Full wwPDB EM Validation Report (i)

Dec 11, 2022 – 09:08 am GMT

PDB ID	:	6RXZ
EMDB ID	:	EMD-10056
Title	:	Cryo-EM structure of the 90S pre-ribosome (Kre33-Noc4) from Chaetomium thermophilum, state b
Authors	:	Cheng, J.; Kellner, N.; Griesel, S.; Berninghausen, O.; Beckmann, R.; Hurt, E.
Deposited on	:	2019-06-10
Resolution	:	4.40 Å(reported)

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

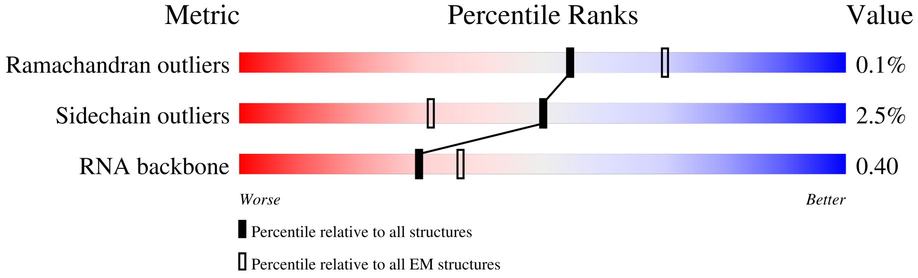
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

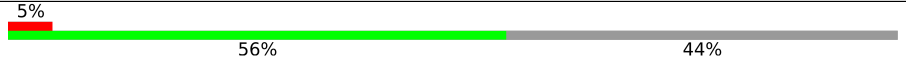
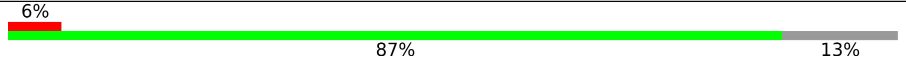
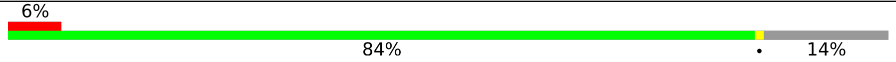
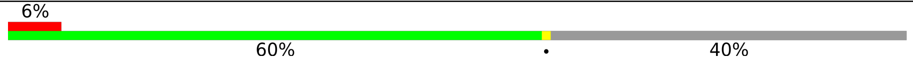
The reported resolution of this entry is 4.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	UA	904	
2	UB	907	
3	UC	648	
4	UD	884	
5	UF	414	
6	UG	558	
7	UJ	1802	
8	UK	270	

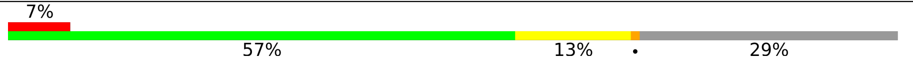
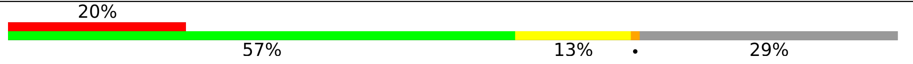
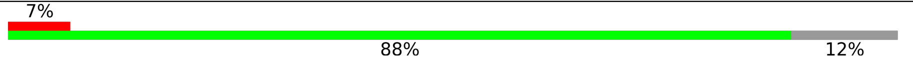
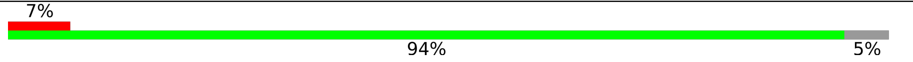
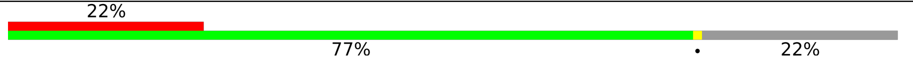
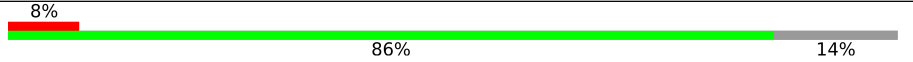
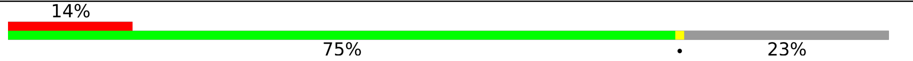
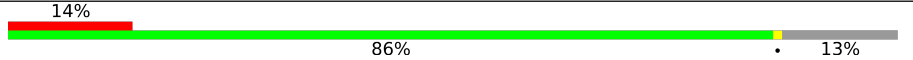
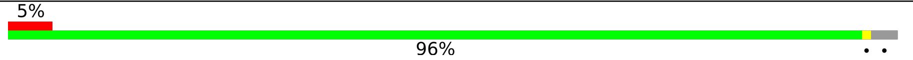
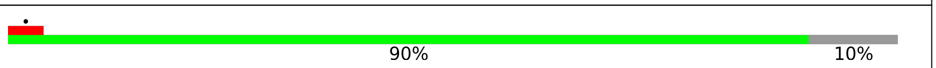
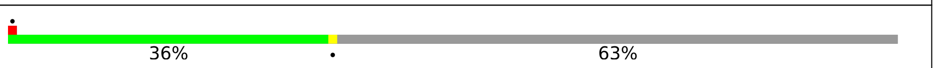
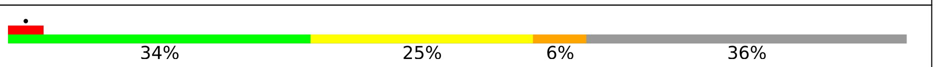
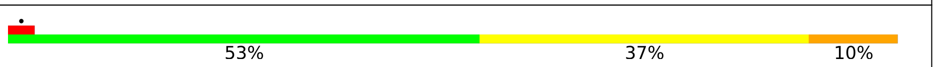
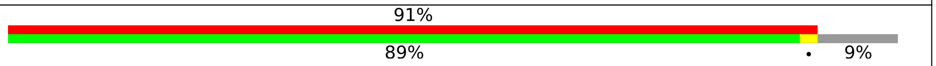
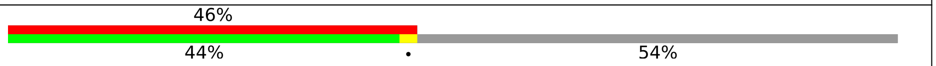
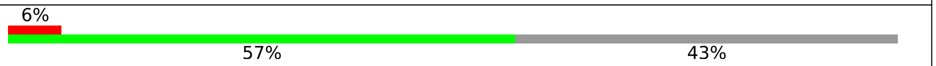
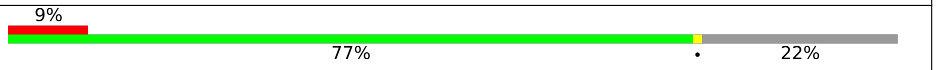
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	UL	962	7% 81% • 18%
10	UM	912	19% 73% • 26%
11	UN	938	• 19% 81%
12	UO	557	• 90% • 10%
13	UQ	960	5% 82% • 18%
14	UR	618	• 72% 28%
15	UU	1049	• 85% • 14%
16	UX	193	• 95% • •
17	UZ	391	• 59% • 40%
18	CA	313	76% • 23%
18	CB	313	5% 75% 24%
19	CC	523	• 74% 26%
20	CD	582	• 72% 28%
21	CE	127	• 94% • 5%
21	CF	127	• 93% • 6%
22	CG	630	• 66% 34%
23	CH	411	• 93% • 5%
24	CI	1163	• 69% • 29%
25	CJ	183	• 96% • •
26	CK	297	97% •
27	CL	785	• 29% 71%
28	CM	446	• 98% •
29	CN	252	6% 90% 10%
29	CO	252	16% 82% • 15%
30	CP	322	19% 57% • 42%

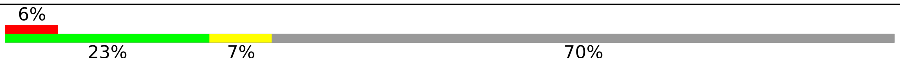
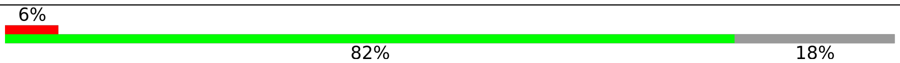
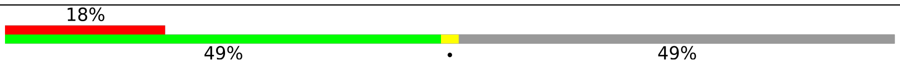
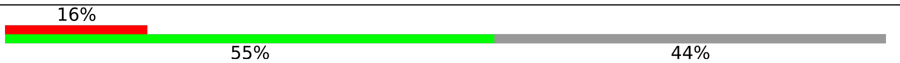
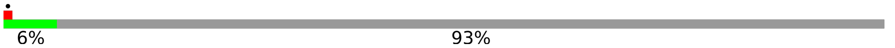
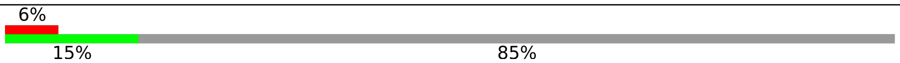
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	CQ	259	
32	CR	1073	
32	CS	1073	
33	CT	203	
34	Cb	264	
35	Cc	212	
36	Cd	239	
37	Ce	203	
38	Cf	202	
39	Cg	190	
40	Ch	151	
41	Ci	150	
42	Cj	143	
43	Ck	161	
44	Cm	130	
45	Cn	145	
46	Co	136	
47	Cp	68	
48	CU	311	
49	C1	2323	
50	C2	230	
51	UV	1171	
52	CV	322	
53	CW	668	
54	UT	2612	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	UH	930	
56	UE	410	
56	UI	410	
57	US	549	
58	Cl	156	
59	CX	480	
60	CY	381	
61	CZ	609	
62	UP	364	
63	Cz	1796	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 218474 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 Periodic tryptophan protein 2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	UA	839	6366	4101	1136	1105	24	0	0

- Molecule 2 is a protein called Utp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	UB	512	4079	2576	781	711	11	0	0

- Molecule 3 is a protein called Utp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	UC	74	588	371	120	97	0	0

- Molecule 4 is a protein called Utp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	UD	772	6071	3851	1093	1103	24	0	0

- Molecule 5 is a protein called Utp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	UF	331	2591	1674	504	399	14	0	0

- Molecule 6 is a protein called Utp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	UG	479	3717	2369	700	636	12	0	0

- Molecule 7 is a protein called UTP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UJ	1090	Total	C	N	O	S	0	0
			8416	5408	1452	1525	31		

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	UK	217	Total	C	N	O	S	0	0
			1687	1062	351	269	5		

- Molecule 9 is a protein called Utp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	UL	785	Total	C	N	O	S	0	0
			6175	3940	1088	1130	17		

- Molecule 10 is a protein called Utp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	UM	679	Total	C	N	O	S	0	0
			5273	3351	924	986	12		

- Molecule 11 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UN	177	Total	C	N	O	S	0	0
			1401	892	263	239	7		

- Molecule 12 is a protein called Utp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	UO	504	Total	C	N	O	S	0	0
			3819	2422	699	684	14		

- Molecule 13 is a protein called Utp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	UQ	789	Total	C	N	O	S	0	0
			6008	3831	1037	1119	21		

- Molecule 14 is a protein called Utp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	UR	447	3491	2209	656	616	10	0	0

- Molecule 15 is a protein called Putative U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	UU	902	6734	4336	1236	1136	26	0	0

- Molecule 16 is a protein called Utp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	UX	190	1470	932	282	246	10	0	0

- Molecule 17 is a protein called Utp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	UZ	235	1815	1184	330	298	3	0	0

- Molecule 18 is a protein called Nop1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	CA	242	1778	1149	327	293	9	0	0
			Total	C	N	O	S		
18	CB	237	1816	1154	318	335	9	0	0

- Molecule 19 is a protein called Putative nucleolar protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	CC	387	2866	1836	527	492	11	0	0

- Molecule 20 is a protein called Nop58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	CD	420	3150	2023	560	557	10	0	0

- Molecule 21 is a protein called Snu13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CE	121	Total 879	C 557	N 165	O 154	S 3	0	0
21	CF	120	Total 864	C 550	N 161	O 150	S 3	0	0

- Molecule 22 is a protein called Rrp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CG	416	Total 3245	C 2065	N 587	O 580	S 13	0	0

- Molecule 23 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CH	389	Total 2888	C 1827	N 526	O 525	S 10	0	0

- Molecule 24 is a protein called Bms1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CI	822	Total 6486	C 4169	N 1213	O 1077	S 27	0	0

- Molecule 25 is a protein called Imp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CJ	179	Total 1434	C 918	N 283	O 226	S 7	0	0

- Molecule 26 is a protein called Putative U3 small nucleolar ribonucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CK	297	Total 2329	C 1476	N 445	O 400	S 8	0	0

- Molecule 27 is a protein called Putative U3 small nucleolar ribonucleoprotein protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CL	231	Total 1786	C 1114	N 339	O 327	S 6	0	0

- Molecule 28 is a protein called Sof1.

Mol	Chain	Residues	Atoms	AltConf	Trace
28	CM	445	Total C N O S 3501 2195 672 619 15	0	0

- Molecule 29 is a protein called Emg1.

Mol	Chain	Residues	Atoms	AltConf	Trace
29	CN	226	Total C N O S 1762 1119 306 327 10	0	0
29	CO	215	Total C N O S 1683 1067 293 313 10	0	0

- Molecule 30 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms	AltConf	Trace
30	CP	187	Total C N O S 1504 961 269 265 9	0	0

- Molecule 31 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms	AltConf	Trace
31	CQ	175	Total C N O S 1361 862 250 242 7	0	0

- Molecule 32 is a protein called Kre33.

Mol	Chain	Residues	Atoms	AltConf	Trace
32	CR	760	Total C N O S 5989 3851 1024 1087 27	0	0
32	CS	760	Total C N O S 5989 3851 1024 1087 27	0	0

- Molecule 33 is a protein called Fcf2.

Mol	Chain	Residues	Atoms	AltConf	Trace
33	CT	131	Total C N O S 1035 656 197 178 4	0	0

- Molecule 34 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms	AltConf	Trace
34	Cb	232	Total C N O S 1851 1179 340 325 7	0	0

- Molecule 35 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Cc	192	Total 1464	C 926	N 278	O 253	S 7	0	0

- Molecule 36 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Cd	226	Total 1819	C 1138	N 363	O 313	S 5	0	0

- Molecule 37 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	Ce	159	Total 1279	C 810	N 237	O 232	0	0

- Molecule 38 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Cf	174	Total 1398	C 872	N 283	O 242	S 1	0	0

- Molecule 39 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Cg	159	Total 1242	C 801	N 255	O 184	S 2	0	0

- Molecule 40 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	Ch	49	Total 406	C 265	N 79	O 62	0	0

- Molecule 41 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ci	115	Total 791	C 492	N 154	O 141	S 4	0	0

- Molecule 42 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Cj	126	Total 943	C 613	N 177	O 151	S 2	0	0

- Molecule 43 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ck	140	Total 1163	C 750	N 224	O 184	S 5	0	0

- Molecule 44 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Cm	126	Total 985	C 632	N 184	O 164	S 5	0	0

- Molecule 45 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Cn	96	Total 702	C 456	N 134	O 110	S 2	0	0

- Molecule 46 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Co	92	Total 741	C 474	N 139	O 126	S 2	0	0

- Molecule 47 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	Cp	61	Total 455	C 284	N 97	O 74	0	0

- Molecule 48 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	CU	114	Total 882	C 544	N 178	O 154	S 6	0	0

- Molecule 49 is a RNA chain called 35S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	C1	1487	Total	C	N	O	P	0	0
			31732	14158	5691	10396	1487		

- Molecule 50 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	C2	230	Total	C	N	O	P	0	0
			4891	2182	856	1623	230		

- Molecule 51 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	UV	1061	Total	C	N	O	S	0	0
			8424	5399	1480	1523	22		

- Molecule 52 is a protein called Rrp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	CV	148	Total	C	N	O	S	0	0
			1145	729	198	216	2		

- Molecule 53 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	CW	382	Total	C	N	O	S	0	0
			2924	1857	530	524	13		

- Molecule 54 is a protein called Utp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	UT	2028	Total	C	N	O	S	0	0
			16000	10303	2813	2816	68		

- Molecule 55 is a protein called Utp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	UH	359	Total	C	N	O	S	0	0
			2809	1773	496	527	13		

- Molecule 56 is a protein called Utp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	UE	125	Total 972	C 608	N 183	O 175	S 6	0	0
56	UI	125	Total 972	C 608	N 183	O 175	S 6	0	0

- Molecule 57 is a protein called Noc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	US	451	Total 3672	C 2389	N 608	O 660	S 15	0	0

- Molecule 58 is a protein called Rps18.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Cl	80	Total 633	C 400	N 115	O 117	S 1	0	0

- Molecule 59 is a protein called Enp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CX	267	Total 2122	C 1380	N 374	O 358	S 10	0	0

- Molecule 60 is a protein called U3 small nucleolar ribonucleoprotein protein lcp5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CY	122	Total 975	C 590	N 194	O 188	S 3	0	0

- Molecule 61 is a protein called Bfr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	CZ	42	Total 354	C 223	N 68	O 62	S 1	0	0

- Molecule 62 is a protein called Utp16.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	UP	54	Total 422	C 264	N 88	O 70	0	0

- Molecule 63 is a protein called Rrp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	Cz	275	2259	1435	401	420	3	0	0

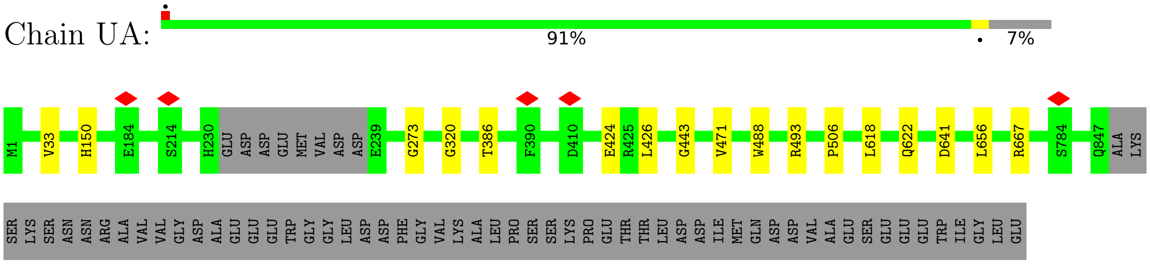
- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
64	UX	1	1	1	0

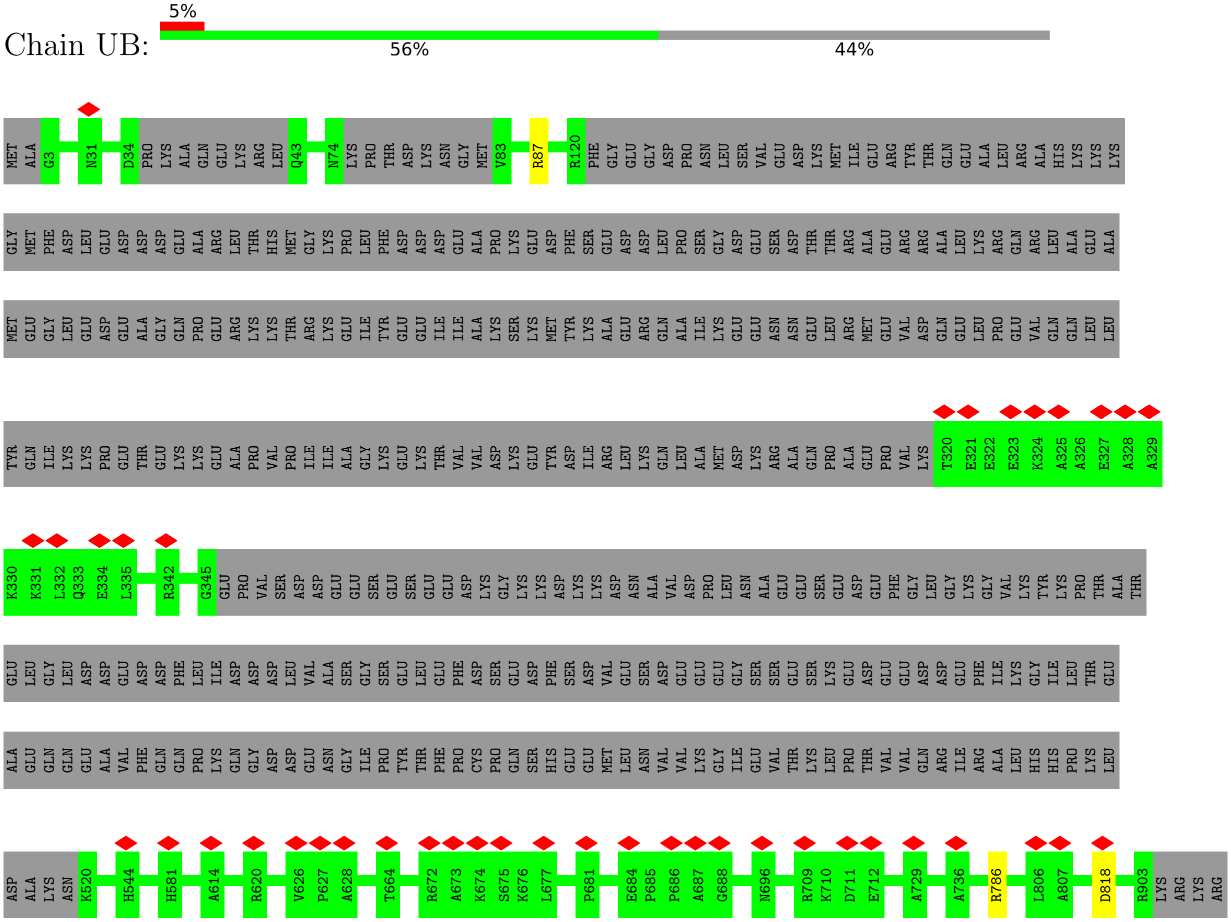
3 Residue-property plots ⓘ

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: Periodic tryptophan protein 2-like protein

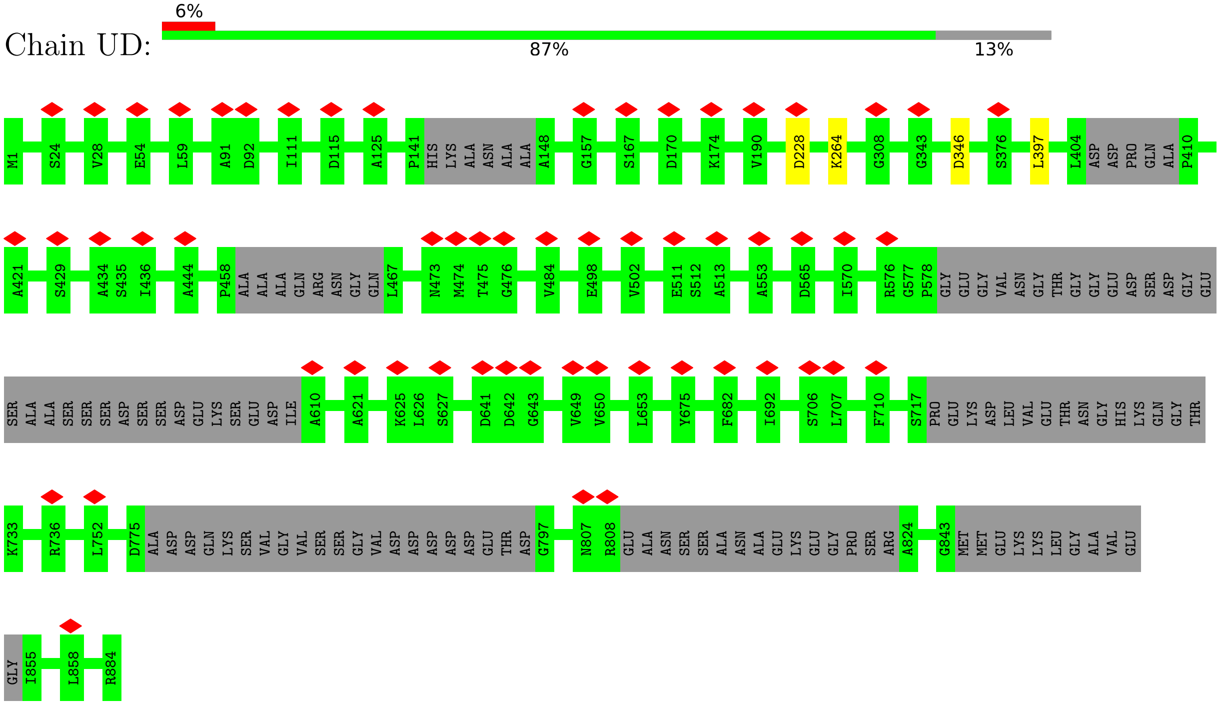


- Molecule 2: Utp2



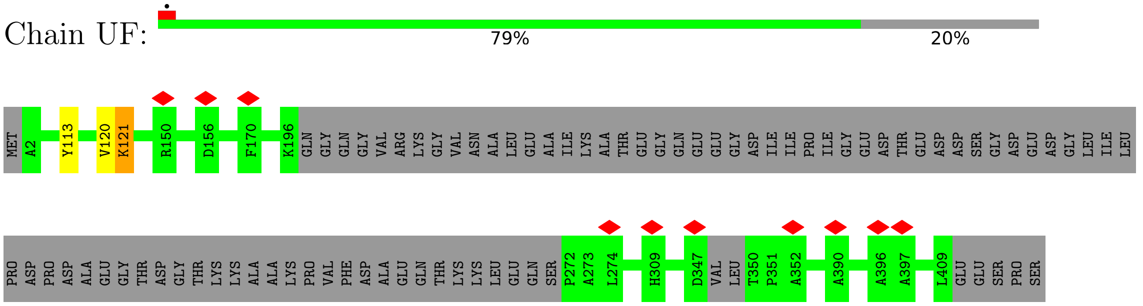
- Molecule 3: Utp3

- Molecule 4: Utp4



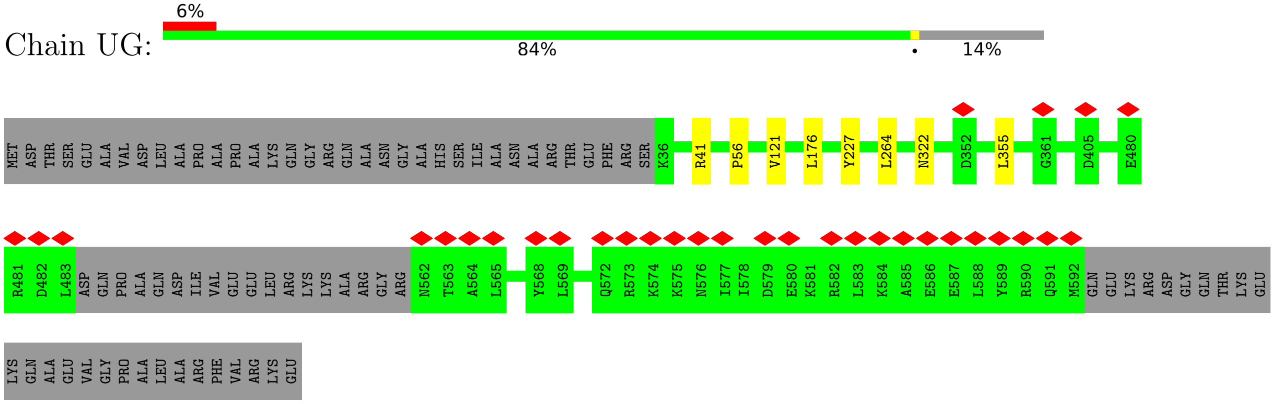
- Molecule 5: Utp6

Chain UF:



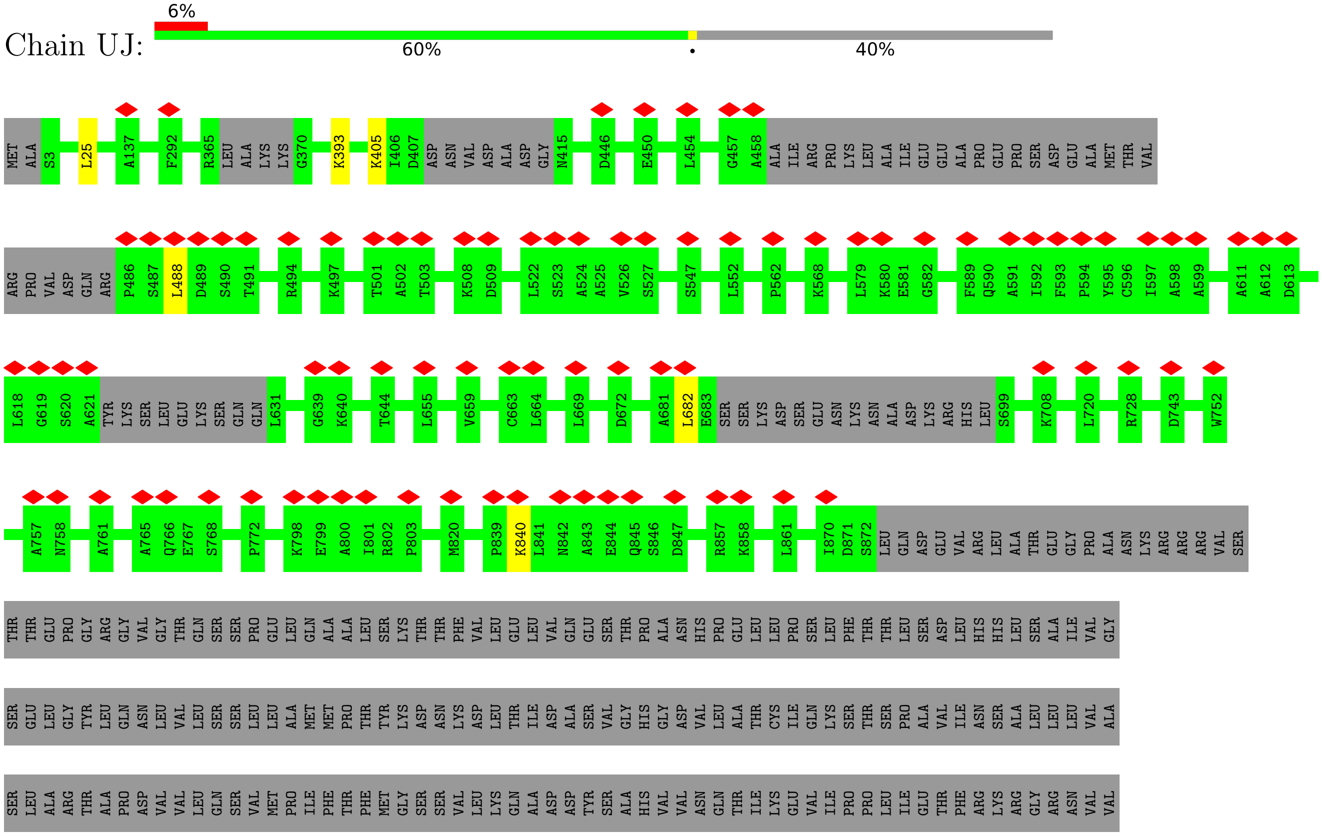
- Molecule 6: Utp7

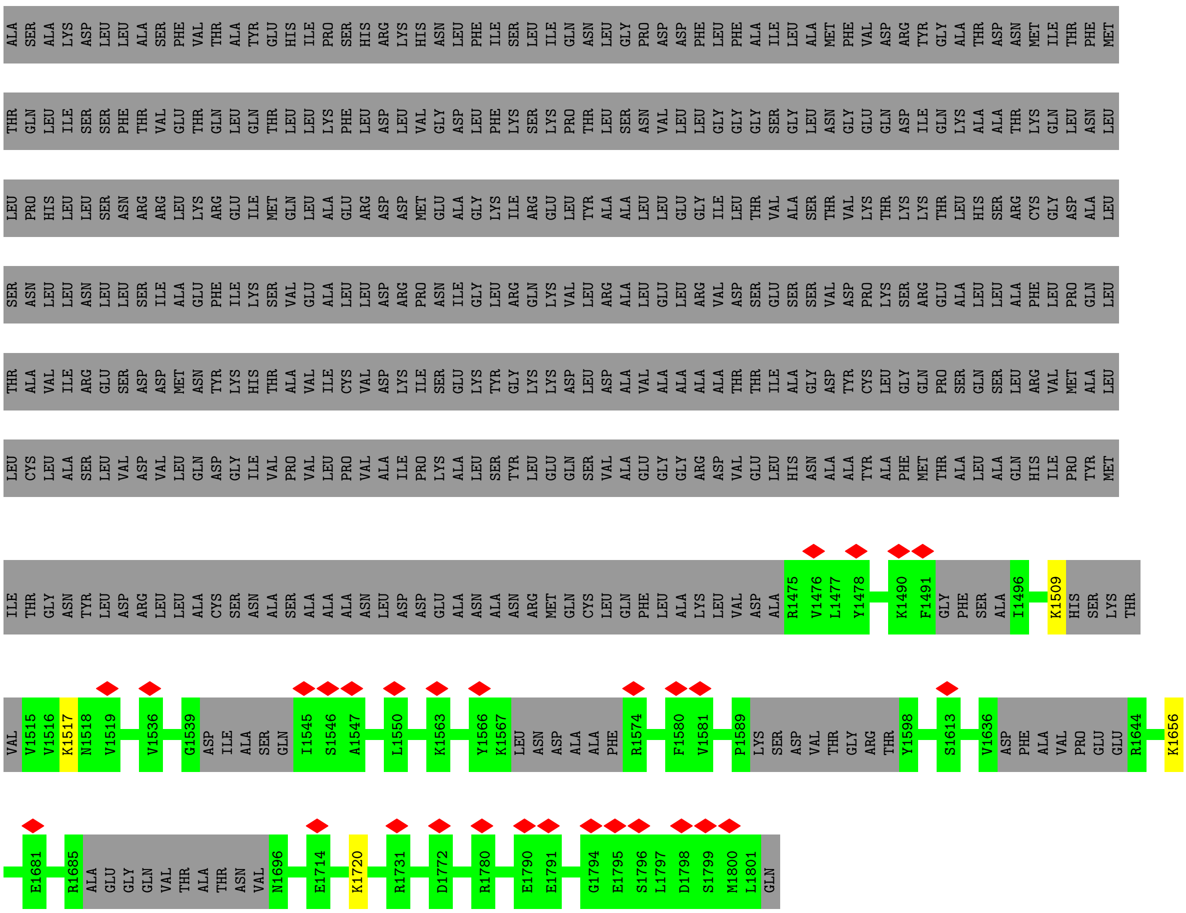
Chain UG:



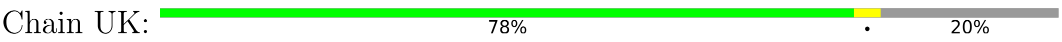
- Molecule 7: UTP10

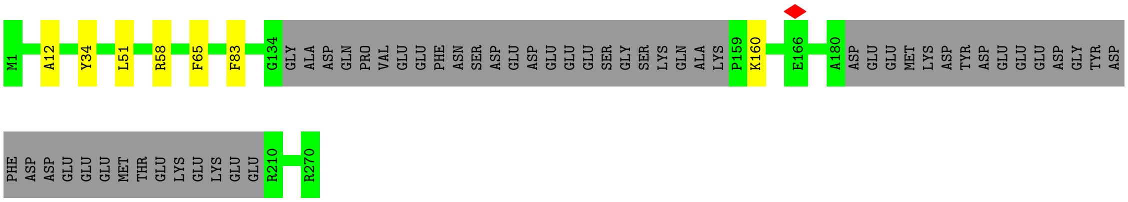
Chain UJ:



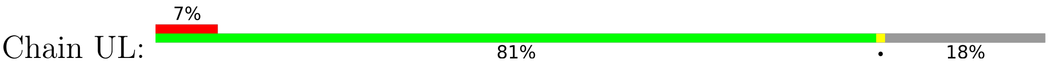


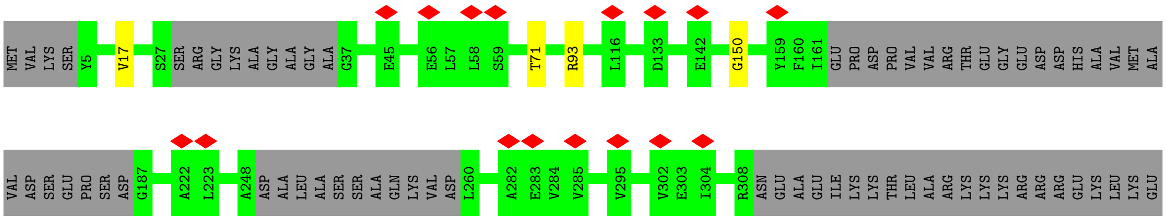
- Molecule 8: U3 small nucleolar RNA-associated protein 11

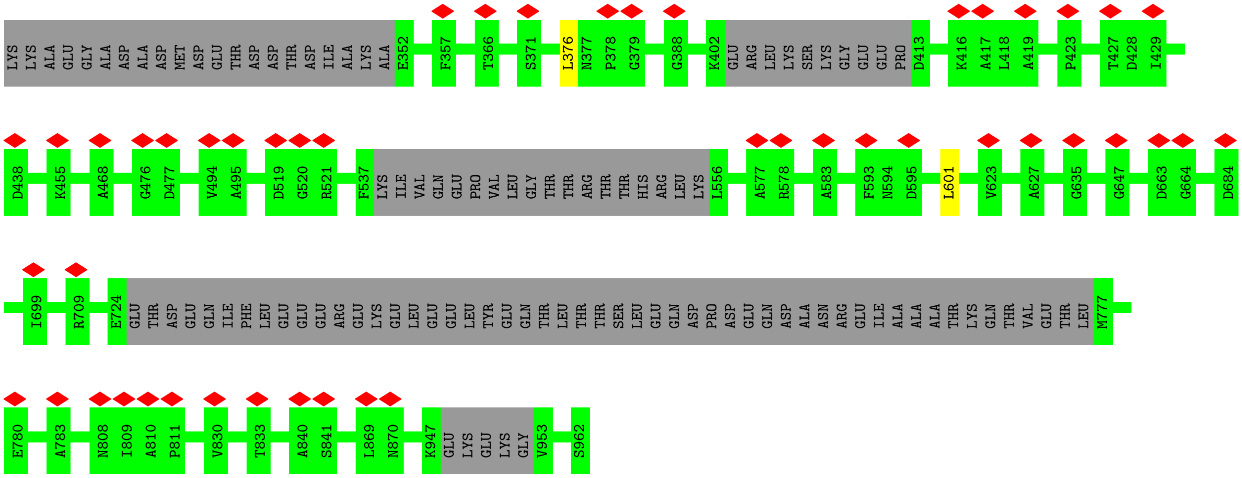




- Molecule 9: Utp12

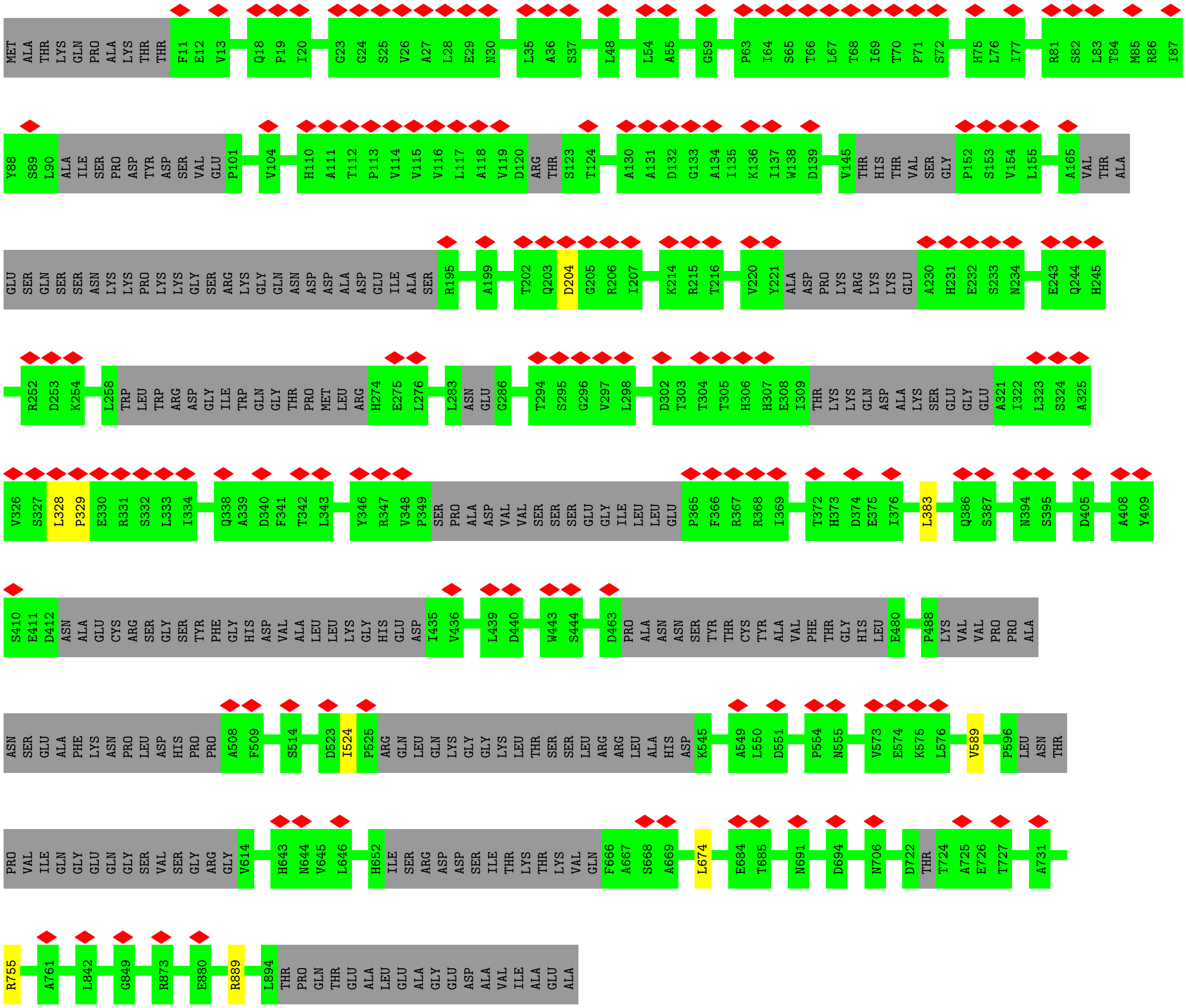




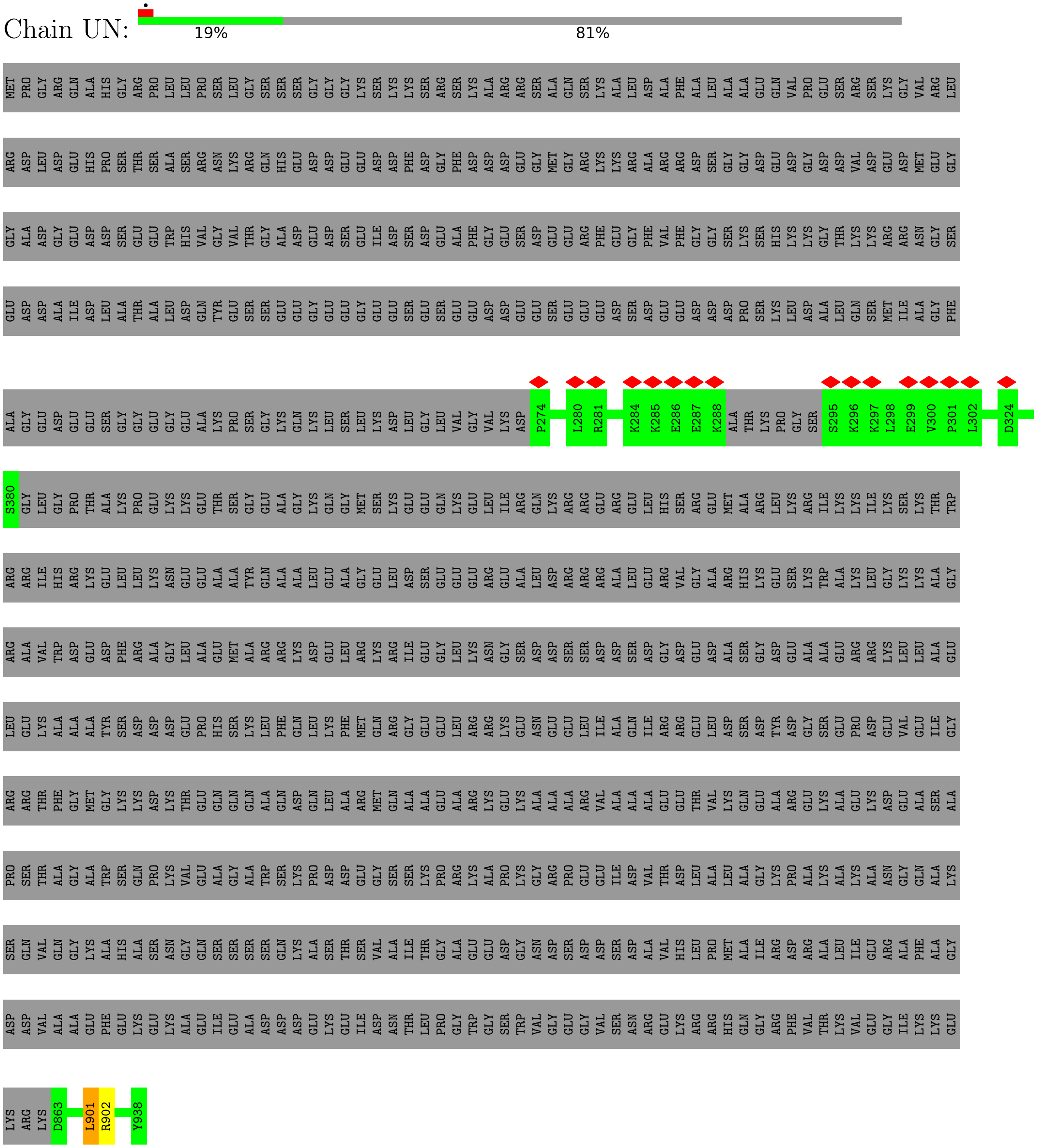


- Molecule 10: Utp13

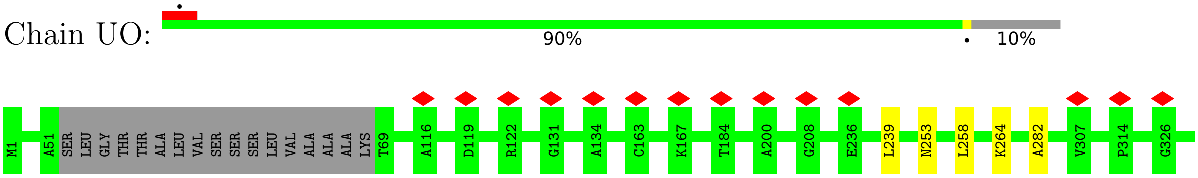
Chain UM:

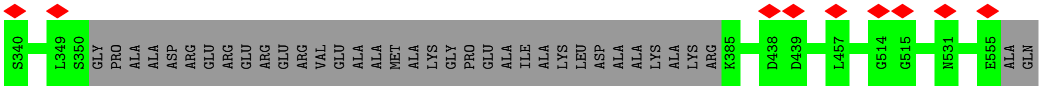


- Molecule 11: Utp14



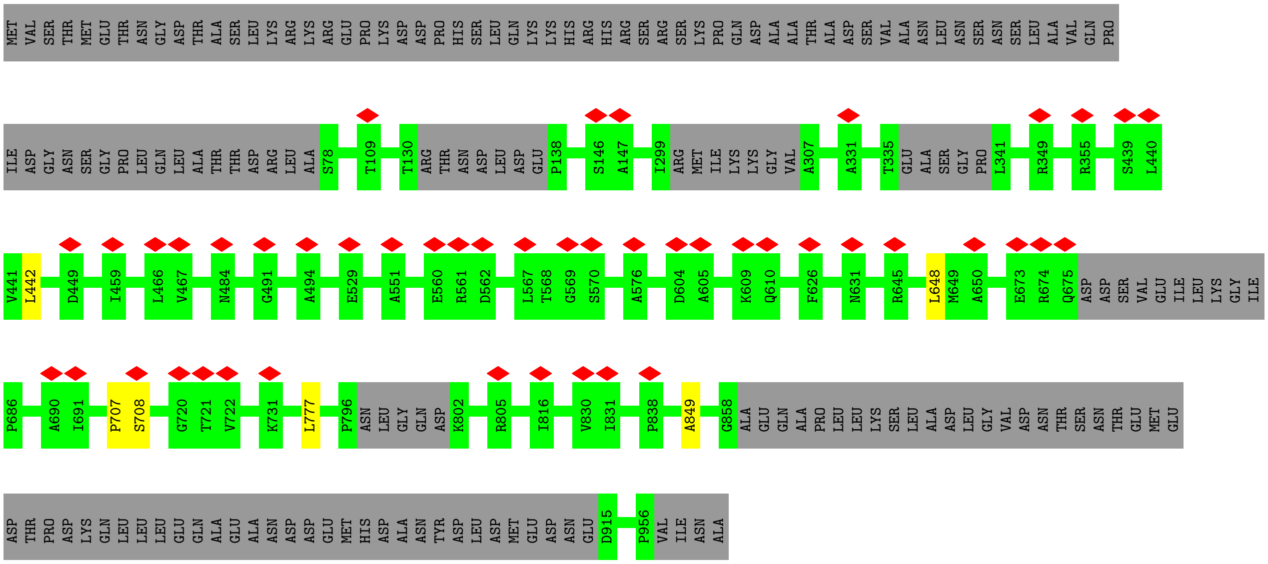
- Molecule 12: Utp15





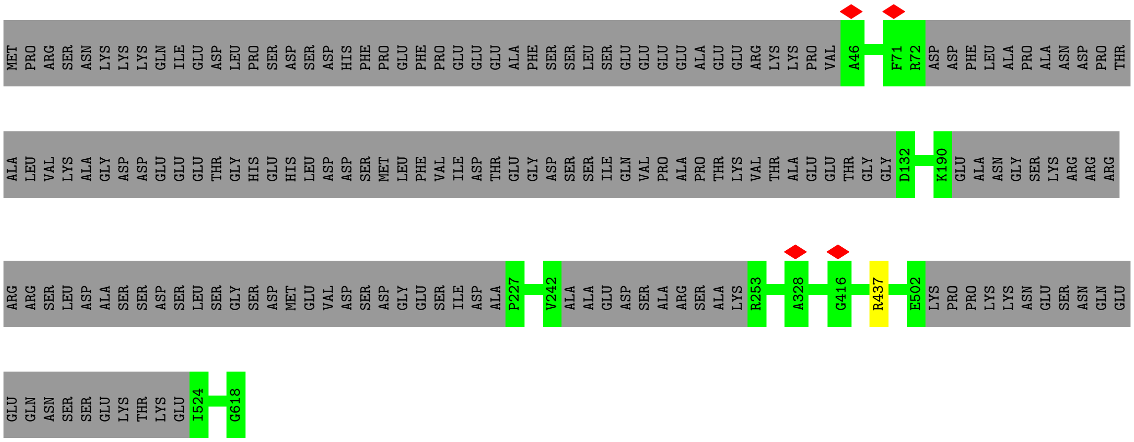
- Molecule 13: Utp17

Chain UQ:



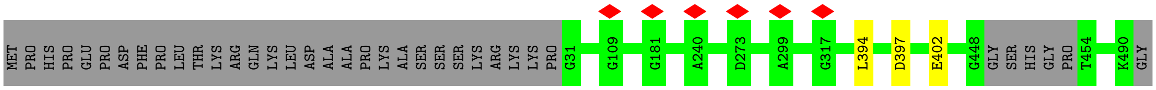
- Molecule 14: Utp18

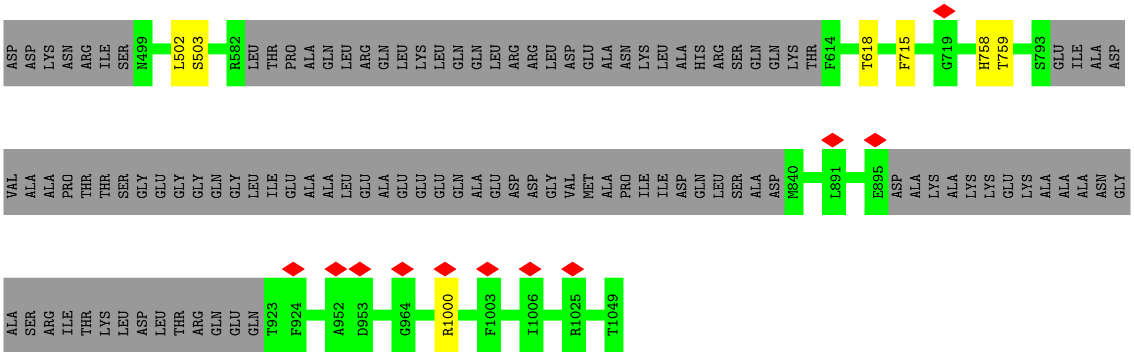
Chain UR:



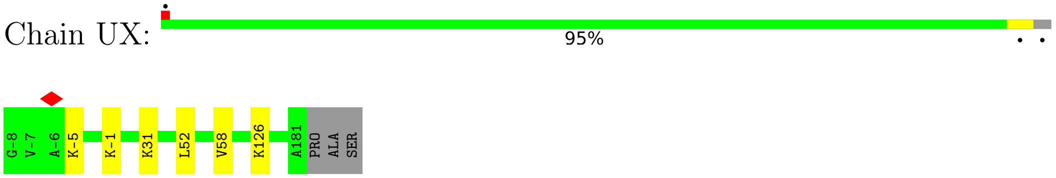
- Molecule 15: Putative U3 snoRNP protein

Chain UU:

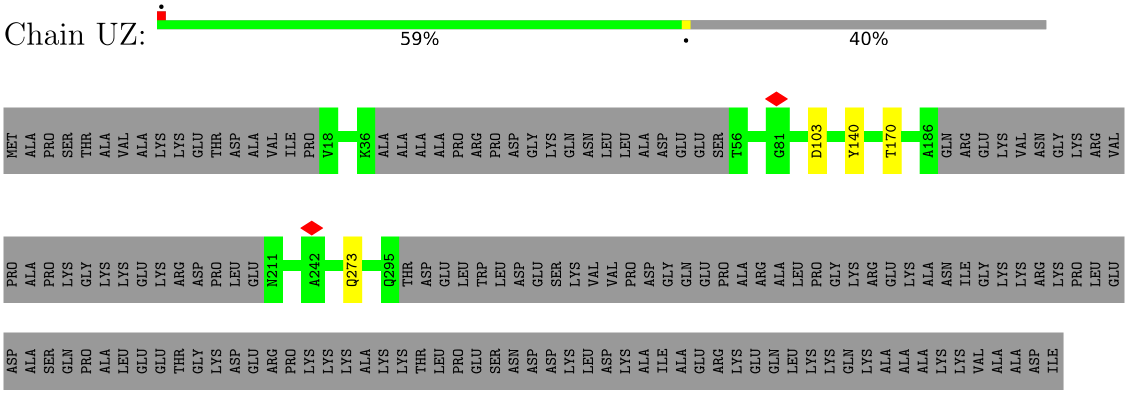




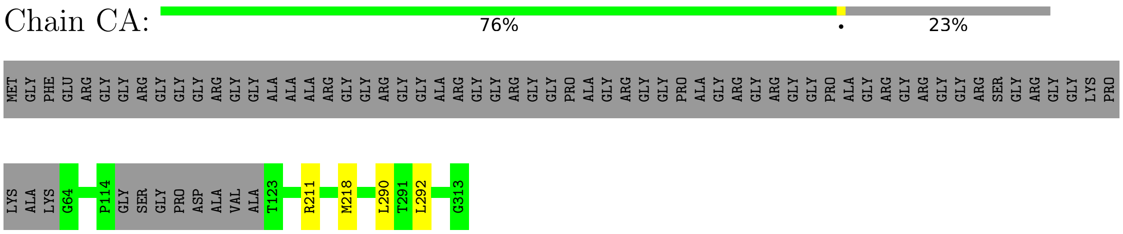
- Molecule 16: Utp24



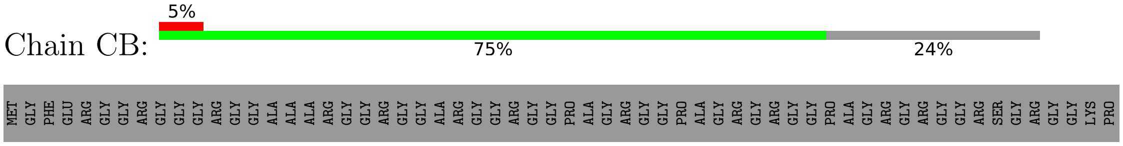
- Molecule 17: Utp30

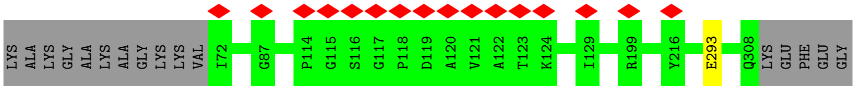


- Molecule 18: Nop1



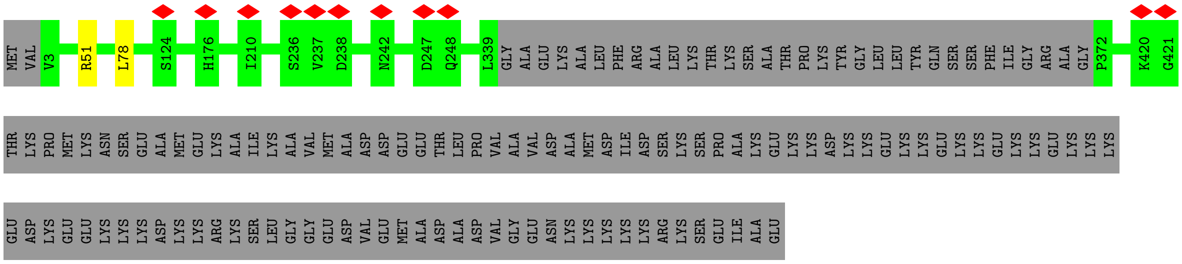
- Molecule 18: Nop1





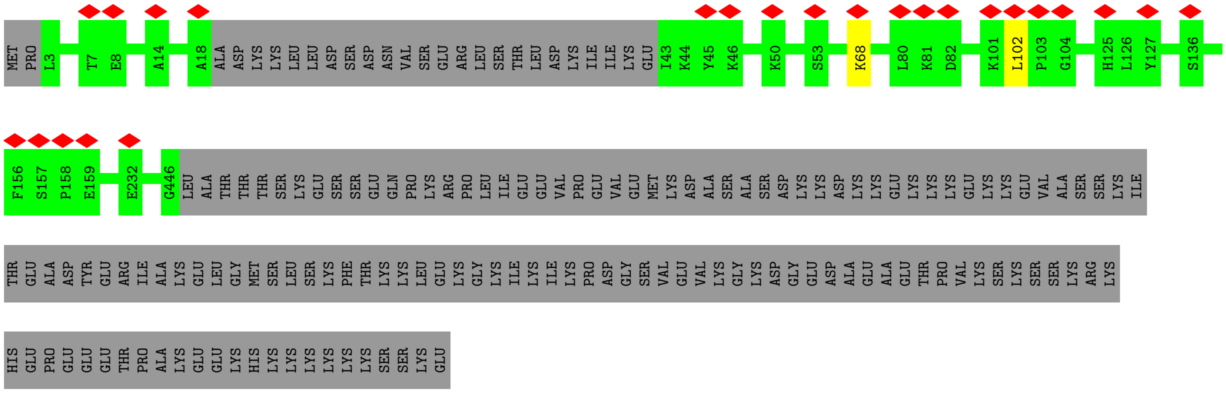
- Molecule 19: Putative nucleolar protein

Chain CC:



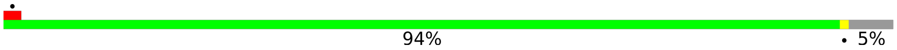
- Molecule 20: Nop58

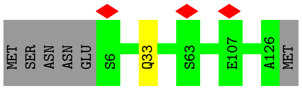
Chain CD:



- Molecule 21: Snu13

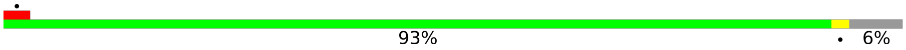
Chain CE:

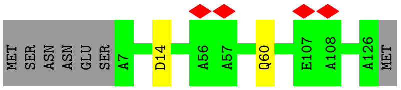




- Molecule 21: Snu13

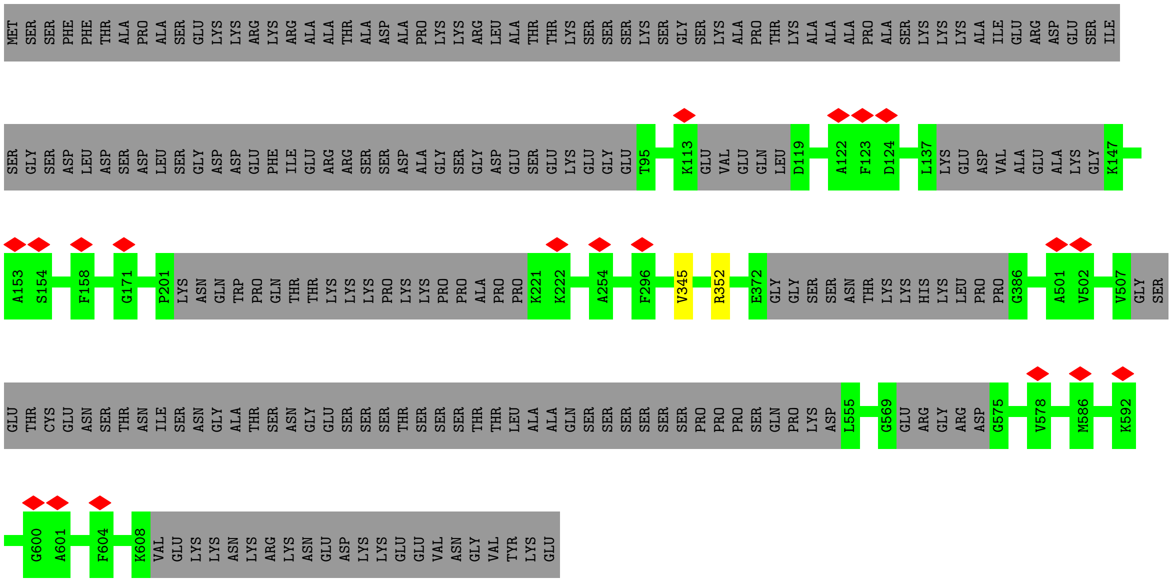
Chain CF:





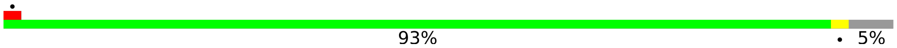
- Molecule 22: Rrp9

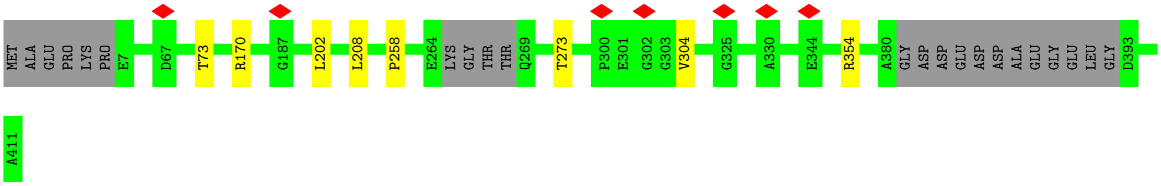
Chain CG:



- Molecule 23: RNA 3'-terminal phosphate cyclase-like protein

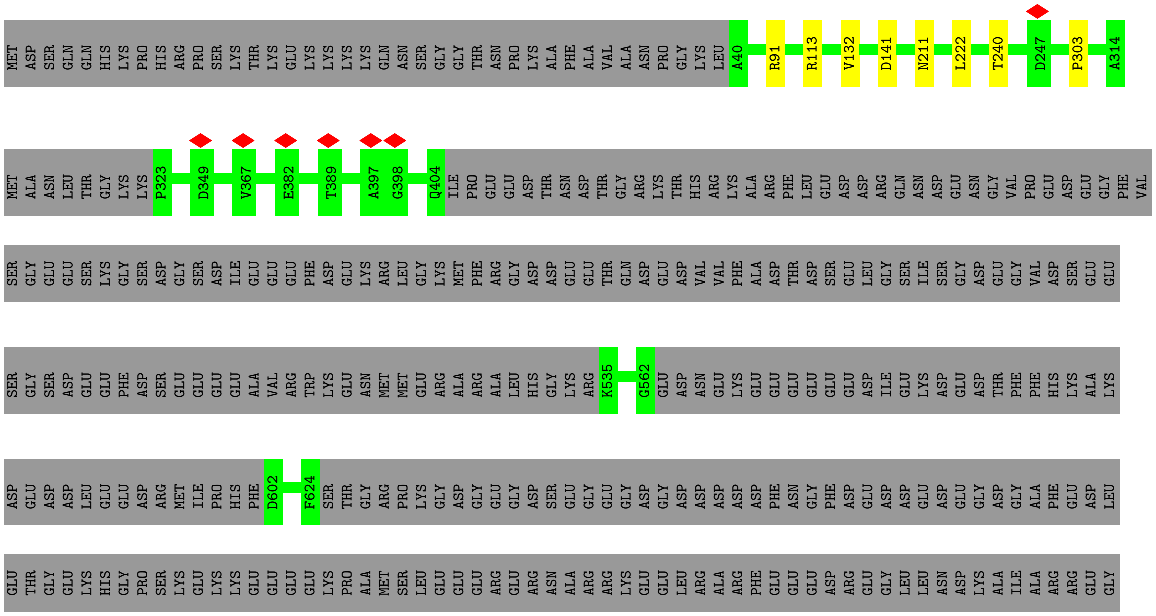
Chain CH:

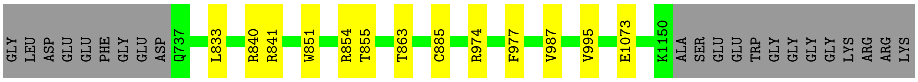




- Molecule 24: Bms1

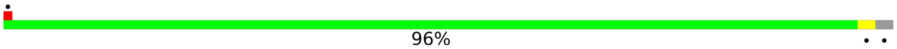
Chain CI:

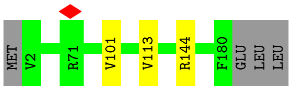




- Molecule 25: Imp3

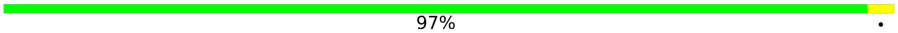
Chain CJ:





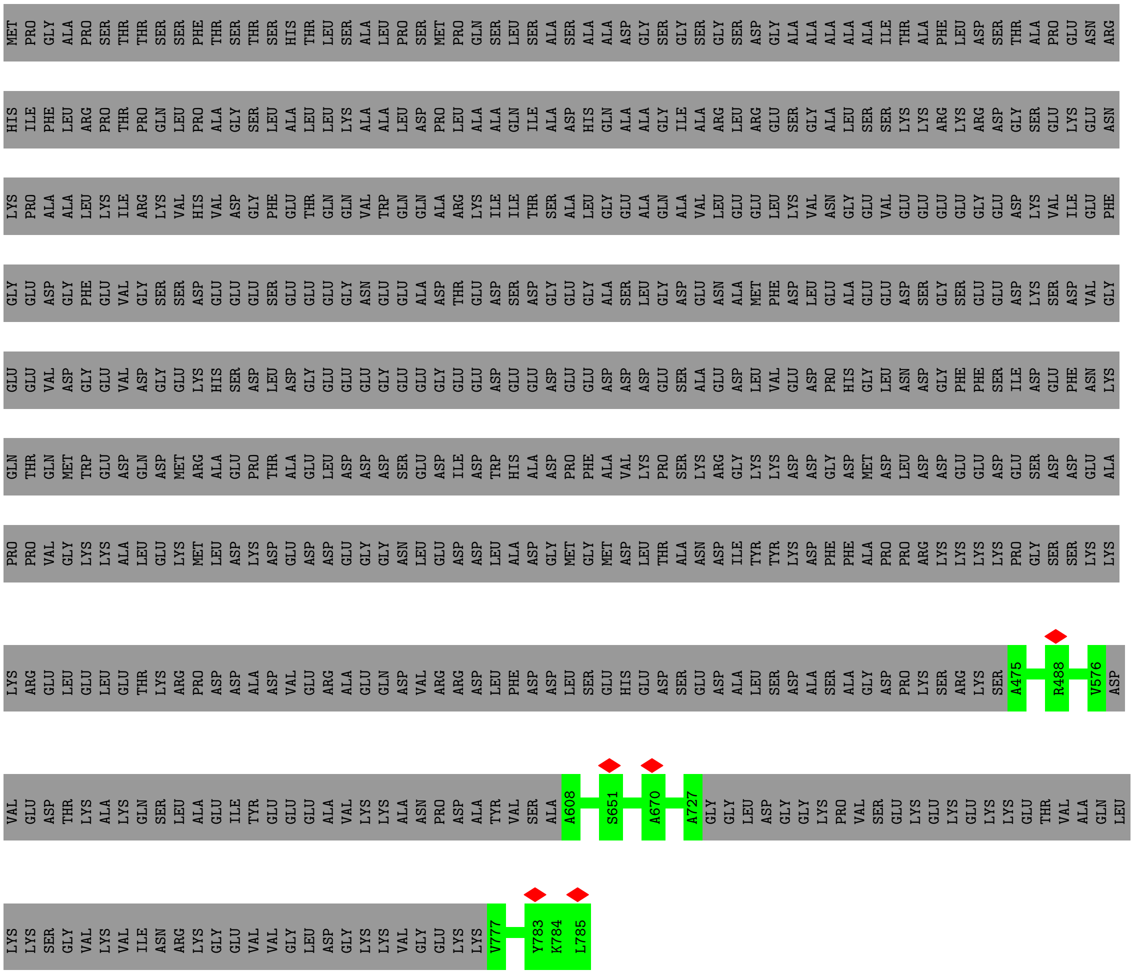
- Molecule 26: Putative U3 small nucleolar ribonucleoprotein

Chain CK:



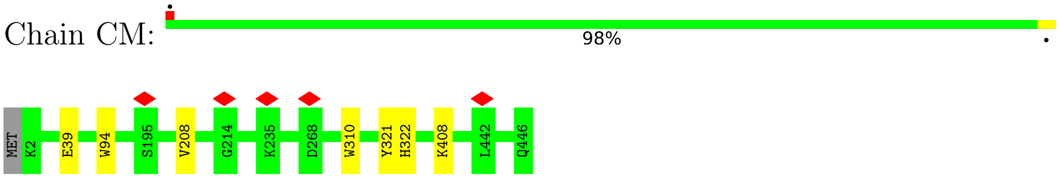
- Molecule 27: Putative U3 small nucleolar ribonucleoprotein protein

Chain CL:



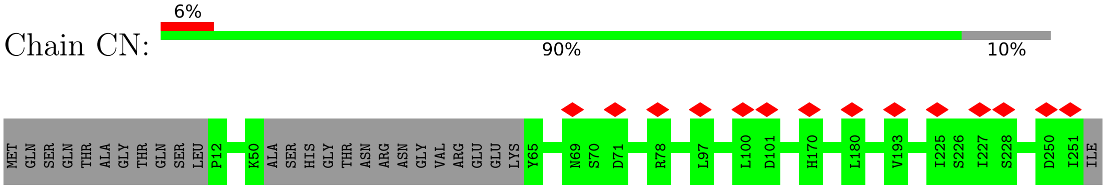
- Molecule 28: Sof1

Chain CM:



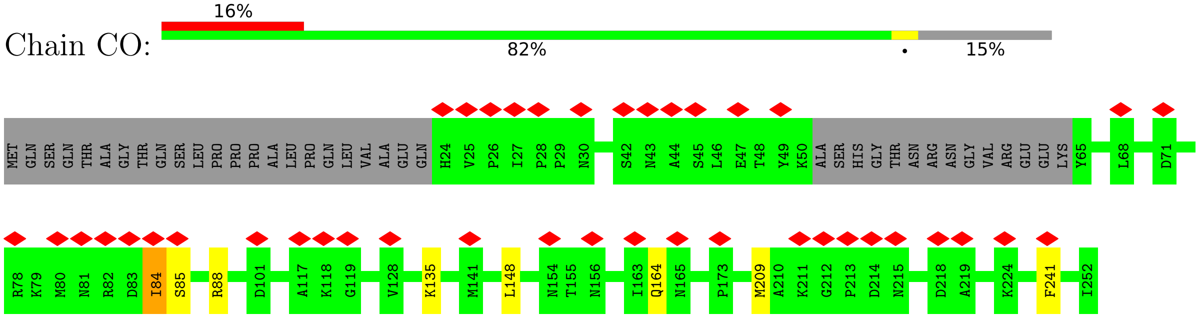
- Molecule 29: Emg1

Chain CN:



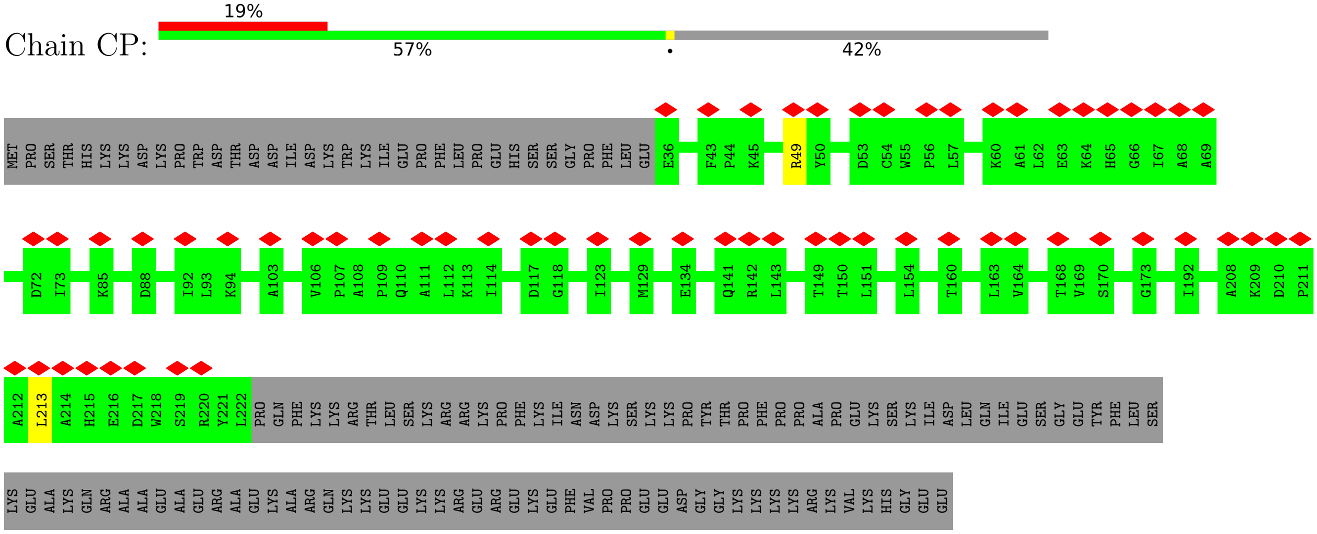
- Molecule 29: Emg1

Chain CO:



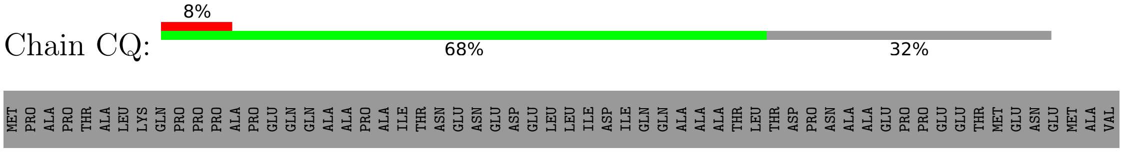
- Molecule 30: KRR1 small subunit processome component

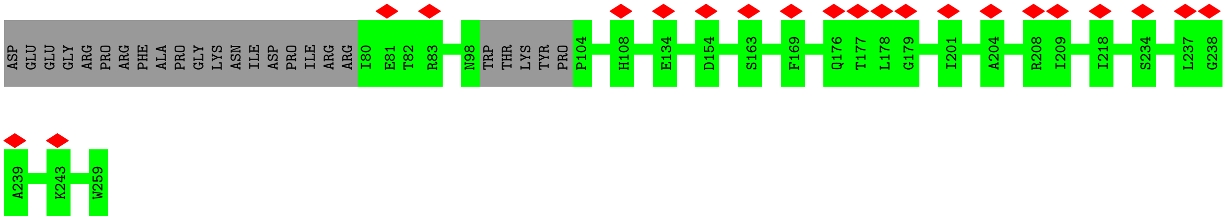
Chain CP:



- Molecule 31: Pre-rRNA-processing protein PNO1

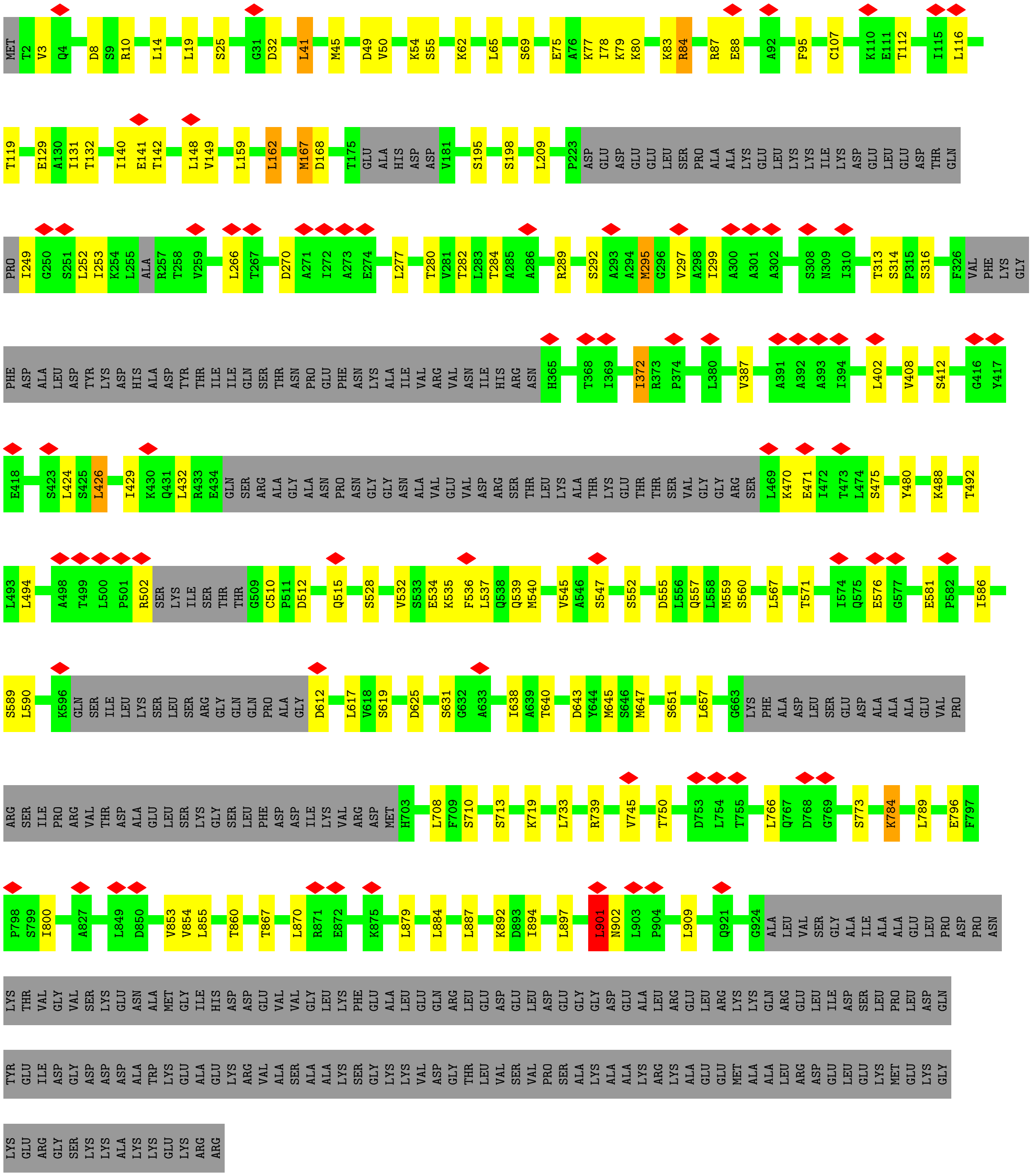
Chain CQ:



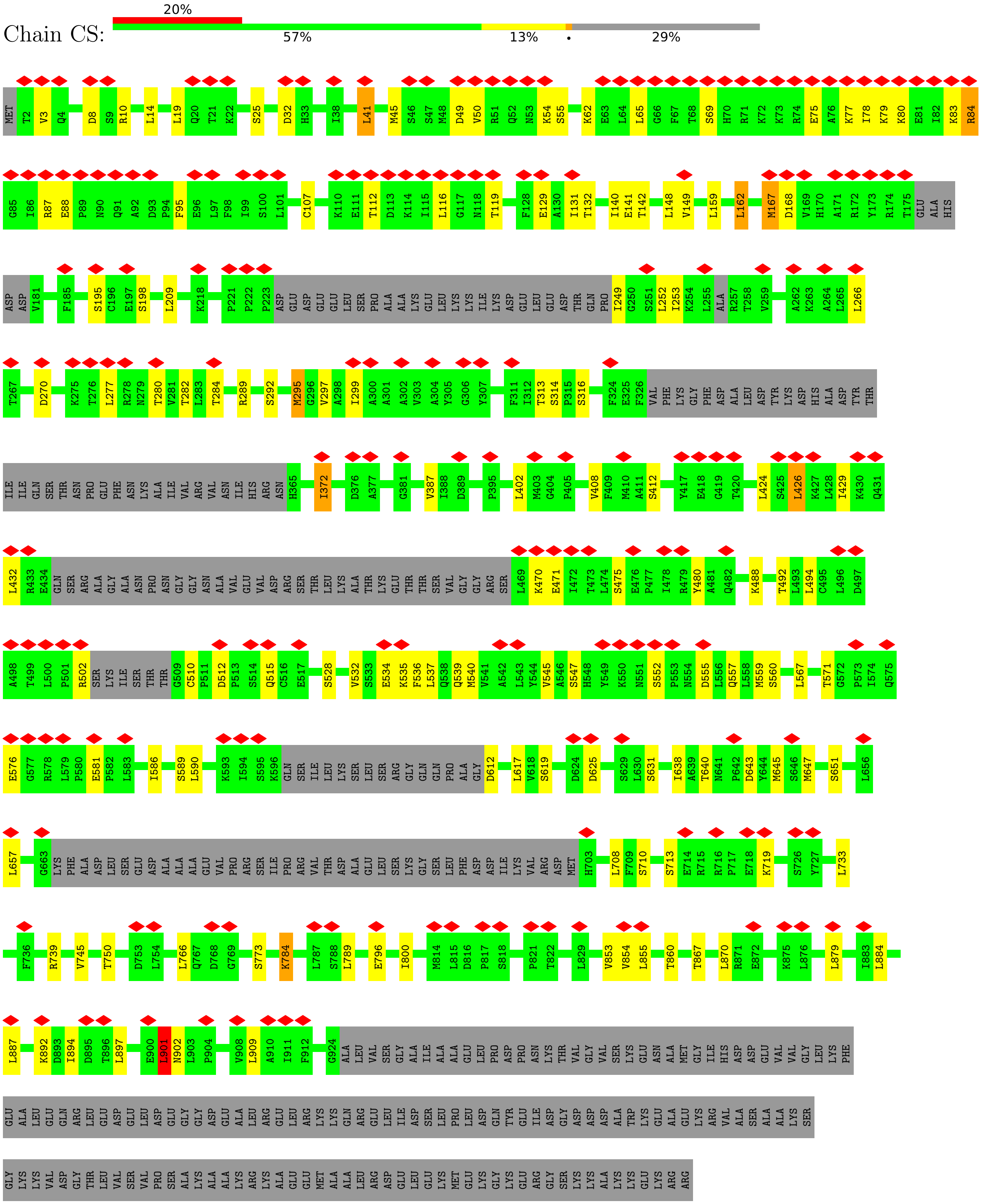


- Molecule 32: Kre33

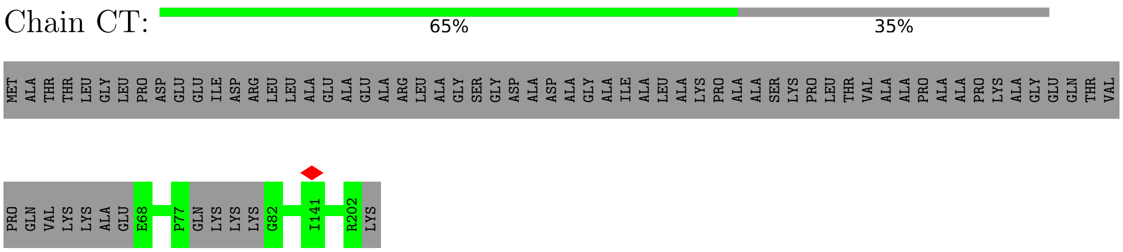
Chain CR:



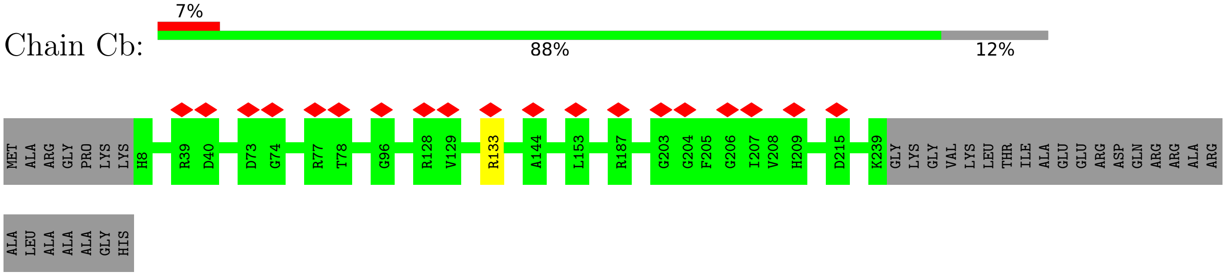
- Molecule 32: Kre33



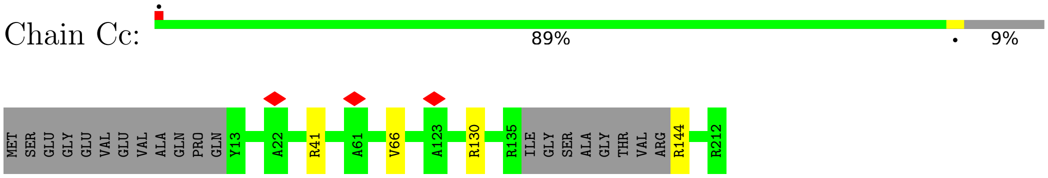
- Molecule 33: Fcf2



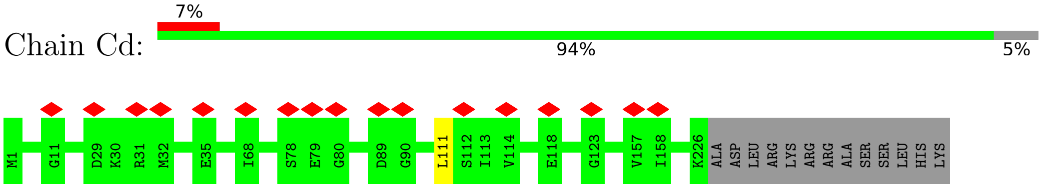
- Molecule 34: 40S ribosomal protein S4



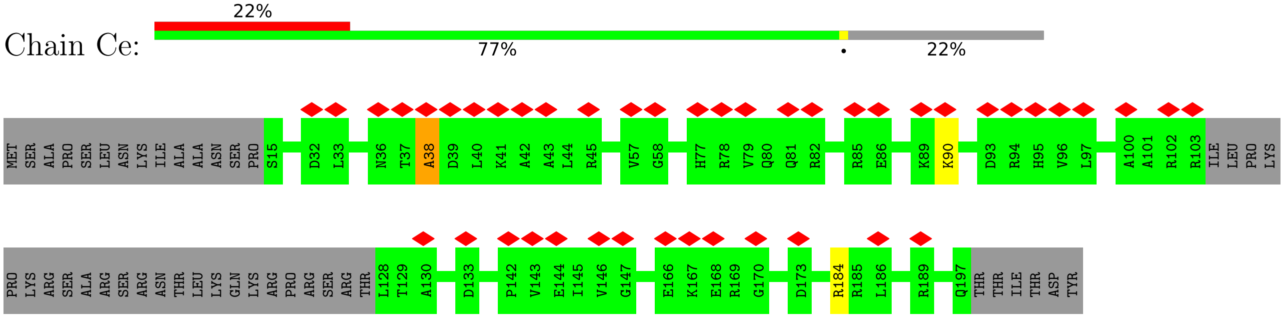
- Molecule 35: 40S ribosomal protein s5-like protein



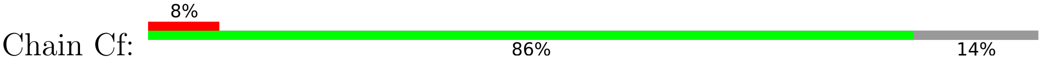
- Molecule 36: 40S ribosomal protein S6

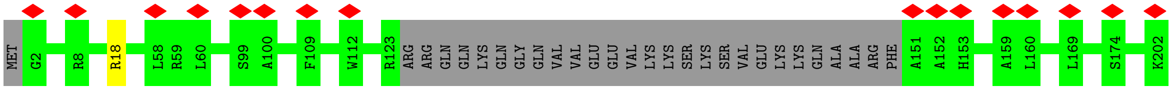


- Molecule 37: 40S ribosomal protein S7



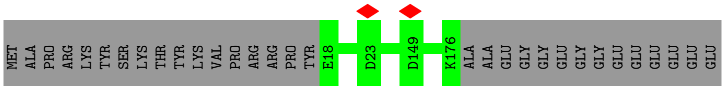
- Molecule 38: 40S ribosomal protein S8





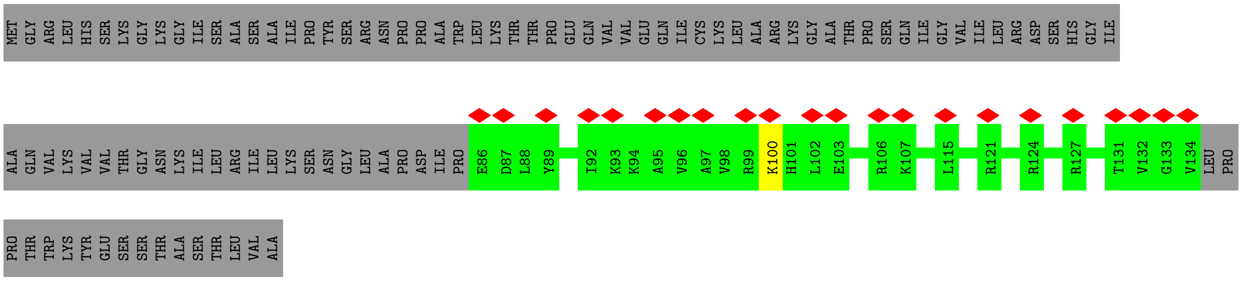
- Molecule 39: 40S ribosomal protein s9-like protein

Chain Cg:



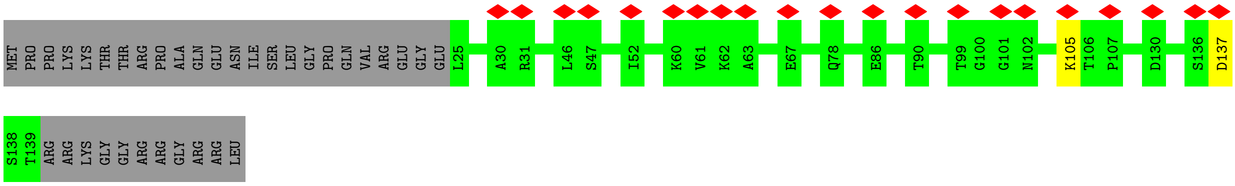
- Molecule 40: 40S ribosomal protein S13-like protein

Chain Ch:



- Molecule 41: 40S ribosomal protein S14-like protein

Chain Ci:

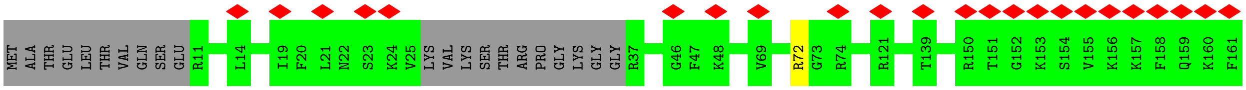


- Molecule 42: 40S ribosomal protein S16-like protein

Chain Cj:

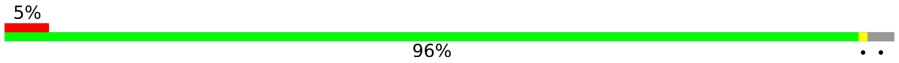
- Molecule 43: 40S ribosomal protein S11-like protein

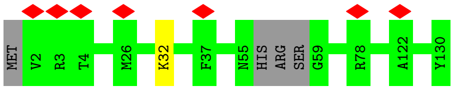
Chain Ck:



- Molecule 44: 40S ribosomal protein S22-like protein

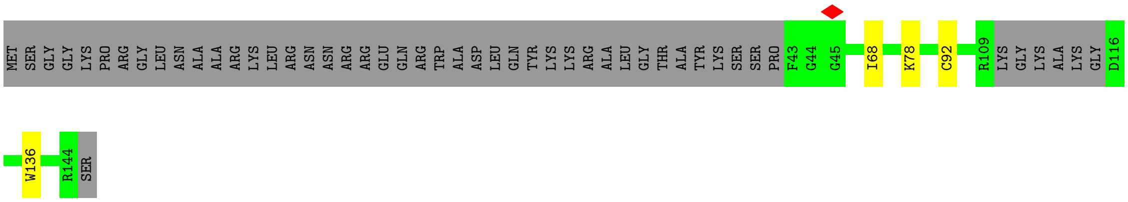
Chain Cm:





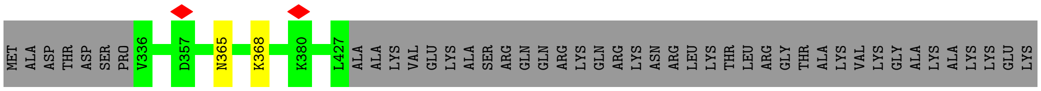
- Molecule 45: 40S ribosomal protein s23-like protein

Chain Cn:



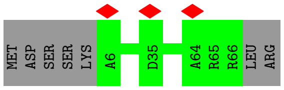
- Molecule 46: 40S ribosomal protein S24

Chain Co:



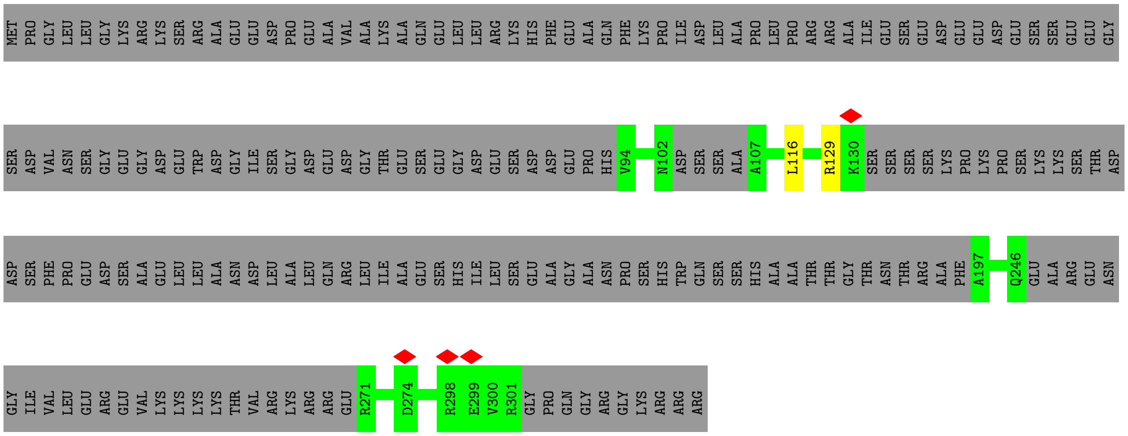
- Molecule 47: 40S ribosomal protein S28-like protein

Chain Cp:

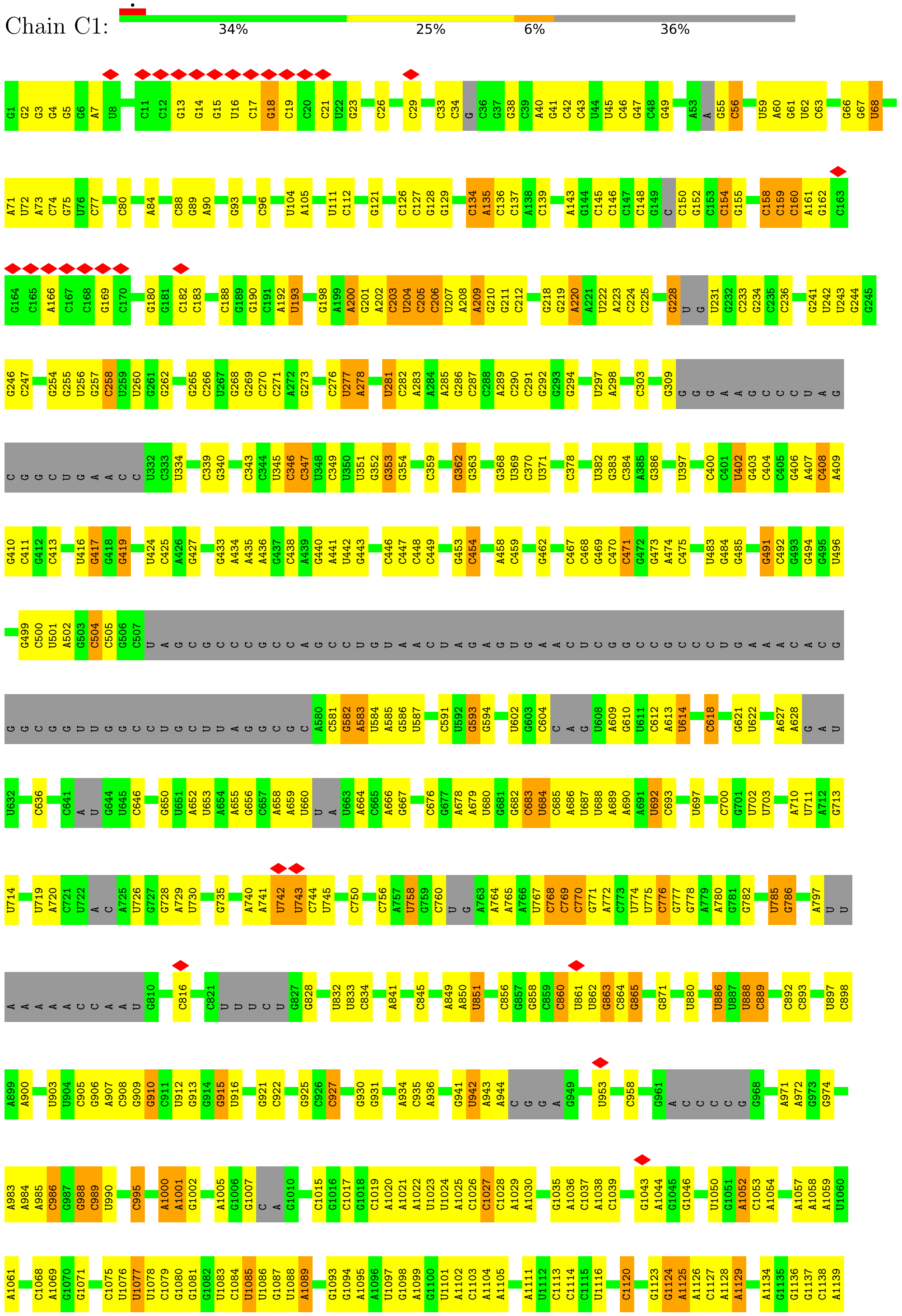


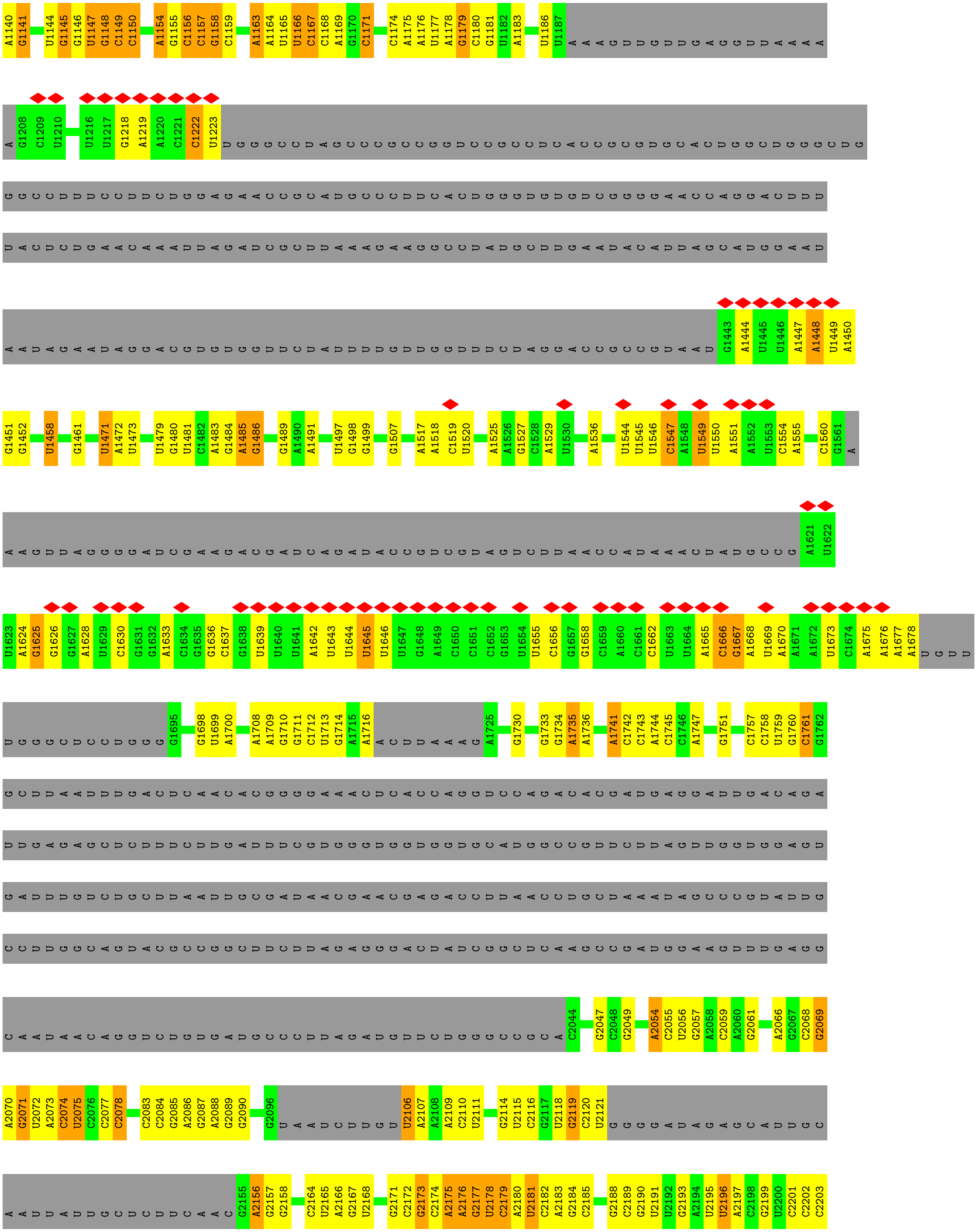
- Molecule 48: Faf1

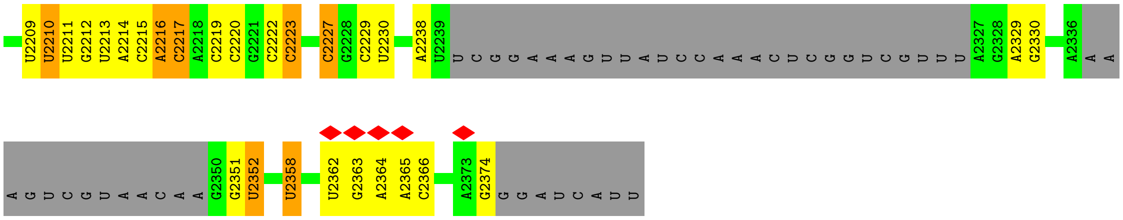
Chain CU:



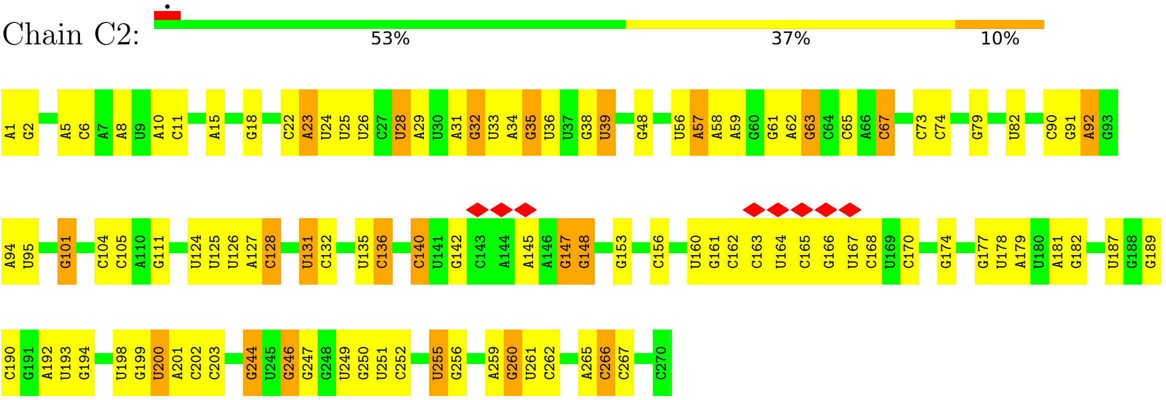
- Molecule 49: 35S ribosomal RNA


Chain C1:
34%
25%
6%
36%
G1 G2 G3 G4 G5 G6 A7 U8 C11 C12 G13 G14 G15 U16 C17 G18 C19 C20 C21 U22 G23 C26 C29 C33 C34 G C36 G37 G38 C39 A40 G41 C42 C43 U44 U45 C46 G47 C48 G49 A53 A G55 C56 U59 A60 G61 U62 C63 G66 G67 U68
A71 U72 A73 C74 G75 U76 C77 C80 A84 C88 G89 A90 G93 C96 U104 A105 U111 C112 G121 C126 C127 G128 G129 C134 A135 C136 C137 A138 C139 A143 G144 C145 C146 C147 C148 G149 C C150 G152 C153 C154 G155 C158 C159 C160 A161 G162 C163
G164 C165 A166 C167 C168 G169 C170 G180 G181 C182 C183 C188 G189 G190 C191 A192 U193 G198 A199 A200 G201 A202 C203 U204 C205 C206 U207 A208 A209 G210 G211 C212 G218 G219 A220 A221 U222 A223 C224 C225 G228 U G U231 G232 C233 G234 C235 C236 G241 U242 U243 G244 G245
G246 C247 G254 G255 U256 G257 C258 U259 U260 G261 G262 G265 C266 U267 G268 G269 C270 C271 A272 G273 C276 U277 A278 U281 C282 A283 A284 A285 G286 C287 C288 A289 C290 C291 G292 G293 G294 U297 A298 C303 G309 G G G A A G C C C U A G
C G G C U G A A C C U332 C333 U334 C339 G340 C343 C344 U345 C346 C347 U348 C349 U350 U351 G352 G353 G354 C359 G362 G363 G368 U369 C370 U371 C378 U382 G383 C384 A385 G386 U397 C400 C401 U402 G403 C404 C405 G406 A407 C408 A409
G410 C411 G412 C413 U416 G417 G418 G419 U424 C425 A426 G427 G433 A434 A435 A436 G437 C438 A439 G440 A441 U442 G443 C446 C447 C448 C449 G453 C454 A458 C459 G462 C467 C468 G469 C470 C471 G472 G473 A474 C475 U483 G484 G485 G491 C492 G493 G494 G495 U496
G499 C500 U501 A502 G503 C504 C505 G506 C507 U A G C G C C C G C C A G C C U G U A A C U A G A G U G A A C U C G G C C G C C U G A A A C A C G
G G C G G U U G G C C U G C C U U A G G C G C A580 C581 G582 A583 U584 A585 G586 U587 C591 U592 G593 G594 U602 G603 C604 C A G U608 A609 G610 U611 C612 A613 U614 C618 G621 U622 A627 A628 G A U
U632 C636 C641 A U G644 U645 C646 G650 U651 A652 U653 A654 A655 G656 C657 A658 A659 U660 U A U663 A664 C665 A666 G667 C676 G677 A678 A679 U680 G681 G682 C683 U684 C685 A686 U687 U688 A689 A690 A691 U692 C693 U697 C700 G701 U702 U703 A710 U711 A712 G713
U714 U719 A720 C721 U722 A C A725 U726 G727 G728 A729 U730 G735 A740 A741 U742 U743 C744 U745 C750 C756 A757 U758 G759 C760 U G A763 A764 A765 A766 U767 C768 C769 C770 G771 A772 C773 U774 U775 C776 G777 G778 A779 A780 G781 G782 U785 G786 A797 U U
A A A A C C A A U G810 C816 C821 U U U C U G827 G828 U832 U833 C834 A841 C845 A849 A850 U851 C856 G857 G858 C859 C860 U861 U862 G863 C864 G865 G871 U880 U886 U887 U888 C889 C892 C893 U897 C898
A899 A900 U903 U904 C905 G906 A907 C908 G909 G910 C911 U912 G913 G914 G915 U916 G921 C922 G925 C926 C927 G930 G931 A934 C935 A936 G941 U942 A943 A944 C G G A G949 U953 C958 G961 A C C C C G G968 A971 A972 G973 G974
A983 A984 A985 C986 G987 G988 C989 U990 C995 A1000 A1001 G1002 A1005 G1006 G1007 C A G1010 C1015 G1016 C1017 G1018 C1019 A1020 A1021 A1022 U1023 U1024 A1025 C1026 C1027 C1028 A1029 A1030 G1035 A1036 C1037 A1038 C1039 G1043 A1044 G1045 G1046 U1050 G1051 A1052 C1053 A1054 A1057 A1058 A1059 U1060
A1061 C1068 A1069 G1070 G1071 C1075 U1076 U1077 U1078 C1079 G1080 G1081 G1082 U1083 C1084 U1085 U1086 G1087 U1088 A1089 G1093 G1094 A1095 A1096 U1097 G1098 A1099 G1100 U1101 A1102 C1103 A1104 A1105 A1111 U1112 C1113 C1114 C1115 U1116 C1120 G1123 G1124 A1125 A1126 C1127 A1128 A1129 A1134 G1135 G1136 C1138 A1139

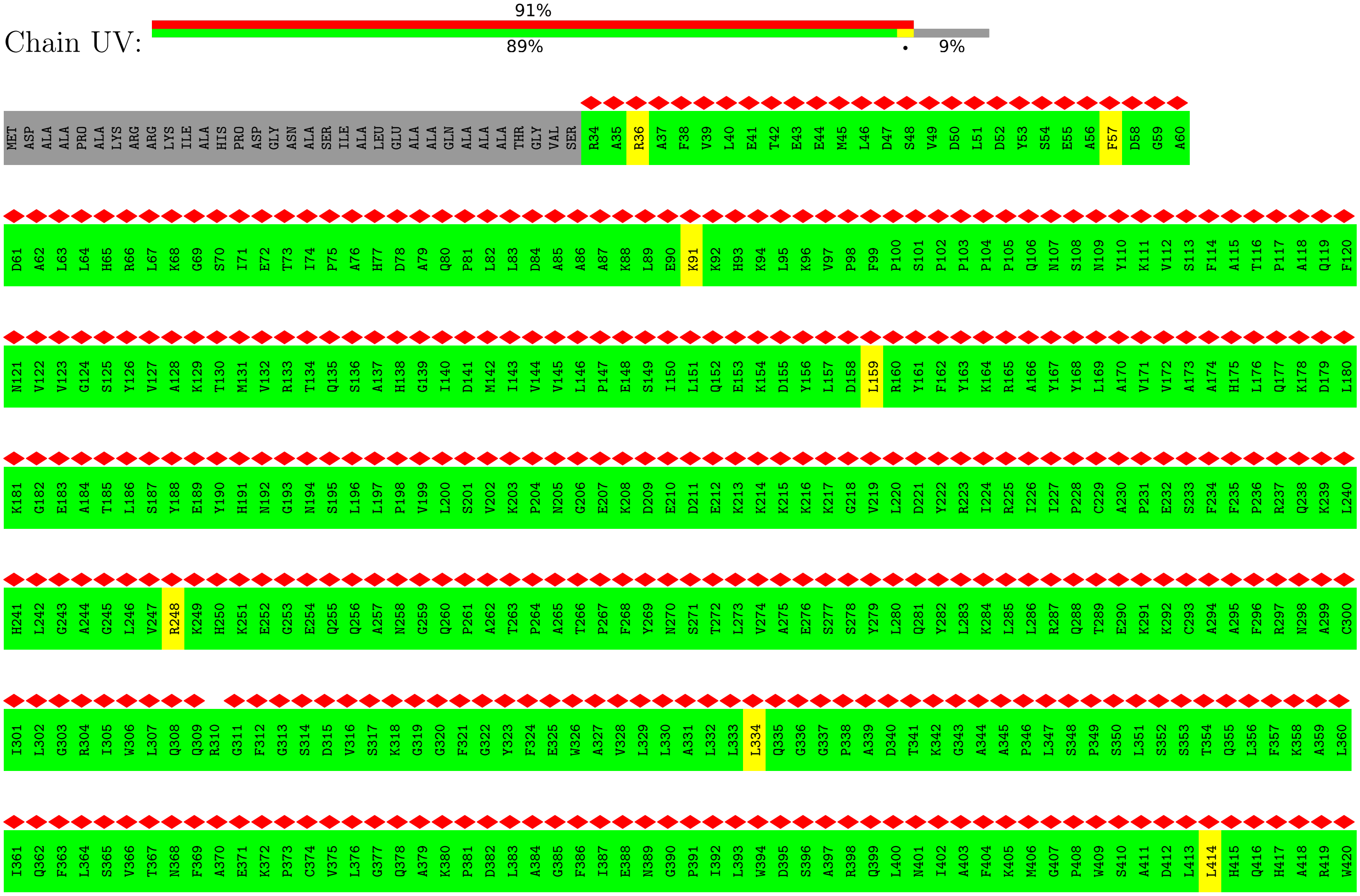

A1140 G1141 U1144 G1145 G1146 U1147 G1148 C1149 C1150 A1154 G1155 C1156 C1157 G1158 C1159 A1163 A1164 U1165 U1166 C1167 C1168 A1169 G1170 C1171 C1174 A1175 A1176 U1177 A1178 G1179 C1180 G1181 U1182 A1183 U1186 U1187 A A A G U U G U U G A G G U U A A A A
A G1208 C1209 U1210 U1216 U1217 G1218 A1219 A1220 C1221 C1222 U1223 U G G G C C U A G C C C G C C G G U C C G C C U C A C C G C G U G C A C U G G C U G G G C U G
G G C C U U U C C U U C U G G A G A A C C G C A U G C C C U U C A C U G G G U G U G U C G G G G A A C C A G G A C U U U
U A C U C U G A A C A A A U U A G A U C G C U U A A A G A A G G C C U A U G C U U G A A U A C A U U A G C A U G G A A U
A A U A G A A U A G G A C G U G U G G U U C U A U U U G U U G G U U U C U A G G A C C G C C G U A A U G1443 A1444 U1445 U1446 A1447 A1448 U1449 A1450
G1451 G1452 U1458 G1461 U1471 A1472 U1473 U1479 G1480 U1481 C1482 A1483 G1484 A1485 G1486 G1489 A1490 A1491 U1497 G1498 G1499 G1507 A1517 A1518 C1519 U1520 A1525 A1526 G1527 C1528 A1529 U1530 A1536 U1544 U1545 U1546 C1547 A1548 U1549 U1550 A1551 A1552 U1553 C1554 A1555 C1560 G1561 A
A A G U U A G G G G A U C G A A G A C G A U C A G A U A C C G U C G U A G U C U U A A C C A U A A A C U A U G C C G A1621 U1622
U1623 A1624 G1625 G1626 G1627 A1628 U1629 C1630 G1631 G1632 A1633 C1634 G1635 G1636 C1637 G1638 U1639 U1640 U1641 A1642 U1643 U1644 U1645 U1646 U1647 G1648 A1649 C1650 C1651 C1652 G1653 U1654 U1655 C1656 G1657 G1658 C1659 A1660 C1661 C1662 U1663 U1664 A1665 C1666 G1667 A1668 U1669 A1670 A1671 A1672 U1673 C1674 A1675 A1676 A1677 A1678 U G U U
U G G G C U C C U G G G G1695 G1698 U1699 A1700 A1708 A1709 G1710 G1711 C1712 U1713 G1714 A1715 A1716 A C U U A A A G A1725 G1730 G1733 G1734 A1735 A1736 A1741 C1742 C1743 A1744 C1745 C1746 A1747 G1751 C1757 C1758 U1759 G1760 C1761 G1762
G C U U A A U U U G A C U C A A C A C G G G G A A A C U C A C C A G G U C C A G A C A C G A U G A G G A U U G A C A G A
U U G A G A G C U C U U U C U U G A U U U C G U G G G U G G U G G U G C A U G G C C G U U C U U A G U U G G U G G A G U
G A U U U G U C U G C U U A A U U G C G A U A A C G A A C G A G A C C U U A A C C U G C U A A A U A G C C C G U A U U G
C C U U G G C A G U A C G C C G G C U U C U U A G A G G G A C U A U C G G C U C A A G C C G A U G G A A G U U U G A G G
C A A U A A C A G G U C U G U G A U G C C C U U A G A U G U U C U G G G C C G C A C2044 G2047 C2048 G2049 A2054 C2055 U2056 G2057 A2058 C2059 A2060 G2061 A2066 G2067 C2068 G2069
A2070 G2071 U2072 A2073 C2074 U2075 C2076 C2077 C2078 C2083 C2084 G2085 A2086 G2087 A2088 G2089 G2090 G2096 U A A U C U U G U U2106 A2107 A2108 A2109 C2110 U2111 G2114 U2115 C2116 G2117 U2118 G2119 C2120 U2121 G G G G A U A G A G C A U U G C
A A U U A U U G C U C U U C A A C G2155 A2156 G2157 G2158 C2164 U2165 A2166 G2167 U2168 G2171 C2172 G2173 C2174 A2175 A2176 G2177 U2178 C2179 A2180 U2181 C2182 A2183 G2184 C2185 G2188 C2189 G2190 U2191 U2192 G2193 A2194 U2195 U2196 A2197 C2198 G2199 U2200 C2201 C2202 C2203

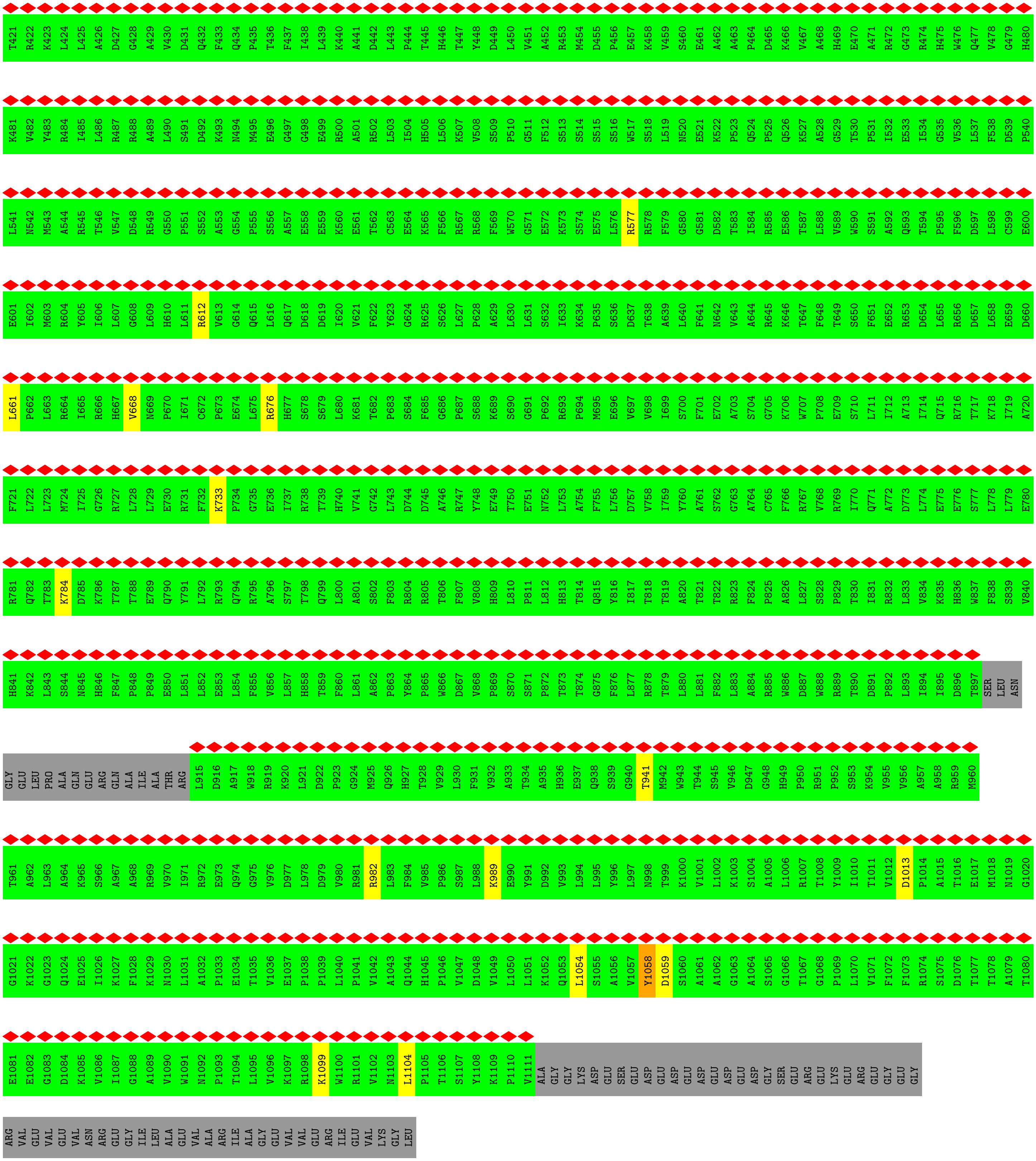


- Molecule 50: U3 snoRNA



- Molecule 51: U3 small nucleolar RNA-associated protein 22





T421 R422 K423 L424 L425 A426 D427 G428 A429 V430 D431 Q432 F433 Q434 P435 T436 F437 I438 L439 K440 A441 D442 L443 P444 T445 H446 T447 Y448 D449 L450 V451 A452 R453 M454 D455 P456 E457 K458 V459 S460 E461 K462 A463 P464 D465 K466 V467 A468 H469 E470 A471 R472 G473 R474 H475 W476 Q477 V478 G479 H480

K481 V482 Y483 R484 I485 L486 R487 R488 A489 L490 S491 D492 K493 N494 M495 E496 G497 G498 E499 R500 A501 R502 L503 I504 H505 L506 K507 V508 S509 P510 G511 F512 S513 S514 S515 S516 W517 S518 L519 N520 E521 K522 P523 Q524 P525 Q526 K527 A528 G529 T530 P531 I532 E533 I534 G535 V536 L537 F538 D539 P540

L541 N542 M543 A544 R545 T546 V547 D548 R549 G550 P551 S552 A553 G554 P555 S556 A557 E558 E559 K560 E561 T562 C563 E564 K565 F566 R567 R568 F569 W570 G571 E572 K573 S574 E575 L576 R577 R578 F579 G580 G581 D582 T583 I584 R585 E586 T587 L588 V589 W590 S591 A592 Q593 T594 P595 F596 D597 L598 C599 E600

E601 I602 M603 R604 Y605 I606 L607 G608 L609 H610 L611 R612 V613 G614 Q615 L616 Q617 D618 D619 I620 V621 F622 Y623 G624 R625 S626 L627 P628 A629 L630 L631 S632 I633 K634 P635 S636 D637 T638 A639 L640 F641 N642 V643 A644 R645 K646 T647 F648 T649 S650 F651 E652 R653 D654 L655 R656 D657 L658 E659 D660

L661 P662 L663 R664 I665 R666 H667 V668 N669 P670 I671 C672 P673 E674 L675 R676 H677 S678 S679 L680 K681 T682 P683 S684 F685 G686 P687 S688 K689 S690 G691 P692 R693 P694 M695 E696 V697 V698 I699 S700 F701 E702 A703 S704 G705 K706 W707 P708 E709 S710 L711 I712 A713 I714 Q715 R716 T717 K718 I719 A720

F721 L722 L723 M724 I725 G726 R727 L728 L729 E730 R731 F732 K733 P734 G735 E736 I737 R738 T739 H740 V741 G742 L743 D744 D745 A746 R747 Y748 E749 T750 E751 N752 L753 A754 F755 L756 D757 V758 I759 Y760 A761 S762 G763 A764 C765 F766 R767 V768 R769 I770 Q771 A772 D773 L774 E775 E776 S777 L778 L779 E780

R781 Q782 T783 K784 D785 K786 T787 T788 E789 Q790 Y791 L792 R793 Q794 R795 A796 S797 T798 Q799 L800 A801 S802 F803 R804 R805 T806 F807 V808 H809 L810 P811 L812 H813 T814 Q815 Y816 I817 T818 T819 A820 T821 T822 R823 F824 P825 A826 L827 S828 P829 T830 I831 R832 L833 V834 K835 H836 W837 F838 S839 V840

H841 K842 L843 S844 N845 H846 F847 P848 P849 E850 L851 L852 E853 L854 F855 V856 L857 H858 T859 F860 L861 A862 P863 Y864 P865 W866 D867 V868 P869 S870 S871 P872 T873 T874 G875 F876 L877 R878 T879 L880 L881 F882 L883 A884 R885 W886 D887 W888 R889 T890 D891 P892 L893 I894 I895 D896 T897 SER LEU ASN

GLY GLU LEU PRO ALA GLN GLU ARG GLN ALA ILE ALA THR ARG L915 D916 A917 W918 R919 K920 L921 D922 P923 G924 M925 Q926 H927 T928 V929 L930 F931 V932 A933 T934 A935 H936 E937 Q938 S939 G940 T941 M942 W943 T944 S945 V946 D947 G948 H949 P950 R951 P952 S953 K954 V955 V956 A957 A958 R959 M960

T961 A962 L963 A964 K965 S966 A967 A968 R969 V970 I971 R972 E973 Q974 G975 V976 D977 L978 D979 V980 R981 R982 L983 F984 V985 P986 S987 L988 K989 E990 Y991 D992 V993 L994 Y995 L996 L997 N998 T999 K1000 V1001 L1002 K1003 S1004 A1005 L1006 R1007 T1008 Y1009 I1010 T1011 V1012 D1013 P1014 A1015 T1016 E1017 M1018 N1019 G1020

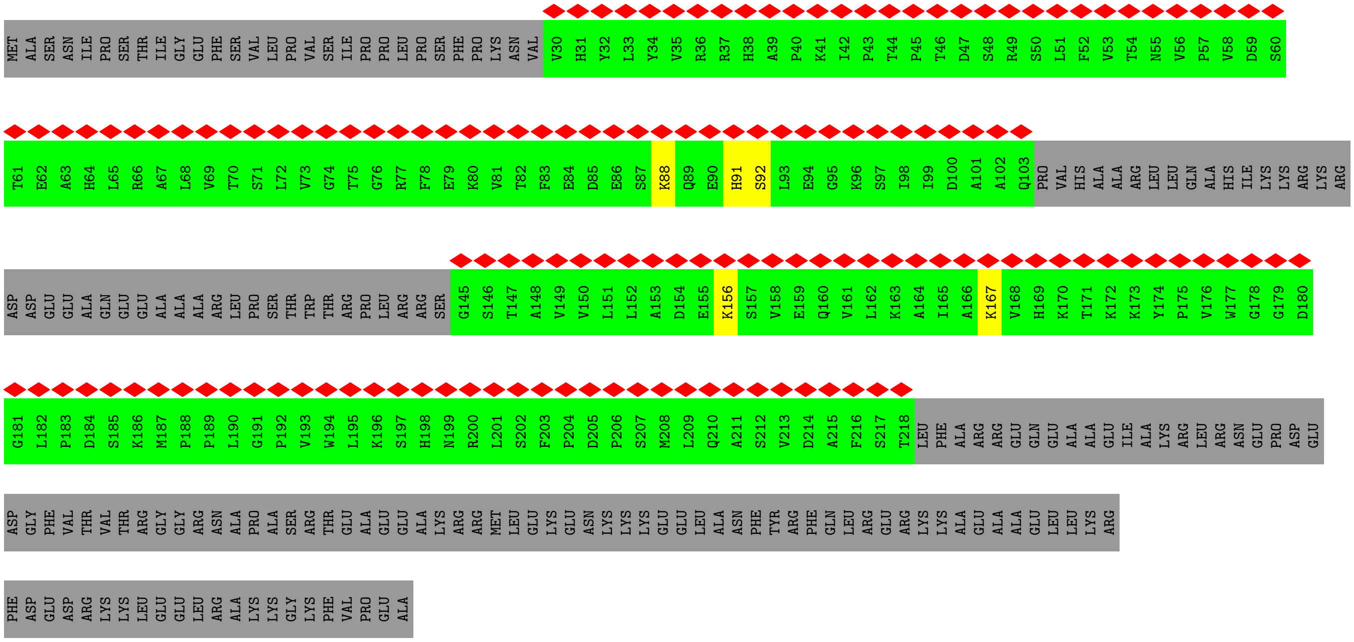
G1021 K1022 G1023 Q1024 E1025 I1026 K1027 F1028 K1029 N1030 L1031 A1032 P1033 E1034 T1035 V1036 E1037 P1038 P1039 L1040 P1041 V1042 A1043 Q1044 H1045 P1046 V1047 D1048 V1049 L1050 L1051 K1052 Q1053 L1054 S1055 A1056 V1057 Y1058 D1059 S1060 A1061 A1062 G1063 A1064 S1065 G1066 T1067 G1068 P1069 L1070 V1071 F1072 F1073 R1074 S1075 D1076 T1077 T1078 A1079 T1080

E1081 E1082 G1083 D1084 K1085 V1086 I1087 G1088 A1089 V1090 W1091 N1092 P1093 T1094 L1095 V1096 K1097 R1098 K1099 W1100 R1101 V1102 N1103 L1104 P1105 T1106 S1107 Y1108 K1109 P1110 V1111 ALA GLY GLY LYS ASP GLU SER GLU ASP GLU ASP GLU ASP GLU ASP GLU ASP GLY SER GLU ARG GLU LYS GLU ARG GLU GLY GLU GLY

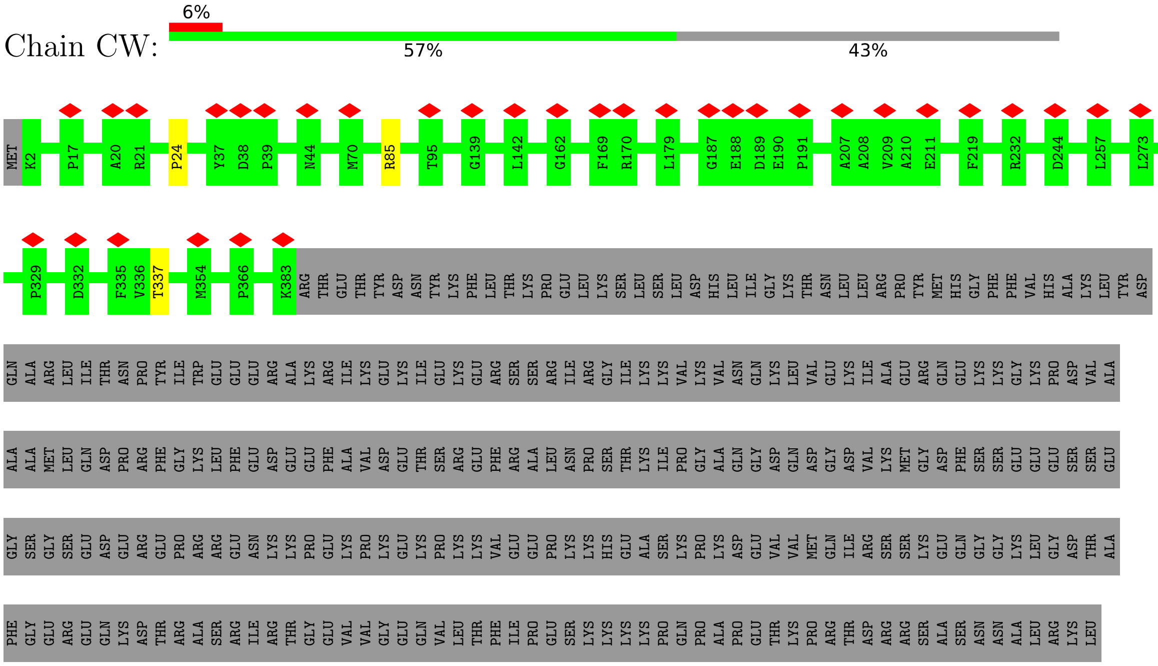
ARG VAL GLU VAL GLU VAL ASN ARG GLU GLY ILE LEU ALA GLU VAL ALA ARG ILE ALA GLY GLU VAL VAL GLU ARG ILE GLU VAL LYS GLY LEU

- Molecule 52: Rrp7

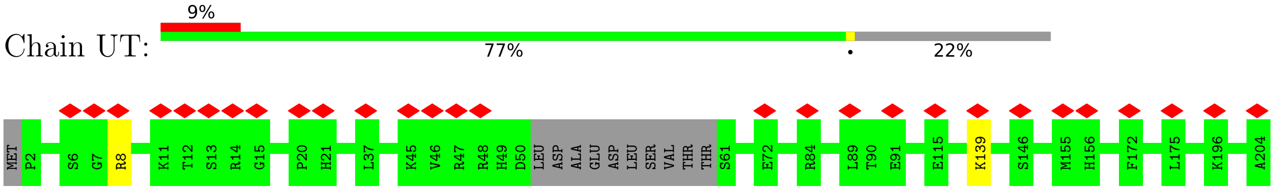
Chain CV:

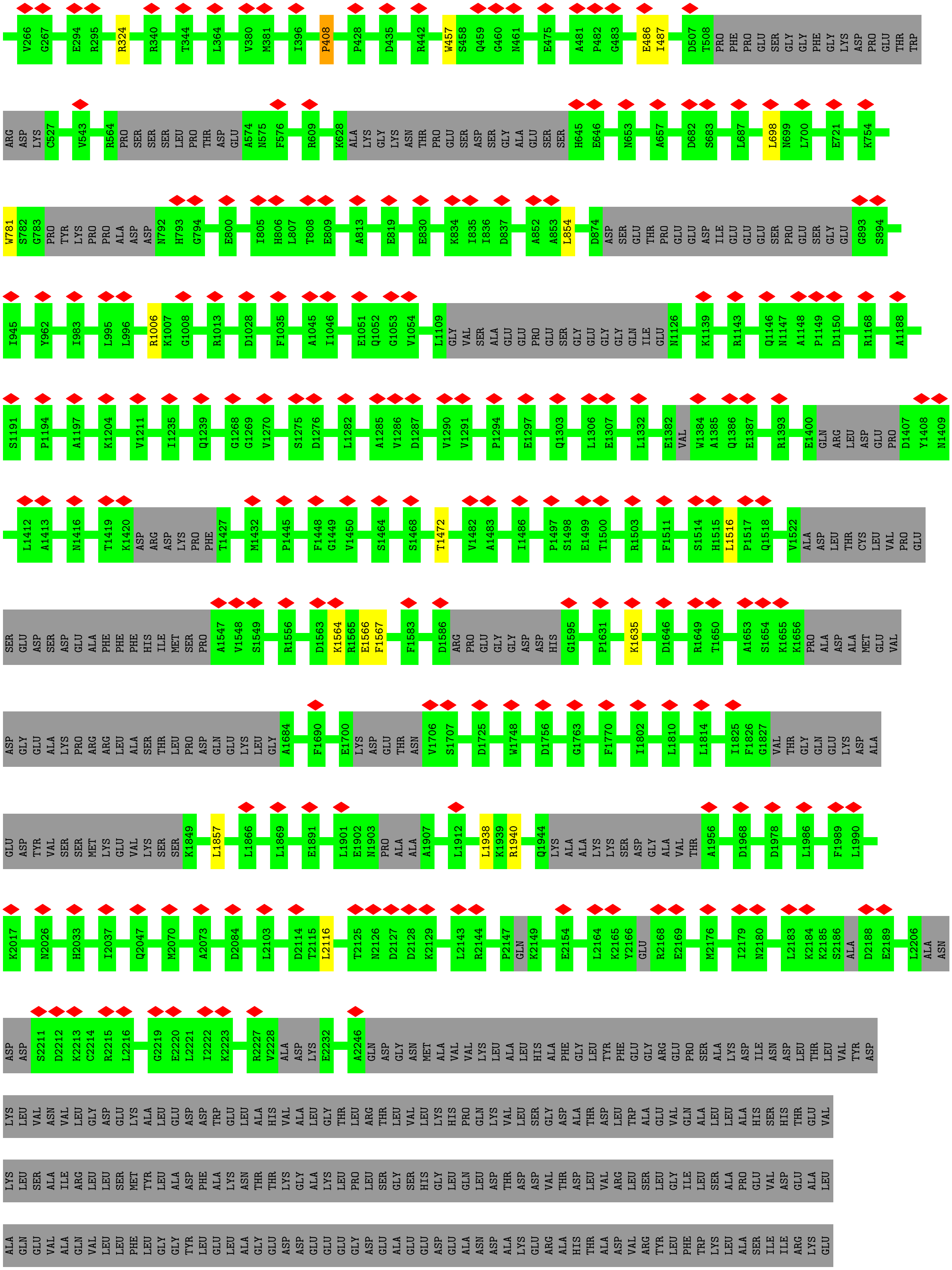


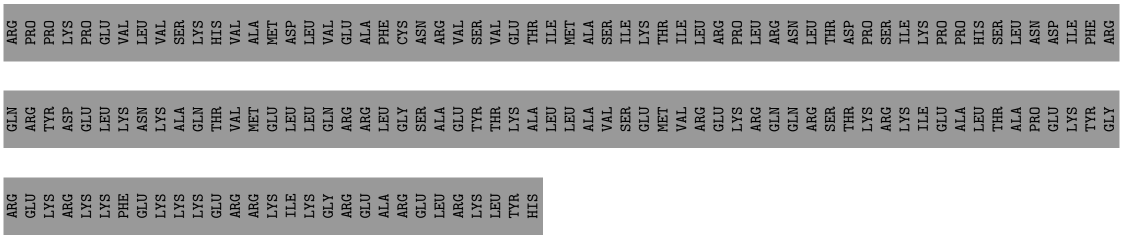
- Molecule 53: Ribosome biogenesis protein ENP2



- Molecule 54: Utp20

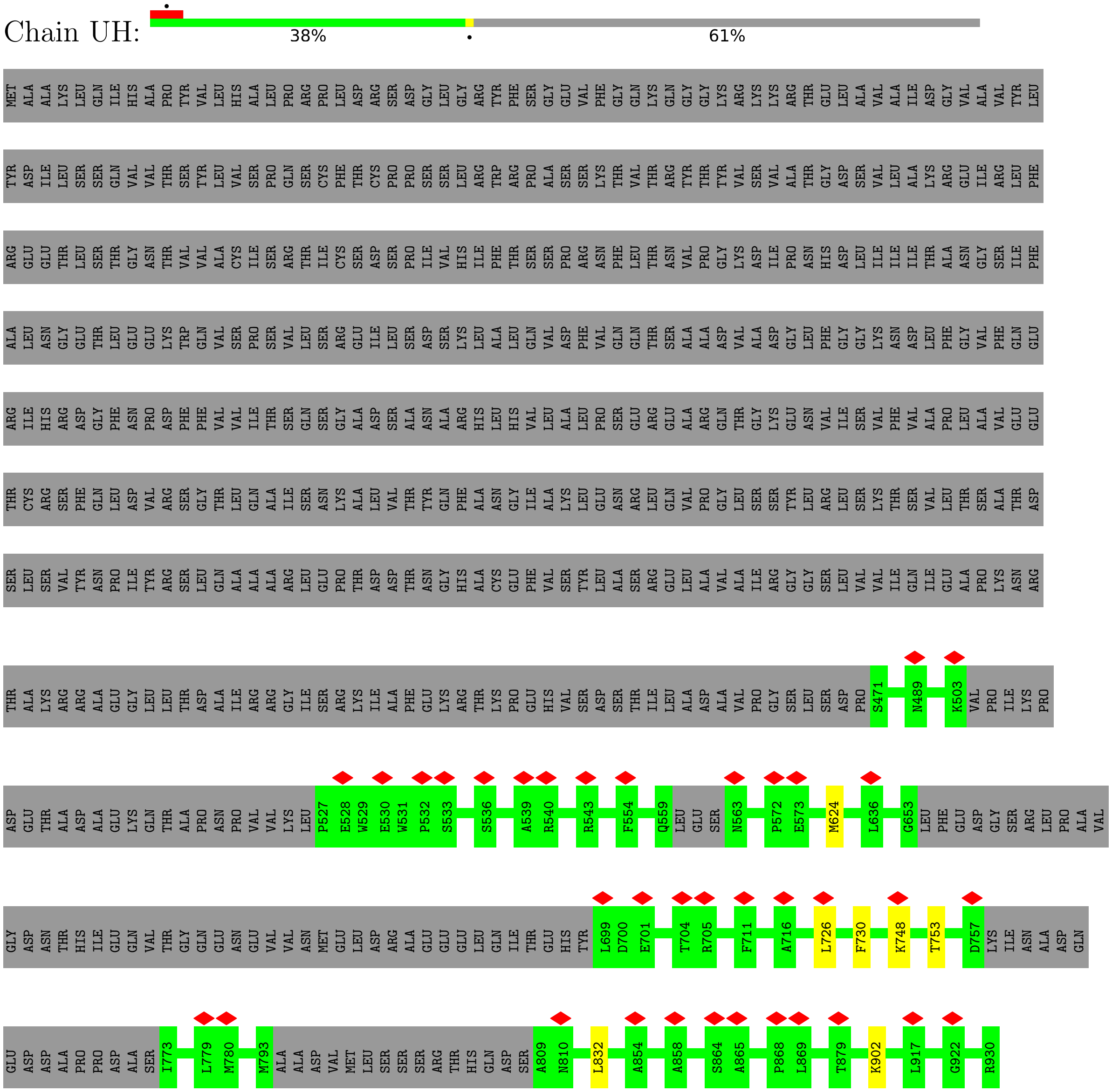



V266 G267 E294 R295 R324 R340 T344 L364 V380 M381 I396 P408 P428 D435 R442 W457 S458 Q459 G460 N461 E475 A481 P482 G483 E486 I487 D507 T508 PRO PHE PRO GLU SER GLY GLY PHE GLY LYS ASP PRO GLU THR TRP
ARG ASP LYS C527 V543 R564 PRO SER SER SER LEU PRO THR ASP GLU A574 N575 F576 R609 K628 ALA LYS GLY LYS ASN THR PRO GLU SER ASP SER GLY ALA GLU SER SER H645 E646 N653 A657 D682 S683 L687 L698 N699 L700 E721 K754
W781 S782 G783 PRO TYR LYS PRO PRO ALA ASP ASP N792 H793 G794 E800 I805 H806 L807 T808 E809 A813 E819 E830 K834 I835 I836 D837 A852 A853 L854 D874 ASP SER GLU THR PRO GLU GLU ASP ILE GLU GLU GLU SER PRO GLU SER GLY GLU G893 S894
I945 Y962 I983 L995 L996 R1006 K1007 G1008 R1013 D1028 F1035 A1045 I1046 E1051 Q1052 G1053 V1054 L1109 GLY VAL SER ALA GLU GLU PRO GLU SER GLY GLU GLY GLY GLN ILE GLU N1126 K1139 R1143 Q1146 N1147 A1148 P1149 D1150 R1168 A1188
S1191 P1194 A1197 K1204 V1211 I1235 Q1239 G1268 G1269 V1270 S1275 D1276 L1282 A1285 V1286 D1287 V1290 V1291 P1294 E1297 Q1303 L1306 E1307 L1332 E1382 VAL W1384 A1385 Q1386 E1387 R1393 E1400 GLN ARG LEU ASP GLU PRO D1407 Y1408 N1409
L1412 A1413 N1416 T1419 K1420 ASP ARG ASP LYS PRO PHE T1427 M1432 P1445 F1448 G1449 V1450 S1464 S1468 T1472 V1482 A1483 I1486 P1497 S1498 E1499 T1500 R1503 F1511 S1514 H1515 L1516 P1517 Q1518 V1522 ALA ASP LEU THR CYS LEU VAL PRO GLU
SER GLU ASP SER ASP GLU ALA PHE PHE PHE HIS ILE MET SER PRO A1547 V1548 S1549 R1556 D1563 K1564 R1565 E1566 F1567 F1583 D1586 ARG PRO GLU GLY GLY ASP ASP HIS G1595 P1631 K1635 D1646 R1649 T1650 A1653 S1654 K1655 K1656 PRO ALA ASP ALA MET GLU VAL
ASP GLY GLU ALA LYS PRO ARG ARG LEU ALA SER THR LEU PRO ASP GLN GLU LYS LEU GLY A1684 F1690 E1700 LYS ASP GLU THR ASN V1706 S1707 D1725 W1748 D1756 G1763 F1770 I1802 L1810 L1814 I1825 F1826 G1827 VAL THR GLY GLN GLU LYS ASP ALA
GLU ASP TYR VAL SER SER MET LYS GLU VAL LYS SER SER K1849 L1857 L1866 L1869 E1891 L1901 E1902 N1903 PRO ALA ALA A1907 L1912 L1938 K1939 R1940 Q1944 LYS ALA ALA LYS LYS SER ASP GLY ALA VAL THR A1956 D1968 D1978 L1986 F1989 L1990
K2017 N2026 H2033 I2037 Q2047 M2070 A2073 D2084 L2103 D2114 T2115 L2116 T2125 N2126 D2127 D2128 K2129 L2143 R2144 P2147 GLN K2149 E2154 L2164 K2165 Y2166 GLU R2168 E2169 M2176 I2179 N2180 L2183 K2184 K2185 S2186 ALA D2188 E2189 L2206 ALA ASN
ASP ASP S2211 D2212 K2213 C2214 R2215 L2216 G2219 E2220 L2221 I2222 K2223 R2227 V2228 ALA ASP LYS E2232 A2246 GLN ASP GLY ASN MET ALA VAL VAL LYS LEU ALA LEU HIS ALA PHE GLY LEU TYR PHE GLU GLY ARG GLU PRO SER ALA LYS ASP ILE ASN ASP LEU THR LEU VAL TYR ASP
LYS LEU VAL ASN VAL LEU GLY ASP GLU LYS ALA LEU GLU ASP ASP TRP GLU LEU ALA HIS VAL ALA LEU GLY THR LEU ARG THR LEU VAL LEU LYS HIS PRO GLN LYS VAL LEU SER GLY ASP ALA THR ASP LEU TRP ALA GLU VAL GLN ALA LEU LEU ALA HIS SER HIS THR GLU VAL
LYS LEU SER ALA ILE ARG LEU LEU SER MET TYR LEU ALA ASP PHE ALA LYS ASN THR THR LYS GLY ALA LYS LEU PRO LEU SER GLY SER HIS GLY LEU GLN LEU ASP THR ASP ASP VAL THR ASP LEU VAL ARG LEU SER LEU GLY ILE LEU SER ALA PRO GLU VAL ASP GLU ALA LEU
ALA GLN GLU VAL ALA GLN VAL LEU LEU PHE LEU GLY GLY TYR LEU GLU LEU ALA GLY GLU ASP ASP GLU GLU GLU GLY ASP GLU ALA GLU GLU ASP GLU ALA ASN ASP ALA LYS GLU ARG ALA HIS THR ALA ASP VAL ARG TYR LEU PHE TRP LYS LEU ALA SER ILE ILE ARG LYS GLU



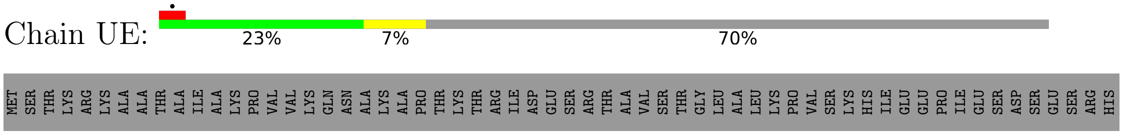
- Molecule 55: Utp8

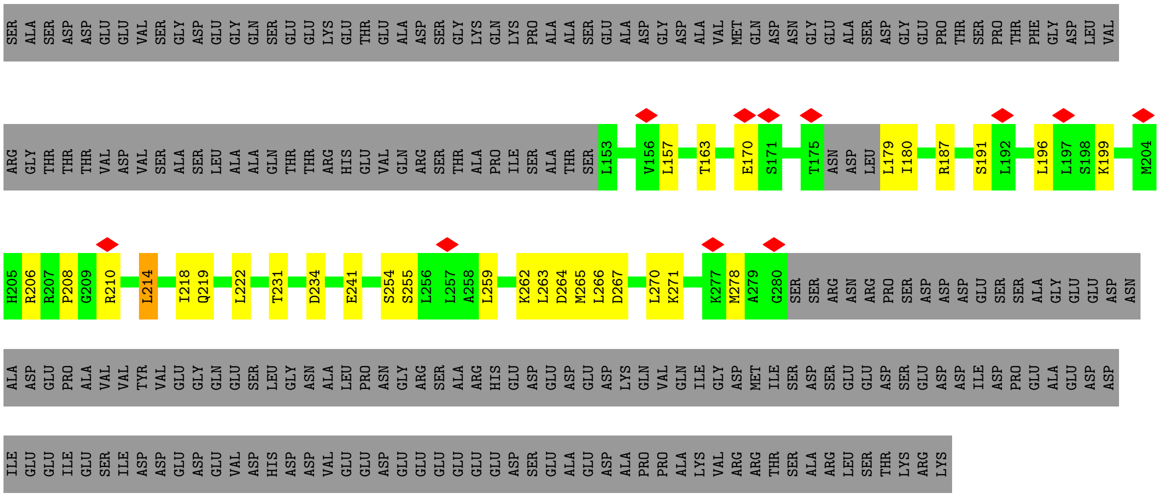
Chain UH:



- Molecule 56: Utp5

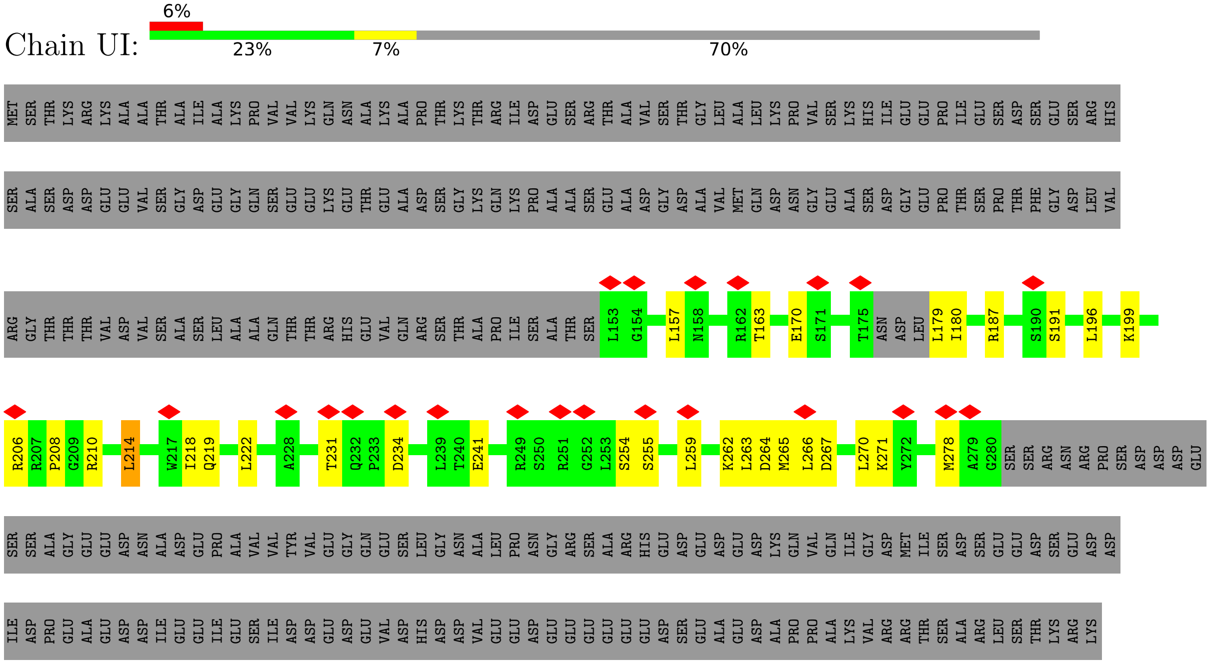
Chain UE:





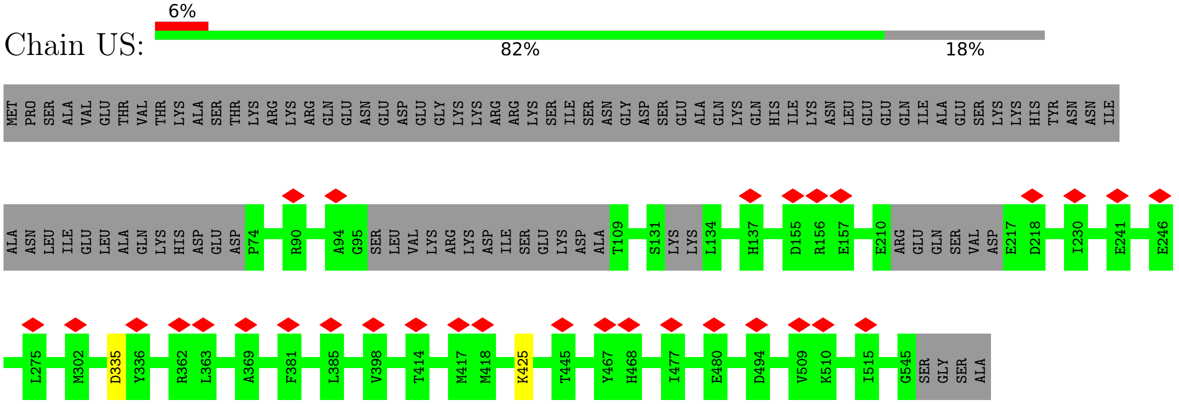
- Molecule 56: Utp5

Chain UI:

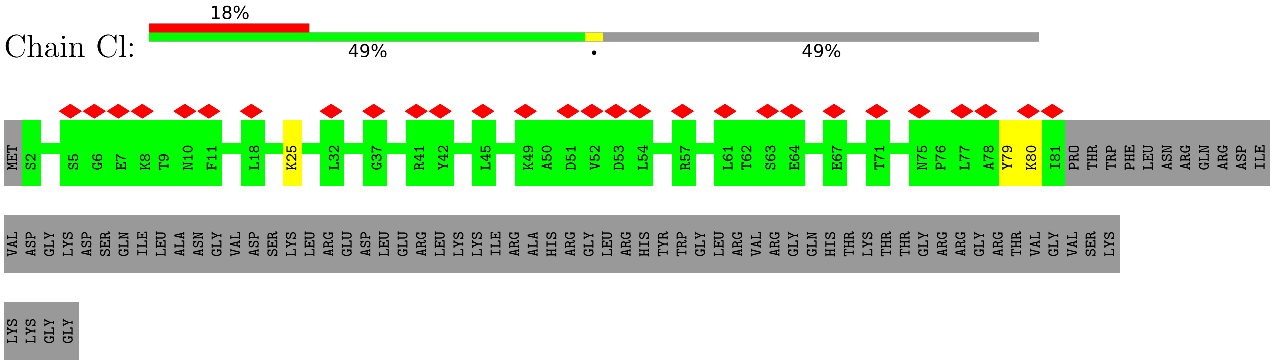


- Molecule 57: Noc4

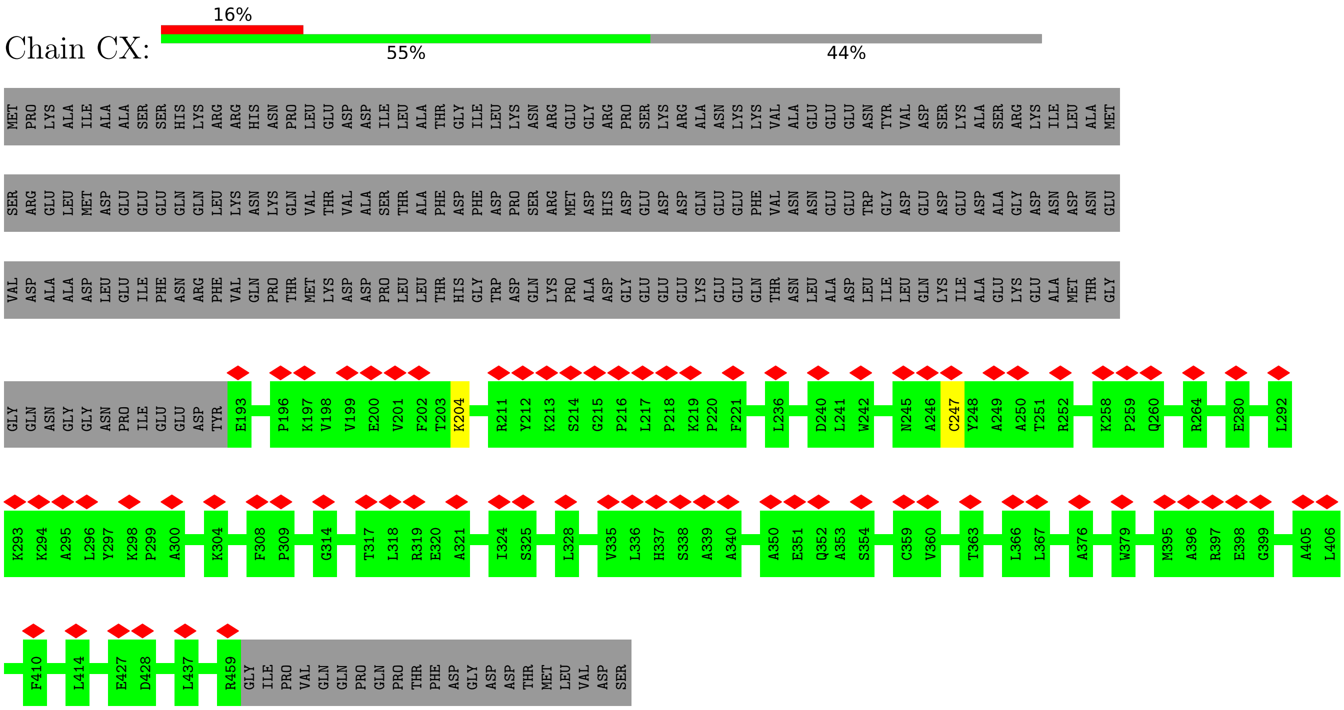
Chain US:



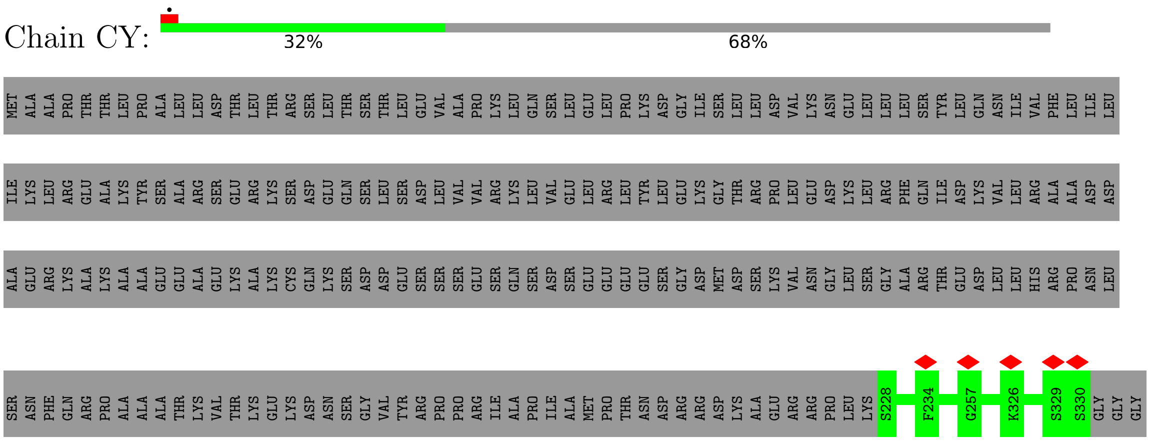
- Molecule 58: Rps18

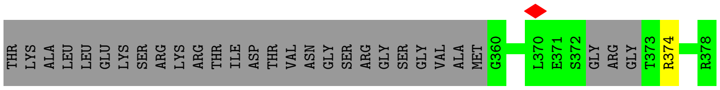


- Molecule 59: Enp1



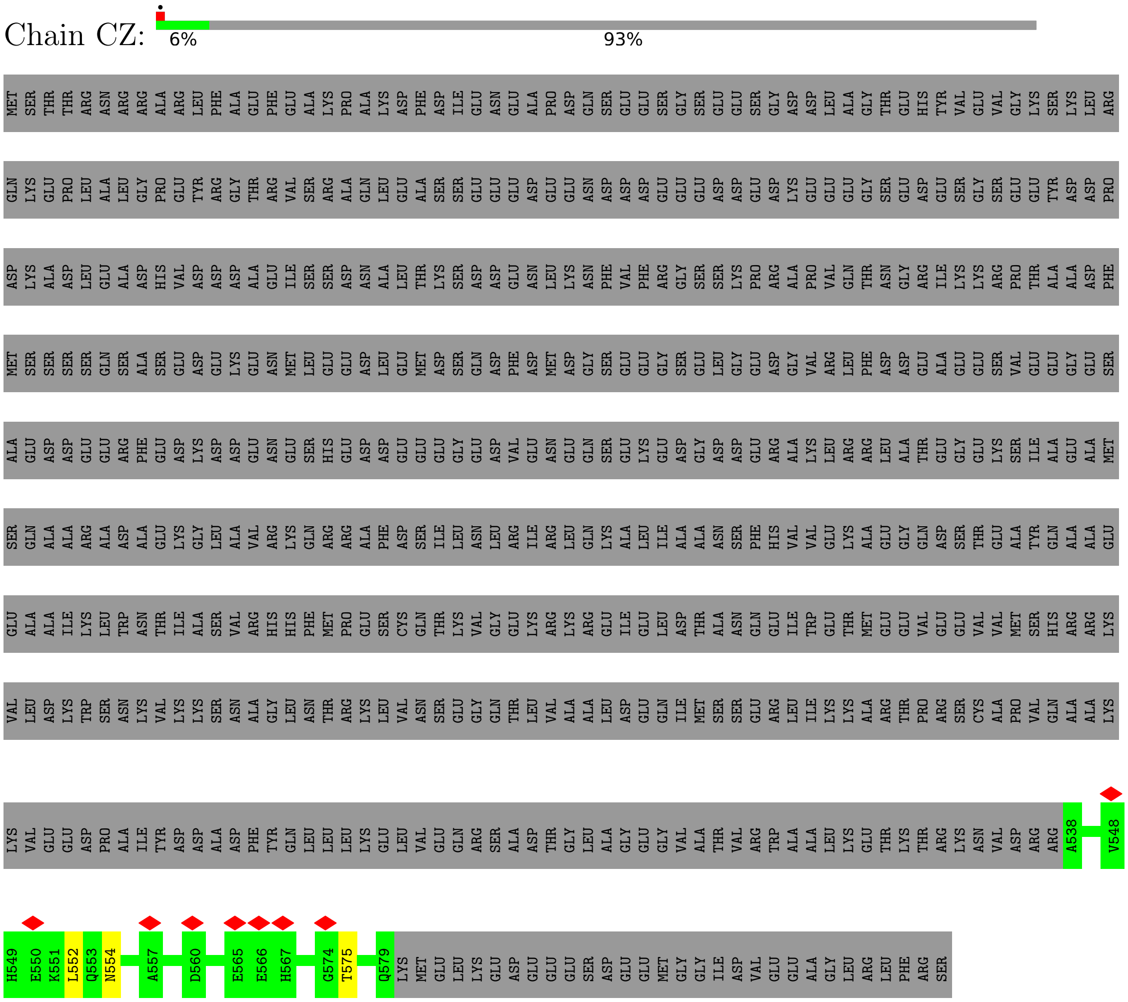
- Molecule 60: U3 small nucleolar ribonucleoprotein protein lcp5-like protein





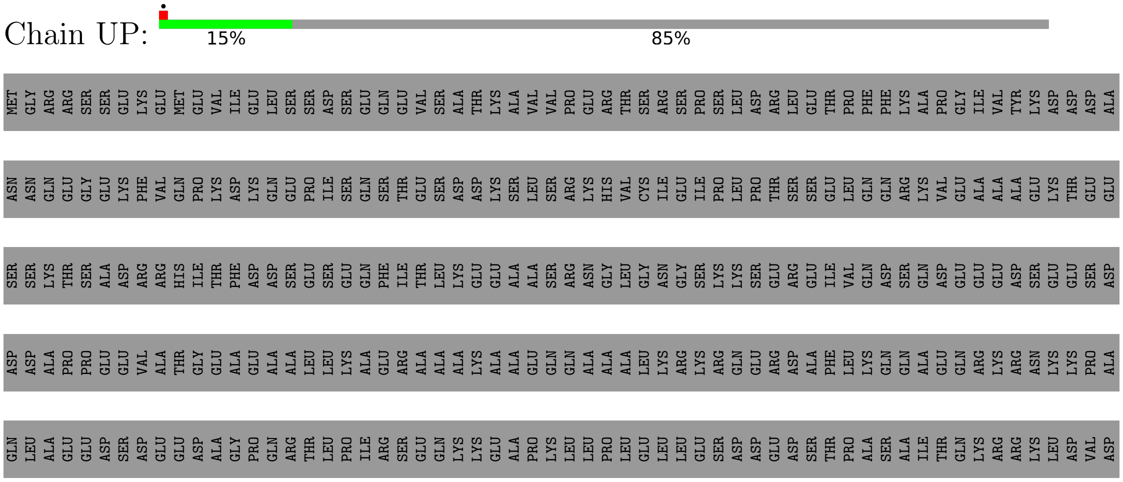
- Molecule 61: Bfr2

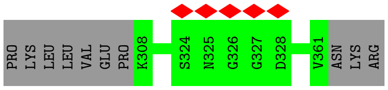
Chain CZ:



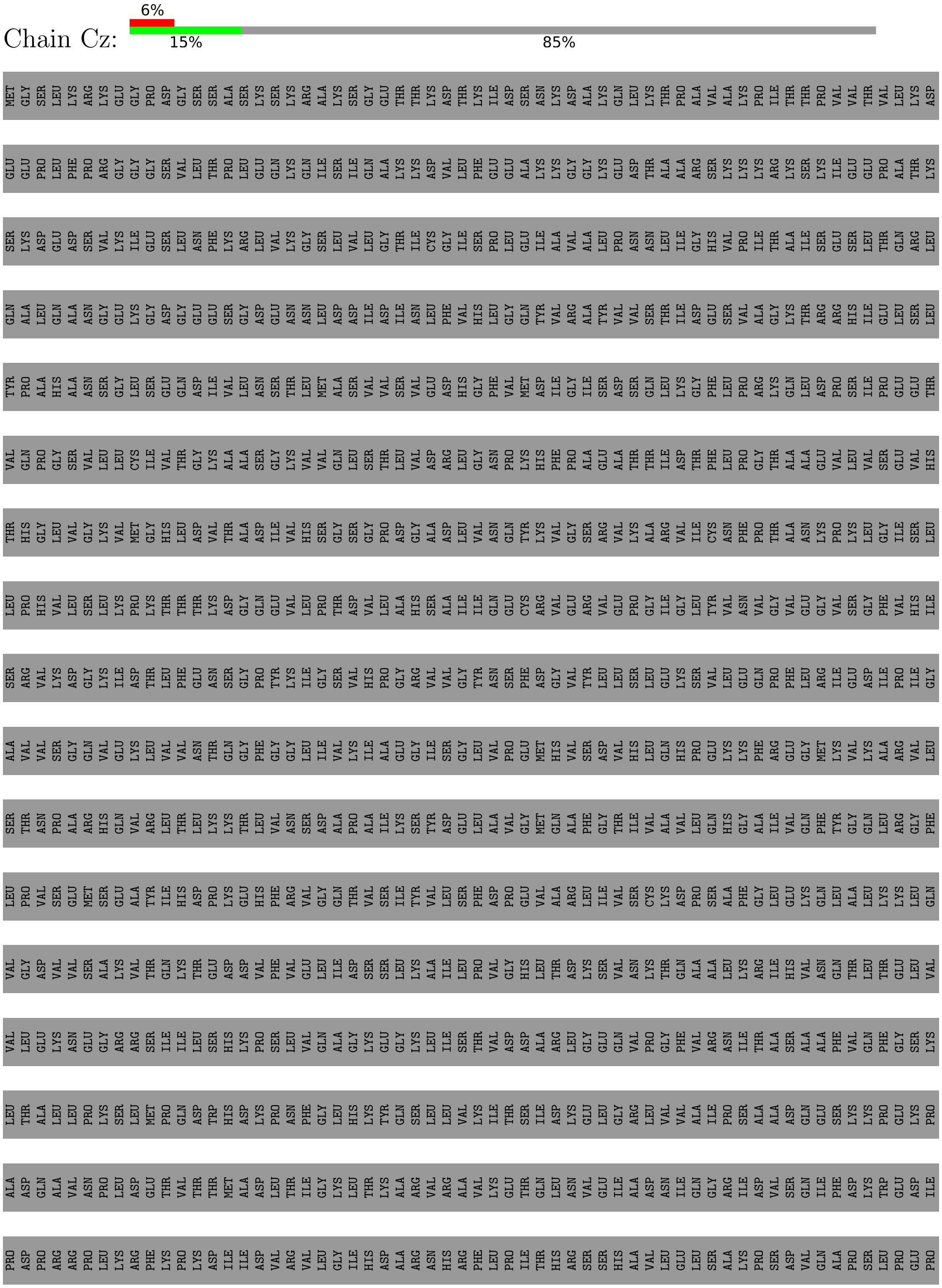
- Molecule 62: Utp16

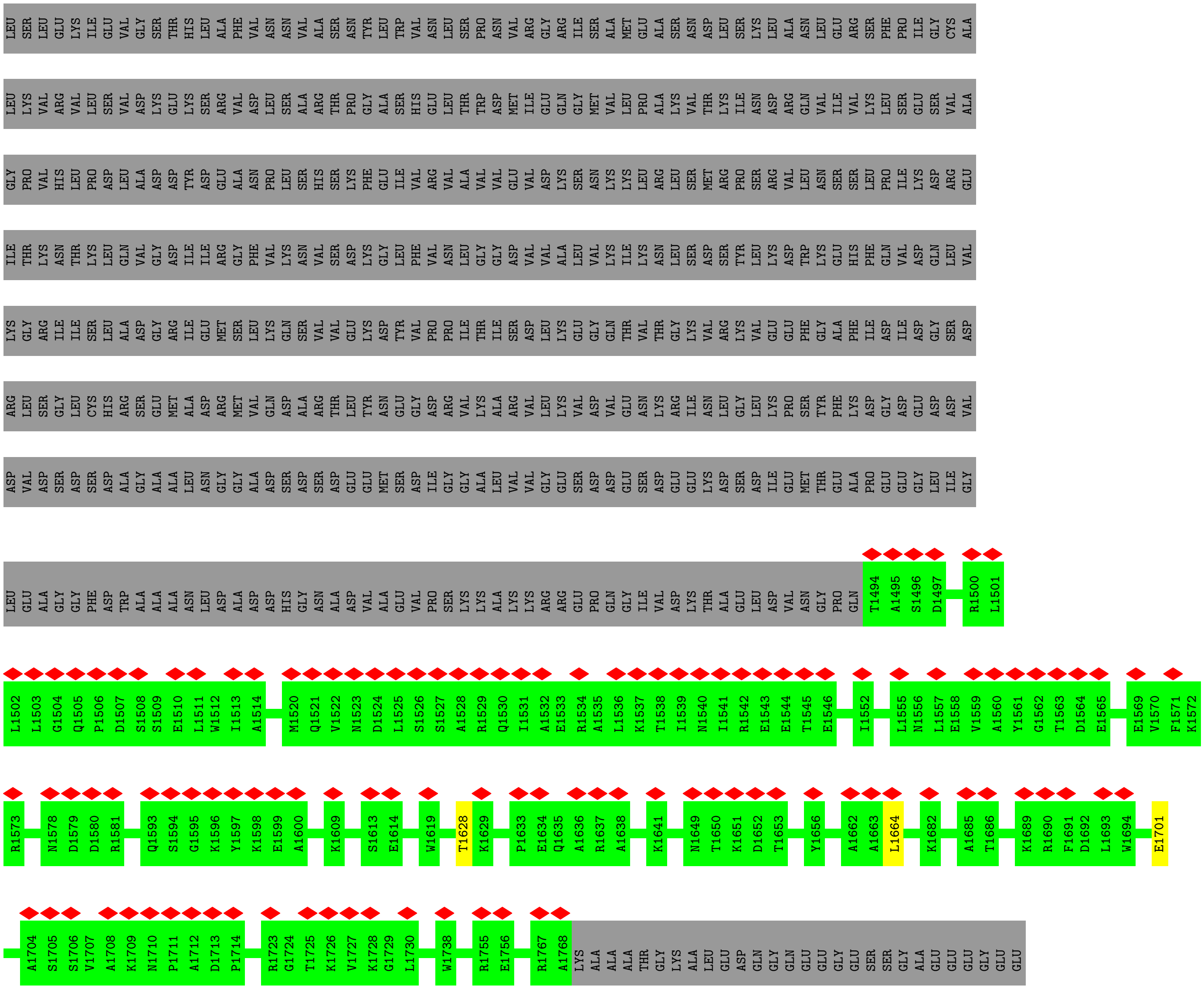
Chain UP:





- Molecule 63: Rrp5




LEU SER LEU GLU LYS ILE GLU VAL GLY SER THR HIS LEU ALA PHE VAL ASN ASN VAL ALA SER ASN TYR LEU TRP VAL ASN LEU SER PRO ASN VAL ARG GLY ARG ILE SER ALA MET GLU ALA SER ASN ASP LEU SER LYS LEU ALA ASN LEU GLU ARG SER PHE PRO ILE GLY CYS ALA
LEU LYS VAL ARG VAL LEU SER VAL ASP LYS GLU LYS SER ARG VAL ASP LEU SER ALA ARG THR PRO GLY ALA SER HIS GLU LEU THR TRP ASP MET ILE GLU GLN GLY MET VAL LEU PRO ALA LYS VAL THR LYS ILE ASN ASP ARG GLN VAL ILE VAL LYS LEU SER GLU SER VAL ALA
GLY PRO VAL HIS LEU PRO ASP LEU ALA ASP ASP TYR ASP GLU ALA ASN PRO LEU SER HIS SER LYS PHE GLU ILE VAL ARG VAL ALA VAL VAL GLU VAL ASP LYS SER ASN LYS LYS LEU ARG LEU SER MET ARG PRO SER ARG VAL LEU ASN SER SER LEU PRO ILE LYS ASP ARG GLU
ILE THR LYS ASN THR LYS LEU GLN VAL GLY ASP ILE ILE ARG GLY PHE VAL LYS ASN VAL SER ASP LYS GLY LEU PHE VAL ASN LEU GLY GLY ASP VAL VAL ALA LEU VAL LYS LYS ILE LYS ASN LEU SER ASP SER TYR LEU LYS ASP TRP LYS GLU HIS PHE GLN VAL ASP GLN LEU VAL
LYS GLY ARG ILE ILE SER LEU ALA ASP GLY ARG ILE GLU MET SER LEU LYS GLN SER VAL VAL GLU LYS ASP TYR VAL PRO PRO ILE THR ILE SER ASP LEU LYS GLU GLY GLN THR VAL THR GLY LYS VAL ARG LYS VAL GLU GLU PHE GLY ALA PHE ILE ASP ILE ASP GLY SER ASP
ARG LEU SER GLY LEU CYS HIS ARG SER GLU MET ALA ASP ARG MET VAL GLN ASP ALA ARG THR LEU TYR ASN GLU GLY ASP ARG VAL LYS ALA ARG VAL LEU LYS VAL ASP VAL GLU ASN LYS ARG ILE ASN LEU GLY LEU LYS PRO SER TYR PHE LYS ASP GLY ASP GLU ASP ASP VAL
ASP VAL ASP SER ASP SER ASP ALA GLY ALA ALA LEU ASN GLY GLY ALA ASP SER ASP SER ASP GLU GLU MET SER ASP ILE GLY GLY ALA LEU VAL VAL GLY GLU SER ASP ASP GLU SER ASP GLU GLU LYS ASP SER ASP ILE GLU MET THR GLU ALA PRO GLU GLU GLY LEU ILE GLY
LEU GLU ALA GLY GLY PHE ASP TRP ALA ALA ALA ASN LEU ASP ALA ASP ASP HIS GLY ASN ALA ASP VAL ALA GLU VAL PRO SER LYS LYS ALA LYS LYS ARG ARG GLU PRO GLN GLY ILE VAL ASP LYS THR ALA GLU LEU ASP VAL ASN GLY PRO GLN T1494 A1495 S1496 D1497 R1500 L1501
L1502 L1503 G1504 Q1505 P1506 D1507 S1508 S1509 E1510 L1511 W1512 I1513 A1514 M1520 Q1521 V1522 N1523 D1524 L1525 S1526 S1527 A1528 R1529 Q1530 I1531 A1532 E1533 R1534 A1535 L1536 K1537 T1538 I1539 N1540 I1541 R1542 E1543 E1544 T1545 E1546 I1552 L1555 N1556 L1557 E1558 V1559 A1560 Y1561 G1562 T1563 D1564 E1565 E1569 V1570 F1571 K1572
R1573 N1578 D1579 D1580 R1581 Q1593 S1594 G1595 K1596 Y1597 K1598 E1599 A1600 K1609 S1613 E1614 W1619 T1628 K1629 P1633 E1634 Q1635 A1636 R1637 A1638 K1641 N1649 T1650 K1651 D1652 T1653 Y1656 A1662 A1663 L1664 K1682 A1685 T1686 K1689 R1690 F1691 D1692 L1693 W1694 E1701
A1704 S1705 S1706 V1707 A1708 K1709 N1710 P1711 A1712 D1713 P1714 R1723 G1724 T1725 K1726 V1727 K1728 G1729 L1730 W1738 R1755 E1756 R1767 A1768 LYS ALA ALA ALA THR GLY LYS ALA LEU GLU ASP GLN GLY GLN GLU GLU GLY GLU SER SER GLY ALA GLU GLU GLY GLU

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24283	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.834	Depositor
Minimum map value	-0.505	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	520.32, 520.32, 520.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	UA	0.55	2/6521 (0.0%)	0.71	2/8867 (0.0%)
2	UB	0.37	0/4154	0.56	1/5583 (0.0%)
3	UC	0.59	0/595	0.65	0/786
4	UD	0.33	0/6211	0.58	1/8408 (0.0%)
5	UF	0.34	0/2657	0.53	0/3596
6	UG	0.49	0/3790	0.65	1/5120 (0.0%)
7	UJ	0.33	0/8567	0.59	2/11619 (0.0%)
8	UK	0.64	2/1701 (0.1%)	0.67	1/2251 (0.0%)
9	UL	0.34	0/6299	0.63	2/8531 (0.0%)
10	UM	0.30	0/5366	0.59	2/7282 (0.0%)
11	UN	0.38	0/1425	0.57	1/1913 (0.1%)
12	UO	0.36	0/3903	0.61	1/5312 (0.0%)
13	UQ	0.32	0/6136	0.59	3/8348 (0.0%)
14	UR	0.40	0/3564	0.61	0/4816
15	UU	0.43	0/6903	0.63	2/9392 (0.0%)
16	UX	0.61	0/1493	0.70	1/2011 (0.0%)
17	UZ	0.40	0/1857	0.62	0/2526
18	CA	0.53	0/1814	0.65	1/2456 (0.0%)
18	CB	0.36	0/1853	0.59	0/2511
19	CC	0.38	0/2911	0.58	1/3937 (0.0%)
20	CD	0.37	0/3205	0.62	1/4338 (0.0%)
21	CE	0.46	0/891	0.60	0/1214
21	CF	0.40	0/876	0.66	0/1195
22	CG	0.34	0/3307	0.60	0/4462
23	CH	0.42	0/2939	0.64	1/3988 (0.0%)
24	CI	0.59	3/6631 (0.0%)	0.70	4/8943 (0.0%)
25	CJ	0.74	1/1462 (0.1%)	0.76	0/1967
26	CK	0.71	1/2376 (0.0%)	0.81	3/3214 (0.1%)
27	CL	0.48	0/1812	0.59	0/2437
28	CM	0.56	3/3573 (0.1%)	0.69	1/4829 (0.0%)
29	CN	0.33	0/1797	0.60	0/2443
29	CO	0.32	0/1714	0.60	2/2325 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	CP	0.30	0/1528	0.63	1/2057 (0.0%)
31	CQ	0.29	0/1379	0.57	0/1850
32	CR	0.37	1/6108 (0.0%)	0.74	13/8266 (0.2%)
32	CS	0.37	1/6108 (0.0%)	0.74	13/8266 (0.2%)
33	CT	0.53	0/1053	0.62	0/1413
34	Cb	0.31	0/1890	0.59	0/2548
35	Cc	0.44	0/1485	0.59	0/2008
36	Cd	0.32	0/1850	0.58	0/2474
37	Ce	0.35	0/1298	0.67	1/1750 (0.1%)
38	Cf	0.30	0/1429	0.56	0/1915
39	Cg	0.46	0/1259	0.60	0/1687
40	Ch	0.28	0/412	0.57	0/549
41	Ci	0.31	0/801	0.60	0/1087
42	Cj	0.58	0/958	0.72	0/1293
43	Ck	0.31	0/1190	0.53	0/1592
44	Cm	0.40	0/1001	0.59	0/1345
45	Cn	0.81	2/712 (0.3%)	0.79	0/954
46	Co	0.34	0/754	0.59	0/1011
47	Cp	0.34	0/458	0.65	0/617
48	CU	0.35	0/887	0.61	1/1178 (0.1%)
49	C1	0.83	45/35454 (0.1%)	1.37	556/55209 (1.0%)
50	C2	0.88	3/5459 (0.1%)	1.47	88/8498 (1.0%)
51	UV	0.33	0/8638	0.66	6/11725 (0.1%)
52	CV	0.34	0/1172	0.71	0/1592
53	CW	0.32	0/2996	0.63	1/4075 (0.0%)
54	UT	0.31	0/16314	0.57	4/22075 (0.0%)
55	UH	0.34	0/2852	0.60	3/3846 (0.1%)
56	UE	0.38	0/980	0.78	2/1316 (0.2%)
56	UI	0.38	0/980	0.78	2/1316 (0.2%)
57	US	0.33	0/3765	0.56	1/5100 (0.0%)
58	Cl	0.32	0/638	0.65	0/857
59	CX	0.27	0/2172	0.51	0/2946
60	CY	0.36	0/982	0.61	0/1298
61	CZ	0.33	0/362	0.73	1/483 (0.2%)
62	UP	0.33	0/428	0.57	0/570
63	Cz	0.31	0/2310	0.54	0/3120
All	All	0.51	64/226365 (0.0%)	0.84	727/314506 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	UA	0	10
5	UF	0	1
6	UG	0	2
8	UK	0	2
9	UL	0	2
10	UM	0	4
11	UN	0	1
12	UO	0	1
13	UQ	0	2
15	UU	0	4
16	UX	0	2
17	UZ	0	2
18	CB	0	1
21	CE	0	1
21	CF	0	2
23	CH	0	1
24	CI	0	6
25	CJ	0	2
26	CK	0	1
28	CM	0	1
29	CO	0	2
32	CR	0	1
32	CS	0	1
37	Ce	0	1
41	Ci	0	1
42	Cj	0	3
45	Cn	0	1
46	Co	0	1
51	UV	0	4
52	CV	0	2
54	UT	0	5
55	UH	0	1
58	Cl	0	1
60	CY	0	1
63	Cz	0	1
All	All	0	74

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	UA	488	TRP	CB-CG	-8.05	1.35	1.50
50	C2	57	A	N7-C5	-7.73	1.34	1.39
32	CS	515	GLN	CA-CB	7.33	1.70	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	CR	515	GLN	CA-CB	7.33	1.70	1.53
49	C1	1154	A	N9-C4	-6.99	1.33	1.37
28	CM	321	TYR	CD2-CE2	-6.89	1.29	1.39
49	C1	1140	A	N7-C5	-6.78	1.35	1.39
49	C1	1129	A	N9-C4	-6.78	1.33	1.37
49	C1	2066	A	N9-C4	-6.78	1.33	1.37
28	CM	94	TRP	CB-CG	-6.71	1.38	1.50
49	C1	255	G	N3-C4	-6.67	1.30	1.35
49	C1	1137	G	N7-C5	-6.61	1.35	1.39
45	Cn	136	TRP	CB-CG	-6.30	1.39	1.50
49	C1	1158	G	N9-C4	-6.30	1.32	1.38
49	C1	2071	G	C6-N1	-6.29	1.35	1.39
49	C1	1140	A	C5-C6	-6.21	1.35	1.41
49	C1	1138	C	N1-C6	-6.11	1.33	1.37
49	C1	2173	G	N7-C5	-6.01	1.35	1.39
49	C1	2172	C	N1-C6	-5.96	1.33	1.37
49	C1	1140	A	N3-C4	-5.95	1.31	1.34
49	C1	2176	A	N3-C4	-5.91	1.31	1.34
49	C1	407	A	N7-C5	-5.91	1.35	1.39
49	C1	2179	C	N3-C4	-5.91	1.29	1.33
49	C1	2177	G	C6-N1	-5.90	1.35	1.39
49	C1	1155	G	C5-C6	-5.88	1.36	1.42
24	CI	987	VAL	CB-CG1	-5.88	1.40	1.52
49	C1	1145	G	C6-N1	-5.86	1.35	1.39
49	C1	2174	C	N1-C6	-5.76	1.33	1.37
24	CI	977	PHE	CB-CG	-5.69	1.41	1.51
1	UA	488	TRP	CA-C	-5.65	1.38	1.52
49	C1	1158	G	C5-C4	-5.63	1.34	1.38
49	C1	2180	A	N7-C5	-5.59	1.35	1.39
49	C1	2180	A	C5-C6	-5.59	1.36	1.41
45	Cn	92	CYS	CB-SG	-5.58	1.72	1.81
49	C1	1138	C	N3-C4	-5.54	1.30	1.33
49	C1	2188	G	N7-C5	-5.51	1.35	1.39
49	C1	2190	G	N7-C5	-5.50	1.35	1.39
49	C1	1156	C	N1-C6	-5.49	1.33	1.37
49	C1	1179	G	C6-N1	-5.47	1.35	1.39
26	CK	287	TYR	CD1-CE1	-5.47	1.31	1.39
49	C1	1146	G	N7-C5	-5.43	1.35	1.39
49	C1	2071	G	N1-C2	-5.42	1.33	1.37
49	C1	1148	G	N9-C4	-5.32	1.33	1.38
24	CI	851	TRP	CB-CG	-5.29	1.40	1.50
49	C1	1148	G	C5-C6	-5.29	1.37	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	C1	1175	A	N7-C5	-5.28	1.36	1.39
49	C1	2177	G	N3-C4	-5.27	1.31	1.35
49	C1	2177	G	N7-C5	-5.24	1.36	1.39
49	C1	363	G	C6-N1	-5.22	1.35	1.39
8	UK	34	TYR	CD1-CE1	-5.21	1.31	1.39
8	UK	34	TYR	CD2-CE2	-5.21	1.31	1.39
49	C1	1140	A	C5-C4	-5.19	1.35	1.38
49	C1	2175	A	C6-N1	-5.16	1.31	1.35
50	C2	32	G	N7-C5	-5.15	1.36	1.39
49	C1	1138	C	C4-C5	-5.13	1.38	1.43
49	C1	1155	G	C5-C4	-5.12	1.34	1.38
49	C1	407	A	N3-C4	-5.10	1.31	1.34
50	C2	59	A	N7-C5	-5.10	1.36	1.39
49	C1	1145	G	C5-C6	-5.10	1.37	1.42
49	C1	353	G	N9-C8	-5.08	1.34	1.37
49	C1	1139	A	N7-C5	-5.07	1.36	1.39
25	CJ	113	VAL	CB-CG2	-5.07	1.42	1.52
49	C1	1146	G	C5-C4	-5.02	1.34	1.38
28	CM	310	TRP	CB-CG	-5.01	1.41	1.50

All (727) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C2	2	G	O5'-P-OP1	-32.38	71.84	110.70
50	C2	2	G	OP1-P-OP2	-26.27	80.19	119.60
24	CI	995	VAL	C-N-CA	19.84	171.29	121.70
50	C2	2	G	O5'-P-OP2	17.99	132.29	110.70
49	C1	2074	C	N1-C2-O2	16.01	128.50	118.90
50	C2	1	A	OP2-P-O3'	-13.64	75.20	105.20
49	C1	1138	C	N3-C2-O2	-13.20	112.66	121.90
49	C1	1155	G	C5-C6-O6	-13.06	120.76	128.60
50	C2	1	A	OP1-P-O3'	13.01	133.82	105.20
49	C1	2168	U	N1-C2-O2	12.86	131.80	122.80
49	C1	1138	C	C2-N1-C1'	12.57	132.63	118.80
49	C1	2168	U	N3-C2-O2	-12.51	113.44	122.20
49	C1	942	U	N3-C2-O2	-12.29	113.60	122.20
49	C1	55	G	OP1-P-O3'	-11.86	79.11	105.20
49	C1	45	U	OP1-P-O3'	-11.29	80.37	105.20
49	C1	2217	C	C2-N1-C1'	11.14	131.05	118.80
49	C1	2217	C	N1-C2-O2	11.00	125.50	118.90
49	C1	2069	G	C8-N9-C4	-10.83	102.07	106.40
32	CR	426	LEU	CA-CB-CG	10.81	140.16	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	CS	426	LEU	CA-CB-CG	10.81	140.16	115.30
49	C1	758	U	N3-C2-O2	-10.75	114.67	122.20
49	C1	2074	C	C2-N1-C1’	10.75	130.62	118.80
49	C1	618	C	N1-C2-O2	10.68	125.31	118.90
49	C1	2074	C	N3-C2-O2	-10.63	114.46	121.90
49	C1	160	C	C6-N1-C2	-10.44	116.12	120.30
49	C1	1547	C	N1-C2-O2	10.40	125.14	118.90
49	C1	160	C	N3-C2-O2	-10.12	114.82	121.90
49	C1	2168	U	C2-N1-C1’	10.10	129.81	117.70
49	C1	785	U	OP1-P-O3’	-10.04	83.10	105.20
49	C1	1155	G	N1-C6-O6	10.03	125.92	119.90
49	C1	1662	C	N3-C2-O2	-9.94	114.94	121.90
49	C1	258	C	N1-C2-O2	9.81	124.78	118.90
49	C1	786	G	OP1-P-OP2	9.79	134.29	119.60
49	C1	1138	C	N1-C2-O2	9.67	124.70	118.90
49	C1	2074	C	C6-N1-C1’	-9.64	109.24	120.80
49	C1	203	C	N1-C2-O2	9.59	124.65	118.90
57	US	335	ASP	C-N-CA	9.57	145.62	121.70
49	C1	505	C	N3-C2-O2	-9.55	115.22	121.90
50	C2	39	U	N3-C2-O2	-9.54	115.52	122.20
26	CK	235	ASP	CB-CG-OD1	9.39	126.75	118.30
32	CS	372	ILE	C-N-CA	9.38	145.15	121.70
32	CR	372	ILE	C-N-CA	9.37	145.12	121.70
49	C1	1138	C	C6-N1-C1’	-9.32	109.62	120.80
49	C1	45	U	OP2-P-O3’	-9.30	84.74	105.20
49	C1	258	C	C2-N1-C1’	9.27	129.00	118.80
50	C2	140	C	N3-C2-O2	-9.14	115.50	121.90
49	C1	758	U	C2-N1-C1’	9.02	128.52	117.70
32	CR	41	LEU	CA-CB-CG	9.00	135.99	115.30
32	CS	41	LEU	CA-CB-CG	8.99	135.98	115.30
49	C1	255	G	C8-N9-C4	-8.99	102.81	106.40
49	C1	255	G	C2-N3-C4	-8.89	107.45	111.90
49	C1	942	U	N1-C2-O2	8.79	128.96	122.80
49	C1	1167	C	N1-C2-O2	8.64	124.08	118.90
49	C1	134	C	C6-N1-C2	-8.64	116.85	120.30
49	C1	618	C	N3-C2-O2	-8.60	115.88	121.90
49	C1	1155	G	C4-C5-N7	8.52	114.21	110.80
49	C1	1550	U	C2-N1-C1’	8.51	127.92	117.70
49	C1	2217	C	C6-N1-C1’	-8.51	110.59	120.80
49	C1	618	C	C2-N1-C1’	8.49	128.14	118.80
49	C1	2181	U	N3-C2-O2	-8.48	116.27	122.20
49	C1	927	C	N3-C2-O2	-8.43	116.00	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	1547	C	C2-N1-C1'	8.38	128.02	118.80
49	C1	1148	G	C4-C5-N7	8.38	114.15	110.80
49	C1	255	G	N3-C2-N2	-8.36	114.05	119.90
49	C1	2173	G	C8-N9-C4	-8.33	103.07	106.40
49	C1	750	C	N1-C2-O2	8.32	123.89	118.90
49	C1	1077	U	N1-C2-O2	8.31	128.62	122.80
49	C1	768	C	C2-N1-C1'	8.29	127.92	118.80
49	C1	2106	U	C2-N1-C1'	8.29	127.65	117.70
49	C1	255	G	N1-C2-N3	8.29	128.87	123.90
49	C1	370	C	N1-C2-O2	8.28	123.87	118.90
49	C1	785	U	OP2-P-O3'	-8.27	87.00	105.20
32	CS	84	ARG	NE-CZ-NH1	8.26	124.43	120.30
53	CW	24	PRO	CA-N-CD	-8.25	99.95	111.50
49	C1	2084	C	N3-C2-O2	-8.24	116.13	121.90
32	CR	84	ARG	NE-CZ-NH1	8.22	124.41	120.30
49	C1	1167	C	C6-N1-C2	-8.19	117.02	120.30
49	C1	159	C	C6-N1-C2	-8.18	117.03	120.30
49	C1	471	C	N3-C2-O2	-8.13	116.21	121.90
50	C2	267	C	N3-C2-O2	-8.13	116.21	121.90
49	C1	413	C	C6-N1-C2	-8.05	117.08	120.30
49	C1	2202	C	N1-C2-O2	8.05	123.73	118.90
49	C1	1747	A	C6-N1-C2	-8.03	113.78	118.60
49	C1	471	C	C6-N1-C2	-7.98	117.11	120.30
49	C1	233	C	C2-N1-C1'	7.97	127.57	118.80
32	CS	162	LEU	CA-CB-CG	7.94	133.56	115.30
32	CR	162	LEU	CA-CB-CG	7.94	133.55	115.30
49	C1	408	C	C5-C6-N1	7.92	124.96	121.00
49	C1	1486	G	C8-N9-C4	-7.92	103.23	106.40
49	C1	1761	C	C6-N1-C2	-7.91	117.14	120.30
49	C1	34	C	N1-C2-O2	7.89	123.64	118.90
49	C1	2182	C	C6-N1-C2	-7.88	117.15	120.30
49	C1	1486	G	N3-C4-C5	-7.87	124.66	128.60
49	C1	68	U	C2-N1-C1'	7.86	127.14	117.70
49	C1	1145	G	C4-C5-N7	7.86	113.94	110.80
49	C1	112	C	N1-C2-O2	7.85	123.61	118.90
49	C1	80	C	N3-C2-O2	-7.85	116.41	121.90
49	C1	408	C	C2-N1-C1'	7.84	127.43	118.80
49	C1	218	G	N3-C4-N9	7.82	130.69	126.00
49	C1	582	G	OP1-P-O3'	7.82	122.39	105.20
49	C1	1145	G	C6-C5-N7	-7.81	125.71	130.40
49	C1	1077	U	N3-C2-O2	-7.80	116.74	122.20
49	C1	1145	G	N3-C4-N9	7.80	130.68	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	1167	C	N3-C2-O2	-7.74	116.48	121.90
49	C1	470	C	N1-C2-O2	7.73	123.54	118.90
54	UT	854	LEU	CA-CB-CG	7.72	133.07	115.30
49	C1	148	C	C6-N1-C2	-7.71	117.22	120.30
49	C1	1027	C	N3-C2-O2	-7.68	116.52	121.90
49	C1	2069	G	N3-C4-C5	-7.66	124.77	128.60
49	C1	2202	C	N3-C2-O2	-7.63	116.56	121.90
49	C1	1138	C	C6-N1-C2	-7.61	117.25	120.30
49	C1	449	C	N3-C2-O2	-7.50	116.65	121.90
49	C1	159	C	N3-C2-O2	-7.49	116.66	121.90
49	C1	692	U	N1-C2-O2	7.48	128.04	122.80
49	C1	2069	G	N7-C8-N9	7.47	116.84	113.10
49	C1	134	C	P-O3'-C3'	7.47	128.66	119.70
49	C1	68	U	N1-C2-O2	7.46	128.02	122.80
49	C1	255	G	N3-C4-N9	-7.45	121.53	126.00
30	CP	213	LEU	CA-CB-CG	7.41	132.35	115.30
49	C1	2179	C	N3-C2-O2	-7.41	116.71	121.90
49	C1	34	C	N3-C2-O2	-7.41	116.71	121.90
50	C2	246	G	C4-N9-C1'	7.41	136.13	126.50
49	C1	134	C	C2-N1-C1'	7.40	126.94	118.80
49	C1	370	C	N3-C2-O2	-7.40	116.72	121.90
49	C1	2217	C	N3-C2-O2	-7.39	116.73	121.90
49	C1	1760	G	N3-C4-N9	7.39	130.43	126.00
51	UV	1058	TYR	CA-CB-CG	7.38	127.41	113.40
50	C2	79	G	C4-C5-N7	7.37	113.75	110.80
49	C1	1662	C	N1-C2-O2	7.35	123.31	118.90
49	C1	2106	U	N1-C2-O2	7.35	127.95	122.80
49	C1	2168	U	C6-N1-C1'	-7.35	110.91	121.20
49	C1	148	C	N3-C2-O2	-7.34	116.76	121.90
15	UU	502	LEU	CA-CB-CG	7.32	132.14	115.30
49	C1	362	G	C8-N9-C4	-7.32	103.47	106.40
49	C1	408	C	C6-N1-C2	-7.32	117.37	120.30
49	C1	989	C	C2-N1-C1'	7.31	126.84	118.80
50	C2	203	C	N3-C2-O2	-7.30	116.79	121.90
49	C1	1145	G	C8-N9-C1'	-7.28	117.53	127.00
49	C1	1758	C	C2-N3-C4	-7.27	116.26	119.90
49	C1	1222	C	N1-C2-O2	7.26	123.26	118.90
49	C1	1114	C	N1-C2-O2	7.26	123.25	118.90
49	C1	137	C	N1-C2-O2	7.22	123.23	118.90
49	C1	995	C	C2-N1-C1'	7.21	126.74	118.80
49	C1	2202	C	C2-N1-C1'	7.21	126.73	118.80
49	C1	1180	C	C6-N1-C2	-7.21	117.42	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	C1	454	C	C2-N1-C1'	7.20	126.72	118.80
49	C1	1167	C	C2-N1-C1'	7.20	126.72	118.80
49	C1	2071	G	C5-C6-N1	7.20	115.10	111.50
50	C2	92	A	C2-N3-C4	7.20	114.20	110.60
49	C1	2182	C	C5-C6-N1	7.19	124.59	121.00
49	C1	1174	C	C6-N1-C2	-7.16	117.44	120.30
49	C1	258	C	C5-C6-N1	7.14	124.57	121.00
49	C1	56	C	OP1-P-OP2	7.12	130.28	119.60
49	C1	1550	U	N1-C2-O2	7.12	127.78	122.80
49	C1	2188	G	C4-N9-C1'	7.11	135.74	126.50
49	C1	158	C	N1-C2-O2	7.11	123.16	118.90
49	C1	346	C	N3-C2-O2	-7.10	116.93	121.90
49	C1	2173	G	N7-C8-N9	7.10	116.65	113.10
50	C2	79	G	N3-C4-N9	7.03	130.22	126.00
49	C1	1486	G	C4-N9-C1'	7.02	135.63	126.50
49	C1	618	C	C6-N1-C2	-7.01	117.50	120.30
49	C1	505	C	N1-C2-O2	6.99	123.09	118.90
49	C1	278	A	O5'-P-OP1	-6.99	99.41	105.70
49	C1	851	U	N3-C2-O2	-6.96	117.33	122.20
49	C1	1081	G	C5-C6-O6	6.96	132.78	128.60
49	C1	1171	C	N1-C2-O2	6.96	123.08	118.90
49	C1	1145	G	C4-N9-C1'	6.95	135.54	126.50
49	C1	258	C	C6-N1-C1'	-6.95	112.46	120.80
49	C1	413	C	C2-N1-C1'	6.95	126.44	118.80
49	C1	886	U	N1-C2-O2	6.94	127.66	122.80
49	C1	1077	U	C2-N1-C1'	6.94	126.03	117.70
49	C1	758	U	N1-C2-O2	6.93	127.65	122.80
50	C2	200	U	N1-C2-O2	6.92	127.64	122.80
50	C2	23	A	C6-N1-C2	-6.90	114.46	118.60
49	C1	400	C	C6-N1-C2	-6.90	117.54	120.30
49	C1	1222	C	C2-N1-C1'	6.89	126.39	118.80
49	C1	1645	U	C2-N1-C1'	6.89	125.97	117.70
50	C2	128	C	O4'-C1'-N1	6.89	113.71	108.20
49	C1	1486	G	N7-C8-N9	6.89	116.54	113.10
50	C2	57	A	N1-C6-N6	6.88	122.73	118.60
50	C2	74	C	N3-C2-O2	-6.87	117.09	121.90
49	C1	1163	A	P-O3'-C3'	6.86	127.93	119.70
49	C1	134	C	N3-C2-O2	-6.85	117.10	121.90
49	C1	345	U	N3-C2-O2	-6.84	117.41	122.20
49	C1	400	C	C2-N1-C1'	6.84	126.33	118.80
49	C1	1626	G	C8-N9-C4	-6.84	103.66	106.40
49	C1	1655	U	N3-C2-O2	-6.84	117.41	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C2	61	G	C8-N9-C1'	6.84	135.89	127.00
49	C1	2173	G	C6-C5-N7	-6.83	126.30	130.40
49	C1	46	C	OP1-P-OP2	6.83	129.84	119.60
50	C2	147	G	N3-C4-N9	6.81	130.09	126.00
49	C1	56	C	C2-N1-C1'	6.80	126.28	118.80
49	C1	255	G	N9-C4-C5	6.79	108.12	105.40
49	C1	1084	C	N3-C2-O2	-6.79	117.15	121.90
49	C1	2180	A	C4-C5-N7	6.79	114.09	110.70
49	C1	203	C	C2-N1-C1'	6.79	126.26	118.80
49	C1	404	C	C2-N1-C1'	6.79	126.26	118.80
49	C1	270	C	N3-C2-O2	-6.78	117.15	121.90
55	UH	832	LEU	CA-CB-CG	-6.77	99.72	115.30
15	UU	715	PHE	C-N-CA	6.77	138.63	121.70
49	C1	692	U	N3-C2-O2	-6.77	117.46	122.20
50	C2	140	C	N1-C2-O2	6.77	122.96	118.90
49	C1	1757	C	N3-C2-O2	-6.76	117.17	121.90
49	C1	218	G	C8-N9-C1'	-6.76	118.22	127.00
49	C1	1145	G	N9-C4-C5	-6.75	102.70	105.40
49	C1	408	C	N1-C2-O2	6.74	122.94	118.90
50	C2	246	G	C8-N9-C1'	-6.74	118.24	127.00
49	C1	491	G	C4-N9-C1'	6.74	135.26	126.50
49	C1	1736	A	N7-C8-N9	6.73	117.17	113.80
50	C2	200	U	C2-N1-C1'	6.72	125.77	117.70
49	C1	2180	A	C6-C5-N7	-6.72	127.59	132.30
50	C2	35	G	C6-C5-N7	-6.72	126.37	130.40
50	C2	260	G	N3-C4-N9	6.71	130.03	126.00
49	C1	1165	U	C2-N1-C1'	6.71	125.75	117.70
49	C1	583	A	O5'-P-OP1	-6.70	99.67	105.70
49	C1	2191	U	C6-N1-C2	-6.70	116.98	121.00
49	C1	55	G	OP2-P-O3'	-6.69	90.49	105.20
49	C1	135	A	C8-N9-C4	-6.68	103.13	105.80
49	C1	1046	G	N1-C6-O6	-6.67	115.90	119.90
55	UH	726	LEU	CA-CB-CG	6.67	130.65	115.30
49	C1	851	U	N1-C2-O2	6.67	127.47	122.80
49	C1	1486	G	C2-N3-C4	6.66	115.23	111.90
50	C2	39	U	N1-C2-O2	6.66	127.46	122.80
49	C1	2229	C	C5-C6-N1	6.65	124.33	121.00
49	C1	1741	A	C8-N9-C4	-6.64	103.14	105.80
24	CI	974	ARG	NE-CZ-NH2	-6.63	116.98	120.30
49	C1	986	C	C2-N1-C1'	6.63	126.09	118.80
49	C1	2071	G	N3-C4-N9	6.63	129.98	126.00
49	C1	915	G	N1-C6-O6	-6.62	115.93	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	C1	218	G	C4-N9-C1’	6.61	135.09	126.50
49	C1	2071	G	N1-C2-N2	-6.61	110.25	116.20
49	C1	2195	U	C2-N1-C1’	6.60	125.62	117.70
49	C1	160	C	N1-C2-O2	6.60	122.86	118.90
49	C1	2047	G	C5-C6-O6	6.57	132.54	128.60
49	C1	449	C	C6-N1-C2	-6.57	117.67	120.30
49	C1	1075	C	N3-C2-O2	-6.56	117.31	121.90
32	CR	167	MET	CA-CB-CG	6.55	124.44	113.30
32	CS	167	MET	CA-CB-CG	6.55	124.43	113.30
49	C1	2047	G	C4-N9-C1’	-6.55	117.99	126.50
49	C1	470	C	C2-N1-C1’	6.53	125.98	118.80
49	C1	2116	C	N3-C2-O2	-6.52	117.33	121.90
49	C1	1471	U	C2-N1-C1’	6.52	125.53	117.70
50	C2	61	G	N3-C4-N9	-6.52	122.09	126.00
49	C1	2176	A	C8-N9-C4	-6.51	103.19	105.80
49	C1	447	C	N3-C2-O2	-6.51	117.34	121.90
49	C1	1758	C	C2-N1-C1’	-6.50	111.65	118.80
49	C1	209	A	P-O3’-C3’	6.50	127.50	119.70
49	C1	2116	C	N1-C2-O2	6.50	122.80	118.90
49	C1	1155	G	C6-C5-N7	-6.50	126.50	130.40
49	C1	2172	C	N3-C2-O2	-6.50	117.35	121.90
49	C1	203	C	N3-C2-O2	-6.50	117.35	121.90
51	UV	159	LEU	CA-CB-CG	6.49	130.23	115.30
49	C1	1747	A	N1-C2-N3	6.49	132.54	129.30
49	C1	1179	G	N9-C4-C5	-6.47	102.81	105.40
50	C2	260	G	C8-N9-C1’	-6.46	118.60	127.00
49	C1	2106	U	N3-C2-O2	-6.46	117.68	122.20
49	C1	2227	C	C2-N1-C1’	6.45	125.90	118.80
49	C1	1736	A	C5-N7-C8	-6.45	100.67	103.90
49	C1	1171	C	N3-C2-O2	-6.44	117.39	121.90
50	C2	56	U	N3-C2-O2	-6.43	117.70	122.20
50	C2	56	U	N1-C2-O2	6.42	127.30	122.80
11	UN	901	LEU	CA-CB-CG	6.42	130.06	115.30
50	C2	57	A	C6-C5-N7	-6.42	127.81	132.30
49	C1	1645	U	N1-C2-O2	6.41	127.29	122.80
49	C1	21	C	N3-C2-O2	-6.41	117.41	121.90
49	C1	2047	G	N3-C4-N9	-6.41	122.15	126.00
49	C1	886	U	N3-C2-O2	-6.41	117.71	122.20
49	C1	2071	G	C6-N1-C2	-6.40	121.26	125.10
50	C2	202	C	N3-C2-O2	-6.40	117.42	121.90
50	C2	128	C	C6-N1-C2	-6.40	117.74	120.30
49	C1	2179	C	N1-C2-O2	6.39	122.73	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	C1	419	G	C8-N9-C1’	-6.38	118.70	127.00
49	C1	419	G	C4-N9-C1’	6.38	134.79	126.50
49	C1	1757	C	N1-C2-O2	6.38	122.73	118.90
50	C2	90	C	O4’-C1’-N1	6.38	113.30	108.20
49	C1	206	C	C2-N1-C1’	6.37	125.81	118.80
49	C1	910	G	C5-C6-O6	6.37	132.42	128.60
49	C1	193	U	N1-C2-O2	6.36	127.25	122.80
49	C1	454	C	N1-C2-O2	6.36	122.72	118.90
49	C1	1166	U	C2-N1-C1’	6.35	125.32	117.70
19	CC	78	LEU	CA-CB-CG	6.34	129.88	115.30
49	C1	2209	U	N3-C2-O2	-6.33	117.77	122.20
49	C1	1156	C	C6-N1-C2	6.33	122.83	120.30
50	C2	267	C	C6-N1-C2	-6.33	117.77	120.30
50	C2	266	C	C2-N1-C1’	6.32	125.75	118.80
49	C1	347	C	C2-N1-C1’	6.31	125.74	118.80
50	C2	260	G	C4-N9-C1’	6.30	134.69	126.50
49	C1	2203	C	N1-C2-O2	6.30	122.68	118.90
49	C1	683	C	C2-N1-C1’	6.30	125.73	118.80
54	UT	698	LEU	CA-CB-CG	6.29	129.78	115.30
49	C1	750	C	N3-C2-O2	-6.29	117.50	121.90
50	C2	266	C	N1-C2-O2	6.28	122.67	118.90
49	C1	190	G	C5-C6-O6	6.28	132.37	128.60
49	C1	1167	C	C5-C6-N1	6.28	124.14	121.00
49	C1	2189	C	N1-C2-O2	6.27	122.66	118.90
49	C1	504	C	N1-C2-O2	6.25	122.65	118.90
49	C1	1145	G	C5-C6-O6	-6.24	124.85	128.60
49	C1	768	C	C6-N1-C1’	-6.24	113.31	120.80
49	C1	255	G	N7-C8-N9	6.24	116.22	113.10
49	C1	370	C	C2-N1-C1’	6.24	125.66	118.80
49	C1	1154	A	C2-N3-C4	-6.24	107.48	110.60
49	C1	129	G	N3-C4-N9	-6.24	122.26	126.00
49	C1	402	U	N1-C2-O2	6.22	127.16	122.80
50	C2	131	U	C2-N1-C1’	6.22	125.17	117.70
49	C1	1550	U	N3-C2-O2	-6.22	117.85	122.20
49	C1	447	C	C6-N1-C2	-6.21	117.81	120.30
49	C1	2217	C	C5-C6-N1	6.21	124.11	121.00
49	C1	233	C	C6-N1-C1’	-6.20	113.36	120.80
49	C1	1148	G	C5-N7-C8	-6.20	101.20	104.30
49	C1	915	G	C5-C6-O6	6.20	132.32	128.60
49	C1	1645	U	N3-C2-O2	-6.20	117.86	122.20
49	C1	618	C	C5-C6-N1	6.18	124.09	121.00
49	C1	1027	C	C6-N1-C2	-6.17	117.83	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	C1	419	G	N3-C4-N9	6.17	129.70	126.00
49	C1	860	C	C2-N1-C1'	-6.17	112.02	118.80
49	C1	1165	U	N1-C2-O2	6.17	127.11	122.80
49	C1	776	C	N1-C2-O2	6.16	122.60	118.90
49	C1	1625	G	N3-C4-N9	6.16	129.70	126.00
49	C1	1046	G	C5-C6-O6	6.15	132.29	128.60
49	C1	1547	C	C5-C6-N1	6.14	124.07	121.00
49	C1	303	C	C5-C6-N1	6.14	124.07	121.00
49	C1	281	U	P-O3'-C3'	6.14	127.06	119.70
32	CR	901	LEU	CA-CB-CG	6.13	129.41	115.30
1	UA	426	LEU	CA-CB-CG	6.13	129.41	115.30
50	C2	82	U	N1-C2-O2	6.13	127.09	122.80
8	UK	51	LEU	CB-CG-CD2	-6.13	100.58	111.00
32	CS	901	LEU	CA-CB-CG	6.13	129.39	115.30
49	C1	2230	U	N3-C2-O2	-6.12	117.91	122.20
7	UJ	488	LEU	CA-CB-CG	6.12	129.38	115.30
49	C1	33	C	N3-C2-O2	-6.12	117.61	121.90
49	C1	1630	C	N3-C2-O2	-6.12	117.61	121.90
49	C1	2047	G	N1-C6-O6	-6.12	116.23	119.90
49	C1	371	U	C2-N1-C1'	6.11	125.03	117.70
49	C1	1120	C	C2-N1-C1'	6.11	125.52	118.80
50	C2	128	C	C5-C6-N1	6.11	124.05	121.00
49	C1	190	G	N3-C4-N9	-6.10	122.34	126.00
49	C1	1113	C	N1-C2-O2	6.08	122.55	118.90
49	C1	1157	C	C2-N1-C1'	6.08	125.49	118.80
49	C1	1179	G	C4-C5-N7	6.07	113.23	110.80
49	C1	277	U	P-O3'-C3'	6.07	126.98	119.70
49	C1	417	G	C6-C5-N7	-6.06	126.77	130.40
50	C2	202	C	N1-C2-O2	6.06	122.53	118.90
49	C1	1147	U	OP2-P-O3'	6.04	118.49	105.20
49	C1	1001	A	OP2-P-O3'	6.04	118.48	105.20
1	UA	656	LEU	CA-CB-CG	-6.04	101.42	115.30
55	UH	730	PHE	C-N-CA	6.03	136.78	121.70
50	C2	57	A	C4-C5-C6	6.03	120.02	117.00
49	C1	1760	G	C8-N9-C1'	-6.03	119.16	127.00
50	C2	23	A	C5-C6-N1	6.03	120.72	117.70
49	C1	622	U	N3-C2-O2	-6.03	117.98	122.20
49	C1	1549	U	N3-C4-C5	6.02	118.21	114.60
49	C1	2071	G	N3-C4-C5	-6.01	125.59	128.60
12	UO	239	LEU	CA-CB-CG	6.01	129.12	115.30
49	C1	2089	G	N3-C4-N9	6.01	129.61	126.00
49	C1	908	C	C5-C6-N1	6.00	124.00	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C2	79	G	C6-C5-N7	-5.99	126.81	130.40
49	C1	2075	U	O5'-P-OP2	-5.99	100.31	105.70
49	C1	683	C	N1-C2-O2	5.98	122.49	118.90
29	CO	164	GLN	C-N-CA	5.98	136.65	121.70
49	C1	258	C	N3-C2-O2	-5.97	117.72	121.90
50	C2	5	A	C8-N9-C4	5.97	108.19	105.80
49	C1	2196	U	N3-C2-O2	-5.96	118.03	122.20
49	C1	1120	C	N1-C2-O2	5.96	122.47	118.90
49	C1	1473	U	C5-C6-N1	5.95	125.67	122.70
26	CK	89	LEU	CB-CG-CD2	-5.95	100.89	111.00
50	C2	61	G	C4-N9-C1'	-5.95	118.77	126.50
49	C1	2069	G	N9-C4-C5	5.94	107.78	105.40
50	C2	63	G	C4-N9-C1'	5.94	134.22	126.50
49	C1	3	G	N3-C4-N9	-5.94	122.44	126.00
49	C1	1141	G	C4-C5-N7	5.93	113.17	110.80
49	C1	1547	C	N3-C2-O2	-5.93	117.75	121.90
49	C1	769	C	C2-N1-C1'	5.92	125.31	118.80
50	C2	252	C	N3-C2-O2	-5.92	117.75	121.90
50	C2	140	C	C6-N1-C2	-5.92	117.93	120.30
49	C1	1735	A	N3-C4-N9	5.91	132.13	127.40
49	C1	1625	G	N3-C4-C5	-5.91	125.64	128.60
49	C1	2047	G	C8-N9-C1'	5.90	134.67	127.00
49	C1	2090	G	C2-N3-C4	-5.90	108.95	111.90
49	C1	1222	C	N3-C2-O2	-5.89	117.78	121.90
49	C1	1138	C	C4-C5-C6	5.88	120.34	117.40
49	C1	1001	A	P-O3'-C3'	5.88	126.75	119.70
49	C1	1760	G	C4-N9-C1'	5.87	134.14	126.50
50	C2	255	U	P-O3'-C3'	5.87	126.74	119.70
48	CU	116	LEU	CA-CB-CG	5.87	128.79	115.30
49	C1	1560	C	N3-C2-O2	-5.86	117.80	121.90
49	C1	80	C	C6-N1-C2	-5.86	117.96	120.30
49	C1	247	C	C6-N1-C2	-5.85	117.96	120.30
49	C1	1758	C	C6-N1-C1'	5.85	127.82	120.80
49	C1	148	C	N1-C2-N3	5.85	123.30	119.20
49	C1	112	C	N3-C2-O2	-5.85	117.81	121.90
49	C1	68	U	C6-N1-C1'	-5.84	113.02	121.20
54	UT	2116	LEU	CA-CB-CG	-5.84	101.87	115.30
49	C1	2180	A	C5-N7-C8	-5.84	100.98	103.90
49	C1	491	G	C8-N9-C1'	-5.83	119.42	127.00
49	C1	910	G	N3-C4-N9	-5.83	122.50	126.00
49	C1	1547	C	C6-N1-C1'	-5.82	113.81	120.80
49	C1	1550	U	C6-N1-C1'	-5.82	113.05	121.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	2173	G	C4-C5-N7	5.82	113.13	110.80
49	C1	2188	G	C8-N9-C1'	-5.82	119.44	127.00
49	C1	347	C	C6-N1-C2	-5.81	117.97	120.30
49	C1	419	G	C6-C5-N7	-5.81	126.91	130.40
49	C1	989	C	N1-C2-O2	5.81	122.39	118.90
49	C1	2049	G	C6-N1-C2	-5.81	121.62	125.10
49	C1	1736	A	C4-C5-N7	5.80	113.60	110.70
49	C1	1175	A	C6-N1-C2	-5.80	115.12	118.60
49	C1	1560	C	N1-C2-O2	5.80	122.38	118.90
56	UI	179	LEU	CA-CB-CG	5.79	128.62	115.30
50	C2	101	G	N3-C4-N9	-5.78	122.53	126.00
49	C1	496	U	N3-C2-O2	-5.78	118.15	122.20
49	C1	886	U	C2-N1-C1'	5.78	124.64	117.70
49	C1	1472	A	N7-C8-N9	5.78	116.69	113.80
49	C1	2177	G	C8-N9-C4	-5.77	104.09	106.40
56	UE	179	LEU	CA-CB-CG	5.77	128.58	115.30
50	C2	136	C	N1-C2-O2	5.77	122.36	118.90
49	C1	470	C	N3-C2-O2	-5.76	117.87	121.90
49	C1	287	C	C5-C6-N1	5.76	123.88	121.00
49	C1	922	C	N3-C2-O2	-5.76	117.87	121.90
49	C1	2223	C	C2-N1-C1'	5.75	125.13	118.80
49	C1	1655	U	N1-C2-N3	5.75	118.35	114.90
50	C2	200	U	N3-C2-O2	-5.74	118.18	122.20
51	UV	1054	LEU	CA-CB-CG	5.74	128.51	115.30
49	C1	2181	U	N1-C2-O2	5.74	126.82	122.80
49	C1	56	C	N1-C2-O2	5.74	122.34	118.90
49	C1	413	C	C5-C6-N1	5.74	123.87	121.00
49	C1	2165	U	C5-C6-N1	5.73	125.57	122.70
49	C1	343	C	C2-N1-C1'	5.73	125.10	118.80
49	C1	1149	C	N3-C4-N4	-5.73	113.99	118.00
49	C1	369	U	C2-N1-C1'	5.72	124.57	117.70
49	C1	190	G	N9-C4-C5	5.72	107.69	105.40
49	C1	1658	G	C5-C6-O6	5.72	132.03	128.60
49	C1	2203	C	C2-N1-C1'	5.72	125.09	118.80
49	C1	1114	C	N3-C2-O2	-5.71	117.91	121.90
49	C1	371	U	N3-C2-O2	-5.70	118.21	122.20
49	C1	1150	C	C2-N1-C1'	5.70	125.08	118.80
49	C1	776	C	C2-N1-C1'	5.70	125.07	118.80
49	C1	1000	A	O4'-C1'-N9	5.70	112.76	108.20
49	C1	2071	G	O4'-C1'-N9	-5.70	103.64	108.20
50	C2	38	G	O4'-C1'-N9	-5.70	103.64	108.20
20	CD	102	LEU	CA-CB-CG	5.69	128.40	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	C1	2195	U	N1-C2-O2	5.69	126.79	122.80
49	C1	986	C	N1-C2-O2	5.69	122.31	118.90
49	C1	228	G	C5-C6-O6	-5.69	125.19	128.60
49	C1	2173	G	C5-N7-C8	-5.68	101.46	104.30
49	C1	1136	G	N1-C6-O6	-5.68	116.49	119.90
49	C1	1140	A	N1-C6-N6	5.68	122.01	118.60
50	C2	79	G	N9-C4-C5	-5.68	103.13	105.40
32	CR	766	LEU	CA-CB-CG	5.68	128.36	115.30
49	C1	758	U	C6-N1-C1’	-5.68	113.25	121.20
49	C1	2110	C	C2-N1-C1’	5.68	125.04	118.80
49	C1	2209	U	N1-C2-O2	5.68	126.77	122.80
49	C1	2164	C	C6-N1-C2	-5.67	118.03	120.30
49	C1	454	C	C6-N1-C1’	-5.67	113.99	120.80
32	CS	766	LEU	CA-CB-CG	5.67	128.34	115.30
49	C1	582	G	P-O3’-C3’	5.66	126.49	119.70
49	C1	2177	G	O4’-C1’-N9	5.65	112.72	108.20
49	C1	1714	G	N3-C4-C5	-5.64	125.78	128.60
49	C1	2210	U	C5-C4-O4	5.64	129.29	125.90
49	C1	190	G	N1-C6-O6	-5.64	116.52	119.90
50	C2	251	U	C2-N1-C1’	5.64	124.47	117.70
49	C1	2106	U	C5-C6-N1	5.64	125.52	122.70
49	C1	2178	U	C5-C4-O4	-5.64	122.52	125.90
49	C1	134	C	N1-C2-O2	5.64	122.28	118.90
49	C1	1120	C	N3-C2-O2	-5.63	117.96	121.90
49	C1	1155	G	C5-N7-C8	-5.63	101.48	104.30
49	C1	1736	A	N9-C4-C5	-5.63	103.55	105.80
49	C1	160	C	C5-C6-N1	5.63	123.81	121.00
49	C1	1136	G	C5-C6-N1	5.62	114.31	111.50
13	UQ	648	LEU	CA-CB-CG	5.62	128.21	115.30
49	C1	1136	G	C2-N3-C4	5.61	114.71	111.90
49	C1	1667	G	C8-N9-C4	-5.61	104.15	106.40
49	C1	1139	A	C8-N9-C4	-5.61	103.56	105.80
49	C1	1625	G	N3-C2-N2	5.61	123.83	119.90
10	UM	674	LEU	CA-CB-CG	5.61	128.19	115.30
50	C2	148	G	C5-C6-O6	5.61	131.96	128.60
49	C1	294	G	N1-C2-N3	5.60	127.26	123.90
49	C1	2227	C	C6-N1-C1’	-5.60	114.08	120.80
32	CS	84	ARG	CG-CD-NE	5.60	123.56	111.80
49	C1	2216	A	N7-C8-N9	5.60	116.60	113.80
49	C1	1759	U	C2-N1-C1’	5.60	124.42	117.70
50	C2	136	C	C2-N1-C1’	5.60	124.95	118.80
37	Ce	38	ALA	C-N-CA	5.59	135.69	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	C1	2047	G	N3-C4-C5	5.59	131.40	128.60
49	C1	2164	C	N3-C2-O2	-5.59	117.98	121.90
51	UV	334	LEU	CA-CB-CG	5.58	128.14	115.30
32	CR	84	ARG	CG-CD-NE	5.58	123.52	111.80
49	C1	676	C	N3-C2-O2	-5.58	118.00	121.90
49	C1	989	C	C6-N1-C1'	-5.58	114.11	120.80
50	C2	67	C	C2-N1-C1'	5.58	124.93	118.80
49	C1	1026	C	N3-C2-O2	-5.55	118.01	121.90
50	C2	246	G	N3-C4-N9	5.55	129.33	126.00
23	CH	202	LEU	CA-CB-CG	5.55	128.07	115.30
49	C1	742	U	P-O3'-C3'	5.55	126.36	119.70
49	C1	1759	U	N3-C2-O2	-5.55	118.31	122.20
49	C1	18	G	C4-N9-C1'	5.55	133.71	126.50
49	C1	2229	C	C6-N1-C2	-5.55	118.08	120.30
49	C1	134	C	OP1-P-O3'	5.54	117.40	105.20
49	C1	18	G	N3-C4-C5	-5.54	125.83	128.60
49	C1	988	G	C8-N9-C1'	-5.54	119.80	127.00
49	C1	2203	C	N3-C2-O2	-5.54	118.02	121.90
49	C1	769	C	C6-N1-C2	-5.54	118.09	120.30
49	C1	1666	C	C2-N1-C1'	5.54	124.89	118.80
49	C1	203	C	C6-N1-C1'	-5.53	114.16	120.80
50	C2	147	G	C8-N9-C1'	-5.53	119.81	127.00
50	C2	251	U	N3-C2-O2	-5.52	118.34	122.20
49	C1	1149	C	C5-C6-N1	-5.51	118.25	121.00
49	C1	485	G	N3-C4-N9	-5.51	122.70	126.00
49	C1	2176	A	C6-N1-C2	-5.51	115.30	118.60
49	C1	254	G	C8-N9-C4	-5.50	104.20	106.40
24	CI	240	THR	C-N-CA	-5.50	107.94	121.70
49	C1	1633	A	N1-C6-N6	-5.50	115.30	118.60
49	C1	2071	G	N3-C2-N2	5.50	123.75	119.90
50	C2	92	A	C4-N9-C1'	5.49	136.19	126.30
49	C1	1166	U	C5-C6-N1	5.49	125.44	122.70
49	C1	446	C	N1-C2-O2	5.48	122.19	118.90
49	C1	1081	G	N1-C6-O6	-5.47	116.62	119.90
49	C1	2054	A	P-O3'-C3'	5.47	126.27	119.70
49	C1	2352	U	N1-C2-O2	5.47	126.63	122.80
49	C1	2069	G	C4-N9-C1'	5.46	133.60	126.50
49	C1	2195	U	N3-C2-O2	-5.46	118.38	122.20
49	C1	1144	U	N3-C4-O4	5.46	123.22	119.40
49	C1	1736	A	C6-C5-N7	-5.46	128.48	132.30
49	C1	860	C	C6-N1-C1'	5.46	127.35	120.80
49	C1	2180	A	N1-C6-N6	5.46	121.87	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C2	131	U	N1-C2-O2	5.45	126.62	122.80
49	C1	135	A	N7-C8-N9	5.45	116.53	113.80
49	C1	204	U	C2-N1-C1’	-5.45	111.16	117.70
49	C1	2084	C	C6-N1-C2	-5.45	118.12	120.30
49	C1	692	U	C2-N1-C1’	5.45	124.23	117.70
49	C1	1757	C	C6-N1-C2	-5.44	118.12	120.30
49	C1	206	C	O4’-C1’-N1	5.43	112.55	108.20
49	C1	2180	A	C4-N9-C1’	5.43	136.08	126.30
6	UG	355	LEU	CA-CB-CG	5.43	127.78	115.30
50	C2	92	A	N3-C4-C5	-5.43	123.00	126.80
28	CM	321	TYR	CB-CG-CD2	-5.42	117.75	121.00
49	C1	2090	G	N3-C4-N9	-5.42	122.75	126.00
49	C1	1547	C	C6-N1-C2	-5.41	118.14	120.30
50	C2	147	G	C4-N9-C1’	5.41	133.53	126.50
29	CO	148	LEU	CA-CB-CG	5.40	127.73	115.30
50	C2	92	A	N3-C4-N9	5.40	131.72	127.40
49	C1	505	C	C6-N1-C2	-5.40	118.14	120.30
49	C1	1761	C	C5-C6-N1	5.40	123.70	121.00
49	C1	462	G	N1-C6-O6	-5.40	116.66	119.90
13	UQ	442	LEU	CA-CB-CG	5.39	127.71	115.30
49	C1	2	G	N3-C4-N9	5.39	129.24	126.00
49	C1	618	C	C6-N1-C1’	-5.39	114.33	120.80
49	C1	1148	G	C2-N3-C4	-5.39	109.20	111.90
49	C1	1165	U	C6-N1-C1’	-5.39	113.65	121.20
49	C1	1486	G	N3-C4-N9	5.39	129.24	126.00
49	C1	2230	U	N1-C2-O2	5.39	126.57	122.80
13	UQ	777	LEU	CA-CB-CG	5.39	127.69	115.30
16	UX	52	LEU	CA-CB-CG	5.39	127.69	115.30
49	C1	863	G	N3-C4-N9	-5.38	122.77	126.00
49	C1	354	G	C4-C5-N7	5.37	112.95	110.80
18	CA	290	LEU	CA-CB-CG	5.37	127.64	115.30
49	C1	2106	U	C6-N1-C1’	-5.37	113.69	121.20
49	C1	2156	A	P-O3’-C3’	5.36	126.14	119.70
49	C1	3	G	C5-C6-O6	5.36	131.82	128.60
49	C1	1760	G	C6-C5-N7	-5.36	127.18	130.40
50	C2	74	C	N1-C2-O2	5.36	122.12	118.90
49	C1	148	C	C6-N1-C1’	5.35	127.22	120.80
51	UV	414	LEU	CA-CB-CG	5.35	127.61	115.30
49	C1	2177	G	C6-C5-N7	-5.35	127.19	130.40
49	C1	205	C	P-O3’-C3’	5.35	126.12	119.70
4	UD	397	LEU	CA-CB-CG	5.34	127.59	115.30
49	C1	68	U	N3-C2-O2	-5.34	118.46	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	C1	1026	C	N1-C2-O2	5.34	122.11	118.90
50	C2	63	G	N3-C4-C5	-5.33	125.93	128.60
50	C2	244	G	C5-C6-O6	5.33	131.80	128.60
49	C1	68	U	C5-C6-N1	5.33	125.36	122.70
49	C1	485	G	C5-C6-O6	5.32	131.79	128.60
49	C1	988	G	N3-C4-N9	5.32	129.19	126.00
49	C1	2203	C	C6-N1-C2	-5.32	118.17	120.30
49	C1	281	U	OP1-P-O3’	5.32	116.90	105.20
50	C2	82	U	C2-N1-C1’	5.32	124.08	117.70
49	C1	658	A	N1-C2-N3	5.31	131.96	129.30
49	C1	988	G	C4-N9-C1’	5.31	133.41	126.50
50	C2	28	U	C5-C6-N1	-5.31	120.04	122.70
49	C1	402	U	C2-N1-C1’	5.31	124.07	117.70
49	C1	1485	A	P-O3’-C3’	5.30	126.06	119.70
49	C1	986	C	C6-N1-C2	-5.30	118.18	120.30
49	C1	1071	G	C6-C5-N7	-5.30	127.22	130.40
49	C1	2171	G	N1-C6-O6	-5.30	116.72	119.90
49	C1	860	C	N3-C2-O2	-5.29	118.19	121.90
49	C1	912	U	N3-C2-O2	-5.29	118.50	122.20
49	C1	1183	A	N7-C8-N9	5.29	116.44	113.80
49	C1	346	C	C6-N1-C2	-5.29	118.18	120.30
49	C1	491	G	N3-C4-N9	5.29	129.17	126.00
49	C1	942	U	O4’-C1’-N1	5.29	112.43	108.20
49	C1	684	U	P-O3’-C3’	5.28	126.04	119.70
49	C1	404	C	C6-N1-C1’	-5.28	114.47	120.80
49	C1	2182	C	O5’-P-OP2	-5.28	100.95	105.70
49	C1	231	U	N1-C2-O2	5.27	126.49	122.80
50	C2	131	U	C5-C6-N1	5.27	125.33	122.70
49	C1	18	G	N3-C4-N9	5.27	129.16	126.00
50	C2	90	C	C2-N1-C1’	-5.27	113.00	118.80
50	C2	79	G	C5-C6-N1	5.27	114.13	111.50
49	C1	910	G	N1-C6-O6	-5.26	116.74	119.90
49	C1	1140	A	C2-N3-C4	-5.26	107.97	110.60
49	C1	865	G	N1-C2-N2	-5.26	111.47	116.20
49	C1	2172	C	N1-C2-O2	5.26	122.05	118.90
49	C1	129	G	C2-N3-C4	-5.25	109.27	111.90
49	C1	218	G	N3-C4-C5	-5.25	125.97	128.60
49	C1	408	C	N3-C2-O2	-5.25	118.22	121.90
49	C1	2071	G	N1-C6-O6	-5.25	116.75	119.90
49	C1	359	C	N3-C2-O2	-5.25	118.22	121.90
49	C1	1124	G	O4’-C1’-N9	5.25	112.40	108.20
50	C2	203	C	C6-N1-C2	-5.25	118.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	C1	228	G	C8-N9-C4	-5.24	104.30	106.40
49	C1	1708	A	N7-C8-N9	5.24	116.42	113.80
49	C1	129	G	N3-C4-C5	5.24	131.22	128.60
49	C1	2111	U	N3-C2-O2	-5.24	118.53	122.20
49	C1	262	G	N3-C4-N9	5.24	129.14	126.00
49	C1	743	U	O5'-P-OP1	-5.24	100.99	105.70
32	CS	295	MET	CA-CB-CG	5.23	122.19	113.30
49	C1	80	C	C6-N1-C1'	5.23	127.08	120.80
49	C1	770	C	C2-N1-C1'	5.23	124.55	118.80
32	CR	784	LYS	CA-CB-CG	5.23	124.90	113.40
50	C2	82	U	N3-C2-O2	-5.23	118.54	122.20
9	UL	601	LEU	CA-CB-CG	5.23	127.32	115.30
49	C1	2180	A	N9-C4-C5	-5.23	103.71	105.80
50	C2	73	C	N3-C2-O2	-5.22	118.24	121.90
49	C1	56	C	C6-N1-C1'	-5.22	114.53	120.80
49	C1	1458	U	N1-C2-O2	5.22	126.45	122.80
49	C1	1745	C	N1-C2-O2	5.22	122.03	118.90
32	CR	295	MET	CA-CB-CG	5.22	122.17	113.30
49	C1	1760	G	N9-C4-C5	-5.22	103.31	105.40
49	C1	2116	C	C6-N1-C2	-5.21	118.21	120.30
50	C2	161	G	C4-N9-C1'	5.21	133.28	126.50
56	UE	214	LEU	CB-CG-CD1	-5.21	102.14	111.00
49	C1	1102	A	O4'-C1'-N9	5.21	112.37	108.20
32	CS	784	LYS	CA-CB-CG	5.21	124.86	113.40
49	C1	246	G	N3-C4-N9	5.21	129.12	126.00
49	C1	909	G	N3-C4-N9	5.21	129.12	126.00
49	C1	1050	U	N3-C2-O2	-5.21	118.56	122.20
56	UI	214	LEU	CB-CG-CD1	-5.21	102.15	111.00
49	C1	995	C	C6-N1-C1'	-5.20	114.56	120.80
49	C1	2173	G	C4-N9-C1'	5.20	133.26	126.50
49	C1	2238	A	N7-C8-N9	5.20	116.40	113.80
49	C1	1125	A	C4-N9-C1'	5.19	135.65	126.30
49	C1	2181	U	O5'-P-OP1	-5.19	101.03	105.70
49	C1	3	G	N9-C4-C5	5.19	107.48	105.40
49	C1	1175	A	C5-C6-N6	-5.19	119.55	123.70
49	C1	593	G	P-O3'-C3'	5.19	125.93	119.70
2	UB	818	ASP	CB-CG-OD2	5.18	122.97	118.30
49	C1	1646	U	O4'-C1'-N1	5.18	112.35	108.20
49	C1	726	U	N3-C2-O2	-5.18	118.57	122.20
49	C1	345	U	N1-C2-O2	5.18	126.43	122.80
49	C1	1448	A	C5-C6-N1	5.18	120.29	117.70
49	C1	2119	G	C4-N9-C1'	5.18	133.24	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	111	U	N3-C2-O2	-5.18	118.58	122.20
49	C1	294	G	C2-N3-C4	-5.18	109.31	111.90
50	C2	61	G	O4'-C1'-N9	5.17	112.34	108.20
49	C1	889	C	C5-C6-N1	5.17	123.58	121.00
9	UL	376	LEU	C-N-CA	-5.16	108.79	121.70
49	C1	112	C	C2-N1-C1'	5.16	124.48	118.80
50	C2	18	G	N1-C6-O6	-5.16	116.80	119.90
49	C1	218	G	N9-C4-C5	-5.16	103.33	105.40
50	C2	147	G	N9-C4-C5	-5.16	103.34	105.40
49	C1	2069	G	N1-C6-O6	-5.16	116.81	119.90
49	C1	2178	U	C4-C5-C6	-5.15	116.61	119.70
49	C1	1101	U	N3-C2-O2	-5.15	118.59	122.20
49	C1	402	U	N3-C2-O2	-5.15	118.60	122.20
49	C1	146	C	N1-C2-O2	5.14	121.98	118.90
49	C1	29	C	C5-C6-N1	5.14	123.57	121.00
49	C1	246	G	N3-C4-C5	-5.13	126.03	128.60
51	UV	661	LEU	CA-CB-CG	5.13	127.11	115.30
49	C1	2216	A	C8-N9-C4	-5.13	103.75	105.80
49	C1	1089	A	N1-C6-N6	-5.13	115.52	118.60
49	C1	2179	C	N3-C4-N4	-5.13	114.41	118.00
49	C1	446	C	N3-C2-O2	-5.13	118.31	121.90
49	C1	614	U	C2-N1-C1'	5.13	123.85	117.70
49	C1	485	G	N9-C4-C5	5.12	107.45	105.40
49	C1	496	U	N1-C2-O2	5.12	126.39	122.80
49	C1	768	C	C5-C6-N1	5.12	123.56	121.00
49	C1	1052	A	C4-C5-N7	5.12	113.26	110.70
26	CK	89	LEU	CA-CB-CG	5.12	127.07	115.30
49	C1	448	C	N3-C2-O2	-5.12	118.32	121.90
49	C1	228	G	C6-C5-N7	-5.11	127.33	130.40
49	C1	1085	U	P-O3'-C3'	5.11	125.83	119.70
49	C1	1626	G	C6-N1-C2	-5.11	122.03	125.10
32	CS	559	MET	CG-SD-CE	5.11	108.37	100.20
50	C2	246	G	C6-C5-N7	-5.11	127.34	130.40
49	C1	343	C	N1-C2-O2	5.11	121.96	118.90
49	C1	1081	G	N1-C2-N3	5.11	126.96	123.90
49	C1	1148	G	N3-C4-C5	5.10	131.15	128.60
49	C1	915	G	N9-C4-C5	5.10	107.44	105.40
50	C2	131	U	N3-C2-O2	-5.10	118.63	122.20
49	C1	1667	G	C6-C5-N7	-5.10	127.34	130.40
32	CR	559	MET	CG-SD-CE	5.10	108.36	100.20
49	C1	137	C	N3-C2-O2	-5.10	118.33	121.90
10	UM	524	ILE	C-N-CD	5.09	139.09	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	C1	2078	C	N3-C2-O2	-5.09	118.34	121.90
49	C1	750	C	C2-N1-C1'	5.09	124.40	118.80
49	C1	434	A	N1-C6-N6	-5.09	115.55	118.60
49	C1	145	C	N1-C2-O2	5.08	121.95	118.90
49	C1	56	C	O5'-P-OP1	5.08	116.79	110.70
49	C1	225	C	C6-N1-C2	-5.07	118.27	120.30
54	UT	1938	LEU	CA-CB-CG	5.07	126.95	115.30
24	CI	833	LEU	CB-CG-CD2	-5.06	102.39	111.00
50	C2	23	A	P-O3'-C3'	5.06	125.77	119.70
32	CR	84	ARG	CD-NE-CZ	5.05	130.68	123.60
49	C1	2180	A	C8-N9-C1'	-5.05	118.61	127.70
49	C1	200	A	C8-N9-C4	5.05	107.82	105.80
49	C1	363	G	C6-C5-N7	-5.05	127.37	130.40
49	C1	1735	A	C2-N3-C4	5.04	113.12	110.60
49	C1	2202	C	C6-N1-C1'	-5.04	114.75	120.80
49	C1	1052	A	N1-C6-N6	5.04	121.62	118.60
49	C1	220	A	C4-N9-C1'	5.04	135.37	126.30
7	UJ	682	LEU	CA-CB-CG	5.03	126.87	115.30
49	C1	1158	G	N3-C4-C5	5.03	131.12	128.60
49	C1	148	C	C5-C4-N4	5.03	123.72	120.20
50	C2	65	C	C6-N1-C2	-5.03	118.29	120.30
50	C2	244	G	N1-C6-O6	-5.02	116.89	119.90
49	C1	1547	C	C2-N3-C4	5.02	122.41	119.90
49	C1	369	U	N3-C2-O2	-5.02	118.69	122.20
49	C1	228	G	N7-C8-N9	5.01	115.61	113.10
49	C1	888	U	N3-C2-O2	-5.01	118.69	122.20
49	C1	2047	G	C6-C5-N7	5.01	133.41	130.40
49	C1	2083	C	N1-C2-O2	5.01	121.91	118.90
49	C1	684	U	N1-C2-O2	5.01	126.31	122.80
32	CS	84	ARG	CD-NE-CZ	5.01	130.61	123.60
49	C1	462	G	C5-C6-O6	5.01	131.60	128.60
61	CZ	552	LEU	CA-CB-CG	5.01	126.81	115.30
49	C1	154	C	C2-N1-C1'	5.00	124.31	118.80
49	C1	1658	G	N9-C4-C5	5.00	107.40	105.40
49	C1	2106	U	OP2-P-O3'	5.00	116.21	105.20
49	C1	2358	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (74) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	CB	293	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	CE	33	GLN	Peptide
21	CF	14	ASP	Peptide
21	CF	60	GLN	Peptide
23	CH	170	ARG	Peptide
24	CI	132	VAL	Peptide
24	CI	141	ASP	Peptide
24	CI	211	ASN	Peptide
24	CI	303	PRO	Peptide
24	CI	855	THR	Peptide
24	CI	885	CYS	Peptide
25	CJ	101	VAL	Peptide
25	CJ	144	ARG	Peptide
26	CK	173	ARG	Peptide
28	CM	322	HIS	Peptide
29	CO	84	ILE	Peptide
29	CO	88	ARG	Peptide
32	CR	901	LEU	Peptide
32	CS	901	LEU	Peptide
52	CV	88	LYS	Peptide
52	CV	91	HIS	Peptide
60	CY	374	ARG	Peptide
37	Ce	38	ALA	Peptide
41	Ci	137	ASP	Peptide
42	Cj	126	PRO	Peptide
42	Cj	39	PHE	Peptide
42	Cj	40	ALA	Peptide
58	Cl	79	TYR	Peptide
45	Cn	68	ILE	Peptide
46	Co	365	ASN	Peptide
63	Cz	1628	THR	Peptide
1	UA	273	GLY	Peptide
1	UA	320	GLY	Peptide
1	UA	386	THR	Peptide
1	UA	424	GLU	Peptide
1	UA	443	GLY	Peptide
1	UA	506	PRO	Peptide
1	UA	618	LEU	Peptide
1	UA	622	GLN	Peptide
1	UA	641	ASP	Peptide
1	UA	667	ARG	Peptide
5	UF	120	VAL	Peptide
6	UG	227	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
6	UG	264	LEU	Peptide
55	UH	753	THR	Peptide
8	UK	12	ALA	Peptide
8	UK	83	PHE	Peptide
9	UL	150	GLY	Peptide
9	UL	17	VAL	Peptide
10	UM	204	ASP	Peptide
10	UM	328	LEU	Peptide
10	UM	383	LEU	Peptide
10	UM	589	VAL	Peptide
11	UN	901	LEU	Peptide
12	UO	282	ALA	Peptide
13	UQ	707	PRO	Peptide
13	UQ	849	ALA	Peptide
54	UT	1516	LEU	Peptide
54	UT	1566	GLU	Peptide
54	UT	408	PRO	Peptide
54	UT	486	GLU	Peptide
54	UT	781	TRP	Peptide
15	UU	397	ASP	Peptide
15	UU	402	GLU	Peptide
15	UU	758	HIS	Peptide
15	UU	759	THR	Peptide
51	UV	1013	ASP	Peptide
51	UV	1058	TYR	Peptide
51	UV	1104	LEU	Peptide
51	UV	57	PHE	Peptide
16	UX	-5	LYS	Peptide
16	UX	126	LYS	Peptide
17	UZ	103	ASP	Peptide
17	UZ	273	GLN	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UA	835/904 (92%)	733 (88%)	102 (12%)	0	100	100
2	UB	502/907 (55%)	472 (94%)	30 (6%)	0	100	100
3	UC	72/648 (11%)	58 (81%)	14 (19%)	0	100	100
4	UD	754/884 (85%)	708 (94%)	46 (6%)	0	100	100
5	UF	325/414 (78%)	303 (93%)	21 (6%)	1 (0%)	41	76
6	UG	475/558 (85%)	433 (91%)	39 (8%)	3 (1%)	25	65
7	UJ	1062/1802 (59%)	1000 (94%)	62 (6%)	0	100	100
8	UK	211/270 (78%)	196 (93%)	15 (7%)	0	100	100
9	UL	767/962 (80%)	704 (92%)	63 (8%)	0	100	100
10	UM	645/912 (71%)	595 (92%)	49 (8%)	1 (0%)	47	81
11	UN	171/938 (18%)	161 (94%)	9 (5%)	1 (1%)	25	65
12	UO	498/557 (89%)	459 (92%)	39 (8%)	0	100	100
13	UQ	775/960 (81%)	703 (91%)	71 (9%)	1 (0%)	51	85
14	UR	437/618 (71%)	400 (92%)	37 (8%)	0	100	100
15	UU	890/1049 (85%)	797 (90%)	93 (10%)	0	100	100
16	UX	188/193 (97%)	172 (92%)	16 (8%)	0	100	100
17	UZ	229/391 (59%)	206 (90%)	23 (10%)	0	100	100
18	CA	238/313 (76%)	218 (92%)	20 (8%)	0	100	100
18	CB	235/313 (75%)	216 (92%)	19 (8%)	0	100	100
19	CC	383/523 (73%)	361 (94%)	22 (6%)	0	100	100
20	CD	416/582 (72%)	384 (92%)	32 (8%)	0	100	100
21	CE	119/127 (94%)	112 (94%)	7 (6%)	0	100	100
21	CF	118/127 (93%)	109 (92%)	9 (8%)	0	100	100
22	CG	402/630 (64%)	366 (91%)	36 (9%)	0	100	100
23	CH	383/411 (93%)	344 (90%)	38 (10%)	1 (0%)	41	76
24	CI	812/1163 (70%)	732 (90%)	80 (10%)	0	100	100
25	CJ	177/183 (97%)	154 (87%)	23 (13%)	0	100	100
26	CK	295/297 (99%)	255 (86%)	40 (14%)	0	100	100
27	CL	225/785 (29%)	205 (91%)	20 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	CM	443/446 (99%)	402 (91%)	41 (9%)	0	100	100
29	CN	222/252 (88%)	202 (91%)	20 (9%)	0	100	100
29	CO	211/252 (84%)	196 (93%)	13 (6%)	2 (1%)	17	56
30	CP	185/322 (58%)	181 (98%)	4 (2%)	0	100	100
31	CQ	171/259 (66%)	165 (96%)	6 (4%)	0	100	100
32	CR	746/1073 (70%)	692 (93%)	54 (7%)	0	100	100
32	CS	746/1073 (70%)	692 (93%)	54 (7%)	0	100	100
33	CT	127/203 (63%)	111 (87%)	16 (13%)	0	100	100
34	Cb	230/264 (87%)	211 (92%)	19 (8%)	0	100	100
35	Cc	188/212 (89%)	166 (88%)	22 (12%)	0	100	100
36	Cd	224/239 (94%)	208 (93%)	16 (7%)	0	100	100
37	Ce	155/203 (76%)	145 (94%)	10 (6%)	0	100	100
38	Cf	170/202 (84%)	162 (95%)	8 (5%)	0	100	100
39	Cg	157/190 (83%)	149 (95%)	8 (5%)	0	100	100
40	Ch	47/151 (31%)	47 (100%)	0	0	100	100
41	Ci	113/150 (75%)	100 (88%)	13 (12%)	0	100	100
42	Cj	124/143 (87%)	109 (88%)	15 (12%)	0	100	100
43	Ck	136/161 (84%)	131 (96%)	5 (4%)	0	100	100
44	Cm	122/130 (94%)	116 (95%)	6 (5%)	0	100	100
45	Cn	92/145 (63%)	83 (90%)	9 (10%)	0	100	100
46	Co	90/136 (66%)	82 (91%)	8 (9%)	0	100	100
47	Cp	59/68 (87%)	55 (93%)	4 (7%)	0	100	100
48	CU	106/311 (34%)	99 (93%)	7 (7%)	0	100	100
51	UV	1057/1171 (90%)	948 (90%)	108 (10%)	1 (0%)	51	85
52	CV	144/322 (45%)	129 (90%)	14 (10%)	1 (1%)	22	62
53	CW	380/668 (57%)	349 (92%)	31 (8%)	0	100	100
54	UT	1982/2612 (76%)	1878 (95%)	100 (5%)	4 (0%)	47	81
55	UH	349/930 (38%)	335 (96%)	14 (4%)	0	100	100
56	UE	121/410 (30%)	111 (92%)	9 (7%)	1 (1%)	19	60
56	UI	121/410 (30%)	111 (92%)	9 (7%)	1 (1%)	19	60
57	US	443/549 (81%)	420 (95%)	23 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	Cl	78/156 (50%)	74 (95%)	4 (5%)	0	100	100
59	CX	265/480 (55%)	251 (95%)	14 (5%)	0	100	100
60	CY	118/381 (31%)	109 (92%)	9 (8%)	0	100	100
61	CZ	40/609 (7%)	32 (80%)	8 (20%)	0	100	100
62	UP	52/364 (14%)	45 (86%)	7 (14%)	0	100	100
63	Cz	273/1796 (15%)	261 (96%)	12 (4%)	0	100	100
All	All	22926/35864 (64%)	21113 (92%)	1795 (8%)	18 (0%)	54	85

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	UG	176	LEU
29	CO	85	SER
51	UV	1059	ASP
54	UT	487	ILE
5	UF	121	LYS
29	CO	84	ILE
54	UT	457	TRP
6	UG	56	PRO
13	UQ	708	SER
54	UT	1567	PHE
6	UG	322	ASN
54	UT	408	PRO
11	UN	902	ARG
52	CV	92	SER
56	UE	208	PRO
10	UM	329	PRO
56	UI	208	PRO
23	CH	258	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	651/775 (84%)	647 (99%)	4 (1%)	86	92
2	UB	425/788 (54%)	423 (100%)	2 (0%)	88	93
3	UC	61/536 (11%)	61 (100%)	0	100	100
4	UD	653/738 (88%)	650 (100%)	3 (0%)	88	93
5	UF	248/341 (73%)	246 (99%)	2 (1%)	81	89
6	UG	373/474 (79%)	371 (100%)	2 (0%)	88	93
7	UJ	898/1526 (59%)	890 (99%)	8 (1%)	78	88
8	UK	159/227 (70%)	156 (98%)	3 (2%)	57	75
9	UL	667/821 (81%)	665 (100%)	2 (0%)	92	95
10	UM	569/770 (74%)	567 (100%)	2 (0%)	91	94
11	UN	146/765 (19%)	146 (100%)	0	100	100
12	UO	404/456 (89%)	401 (99%)	3 (1%)	84	90
13	UQ	650/817 (80%)	650 (100%)	0	100	100
14	UR	360/524 (69%)	359 (100%)	1 (0%)	92	95
15	UU	672/863 (78%)	668 (99%)	4 (1%)	86	92
16	UX	150/167 (90%)	147 (98%)	3 (2%)	55	73
17	UZ	186/329 (56%)	184 (99%)	2 (1%)	73	85
18	CA	175/228 (77%)	172 (98%)	3 (2%)	60	78
18	CB	195/228 (86%)	195 (100%)	0	100	100
19	CC	287/435 (66%)	286 (100%)	1 (0%)	92	95
20	CD	319/489 (65%)	318 (100%)	1 (0%)	92	95
21	CE	91/108 (84%)	91 (100%)	0	100	100
21	CF	88/108 (82%)	88 (100%)	0	100	100
22	CG	331/525 (63%)	329 (99%)	2 (1%)	86	92
23	CH	303/320 (95%)	298 (98%)	5 (2%)	60	78
24	CI	661/1009 (66%)	653 (99%)	8 (1%)	71	84
25	CJ	147/169 (87%)	147 (100%)	0	100	100
26	CK	245/266 (92%)	241 (98%)	4 (2%)	62	79
27	CL	181/642 (28%)	181 (100%)	0	100	100
28	CM	364/383 (95%)	361 (99%)	3 (1%)	81	89
29	CN	202/223 (91%)	202 (100%)	0	100	100
29	CO	193/223 (86%)	190 (98%)	3 (2%)	62	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	CP	164/287 (57%)	163 (99%)	1 (1%)	86	92
31	CQ	145/215 (67%)	145 (100%)	0	100	100
32	CR	654/916 (71%)	512 (78%)	142 (22%)	1	6
32	CS	654/916 (71%)	512 (78%)	142 (22%)	1	6
33	CT	108/167 (65%)	108 (100%)	0	100	100
34	Cb	199/221 (90%)	198 (100%)	1 (0%)	88	93
35	Cc	149/178 (84%)	145 (97%)	4 (3%)	44	66
36	Cd	192/204 (94%)	191 (100%)	1 (0%)	88	93
37	Ce	137/177 (77%)	135 (98%)	2 (2%)	65	80
38	Cf	139/164 (85%)	138 (99%)	1 (1%)	84	90
39	Cg	122/162 (75%)	122 (100%)	0	100	100
40	Ch	41/130 (32%)	40 (98%)	1 (2%)	49	69
41	Ci	74/117 (63%)	73 (99%)	1 (1%)	67	81
42	Cj	92/115 (80%)	91 (99%)	1 (1%)	73	85
43	Ck	126/143 (88%)	125 (99%)	1 (1%)	81	89
44	Cm	103/113 (91%)	102 (99%)	1 (1%)	76	86
45	Cn	70/116 (60%)	69 (99%)	1 (1%)	67	81
46	Co	79/115 (69%)	78 (99%)	1 (1%)	69	82
47	Cp	46/61 (75%)	46 (100%)	0	100	100
48	CU	92/260 (35%)	91 (99%)	1 (1%)	73	85
51	UV	908/989 (92%)	895 (99%)	13 (1%)	67	81
52	CV	129/276 (47%)	127 (98%)	2 (2%)	62	79
53	CW	309/587 (53%)	307 (99%)	2 (1%)	86	92
54	UT	1724/2276 (76%)	1715 (100%)	9 (0%)	88	93
55	UH	301/788 (38%)	298 (99%)	3 (1%)	76	86
56	UE	105/346 (30%)	76 (72%)	29 (28%)	0	3
56	UI	105/346 (30%)	76 (72%)	29 (28%)	0	3
57	US	404/493 (82%)	403 (100%)	1 (0%)	93	96
58	Cl	71/135 (53%)	69 (97%)	2 (3%)	43	65
59	CX	225/411 (55%)	223 (99%)	2 (1%)	78	88
60	CY	100/322 (31%)	100 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	CZ	36/519 (7%)	34 (94%)	2 (6%)	21	48
62	UP	44/314 (14%)	44 (100%)	0	100	100
63	Cz	235/1533 (15%)	233 (99%)	2 (1%)	78	88
All	All	19136/30385 (63%)	18667 (98%)	469 (2%)	50	68

All (469) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	UA	33	VAL
1	UA	150	HIS
1	UA	471	VAL
1	UA	493	ARG
2	UB	87	ARG
2	UB	786	ARG
4	UD	228	ASP
4	UD	264	LYS
4	UD	346	ASP
5	UF	113	TYR
5	UF	121	LYS
6	UG	41	ARG
6	UG	121	VAL
7	UJ	25	LEU
7	UJ	393	LYS
7	UJ	405	LYS
7	UJ	840	LYS
7	UJ	1509	LYS
7	UJ	1517	LYS
7	UJ	1656	LYS
7	UJ	1720	LYS
8	UK	58	ARG
8	UK	65	PHE
8	UK	160	LYS
9	UL	71	THR
9	UL	93	ARG
10	UM	755	ARG
10	UM	889	ARG
12	UO	253	ASN
12	UO	258	LEU
12	UO	264	LYS
14	UR	437	ARG
15	UU	394	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	UU	503	SER
15	UU	618	THR
15	UU	1000	ARG
16	UX	-1	LYS
16	UX	31	LYS
16	UX	58	VAL
17	UZ	140	TYR
17	UZ	170	THR
18	CA	211	ARG
18	CA	218	MET
18	CA	292	LEU
19	CC	51	ARG
20	CD	68	LYS
22	CG	345	VAL
22	CG	352	ARG
23	CH	73	THR
23	CH	208	LEU
23	CH	273	THR
23	CH	304	VAL
23	CH	354	ARG
24	CI	91	ARG
24	CI	113	ARG
24	CI	222	LEU
24	CI	840	ARG
24	CI	841	ARG
24	CI	854	ARG
24	CI	863	THR
24	CI	1073	GLU
26	CK	92	THR
26	CK	108	ARG
26	CK	246	ARG
26	CK	280	VAL
28	CM	39	GLU
28	CM	208	VAL
28	CM	408	LYS
29	CO	135	LYS
29	CO	209	MET
29	CO	241	PHE
30	CP	49	ARG
32	CR	3	VAL
32	CR	8	ASP
32	CR	10	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	14	LEU
32	CR	19	LEU
32	CR	25	SER
32	CR	32	ASP
32	CR	41	LEU
32	CR	45	MET
32	CR	49	ASP
32	CR	50	VAL
32	CR	54	LYS
32	CR	55	SER
32	CR	62	LYS
32	CR	65	LEU
32	CR	69	SER
32	CR	75	GLU
32	CR	77	LYS
32	CR	78	ILE
32	CR	79	LYS
32	CR	80	LYS
32	CR	83	LYS
32	CR	84	ARG
32	CR	87	ARG
32	CR	88	GLU
32	CR	95	PHE
32	CR	107	CYS
32	CR	112	THR
32	CR	116	LEU
32	CR	119	THR
32	CR	129	GLU
32	CR	131	ILE
32	CR	132	THR
32	CR	140	ILE
32	CR	141	GLU
32	CR	142	THR
32	CR	148	LEU
32	CR	149	VAL
32	CR	159	LEU
32	CR	162	LEU
32	CR	167	MET
32	CR	168	ASP
32	CR	195	SER
32	CR	198	SER
32	CR	209	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	249	ILE
32	CR	252	LEU
32	CR	253	ILE
32	CR	266	LEU
32	CR	270	ASP
32	CR	277	LEU
32	CR	280	THR
32	CR	282	THR
32	CR	284	THR
32	CR	289	ARG
32	CR	292	SER
32	CR	295	MET
32	CR	297	VAL
32	CR	299	ILE
32	CR	313	THR
32	CR	314	SER
32	CR	316	SER
32	CR	372	ILE
32	CR	387	VAL
32	CR	402	LEU
32	CR	408	VAL
32	CR	412	SER
32	CR	424	LEU
32	CR	426	LEU
32	CR	429	ILE
32	CR	432	LEU
32	CR	470	LYS
32	CR	471	GLU
32	CR	475	SER
32	CR	480	TYR
32	CR	488	LYS
32	CR	492	THR
32	CR	494	LEU
32	CR	502	ARG
32	CR	510	CYS
32	CR	512	ASP
32	CR	528	SER
32	CR	532	VAL
32	CR	534	GLU
32	CR	535	LYS
32	CR	536	PHE
32	CR	537	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	539	GLN
32	CR	540	MET
32	CR	545	VAL
32	CR	547	SER
32	CR	552	SER
32	CR	555	ASP
32	CR	557	GLN
32	CR	560	SER
32	CR	567	LEU
32	CR	571	THR
32	CR	576	GLU
32	CR	581	GLU
32	CR	586	ILE
32	CR	589	SER
32	CR	590	LEU
32	CR	612	ASP
32	CR	617	LEU
32	CR	619	SER
32	CR	625	ASP
32	CR	631	SER
32	CR	638	ILE
32	CR	640	THR
32	CR	643	ASP
32	CR	645	MET
32	CR	647	MET
32	CR	651	SER
32	CR	657	LEU
32	CR	708	LEU
32	CR	710	SER
32	CR	713	SER
32	CR	719	LYS
32	CR	733	LEU
32	CR	739	ARG
32	CR	745	VAL
32	CR	750	THR
32	CR	773	SER
32	CR	784	LYS
32	CR	789	LEU
32	CR	796	GLU
32	CR	800	ILE
32	CR	853	VAL
32	CR	854	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	855	LEU
32	CR	860	THR
32	CR	867	THR
32	CR	870	LEU
32	CR	879	LEU
32	CR	884	LEU
32	CR	887	LEU
32	CR	892	LYS
32	CR	894	ILE
32	CR	897	LEU
32	CR	901	LEU
32	CR	902	ASN
32	CR	909	LEU
32	CS	3	VAL
32	CS	8	ASP
32	CS	10	ARG
32	CS	14	LEU
32	CS	19	LEU
32	CS	25	SER
32	CS	32	ASP
32	CS	41	LEU
32	CS	45	MET
32	CS	49	ASP
32	CS	50	VAL
32	CS	54	LYS
32	CS	55	SER
32	CS	62	LYS
32	CS	65	LEU
32	CS	69	SER
32	CS	75	GLU
32	CS	77	LYS
32	CS	78	ILE
32	CS	79	LYS
32	CS	80	LYS
32	CS	83	LYS
32	CS	84	ARG
32	CS	87	ARG
32	CS	88	GLU
32	CS	95	PHE
32	CS	107	CYS
32	CS	112	THR
32	CS	116	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CS	119	THR
32	CS	129	GLU
32	CS	131	ILE
32	CS	132	THR
32	CS	140	ILE
32	CS	141	GLU
32	CS	142	THR
32	CS	148	LEU
32	CS	149	VAL
32	CS	159	LEU
32	CS	162	LEU
32	CS	167	MET
32	CS	168	ASP
32	CS	195	SER
32	CS	198	SER
32	CS	209	LEU
32	CS	249	ILE
32	CS	252	LEU
32	CS	253	ILE
32	CS	266	LEU
32	CS	270	ASP
32	CS	277	LEU
32	CS	280	THR
32	CS	282	THR
32	CS	284	THR
32	CS	289	ARG
32	CS	292	SER
32	CS	295	MET
32	CS	297	VAL
32	CS	299	ILE
32	CS	313	THR
32	CS	314	SER
32	CS	316	SER
32	CS	372	ILE
32	CS	387	VAL
32	CS	402	LEU
32	CS	408	VAL
32	CS	412	SER
32	CS	424	LEU
32	CS	426	LEU
32	CS	429	ILE
32	CS	432	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CS	470	LYS
32	CS	471	GLU
32	CS	475	SER
32	CS	480	TYR
32	CS	488	LYS
32	CS	492	THR
32	CS	494	LEU
32	CS	502	ARG
32	CS	510	CYS
32	CS	512	ASP
32	CS	528	SER
32	CS	532	VAL
32	CS	534	GLU
32	CS	535	LYS
32	CS	536	PHE
32	CS	537	LEU
32	CS	539	GLN
32	CS	540	MET
32	CS	545	VAL
32	CS	547	SER
32	CS	552	SER
32	CS	555	ASP
32	CS	557	GLN
32	CS	560	SER
32	CS	567	LEU
32	CS	571	THR
32	CS	576	GLU
32	CS	581	GLU
32	CS	586	ILE
32	CS	589	SER
32	CS	590	LEU
32	CS	612	ASP
32	CS	617	LEU
32	CS	619	SER
32	CS	625	ASP
32	CS	631	SER
32	CS	638	ILE
32	CS	640	THR
32	CS	643	ASP
32	CS	645	MET
32	CS	647	MET
32	CS	651	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CS	657	LEU
32	CS	708	LEU
32	CS	710	SER
32	CS	713	SER
32	CS	719	LYS
32	CS	733	LEU
32	CS	739	ARG
32	CS	745	VAL
32	CS	750	THR
32	CS	773	SER
32	CS	784	LYS
32	CS	789	LEU
32	CS	796	GLU
32	CS	800	ILE
32	CS	853	VAL
32	CS	854	VAL
32	CS	855	LEU
32	CS	860	THR
32	CS	867	THR
32	CS	870	LEU
32	CS	879	LEU
32	CS	884	LEU
32	CS	887	LEU
32	CS	892	LYS
32	CS	894	ILE
32	CS	897	LEU
32	CS	901	LEU
32	CS	902	ASN
32	CS	909	LEU
34	Cb	133	ARG
35	Cc	41	ARG
35	Cc	66	VAL
35	Cc	130	ARG
35	Cc	144	ARG
36	Cd	111	LEU
37	Ce	90	LYS
37	Ce	184	ARG
38	Cf	18	ARG
40	Ch	100	LYS
41	Ci	105	LYS
42	Cj	111	GLN
43	Ck	72	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	Cm	32	LYS
45	Cn	78	LYS
46	Co	368	LYS
48	CU	129	ARG
51	UV	36	ARG
51	UV	91	LYS
51	UV	248	ARG
51	UV	577	ARG
51	UV	612	ARG
51	UV	668	VAL
51	UV	676	ARG
51	UV	733	LYS
51	UV	784	LYS
51	UV	941	THR
51	UV	982	ARG
51	UV	989	LYS
51	UV	1099	LYS
52	CV	156	LYS
52	CV	167	LYS
53	CW	85	ARG
53	CW	337	THR
54	UT	8	ARG
54	UT	139	LYS
54	UT	324	ARG
54	UT	1006	ARG
54	UT	1472	THR
54	UT	1564	LYS
54	UT	1635	LYS
54	UT	1857	LEU
54	UT	1940	ARG
55	UH	624	MET
55	UH	748	LYS
55	UH	902	LYS
56	UE	157	LEU
56	UE	163	THR
56	UE	170	GLU
56	UE	180	ILE
56	UE	187	ARG
56	UE	191	SER
56	UE	196	LEU
56	UE	199	LYS
56	UE	206	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	UE	210	ARG
56	UE	214	LEU
56	UE	218	ILE
56	UE	219	GLN
56	UE	222	LEU
56	UE	231	THR
56	UE	234	ASP
56	UE	241	GLU
56	UE	254	SER
56	UE	255	SER
56	UE	259	LEU
56	UE	262	LYS
56	UE	263	LEU
56	UE	264	ASP
56	UE	265	MET
56	UE	266	LEU
56	UE	267	ASP
56	UE	270	LEU
56	UE	271	LYS
56	UE	278	MET
57	US	425	LYS
58	Cl	25	LYS
58	Cl	80	LYS
59	CX	204	LYS
59	CX	247	CYS
61	CZ	554	ASN
61	CZ	575	THR
56	UI	157	LEU
56	UI	163	THR
56	UI	170	GLU
56	UI	180	ILE
56	UI	187	ARG
56	UI	191	SER
56	UI	196	LEU
56	UI	199	LYS
56	UI	206	ARG
56	UI	210	ARG
56	UI	214	LEU
56	UI	218	ILE
56	UI	219	GLN
56	UI	222	LEU
56	UI	231	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	UI	234	ASP
56	UI	241	GLU
56	UI	254	SER
56	UI	255	SER
56	UI	259	LEU
56	UI	262	LYS
56	UI	263	LEU
56	UI	264	ASP
56	UI	265	MET
56	UI	266	LEU
56	UI	267	ASP
56	UI	270	LEU
56	UI	271	LYS
56	UI	278	MET
63	Cz	1664	LEU
63	Cz	1701	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (279) such sidechains are listed below:

Mol	Chain	Res	Type
1	UA	19	ASN
1	UA	45	ASN
1	UA	131	ASN
1	UA	207	GLN
1	UA	328	GLN
1	UA	344	ASN
1	UA	353	GLN
1	UA	508	GLN
1	UA	576	ASN
1	UA	846	ASN
2	UB	5	GLN
2	UB	525	ASN
2	UB	683	HIS
4	UD	176	GLN
4	UD	195	GLN
4	UD	277	GLN
4	UD	324	HIS
4	UD	416	ASN
4	UD	473	ASN
4	UD	532	GLN
4	UD	536	HIS
4	UD	673	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	UD	697	GLN
4	UD	755	GLN
4	UD	828	HIS
5	UF	154	ASN
6	UG	95	ASN
6	UG	216	HIS
6	UG	243	GLN
6	UG	278	GLN
6	UG	331	ASN
6	UG	378	GLN
6	UG	427	ASN
7	UJ	15	ASN
7	UJ	51	GLN
7	UJ	158	GLN
7	UJ	250	GLN
7	UJ	448	ASN
7	UJ	515	ASN
7	UJ	731	ASN
7	UJ	785	ASN
7	UJ	842	ASN
7	UJ	1645	ASN
7	UJ	1723	ASN
7	UJ	1745	GLN
8	UK	9	GLN
9	UL	21	ASN
9	UL	151	HIS
9	UL	154	GLN
9	UL	207	HIS
9	UL	215	GLN
9	UL	296	HIS
9	UL	453	ASN
9	UL	506	HIS
9	UL	630	ASN
9	UL	688	GLN
9	UL	832	ASN
10	UM	231	HIS
10	UM	236	GLN
10	UM	338	GLN
10	UM	628	ASN
10	UM	644	ASN
10	UM	706	ASN
10	UM	741	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	UM	743	GLN
10	UM	747	ASN
10	UM	772	ASN
11	UN	332	HIS
11	UN	333	ASN
11	UN	362	GLN
11	UN	916	GLN
12	UO	393	ASN
13	UQ	209	ASN
13	UQ	262	HIS
13	UQ	473	GLN
13	UQ	477	HIS
13	UQ	783	ASN
13	UQ	924	GLN
14	UR	177	GLN
14	UR	185	GLN
14	UR	440	GLN
14	UR	493	ASN
14	UR	498	ASN
15	UU	62	GLN
15	UU	89	GLN
15	UU	143	GLN
15	UU	197	ASN
15	UU	314	ASN
15	UU	577	GLN
15	UU	634	ASN
15	UU	727	GLN
15	UU	740	HIS
15	UU	963	ASN
15	UU	1023	GLN
16	UX	63	ASN
17	UZ	79	GLN
17	UZ	90	ASN
17	UZ	110	ASN
17	UZ	143	GLN
18	CB	195	ASN
18	CB	232	GLN
18	CB	235	GLN
18	CB	277	GLN
18	CB	289	GLN
20	CD	106	ASN
20	CD	147	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	CD	219	ASN
20	CD	404	ASN
20	CD	422	ASN
21	CE	112	ASN
22	CG	243	GLN
22	CG	274	ASN
22	CG	330	GLN
22	CG	430	HIS
23	CH	90	ASN
23	CH	127	HIS
23	CH	233	ASN
23	CH	244	ASN
23	CH	316	GLN
23	CH	323	GLN
24	CI	55	HIS
24	CI	165	ASN
24	CI	823	HIS
24	CI	888	GLN
24	CI	930	ASN
24	CI	1030	ASN
25	CJ	8	HIS
25	CJ	30	HIS
25	CJ	39	GLN
25	CJ	59	HIS
25	CJ	135	HIS
25	CJ	169	ASN
26	CK	5	GLN
26	CK	8	GLN
26	CK	48	ASN
26	CK	121	ASN
26	CK	132	GLN
26	CK	159	HIS
26	CK	168	HIS
26	CK	169	ASN
26	CK	242	HIS
27	CL	525	HIS
28	CM	65	HIS
28	CM	77	ASN
28	CM	120	ASN
28	CM	151	GLN
28	CM	206	ASN
28	CM	262	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	CM	282	HIS
28	CM	376	ASN
29	CN	81	ASN
29	CN	111	GLN
29	CO	94	GLN
29	CO	105	ASN
30	CP	110	GLN
30	CP	190	ASN
31	CQ	203	ASN
31	CQ	247	ASN
32	CR	102	ASN
32	CR	126	GLN
32	CR	279	ASN
32	CR	485	ASN
32	CR	655	GLN
32	CR	749	GLN
32	CR	810	ASN
32	CS	102	ASN
32	CS	126	GLN
32	CS	279	ASN
32	CS	485	ASN
32	CS	557	GLN
32	CS	655	GLN
32	CS	749	GLN
32	CS	810	ASN
34	Cb	57	ASN
34	Cb	67	GLN
34	Cb	197	HIS
35	Cc	31	ASN
35	Cc	82	ASN
35	Cc	87	HIS
35	Cc	109	HIS
35	Cc	115	ASN
35	Cc	211	ASN
36	Cd	129	HIS
36	Cd	163	GLN
36	Cd	179	GLN
36	Cd	189	HIS
36	Cd	200	GLN
37	Ce	36	ASN
38	Cf	94	ASN
39	Cg	121	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	Cg	140	ASN
42	Cj	77	GLN
42	Cj	107	GLN
43	Ck	22	ASN
43	Ck	111	ASN
43	Ck	115	HIS
43	Ck	132	GLN
43	Ck	143	ASN
44	Cm	42	GLN
44	Cm	64	GLN
44	Cm	113	HIS
45	Cn	48	HIS
45	Cn	79	ASN
46	Co	353	GLN
46	Co	360	HIS
48	CU	211	GLN
51	UV	106	GLN
51	UV	107	ASN
51	UV	260	GLN
51	UV	355	GLN
51	UV	368	ASN
51	UV	378	GLN
51	UV	494	ASN
51	UV	526	GLN
51	UV	542	ASN
51	UV	615	GLN
51	UV	809	HIS
51	UV	813	HIS
51	UV	841	HIS
51	UV	974	GLN
51	UV	1092	ASN
52	CV	198	HIS
53	CW	80	HIS
53	CW	177	GLN
53	CW	243	GLN
53	CW	361	ASN
54	UT	24	ASN
54	UT	25	HIS
54	UT	87	ASN
54	UT	311	HIS
54	UT	365	ASN
54	UT	377	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	UT	389	HIS
54	UT	495	GLN
54	UT	768	ASN
54	UT	780	GLN
54	UT	803	ASN
54	UT	909	GLN
54	UT	971	ASN
54	UT	1026	GLN
54	UT	1272	HIS
54	UT	1314	ASN
54	UT	1315	GLN
54	UT	1345	GLN
54	UT	1416	ASN
54	UT	1437	ASN
54	UT	1454	ASN
54	UT	1599	GLN
54	UT	1602	ASN
54	UT	1795	HIS
54	UT	1874	GLN
54	UT	1909	GLN
54	UT	1985	ASN
54	UT	2052	GLN
54	UT	2097	ASN
54	UT	2141	GLN
54	UT	2163	ASN
55	UH	590	ASN
56	UE	186	ASN
56	UE	237	ASN
57	US	152	HIS
57	US	184	HIS
57	US	225	ASN
57	US	253	HIS
57	US	391	ASN
57	US	468	HIS
58	Cl	21	ASN
58	Cl	74	GLN
59	CX	290	ASN
59	CX	355	GLN
59	CX	364	ASN
59	CX	423	ASN
56	UI	186	ASN
56	UI	237	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
62	UP	325	ASN
62	UP	341	ASN
63	Cz	1556	ASN
63	Cz	1578	ASN
63	Cz	1617	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	C1	1461/2323 (62%)	559 (38%)	35 (2%)
50	C2	226/230 (98%)	86 (38%)	6 (2%)
All	All	1687/2553 (66%)	645 (38%)	41 (2%)

All (645) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
49	C1	4	G
49	C1	5	G
49	C1	7	A
49	C1	13	G
49	C1	14	G
49	C1	15	G
49	C1	16	U
49	C1	17	C
49	C1	18	G
49	C1	19	C
49	C1	23	G
49	C1	26	C
49	C1	38	G
49	C1	40	A
49	C1	41	G
49	C1	42	C
49	C1	43	C
49	C1	47	G
49	C1	49	G
49	C1	56	C
49	C1	59	U
49	C1	60	A
49	C1	61	G
49	C1	62	U
49	C1	63	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	66	G
49	C1	68	U
49	C1	71	A
49	C1	72	U
49	C1	73	A
49	C1	74	C
49	C1	75	G
49	C1	77	C
49	C1	84	A
49	C1	88	C
49	C1	89	G
49	C1	90	A
49	C1	93	G
49	C1	96	C
49	C1	104	U
49	C1	105	A
49	C1	121	G
49	C1	126	C
49	C1	127	C
49	C1	128	G
49	C1	134	C
49	C1	135	A
49	C1	136	C
49	C1	139	C
49	C1	143	A
49	C1	152	G
49	C1	154	C
49	C1	155	G
49	C1	158	C
49	C1	159	C
49	C1	160	C
49	C1	161	A
49	C1	162	G
49	C1	166	A
49	C1	169	G
49	C1	180	G
49	C1	182	C
49	C1	183	C
49	C1	188	C
49	C1	192	A
49	C1	193	U
49	C1	198	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	201	G
49	C1	202	A
49	C1	203	C
49	C1	204	U
49	C1	205	C
49	C1	206	C
49	C1	207	U
49	C1	208	A
49	C1	209	A
49	C1	210	G
49	C1	211	G
49	C1	212	C
49	C1	219	G
49	C1	220	A
49	C1	222	U
49	C1	223	A
49	C1	224	C
49	C1	228	G
49	C1	234	G
49	C1	236	C
49	C1	241	G
49	C1	242	U
49	C1	243	U
49	C1	244	G
49	C1	256	U
49	C1	257	G
49	C1	258	C
49	C1	260	U
49	C1	265	G
49	C1	266	C
49	C1	268	G
49	C1	269	G
49	C1	271	C
49	C1	273	G
49	C1	276	C
49	C1	277	U
49	C1	278	A
49	C1	282	C
49	C1	283	A
49	C1	285	A
49	C1	286	G
49	C1	289	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	290	C
49	C1	291	C
49	C1	292	G
49	C1	297	U
49	C1	298	A
49	C1	309	G
49	C1	334	U
49	C1	339	C
49	C1	340	G
49	C1	346	C
49	C1	347	C
49	C1	349	C
49	C1	351	U
49	C1	352	G
49	C1	353	G
49	C1	362	G
49	C1	368	G
49	C1	378	C
49	C1	382	U
49	C1	383	G
49	C1	384	C
49	C1	386	G
49	C1	397	U
49	C1	402	U
49	C1	403	G
49	C1	406	G
49	C1	408	C
49	C1	409	A
49	C1	410	G
49	C1	411	C
49	C1	416	U
49	C1	417	G
49	C1	419	G
49	C1	425	C
49	C1	427	G
49	C1	433	G
49	C1	435	A
49	C1	436	A
49	C1	438	C
49	C1	440	G
49	C1	441	A
49	C1	442	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	443	G
49	C1	453	G
49	C1	454	C
49	C1	458	A
49	C1	459	C
49	C1	467	C
49	C1	468	C
49	C1	469	G
49	C1	471	C
49	C1	473	G
49	C1	474	A
49	C1	475	C
49	C1	483	U
49	C1	484	G
49	C1	491	G
49	C1	492	C
49	C1	494	G
49	C1	499	G
49	C1	500	C
49	C1	501	U
49	C1	502	A
49	C1	504	C
49	C1	581	C
49	C1	582	G
49	C1	583	A
49	C1	584	U
49	C1	585	A
49	C1	586	G
49	C1	587	U
49	C1	591	C
49	C1	594	G
49	C1	602	U
49	C1	604	C
49	C1	609	A
49	C1	610	G
49	C1	612	C
49	C1	613	A
49	C1	614	U
49	C1	618	C
49	C1	621	G
49	C1	627	A
49	C1	628	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	636	C
49	C1	646	C
49	C1	650	G
49	C1	652	A
49	C1	653	U
49	C1	655	A
49	C1	656	G
49	C1	659	A
49	C1	660	U
49	C1	664	A
49	C1	666	A
49	C1	667	G
49	C1	678	A
49	C1	679	A
49	C1	680	U
49	C1	682	G
49	C1	683	C
49	C1	685	C
49	C1	686	A
49	C1	687	U
49	C1	688	U
49	C1	689	A
49	C1	690	A
49	C1	692	U
49	C1	693	C
49	C1	697	U
49	C1	700	C
49	C1	702	U
49	C1	703	U
49	C1	710	A
49	C1	711	U
49	C1	713	G
49	C1	714	U
49	C1	719	U
49	C1	720	A
49	C1	728	G
49	C1	729	A
49	C1	730	U
49	C1	735	G
49	C1	740	A
49	C1	741	A
49	C1	742	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	743	U
49	C1	744	C
49	C1	745	U
49	C1	756	C
49	C1	758	U
49	C1	760	C
49	C1	764	A
49	C1	765	A
49	C1	767	U
49	C1	768	C
49	C1	769	C
49	C1	770	C
49	C1	771	G
49	C1	772	A
49	C1	774	U
49	C1	775	U
49	C1	776	C
49	C1	777	G
49	C1	778	G
49	C1	780	A
49	C1	782	G
49	C1	785	U
49	C1	786	G
49	C1	797	A
49	C1	816	C
49	C1	828	G
49	C1	832	U
49	C1	833	U
49	C1	834	C
49	C1	841	A
49	C1	845	C
49	C1	849	A
49	C1	850	A
49	C1	851	U
49	C1	856	C
49	C1	858	G
49	C1	860	C
49	C1	861	U
49	C1	862	U
49	C1	863	G
49	C1	864	C
49	C1	865	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	871	G
49	C1	880	U
49	C1	886	U
49	C1	888	U
49	C1	889	C
49	C1	892	C
49	C1	893	C
49	C1	897	U
49	C1	898	C
49	C1	900	A
49	C1	903	U
49	C1	905	C
49	C1	906	G
49	C1	907	A
49	C1	910	G
49	C1	913	G
49	C1	915	G
49	C1	916	U
49	C1	921	G
49	C1	925	G
49	C1	927	C
49	C1	930	G
49	C1	931	G
49	C1	934	A
49	C1	935	C
49	C1	936	A
49	C1	941	G
49	C1	942	U
49	C1	943	A
49	C1	944	A
49	C1	953	U
49	C1	958	C
49	C1	971	A
49	C1	972	A
49	C1	974	G
49	C1	983	A
49	C1	984	A
49	C1	985	A
49	C1	986	C
49	C1	988	G
49	C1	989	C
49	C1	990	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	995	C
49	C1	1000	A
49	C1	1001	A
49	C1	1002	G
49	C1	1005	A
49	C1	1007	G
49	C1	1015	C
49	C1	1017	C
49	C1	1019	C
49	C1	1020	A
49	C1	1021	A
49	C1	1022	A
49	C1	1023	U
49	C1	1024	U
49	C1	1025	A
49	C1	1027	C
49	C1	1028	C
49	C1	1029	A
49	C1	1030	A
49	C1	1035	G
49	C1	1036	A
49	C1	1037	C
49	C1	1038	A
49	C1	1039	C
49	C1	1043	G
49	C1	1044	A
49	C1	1052	A
49	C1	1053	C
49	C1	1054	A
49	C1	1057	A
49	C1	1059	A
49	C1	1061	A
49	C1	1069	A
49	C1	1076	U
49	C1	1077	U
49	C1	1078	U
49	C1	1079	C
49	C1	1080	G
49	C1	1083	U
49	C1	1085	U
49	C1	1086	U
49	C1	1087	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	1088	U
49	C1	1089	A
49	C1	1093	G
49	C1	1094	G
49	C1	1095	A
49	C1	1097	U
49	C1	1098	G
49	C1	1099	A
49	C1	1103	C
49	C1	1104	A
49	C1	1105	A
49	C1	1111	A
49	C1	1116	U
49	C1	1120	C
49	C1	1123	G
49	C1	1124	G
49	C1	1125	A
49	C1	1126	A
49	C1	1127	C
49	C1	1128	A
49	C1	1129	A
49	C1	1134	A
49	C1	1141	G
49	C1	1145	G
49	C1	1147	U
49	C1	1148	G
49	C1	1149	C
49	C1	1150	C
49	C1	1154	A
49	C1	1156	C
49	C1	1157	C
49	C1	1158	G
49	C1	1159	C
49	C1	1163	A
49	C1	1164	A
49	C1	1166	U
49	C1	1167	C
49	C1	1168	C
49	C1	1169	A
49	C1	1171	C
49	C1	1177	U
49	C1	1178	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	1179	G
49	C1	1181	G
49	C1	1186	U
49	C1	1218	G
49	C1	1219	A
49	C1	1222	C
49	C1	1223	U
49	C1	1444	A
49	C1	1447	A
49	C1	1448	A
49	C1	1449	U
49	C1	1450	A
49	C1	1451	G
49	C1	1452	G
49	C1	1458	U
49	C1	1461	G
49	C1	1471	U
49	C1	1479	U
49	C1	1480	G
49	C1	1481	U
49	C1	1483	A
49	C1	1484	G
49	C1	1486	G
49	C1	1489	G
49	C1	1491	A
49	C1	1497	U
49	C1	1498	G
49	C1	1499	G
49	C1	1507	G
49	C1	1517	A
49	C1	1518	A
49	C1	1519	C
49	C1	1520	U
49	C1	1525	A
49	C1	1527	G
49	C1	1529	A
49	C1	1536	A
49	C1	1544	U
49	C1	1545	U
49	C1	1546	U
49	C1	1547	C
49	C1	1549	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	1551	A
49	C1	1554	C
49	C1	1555	A
49	C1	1624	A
49	C1	1625	G
49	C1	1628	A
49	C1	1636	G
49	C1	1637	C
49	C1	1639	U
49	C1	1642	A
49	C1	1643	U
49	C1	1644	U
49	C1	1645	U
49	C1	1656	C
49	C1	1665	A
49	C1	1666	C
49	C1	1667	G
49	C1	1668	A
49	C1	1669	U
49	C1	1670	A
49	C1	1673	U
49	C1	1675	A
49	C1	1676	A
49	C1	1677	A
49	C1	1678	A
49	C1	1698	G
49	C1	1699	U
49	C1	1700	A
49	C1	1709	A
49	C1	1710	G
49	C1	1711	G
49	C1	1712	C
49	C1	1713	U
49	C1	1716	A
49	C1	1730	G
49	C1	1733	G
49	C1	1734	G
49	C1	1735	A
49	C1	1741	A
49	C1	1742	C
49	C1	1743	C
49	C1	1744	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	1751	G
49	C1	1761	C
49	C1	2054	A
49	C1	2055	C
49	C1	2056	U
49	C1	2057	G
49	C1	2059	C
49	C1	2061	G
49	C1	2068	C
49	C1	2069	G
49	C1	2070	A
49	C1	2071	G
49	C1	2072	U
49	C1	2073	A
49	C1	2074	C
49	C1	2075	U
49	C1	2077	C
49	C1	2078	C
49	C1	2085	G
49	C1	2086	A
49	C1	2087	G
49	C1	2088	A
49	C1	2107	A
49	C1	2109	A
49	C1	2114	G
49	C1	2115	U
49	C1	2118	U
49	C1	2119	G
49	C1	2120	C
49	C1	2121	U
49	C1	2157	G
49	C1	2158	G
49	C1	2166	A
49	C1	2167	G
49	C1	2173	G
49	C1	2175	A
49	C1	2176	A
49	C1	2177	G
49	C1	2178	U
49	C1	2179	C
49	C1	2181	U
49	C1	2183	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	2184	G
49	C1	2185	C
49	C1	2193	G
49	C1	2196	U
49	C1	2197	A
49	C1	2199	G
49	C1	2201	C
49	C1	2210	U
49	C1	2211	U
49	C1	2212	G
49	C1	2213	U
49	C1	2214	A
49	C1	2215	C
49	C1	2216	A
49	C1	2217	C
49	C1	2220	C
49	C1	2222	C
49	C1	2223	C
49	C1	2227	C
49	C1	2329	A
49	C1	2330	G
49	C1	2351	G
49	C1	2352	U
49	C1	2358	U
49	C1	2362	U
49	C1	2363	G
49	C1	2364	A
49	C1	2365	A
49	C1	2366	C
49	C1	2374	G
50	C2	6	C
50	C2	8	A
50	C2	10	A
50	C2	11	C
50	C2	15	A
50	C2	22	C
50	C2	23	A
50	C2	24	U
50	C2	25	U
50	C2	26	U
50	C2	28	U
50	C2	29	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	C2	31	A
50	C2	32	G
50	C2	33	U
50	C2	34	A
50	C2	36	U
50	C2	39	U
50	C2	48	G
50	C2	57	A
50	C2	58	A
50	C2	62	A
50	C2	63	G
50	C2	67	C
50	C2	91	G
50	C2	92	A
50	C2	94	A
50	C2	95	U
50	C2	101	G
50	C2	104	C
50	C2	105	C
50	C2	111	G
50	C2	124	U
50	C2	125	U
50	C2	126	U
50	C2	127	A
50	C2	128	C
50	C2	131	U
50	C2	132	C
50	C2	135	U
50	C2	136	C
50	C2	140	C
50	C2	142	G
50	C2	145	A
50	C2	147	G
50	C2	148	G
50	C2	153	G
50	C2	156	C
50	C2	160	U
50	C2	162	C
50	C2	163	C
50	C2	164	U
50	C2	165	C
50	C2	166	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	C2	167	U
50	C2	168	C
50	C2	170	C
50	C2	174	G
50	C2	177	G
50	C2	178	U
50	C2	179	A
50	C2	181	A
50	C2	182	G
50	C2	187	U
50	C2	189	G
50	C2	190	C
50	C2	192	A
50	C2	193	U
50	C2	194	G
50	C2	198	U
50	C2	199	G
50	C2	200	U
50	C2	201	A
50	C2	244	G
50	C2	246	G
50	C2	247	G
50	C2	249	U
50	C2	250	G
50	C2	255	U
50	C2	256	G
50	C2	259	A
50	C2	260	G
50	C2	261	U
50	C2	262	C
50	C2	265	A
50	C2	266	C

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
49	C1	67	G
49	C1	89	G
49	C1	134	C
49	C1	135	A
49	C1	150	C
49	C1	200	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	205	C
49	C1	209	A
49	C1	257	G
49	C1	277	U
49	C1	281	U
49	C1	290	C
49	C1	424	U
49	C1	582	G
49	C1	593	G
49	C1	684	U
49	C1	742	U
49	C1	771	G
49	C1	1001	A
49	C1	1058	A
49	C1	1068	C
49	C1	1077	U
49	C1	1085	U
49	C1	1087	G
49	C1	1163	A
49	C1	1176	A
49	C1	1485	A
49	C1	1712	C
49	C1	1734	G
49	C1	2054	A
49	C1	2070	A
49	C1	2106	U
49	C1	2156	A
49	C1	2166	A
49	C1	2219	C
50	C2	23	A
50	C2	33	U
50	C2	35	G
50	C2	91	G
50	C2	255	U
50	C2	259	A

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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
50	C2	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C2	206:G	O3'	240:C	P	18.94
1	C2	105:C	O3'	110:A	P	15.09
1	C2	119:C	O3'	123:A	P	11.47

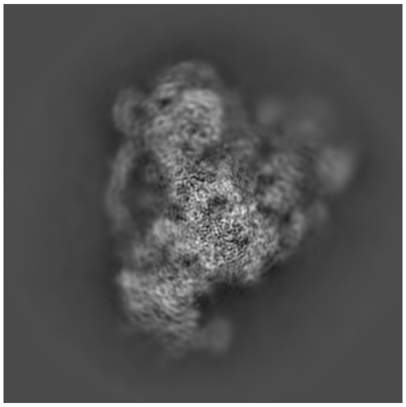
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10056. These allow visual inspection of the internal detail of the map and identification of artifacts.

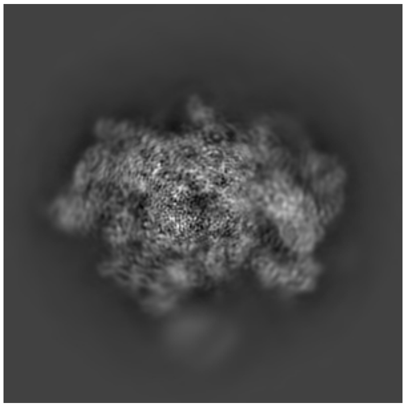
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

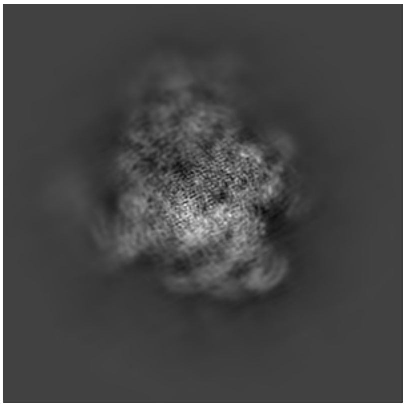
6.1.1 Primary map



X



Y

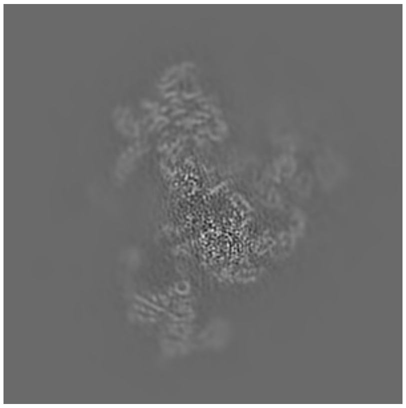


Z

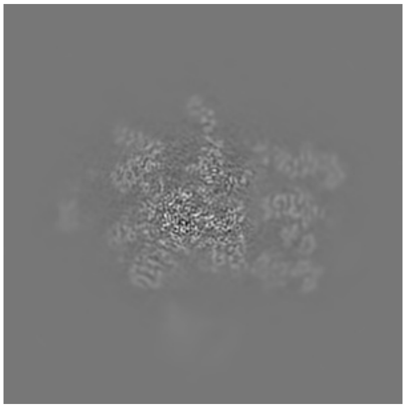
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 240



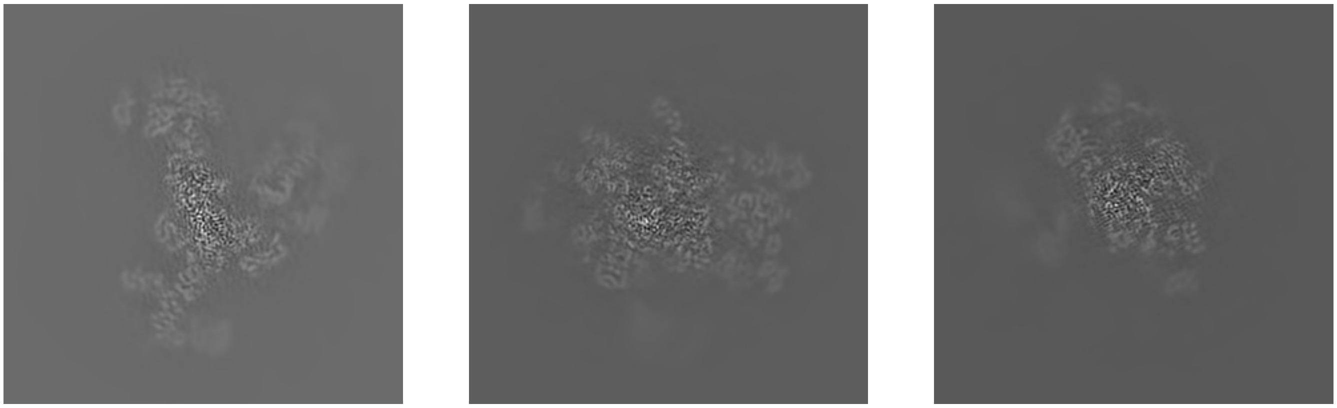
Y Index: 240

Z Index: 240

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

6.3 Largest variance slices

6.3.1 Primary map



X Index: 217 Y Index: 238 Z Index: 214

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

6.4 Orthogonal surface views

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

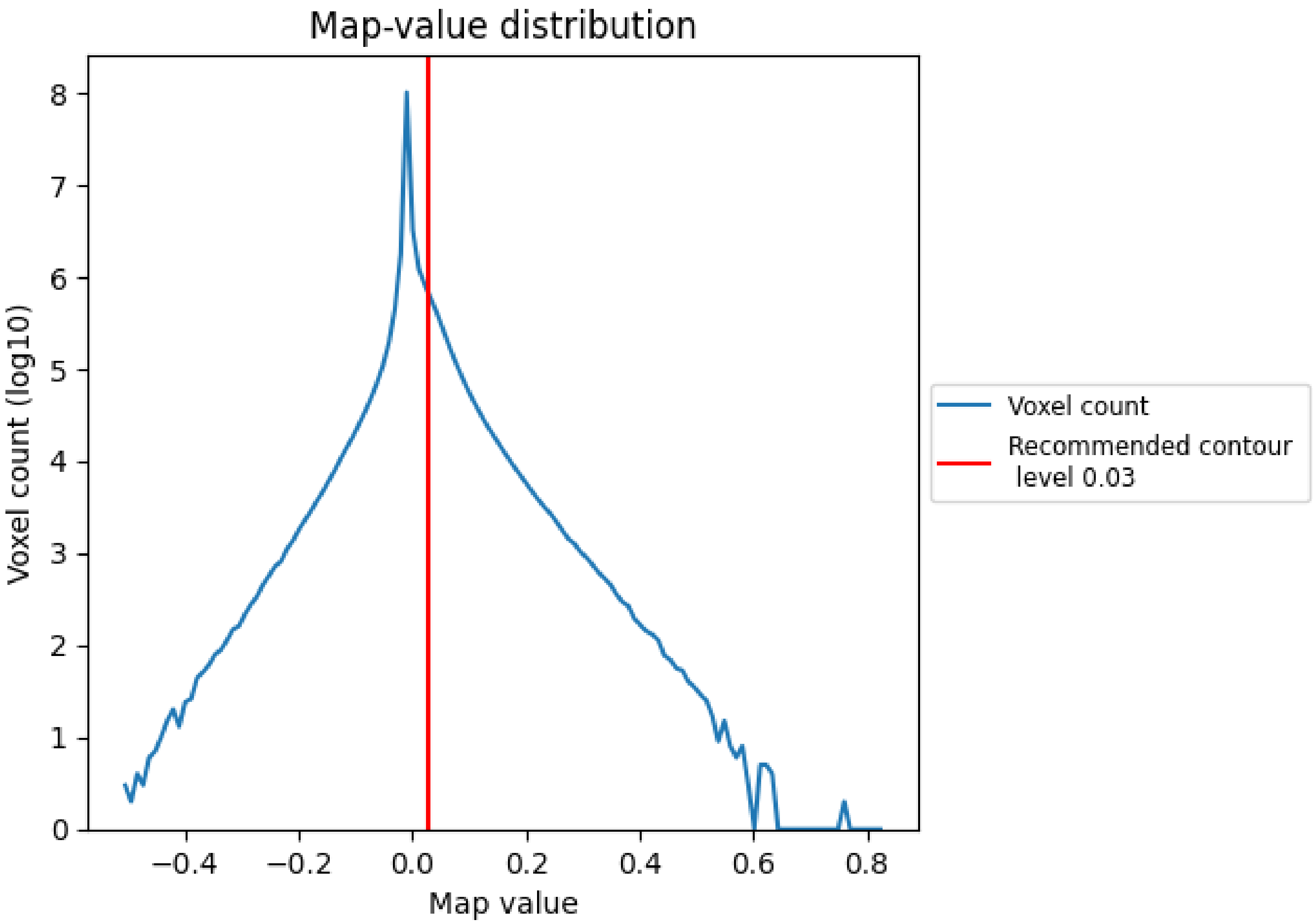
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

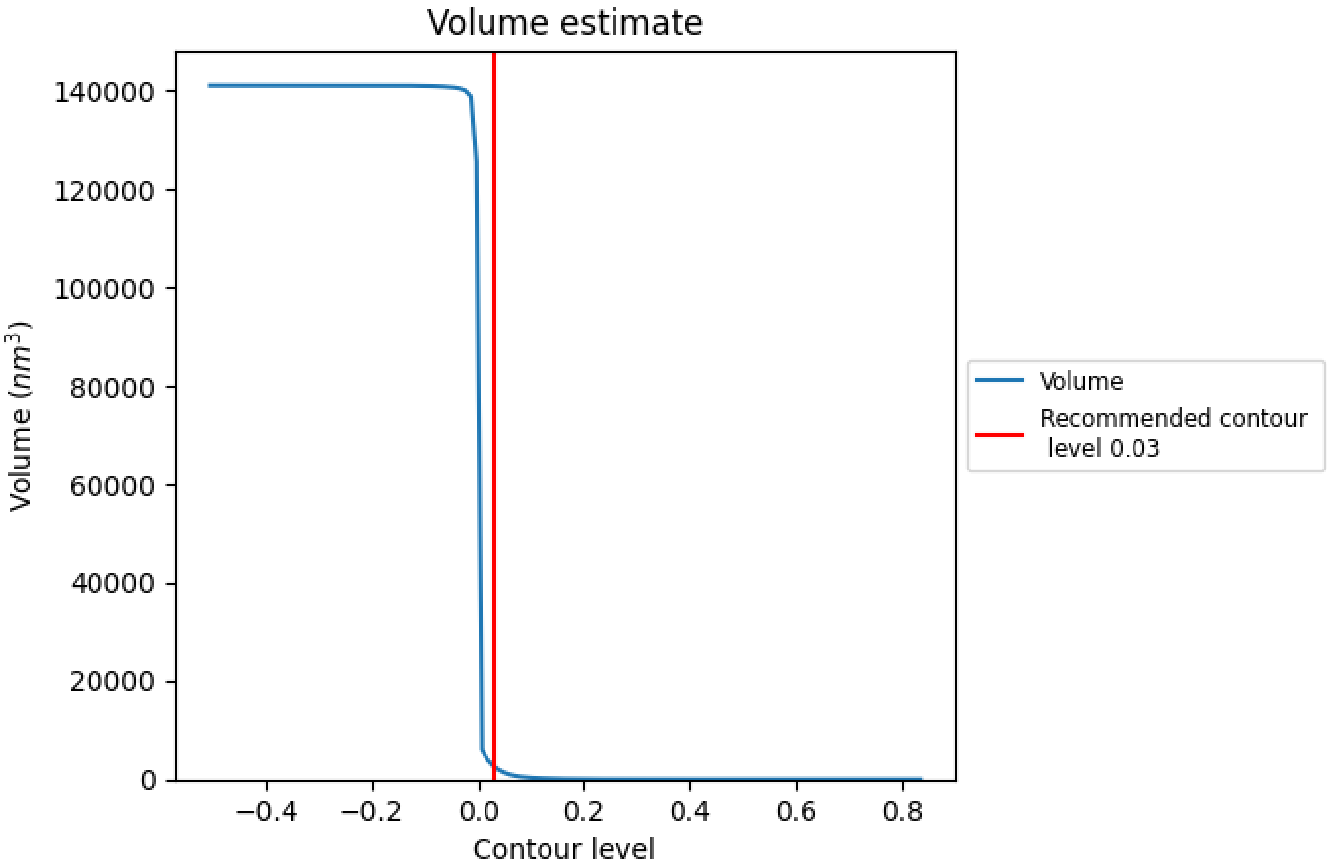
This section contains the results of statistical analysis of the map.

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.

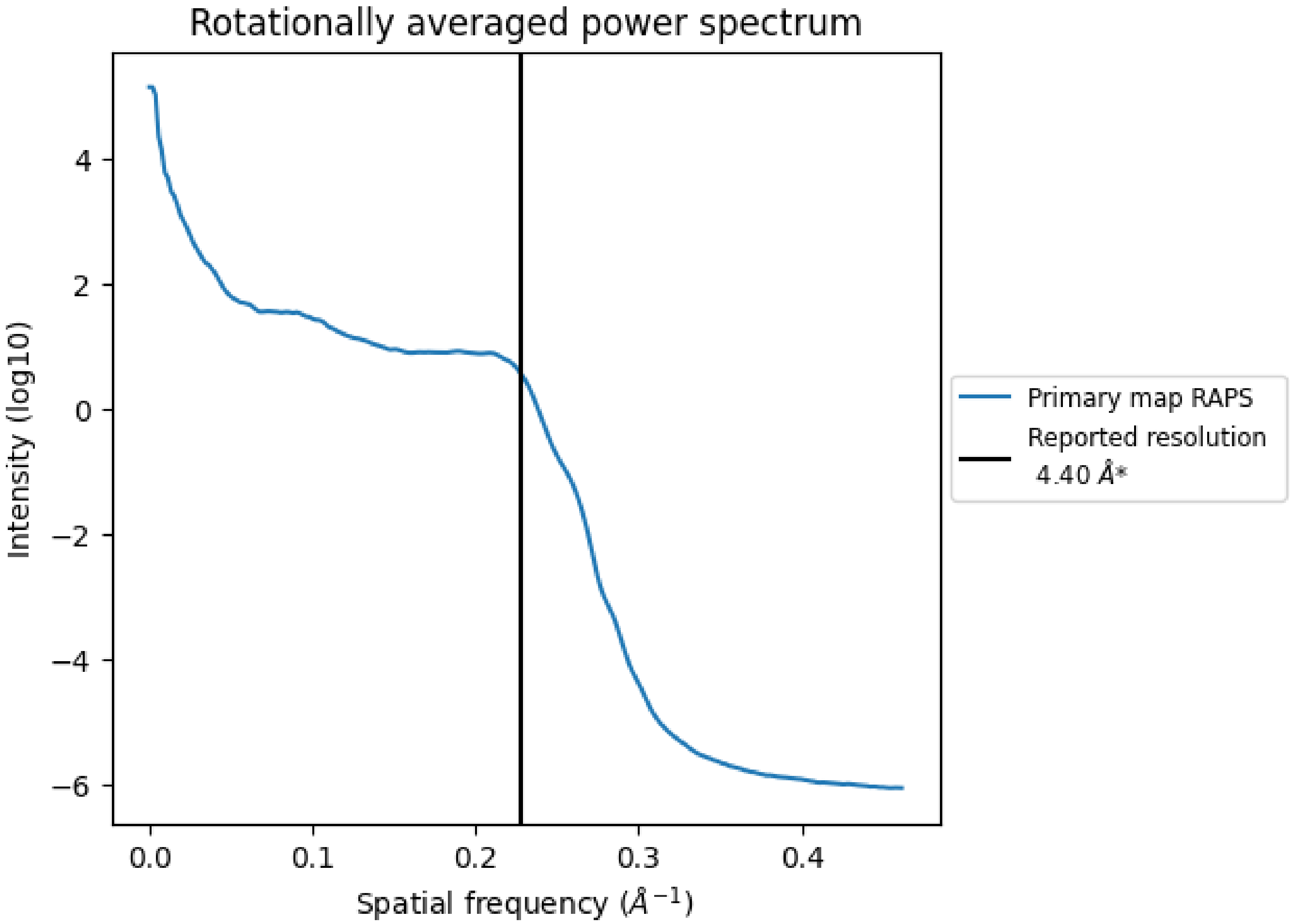
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2721 nm^3; this corresponds to an approximate mass of 2458 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 ⓘ

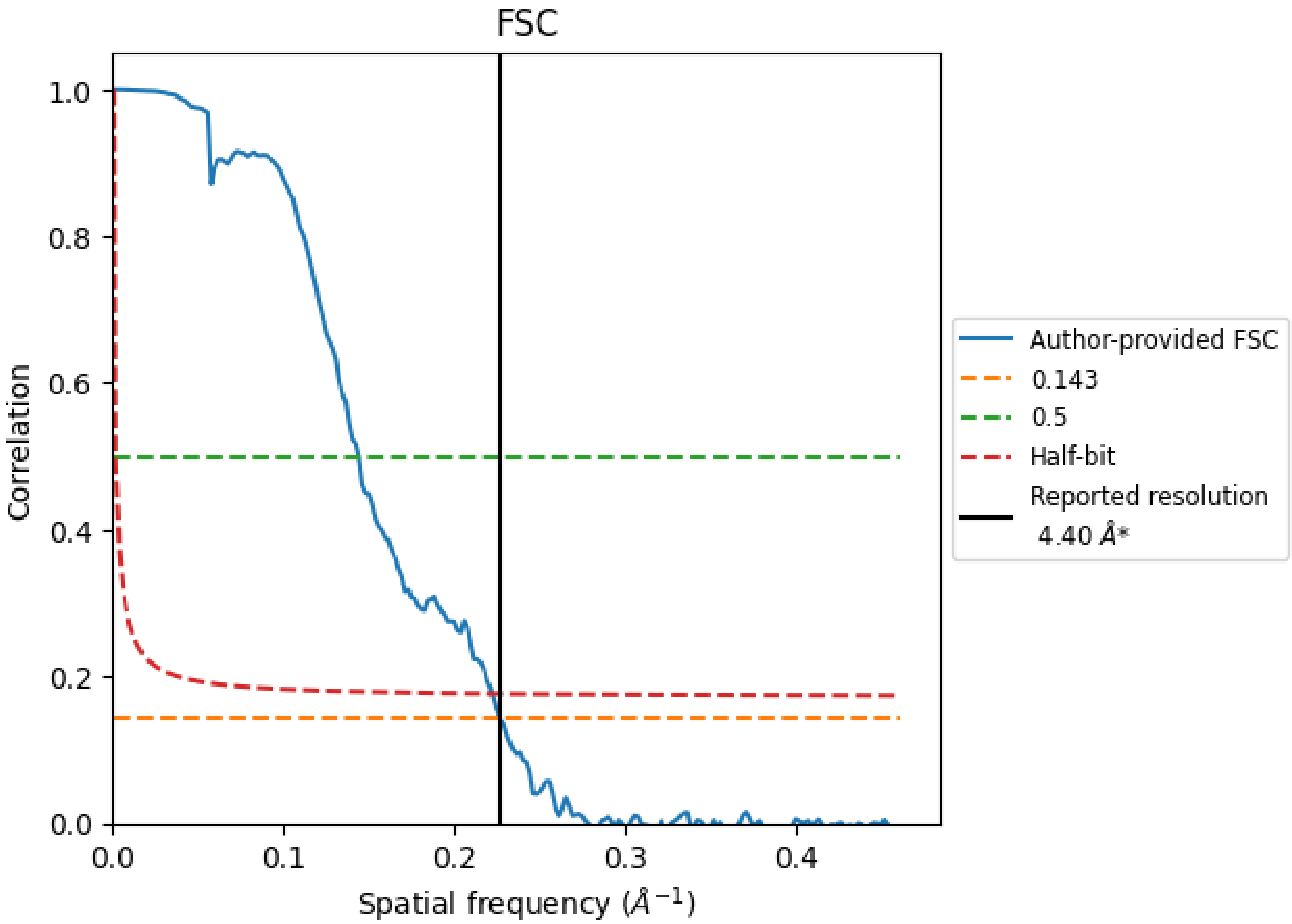


*Reported resolution corresponds to spatial frequency of 0.227 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.227 $Å^{-1}$

8.2 Resolution estimates ⓘ

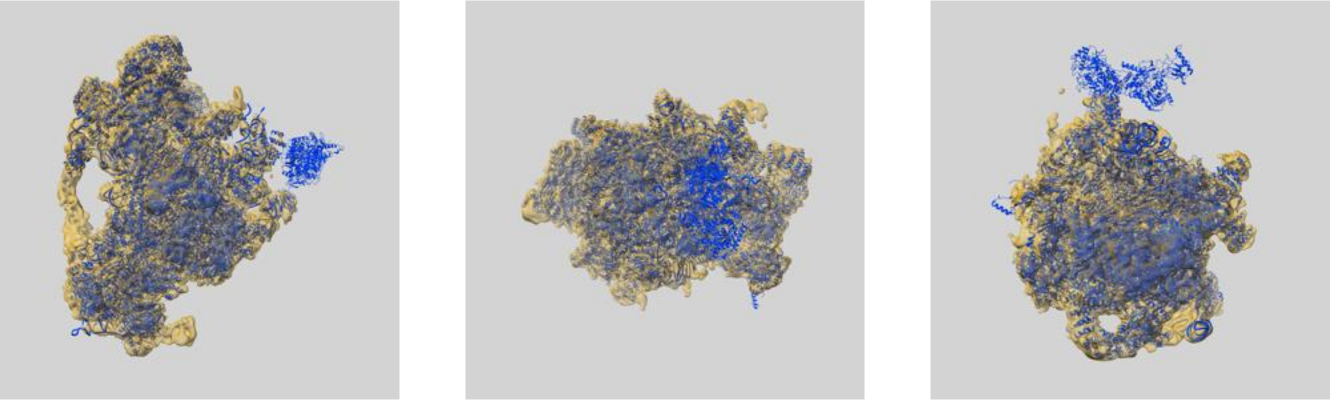
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.42	6.93	4.50
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10056 and PDB model 6RXZ. Per-residue inclusion information can be found in section 3 on page 16.

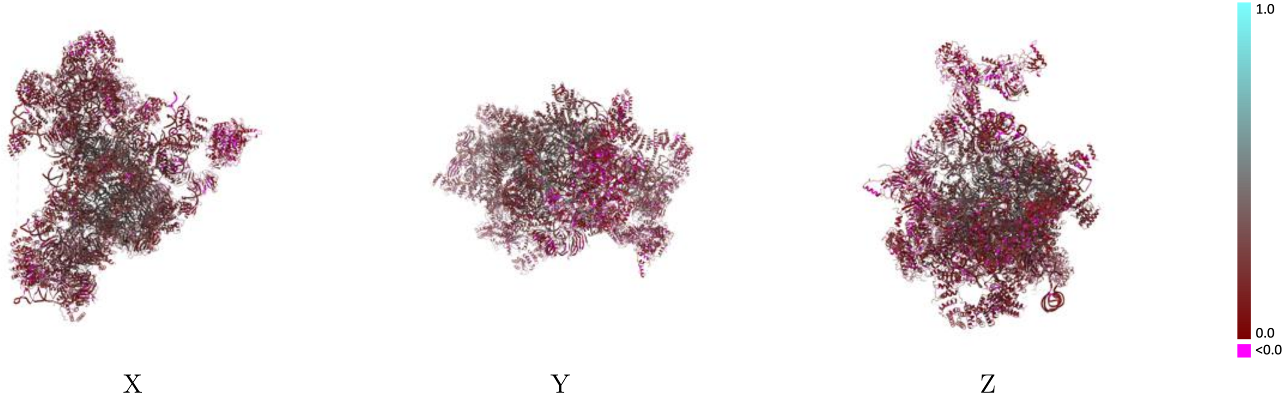
9.1 Map-model overlay



X Y Z

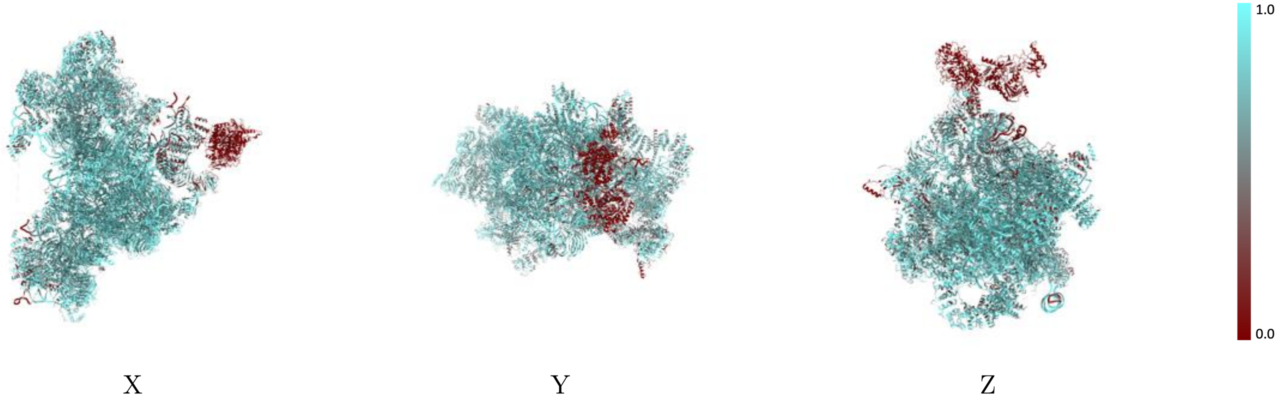
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



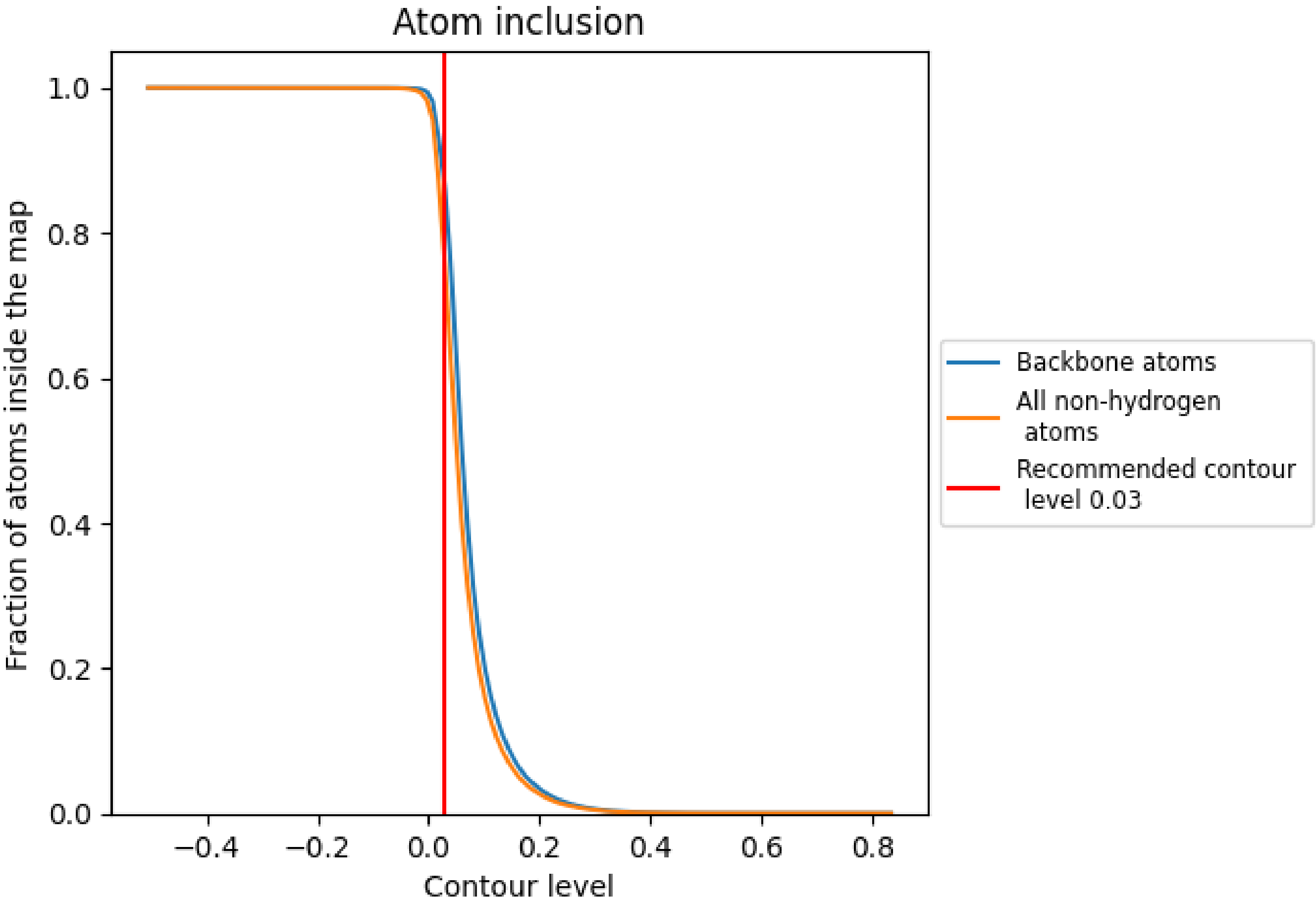
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.03).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7524	0.2270
C1	0.8699	0.2580
C2	0.9053	0.2760
CA	0.8723	0.3590
CB	0.7423	0.2130
CC	0.8126	0.2470
CD	0.7939	0.2420
CE	0.8606	0.3370
CF	0.8184	0.2680
CG	0.7831	0.2070
CH	0.8128	0.2770
CI	0.8791	0.3550
CJ	0.9151	0.4170
CK	0.8977	0.4110
CL	0.8385	0.3190
CM	0.8583	0.3350
CN	0.7369	0.2190
CO	0.6651	0.1760
CP	0.5345	0.1610
CQ	0.7254	0.1670
CR	0.7263	0.1710
CS	0.6115	0.1210
CT	0.8942	0.3680
CU	0.7963	0.2810
CV	0.0000	0.0660
CW	0.7382	0.1660
CX	0.6185	0.1010
CY	0.7508	0.2410
CZ	0.6959	0.1540
Cb	0.7137	0.1810
Cc	0.8225	0.2950
Cd	0.7366	0.1700
Ce	0.5815	0.1730
Cf	0.7440	0.1410
Cg	0.8543	0.3460

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ch	0.5345	0.1030
Ci	0.6464	0.1590
Cj	0.8915	0.4000
Ck	0.6735	0.1430
Cl	0.5032	0.2250
Cm	0.7765	0.2740
Cn	0.9175	0.4400
Co	0.7559	0.2010
Cp	0.8023	0.2540
Cz	0.4379	0.1550
UA	0.8579	0.3350
UB	0.7750	0.2200
UC	0.8881	0.3970
UD	0.7717	0.2150
UE	0.7196	0.1650
UF	0.8260	0.2180
UG	0.8044	0.3170
UH	0.7483	0.1680
UI	0.6508	0.1390
UJ	0.7461	0.2010
UK	0.8757	0.3630
UL	0.7576	0.1780
UM	0.6520	0.1240
UN	0.7668	0.2770
UO	0.7735	0.2240
UP	0.7543	0.2410
UQ	0.7901	0.2070
UR	0.8518	0.3000
US	0.7560	0.1660
UT	0.7437	0.1570
UU	0.8530	0.2850
UV	0.0029	0.0740
UX	0.8962	0.4090
UZ	0.8146	0.2630