Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 08:41 AM JST

PDB ID	:	5YZG
EMDB ID	:	EMD-6864
Title	:	The Cryo-EM Structure of Human Catalytic Step I Spliceosome (C complex) at 4.1 angstrom resolution
Authors	:	Zhan, X.; Yan, C.; Zhang, X.; Lei, J.; Shi, Y.
Deposited on	:	2017-12-14
Resolution	:	4.10 Å(reported)

This is a Full wwPDB EM Validation 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:

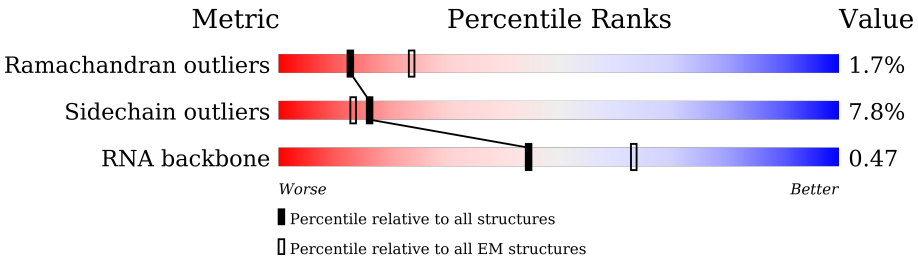
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 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.



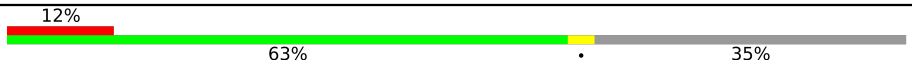
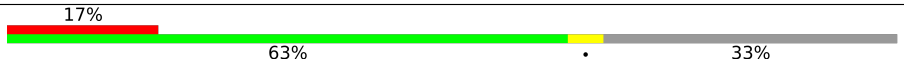
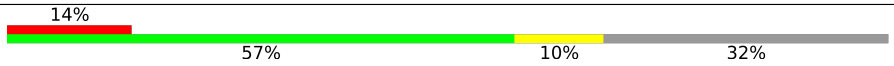
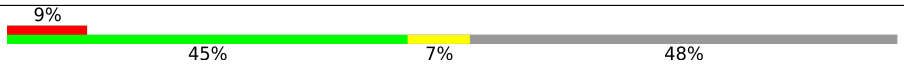
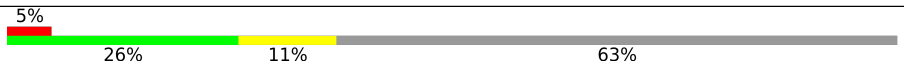
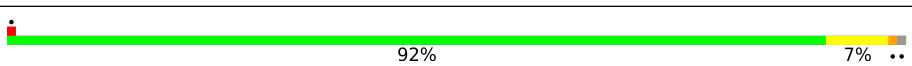
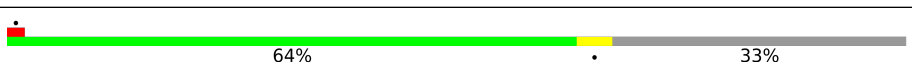
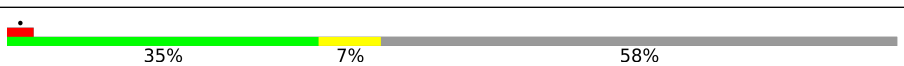
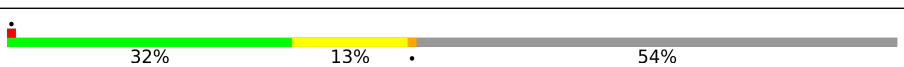
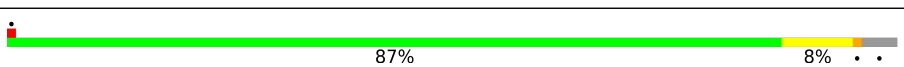
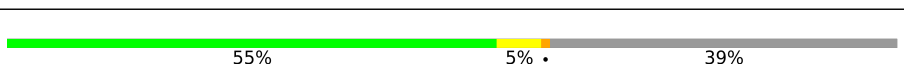
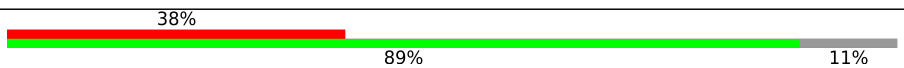
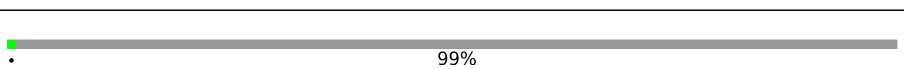
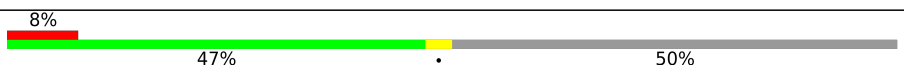
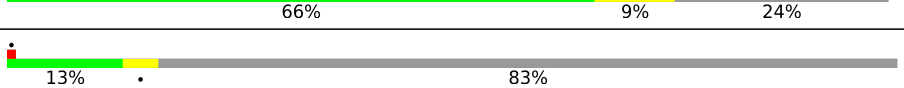
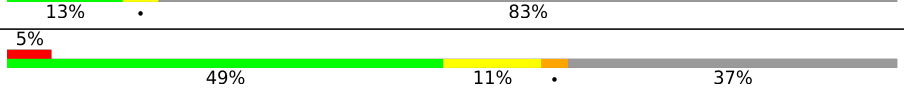
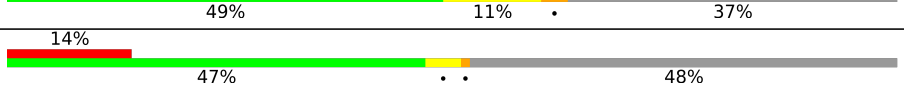
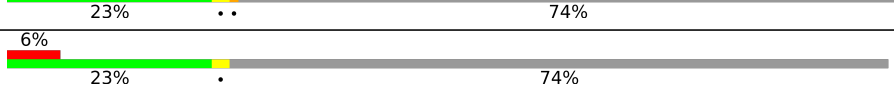
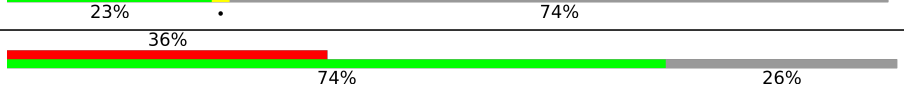
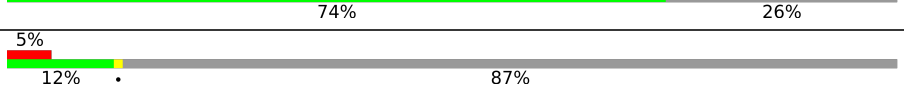
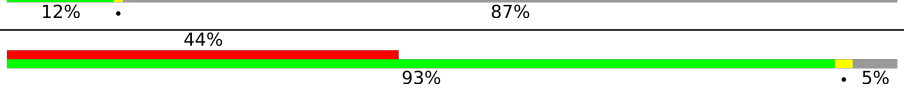
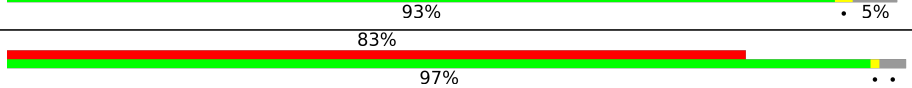
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	6% 87% 9%
2	B	117	8% 52% 16% 28%
3	C	972	79% 9% 11%
4	D	2136	74% 89% 11%
5	E	357	78% 5% 16%
6	F	107	7% 46% 43% 9%
7	G	275	9% 23% 68%
8	H	188	17% 29% 41% 26%

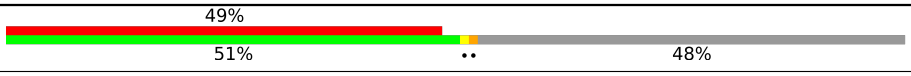
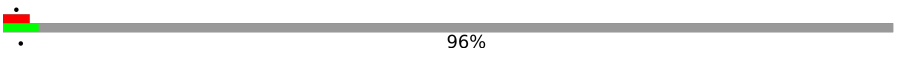
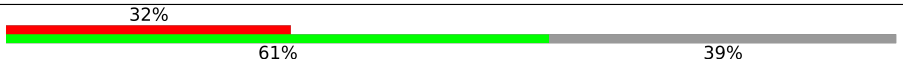
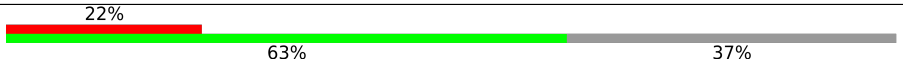
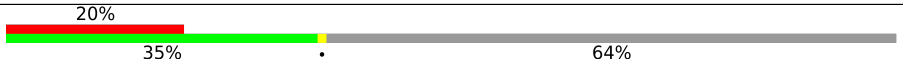
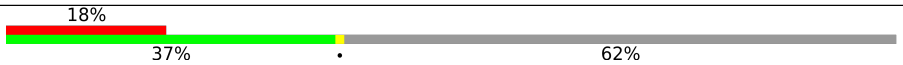
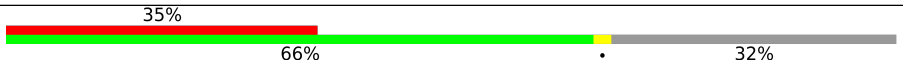
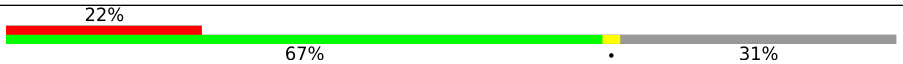
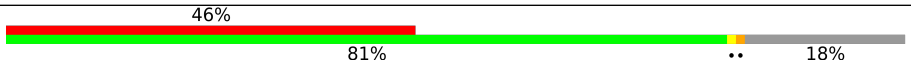
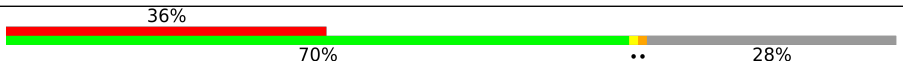
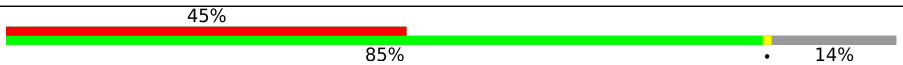
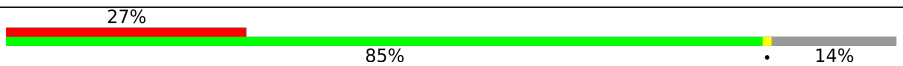
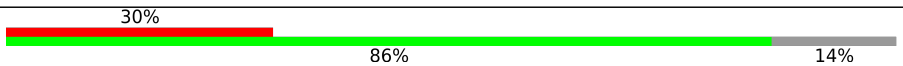
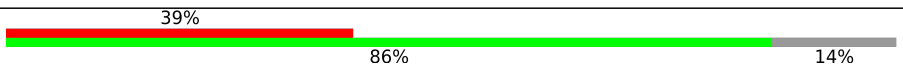
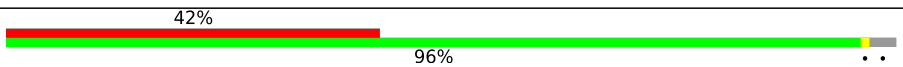
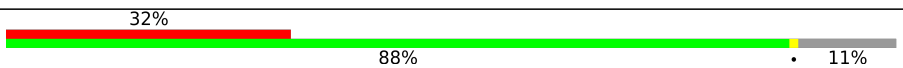
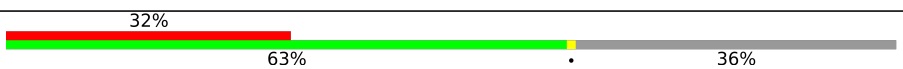
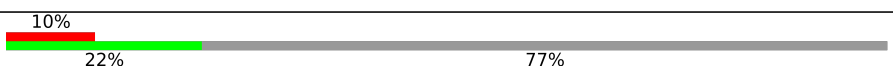
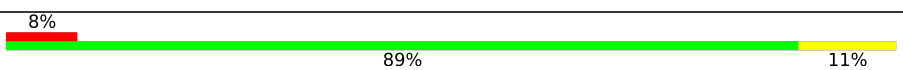
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	855	
10	J	848	
11	K	225	
12	L	802	
13	y	307	
14	M	243	
15	N	144	
16	O	420	
17	P	229	
18	R	536	
19	S	166	
20	T	514	
21	Q	1485	
22	U	2752	
23	V	908	
24	W	579	
25	X	425	
26	Y	323	
27	Z	1227	
28	q	504	
28	r	504	
28	s	504	
28	t	504	
29	u	411	
30	v	148	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	w	174	
32	x	703	
33	a	126	
33	h	126	
34	b	229	
34	i	229	
35	c	119	
35	j	119	
36	d	118	
36	k	118	
37	f	86	
37	m	86	
38	e	92	
38	l	92	
39	g	76	
39	n	76	
40	o	255	
41	p	225	
42	1	301	
43	2	646	
44	3	754	
45	4	37	

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 103906 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	2253	17519	11136	3147	3166	70	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	84	1768	792	295	597	84	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	862	6795	4344	1138	1281	32	0	0

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	1908	7632	3816	1908	1908	0	0

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	299	2338	1470	410	445	13	0	0

- Molecule 6 is a RNA chain called U6 snRNA.

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

- Molecule 7 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	88	Total	C	N	O	P	0	0
			1641	727	238	589	87		

- Molecule 8 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	139	Total	C	N	O	P	0	0
			2946	1317	507	983	139		

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	559	Total	C	N	O	0	0
			2757	1639	559	559		

- Molecule 10 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	571	Total	C	N	O	S	0	0
			3829	2385	720	718	6		

- Molecule 11 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	152	Total	C	N	O	S	0	0
			979	611	177	189	2		

- Molecule 12 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	419	Total	C	N	O	S	0	0
			2885	1809	534	537	5		

- Molecule 13 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	y	112	Total	C	N	O	S	0	0
			704	440	130	133	1		

- Molecule 14 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	91	Total	C	N	O	S	0	0
			775	482	146	145	2		

- Molecule 15 is a protein called Protein BUD31 homolog.

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

- Molecule 16 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	283	Total	C	N	O	S	0	0
			2277	1430	403	424	20		

- Molecule 17 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	96	Total	C	N	O	S	0	0
			829	508	162	157	2		

- Molecule 18 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	245	Total	C	N	O	P	S	0	0
			1962	1231	353	364	2	12		

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

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

- Molecule 20 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	313	Total	C	N	O	S	0	0
			2461	1554	447	452	8		

- Molecule 21 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Q	1322	Total 5288	C 2644	N 1322	O 1322	0	0

- Molecule 22 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	26	Total 193	C 120	N 36	O 36	S 1	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	452	Total 3410	C 2194	N 590	O 611	S 15	0	0

- Molecule 24 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	440	Total 2310	C 1296	N 487	O 523	S 4	0	0

- Molecule 25 is a protein called Pre-mRNA-splicing factor CWC25 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	71	Total 480	C 297	N 95	O 88	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	145	GLN	LYS	conflict	UNP Q9NXE8
X	149	PRO	LYS	conflict	UNP Q9NXE8

- Molecule 26 is a protein called Coiled-coil domain-containing protein 94.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	204	Total 1426	C 898	N 259	O 261	S 8	0	0

- Molecule 27 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Z	635	Total	C	N	O	0	0
			2540	1270	635	635		

- Molecule 28 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	q	132	Total	C	N	O	S	0	0
			918	581	156	178	3		
28	r	131	Total	C	N	O	S	0	0
			901	572	149	177	3		
28	s	374	Total	C	N	O		1	0
			1497	749	374	374			
28	t	67	Total	C	N	O	S	0	0
			476	300	83	92	1		

- Molecule 29 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	u	390	Total	C	N	O	S	0	0
			3126	1974	545	588	19		

- Molecule 30 is a protein called Protein mago nashi homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	v	144	Total	C	N	O	S	0	0
			1196	772	200	221	3		

- Molecule 31 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	w	91	Total	C	N	O	S	0	0
			730	463	122	142	3		

- Molecule 32 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	x	25	Total	C	N	O	0	0
			216	136	39	41		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	80	Total	C	N	O	S	0	0
			621	388	110	117	6		
33	a	77	Total	C	N	O	S	0	0
			609	381	108	115	5		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	86	Total	C	N	O	S	0	0
			690	434	126	123	7		
34	b	83	Total	C	N	O	S	0	0
			675	426	123	119	7		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	82	Total	C	N	O	S	0	0
			649	413	113	119	4		
35	c	81	Total	C	N	O	S	0	0
			641	409	112	116	4		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	85	Total	C	N	O	S	0	0
			688	432	125	126	5		
36	d	97	Total	C	N	O	S	0	0
			768	482	141	140	5		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	74	Total	C	N	O	S	0	0
			576	373	95	103	5		
37	f	74	Total	C	N	O	S	0	0
			576	373	95	103	5		

- Molecule 38 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	79	Total	C	N	O	S	0	0
			652	412	116	119	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	79	Total 652	C 412	N 116	O 119	S 5	0	0

- Molecule 39 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	68	Total 533	C 339	N 95	O 93	S 6	0	0
39	g	74	Total 569	C 358	N 102	O 103	S 6	0	0

- Molecule 40 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	162	Total 1277	C 817	N 219	O 238	S 3	0	0

- Molecule 41 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	94	Total 760	C 488	N 135	O 132	S 5	0	0

- Molecule 42 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	1	243	Total 972	C 486	N 243	O 243	0	0

- Molecule 43 is a protein called Peptidylprolyl isomerase domain and WD repeat-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	2	416	Total 1664	C 832	N 416	O 416	0	0

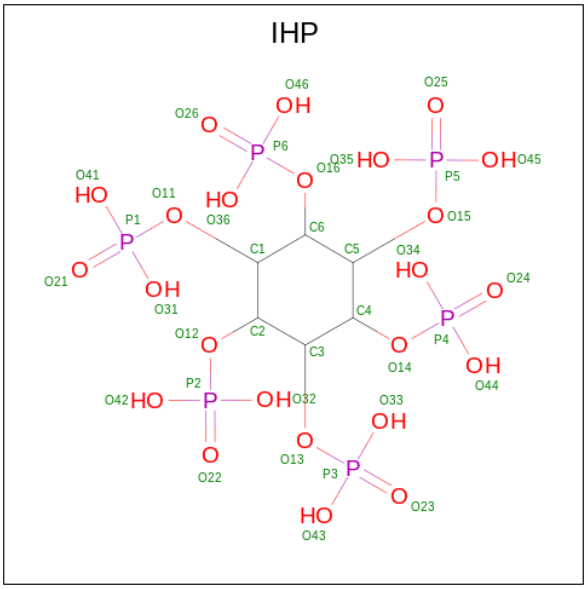
- Molecule 44 is a protein called Peptidyl-prolyl cis-trans isomerase G.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	3	171	Total 684	C 342	N 171	O 171	0	0

- Molecule 45 is a protein called UNKNOW.

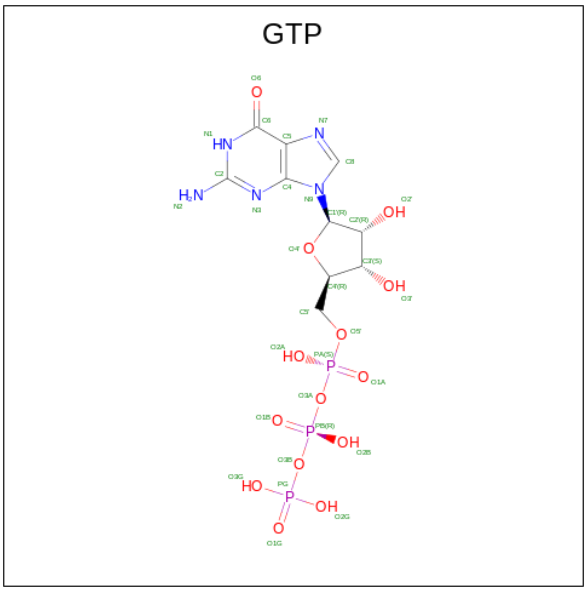
Mol	Chain	Residues	Atoms				AltConf	Trace
45	4	37	Total	C	N	O	0	0
			184	110	37	37		

- Molecule 46 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 47 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

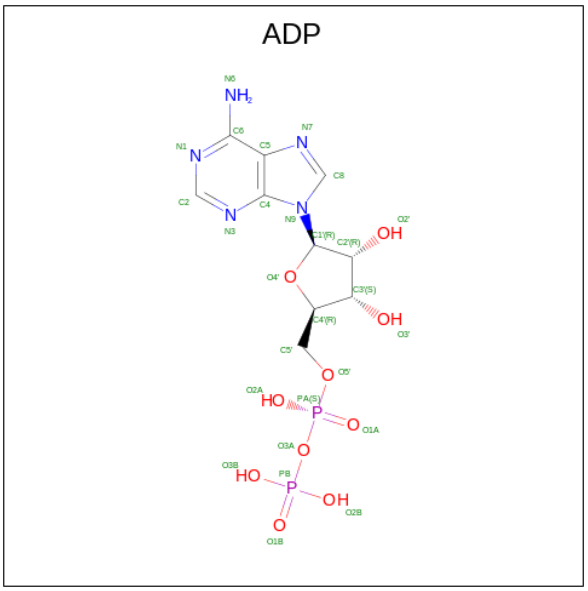


Mol	Chain	Residues	Atoms					AltConf
47	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	C	1	Total	Mg	0
			1	1	
48	F	5	Total	Mg	0
			5	5	
48	u	1	Total	Mg	0
			1	1	

- Molecule 49 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

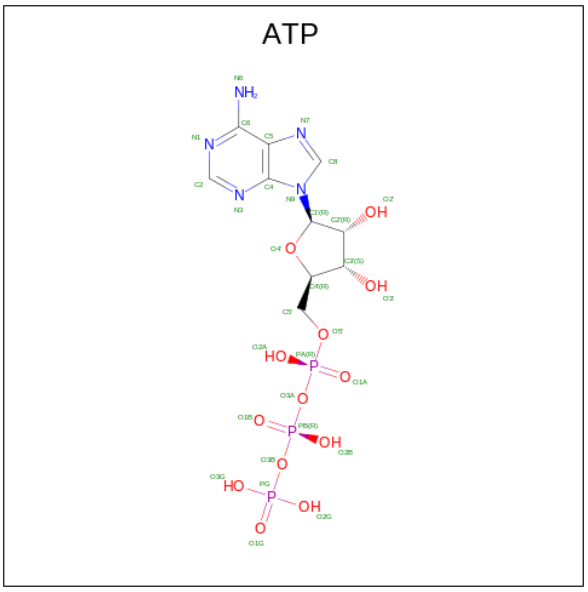


Mol	Chain	Residues	Atoms					AltConf
49	D	1	Total	C	N	O	P	0
			54	20	10	20	4	
49	D	1	Total	C	N	O	P	0
			54	20	10	20	4	

- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
50	N	3	Total	Zn	0
			3	3	
50	O	3	Total	Zn	0
			3	3	
50	Y	1	Total	Zn	0
			1	1	

- Molecule 51 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

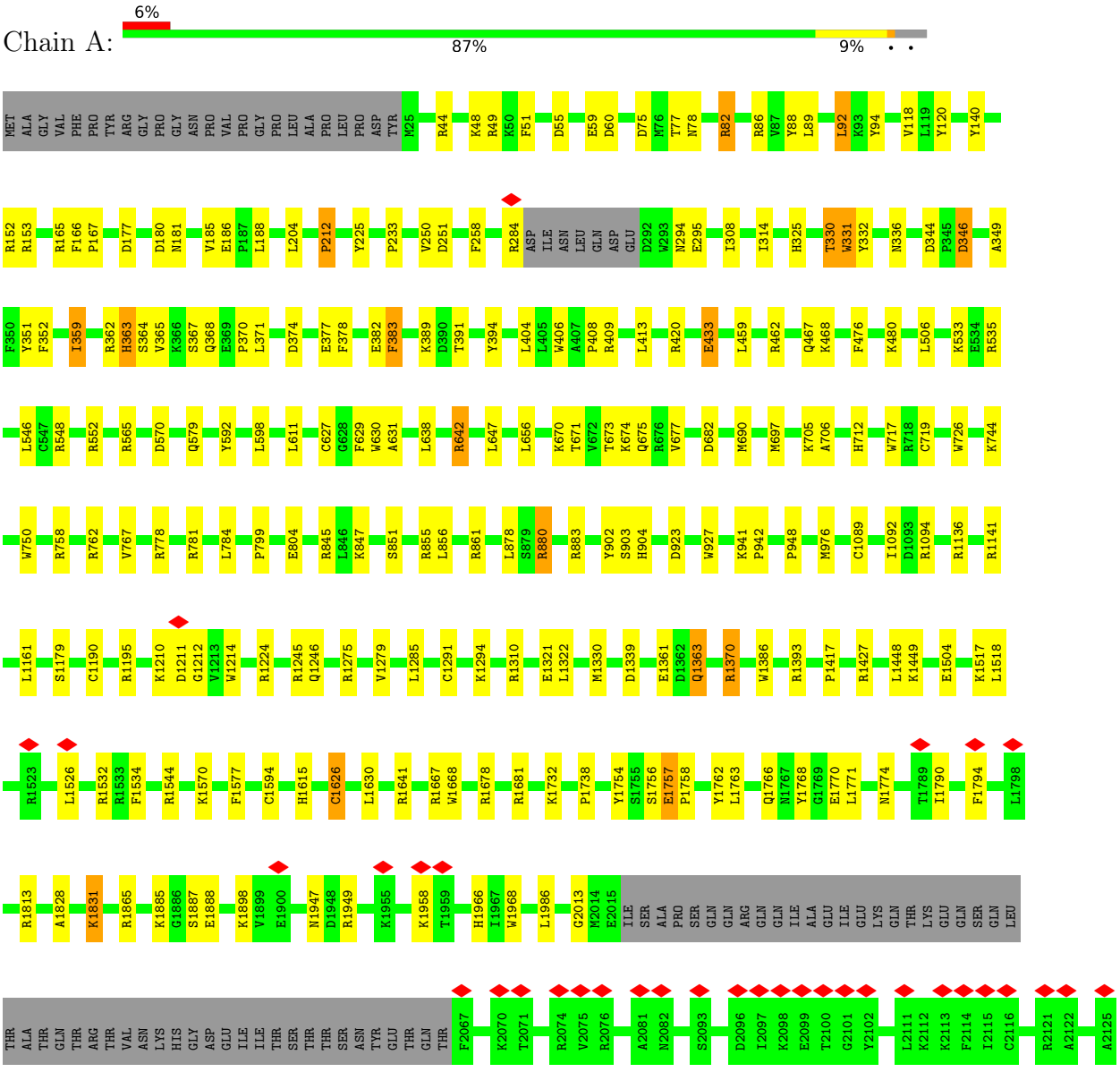


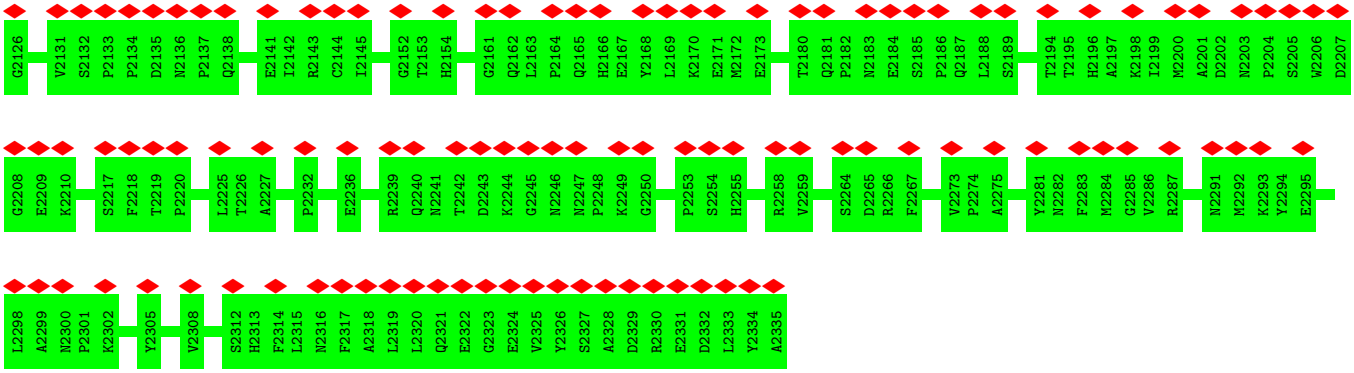
Mol	Chain	Residues	Atoms					AltConf
51	u	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

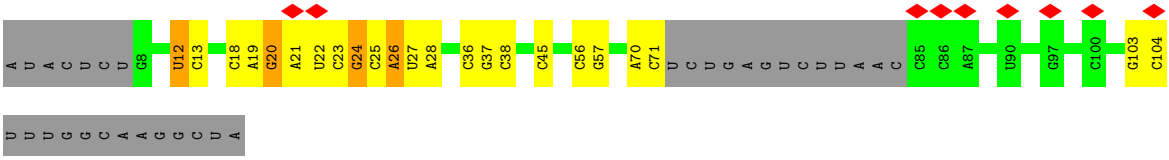
• Molecule 1: Pre-mRNA-processing-splicing factor 8





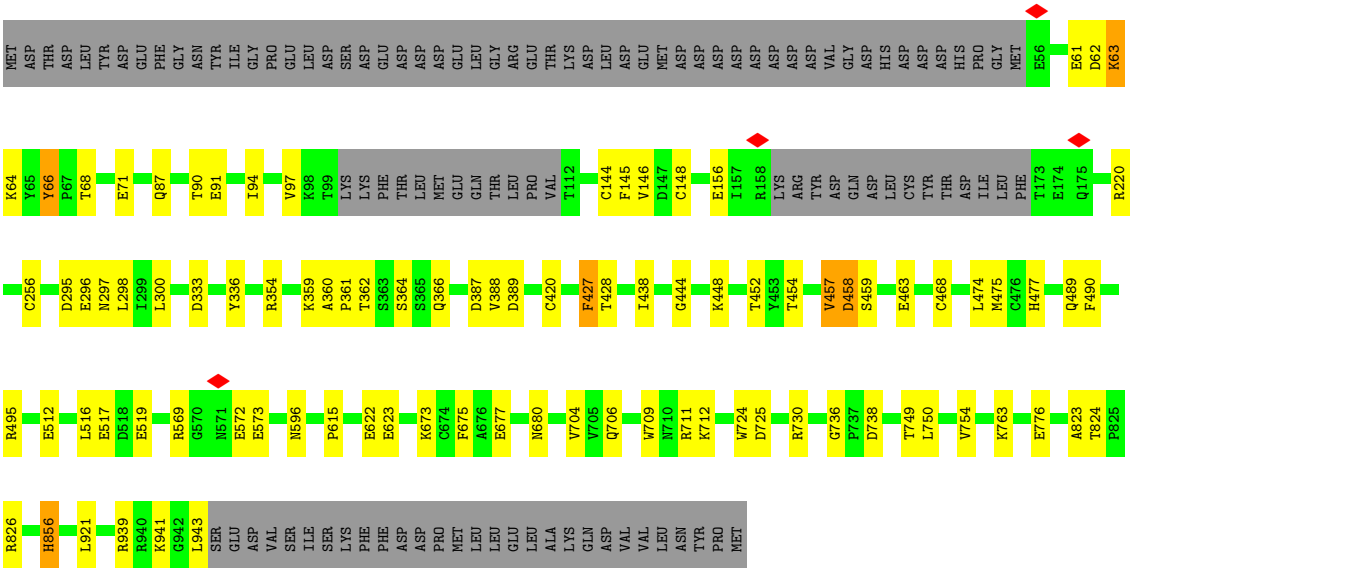
• Molecule 2: U5 snRNA

Chain B:



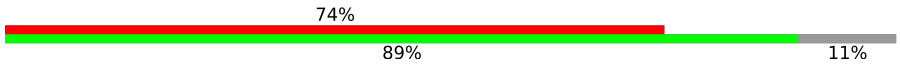
• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

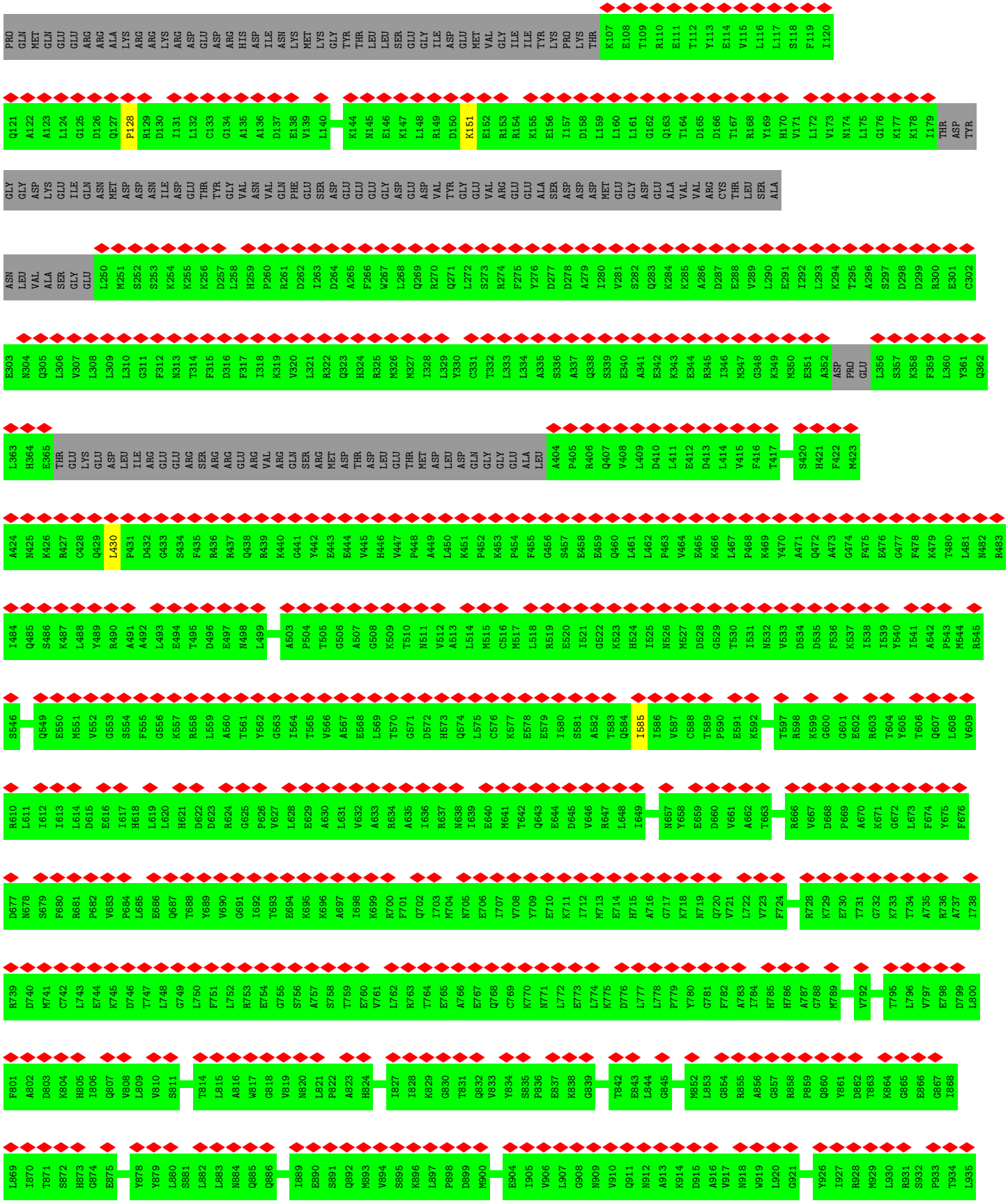
Chain C:

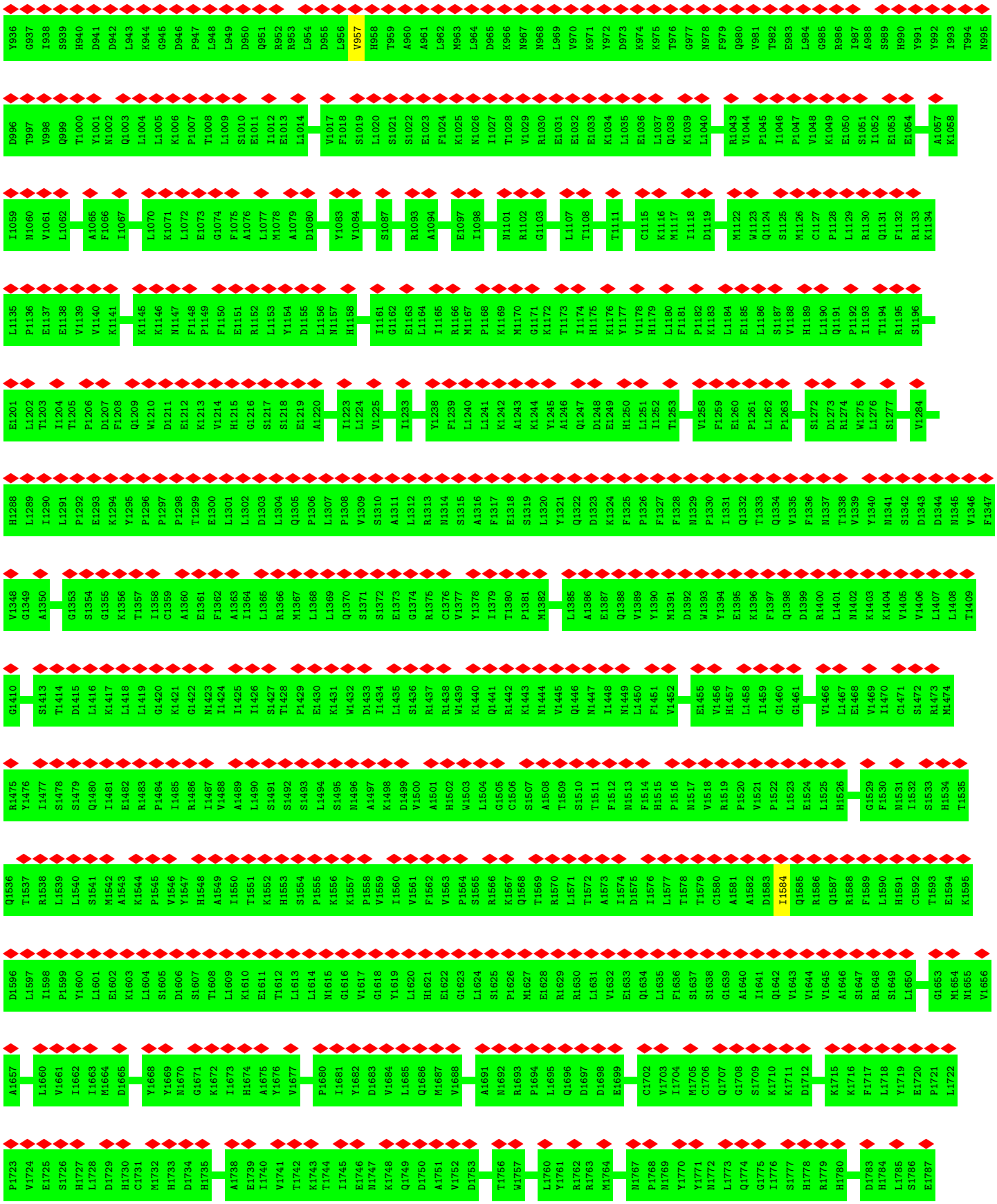


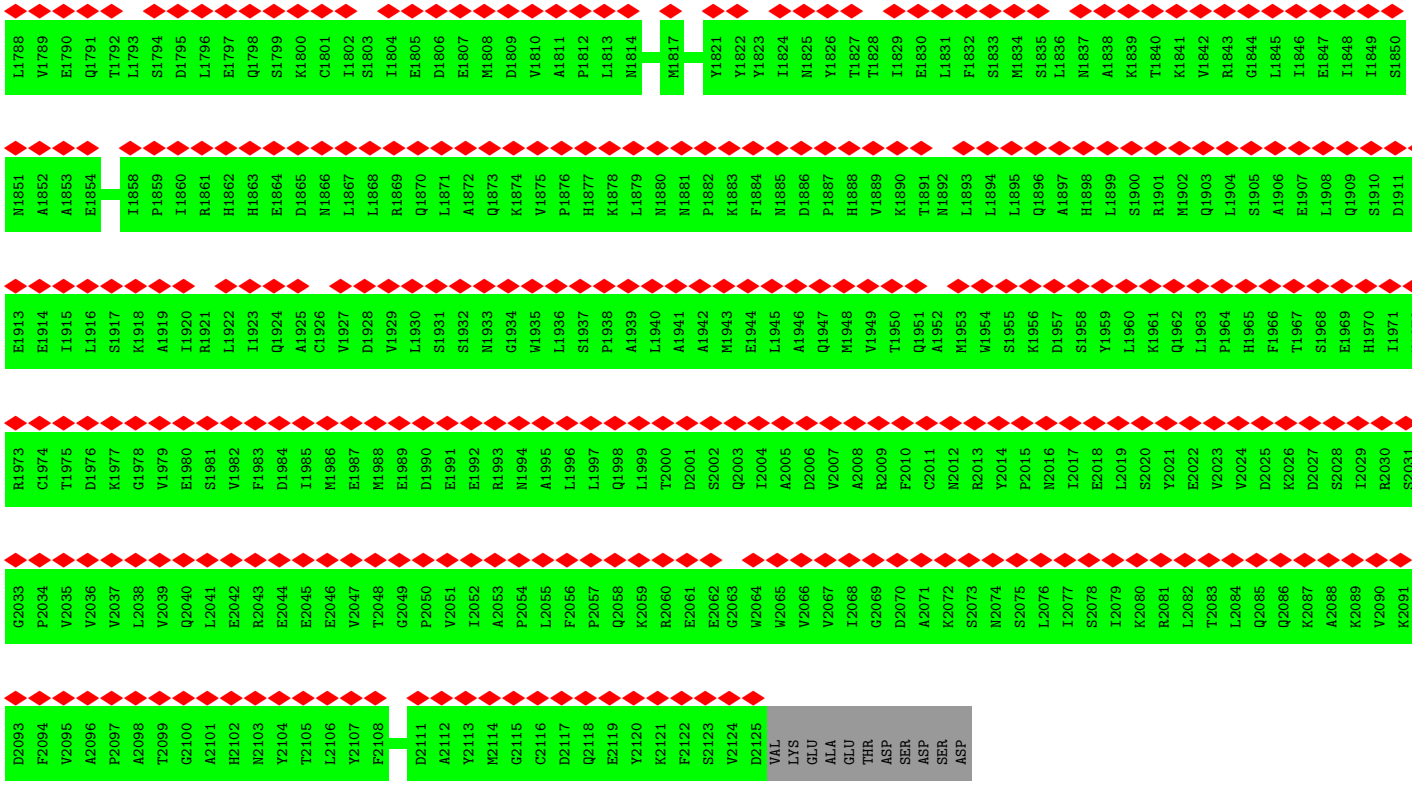
• Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain D:



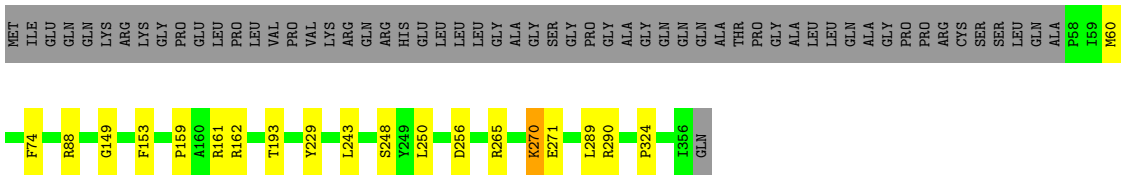

PRO GLN MET GLN GLU GLU ARG ARG ALA LYS ARG ARG LYS ARG ASP GLU ASP ARG HIS ASP ILE ASN LYS MET LYS GLY TYR THR LEU LEU SER GLU GLY ILE ASP GLU MET VAL GLY ILE ILE TYR LYS PRO LYS THR
K107 E108 T109 R110 E111 T112 Y113 E114 V115 L116 L117 S118 F119 I120
Q121 A122 A123 L124 G125 D126 Q127 P128 R129 D130 I131 L132 C133 G134 A135 A136 D137 E138 V139 L140
K144 N145 E146 K147 L148 R149 D150 K151 E152 R153 R154 K155 E156 I157 D158 L159 L160 L161 G162 Q163 T164 D165 D166 T167 R168 Y169 H170 V171 L172 V173 N174 L175 G176 K177 K178 I179 THR ASP TYR
GLY GLY ASP LYS GLU ILE GLN ASN MET ASP ASP ASN ILE ASP GLU THR TYR GLY VAL ASN VAL GLN PHE GLU SER ASP GLU GLU GLU GLY ASP GLU ASP VAL TYR GLY GLU VAL ARG GLU GLU ALA SER ASP ASP ASP MET GLU GLY ASP GLU ALA VAL VAL ARG CYS THR LEU SER ALA
ASN LEU VAL ALA SER GLY GLU
L250 M251 S252 S253 K254 K255 K256 D257 L258 H259 P260 R261 D262 I263 D264 A265 F266 W267 L268 Q269 R270 Q271 L272 S273 R274 F275 Y276 D277 D278 A279 I280 V281 S282 Q283 K284 K285 A286 D287 E288 V289 L290 E291 I292 L293 K294 T295 A296 S297 D298 D299 R300 E301 C302
E303 N304 Q305 L306 V307 L308 L309 L310 G311 F312 N313 T314 F315 D316 F317 I318 K319 V320 L321 R322 Q323 H324 R325 M326 M327 I328 L329 Y330 C331 T332 L333 L334 A335 S336 A337 Q338 S339 E340 A341 E342 K343 E344 R345 I346 M347 G348 K349 M350 E351 A352 ASP PRO GLU L356 S357 K358 F359 L360 Y361 Q362
L363 H364 E365 THR GLU LYS GLU ASP LEU ILE ARG GLU GLU ARG SER ARG ARG GLU ARG VAL ARG GLN SER ARG MET ASP THR ASP LEU GLU THR MET ASP LEU ASP GLN GLY GLY GLU ALA LEU
A404 P405 R406 Q407 V408 L409 D410 L411 E412 D413 L414 V415 F416 T417 S420 H421 F422 M423
A424 N425 K426 R427 C428 Q429 L430 P431 D432 G433 S434 F435 R436 R437 Q438 R439 K440 G441 Y442 E443 E444 V445 H446 V447 P448 A449 L450 K451 P452 K453 P454 F455 G456 S457 E458 E459 Q460 L461 L462 P463 V464 E465 K466 L467 P468 K469 Y470 A471 Q472 A473 G474 F475 E476 G477 F478 K479 T480 L481 N482 R483
I484 Q485 S486 K487 L488 Y489 R490 A491 A492 L493 E494 T495 D496 E497 N498 L499
A503 P504 T505 G506 A507 G508 K509 T510 N511 V512 A513 L514 M515 C516 M517 L518 R519 E520 I521 G522 K523 H524 I525 N526 M527 D528 G529 T530 I531 N532 V533 D534 D535 F536 K537 I538 I539 Y540 I541 A542 P543 M544 R545
S546
Q549 E550 M551 V552 G553 S554 F555 G556 K557 R558 L559 A560 T561 Y562 G563 I564 T565 V566 A567 E568 L569 T570 G571 D572 H573 Q574 L575 C576 K577 E578 E579 I580 S581 A582 T583 Q584
I585
I586 V587 C588 T589 P590 E591 K592
T597 R598 K599 G600 G601 E602 R603 T604 Y605 T606 Q607 L608 V609
R610 L611 I612 I613 L614 D615 E616 I617 H618 L619 L620 H621 D622 D623 R624 G625 P626 V627 L628 E629 A630 L631 V632 A633 R634 A635 I636 R637 N638 I639 E640 M641 T642 Q643 E644 D645 V646 R647 L648 I649
N657 Y658 E659 D660 V661 A662 T663
R666 V667 D668 P669 A670 K671 G672 L673 F674 Y675 F676
D677 N678 S679 F680 R681 P682 V683 P684 L685 E686 Q687 T688 Y689 V690 G691 I692 T693 E694 K695 K696 A697 I698 K699 R700 F701 Q702 I703 M704 N705 E706 I707 V708 Y709 E710 K711 I712 M713 E714 H715 A716 G717 K718 W719 Q720 V721 L722 V723 F724
R728 K729 E730 T731 G732 K733 T734 A735 R736 A737 I738
R739 D740 M741 C742 L743 E744 K745 D746 T747 L748 G749 L750 F751 L752 R753 E754 G755 S756 A757 S758 T759 E760 V761 L762 R763 T764 E765 A766 E767 Q768 C769 K770 N771 L772 E773 L774 K775 D776 L777 L778 P779 Y780 G781 F782 A783 I784 H785 H786 A787 G788 M789 V792 T795 L796 V797 E798 D799 L800
F801 A802 D803 K804 H805 I806 Q807 V808 L809 V810 S811 T814 L815 A816 W817 G818 V819 N820 L821 P822 A823 H824 I827 I828 K829 G830 T831 Q832 V833 Y834 S835 P836 E837 K838 G839 T842 E843 L844 G845 M852 L853 G854 R855 A856 G857 R858 P859 Q860 Y861 D862 T863 K864 G865 E866 G867 I868
L869 I870 T871 S872 H873 G874 E875 Y878 Y879 L880 S881 L882 L883 N884 Q885 Q886 I889 E890 S891 Q892 M893 V894 S895 K896 L897 P898 D899 M900 E904 I905 V906 L907 G908 N909 V910 Q911 N912 A913 K914 D915 A916 V917 N918 W919 L920 G921 Y926 I927 R928 M929 L930 R931 S932 P933 T934 L935


Y936 G937 I938 S939 H940 D941 D942 L943 K944 G945 D946 P947 L948 L949 D950 Q951 R952 R953 L954 D955 L956 V957 H958 T959 A960 A961 L962 M963 L964 D965 K966 N967 N968 L969 V970 K971 Y972 D973 K974 K975 T976 G977 N978 F979 Q980 V981 T982 E983 L984 G985 R986 I987 A988 S989 H990 Y991 Y992 I993 T994 N995
D996 T997 V998 Q999 T1000 Y1001 N1002 Q1003 L1004 L1005 K1006 P1007 T1008 L1009 S1010 E1011 I1012 E1013 L1014 V1017 F1018 S1019 L1020 S1021 S1022 E1023 F1024 K1025 N1026 I1027 T1028 V1029 R1030 E1031 E1032 E1033 K1034 L1035 E1036 L1037 Q1038 K1039 L1040 R1043 V1044 P1045 I1046 P1047 V1048 K1049 E1050 S1051 I1052 E1053 E1054 A1057 K1058
I1059 N1060 V1061 L1062 A1065 F1066 I1067 L1070 K1071 L1072 E1073 G1074 P1075 A1076 L1077 M1078 A1079 D1080 Y1083 V1084 S1087 R1093 A1094 E1097 I1098 N1101 R1102 G1103 L1107 T1108 T1111 C1115 K1116 M1117 I1118 D1119 M1122 W1123 Q1124 S1125 M1126 C1127 P1128 L1129 R1130 Q1131 F1132 R1133 K1134
L1135 P1136 E1137 E1138 V1139 V1140 K1141 K1145 K1146 N1147 F1148 P1149 F1150 E1151 R1152 L1153 Y1154 D1155 L1156 N1157 H1158 I1161 G1162 E1163 L1164 I1165 R1166 M1167 P1168 K1169 M1170 G1171 K1172 T1173 I1174 H1175 K1176 Y1177 V1178 H1179 L1180 F1181 P1182 K1183 L1184 E1185 L1186 S1187 V1188 H1189 L1190 Q1191 P1192 I1193 T1194 R1195 S1196
E1201 L1202 T1203 I1204 T1205 P1206 D1207 F1208 Q1209 W1210 D1211 E1212 K1213 V1214 H1215 G1216 S1217 S1218 E1219 A1220 I1223 L1224 V1225 I1233 Y1238 F1239 L1240 L1241 K1242 A1243 K1244 Y1245 A1246 Q1247 D1248 E1249 H1250 L1251 T1252 T1253 V1258 F1259 E1260 P1261 L1262 P1263 S1272 D1273 R1274 W1275 L1276 S1277 V1284
H1288 L1289 I1290 L1291 P1292 E1293 K1294 Y1295 P1296 P1297 P1298 T1299 E1300 L1301 L1302 D1303 L1304 Q1305 P1306 L1307 P1308 V1309 S1310 A1311 L1312 R1313 N1314 S1315 A1316 F1317 E1318 S1319 L1320 Y1321 Q1322 D1323 K1324 F1325 P1326 F1327 F1328 N1329 P1330 I1331 Q1332 T1333 Q1334 V1335 F1336 N1337 T1338 V1339 Y1340 N1341 S1342 D1343 D1344 N1345 V1346 F1347
V1348 G1349 A1350 G1353 S1354 G1355 K1356 T1357 I1358 C1359 A1360 E1361 F1362 A1363 I1364 L1365 R1366 M1367 L1368 L1369 Q1370 S1371 S1372 E1373 G1374 R1375 C1376 V1377 Y1378 I1379 T1380 P1381 M1382 L1385 A1386 E1387 Q1388 V1389 Y1390 M1391 D1392 W1393 Y1394 E1395 K1396 F1397 Q1398 D1399 R1400 L1401 N1402 K1403 K1404 V1405 V1406 L1407 L1408 T1409
G1410 S1413 T1414 D1415 L1416 K1417 L1418 L1419 G1420 K1421 G1422 N1423 I1424 I1425 I1426 S1427 T1428 P1429 E1430 K1431 W1432 D1433 I1434 L1435 S1436 R1437 R1438 W1439 K1440 Q1441 R1442 K1443 N1444 V1445 Q1446 N1447 I1448 N1449 L1450 F1451 V1452 E1455 V1456 H1457 L1458 I1459 G1460 G1461 V1466 L1467 E1468 V1469 I1470 C1471 S1472 R1473 M1474
R1475 Y1476 I1477 S1478 S1479 Q1480 I1481 E1482 R1483 P1484 I1485 R1486 I1487 V1488 A1489 L1490 S1491 S1492 S1493 L1494 S1495 N1496 A1497 K1498 D1499 V1500 A1501 H1502 W1503 L1504 G1505 C1506 S1507 A1508 T1509 S1510 T1511 F1512 N1513 F1514 H1515 P1516 N1517 V1518 R1519 P1520 V1521 P1522 L1523 E1524 L1525 H1526 G1529 F1530 N1531 I1532 S1533 H1534 T1535
Q1536 T1537 R1538 L1539 L1540 S1541 M1542 A1543 K1544 P1545 Y1546 Y1547 H1548 A1549 I1550 T1551 K1552 H1553 S1554 P1555 K1556 K1557 P1558 V1559 I1560 V1561 F1562 V1563 P1564 S1565 R1566 K1567 Q1568 T1569 R1570 L1571 T1572 A1573 I1574 D1575 I1576 L1577 T1578 T1579 C1580 A1581 A1582 D1583 I1584 Q1585 R1586 Q1587 R1588 F1589 L1590 H1591 C1592 T1593 E1594 K1595
D1596 L1597 I1598 P1599 Y1600 L1601 E1602 K1603 L1604 S1605 D1606 S1607 T1608 L1609 K1610 E1611 T1612 L1613 L1614 N1615 G1616 V1617 G1618 Y1619 L1620 H1621 E1622 G1623 L1624 S1625 P1626 M1627 E1628 R1629 R1630 L1631 V1632 E1633 Q1634 L1635 F1636 S1637 S1638 G1639 A1640 I1641 Q1642 V1643 V1644 V1645 A1646 S1647 R1648 S1649 L1650 G1653 M1654 N1655 V1656
A1657 L1660 V1661 I1662 I1663 M1664 D1665 Y1668 Y1669 N1670 G1671 K1672 I1673 H1674 A1675 Y1676 V1677 P1680 I1681 Y1682 D1683 V1684 L1685 Q1686 M1687 V1688 A1691 N1692 R1693 P1694 L1695 Q1696 D1697 D1698 E1699 C1702 V1703 I1704 M1705 C1706 Q1707 G1708 S1709 K1710 K1711 D1712 K1715 K1716 F1717 L1718 Y1719 E1720 P1721 L1722
P1723 V1724 E1725 S1726 H1727 L1728 D1729 H1730 C1731 M1732 H1733 D1734 H1735 A1738 E1739 I1740 V1741 T1742 K1743 T1744 I1745 E1746 N1747 K1748 Q1749 D1750 A1751 V1752 D1753 T1756 W1757 L1760 Y1761 R1762 R1763 M1764 N1767 P1768 N1769 Y1770 Y1771 N1772 L1773 Q1774 G1775 I1776 S1777 H1778 R1779 H1780 D1783 H1784 L1785 S1786 E1787



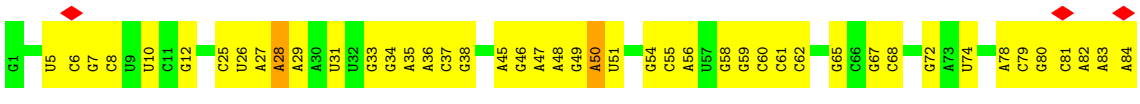
• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:



• Molecule 6: U6 snRNA

Chain F:

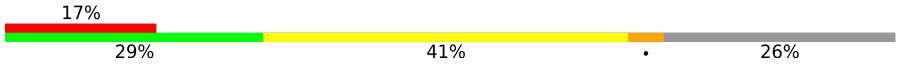


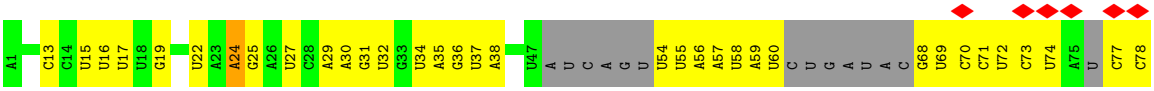
• Molecule 7: Pre-mRNA

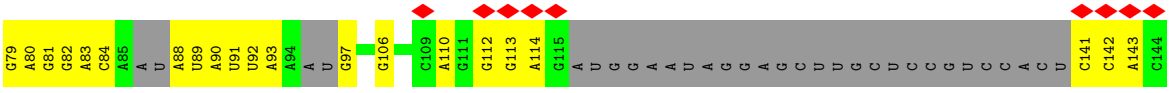
Chain G:

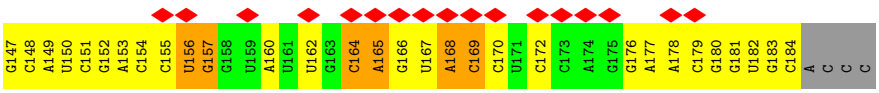
• Molecule 8: U2 snRNA

Chain H:



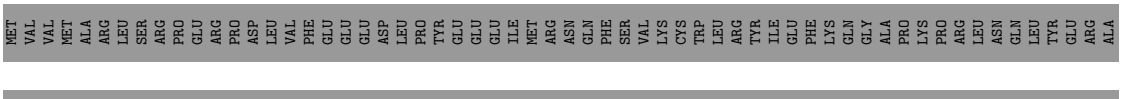


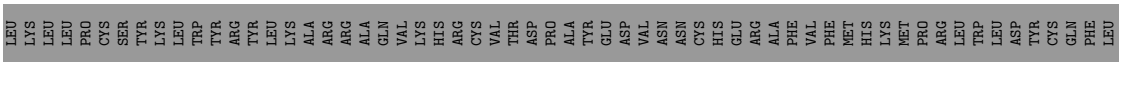


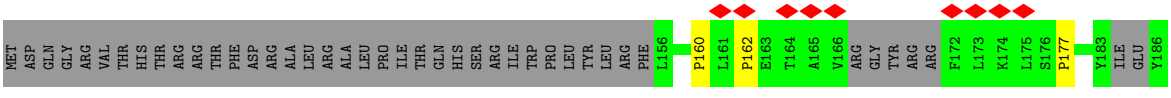


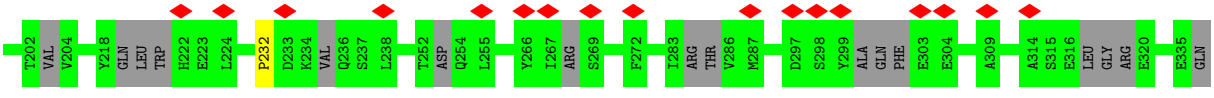
• Molecule 9: Pre-mRNA-splicing factor SYF1

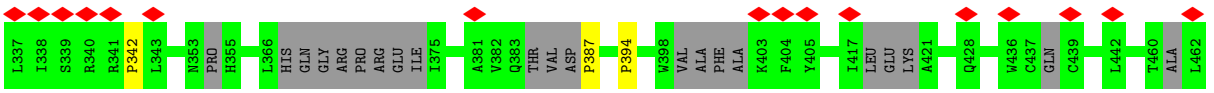
Chain I:

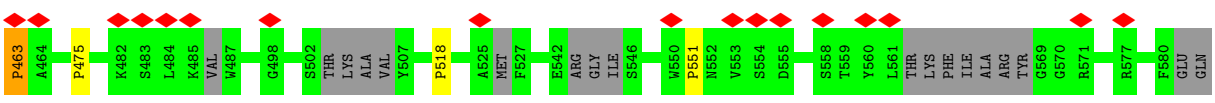


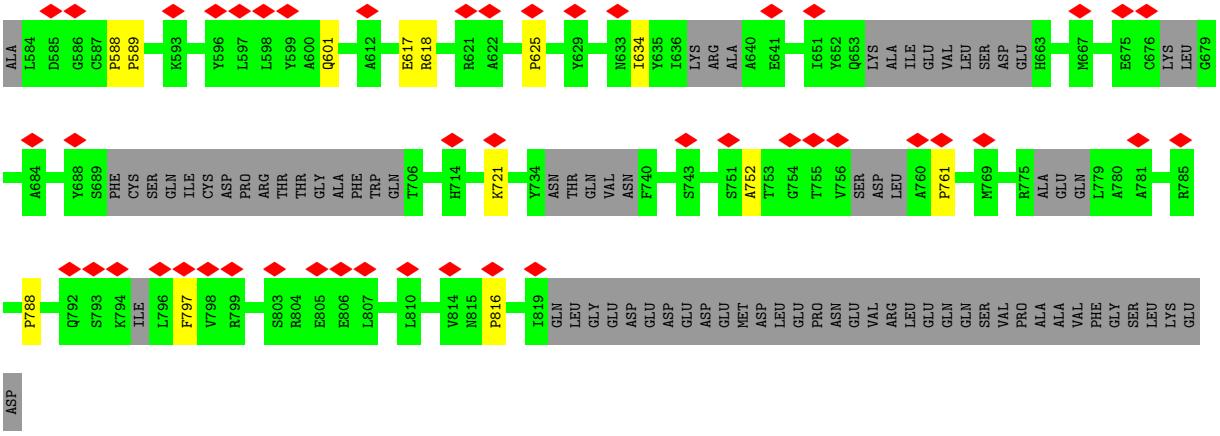






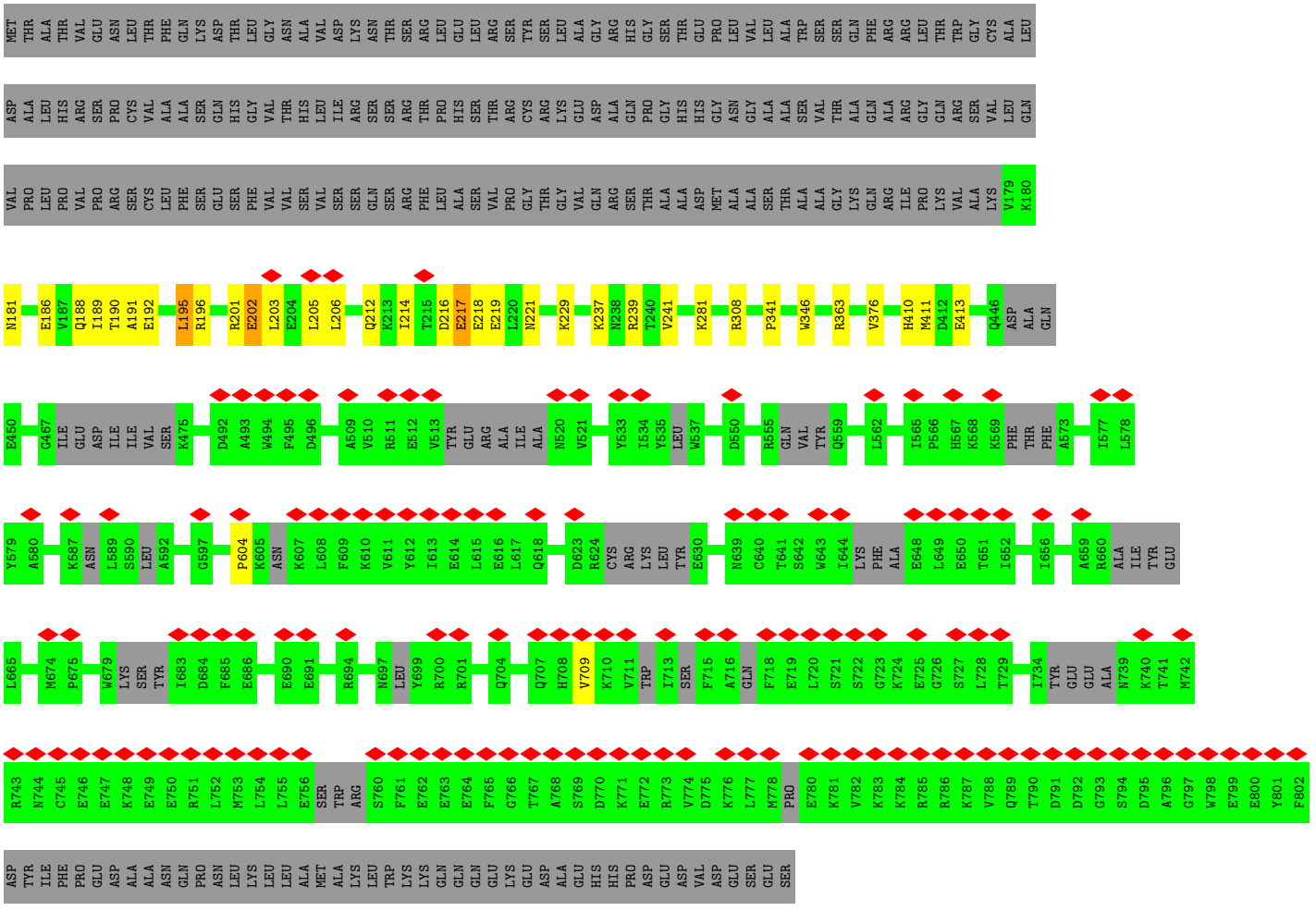






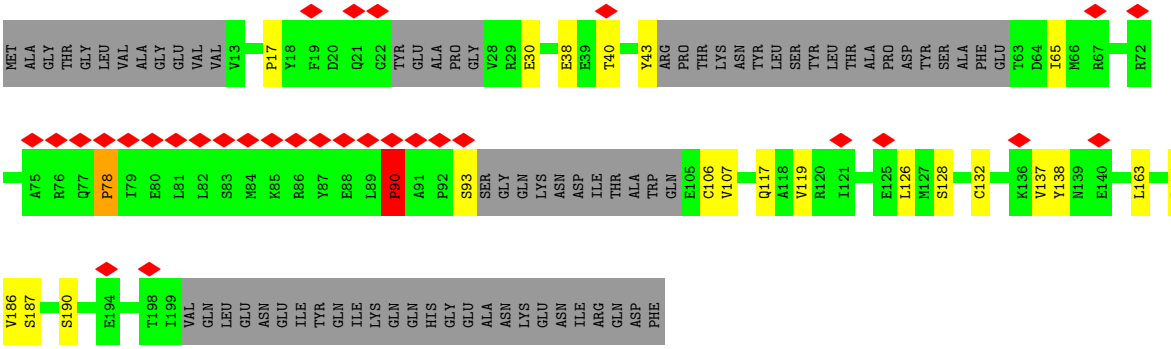
• Molecule 10: Crooked neck-like protein 1

Chain J:



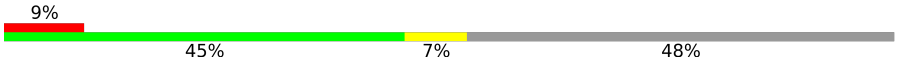
• Molecule 11: Pre-mRNA-splicing factor SPF27

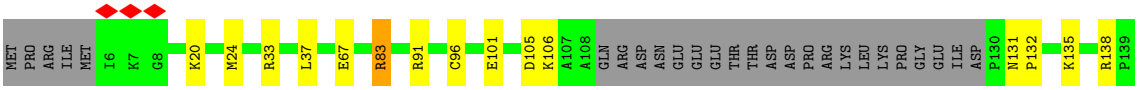
Chain K:

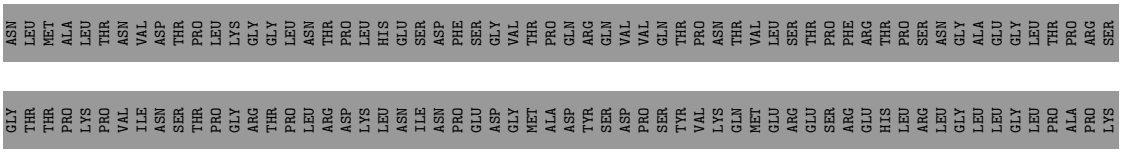


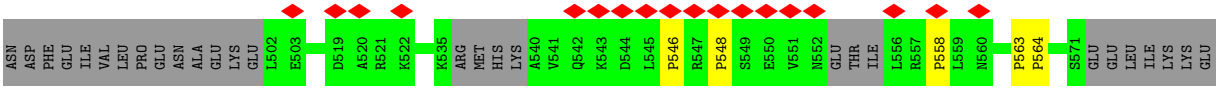
• Molecule 12: Cell division cycle 5-like protein

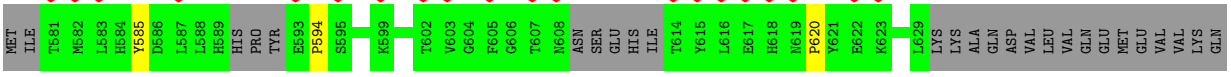
Chain L:

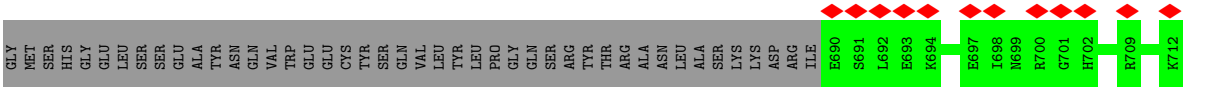


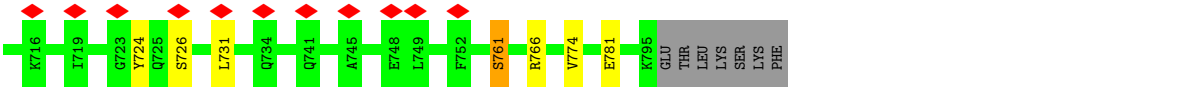






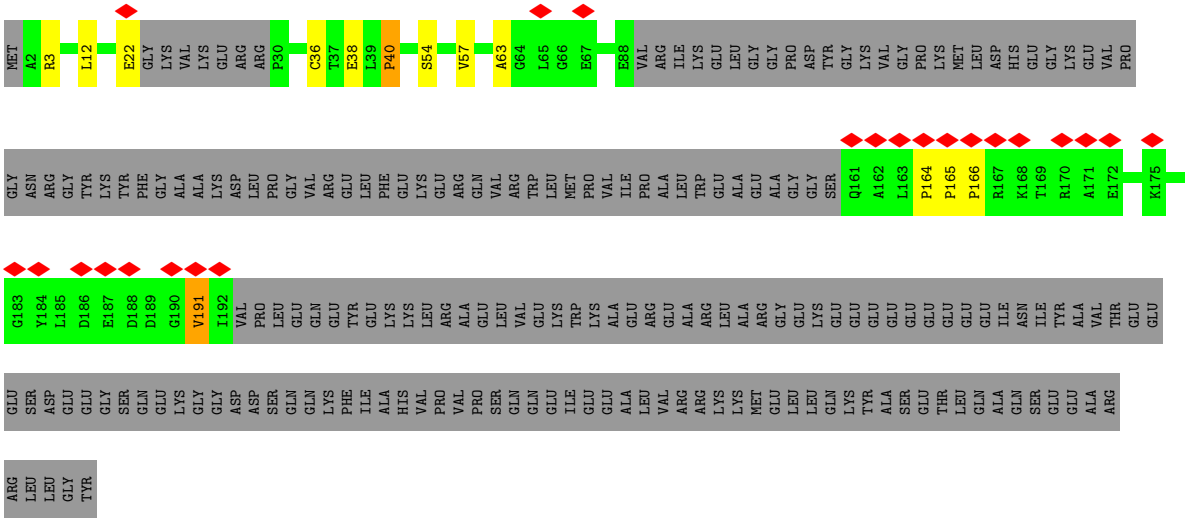






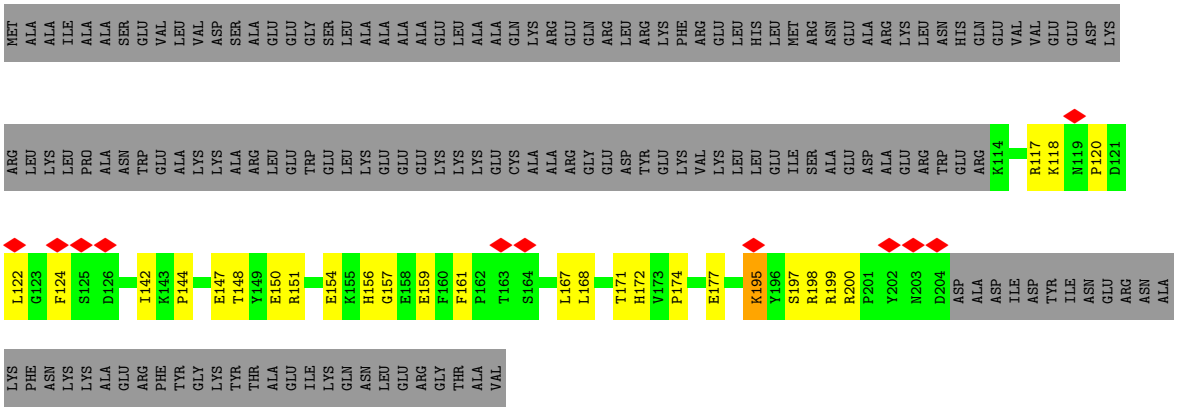
• Molecule 13: Pre-mRNA-splicing factor ISY1 homolog

Chain y:



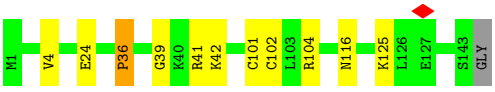
• Molecule 14: Pre-mRNA-splicing factor SYF2

Chain M:



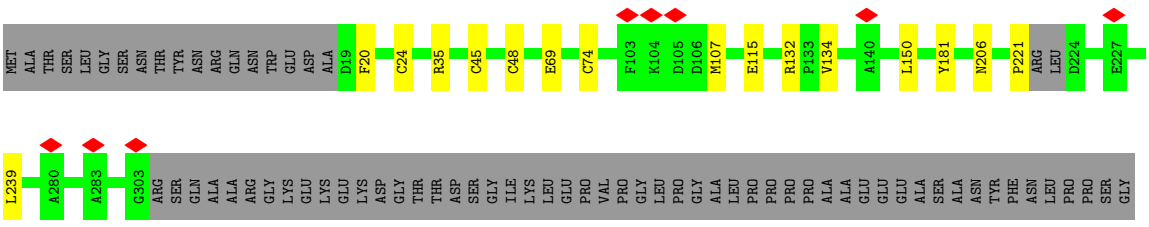
• Molecule 15: Protein BUD31 homolog

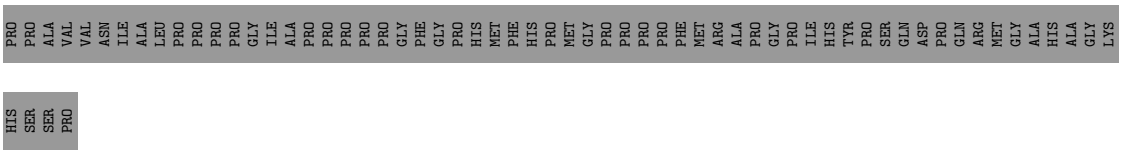
Chain N:



• Molecule 16: Pre-mRNA-splicing factor RBM22

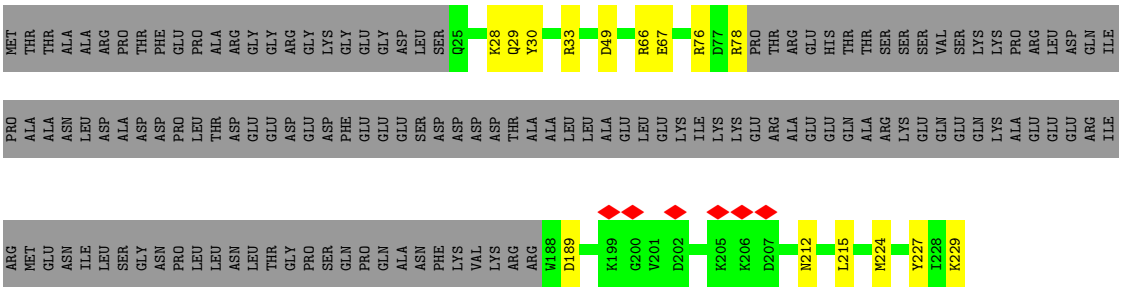
Chain O:





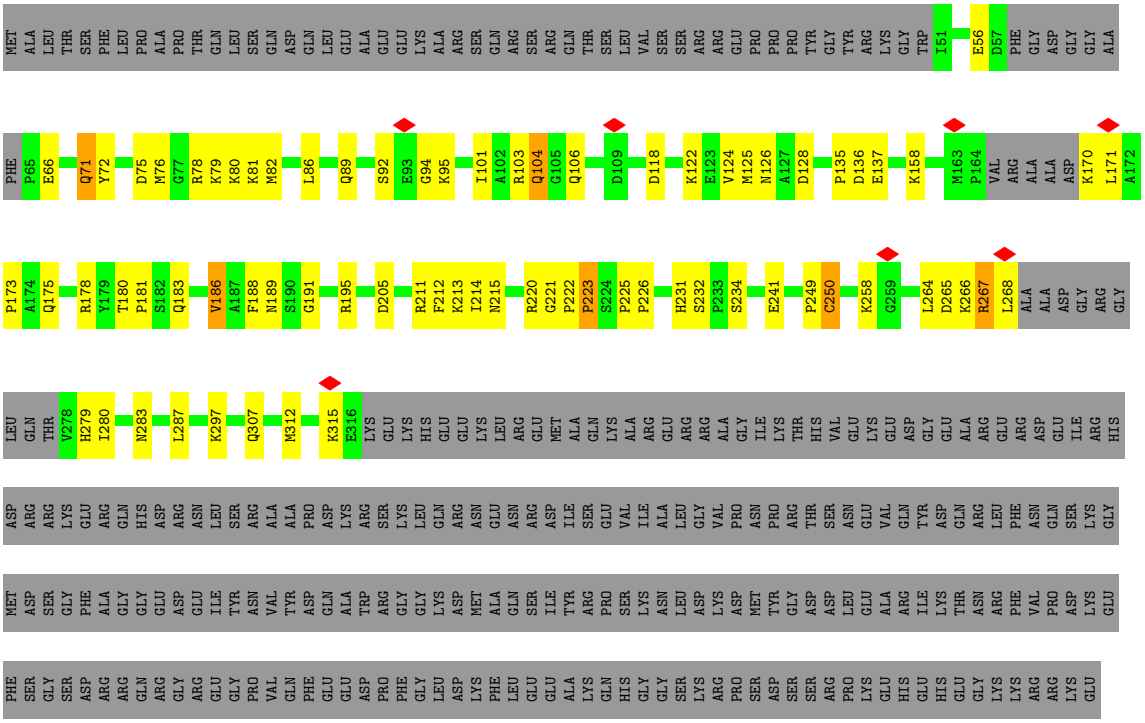
• Molecule 17: Spliceosome-associated protein CWC15 homolog

Chain P:



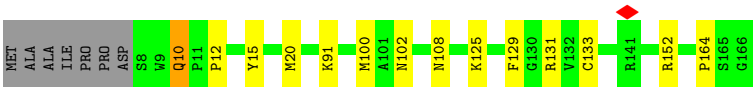
• Molecule 18: SNW domain-containing protein 1

Chain R:



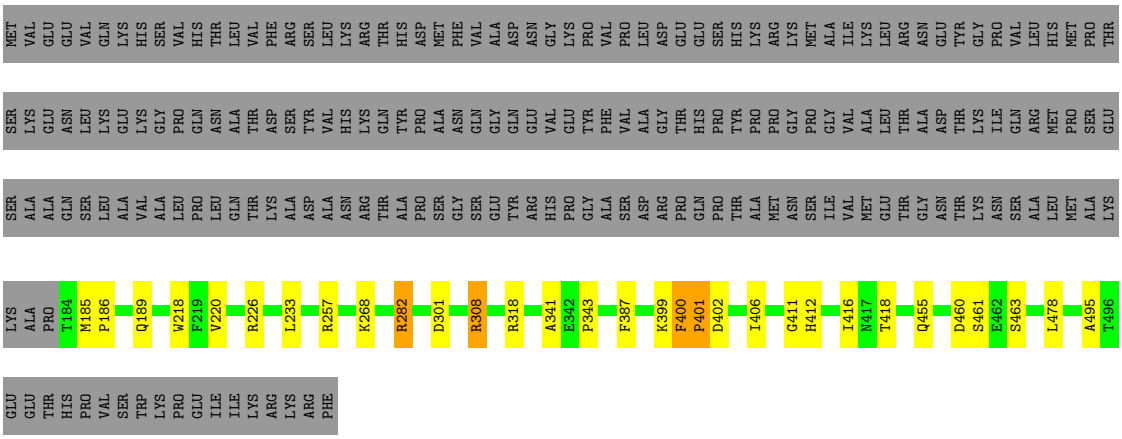
• Molecule 19: Peptidyl-prolyl cis-trans isomerase-like 1

Chain S:



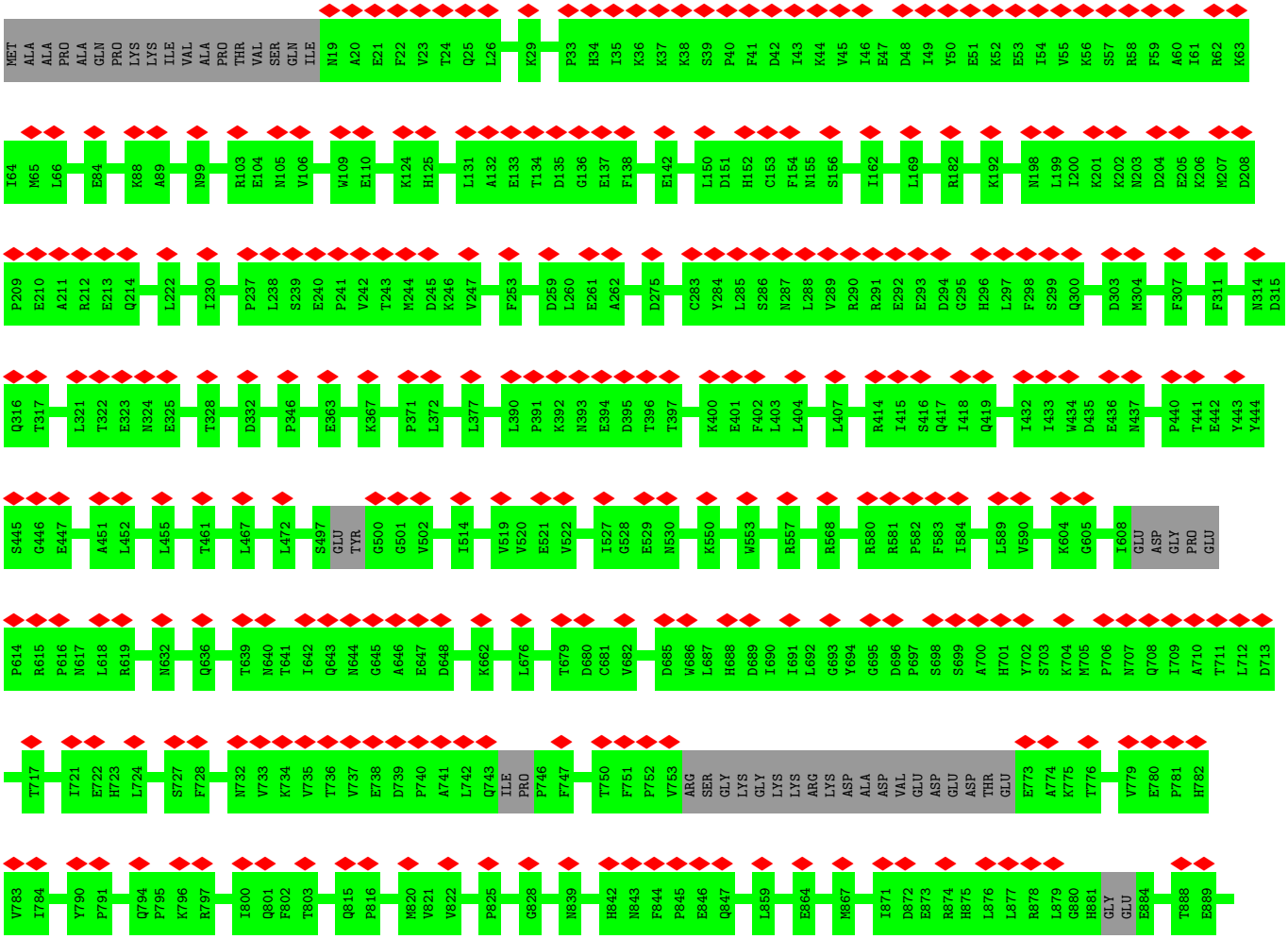
• Molecule 20: Pleiotropic regulator 1

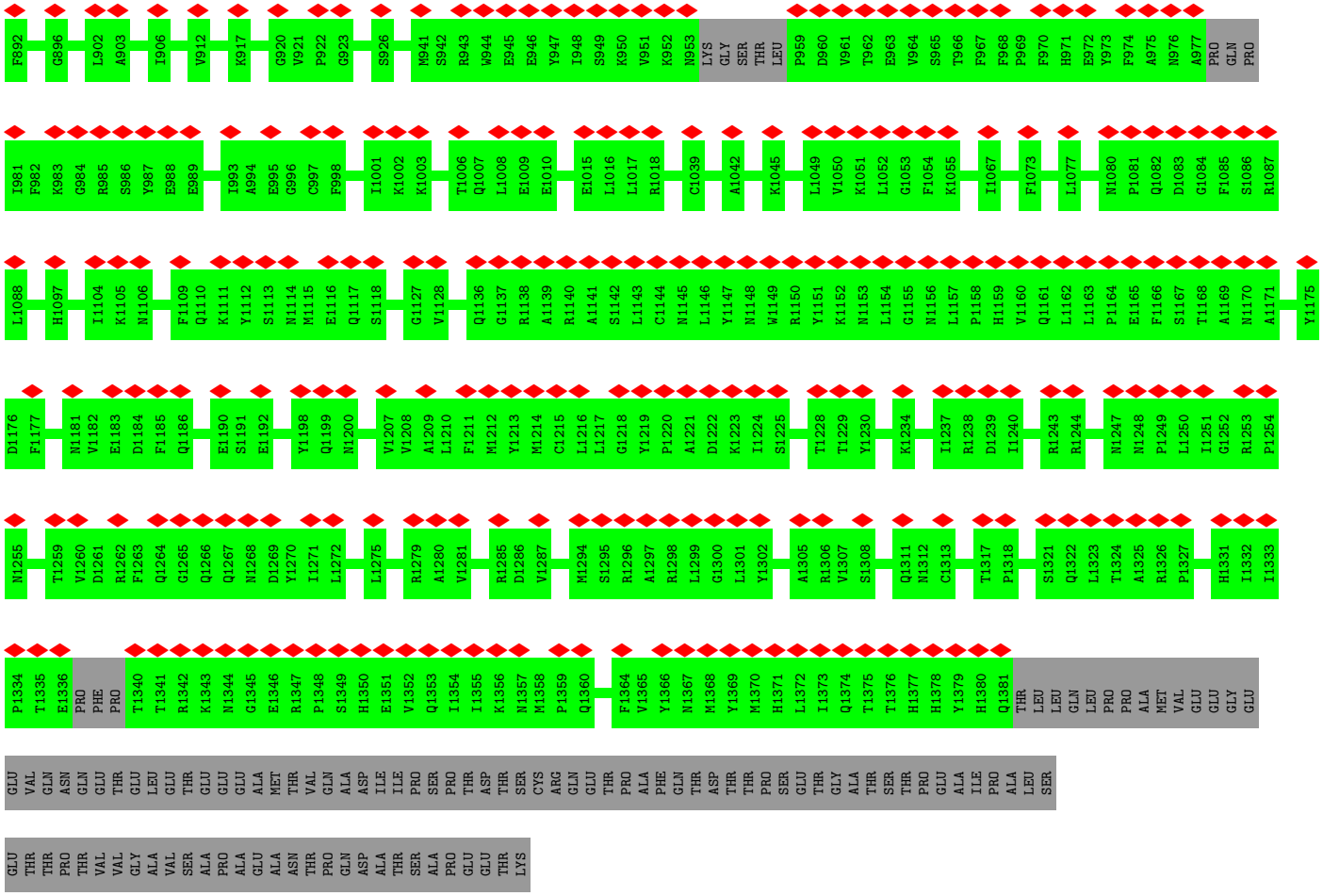
Chain T:



• Molecule 21: Intron-binding protein aquarius

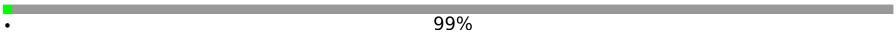
Chain Q:

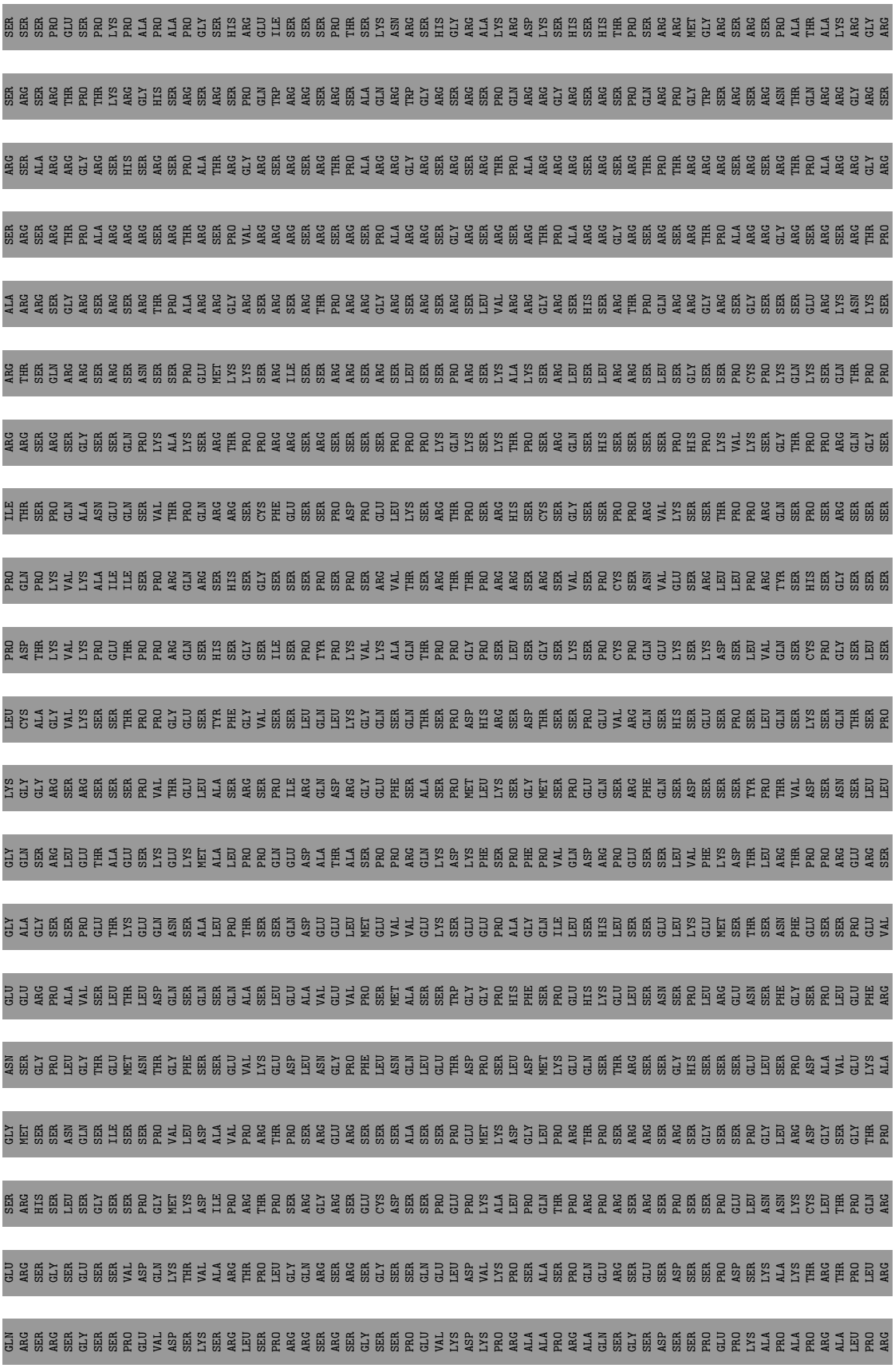


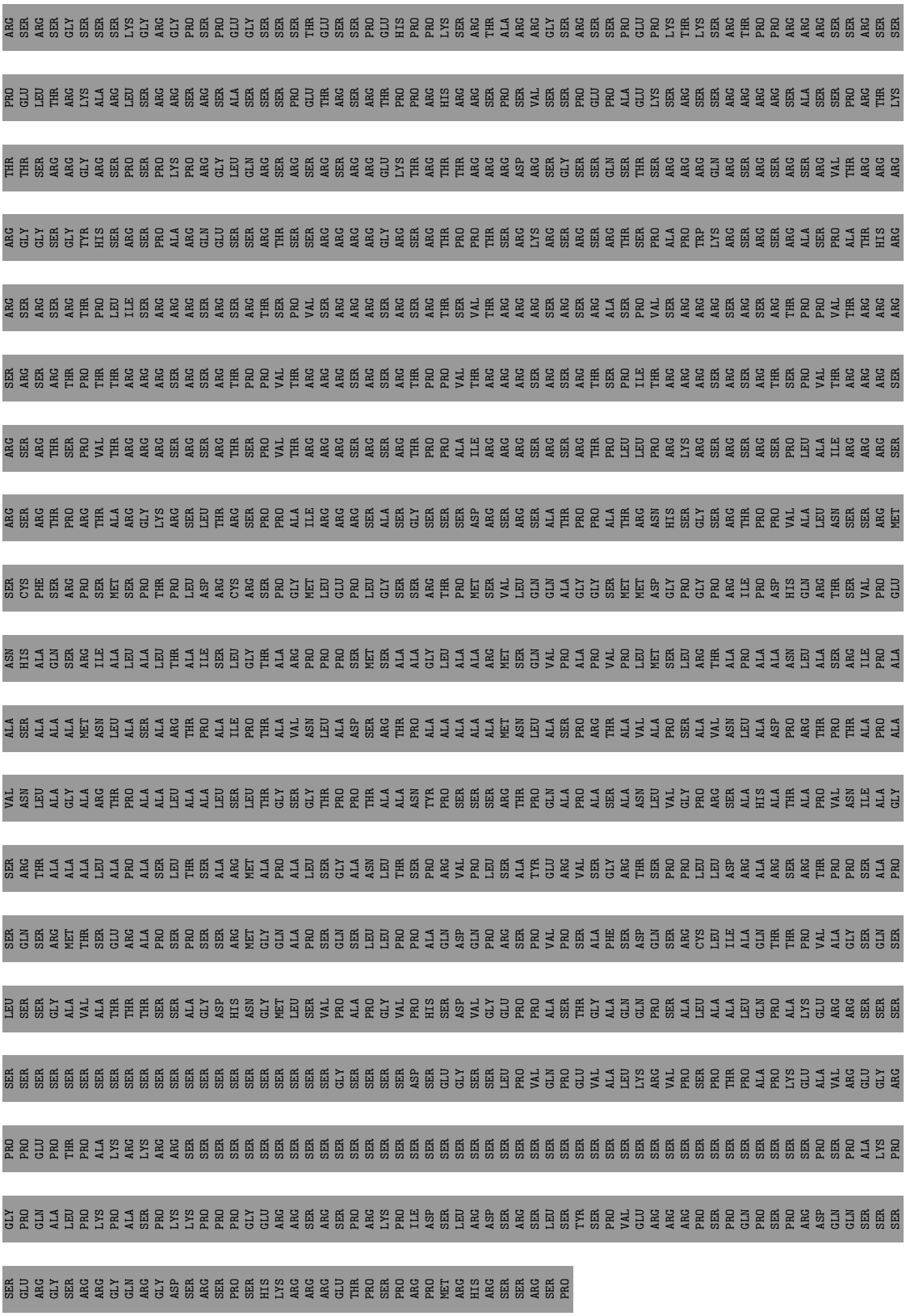


• Molecule 22: Serine/arginine repetitive matrix protein 2

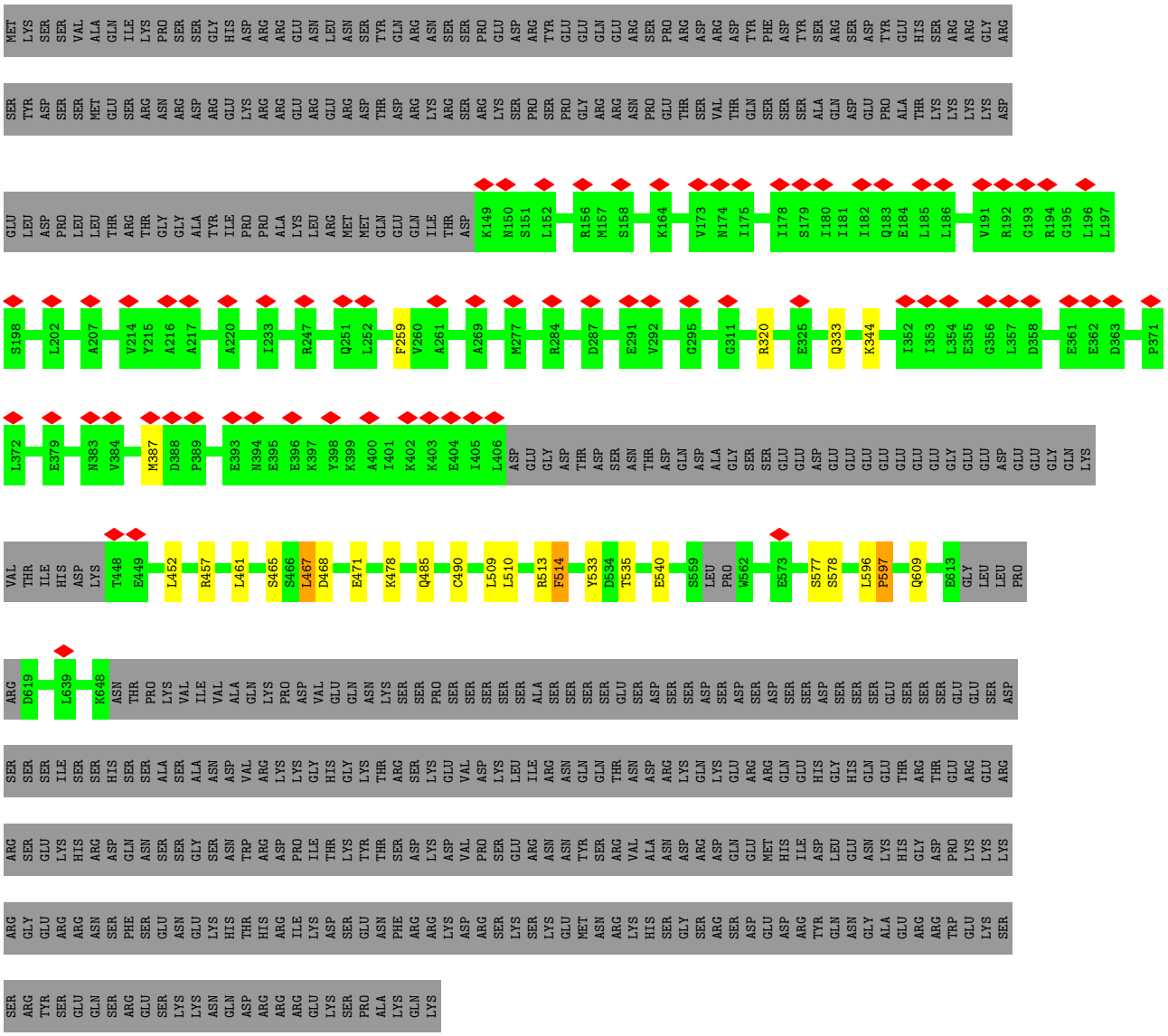
Chain U:





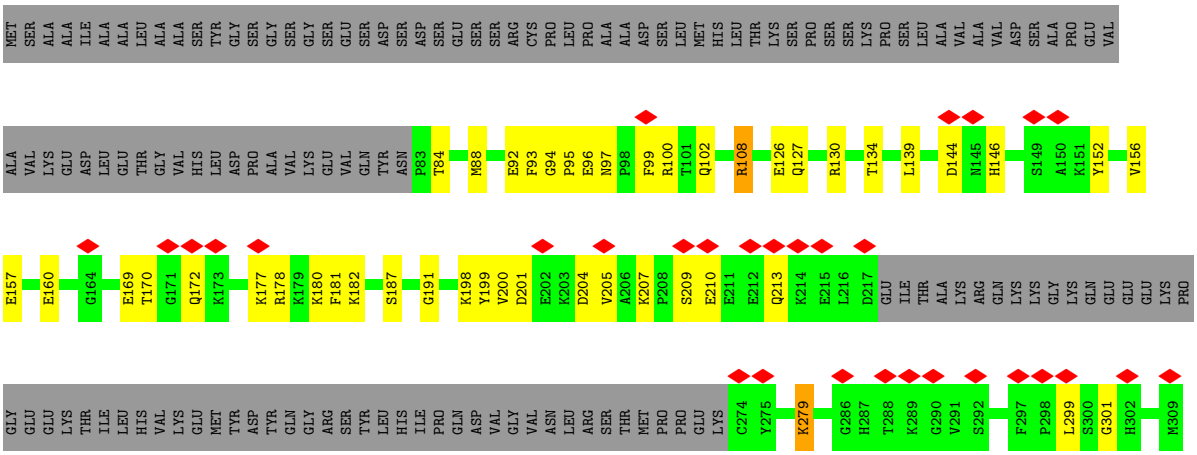


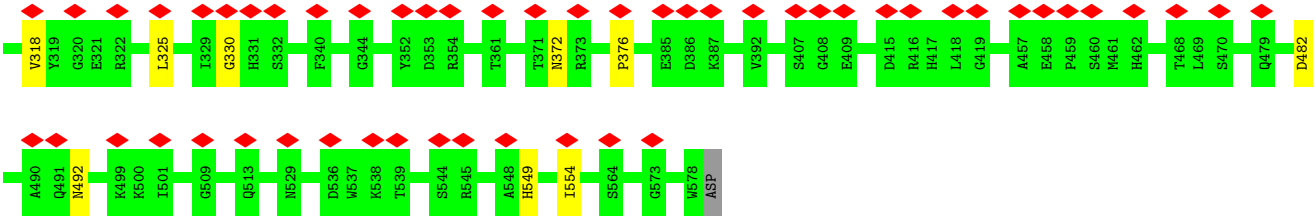
• Molecule 23: Pre-mRNA-splicing factor CWC22 homolog



• Molecule 24: Pre-mRNA-processing factor 17

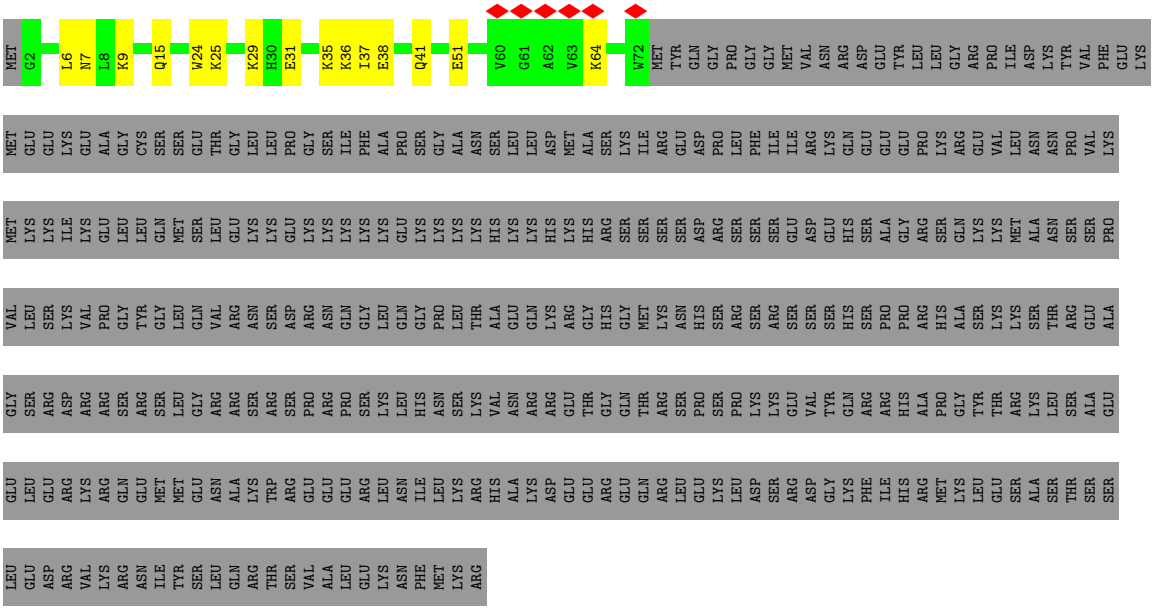
Chain W:





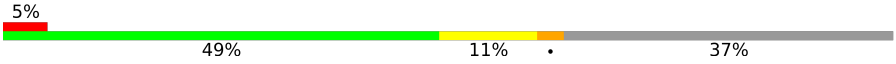
• Molecule 25: Pre-mRNA-splicing factor CWC25 homolog

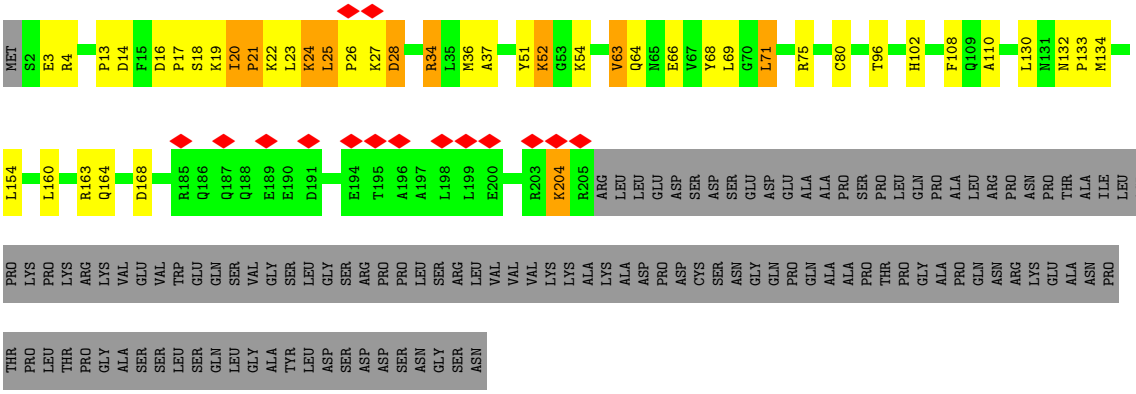
Chain X:



• Molecule 26: Coiled-coil domain-containing protein 94

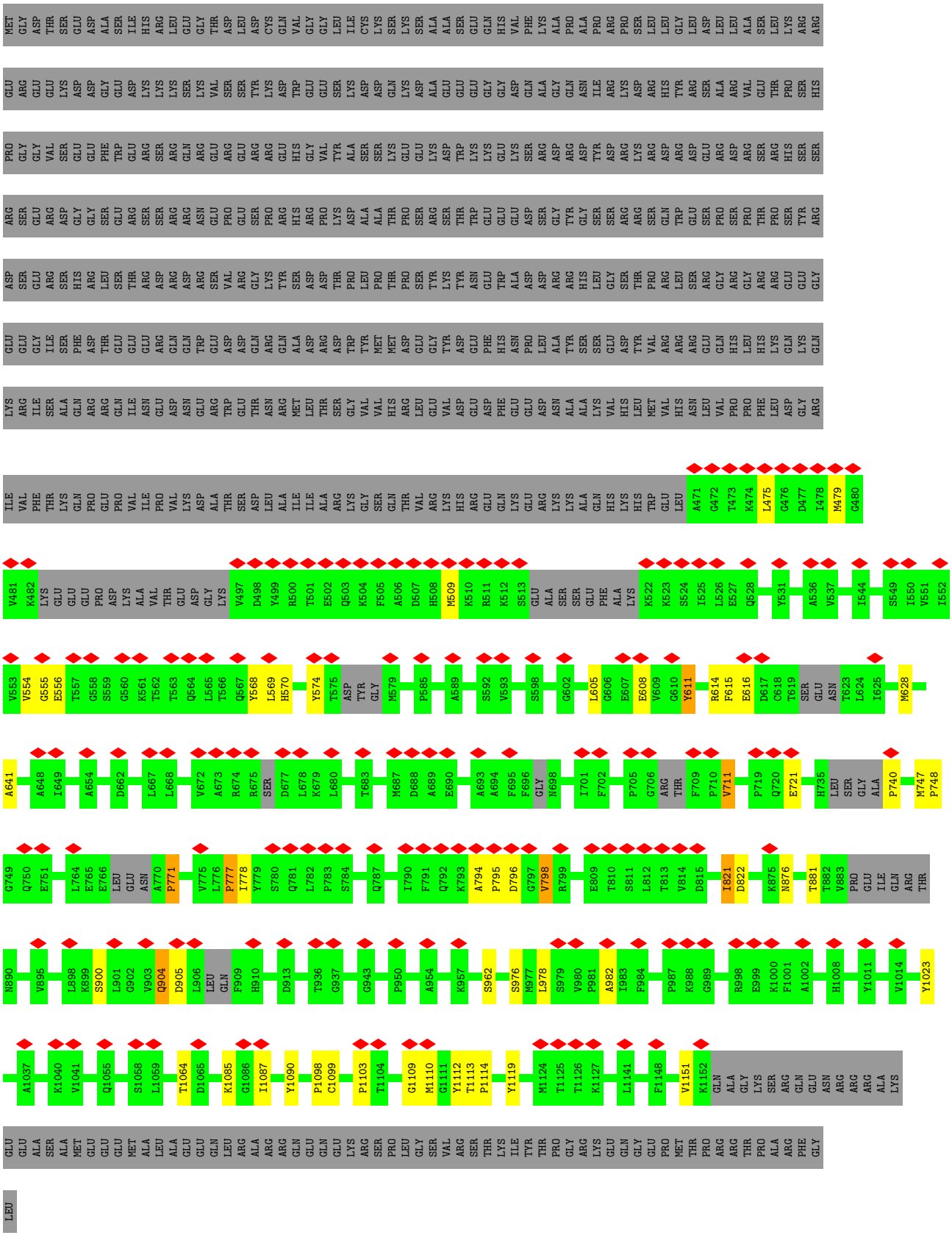
Chain Y:





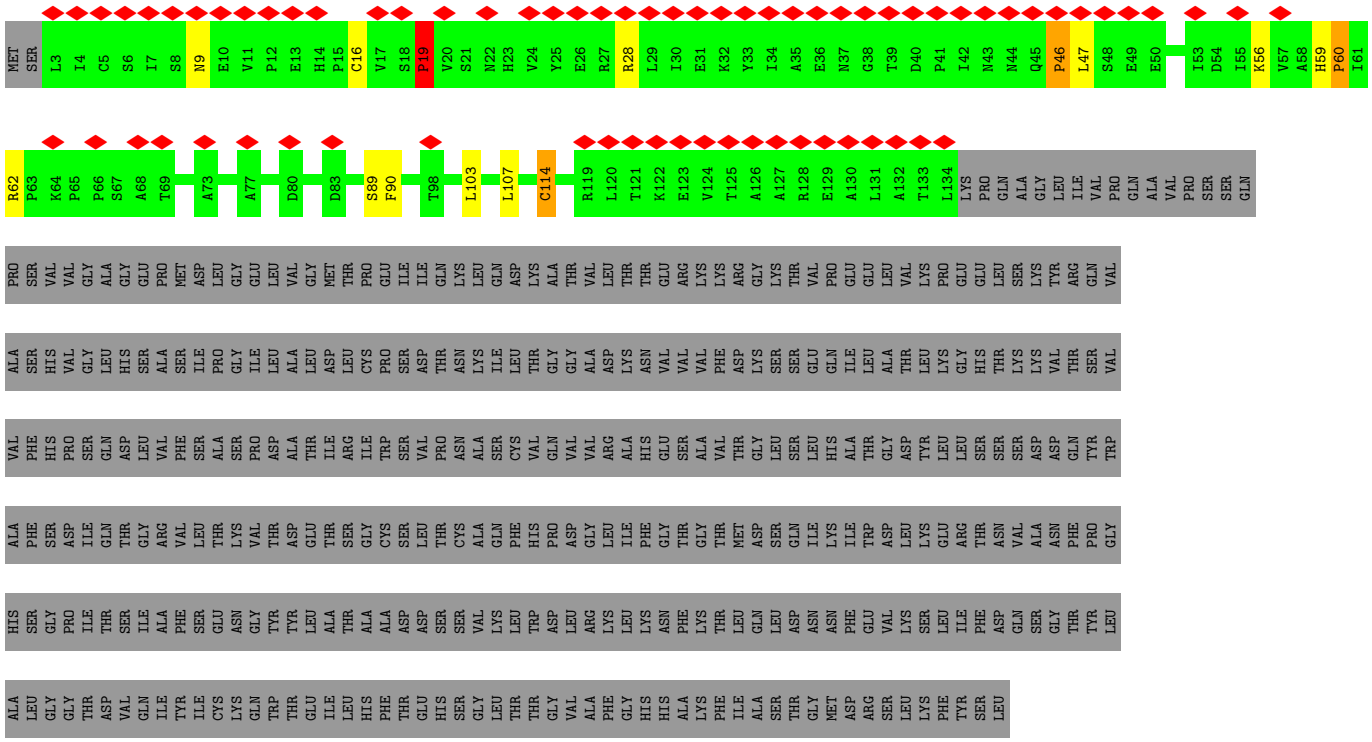
• Molecule 27: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16

Chain Z:



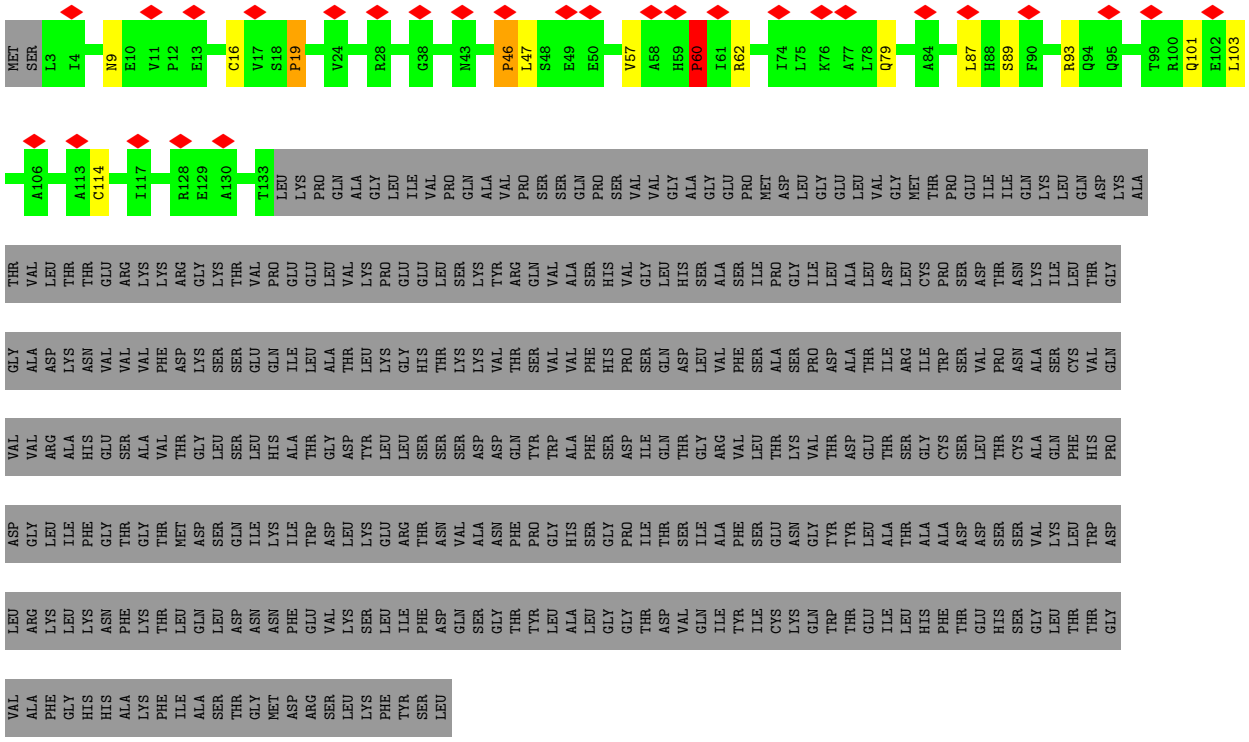
• Molecule 28: Pre-mRNA-processing factor 19

Chain q:



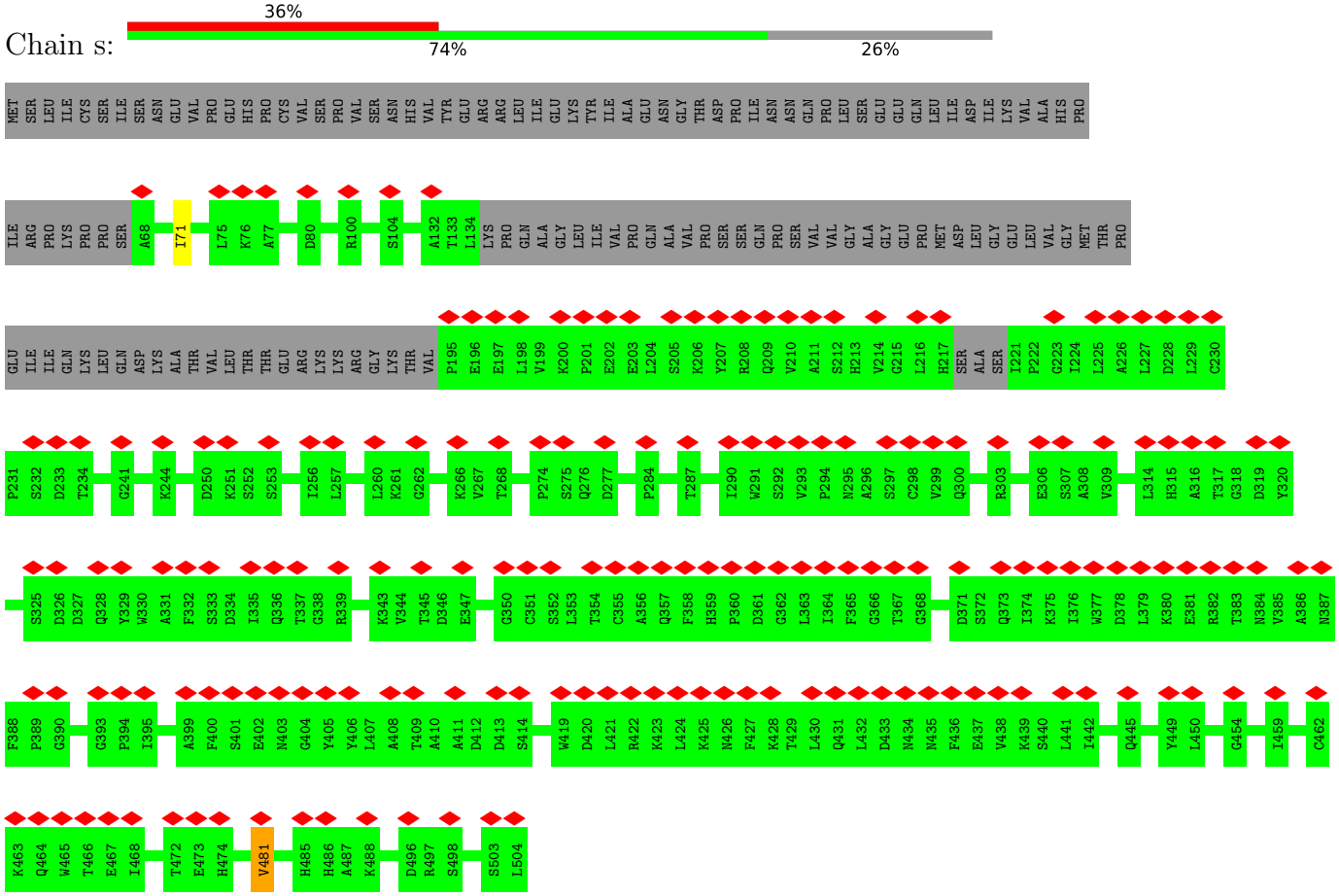
• Molecule 28: Pre-mRNA-processing factor 19

Chain r:



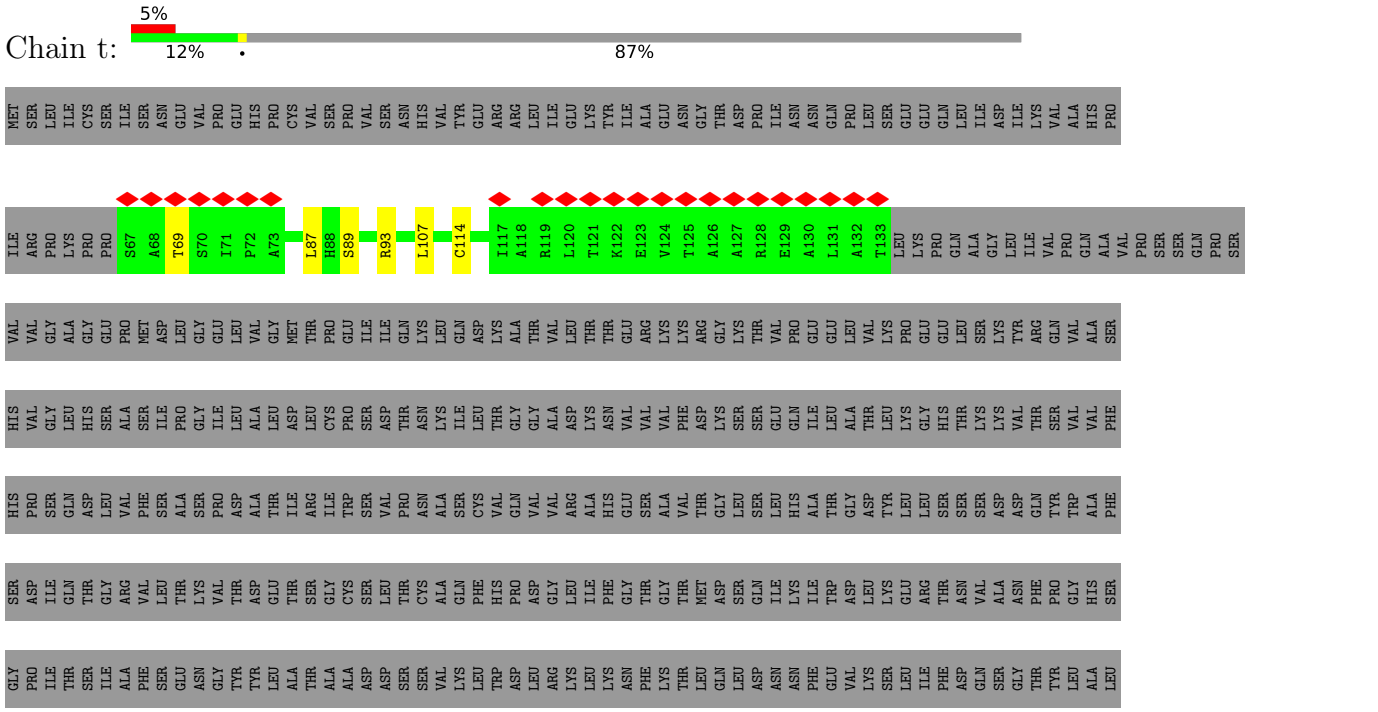
• Molecule 28: Pre-mRNA-processing factor 19

Chain s:



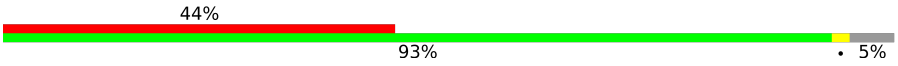
• Molecule 28: Pre-mRNA-processing factor 19

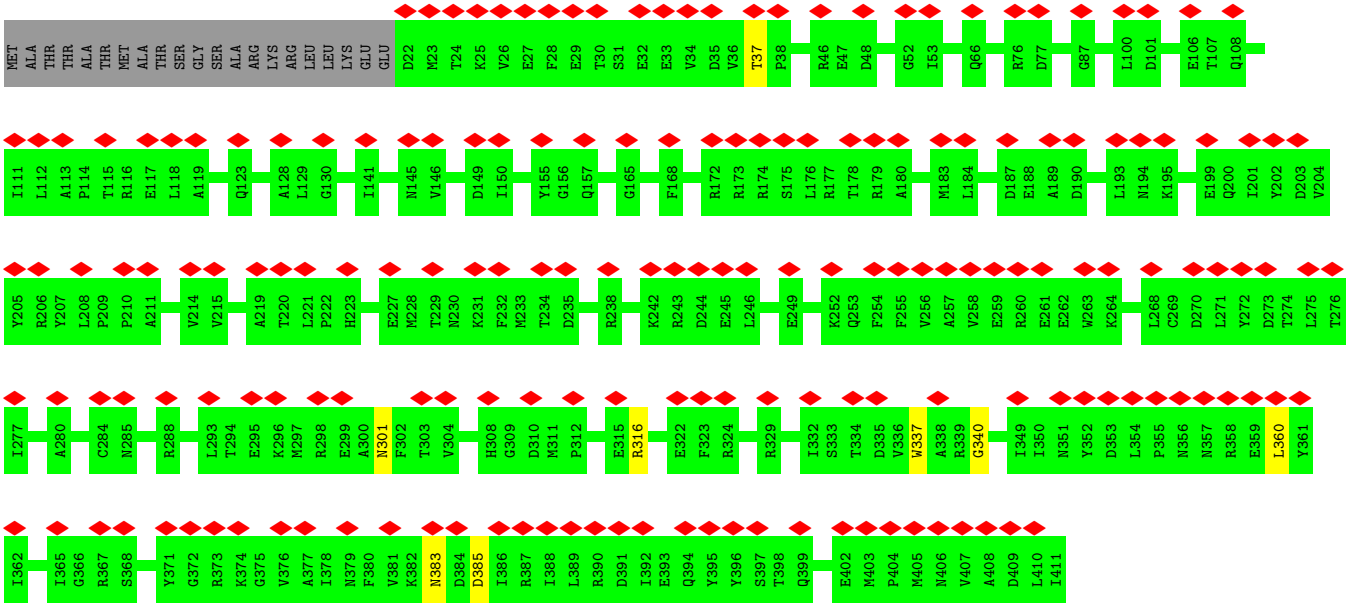
Chain t:



• Molecule 29: Eukaryotic initiation factor 4A-III

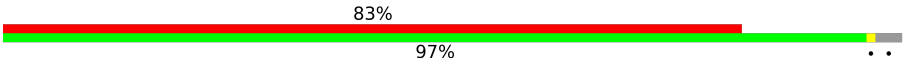
Chain u:

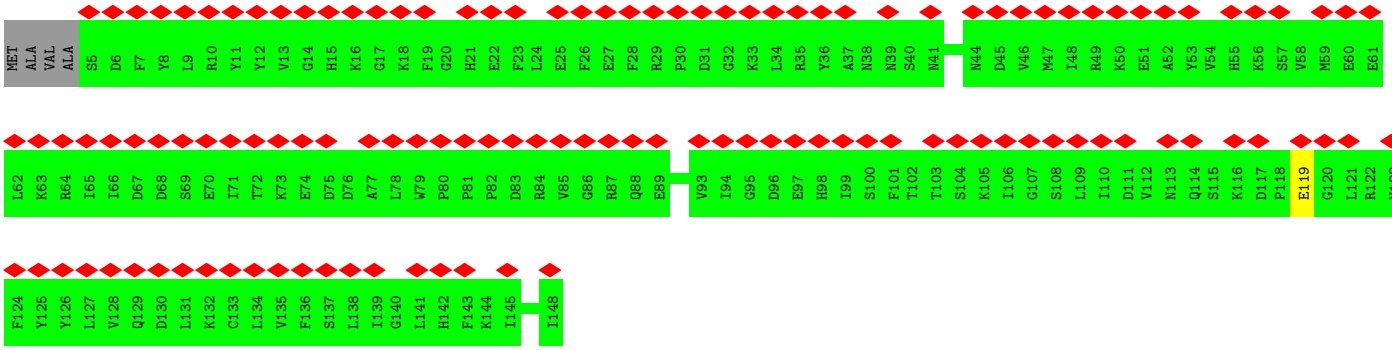




• Molecule 30: Protein mago nashi homolog 2

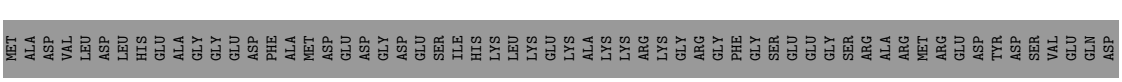
Chain v:

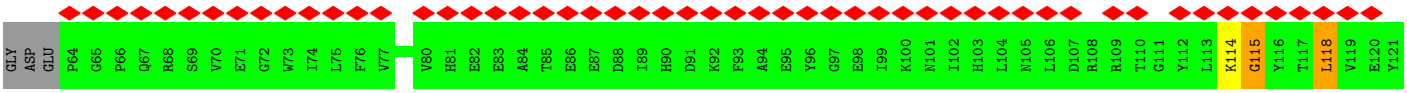


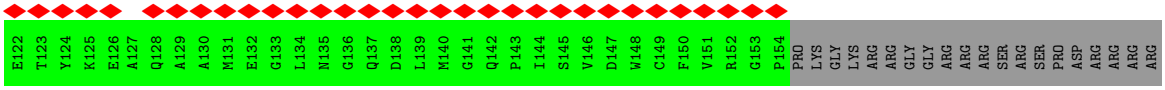


• Molecule 31: RNA-binding protein 8A

Chain w:

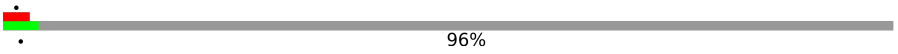


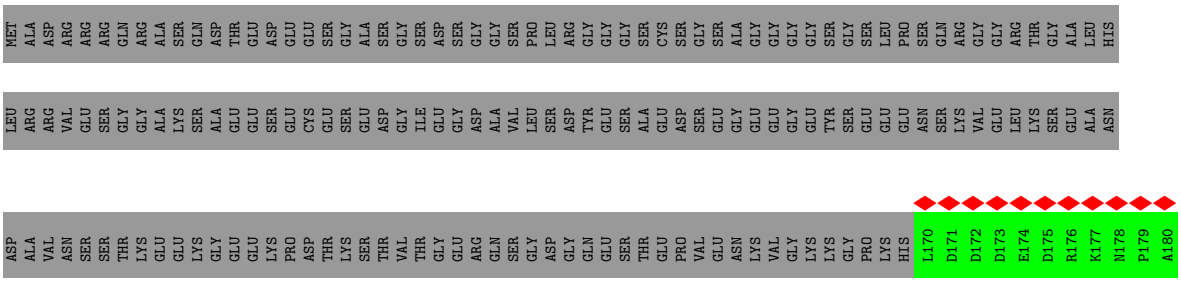




• Molecule 32: Protein CASC3

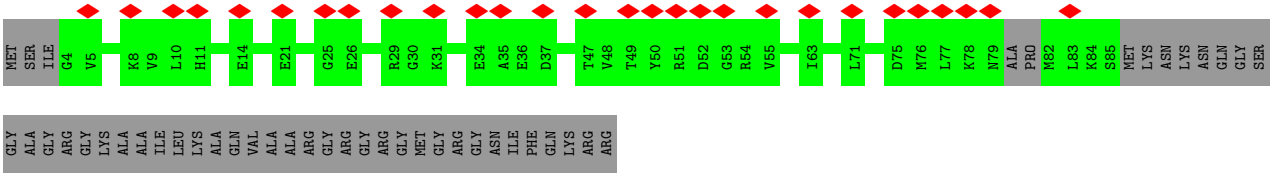
Chain x:





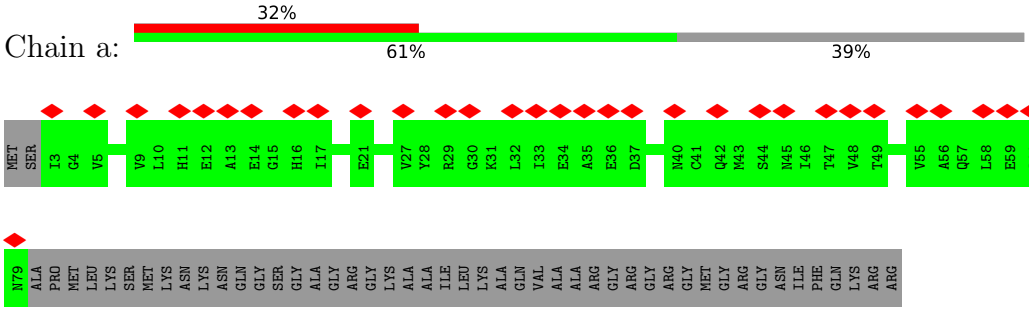
• Molecule 33: Small nuclear ribonucleoprotein Sm D3

Chain h:



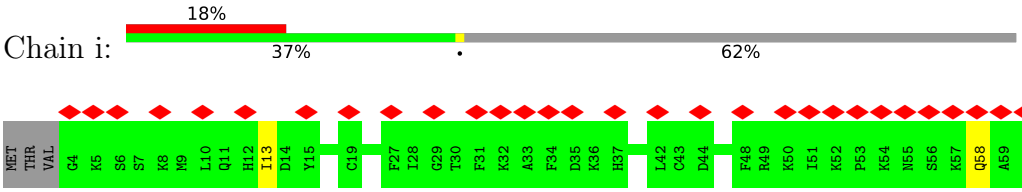
• Molecule 33: Small nuclear ribonucleoprotein Sm D3

Chain a:



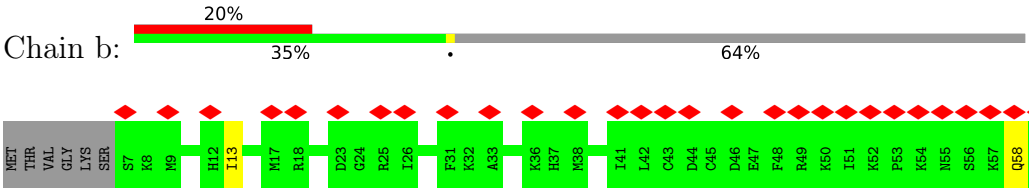
• Molecule 34: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain i:



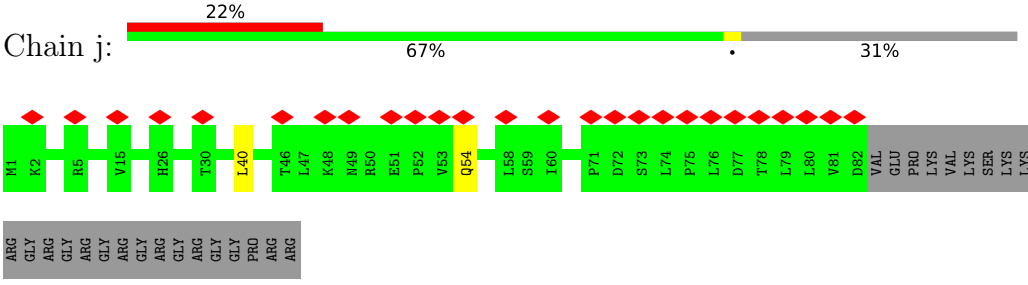
• Molecule 34: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain b:



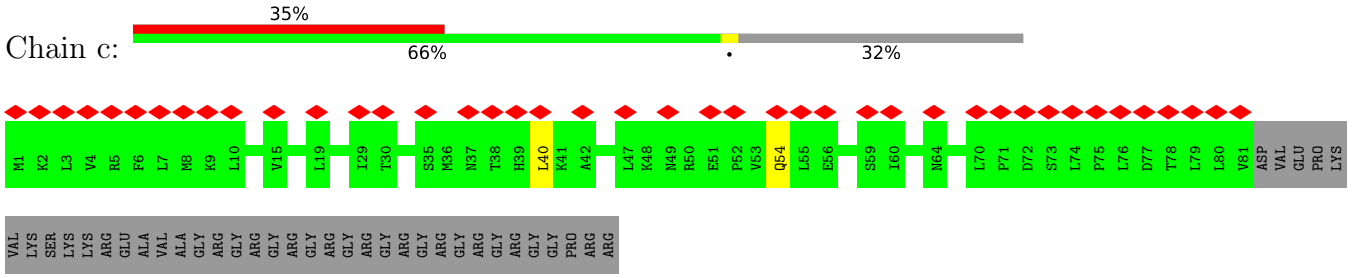
• Molecule 35: Small nuclear ribonucleoprotein Sm D1

Chain j:



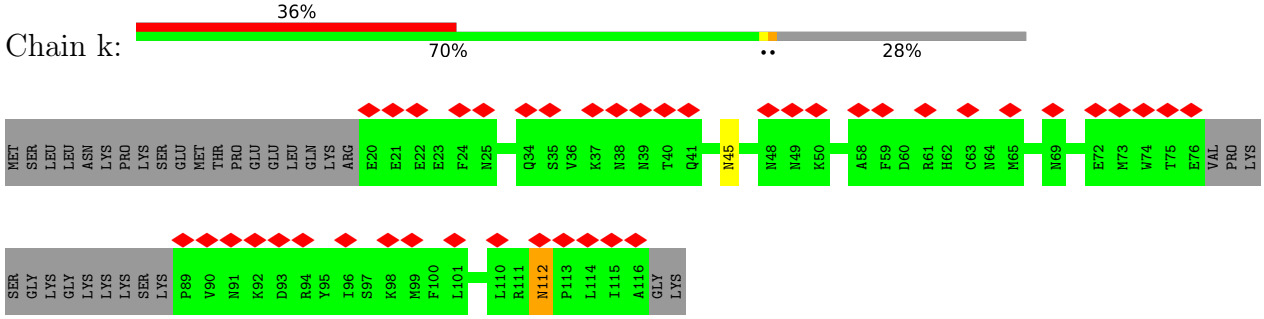
• Molecule 35: Small nuclear ribonucleoprotein Sm D1

Chain c:



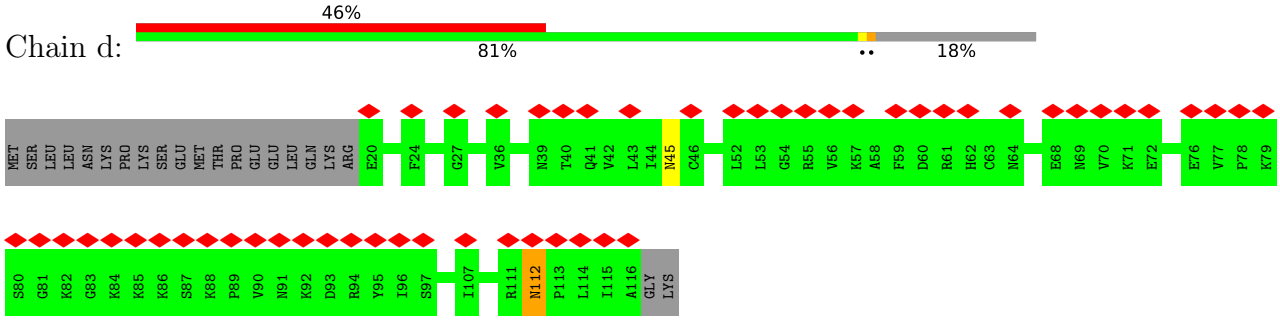
• Molecule 36: Small nuclear ribonucleoprotein Sm D2

Chain k:



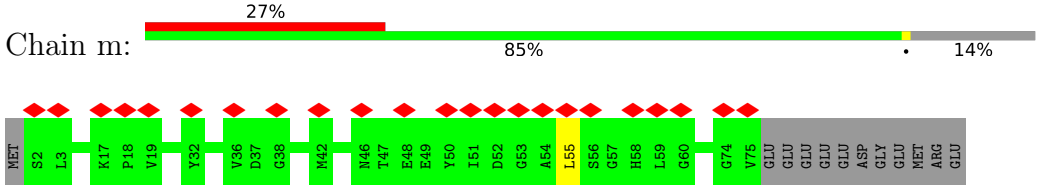
• Molecule 36: Small nuclear ribonucleoprotein Sm D2

Chain d:



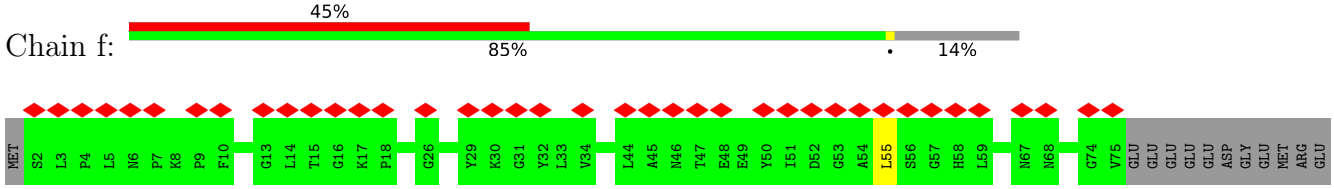
• Molecule 37: Small nuclear ribonucleoprotein F

Chain m:



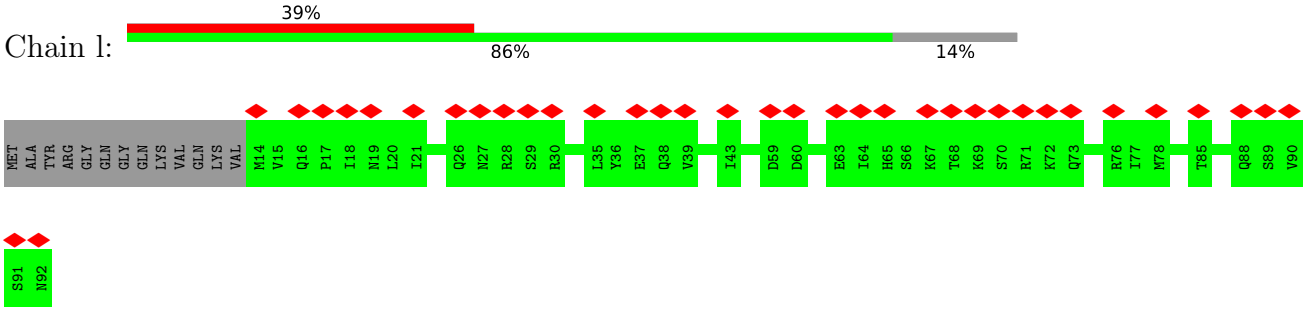
• Molecule 37: Small nuclear ribonucleoprotein F

Chain f:



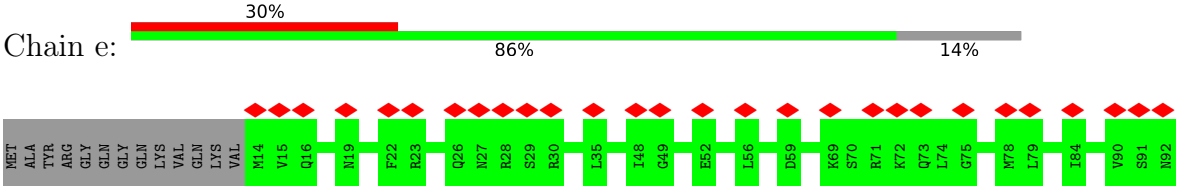
• Molecule 38: Small nuclear ribonucleoprotein E

Chain l:



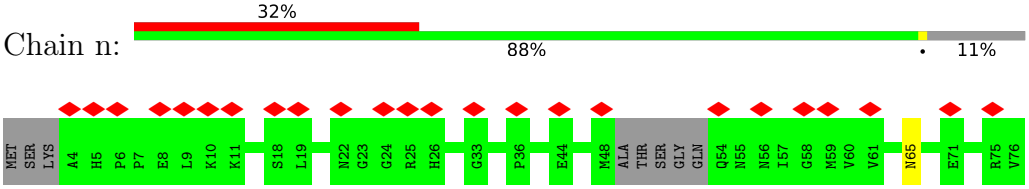
• Molecule 38: Small nuclear ribonucleoprotein E

Chain e:



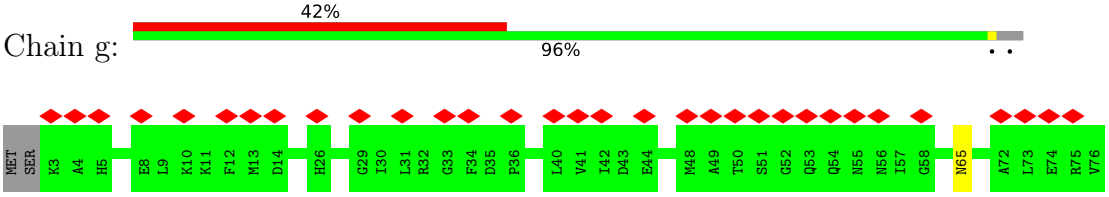
• Molecule 39: Small nuclear ribonucleoprotein G

Chain n:



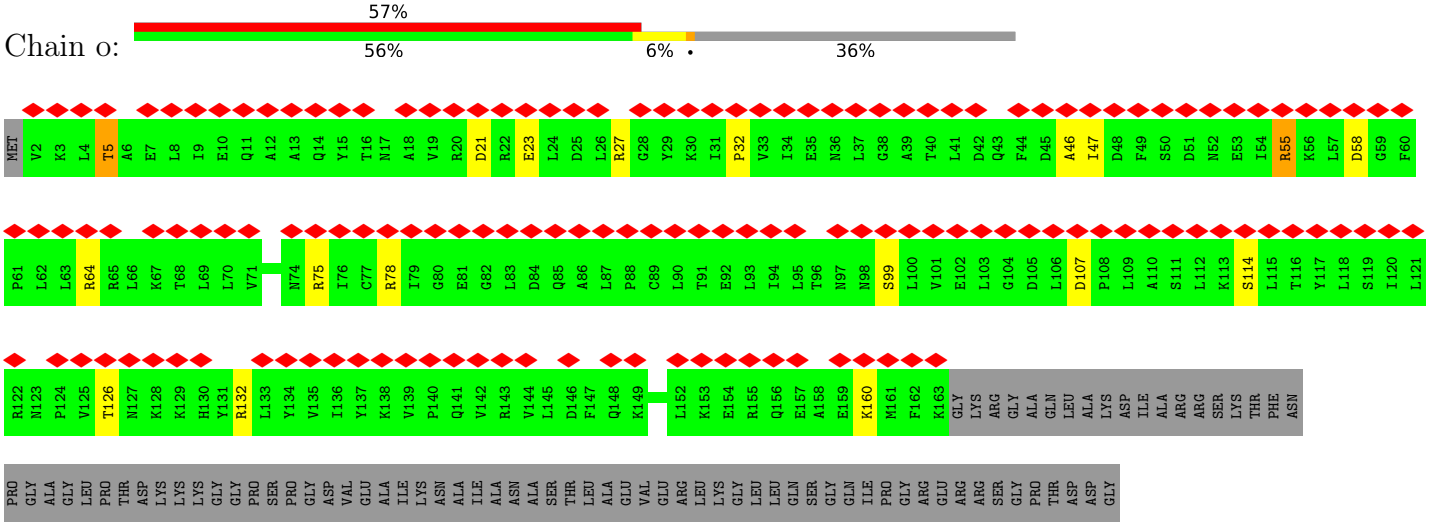
• Molecule 39: Small nuclear ribonucleoprotein G

Chain g:



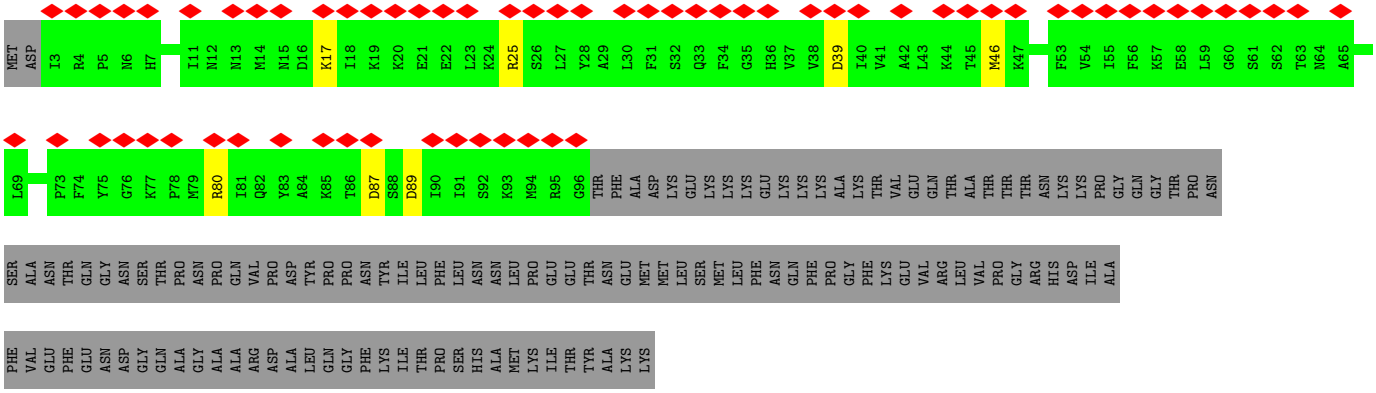
• Molecule 40: U2 small nuclear ribonucleoprotein A'

Chain o:



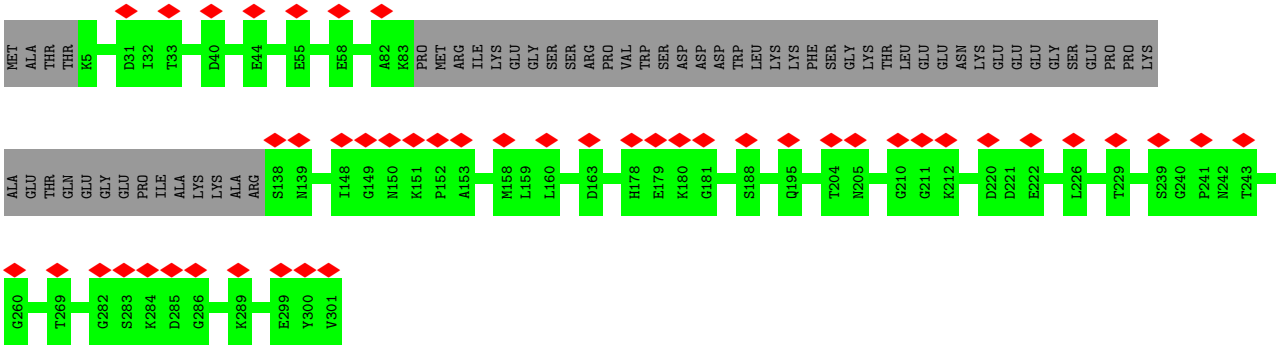
• Molecule 41: U2 small nuclear ribonucleoprotein B"

Chain p:



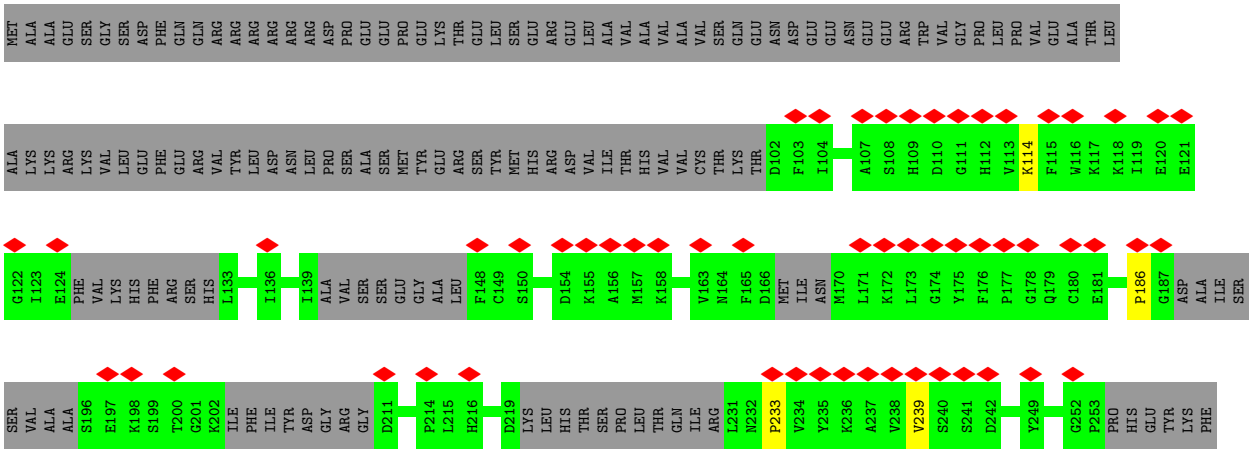
• Molecule 42: Peptidyl-prolyl cis-trans isomerase E

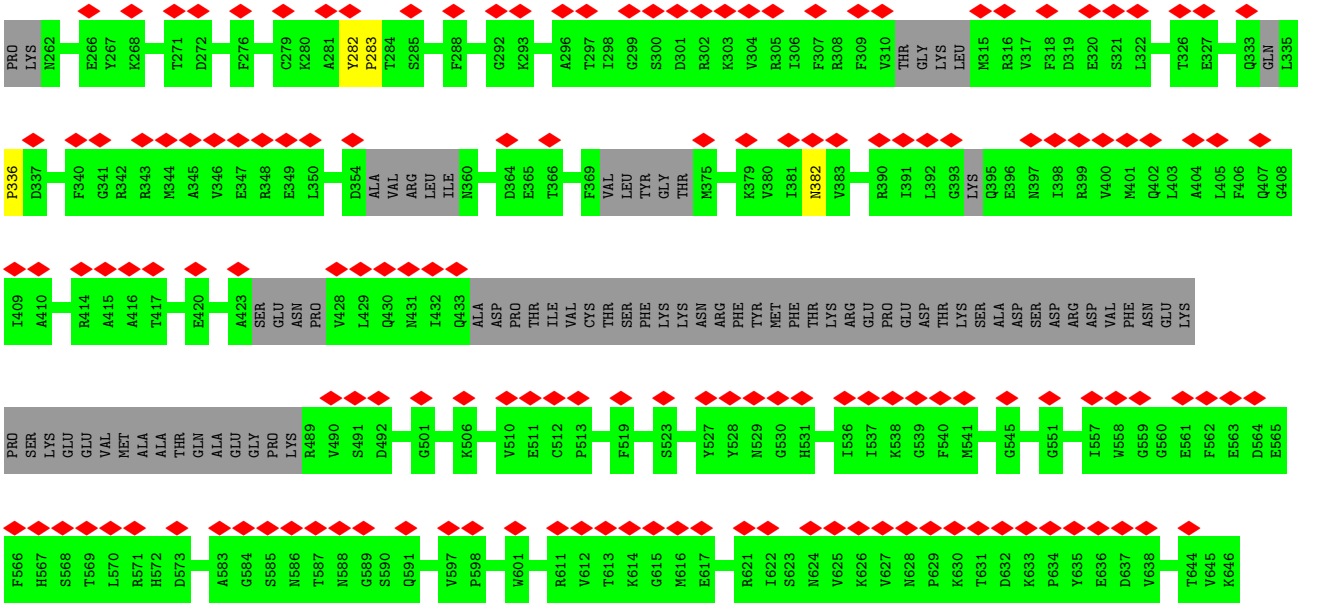
Chain 1:



• Molecule 43: Peptidylprolyl isomerase domain and WD repeat-containing protein 1

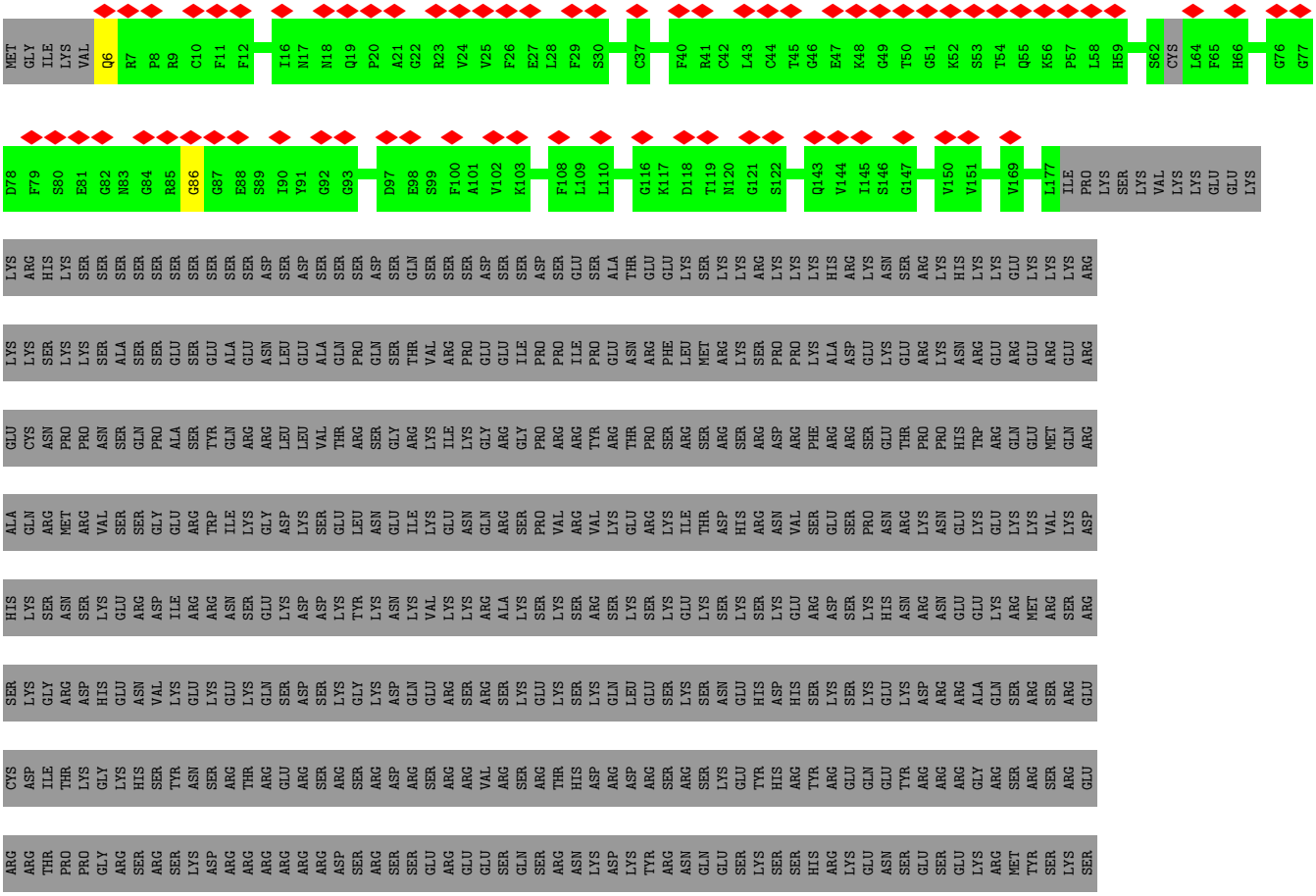
Chain 2:





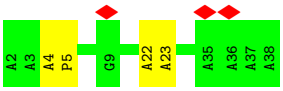
• Molecule 44: Peptidyl-prolyl cis-trans isomerase G

Chain 3:



• Molecule 45: UNKNOW

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53633	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 ($e^-/Å^2$)	50	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	0.209	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.029	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, ADP, IHP, SEP, ATP, 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	1.00	25/17966 (0.1%)	1.07	63/24251 (0.3%)
2	B	0.78	3/1970 (0.2%)	0.91	6/3060 (0.2%)
3	C	0.80	1/6946 (0.0%)	0.97	10/9436 (0.1%)
4	D	0.32	0/7628	0.56	0/9528
5	E	0.64	0/2392	0.79	0/3242
6	F	0.68	3/2323 (0.1%)	0.86	3/3619 (0.1%)
7	G	0.76	8/1820 (0.4%)	0.90	2/2819 (0.1%)
8	H	0.98	28/3283 (0.9%)	1.65	117/5096 (2.3%)
9	I	0.39	0/2724	0.56	17/3738 (0.5%)
10	J	0.63	1/3870 (0.0%)	0.75	1/5252 (0.0%)
11	K	1.32	15/981 (1.5%)	0.69	5/1317 (0.4%)
12	L	0.70	4/2914 (0.1%)	0.86	14/3929 (0.4%)
13	y	0.96	5/707 (0.7%)	0.77	6/953 (0.6%)
14	M	0.53	0/791	0.80	0/1058
15	N	0.88	1/1210 (0.1%)	1.00	3/1622 (0.2%)
16	O	0.80	2/2324 (0.1%)	0.92	5/3135 (0.2%)
17	P	0.86	1/841 (0.1%)	1.05	2/1117 (0.2%)
18	R	0.78	4/1976 (0.2%)	1.03	10/2651 (0.4%)
19	S	0.59	0/1268	0.80	1/1714 (0.1%)
20	T	1.05	1/2526 (0.0%)	1.11	4/3443 (0.1%)
21	Q	0.20	0/5279	0.40	0/6583
22	U	1.03	0/196	1.09	1/265 (0.4%)
23	V	0.55	0/3453	0.76	4/4640 (0.1%)
24	W	0.57	1/2336 (0.0%)	0.73	3/3027 (0.1%)
25	X	0.46	0/486	0.54	0/658
26	Y	0.65	2/1450 (0.1%)	0.88	9/1975 (0.5%)
27	Z	0.50	0/2528	0.99	3/3139 (0.1%)
28	q	1.07	4/929 (0.4%)	0.70	3/1260 (0.2%)
28	r	1.08	4/912 (0.4%)	0.71	3/1239 (0.2%)
28	s	1.91	4/1497 (0.3%)	0.83	4/1866 (0.2%)
28	t	1.06	2/480 (0.4%)	0.57	0/650
29	u	0.38	0/3175	0.65	0/4286

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	v	0.38	0/1225	0.60	0/1648
31	w	0.36	0/748	0.71	3/1012 (0.3%)
32	x	0.43	0/221	0.66	0/296
33	a	0.46	0/616	0.66	0/830
33	h	0.46	0/627	0.68	0/842
34	b	0.52	0/685	0.82	0/913
34	i	0.53	0/700	0.82	0/933
35	c	0.56	0/649	0.78	0/877
35	j	0.56	0/657	0.77	0/888
36	d	0.69	0/778	0.86	0/1045
36	k	0.69	0/696	0.86	0/935
37	f	0.82	0/588	0.84	0/795
37	m	0.82	0/588	0.84	0/795
38	e	0.62	0/660	0.83	0/886
38	l	0.61	0/660	0.83	0/886
39	g	0.53	0/576	0.78	0/771
39	n	0.53	0/539	0.80	0/718
40	o	0.59	0/1294	1.63	18/1754 (1.0%)
41	p	0.56	0/774	1.35	6/1035 (0.6%)
42	1	0.34	0/970	0.60	0/1209
43	2	0.54	0/1649	0.64	0/2035
44	3	0.68	0/682	0.89	3/849 (0.4%)
45	4	0.35	0/184	0.70	0/255
All	All	0.76	119/105947 (0.1%)	0.91	329/142775 (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
1	A	0	6
3	C	0	3
4	D	0	1
10	J	0	1
12	L	0	1
13	y	0	1
14	M	0	1
15	N	0	1
18	R	0	1
20	T	0	2
26	Y	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
27	Z	0	29
28	s	0	4
36	d	0	1
36	k	0	1
All	All	0	56

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	s	481[A]	VAL	N-CA	48.51	2.43	1.46
28	s	481[B]	VAL	N-CA	48.51	2.43	1.46
11	K	106	CYS	CB-SG	-23.18	1.42	1.82
13	y	36	CYS	CB-SG	-18.29	1.51	1.82
11	K	132	CYS	CB-SG	-17.41	1.52	1.82
28	q	16	CYS	CB-SG	-17.36	1.52	1.82
28	r	16	CYS	CB-SG	-17.20	1.53	1.82
28	r	114	CYS	CB-SG	-16.92	1.53	1.82
28	t	114	CYS	CB-SG	-16.72	1.53	1.82
28	q	114	CYS	CB-SG	-16.54	1.54	1.82
1	A	642	ARG	CD-NE	12.17	1.67	1.46
1	A	642	ARG	NE-CZ	11.22	1.47	1.33
28	q	47	LEU	CB-CG	9.98	1.81	1.52
7	G	-10	C	C4-C5	-9.95	1.34	1.43
28	r	47	LEU	CB-CG	9.92	1.81	1.52
11	K	163	LEU	CB-CG	9.81	1.81	1.52
12	L	761	SER	CB-OG	8.97	1.53	1.42
11	K	128	SER	CB-OG	8.36	1.53	1.42
11	K	183	SER	CB-OG	8.29	1.53	1.42
1	A	750	TRP	CE3-CZ3	-8.28	1.24	1.38
16	O	221	PRO	CA-C	-8.24	1.36	1.52
28	t	89	SER	CB-OG	8.24	1.52	1.42
28	r	89	SER	CB-OG	8.21	1.52	1.42
16	O	181	TYR	CE1-CZ	-8.18	1.27	1.38
28	q	89	SER	CB-OG	8.08	1.52	1.42
11	K	190	SER	CB-OG	8.05	1.52	1.42
11	K	187	SER	CB-OG	8.03	1.52	1.42
12	L	726	SER	CB-OG	7.95	1.52	1.42
13	y	54	SER	CB-OG	7.84	1.52	1.42
8	H	142	C	C1'-N1	7.46	1.59	1.48
8	H	77	C	C1'-N1	7.40	1.59	1.48
15	N	102	CYS	CB-SG	-7.34	1.69	1.82
1	A	406	TRP	CB-CG	-7.02	1.37	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	55	U	C1'-N1	6.97	1.59	1.48
8	H	92	U	C1'-N1	6.96	1.59	1.48
8	H	89	U	C1'-N1	6.92	1.59	1.48
8	H	54	U	C1'-N1	6.90	1.59	1.48
8	H	72	U	C1'-N1	6.90	1.59	1.48
7	G	-22	G	C1'-N9	-6.88	1.37	1.46
8	H	74	U	C1'-N1	6.88	1.59	1.48
8	H	69	U	C1'-N1	6.86	1.59	1.48
2	B	103	G	C1'-N9	-6.86	1.37	1.46
8	H	182	U	C1'-N1	6.83	1.59	1.48
8	H	60	U	C1'-N1	6.80	1.58	1.48
8	H	150	U	C1'-N1	6.80	1.58	1.48
1	A	1668	TRP	CB-CG	-6.80	1.38	1.50
8	H	91	U	C1'-N1	6.79	1.58	1.48
17	P	227	TYR	CG-CD2	-6.74	1.30	1.39
8	H	58	U	C1'-N1	6.73	1.58	1.48
1	A	476	PHE	CG-CD2	6.61	1.48	1.38
1	A	750	TRP	CE2-CZ2	-6.59	1.28	1.39
7	G	-23	G	C1'-N9	-6.53	1.37	1.46
1	A	927	TRP	CB-CG	-6.48	1.38	1.50
12	L	724	TYR	CB-CG	-6.48	1.42	1.51
10	J	346	TRP	CB-CG	-6.44	1.38	1.50
8	H	97	G	C1'-N9	-6.42	1.37	1.46
8	H	151	C	C1'-N1	6.41	1.58	1.48
8	H	184	C	C1'-N1	6.35	1.58	1.48
11	K	138	TYR	CB-CG	-6.34	1.42	1.51
8	H	73	C	C1'-N1	6.33	1.58	1.48
8	H	141	C	C1'-N1	6.33	1.58	1.48
11	K	93	SER	CB-OG	6.32	1.50	1.42
8	H	148	C	C1'-N1	6.29	1.58	1.48
8	H	84	C	C1'-N1	6.27	1.58	1.48
1	A	592	TYR	CB-CG	-6.25	1.42	1.51
11	K	43	TYR	CB-CG	-6.25	1.42	1.51
8	H	71	C	C1'-N1	6.24	1.58	1.48
8	H	78	C	C1'-N1	6.24	1.58	1.48
8	H	70	C	C1'-N1	6.23	1.58	1.48
7	G	-19	A	C1'-N9	-6.21	1.38	1.46
7	G	-20	A	C1'-N9	-6.20	1.38	1.46
2	B	24	G	O3'-P	-6.18	1.53	1.61
1	A	719	CYS	CB-SG	6.15	1.92	1.82
1	A	717	TRP	CB-CG	-6.15	1.39	1.50
1	A	1577	PHE	CG-CD2	-6.02	1.29	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	902	TYR	CG-CD2	-5.95	1.31	1.39
1	A	1294	LYS	CE-NZ	5.93	1.63	1.49
7	G	-21	A	C1'-N9	-5.84	1.38	1.46
1	A	1214	TRP	CB-CG	-5.82	1.39	1.50
6	F	28	A	N1-C2	5.80	1.39	1.34
20	T	218	TRP	CB-CG	-5.72	1.40	1.50
11	K	40	THR	CB-OG1	5.63	1.54	1.43
6	F	72	G	O3'-P	-5.58	1.54	1.61
1	A	592	TYR	CG-CD1	-5.56	1.31	1.39
8	H	36	G	O3'-P	-5.48	1.54	1.61
28	s	481[A]	VAL	CA-C	5.48	1.67	1.52
28	s	481[B]	VAL	CA-C	5.48	1.67	1.52
1	A	1386	TRP	CB-CG	-5.46	1.40	1.50
8	H	37	U	O3'-P	-5.46	1.54	1.61
7	G	4	A	C1'-N9	-5.44	1.39	1.46
12	L	96	CYS	CB-SG	-5.41	1.73	1.81
24	W	95	PRO	N-CD	5.41	1.55	1.47
1	A	212	PRO	N-CA	-5.39	1.38	1.47
1	A	120	TYR	CG-CD1	5.39	1.46	1.39
13	y	38	GLU	CB-CG	-5.35	1.42	1.52
2	B	56	C	O3'-P	-5.35	1.54	1.61
13	y	57	VAL	CB-CG2	-5.33	1.41	1.52
1	A	94	TYR	CB-CG	-5.30	1.43	1.51
1	A	1291	CYS	CB-SG	5.29	1.91	1.82
13	y	22	GLU	CB-CG	-5.25	1.42	1.52
8	H	27	U	O3'-P	-5.24	1.54	1.61
11	K	30	GLU	CB-CG	-5.24	1.42	1.52
6	F	28	A	C6-N6	5.23	1.38	1.33
1	A	140	TYR	CG-CD2	-5.18	1.32	1.39
11	K	119	VAL	CB-CG2	-5.18	1.42	1.52
8	H	110	A	C1'-N9	-5.17	1.39	1.46
26	Y	133	PRO	N-CD	5.17	1.55	1.47
7	G	136	U	C1'-N1	5.15	1.56	1.48
11	K	186	VAL	CA-CB	-5.15	1.44	1.54
11	K	137	VAL	CB-CG2	-5.14	1.42	1.52
18	R	226	PRO	N-CD	5.13	1.55	1.47
26	Y	17	PRO	N-CD	5.12	1.55	1.47
18	R	223	PRO	N-CD	5.11	1.55	1.47
18	R	222	PRO	N-CD	5.08	1.54	1.47
1	A	225	TYR	CB-CG	-5.07	1.44	1.51
1	A	351	TYR	CB-CG	-5.07	1.44	1.51
18	R	225	PRO	N-CD	5.06	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	145	PHE	CB-CG	-5.05	1.42	1.51
1	A	1758	PRO	N-CD	5.05	1.54	1.47

All (329) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	s	481[A]	VAL	N-CA-C	-15.66	68.71	111.00
28	s	481[B]	VAL	N-CA-C	-15.66	68.71	111.00
40	o	55	ARG	NE-CZ-NH1	15.07	127.83	120.30
1	A	642	ARG	NE-CZ-NH2	-14.47	113.06	120.30
40	o	55	ARG	CD-NE-CZ	13.79	142.90	123.60
8	H	27	U	P-O3'-C3'	-12.86	104.26	119.70
8	H	167	U	C5-C4-O4	11.87	133.02	125.90
12	L	158	ARG	NE-CZ-NH1	11.62	126.11	120.30
40	o	55	ARG	NE-CZ-NH2	-11.37	114.61	120.30
40	o	75	ARG	NE-CZ-NH1	-11.30	114.65	120.30
16	O	221	PRO	CA-C-O	10.98	146.55	120.20
26	Y	13	PRO	N-CA-C	10.44	139.25	112.10
1	A	1370	ARG	NE-CZ-NH2	10.32	125.46	120.30
8	H	164	C	N1-C2-O2	-10.08	112.85	118.90
1	A	1370	ARG	NE-CZ-NH1	-9.22	115.69	120.30
12	L	158	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	A	781	ARG	NE-CZ-NH1	9.12	124.86	120.30
26	Y	14	ASP	N-CA-CB	-9.10	94.22	110.60
41	p	80	ARG	CD-NE-CZ	8.96	136.14	123.60
41	p	25	ARG	NE-CZ-NH1	8.94	124.77	120.30
8	H	162	U	N3-C2-O2	-8.86	116.00	122.20
11	K	90	PRO	CA-CB-CG	8.65	121.24	104.80
1	A	1245	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	A	1291	CYS	CB-CA-C	8.30	127.00	110.40
8	H	164	C	C5'-C4'-O4'	-8.28	99.17	109.10
8	H	169	C	P-O3'-C3'	8.19	129.53	119.70
26	Y	204	LYS	O-C-N	-8.13	109.69	122.70
13	y	191	VAL	O-C-N	-8.11	109.72	122.70
1	A	404	LEU	CB-CG-CD1	8.09	124.75	111.00
8	H	34	U	O5'-P-OP1	-8.07	98.43	105.70
8	H	166	G	O4'-C1'-N9	8.01	114.61	108.20
27	Z	555	GLY	O-C-N	7.97	135.45	122.70
8	H	167	U	N3-C4-O4	-7.94	113.84	119.40
1	A	1667	ARG	NE-CZ-NH2	-7.88	116.36	120.30
16	O	35	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	552	ARG	NE-CZ-NH1	7.70	124.15	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1195	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	A	1310	ARG	NE-CZ-NH2	-7.66	116.47	120.30
40	o	107	ASP	CB-CG-OD1	7.65	125.19	118.30
1	A	778	ARG	NE-CZ-NH1	7.63	124.11	120.30
8	H	34	U	O5'-P-OP2	7.63	119.85	110.70
3	C	939	ARG	NE-CZ-NH1	7.57	124.09	120.30
8	H	35	A	O5'-P-OP2	-7.57	98.89	105.70
8	H	164	C	P-O3'-C3'	7.53	128.73	119.70
1	A	642	ARG	NH1-CZ-NH2	7.50	127.65	119.40
40	o	27	ARG	NE-CZ-NH2	-7.48	116.56	120.30
8	H	167	U	N1-C2-O2	7.46	128.02	122.80
1	A	153	ARG	NE-CZ-NH2	-7.40	116.60	120.30
8	H	164	C	N3-C2-O2	7.37	127.06	121.90
2	B	20	G	N9-C1'-C2'	7.31	123.50	114.00
8	H	77	C	OP2-P-O3'	7.29	121.24	105.20
8	H	89	U	OP2-P-O3'	7.25	121.14	105.20
8	H	70	C	OP2-P-O3'	7.24	121.13	105.20
8	H	114	A	OP2-P-O3'	7.24	121.13	105.20
8	H	92	U	OP2-P-O3'	7.24	121.13	105.20
8	H	180	G	OP2-P-O3'	7.24	121.12	105.20
8	H	81	G	OP2-P-O3'	7.23	121.11	105.20
8	H	141	C	OP2-P-O3'	7.23	121.10	105.20
8	H	71	C	OP2-P-O3'	7.23	121.10	105.20
8	H	84	C	OP2-P-O3'	7.23	121.10	105.20
8	H	59	A	OP2-P-O3'	7.22	121.09	105.20
8	H	150	U	OP2-P-O3'	7.22	121.09	105.20
8	H	58	U	OP2-P-O3'	7.22	121.08	105.20
8	H	91	U	OP2-P-O3'	7.21	121.07	105.20
8	H	57	A	OP2-P-O3'	7.21	121.07	105.20
8	H	113	G	OP2-P-O3'	7.21	121.06	105.20
8	H	149	A	OP2-P-O3'	7.21	121.06	105.20
8	H	54	U	OP2-P-O3'	7.21	121.06	105.20
8	H	83	A	OP2-P-O3'	7.21	121.06	105.20
8	H	148	C	OP2-P-O3'	7.21	121.06	105.20
8	H	183	G	OP2-P-O3'	7.20	121.05	105.20
8	H	79	G	OP2-P-O3'	7.20	121.05	105.20
8	H	68	G	OP2-P-O3'	7.20	121.04	105.20
8	H	73	C	OP2-P-O3'	7.20	121.04	105.20
8	H	88	A	OP2-P-O3'	7.20	121.03	105.20
8	H	55	U	OP2-P-O3'	7.19	121.02	105.20
8	H	82	G	OP2-P-O3'	7.19	121.02	105.20
8	H	80	A	OP2-P-O3'	7.19	121.02	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	3	6	GLN	CA-C-O	7.19	135.19	120.10
3	C	144	CYS	N-CA-CB	7.18	123.53	110.60
8	H	69	U	OP2-P-O3'	7.18	121.01	105.20
8	H	181	G	OP2-P-O3'	7.18	121.00	105.20
8	H	182	U	OP2-P-O3'	7.18	121.00	105.20
8	H	56	A	OP2-P-O3'	7.18	121.00	105.20
8	H	72	U	OP2-P-O3'	7.18	120.99	105.20
8	H	74	U	OP2-P-O3'	7.18	120.99	105.20
8	H	93	A	OP2-P-O3'	7.18	120.99	105.20
8	H	78	C	OP2-P-O3'	7.17	120.98	105.20
8	H	90	A	OP2-P-O3'	7.17	120.98	105.20
12	L	83	ARG	NE-CZ-NH2	7.16	123.88	120.30
18	R	180	THR	C-N-CD	-7.15	104.87	120.60
1	A	611	LEU	CB-CG-CD1	-7.14	98.87	111.00
8	H	168	A	P-O5'-C5'	-7.12	109.51	120.90
8	H	24	A	O5'-P-OP1	7.09	119.21	110.70
1	A	1544	ARG	NE-CZ-NH1	7.02	123.81	120.30
8	H	167	U	N3-C2-O2	-7.02	117.29	122.20
1	A	565	ARG	NE-CZ-NH2	-6.87	116.87	120.30
8	H	82	G	O3'-P-O5'	-6.83	91.03	104.00
8	H	84	C	O3'-P-O5'	-6.82	91.04	104.00
8	H	88	A	O3'-P-O5'	-6.82	91.05	104.00
8	H	56	A	O3'-P-O5'	-6.81	91.06	104.00
8	H	91	U	O3'-P-O5'	-6.81	91.06	104.00
8	H	73	C	O3'-P-O5'	-6.80	91.07	104.00
8	H	180	G	O3'-P-O5'	-6.80	91.07	104.00
8	H	183	G	O3'-P-O5'	-6.80	91.08	104.00
8	H	181	G	O3'-P-O5'	-6.80	91.08	104.00
8	H	72	U	O3'-P-O5'	-6.80	91.08	104.00
8	H	93	A	O3'-P-O5'	-6.80	91.08	104.00
8	H	78	C	O3'-P-O5'	-6.80	91.09	104.00
8	H	182	U	O3'-P-O5'	-6.79	91.09	104.00
8	H	70	C	O3'-P-O5'	-6.79	91.10	104.00
8	H	150	U	O3'-P-O5'	-6.79	91.10	104.00
8	H	141	C	O3'-P-O5'	-6.78	91.11	104.00
8	H	59	A	O3'-P-O5'	-6.78	91.12	104.00
8	H	79	G	O3'-P-O5'	-6.78	91.11	104.00
27	Z	555	GLY	C-N-CA	6.78	138.65	121.70
8	H	55	U	O3'-P-O5'	-6.77	91.13	104.00
8	H	81	G	O3'-P-O5'	-6.77	91.13	104.00
8	H	80	A	O3'-P-O5'	-6.77	91.14	104.00
8	H	54	U	O3'-P-O5'	-6.77	91.14	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	92	U	O3'-P-O5'	-6.77	91.14	104.00
2	B	104	C	C2'-C3'-O3'	-6.77	94.61	109.50
8	H	89	U	O3'-P-O5'	-6.77	91.14	104.00
8	H	149	A	O3'-P-O5'	-6.77	91.14	104.00
40	o	23	GLU	OE1-CD-OE2	-6.77	115.18	123.30
8	H	90	A	O3'-P-O5'	-6.76	91.15	104.00
8	H	83	A	O3'-P-O5'	-6.76	91.16	104.00
8	H	68	G	O3'-P-O5'	-6.75	91.17	104.00
8	H	113	G	O3'-P-O5'	-6.75	91.17	104.00
8	H	69	U	O3'-P-O5'	-6.75	91.17	104.00
8	H	57	A	O3'-P-O5'	-6.75	91.17	104.00
8	H	71	C	O3'-P-O5'	-6.75	91.18	104.00
8	H	155	C	P-O3'-C3'	6.75	127.80	119.70
8	H	114	A	O3'-P-O5'	-6.75	91.18	104.00
8	H	148	C	O3'-P-O5'	-6.75	91.18	104.00
8	H	74	U	O3'-P-O5'	-6.74	91.20	104.00
1	A	1667	ARG	NE-CZ-NH1	6.73	123.66	120.30
8	H	77	C	O3'-P-O5'	-6.72	91.22	104.00
2	B	26	A	O5'-P-OP2	6.72	118.76	110.70
41	p	89	ASP	CB-CG-OD1	6.71	124.34	118.30
8	H	58	U	O3'-P-O5'	-6.69	91.29	104.00
17	P	215	LEU	CB-CG-CD1	-6.63	99.73	111.00
28	q	46	PRO	N-CA-CB	6.62	111.24	103.30
3	C	420	CYS	CA-CB-SG	-6.62	102.09	114.00
28	s	481[A]	VAL	CA-C-N	-6.60	102.68	117.20
28	s	481[B]	VAL	CA-C-N	-6.60	102.68	117.20
1	A	1630	LEU	CB-CG-CD2	-6.60	99.79	111.00
2	B	12	U	N1-C1'-C2'	-6.58	104.76	112.00
24	W	279	LYS	N-CA-C	-6.58	93.25	111.00
8	H	24	A	O5'-P-OP2	-6.56	99.80	105.70
11	K	90	PRO	N-CA-CB	6.56	111.17	103.30
23	V	320	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	535	ARG	NE-CZ-NH1	-6.50	117.05	120.30
8	H	166	G	C8-N9-C4	-6.49	103.80	106.40
28	r	46	PRO	N-CA-CB	6.49	111.09	103.30
17	P	215	LEU	CB-CG-CD2	6.48	122.02	111.00
1	A	598	LEU	CB-CG-CD2	-6.47	100.00	111.00
1	A	1330	MET	CA-CB-CG	-6.44	102.35	113.30
28	q	60	PRO	N-CA-CB	6.44	111.03	103.30
31	w	114	LYS	N-CA-C	-6.43	93.65	111.00
15	N	101	CYS	CB-CA-C	-6.42	97.57	110.40
10	J	195	LEU	CB-CG-CD2	-6.40	100.13	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	3	86	GLY	CA-C-O	6.36	132.05	120.60
3	C	921	LEU	CB-CG-CD1	6.34	121.77	111.00
11	K	78	PRO	N-CA-CB	6.33	110.89	103.30
9	I	475	PRO	N-CA-CB	6.32	110.89	103.30
40	o	5	THR	N-CA-CB	-6.31	98.32	110.30
9	I	589	PRO	N-CA-CB	6.30	110.86	103.30
19	S	152	ARG	NE-CZ-NH2	-6.29	117.15	120.30
31	w	118	LEU	CA-CB-CG	6.27	129.72	115.30
18	R	205	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	1190	CYS	CA-CB-SG	-6.26	102.72	114.00
8	H	165	A	O4'-C1'-N9	-6.26	103.19	108.20
1	A	153	ARG	NE-CZ-NH1	6.26	123.43	120.30
16	O	181	TYR	CG-CD2-CE2	-6.24	116.30	121.30
20	T	282	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	506	LEU	CB-CG-CD1	-6.23	100.40	111.00
11	K	107	VAL	CA-CB-CG1	6.22	120.23	110.90
8	H	166	G	N9-C4-C5	6.21	107.89	105.40
24	W	108	ARG	NE-CZ-NH2	-6.20	117.20	120.30
20	T	220	VAL	CB-CA-C	-6.18	99.66	111.40
9	I	551	PRO	N-CA-CB	6.17	110.71	103.30
9	I	162	PRO	N-CA-CB	6.17	110.70	103.30
1	A	476	PHE	CB-CG-CD1	6.16	125.11	120.80
1	A	1544	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	1322	LEU	CB-CG-CD2	-6.14	100.56	111.00
1	A	976	MET	CG-SD-CE	-6.14	90.38	100.20
8	H	166	G	N3-C4-C5	-6.12	125.54	128.60
9	I	232	PRO	N-CA-CB	6.12	110.64	103.30
44	3	6	GLN	O-C-N	-6.12	112.91	122.70
1	A	719	CYS	CA-CB-SG	6.10	124.98	114.00
26	Y	25	LEU	C-N-CD	6.10	141.21	128.40
12	L	546	PRO	N-CA-CB	6.08	110.60	103.30
1	A	1285	LEU	CA-CB-CG	-6.08	101.31	115.30
9	I	788	PRO	N-CA-CB	6.08	110.60	103.30
9	I	177	PRO	N-CA-CB	6.07	110.58	103.30
12	L	558	PRO	N-CA-CB	6.06	110.57	103.30
40	o	132	ARG	CD-NE-CZ	6.04	132.05	123.60
1	A	1626	CYS	CA-CB-SG	6.02	124.83	114.00
18	R	222	PRO	C-N-CD	6.01	141.03	128.40
9	I	394	PRO	N-CA-CB	6.00	110.50	103.30
8	H	162	U	N1-C2-O2	6.00	127.00	122.80
23	V	509	LEU	CA-CB-CG	5.98	129.06	115.30
9	I	160	PRO	N-CA-CB	5.97	110.46	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	816	PRO	N-CA-CB	5.97	110.46	103.30
40	o	21	ASP	CB-CG-OD1	5.97	123.67	118.30
41	p	25	ARG	CD-NE-CZ	5.96	131.94	123.60
8	H	32	U	C5'-C4'-C3'	-5.94	106.49	116.00
8	H	168	A	C5'-C4'-C3'	-5.91	106.55	116.00
12	L	563	PRO	N-CA-CB	5.91	110.39	103.30
26	Y	71	LEU	C-N-CD	5.90	140.79	128.40
9	I	387	PRO	N-CA-CB	5.90	110.38	103.30
1	A	1245	ARG	NE-CZ-NH2	-5.89	117.36	120.30
9	I	342	PRO	N-CA-CB	5.86	110.34	103.30
8	H	164	C	C5-C4-N4	-5.84	116.11	120.20
12	L	564	PRO	N-CA-CB	5.84	110.31	103.30
40	o	27	ARG	CB-CA-C	-5.84	98.71	110.40
6	F	28	A	C4-C5-C6	5.84	119.92	117.00
26	Y	20	ILE	C-N-CD	5.83	140.64	128.40
3	C	148	CYS	CB-CA-C	5.82	122.04	110.40
28	q	19	PRO	N-CA-CB	5.82	110.28	103.30
40	o	64	ARG	NE-CZ-NH1	5.82	123.21	120.30
8	H	172	C	P-O3'-C3'	5.81	126.67	119.70
1	A	1448	LEU	CB-CG-CD2	-5.79	101.15	111.00
12	L	620	PRO	N-CA-CB	5.78	110.24	103.30
27	Z	611	TYR	C-N-CA	5.78	136.15	121.70
28	r	19	PRO	N-CA-CB	5.77	110.23	103.30
12	L	548	PRO	N-CA-CB	5.77	110.22	103.30
9	I	518	PRO	N-CA-CB	5.76	110.21	103.30
26	Y	16	ASP	C-N-CD	5.76	140.49	128.40
18	R	225	PRO	C-N-CD	5.75	140.47	128.40
1	A	1757	GLU	C-N-CD	5.74	140.46	128.40
8	H	167	U	O3'-P-O5'	-5.74	93.10	104.00
12	L	594	PRO	N-CA-CB	5.74	110.18	103.30
13	y	40	PRO	N-CA-CB	5.74	110.18	103.30
18	R	221	GLY	C-N-CD	5.73	140.43	128.40
1	A	565	ARG	NE-CZ-NH1	5.72	123.16	120.30
8	H	156	U	P-O3'-C3'	-5.72	112.84	119.70
9	I	588	PRO	N-CA-CB	5.70	110.14	103.30
16	O	48	CYS	CA-CB-SG	5.70	124.26	114.00
40	o	75	ARG	NH1-CZ-NH2	5.68	125.65	119.40
1	A	845	ARG	NE-CZ-NH2	5.64	123.12	120.30
40	o	78	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	332	TYR	N-CA-C	-5.62	95.83	111.00
11	K	93	SER	N-CA-CB	-5.62	102.08	110.50
7	G	-10	C	C2-N3-C4	5.60	122.70	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	65	G	P-O5'-C5'	-5.59	111.95	120.90
1	A	1190	CYS	CB-CA-C	5.58	121.56	110.40
1	A	420	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	923	ASP	CB-CG-OD1	5.57	123.31	118.30
40	o	58	ASP	N-CA-CB	-5.56	100.59	110.60
24	W	94	GLY	C-N-CD	5.56	140.08	128.40
8	H	166	G	C6-N1-C2	-5.56	121.77	125.10
6	F	50	A	C4'-C3'-C2'	-5.55	97.05	102.60
9	I	463	PRO	N-CA-CB	5.54	109.94	103.30
1	A	1330	MET	CG-SD-CE	-5.52	91.37	100.20
12	L	774	VAL	CA-CB-CG2	5.51	119.16	110.90
1	A	251	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	1594	CYS	CA-CB-SG	5.50	123.89	114.00
9	I	761	PRO	N-CA-CB	5.50	109.90	103.30
26	Y	132	ASN	C-N-CD	5.50	139.94	128.40
1	A	656	LEU	CB-CG-CD1	-5.49	101.67	111.00
13	y	63	ALA	N-CA-CB	-5.48	102.43	110.10
9	I	625	PRO	N-CA-CB	5.46	109.85	103.30
15	N	104	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	118	VAL	CB-CA-C	-5.45	101.05	111.40
3	C	146	VAL	CA-CB-CG2	-5.44	102.74	110.90
28	r	60	PRO	N-CA-CB	5.44	109.83	103.30
3	C	91	GLU	C-N-CD	-5.41	108.71	120.60
1	A	535	ARG	NE-CZ-NH2	5.40	123.00	120.30
7	G	-4	A	O5'-P-OP1	-5.40	100.84	105.70
22	U	19	VAL	CB-CA-C	-5.39	101.15	111.40
18	R	287	LEU	CB-CG-CD2	5.39	120.17	111.00
15	N	102	CYS	CB-CA-C	-5.38	99.63	110.40
8	H	157	G	O4'-C1'-N9	-5.37	103.91	108.20
1	A	712	HIS	CB-CA-C	-5.35	99.70	110.40
8	H	106	G	O5'-P-OP1	5.35	117.12	110.70
23	V	514	PHE	CB-CG-CD2	-5.35	117.05	120.80
12	L	144	MET	N-CA-C	-5.35	96.56	111.00
40	o	47	ILE	N-CA-CB	5.34	123.07	110.80
20	T	308	ARG	NE-CZ-NH2	-5.33	117.63	120.30
18	R	178	ARG	NE-CZ-NH2	-5.33	117.64	120.30
8	H	156	U	OP2-P-O3'	5.33	116.92	105.20
26	Y	21	PRO	CA-N-CD	-5.32	104.05	111.50
8	H	170	C	N3-C4-C5	-5.31	119.78	121.90
1	A	1161	LEU	CB-CG-CD1	-5.30	101.98	111.00
1	A	656	LEU	CA-CB-CG	-5.29	103.13	115.30
1	A	92	LEU	CB-CG-CD1	-5.28	102.02	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	314	ILE	CA-CB-CG1	-5.28	100.97	111.00
2	B	37	G	O5'-P-OP2	-5.28	100.95	105.70
3	C	921	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	A	682	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	656	LEU	CB-CG-CD2	5.24	119.90	111.00
41	p	39	ASP	CB-CG-OD2	-5.24	113.59	118.30
31	w	115	GLY	N-CA-C	5.23	126.17	113.10
1	A	880	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	799	PRO	N-CA-C	-5.19	98.61	112.10
1	A	878	LEU	CB-CG-CD1	-5.18	102.19	111.00
18	R	267	ARG	NE-CZ-NH2	-5.17	117.71	120.30
8	H	160	A	P-O5'-C5'	-5.17	112.63	120.90
16	O	24	CYS	CA-CB-SG	5.17	123.30	114.00
1	A	647	LEU	CB-CG-CD1	-5.16	102.23	111.00
23	V	467	LEU	CB-CA-C	-5.16	100.40	110.20
3	C	776	GLU	N-CA-C	5.16	124.93	111.00
41	p	39	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	330	THR	CA-CB-CG2	-5.14	105.20	112.40
8	H	160	A	C4'-C3'-C2'	-5.13	97.47	102.60
8	H	157	G	P-O5'-C5'	-5.12	112.70	120.90
8	H	170	C	O4'-C1'-C2'	-5.12	100.68	105.80
1	A	638	LEU	CA-CB-CG	-5.12	103.52	115.30
2	B	20	G	O4'-C1'-N9	5.11	112.29	108.20
8	H	162	U	C2-N3-C4	-5.11	123.93	127.00
1	A	784	LEU	CA-CB-CG	-5.11	103.56	115.30
3	C	220	ARG	NE-CZ-NH2	-5.09	117.75	120.30
18	R	178	ARG	NE-CZ-NH1	5.09	122.85	120.30
12	L	189	ARG	NE-CZ-NH1	5.09	122.84	120.30
8	H	156	U	C4'-C3'-C2'	5.08	107.68	102.60
12	L	83	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	677	VAL	CB-CA-C	-5.08	101.75	111.40
13	y	165	PRO	N-CA-CB	5.07	109.39	103.30
13	y	164	PRO	N-CA-CB	5.06	109.37	103.30
13	y	166	PRO	N-CA-CB	5.06	109.37	103.30
20	T	233	LEU	CB-CG-CD1	-5.06	102.40	111.00
8	H	176	G	OP1-P-OP2	-5.05	112.02	119.60
40	o	99	SER	N-CA-CB	-5.03	102.95	110.50
18	R	101	ILE	CB-CA-C	-5.03	101.54	111.60
8	H	38	A	O5'-P-OP1	5.03	116.73	110.70
40	o	46	ALA	CB-CA-C	-5.00	102.59	110.10
1	A	548	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	PHE	Peptide
1	A	346	ASP	Peptide
1	A	408	PRO	Peptide
1	A	433	GLU	Peptide
1	A	642	ARG	Sidechain
1	A	941	LYS	Peptide
3	C	622	GLU	Peptide
3	C	736	GLY	Peptide
3	C	823	ALA	Peptide
4	D	430	LEU	Peptide
10	J	202	GLU	Peptide
12	L	202	ARG	Peptide
14	M	171	THR	Peptide
15	N	36	PRO	Peptide
18	R	94	GLY	Peptide
20	T	400	PHE	Peptide,Mainchain
26	Y	204	LYS	Mainchain
26	Y	34	ARG	Sidechain
26	Y	63	VAL	Peptide
27	Z	1023	TYR	Peptide
27	Z	1064	THR	Peptide
27	Z	1090	TYR	Peptide
27	Z	1113	THR	Peptide
27	Z	1119	TYR	Peptide
27	Z	475	LEU	Peptide
27	Z	479	MET	Peptide
27	Z	554	VAL	Peptide
27	Z	568	TYR	Peptide
27	Z	569	LEU	Peptide
27	Z	611	TYR	Peptide
27	Z	616	GLU	Peptide
27	Z	628	MET	Peptide
27	Z	711	VAL	Peptide
27	Z	721	GLU	Peptide
27	Z	740	PRO	Peptide
27	Z	747	MET	Peptide
27	Z	771	PRO	Peptide
27	Z	777	PRO	Peptide
27	Z	794	ALA	Peptide
27	Z	798	VAL	Peptide,Mainchain
27	Z	821	ILE	Peptide
27	Z	876	ASN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
27	Z	900	SER	Peptide
27	Z	904	GLN	Peptide
27	Z	905	ASP	Peptide
27	Z	962	SER	Peptide
27	Z	976	SER	Peptide
36	d	112	ASN	Peptide
36	k	112	ASN	Peptide
28	s	481[A]	VAL	Peptide,Mainchain
28	s	481[B]	VAL	Peptide,Mainchain
13	y	191	VAL	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	2247/2335 (96%)	2100 (94%)	107 (5%)	40 (2%)	8 40
3	C	856/972 (88%)	779 (91%)	57 (7%)	20 (2%)	6 36
4	D	1900/2136 (89%)	1799 (95%)	96 (5%)	5 (0%)	41 75
5	E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	4 31
9	I	493/855 (58%)	475 (96%)	10 (2%)	8 (2%)	9 43
10	J	530/848 (62%)	483 (91%)	30 (6%)	17 (3%)	4 30
11	K	144/225 (64%)	134 (93%)	6 (4%)	4 (3%)	5 32
12	L	401/802 (50%)	375 (94%)	19 (5%)	7 (2%)	9 42
13	y	106/307 (34%)	98 (92%)	8 (8%)	0	100 100
14	M	89/243 (37%)	80 (90%)	3 (3%)	6 (7%)	1 17
15	N	141/144 (98%)	126 (89%)	12 (8%)	3 (2%)	7 38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	O	279/420 (66%)	247 (88%)	26 (9%)	6 (2%)	6 37
17	P	92/229 (40%)	82 (89%)	9 (10%)	1 (1%)	14 50
18	R	235/536 (44%)	207 (88%)	14 (6%)	14 (6%)	1 19
19	S	157/166 (95%)	144 (92%)	10 (6%)	3 (2%)	8 39
20	T	311/514 (60%)	282 (91%)	17 (6%)	12 (4%)	3 26
21	Q	1304/1485 (88%)	1279 (98%)	25 (2%)	0	100 100
22	U	24/2752 (1%)	20 (83%)	3 (12%)	1 (4%)	3 24
23	V	444/908 (49%)	413 (93%)	26 (6%)	5 (1%)	14 50
24	W	436/579 (75%)	385 (88%)	32 (7%)	19 (4%)	2 24
25	X	69/425 (16%)	65 (94%)	2 (3%)	2 (3%)	4 32
26	Y	202/323 (62%)	182 (90%)	6 (3%)	14 (7%)	1 16
27	Z	611/1227 (50%)	517 (85%)	61 (10%)	33 (5%)	2 21
28	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	4 31
28	r	129/504 (26%)	118 (92%)	9 (7%)	2 (2%)	9 43
28	s	369/504 (73%)	352 (95%)	16 (4%)	1 (0%)	41 75
28	t	65/504 (13%)	64 (98%)	0	1 (2%)	10 44
29	u	388/411 (94%)	376 (97%)	9 (2%)	3 (1%)	19 58
30	v	142/148 (96%)	138 (97%)	4 (3%)	0	100 100
31	w	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	14 50
32	x	23/703 (3%)	22 (96%)	1 (4%)	0	100 100
33	a	75/126 (60%)	74 (99%)	1 (1%)	0	100 100
33	h	76/126 (60%)	75 (99%)	1 (1%)	0	100 100
34	b	81/229 (35%)	79 (98%)	2 (2%)	0	100 100
34	i	84/229 (37%)	82 (98%)	2 (2%)	0	100 100
35	c	79/119 (66%)	76 (96%)	3 (4%)	0	100 100
35	j	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
36	d	95/118 (80%)	91 (96%)	4 (4%)	0	100 100
36	k	81/118 (69%)	78 (96%)	3 (4%)	0	100 100
37	f	72/86 (84%)	69 (96%)	3 (4%)	0	100 100
37	m	72/86 (84%)	68 (94%)	4 (6%)	0	100 100
38	e	77/92 (84%)	76 (99%)	1 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
38	l	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
39	g	72/76 (95%)	70 (97%)	2 (3%)	0	100 100
39	n	64/76 (84%)	62 (97%)	2 (3%)	0	100 100
40	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	12 47
41	p	92/225 (41%)	90 (98%)	2 (2%)	0	100 100
42	1	239/301 (79%)	232 (97%)	7 (3%)	0	100 100
43	2	386/646 (60%)	358 (93%)	20 (5%)	8 (2%)	7 38
44	3	167/754 (22%)	165 (99%)	2 (1%)	0	100 100
45	4	35/37 (95%)	29 (83%)	2 (6%)	4 (11%)	0 6
All	All	14867/26150 (57%)	13893 (93%)	719 (5%)	255 (2%)	13 42

All (255) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	92	LEU
1	A	167	PRO
1	A	188	LEU
1	A	331	TRP
1	A	346	ASP
1	A	365	VAL
1	A	367	SER
1	A	368	GLN
1	A	570	ASP
1	A	629	PHE
1	A	706	ALA
1	A	942	PRO
1	A	1518	LEU
1	A	1762	TYR
1	A	1828	ALA
3	C	156	GLU
3	C	388	VAL
3	C	427	PHE
3	C	444	GLY
3	C	457	VAL
3	C	458	ASP
3	C	516	LEU
3	C	824	THR
4	D	128	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	957	VAL
4	D	1584	ILE
5	E	193	THR
9	I	463	PRO
9	I	721	LYS
9	I	797	PHE
10	J	188	GLN
10	J	191	ALA
10	J	192	GLU
10	J	202	GLU
10	J	203	LEU
10	J	205	LEU
10	J	216	ASP
10	J	413	GLU
11	K	78	PRO
11	K	90	PRO
12	L	138	ARG
12	L	146	GLU
12	L	201	LYS
12	L	203	LYS
14	M	157	GLY
14	M	195	LYS
15	N	36	PRO
16	O	20	PHE
16	O	107	MET
17	P	49	ASP
18	R	71	GLN
18	R	135	PRO
18	R	136	ASP
18	R	186	VAL
18	R	223	PRO
19	S	164	PRO
20	T	186	PRO
20	T	268	LYS
20	T	341	ALA
20	T	343	PRO
20	T	495	ALA
23	V	596	LEU
23	V	597	PRO
24	W	156	VAL
24	W	199	TYR
24	W	205	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	W	213	GLN
24	W	279	LYS
24	W	299	LEU
24	W	325	LEU
24	W	372	ASN
24	W	492	ASN
25	X	51	GLU
25	X	64	LYS
26	Y	24	LYS
26	Y	25	LEU
26	Y	27	LYS
26	Y	37	ALA
26	Y	69	LEU
26	Y	110	ALA
27	Z	556	GLU
27	Z	574	TYR
27	Z	614	ARG
27	Z	711	VAL
27	Z	748	PRO
27	Z	771	PRO
27	Z	795	PRO
27	Z	821	ILE
27	Z	881	THR
27	Z	978	LEU
27	Z	1087	ILE
27	Z	1099	CYS
27	Z	1114	PRO
28	q	59	HIS
28	q	60	PRO
28	s	71	ILE
28	t	69	THR
29	u	383	ASN
43	2	114	LYS
43	2	186	PRO
43	2	233	PRO
43	2	239	VAL
43	2	282	TYR
43	2	382	ASN
45	4	4	ALA
45	4	22	ALA
45	4	23	ALA
1	A	308	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	349	ALA
1	A	370	PRO
1	A	374	ASP
1	A	382	GLU
1	A	383	PHE
1	A	631	ALA
1	A	1212	GLY
3	C	90	THR
3	C	364	SER
3	C	711	ARG
4	D	151	LYS
9	I	618	ARG
9	I	634	ILE
10	J	217	GLU
10	J	341	PRO
10	J	376	VAL
10	J	709	VAL
14	M	120	PRO
15	N	39	GLY
16	O	132	ARG
16	O	206	ASN
18	R	191	GLY
19	S	12	PRO
20	T	301	ASP
22	U	2	TYR
23	V	485	GLN
24	W	177	LYS
24	W	191	GLY
24	W	318	VAL
24	W	482	ASP
26	Y	96	THR
27	Z	570	HIS
27	Z	608	GLU
27	Z	778	ILE
27	Z	796	ASP
27	Z	798	VAL
27	Z	1085	LYS
27	Z	1098	PRO
28	q	9	ASN
29	u	340	GLY
29	u	385	ASP
31	w	115	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	o	160	LYS
1	A	51	PHE
1	A	212	PRO
1	A	378	PHE
1	A	1092	ILE
1	A	1831	LYS
1	A	1947	ASN
3	C	63	LYS
5	E	60	MET
5	E	88	ARG
5	E	256	ASP
9	I	601	GLN
9	I	752	ALA
10	J	190	THR
18	R	104	GLN
18	R	173	PRO
18	R	250	CYS
20	T	406	ILE
23	V	578	SER
24	W	102	GLN
26	Y	21	PRO
26	Y	52	LYS
26	Y	102	HIS
27	Z	615	PHE
27	Z	641	ALA
27	Z	822	ASP
27	Z	982	ALA
28	q	19	PRO
28	r	9	ASN
43	2	336	PRO
1	A	363	HIS
1	A	480	LYS
1	A	1363	GLN
3	C	754	VAL
3	C	856	HIS
5	E	162	ARG
9	I	617	GLU
10	J	189	ILE
10	J	206	LEU
10	J	604	PRO
11	K	65	ILE
12	L	132	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	585	TYR
16	O	134	VAL
18	R	124	VAL
18	R	234	SER
18	R	283	ASN
19	S	10	GLN
20	T	401	PRO
24	W	554	ILE
26	Y	28	ASP
26	Y	66	GLU
27	Z	509	MET
27	Z	605	LEU
27	Z	777	PRO
27	Z	904	GLN
27	Z	1110	MET
27	Z	1112	TYR
27	Z	1151	VAL
40	o	32	PRO
1	A	359	ILE
1	A	1339	ASP
1	A	1517	LYS
3	C	361	PRO
3	C	615	PRO
5	E	159	PRO
16	O	239	LEU
18	R	126	ASN
20	T	185	MET
20	T	189	GLN
20	T	226	ARG
24	W	301	GLY
24	W	330	GLY
26	Y	20	ILE
43	2	283	PRO
1	A	903	SER
1	A	1275	ARG
1	A	2013	GLY
3	C	94	ILE
3	C	360	ALA
3	C	623	GLU
5	E	270	LYS
14	M	161	PHE
18	R	249	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	V	609	GLN
24	W	376	PRO
24	W	549	HIS
27	Z	1103	PRO
3	C	66	TYR
5	E	149	GLY
12	L	215	PRO
11	K	17	PRO
1	A	186	GLU
10	J	241	VAL
14	M	174	PRO
20	T	411	GLY
26	Y	26	PRO
27	Z	1109	GLY
4	D	585	ILE
5	E	324	PRO
14	M	144	PRO
15	N	4	VAL
28	r	60	PRO
45	4	5	PRO

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	1778/2108 (84%)	1648 (93%)	130 (7%)	14 41
3	C	760/866 (88%)	694 (91%)	66 (9%)	10 35
5	E	256/300 (85%)	244 (95%)	12 (5%)	26 53
10	J	241/751 (32%)	222 (92%)	19 (8%)	12 39
11	K	54/196 (28%)	49 (91%)	5 (9%)	9 32
12	L	193/709 (27%)	156 (81%)	37 (19%)	1 9
13	y	33/256 (13%)	30 (91%)	3 (9%)	9 33
14	M	85/209 (41%)	64 (75%)	21 (25%)	0 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	N	130/130 (100%)	125 (96%)	5 (4%)	33 59
16	O	253/361 (70%)	248 (98%)	5 (2%)	55 73
17	P	90/203 (44%)	78 (87%)	12 (13%)	4 21
18	R	210/457 (46%)	156 (74%)	54 (26%)	0 4
19	S	129/134 (96%)	118 (92%)	11 (8%)	10 37
20	T	269/441 (61%)	252 (94%)	17 (6%)	18 46
22	U	21/2432 (1%)	16 (76%)	5 (24%)	0 5
23	V	324/838 (39%)	303 (94%)	21 (6%)	17 45
24	W	115/502 (23%)	81 (70%)	34 (30%)	0 2
25	X	33/381 (9%)	20 (61%)	13 (39%)	0 0
26	Y	114/289 (39%)	87 (76%)	27 (24%)	1 5
28	q	78/435 (18%)	69 (88%)	9 (12%)	5 24
28	r	76/435 (18%)	66 (87%)	10 (13%)	4 21
28	t	40/435 (9%)	37 (92%)	3 (8%)	13 40
29	u	344/361 (95%)	339 (98%)	5 (2%)	65 79
30	v	132/134 (98%)	131 (99%)	1 (1%)	81 88
31	w	76/143 (53%)	75 (99%)	1 (1%)	69 81
32	x	23/581 (4%)	23 (100%)	0	100 100
33	a	68/101 (67%)	68 (100%)	0	100 100
33	h	68/101 (67%)	68 (100%)	0	100 100
34	b	76/167 (46%)	74 (97%)	2 (3%)	46 67
34	i	77/167 (46%)	75 (97%)	2 (3%)	46 67
35	c	76/101 (75%)	74 (97%)	2 (3%)	46 67
35	j	77/101 (76%)	75 (97%)	2 (3%)	46 67
36	d	88/110 (80%)	86 (98%)	2 (2%)	50 70
36	k	80/110 (73%)	78 (98%)	2 (2%)	47 68
37	f	63/74 (85%)	62 (98%)	1 (2%)	62 78
37	m	63/74 (85%)	62 (98%)	1 (2%)	62 78
38	e	74/84 (88%)	74 (100%)	0	100 100
38	l	74/84 (88%)	74 (100%)	0	100 100
39	g	62/66 (94%)	61 (98%)	1 (2%)	62 78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	n	59/66 (89%)	58 (98%)	1 (2%)	60 78
40	o	138/218 (63%)	134 (97%)	4 (3%)	42 64
41	p	82/195 (42%)	79 (96%)	3 (4%)	34 59
45	4	1/1 (100%)	1 (100%)	0	100 100
All	All	7083/15907 (44%)	6534 (92%)	549 (8%)	16 39

All (549) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	48	LYS
1	A	49	ARG
1	A	55	ASP
1	A	59	GLU
1	A	60	ASP
1	A	75	ASP
1	A	77	THR
1	A	78	ASN
1	A	82	ARG
1	A	86	ARG
1	A	88	TYR
1	A	89	LEU
1	A	152	ARG
1	A	165	ARG
1	A	177	ASP
1	A	180	ASP
1	A	181	ASN
1	A	185	VAL
1	A	204	LEU
1	A	233	PRO
1	A	250	VAL
1	A	258	PHE
1	A	284	ARG
1	A	294	ASN
1	A	295	GLU
1	A	325	HIS
1	A	330	THR
1	A	331	TRP
1	A	336	ASN
1	A	344	ASP
1	A	352	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	359	ILE
1	A	362	ARG
1	A	363	HIS
1	A	364	SER
1	A	371	LEU
1	A	377	GLU
1	A	383	PHE
1	A	389	LYS
1	A	391	THR
1	A	394	TYR
1	A	409	ARG
1	A	413	LEU
1	A	433	GLU
1	A	459	LEU
1	A	462	ARG
1	A	467	GLN
1	A	468	LYS
1	A	533	LYS
1	A	546	LEU
1	A	579	GLN
1	A	627	CYS
1	A	630	TRP
1	A	670	LYS
1	A	671	THR
1	A	673	THR
1	A	674	LYS
1	A	675	GLN
1	A	690	MET
1	A	697	MET
1	A	705	LYS
1	A	726	TRP
1	A	744	LYS
1	A	758	ARG
1	A	762	ARG
1	A	767	VAL
1	A	804	GLU
1	A	847	LYS
1	A	851	SER
1	A	855	ARG
1	A	856	LEU
1	A	861	ARG
1	A	880	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	883	ARG
1	A	904	HIS
1	A	948	PRO
1	A	1089	CYS
1	A	1094	ARG
1	A	1136	ARG
1	A	1141	ARG
1	A	1179	SER
1	A	1210	LYS
1	A	1211	ASP
1	A	1224	ARG
1	A	1246	GLN
1	A	1279	VAL
1	A	1321	GLU
1	A	1361	GLU
1	A	1363	GLN
1	A	1370	ARG
1	A	1393	ARG
1	A	1417	PRO
1	A	1427	ARG
1	A	1449	LYS
1	A	1504	GLU
1	A	1526	LEU
1	A	1532	ARG
1	A	1534	PHE
1	A	1570	LYS
1	A	1615	HIS
1	A	1626	CYS
1	A	1641	ARG
1	A	1678	ARG
1	A	1681	ARG
1	A	1732	LYS
1	A	1738	PRO
1	A	1754	TYR
1	A	1756	SER
1	A	1757	GLU
1	A	1763	LEU
1	A	1766	GLN
1	A	1768	TYR
1	A	1770	GLU
1	A	1771	LEU
1	A	1774	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1790	ILE
1	A	1794	PHE
1	A	1813	ARG
1	A	1831	LYS
1	A	1865	ARG
1	A	1885	LYS
1	A	1887	SER
1	A	1888	GLU
1	A	1898	LYS
1	A	1949	ARG
1	A	1958	LYS
1	A	1966	HIS
1	A	1968	TRP
1	A	1986	LEU
3	C	61	GLU
3	C	62	ASP
3	C	63	LYS
3	C	64	LYS
3	C	66	TYR
3	C	68	THR
3	C	71	GLU
3	C	87	GLN
3	C	97	VAL
3	C	256	CYS
3	C	295	ASP
3	C	296	GLU
3	C	297	ASN
3	C	298	LEU
3	C	300	LEU
3	C	333	ASP
3	C	336	TYR
3	C	354	ARG
3	C	359	LYS
3	C	362	THR
3	C	366	GLN
3	C	387	ASP
3	C	389	ASP
3	C	427	PHE
3	C	428	THR
3	C	438	ILE
3	C	448	LYS
3	C	452	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	454	THR
3	C	457	VAL
3	C	458	ASP
3	C	459	SER
3	C	463	GLU
3	C	468	CYS
3	C	474	LEU
3	C	475	MET
3	C	477	HIS
3	C	489	GLN
3	C	490	PHE
3	C	495	ARG
3	C	512	GLU
3	C	517	GLU
3	C	519	GLU
3	C	569	ARG
3	C	572	GLU
3	C	573	GLU
3	C	596	ASN
3	C	673	LYS
3	C	675	PHE
3	C	677	GLU
3	C	680	ASN
3	C	704	VAL
3	C	706	GLN
3	C	709	TRP
3	C	712	LYS
3	C	724	TRP
3	C	725	ASP
3	C	730	ARG
3	C	738	ASP
3	C	749	THR
3	C	750	LEU
3	C	763	LYS
3	C	826	ARG
3	C	856	HIS
3	C	941	LYS
3	C	943	LEU
5	E	74	PHE
5	E	153	PHE
5	E	161	ARG
5	E	229	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	243	LEU
5	E	248	SER
5	E	250	LEU
5	E	265	ARG
5	E	270	LYS
5	E	271	GLU
5	E	289	LEU
5	E	290	ARG
10	J	181	ASN
10	J	186	GLU
10	J	195	LEU
10	J	196	ARG
10	J	201	ARG
10	J	212	GLN
10	J	214	ILE
10	J	217	GLU
10	J	218	GLU
10	J	219	GLU
10	J	221	ASN
10	J	229	LYS
10	J	237	LYS
10	J	239	ARG
10	J	281	LYS
10	J	308	ARG
10	J	363	ARG
10	J	410	HIS
10	J	411	MET
11	K	38	GLU
11	K	90	PRO
11	K	117	GLN
11	K	126	LEU
11	K	171	GLN
12	L	20	LYS
12	L	24	MET
12	L	33	ARG
12	L	37	LEU
12	L	67	GLU
12	L	83	ARG
12	L	91	ARG
12	L	101	GLU
12	L	105	ASP
12	L	106	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	131	ASN
12	L	135	LYS
12	L	140	ASP
12	L	147	ASP
12	L	154	GLU
12	L	158	ARG
12	L	159	LEU
12	L	161	ASN
12	L	165	LYS
12	L	175	GLN
12	L	176	LEU
12	L	178	GLU
12	L	181	ARG
12	L	185	LEU
12	L	188	ARG
12	L	203	LYS
12	L	204	ARG
12	L	206	ARG
12	L	219	LYS
12	L	222	LEU
12	L	227	THR
12	L	228	SER
12	L	235	LEU
12	L	731	LEU
12	L	761	SER
12	L	766	ARG
12	L	781	GLU
13	y	3	ARG
13	y	12	LEU
13	y	40	PRO
14	M	117	ARG
14	M	118	LYS
14	M	122	LEU
14	M	124	PHE
14	M	142	ILE
14	M	147	GLU
14	M	148	THR
14	M	150	GLU
14	M	151	ARG
14	M	154	GLU
14	M	156	HIS
14	M	159	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	M	167	LEU
14	M	168	LEU
14	M	172	HIS
14	M	177	GLU
14	M	195	LYS
14	M	197	SER
14	M	198	ARG
14	M	199	ARG
14	M	200	ARG
15	N	24	GLU
15	N	41	ARG
15	N	42	LYS
15	N	116	ASN
15	N	125	LYS
16	O	45	CYS
16	O	69	GLU
16	O	74	CYS
16	O	115	GLU
16	O	150	LEU
17	P	28	LYS
17	P	29	GLN
17	P	30	TYR
17	P	33	ARG
17	P	66	ARG
17	P	67	GLU
17	P	76	ARG
17	P	78	ARG
17	P	189	ASP
17	P	212	ASN
17	P	224	MET
17	P	229	LYS
18	R	56	GLU
18	R	66	GLU
18	R	71	GLN
18	R	72	TYR
18	R	75	ASP
18	R	76	MET
18	R	78	ARG
18	R	79	LYS
18	R	80	LYS
18	R	81	LYS
18	R	82	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	86	LEU
18	R	89	GLN
18	R	92	SER
18	R	95	LYS
18	R	103	ARG
18	R	104	GLN
18	R	106	GLN
18	R	118	ASP
18	R	122	LYS
18	R	125	MET
18	R	128	ASP
18	R	137	GLU
18	R	158	LYS
18	R	170	LYS
18	R	171	LEU
18	R	175	GLN
18	R	181	PRO
18	R	183	GLN
18	R	186	VAL
18	R	188	PHE
18	R	189	ASN
18	R	195	ARG
18	R	211	ARG
18	R	212	PHE
18	R	213	LYS
18	R	214	ILE
18	R	215	ASN
18	R	220	ARG
18	R	231	HIS
18	R	241	GLU
18	R	250	CYS
18	R	258	LYS
18	R	264	LEU
18	R	265	ASP
18	R	266	LYS
18	R	267	ARG
18	R	268	LEU
18	R	279	HIS
18	R	280	ILE
18	R	297	LYS
18	R	307	GLN
18	R	312	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	315	LYS
19	S	10	GLN
19	S	15	TYR
19	S	20	MET
19	S	91	LYS
19	S	100	MET
19	S	102	ASN
19	S	108	ASN
19	S	125	LYS
19	S	129	PHE
19	S	131	ARG
19	S	133	CYS
20	T	257	ARG
20	T	282	ARG
20	T	308	ARG
20	T	318	ARG
20	T	387	PHE
20	T	399	LYS
20	T	400	PHE
20	T	401	PRO
20	T	402	ASP
20	T	412	HIS
20	T	416	ILE
20	T	418	THR
20	T	455	GLN
20	T	460	ASP
20	T	461	SER
20	T	463	SER
20	T	478	LEU
22	U	1	MET
22	U	11	ARG
22	U	20	GLN
22	U	23	LEU
22	U	25	LEU
23	V	259	PHE
23	V	333	GLN
23	V	344	LYS
23	V	387	MET
23	V	452	LEU
23	V	457	ARG
23	V	461	LEU
23	V	465	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	V	467	LEU
23	V	468	ASP
23	V	471	GLU
23	V	478	LYS
23	V	490	CYS
23	V	510	LEU
23	V	513	ARG
23	V	514	PHE
23	V	533	TYR
23	V	535	THR
23	V	540	GLU
23	V	577	SER
23	V	597	PRO
24	W	84	THR
24	W	88	MET
24	W	92	GLU
24	W	93	PHE
24	W	96	GLU
24	W	97	ASN
24	W	99	PHE
24	W	100	ARG
24	W	108	ARG
24	W	126	GLU
24	W	127	GLN
24	W	130	ARG
24	W	134	THR
24	W	139	LEU
24	W	144	ASP
24	W	146	HIS
24	W	152	TYR
24	W	157	GLU
24	W	160	GLU
24	W	169	GLU
24	W	170	THR
24	W	172	GLN
24	W	178	ARG
24	W	180	LYS
24	W	181	PHE
24	W	182	LYS
24	W	187	SER
24	W	198	LYS
24	W	200	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	W	201	ASP
24	W	204	ASP
24	W	207	LYS
24	W	209	SER
24	W	210	GLU
25	X	6	LEU
25	X	7	ASN
25	X	9	LYS
25	X	15	GLN
25	X	24	TRP
25	X	25	LYS
25	X	29	LYS
25	X	31	GLU
25	X	35	LYS
25	X	36	LYS
25	X	37	ILE
25	X	38	GLU
25	X	41	GLN
26	Y	3	GLU
26	Y	4	ARG
26	Y	18	SER
26	Y	19	LYS
26	Y	22	LYS
26	Y	23	LEU
26	Y	24	LYS
26	Y	28	ASP
26	Y	34	ARG
26	Y	36	MET
26	Y	51	TYR
26	Y	52	LYS
26	Y	54	LYS
26	Y	63	VAL
26	Y	64	GLN
26	Y	68	TYR
26	Y	71	LEU
26	Y	75	ARG
26	Y	80	CYS
26	Y	108	PHE
26	Y	130	LEU
26	Y	134	MET
26	Y	154	LEU
26	Y	160	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	Y	163	ARG
26	Y	164	GLN
26	Y	168	ASP
28	q	19	PRO
28	q	28	ARG
28	q	46	PRO
28	q	56	LYS
28	q	62	ARG
28	q	90	PHE
28	q	103	LEU
28	q	107	LEU
28	q	114	CYS
28	r	19	PRO
28	r	46	PRO
28	r	57	VAL
28	r	60	PRO
28	r	62	ARG
28	r	79	GLN
28	r	87	LEU
28	r	93	ARG
28	r	101	GLN
28	r	103	LEU
28	t	87	LEU
28	t	93	ARG
28	t	107	LEU
29	u	37	THR
29	u	301	ASN
29	u	316	ARG
29	u	337	TRP
29	u	360	LEU
30	v	119	GLU
31	w	118	LEU
34	i	13	ILE
34	i	58	GLN
35	j	40	LEU
35	j	54	GLN
36	k	45	ASN
36	k	112	ASN
37	m	55	LEU
39	n	65	ASN
40	o	5	THR
40	o	55	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	o	114	SER
40	o	126	THR
41	p	17	LYS
41	p	46	MET
41	p	87	ASP
34	b	13	ILE
34	b	58	GLN
35	c	40	LEU
35	c	54	GLN
36	d	45	ASN
36	d	112	ASN
37	f	55	LEU
39	g	65	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	73	HIS
1	A	78	ASN
1	A	97	HIS
1	A	210	HIS
1	A	270	ASN
1	A	294	ASN
1	A	297	ASN
1	A	325	HIS
1	A	333	HIS
1	A	573	GLN
1	A	584	HIS
1	A	601	GLN
1	A	675	GLN
1	A	703	GLN
1	A	775	ASN
1	A	792	HIS
1	A	904	HIS
1	A	924	GLN
1	A	1096	HIS
1	A	1359	HIS
1	A	1527	ASN
1	A	1717	ASN
1	A	1784	ASN
1	A	1946	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	82	GLN
3	C	245	HIS
3	C	297	ASN
3	C	437	HIS
3	C	513	ASN
3	C	575	GLN
3	C	583	ASN
3	C	596	ASN
3	C	706	GLN
3	C	890	HIS
3	C	892	GLN
3	C	924	GLN
5	E	165	GLN
5	E	253	ASN
10	J	181	ASN
10	J	212	GLN
10	J	221	ASN
11	K	117	GLN
11	K	171	GLN
12	L	13	ASN
12	L	39	HIS
12	L	175	GLN
12	L	199	GLN
12	L	211	ASN
14	M	119	ASN
14	M	134	GLN
14	M	156	HIS
14	M	172	HIS
14	M	189	GLN
15	N	27	GLN
15	N	54	HIS
15	N	99	ASN
15	N	107	GLN
16	O	113	ASN
16	O	163	HIS
16	O	196	GLN
16	O	254	GLN
16	O	267	GLN
16	O	268	GLN
16	O	294	ASN
18	R	89	GLN
18	R	104	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	126	ASN
18	R	133	GLN
18	R	189	ASN
18	R	194	GLN
18	R	215	ASN
18	R	231	HIS
18	R	242	GLN
18	R	314	GLN
19	S	13	ASN
20	T	217	GLN
20	T	285	HIS
20	T	297	HIS
20	T	413	ASN
20	T	417	ASN
20	T	446	ASN
20	T	451	HIS
20	T	455	GLN
22	U	20	GLN
23	V	474	HIS
23	V	553	HIS
24	W	162	ASN
24	W	172	GLN
24	W	188	ASN
25	X	15	GLN
25	X	41	GLN
26	Y	57	ASN
26	Y	64	GLN
29	u	301	ASN
29	u	356	ASN
29	u	394	GLN
33	h	60	GLN
34	i	22	GLN
34	i	76	ASN
35	j	64	ASN
36	k	69	ASN
37	m	58	HIS
39	n	65	ASN
40	o	130	HIS
41	p	7	HIS
33	a	60	GLN
34	b	11	GLN
34	b	22	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	b	76	ASN
35	c	64	ASN
36	d	69	ASN
37	f	58	HIS
39	g	65	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	82/117 (70%)	17 (20%)	6 (7%)
6	F	96/107 (89%)	43 (44%)	17 (17%)
7	G	85/275 (30%)	50 (58%)	8 (9%)
8	H	132/188 (70%)	26 (19%)	4 (3%)
All	All	395/687 (57%)	136 (34%)	35 (8%)

All (136) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	U
2	B	13	C
2	B	19	A
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	24	G
2	B	25	C
2	B	26	A
2	B	28	A
2	B	36	C
2	B	38	C
2	B	45	C
2	B	57	G
2	B	70	A
2	B	71	C
6	F	6	C
6	F	7	G
6	F	8	C
6	F	10	U
6	F	12	G
6	F	25	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	26	U
6	F	27	A
6	F	28	A
6	F	29	A
6	F	31	U
6	F	33	G
6	F	34	G
6	F	35	A
6	F	36	A
6	F	37	C
6	F	38	G
6	F	45	A
6	F	46	G
6	F	47	A
6	F	48	A
6	F	49	G
6	F	51	U
6	F	54	G
6	F	55	C
6	F	56	A
6	F	59	G
6	F	60	C
6	F	61	C
6	F	62	C
6	F	67	G
6	F	68	C
6	F	74	U
6	F	78	A
6	F	79	C
6	F	80	G
6	F	81	C
6	F	82	A
6	F	83	A
6	F	84	A
6	F	85	U
6	F	86	U
6	F	87	C
7	G	-11	G
7	G	-6	C
7	G	-1	G
7	G	2	U
7	G	3	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	5	G
7	G	6	A
7	G	7	G
7	G	8	C
7	G	10	U
7	G	11	A
7	G	12	G
7	G	13	C
7	G	14	A
7	G	17	U
7	G	21	A
7	G	22	C
7	G	23	U
7	G	24	G
7	G	25	G
7	G	26	U
7	G	27	U
7	G	28	A
7	G	29	C
7	G	30	C
7	G	31	U
7	G	120	G
7	G	121	G
7	G	122	U
7	G	123	U
7	G	124	U
7	G	125	C
7	G	126	C
7	G	127	U
7	G	128	U
7	G	129	G
7	G	130	A
7	G	138	A
7	G	142	U
7	G	143	U
7	G	145	U
7	G	146	C
7	G	147	C
7	G	148	U
7	G	149	G
7	G	150	U
7	G	151	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	152	C
7	G	153	C
7	G	154	U
8	H	13	C
8	H	15	U
8	H	16	U
8	H	17	U
8	H	19	G
8	H	22	U
8	H	24	A
8	H	25	G
8	H	29	A
8	H	30	A
8	H	31	G
8	H	112	G
8	H	143	A
8	H	147	G
8	H	152	G
8	H	153	A
8	H	154	C
8	H	156	U
8	H	157	G
8	H	164	C
8	H	165	A
8	H	168	A
8	H	169	C
8	H	177	A
8	H	178	A
8	H	179	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	12	U
2	B	18	C
2	B	19	A
2	B	20	G
2	B	25	C
2	B	27	U
6	F	5	U
6	F	7	G
6	F	25	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	26	U
6	F	33	G
6	F	34	G
6	F	35	A
6	F	36	A
6	F	45	A
6	F	47	A
6	F	48	A
6	F	50	A
6	F	58	G
6	F	59	G
6	F	81	C
6	F	84	A
6	F	86	U
7	G	-12	G
7	G	16	G
7	G	20	A
7	G	21	A
7	G	22	C
7	G	23	U
7	G	146	C
7	G	152	C
8	H	15	U
8	H	156	U
8	H	164	C
8	H	168	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	$\#\|Z\| > 2$
18	SEP	R	224	18	8,9,10	0.81	0	8,12,14	1.14	0
18	SEP	R	232	18	8,9,10	0.73	0	8,12,14	1.38	1 (12%)

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
18	SEP	R	224	18	-	3/5/8/10	-
18	SEP	R	232	18	-	2/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	232	SEP	OG-CB-CA	-2.55	105.67	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	224	SEP	CB-OG-P-O1P
18	R	224	SEP	CB-OG-P-O2P
18	R	224	SEP	CB-OG-P-O3P
18	R	232	SEP	N-CA-CB-OG
18	R	232	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 14 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
46	IHP	A	3000	-	36,36,36	1.01	2 (5%)	54,60,60	1.62	12 (22%)
49	ADP	D	2202	-	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)
51	ATP	u	702	48	26,33,33	0.92	0	31,52,52	1.54	5 (16%)
49	ADP	D	2201	-	24,29,29	0.97	1 (4%)	29,45,45	1.34	4 (13%)
47	GTP	C	1500	48	26,34,34	1.17	1 (3%)	32,54,54	1.81	8 (25%)

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
46	IHP	A	3000	-	-	6/30/54/54	0/1/1/1
49	ADP	D	2202	-	-	2/12/32/32	0/3/3/3
51	ATP	u	702	48	-	0/18/38/38	0/3/3/3
49	ADP	D	2201	-	-	8/12/32/32	0/3/3/3
47	GTP	C	1500	48	-	7/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	C	1500	GTP	C6-N1	-3.48	1.32	1.37
46	A	3000	IHP	P5-O45	-2.84	1.43	1.54
46	A	3000	IHP	P2-O12	2.65	1.64	1.59
49	D	2201	ADP	C5-C4	2.52	1.47	1.40
49	D	2202	ADP	C5-C4	2.31	1.47	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	u	702	ATP	PB-O3B-PG	-4.33	117.98	132.83
46	A	3000	IHP	O45-P5-O35	4.09	123.25	107.64
51	u	702	ATP	N3-C2-N1	-4.08	122.30	128.68
49	D	2202	ADP	PA-O3A-PB	-4.02	119.02	132.83
46	A	3000	IHP	O35-P5-O15	-3.97	88.20	105.99
47	C	1500	GTP	PA-O3A-PB	-3.79	119.83	132.83
47	C	1500	GTP	C5-C6-N1	3.78	120.62	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	C	1500	GTP	O6-C6-C5	-3.71	117.12	124.37
46	A	3000	IHP	O16-C6-C1	3.31	116.50	108.69
51	u	702	ATP	C4-C5-N7	-3.31	105.95	109.40
46	A	3000	IHP	C6-C1-C2	-3.22	103.36	110.41
49	D	2201	ADP	N3-C2-N1	-3.18	123.71	128.68
47	C	1500	GTP	PB-O3B-PG	-3.15	122.01	132.83
49	D	2202	ADP	C3'-C2'-C1'	3.11	105.66	100.98
47	C	1500	GTP	C2-N1-C6	-3.01	119.56	125.10
49	D	2202	ADP	N3-C2-N1	-2.97	124.04	128.68
47	C	1500	GTP	O2G-PG-O3B	2.91	114.38	104.64
49	D	2202	ADP	C4-C5-N7	-2.87	106.41	109.40
49	D	2201	ADP	C3'-C2'-C1'	2.76	105.13	100.98
46	A	3000	IHP	O44-P4-O34	2.73	118.08	107.64
51	u	702	ATP	PA-O3A-PB	-2.73	123.47	132.83
46	A	3000	IHP	C5-C6-C1	-2.66	104.58	110.41
49	D	2201	ADP	PA-O3A-PB	-2.45	124.43	132.83
49	D	2201	ADP	C4-C5-N7	-2.35	106.95	109.40
47	C	1500	GTP	C3'-C2'-C1'	2.31	104.46	100.98
47	C	1500	GTP	O4'-C4'-C3'	2.30	109.67	105.11
51	u	702	ATP	O4'-C1'-C2'	-2.28	103.59	106.93
46	A	3000	IHP	O35-P5-O25	2.27	119.57	110.68
46	A	3000	IHP	O12-C2-C3	2.13	113.72	108.69
46	A	3000	IHP	O15-C5-C4	-2.13	103.68	108.69
46	A	3000	IHP	O31-P1-O11	-2.09	96.62	105.99
46	A	3000	IHP	C4-C3-C2	2.09	114.98	110.41
46	A	3000	IHP	O42-P2-O22	2.08	118.84	110.68

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	3000	IHP	C4-C5-O15-P5
46	A	3000	IHP	C6-C5-O15-P5
47	C	1500	GTP	PB-O3B-PG-O3G
47	C	1500	GTP	C5'-O5'-PA-O3A
47	C	1500	GTP	C5'-O5'-PA-O1A
47	C	1500	GTP	C5'-O5'-PA-O2A
49	D	2201	ADP	PA-O3A-PB-O2B
49	D	2201	ADP	C5'-O5'-PA-O1A
49	D	2201	ADP	C5'-O5'-PA-O2A
49	D	2201	ADP	C3'-C4'-C5'-O5'
47	C	1500	GTP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

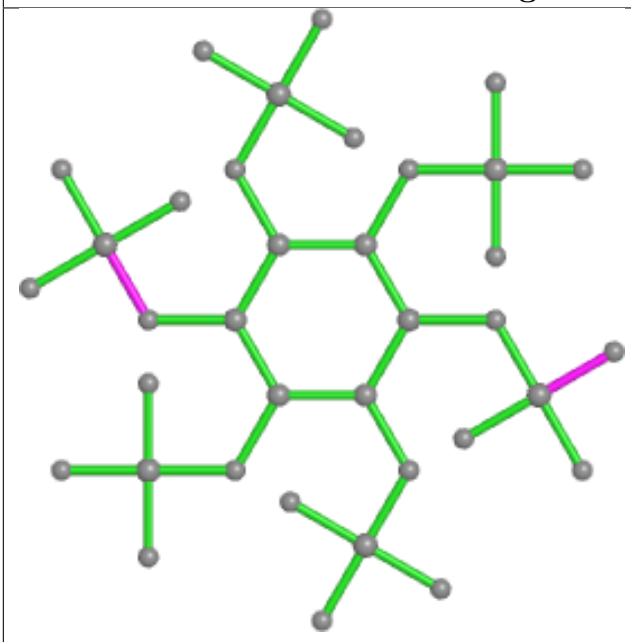
Mol	Chain	Res	Type	Atoms
47	C	1500	GTP	C3'-C4'-C5'-O5'
49	D	2201	ADP	O4'-C4'-C5'-O5'
49	D	2202	ADP	C3'-C4'-C5'-O5'
49	D	2202	ADP	O4'-C4'-C5'-O5'
46	A	3000	IHP	C2-O12-P2-O22
46	A	3000	IHP	C1-O11-P1-O21
49	D	2201	ADP	PA-O3A-PB-O1B
49	D	2201	ADP	PA-O3A-PB-O3B
46	A	3000	IHP	C1-O11-P1-O31
46	A	3000	IHP	C5-O15-P5-O35
49	D	2201	ADP	C5'-O5'-PA-O3A
47	C	1500	GTP	PG-O3B-PB-O2B

There are no ring outliers.

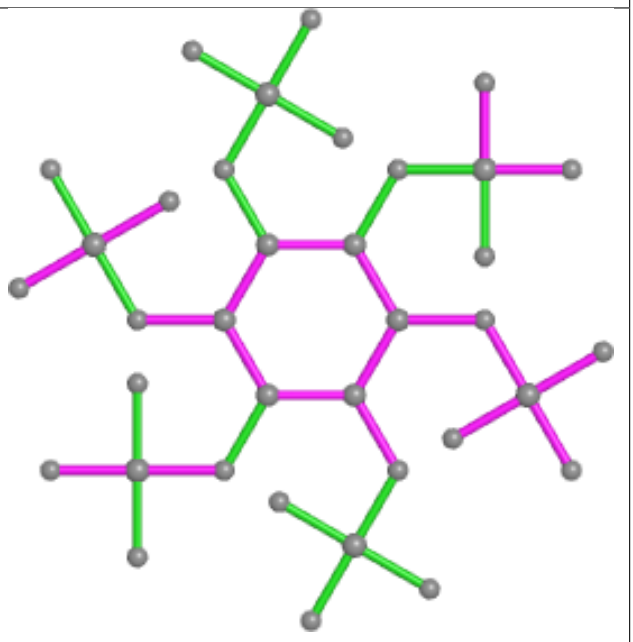
No monomer is involved in short contacts.

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.

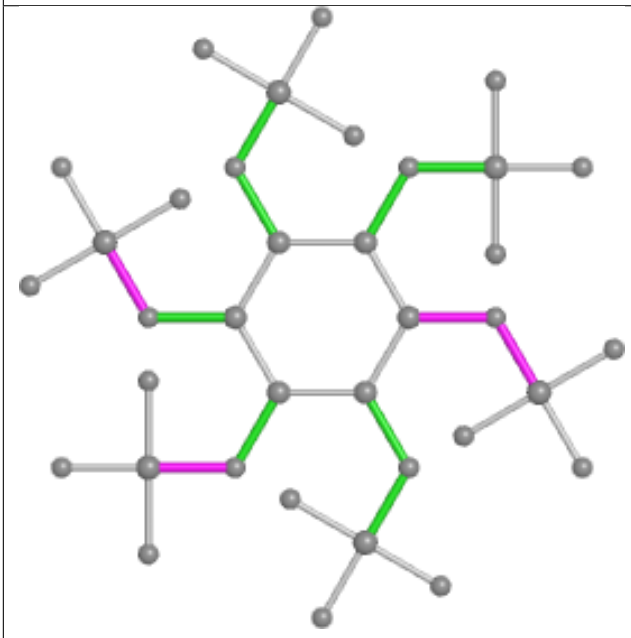
Ligand IHP A 3000



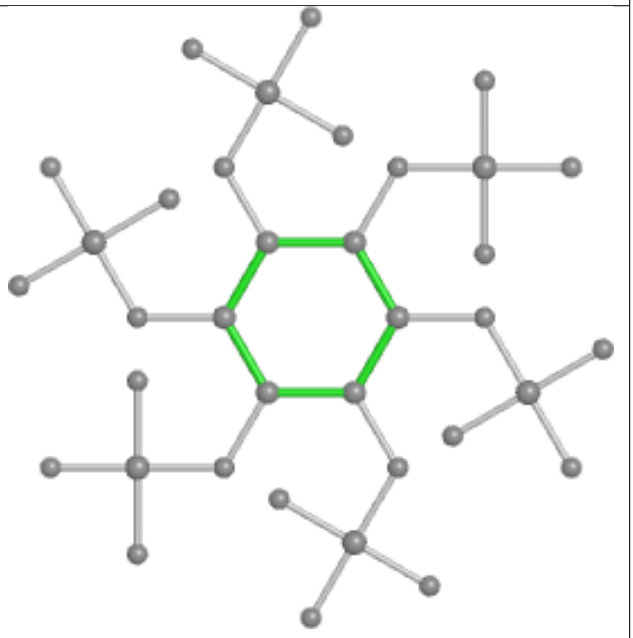
Bond lengths



Bond angles

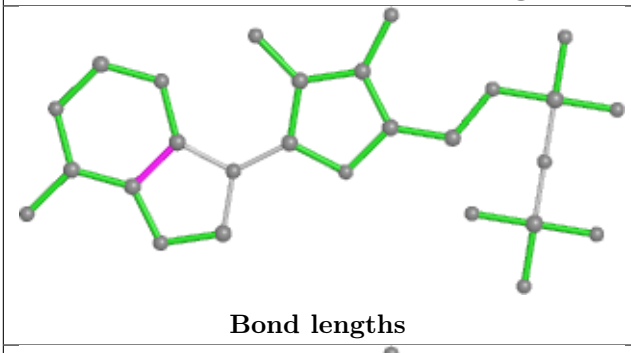


Torsions

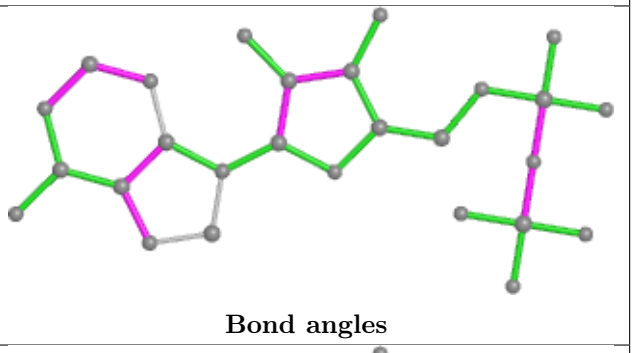


Rings

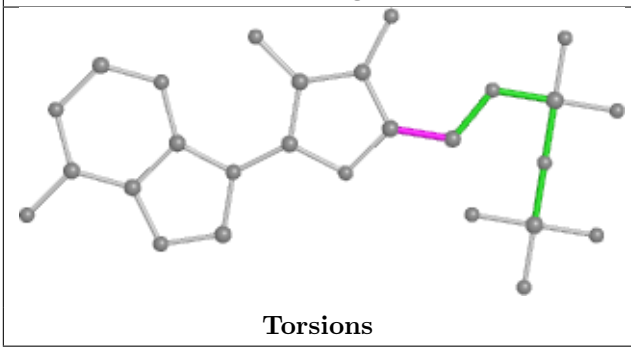
Ligand ADP D 2202



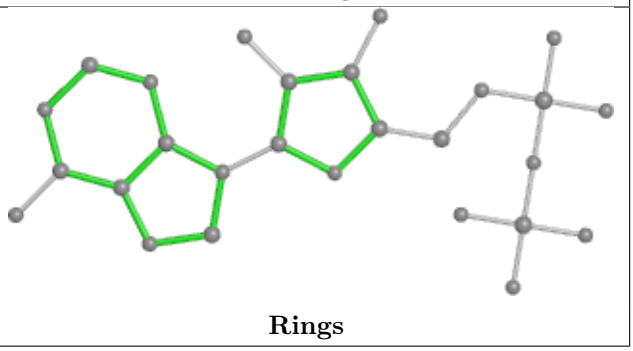
Bond lengths



Bond angles

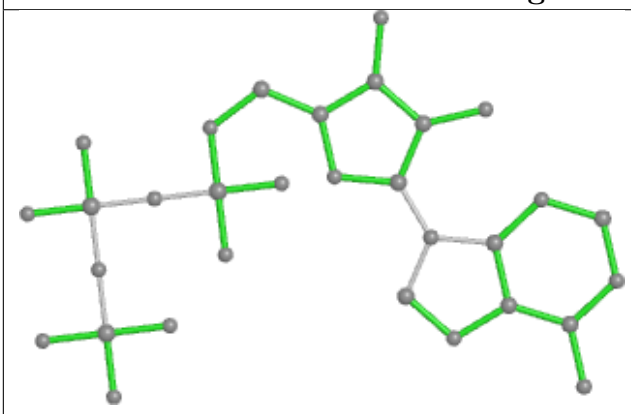


Torsions

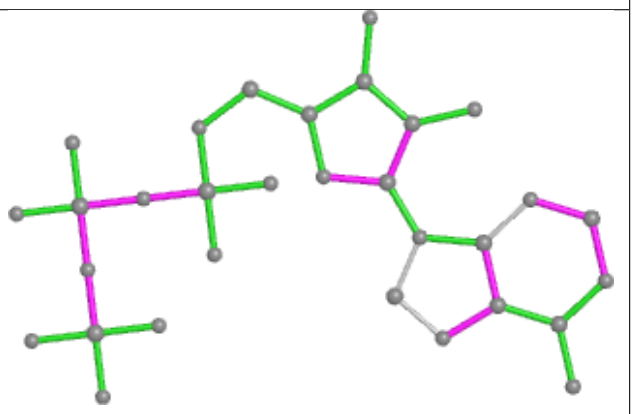


Rings

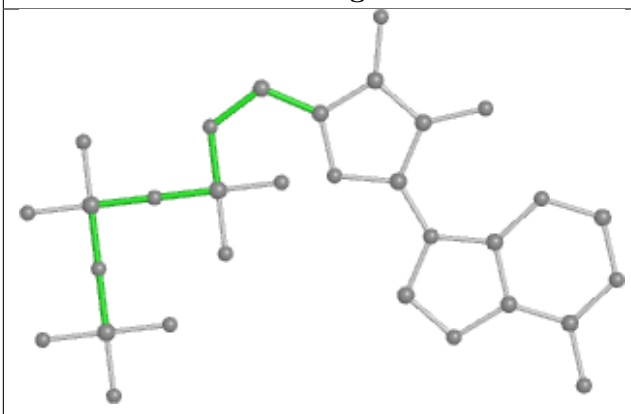
Ligand ATP u 702



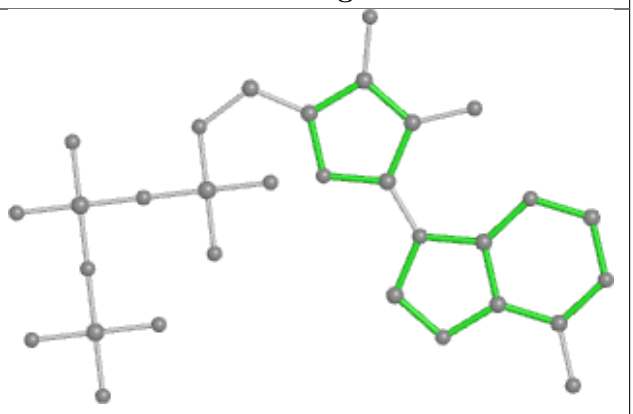
Bond lengths



Bond angles

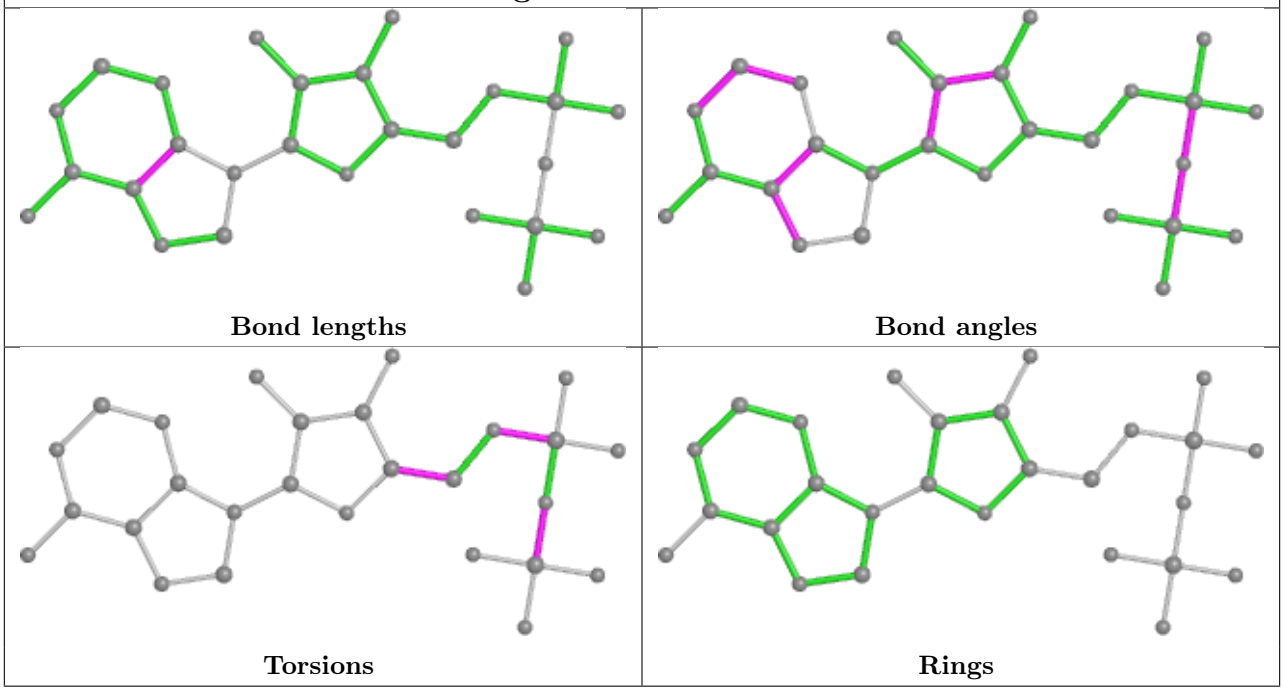


Torsions

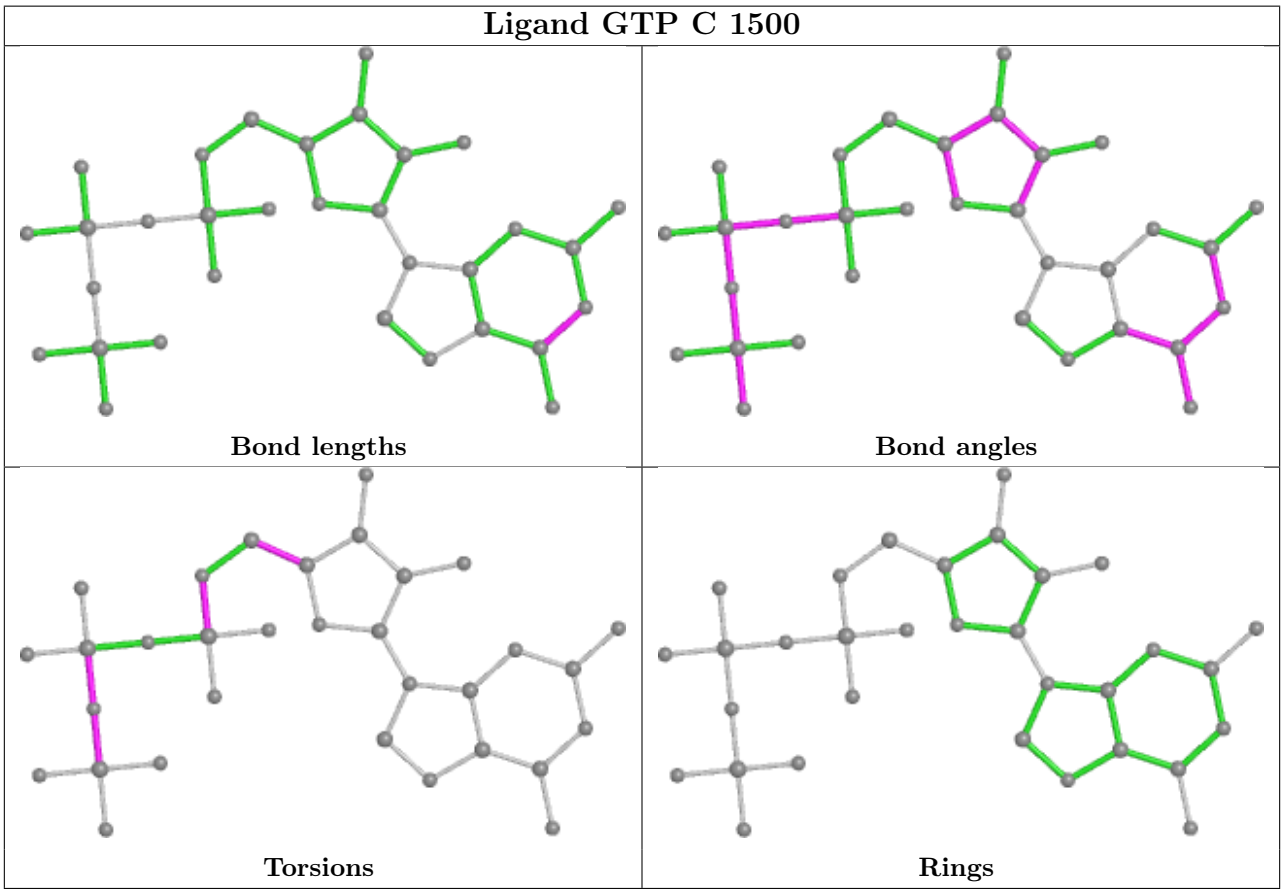


Rings

Ligand ADP D 2201



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.

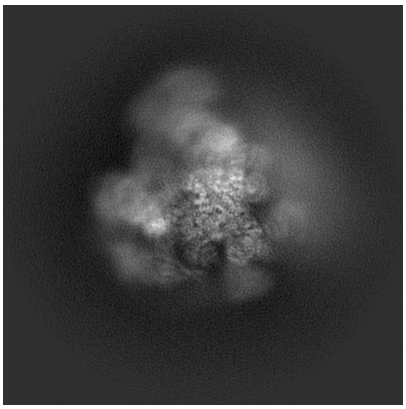
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6864. These allow visual inspection of the internal detail of the map and identification of artifacts.

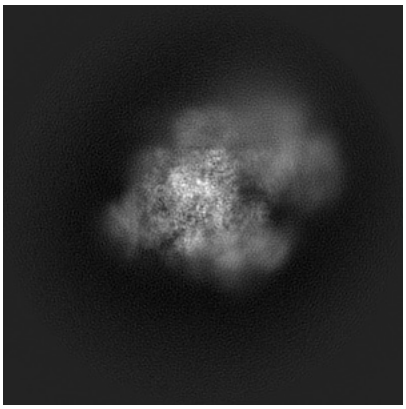
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

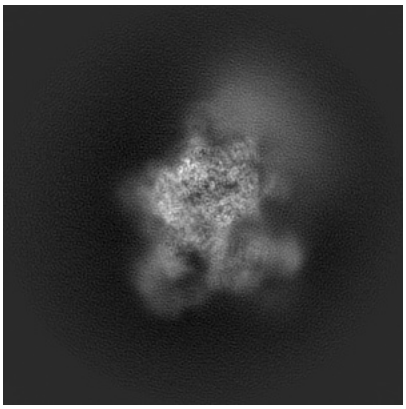
6.1.1 Primary map



X

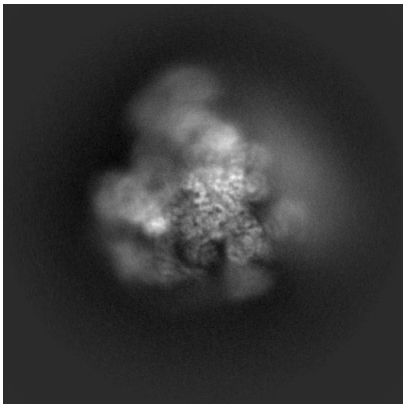


Y

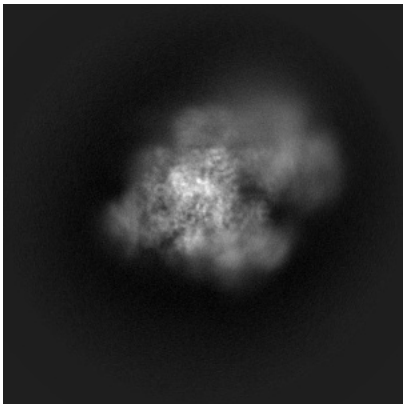


Z

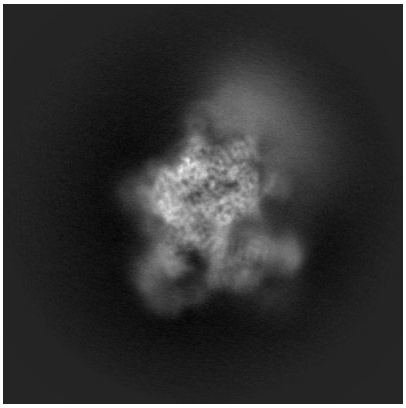
6.1.2 Raw map



X



Y

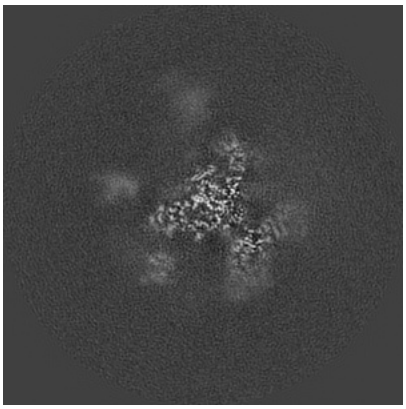


Z

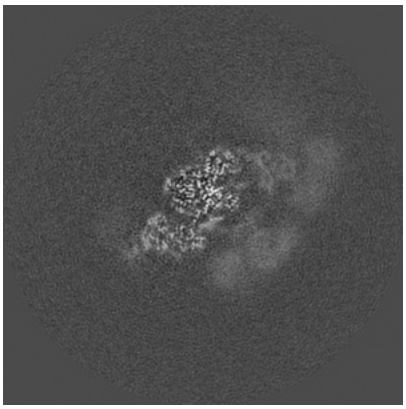
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

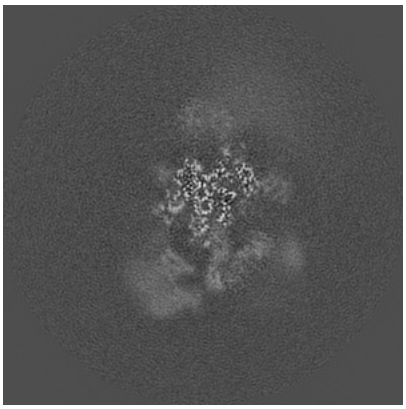
6.2.1 Primary map



X Index: 200

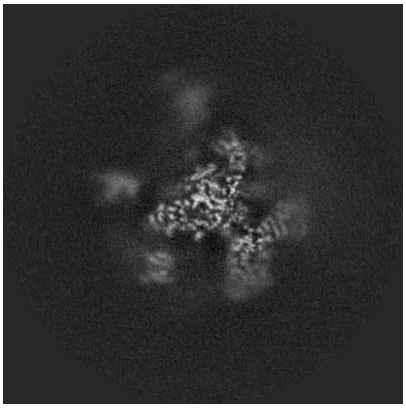


Y Index: 200

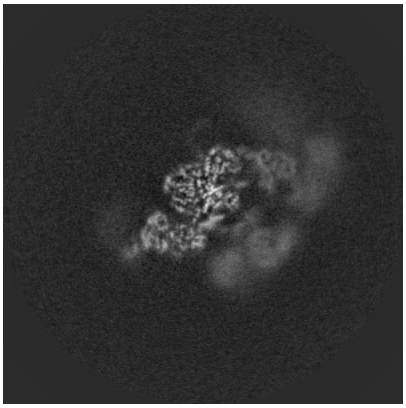


Z Index: 200

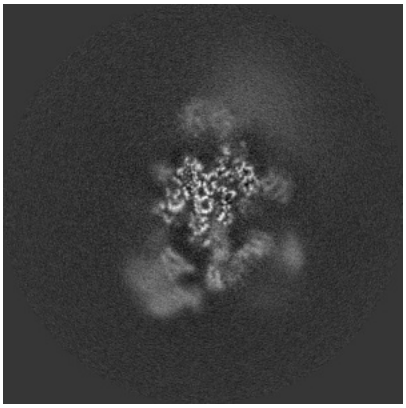
6.2.2 Raw map



X Index: 200



Y Index: 200

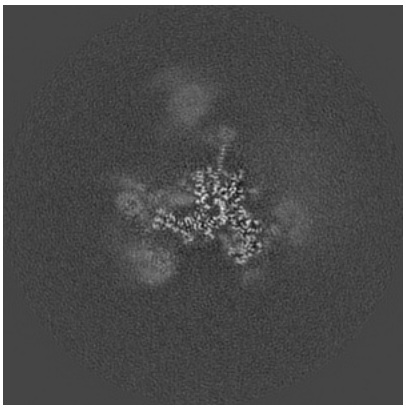


Z Index: 200

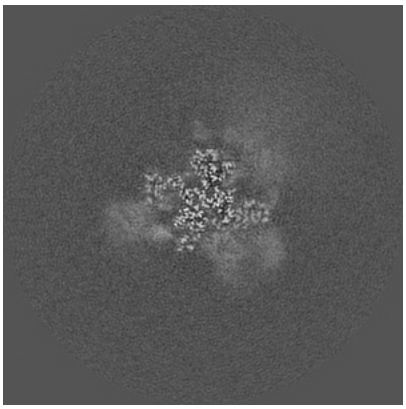
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

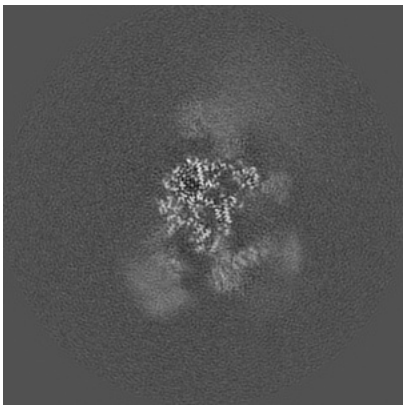
6.3.1 Primary map



X Index: 210

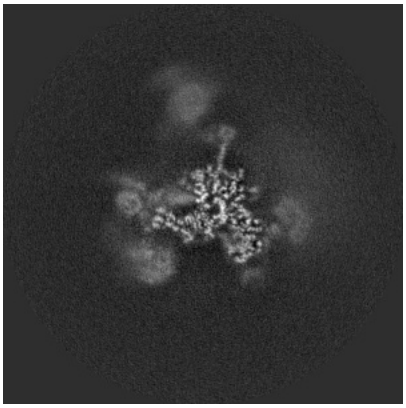


Y Index: 229

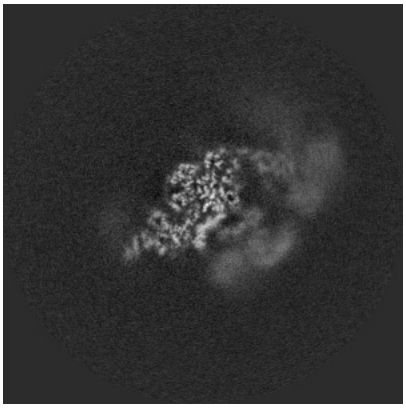


Z Index: 194

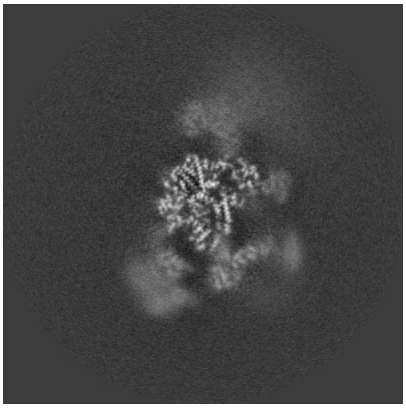
6.3.2 Raw map



X Index: 210



Y Index: 197



Z Index: 195

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

6.4.2 Raw map

X Y Z

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

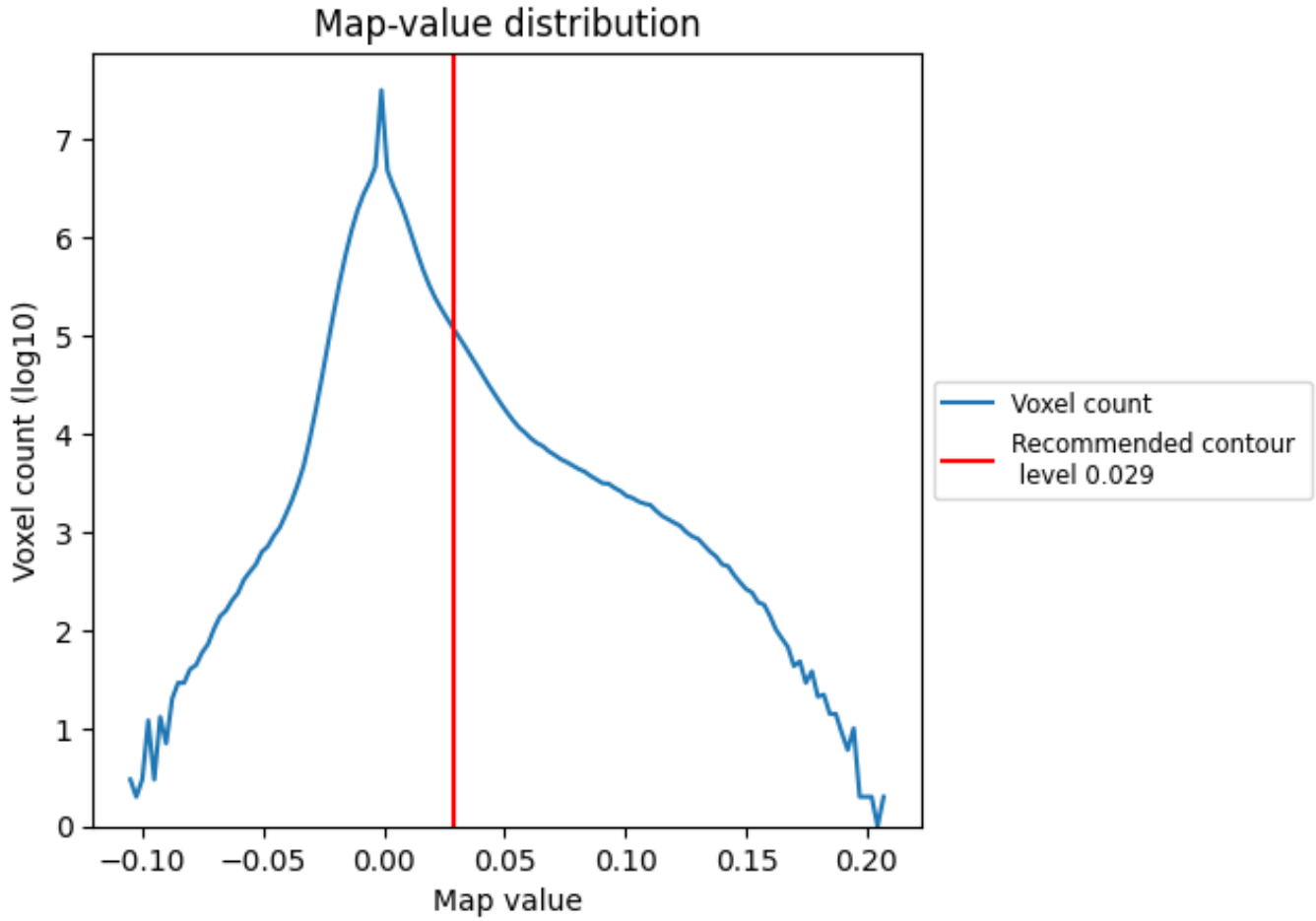
6.5 Mask visualisation (i)

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

7 Map analysis

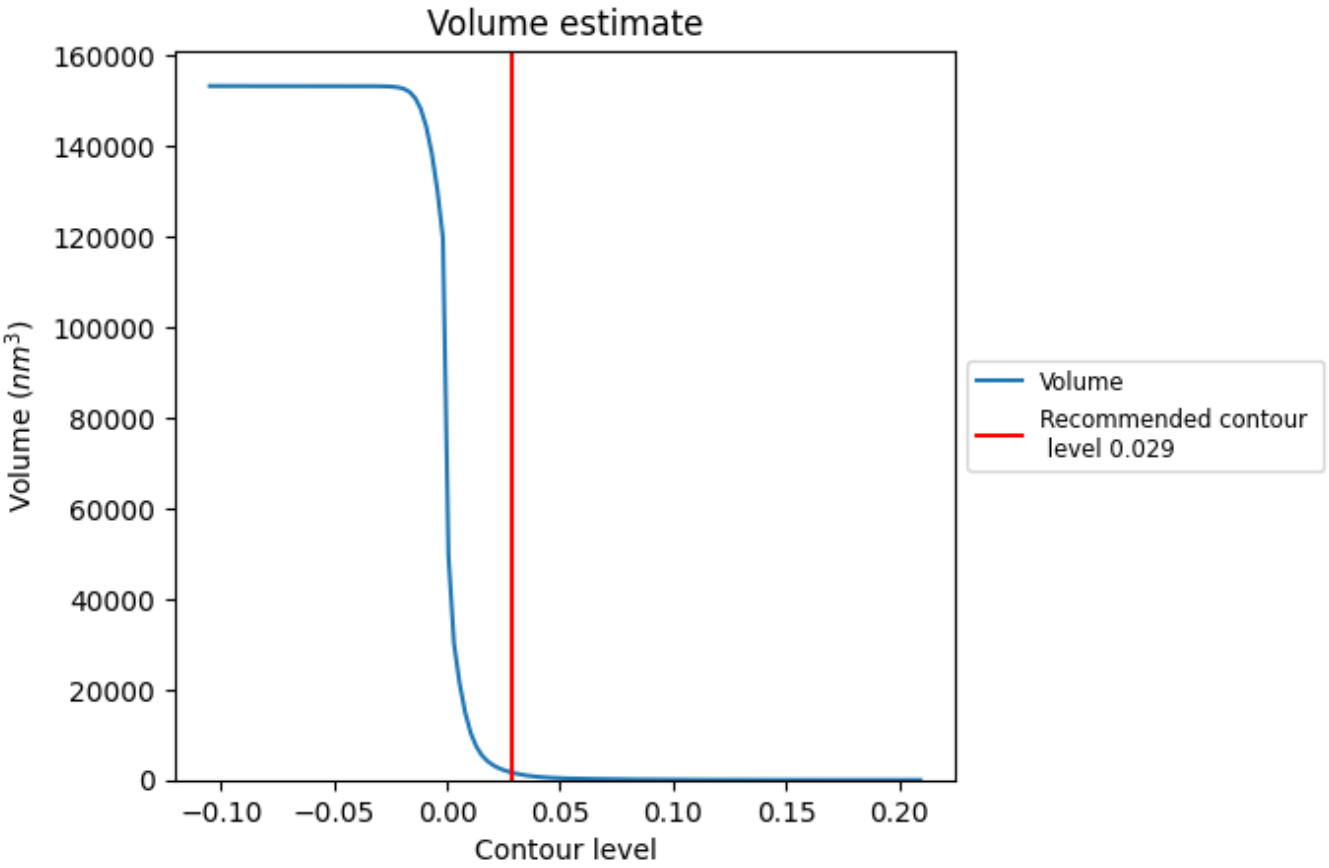
This section contains the results of statistical analysis of the map.

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.

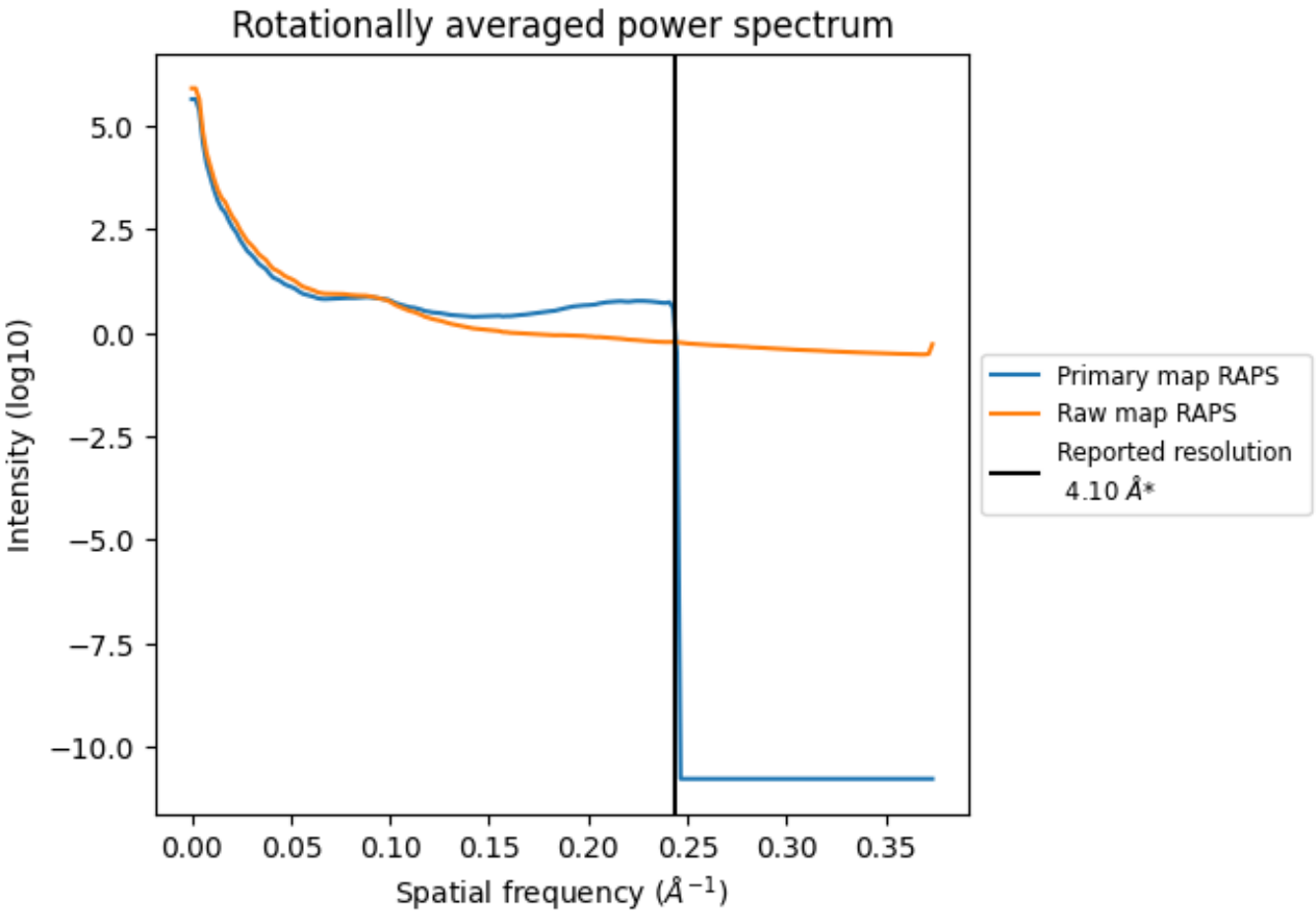
7.2 Volume estimate



The volume at the recommended contour level is 1595 nm^3; this corresponds to an approximate mass of 1441 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)

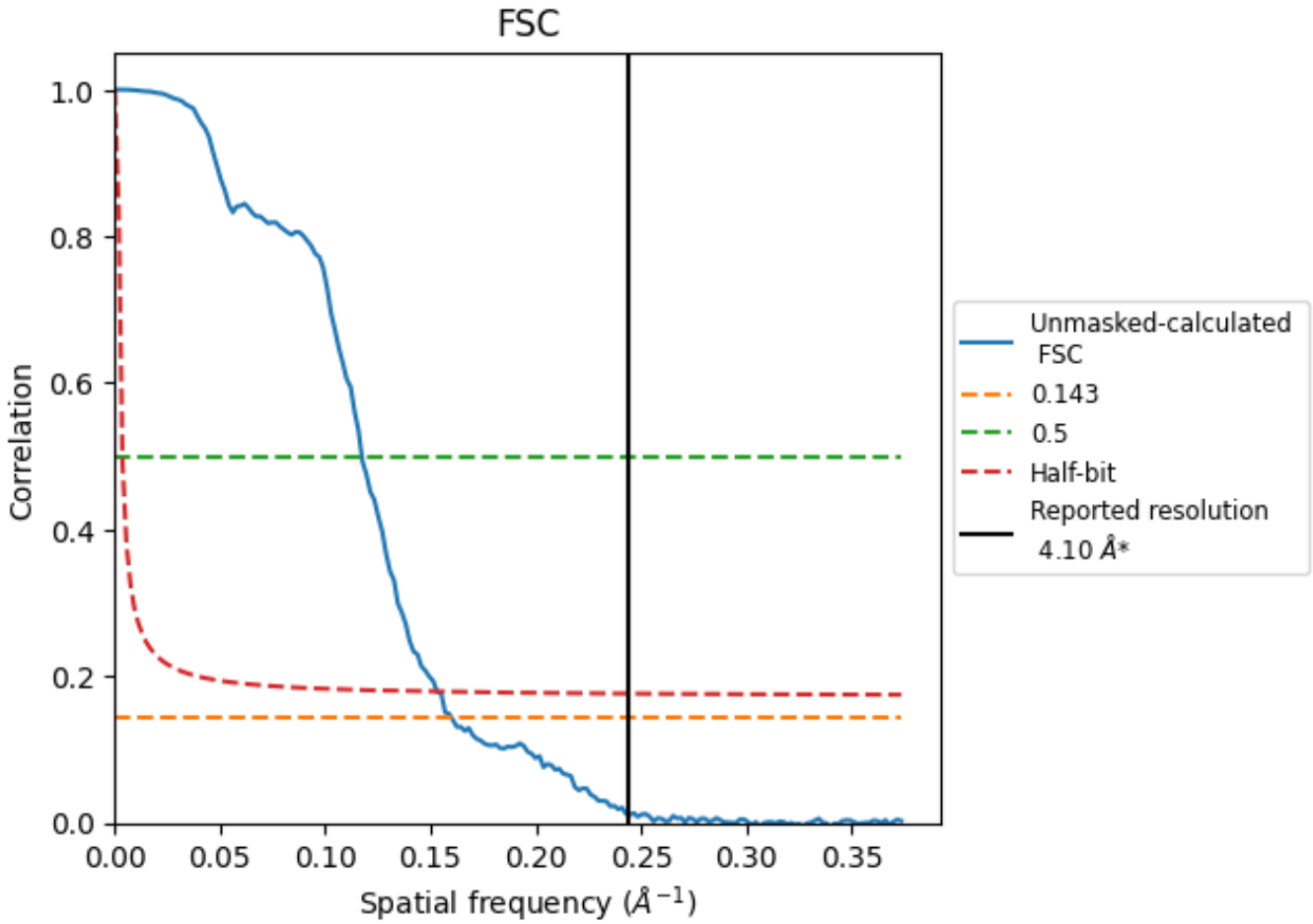


*Reported resolution corresponds to spatial frequency of 0.244 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8.2 Resolution estimates (i)

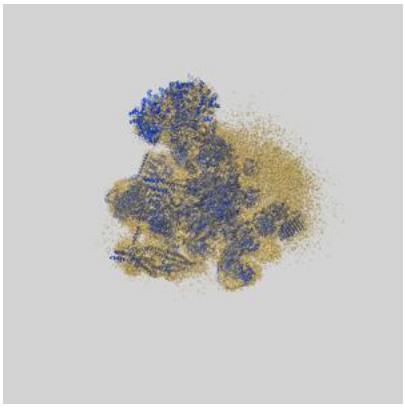
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.25	8.52	6.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.25 differs from the reported value 4.1 by more than 10 %

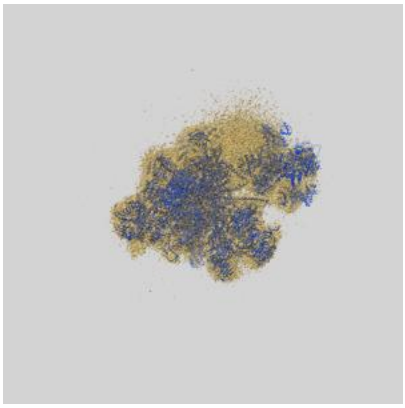
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6864 and PDB model 5YZG. Per-residue inclusion information can be found in section 3 on page 16.

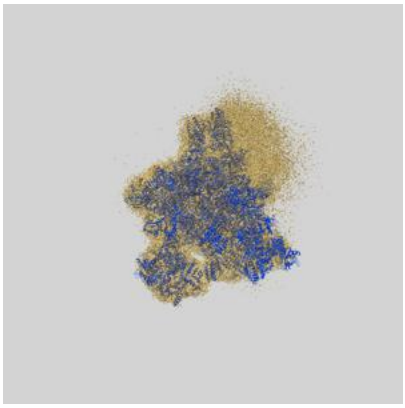
9.1 Map-model overlay



X



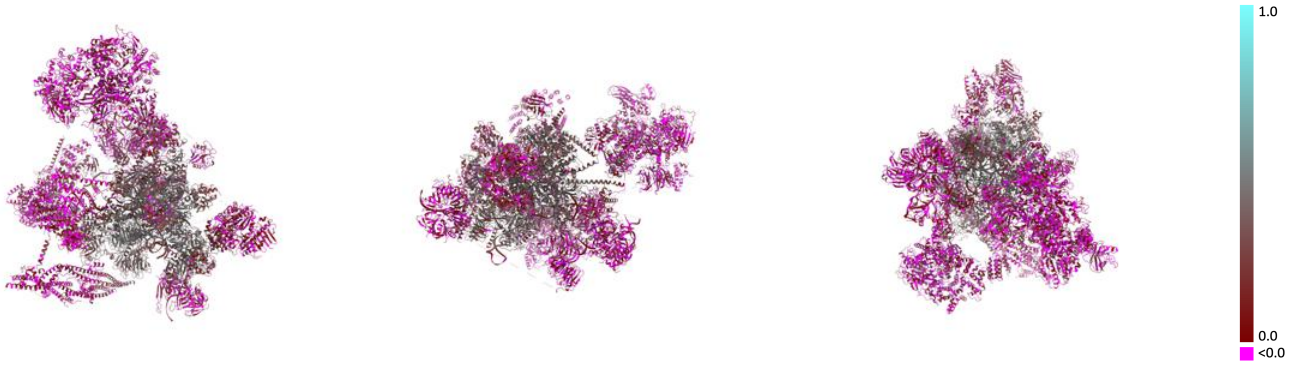
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.029 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.

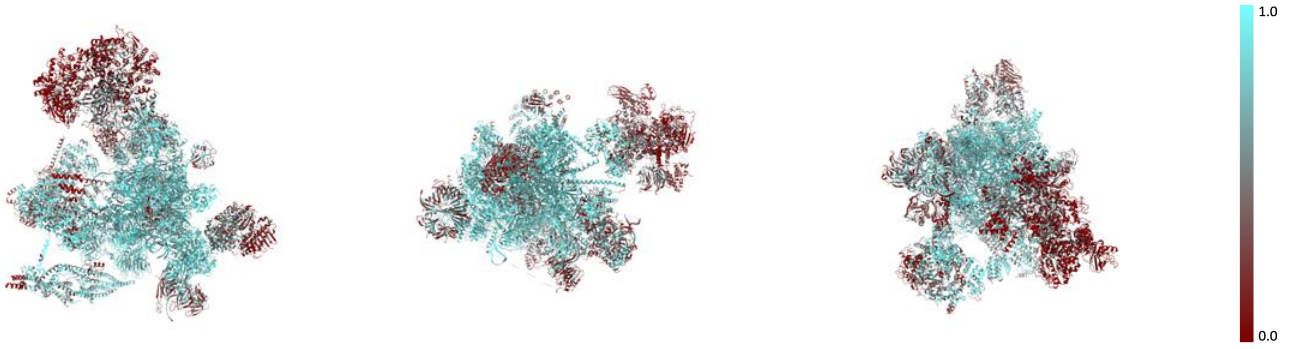
9.2 Q-score mapped to coordinate model



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.

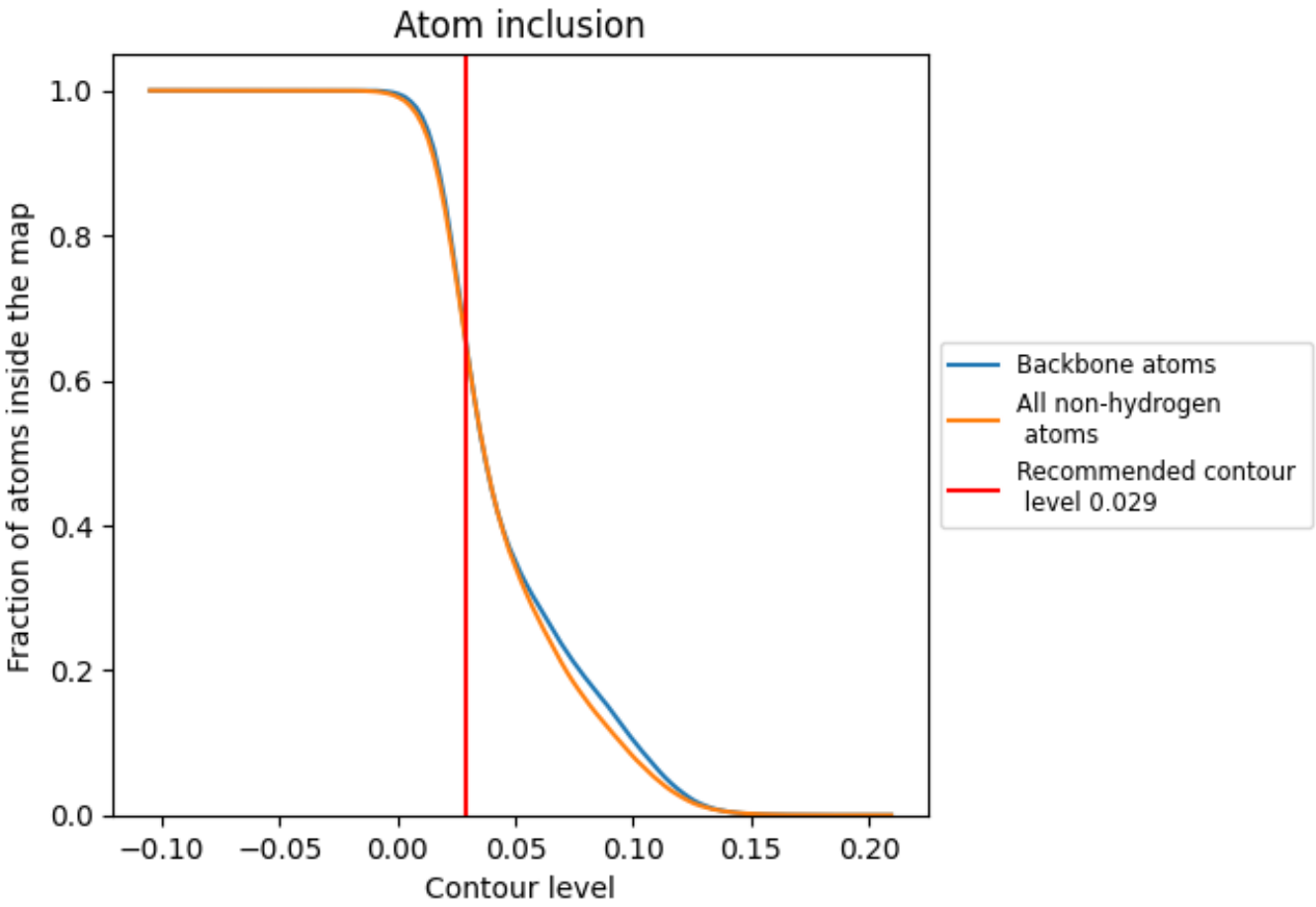
9.3 Atom inclusion mapped to coordinate model



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 (0.029).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 65% 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 (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6506	0.2050
1	0.7202	0.1430
2	0.4002	0.0390
3	0.4678	0.1560
4	0.8696	0.3750
A	0.8373	0.3780
B	0.8518	0.2730
C	0.8681	0.3820
D	0.1458	0.0280
E	0.8899	0.3500
F	0.8649	0.2960
G	0.8507	0.2700
H	0.6307	0.0890
I	0.7740	0.0680
J	0.7230	0.2200
K	0.7125	0.0690
L	0.7545	0.2330
M	0.6960	0.2110
N	0.8733	0.4120
O	0.8471	0.3230
P	0.8098	0.3700
Q	0.4888	0.0330
R	0.8266	0.3610
S	0.8434	0.3040
T	0.9239	0.4440
U	0.9358	0.4430
V	0.6770	0.2120
W	0.7043	0.1780
X	0.8270	0.3130
Y	0.8358	0.3570
Z	0.6213	0.1250
a	0.3926	0.0090
b	0.3742	0.0240
c	0.4241	0.0370
d	0.4005	0.0410

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	0.5362	0.0140
f	0.4081	0.0310
g	0.4813	0.0080
h	0.5263	0.0240
i	0.4030	-0.0170
j	0.4984	0.0360
k	0.4199	0.0330
l	0.4906	-0.0020
m	0.5671	0.0230
n	0.5657	0.0530
o	0.1711	0.0460
p	0.3105	-0.0180
q	0.4197	0.0250
r	0.6584	0.0370
s	0.4311	0.0090
t	0.5923	0.0430
u	0.4448	0.0850
v	0.1648	0.0720
w	0.1538	0.0230
x	0.0861	0.0040
y	0.7299	0.1960