Full wwPDB EM Validation Report ⓘ

Mar 19, 2024 – 05:50 PM JST

PDB ID	:	6AH0
EMDB ID	:	EMD-9621
Title	:	The Cryo-EM Structure of the Precusor of Human Pre-catalytic Spliceosome (pre-B complex)
Authors	:	Zhan, X.; Yan, C.; Zhang, X.; Shi, Y.
Deposited on	:	2018-08-15
Resolution	:	5.70 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:

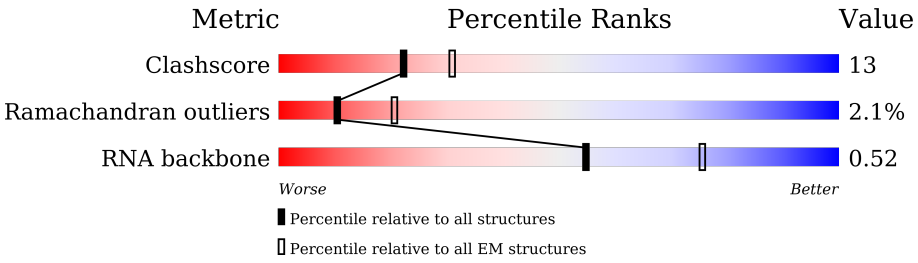
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 5.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
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	B	117	38% 44% 16%
2	D	2136	86% 12%
3	E	357	18% 81% 16%
4	P	118	61% 37%
4	a	118	66% 34%
4	k	118	72% 71% 28%
5	Q	86	6% 81% 17%
5	b	86	10% 85% 15%

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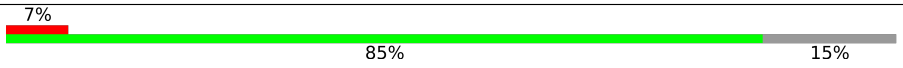
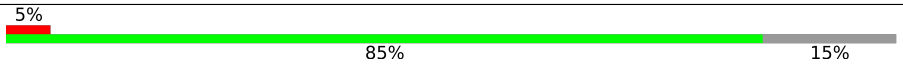
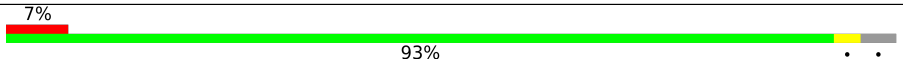
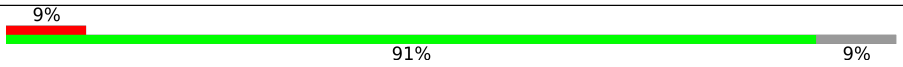
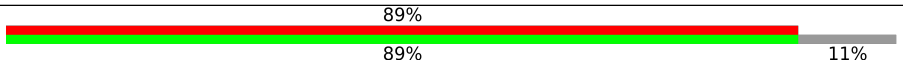
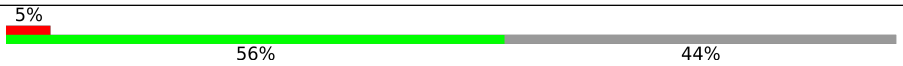
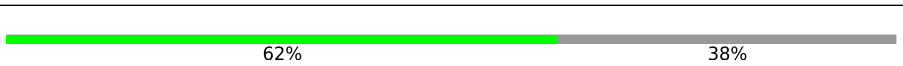
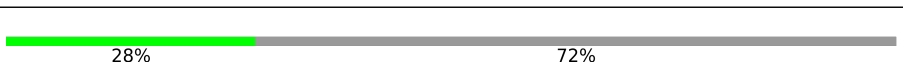
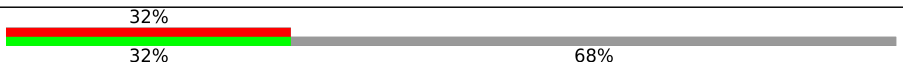
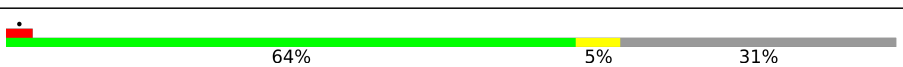
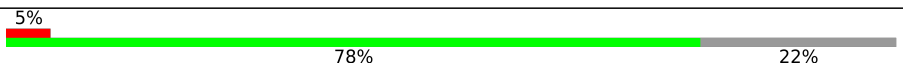
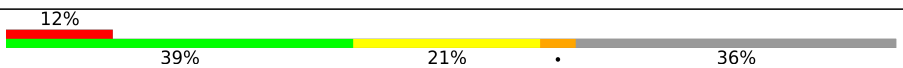
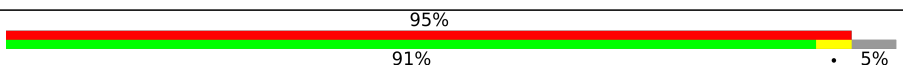
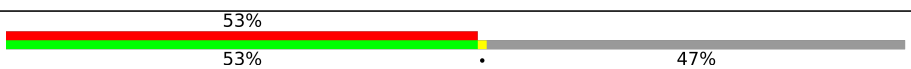
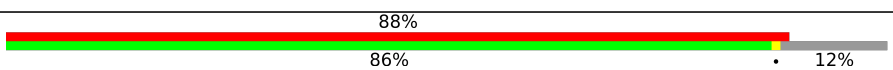
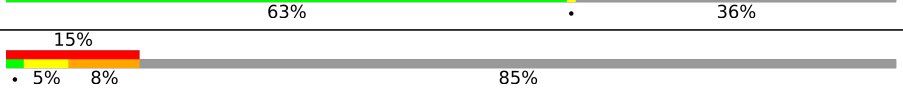
Mol	Chain	Length	Quality of chain
5	m	86	
6	R	92	
6	c	92	
6	l	92	
7	S	76	
7	d	76	
7	n	76	
8	T	126	
8	e	126	
8	h	126	
9	U	231	
9	f	231	
9	i	231	
10	V	119	
10	g	119	
10	j	119	
11	F	107	
12	q	95	
13	r	102	
14	s	139	
15	t	91	
16	x	80	
17	y	103	
18	z	96	
19	G	274	

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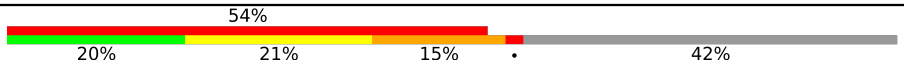
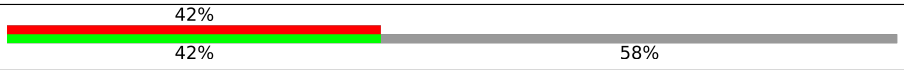
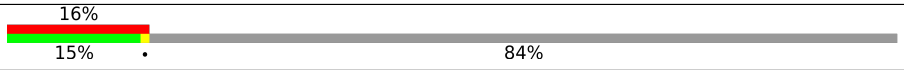
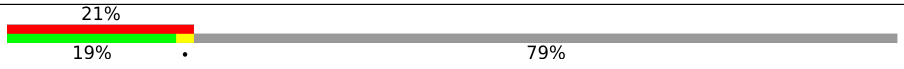
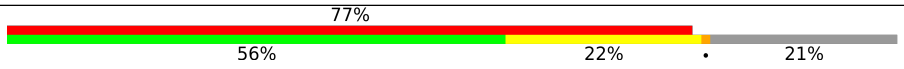
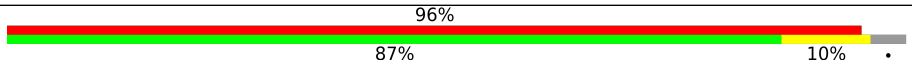
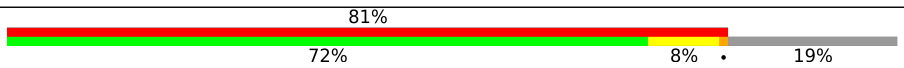
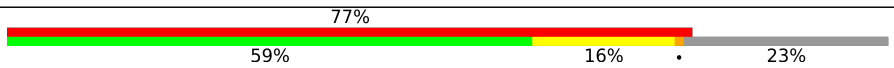
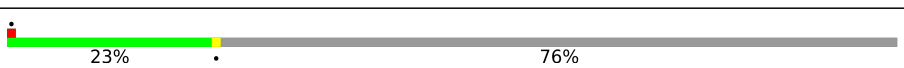
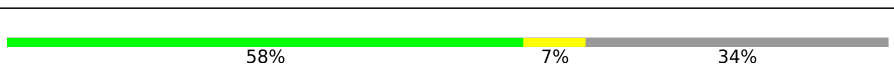
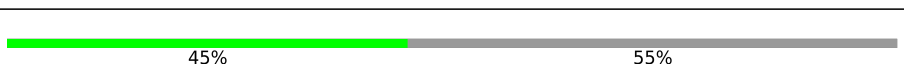
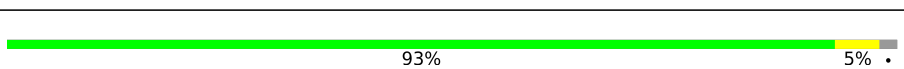
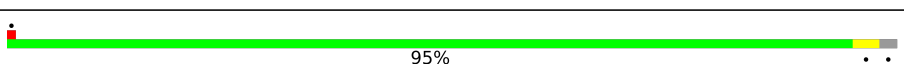
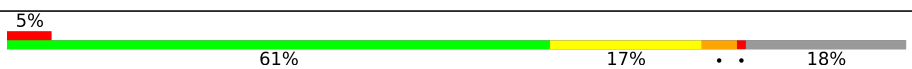
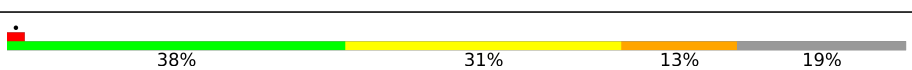
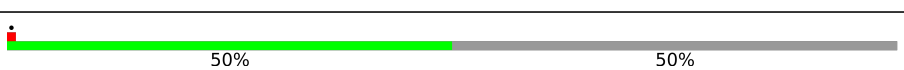
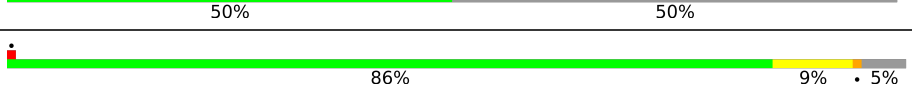
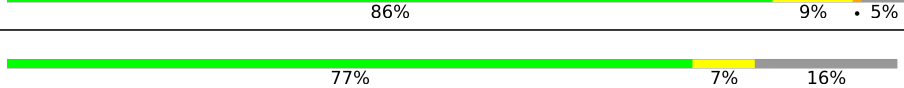
Mol	Chain	Length	Quality of chain
20	H	188	
21	o	255	
22	p	225	
23	u	793	
24	v	464	
25	w	501	
26	1	1304	
27	2	895	
28	3	1217	
29	4	424	
30	5	125	
31	6	110	
32	7	86	
33	J	683	
34	K	522	
35	N	941	
36	L	499	
37	M	128	
38	O	142	
39	W	565	
40	I	144	
41	X	820	
42	A	2335	
43	C	972	

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 63369 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	B	115	2419	1084	402	818	115	0	0

- Molecule 2 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	1874	7496	3748	1874	1874	0	0

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	299	1196	598	299	299	0	0

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	a	78	318	162	78	78	0	0
4	k	85	340	170	85	85	0	0
4	P	74	300	152	74	74	0	0

- Molecule 5 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	b	73	300	154	73	73	0	0
5	m	74	296	148	74	74	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	Q	71	Total 292	C 150	N 71	O 71	0	0

- Molecule 6 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	c	78	Total 314	C 158	N 78	O 78	0	0
6	l	79	Total 316	C 158	N 79	O 79	0	0
6	R	78	Total 314	C 158	N 78	O 78	0	0

- Molecule 7 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	d	69	Total 282	C 144	N 69	O 69	0	0
7	n	68	Total 272	C 136	N 68	O 68	0	0
7	S	73	Total 298	C 152	N 73	O 73	0	0

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	e	78	Total 318	C 162	N 78	O 78	0	0
8	h	80	Total 320	C 160	N 80	O 80	0	0
8	T	71	Total 288	C 146	N 71	O 71	0	0

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	f	64	Total 260	C 132	N 64	O 64	0	0
9	i	73	Total 292	C 146	N 73	O 73	0	0
9	U	64	Total 256	C 128	N 64	O 64	0	0

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	g	93	Total 380	C 194	N 93	O 93	0	0
10	j	82	Total 328	C 164	N 82	O 82	0	0
10	V	82	Total 334	C 170	N 82	O 82	0	0

- Molecule 11 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	69	Total 1470	C 656	N 259	O 486	P 69	0	0

- Molecule 12 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	q	90	Total 360	C 180	N 90	O 90	0	0

- Molecule 13 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	r	75	Total 300	C 150	N 75	O 75	0	0

- Molecule 14 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	s	74	Total 296	C 148	N 74	O 74	0	0

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	t	75	Total 300	C 150	N 75	O 75	0	0

- Molecule 16 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	x	70	Total 280	C 140	N 70	O 70	0	0

- Molecule 17 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	y	65	Total 260	C 130	N 65	O 65	0	0

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	z	61	Total 244	C 122	N 61	O 61	0	0

- Molecule 19 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	42	Total 862	C 387	N 122	O 311	P 42	0	0

- Molecule 20 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	109	Total 2311	C 1032	N 396	O 774	P 109	0	0

- Molecule 21 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	o	162	Total 648	C 324	N 162	O 162	0	0

- Molecule 22 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
22	p	94	Total 376	C 188	N 94	O 94	0	0

- Molecule 23 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	u	124	Total 496	C 248	N 124	O 124	0	0

- Molecule 24 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	v	99	Total 396	C 198	N 99	O 99	0	0

- Molecule 25 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	w	443	Total 1773	C 887	N 443	O 443	0	0

- Molecule 26 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	1	1030	Total 4120	C 2060	N 1030	O 1030	0	0

- Molecule 27 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	2	186	Total 744	C 372	N 186	O 186	0	0

- Molecule 28 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	3	1174	Total 4696	C 2348	N 1174	O 1174	0	0

- Molecule 29 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	4	78	Total 312	C 156	N 78	O 78	0	0

- Molecule 30 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	5	108	Total 432	C 216	N 108	O 108	0	0

- Molecule 31 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	6	89	Total 356	C 178	N 89	O 89	0	0

- Molecule 32 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	7	66	Total 264	C 132	N 66	O 66	0	0

- Molecule 33 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	J	167	Total 668	C 334	N 167	O 167	0	0

- Molecule 34 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	K	343	Total 1371	C 686	N 343	O 342	0	0

- Molecule 35 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	N	579	Total 2316	C 1158	N 579	O 579	0	0

- Molecule 36 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	L	226	Total 904	C 452	N 226	O 226	0	0

- Molecule 37 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	M	125	Total 500	C 250	N 125	O 125	0	0

- Molecule 38 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	O	139	Total 556	C 278	N 139	O 139	0	0

- Molecule 39 is a protein called U4/U6.U5 tri-snRNP-associated protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	W	463	Total 1852	C 926	N 463	O 463	0	0

- Molecule 40 is a RNA chain called U4snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	I	117	Total 2491	C 1112	N 439	O 823	P 117	0	0

- Molecule 41 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	X	414	Total 1661	C 833	N 414	O 414	0	0

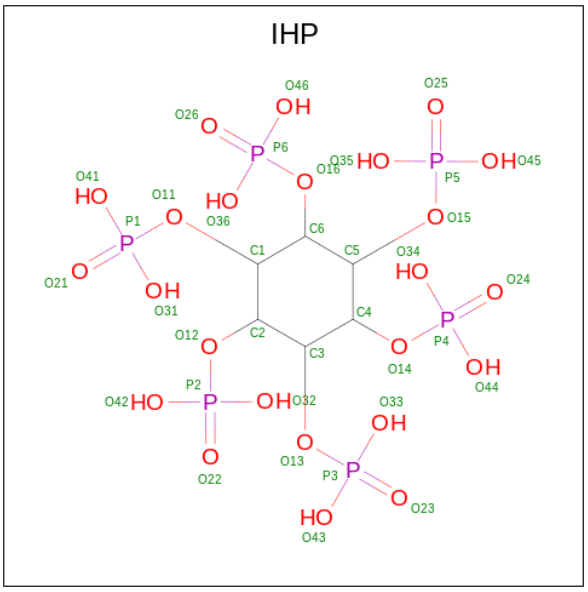
- Molecule 42 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	A	2221	Total 8884	C 4442	N 2221	O 2221	0	0

- Molecule 43 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

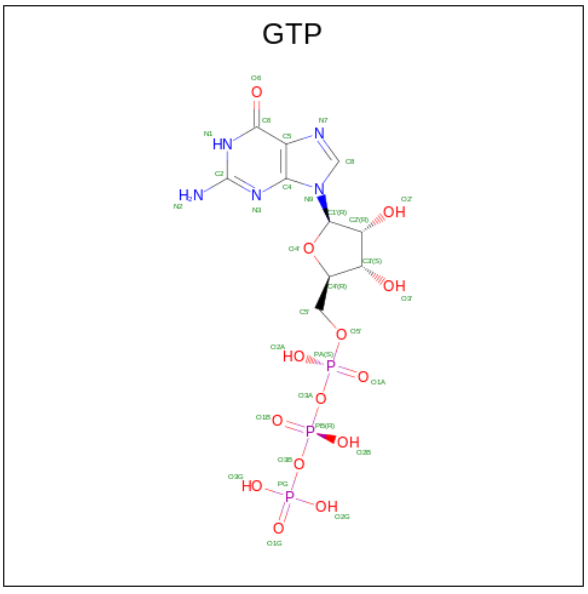
Mol	Chain	Residues	Atoms				AltConf	Trace
43	C	818	Total 3272	C 1636	N 818	O 818	0	0

- Molecule 44 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 45 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

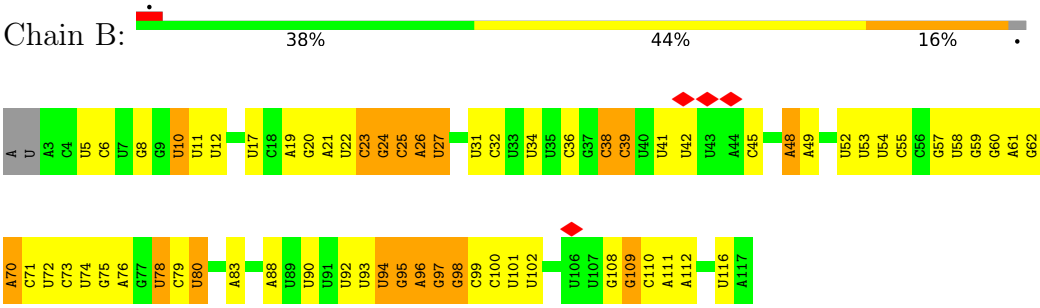
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
46	C	1	1	1	0

3 Residue-property plots (i)

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

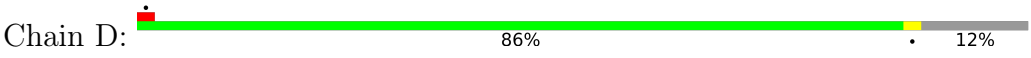
• Molecule 1: U5snRNA

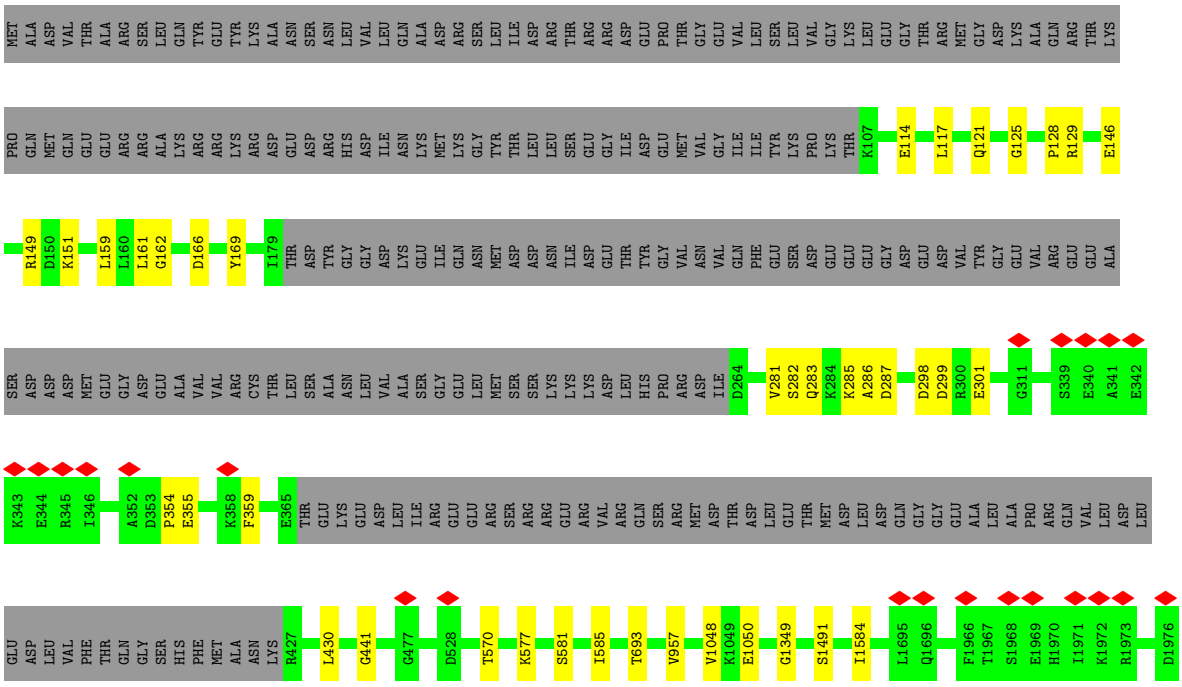
Chain B:

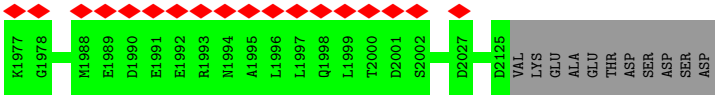


• Molecule 2: U5 small nuclear ribonucleoprotein 200 kDa helicase

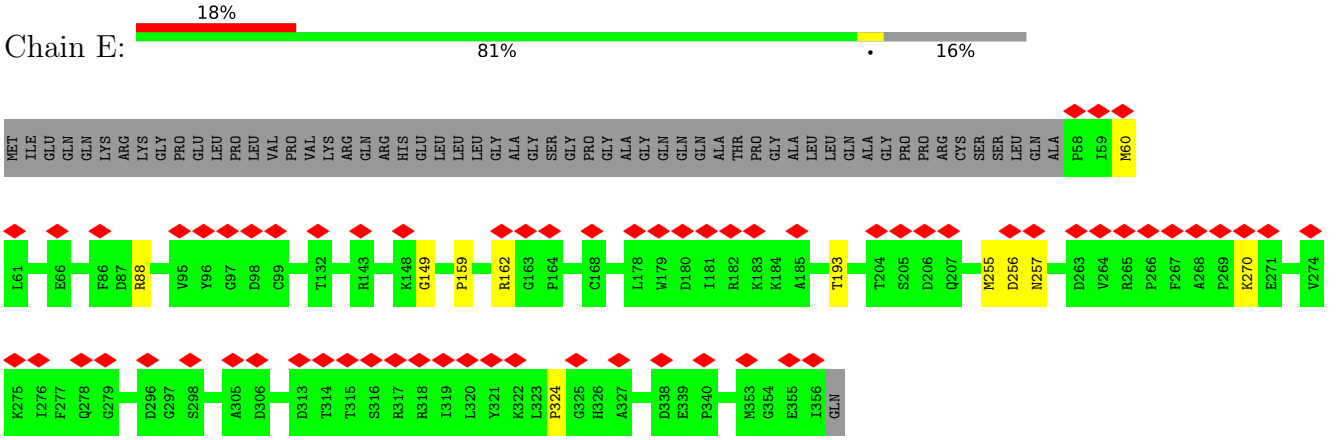
Chain D:



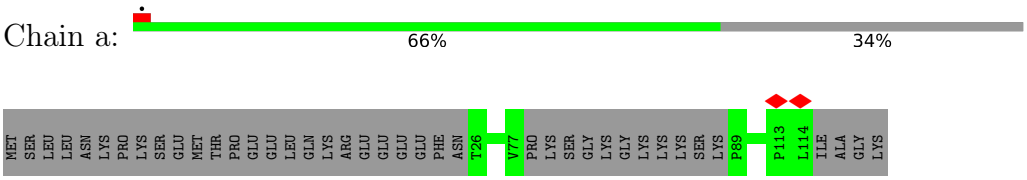




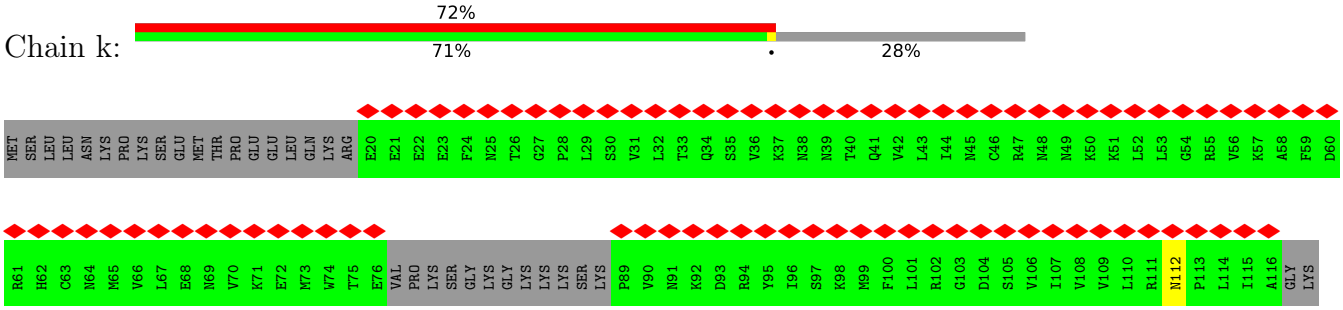
• Molecule 3: U5 small nuclear ribonucleoprotein 40 kDa protein



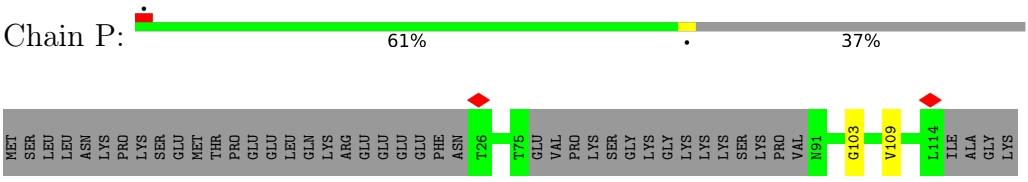
• Molecule 4: Small nuclear ribonucleoprotein Sm D2



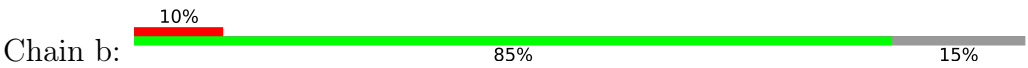
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

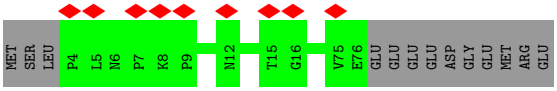


• Molecule 4: Small nuclear ribonucleoprotein Sm D2

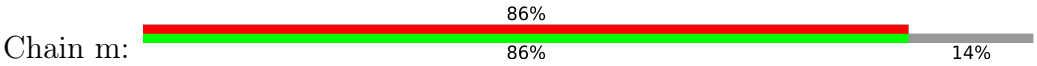


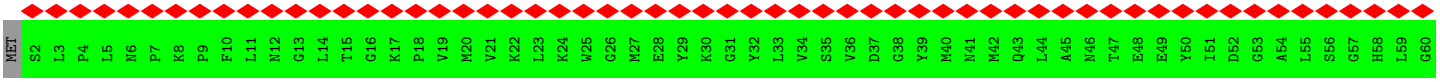
• Molecule 5: Small nuclear ribonucleoprotein F

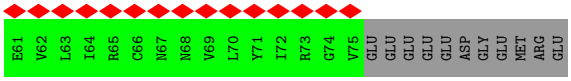




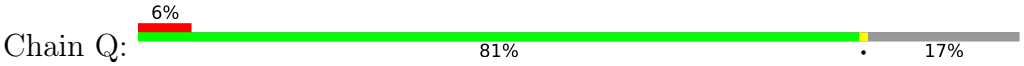
• Molecule 5: Small nuclear ribonucleoprotein F

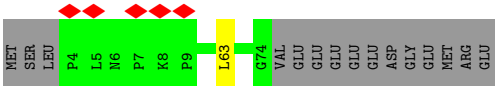




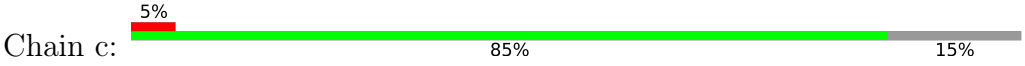


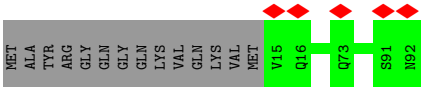
• Molecule 5: Small nuclear ribonucleoprotein F



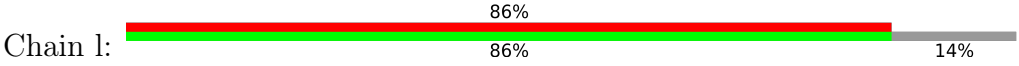


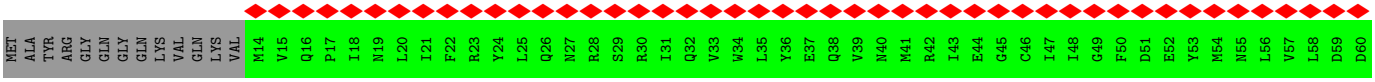
• Molecule 6: Small nuclear ribonucleoprotein E

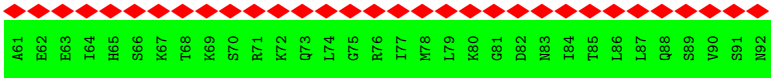




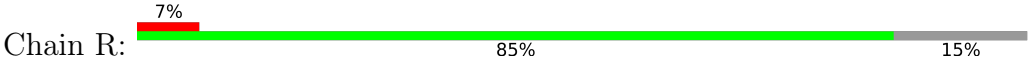
• Molecule 6: Small nuclear ribonucleoprotein E

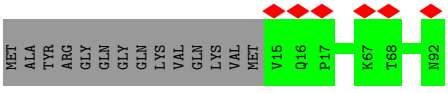






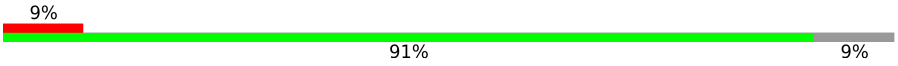
• Molecule 6: Small nuclear ribonucleoprotein E

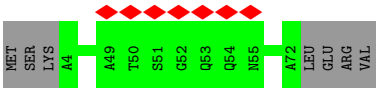




• Molecule 7: Small nuclear ribonucleoprotein G

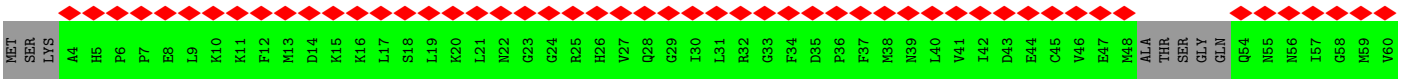
Chain d:

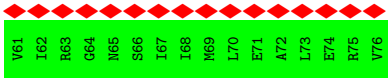




• Molecule 7: Small nuclear ribonucleoprotein G

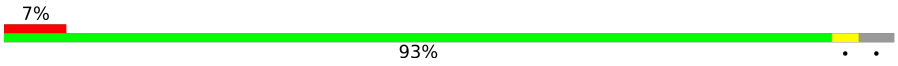
Chain n:

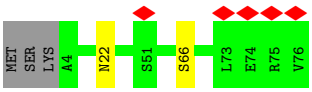




• Molecule 7: Small nuclear ribonucleoprotein G

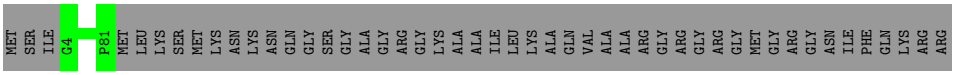
Chain S:





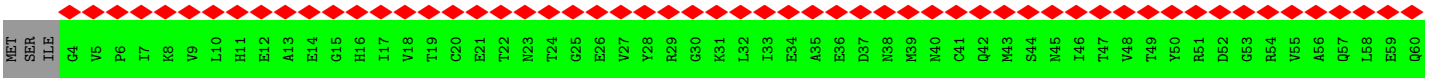
• Molecule 8: Small nuclear ribonucleoprotein Sm D3

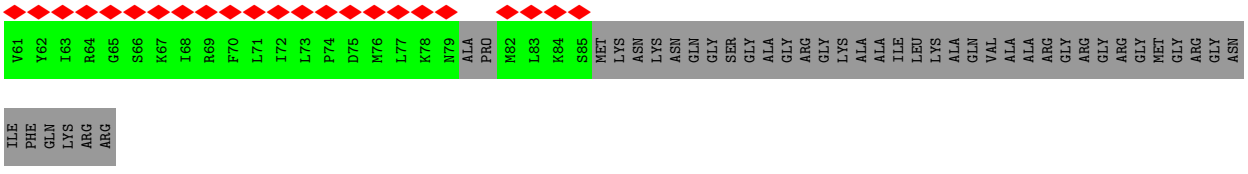
Chain e:



• Molecule 8: Small nuclear ribonucleoprotein Sm D3

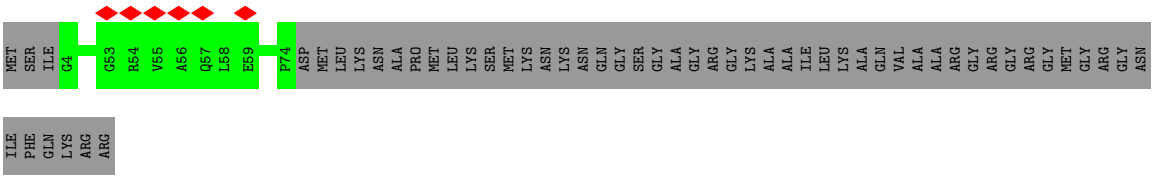
Chain h:





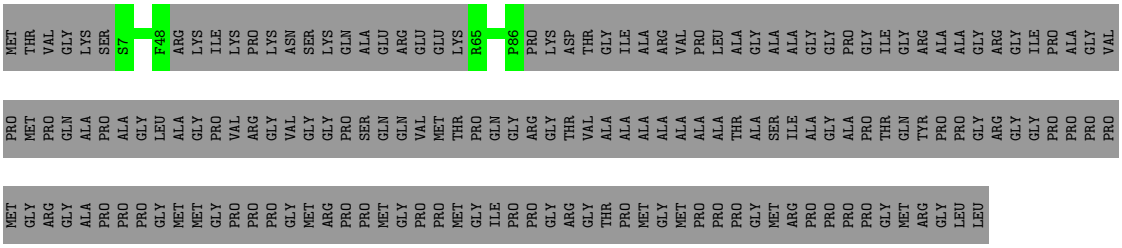
• Molecule 8: Small nuclear ribonucleoprotein Sm D3

Chain T:



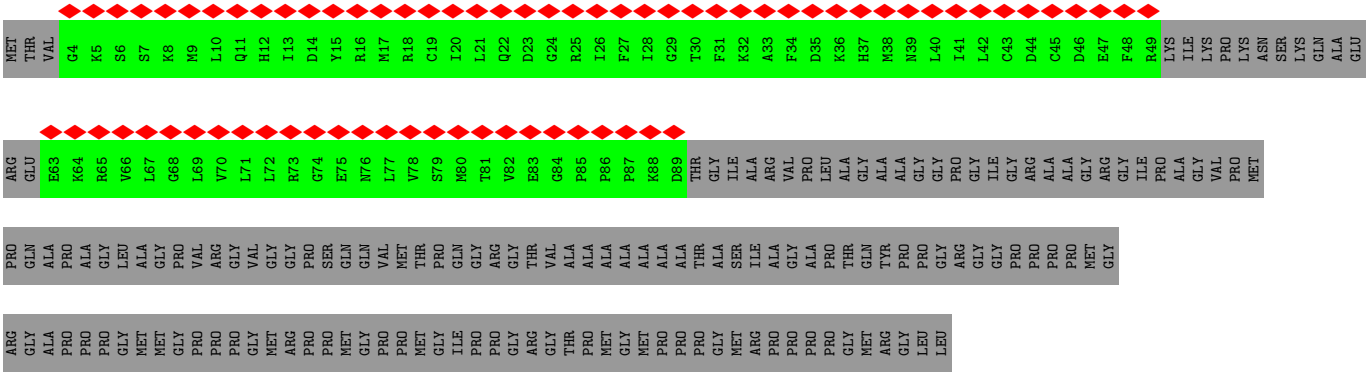
• Molecule 9: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain f:



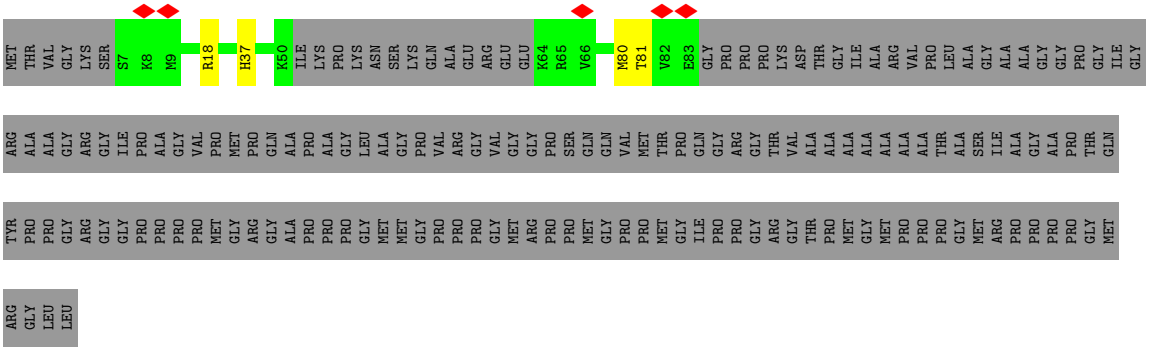
• Molecule 9: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain i:



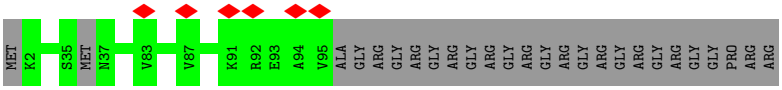
• Molecule 9: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain U:



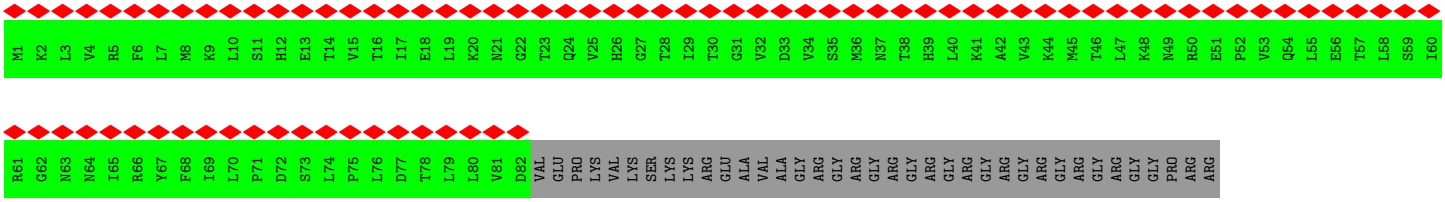
• Molecule 10: Small nuclear ribonucleoprotein Sm D1

Chain g:



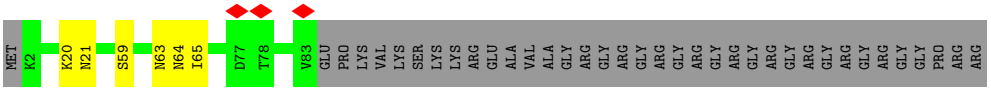
• Molecule 10: Small nuclear ribonucleoprotein Sm D1

Chain j:



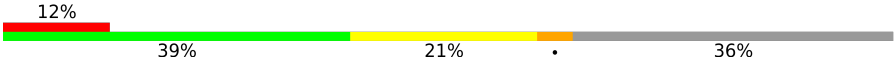
• Molecule 10: Small nuclear ribonucleoprotein Sm D1

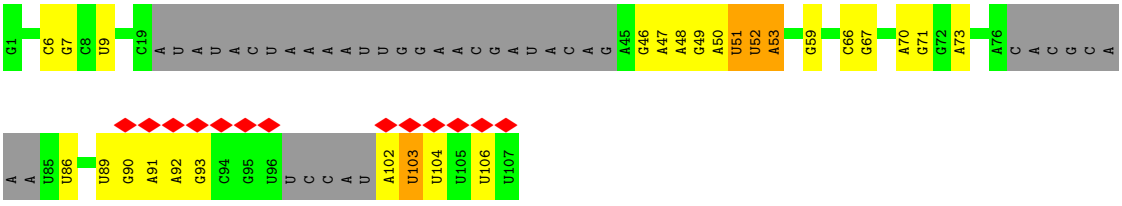
Chain V:



• Molecule 11: U6snRNA

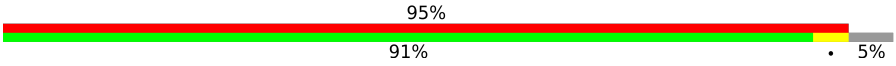
Chain F:

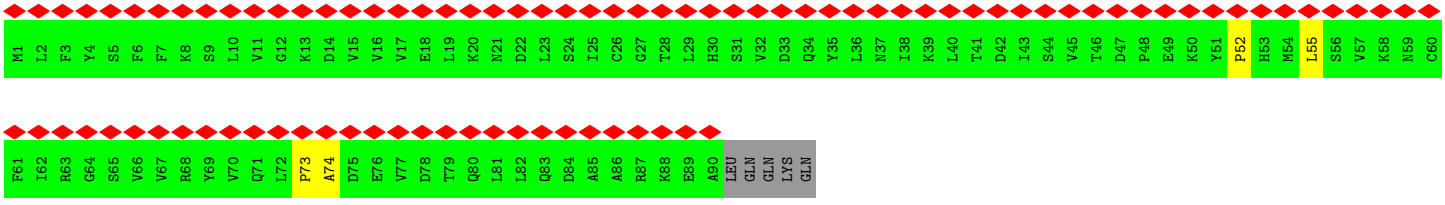




• Molecule 12: U6 snRNA-associated Sm-like protein LSm2

Chain q:

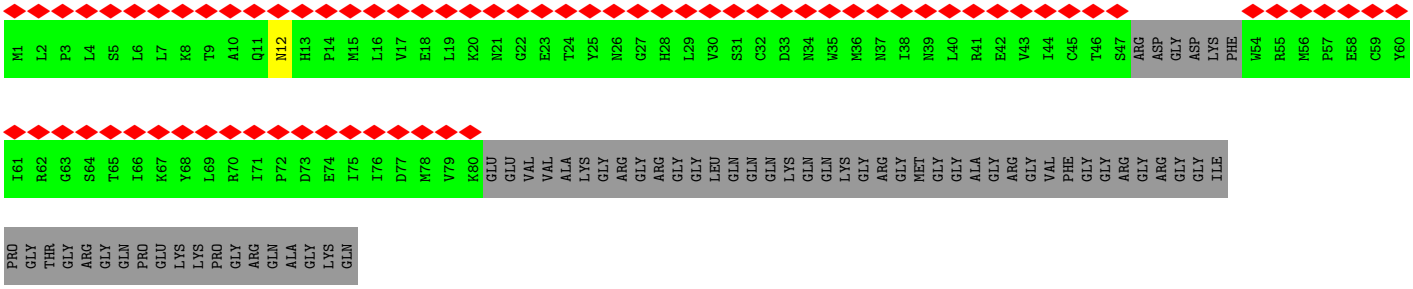




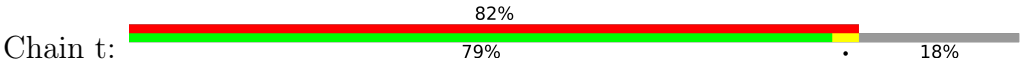
• Molecule 13: U6 snRNA-associated Sm-like protein LSm3

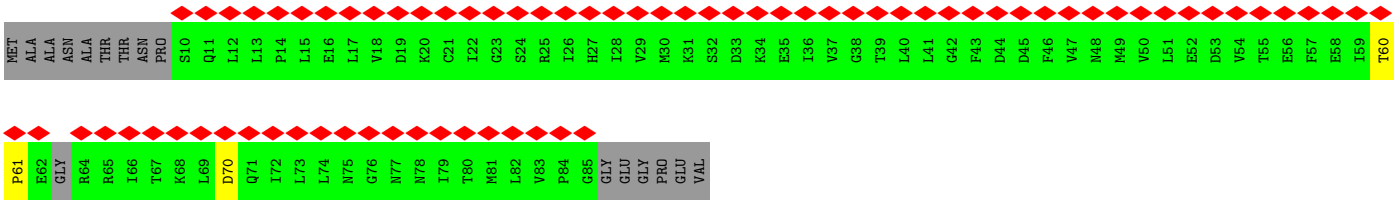
Chain r:

• Molecule 14: U6 snRNA-associated Sm-like protein LSm4

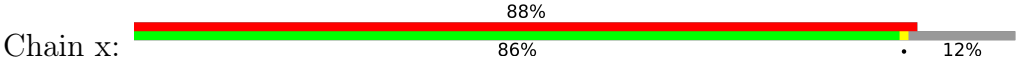


• Molecule 15: U6 snRNA-associated Sm-like protein LSm5

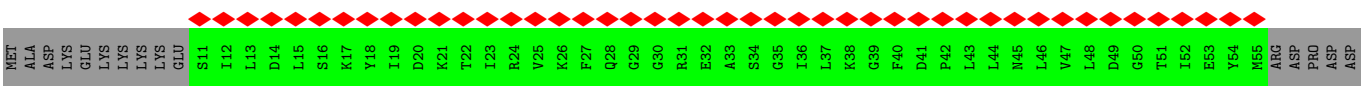


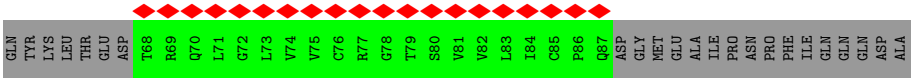


• Molecule 16: U6 snRNA-associated Sm-like protein LSm6



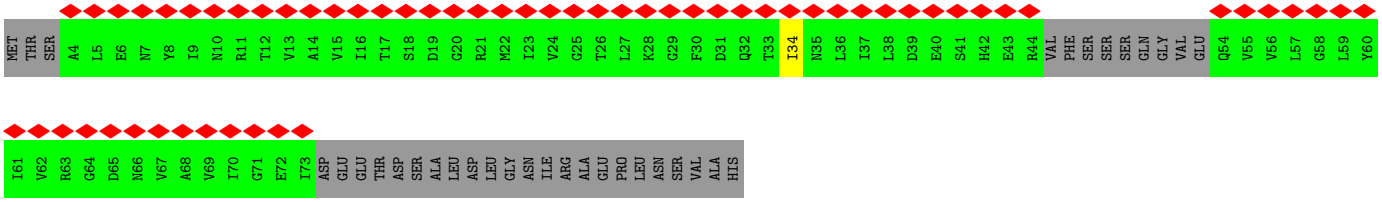
• Molecule 17: U6 snRNA-associated Sm-like protein LSm7





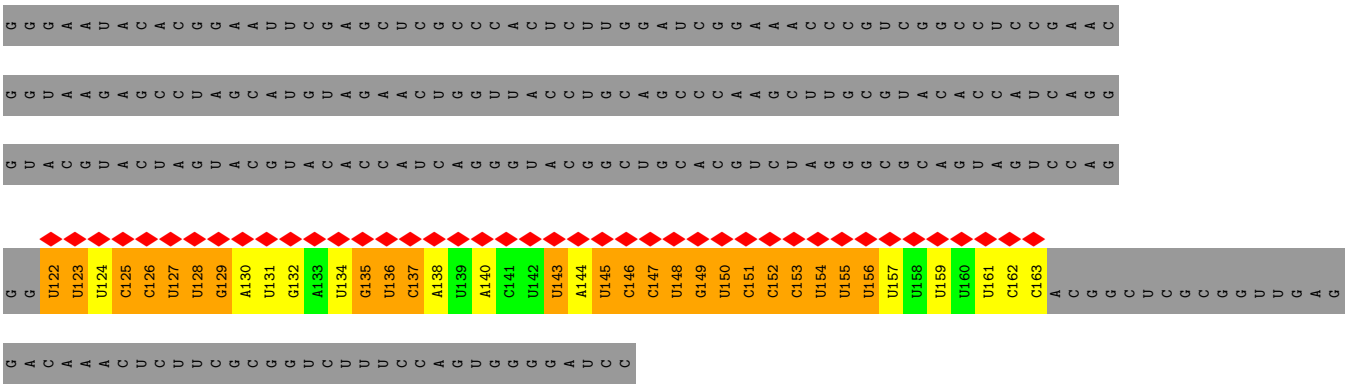
• Molecule 18: U6 snRNA-associated Sm-like protein LSm8

Chain z:



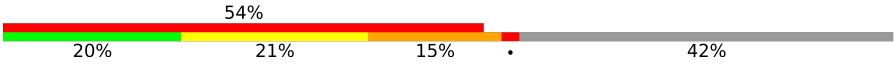
• Molecule 19: pre-mRNA

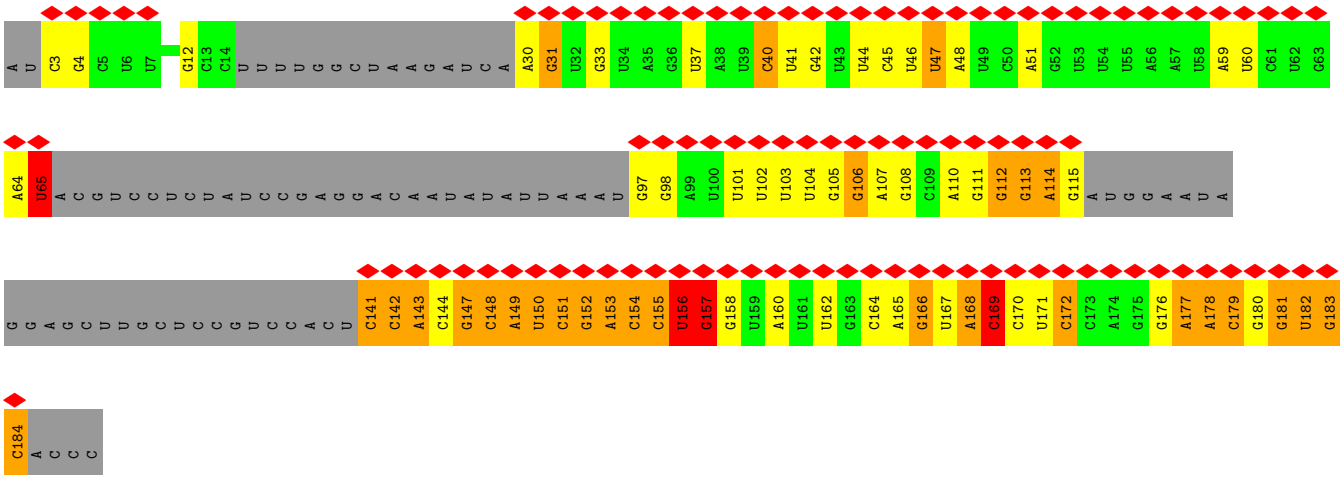
Chain G:



• Molecule 20: U2snRNA

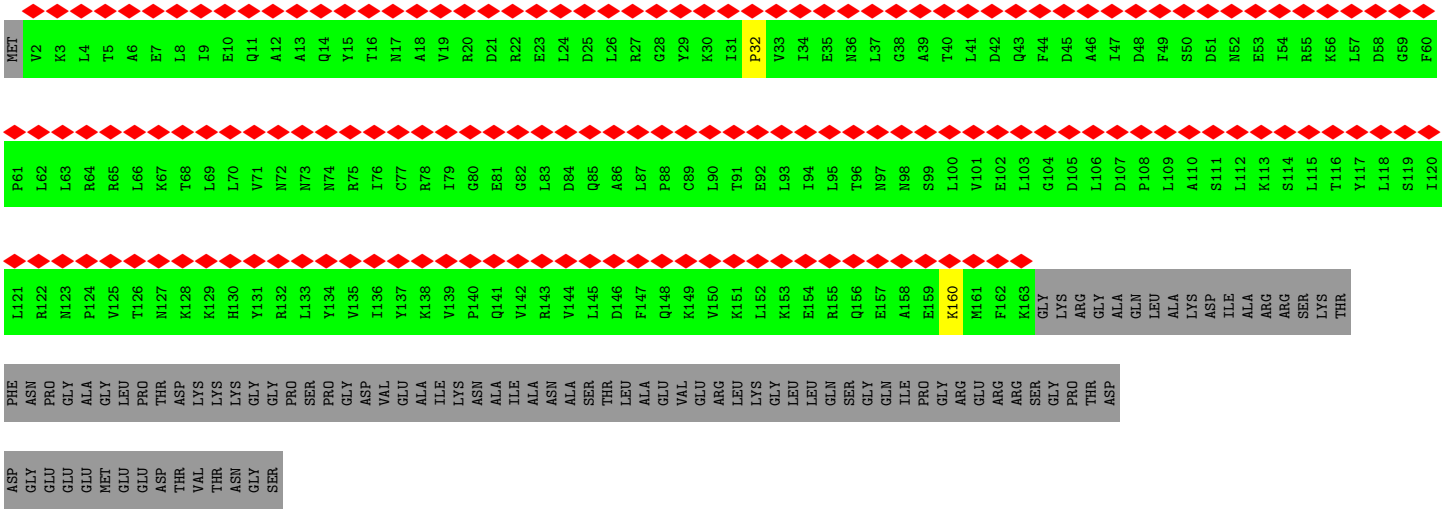
Chain H:





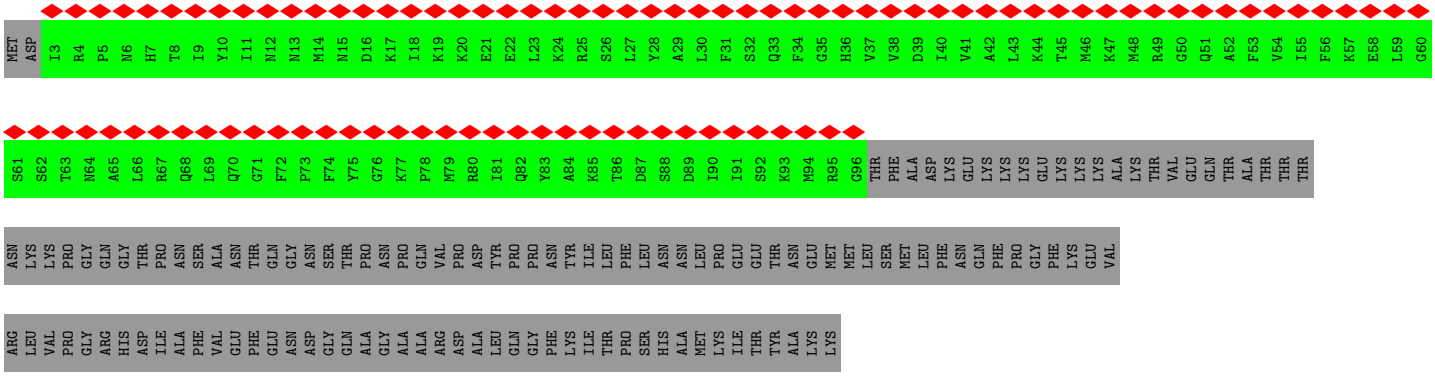
• Molecule 21: U2 small nuclear ribonucleoprotein A'

Chain o:



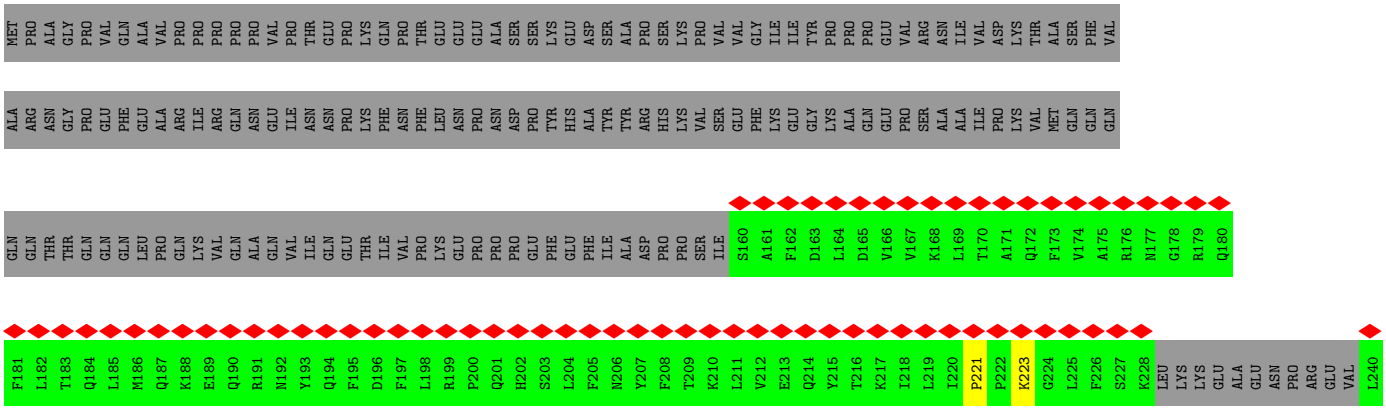
• Molecule 22: U2 small nuclear ribonucleoprotein B”

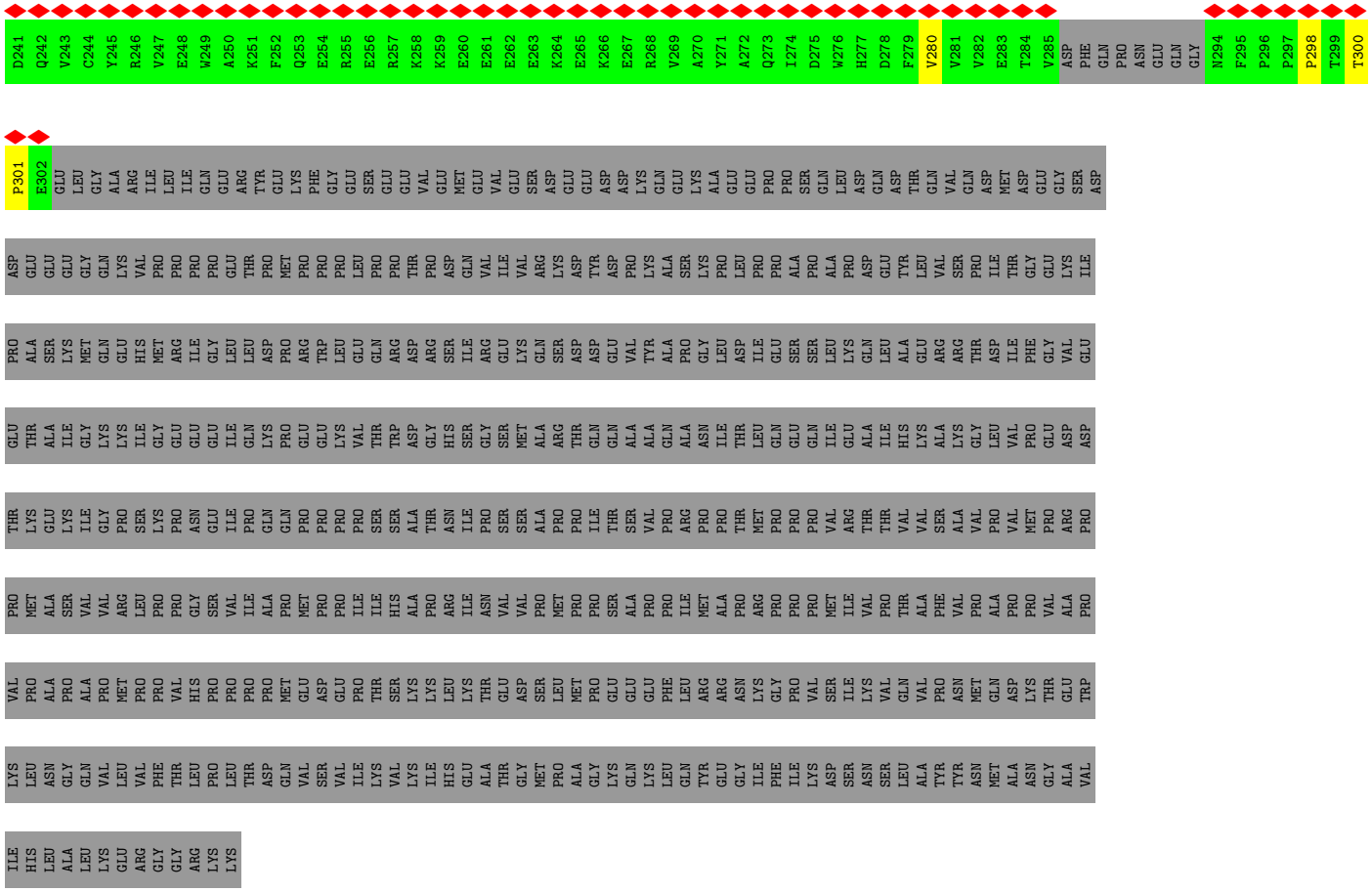
Chain p:



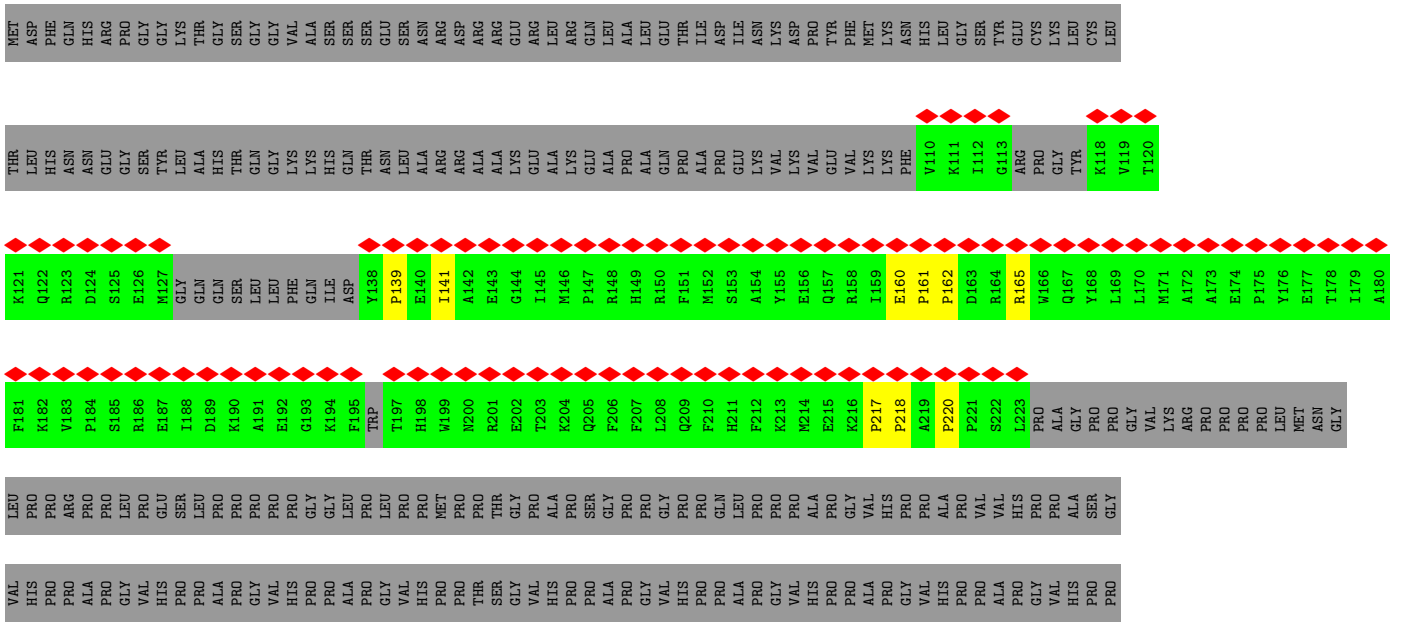
• Molecule 23: Splicing factor 3A subunit 1

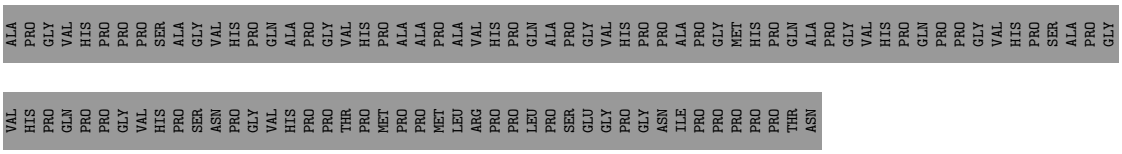
Chain u:





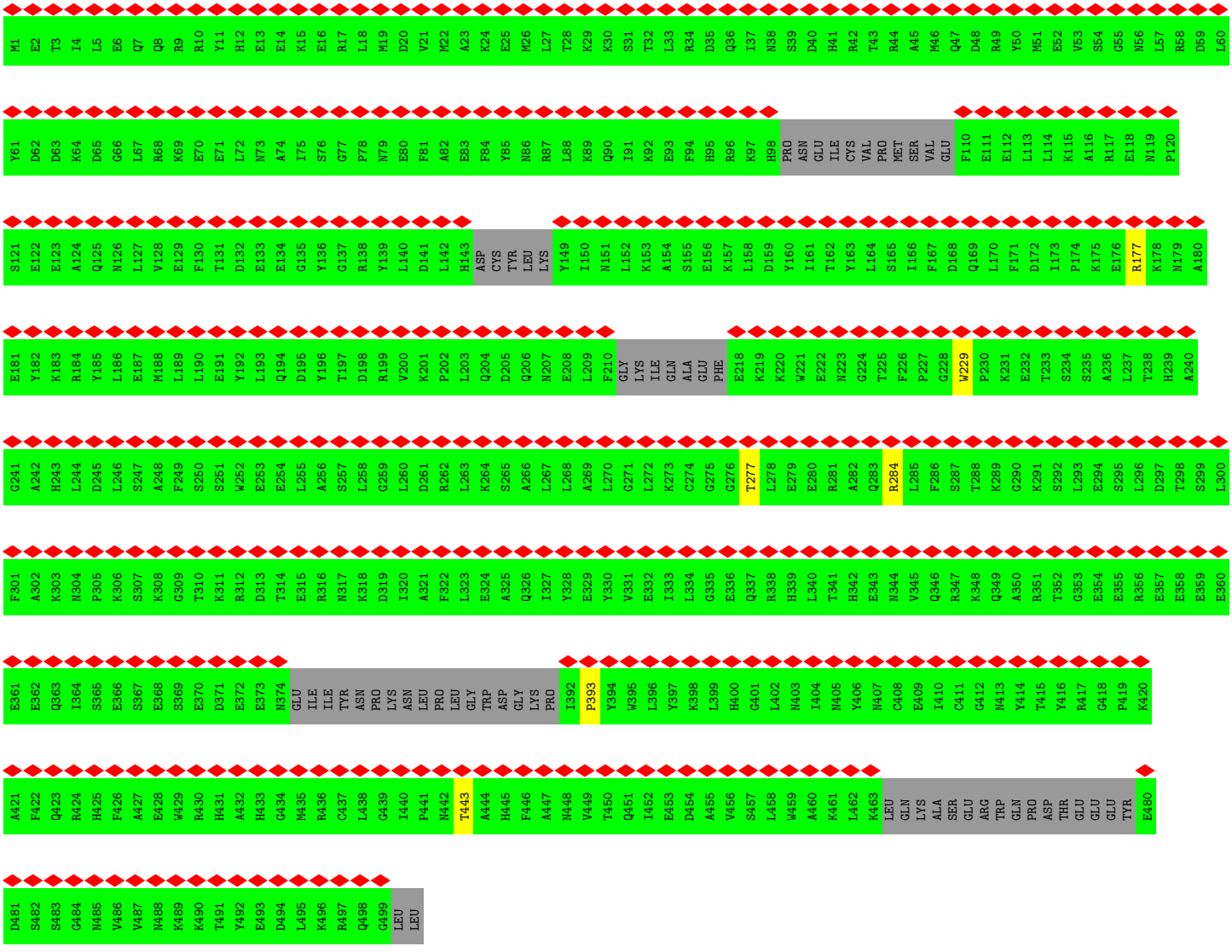
- Molecule 24: Splicing factor 3A subunit 2





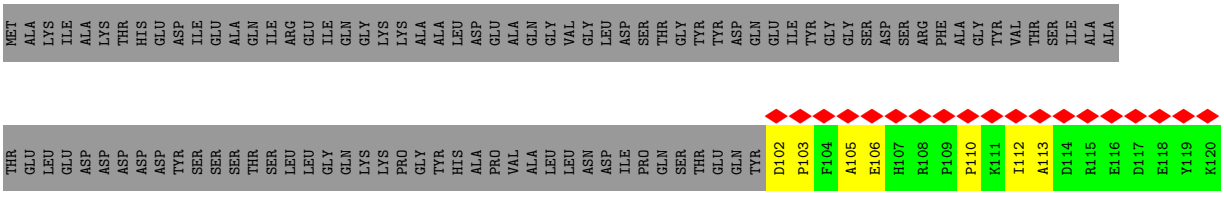
• Molecule 25: Splicing factor 3A subunit 3

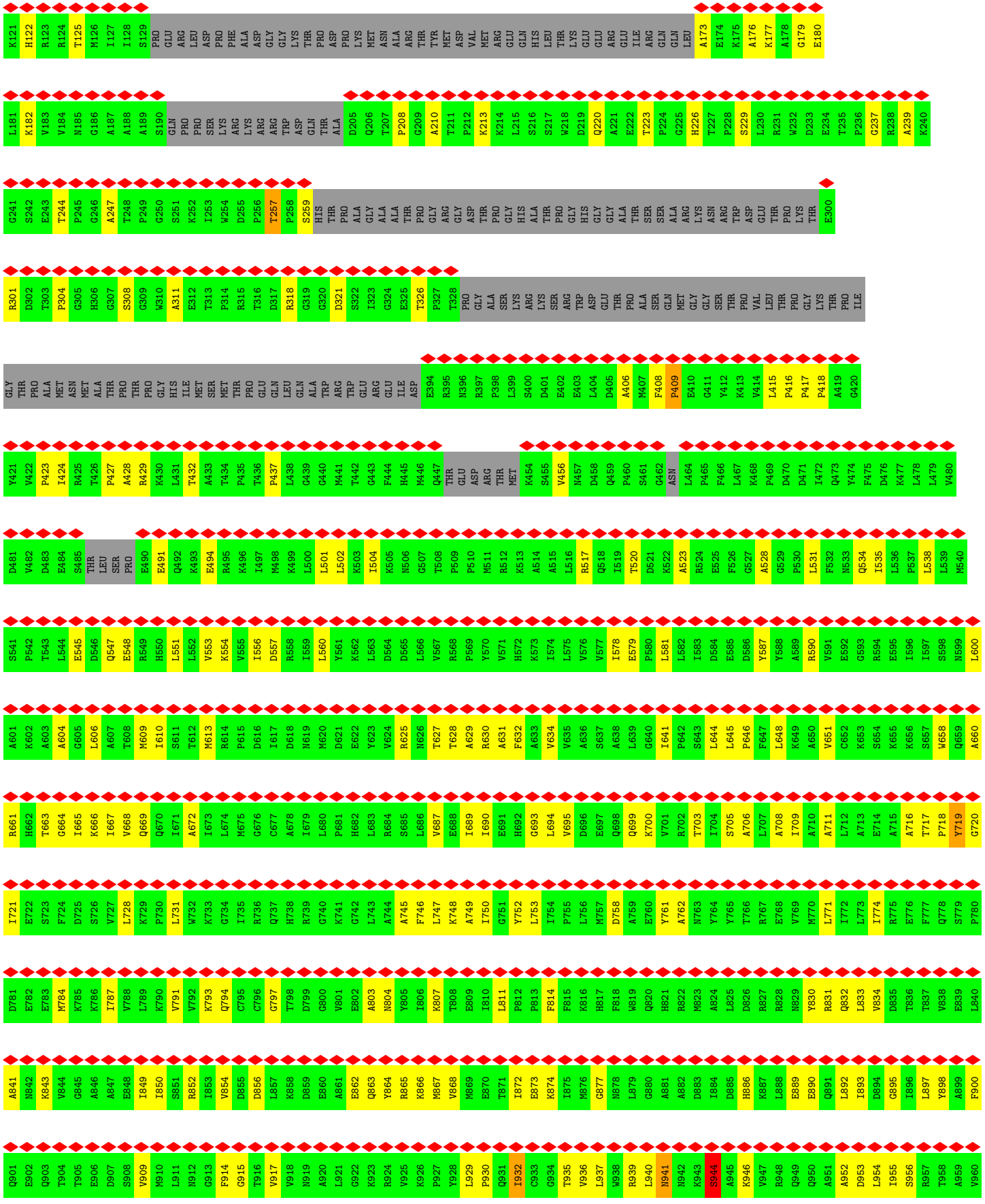
Chain w:



• Molecule 26: Splicing factor 3B subunit 1

Chain 1:

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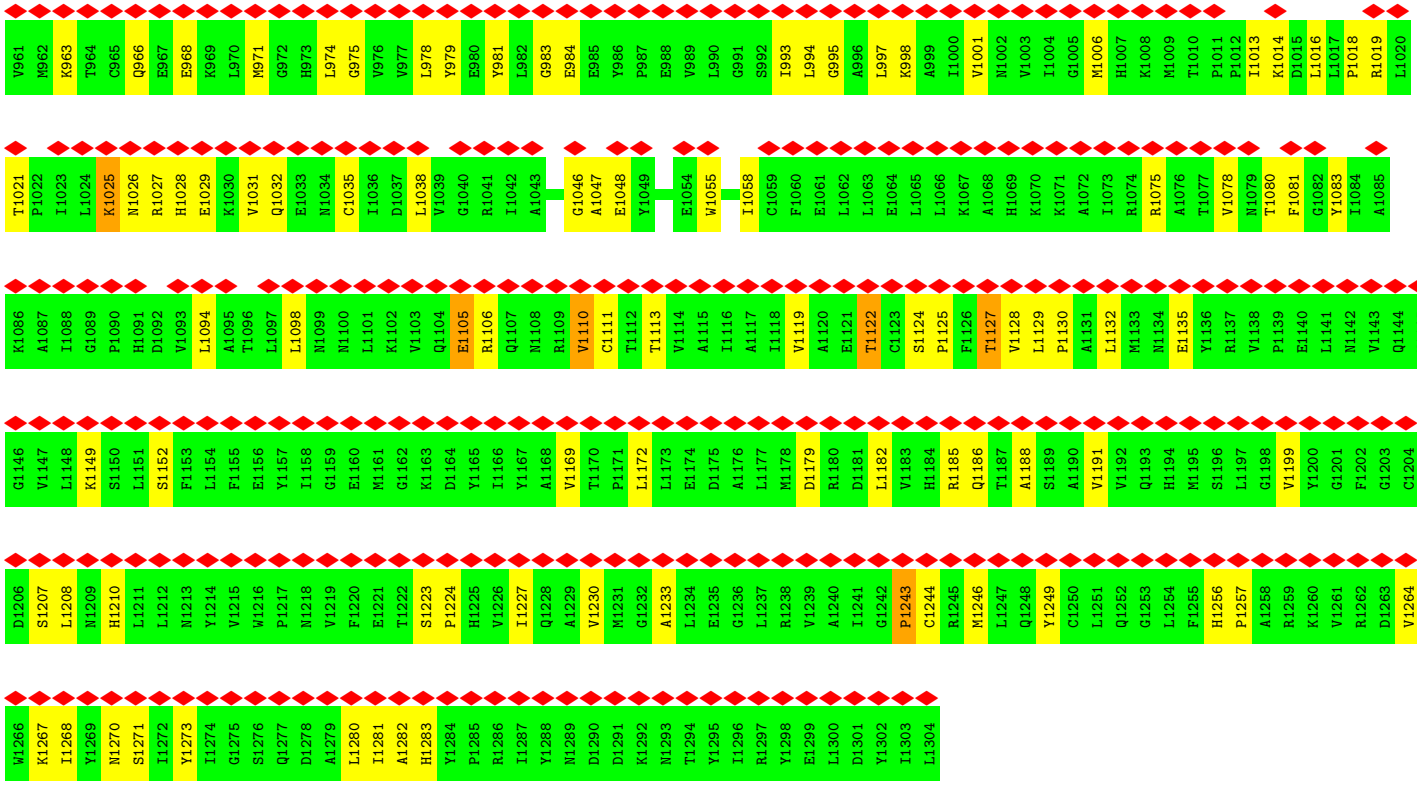
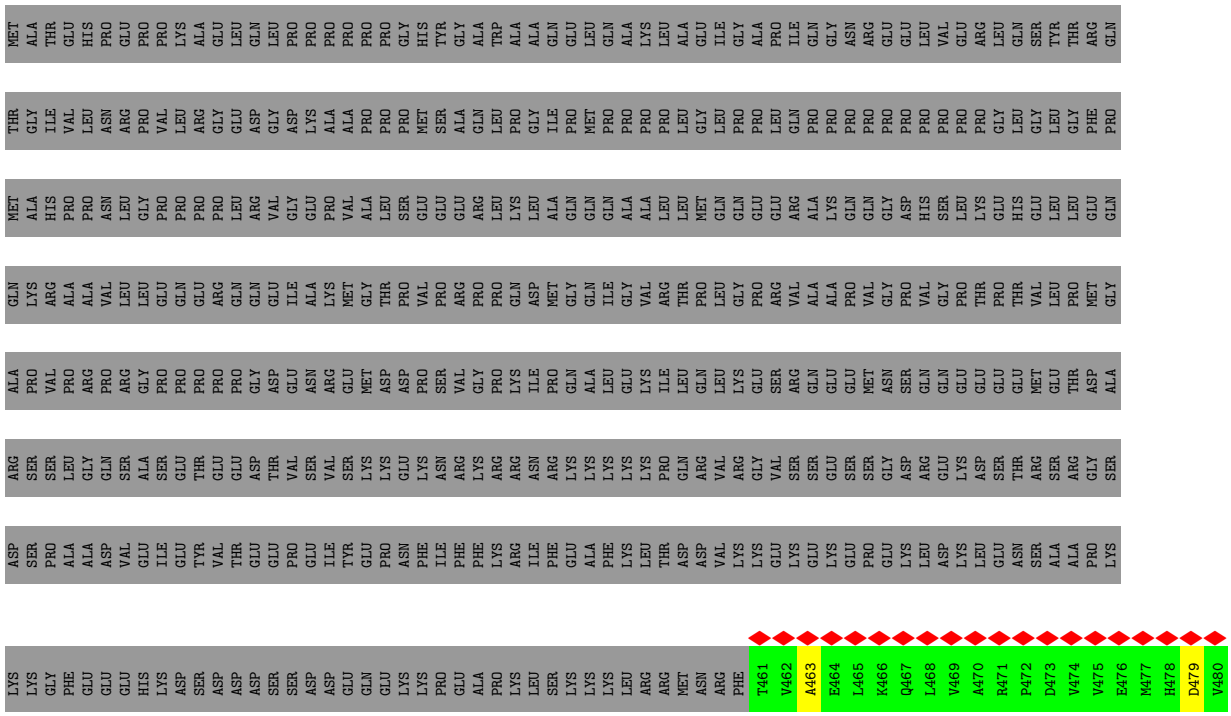
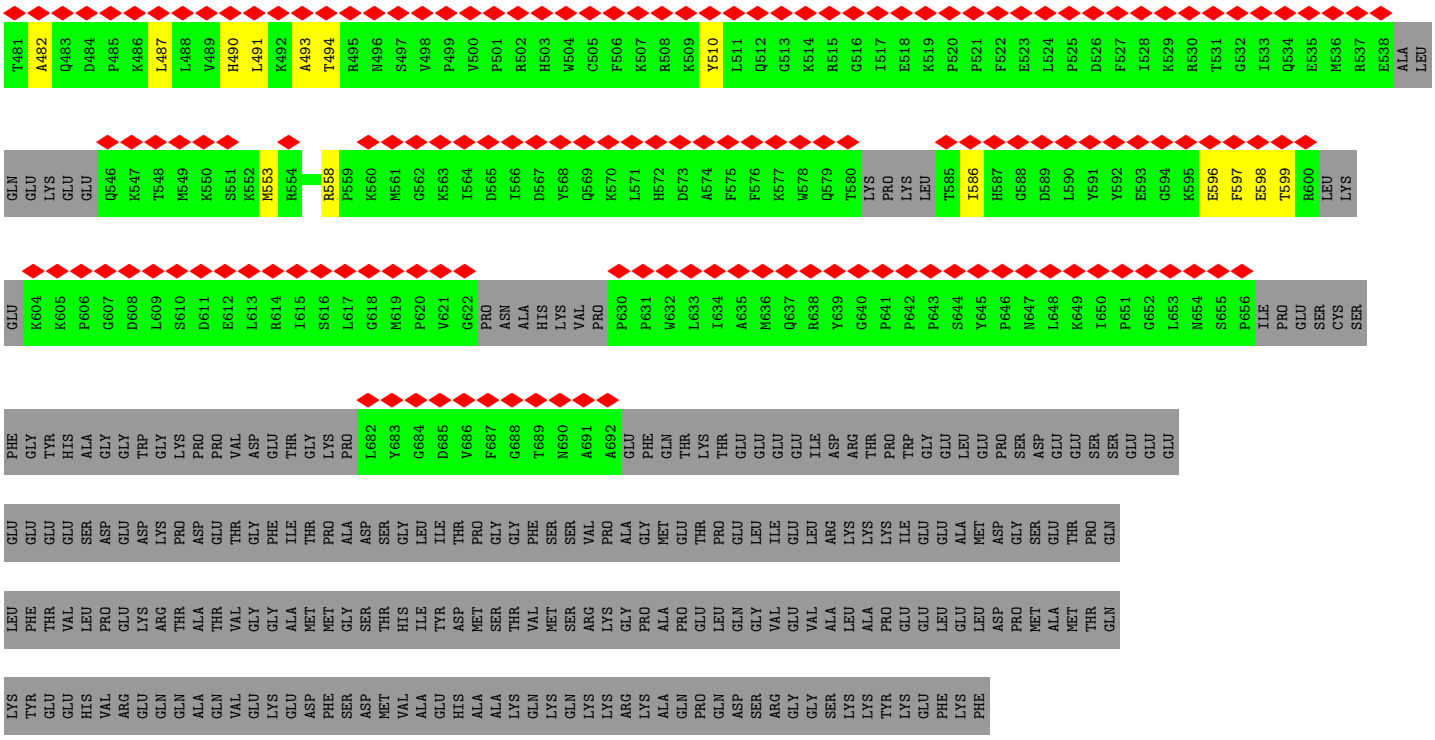
L181 K182 V183 V184 N185 G186 A187 A188 A189 S190 GLN PRO PRO SER LYS ARG LYS ARG ARG TRP ASP GLN THR ALA D205 Q206 T207 P208 G209 A210 T211 P212 K213 K214 L215 S216 S217 W218 D219 Q220 A221 E222 T223 P224 G225 H226 T227 P228 S229 L230 R231 W232 D233 E234 T235 P236 G237 R238 A239 K240
G241 S242 E243 T244 P245 G246 A247 T248 P249 G250 S251 K252 I253 W254 D255 P256 T257 P258 S259 HIS THR PRO ALA GLY ALA ALA THR PRO GLY ARG GLY ASP THR PRO GLY HIS ALA THR PRO GLY HIS GLY GLY ALA THR SER SER ALA ARG LYS ASN ARG TRP ASP GLU THR PRO LYS THR E300
R301 D302 T303 P304 G305 H306 G307 S308 G309 W310 A311 E312 T313 P314 R315 T316 D317 R318 G319 G320 D321 S322 I323 G324 E325 T326 P327 T328 PRO GLY ALA SER LYS ARG LYS SER ARG TRP ASP GLU THR PRO ALA SER GLN MET GLY GLY SER THR PRO VAL LEU THR PRO GLY LYS THR PRO ILE
GLY THR PRO ALA MET ASN MET ALA THR PRO THR PRO GLY HIS ILE MET SER MET THR PRO GLU GLN LEU GLN ALA TRP ARG TRP GLU ARG GLU ILE ASP E394 R395 N396 R397 P398 L399 S400 D401 E402 E403 L404 D405 A406 M407 F408 P409 E410 G411 Y412 K413 V414 L415 P416 P417 P418 A419 G420
Y421 V422 P423 I424 R425 T426 P427 A428 R429 K430 L431 T432 A433 T434 P435 T436 P437 L438 G439 G440 M441 T442 G443 F444 H445 M446 Q447 THR GLU ASP ARG THR MET K454 S455 V456 N457 D458 Q459 P460 S461 G462 ASN L464 P465 F466 L467 K468 P469 D470 D471 I472 Q473 Y474 F475 D476 K477 L478 L479 V480
D481 V482 D483 E484 S485 THR LEU SER PRO E490 E491 Q492 K493 E494 R495 K496 I497 M498 K499 L500 L501 L502 K503 I504 K505 N506 G507 T508 P509 P510 M511 R512 K513 A514 A515 L516 R517 Q518 I519 T520 D521 K522 A523 R524 E525 F526 G527 A528 G529 P530 L531 F532 N533 Q534 I535 L536 P537 L538 L539 N540
S541 P542 T543 L544 E545 D546 Q547 E548 R549 H550 L551 L552 V553 K554 V555 I556 D557 R558 I559 L560 Y561 K562 L563 D564 D565 L566 V567 R568 P569 Y570 V571 H572 K573 I574 L575 V576 V577 I578 E579 P580 L581 L582 I583 D584 E585 D586 Y587 Y588 A589 R590 V591 E592 G593 R594 E595 I596 I597 S598 N599 L600
A601 K602 A603 A604 G605 L606 A607 T608 M609 I610 S611 T612 M613 R614 P615 D616 I617 D618 N619 M620 D621 E622 Y623 V624 R625 N626 T627 T628 A629 R630 A631 F632 A633 V634 V635 A636 S637 A638 L639 G640 I641 P642 S643 L644 L645 P646 F647 L648 K649 A650 V651 C652 K653 S654 K655 K656 S657 W658 Q659 A660
R661 H662 T663 G664 I665 K666 I667 V668 Q669 Q670 I671 A672 I673 L674 M675 G676 C677 A678 I679 L680 P681 H682 L683 R684 S685 L686 V687 E688 I689 I690 E691 H692 G693 L694 V695 D696 E697 Q698 Q699 K700 V701 R702 T703 I704 S705 A706 L707 A708 I709 A710 A711 L712 A713 E714 A715 A716 T717 P718 Y719 G720
I721 E722 S723 F724 D725 S726 V727 L728 K729 P730 L731 W732 K733 G734 I735 R736 Q737 H738 R739 G740 K741 G742 L743 A744 A745 F746 L747 K748 A749 I750 G751 Y752 L753 I754 P755 L756 M757 D758 A759 E760 Y761 A762 N763 Y764 Y765 T766 R767 E768 V769 M770 L771 I772 L773 I774 R775 E776 F777 Q778 S779 P780
D781 E782 E783 M784 K785 K786 I787 V788 L789 K790 V791 V792 K793 Q794 C795 C796 G797 T798 D799 G800 V801 E802 A803 N804 Y805 I806 K807 T808 E809 I810 L811 P812 P813 F814 F815 K816 H817 F818 W819 Q820 H821 R822 M823 A824 L825 D826 R827 R828 N829 Y830 R831 Q832 L833 V834 D835 T836 T837 V838 E839 L840
A841 N842 K843 V844 Q845 A846 A847 E848 I849 I850 S851 R852 I853 V854 D855 D856 L857 K858 D859 E860 A861 E862 Q863 Y864 R865 K866 M867 V868 M869 E870 T871 I872 E873 K874 I875 M876 G877 N878 L879 G880 A881 A882 D883 I884 D885 H886 K887 L888 E889 E890 Q891 L892 I893 D894 G895 I896 L897 Y898 A899 F900
Q901 E902 Q903 T904 T905 E906 D907 S908 V909 M910 L911 N912 G913 F914 G915 T916 V917 V918 N919 A920 L921 G922 K923 R924 V925 K926 P927 Y928 L929 P930 Q931 I932 C933 G934 T935 V936 L937 W938 R939 L940 N941 N942 K943 S944 A945 K946 V947 R948 Q949 Q950 A951 A952 D953 L954 I955 S956 R957 T958 A959 V960



- Molecule 27: Splicing factor 3B subunit 2

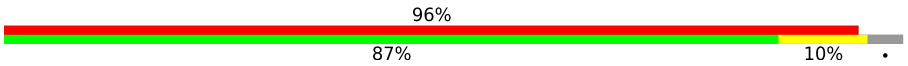
Chain 2: 20% 19% 79%

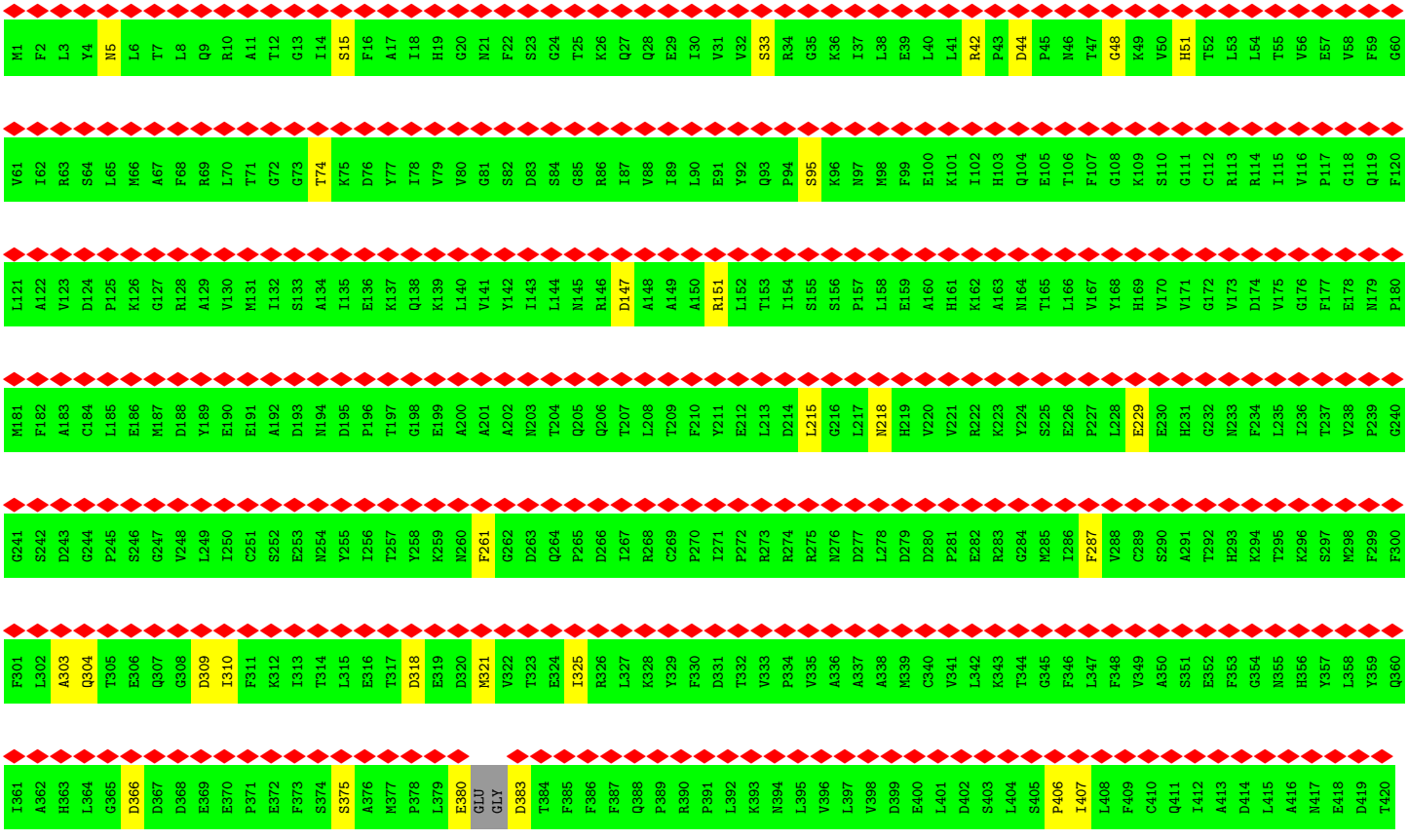


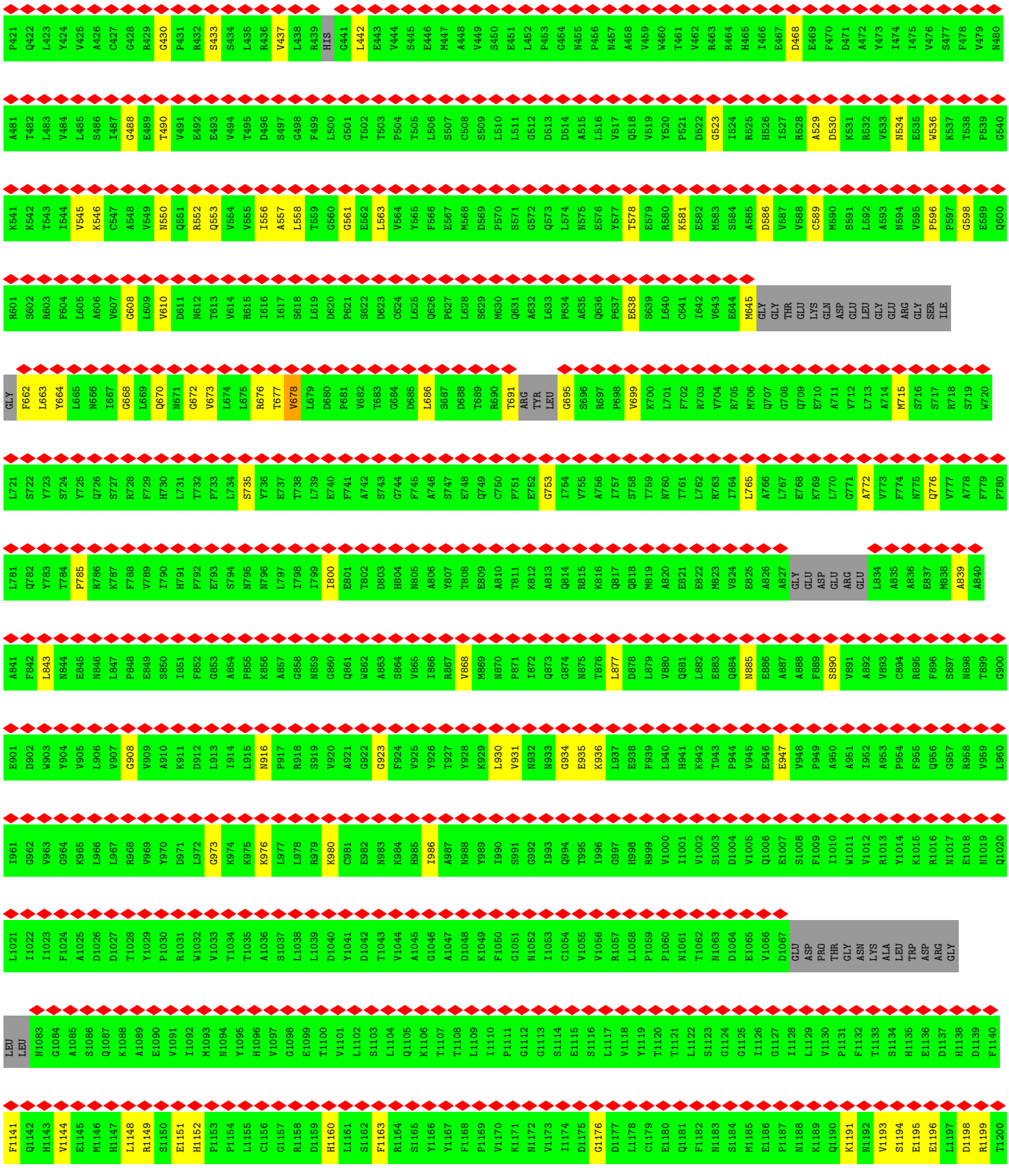


• Molecule 28: Splicing factor 3B subunit 3

Chain 3:



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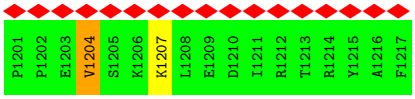
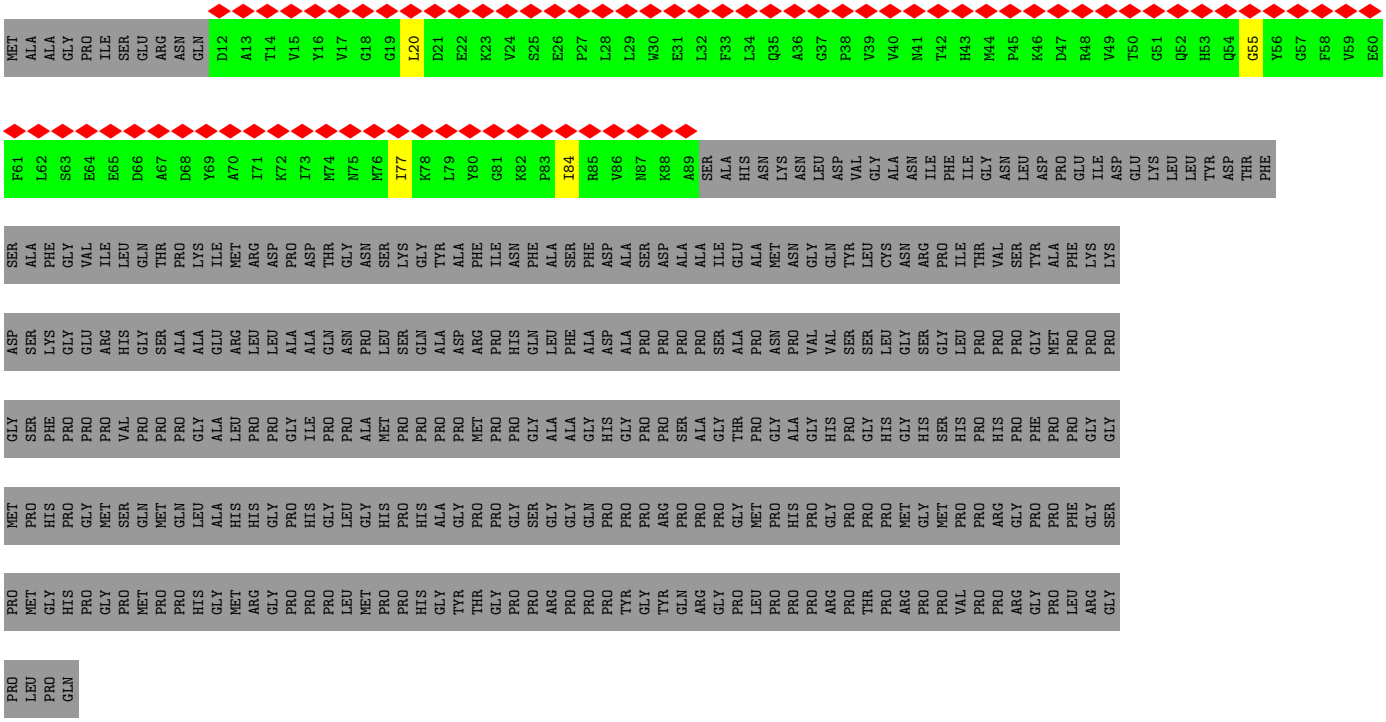
A481 T482 L483 V484 L485 S486 I487 G488 E489 T490 V491 E492 E493 V494 T495 D496 S497 G498 F499 L500 G501 T502 T503 P504 T505 L506 S507 C508 S509 L510 L511 G512 D513 D514 A515 L516 V517 Q518 V519 Y520 P521 D522 G523 I524 R525 H526 I527 R528 A529 D530 K531 R532 V533 N534 E535 W536 K537 T538 P539 G540
K541 K542 T543 I544 V545 K546 C547 A548 V549 N550 Q551 R552 Q553 V554 V555 I556 A557 L558 T559 G560 G561 E562 L563 V564 Y565 F566 E567 M568 D569 P570 S571 G572 Q573 L574 N575 E576 Y577 T578 E579 R580 K581 E582 M583 S584 A585 D586 V587 V588 C589 M590 S591 L592 A593 N594 V595 P596 P597 G598 E599 Q600
R601 S602 R603 F604 L605 A606 V607 G608 L609 V610 D611 N612 T613 V614 R615 I616 I617 S618 L619 D620 P621 S622 D623 G624 L625 Q626 P627 L628 S629 M630 Q631 A632 L633 P634 A635 Q636 P637 E638 S639 L640 C641 I642 V643 E644 M645 GLY GLY THR GLU LYS GLN ASP GLU LEU GLY GLU ARG GLY SER ILE
GLY F662 L663 Y664 L665 N666 I667 G668 L669 Q670 N671 G672 V673 L674 L675 R676 T677 V678 L679 D680 P681 V682 T683 G684 D685 L686 S687 D688 T689 R690 T691 ARG TYR LEU G695 S696 R697 P698 V699 K700 L701 F702 R703 V704 R705 M706 Q707 G708 Q709 E710 A711 V712 L713 A714 M715 S716 S717 R718 S719 W720
L721 S722 Y723 S724 Y725 Q726 S727 R728 F729 H730 L731 T732 P733 L734 S735 Y736 E737 T738 L739 E740 F741 A742 S743 G744 F745 A746 S747 E748 Q749 C750 P751 E752 G753 I764 V755 A756 I757 S758 T759 N760 T761 L762 R763 I764 L765 A766 L767 E768 K769 L770 G771 A772 V773 F774 N775 Q776 V777 A778 F779 P780
L781 Q782 Y783 T784 P785 R786 K787 F788 V789 I790 H791 P792 E793 S794 N795 N796 L797 T798 I799 I800 E801 T802 D803 H804 N805 A806 Y807 T808 E809 A810 T811 K812 A813 Q814 R815 K816 Q817 Q818 M819 A820 E821 E822 M823 V824 E825 A826 A827 GLY GLU ASP GLU ARG GLU L834 A835 A836 E837 M838 A839 A840
A841 F842 L843 N844 E845 N846 L847 P848 E849 S850 I851 F852 G853 A854 P855 K856 A857 G858 N859 G860 Q861 W862 A863 S864 V865 I866 R867 V868 M869 N870 P871 I872 Q873 G874 N875 T876 L877 D878 L879 V880 Q881 L882 E883 Q884 N885 E886 A887 A888 F889 S890 V891 A892 V893 C894 R895 F896 S897 N898 T899 G900
E901 D902 W903 Y904 V905 L906 V907 G908 V909 A910 K911 D912 L913 I914 L915 N916 P917 R918 S919 V920 A921 G922 G923 F924 V925 Y926 T927 Y928 K929 L930 V931 N932 N933 G934 E935 K936 L937 E938 F939 L940 H941 K942 T943 P944 V945 E946 E947 V948 P949 A950 A951 I952 A953 P954 F955 Q956 G957 R958 V959 L960
I961 G962 V963 G964 K965 L966 L967 R968 V969 Y970 D971 L972 G973 K974 K975 K976 L977 L978 R979 K980 C981 E982 N983 K984 H985 I986 A987 N988 Y989 I990 S991 G992 I993 Q994 T995 I996 G997 H998 R999 V1000 I1001 H1002 S1003 D1004 V1005 Q1006 E1007 S1008 F1009 I1010 W1011 V1012 R1013 Y1014 K1015 R1016 N1017 E1018 N1019 Q1020
L1021 I1022 I1023 F1024 A1025 D1026 D1027 T1028 Y1029 P1030 R1031 W1032 V1033 T1034 T1035 A1036 S1037 L1038 L1039 D1040 Y1041 D1042 T1043 V1044 A1045 G1046 A1047 D1048 K1049 F1050 G1051 N1052 I1053 C1054 V1055 V1056 R1057 L1058 P1059 P1060 N1061 T1062 N1063 D1064 E1065 V1066 D1067 GLU ASP PRO THR GLY ASN LYS ALA LEU TRP ASP ARG GLY
LEU LEU N1083 G1084 A1085 S1086 Q1087 K1088 A1089 E1090 V1091 I1092 M1093 N1094 Y1095 H1096 V1097 G1098 E1099 T1100 V1101 L1102 S1103 L1104 Q1105 K1106 T1107 T1108 L1109 I1110 P1111 G1112 G1113 S1114 E1115 S1116 L1117 V1118 Y1119 T1120 T1121 L1122 S1123 G1124 G1125 I1126 G1127 I1128 L1129 V1130 P1131 F1132 T1133 S1134 H1135 E1136 D1137 H1138 D1139 F1140
F1141 Q1142 H1143 V1144 E1145 M1146 H1147 L1148 R1149 S1150 E1151 H1152 P1153 P1154 L1155 C1156 G1157 R1158 D1159 H1160 L1161 S1162 F1163 R1164 S1165 Y1166 Y1167 F1168 P1169 V1170 K1171 N1172 V1173 I1174 D1175 G1176 D1177 L1178 C1179 E1180 Q1181 F1182 N1183 S1184 M1185 E1186 P1187 N1188 K1189 Q1190 K1191 N1192 V1193 S1194 E1195 E1196 L1197 D1198 R1199 T1200



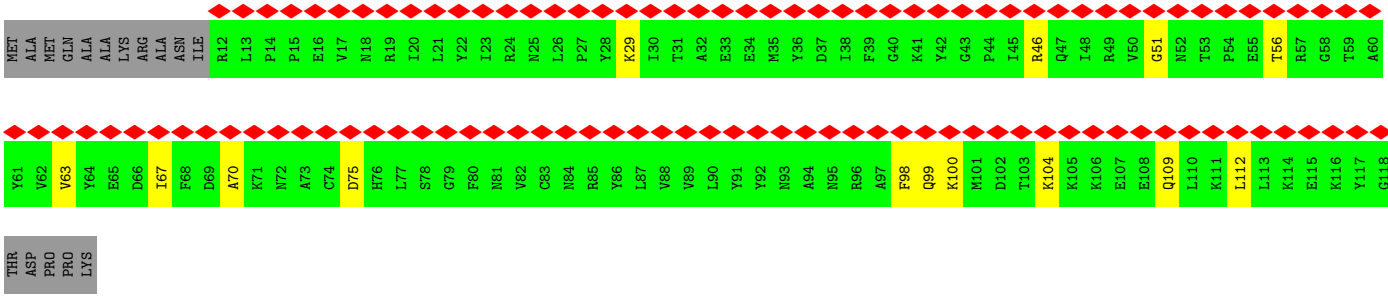
• Molecule 29: Splicing factor 3B subunit 4

Chain 4:



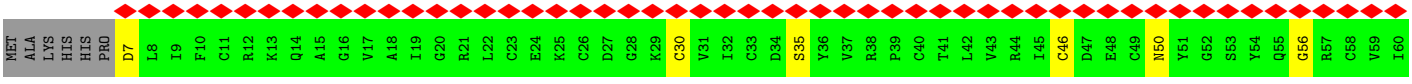
• Molecule 30: Splicing factor 3B subunit 6

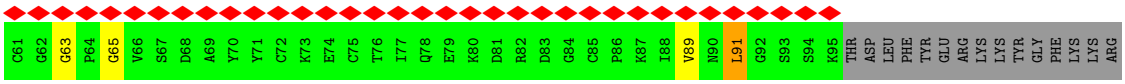
Chain 5:



• Molecule 31: PHD finger-like domain-containing protein 5A

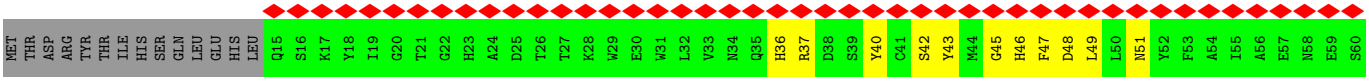
Chain 6:

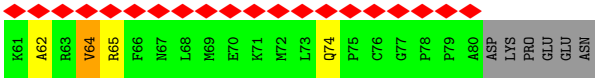




• Molecule 32: Splicing factor 3B subunit 5

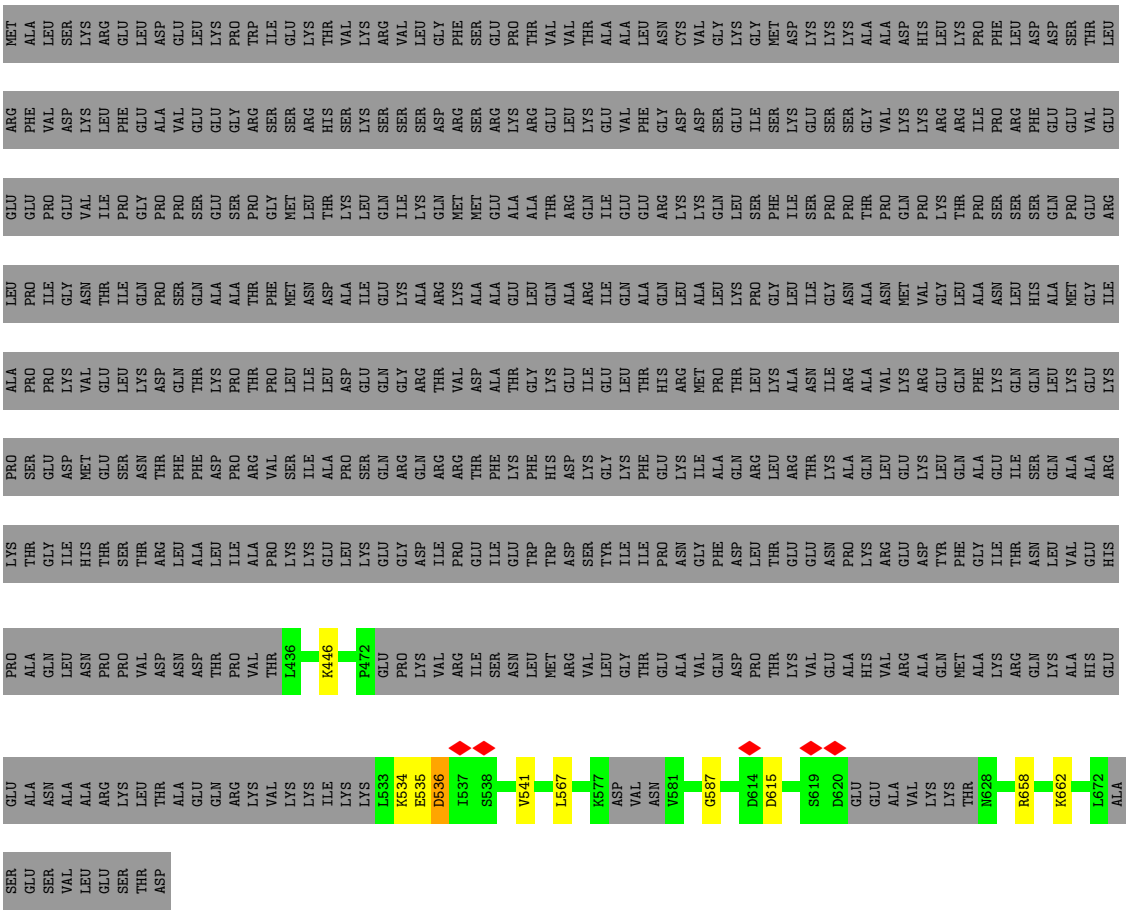
Chain 7:





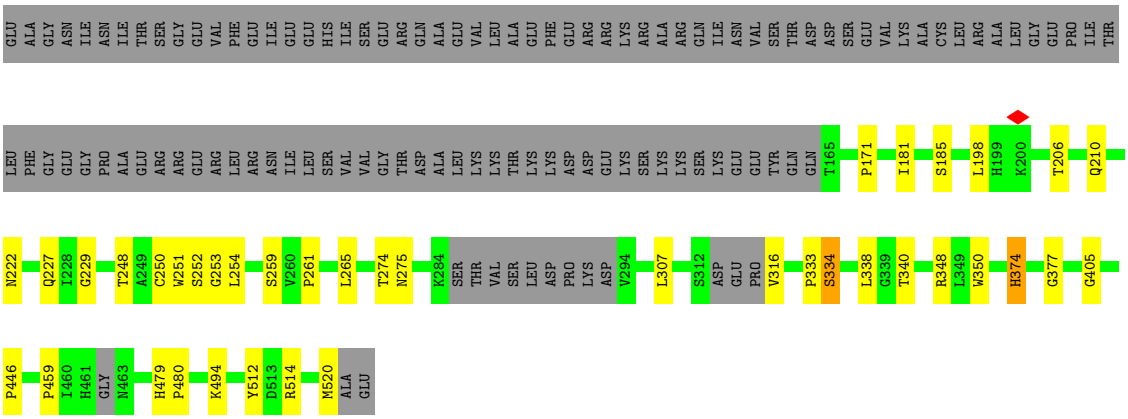
• Molecule 33: U4/U6 small nuclear ribonucleoprotein Prp3

Chain J:



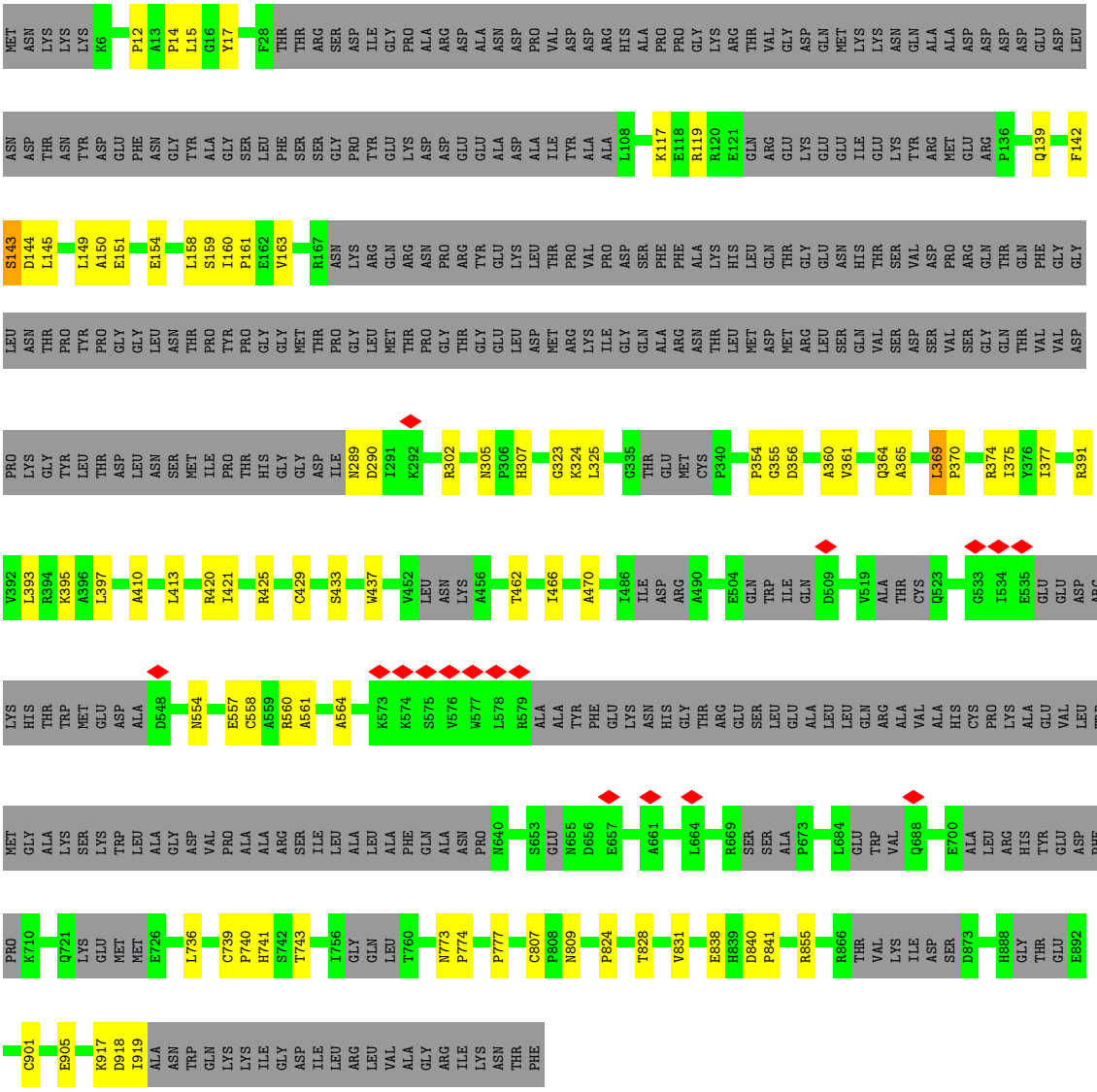
• Molecule 34: U4/U6 small nuclear ribonucleoprotein Prp4

Chain K:



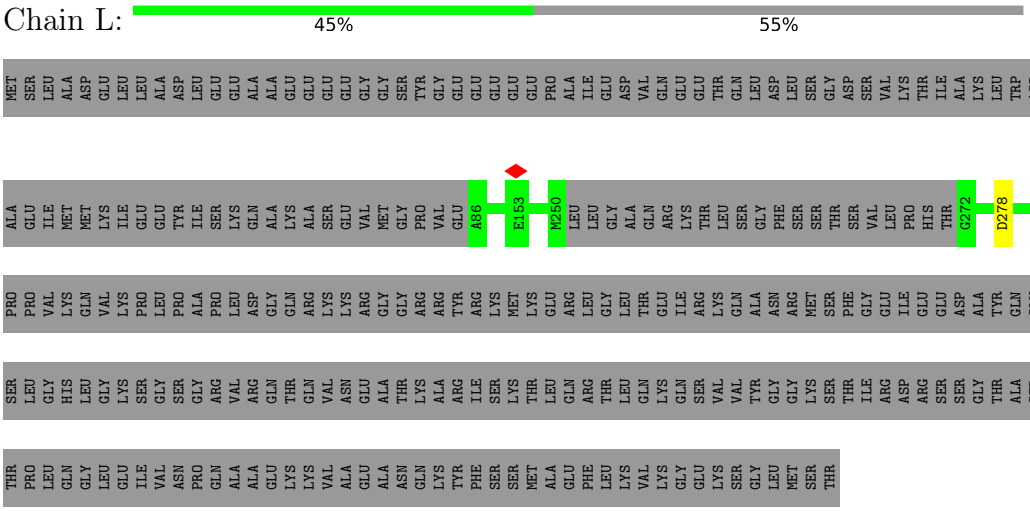
• Molecule 35: Pre-mRNA-processing factor 6

Chain N:



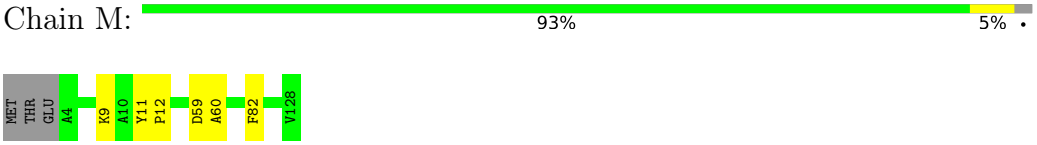
• Molecule 36: U4/U6 small nuclear ribonucleoprotein Prp31

Chain L:



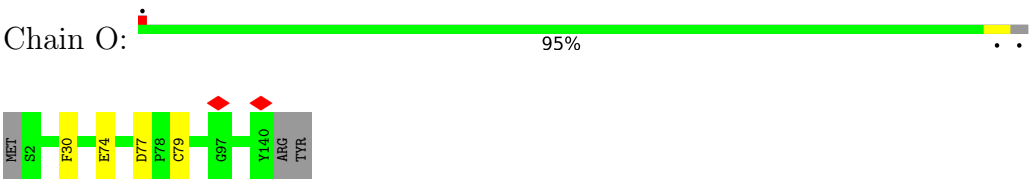
• Molecule 37: NHP2-like protein 1

Chain M:



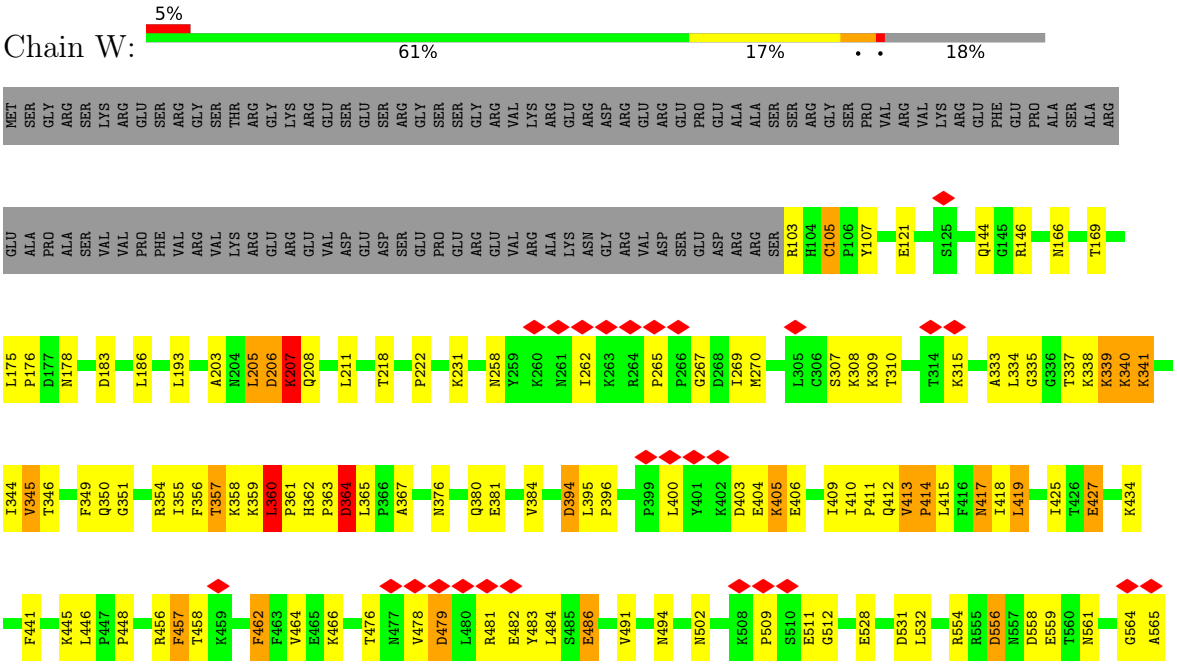
• Molecule 38: Thioredoxin-like protein 4A

Chain O:



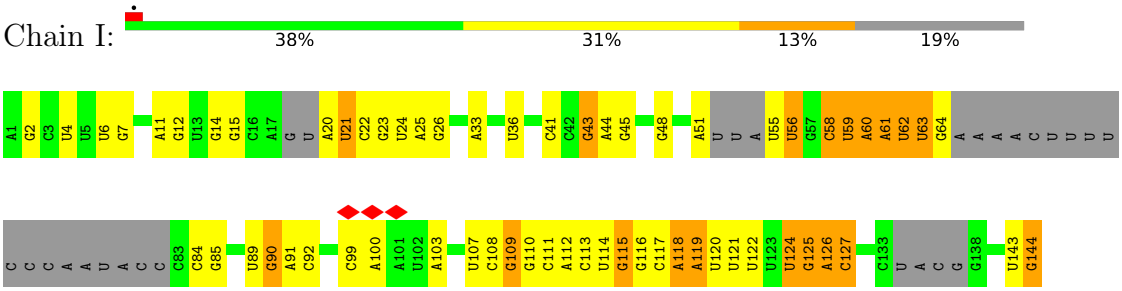
• Molecule 39: U4/U6.U5 tri-snRNP-associated protein 2

Chain W:



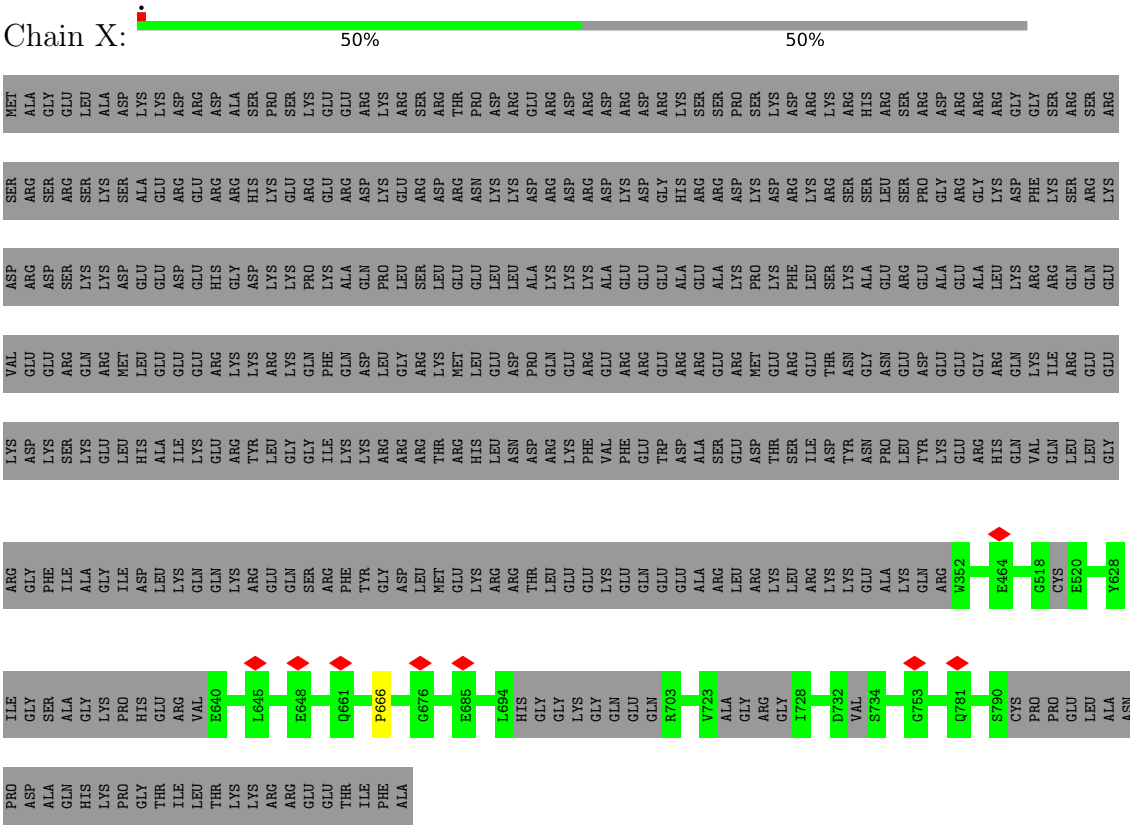
• Molecule 40: U4snRNA

Chain I:



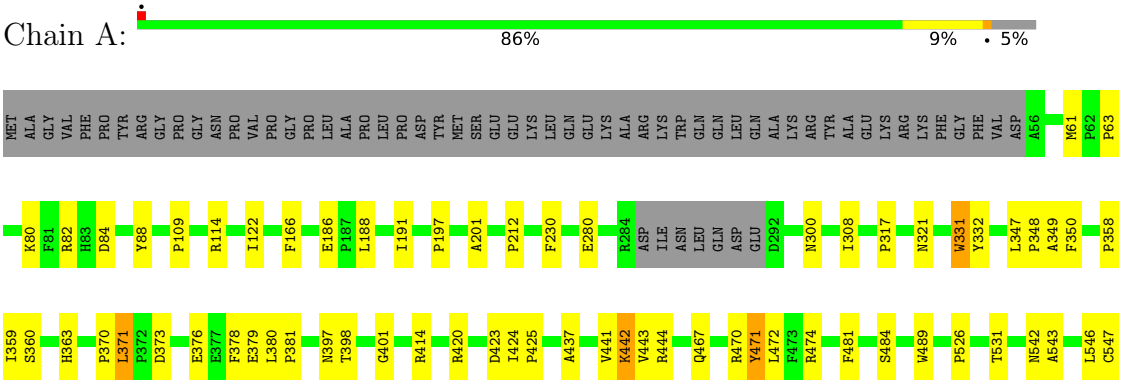
• Molecule 41: Probable ATP-dependent RNA helicase DDX23

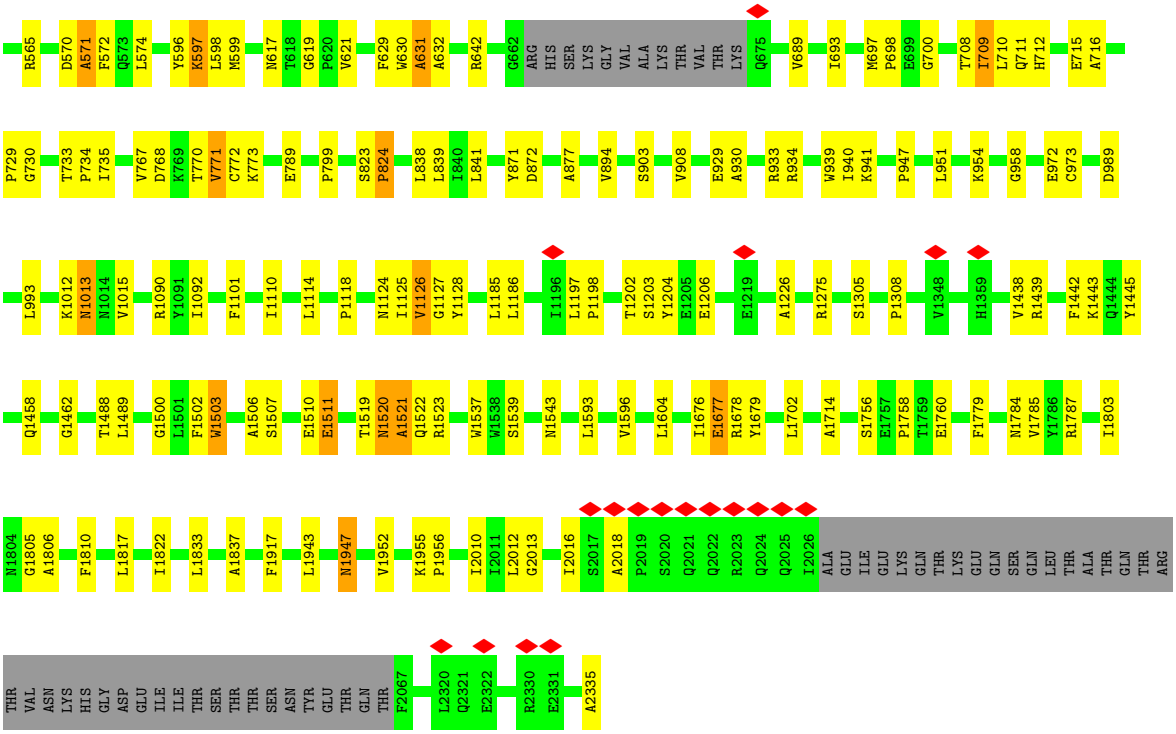
Chain X:



• Molecule 42: Pre-mRNA-processing-splicing factor 8

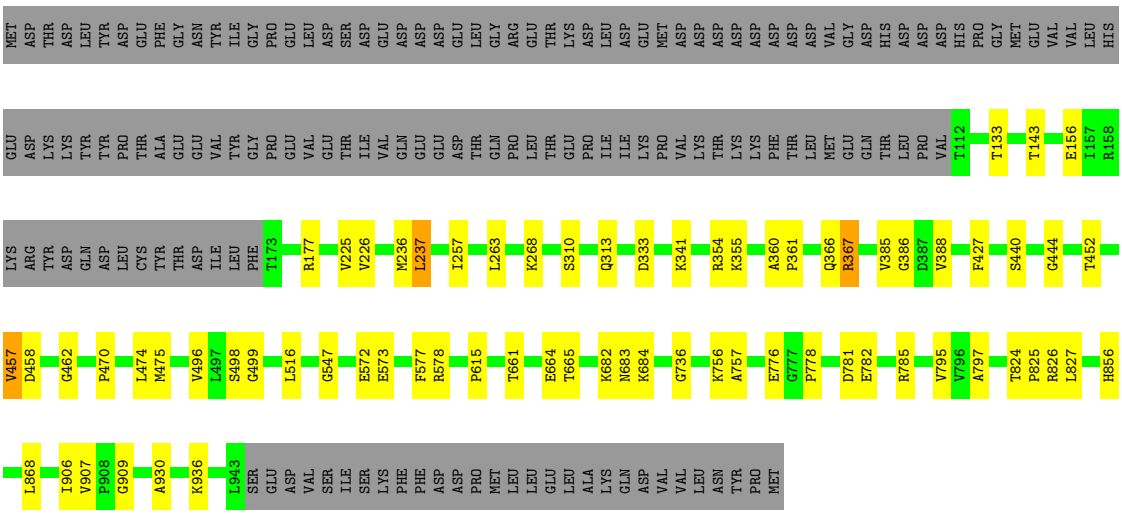
Chain A:





• Molecule 43: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.18	0/2697	0.76	0/4193
2	D	0.32	0/7493	0.57	0/9361
3	E	0.67	0/1195	0.71	0/1492
4	P	0.23	0/298	0.48	0/370
4	a	0.23	0/316	0.48	0/392
4	k	0.70	0/338	0.73	0/419
5	Q	0.24	0/291	0.49	0/363
5	b	0.24	0/299	0.49	0/373
5	m	0.78	0/295	0.76	0/367
6	R	0.22	0/313	0.49	0/390
6	c	0.22	0/313	0.49	0/390
6	l	0.63	0/315	0.75	0/392
7	S	0.24	0/297	0.51	0/371
7	d	0.24	0/281	0.52	0/351
7	n	0.55	0/270	0.63	0/334
8	T	0.23	0/287	0.49	0/358
8	e	0.23	0/317	0.52	0/396
8	h	0.47	0/318	0.56	0/394
9	U	0.22	0/254	0.48	0/314
9	f	0.23	0/258	0.48	0/320
9	i	0.47	0/290	0.65	0/359
10	V	0.22	0/333	0.47	0/416
10	g	0.22	0/378	0.46	0/471
10	j	0.56	0/327	0.68	0/407
11	F	0.26	0/1639	0.72	0/2545
12	q	0.42	0/359	0.67	0/447
13	r	0.46	0/298	0.77	0/369
14	s	0.34	0/294	0.61	0/364
15	t	0.42	0/298	0.57	0/369
16	x	0.43	0/279	0.66	0/347
17	y	0.38	0/258	0.61	0/319
18	z	0.42	0/242	0.65	0/299

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	G	0.62	2/954 (0.2%)	0.87	0/1477
20	H	0.77	11/2576 (0.4%)	1.24	32/4003 (0.8%)
21	o	0.63	0/647	1.42	0/807
22	p	0.62	0/375	1.20	0/467
23	u	0.22	0/493	0.42	0/611
24	v	0.23	0/392	0.55	0/483
25	w	0.24	0/1767	0.46	0/2199
26	1	1.03	4/4112 (0.1%)	0.81	0/5126
27	2	0.72	0/738	0.72	0/912
28	3	0.85	0/4689	0.76	0/5849
29	4	0.66	0/311	0.70	0/387
30	5	0.77	0/431	0.77	0/537
31	6	0.75	0/355	0.70	0/442
32	7	1.01	0/263	0.77	0/327
33	J	0.68	0/664	0.66	0/823
34	K	0.73	0/1367	0.79	0/1702
35	N	0.55	0/2297	0.68	1/2838 (0.0%)
36	L	0.34	0/902	0.51	0/1124
37	M	0.38	0/499	0.62	0/622
38	O	0.74	0/555	0.73	0/692
39	W	0.50	0/1851	1.16	7/2312 (0.3%)
40	I	0.23	1/2779 (0.0%)	0.70	0/4319
41	X	0.43	0/1655	0.56	0/2062
42	A	0.62	2/8880 (0.0%)	0.72	2/11093 (0.0%)
43	C	0.65	1/3270 (0.0%)	0.73	0/4084
All	All	0.59	21/64262 (0.0%)	0.75	42/83350 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
4	k	0	1
16	x	0	1
25	w	0	1
26	1	0	15
27	2	0	2
28	3	0	13
30	5	0	1
31	6	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	7	0	1
34	K	0	1
35	N	0	6
39	W	0	62
43	C	0	1
All	All	0	108

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	A	597	LYS	C-N	10.75	1.58	1.34
20	H	142	C	C1'-N1	7.31	1.59	1.48
26	1	1243	PRO	N-CA	-7.12	1.35	1.47
42	A	877	ALA	C-N	7.10	1.50	1.34
20	H	182	U	C1'-N1	6.93	1.59	1.48
20	H	150	U	C1'-N1	6.69	1.58	1.48
20	H	151	C	C1'-N1	6.50	1.58	1.48
20	H	141	C	C1'-N1	6.43	1.58	1.48
20	H	148	C	C1'-N1	6.40	1.58	1.48
20	H	97	G	C1'-N9	-6.38	1.38	1.46
20	H	184	C	C1'-N1	6.38	1.58	1.48
26	1	719	TYR	C-O	-6.29	1.11	1.23
26	1	944	SER	N-CA	-5.69	1.34	1.46
40	I	63	U	C1'-N1	5.68	1.57	1.48
26	1	718	PRO	CA-C	-5.58	1.41	1.52
20	H	48	A	C1'-N9	-5.49	1.39	1.46
19	G	131	U	C1'-N1	5.47	1.56	1.48
20	H	65	U	C1'-N1	5.45	1.56	1.48
43	C	661	THR	C-N	-5.12	1.22	1.34
19	G	122	U	C1'-N1	5.09	1.56	1.48
20	H	110	A	C1'-N9	-5.06	1.39	1.46

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	H	162	U	N3-C2-O2	-9.04	115.88	122.20
20	H	169	C	P-O3'-C3'	8.24	129.58	119.70
35	N	369	LEU	C-N-CA	-8.00	88.41	122.00
42	A	877	ALA	O-C-N	7.84	135.24	122.70
20	H	114	A	OP2-P-O3'	7.27	121.19	105.20
20	H	149	A	OP2-P-O3'	7.26	121.18	105.20
20	H	183	G	OP2-P-O3'	7.24	121.12	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	H	181	G	OP2-P-O3'	7.23	121.10	105.20
20	H	141	C	OP2-P-O3'	7.22	121.08	105.20
20	H	113	G	OP2-P-O3'	7.21	121.07	105.20
20	H	182	U	OP2-P-O3'	7.19	121.02	105.20
20	H	148	C	OP2-P-O3'	7.18	121.00	105.20
20	H	150	U	OP2-P-O3'	7.18	121.00	105.20
20	H	149	A	O3'-P-O5'	-6.86	90.97	104.00
20	H	155	C	P-O3'-C3'	6.84	127.91	119.70
20	H	183	G	O3'-P-O5'	-6.82	91.05	104.00
20	H	182	U	O3'-P-O5'	-6.80	91.08	104.00
20	H	141	C	O3'-P-O5'	-6.79	91.09	104.00
20	H	148	C	O3'-P-O5'	-6.79	91.11	104.00
20	H	113	G	O3'-P-O5'	-6.75	91.18	104.00
20	H	181	G	O3'-P-O5'	-6.75	91.18	104.00
20	H	114	A	O3'-P-O5'	-6.74	91.20	104.00
20	H	150	U	O3'-P-O5'	-6.72	91.23	104.00
39	W	354	ARG	O-C-N	6.56	133.19	122.70
39	W	427	GLU	N-CA-C	6.51	128.57	111.00
20	H	162	U	N1-C2-O2	6.20	127.14	122.80
42	A	877	ALA	CA-C-N	-5.99	104.01	117.20
20	H	172	C	P-O3'-C3'	5.80	126.66	119.70
39	W	457	PHE	N-CA-C	5.78	126.61	111.00
20	H	156	U	P-O3'-C3'	-5.78	112.77	119.70
39	W	457	PHE	C-N-CA	5.55	135.59	121.70
20	H	157	G	O4'-C1'-N9	-5.38	103.90	108.20
39	W	364	ASP	N-CA-C	5.33	125.40	111.00
20	H	156	U	OP2-P-O3'	5.28	116.83	105.20
20	H	160	A	P-O5'-C5'	-5.27	112.47	120.90
20	H	170	C	N3-C4-C5	-5.18	119.83	121.90
39	W	394	ASP	C-N-CA	5.17	134.63	121.70
20	H	170	C	O4'-C1'-C2'	-5.16	100.64	105.80
20	H	162	U	C2-N3-C4	-5.13	123.92	127.00
20	H	157	G	P-O5'-C5'	-5.10	112.75	120.90
39	W	427	GLU	C-N-CA	-5.09	108.98	121.70
20	H	156	U	C4'-C3'-C2'	5.01	107.61	102.60

There are no chirality outliers.

All (108) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	1	1025	LYS	Peptide
26	1	110	PRO	Peptide

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Mol	Chain	Res	Type	Group
26	1	1122	THR	Peptide
26	1	1127	THR	Peptide
26	1	1179	ASP	Peptide
26	1	1199	VAL	Peptide
26	1	220	GLN	Peptide
26	1	257	THR	Peptide
26	1	415	LEU	Peptide,Mainchain
26	1	545	GLU	Peptide
26	1	689	ILE	Peptide
26	1	717	THR	Peptide
26	1	941	ASN	Peptide
26	1	944	SER	Peptide
27	2	553	MET	Peptide
27	2	558	ARG	Peptide
28	3	261	PHE	Peptide
28	3	366	ASP	Peptide
28	3	468	ASP	Peptide
28	3	530	ASP	Peptide
28	3	534	ASN	Peptide
28	3	552	ARG	Peptide
28	3	670	GLN	Peptide
28	3	678	VAL	Peptide
28	3	74	THR	Peptide
28	3	885	ASN	Peptide
28	3	916	ASN	Peptide
28	3	980	LYS	Peptide
28	3	986	ILE	Peptide
30	5	29	LYS	Peptide
31	6	89	VAL	Peptide
31	6	91	LEU	Peptide
32	7	74	GLN	Peptide
43	C	736	GLY	Peptide
2	D	430	LEU	Peptide
34	K	374	HIS	Peptide
35	N	14	PRO	Peptide
35	N	773	ASN	Peptide,Mainchain
35	N	807	CYS	Peptide,Mainchain
35	N	838	GLU	Peptide
39	W	103	ARG	Peptide,Mainchain
39	W	105	CYS	Peptide
39	W	121	GLU	Peptide
39	W	144	GLN	Peptide

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Mol	Chain	Res	Type	Group
39	W	175	LEU	Peptide
39	W	193	LEU	Peptide
39	W	203	ALA	Peptide
39	W	205	LEU	Peptide
39	W	206	ASP	Peptide
39	W	207	LYS	Peptide
39	W	218	THR	Peptide
39	W	258	ASN	Peptide
39	W	267	GLY	Peptide
39	W	269	ILE	Peptide
39	W	270	MET	Peptide
39	W	308	LYS	Peptide
39	W	309	LYS	Peptide
39	W	310	THR	Peptide
39	W	315	LYS	Peptide
39	W	333	ALA	Peptide
39	W	346	THR	Peptide
39	W	356	PHE	Peptide
39	W	357	THR	Peptide
39	W	360	LEU	Peptide
39	W	362	HIS	Peptide
39	W	363	PRO	Peptide
39	W	364	ASP	Peptide
39	W	381	GLU	Peptide
39	W	384	VAL	Peptide
39	W	396	PRO	Peptide
39	W	403	ASP	Peptide
39	W	404	GLU	Peptide
39	W	405	LYS	Peptide
39	W	409	ILE	Peptide
39	W	412	GLN	Peptide
39	W	413	VAL	Peptide
39	W	414	PRO	Peptide
39	W	417	ASN	Peptide
39	W	419	LEU	Peptide
39	W	445	LYS	Peptide
39	W	446	LEU	Peptide
39	W	448	PRO	Peptide
39	W	456	ARG	Peptide
39	W	462	PHE	Peptide
39	W	464	VAL	Peptide
39	W	476	THR	Peptide

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Mol	Chain	Res	Type	Group
39	W	478	VAL	Peptide
39	W	479	ASP	Peptide
39	W	481	ARG	Peptide
39	W	482	GLU	Peptide
39	W	483	TYR	Peptide
39	W	486	GLU	Peptide
39	W	494	ASN	Peptide
39	W	511	GLU	Peptide
39	W	512	GLY	Peptide
39	W	528	GLU	Peptide
39	W	554	ARG	Peptide
39	W	556	ASP	Peptide
39	W	558	ASP	Peptide
39	W	559	GLU	Peptide
39	W	561	ASN	Peptide
4	k	112	ASN	Peptide
25	w	443	THR	Peptide
16	x	51	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2419	0	1224	60	0
2	D	7496	0	1961	18	0
3	E	1196	0	337	2	0
4	P	300	0	80	9	0
4	a	318	0	86	0	0
4	k	340	0	87	0	0
5	Q	292	0	93	1	0
5	b	300	0	95	0	0
5	m	296	0	87	0	0
6	R	314	0	86	0	0
6	c	314	0	86	0	0
6	l	316	0	85	0	0
7	S	298	0	89	1	0
7	d	282	0	85	0	0
7	n	272	0	75	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	T	288	0	84	0	0
8	e	318	0	92	0	0
8	h	320	0	88	0	0
9	U	256	0	70	3	0
9	f	260	0	74	0	0
9	i	292	0	80	0	0
10	V	334	0	92	16	0
10	g	380	0	103	0	0
10	j	328	0	89	0	0
11	F	1470	0	745	49	0
12	q	360	0	95	0	0
13	r	300	0	77	0	0
14	s	296	0	77	0	0
15	t	300	0	80	0	0
16	x	280	0	81	0	0
17	y	260	0	75	0	0
18	z	244	0	71	0	0
19	G	862	0	441	136	0
20	H	2311	0	1170	139	0
21	o	648	0	167	0	0
22	p	376	0	102	0	0
23	u	496	0	118	0	0
24	v	396	0	91	0	0
25	w	1773	0	477	0	0
26	1	4120	0	1091	171	0
27	2	744	0	189	5	0
28	3	4696	0	1266	59	0
29	4	312	0	87	2	0
30	5	432	0	114	7	0
31	6	356	0	105	5	0
32	7	264	0	70	9	0
33	J	668	0	179	8	0
34	K	1371	0	384	17	0
35	N	2316	0	581	45	0
36	L	904	0	235	1	0
37	M	500	0	128	4	0
38	O	556	0	147	1	0
39	W	1852	0	477	30	0
40	I	2491	0	1262	118	0
41	X	1661	0	440	0	0
42	A	8884	0	2283	148	0
43	C	3272	0	874	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	A	36	0	6	0	0
45	C	32	0	12	4	0
46	C	1	0	0	0	0
All	All	63369	0	19125	1003	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1003) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:145:U:C2'	19:G:146:C:H5"	1.54	1.37
33:J:536:ASP:CA	33:J:587:GLY:CA	2.11	1.28
43:C:470:PRO:CA	43:C:499:GLY:HA2	1.64	1.27
40:I:63:U:H2'	40:I:64:G:C8	1.69	1.26
33:J:536:ASP:CA	33:J:587:GLY:HA3	1.64	1.25
39:W:341:LYS:CA	39:W:359:LYS:H	1.51	1.24
19:G:135:G:N2	20:H:42:G:C4	2.07	1.21
19:G:153:C:H4'	19:G:154:U:OP1	1.42	1.18
19:G:145:U:C4	19:G:146:C:C5	2.32	1.18
19:G:137:C:O2'	19:G:138:A:H5'	1.45	1.15
19:G:149:G:C8	19:G:150:U:C5	2.34	1.15
33:J:536:ASP:CA	33:J:587:GLY:N	2.10	1.15
19:G:145:U:H2'	19:G:146:C:C5'	1.78	1.14
40:I:51:A:O2'	40:I:56:U:H5"	1.46	1.14
42:A:398:THR:CA	43:C:386:GLY:HA2	1.79	1.11
42:A:1458:GLN:O	42:A:1462:GLY:CA	1.99	1.11
20:H:156:U:H6	20:H:156:U:H5"	1.10	1.09
43:C:665:THR:O	43:C:826:ARG:CA	2.00	1.08
42:A:1833:LEU:O	42:A:1837:ALA:N	1.86	1.07
19:G:145:U:C3'	19:G:146:C:H5"	1.84	1.07
40:I:119:A:N3	4:P:103:GLY:O	1.87	1.06
19:G:145:U:O4	19:G:146:C:C4	2.09	1.06
34:K:250:CYS:N	34:K:253:GLY:O	1.88	1.06
42:A:1458:GLN:O	42:A:1462:GLY:N	1.88	1.05
40:I:126:A:N1	10:V:65:ILE:O	1.91	1.04
11:F:59:G:H1'	40:I:21:U:H4'	1.41	1.03
19:G:155:U:H4'	19:G:156:U:H5'	1.38	1.03
39:W:344:ILE:C	39:W:360:LEU:CA	2.26	1.03
19:G:149:G:C8	19:G:150:U:C4	2.47	1.02
11:F:59:G:H5'	40:I:22:C:H5"	1.36	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:145:U:H2'	19:G:146:C:H5"	1.03	1.01
19:G:135:G:N2	20:H:42:G:N3	2.06	1.01
33:J:536:ASP:CA	33:J:587:GLY:H	1.72	1.01
26:1:102:ASP:O	26:1:105:ALA:N	1.94	1.00
40:I:119:A:N3	4:P:103:GLY:C	2.14	1.00
19:G:145:U:C3'	19:G:146:C:C5'	2.39	0.99
40:I:60:A:H2'	40:I:61:A:H1'	1.40	0.99
35:N:901:CYS:O	35:N:905:GLU:CA	2.09	0.99
40:I:127:C:H1'	10:V:21:ASN:CA	1.91	0.99
40:I:58:C:O2'	40:I:59:U:C5'	2.10	0.99
40:I:91:A:H2	40:I:110:G:N2	1.61	0.99
19:G:146:C:C2	20:H:33:G:N1	2.32	0.97
19:G:135:G:N3	20:H:42:G:C2	2.33	0.97
42:A:1519:THR:O	42:A:1521:ALA:N	1.96	0.97
26:1:501:LEU:O	26:1:504:ILE:N	1.98	0.97
40:I:58:C:H2'	40:I:59:U:O5'	1.65	0.96
19:G:143:U:H6	19:G:143:U:H5'	1.30	0.96
42:A:1458:GLN:O	42:A:1462:GLY:HA2	1.64	0.96
19:G:146:C:C2	20:H:33:G:C6	2.53	0.96
34:K:251:TRP:O	34:K:275:ASN:CA	2.14	0.95
19:G:145:U:C2'	19:G:146:C:C5'	2.38	0.95
42:A:378:PHE:O	43:C:355:LYS:CA	2.14	0.95
39:W:345:VAL:N	39:W:360:LEU:N	2.15	0.95
43:C:776:GLU:O	43:C:781:ASP:C	2.06	0.94
35:N:901:CYS:O	35:N:905:GLU:N	2.01	0.94
11:F:71:G:H1	40:I:4:U:H3	0.98	0.94
34:K:494:LYS:O	34:K:512:TYR:N	2.01	0.94
20:H:156:U:H5"	20:H:156:U:C6	2.02	0.94
19:G:146:C:O2	20:H:33:G:C6	2.20	0.94
35:N:560:ARG:O	35:N:564:ALA:C	2.06	0.93
11:F:52:U:H5"	11:F:52:U:H6	1.34	0.93
19:G:135:G:C2	20:H:42:G:C2	2.57	0.93
35:N:354:PRO:O	35:N:356:ASP:N	2.02	0.92
40:I:51:A:HO2'	40:I:56:U:H5"	1.29	0.92
1:B:94:U:H1'	1:B:95:G:OP1	1.70	0.92
40:I:63:U:H2'	40:I:64:G:H8	1.13	0.91
1:B:12:U:H3	1:B:65:G:H1	1.12	0.91
42:A:1785:VAL:CA	42:A:1806:ALA:O	2.18	0.91
42:A:1676:ILE:O	42:A:1679:TYR:N	2.03	0.91
35:N:560:ARG:O	35:N:564:ALA:N	2.04	0.91
35:N:375:ILE:O	35:N:377:ILE:N	2.03	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:I:58:C:C2’	40:I:59:U:O5’	2.15	0.90
19:G:143:U:H5’	19:G:143:U:C6	2.06	0.90
39:W:341:LYS:CA	39:W:359:LYS:N	2.34	0.90
40:I:119:A:N3	4:P:103:GLY:CA	2.35	0.90
42:A:398:THR:CA	43:C:386:GLY:CA	2.49	0.89
19:G:149:G:N7	19:G:150:U:C4	2.40	0.89
26:1:793:LYS:O	26:1:797:GLY:HA3	1.72	0.89
42:A:711:GLN:O	42:A:715:GLU:N	2.05	0.89
19:G:155:U:O2’	19:G:156:U:OP2	1.89	0.89
42:A:379:GLU:O	43:C:355:LYS:N	2.07	0.88
42:A:109:PRO:O	42:A:191:ILE:N	2.06	0.88
42:A:1784:ASN:C	42:A:1806:ALA:O	2.12	0.88
19:G:145:U:H3’	19:G:146:C:C5’	2.04	0.88
42:A:941:LYS:N	42:A:1090:ARG:O	2.07	0.88
35:N:560:ARG:O	35:N:564:ALA:CA	2.23	0.86
40:I:58:C:O2’	40:I:59:U:H5’	1.73	0.86
20:H:154:C:O2	20:H:176:G:N2	2.07	0.86
11:F:59:G:H5’	40:I:22:C:C5’	2.05	0.86
42:A:1520:ASN:O	42:A:1523:ARG:N	2.08	0.86
35:N:160:ILE:CA	42:A:730:GLY:O	2.24	0.86
19:G:153:C:OP1	19:G:154:U:P	2.34	0.86
20:H:40:C:H5”	20:H:40:C:H6	1.39	0.86
40:I:63:U:C2’	40:I:64:G:H8	1.89	0.85
40:I:21:U:O2’	40:I:22:C:H5’	1.75	0.85
42:A:197:PRO:O	42:A:201:ALA:CA	2.24	0.85
20:H:156:U:H6	20:H:156:U:C5’	1.88	0.85
34:K:494:LYS:O	34:K:512:TYR:CA	2.25	0.85
26:1:728:LEU:O	26:1:731:LEU:N	2.10	0.84
42:A:733:THR:C	42:A:735:ILE:H	1.78	0.84
40:I:59:U:O2’	40:I:60:A:O5’	1.95	0.84
42:A:973:CYS:N	42:A:1101:PHE:O	2.11	0.83
19:G:137:C:HO2’	19:G:138:A:H5’	1.37	0.83
19:G:151:C:H1’	19:G:152:C:OP1	1.78	0.83
40:I:58:C:C2’	40:I:59:U:C5’	2.57	0.83
19:G:151:C:H4’	19:G:152:C:H5	1.44	0.83
42:A:1785:VAL:N	42:A:1806:ALA:O	2.11	0.82
40:I:62:U:H2’	40:I:63:U:H6	1.44	0.82
20:H:152:G:N2	20:H:153:A:N7	2.27	0.82
19:G:145:U:C5	19:G:146:C:C5	2.66	0.82
19:G:146:C:O2	20:H:33:G:N1	2.13	0.82
26:1:406:ALA:O	30:5:98:PHE:CA	2.28	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:152:G:H5”	20:H:153:A:OP2	1.80	0.82
19:G:135:G:C2	20:H:42:G:C4	2.68	0.81
26:1:648:LEU:O	26:1:651:VAL:N	2.13	0.81
40:I:59:U:HO2’	40:I:60:A:P	2.02	0.81
43:C:470:PRO:CA	43:C:499:GLY:CA	2.54	0.81
19:G:145:U:C4	19:G:146:C:C4	2.63	0.81
40:I:108:C:O2’	40:I:109:G:H5’	1.81	0.81
29:4:77:ILE:O	29:4:84:ILE:N	2.14	0.81
35:N:142:PHE:O	35:N:145:LEU:N	2.14	0.81
31:6:56:GLY:O	31:6:65:GLY:N	2.12	0.81
42:A:929:GLU:O	42:A:933:ARG:N	2.13	0.81
19:G:149:G:C2	19:G:150:U:H2’	2.16	0.80
20:H:165:A:O2’	20:H:166:G:H5’	1.81	0.80
19:G:149:G:N9	19:G:150:U:C5	2.49	0.80
43:C:827:LEU:O	43:C:906:ILE:CA	2.30	0.80
42:A:712:HIS:O	42:A:716:ALA:N	2.13	0.80
40:I:119:A:C2	4:P:103:GLY:O	2.34	0.80
2:D:570:THR:CA	42:A:2335:ALA:O	2.29	0.80
39:W:334:LEU:C	39:W:340:LYS:CA	2.50	0.80
28:3:523:GLY:HA3	28:3:536:TRP:O	1.83	0.79
39:W:345:VAL:N	39:W:360:LEU:H	1.81	0.79
42:A:973:CYS:O	42:A:1101:PHE:N	2.13	0.79
1:B:17:U:H3	1:B:60:G:H1	0.83	0.79
11:F:52:U:H5”	11:F:52:U:C6	2.17	0.79
19:G:147:C:O2	20:H:31:G:N1	2.11	0.79
20:H:177:A:H5”	20:H:178:A:OP1	1.84	0.78
26:1:669:GLN:O	26:1:672:ALA:N	2.16	0.78
11:F:59:G:H4’	40:I:22:C:OP1	1.84	0.78
19:G:149:G:H2’	19:G:150:U:C6	2.19	0.77
26:1:428:ALA:O	26:1:432:THR:N	2.17	0.77
19:G:146:C:H1’	20:H:33:G:N2	1.99	0.77
20:H:101:U:H5”	20:H:102:U:H5’	1.64	0.77
19:G:151:C:H4’	19:G:152:C:C5	2.18	0.77
11:F:59:G:C1’	40:I:21:U:H4’	2.14	0.77
28:3:839:ALA:O	28:3:843:LEU:N	2.13	0.77
19:G:146:C:O2	20:H:33:G:C2	2.37	0.77
19:G:145:U:H3	20:H:33:G:H1	1.33	0.77
19:G:155:U:H4’	19:G:156:U:C5’	2.13	0.77
42:A:908:VAL:CA	42:A:1445:TYR:O	2.33	0.77
19:G:146:C:H1’	20:H:33:G:C2	2.20	0.76
19:G:135:G:C2	20:H:42:G:N3	2.52	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:I:58:C:H2'	40:I:59:U:C5'	2.14	0.76
42:A:1125:ILE:O	42:A:1126:VAL:C	2.24	0.76
11:F:52:U:H6	11:F:52:U:C5'	1.97	0.76
26:1:102:ASP:O	26:1:105:ALA:CA	2.34	0.76
19:G:132:G:H1	20:H:44:U:H3	1.33	0.76
20:H:143:A:H3'	20:H:143:A:N3	2.01	0.76
20:H:153:A:H2'	20:H:154:C:H5'	1.65	0.76
40:I:62:U:H2'	40:I:63:U:C6	2.21	0.76
11:F:102:A:H2'	11:F:103:U:H5'	1.68	0.76
43:C:683:ASN:CA	43:C:795:VAL:O	2.34	0.76
42:A:630:TRP:O	42:A:632:ALA:N	2.18	0.76
19:G:149:G:H3'	19:G:150:U:H5"	1.67	0.76
26:1:1016:LEU:O	26:1:1019:ARG:N	2.19	0.76
39:W:340:LYS:O	39:W:358:LYS:CA	2.34	0.75
42:A:708:THR:O	42:A:711:GLN:N	2.19	0.75
11:F:59:G:C5'	40:I:22:C:H5"	2.15	0.75
2:D:282:SER:O	2:D:286:ALA:N	2.18	0.75
40:I:91:A:H2	40:I:110:G:H22	0.83	0.75
42:A:1702:LEU:O	42:A:1714:ALA:CA	2.34	0.75
19:G:149:G:H2'	19:G:150:U:H6	1.52	0.75
40:I:126:A:H2	10:V:64:ASN:O	1.70	0.75
26:1:1246:MET:O	26:1:1249:TYR:N	2.18	0.74
42:A:1833:LEU:O	42:A:1837:ALA:CA	2.36	0.74
26:1:874:LYS:O	26:1:877:GLY:N	2.20	0.74
1:B:48:A:P	42:A:280:GLU:H	2.11	0.74
1:B:95:G:H5'	1:B:96:A:OP2	1.87	0.74
19:G:153:C:OP1	19:G:154:U:OP1	2.05	0.74
20:H:153:A:C2'	20:H:154:C:H5'	2.17	0.74
42:A:84:ASP:O	42:A:88:TYR:N	2.20	0.74
42:A:317:PRO:O	42:A:321:ASN:O	2.05	0.74
28:3:442:LEU:O	28:3:735:SER:N	2.19	0.74
40:I:119:A:C4	4:P:103:GLY:HA3	2.22	0.74
43:C:143:THR:CA	45:C:1500:GTP:O1B	2.36	0.74
1:B:26:A:C5	42:A:423:ASP:CA	2.71	0.74
1:B:26:A:H5"	1:B:26:A:N3	2.02	0.74
28:3:304:GLN:CA	28:3:309:ASP:O	2.36	0.73
28:3:753:GLY:HA3	28:3:765:LEU:O	1.88	0.73
42:A:80:LYS:C	42:A:82:ARG:H	1.92	0.73
42:A:1500:GLY:O	42:A:1756:SER:CA	2.37	0.73
26:1:1270:ASN:O	26:1:1273:TYR:N	2.21	0.73
42:A:441:VAL:O	42:A:444:ARG:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:153:A:H2'	20:H:154:C:C5'	2.19	0.73
40:I:126:A:H2	10:V:64:ASN:C	1.93	0.73
19:G:136:U:H1'	19:G:137:C:OP1	1.89	0.72
19:G:146:C:O2	20:H:33:G:C5	2.41	0.72
26:1:994:LEU:O	26:1:997:LEU:N	2.22	0.72
42:A:733:THR:O	42:A:735:ILE:N	2.21	0.72
26:1:660:ALA:O	26:1:663:THR:N	2.22	0.72
28:3:380:GLU:O	28:3:383:ASP:N	2.22	0.72
40:I:127:C:H1'	10:V:21:ASN:C	2.08	0.72
40:I:127:C:O2	10:V:21:ASN:O	2.08	0.72
39:W:344:ILE:C	39:W:360:LEU:N	2.40	0.72
40:I:58:C:C2'	40:I:59:U:H5'	2.20	0.72
26:1:531:LEU:O	26:1:534:GLN:N	2.18	0.72
42:A:186:GLU:O	42:A:565:ARG:O	2.08	0.72
19:G:145:U:C4	19:G:146:C:C6	2.77	0.72
26:1:1055:TRP:O	26:1:1058:ILE:N	2.22	0.71
26:1:535:ILE:O	26:1:538:LEU:N	2.23	0.71
42:A:470:ARG:O	42:A:472:LEU:N	2.23	0.71
26:1:122:HIS:O	26:1:125:THR:N	2.22	0.71
1:B:26:A:N3	1:B:26:A:H3'	2.05	0.71
42:A:471:TYR:O	42:A:474:ARG:N	2.24	0.71
26:1:700:LYS:O	26:1:703:THR:N	2.24	0.71
19:G:153:C:OP1	19:G:154:U:OP2	2.09	0.70
26:1:791:VAL:O	26:1:794:GLN:N	2.23	0.70
11:F:102:A:C2'	11:F:103:U:H5'	2.21	0.70
42:A:1520:ASN:O	42:A:1522:GLN:N	2.24	0.70
19:G:134:U:H3	20:H:42:G:H1	1.37	0.70
20:H:154:C:H2'	20:H:155:C:C6	2.27	0.70
42:A:114:ARG:O	42:A:489:TRP:N	2.25	0.70
43:C:909:GLY:HA3	43:C:930:ALA:H	1.56	0.70
40:I:21:U:H2'	40:I:22:C:H6	1.57	0.70
42:A:939:TRP:O	42:A:1090:ARG:N	2.17	0.70
20:H:153:A:N6	20:H:177:A:C2	2.60	0.69
20:H:168:A:C8	20:H:168:A:H5"	2.27	0.69
43:C:776:GLU:O	43:C:781:ASP:CA	2.40	0.69
11:F:86:U:H3	20:H:12:G:H1	1.39	0.69
20:H:30:A:N3	20:H:30:A:H2'	2.06	0.69
42:A:331:TRP:O	43:C:177:ARG:O	2.10	0.69
42:A:930:ALA:O	42:A:934:ARG:O	2.10	0.69
27:2:479:ASP:O	27:2:482:ALA:N	2.25	0.69
42:A:930:ALA:O	42:A:934:ARG:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:LEU:O	2:D:162:GLY:N	2.24	0.69
20:H:150:U:H3	20:H:181:G:H1	1.41	0.69
28:3:545:VAL:N	28:3:557:ALA:O	2.25	0.69
35:N:361:VAL:O	35:N:365:ALA:N	2.26	0.69
42:A:61:MET:N	42:A:484:SER:O	2.26	0.69
20:H:40:C:H6	20:H:40:C:C5'	2.05	0.69
20:H:180:G:H2'	20:H:181:G:H8	1.57	0.69
40:I:119:A:C2	4:P:103:GLY:CA	2.76	0.69
35:N:154:GLU:O	42:A:700:GLY:HA3	1.94	0.68
39:W:166:ASN:O	39:W:169:THR:O	2.11	0.68
40:I:63:U:C2'	40:I:64:G:C8	2.61	0.68
42:A:1125:ILE:O	42:A:1128:TYR:N	2.21	0.68
39:W:335:GLY:N	39:W:340:LYS:CA	2.56	0.68
42:A:80:LYS:O	42:A:82:ARG:N	2.25	0.68
11:F:49:G:H1	40:I:63:U:H3	1.41	0.68
28:3:558:LEU:O	28:3:561:GLY:N	2.24	0.68
40:I:127:C:H1'	10:V:21:ASN:O	1.93	0.68
11:F:73:A:N1	40:I:2:G:O6	2.27	0.68
20:H:143:A:H2'	20:H:144:C:H6	1.59	0.68
20:H:152:G:O3'	20:H:153:A:O4'	2.11	0.68
42:A:570:ASP:O	42:A:572:PHE:N	2.26	0.67
19:G:146:C:H6	19:G:146:C:H5'	1.58	0.67
19:G:151:C:C4'	19:G:152:C:H5	2.07	0.67
40:I:24:U:H3	40:I:48:G:H1	1.42	0.67
40:I:21:U:H2'	40:I:22:C:C6	2.29	0.67
40:I:60:A:H2'	40:I:61:A:C1'	2.20	0.67
40:I:55:U:H5'	40:I:56:U:OP2	1.93	0.67
43:C:474:LEU:CA	43:C:498:SER:O	2.42	0.67
20:H:106:G:H21	20:H:107:A:N6	1.92	0.67
27:2:487:LEU:O	27:2:490:HIS:N	2.28	0.67
42:A:1519:THR:O	42:A:1520:ASN:C	2.31	0.67
20:H:151:C:H2'	20:H:152:G:H8	1.60	0.67
20:H:151:C:O2	20:H:152:G:C8	2.48	0.66
42:A:733:THR:C	42:A:735:ILE:N	2.49	0.66
2:D:166:ASP:O	2:D:169:TYR:N	2.26	0.66
40:I:20:A:H2'	40:I:21:U:C6	2.31	0.66
19:G:147:C:OP2	19:G:147:C:H3'	1.96	0.66
40:I:119:A:N3	4:P:103:GLY:HA3	2.09	0.66
20:H:151:C:C2	20:H:152:G:C8	2.83	0.66
20:H:153:A:C3'	20:H:154:C:H5'	2.25	0.66
28:3:753:GLY:CA	28:3:765:LEU:O	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:A:1539:SER:O	42:A:1543:ASN:N	2.17	0.66
34:K:251:TRP:O	34:K:274:THR:O	2.13	0.66
19:G:128:U:H6	19:G:128:U:O5'	1.78	0.65
11:F:59:G:H4'	40:I:22:C:P	2.37	0.65
19:G:127:U:O2'	19:G:128:U:O4'	2.13	0.65
26:1:1243:PRO:O	26:1:1246:MET:N	2.29	0.65
27:2:491:LEU:O	27:2:494:THR:N	2.30	0.65
40:I:6:U:H2'	40:I:7:G:H8	1.62	0.65
42:A:1110:ILE:O	42:A:1114:LEU:N	2.29	0.65
35:N:161:PRO:N	42:A:730:GLY:O	2.29	0.65
1:B:58:U:H2'	1:B:59:G:H8	1.62	0.65
19:G:137:C:H6	19:G:137:C:O5'	1.78	0.65
26:1:886:HIS:O	26:1:889:GLU:N	2.30	0.65
40:I:111:C:H6	40:I:111:C:O5'	1.78	0.65
19:G:151:C:H1'	19:G:152:C:P	2.36	0.65
42:A:543:ALA:O	42:A:547:CYS:N	2.17	0.65
19:G:151:C:C4'	19:G:152:C:C5	2.79	0.65
42:A:441:VAL:O	42:A:442:LYS:C	2.36	0.65
20:H:153:A:H3'	20:H:154:C:H5'	1.79	0.65
28:3:1148:LEU:O	28:3:1152:HIS:N	2.27	0.65
42:A:441:VAL:O	42:A:443:VAL:N	2.30	0.65
1:B:78:U:O2'	1:B:80:U:OP1	2.13	0.64
39:W:344:ILE:O	39:W:360:LEU:CA	2.44	0.64
1:B:97:G:H1	1:B:116:U:H3	1.44	0.64
40:I:117:C:H6	40:I:117:C:O5'	1.80	0.64
26:1:758:ASP:O	26:1:762:ALA:N	2.28	0.64
28:3:868:VAL:O	28:3:877:LEU:N	2.30	0.64
42:A:1676:ILE:O	42:A:1677:GLU:C	2.33	0.64
19:G:146:C:N3	20:H:33:G:C6	2.66	0.64
26:1:1280:LEU:O	26:1:1283:HIS:N	2.22	0.64
19:G:153:C:C4'	19:G:154:U:OP1	2.35	0.64
26:1:749:ALA:O	26:1:752:TYR:N	2.31	0.64
40:I:51:A:O2'	40:I:56:U:C5'	2.35	0.64
26:1:1018:PRO:O	26:1:1021:THR:N	2.30	0.64
42:A:1438:VAL:O	42:A:1442:PHE:N	2.31	0.64
26:1:658:TRP:O	26:1:661:ARG:N	2.30	0.63
32:7:40:TYR:O	32:7:43:TYR:N	2.31	0.63
42:A:397:ASN:C	43:C:386:GLY:O	2.37	0.63
19:G:145:U:O4	19:G:146:C:N4	2.31	0.63
19:G:150:U:OP1	31:6:63:GLY:HA3	1.98	0.63
33:J:658:ARG:O	33:J:662:LYS:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:K:248:THR:O	34:K:254:LEU:CA	2.46	0.63
34:K:338:LEU:O	34:K:350:TRP:N	2.29	0.63
42:A:1784:ASN:O	42:A:1806:ALA:N	2.30	0.63
20:H:152:G:C2	20:H:153:A:C5	2.87	0.63
28:3:931:VAL:O	28:3:936:LYS:N	2.31	0.63
20:H:147:G:H2'	20:H:148:C:H6	1.63	0.63
26:1:1264:VAL:O	26:1:1267:LYS:N	2.32	0.63
19:G:135:G:H5'	19:G:136:U:OP2	1.99	0.63
20:H:114:A:H61	20:H:142:C:H42	1.44	0.63
28:3:325:ILE:O	28:3:375:SER:N	2.30	0.63
40:I:89:U:C2'	40:I:90:G:H5'	2.29	0.63
40:I:126:A:C2	10:V:20:LYS:CA	2.82	0.63
42:A:1784:ASN:O	42:A:1806:ALA:O	2.16	0.63
19:G:137:C:C2'	19:G:138:A:H5'	2.28	0.63
40:I:89:U:O2'	40:I:90:G:H5'	1.99	0.63
42:A:1125:ILE:O	42:A:1127:GLY:N	2.31	0.62
20:H:106:G:H4'	20:H:107:A:O4'	1.99	0.62
1:B:98:G:H2'	1:B:99:C:C6	2.34	0.62
19:G:127:U:OP2	19:G:127:U:H2'	1.99	0.62
19:G:146:C:C2	19:G:147:C:C5	2.87	0.62
26:1:914:PHE:O	26:1:917:VAL:N	2.32	0.62
40:I:91:A:O5'	40:I:91:A:H8	1.82	0.62
26:1:179:GLY:O	26:1:182:LYS:N	2.33	0.62
35:N:410:ALA:O	35:N:413:LEU:N	2.33	0.62
42:A:542:ASN:O	42:A:546:LEU:N	2.30	0.62
20:H:154:C:H2'	20:H:155:C:H6	1.63	0.62
35:N:828:THR:O	35:N:831:VAL:N	2.31	0.62
40:I:126:A:N1	10:V:65:ILE:C	2.53	0.62
42:A:371:LEU:CA	43:C:341:LYS:O	2.47	0.62
20:H:157:G:H8	20:H:157:G:H5"	1.65	0.62
28:3:973:GLY:HA3	28:3:976:LYS:O	2.00	0.62
19:G:146:C:O2'	19:G:147:C:H5'	2.00	0.62
28:3:1191:LYS:O	28:3:1194:SER:N	2.32	0.62
42:A:1519:THR:C	42:A:1521:ALA:N	2.53	0.62
1:B:98:G:H2'	1:B:99:C:H6	1.65	0.62
42:A:471:TYR:O	42:A:472:LEU:C	2.38	0.62
11:F:49:G:H2'	11:F:50:A:H8	1.64	0.61
19:G:150:U:H4'	19:G:151:C:OP2	1.98	0.61
40:I:119:A:C2	4:P:103:GLY:HA2	2.35	0.61
19:G:146:C:C2'	19:G:147:C:H5'	2.30	0.61
20:H:143:A:H2'	20:H:144:C:C6	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:I:108:C:H2'	40:I:109:G:H8	1.63	0.61
19:G:155:U:H5"	19:G:156:U:H5"	1.83	0.61
26:1:895:GLY:O	26:1:898:TYR:N	2.34	0.61
19:G:146:C:H2'	19:G:147:C:C6	2.36	0.61
20:H:112:G:H2'	20:H:113:G:H8	1.65	0.61
28:3:586:ASP:O	28:3:610:VAL:N	2.32	0.61
40:I:127:C:C1'	10:V:21:ASN:CA	2.74	0.61
26:1:551:LEU:O	26:1:554:LYS:N	2.34	0.61
26:1:862:GLU:O	26:1:865:ARG:N	2.33	0.61
1:B:12:U:O4	1:B:65:G:O6	2.19	0.61
20:H:153:A:N6	20:H:177:A:H2	1.98	0.61
20:H:156:U:C6	20:H:156:U:C5'	2.72	0.61
34:K:252:SER:CA	34:K:274:THR:O	2.49	0.61
20:H:142:C:C2'	20:H:143:A:H5'	2.30	0.61
26:1:953:ASP:O	26:1:956:SER:N	2.34	0.61
19:G:136:U:H1'	19:G:137:C:P	2.41	0.60
28:3:638:GLU:N	28:3:668:GLY:O	2.32	0.60
42:A:768:ASP:O	42:A:772:CYS:N	2.34	0.60
26:1:491:GLU:O	26:1:494:GLU:N	2.32	0.60
39:W:345:VAL:N	39:W:360:LEU:CA	2.62	0.60
26:1:897:LEU:O	26:1:900:PHE:N	2.34	0.60
40:I:33:A:H62	40:I:43:G:H21	1.49	0.60
42:A:1489:LEU:N	42:A:1537:TRP:O	2.33	0.60
28:3:563:LEU:N	28:3:581:LYS:O	2.27	0.60
39:W:344:ILE:C	39:W:360:LEU:H	2.03	0.60
43:C:143:THR:N	45:C:1500:GTP:O1B	2.34	0.60
26:1:784:MET:O	26:1:787:ILE:N	2.34	0.60
26:1:929:LEU:O	26:1:932:ILE:N	2.34	0.60
26:1:1094:LEU:O	26:1:1098:LEU:N	2.32	0.60
40:I:59:U:C2	40:I:60:A:C8	2.90	0.60
19:G:146:C:H2'	19:G:147:C:H6	1.65	0.60
26:1:610:ILE:O	26:1:613:MET:N	2.34	0.60
39:W:341:LYS:C	39:W:359:LYS:H	2.04	0.60
43:C:313:GLN:N	45:C:1500:GTP:O6	2.24	0.60
37:M:12:PRO:O	37:M:82:PHE:CA	2.50	0.59
1:B:94:U:C1'	1:B:95:G:OP1	2.47	0.59
26:1:1182:LEU:O	26:1:1185:ARG:N	2.35	0.59
39:W:338:LYS:O	39:W:339:LYS:C	2.37	0.59
2:D:281:VAL:O	2:D:285:LYS:N	2.30	0.59
28:3:550:ASN:N	28:3:553:GLN:O	2.27	0.59
34:K:181:ILE:O	34:K:185:SER:N	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:917:LYS:O	35:N:919:ILE:N	2.36	0.59
42:A:300:ASN:O	43:C:936:LYS:CA	2.50	0.59
42:A:1676:ILE:O	42:A:1678:ARG:N	2.35	0.59
42:A:1779:PHE:N	42:A:1810:PHE:O	2.29	0.59
28:3:664:TYR:CA	28:3:677:THR:O	2.50	0.59
33:J:536:ASP:N	33:J:587:GLY:HA3	2.17	0.59
39:W:344:ILE:CA	39:W:360:LEU:H	2.16	0.59
26:1:1125:PRO:O	26:1:1128:VAL:N	2.35	0.59
35:N:466:ILE:O	35:N:470:ALA:N	2.35	0.59
39:W:427:GLU:N	39:W:441:PHE:H	2.01	0.59
19:G:145:U:H3'	19:G:146:C:H5'	1.82	0.59
26:1:308:SER:O	26:1:311:ALA:N	2.35	0.59
28:3:645:MET:N	28:3:662:PHE:O	2.28	0.59
40:I:62:U:C2	40:I:63:U:C5	2.91	0.59
30:5:67:ILE:O	30:5:70:ALA:N	2.36	0.59
42:A:770:THR:O	42:A:773:LYS:N	2.32	0.58
11:F:59:G:H4'	40:I:21:U:O3'	2.04	0.58
19:G:135:G:N3	20:H:42:G:N2	2.50	0.58
19:G:146:C:O2	20:H:33:G:C4	2.55	0.58
37:M:12:PRO:O	37:M:82:PHE:N	2.36	0.58
1:B:96:A:H3'	1:B:96:A:OP1	2.03	0.58
42:A:80:LYS:C	42:A:82:ARG:N	2.54	0.58
42:A:2010:ILE:O	42:A:2013:GLY:O	2.21	0.58
43:C:496:VAL:O	43:C:547:GLY:N	2.30	0.58
26:1:745:ALA:O	26:1:748:LYS:N	2.36	0.58
26:1:1149:LYS:O	26:1:1152:SER:N	2.36	0.58
26:1:811:LEU:O	26:1:814:PHE:N	2.36	0.58
20:H:154:C:O2'	20:H:155:C:H5'	2.04	0.58
1:B:96:A:H3'	1:B:96:A:P	2.43	0.58
19:G:145:U:N3	19:G:146:C:C6	2.71	0.58
40:I:59:U:C2	40:I:60:A:N7	2.71	0.58
42:A:1506:ALA:O	42:A:1510:GLU:N	2.34	0.58
42:A:689:VAL:O	42:A:693:ILE:N	2.32	0.58
35:N:361:VAL:O	35:N:365:ALA:CA	2.52	0.58
1:B:95:G:H3'	1:B:95:G:N3	2.19	0.58
19:G:149:G:N9	19:G:150:U:C6	2.72	0.58
19:G:151:C:C5'	19:G:152:C:H5	2.17	0.58
28:3:1204:VAL:O	28:3:1207:LYS:N	2.37	0.58
40:I:108:C:C2'	40:I:109:G:H5'	2.34	0.58
26:1:424:ILE:O	26:1:428:ALA:N	2.36	0.57
32:7:48:ASP:O	32:7:51:ASN:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:125:C:O2'	19:G:126:C:P	2.62	0.57
40:I:113:C:H6	40:I:113:C:O5'	1.88	0.57
19:G:149:G:C4	19:G:150:U:C6	2.93	0.57
42:A:122:ILE:N	42:A:481:PHE:O	2.25	0.57
19:G:150:U:O2	19:G:150:U:O2'	2.22	0.57
20:H:152:G:N2	20:H:153:A:C5	2.73	0.57
39:W:335:GLY:HA2	39:W:340:LYS:O	2.05	0.57
42:A:379:GLU:C	43:C:355:LYS:CA	2.73	0.57
26:1:892:LEU:O	26:1:895:GLY:N	2.37	0.57
35:N:139:GLN:O	35:N:143:SER:N	2.35	0.57
20:H:165:A:C6	20:H:166:G:O6	2.57	0.57
40:I:110:G:O5'	40:I:110:G:H8	1.86	0.57
11:F:50:A:H2'	11:F:51:U:H6	1.69	0.57
26:1:578:ILE:O	26:1:581:LEU:N	2.37	0.57
26:1:937:LEU:O	26:1:940:LEU:N	2.38	0.57
40:I:111:C:H2'	40:I:112:A:H8	1.69	0.56
1:B:110:C:H2'	1:B:111:A:H8	1.70	0.56
19:G:146:C:N4	19:G:147:C:H41	2.03	0.56
28:3:287:PHE:CA	28:3:304:GLN:O	2.53	0.56
42:A:630:TRP:O	42:A:631:ALA:C	2.43	0.56
43:C:682:LYS:O	43:C:797:ALA:N	2.38	0.56
26:1:849:ILE:O	26:1:852:ARG:N	2.38	0.56
28:3:1160:HIS:O	28:3:1163:PHE:N	2.37	0.56
39:W:341:LYS:CA	39:W:358:LYS:CA	2.83	0.56
40:I:20:A:H2'	40:I:21:U:C5	2.40	0.56
42:A:1012:LYS:O	42:A:1013:ASN:O	2.23	0.56
11:F:59:G:C4'	40:I:21:U:O3'	2.53	0.56
19:G:149:G:C2'	19:G:150:U:C6	2.89	0.56
28:3:15:SER:N	28:3:33:SER:O	2.35	0.56
20:H:141:C:H2'	20:H:142:C:H6	1.71	0.56
42:A:940:ILE:CA	42:A:1090:ARG:O	2.54	0.56
19:G:136:U:C1'	19:G:137:C:P	2.94	0.56
20:H:141:C:C2	20:H:142:C:C5	2.93	0.56
42:A:930:ALA:O	42:A:934:ARG:CA	2.54	0.56
1:B:69:A:O2'	1:B:70:A:N3	2.39	0.56
20:H:149:A:H2'	20:H:150:U:H6	1.70	0.56
20:H:152:G:N2	20:H:153:A:C8	2.73	0.56
26:1:716:ALA:O	26:1:719:TYR:N	2.39	0.56
40:I:108:C:H2'	40:I:109:G:C8	2.41	0.56
42:A:371:LEU:CA	43:C:341:LYS:C	2.74	0.56
19:G:151:C:C1'	19:G:152:C:P	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:150:U:H2'	20:H:151:C:H6	1.71	0.56
42:A:331:TRP:O	43:C:177:ARG:CA	2.54	0.56
42:A:1787:ARG:O	42:A:1803:ILE:O	2.24	0.56
1:B:61:A:H2'	1:B:62:G:H8	1.69	0.55
26:1:968:GLU:O	26:1:971:MET:N	2.39	0.55
11:F:50:A:C4	11:F:51:U:C5	2.94	0.55
19:G:149:G:C3'	19:G:150:U:H5"	2.35	0.55
20:H:147:G:C4	20:H:148:C:C5	2.94	0.55
28:3:523:GLY:CA	28:3:536:TRP:O	2.51	0.55
20:H:150:U:C2	20:H:151:C:C5	2.94	0.55
26:1:874:LYS:O	26:1:877:GLY:CA	2.54	0.55
26:1:1124:SER:O	26:1:1127:THR:N	2.34	0.55
28:3:931:VAL:O	28:3:935:GLU:N	2.39	0.55
19:G:135:G:N2	20:H:42:G:N9	2.53	0.55
20:H:181:G:H2'	20:H:182:U:H6	1.71	0.55
40:I:125:G:H1'	10:V:63:ASN:C	2.27	0.55
26:1:173:ALA:C	26:1:176:ALA:H	2.09	0.55
28:3:303:ALA:O	28:3:310:ILE:CA	2.55	0.55
30:5:98:PHE:O	30:5:100:LYS:N	2.39	0.55
28:3:1194:SER:O	28:3:1199:ARG:N	2.36	0.55
2:D:128:PRO:O	2:D:129:ARG:C	2.45	0.55
2:D:146:GLU:O	2:D:149:ARG:N	2.40	0.55
19:G:137:C:O2'	19:G:138:A:C5'	2.37	0.55
20:H:183:G:C4	20:H:184:C:C5	2.94	0.55
20:H:183:G:H2'	20:H:184:C:H6	1.71	0.55
30:5:109:GLN:O	30:5:112:LEU:N	2.39	0.55
40:I:21:U:C2'	40:I:22:C:H5'	2.37	0.55
40:I:59:U:H1'	40:I:60:A:H5'	1.89	0.55
11:F:51:U:H2'	11:F:51:U:O2	2.06	0.55
20:H:181:G:C4	20:H:182:U:C5	2.95	0.55
19:G:151:C:O2'	19:G:151:C:O2	2.24	0.54
42:A:359:ILE:O	42:A:360:SER:C	2.44	0.54
2:D:283:GLN:O	2:D:287:ASP:N	2.33	0.54
20:H:149:A:C4	20:H:150:U:C5	2.95	0.54
26:1:517:ARG:O	26:1:520:THR:N	2.41	0.54
26:1:557:ASP:O	26:1:560:LEU:N	2.40	0.54
40:I:55:U:H3'	40:I:56:U:C6	2.42	0.54
40:I:55:U:H2'	40:I:55:U:O2	2.07	0.54
40:I:124:U:H1'	9:U:37:HIS:O	2.06	0.54
43:C:664:GLU:O	43:C:785:ARG:N	2.27	0.54
1:B:17:U:O2	1:B:60:G:N2	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:G:H3'	1:B:109:G:H8	1.73	0.54
2:D:1048:VAL:O	2:D:1050:GLU:N	2.40	0.54
11:F:52:U:C6	11:F:52:U:C5'	2.85	0.54
19:G:146:C:C2	20:H:33:G:C2	2.95	0.54
20:H:153:A:C3'	20:H:154:C:C5'	2.86	0.54
35:N:142:PHE:O	35:N:143:SER:C	2.45	0.54
43:C:776:GLU:O	43:C:782:GLU:N	2.41	0.54
1:B:26:A:H2	1:B:27:U:C5	2.26	0.54
19:G:146:C:N3	20:H:33:G:O6	2.40	0.54
1:B:110:C:H2'	1:B:111:A:C8	2.41	0.54
19:G:146:C:C1'	20:H:33:G:N2	2.68	0.54
19:G:151:C:O2'	19:G:152:C:OP1	2.24	0.54
1:B:99:C:H2'	1:B:100:C:C6	2.43	0.54
20:H:147:G:H2'	20:H:148:C:C6	2.43	0.54
26:1:1026:ASN:O	26:1:1028:HIS:N	2.41	0.54
26:1:1205:GLU:O	26:1:1208:LEU:N	2.41	0.54
31:6:7:ASP:O	31:6:91:LEU:N	2.39	0.54
19:G:151:C:C5'	19:G:152:C:C5	2.91	0.54
26:1:641:ILE:O	26:1:644:LEU:N	2.40	0.54
37:M:9:LYS:O	37:M:11:TYR:N	2.40	0.54
26:1:981:TYR:O	26:1:984:GLU:N	2.20	0.53
28:3:785:PRO:CA	28:3:800:ILE:O	2.56	0.53
11:F:47:A:H2'	11:F:48:A:H8	1.72	0.53
26:1:1132:LEU:O	26:1:1135:GLU:N	2.41	0.53
42:A:1817:LEU:N	42:A:1917:PHE:O	2.40	0.53
19:G:153:C:H2'	19:G:153:C:O2	2.08	0.53
20:H:153:A:H3'	20:H:154:C:C5'	2.38	0.53
34:K:222:ASN:O	34:K:520:MET:N	2.39	0.53
35:N:159:SER:O	42:A:730:GLY:HA3	2.08	0.53
35:N:142:PHE:O	35:N:144:ASP:N	2.41	0.53
40:I:58:C:H2'	40:I:59:U:H5'	1.85	0.53
40:I:61:A:H2'	40:I:62:U:C6	2.44	0.53
26:1:841:ALA:O	26:1:843:LYS:N	2.42	0.53
43:C:457:VAL:CA	43:C:462:GLY:HA3	2.39	0.53
28:3:1195:GLU:O	28:3:1198:ASP:N	2.41	0.53
35:N:290:ASP:H	42:A:872:ASP:CA	2.21	0.53
40:I:55:U:H3'	40:I:56:U:C5	2.44	0.53
40:I:126:A:C2	10:V:64:ASN:C	2.79	0.53
42:A:570:ASP:C	42:A:572:PHE:N	2.61	0.53
11:F:73:A:C2	40:I:2:G:N1	2.75	0.53
19:G:137:C:C2'	19:G:138:A:C5'	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:963:LYS:O	26:1:966:GLN:N	2.30	0.52
35:N:117:LYS:C	35:N:119:ARG:H	2.12	0.52
2:D:298:ASP:O	2:D:301:GLU:N	2.41	0.52
26:1:244:THR:O	26:1:247:ALA:N	2.42	0.52
33:J:534:LYS:O	33:J:567:LEU:O	2.26	0.52
34:K:206:THR:O	34:K:210:GLN:N	2.37	0.52
42:A:823:SER:O	42:A:824:PRO:C	2.47	0.52
26:1:929:LEU:O	26:1:930:PRO:C	2.45	0.52
26:1:1280:LEU:O	26:1:1282:ALA:N	2.42	0.52
35:N:302:ARG:O	35:N:305:ASN:O	2.28	0.52
26:1:747:LEU:O	26:1:748:LYS:C	2.48	0.52
27:2:596:GLU:O	27:2:598:GLU:N	2.43	0.52
40:I:21:U:HO2'	40:I:22:C:H5'	1.73	0.52
26:1:663:THR:O	26:1:666:LYS:N	2.42	0.52
35:N:425:ARG:O	35:N:429:CYS:N	2.38	0.52
42:A:347:LEU:O	42:A:348:PRO:C	2.47	0.52
28:3:430:GLY:O	28:3:433:SER:N	2.31	0.52
28:3:546:LYS:O	28:3:556:ILE:CA	2.58	0.52
40:I:118:A:H8	40:I:118:A:OP2	1.92	0.52
42:A:1943:LEU:O	42:A:1947:ASN:CA	2.58	0.52
1:B:19:A:H62	42:A:467:GLN:CA	2.22	0.52
1:B:48:A:O5'	42:A:280:GLU:N	2.42	0.52
28:3:589:CYS:O	28:3:608:GLY:N	2.30	0.52
42:A:708:THR:O	42:A:709:ILE:C	2.48	0.52
42:A:1439:ARG:O	42:A:1443:LYS:N	2.43	0.52
19:G:146:C:H2'	19:G:147:C:H5'	1.91	0.51
26:1:699:GLN:O	26:1:700:LYS:C	2.48	0.51
20:H:30:A:N3	20:H:30:A:C2'	2.73	0.51
20:H:107:A:C6	20:H:108:G:C5	2.99	0.51
26:1:771:LEU:O	26:1:774:ILE:N	2.44	0.51
26:1:793:LYS:O	26:1:797:GLY:CA	2.54	0.51
26:1:1110:VAL:O	26:1:1113:THR:N	2.43	0.51
32:7:37:ARG:O	32:7:40:TYR:N	2.44	0.51
34:K:340:THR:O	34:K:348:ARG:N	2.40	0.51
35:N:393:LEU:O	35:N:397:LEU:N	2.39	0.51
42:A:617:ASN:CA	42:A:621:VAL:O	2.59	0.51
11:F:52:U:O4	11:F:53:A:N6	2.43	0.51
19:G:152:C:H6	19:G:152:C:H3'	1.76	0.51
28:3:673:VAL:CA	28:3:691:THR:H	2.24	0.51
35:N:375:ILE:C	35:N:377:ILE:N	2.63	0.51
11:F:46:G:H2'	11:F:47:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:699:VAL:CA	28:3:715:MET:O	2.59	0.51
28:3:973:GLY:HA3	28:3:976:LYS:C	2.31	0.51
39:W:344:ILE:CA	39:W:360:LEU:CA	2.89	0.51
26:1:423:PRO:O	26:1:427:PRO:N	2.43	0.51
1:B:95:G:N3	1:B:95:G:C2'	2.73	0.51
26:1:1025:LYS:O	26:1:1027:ARG:N	2.42	0.51
42:A:838:LEU:O	42:A:841:LEU:N	2.44	0.51
19:G:156:U:H2'	19:G:156:U:O2	2.08	0.51
28:3:488:GLY:C	28:3:490:THR:H	2.14	0.51
30:5:46:ARG:N	30:5:63:VAL:O	2.44	0.51
42:A:1520:ASN:C	42:A:1522:GLN:N	2.63	0.51
19:G:126:C:H2'	19:G:126:C:O2	2.09	0.51
40:I:111:C:H2'	40:I:112:A:C8	2.46	0.51
42:A:398:THR:CA	43:C:386:GLY:HA3	2.38	0.51
26:1:1035:CYS:O	26:1:1038:LEU:N	2.44	0.51
2:D:114:GLU:O	2:D:117:LEU:N	2.44	0.51
20:H:111:G:O3'	20:H:112:G:O4'	2.29	0.51
26:1:1080:THR:O	26:1:1083:TYR:N	2.44	0.51
26:1:1188:ALA:O	26:1:1191:VAL:N	2.44	0.51
26:1:1207:SER:O	26:1:1210:HIS:N	2.43	0.51
28:3:147:ASP:N	28:3:151:ARG:O	2.42	0.51
28:3:318:ASP:N	28:3:321:MET:O	2.27	0.51
26:1:804:ASN:O	26:1:807:LYS:N	2.44	0.50
40:I:143:U:H2'	40:I:144:G:H5"	1.92	0.50
26:1:1129:LEU:O	26:1:1132:LEU:N	2.44	0.50
26:1:629:ALA:O	26:1:632:PHE:N	2.45	0.50
42:A:1488:THR:C	42:A:1537:TRP:O	2.49	0.50
19:G:143:U:C6	19:G:143:U:C5'	2.89	0.50
9:U:18:ARG:N	9:U:81:THR:O	2.40	0.50
1:B:26:A:N3	1:B:26:A:C3'	2.73	0.50
19:G:149:G:H21	19:G:150:U:H5'	1.77	0.50
20:H:143:A:N3	20:H:143:A:C3'	2.73	0.50
40:I:20:A:O2'	40:I:21:U:H5'	2.12	0.50
42:A:332:TYR:CA	43:C:177:ARG:O	2.60	0.50
19:G:146:C:C4	19:G:147:C:N4	2.73	0.50
40:I:58:C:O2'	40:I:59:U:H5"	2.09	0.50
42:A:972:GLU:CA	42:A:1101:PHE:O	2.60	0.50
43:C:452:THR:O	43:C:577:PHE:CA	2.60	0.50
26:1:1268:ILE:O	26:1:1271:SER:N	2.44	0.50
28:3:1195:GLU:C	28:3:1198:ASP:H	2.14	0.50
42:A:823:SER:O	42:A:824:PRO:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:360:ALA:O	35:N:364:GLN:N	2.38	0.50
1:B:100:C:H2'	1:B:101:U:C6	2.46	0.50
34:K:250:CYS:O	34:K:251:TRP:C	2.50	0.50
1:B:58:U:H2'	1:B:59:G:C8	2.46	0.49
39:W:564:GLY:O	39:W:565:ALA:O	2.29	0.49
26:1:528:ALA:O	26:1:531:LEU:N	2.44	0.49
39:W:349:PHE:N	39:W:364:ASP:H	2.10	0.49
42:A:401:GLY:HA3	43:C:385:VAL:O	2.12	0.49
42:A:929:GLU:O	42:A:933:ARG:CA	2.59	0.49
11:F:102:A:O2'	11:F:103:U:C5'	2.60	0.49
26:1:587:TYR:O	26:1:590:ARG:N	2.45	0.49
11:F:47:A:H2'	11:F:48:A:C8	2.47	0.49
26:1:237:GLY:O	26:1:239:ALA:N	2.45	0.49
33:J:446:LYS:CA	40:I:23:G:OP1	2.61	0.49
39:W:334:LEU:CA	39:W:340:LYS:CA	2.90	0.49
43:C:470:PRO:C	43:C:499:GLY:HA2	2.29	0.49
1:B:48:A:O5'	42:A:280:GLU:CA	2.60	0.49
20:H:106:G:N2	20:H:107:A:C6	2.72	0.49
20:H:46:U:H5"	20:H:47:U:H2'	1.93	0.49
26:1:1227:ILE:O	26:1:1230:VAL:N	2.46	0.49
28:3:596:PRO:O	28:3:598:GLY:N	2.45	0.49
42:A:597:LYS:C	42:A:599:MET:H	2.16	0.49
1:B:48:A:H2'	1:B:49:A:H8	1.76	0.49
19:G:149:G:H3'	19:G:149:G:N3	2.28	0.49
35:N:158:LEU:O	35:N:160:ILE:N	2.44	0.49
42:A:596:TYR:O	42:A:597:LYS:C	2.50	0.49
11:F:102:A:O2'	11:F:103:U:H5"	2.12	0.49
19:G:146:C:C2	19:G:147:C:H5	2.30	0.49
20:H:40:C:C5'	20:H:40:C:C6	2.92	0.49
26:1:553:VAL:O	26:1:556:ILE:N	2.46	0.49
39:W:341:LYS:O	39:W:359:LYS:CA	2.61	0.49
19:G:151:C:C1'	19:G:152:C:OP1	2.55	0.48
20:H:107:A:C2	20:H:108:G:C4	3.01	0.48
42:A:708:THR:O	42:A:710:LEU:N	2.46	0.48
26:1:625:ARG:O	26:1:628:THR:N	2.46	0.48
26:1:631:ALA:O	26:1:634:VAL:N	2.47	0.48
43:C:133:THR:O	43:C:225:VAL:CA	2.62	0.48
19:G:135:G:H1	20:H:41:U:H3	1.60	0.48
42:A:1197:LEU:O	42:A:1226:ALA:CA	2.62	0.48
19:G:135:G:C2	20:H:42:G:C5	3.02	0.48
26:1:177:LYS:O	26:1:180:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:672:GLY:O	28:3:695:GLY:N	2.46	0.48
35:N:160:ILE:CA	42:A:730:GLY:C	2.82	0.48
42:A:947:PRO:O	42:A:951:LEU:N	2.41	0.48
1:B:72:U:H2'	1:B:73:C:H6	1.78	0.48
27:2:491:LEU:O	27:2:493:ALA:N	2.46	0.48
26:1:939:ARG:O	26:1:940:LEU:C	2.51	0.48
11:F:73:A:H2	40:I:2:G:H1	1.56	0.48
19:G:152:C:O2'	19:G:153:C:O5'	2.30	0.48
26:1:408:PHE:O	26:1:409:PRO:C	2.50	0.48
43:C:263:LEU:O	43:C:268:LYS:N	2.47	0.48
1:B:17:U:O4	1:B:60:G:O6	2.31	0.47
1:B:25:C:H42	42:A:420:ARG:H	1.62	0.47
1:B:95:G:N3	1:B:95:G:H2'	2.28	0.47
11:F:49:G:H2'	11:F:50:A:C8	2.48	0.47
19:G:125:C:HO2'	19:G:126:C:P	2.36	0.47
20:H:151:C:C2	20:H:152:G:N7	2.82	0.47
1:B:23:C:H3'	1:B:24:G:H4'	1.96	0.47
19:G:149:G:C2'	19:G:150:U:H6	2.23	0.47
26:1:944:SER:O	26:1:946:LYS:N	2.38	0.47
26:1:978:LEU:O	26:1:979:TYR:C	2.51	0.47
28:3:923:GLY:HA3	28:3:947:GLU:O	2.14	0.47
40:I:110:G:H2'	40:I:111:C:C6	2.49	0.47
43:C:143:THR:H	45:C:1500:GTP:PB	2.37	0.47
43:C:366:GLN:O	43:C:367:ARG:C	2.51	0.47
26:1:102:ASP:O	26:1:106:GLU:N	2.47	0.47
11:F:73:A:N1	40:I:2:G:C6	2.82	0.47
19:G:135:G:O6	20:H:41:U:O4	2.32	0.47
28:3:558:LEU:O	28:3:561:GLY:CA	2.63	0.47
40:I:109:G:H2'	40:I:110:G:C8	2.49	0.47
20:H:153:A:C2'	20:H:154:C:C5'	2.86	0.47
26:1:226:HIS:O	26:1:229:SER:N	2.47	0.47
26:1:660:ALA:O	26:1:661:ARG:C	2.53	0.47
39:W:351:GLY:HA2	39:W:367:ALA:C	2.35	0.47
26:1:103:PRO:C	26:1:106:GLU:H	2.18	0.47
28:3:42:ARG:N	28:3:51:HIS:O	2.32	0.47
35:N:433:SER:O	35:N:437:TRP:N	2.47	0.47
43:C:452:THR:O	43:C:578:ARG:N	2.46	0.47
28:3:44:ASP:O	28:3:48:GLY:HA2	2.15	0.47
34:K:333:PRO:O	34:K:334:SER:O	2.33	0.47
35:N:410:ALA:O	35:N:413:LEU:CA	2.62	0.47
20:H:153:A:C8	20:H:154:C:H5'	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:183:G:H2'	20:H:184:C:C6	2.50	0.47
35:N:15:LEU:O	35:N:17:TYR:N	2.48	0.47
42:A:230:PHE:N	42:A:414:ARG:O	2.45	0.47
2:D:355:GLU:O	2:D:359:PHE:N	2.40	0.47
26:1:210:ALA:O	26:1:213:LYS:N	2.48	0.47
26:1:693:GLY:O	26:1:695:VAL:N	2.48	0.47
32:7:36:HIS:O	32:7:37:ARG:C	2.53	0.47
34:K:307:LEU:O	34:K:316:VAL:N	2.48	0.47
1:B:111:A:H2'	1:B:112:A:C8	2.49	0.46
11:F:50:A:H2'	11:F:51:U:C6	2.50	0.46
19:G:122:U:H4'	19:G:123:U:OP1	2.14	0.46
26:1:667:ILE:O	26:1:668:VAL:C	2.53	0.46
11:F:66:C:H2'	11:F:67:G:C8	2.50	0.46
32:7:42:SER:O	32:7:45:GLY:N	2.48	0.46
40:I:61:A:H2'	40:I:62:U:H6	1.80	0.46
20:H:107:A:C6	20:H:108:G:C6	3.04	0.46
26:1:705:SER:O	26:1:706:ALA:C	2.54	0.46
19:G:153:C:H4'	19:G:153:C:OP1	2.14	0.46
35:N:557:GLU:O	35:N:561:ALA:N	2.48	0.46
40:I:51:A:C2	40:I:55:U:O2'	2.64	0.46
40:I:126:A:C2	10:V:64:ASN:O	2.60	0.46
26:1:974:LEU:O	26:1:975:GLY:C	2.54	0.46
37:M:59:ASP:O	37:M:60:ALA:C	2.53	0.46
40:I:11:A:H2'	40:I:12:G:C8	2.50	0.46
26:1:1280:LEU:O	26:1:1281:ILE:C	2.51	0.46
35:N:391:ARG:O	35:N:395:LYS:N	2.37	0.46
20:H:141:C:H2'	20:H:142:C:C6	2.50	0.46
20:H:150:U:H2'	20:H:151:C:C6	2.50	0.46
20:H:168:A:H3'	20:H:169:C:H6	1.80	0.46
31:6:46:CYS:O	31:6:50:ASN:N	2.43	0.46
43:C:827:LEU:C	43:C:907:VAL:H	2.18	0.46
20:H:149:A:H2'	20:H:150:U:C6	2.50	0.46
26:1:257:THR:O	26:1:259:SER:N	2.49	0.46
32:7:48:ASP:O	32:7:49:LEU:C	2.54	0.46
1:B:26:A:H2	1:B:27:U:C6	2.34	0.46
1:B:99:C:H2'	1:B:100:C:H6	1.79	0.46
20:H:3:C:H2'	20:H:4:G:C8	2.51	0.46
20:H:181:G:H2'	20:H:182:U:C6	2.50	0.46
26:1:708:ALA:O	26:1:711:ALA:N	2.49	0.46
35:N:429:CYS:O	35:N:433:SER:N	2.38	0.46
42:A:1520:ASN:C	42:A:1522:GLN:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:180:G:H2'	20:H:181:G:C8	2.44	0.45
28:3:890:SER:O	28:3:908:GLY:N	2.41	0.45
20:H:59:A:H2'	20:H:60:U:O4'	2.17	0.45
42:A:570:ASP:O	42:A:571:ALA:C	2.54	0.45
2:D:159:LEU:C	2:D:161:LEU:N	2.68	0.45
20:H:113:G:H2'	20:H:114:A:H8	1.82	0.45
28:3:1141:PHE:O	28:3:1144:VAL:N	2.49	0.45
32:7:62:ALA:O	32:7:65:ARG:N	2.50	0.45
20:H:112:G:H2'	20:H:113:G:C8	2.50	0.45
26:1:687:VAL:O	26:1:690:ILE:N	2.50	0.45
35:N:554:ASN:O	35:N:558:CYS:N	2.43	0.45
20:H:148:C:H2'	20:H:149:A:H8	1.82	0.45
40:I:125:G:H1'	10:V:63:ASN:O	2.17	0.45
42:A:770:THR:O	42:A:771:VAL:C	2.51	0.45
2:D:1349:GLY:HA2	2:D:1491:SER:O	2.16	0.45
9:U:80:MET:O	10:V:59:SER:N	2.44	0.45
11:F:52:U:C5	11:F:52:U:OP2	2.70	0.45
19:G:149:G:N3	19:G:150:U:H5"	2.31	0.45
28:3:672:GLY:O	28:3:691:THR:N	2.49	0.45
40:I:115:G:H2'	40:I:116:G:C8	2.52	0.45
20:H:142:C:H2'	20:H:143:A:H5'	1.98	0.45
26:1:862:GLU:O	26:1:863:GLN:C	2.55	0.45
1:B:74:U:H2'	1:B:75:G:C8	2.52	0.45
28:3:215:LEU:O	28:3:218:ASN:N	2.50	0.45
43:C:133:THR:O	43:C:226:VAL:N	2.46	0.45
26:1:1119:VAL:O	26:1:1122:THR:N	2.49	0.45
28:3:663:LEU:O	28:3:678:VAL:CA	2.65	0.45
26:1:849:ILE:O	26:1:850:ILE:C	2.54	0.44
26:1:1243:PRO:O	26:1:1244:CYS:C	2.55	0.44
40:I:118:A:OP2	40:I:118:A:C8	2.71	0.44
42:A:350:PHE:O	43:C:268:LYS:O	2.35	0.44
1:B:98:G:OP2	1:B:98:G:C8	2.70	0.44
19:G:127:U:O2'	19:G:127:U:O2	2.31	0.44
19:G:147:C:N3	20:H:31:G:O6	2.50	0.44
19:G:150:U:O2'	19:G:151:C:C5	2.71	0.44
35:N:289:ASN:N	42:A:871:TYR:C	2.71	0.44
42:A:989:ASP:O	42:A:993:LEU:N	2.41	0.44
11:F:102:A:C2'	11:F:103:U:C5'	2.93	0.44
20:H:114:A:H2'	20:H:115:G:H8	1.81	0.44
20:H:152:G:O2'	20:H:153:A:H1'	2.16	0.44
35:N:149:LEU:O	35:N:151:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:606:LEU:O	26:1:609:MET:N	2.51	0.44
40:I:91:A:H2'	40:I:92:C:C6	2.53	0.44
4:P:109:VAL:N	5:Q:63:LEU:O	2.42	0.44
34:K:374:HIS:O	34:K:377:GLY:N	2.46	0.44
42:A:1520:ASN:O	42:A:1521:ALA:C	2.56	0.44
1:B:10:U:H2'	1:B:11:U:C6	2.52	0.44
19:G:148:U:O3'	19:G:149:G:O4'	2.35	0.44
20:H:178:A:C5'	20:H:179:C:OP2	2.66	0.44
20:H:182:U:H2'	20:H:183:G:H8	1.81	0.44
26:1:693:GLY:O	26:1:694:LEU:C	2.55	0.44
26:1:708:ALA:O	26:1:709:ILE:C	2.54	0.44
26:1:892:LEU:O	26:1:893:ILE:C	2.54	0.44
42:A:570:ASP:O	42:A:574:LEU:N	2.38	0.44
2:D:121:GLN:O	2:D:125:GLY:N	2.40	0.44
11:F:52:U:C6	11:F:52:U:OP2	2.71	0.44
11:F:90:G:H2'	11:F:91:A:H8	1.82	0.44
11:F:91:A:H2'	11:F:92:A:C8	2.53	0.44
19:G:149:G:C5	19:G:150:U:C4	3.05	0.44
28:3:676:ARG:O	28:3:686:LEU:CA	2.65	0.44
28:3:930:LEU:C	28:3:934:GLY:HA2	2.38	0.44
39:W:334:LEU:O	39:W:340:LYS:O	2.35	0.44
40:I:59:U:O2	40:I:60:A:C8	2.70	0.44
7:S:22:ASN:N	7:S:66:SER:O	2.49	0.44
1:B:61:A:H2'	1:B:62:G:C8	2.50	0.44
19:G:126:C:C2	19:G:126:C:OP2	2.70	0.44
20:H:142:C:O2'	20:H:143:A:H5'	2.18	0.44
20:H:143:A:OP2	20:H:143:A:C2	2.71	0.44
26:1:663:THR:O	26:1:664:GLY:C	2.56	0.44
26:1:953:ASP:O	26:1:954:LEU:C	2.56	0.44
43:C:257:ILE:O	43:C:310:SER:O	2.36	0.44
35:N:560:ARG:C	35:N:564:ALA:H	2.21	0.44
26:1:889:GLU:O	26:1:892:LEU:N	2.51	0.43
26:1:1078:VAL:O	26:1:1081:PHE:N	2.50	0.43
28:3:1148:LEU:O	28:3:1151:GLU:N	2.51	0.43
40:I:59:U:HO2'	40:I:60:A:C5'	2.19	0.43
26:1:665:ILE:O	26:1:666:LYS:C	2.55	0.43
40:I:21:U:C5	40:I:21:U:OP2	2.70	0.43
42:A:770:THR:O	42:A:772:CYS:N	2.51	0.43
26:1:865:ARG:O	26:1:866:LYS:C	2.56	0.43
26:1:955:ILE:O	26:1:956:SER:C	2.57	0.43
26:1:1264:VAL:O	26:1:1265:TYR:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:G:N3	1:B:95:G:C3'	2.81	0.43
26:1:629:ALA:O	26:1:630:ARG:C	2.56	0.43
26:1:1230:VAL:O	26:1:1233:ALA:N	2.52	0.43
40:I:110:G:O5'	40:I:110:G:C8	2.70	0.43
1:B:31:U:H2'	1:B:32:C:C6	2.54	0.43
1:B:72:U:H2'	1:B:73:C:C6	2.53	0.43
20:H:98:G:H5'	20:H:104:U:OP2	2.19	0.43
26:1:994:LEU:O	26:1:995:GLY:C	2.56	0.43
20:H:154:C:O2'	20:H:155:C:C5'	2.66	0.43
26:1:803:ALA:O	26:1:804:ASN:C	2.54	0.43
26:1:1029:GLU:O	26:1:1032:GLN:N	2.51	0.43
26:1:1110:VAL:O	26:1:1111:CYS:C	2.57	0.43
28:3:5:ASN:O	28:3:1176:GLY:HA3	2.19	0.43
35:N:560:ARG:O	35:N:564:ALA:O	2.33	0.43
2:D:298:ASP:O	2:D:299:ASP:C	2.56	0.43
20:H:64:A:H2'	20:H:65:U:C6	2.54	0.43
20:H:157:G:H2'	20:H:158:G:O4'	2.19	0.43
26:1:720:GLY:O	26:1:721:ILE:C	2.54	0.43
26:1:872:ILE:O	26:1:873:GLU:C	2.57	0.43
42:A:84:ASP:O	42:A:88:TYR:CA	2.66	0.43
42:A:379:GLU:O	43:C:355:LYS:CA	2.67	0.43
43:C:474:LEU:CA	43:C:498:SER:C	2.86	0.43
30:5:98:PHE:C	30:5:100:LYS:N	2.72	0.43
42:A:1502:PHE:O	42:A:1503:TRP:O	2.36	0.43
26:1:998:LYS:O	26:1:1001:VAL:N	2.51	0.43
3:E:255:MET:C	3:E:257:ASN:H	2.22	0.43
11:F:48:A:H2'	11:F:49:G:H8	1.84	0.43
11:F:91:A:H2'	11:F:92:A:H8	1.82	0.43
26:1:501:LEU:O	26:1:502:LEU:C	2.55	0.43
26:1:993:ILE:O	26:1:994:LEU:C	2.57	0.43
42:A:597:LYS:C	42:A:599:MET:N	2.72	0.43
11:F:89:U:H2'	11:F:90:G:C8	2.53	0.42
20:H:3:C:H2'	20:H:4:G:H8	1.84	0.42
26:1:665:ILE:O	26:1:668:VAL:N	2.52	0.42
26:1:833:LEU:O	26:1:834:VAL:C	2.56	0.42
42:A:838:LEU:O	42:A:839:LEU:C	2.57	0.42
42:A:1805:GLY:O	42:A:1822:ILE:N	2.45	0.42
19:G:128:U:H2'	19:G:129:G:H8	1.84	0.42
19:G:149:G:C8	19:G:150:U:O4	2.70	0.42
19:G:152:C:C2'	19:G:153:C:O5'	2.67	0.42
26:1:627:THR:O	26:1:630:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:137:C:H2'	19:G:138:A:C5'	2.49	0.42
26:1:981:TYR:O	26:1:983:GLY:N	2.52	0.42
40:I:21:U:OP2	40:I:21:U:H5	2.03	0.42
42:A:597:LYS:O	42:A:599:MET:N	2.51	0.42
11:F:92:A:H2'	11:F:93:G:C8	2.54	0.42
20:H:179:C:H2'	20:H:180:G:H8	1.83	0.42
26:1:889:GLU:O	26:1:890:GLU:C	2.57	0.42
40:I:90:G:H2'	40:I:91:A:C8	2.55	0.42
19:G:152:C:O2'	19:G:153:C:O4'	2.38	0.42
20:H:178:A:N3	20:H:178:A:H2'	2.34	0.42
26:1:429:ARG:O	26:1:432:THR:N	2.46	0.42
26:1:935:THR:O	26:1:936:VAL:C	2.58	0.42
1:B:31:U:H2'	1:B:32:C:H6	1.84	0.42
11:F:92:A:H2'	11:F:93:G:H8	1.83	0.42
30:5:51:GLY:HA3	30:5:56:THR:O	2.20	0.42
1:B:59:G:C2	1:B:60:G:C8	3.08	0.42
11:F:71:G:N2	40:I:4:U:O2	2.33	0.42
11:F:89:U:H2'	11:F:90:G:H8	1.84	0.42
20:H:107:A:N1	20:H:108:G:C5	2.88	0.42
26:1:854:VAL:O	26:1:856:ASP:N	2.52	0.42
40:I:125:G:N3	10:V:63:ASN:O	2.53	0.42
1:B:98:G:OP2	1:B:98:G:H8	2.03	0.42
19:G:155:U:O4'	19:G:156:U:C5	2.73	0.42
26:1:831:ARG:O	26:1:832:GLN:C	2.58	0.42
26:1:867:MET:O	26:1:868:VAL:C	2.57	0.42
34:K:333:PRO:O	34:K:334:SER:C	2.58	0.42
35:N:462:THR:O	35:N:466:ILE:N	2.38	0.42
40:I:14:G:H2'	40:I:15:G:C8	2.55	0.42
1:B:55:C:O2'	42:A:642:ARG:O	2.23	0.42
2:D:441:GLY:O	2:D:693:THR:N	2.36	0.42
19:G:135:G:C2	20:H:42:G:N1	2.87	0.42
26:1:578:ILE:O	26:1:579:GLU:C	2.57	0.42
42:A:1507:SER:O	42:A:1511:GLU:N	2.48	0.42
43:C:909:GLY:HA3	43:C:930:ALA:N	2.29	0.42
20:H:168:A:H3'	20:H:169:C:C6	2.54	0.42
26:1:631:ALA:O	26:1:632:PHE:C	2.58	0.42
39:W:344:ILE:CA	39:W:360:LEU:N	2.81	0.42
20:H:155:C:H2'	20:H:156:U:H5"	2.02	0.41
36:L:278:ASP:O	36:L:281:GLN:N	2.53	0.41
39:W:205:LEU:C	39:W:207:LYS:H	2.23	0.41
39:W:405:LYS:CA	42:A:789:GLU:CA	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:952:ALA:O	26:1:953:ASP:C	2.57	0.41
42:A:1593:LEU:O	42:A:1596:VAL:N	2.53	0.41
1:B:38:C:N4	1:B:39:C:N3	2.68	0.41
11:F:66:C:H2'	11:F:67:G:H8	1.85	0.41
20:H:153:A:H62	20:H:177:A:H2	1.67	0.41
26:1:318:ARG:O	26:1:321:ASP:N	2.52	0.41
26:1:1046:GLY:O	26:1:1048:GLU:N	2.52	0.41
39:W:338:LYS:O	39:W:339:LYS:O	2.38	0.41
19:G:125:C:OP2	19:G:125:C:C2	2.73	0.41
20:H:112:G:H8	20:H:112:G:O5'	2.04	0.41
26:1:1256:HIS:O	26:1:1257:PRO:C	2.58	0.41
1:B:26:A:N7	42:A:423:ASP:CA	2.83	0.41
20:H:152:G:H2'	20:H:153:A:C1'	2.51	0.41
26:1:758:ASP:O	26:1:761:TYR:N	2.54	0.41
28:3:437:VAL:O	28:3:776:GLN:CA	2.69	0.41
35:N:117:LYS:C	35:N:119:ARG:N	2.74	0.41
26:1:600:LEU:O	26:1:604:ALA:N	2.35	0.41
43:C:236:MET:O	43:C:237:LEU:C	2.59	0.41
20:H:153:A:H2'	20:H:154:C:H5"	1.99	0.41
26:1:841:ALA:C	26:1:843:LYS:N	2.73	0.41
26:1:1105:GLU:O	26:1:1106:ARG:C	2.59	0.41
32:7:64:VAL:O	32:7:65:ARG:C	2.59	0.41
1:B:26:A:N3	1:B:26:A:C5'	2.80	0.41
20:H:103:U:C3'	20:H:104:U:H5'	2.50	0.41
20:H:183:G:C6	20:H:184:C:N4	2.89	0.41
26:1:301:ARG:O	26:1:304:PRO:N	2.53	0.41
26:1:745:ALA:O	26:1:746:PHE:C	2.59	0.41
1:B:5:U:H2'	1:B:6:C:C6	2.56	0.41
1:B:75:G:H2'	1:B:76:A:C8	2.55	0.41
2:D:577:LYS:O	2:D:581:SER:N	2.54	0.41
3:E:255:MET:O	3:E:257:ASN:N	2.54	0.41
19:G:145:U:C3'	19:G:146:C:H5'	2.42	0.41
19:G:146:C:N3	19:G:147:C:N4	2.69	0.41
20:H:171:U:H2'	20:H:172:C:O4'	2.21	0.41
26:1:645:LEU:O	26:1:646:PRO:C	2.56	0.41
26:1:750:ILE:O	26:1:753:LEU:N	2.54	0.41
26:1:830:TYR:O	26:1:831:ARG:C	2.57	0.41
26:1:1169:VAL:O	26:1:1172:LEU:N	2.54	0.41
28:3:1148:LEU:O	28:3:1149:ARG:C	2.58	0.41
42:A:331:TRP:O	43:C:177:ARG:C	2.59	0.41
42:A:1952:VAL:O	42:A:1956:PRO:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:547:GLN:O	26:1:548:GLU:C	2.58	0.41
26:1:862:GLU:O	26:1:864:TYR:N	2.53	0.41
26:1:914:PHE:O	26:1:915:GLY:C	2.58	0.41
26:1:1129:LEU:O	26:1:1130:PRO:C	2.59	0.41
32:7:46:HIS:O	32:7:47:PHE:C	2.59	0.41
40:I:107:U:H2'	40:I:108:C:H6	1.85	0.41
43:C:756:LYS:O	43:C:757:ALA:C	2.58	0.41
1:B:101:U:H2'	1:B:102:U:C6	2.56	0.40
26:1:1128:VAL:O	26:1:1129:LEU:C	2.60	0.40
26:1:1223:SER:O	26:1:1224:PRO:C	2.60	0.40
43:C:684:LYS:O	43:C:795:VAL:N	2.45	0.40
28:3:1193:VAL:O	28:3:1196:GLU:N	2.54	0.40
35:N:736:LEU:O	35:N:740:PRO:N	2.54	0.40
38:O:30:PHE:O	38:O:79:CYS:CA	2.69	0.40
40:I:60:A:P	40:I:61:A:OP1	2.79	0.40
29:4:20:LEU:O	29:4:55:GLY:HA2	2.21	0.40
31:6:30:CYS:N	31:6:35:SER:O	2.38	0.40
42:A:570:ASP:C	42:A:572:PHE:H	2.22	0.40
43:C:684:LYS:N	43:C:795:VAL:O	2.55	0.40
1:B:71:C:H2'	1:B:72:U:C6	2.55	0.40
11:F:90:G:H2'	11:F:91:A:C8	2.57	0.40
26:1:1013:ILE:O	26:1:1014:LYS:C	2.60	0.40
35:N:289:ASN:N	42:A:871:TYR:O	2.54	0.40
42:A:954:LYS:O	42:A:958:GLY:N	2.46	0.40
42:A:1519:THR:C	42:A:1521:ALA:H	2.22	0.40
19:G:149:G:C4	19:G:150:U:C5	3.09	0.40
20:H:152:G:H2'	20:H:152:G:N3	2.36	0.40
20:H:166:G:N3	20:H:166:G:H2'	2.37	0.40
26:1:874:LYS:O	26:1:877:GLY:HA3	2.21	0.40
40:I:14:G:H2'	40:I:15:G:H8	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	1868/2136 (88%)	1770 (95%)	93 (5%)	5 (0%)	41 76
3	E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	4 28
4	P	70/118 (59%)	68 (97%)	2 (3%)	0	100 100
4	a	74/118 (63%)	71 (96%)	3 (4%)	0	100 100
4	k	81/118 (69%)	78 (96%)	3 (4%)	0	100 100
5	Q	69/86 (80%)	67 (97%)	2 (3%)	0	100 100
5	b	71/86 (83%)	70 (99%)	1 (1%)	0	100 100
5	m	72/86 (84%)	68 (94%)	4 (6%)	0	100 100
6	R	76/92 (83%)	70 (92%)	6 (8%)	0	100 100
6	c	76/92 (83%)	70 (92%)	6 (8%)	0	100 100
6	l	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
7	S	71/76 (93%)	67 (94%)	4 (6%)	0	100 100
7	d	67/76 (88%)	63 (94%)	4 (6%)	0	100 100
7	n	64/76 (84%)	62 (97%)	2 (3%)	0	100 100
8	T	69/126 (55%)	69 (100%)	0	0	100 100
8	e	76/126 (60%)	73 (96%)	3 (4%)	0	100 100
8	h	76/126 (60%)	75 (99%)	1 (1%)	0	100 100
9	U	60/231 (26%)	57 (95%)	3 (5%)	0	100 100
9	f	60/231 (26%)	57 (95%)	3 (5%)	0	100 100
9	i	69/231 (30%)	68 (99%)	1 (1%)	0	100 100
10	V	80/119 (67%)	76 (95%)	4 (5%)	0	100 100
10	g	89/119 (75%)	84 (94%)	5 (6%)	0	100 100
10	j	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
12	q	88/95 (93%)	77 (88%)	7 (8%)	4 (4%)	2 22
13	r	71/102 (70%)	66 (93%)	3 (4%)	2 (3%)	5 30
14	s	70/139 (50%)	64 (91%)	5 (7%)	1 (1%)	11 46
15	t	71/91 (78%)	64 (90%)	4 (6%)	3 (4%)	3 22
16	x	68/80 (85%)	66 (97%)	2 (3%)	0	100 100
17	y	61/103 (59%)	56 (92%)	5 (8%)	0	100 100
18	z	57/96 (59%)	52 (91%)	4 (7%)	1 (2%)	8 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	12 48
22	p	92/225 (41%)	90 (98%)	2 (2%)	0	100 100
23	u	118/793 (15%)	106 (90%)	6 (5%)	6 (5%)	2 19
24	v	91/464 (20%)	66 (72%)	16 (18%)	9 (10%)	0 9
25	w	431/501 (86%)	385 (89%)	41 (10%)	5 (1%)	13 49
26	1	1014/1304 (78%)	821 (81%)	171 (17%)	22 (2%)	6 35
27	2	174/895 (19%)	155 (89%)	14 (8%)	5 (3%)	4 29
28	3	1160/1217 (95%)	1062 (92%)	90 (8%)	8 (1%)	22 62
29	4	76/424 (18%)	74 (97%)	2 (3%)	0	100 100
30	5	106/125 (85%)	83 (78%)	20 (19%)	3 (3%)	5 30
31	6	87/110 (79%)	76 (87%)	11 (13%)	0	100 100
32	7	64/86 (74%)	55 (86%)	8 (12%)	1 (2%)	9 43
33	J	159/683 (23%)	148 (93%)	7 (4%)	4 (2%)	5 32
34	K	335/522 (64%)	295 (88%)	26 (8%)	14 (4%)	3 22
35	N	541/941 (58%)	475 (88%)	41 (8%)	25 (5%)	2 21
36	L	222/499 (44%)	214 (96%)	8 (4%)	0	100 100
37	M	123/128 (96%)	117 (95%)	6 (5%)	0	100 100
38	O	137/142 (96%)	126 (92%)	9 (7%)	2 (2%)	10 45
39	W	461/565 (82%)	327 (71%)	77 (17%)	57 (12%)	0 5
41	X	402/820 (49%)	393 (98%)	8 (2%)	1 (0%)	47 81
42	A	2213/2335 (95%)	2046 (92%)	100 (4%)	67 (3%)	4 28
43	C	814/972 (84%)	751 (92%)	40 (5%)	23 (3%)	5 30
All	All	13158/19749 (67%)	11964 (91%)	915 (7%)	279 (2%)	10 36

All (279) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	354	PRO
2	D	957	VAL
2	D	1584	ILE
3	E	193	THR
12	q	55	LEU
15	t	60	THR
15	t	61	PRO

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Mol	Chain	Res	Type
15	t	70	ASP
23	u	301	PRO
24	v	139	PRO
24	v	160	GLU
24	v	161	PRO
24	v	162	PRO
24	v	165	ARG
24	v	218	PRO
25	w	284	ARG
26	1	113	ALA
26	1	208	PRO
26	1	416	PRO
26	1	418	PRO
26	1	456	VAL
26	1	941	ASN
26	1	1105	GLU
26	1	1110	VAL
27	2	597	PHE
28	3	406	PRO
30	5	99	GLN
33	J	541	VAL
34	K	171	PRO
34	K	227	GLN
34	K	334	SER
34	K	480	PRO
34	K	514	ARG
35	N	12	PRO
35	N	163	VAL
35	N	355	GLY
35	N	370	PRO
35	N	420	ARG
35	N	741	HIS
35	N	841	PRO
35	N	918	ASP
39	W	146	ARG
39	W	178	ASN
39	W	183	ASP
39	W	206	ASP
39	W	207	LYS
39	W	208	GLN
39	W	231	LYS
39	W	265	PRO

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Mol	Chain	Res	Type
39	W	307	SER
39	W	340	LYS
39	W	345	VAL
39	W	350	GLN
39	W	355	ILE
39	W	360	LEU
39	W	361	PRO
39	W	364	ASP
39	W	394	ASP
39	W	406	GLU
39	W	411	PRO
39	W	414	PRO
39	W	415	LEU
39	W	419	LEU
39	W	458	THR
39	W	479	ASP
39	W	484	LEU
39	W	486	GLU
39	W	532	LEU
39	W	556	ASP
42	A	63	PRO
42	A	166	PHE
42	A	308	ILE
42	A	331	TRP
42	A	363	HIS
42	A	371	LEU
42	A	373	ASP
42	A	424	ILE
42	A	425	PRO
42	A	442	LYS
42	A	471	TYR
42	A	571	ALA
42	A	598	LEU
42	A	629	PHE
42	A	631	ALA
42	A	697	MET
42	A	698	PRO
42	A	799	PRO
42	A	1013	ASN
42	A	1124	ASN
42	A	1186	LEU
42	A	1202	THR

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Mol	Chain	Res	Type
42	A	1511	GLU
42	A	1520	ASN
42	A	1521	ALA
42	A	1604	LEU
42	A	1760	GLU
42	A	2016	ILE
42	A	2018	ALA
43	C	333	ASP
43	C	388	VAL
43	C	427	PHE
43	C	444	GLY
43	C	457	VAL
43	C	458	ASP
43	C	475	MET
43	C	516	LEU
43	C	572	GLU
43	C	825	PRO
2	D	151	LYS
12	q	74	ALA
13	r	97	PRO
14	s	12	ASN
21	o	160	LYS
23	u	223	LYS
23	u	280	VAL
25	w	277	THR
28	3	772	ALA
30	5	104	LYS
34	K	198	LEU
34	K	265	LEU
35	N	150	ALA
35	N	824	PRO
35	N	840	ASP
39	W	105	CYS
39	W	107	TYR
39	W	186	LEU
39	W	211	LEU
39	W	339	LYS
39	W	341	LYS
39	W	365	LEU
39	W	380	GLN
39	W	395	LEU
39	W	457	PHE

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Mol	Chain	Res	Type
39	W	462	PHE
39	W	502	ASN
39	W	531	ASP
41	X	666	PRO
42	A	531	THR
42	A	729	PRO
42	A	767	VAL
42	A	1015	VAL
42	A	1092	ILE
42	A	1126	VAL
42	A	1185	LEU
42	A	1308	PRO
43	C	156	GLU
43	C	354	ARG
43	C	367	ARG
43	C	440	SER
43	C	824	THR
43	C	868	LEU
3	E	60	MET
3	E	88	ARG
3	E	256	ASP
25	w	177	ARG
25	w	393	PRO
26	1	437	PRO
27	2	510	TYR
34	K	261	PRO
35	N	143	SER
35	N	774	PRO
38	O	74	GLU
39	W	400	LEU
39	W	410	ILE
39	W	417	ASN
39	W	466	LYS
39	W	509	PRO
42	A	212	PRO
42	A	376	GLU
42	A	381	PRO
42	A	709	ILE
42	A	734	PRO
42	A	824	PRO
42	A	1203	SER
42	A	1204	TYR

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Mol	Chain	Res	Type
42	A	1503	TRP
42	A	1677	GLU
42	A	1758	PRO
42	A	1947	ASN
43	C	237	LEU
43	C	615	PRO
3	E	162	ARG
13	r	96	ALA
21	o	32	PRO
23	u	300	THR
26	1	112	ILE
26	1	523	ALA
26	1	909	VAL
26	1	1006	MET
27	2	463	ALA
27	2	599	THR
28	3	529	ALA
28	3	578	THR
30	5	75	ASP
33	J	535	GLU
33	J	536	ASP
33	J	615	ASP
34	K	229	GLY
34	K	259	SER
34	K	405	GLY
35	N	324	LYS
35	N	374	ARG
35	N	777	PRO
35	N	809	ASN
35	N	855	ARG
39	W	176	PRO
39	W	376	ASN
39	W	418	ILE
39	W	425	ILE
39	W	491	VAL
42	A	188	LEU
42	A	380	LEU
42	A	526	PRO
42	A	903	SER
42	A	1305	SER
43	C	856	HIS
3	E	159	PRO

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Mol	Chain	Res	Type
12	q	73	PRO
24	v	141	ILE
24	v	217	PRO
26	1	1075	ARG
26	1	1186	GLN
28	3	95	SER
28	3	229	GLU
35	N	421	ILE
39	W	337	THR
39	W	434	LYS
42	A	349	ALA
42	A	437	ALA
42	A	1206	GLU
43	C	360	ALA
43	C	573	GLU
3	E	270	LYS
18	z	34	ILE
24	v	220	PRO
26	1	326	THR
26	1	932	ILE
26	1	1047	ALA
28	3	407	ILE
35	N	307	HIS
35	N	325	LEU
38	O	77	ASP
39	W	357	THR
39	W	413	VAL
42	A	370	PRO
42	A	619	GLY
42	A	1198	PRO
42	A	1275	ARG
42	A	1955	LYS
42	A	2012	LEU
43	C	361	PRO
3	E	149	GLY
26	1	417	PRO
34	K	459	PRO
34	K	479	HIS
35	N	739	CYS
39	W	222	PRO
39	W	262	ILE
42	A	771	VAL

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Mol	Chain	Res	Type
23	u	221	PRO
26	1	223	THR
42	A	358	PRO
42	A	1118	PRO
25	w	229	TRP
26	1	409	PRO
27	2	586	ILE
28	3	1204	VAL
34	K	446	PRO
35	N	323	GLY
35	N	369	LEU
2	D	585	ILE
3	E	324	PRO
23	u	298	PRO
26	1	1031	VAL
32	7	64	VAL
42	A	894	VAL
12	q	52	PRO
35	N	743	THR
43	C	778	PRO

5.3.2 Protein sidechains

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

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	114/117 (97%)	38 (33%)	2 (1%)
11	F	65/107 (60%)	10 (15%)	2 (3%)
19	G	41/274 (14%)	28 (68%)	9 (21%)
20	H	105/188 (55%)	25 (23%)	2 (1%)
40	I	112/144 (77%)	31 (27%)	4 (3%)
All	All	437/830 (52%)	132 (30%)	19 (4%)

All (132) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	8	G
1	B	10	U
1	B	20	G

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Mol	Chain	Res	Type
1	B	21	A
1	B	22	U
1	B	23	C
1	B	24	G
1	B	25	C
1	B	26	A
1	B	27	U
1	B	34	U
1	B	36	C
1	B	38	C
1	B	39	C
1	B	41	U
1	B	42	U
1	B	45	C
1	B	48	A
1	B	52	U
1	B	53	U
1	B	54	U
1	B	57	G
1	B	68	C
1	B	69	A
1	B	70	A
1	B	79	C
1	B	80	U
1	B	83	A
1	B	88	A
1	B	90	U
1	B	92	U
1	B	93	U
1	B	94	U
1	B	95	G
1	B	96	A
1	B	97	G
1	B	98	G
1	B	109	G
11	F	6	C
11	F	7	G
11	F	9	U
11	F	51	U
11	F	52	U
11	F	53	A
11	F	70	A

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Mol	Chain	Res	Type
11	F	103	U
11	F	104	U
11	F	106	U
19	G	123	U
19	G	124	U
19	G	125	C
19	G	126	C
19	G	127	U
19	G	128	U
19	G	129	G
19	G	130	A
19	G	135	G
19	G	136	U
19	G	137	C
19	G	140	A
19	G	144	A
19	G	145	U
19	G	146	C
19	G	147	C
19	G	148	U
19	G	149	G
19	G	150	U
19	G	151	C
19	G	152	C
19	G	154	U
19	G	156	U
19	G	157	U
19	G	159	U
19	G	161	U
19	G	162	C
19	G	163	C
20	H	31	G
20	H	37	U
20	H	40	C
20	H	45	C
20	H	47	U
20	H	51	A
20	H	65	U
20	H	105	G
20	H	106	G
20	H	112	G
20	H	143	A

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Mol	Chain	Res	Type
20	H	147	G
20	H	152	G
20	H	153	A
20	H	154	C
20	H	156	U
20	H	157	G
20	H	164	C
20	H	166	G
20	H	167	U
20	H	168	A
20	H	169	C
20	H	177	A
20	H	178	A
20	H	179	C
40	I	21	U
40	I	25	A
40	I	26	G
40	I	36	U
40	I	41	C
40	I	44	A
40	I	45	G
40	I	56	U
40	I	58	C
40	I	59	U
40	I	60	A
40	I	61	A
40	I	62	U
40	I	84	C
40	I	85	G
40	I	90	G
40	I	100	A
40	I	103	A
40	I	109	G
40	I	114	U
40	I	115	G
40	I	118	A
40	I	119	A
40	I	120	U
40	I	121	U
40	I	122	U
40	I	124	U
40	I	125	G

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Mol	Chain	Res	Type
40	I	126	A
40	I	127	C
40	I	144	G

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	78	U
1	B	94	U
11	F	51	U
11	F	52	U
19	G	123	U
19	G	136	U
19	G	143	U
19	G	148	U
19	G	150	U
19	G	151	C
19	G	153	C
19	G	155	U
19	G	156	U
20	H	156	U
20	H	168	A
40	I	43	G
40	I	58	C
40	I	99	C
40	I	114	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	GTP	C	1500	46	26,34,34	1.27	1 (3%)	32,54,54	1.62	3 (9%)
44	IHP	A	3000	-	36,36,36	0.82	0	54,60,60	1.20	2 (3%)

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
45	GTP	C	1500	46	-	3/18/38/38	0/3/3/3
44	IHP	A	3000	-	-	6/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	1500	GTP	C6-N1	-3.66	1.32	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C	1500	GTP	PB-O3B-PG	-5.86	112.72	132.83
44	A	3000	IHP	C6-C5-C4	3.80	118.73	110.41
45	C	1500	GTP	PA-O3A-PB	-3.76	119.91	132.83
44	A	3000	IHP	C5-C4-C3	2.46	115.80	110.41
45	C	1500	GTP	C5-C6-N1	2.40	118.19	113.95

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	A	3000	IHP	C2-O12-P2-O42
44	A	3000	IHP	C3-O13-P3-O23
45	C	1500	GTP	C5'-O5'-PA-O3A
44	A	3000	IHP	C6-O16-P6-O46
44	A	3000	IHP	C5-O15-P5-O25

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Mol	Chain	Res	Type	Atoms
44	A	3000	IHP	C1-O11-P1-O31
44	A	3000	IHP	C4-O14-P4-O34
45	C	1500	GTP	PG-O3B-PB-O2B
45	C	1500	GTP	C5'-O5'-PA-O1A

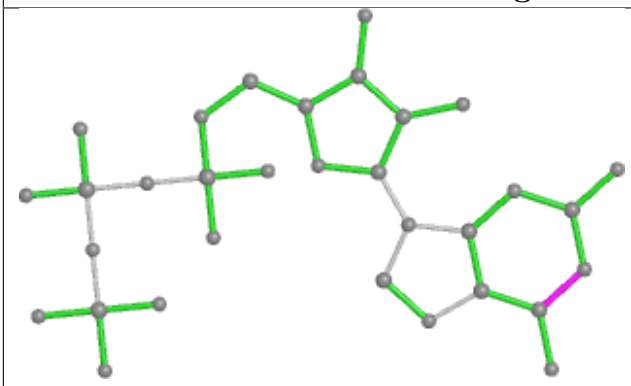
There are no ring outliers.

1 monomer is involved in 4 short contacts:

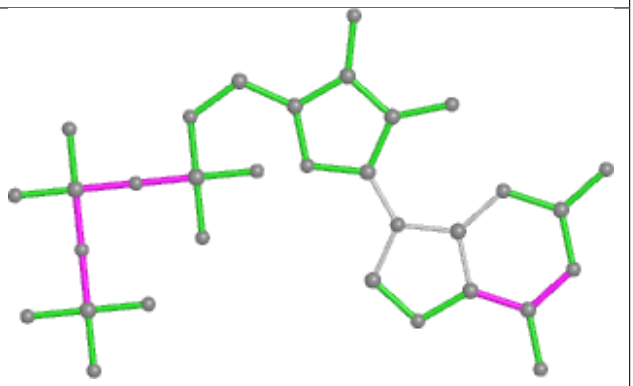
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	C	1500	GTP	4	0

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

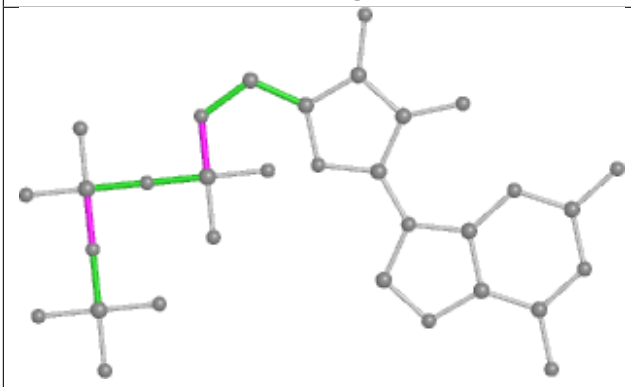
Ligand GTP C 1500



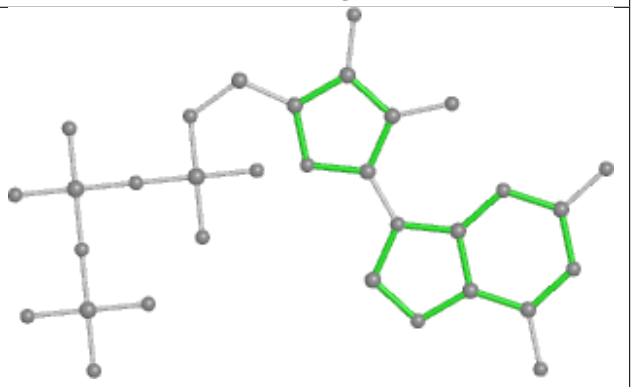
Bond lengths



Bond angles

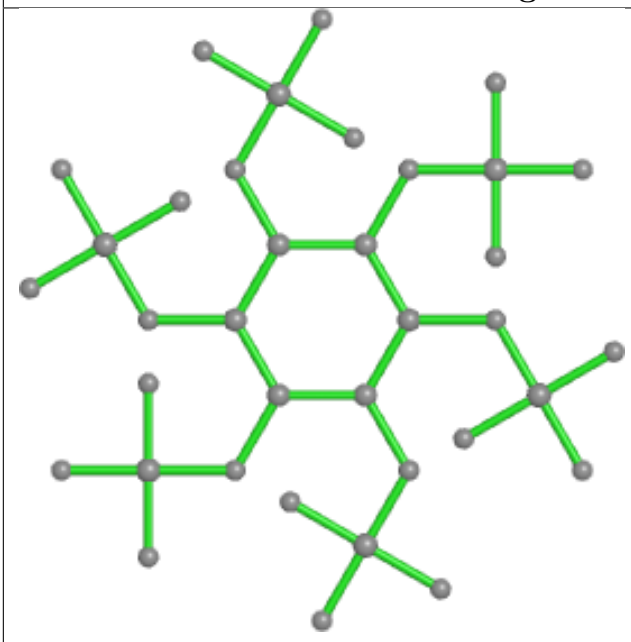


Torsions

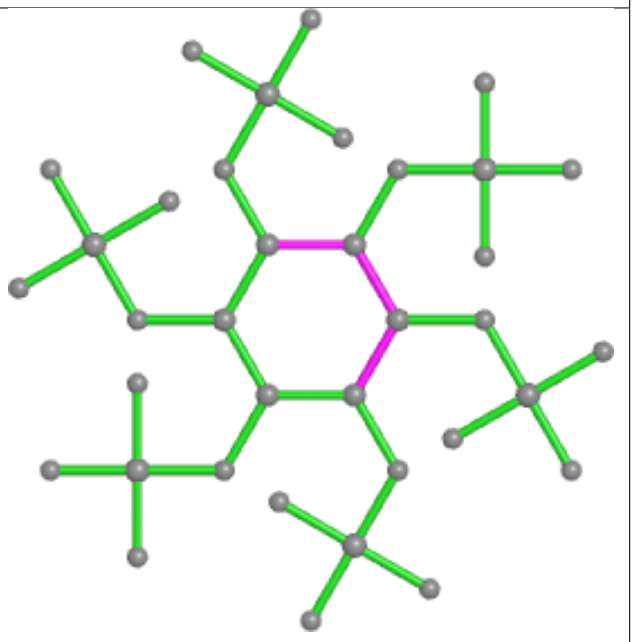


Rings

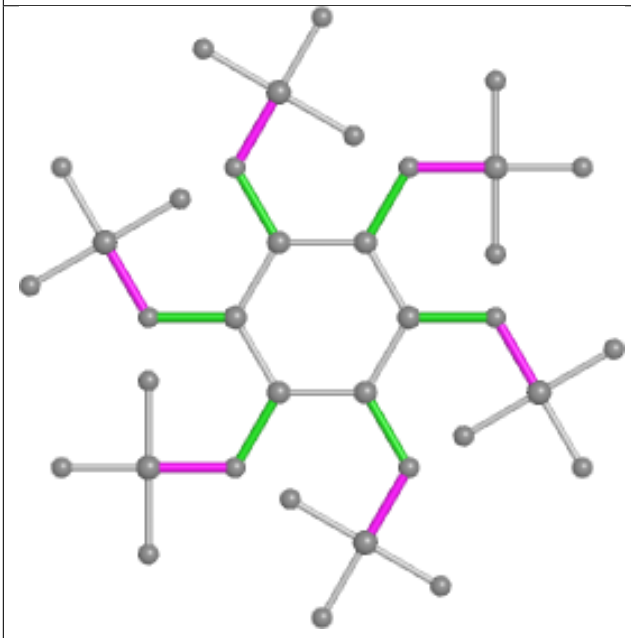
Ligand IHP A 3000



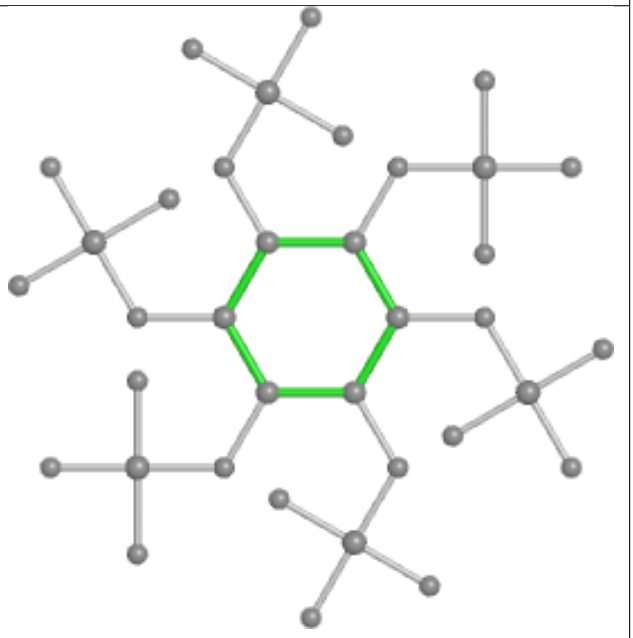
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

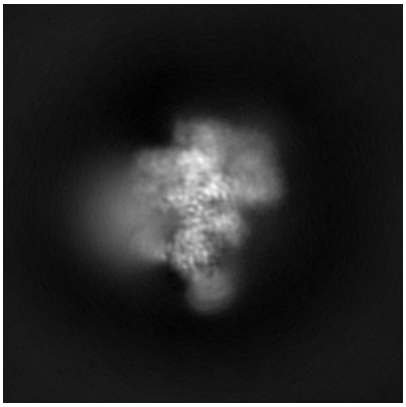
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9621. These allow visual inspection of the internal detail of the map and identification of artifacts.

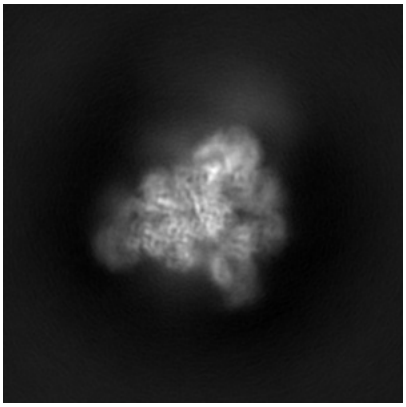
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

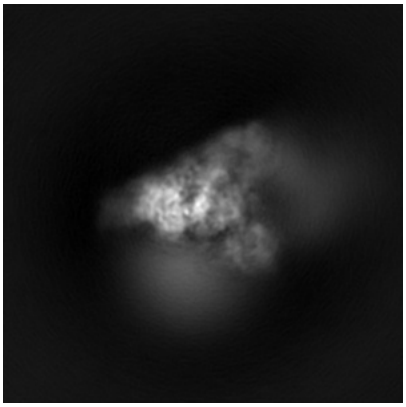
6.1.1 Primary map



X



Y

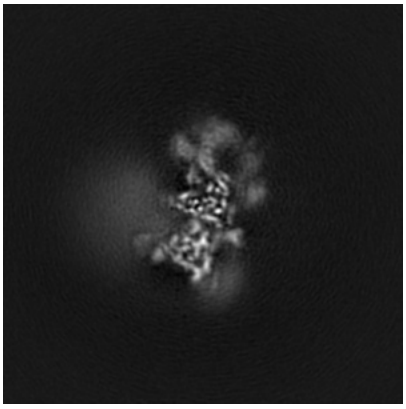


Z

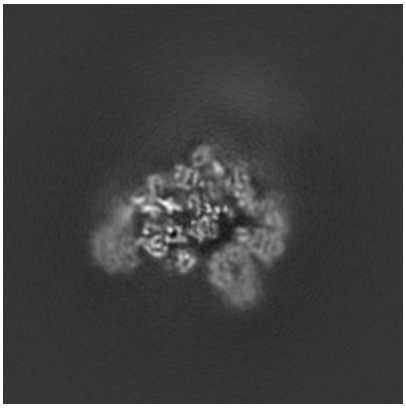
The images above show the map projected in three orthogonal directions.

6.2 Central slices

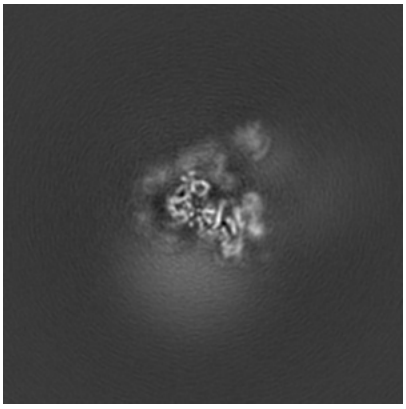
6.2.1 Primary map



X Index: 200



Y Index: 200

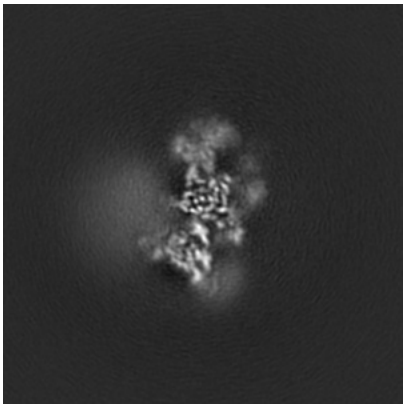


Z Index: 200

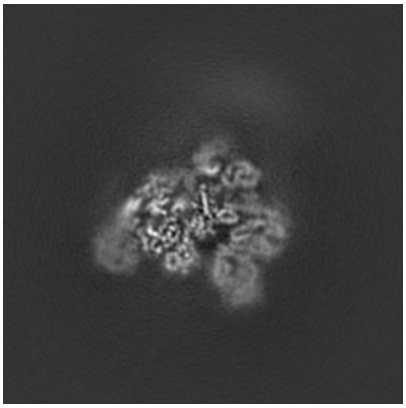
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

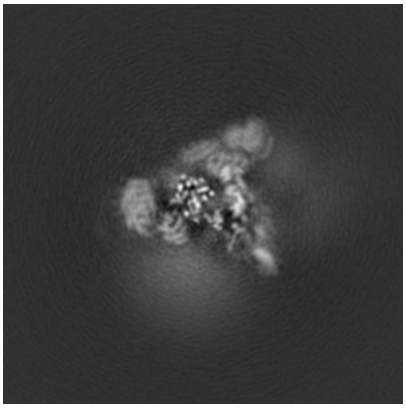
6.3.1 Primary map



X Index: 197



Y Index: 193

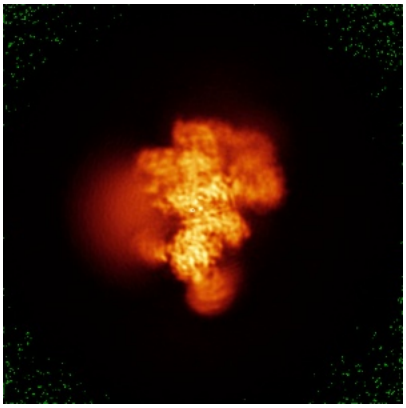


Z Index: 213

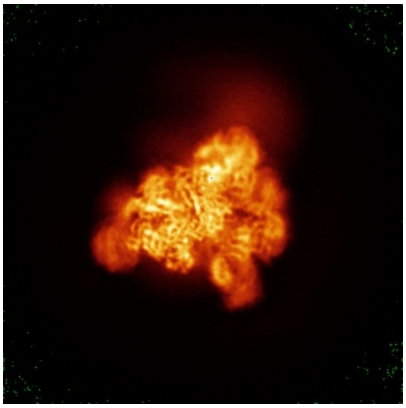
The images above show the largest variance slices of the map in three orthogonal directions.

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

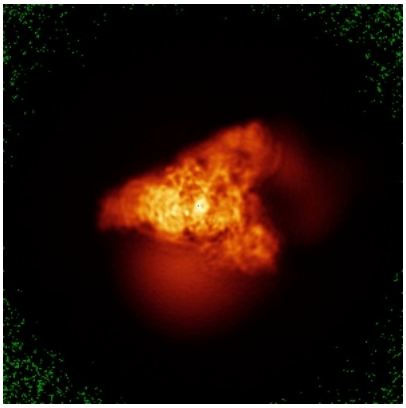
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

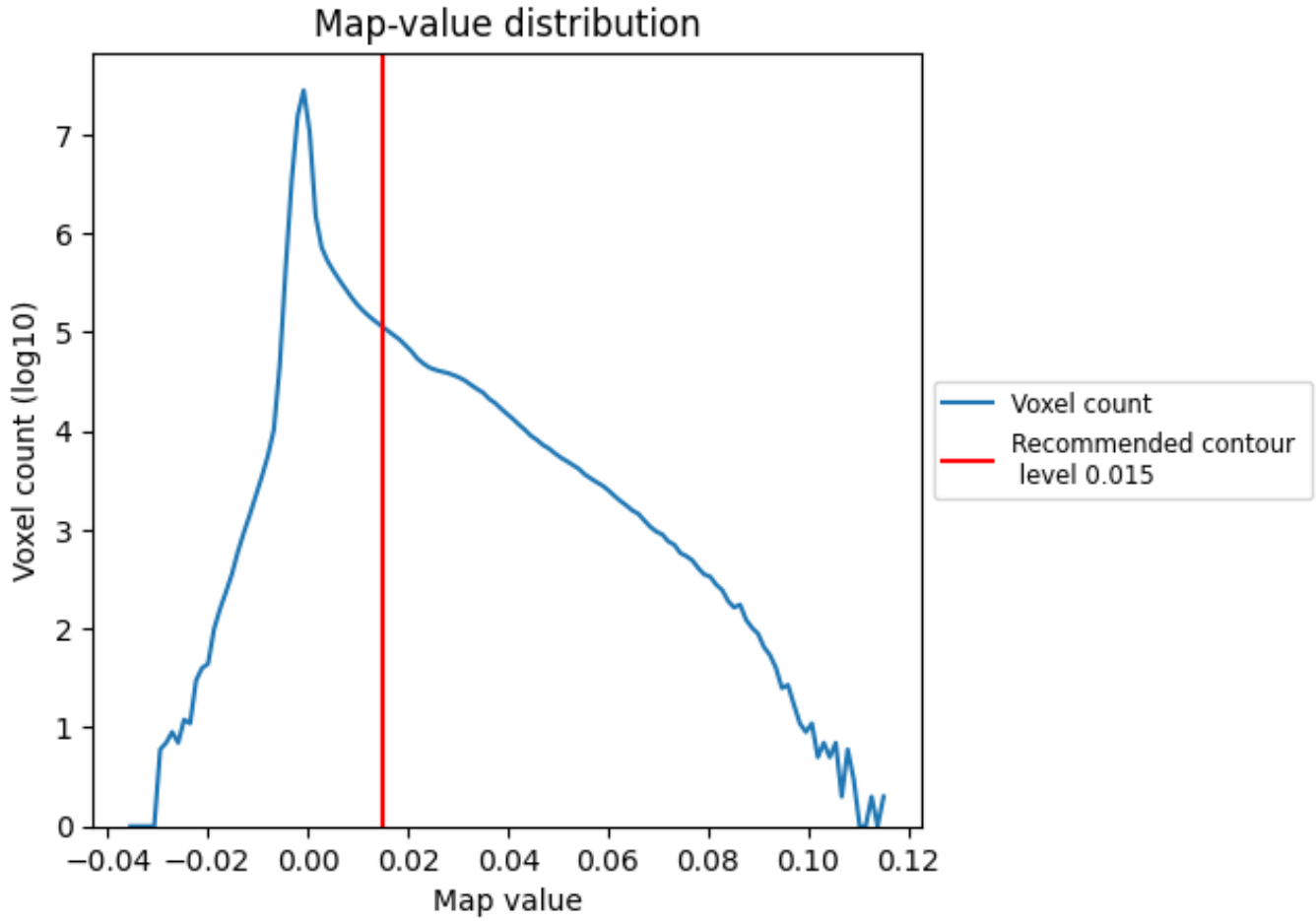
6.6 Mask visualisation (i)

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

7 Map analysis

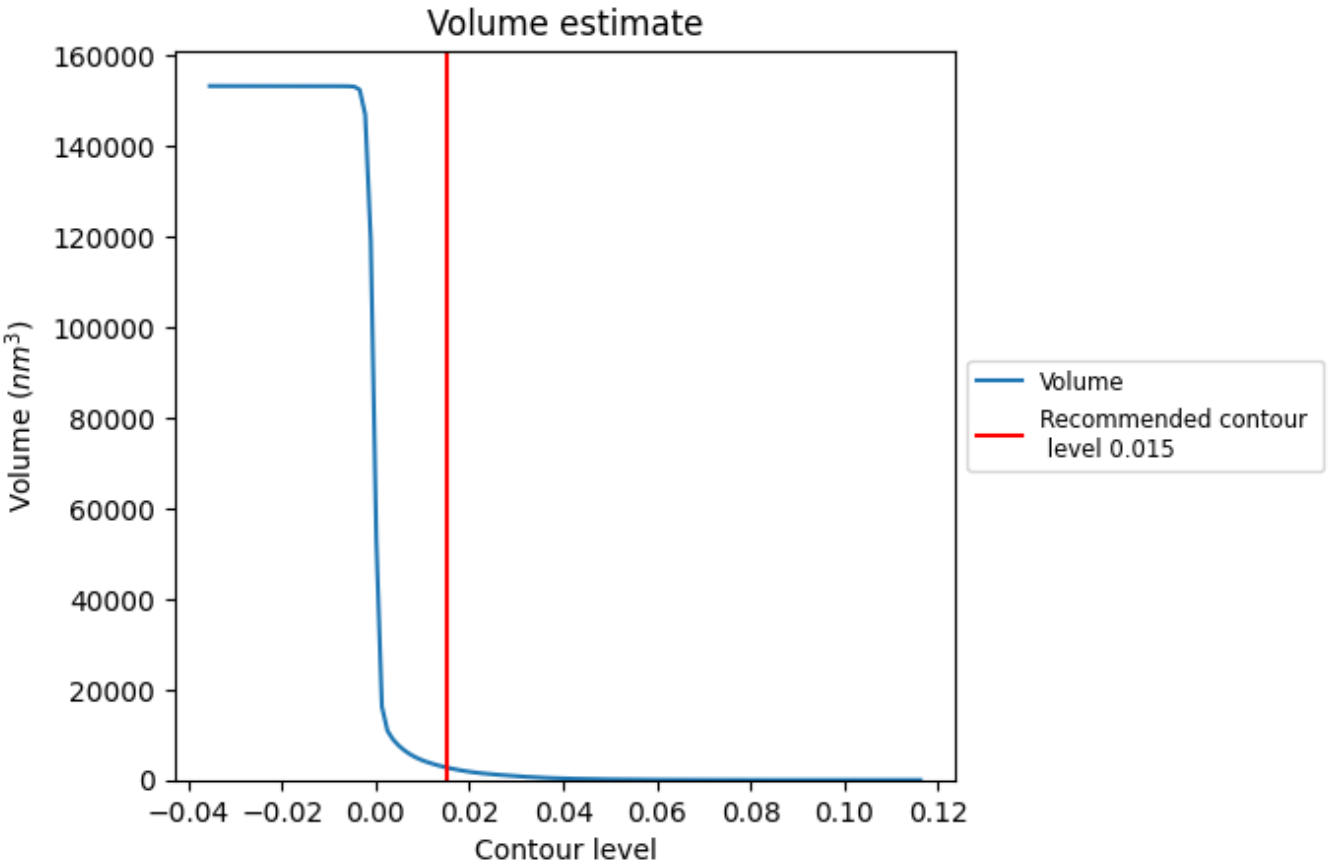
This section contains the results of statistical analysis of the map.

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.

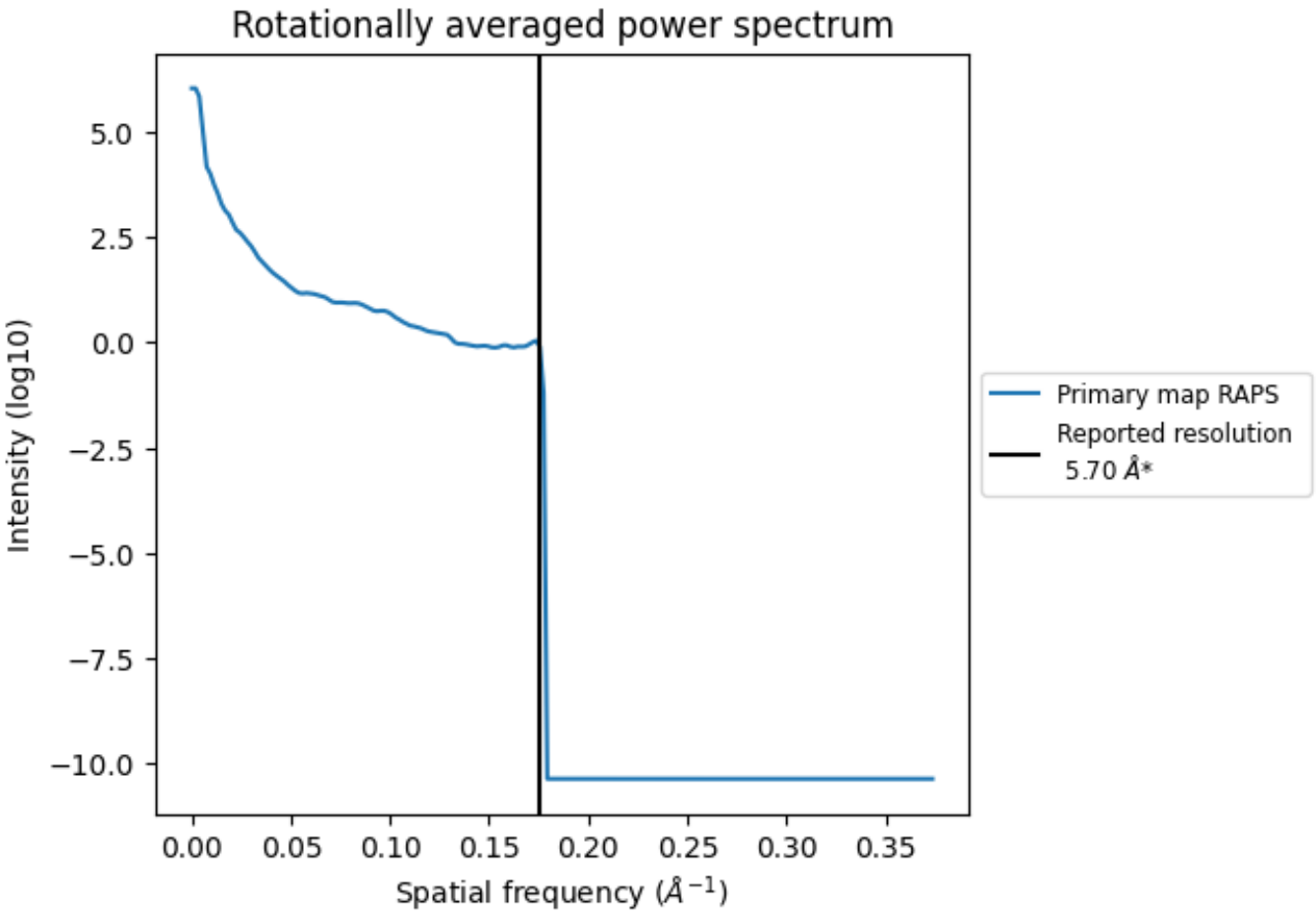
7.2 Volume estimate



The volume at the recommended contour level is 2784 nm^3; this corresponds to an approximate mass of 2515 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 0.175 $Å^{-1}$

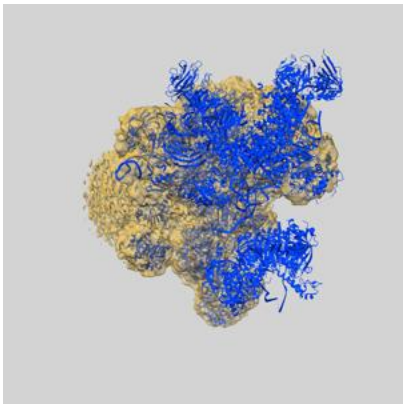
8 Fourier-Shell correlation (i)

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

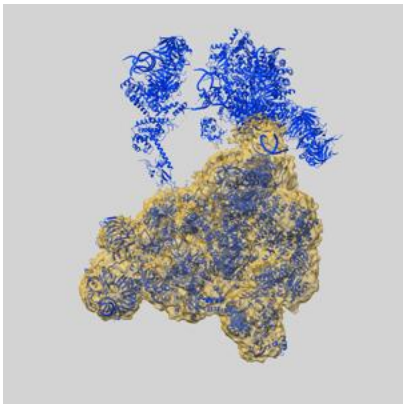
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9621 and PDB model 6AH0. Per-residue inclusion information can be found in section 3 on page 14.

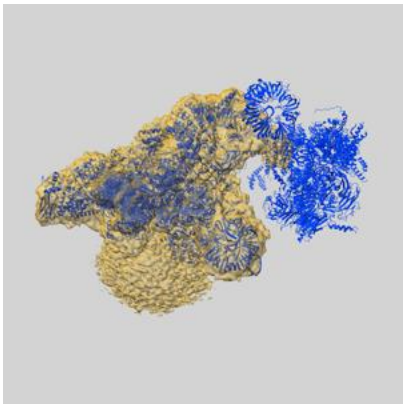
9.1 Map-model overlay



X



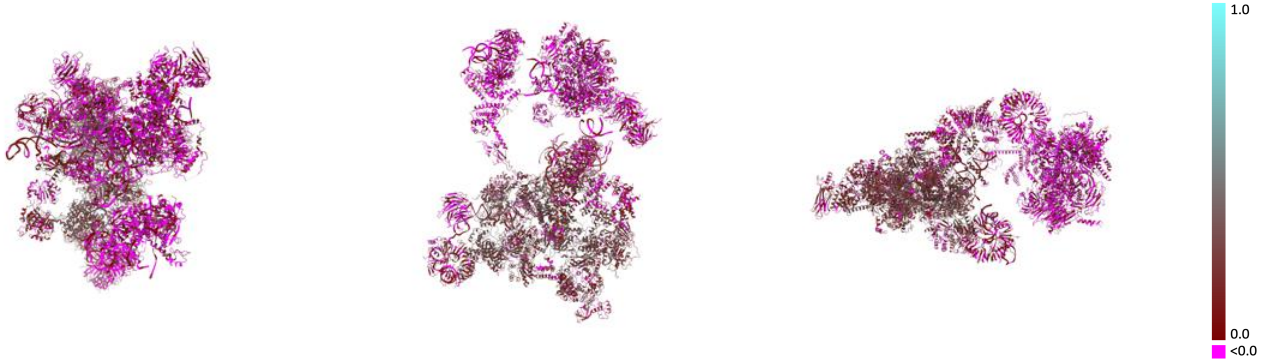
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

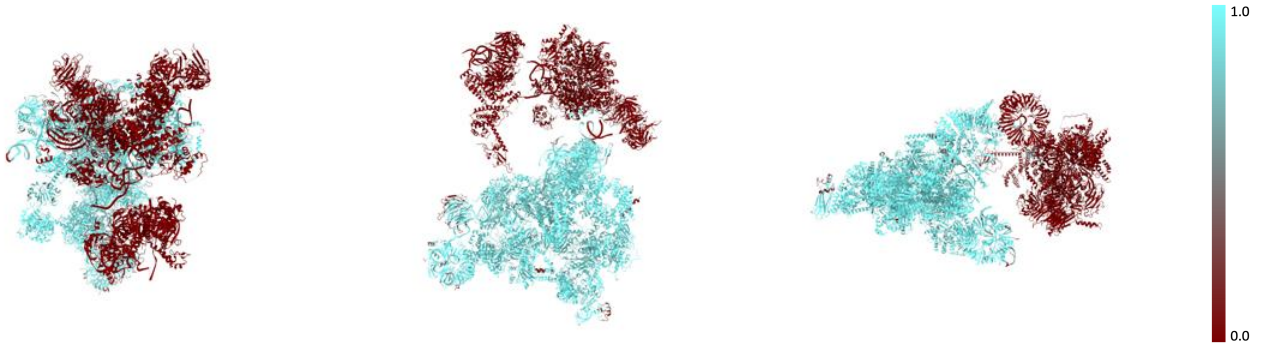
9.2 Q-score mapped to coordinate model



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.

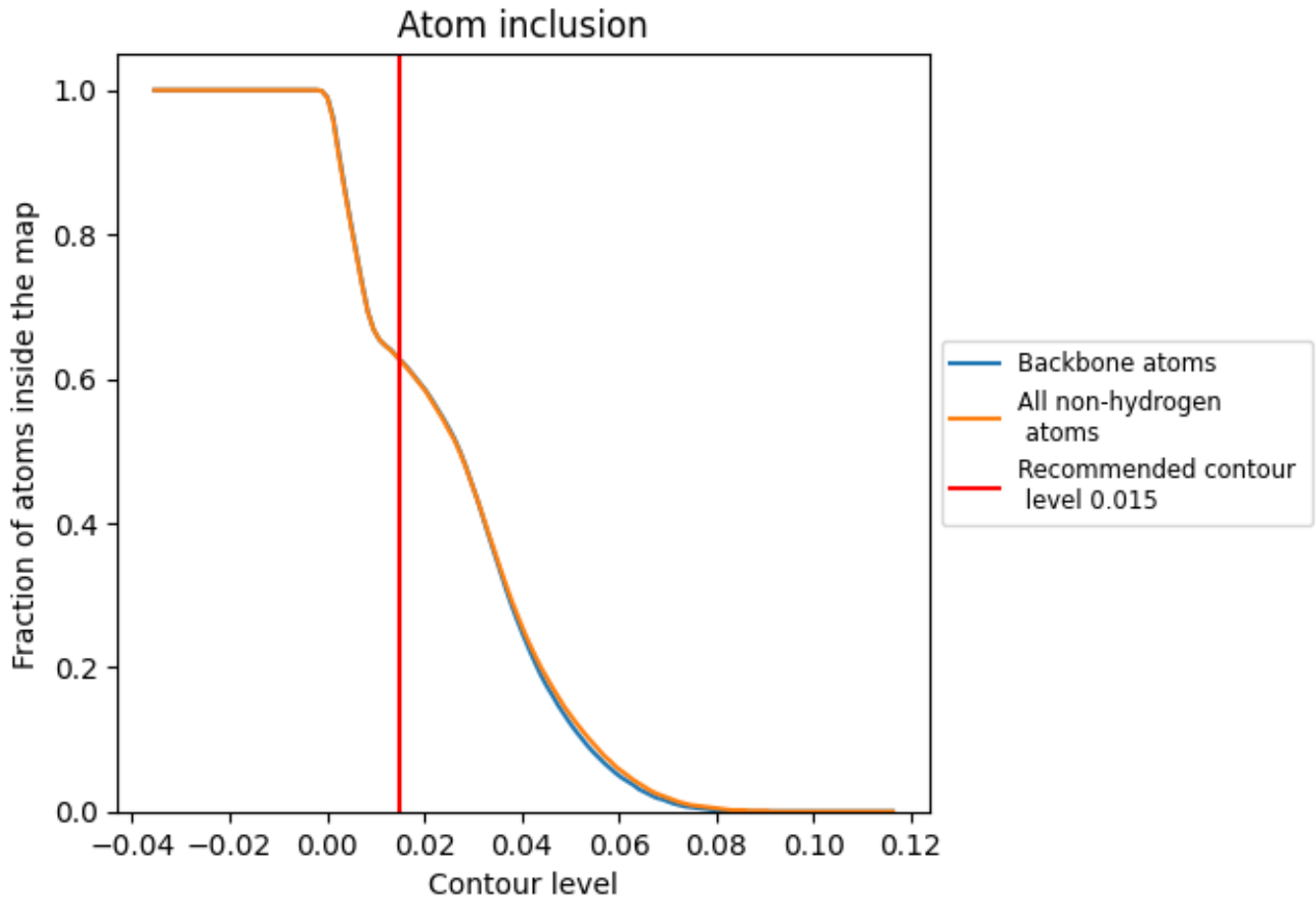
9.3 Atom inclusion mapped to coordinate model



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 63% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6260	0.1190
1	0.0190	0.0020
2	0.0360	0.0050
3	0.0000	-0.0030
4	0.0000	-0.0090
5	0.0000	-0.0110
6	0.0000	-0.0050
7	0.0000	0.0920
A	0.9900	0.2830
B	0.9360	0.1220
C	1.0000	0.2810
D	0.9740	0.1980
E	0.7270	-0.0190
F	0.7860	0.1010
G	0.0000	0.0150
H	0.0530	-0.0000
I	0.9330	0.1200
J	0.9580	0.0740
K	0.9940	0.0920
L	0.9870	0.1530
M	0.9900	0.2130
N	0.9580	0.1260
O	0.9750	0.2170
P	0.9570	0.1190
Q	0.9210	0.0870
R	0.8920	0.0800
S	0.9230	0.1050
T	0.9060	0.0760
U	0.9100	0.0820
V	0.9550	0.1500
W	0.9250	0.1840
X	0.9610	0.1200
a	0.9650	0.1010
b	0.8400	0.0480
c	0.9040	0.0990

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Chain	Atom inclusion	Q-score
d	0.8760	0.1480
e	1.0000	0.2090
f	1.0000	0.1490
g	0.9290	0.1560
h	0.0000	0.0120
i	0.0000	-0.0140
j	0.0000	-0.0180
k	0.0000	0.0390
l	0.0000	0.0120
m	0.0000	0.0380
n	0.0000	0.0170
o	0.0000	-0.0050
p	0.0000	0.0060
q	0.0000	0.0370
r	0.0000	0.0420
s	0.0000	-0.0520
t	0.0000	-0.0050
u	0.0000	0.0100
v	0.0000	0.0170
w	0.0000	-0.0140
x	0.0000	0.0050
y	0.0000	0.0190
z	0.0000	-0.0140