Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 07:37 pm GMT

PDB ID	:	5JCS
EMDB ID	:	EMD-3199
Title	:	CRYO-EM STRUCTURE OF THE RIX1-REA1 PRE-60S PARTICLE
Authors	:	Barrio-Garcia, C.; Thoms, M.; Flemming, D.; Kater, L.; Berninghausen, O.; Bassler, J.; Beckmann, R.; Hurt, E.
Deposited on	:	2016-04-15
Resolution	:	9.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

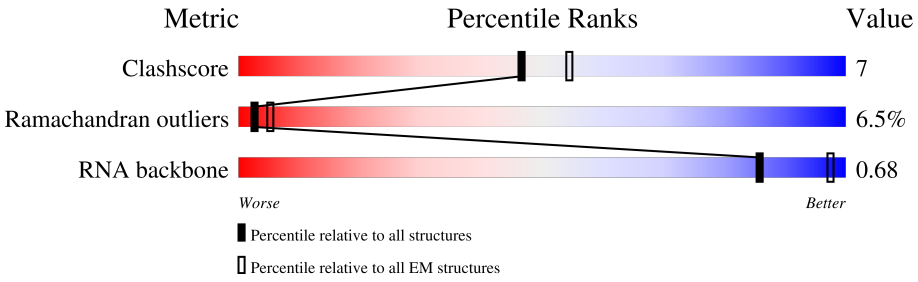
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.50 Å.

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



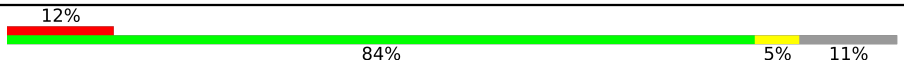
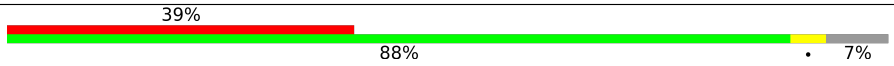
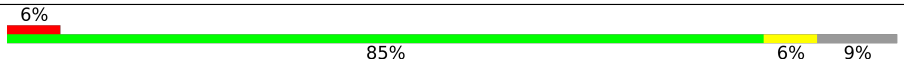
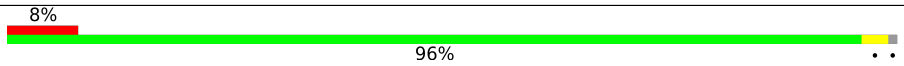
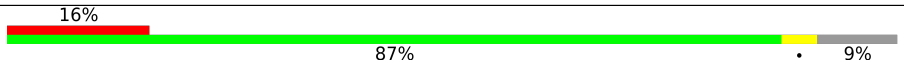
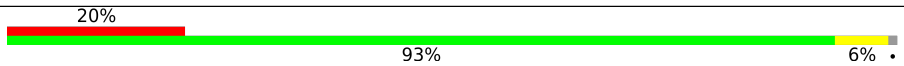
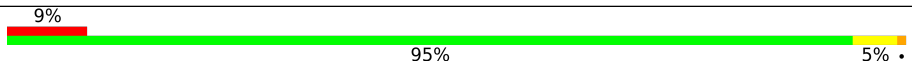
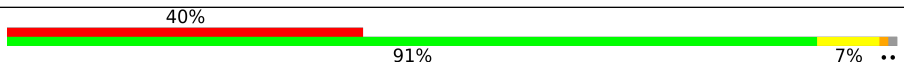
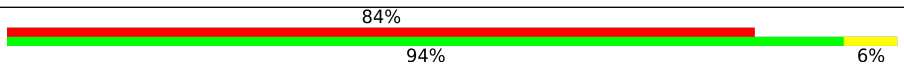
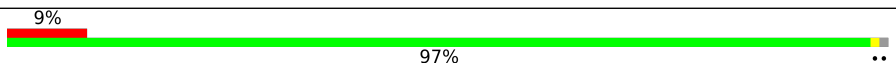
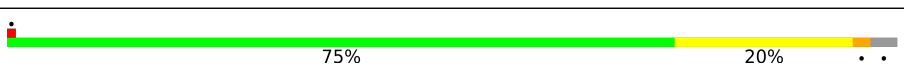
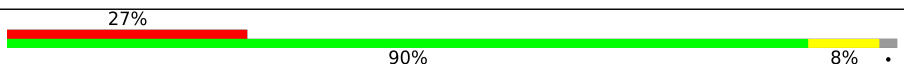
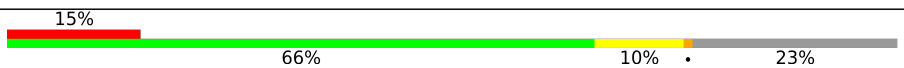
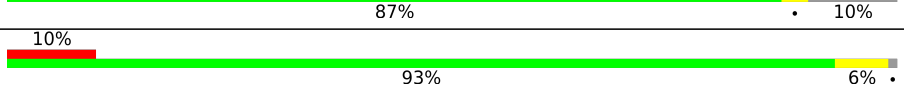
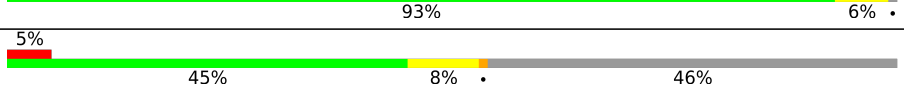
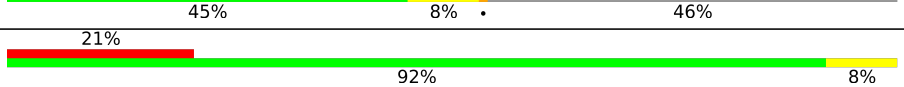
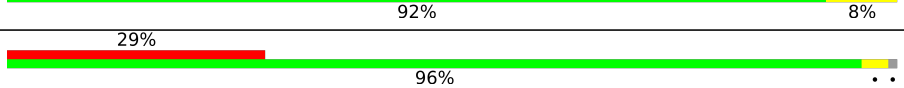
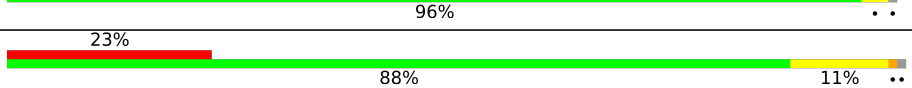
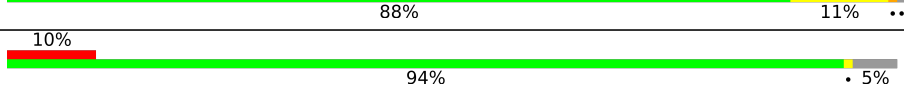
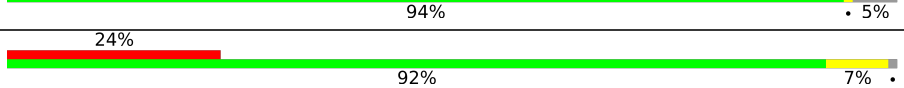
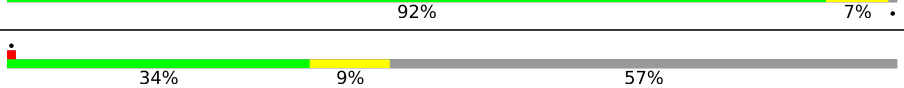
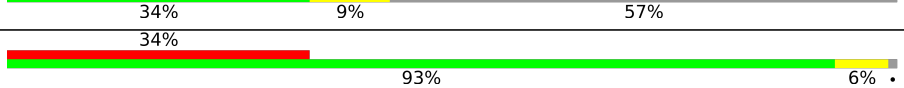
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
RNA backbone	4643	859

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	A	254	39% 85% 13%
2	c	105	12% 91% 8%
3	B	387	18% 92% 7%
4	d	113	15% 93%
5	C	362	25% 90% 9%
6	e	130	22% 96%
7	D	297	13% 95%
8	f	107	15% 92% 6%

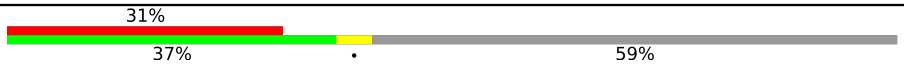
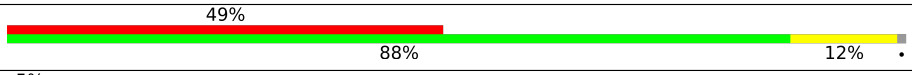
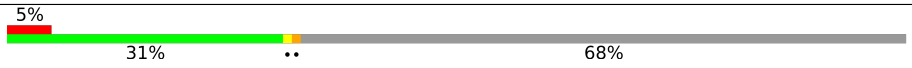
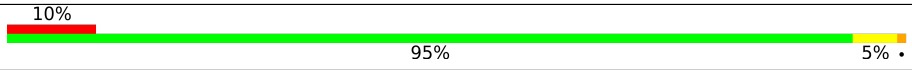
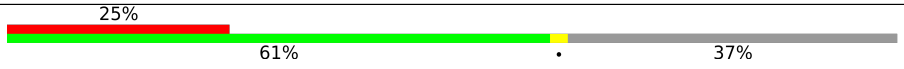
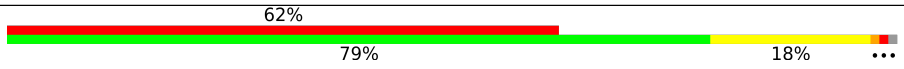
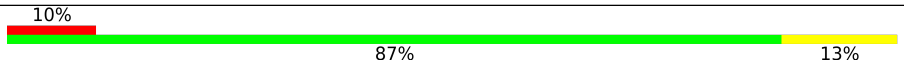
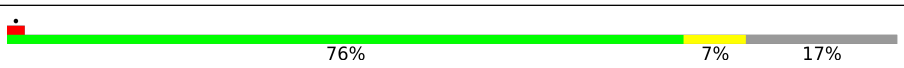
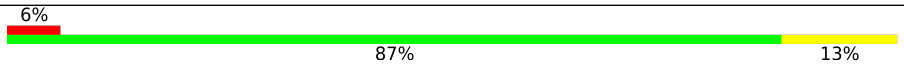
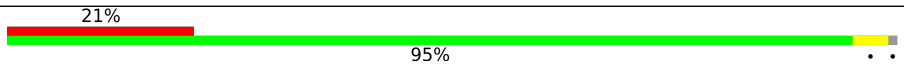
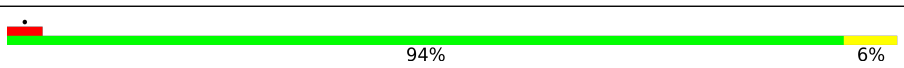
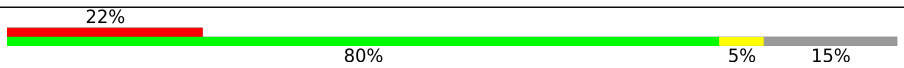
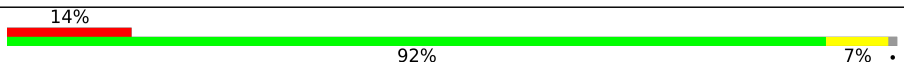
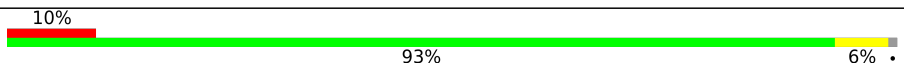
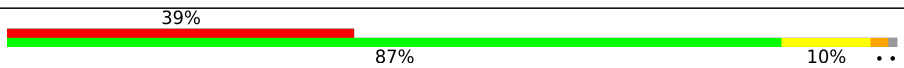
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	E	176	
10	g	121	
11	F	244	
12	h	120	
13	G	256	
14	i	100	
15	H	191	
16	j	88	
17	I	217	
18	k	78	
19	J	174	
20	l	51	
21	K	165	
22	m	245	
23	L	199	
24	n	236	
25	M	138	
26	o	647	
27	N	204	
28	p	92	
29	O	199	
30	q	515	
31	P	184	
32	r	767	
33	Q	186	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	s	4910	
35	R	189	
36	t	199	
37	S	172	
38	u	593	
39	T	160	
40	x	3396	
41	U	121	
42	y	158	
43	V	137	
44	z	121	
45	X	142	
46	Y	127	
47	Z	136	
48	a	149	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 118855 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	252	Total 1007	C 504	N 252	O 251	0	0

- Molecule 2 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	c	97	Total 387	C 194	N 97	O 96	0	0

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	386	Total 1543	C 772	N 386	O 385	0	0

- Molecule 4 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	d	109	Total 435	C 218	N 109	O 108	0	0

- Molecule 5 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	361	Total 1443	C 722	N 361	O 360	0	0

- Molecule 6 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	127	Total 507	C 254	N 127	O 126	0	0

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	D	296	Total 1183	C 592	N 296	O 295	0	0

- Molecule 8 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	f	106	Total 423	C 212	N 106	O 105	0	0

- Molecule 9 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	156	Total 622	C 312	N 156	O 154	0	0

- Molecule 10 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	g	112	Total 447	C 224	N 112	O 111	0	0

- Molecule 11 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	F	222	Total 887	C 444	N 222	O 221	0	0

- Molecule 12 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	h	119	Total 475	C 238	N 119	O 118	0	0

- Molecule 13 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	G	233	Total 931	C 466	N 233	O 232	0	0

- Molecule 14 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	i	99	Total 395	C 198	N 99	O 98	0	0

- Molecule 15 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	H	191	Total 763	C 382	N 191	O 190	0	0

- Molecule 16 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	j	87	Total 347	C 174	N 87	O 86	0	0

- Molecule 17 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	I	217	Total 867	C 434	N 217	O 216	0	0

- Molecule 18 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	k	77	Total 307	C 154	N 77	O 76	0	0

- Molecule 19 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	J	169	Total 675	C 338	N 169	O 168	0	0

- Molecule 20 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	l	50	Total 199	C 100	N 50	O 49	0	0

- Molecule 21 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	K	127	Total 507	C 254	N 127	O 126	0	0

- Molecule 22 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	m	224	Total 895	C 448	N 224	O 223	0	0

- Molecule 23 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	L	193	Total 771	C 386	N 193	O 192	0	0

- Molecule 24 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	n	212	Total 847	C 424	N 212	O 211	0	0

- Molecule 25 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	M	136	Total 543	C 272	N 136	O 135	0	0

- Molecule 26 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	o	347	Total 1387	C 694	N 347	O 346	0	0

- Molecule 27 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	N	203	Total 811	C 406	N 203	O 202	0	0

- Molecule 28 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	p	91	Total 363	C 182	N 91	O 90	0	0

- Molecule 29 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	O	197	Total 787	C 394	N 197	O 196	0	0

- Molecule 30 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	q	488	Total 1951	C 976	N 488	O 487	0	0

- Molecule 31 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	P	183	Total 731	C 366	N 183	O 182	0	0

- Molecule 32 is a protein called Protein SDA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	r	333	Total 1304	C 666	N 333	O 305	0	0

- Molecule 33 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Q	185	Total 739	C 370	N 185	O 184	0	0

- Molecule 34 is a protein called Midasin.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	2003	Total 8007	C 4006	N 2003	O 1998	0	0

- Molecule 35 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	R	188	Total 751	C 376	N 188	O 187	0	0

- Molecule 36 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	t	63	Total 251	C 126	N 63	O 62	0	0

- Molecule 37 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	S	172	Total 687	C 344	N 172	O 171	0	0

- Molecule 38 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	u	373	Total 1491	C 746	N 373	O 372	0	0

- Molecule 39 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	T	159	Total 635	C 318	N 159	O 158	0	0

- Molecule 40 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	x	3394	Total 72570	C 32410	N 13042	O 23725	P 3393	0	0

- Molecule 41 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	U	100	Total 399	C 200	N 100	O 99	0	0

- Molecule 42 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	y	158	Total	C	N	O	P	0	0
			3350	1500	586	1107	157		

- Molecule 43 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	V	136	Total	C	N	O	0	0
			543	272	136	135		

- Molecule 44 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	121	Total	C	N	O	P	0	0
			2576	1152	461	843	120		

- Molecule 45 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	X	121	Total	C	N	O	0	0
			483	242	121	120		

- Molecule 46 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	Y	126	Total	C	N	O	0	0
			503	252	126	125		

- Molecule 47 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	Z	135	Total	C	N	O	0	0
			539	270	135	134		

- Molecule 48 is a protein called 60S ribosomal protein L28.

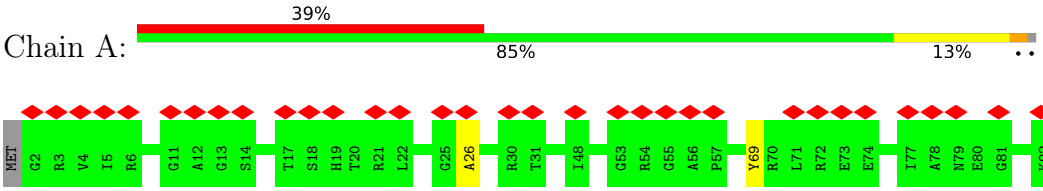
Mol	Chain	Residues	Atoms				AltConf	Trace
48	a	148	Total	C	N	O	0	0
			591	296	148	147		

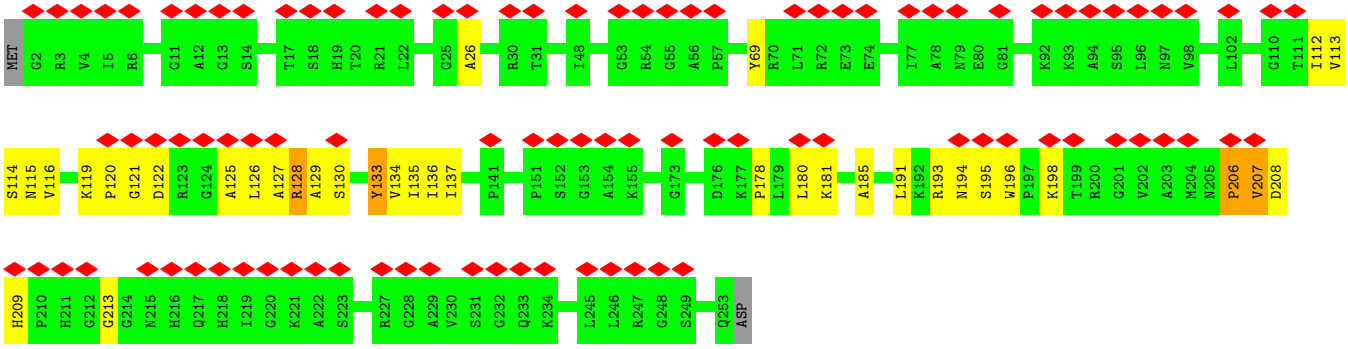
3 Residue-property plots (i)

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: 60S ribosomal protein L2-A

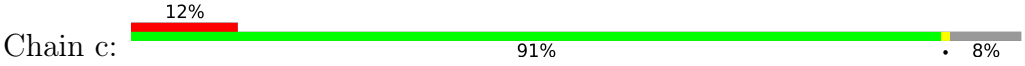
Chain A:

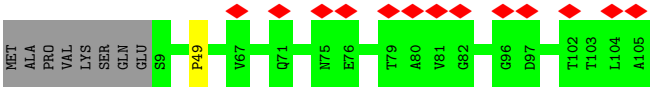




• Molecule 2: 60S ribosomal protein L30

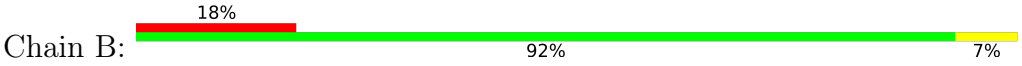
Chain c:

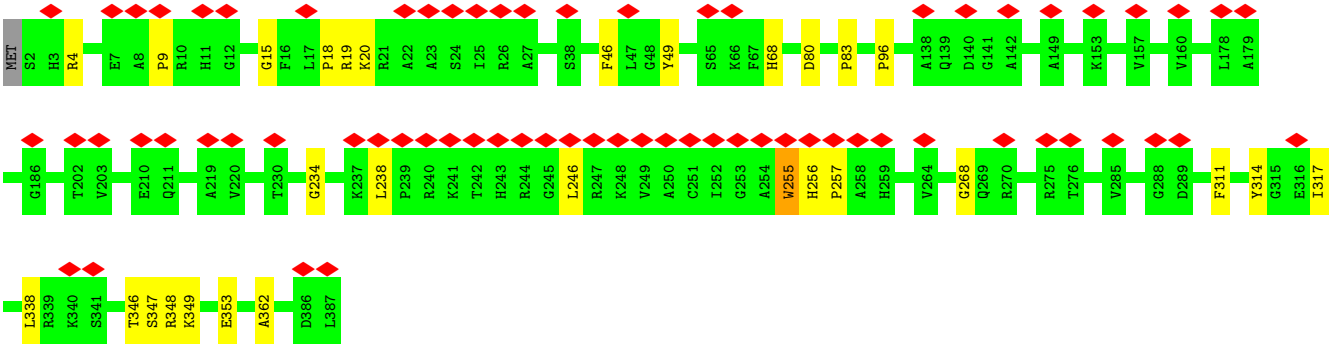




• Molecule 3: 60S ribosomal protein L3

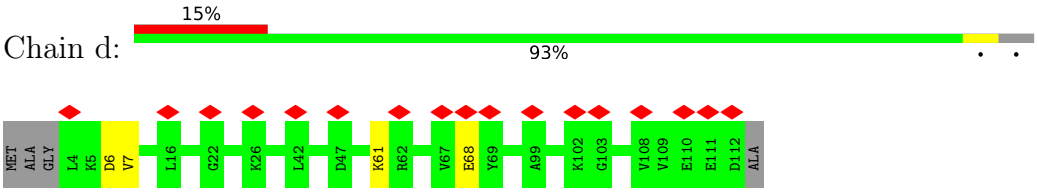
Chain B:





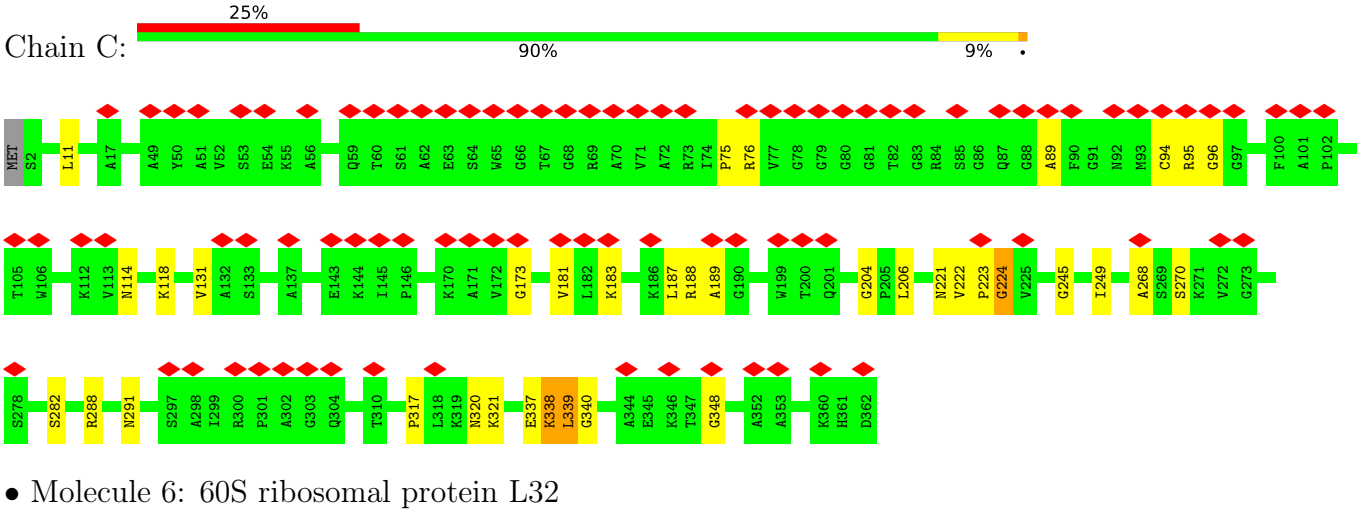
• Molecule 4: 60S ribosomal protein L31-A

Chain d:



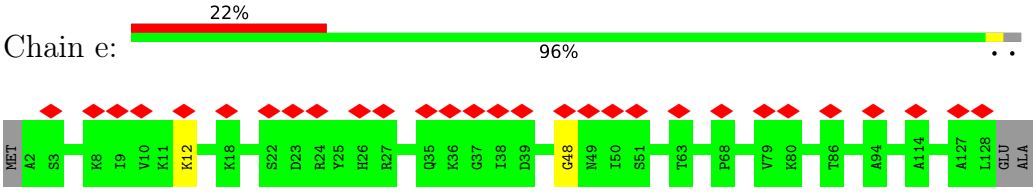
• Molecule 5: 60S ribosomal protein L4-A

Chain C:



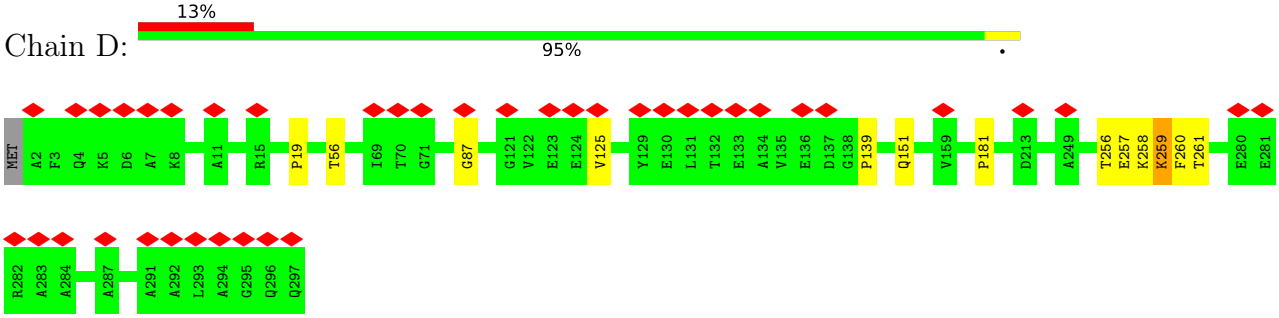
• Molecule 6: 60S ribosomal protein L32

Chain e:



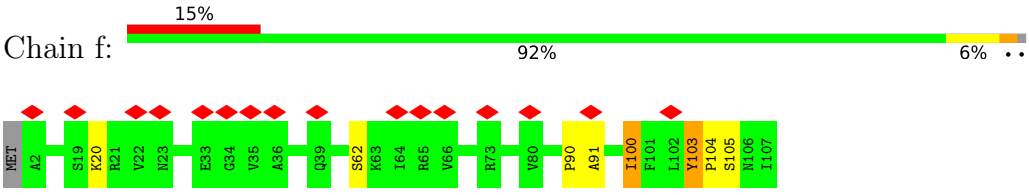
• Molecule 7: 60S ribosomal protein L5

Chain D:



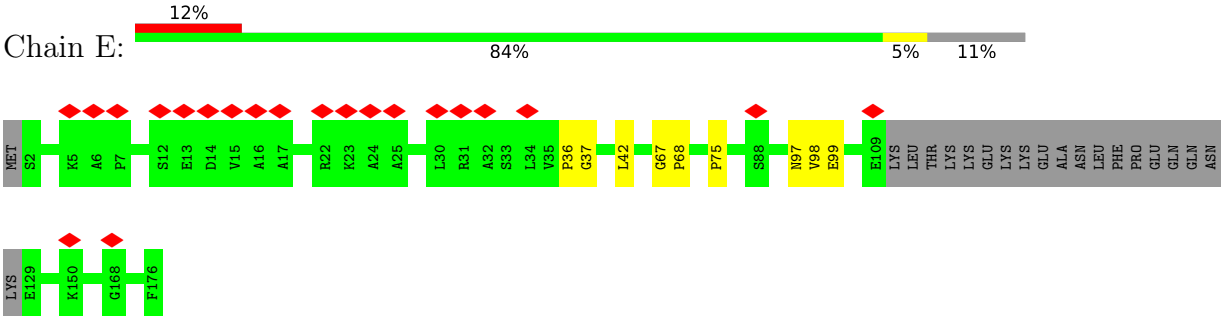
• Molecule 8: 60S ribosomal protein L33-A

Chain f:



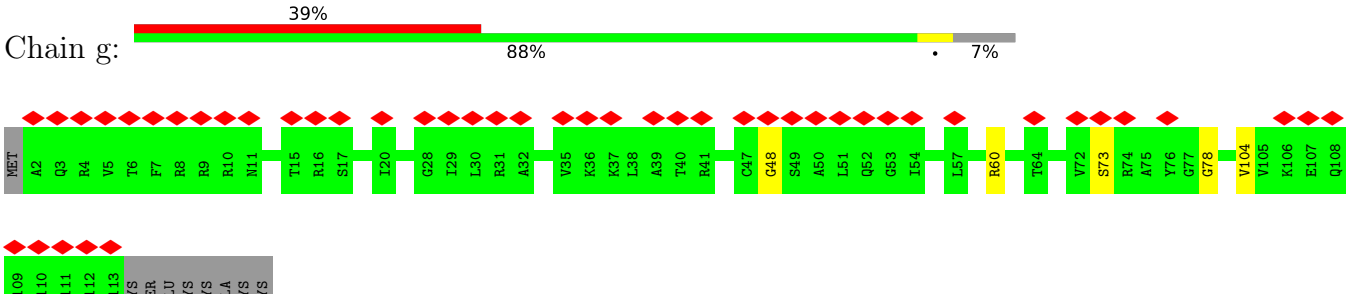
• Molecule 9: 60S ribosomal protein L6-A

Chain E:



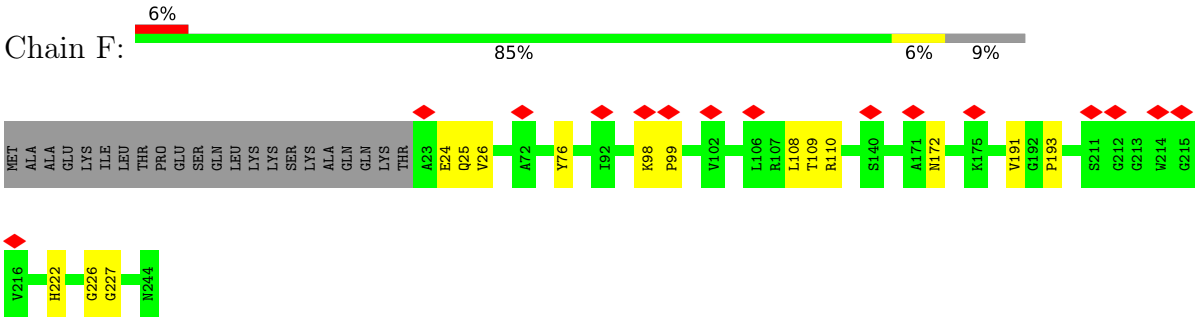
• Molecule 10: 60S ribosomal protein L34-A

Chain g:



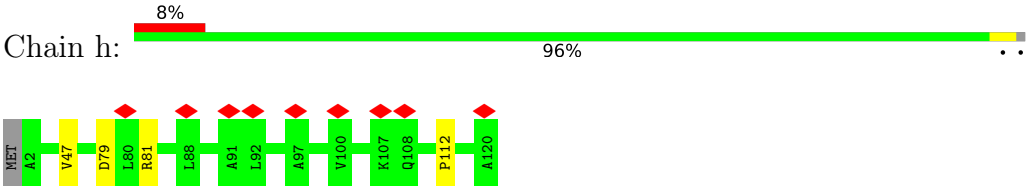
• Molecule 11: 60S ribosomal protein L7-A

Chain F:



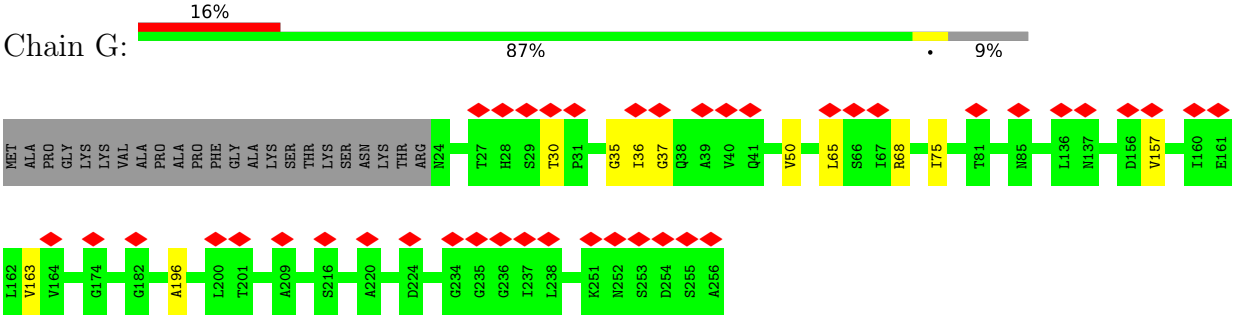
• Molecule 12: 60S ribosomal protein L35-A

Chain h:



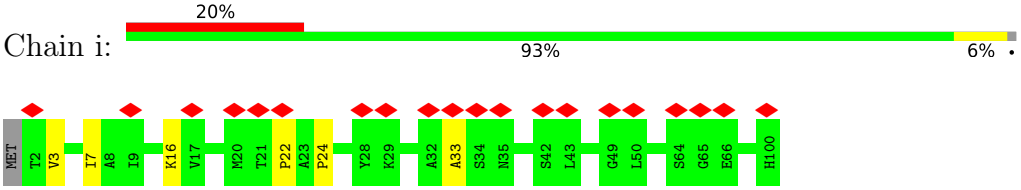
• Molecule 13: 60S ribosomal protein L8-A

Chain G:



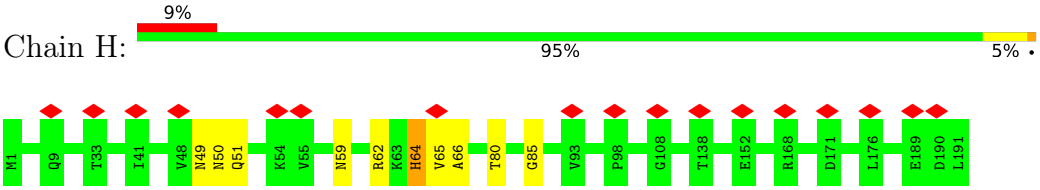
• Molecule 14: 60S ribosomal protein L36-A

Chain i:



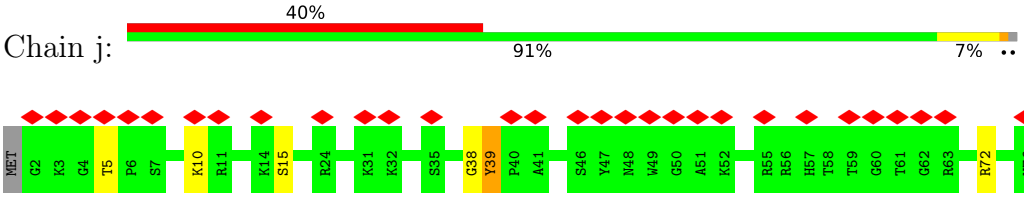
• Molecule 15: 60S ribosomal protein L9-A

Chain H:



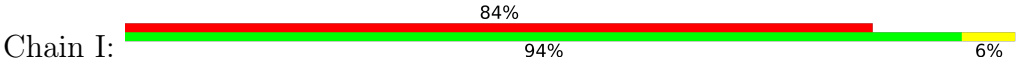
• Molecule 16: 60S ribosomal protein L37-A

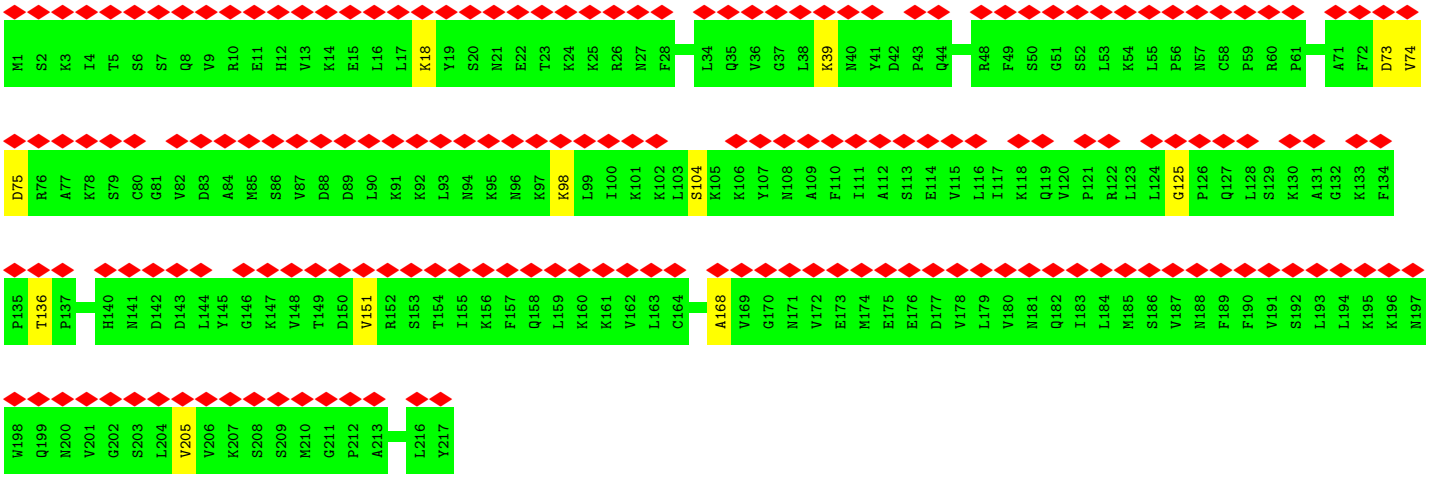
Chain j:



• Molecule 17: 60S ribosomal protein L1-A

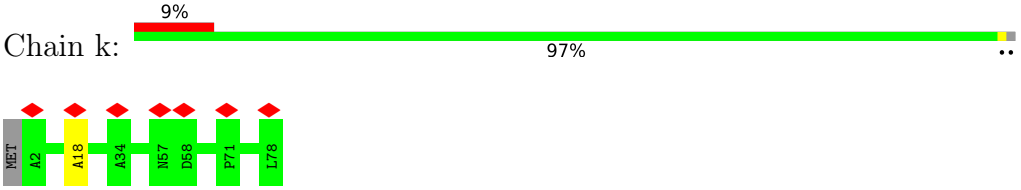
Chain I:





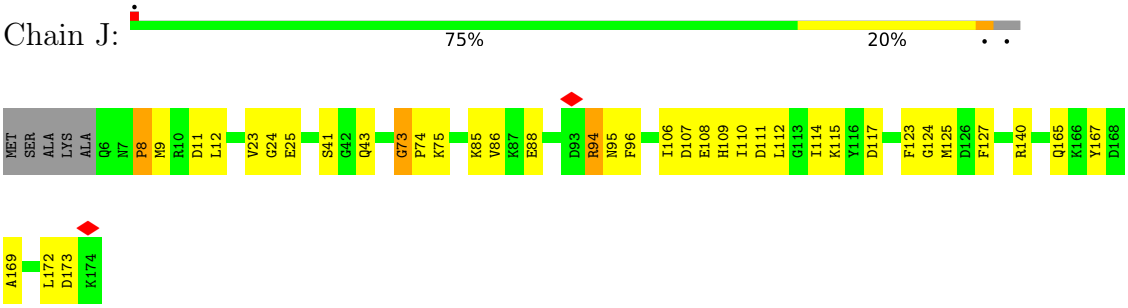
• Molecule 18: 60S ribosomal protein L38

Chain k:



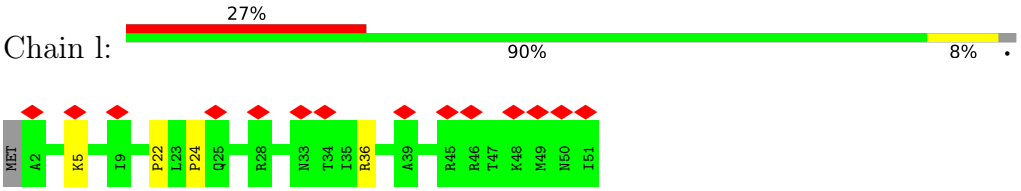
• Molecule 19: 60S ribosomal protein L11-A

Chain J:



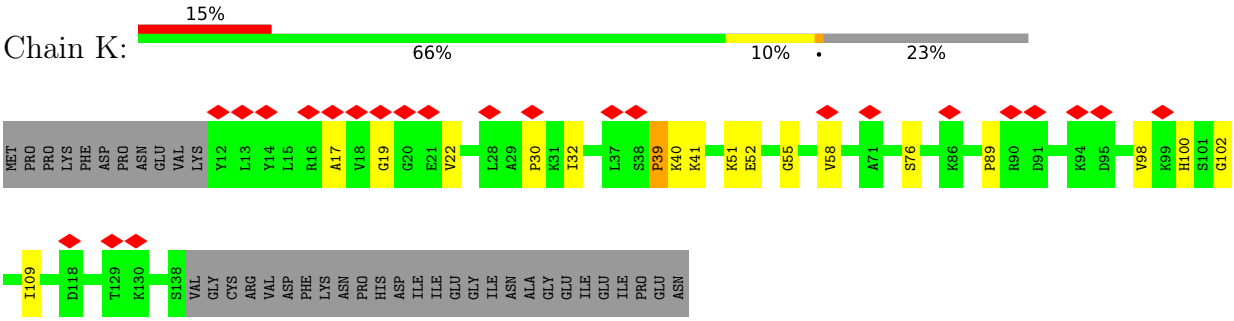
• Molecule 20: 60S ribosomal protein L39

Chain l:



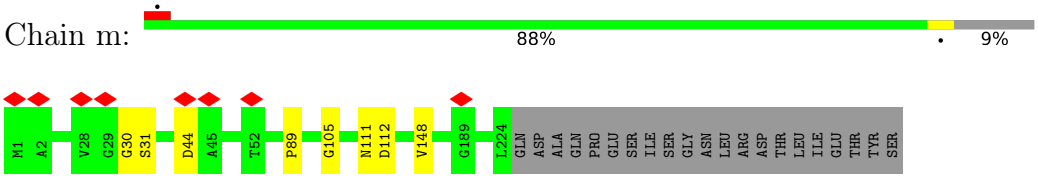
• Molecule 21: 60S ribosomal protein L12-A

Chain K:



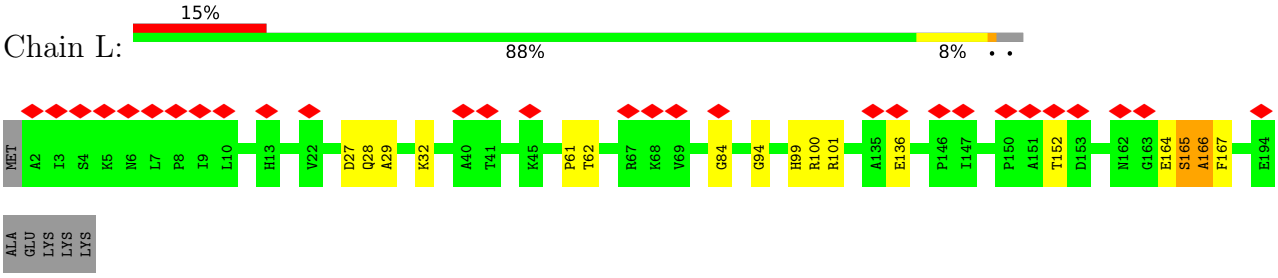
• Molecule 22: Eukaryotic translation initiation factor 6

Chain m:



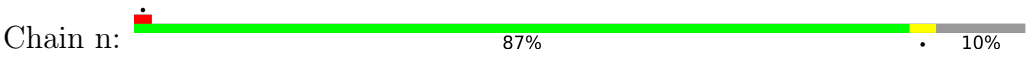
• Molecule 23: 60S ribosomal protein L13-A

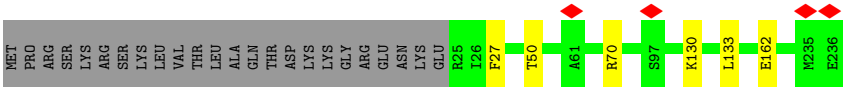
Chain L:



• Molecule 24: Ribosome assembly factor MRT4

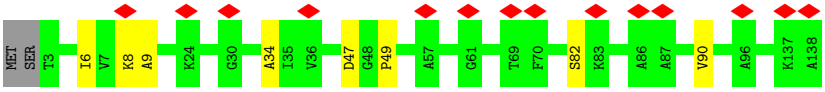
Chain n:





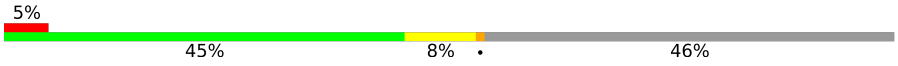
• Molecule 25: 60S ribosomal protein L14-A

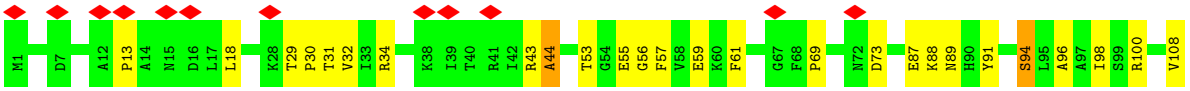
Chain M:

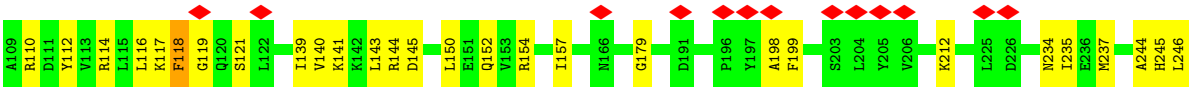


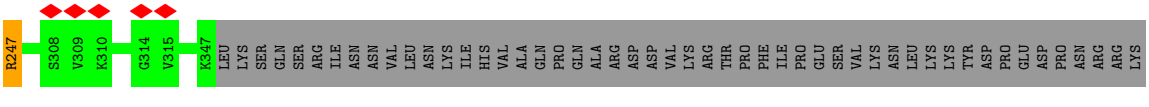
• Molecule 26: Nucleolar GTP-binding protein 1

Chain o:



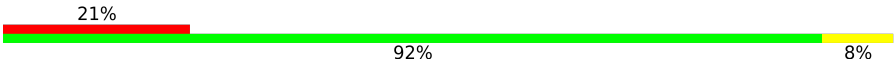


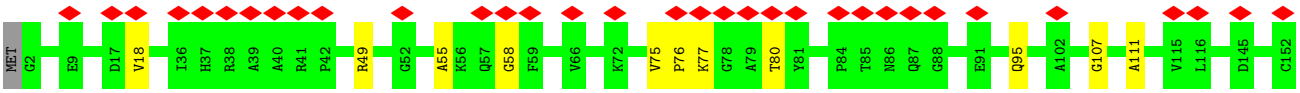


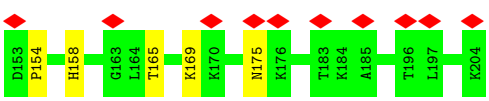


• Molecule 27: 60S ribosomal protein L15-A

Chain N:

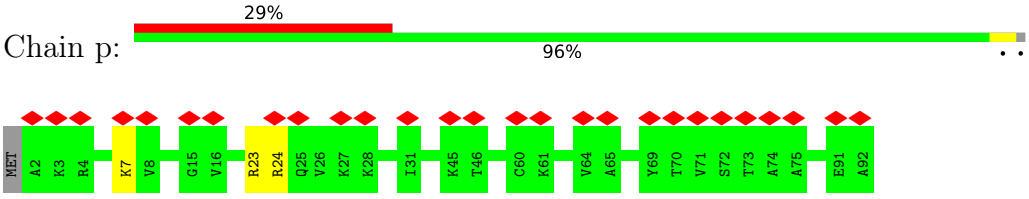






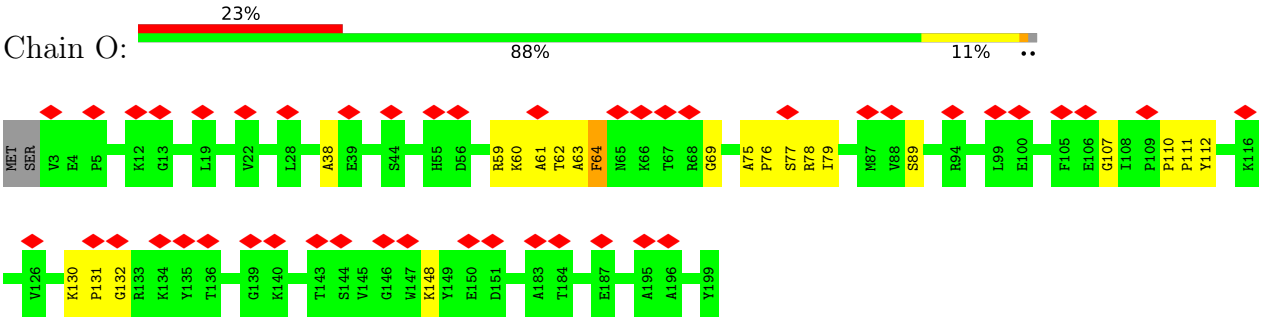
• Molecule 28: 60S ribosomal protein L43-A

Chain p:



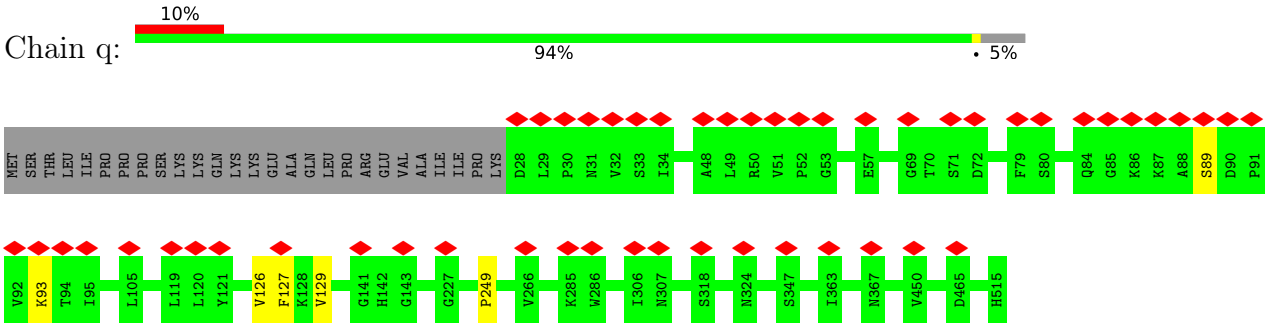
• Molecule 29: 60S ribosomal protein L16-A

Chain O:



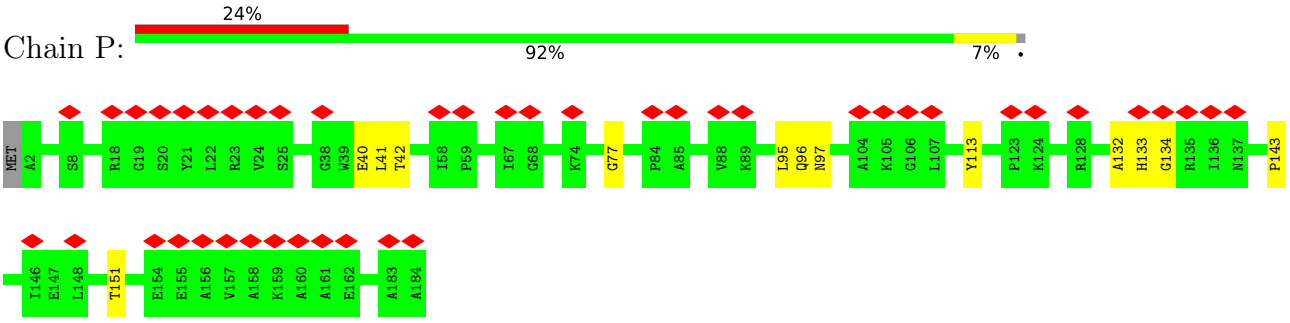
• Molecule 30: Ribosome assembly protein 4

Chain q:



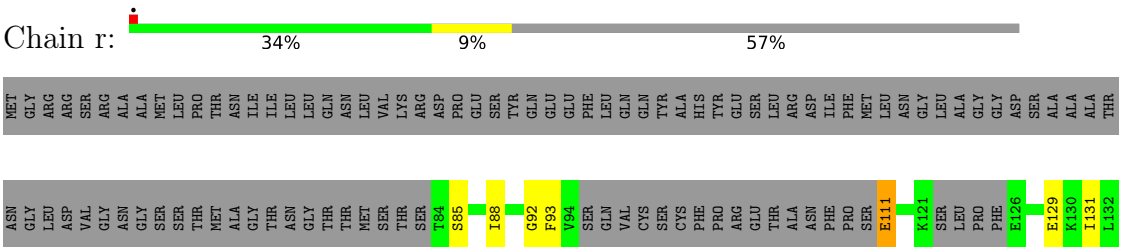
• Molecule 31: 60S ribosomal protein L17-A

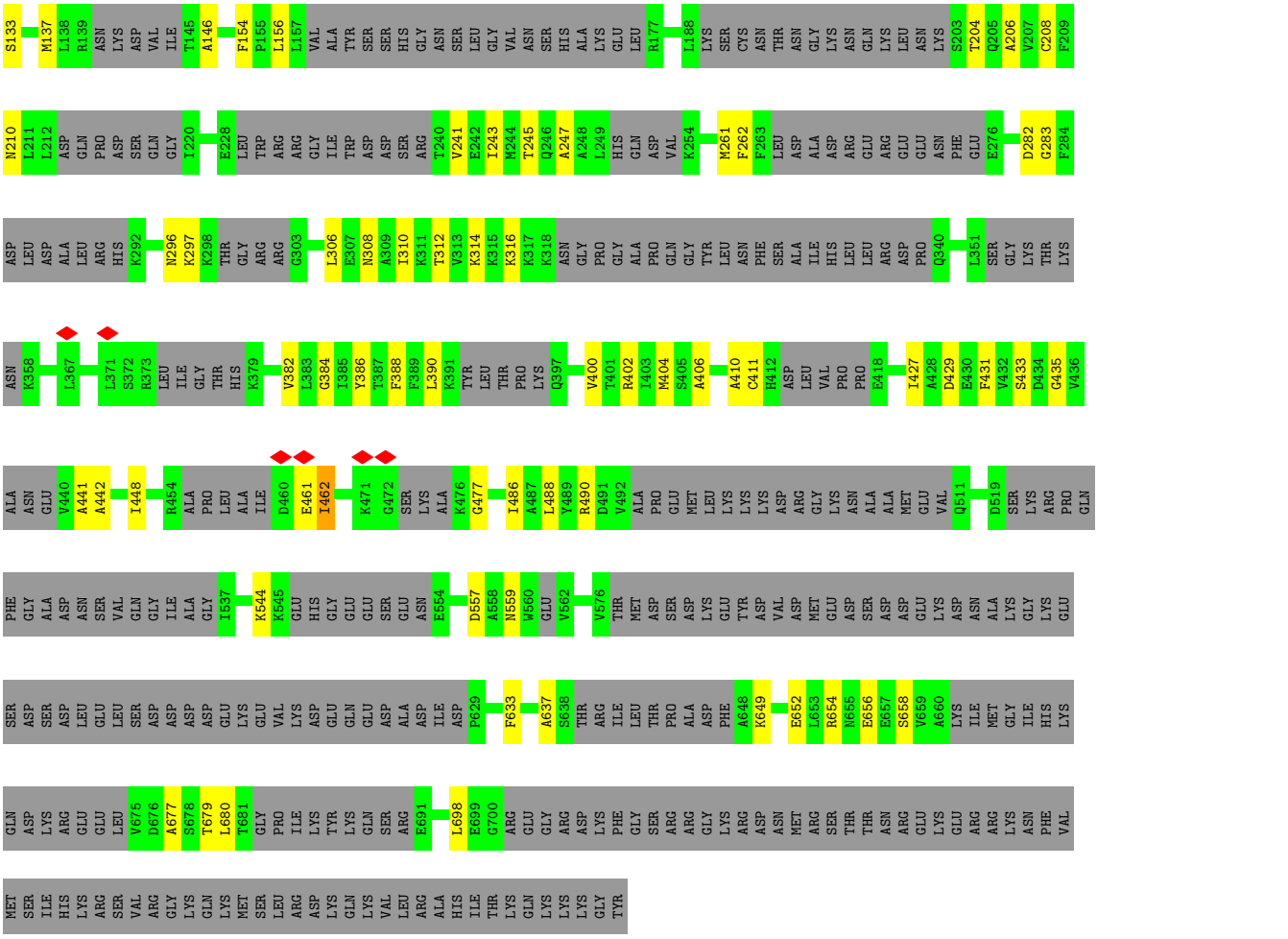
Chain P:



• Molecule 32: Protein SDA1

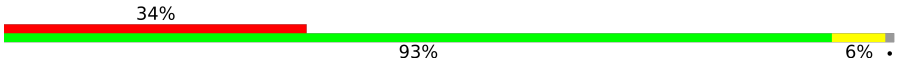
Chain r:

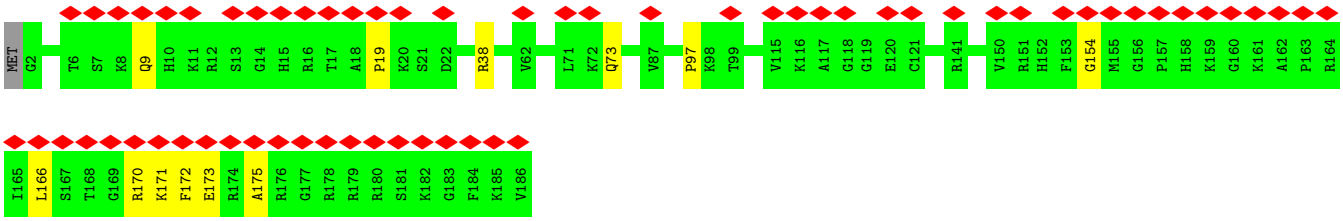




• Molecule 33: 60S ribosomal protein L18-A

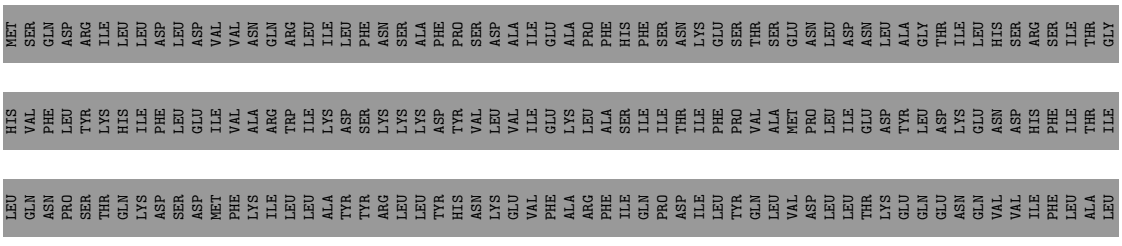
Chain Q:

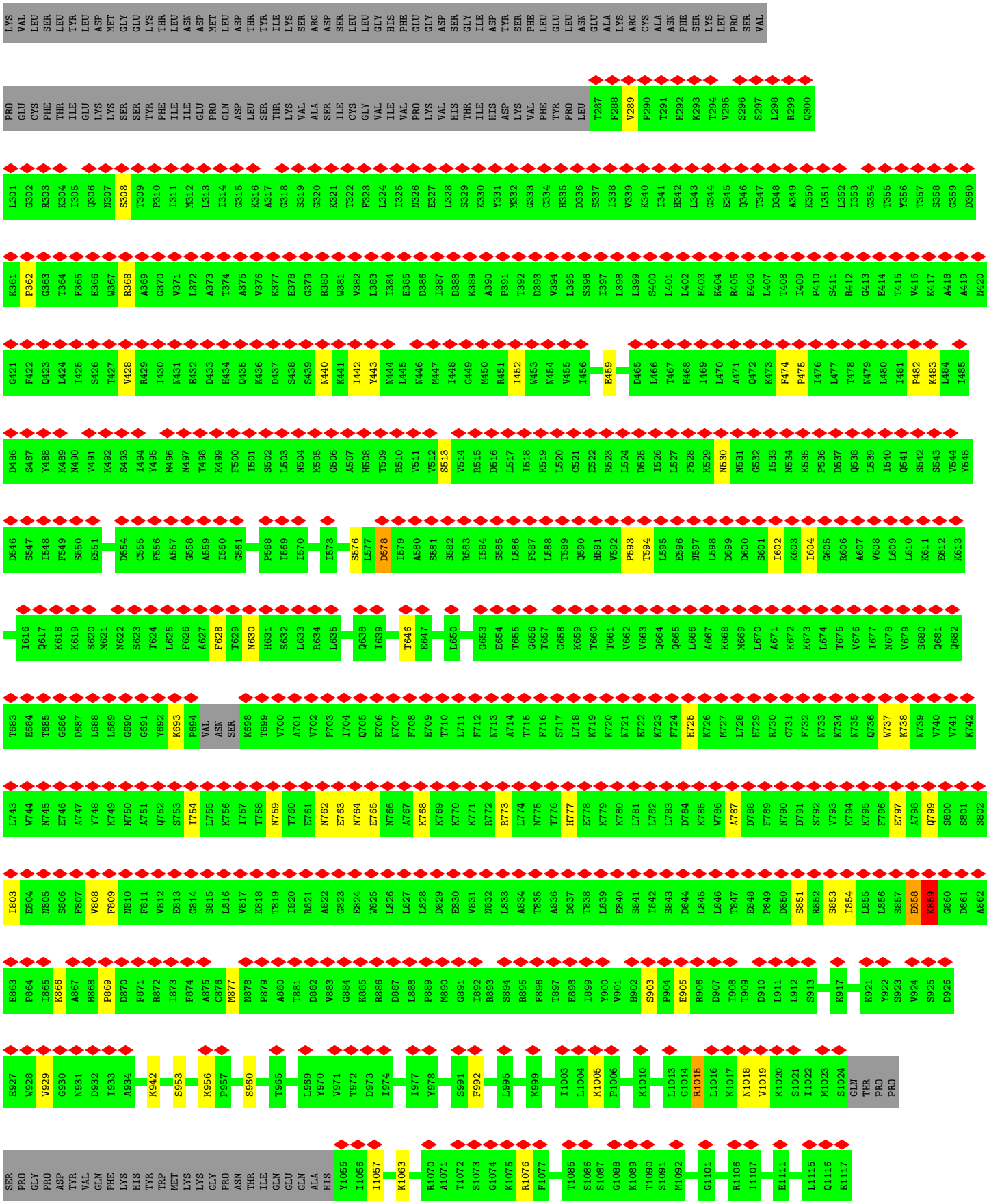


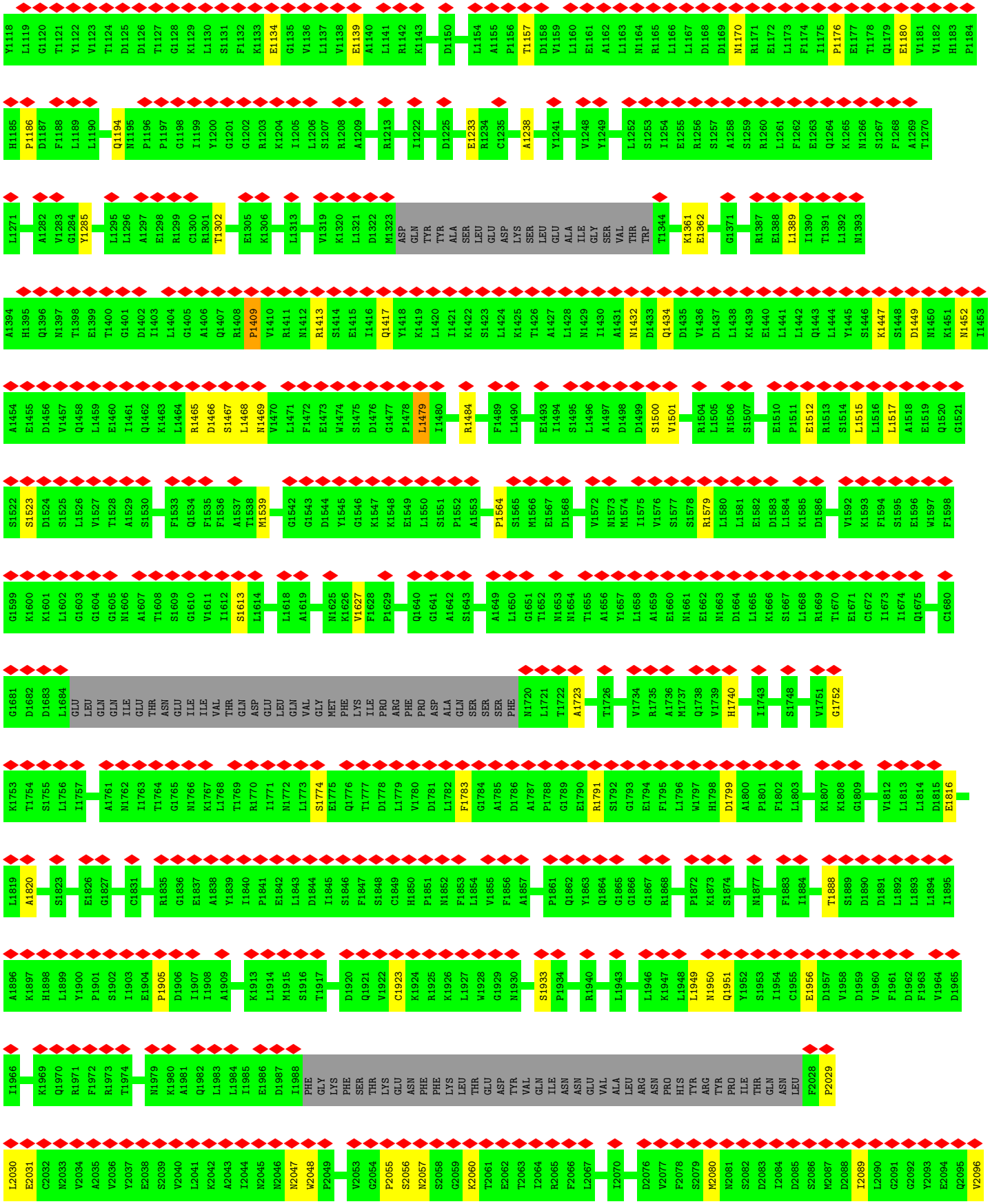


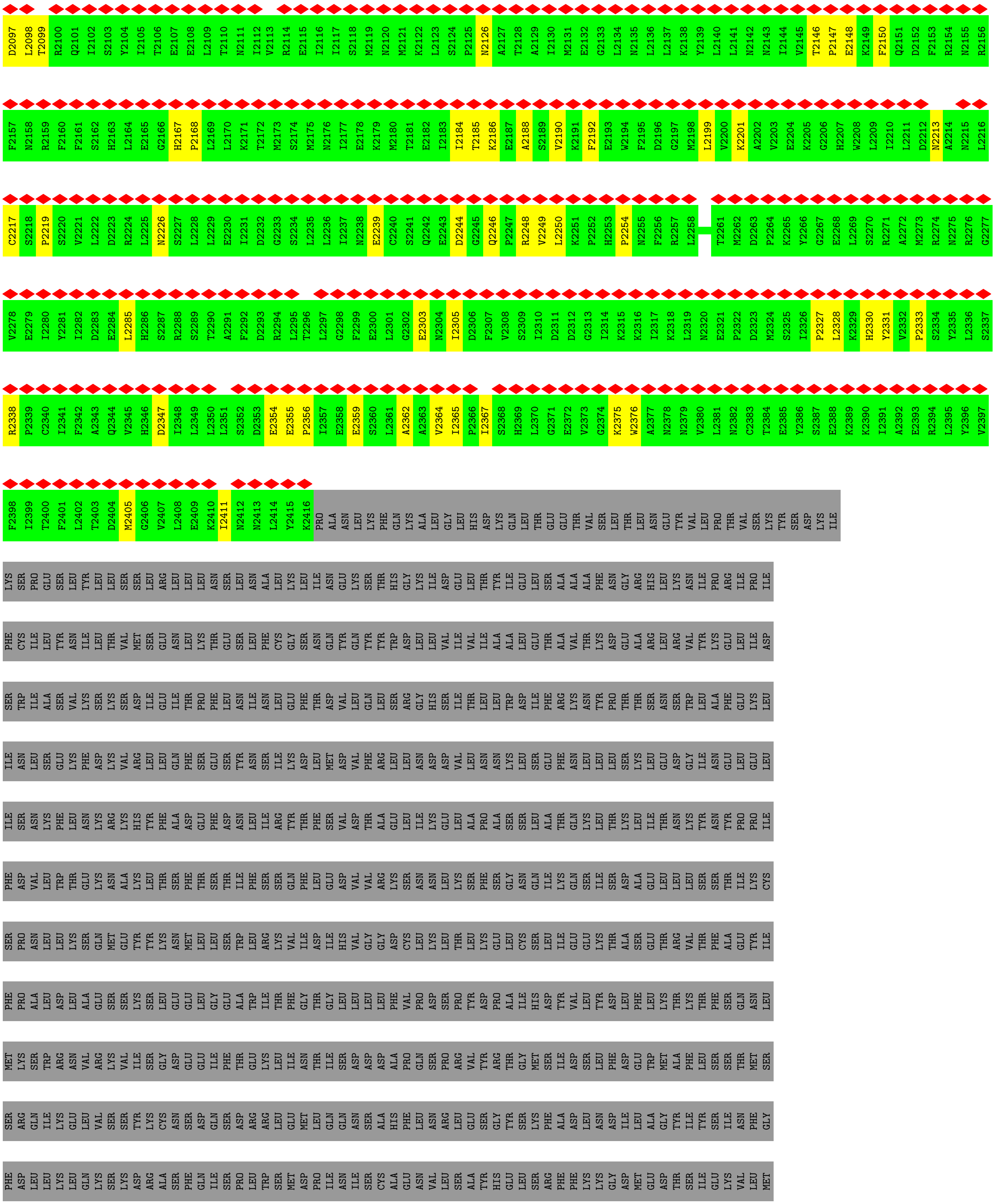
• Molecule 34: Midasin

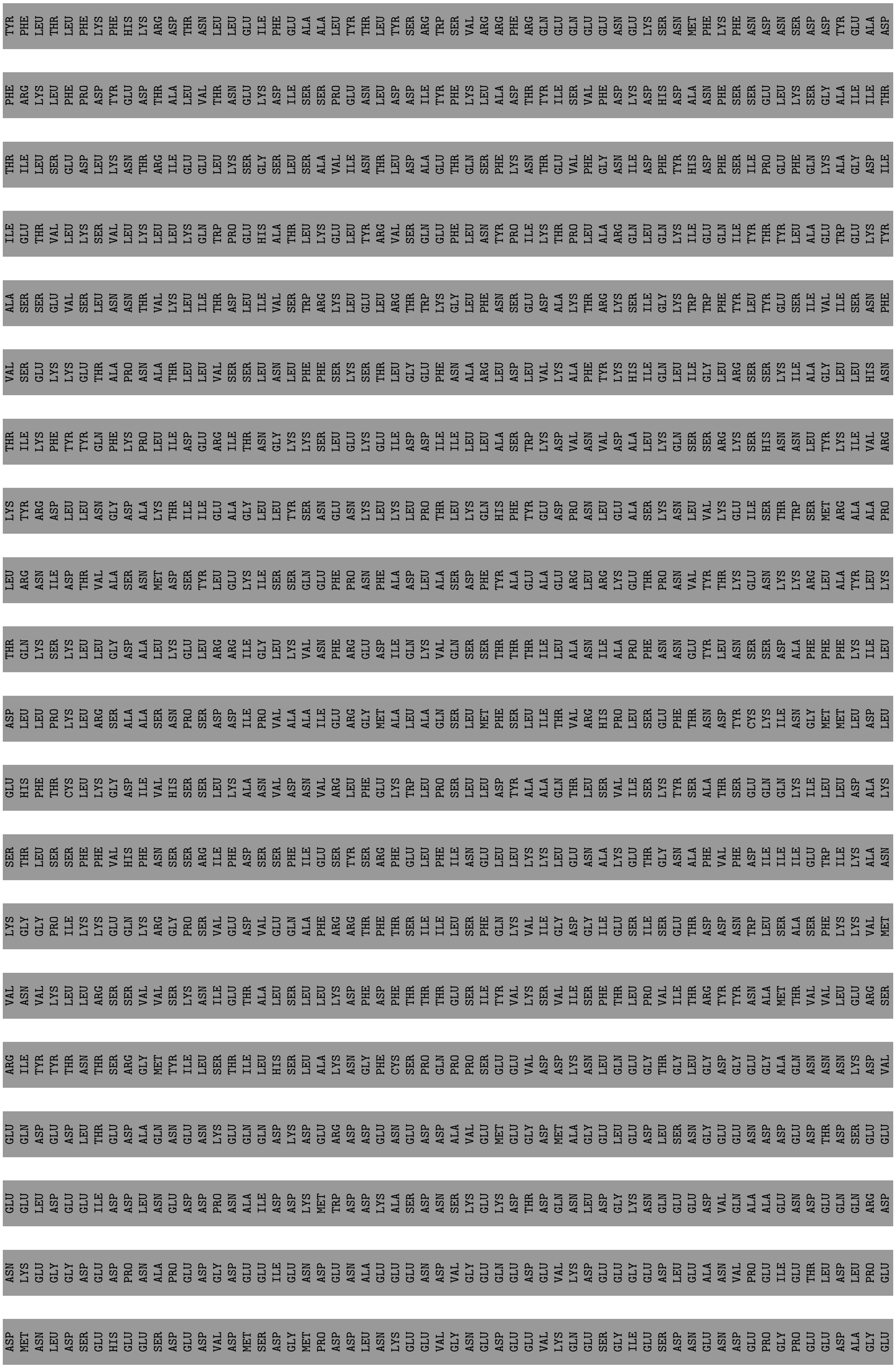
Chain s:

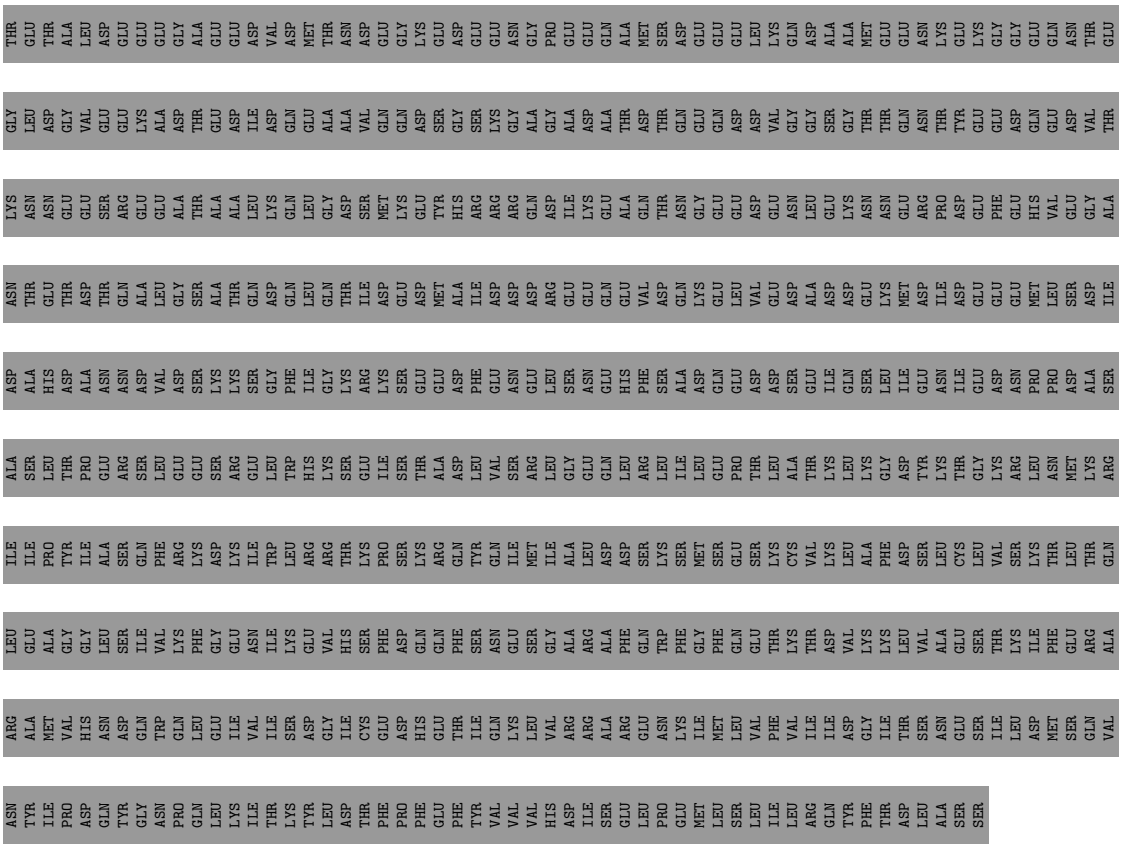



LYS VAL LEU SER LEU TYR LEU ASP MET GLY GLU LYS THR LEU ASN ASP MET LEU ASP THR TYR ILE LYS SER ARG ASP SER LEU LEU GLY HIS PHE GLU GLY ASP SER GLY ILE ASP TYR SER PHE LEU GLU LEU ASN GLU ALA LYS ARG CYS ALA ASN PHE SER LYS LEU PRO SER VAL
PRO GLU CYS PHE THR ILE GLU LYS LYS SER SER TYR PHE ILE ILE GLU PRO GLN ASP LEU SER THR LYS VAL ALA SER ILE CYS GLY VAL ILE VAL PRO LYS VAL HIS THR ILE HIS ASP LYS VAL PHE TYR PRO LEU T287 F288 V289 P290 T291 H292 K293 T294 V295 S296 S297 L298 R299 Q300
L301 G302 R303 K304 I305 Q306 N307 S308 T309 P310 I311 M312 L313 I314 G315 K316 A317 G318 S319 G320 K321 T322 F323 L324 I325 N326 E327 L328 S329 K330 Y331 M332 G333 C334 H335 D336 S337 I338 V339 K340 I341 H342 L343 G344 E345 Q346 T347 D348 A349 K350 L351 L352 I353 G354 T355 Y356 T357 S358 G359 D360
K361 P362 G363 T364 F365 E366 W367 R368 A369 G370 V371 L372 A373 T374 A375 V376 K377 E378 G379 R380 W381 V382 L383 I384 E385 D386 I387 D388 K389 A390 P391 T392 D393 V394 L395 S396 I397 L398 L399 S400 L401 L402 E403 K404 R405 E406 L407 T408 I409 P410 S411 R412 G413 E414 T415 V416 K417 A418 A419 N420
G421 F422 Q423 L424 I425 S426 T427 V428 R429 I430 N431 E432 D433 H434 Q435 K436 D437 S438 S439 N440 K441 I442 Y443 N444 L445 N446 M447 I448 G449 M450 R451 I452 W453 N454 V455 I456 E459 D465 L466 T467 H468 I469 L470 A471 Q472 K473 F474 P475 I476 L477 T478 N479 L480 I481 P482 K483 L484 I485
D486 S487 Y488 K489 N490 V491 K492 S493 I494 Y495 M496 N497 T498 K499 F500 I501 S502 L503 N504 K505 G506 A507 H508 T509 R510 V511 V512 S513 V514 R515 D516 L517 I518 K519 L520 C521 E522 R523 L524 D525 I526 L527 F528 K529 N530 N531 G532 I533 N534 K535 P536 D537 Q538 L539 I540 Q541 S542 S543 V544 Y545
D546 S547 I548 F549 S550 E551 D554 C555 F556 A557 G558 A559 I560 G561 P568 I569 I570 I573 S576 L577 D578 I579 A580 S581 S582 R583 I584 S585 L586 F587 L588 T589 Q590 H591 V592 P593 T594 L595 E596 N597 L598 D599 D600 S601 I602 K603 I604 G605 R606 A607 V608 L609 L610 K611 E612 K613
I616 Q617 K618 K619 S620 M621 N622 S623 T624 L625 F626 A627 F628 T629 N630 H631 S632 L633 R634 L635 Q638 I639 T646 E647 L650 G653 E654 T655 G656 T657 G658 K659 T660 T661 V662 V663 Q664 Q665 L666 A667 K668 M669 L670 A671 K672 K673 L674 T675 V676 I677 N678 V679 S680 Q681 Q682
T683 E684 T685 G686 D687 L688 L689 G690 G691 Y692 K693 P694 VAL ASN SER K698 T699 V700 A701 V702 P703 I704 Q705 E706 N707 F708 E709 T710 L711 F712 N713 A714 T715 F716 S717 L718 K719 K720 N721 E722 K723 F724 H725 K726 M727 L728 H729 R730 C731 F732 N733 K734 N735 Q736 W737 K738 N739 V740 V741 K742
L743 W744 N745 E746 A747 Y748 K749 M750 A751 Q752 S753 I754 L755 K756 I757 T758 N759 T760 E761 N762 E763 N764 E765 N766 A767 K768 K769 K770 K771 R772 R773 L774 N775 T776 H777 E778 K779 K780 L781 L782 L783 D784 K785 W786 A787 D788 F789 N790 D791 S792 V793 K794 K795 F796 E797 A798 Q799 S800 S801 S802
I803 E804 N805 S806 F807 V808 F809 N810 F811 V812 E813 G814 S815 L816 V817 K818 T819 I820 R821 A822 G823 E824 W825 L826 L827 L828 D829 E830 V831 N832 L833 A834 T835 A836 D837 T838 L839 E840 S841 I842 S843 D844 L845 L846 T847 E848 P849 D850 S851 R852 S853 I854 L855 L856 S857 E858 K859 G860 D861 A862
E863 P864 I865 K866 A867 H868 P869 D870 F871 R872 I873 F874 A875 C876 M877 N878 P879 A880 T881 D882 V883 G884 K885 R886 D887 L888 P889 M890 G891 I892 R893 S894 R895 F896 T897 E898 I899 Y900 Y901 H902 S903 P904 E905 R906 D907 I908 T909 D910 L911 L912 S913 K917 K921 Y922 S923 Y924 S925 D926
E927 W928 V929 G930 N931 D932 I933 A934 K942 S953 K956 P957 S960 T965 L969 Y970 V971 T972 D973 I974 I977 Y978 S991 F992 L995 K999 I1003 L1004 K1005 P1006 K1010 L1013 G1014 R1015 L1016 K1017 N1018 V1019 K1020 S1021 I1022 M1023 S1024 GLN THR PRO PRO
SER PRO GLY PRO ASP TYR VAL GLN PHE LYS HIS TYR TRP MET LYS LYS GLY PRO ASN THR ILE GLN GLU GLN ALA HIS Y1055 I1056 I1057 K1063 R1070 A1071 T1072 S1073 G1074 K1075 R1076 F1077 T1085 S1086 S1087 G1088 K1089 T1090 S1091 M1092 G1101 R1106 I1107 E1111 L1115 Q1116 E1117

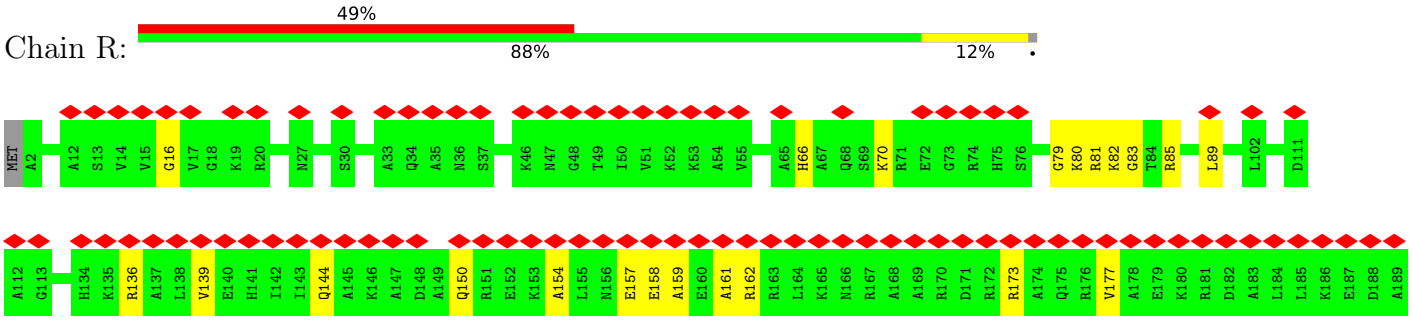



D2097 L2098 T2099 R2100 Q2101 I2102 S2103 Y2104 I2105 T2106 E2107 E2108 L2109 T2110 N2111 I2112 V2113 R2114 E2115 I2116 I2117 S2118 M2119 N2120 M2121 K2122 L2123 S2124 P2125 N2126 A2127 T2128 A2129 I2130 M2131 E2132 G2133 L2134 N2135 L2136 L2137 K2138 Y2139 L2140 L2141 N2142 N2143 I2144 V2145 T2146 P2147 E2148 K2149 F2150 Q2151 D2152 F2153 R2154 N2155 R2156
F2157 N2158 R2159 F2160 F2161 S2162 H2163 L2164 E2165 G2166 H2167 P2168 L2169 L2170 K2171 T2172 M2173 S2174 M2175 N2176 I2177 E2178 K2179 M2180 T2181 E2182 I2183 I2184 T2185 K2186 E2187 A2188 S2189 V2190 K2191 F2192 E2193 W2194 F2195 D2196 G2197 M2198 L2199 V2200 K2201 A2202 V2203 E2204 K2205 G2206 H2207 W2208 L2209 I2210 L2211 D2212 N2213 A2214 N2215 L2216
C2217 S2218 P2219 S2220 V2221 L2222 D2223 R2224 L2225 N2226 S2227 L2228 L2229 E2230 I2231 D2232 G2233 S2234 L2235 I2236 I2237 N2238 E2239 C2240 S2241 Q2242 E2243 D2244 G2245 Q2246 P2247 R2248 V2249 L2250 K2251 P2252 H2253 P2254 N2255 F2256 R2257 L2258 T2261 M2262 D2263 P2264 K2265 Y2266 G2267 E2268 L2269 S2270 R2271 A2272 M2273 R2274 N2275 R2276 G2277
V2278 E2279 I2280 Y2281 I2282 D2283 E2284 L2285 H2286 S2287 R2288 S2289 T2290 A2291 F2292 D2293 R2294 L2295 T2296 L2297 G2298 F2299 E2300 L2301 G2302 E2303 N2304 I2305 D2306 F2307 V2308 S2309 I2310 D2311 D2312 G2313 I2314 K2315 K2316 I2317 K2318 L2319 N2320 E2321 P2322 D2323 M2324 S2325 I2326 P2327 L2328 K2329 H2330 Y2331 V2332 P2333 S2334 Y2335 L2336 S2337
R2338 P2339 C2340 I2341 F2342 A2343 Q2344 V2345 H2346 D2347 I2348 L2349 L2350 L2351 S2352 D2353 E2354 E2355 P2356 I2357 E2358 E2359 S2360 L2361 A2362 A2363 V2364 I2365 P2366 I2367 S2368 H2369 L2370 G2371 E2372 V2373 G2374 K2375 W2376 A2377 N2378 N2379 V2380 L2381 N2382 C2383 T2384 E2385 Y2386 S2387 E2388 K2389 K2390 I2391 A2392 E2393 R2394 L2395 Y2396 V2397
F2398 I2399 T2400 F2401 L2402 T2403 D2404 M2405 G2406 V2407 L2408 E2409 K2410 I2411 N2412 N2413 L2414 Y2415 K2416 PRO ALA ASN LEU LYS PHE GLN LYS ALA LEU GLY LEU HIS ASP LYS GLN LEU THR GLU GLU THR VAL SER LEU THR LEU ASN GLU TYR VAL LEU PRO THR VAL SER LYS TYR SER ASP LYS ILE
LYS SER PRO GLU SER LEU TYR LEU LEU SER SER LEU ARG LEU LEU LEU ASN SER LEU ASN ALA LEU LYS LEU ILE ASN GLU LYS SER THR HIS GLY LYS ILE ASP GLU LEU THR TYR ILE GLU LEU SER ALA ALA ALA PHE ASN GLY ARG HIS LEU LYS ASN ILE PRO ARG ILE PRO ILE
PHE CYS ILE LEU TYR ASN ILE LEU THR VAL MET SER GLU ASN LEU LYS THR GLU SER LEU PHE CYS GLY SER ASN GLN TYR GLN TYR TRP ASP LEU LEU VAL ILE VAL ILE ALA ALA LEU GLU THR ALA VAL THR LYS ASP GLU ALA ARG LEU ARG VAL TYR LYS GLU LEU ILE ASP
SER TRP ILE ALA SER VAL LYS SER LYS SER ASP ILE GLU ILE THR PRO PHE LEU ASN ILE ASN LEU GLU PHE THR ASP VAL LEU GLN LEU SER ARG GLY HIS SER ILE THR LEU LEU TRP ASP ILE PHE ARG LYS ASN TYR PRO THR THR SER ASN SER TRP LEU ALA PHE GLU LYS LEU
ILE ASN LEU SER GLU LYS PHE ASP LYS VAL ARG LEU LEU GLN PHE SER GLU SER TYR ASN SER ILE LYS ASP LEU MET ASP VAL PHE ARG LEU LEU ASN ASP ASP VAL LEU ASN ASN LYS LEU SER GLU PHE ASN LEU LEU LEU SER LYS LEU GLU ASP GLY ILE ASN GLU LEU GLU LEU
ILE SER ASN LYS PHE LEU ASN LYS ARG LYS HIS TYR PHE ALA ASP GLU PHE ASP ASN LEU ILE ARG TYR THR PHE SER VAL ASP THR ALA GLU LEU ILE LYS GLU LEU ALA PRO ALA SER SER LEU ALA THR GLN LYS LEU THR LYS LEU ILE THR ASN LYS TYR ASN TYR PRO PRO ILE
PHE ASP VAL LEU TRP THR GLU LYS ASN ALA LYS LEU THR SER PHE THR SER THR ILE PHE SER SER GLN PHE LEU GLU ASP VAL VAL ARG LYS SER ASN ASN LEU LYS SER PHE SER GLY ASN GLN ILE LYS GLN SER ILE SER ASP ALA GLU LEU LEU LEU SER SER THR ILE LYS CYS
SER PRO ASN LEU LEU LYS SER GLN MET GLU TYR TYR LYS ASN MET LEU LEU SER TRP LEU ARG LYS VAL ILE ASP ILE HIS VAL GLY GLY ASP CYS LEU LYS LEU THR LEU LYS GLU LEU CYS SER LEU ILE GLU GLU LYS THR ALA SER GLU THR ARG VAL THR PHE ALA GLU TYR ILE
PHE PRO ALA LEU ASP LEU ALA GLU SER SER LYS SER LEU GLU GLU LEU GLY GLU ALA TRP ILE THR PHE GLY THR GLY LEU LEU LEU LEU PHE VAL PRO ASP SER PRO TYR ASP PRO ALA ILE HIS ASP TYR VAL LEU TYR ASP LEU PHE LEU LYS THR LYS THR PHE SER GLN ASN LEU
MET LYS SER TRP ARG ASN VAL ARG LYS VAL ILE SER GLY ASP GLU GLU ILE PHE THR GLU LYS LEU ILE ASN THR ILE SER ASP ASP ALA PRO GLN SER PRO ARG VAL TYR ARG THR GLY MET SER ILE ASP SER LEU PHE ASP GLU TRP MET ALA PHE LEU SER SER THR MET SER
SER ARG GLN ILE LYS GLU LEU VAL SER SER TYR LYS CYS ASN SER ASP GLN SER ASP ARG ARG LEU GLU MET LEU GLN GLN ASN SER ALA HIS PHE LEU ASN ARG LEU GLU SER GLY TYR SER LYS PHE ALA ASP LEU ASN ASP ILE LEU ALA GLY TYR ILE TYR SER ILE ASN PHE GLY
PHE ASP LEU LEU LYS LEU GLN LYS SER LYS ASP ARG ALA SER PHE GLN ILE SER PRO LEU TRP SER MET ASP PRO ILE ASN ILE SER CYS ALA GLU ASN VAL LEU SER ALA TYR HIS GLU LEU SER ARG PHE PHE LYS LYS GLY ASP MET GLU ASP THR SER ILE GLU LYS VAL LEU MET

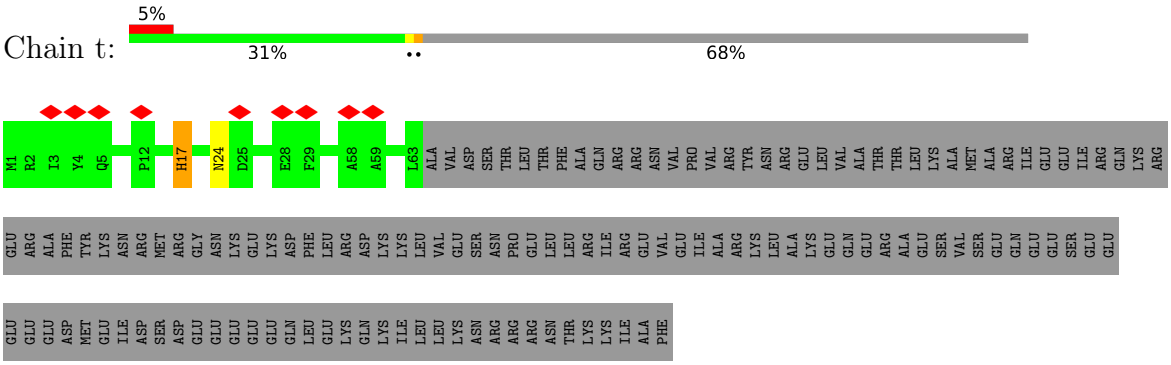

TYR PHE LEU THR LEU PHE LYS PHE HIS LYS ARG ASP THR ASN LEU LEU GLU ILE PHE GLU ALA ALA LEU TYR THR LEU TYR SER ARG TRP SER VAL ARG ARG PHE ARG GLN GLU GLN GLU GLU ASN GLU LYS SER ASN MET PHE LYS PHE ASN ASP ASN SER ASP ASP TYR GLU ALA ASP
PHE ARG LYS LEU PHE PRO ASP TYR GLU ASP THR ALA LEU VAL THR ASN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



• Molecule 35: 60S ribosomal protein L19-A

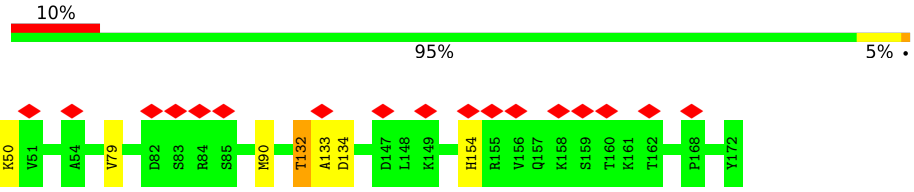


• Molecule 36: Ribosome biogenesis protein RLP24



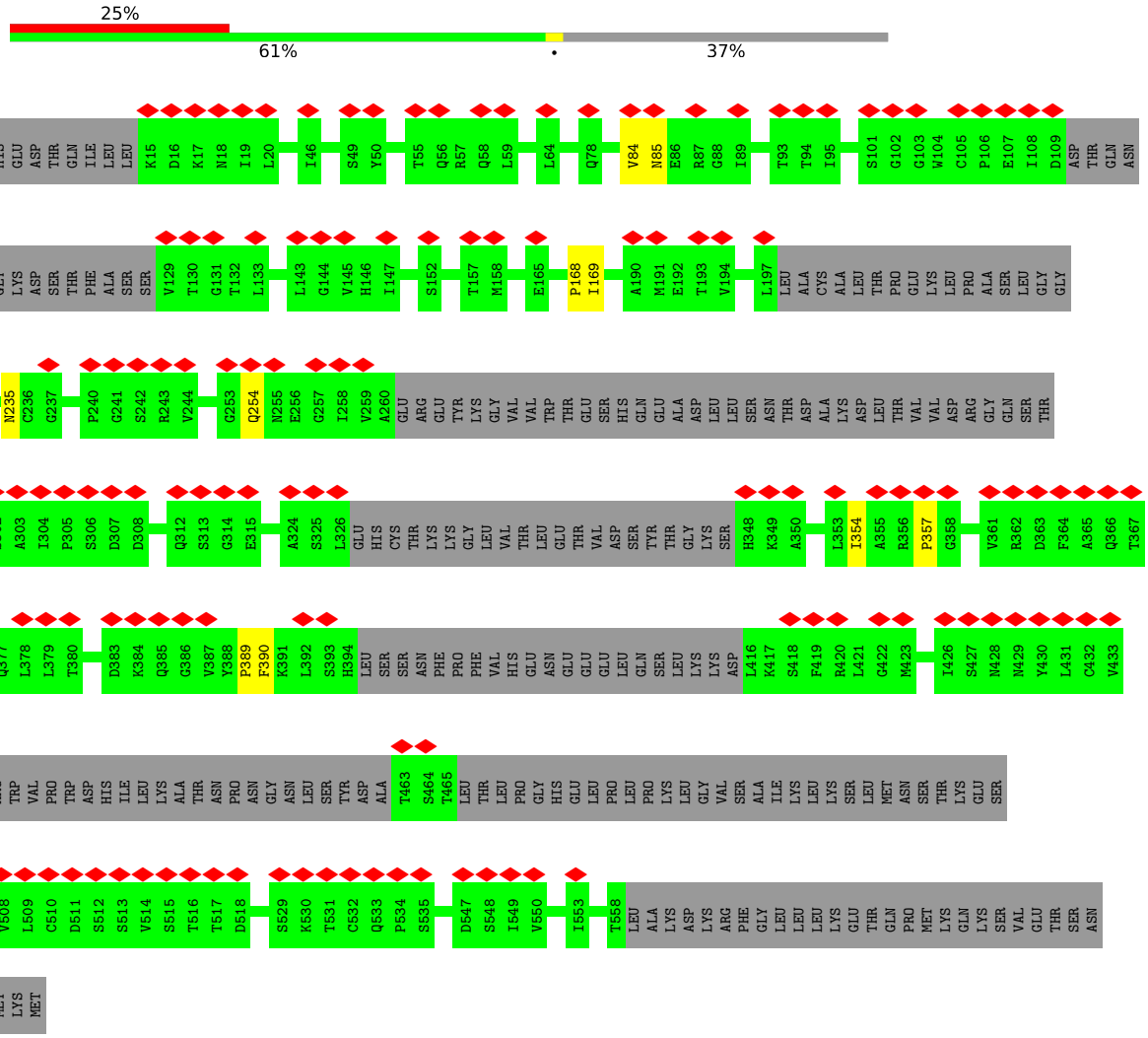
• Molecule 37: 60S ribosomal protein L20-A

Chain S:



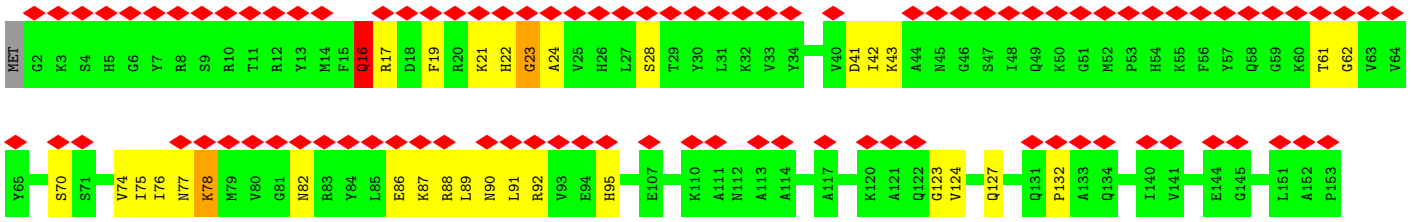
• Molecule 38: Probable metalloprotease ARX1

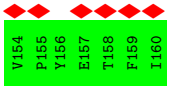
Chain u:



• Molecule 39: 60S ribosomal protein L21-A

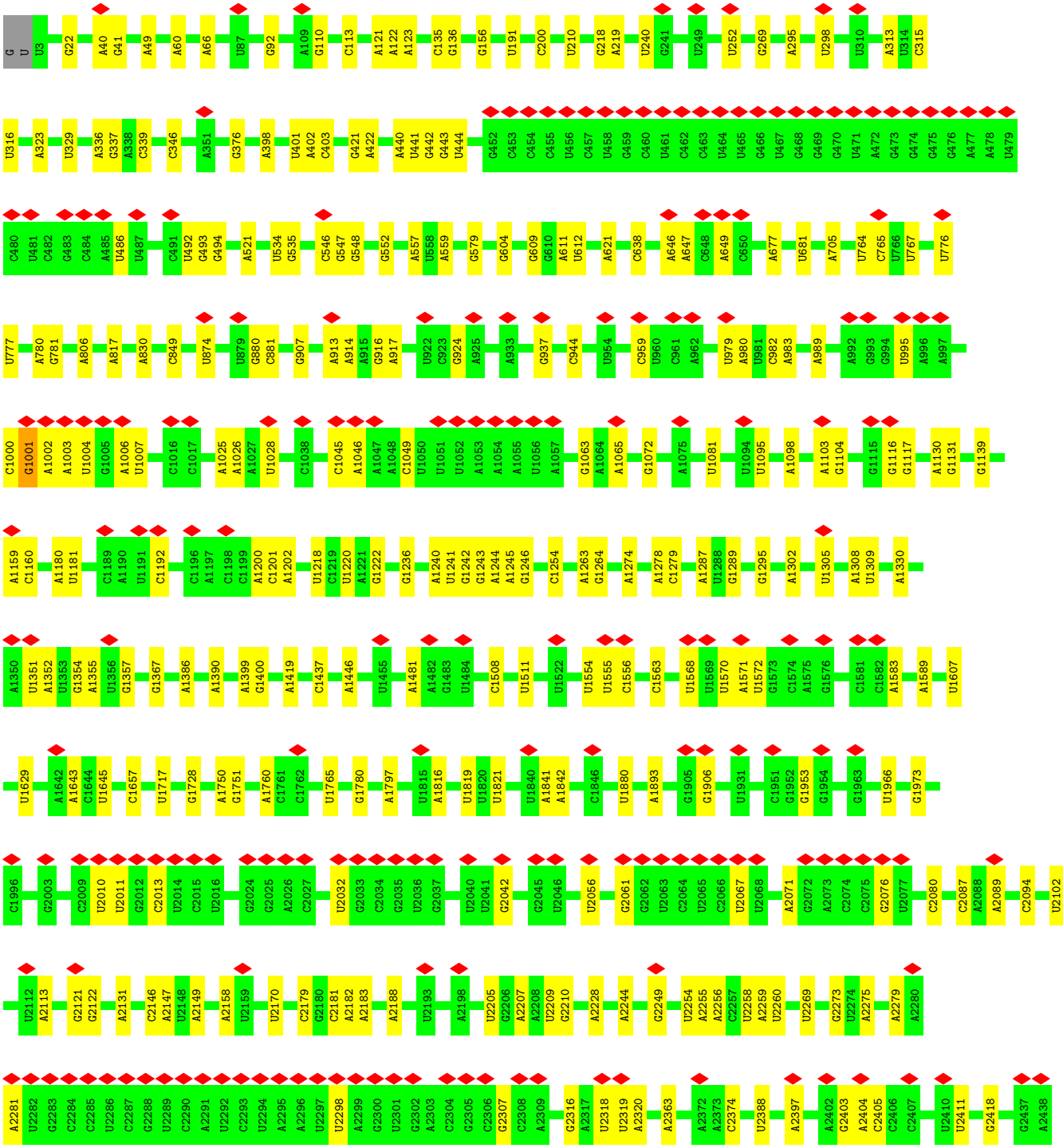
Chain T:

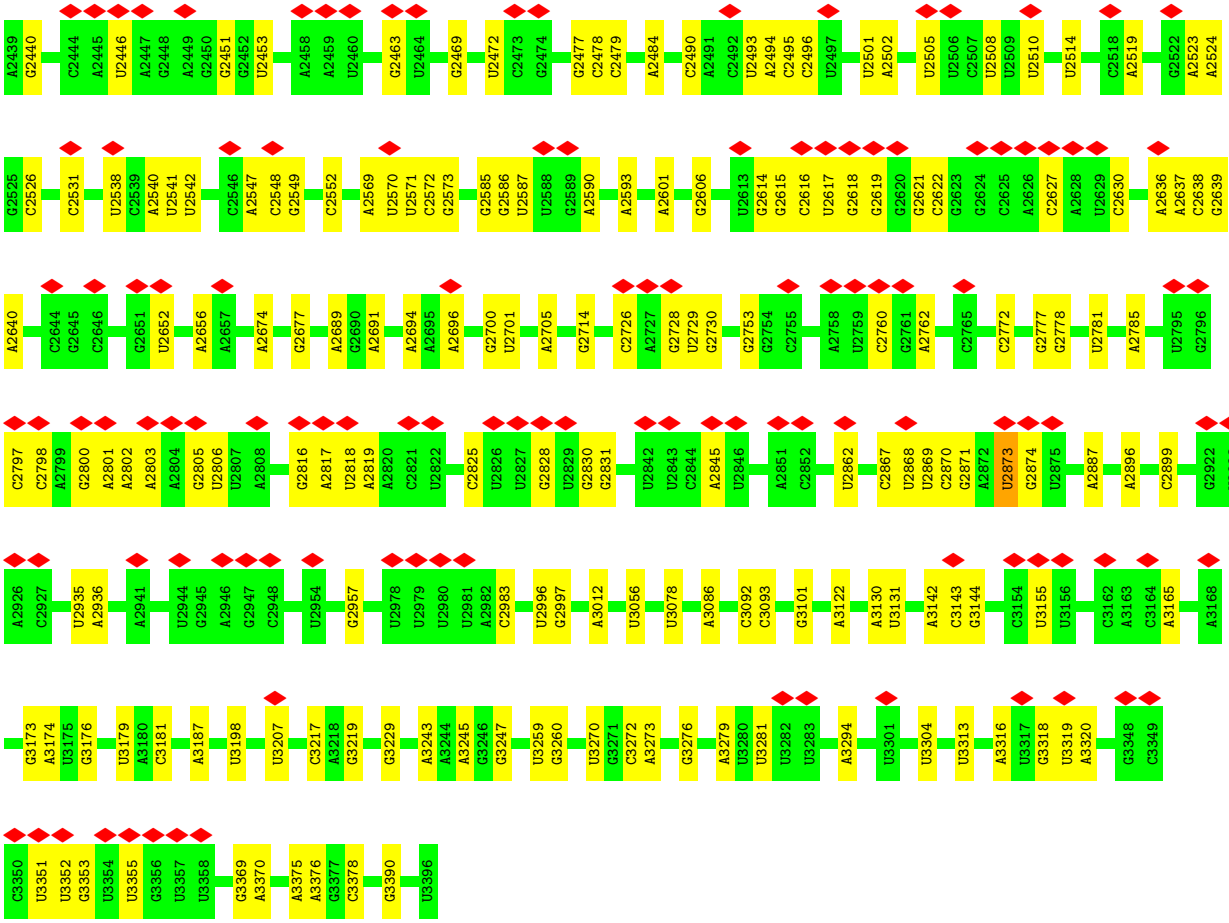




• Molecule 40: 25S ribosomal RNA

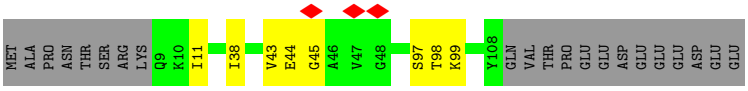
Chain x:





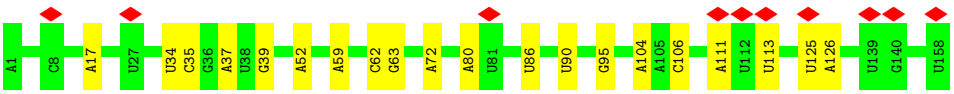
• Molecule 41: 60S ribosomal protein L22-A

Chain U:



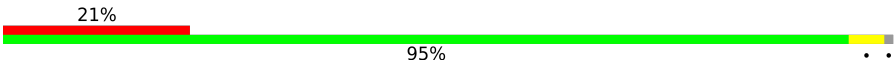
• Molecule 42: 5.8S ribosomal RNA

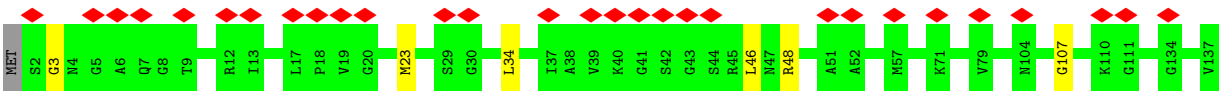
Chain y:



• Molecule 43: 60S ribosomal protein L23-A

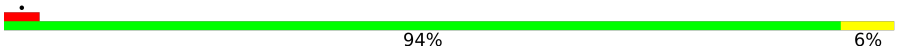
Chain V:

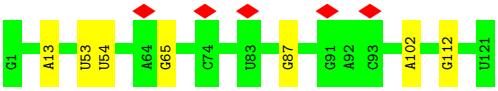




• Molecule 44: 5S ribosomal RNA

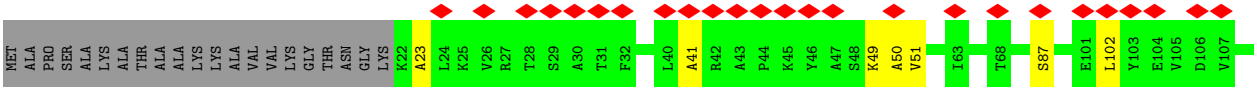
Chain z:

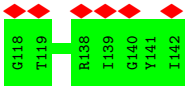




• Molecule 45: 60S ribosomal protein L25

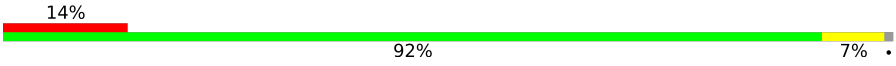
Chain X:

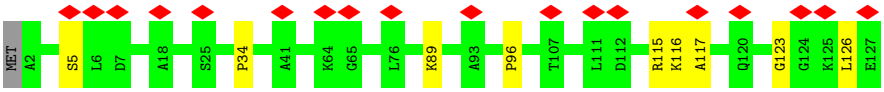




• Molecule 46: 60S ribosomal protein L26-A

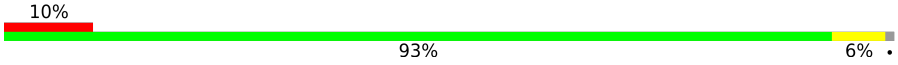
Chain Y:

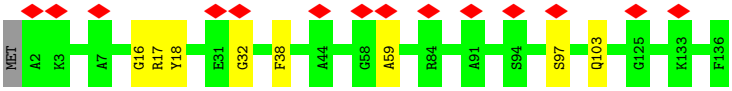




• Molecule 47: 60S ribosomal protein L27-A

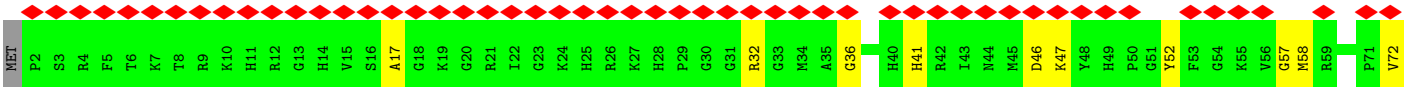
Chain Z:

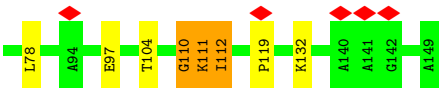




• Molecule 48: 60S ribosomal protein L28

Chain a:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15749	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor
Maximum map value	1.479	Depositor
Minimum map value	-0.721	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	827.6, 827.6, 827.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.069, 2.069, 2.069	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.35	1/1006 (0.1%)	0.47	0/1256
2	c	0.17	0/386	0.27	0/481
3	B	0.19	0/1542	0.36	0/1926
4	d	0.18	0/434	0.31	0/541
5	C	0.19	0/1442	0.37	1/1801 (0.1%)
6	e	0.17	0/506	0.32	0/631
7	D	0.18	0/1182	0.32	0/1476
8	f	0.49	1/422 (0.2%)	0.71	1/526 (0.2%)
9	E	0.55	1/620 (0.2%)	0.70	4/772 (0.5%)
10	g	0.18	0/446	0.32	0/556
11	F	0.18	0/886	0.32	0/1106
12	h	0.17	0/474	0.29	0/591
13	G	0.18	0/930	0.32	0/1161
14	i	0.18	0/394	0.31	0/491
15	H	0.17	0/762	0.30	0/951
16	j	0.57	1/346 (0.3%)	0.57	1/431 (0.2%)
17	I	0.18	0/866	0.31	0/1081
18	k	0.17	0/306	0.29	0/381
19	J	0.54	0/674	0.78	0/841
20	l	0.17	0/198	0.36	0/246
21	K	0.18	0/506	0.34	0/631
22	m	0.18	0/894	0.30	0/1116
23	L	0.18	0/770	0.35	0/961
24	n	0.18	0/846	0.31	0/1056
25	M	0.17	0/542	0.30	0/676
26	o	0.59	2/1386 (0.1%)	0.85	9/1731 (0.5%)
27	N	0.19	0/810	0.38	0/1011
28	p	0.18	0/362	0.30	0/451
29	O	0.20	0/786	0.47	1/981 (0.1%)
30	q	0.92	0/1950	0.88	0/2436
31	P	0.17	0/730	0.33	0/911
32	r	0.55	1/1276 (0.1%)	0.90	4/1553 (0.3%)
33	Q	0.17	0/738	0.30	0/921
34	s	0.29	1/8001 (0.0%)	0.49	8/9992 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	R	0.20	0/750	0.41	0/936
36	t	0.34	0/250	0.52	0/311
37	S	0.16	0/686	0.32	0/856
38	u	0.92	0/1483	0.86	1/1840 (0.1%)
39	T	0.44	1/634 (0.2%)	0.64	2/791 (0.3%)
40	x	0.20	5/81221 (0.0%)	0.74	168/126638 (0.1%)
41	U	0.18	0/398	0.31	0/496
42	y	0.13	0/3743	0.64	0/5828
43	V	0.22	0/542	0.35	0/676
44	z	0.13	0/2880	0.64	0/4487
45	X	0.17	0/482	0.29	0/601
46	Y	0.17	0/502	0.30	0/626
47	Z	0.18	0/538	0.31	0/671
48	a	0.80	3/590 (0.5%)	0.71	3/736 (0.4%)
All	All	0.28	17/128118 (0.0%)	0.68	203/187166 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	B	0	2
8	f	0	2
9	E	0	1
19	J	0	1
26	o	0	1
32	r	0	3
34	s	0	11
36	t	0	1
39	T	0	3
48	a	0	1
All	All	0	27

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	a	111	LYS	N-CA	14.13	1.74	1.46
48	a	110	GLY	C-N	10.00	1.57	1.34
9	E	67	GLY	CA-C	-9.76	1.36	1.51
16	j	39	TYR	C-O	-8.62	1.06	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	x	2638	C	O3'-P	-7.47	1.52	1.61
8	f	100	ILE	C-N	7.04	1.50	1.34
34	s	2362	ALA	C-O	7.02	1.36	1.23
40	x	2781	U	O3'-P	-6.79	1.53	1.61
26	o	56	GLY	C-O	6.14	1.33	1.23
39	T	16	GLN	N-CA	6.11	1.58	1.46
40	x	443	G	O3'-P	5.87	1.68	1.61
26	o	44	ALA	CA-C	5.81	1.68	1.52
40	x	1025	A	C6-N6	5.56	1.38	1.33
40	x	1130	A	O3'-P	5.55	1.67	1.61
32	r	111	GLU	C-N	5.49	1.46	1.34
48	a	112	ILE	N-CA	-5.43	1.35	1.46
1	A	207	VAL	N-CA	5.27	1.56	1.46

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	s	858	GLU	O-C-N	-21.28	88.65	122.70
40	x	440	A	O5'-P-OP1	-19.65	87.12	110.70
40	x	440	A	O5'-P-OP2	17.48	131.68	110.70
40	x	2638	C	P-O3'-C3'	-16.82	99.52	119.70
40	x	2873	U	C5'-C4'-O4'	-15.31	90.73	109.10
40	x	440	A	P-O5'-C5'	14.20	143.62	120.90
40	x	494	G	P-O5'-C5'	13.60	142.66	120.90
40	x	2873	U	P-O5'-C5'	13.29	142.16	120.90
40	x	2873	U	C5'-C4'-C3'	13.19	137.10	116.00
40	x	1026	A	N1-C6-N6	12.33	126.00	118.60
40	x	2819	A	O5'-P-OP2	12.13	125.26	110.70
40	x	913	A	N1-C6-N6	12.08	125.85	118.60
40	x	2705	A	N1-C6-N6	11.74	125.64	118.60
40	x	2183	A	N1-C6-N6	11.71	125.62	118.60
40	x	2182	A	N1-C6-N6	11.69	125.62	118.60
40	x	1025	A	N1-C6-N6	11.68	125.61	118.60
40	x	494	G	C4'-C3'-O3'	11.52	136.04	113.00
40	x	2149	A	N1-C6-N6	11.40	125.44	118.60
40	x	2147	A	N1-C6-N6	11.30	125.38	118.60
40	x	2617	U	C4'-C3'-O3'	-11.24	85.79	109.40
40	x	2870	C	C4'-C3'-O3'	11.14	135.28	113.00
9	E	67	GLY	N-CA-C	-11.04	85.50	113.10
40	x	1218	U	P-O5'-C5'	10.86	138.28	120.90
40	x	1002	A	P-O5'-C5'	10.69	138.00	120.90
48	a	110	GLY	CA-C-O	-10.67	101.40	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	x	2873	U	P-O3'-C3'	10.64	132.47	119.70
40	x	2873	U	C2'-C3'-O3'	10.31	132.19	109.50
8	f	100	ILE	O-C-N	-10.18	106.41	122.70
34	s	1015	ARG	O-C-N	-10.16	106.44	122.70
40	x	2819	A	C4'-C3'-O3'	10.11	133.21	113.00
40	x	2867	C	C4'-C3'-O3'	10.09	133.17	113.00
40	x	313	A	P-O3'-C3'	-10.07	107.62	119.70
40	x	442	G	C4'-C3'-O3'	9.86	132.72	113.00
40	x	2874	G	O5'-C5'-C4'	9.59	129.91	111.70
40	x	2403	G	C4'-C3'-O3'	-9.56	89.32	109.40
40	x	2874	G	C4'-C3'-O3'	-9.40	89.67	109.40
40	x	1131	G	O4'-C4'-C3'	-9.31	94.69	104.00
40	x	2637	A	C4'-C3'-O3'	-9.07	90.34	109.40
40	x	2639	G	P-O5'-C5'	8.91	135.16	120.90
40	x	315	C	C5'-C4'-O4'	-8.89	98.43	109.10
40	x	2638	C	C4'-C3'-O3'	8.84	130.68	113.00
40	x	2869	U	C2'-C3'-O3'	8.74	128.73	109.50
40	x	2818	U	N1-C1'-C2'	-8.70	102.44	112.00
40	x	315	C	C2'-C3'-O3'	8.60	128.42	109.50
40	x	2818	U	O4'-C4'-C3'	-8.57	95.43	104.00
40	x	315	C	P-O5'-C5'	-8.50	107.30	120.90
40	x	1000	C	C4'-C3'-O3'	8.48	129.96	113.00
40	x	2259	A	C4'-C3'-O3'	8.42	129.84	113.00
40	x	2874	G	P-O5'-C5'	-8.35	107.54	120.90
40	x	1130	A	C4'-C3'-O3'	8.26	129.52	113.00
40	x	2403	G	P-O3'-C3'	8.26	129.61	119.70
26	o	247	ARG	N-CA-C	8.24	133.26	111.00
40	x	2319	U	C2'-C3'-O3'	-8.24	91.36	109.50
40	x	1001	G	C2'-C3'-O3'	-8.21	91.45	109.50
40	x	1001	G	C4'-C3'-O3'	8.18	129.37	113.00
40	x	2254	U	C4'-C3'-O3'	7.93	128.87	113.00
40	x	2181	C	O4'-C1'-N1	7.88	114.50	108.20
26	o	119	GLY	O-C-N	7.80	135.18	122.70
40	x	2818	U	O4'-C1'-N1	7.72	114.38	108.20
40	x	1003	A	N9-C1'-C2'	-7.71	103.52	112.00
40	x	2319	U	C4'-C3'-O3'	7.71	128.41	113.00
48	a	110	GLY	CA-C-N	7.64	134.01	117.20
40	x	2404	A	C5'-C4'-C3'	7.61	128.17	116.00
40	x	1554	U	P-O3'-C3'	7.58	128.79	119.70
40	x	1025	A	O4'-C1'-N9	7.45	114.16	108.20
48	a	110	GLY	C-N-CA	7.35	140.08	121.70
26	o	119	GLY	CA-C-N	-7.31	101.12	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	x	2319	U	C5'-C4'-O4'	7.24	117.78	109.10
40	x	2874	G	O4'-C1'-N9	7.22	113.97	108.20
40	x	2256	A	C2'-C3'-O3'	7.21	125.36	109.50
40	x	2818	U	OP2-P-O3'	-7.15	89.47	105.20
26	o	119	GLY	C-N-CA	7.14	139.56	121.70
40	x	2617	U	P-O5'-C5'	7.11	132.28	120.90
40	x	1130	A	O3'-P-O5'	7.03	117.35	104.00
38	u	389	PRO	N-CA-C	7.02	130.34	112.10
34	s	630	ASN	C-N-CA	-6.97	104.27	121.70
40	x	2146	C	P-O3'-C3'	-6.87	111.46	119.70
40	x	2640	A	P-O5'-C5'	-6.84	109.96	120.90
40	x	2617	U	C2'-C3'-O3'	6.83	124.63	113.70
40	x	2585	G	C4'-C3'-O3'	-6.79	95.13	109.40
40	x	983	A	C4'-C3'-O3'	-6.74	95.24	109.40
40	x	2585	G	P-O5'-C5'	6.72	131.66	120.90
40	x	2817	A	P-O3'-C3'	6.71	127.76	119.70
39	T	16	GLN	N-CA-C	6.70	129.08	111.00
40	x	2873	U	O4'-C1'-N1	6.69	113.55	108.20
40	x	2874	G	C5'-C4'-O4'	6.65	117.08	109.10
40	x	313	A	O3'-P-O5'	6.56	116.47	104.00
40	x	2705	A	C4-C5-C6	6.53	120.26	117.00
29	O	59	ARG	N-CA-C	6.44	128.39	111.00
26	o	44	ALA	N-CA-C	6.43	128.37	111.00
40	x	444	U	P-O5'-C5'	6.42	131.18	120.90
40	x	1025	A	C4-C5-C6	6.42	120.21	117.00
40	x	2639	G	O5'-C5'-C4'	-6.41	99.53	111.70
40	x	2183	A	C4-C5-C6	6.40	120.20	117.00
40	x	2182	A	O4'-C1'-N9	6.40	113.32	108.20
39	T	16	GLN	C-N-CA	6.40	137.69	121.70
40	x	1002	A	O5'-C5'-C4'	-6.39	99.56	111.70
40	x	2210	G	C4'-C3'-O3'	6.39	125.78	113.00
40	x	494	G	O5'-C5'-C4'	-6.37	99.60	111.70
40	x	440	A	O5'-C5'-C4'	-6.35	99.63	111.70
40	x	2586	G	C4'-C3'-O3'	6.35	125.69	113.00
40	x	1003	A	O3'-P-O5'	-6.21	92.20	104.00
40	x	1218	U	O5'-C5'-C4'	-6.21	99.90	111.70
16	j	38	GLY	O-C-N	-6.20	112.78	122.70
40	x	2258	U	O5'-P-OP2	-6.18	100.14	105.70
40	x	1554	U	C4'-C3'-O3'	6.14	125.29	113.00
40	x	913	A	C4-C5-C6	6.13	120.07	117.00
40	x	2868	U	O4'-C1'-N1	6.13	113.10	108.20
26	o	117	LYS	C-N-CA	6.10	136.96	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	67	GLY	C-N-CA	-6.08	96.46	122.00
40	x	2816	G	C2'-C3'-O3'	-6.08	96.14	109.50
40	x	2182	A	C4-C5-C6	6.05	120.03	117.00
40	x	1026	A	C4-C5-C6	5.97	119.98	117.00
9	E	68	PRO	CA-C-N	-5.96	104.08	117.20
40	x	1004	U	C5'-C4'-C3'	5.93	125.49	116.00
40	x	2316	G	C4'-C3'-O3'	5.92	124.83	113.00
40	x	2586	G	O4'-C1'-N9	-5.91	103.47	108.20
40	x	1026	A	C5-C6-N6	-5.91	118.98	123.70
40	x	1131	G	P-O5'-C5'	5.90	130.33	120.90
40	x	2318	U	O4'-C1'-N1	5.88	112.91	108.20
40	x	2147	A	O4'-C1'-N9	5.88	112.90	108.20
40	x	1556	C	O4'-C1'-N1	5.86	112.89	108.20
40	x	441	U	P-O3'-C3'	5.86	126.73	119.70
40	x	2587	U	C4'-C3'-O3'	-5.83	97.16	109.40
40	x	2183	A	O4'-C1'-N9	5.82	112.85	108.20
9	E	68	PRO	N-CA-C	-5.80	97.02	112.10
40	x	2616	C	C2'-C3'-O3'	5.78	122.95	113.70
40	x	1000	C	P-O3'-C3'	5.78	126.63	119.70
40	x	443	G	C4'-C3'-O3'	5.77	124.54	113.00
40	x	2319	U	P-O3'-C3'	5.76	126.62	119.70
40	x	1556	C	N1-C1'-C2'	5.76	121.49	114.00
40	x	493	G	O3'-P-O5'	5.75	114.93	104.00
40	x	2818	U	O5'-C5'-C4'	5.74	122.61	111.70
40	x	1025	A	C5-C6-N6	-5.74	119.11	123.70
40	x	1002	A	P-O3'-C3'	5.74	126.58	119.70
40	x	913	A	C5-C6-N6	-5.70	119.14	123.70
32	r	442	ALA	N-CA-C	-5.69	95.64	111.00
40	x	2825	C	C5'-C4'-C3'	5.69	125.10	116.00
40	x	2320	A	C5'-C4'-C3'	5.65	125.04	116.00
34	s	1479	LEU	O-C-N	-5.65	113.67	122.70
40	x	2147	A	C4-C5-C6	5.64	119.82	117.00
40	x	2818	U	O3'-P-O5'	5.63	114.70	104.00
34	s	630	ASN	N-CA-C	-5.62	95.82	111.00
40	x	2637	A	C2'-C3'-O3'	5.62	122.69	113.70
40	x	1131	G	O4'-C1'-N9	5.62	112.69	108.20
40	x	2617	U	N1-C1'-C2'	-5.62	105.82	112.00
40	x	2705	A	C5-C6-N1	-5.62	114.89	117.70
26	o	237	MET	N-CA-C	-5.61	95.86	111.00
40	x	2256	A	C4'-C3'-O3'	-5.58	97.69	109.40
40	x	2207	A	C4'-C3'-O3'	5.57	124.14	113.00
40	x	2181	C	N3-C4-N4	5.57	121.90	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	x	2586	G	C2'-C3'-O3'	5.56	122.59	113.70
40	x	2405	C	O5'-C5'-C4'	-5.55	101.15	111.70
40	x	2404	A	O5'-C5'-C4'	5.55	122.25	111.70
40	x	2403	G	N9-C1'-C2'	5.54	121.19	114.00
40	x	2149	A	C5-C6-N6	-5.53	119.28	123.70
40	x	2868	U	C5'-C4'-O4'	5.52	115.72	109.10
40	x	2616	C	P-O3'-C3'	5.51	126.31	119.70
40	x	913	A	O4'-C1'-N9	5.50	112.60	108.20
5	C	187	LEU	N-CA-C	-5.49	96.17	111.00
40	x	1220	U	O4'-C1'-N1	5.49	112.59	108.20
40	x	1220	U	P-O3'-C3'	-5.47	113.13	119.70
40	x	2873	U	O4'-C4'-C3'	-5.46	98.54	104.00
40	x	443	G	O3'-P-O5'	5.45	114.36	104.00
40	x	494	G	C2'-C3'-O3'	-5.43	97.55	109.50
40	x	2183	A	C5-C6-N6	-5.43	119.35	123.70
40	x	2182	A	C5-C6-N6	-5.42	119.36	123.70
40	x	2181	C	N3-C4-C5	-5.41	119.74	121.90
40	x	913	A	C5-C6-N1	-5.38	115.01	117.70
40	x	2873	U	C2-N1-C1'	5.38	124.15	117.70
40	x	2869	U	P-O5'-C5'	5.37	129.50	120.90
34	s	1409	PRO	CA-C-N	-5.37	105.39	117.20
40	x	2182	A	C5-C6-N1	-5.36	115.02	117.70
40	x	2183	A	C5-C6-N1	-5.36	115.02	117.70
40	x	1026	A	C5-C6-N1	-5.35	115.03	117.70
40	x	2615	G	C4'-C3'-O3'	5.35	123.69	113.00
40	x	2147	A	C5-C6-N1	-5.34	115.03	117.70
40	x	2585	G	P-O3'-C3'	5.34	126.10	119.70
34	s	578	ASP	N-CA-C	-5.33	96.60	111.00
32	r	306	LEU	N-CA-C	-5.33	96.60	111.00
40	x	2705	A	C5-C6-N6	-5.30	119.46	123.70
26	o	118	PHE	CA-C-N	5.29	126.79	116.20
32	r	88	ILE	N-CA-C	-5.29	96.72	111.00
40	x	2870	C	C2'-C3'-O3'	-5.26	97.94	109.50
40	x	2209	U	C5'-C4'-O4'	-5.25	102.81	109.10
40	x	2319	U	O4'-C4'-C3'	-5.24	98.76	104.00
40	x	2258	U	C4'-C3'-O3'	5.22	123.43	113.00
40	x	2817	A	C4'-C3'-O3'	-5.22	98.44	109.40
40	x	2871	G	P-O3'-C3'	-5.19	113.47	119.70
32	r	129	GLU	N-CA-C	-5.19	97.00	111.00
26	o	94	SER	N-CA-C	-5.17	97.04	111.00
40	x	2868	U	P-O5'-C5'	-5.17	112.63	120.90
40	x	2618	G	P-O5'-C5'	5.16	129.16	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	x	2147	A	C5-C6-N6	-5.14	119.59	123.70
40	x	2149	A	C4-C5-C6	5.13	119.57	117.00
40	x	441	U	O5'-C5'-C4'	-5.13	101.95	111.70
40	x	2862	U	P-O3'-C3'	-5.12	113.56	119.70
40	x	2269	U	P-O5'-C5'	5.10	129.06	120.90
40	x	1556	C	C5'-C4'-O4'	5.08	115.20	109.10
40	x	1555	U	C4'-C3'-O3'	5.07	123.14	113.00
40	x	2781	U	P-O3'-C3'	5.06	125.77	119.70
40	x	2618	G	O5'-C5'-C4'	-5.05	102.11	111.70
34	s	859	LYS	C-N-CA	-5.04	111.71	122.30

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	LYS	Peptide
3	B	255	TRP	Peptide
3	B	256	HIS	Peptide
9	E	42	LEU	Mainchain
19	J	8	PRO	Peptide
39	T	16	GLN	Mainchain
39	T	23	GLY	Peptide
39	T	86	GLU	Peptide
48	a	111	LYS	Peptide
8	f	100	ILE	Mainchain
8	f	103	TYR	Peptide
26	o	43	ARG	Mainchain
32	r	111	GLU	Mainchain
32	r	461	GLU	Peptide
32	r	462	ILE	Peptide
34	s	1015	ARG	Mainchain
34	s	1018	ASN	Peptide
34	s	1466	ASP	Peptide
34	s	1479	LEU	Mainchain
34	s	576	SER	Peptide,Mainchain
34	s	578	ASP	Peptide
34	s	628	PHE	Peptide
34	s	858	GLU	Mainchain
34	s	859	LYS	Peptide
34	s	903	SER	Peptide
36	t	17	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1007	0	310	18	0
2	c	387	0	113	0	0
3	B	1543	0	433	4	0
4	d	435	0	114	0	0
5	C	1443	0	399	7	0
6	e	507	0	135	0	0
7	D	1183	0	325	1	0
8	f	423	0	117	0	0
9	E	622	0	160	1	0
10	g	447	0	121	0	0
11	F	887	0	241	3	0
12	h	475	0	118	0	0
13	G	931	0	242	1	0
14	i	395	0	109	0	0
15	H	763	0	215	3	0
16	j	347	0	104	0	0
17	I	867	0	230	2	0
18	k	307	0	79	0	0
19	J	675	0	191	11	0
20	l	199	0	47	0	0
21	K	507	0	140	1	0
22	m	895	0	257	0	0
23	L	771	0	199	4	0
24	n	847	0	224	0	0
25	M	543	0	145	2	0
26	o	1387	0	358	0	0
27	N	811	0	221	3	0
28	p	363	0	108	0	0
29	O	787	0	214	5	0
30	q	1951	0	540	0	0
31	P	731	0	197	4	0
32	r	1304	0	332	0	0
33	Q	739	0	205	1	0
34	s	8007	0	2136	0	0
35	R	751	0	203	14	0
36	t	251	0	68	0	0
37	S	687	0	175	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	u	1491	0	399	0	0
39	T	635	0	174	14	0
40	x	72570	0	36462	0	0
41	U	399	0	109	2	0
42	y	3350	0	1696	0	0
43	V	543	0	162	2	0
44	z	2576	0	1304	0	0
45	X	483	0	121	1	0
46	Y	503	0	134	1	0
47	Z	539	0	144	1	0
48	a	591	0	176	0	0
All	All	118855	0	50406	109	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 7.

All (109) 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)
39:T:62:GLY:N	39:T:75:ILE:H	1.51	1.07
39:T:43:LYS:O	39:T:95:HIS:CA	2.03	1.06
35:R:158:GLU:O	35:R:162:ARG:N	1.90	1.03
39:T:62:GLY:CA	39:T:75:ILE:H	1.72	1.03
39:T:62:GLY:HA3	39:T:75:ILE:N	1.80	0.96
39:T:41:ASP:O	39:T:43:LYS:N	2.00	0.93
1:A:114:SER:CA	1:A:134:VAL:H	1.81	0.89
1:A:206:PRO:O	1:A:208:ASP:N	2.06	0.88
35:R:158:GLU:O	35:R:161:ALA:N	2.08	0.86
1:A:119:LYS:O	1:A:121:GLY:N	2.12	0.82
1:A:115:ASN:CA	1:A:133:TYR:CA	2.58	0.81
39:T:62:GLY:CA	39:T:75:ILE:N	2.42	0.81
1:A:115:ASN:N	1:A:133:TYR:CA	2.45	0.80
19:J:106:ILE:O	19:J:125:MET:N	2.14	0.79
35:R:157:GLU:O	35:R:161:ALA:N	2.16	0.78
1:A:113:VAL:N	1:A:134:VAL:C	2.39	0.73
19:J:94:ARG:O	19:J:96:PHE:N	2.22	0.71
39:T:74:VAL:O	39:T:89:LEU:N	2.25	0.69
35:R:173:ARG:O	35:R:177:VAL:N	2.24	0.68
39:T:62:GLY:H	39:T:75:ILE:H	1.42	0.68
1:A:114:SER:C	1:A:133:TYR:CA	2.63	0.67
1:A:113:VAL:N	1:A:134:VAL:O	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:85:LYS:O	19:J:88:GLU:N	2.28	0.66
1:A:206:PRO:C	1:A:208:ASP:H	1.98	0.65
23:L:99:HIS:O	23:L:101:ARG:N	2.28	0.63
35:R:158:GLU:O	35:R:159:ALA:C	2.36	0.63
39:T:62:GLY:N	39:T:75:ILE:N	2.36	0.62
39:T:76:ILE:O	39:T:78:LYS:N	2.34	0.60
3:B:238:LEU:N	3:B:246:LEU:O	2.36	0.59
35:R:81:ARG:O	35:R:83:GLY:N	2.35	0.59
1:A:134:VAL:O	1:A:136:ILE:N	2.35	0.59
29:O:62:THR:O	29:O:64:PHE:N	2.29	0.58
35:R:79:GLY:O	35:R:81:ARG:N	2.36	0.58
13:G:35:GLY:O	13:G:37:GLY:N	2.37	0.58
1:A:125:ALA:O	1:A:127:ALA:N	2.37	0.58
35:R:158:GLU:O	35:R:161:ALA:CA	2.52	0.57
1:A:114:SER:C	1:A:134:VAL:H	2.07	0.56
19:J:94:ARG:C	19:J:96:PHE:H	2.09	0.56
31:P:95:LEU:O	31:P:97:ASN:N	2.38	0.55
1:A:125:ALA:C	1:A:127:ALA:H	2.10	0.54
39:T:61:THR:CA	39:T:75:ILE:O	2.55	0.54
29:O:110:PRO:O	29:O:112:TYR:N	2.41	0.54
39:T:43:LYS:C	39:T:95:HIS:CA	2.75	0.54
43:V:46:LEU:O	43:V:48:ARG:N	2.41	0.53
27:N:107:GLY:O	27:N:111:ALA:N	2.41	0.53
35:R:150:GLN:O	35:R:154:ALA:N	2.40	0.53
39:T:61:THR:C	39:T:75:ILE:O	2.46	0.53
1:A:114:SER:CA	1:A:134:VAL:N	2.64	0.52
1:A:114:SER:C	1:A:134:VAL:N	2.63	0.52
5:C:94:CYS:O	5:C:96:GLY:N	2.42	0.52
27:N:75:VAL:O	27:N:77:LYS:N	2.43	0.52
37:S:132:THR:O	37:S:134:ASP:N	2.43	0.52
31:P:40:GLU:O	31:P:42:THR:N	2.42	0.52
39:T:74:VAL:O	39:T:88:ARG:CA	2.58	0.51
1:A:112:ILE:CA	1:A:134:VAL:O	2.59	0.51
1:A:125:ALA:C	1:A:127:ALA:N	2.63	0.51
17:I:39:LYS:N	17:I:205:VAL:O	2.41	0.50
27:N:165:THR:O	27:N:169:LYS:N	2.28	0.50
3:B:46:PHE:O	3:B:338:LEU:N	2.45	0.50
3:B:346:THR:O	3:B:348:ARG:N	2.45	0.49
7:D:257:GLU:O	7:D:259:LYS:N	2.44	0.49
31:P:132:ALA:O	31:P:134:GLY:N	2.45	0.49
19:J:23:VAL:O	19:J:25:GLU:N	2.39	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:73:GLY:O	19:J:75:LYS:N	2.46	0.49
5:C:181:VAL:O	5:C:183:LYS:N	2.43	0.49
23:L:164:GLU:O	23:L:166:ALA:N	2.45	0.49
25:M:34:ALA:O	25:M:47:ASP:N	2.46	0.48
15:H:80:THR:O	15:H:85:GLY:N	2.47	0.48
3:B:49:TYR:O	3:B:80:ASP:N	2.46	0.48
37:S:79:VAL:N	37:S:90:MET:O	2.45	0.48
5:C:337:GLU:O	5:C:339:LEU:N	2.48	0.47
1:A:128:ARG:C	1:A:130:SER:H	2.17	0.47
46:Y:115:ARG:O	46:Y:117:ALA:N	2.48	0.47
21:K:39:PRO:O	21:K:41:LYS:N	2.47	0.47
35:R:81:ARG:C	35:R:83:GLY:H	2.18	0.47
35:R:85:ARG:O	35:R:89:LEU:N	2.47	0.47
11:F:108:LEU:O	11:F:110:ARG:N	2.48	0.46
47:Z:16:GLY:O	47:Z:18:TYR:N	2.48	0.46
23:L:27:ASP:O	23:L:29:ALA:N	2.49	0.46
5:C:114:ASN:O	5:C:118:LYS:N	2.42	0.46
23:L:165:SER:O	23:L:167:PHE:N	2.47	0.46
35:R:66:HIS:O	35:R:70:LYS:N	2.41	0.45
5:C:206:LEU:O	5:C:249:ILE:N	2.39	0.45
11:F:24:GLU:O	11:F:26:VAL:N	2.50	0.45
19:J:109:HIS:N	19:J:123:PHE:O	2.49	0.44
5:C:338:LYS:O	5:C:340:GLY:N	2.50	0.44
37:S:79:VAL:O	37:S:90:MET:N	2.49	0.44
45:X:49:LYS:O	45:X:51:VAL:N	2.51	0.44
11:F:222:HIS:O	11:F:227:GLY:N	2.51	0.44
33:Q:170:ARG:O	33:Q:172:PHE:N	2.51	0.43
5:C:222:VAL:O	5:C:224:GLY:N	2.52	0.43
15:H:49:ASN:O	15:H:51:GLN:N	2.51	0.43
17:I:73:ASP:O	17:I:75:ASP:N	2.51	0.43
19:J:110:ILE:C	19:J:112:LEU:H	2.21	0.43
41:U:97:SER:O	41:U:99:LYS:N	2.52	0.43
41:U:43:VAL:O	41:U:45:GLY:N	2.52	0.43
43:V:23:MET:O	43:V:34:LEU:N	2.43	0.42
15:H:64:HIS:O	15:H:66:ALA:N	2.52	0.42
35:R:158:GLU:C	35:R:161:ALA:H	2.22	0.42
19:J:107:ASP:CA	19:J:124:GLY:HA2	2.50	0.42
31:P:113:TYR:O	31:P:151:THR:N	2.48	0.42
29:O:130:LYS:O	29:O:132:GLY:N	2.53	0.42
9:E:97:ASN:O	9:E:99:GLU:N	2.53	0.41
19:J:41:SER:C	19:J:43:GLN:H	2.24	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:O:38:ALA:H	29:O:107:GLY:HA2	1.85	0.41
25:M:34:ALA:N	25:M:47:ASP:O	2.52	0.41
19:J:110:ILE:O	19:J:112:LEU:N	2.53	0.40
29:O:62:THR:N	29:O:69:GLY:HA2	2.36	0.40
35:R:158:GLU:O	35:R:161:ALA:C	2.54	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	
1	A	250/254 (98%)	156 (62%)	70 (28%)	24 (10%)	0	10
2	c	95/105 (90%)	84 (88%)	10 (10%)	1 (1%)	14	52
3	B	384/387 (99%)	294 (77%)	70 (18%)	20 (5%)	2	19
4	d	107/113 (95%)	88 (82%)	15 (14%)	4 (4%)	3	24
5	C	359/362 (99%)	254 (71%)	80 (22%)	25 (7%)	1	14
6	e	125/130 (96%)	99 (79%)	24 (19%)	2 (2%)	9	44
7	D	294/297 (99%)	229 (78%)	53 (18%)	12 (4%)	3	23
8	f	104/107 (97%)	78 (75%)	19 (18%)	7 (7%)	1	15
9	E	152/176 (86%)	113 (74%)	35 (23%)	4 (3%)	5	31
10	g	110/121 (91%)	78 (71%)	27 (24%)	5 (4%)	2	22
11	F	220/244 (90%)	181 (82%)	30 (14%)	9 (4%)	3	23
12	h	117/120 (98%)	92 (79%)	21 (18%)	4 (3%)	3	26
13	G	231/256 (90%)	180 (78%)	42 (18%)	9 (4%)	3	23
14	i	97/100 (97%)	78 (80%)	13 (13%)	6 (6%)	1	17
15	H	189/191 (99%)	147 (78%)	37 (20%)	5 (3%)	5	31
16	j	85/88 (97%)	53 (62%)	26 (31%)	6 (7%)	1	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	I	215/217 (99%)	159 (74%)	48 (22%)	8 (4%)	3 24
18	k	75/78 (96%)	66 (88%)	8 (11%)	1 (1%)	12 48
19	J	167/174 (96%)	116 (70%)	29 (17%)	22 (13%)	0 5
20	l	48/51 (94%)	33 (69%)	11 (23%)	4 (8%)	1 12
21	K	125/165 (76%)	81 (65%)	27 (22%)	17 (14%)	0 4
22	m	222/245 (91%)	170 (77%)	44 (20%)	8 (4%)	3 25
23	L	191/199 (96%)	141 (74%)	39 (20%)	11 (6%)	1 18
24	n	210/236 (89%)	156 (74%)	48 (23%)	6 (3%)	4 29
25	M	134/138 (97%)	106 (79%)	22 (16%)	6 (4%)	2 22
26	o	345/647 (53%)	223 (65%)	72 (21%)	50 (14%)	0 4
27	N	201/204 (98%)	147 (73%)	44 (22%)	10 (5%)	2 20
28	p	89/92 (97%)	72 (81%)	14 (16%)	3 (3%)	3 26
29	O	195/199 (98%)	143 (73%)	39 (20%)	13 (7%)	1 15
30	q	486/515 (94%)	458 (94%)	22 (4%)	6 (1%)	13 50
31	P	181/184 (98%)	141 (78%)	35 (19%)	5 (3%)	5 30
32	r	277/767 (36%)	155 (56%)	57 (21%)	65 (24%)	0 1
33	Q	183/186 (98%)	143 (78%)	30 (16%)	10 (6%)	2 19
34	s	1991/4910 (40%)	1585 (80%)	229 (12%)	177 (9%)	1 11
35	R	186/189 (98%)	136 (73%)	44 (24%)	6 (3%)	4 26
36	t	61/199 (31%)	52 (85%)	7 (12%)	2 (3%)	4 26
37	S	170/172 (99%)	133 (78%)	31 (18%)	6 (4%)	3 25
38	u	357/593 (60%)	342 (96%)	6 (2%)	9 (2%)	5 32
39	T	157/160 (98%)	90 (57%)	46 (29%)	21 (13%)	0 5
41	U	98/121 (81%)	77 (79%)	17 (17%)	4 (4%)	3 23
43	V	134/137 (98%)	95 (71%)	37 (28%)	2 (2%)	10 46
45	X	119/142 (84%)	91 (76%)	23 (19%)	5 (4%)	3 22
46	Y	124/127 (98%)	91 (73%)	26 (21%)	7 (6%)	2 19
47	Z	133/136 (98%)	97 (73%)	30 (23%)	6 (4%)	2 22
48	a	146/149 (98%)	89 (61%)	40 (27%)	17 (12%)	0 6
All	All	9939/14383 (69%)	7592 (76%)	1697 (17%)	650 (6%)	2 16

All (650) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	128	ARG
1	A	133	TYR
1	A	135	ILE
1	A	137	ILE
1	A	196	TRP
1	A	206	PRO
1	A	207	VAL
5	C	95	ARG
5	C	188	ARG
5	C	317	PRO
8	f	103	TYR
8	f	104	PRO
11	F	99	PRO
16	j	5	THR
19	J	8	PRO
19	J	11	ASP
19	J	12	LEU
19	J	74	PRO
19	J	94	ARG
19	J	127	PHE
19	J	165	GLN
20	l	22	PRO
21	K	30	PRO
21	K	58	VAL
23	L	100	ARG
25	M	49	PRO
26	o	13	PRO
26	o	18	LEU
26	o	30	PRO
26	o	31	THR
26	o	32	VAL
26	o	55	GLU
26	o	59	GLU
26	o	61	PHE
26	o	88	LYS
26	o	98	ILE
26	o	100	ARG
26	o	108	VAL
26	o	110	ARG
26	o	112	TYR
26	o	114	ARG
26	o	116	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	o	139	ILE
26	o	143	LEU
26	o	145	ASP
26	o	157	ILE
26	o	234	ASN
26	o	245	HIS
26	o	246	LEU
26	o	247	ARG
29	O	63	ALA
29	O	75	ALA
29	O	76	PRO
29	O	79	ILE
30	q	249	PRO
31	P	143	PRO
32	r	131	ILE
32	r	137	MET
32	r	154	PHE
32	r	156	LEU
32	r	243	ILE
32	r	382	VAL
32	r	390	LEU
32	r	400	VAL
32	r	402	ARG
32	r	404	MET
32	r	406	ALA
32	r	410	ALA
32	r	441	ALA
32	r	486	ILE
32	r	490	ARG
32	r	559	ASN
32	r	649	LYS
32	r	654	ARG
32	r	679	THR
34	s	368	ARG
34	s	428	VAL
34	s	442	ILE
34	s	443	TYR
34	s	452	ILE
34	s	474	PHE
34	s	475	PRO
34	s	513	SER
34	s	737	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	s	738	LYS
34	s	754	ILE
34	s	759	ASN
34	s	762	ASN
34	s	773	ARG
34	s	777	HIS
34	s	808	VAL
34	s	809	PHE
34	s	853	SER
34	s	854	ILE
34	s	859	LYS
34	s	866	LYS
34	s	869	PRO
34	s	877	MET
34	s	929	VAL
34	s	1019	VAL
34	s	1076	ARG
34	s	1157	THR
34	s	1285	TYR
34	s	1361	LYS
34	s	1362	GLU
34	s	1409	PRO
34	s	1432	ASN
34	s	1434	GLN
34	s	1467	SER
34	s	1468	LEU
34	s	1500	SER
34	s	1501	VAL
34	s	1517	LEU
34	s	1539	MET
34	s	1613	SER
34	s	1774	SER
34	s	1791	ARG
34	s	1905	PRO
34	s	1933	SER
34	s	2030	LEU
34	s	2047	ASN
34	s	2048	TRP
34	s	2055	PRO
34	s	2060	LYS
34	s	2089	ILE
34	s	2099	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	s	2126	ASN
34	s	2146	THR
34	s	2147	PRO
34	s	2167	HIS
34	s	2184	ILE
34	s	2186	LYS
34	s	2190	VAL
34	s	2192	PHE
34	s	2201	LYS
34	s	2239	GLU
34	s	2244	ASP
34	s	2248	ARG
34	s	2250	LEU
34	s	2303	GLU
34	s	2327	PRO
34	s	2328	LEU
34	s	2356	PRO
34	s	2364	VAL
34	s	2367	ILE
34	s	2375	LYS
34	s	2405	MET
35	R	80	LYS
35	R	144	GLN
38	u	84	VAL
38	u	168	PRO
38	u	235	ASN
38	u	254	GLN
38	u	354	ILE
39	T	17	ARG
39	T	42	ILE
39	T	70	SER
39	T	77	ASN
39	T	87	LYS
39	T	90	ASN
39	T	91	LEU
39	T	92	ARG
39	T	132	PRO
48	a	112	ILE
48	a	119	PRO
1	A	116	VAL
1	A	126	LEU
1	A	185	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	194	ASN
2	c	49	PRO
3	B	4	ARG
3	B	18	PRO
3	B	19	ARG
3	B	20	LYS
3	B	96	PRO
4	d	68	GLU
5	C	76	ARG
5	C	189	ALA
5	C	224	GLY
5	C	270	SER
5	C	282	SER
5	C	338	LYS
7	D	56	THR
7	D	259	LYS
7	D	261	THR
11	F	25	GLN
11	F	109	THR
12	h	112	PRO
13	G	65	LEU
13	G	163	VAL
14	i	22	PRO
14	i	24	PRO
15	H	65	VAL
17	I	98	LYS
19	J	9	MET
19	J	73	GLY
19	J	86	VAL
19	J	115	LYS
19	J	167	TYR
20	l	24	PRO
22	m	30	GLY
22	m	89	PRO
23	L	28	GLN
24	n	27	PHE
25	M	8	LYS
26	o	44	ALA
26	o	57	PHE
26	o	69	PRO
26	o	73	ASP
26	o	89	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	o	94	SER
26	o	118	PHE
26	o	141	LYS
26	o	144	ARG
26	o	152	GLN
26	o	154	ARG
27	N	18	VAL
27	N	76	PRO
29	O	60	LYS
29	O	61	ALA
29	O	64	PHE
29	O	77	SER
29	O	78	ARG
29	O	111	PRO
29	O	148	LYS
30	q	126	VAL
30	q	127	PHE
32	r	85	SER
32	r	93	PHE
32	r	206	ALA
32	r	208	CYS
32	r	210	ASN
32	r	241	VAL
32	r	245	THR
32	r	261	MET
32	r	262	PHE
32	r	282	ASP
32	r	283	GLY
32	r	296	ASN
32	r	297	LYS
32	r	310	ILE
32	r	312	THR
32	r	386	TYR
32	r	388	PHE
32	r	427	ILE
32	r	429	ASP
32	r	431	PHE
32	r	433	SER
32	r	448	ILE
32	r	477	GLY
32	r	488	LEU
32	r	557	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	r	633	PHE
32	r	656	GLU
32	r	658	SER
33	Q	19	PRO
33	Q	97	PRO
33	Q	171	LYS
33	Q	173	GLU
34	s	440	ASN
34	s	482	PRO
34	s	483	LYS
34	s	594	THR
34	s	725	HIS
34	s	763	GLU
34	s	768	LYS
34	s	799	GLN
34	s	942	LYS
34	s	960	SER
34	s	992	PHE
34	s	1057	ILE
34	s	1134	GLU
34	s	1139	GLU
34	s	1417	GLN
34	s	1452	ASN
34	s	1465	ARG
34	s	1579	ARG
34	s	1740	HIS
34	s	1950	ASN
34	s	1951	GLN
34	s	2031	GLU
34	s	2056	SER
34	s	2148	GLU
34	s	2185	THR
34	s	2226	ASN
34	s	2246	GLN
34	s	2249	VAL
34	s	2285	LEU
34	s	2305	ILE
34	s	2333	PRO
34	s	2354	GLU
34	s	2359	GLU
34	s	2376	TRP
35	R	82	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	t	17	HIS
36	t	24	ASN
37	S	22	PRO
37	S	50	LYS
38	u	169	ILE
38	u	390	PHE
39	T	16	GLN
39	T	19	PHE
39	T	21	LYS
39	T	24	ALA
39	T	78	LYS
39	T	124	VAL
41	U	44	GLU
41	U	98	THR
45	X	50	ALA
45	X	87	SER
45	X	102	LEU
46	Y	116	LYS
46	Y	126	LEU
47	Z	17	ARG
48	a	17	ALA
48	a	41	HIS
48	a	104	THR
1	A	120	PRO
1	A	181	LYS
1	A	191	LEU
1	A	193	ARG
1	A	195	SER
3	B	68	HIS
3	B	255	TRP
3	B	257	PRO
3	B	311	PHE
3	B	347	SER
4	d	6	ASP
4	d	61	LYS
5	C	11	LEU
5	C	223	PRO
5	C	268	ALA
5	C	320	ASN
5	C	321	LYS
5	C	339	LEU
6	e	12	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	D	151	GLN
8	f	20	LYS
8	f	91	ALA
9	E	37	GLY
9	E	98	VAL
10	g	48	GLY
10	g	60	ARG
10	g	78	GLY
11	F	98	LYS
11	F	193	PRO
11	F	226	GLY
14	i	16	LYS
15	H	50	ASN
16	j	10	LYS
16	j	39	TYR
16	j	72	ARG
16	j	77	GLY
17	I	18	LYS
17	I	74	VAL
17	I	136	THR
18	k	18	ALA
19	J	140	ARG
19	J	169	ALA
19	J	173	ASP
20	l	36	ARG
21	K	17	ALA
21	K	39	PRO
21	K	40	LYS
21	K	76	SER
21	K	89	PRO
21	K	98	VAL
21	K	102	GLY
23	L	61	PRO
23	L	62	THR
23	L	165	SER
23	L	166	ALA
24	n	50	THR
26	o	34	ARG
26	o	53	THR
26	o	91	TYR
26	o	96	ALA
26	o	150	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	o	199	PHE
26	o	244	ALA
27	N	80	THR
27	N	158	HIS
27	N	175	ASN
28	p	23	ARG
28	p	24	ARG
29	O	89	SER
30	q	89	SER
30	q	93	LYS
30	q	129	VAL
31	P	41	LEU
31	P	96	GLN
31	P	133	HIS
32	r	133	SER
32	r	204	THR
32	r	247	ALA
32	r	314	LYS
32	r	316	LYS
32	r	637	ALA
32	r	652	GLU
32	r	698	LEU
33	Q	73	GLN
34	s	308	SER
34	s	362	PRO
34	s	459	GLU
34	s	765	GLU
34	s	787	ALA
34	s	851	SER
34	s	905	GLU
34	s	1063	LYS
34	s	1194	GLN
34	s	1233	GLU
34	s	1469	ASN
34	s	1512	GLU
34	s	1515	LEU
34	s	1523	SER
34	s	1723	ALA
34	s	1752	GLY
34	s	1820	ALA
34	s	1888	THR
34	s	1923	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	s	2029	PRO
34	s	2098	LEU
34	s	2168	PRO
34	s	2188	ALA
35	R	16	GLY
35	R	136	ARG
35	R	139	VAL
37	S	133	ALA
37	S	154	HIS
38	u	85	ASN
39	T	22	HIS
45	X	41	ALA
46	Y	5	SER
46	Y	89	LYS
47	Z	59	ALA
48	a	32	ARG
48	a	46	ASP
48	a	47	LYS
48	a	52	TYR
48	a	58	MET
48	a	97	GLU
48	a	132	LYS
1	A	69	TYR
1	A	180	LEU
3	B	9	PRO
3	B	15	GLY
3	B	234	GLY
3	B	314	TYR
3	B	353	GLU
3	B	362	ALA
5	C	89	ALA
5	C	288	ARG
5	C	291	ASN
7	D	87	GLY
7	D	256	THR
7	D	258	LYS
8	f	105	SER
9	E	75	PRO
10	g	73	SER
11	F	76	TYR
11	F	172	ASN
12	h	81	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	G	36	ILE
13	G	196	ALA
15	H	62	ARG
15	H	64	HIS
16	j	15	SER
19	J	95	ASN
19	J	108	GLU
19	J	114	ILE
19	J	117	ASP
21	K	19	GLY
21	K	51	LYS
21	K	52	GLU
21	K	55	GLY
22	m	31	SER
22	m	111	ASN
23	L	152	THR
24	n	133	LEU
24	n	162	GLU
25	M	9	ALA
26	o	87	GLU
26	o	179	GLY
26	o	198	ALA
26	o	212	LYS
26	o	235	ILE
27	N	95	GLN
32	r	92	GLY
32	r	146	ALA
32	r	544	LYS
32	r	677	ALA
33	Q	154	GLY
33	Q	166	LEU
34	s	797	GLU
34	s	1180	GLU
34	s	1389	LEU
34	s	1413	ARG
34	s	1484	ARG
34	s	1564	PRO
34	s	1783	PHE
34	s	1816	GLU
34	s	1949	LEU
34	s	1956	GLU
34	s	2057	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	s	2097	ASP
37	S	32	SER
38	u	357	PRO
39	T	82	ASN
48	a	78	LEU
1	A	26	ALA
1	A	129	ALA
1	A	209	HIS
1	A	213	GLY
3	B	317	ILE
3	B	349	LYS
5	C	75	PRO
5	C	131	VAL
5	C	221	ASN
6	e	48	GLY
7	D	125	VAL
7	D	260	PHE
8	f	62	SER
11	F	191	VAL
12	h	79	ASP
13	G	50	VAL
13	G	68	ARG
14	i	3	VAL
15	H	59	ASN
17	I	151	VAL
17	I	168	ALA
19	J	24	GLY
19	J	111	ASP
19	J	172	LEU
20	l	5	LYS
21	K	32	ILE
21	K	100	HIS
21	K	109	ILE
22	m	112	ASP
23	L	84	GLY
23	L	94	GLY
23	L	136	GLU
24	n	130	LYS
25	M	6	ILE
25	M	82	SER
25	M	90	VAL
27	N	49	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	N	55	ALA
27	N	58	GLY
28	p	7	LYS
29	O	131	PRO
32	r	308	ASN
32	r	680	LEU
33	Q	9	GLN
33	Q	38	ARG
34	s	530	ASN
34	s	803	ILE
34	s	1176	PRO
34	s	1238	ALA
34	s	1302	THR
34	s	1447	LYS
34	s	1449	ASP
34	s	1799	ASP
34	s	2080	MET
34	s	2199	LEU
34	s	2213	ASN
34	s	2219	PRO
34	s	2331	TYR
34	s	2347	ASP
34	s	2411	ILE
39	T	28	SER
39	T	127	GLN
41	U	11	ILE
41	U	38	ILE
45	X	23	ALA
46	Y	34	PRO
47	Z	32	GLY
47	Z	38	PHE
47	Z	97	SER
3	B	83	PRO
4	d	7	VAL
7	D	19	PRO
8	f	90	PRO
9	E	36	PRO
13	G	157	VAL
14	i	33	ALA
17	I	104	SER
22	m	44	ASP
23	L	32	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	n	70	ARG
26	o	121	SER
26	o	140	VAL
32	r	384	GLY
32	r	411	CYS
33	Q	175	ALA
34	s	593	PRO
34	s	602	ILE
34	s	646	THR
34	s	764	ASN
34	s	953	SER
34	s	1170	ASN
34	s	2150	PHE
34	s	2217	CYS
34	s	2330	HIS
37	S	132	THR
43	V	3	GLY
5	C	173	GLY
10	g	104	VAL
12	h	47	VAL
13	G	30	THR
34	s	289	VAL
34	s	604	ILE
34	s	956	LYS
47	Z	103	GLN
21	K	22	VAL
26	o	29	THR
31	P	77	GLY
32	r	462	ILE
34	s	2096	VAL
39	T	23	GLY
39	T	123	GLY
1	A	178	PRO
5	C	204	GLY
5	C	245	GLY
5	C	348	GLY
7	D	181	PRO
34	s	1186	PRO
34	s	1627	VAL
34	s	2338	ARG
46	Y	96	PRO
48	a	57	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	G	75	ILE
14	i	7	ILE
22	m	105	GLY
22	m	148	VAL
34	s	2365	ILE
46	Y	123	GLY
48	a	72	VAL
3	B	268	GLY
7	D	139	PRO
17	I	125	GLY
27	N	154	PRO
32	r	435	GLY
34	s	693	LYS
34	s	1005	LYS
34	s	2254	PRO
34	s	2355	GLU
43	V	107	GLY
48	a	36	GLY
48	a	110	GLY

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
40	x	3393/3396 (99%)	376 (11%)	0
42	y	157/158 (99%)	20 (12%)	0
44	z	120/121 (99%)	7 (5%)	0
All	All	3670/3675 (99%)	403 (10%)	0

All (403) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
40	x	22	G
40	x	40	A
40	x	41	G
40	x	49	A
40	x	60	A
40	x	66	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	x	92	G
40	x	110	G
40	x	113	C
40	x	121	A
40	x	122	A
40	x	123	A
40	x	135	C
40	x	136	G
40	x	156	G
40	x	191	U
40	x	200	C
40	x	210	U
40	x	218	G
40	x	219	A
40	x	240	U
40	x	252	U
40	x	269	G
40	x	295	A
40	x	298	U
40	x	316	U
40	x	323	A
40	x	329	U
40	x	336	A
40	x	337	G
40	x	339	C
40	x	346	C
40	x	376	G
40	x	398	A
40	x	401	U
40	x	402	A
40	x	403	C
40	x	421	G
40	x	422	A
40	x	486	U
40	x	492	U
40	x	521	A
40	x	534	U
40	x	535	G
40	x	546	C
40	x	547	G
40	x	548	G
40	x	552	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	x	557	A
40	x	559	A
40	x	579	G
40	x	604	G
40	x	609	G
40	x	611	A
40	x	612	U
40	x	621	A
40	x	638	C
40	x	646	A
40	x	647	A
40	x	649	A
40	x	677	A
40	x	681	U
40	x	705	A
40	x	764	U
40	x	765	C
40	x	767	U
40	x	776	U
40	x	777	U
40	x	780	A
40	x	781	G
40	x	806	A
40	x	817	A
40	x	830	A
40	x	849	C
40	x	874	U
40	x	880	G
40	x	881	C
40	x	907	G
40	x	914	A
40	x	916	G
40	x	917	A
40	x	924	G
40	x	937	G
40	x	944	C
40	x	959	C
40	x	979	U
40	x	980	A
40	x	982	C
40	x	989	A
40	x	995	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	x	1001	G
40	x	1006	A
40	x	1007	U
40	x	1028	U
40	x	1045	C
40	x	1046	A
40	x	1049	C
40	x	1063	G
40	x	1065	A
40	x	1072	G
40	x	1081	U
40	x	1095	U
40	x	1098	A
40	x	1103	A
40	x	1104	G
40	x	1116	G
40	x	1117	G
40	x	1139	G
40	x	1159	A
40	x	1160	C
40	x	1180	A
40	x	1181	U
40	x	1192	C
40	x	1200	A
40	x	1201	C
40	x	1202	A
40	x	1222	G
40	x	1236	G
40	x	1240	A
40	x	1241	U
40	x	1242	G
40	x	1243	G
40	x	1244	A
40	x	1245	A
40	x	1246	G
40	x	1254	C
40	x	1263	A
40	x	1264	G
40	x	1274	A
40	x	1278	A
40	x	1279	C
40	x	1287	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	x	1289	G
40	x	1295	G
40	x	1302	A
40	x	1305	U
40	x	1308	A
40	x	1309	U
40	x	1330	A
40	x	1351	U
40	x	1352	A
40	x	1354	G
40	x	1355	A
40	x	1357	G
40	x	1367	G
40	x	1386	A
40	x	1390	A
40	x	1399	A
40	x	1400	G
40	x	1419	A
40	x	1437	C
40	x	1446	A
40	x	1481	A
40	x	1508	C
40	x	1511	U
40	x	1563	C
40	x	1568	U
40	x	1570	U
40	x	1571	A
40	x	1572	U
40	x	1583	A
40	x	1589	A
40	x	1607	U
40	x	1629	U
40	x	1643	A
40	x	1645	U
40	x	1657	C
40	x	1717	U
40	x	1728	G
40	x	1750	A
40	x	1751	G
40	x	1760	A
40	x	1765	U
40	x	1780	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	x	1797	A
40	x	1816	A
40	x	1819	U
40	x	1821	U
40	x	1841	A
40	x	1842	A
40	x	1880	U
40	x	1893	A
40	x	1906	G
40	x	1953	G
40	x	1966	U
40	x	1973	G
40	x	2010	U
40	x	2011	U
40	x	2013	C
40	x	2032	U
40	x	2042	G
40	x	2056	U
40	x	2061	G
40	x	2067	U
40	x	2071	A
40	x	2076	G
40	x	2080	C
40	x	2087	C
40	x	2089	A
40	x	2094	C
40	x	2102	U
40	x	2113	A
40	x	2121	G
40	x	2122	G
40	x	2131	A
40	x	2158	A
40	x	2170	U
40	x	2179	C
40	x	2188	A
40	x	2205	U
40	x	2228	A
40	x	2244	A
40	x	2249	G
40	x	2255	A
40	x	2260	U
40	x	2273	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	x	2275	A
40	x	2279	A
40	x	2281	A
40	x	2298	U
40	x	2307	G
40	x	2363	A
40	x	2374	C
40	x	2388	U
40	x	2397	A
40	x	2411	U
40	x	2418	G
40	x	2440	G
40	x	2446	U
40	x	2451	G
40	x	2453	U
40	x	2463	G
40	x	2469	G
40	x	2472	U
40	x	2477	G
40	x	2478	C
40	x	2479	C
40	x	2484	A
40	x	2490	C
40	x	2493	U
40	x	2494	A
40	x	2495	C
40	x	2496	C
40	x	2501	U
40	x	2502	A
40	x	2505	U
40	x	2508	U
40	x	2510	U
40	x	2514	U
40	x	2519	A
40	x	2523	A
40	x	2524	A
40	x	2526	C
40	x	2531	C
40	x	2538	U
40	x	2540	A
40	x	2541	U
40	x	2542	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	x	2547	A
40	x	2548	C
40	x	2549	G
40	x	2552	C
40	x	2569	A
40	x	2570	U
40	x	2571	U
40	x	2572	C
40	x	2573	G
40	x	2590	A
40	x	2593	A
40	x	2601	A
40	x	2606	G
40	x	2614	G
40	x	2619	G
40	x	2621	G
40	x	2622	C
40	x	2627	C
40	x	2630	C
40	x	2636	A
40	x	2652	U
40	x	2656	A
40	x	2674	A
40	x	2677	G
40	x	2689	A
40	x	2691	A
40	x	2694	A
40	x	2696	A
40	x	2700	G
40	x	2701	U
40	x	2714	G
40	x	2726	C
40	x	2728	G
40	x	2729	U
40	x	2730	G
40	x	2753	G
40	x	2760	C
40	x	2762	A
40	x	2772	C
40	x	2777	G
40	x	2778	G
40	x	2785	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	x	2797	C
40	x	2798	C
40	x	2800	G
40	x	2801	A
40	x	2802	A
40	x	2803	A
40	x	2805	G
40	x	2806	U
40	x	2828	G
40	x	2830	G
40	x	2831	G
40	x	2845	A
40	x	2873	U
40	x	2887	A
40	x	2896	A
40	x	2899	C
40	x	2935	U
40	x	2936	A
40	x	2957	G
40	x	2983	C
40	x	2996	U
40	x	2997	G
40	x	3012	A
40	x	3056	U
40	x	3078	U
40	x	3086	A
40	x	3092	C
40	x	3093	C
40	x	3101	G
40	x	3122	A
40	x	3130	A
40	x	3131	U
40	x	3142	A
40	x	3143	C
40	x	3144	G
40	x	3155	U
40	x	3165	A
40	x	3173	G
40	x	3174	A
40	x	3176	G
40	x	3179	U
40	x	3181	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	x	3187	A
40	x	3198	U
40	x	3207	U
40	x	3217	C
40	x	3219	G
40	x	3229	G
40	x	3243	A
40	x	3245	A
40	x	3247	G
40	x	3259	U
40	x	3260	G
40	x	3270	U
40	x	3272	C
40	x	3273	A
40	x	3276	G
40	x	3279	A
40	x	3281	U
40	x	3294	A
40	x	3304	U
40	x	3313	U
40	x	3316	A
40	x	3318	G
40	x	3319	U
40	x	3320	A
40	x	3351	U
40	x	3352	U
40	x	3353	G
40	x	3355	U
40	x	3369	G
40	x	3370	A
40	x	3375	A
40	x	3376	A
40	x	3378	C
40	x	3390	G
42	y	17	A
42	y	34	U
42	y	35	C
42	y	37	A
42	y	39	G
42	y	52	A
42	y	59	A
42	y	62	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	y	63	G
42	y	72	A
42	y	80	A
42	y	86	U
42	y	90	U
42	y	95	G
42	y	104	A
42	y	106	C
42	y	111	A
42	y	113	U
42	y	125	U
42	y	126	A
44	z	13	A
44	z	53	U
44	z	54	U
44	z	65	G
44	z	87	G
44	z	102	A
44	z	112	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

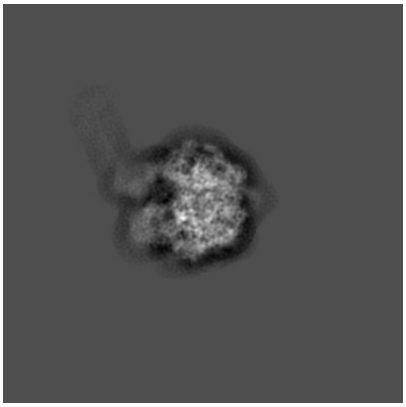
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3199. These allow visual inspection of the internal detail of the map and identification of artifacts.

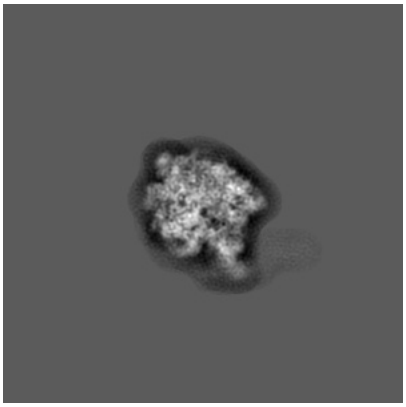
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

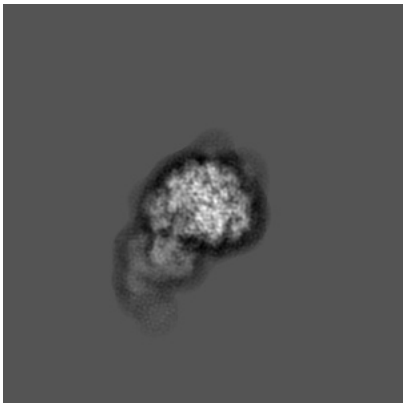
6.1.1 Primary map



X



Y

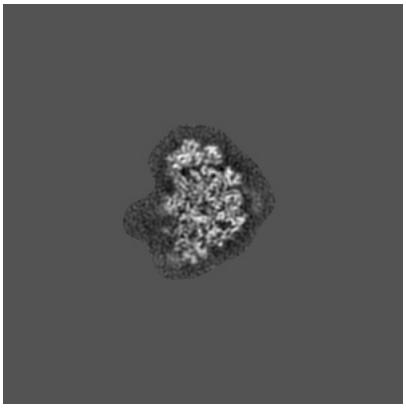


Z

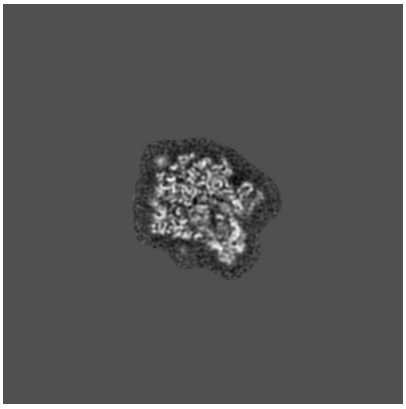
The images above show the map projected in three orthogonal directions.

6.2 Central slices

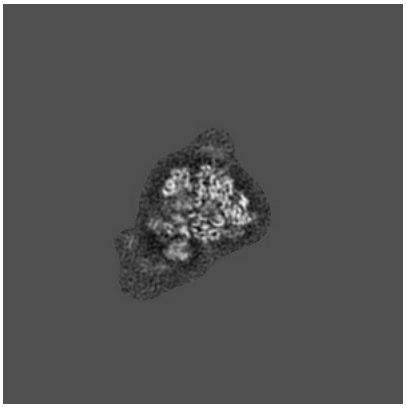
6.2.1 Primary map



X Index: 200



Y Index: 200

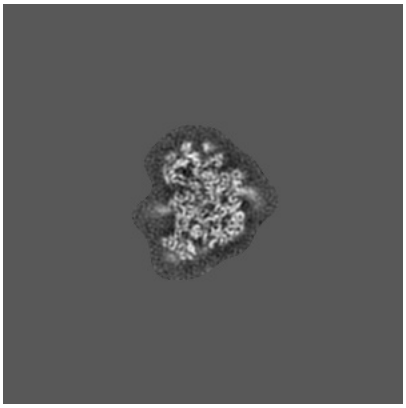


Z Index: 200

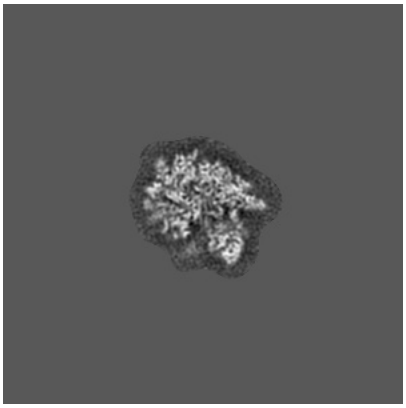
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

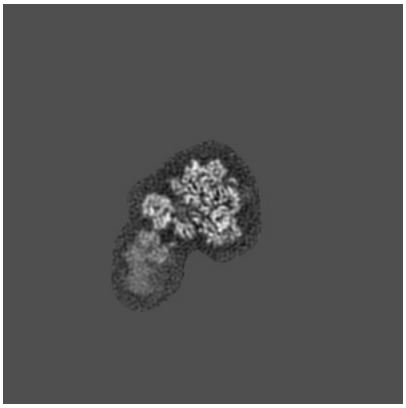
6.3.1 Primary map



X Index: 206



Y Index: 192

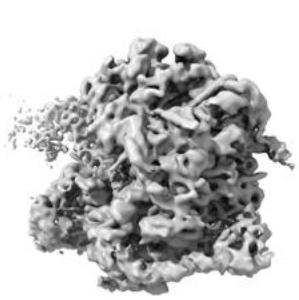


Z Index: 226

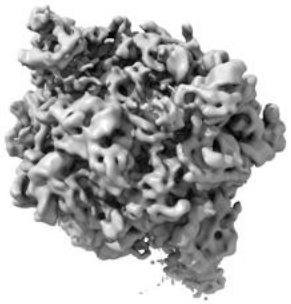
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

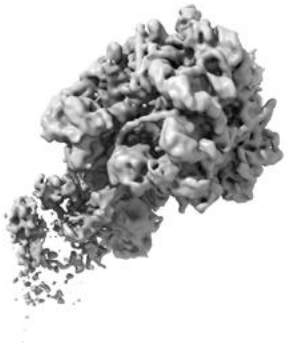
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

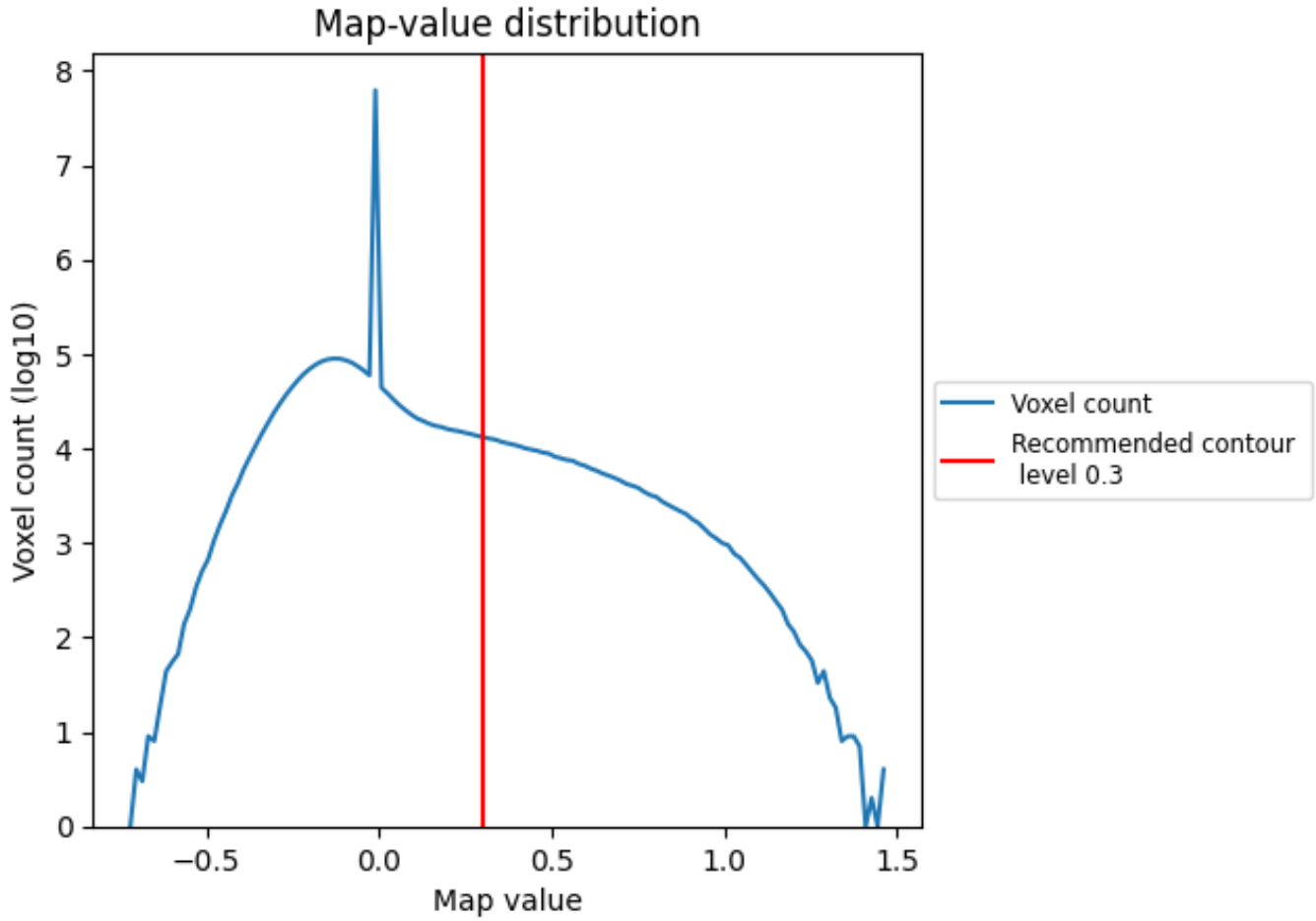
6.5 Mask visualisation (i)

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

7 Map analysis

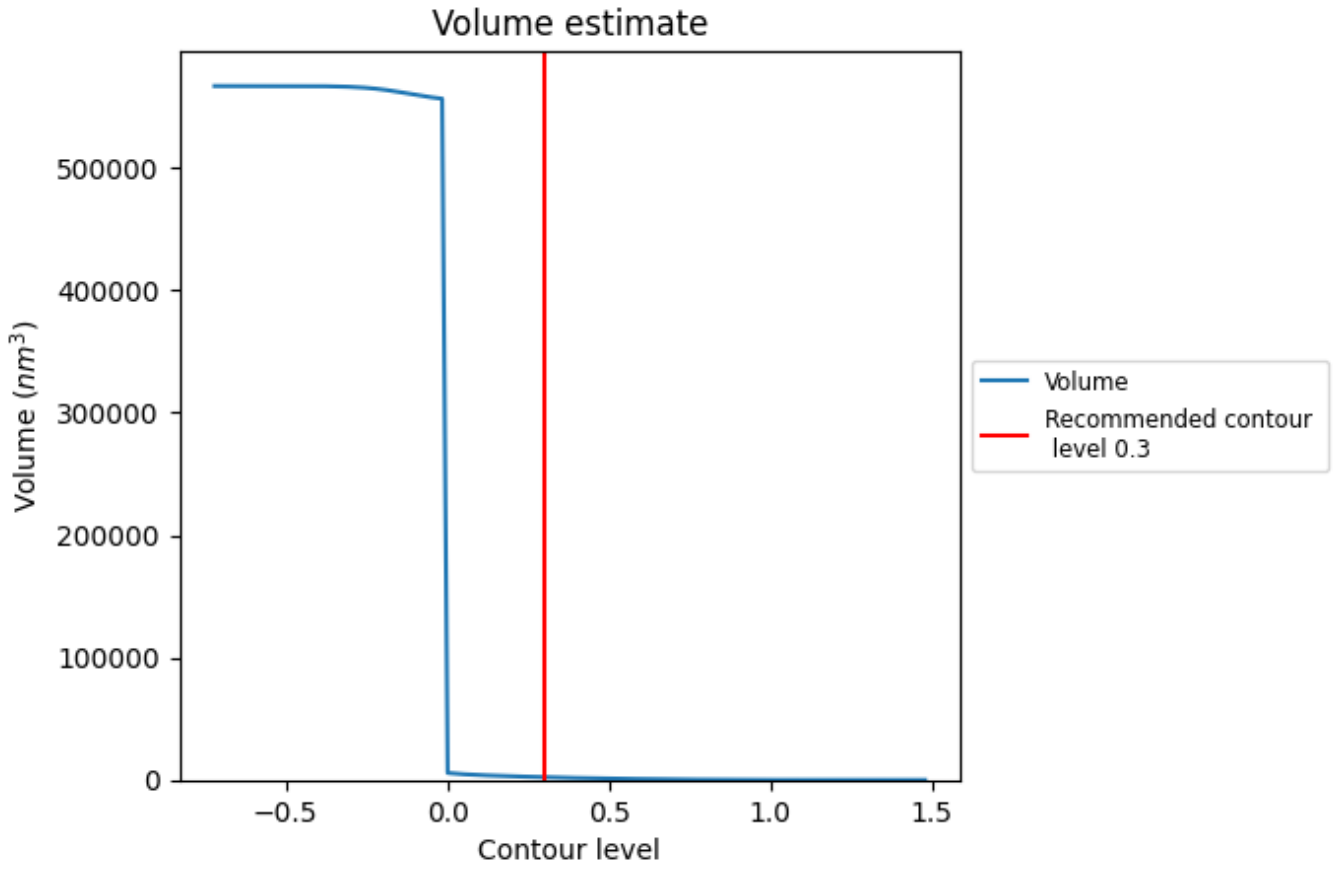
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

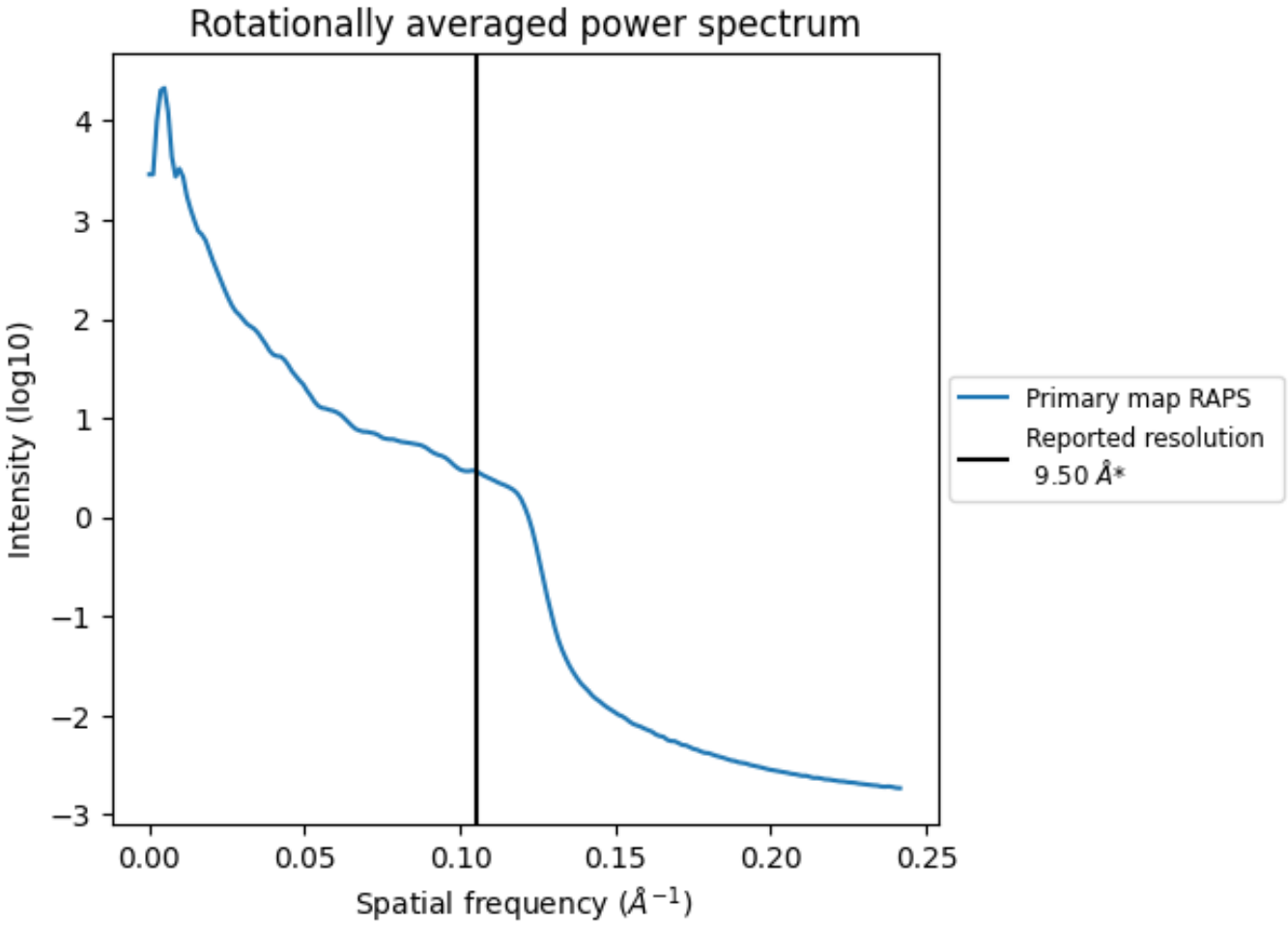
7.2 Volume estimate



The volume at the recommended contour level is 2263 nm^3; this corresponds to an approximate mass of 2044 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 0.105 Å^{-1}

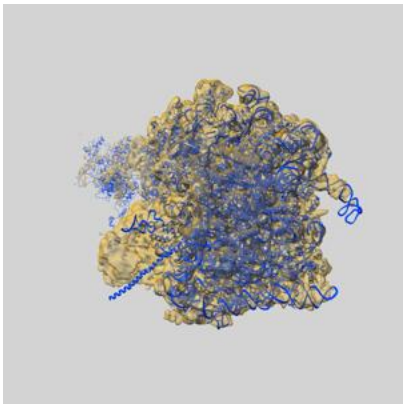
8 Fourier-Shell correlation

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

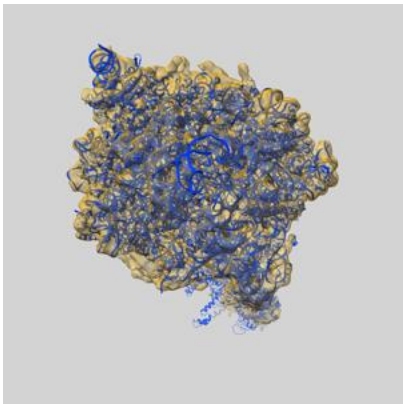
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3199 and PDB model 5JCS. Per-residue inclusion information can be found in section 3 on page 12.

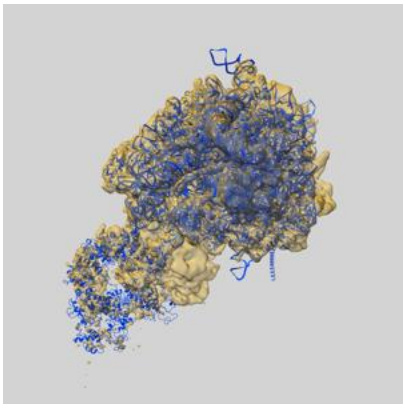
9.1 Map-model overlay



X



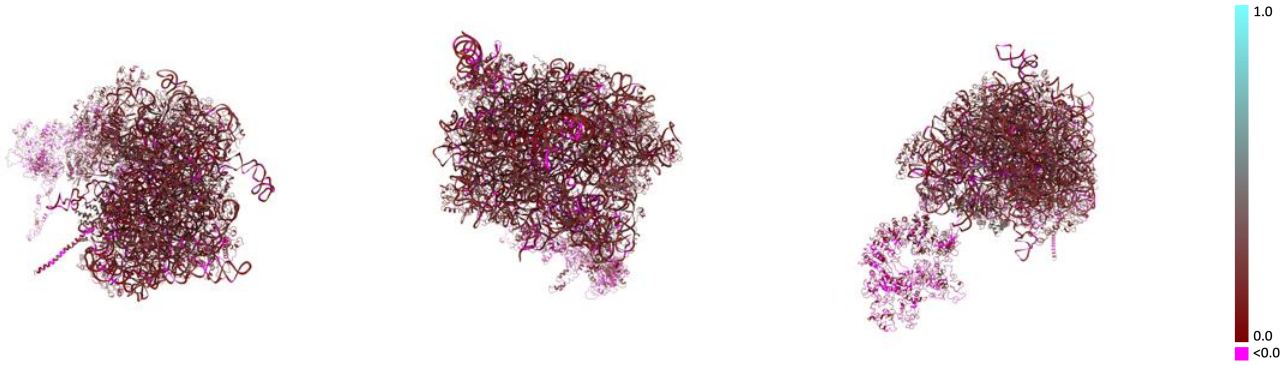
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

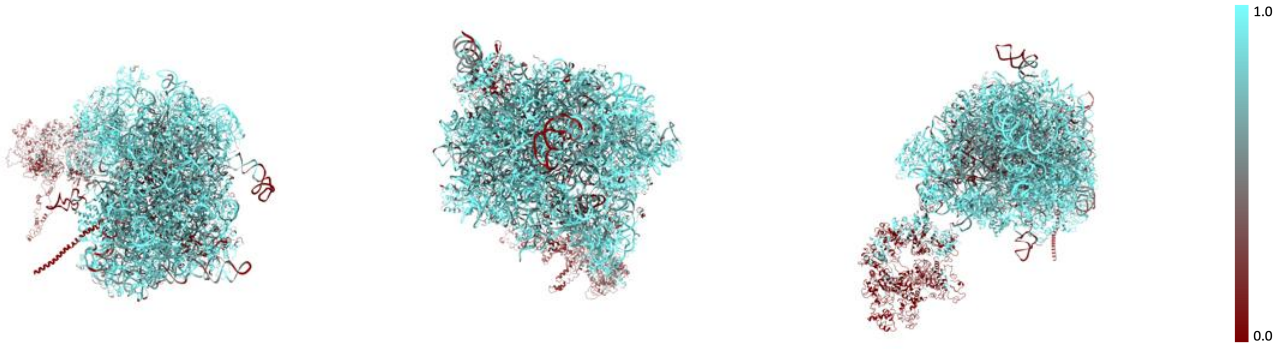
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

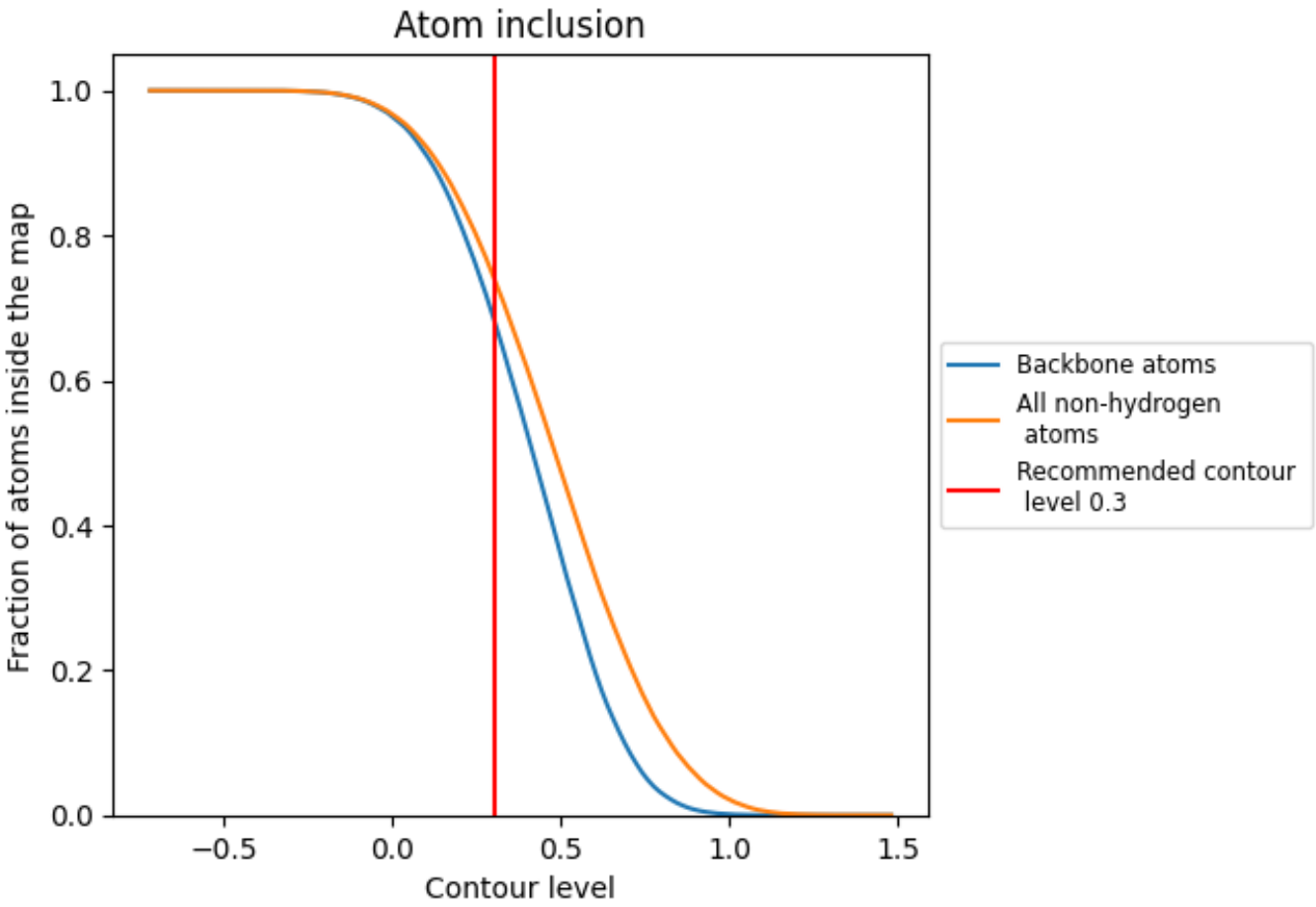
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 74% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7414	0.1460
A	0.5511	0.1300
B	0.7680	0.1560
C	0.6972	0.1620
D	0.8292	0.1880
E	0.8119	0.1930
F	0.8749	0.2170
G	0.7938	0.1700
H	0.8716	0.2110
I	0.1442	0.0270
J	0.9733	0.2200
K	0.7732	0.1550
L	0.8145	0.2240
M	0.8545	0.2100
N	0.7164	0.1600
O	0.7522	0.1850
P	0.7004	0.1780
Q	0.6292	0.1620
R	0.4967	0.1260
S	0.8603	0.2170
T	0.3449	0.0350
U	0.9223	0.2360
V	0.7274	0.1850
X	0.6832	0.1650
Y	0.8091	0.1760
Z	0.8534	0.1750
a	0.5787	0.1180
c	0.8346	0.2030
d	0.7770	0.1850
e	0.7101	0.1950
f	0.7707	0.1620
g	0.5347	0.1170
h	0.8695	0.2310
i	0.7519	0.1900
j	0.5591	0.1000

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	0.8827	0.2150
l	0.6432	0.1760
m	0.9352	0.1940
n	0.9516	0.2070
o	0.8745	0.2300
p	0.6419	0.1540
q	0.8606	0.1840
r	0.9716	0.3470
s	0.2121	0.0620
t	0.8127	0.1450
u	0.5513	0.1670
x	0.7877	0.1400
y	0.8107	0.1410
z	0.8855	0.1520