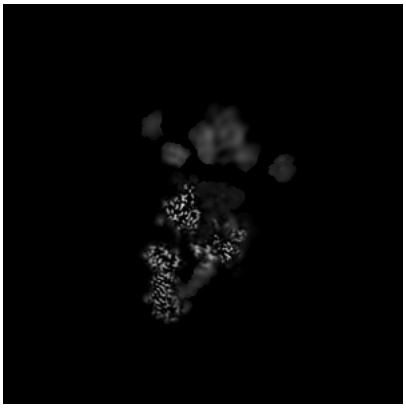


Z Index: 210

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

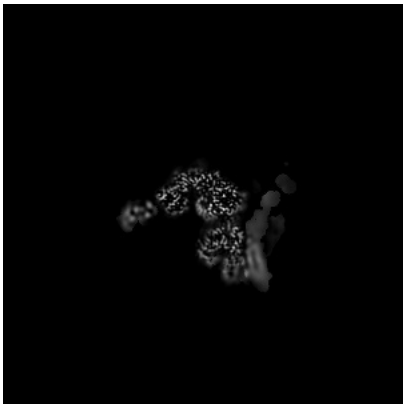
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 208

Y Index: 181

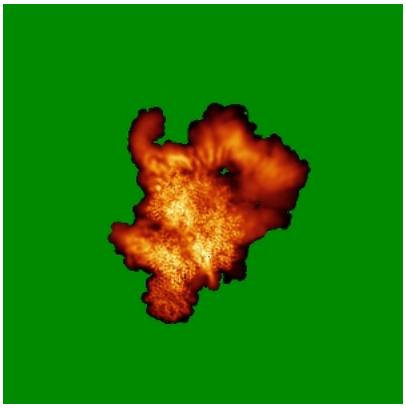


Z Index: 164

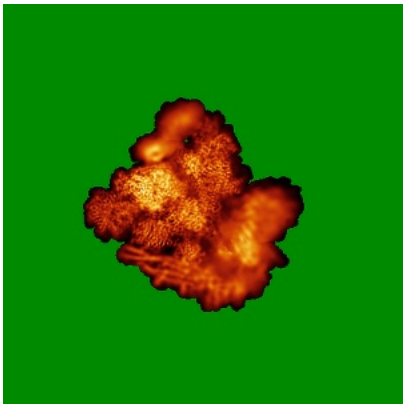
The images above show the largest variance slices of the map in three orthogonal directions.

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

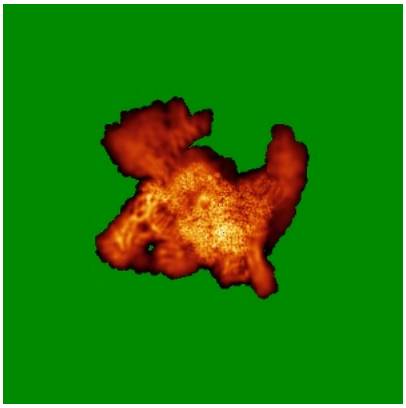
6.4.1 Primary map



X



Y

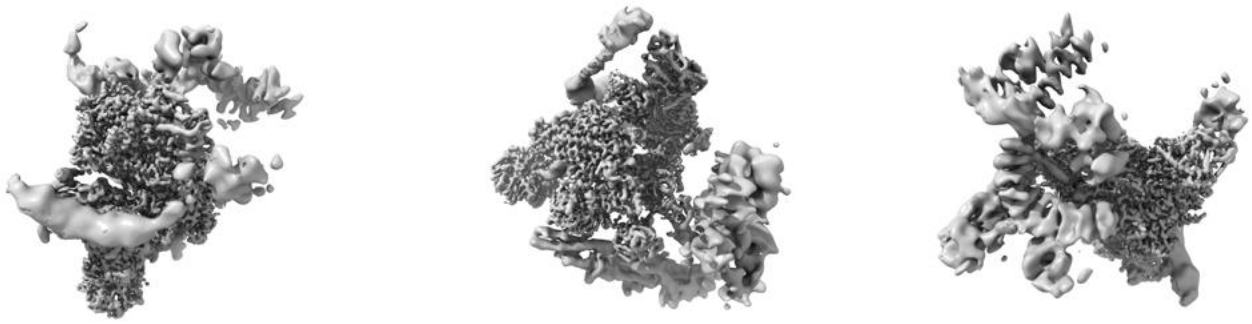


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.975. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

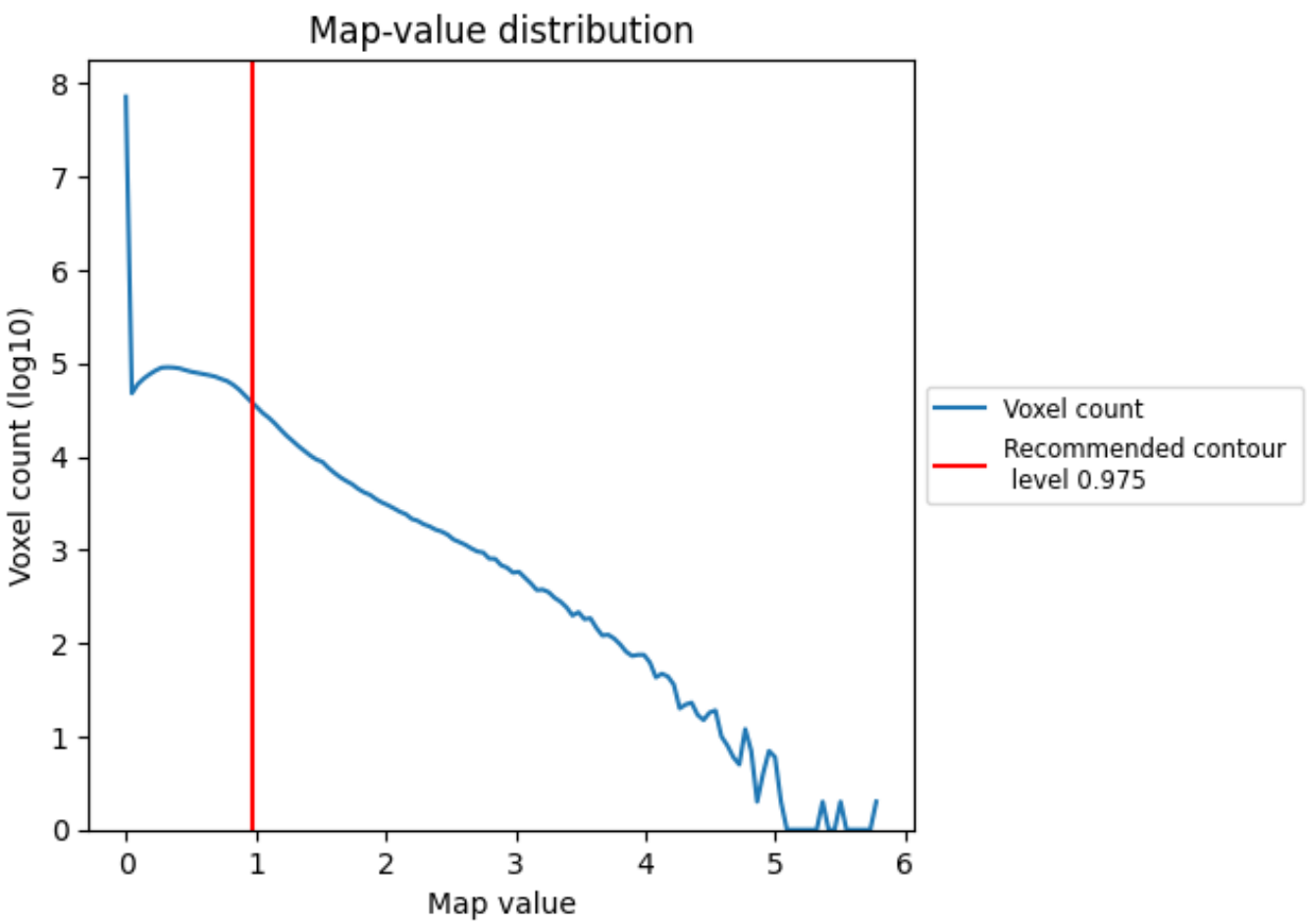
6.6 Mask visualisation (i)

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

7 Map analysis (i)

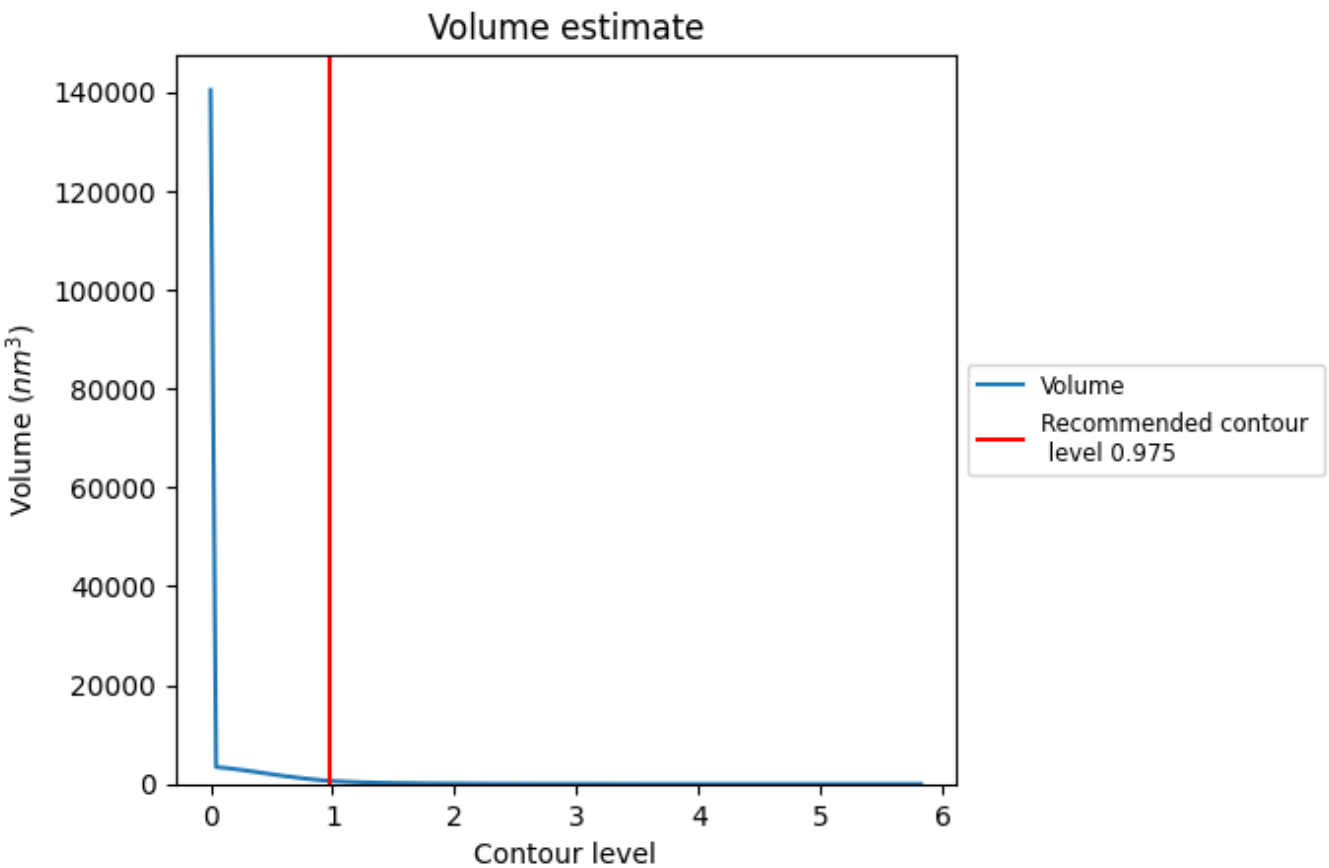
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

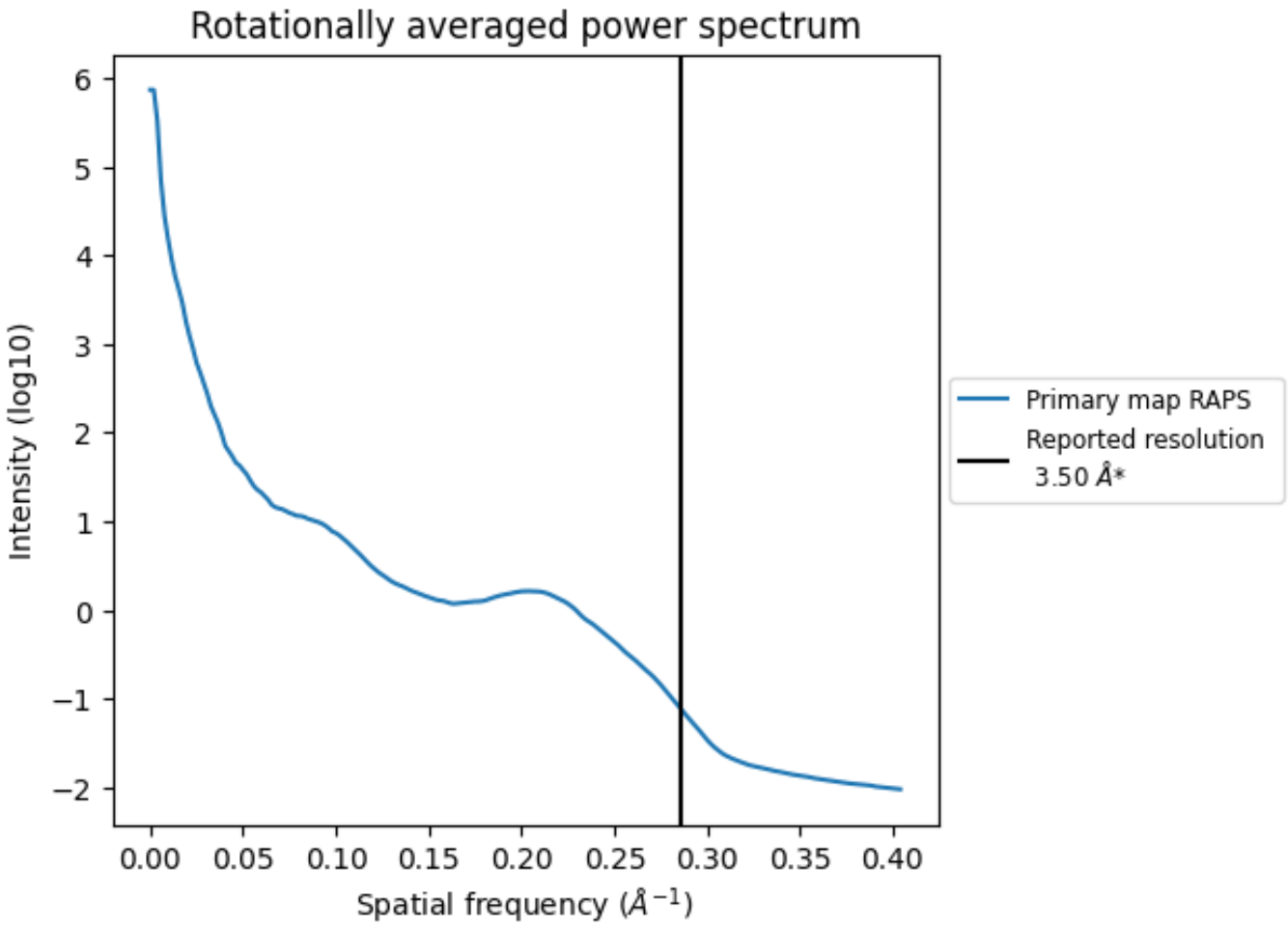
7.2 Volume estimate (i)



The volume at the recommended contour level is 632 nm^3; this corresponds to an approximate mass of 571 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 0.286 Å^{-1}

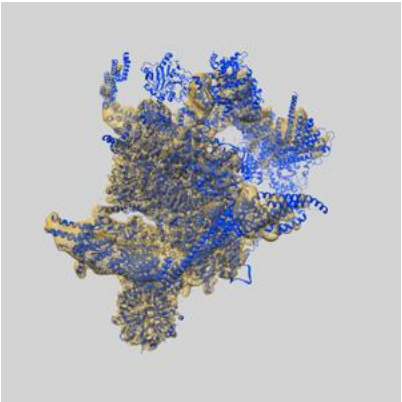
8 Fourier-Shell correlation (i)

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

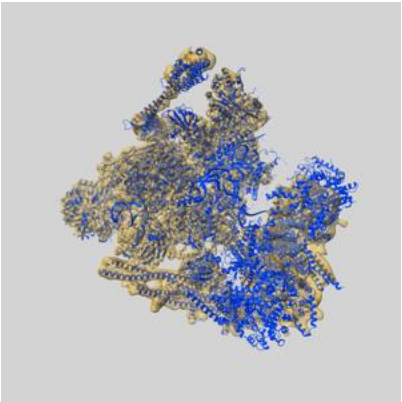
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-19399 and PDB model 8RO2. Per-residue inclusion information can be found in section 3 on page 12.

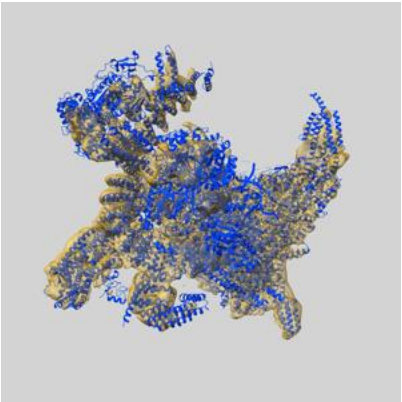
9.1 Map-model overlay (i)



X



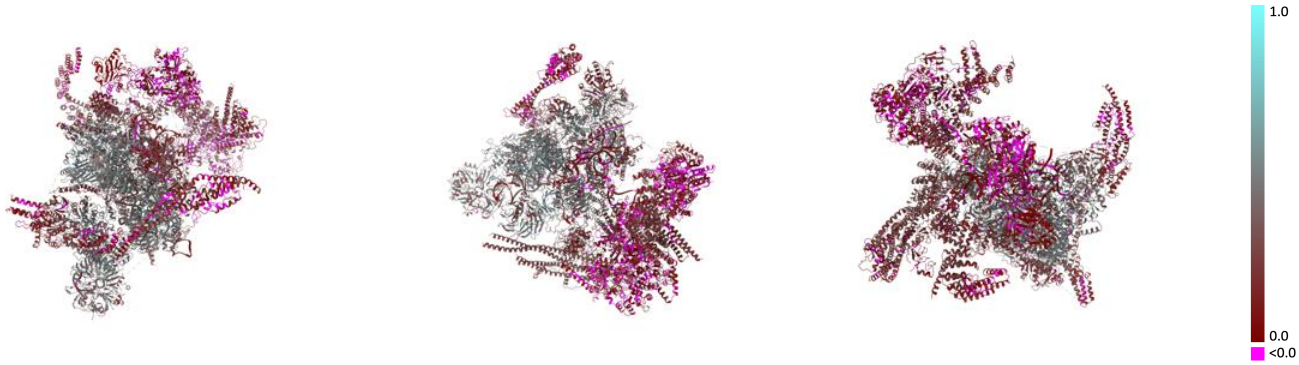
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.975 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.

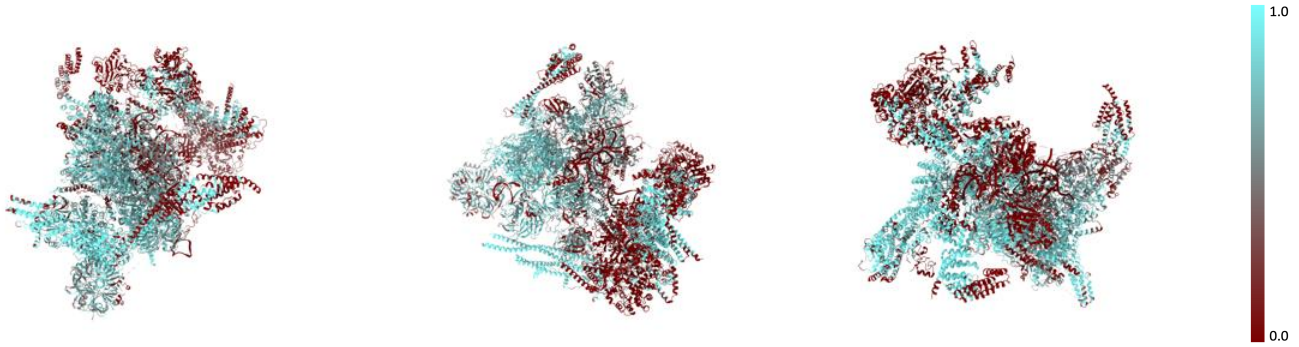
9.2 Q-score mapped to coordinate model (i)



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.

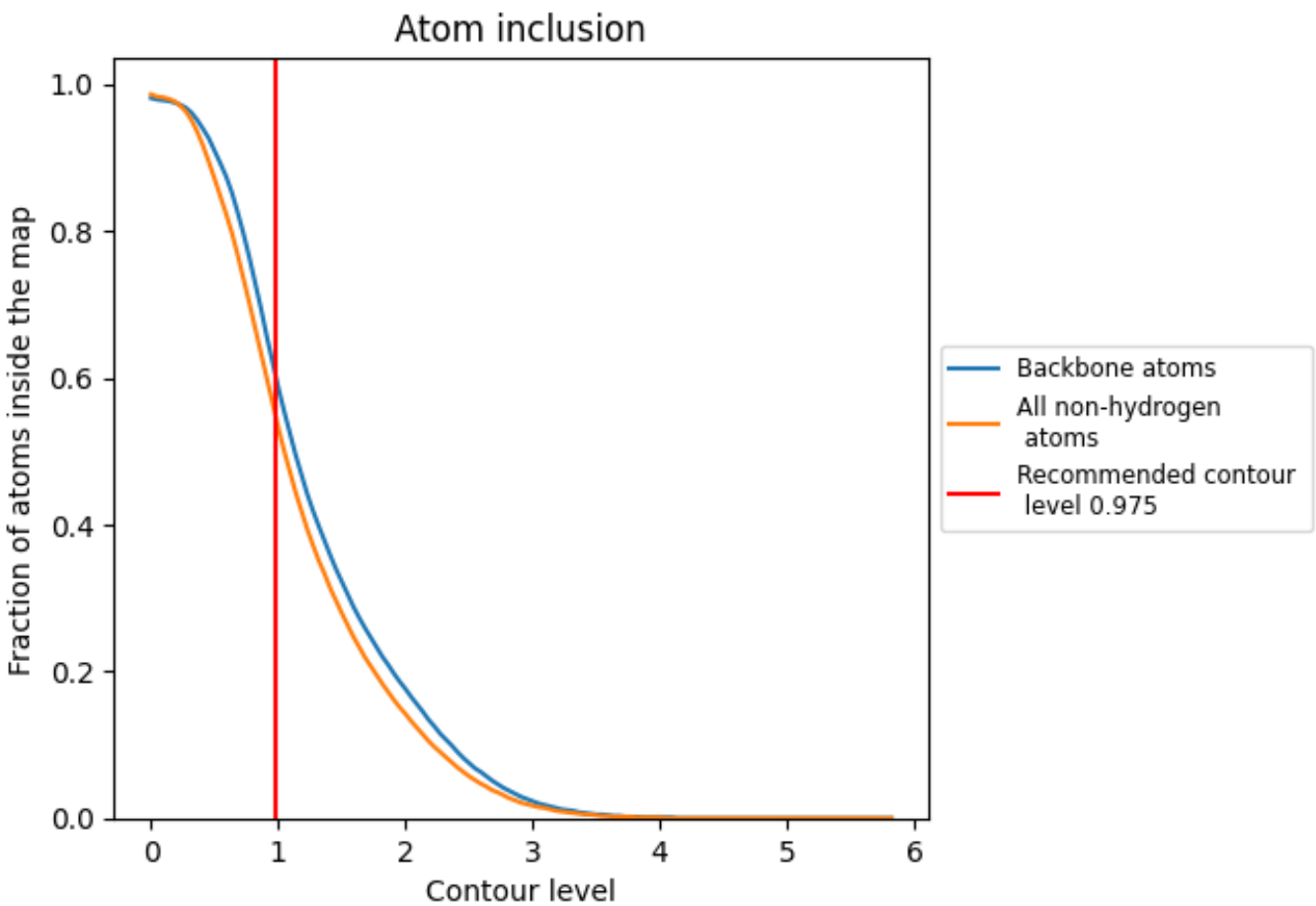
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.975).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.975) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5500	0.2970
2	0.1030	0.1420
3	0.1130	0.2610
5	0.7420	0.3420
6	0.1140	0.1380
A	0.6610	0.4410
C	0.7990	0.4230
D	0.3200	0.1480
DX	0.3170	0.0420
E	0.7530	0.4590
I	0.7640	0.2170
IN	0.1340	0.1400
J	0.4970	0.2040
K	0.8930	0.2380
L	0.5120	0.2490
L1	0.0050	-0.0160
L2	0.5040	0.3570
M	0.3880	0.2140
N	0.7100	0.4570
O	0.4830	0.3360
P	0.3950	0.3060
PX	0.3900	0.0850
Q	0.1440	0.0730
R	0.5260	0.3470
S	0.6770	0.3700
T	0.8480	0.4350
TF	0.6370	0.1070
W	0.4190	0.3350
Z	0.5930	0.1980
a	0.7150	0.4790
b	0.5820	0.4170
c	0.5730	0.4140
d	0.4780	0.3430
e	0.5900	0.4110
f	0.6080	0.4210

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Chain	Atom inclusion	Q-score
g	0.5840	0.4440
q	0.6130	0.2030
r	0.5660	0.1850
s	0.9060	0.2290
t	0.5800	0.1830
z	0.0260	-0.0320