Full wwPDB EM Validation Report ⓘ

May 18, 2024 – 05:35 pm BST

PDB ID	:	6RXY
EMDB ID	:	EMD-10055
Title	:	Cryo-EM structure of the 90S pre-ribosome (Kre33-Noc4) from Chaetomium thermophilum, state a
Authors	:	Cheng, J.; Kellner, N.; Griesel, S.; Berninghausen, O.; Beckmann, R.; Hurt, E.
Deposited on	:	2019-06-10
Resolution	:	4.70 Å(reported)

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

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

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

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

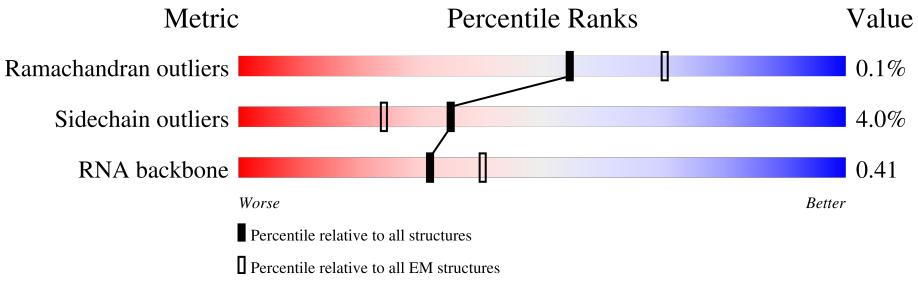
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 Å.

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



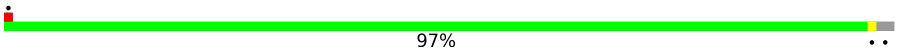
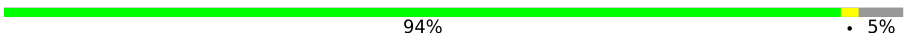
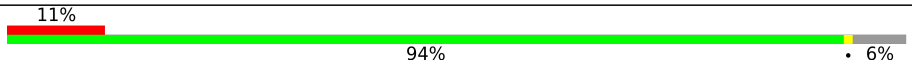
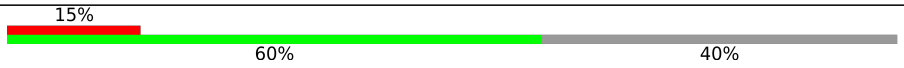
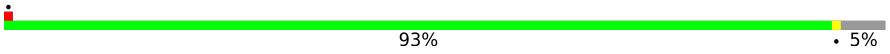
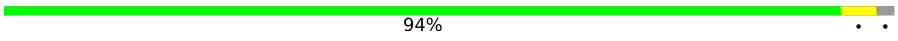
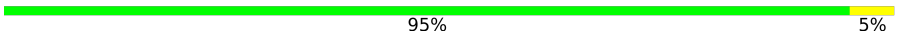
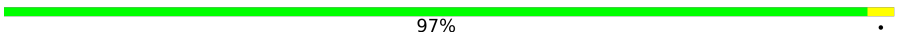
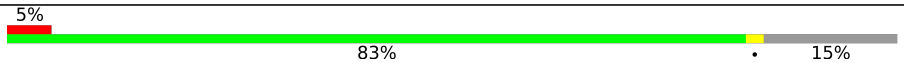
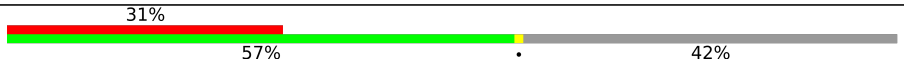
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	89% · 7%
2	UB	907	56% · 44%
3	UC	648	11% 89%
4	UD	884	86% · 13%
5	UF	414	80% 20%
6	UG	558	76% · 20%
7	UJ	1802	20% 44% · 55%
8	UK	270	79% · 20%

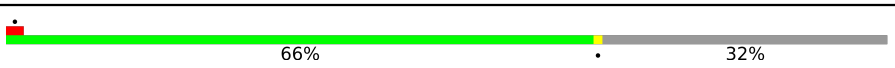
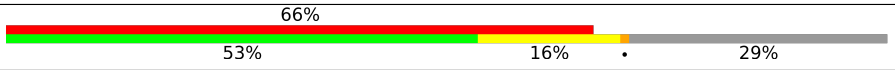
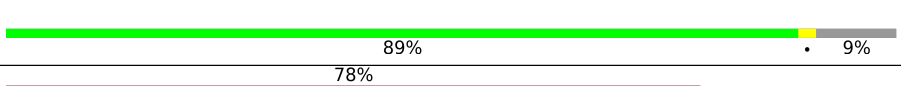
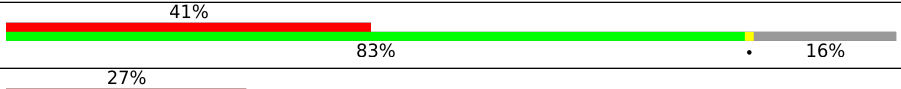
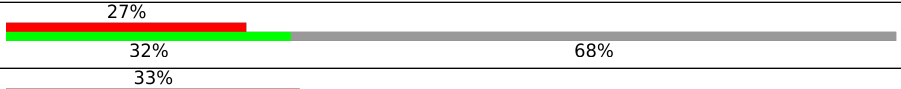
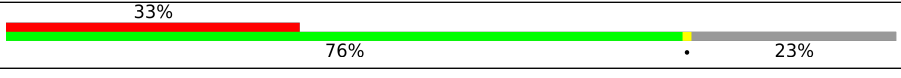
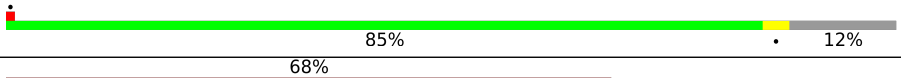
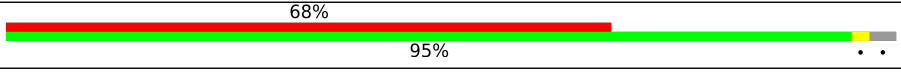
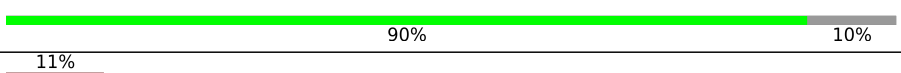
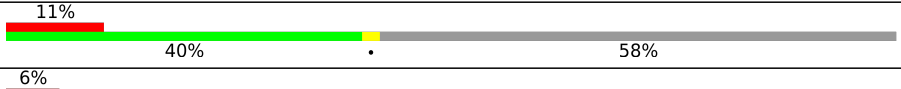
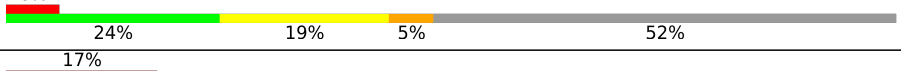
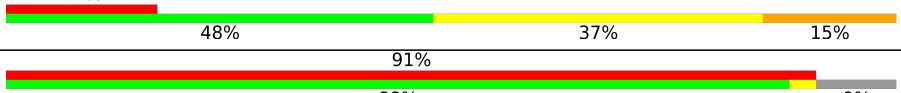
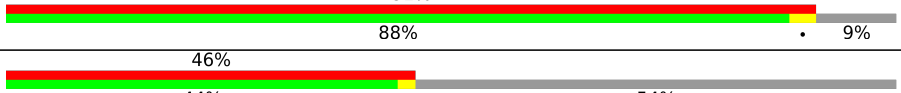
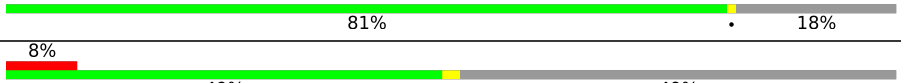
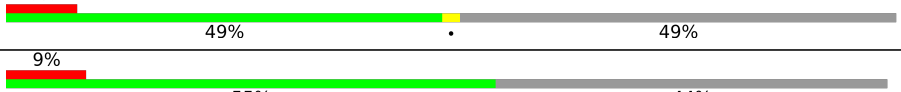
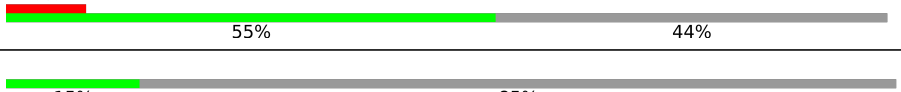
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	UL	962	
10	UM	912	
11	UN	938	
12	UO	557	
13	UQ	960	
14	UR	618	
15	UU	1049	
16	UX	193	
17	UZ	391	
18	CA	313	
18	CB	313	
19	CC	523	
20	CD	582	
21	CE	127	
21	CF	127	
22	CG	630	
23	CH	411	
24	CI	1163	
25	CJ	183	
26	CK	297	
27	CL	785	
28	CM	446	
29	CN	252	
29	CO	252	
30	CP	322	

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	Cc	212	
35	Ce	203	
36	Cg	190	
37	Ch	151	
38	Ci	150	
39	Cj	143	
40	Cm	130	
41	Cn	145	
42	Cp	68	
43	CU	311	
44	C1	2323	
45	C2	230	
46	UV	1171	
47	CV	322	
48	UH	930	
49	UE	410	
49	UI	410	
50	US	549	
51	Cl	156	
52	CX	480	
53	UP	364	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	Cz	1796	13% 15% 85%

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 180242 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
1	UA	839	Total	C	N	O	S	0	0
			6366	4101	1136	1105	24		

- Molecule 2 is a protein called Utp2.

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

- Molecule 3 is a protein called Utp3.

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

- Molecule 4 is a protein called Utp4.

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

- Molecule 5 is a protein called Utp6.

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

- Molecule 6 is a protein called Utp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	UG	448	Total	C	N	O	S	0	0
			3444	2197	646	590	11		

- Molecule 7 is a protein called Utp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UJ	808	Total	C	N	O	S	0	0
			6180	3965	1077	1115	23		

- 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	154	Total	C	N	O	S	0	0
			1209	770	228	206	5		

- 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
14	UR	447	Total	C	N	O	S	0	0
			3491	2209	656	616	10		

- Molecule 15 is a protein called Utp21.

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

- Molecule 16 is a protein called Utp24.

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

- Molecule 17 is a protein called Utp30.

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

- Molecule 18 is a protein called Nop1.

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

- Molecule 19 is a protein called Nop56.

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

- Molecule 20 is a protein called Nop58.

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

- Molecule 21 is a protein called Snu13.

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

- Molecule 22 is a protein called Rrp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CG	378	Total	C	N	O	S	0	0
			2922	1865	527	517	13		

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

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

- Molecule 24 is a protein called Bms1.

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

- Molecule 25 is a protein called Imp3.

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

- Molecule 26 is a protein called Imp4.

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

- Molecule 27 is a protein called Mpp10.

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

- Molecule 28 is a protein called Sof1.

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

- Molecule 29 is a protein called Emg1.

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

- 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	0	0
			1504	961	269	265	9		

- 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	0	0
			1361	862	250	242	7		

- Molecule 32 is a protein called Kre33.

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

- Molecule 33 is a protein called Fcf2.

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

- Molecule 34 is a protein called 40S ribosomal protein s5-like protein.

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

- Molecule 35 is a protein called 40S ribosomal protein S7.

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

- Molecule 36 is a protein called 40S ribosomal protein s9-like protein.

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

- Molecule 37 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	Ch	49	Total	C	N	O	0	0
			416	270	82	64		

- Molecule 38 is a protein called 40S ribosomal protein S14-like protein.

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

- Molecule 39 is a protein called 40S ribosomal protein S16-like protein.

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

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

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

- Molecule 41 is a protein called 40S ribosomal protein s23-like protein.

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

- Molecule 42 is a protein called 40S ribosomal protein S28-like protein.

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

- Molecule 43 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	CU	131	Total	C	N	O	S	0	0
			1009	623	205	175	6		

- Molecule 44 is a RNA chain called 35S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	C1	1106	Total	C	N	O	P	0	0
			23604	10525	4233	7740	1106		

- Molecule 45 is a RNA chain called U3 snoRNA.

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

- Molecule 46 is a protein called U3 small nucleolar RNA-associated protein 22.

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

- Molecule 47 is a protein called Rrp7.

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

- Molecule 48 is a protein called Utp8.

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

- Molecule 49 is a protein called Utp5.

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

- Molecule 50 is a protein called Noc4.

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

- Molecule 51 is a protein called Rps18.

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

- Molecule 52 is a protein called Enp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	CX	267	Total	C	N	O	S	0	0
			2130	1384	374	362	10		

- Molecule 53 is a protein called Utp16.

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

- Molecule 54 is a protein called Rrp5.

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

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

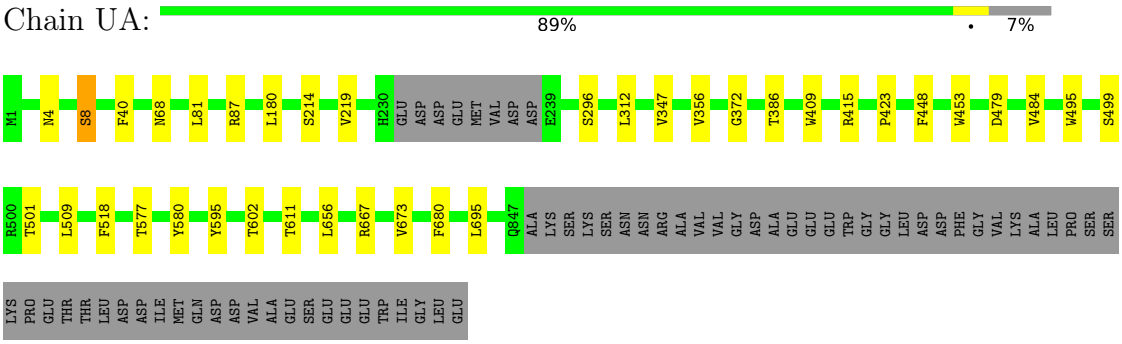
Mol	Chain	Residues	Atoms		AltConf
55	UX	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

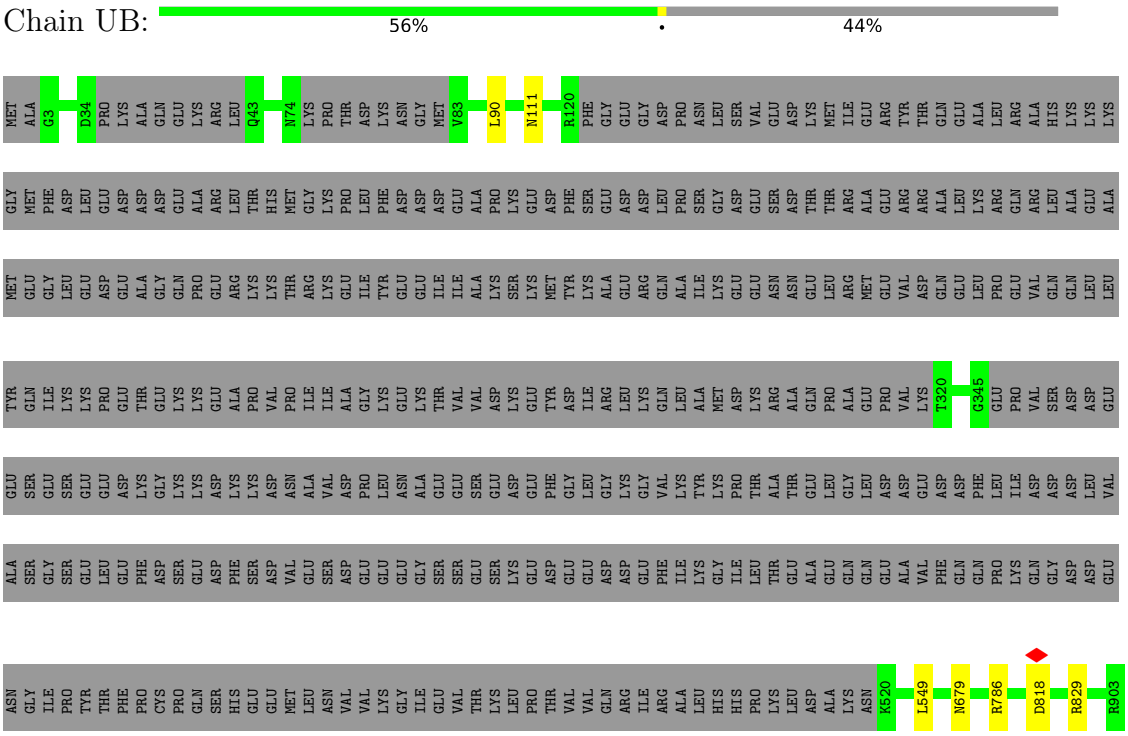
• Molecule 1: Periodic tryptophan protein 2-like protein

Chain UA:



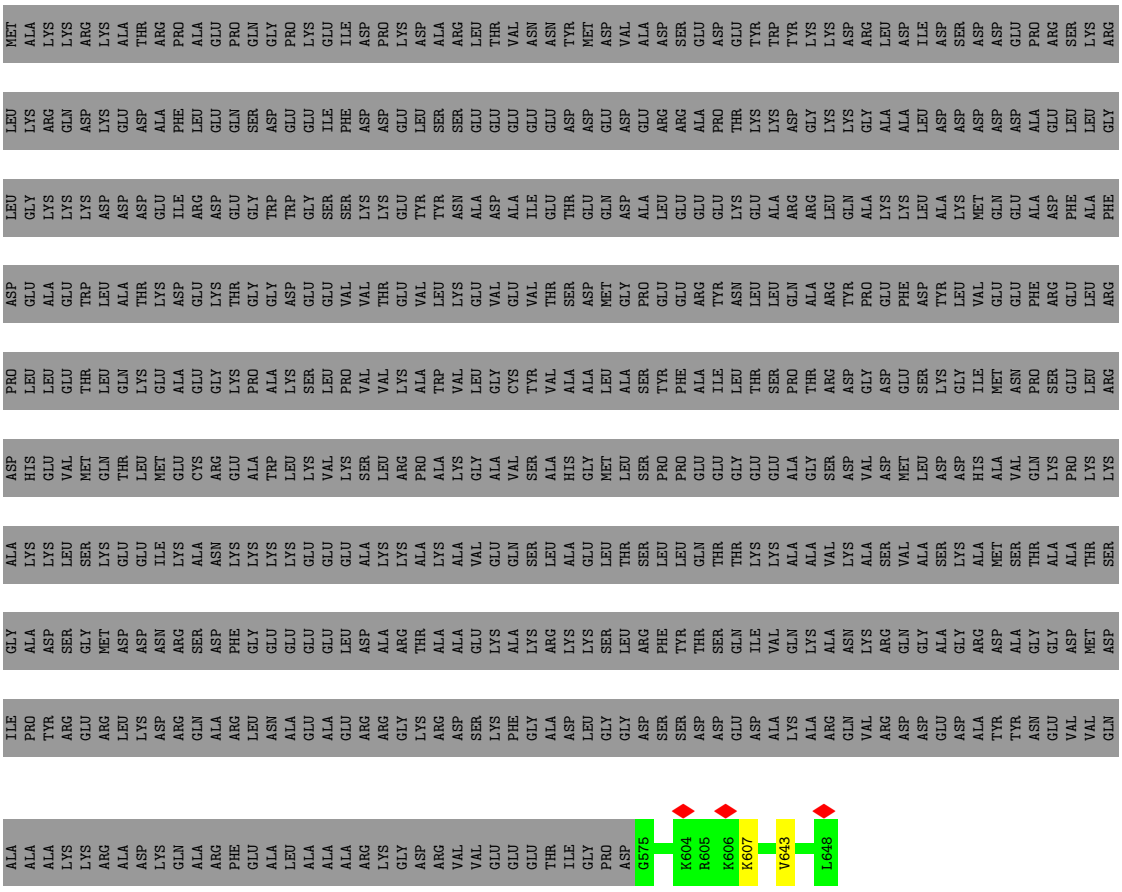
• Molecule 2: Utp2

Chain UB:



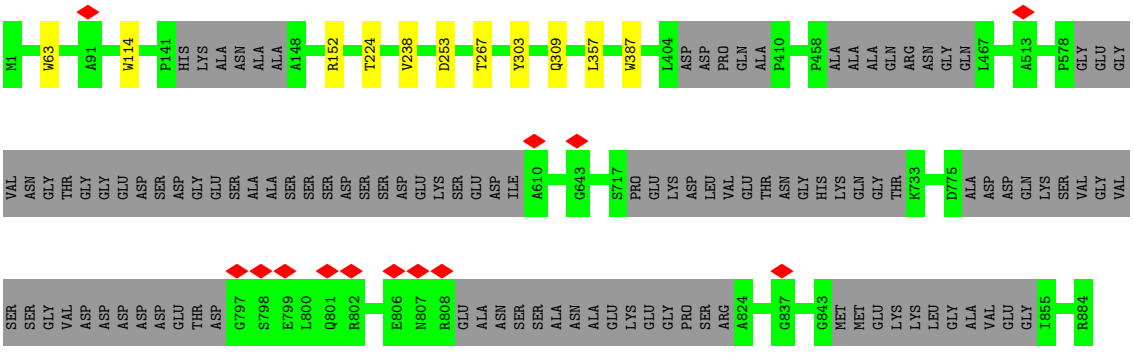
• Molecule 3: Utp3

Chain UC:



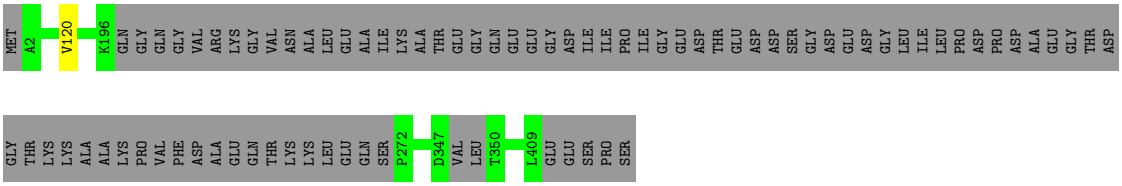
• Molecule 4: Utp4

Chain UD:



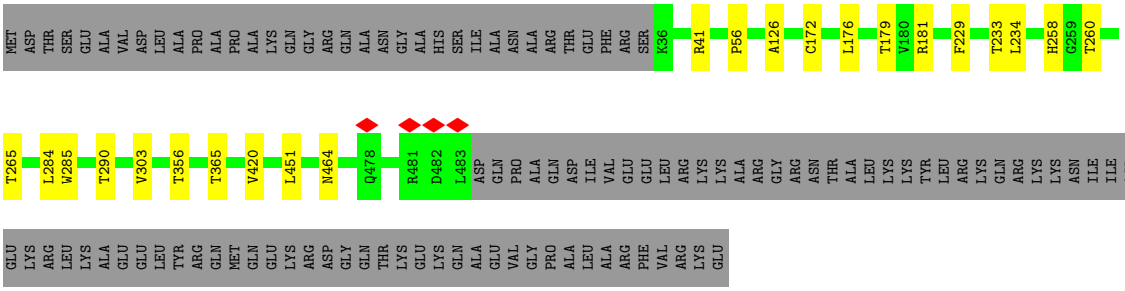
• Molecule 5: Utp6

Chain UF:



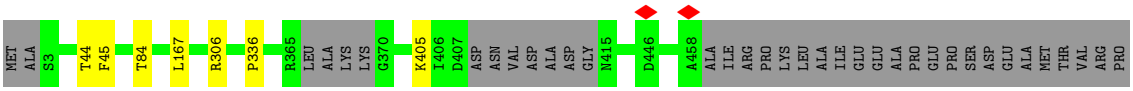
• Molecule 6: Utp7

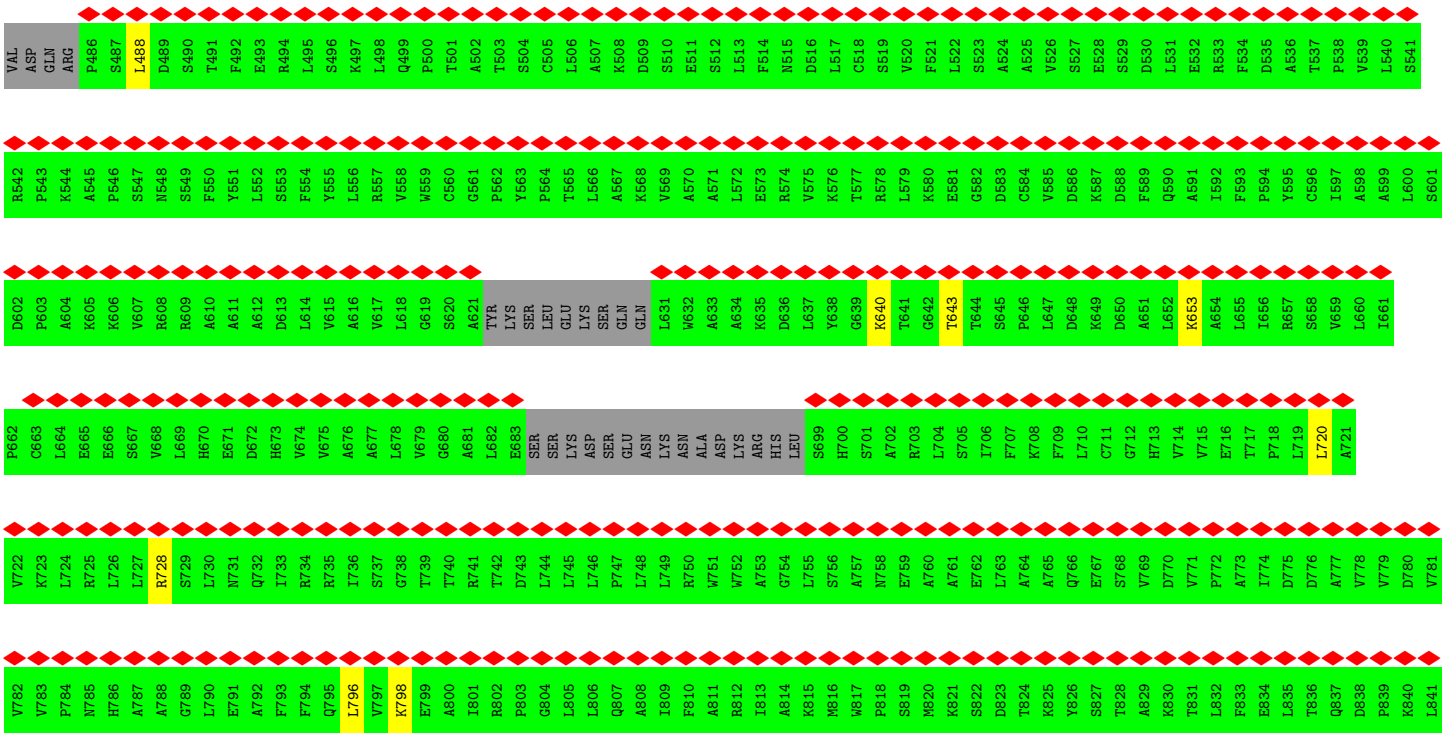
Chain UG:

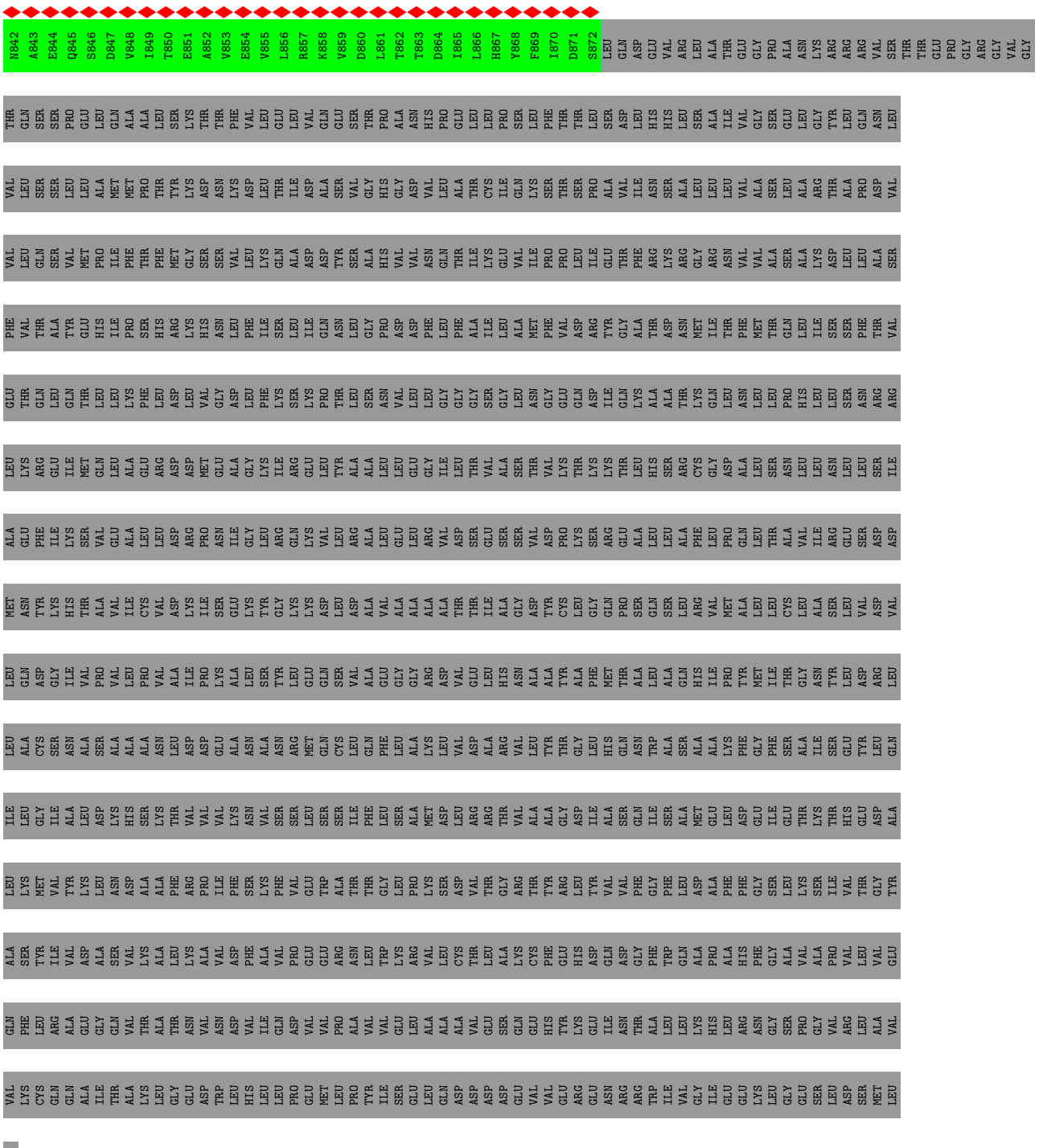


• Molecule 7: Utp10

Chain UJ:

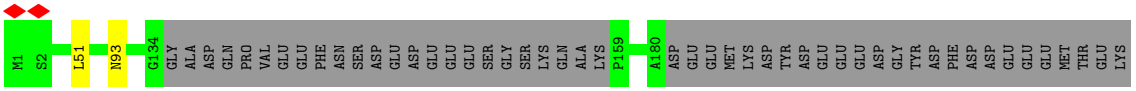






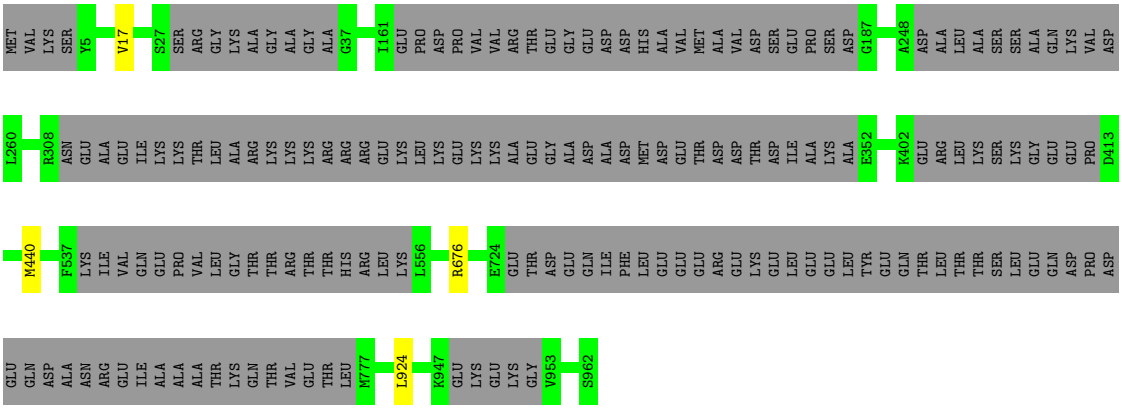
• Molecule 8: U3 small nucleolar RNA-associated protein 11

Chain UK:



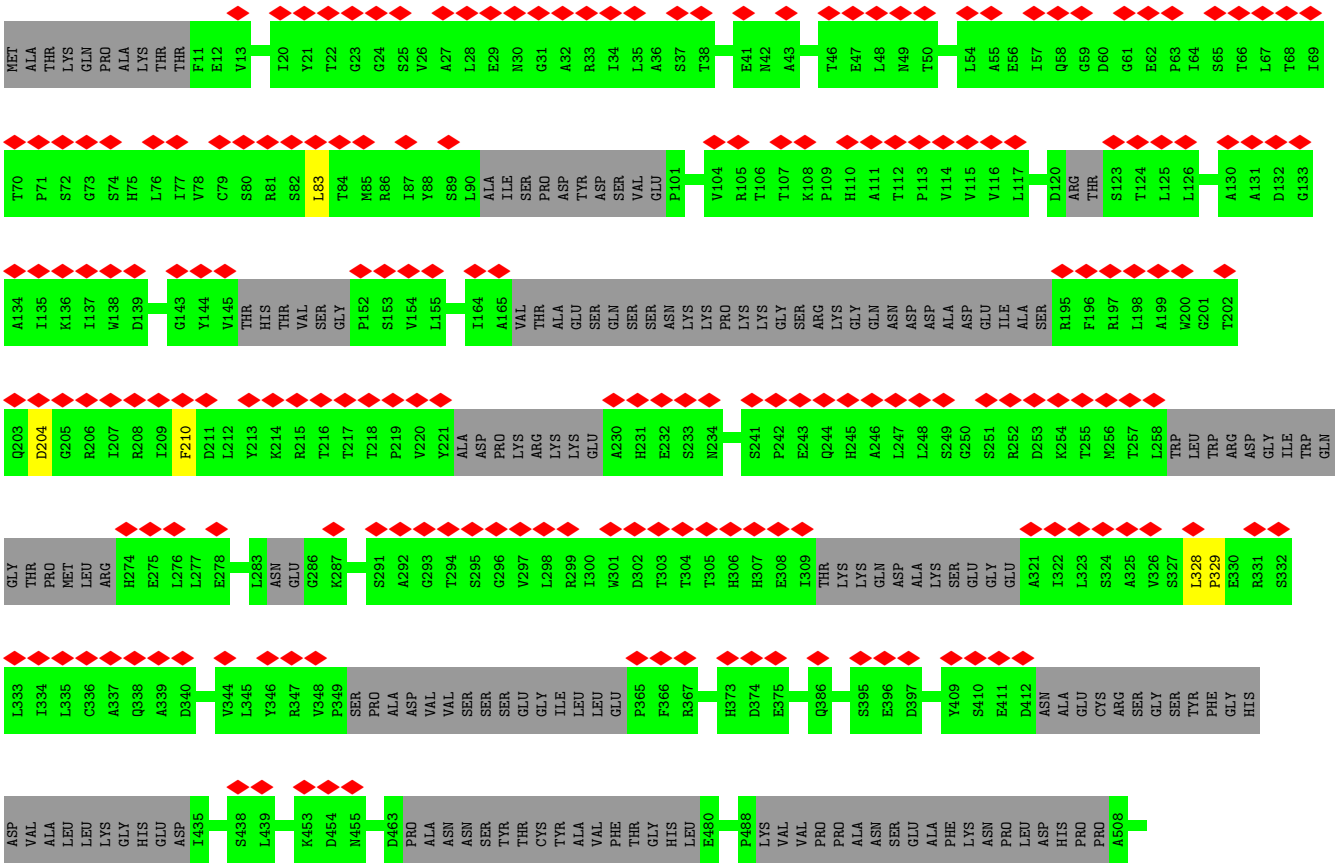
• Molecule 9: Utp12

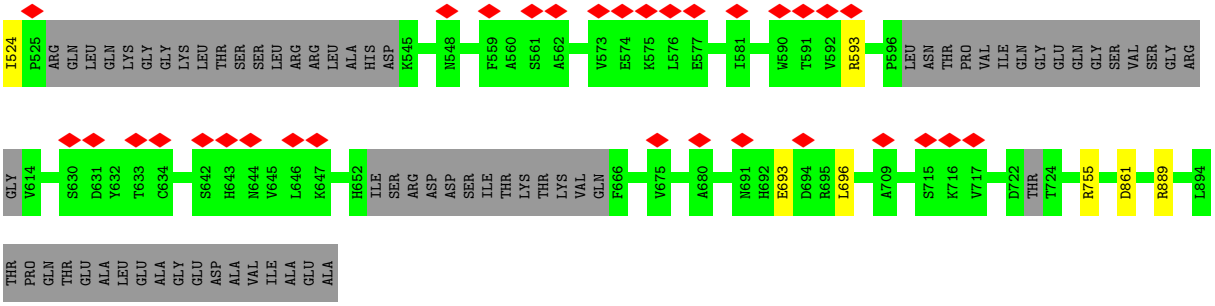
Chain UL:



• Molecule 10: Utp13

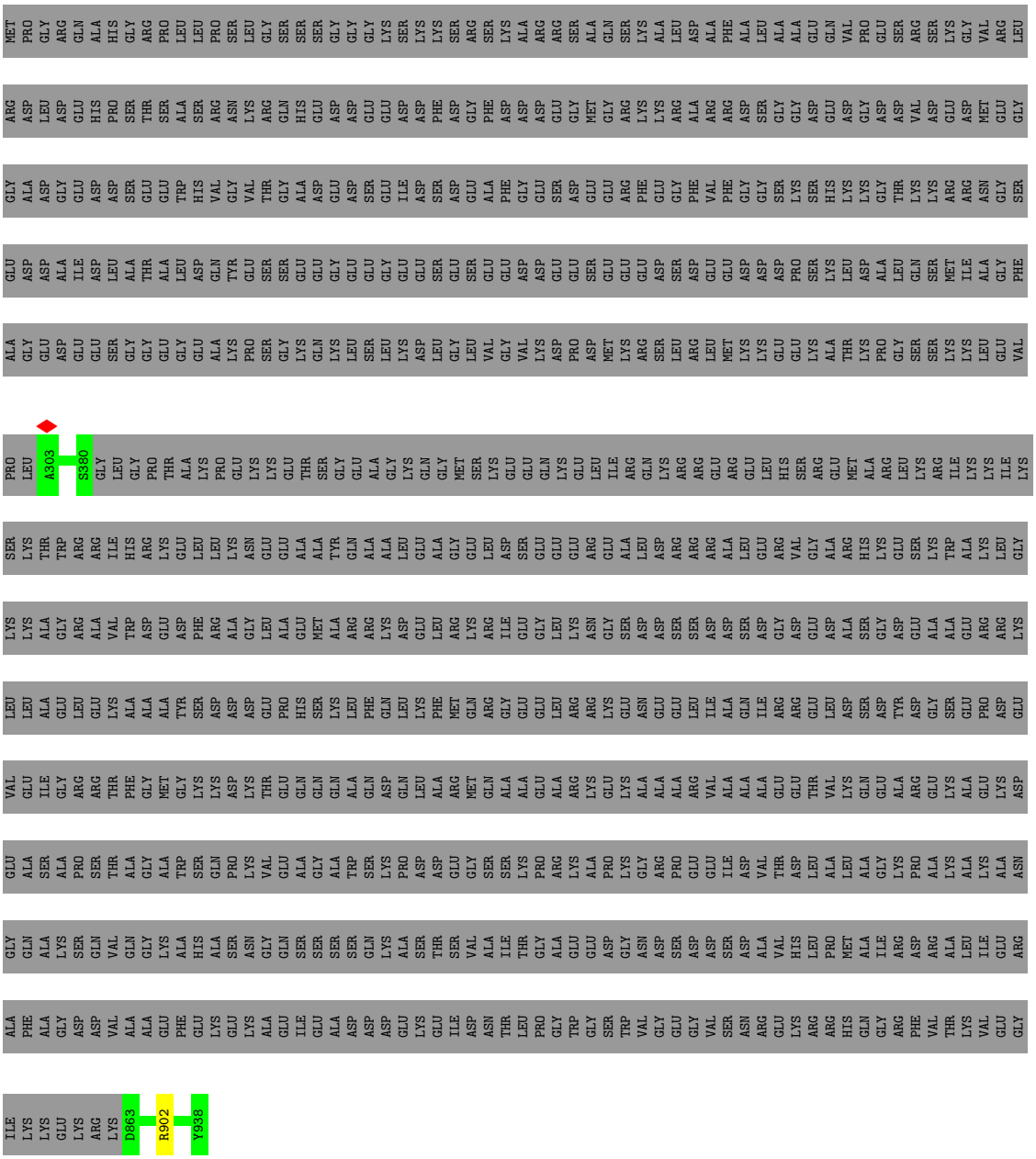
Chain UM:





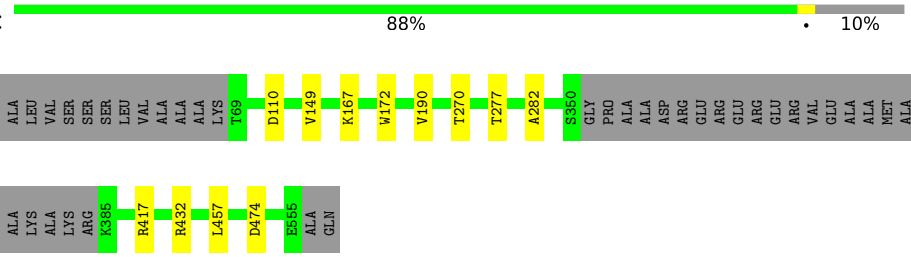
• Molecule 11: Utp14

Chain UN:



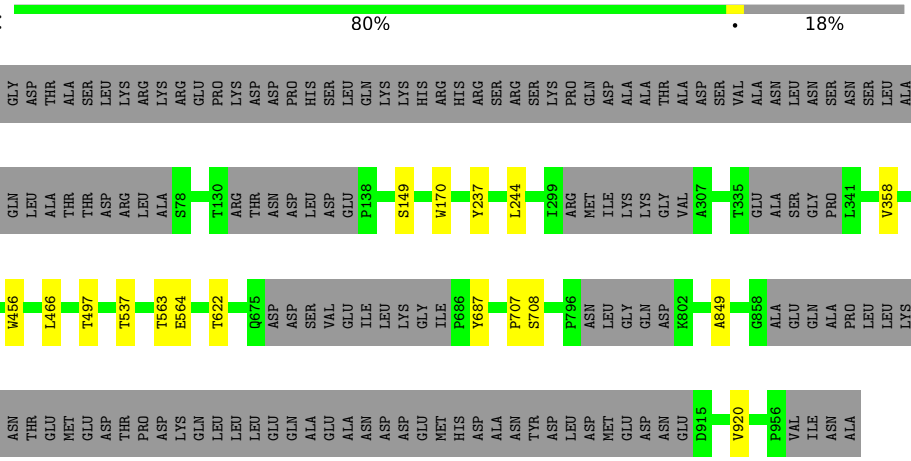
• Molecule 12: Utp15

Chain UO:



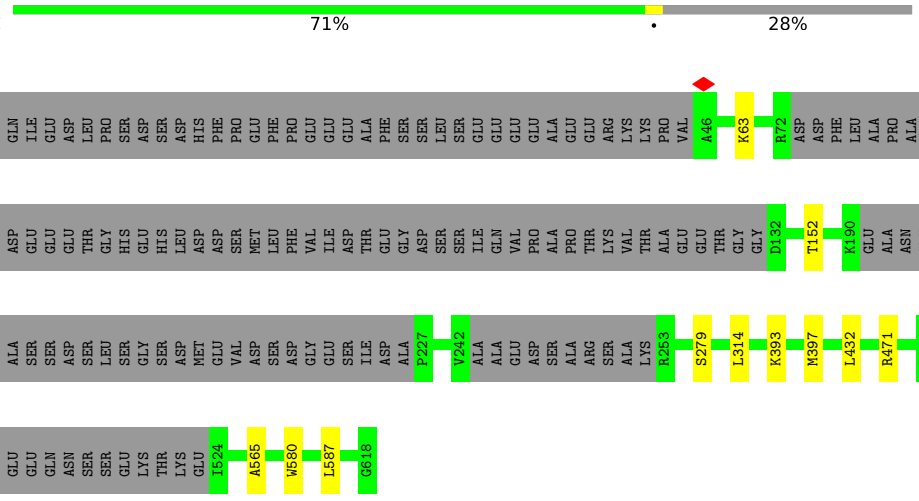
• Molecule 13: Utp17

Chain UQ:



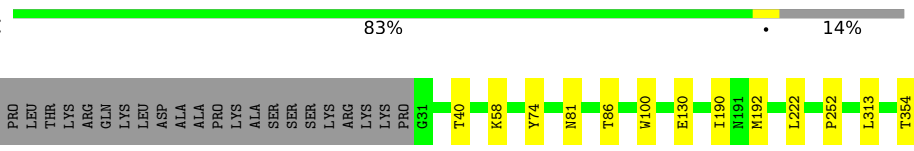
• Molecule 14: Utp18

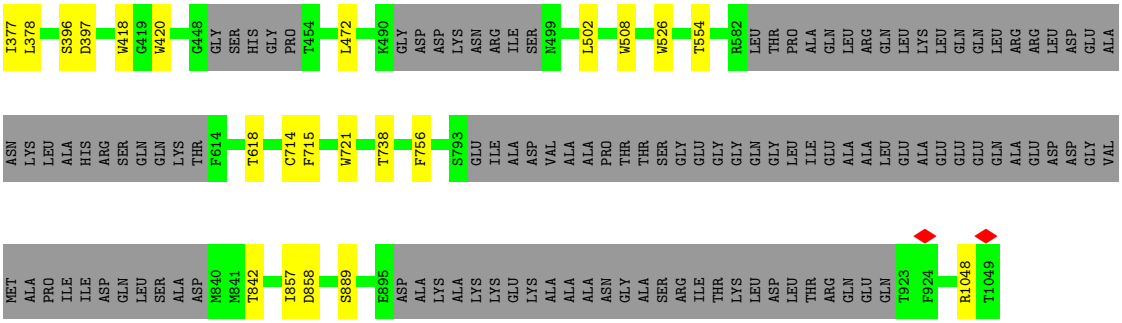
Chain UR:



• Molecule 15: Utp21

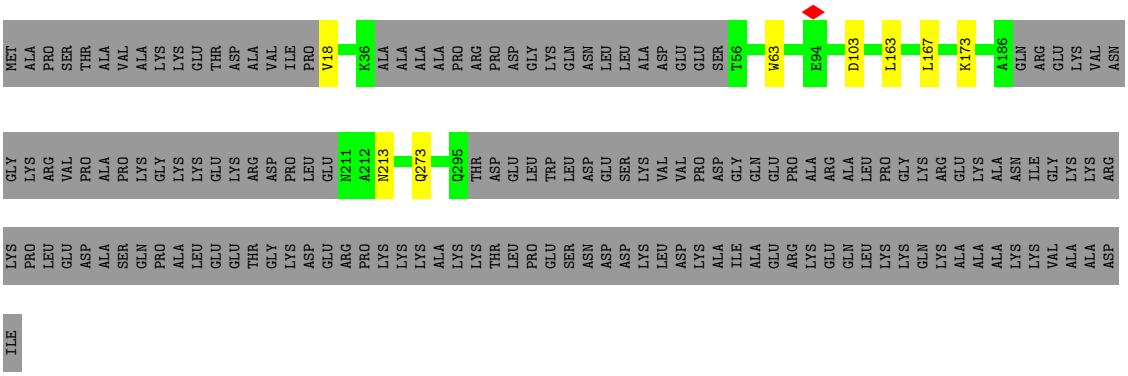
Chain UU:



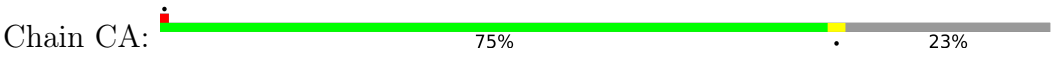


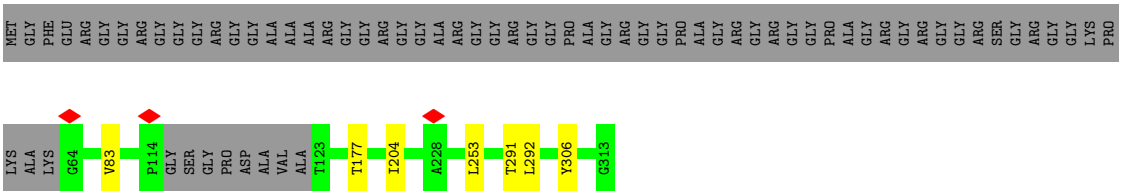
• Molecule 16: Utp24

• Molecule 17: Utp30

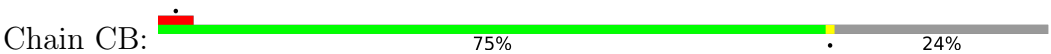


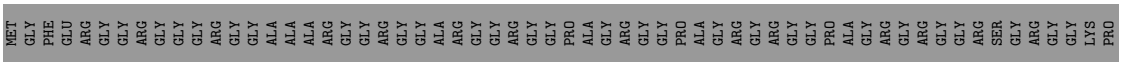
• Molecule 18: Nop1

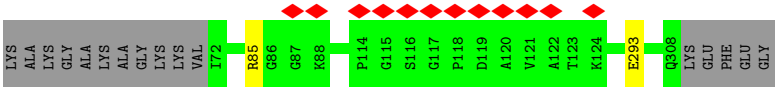




• Molecule 18: Nop1

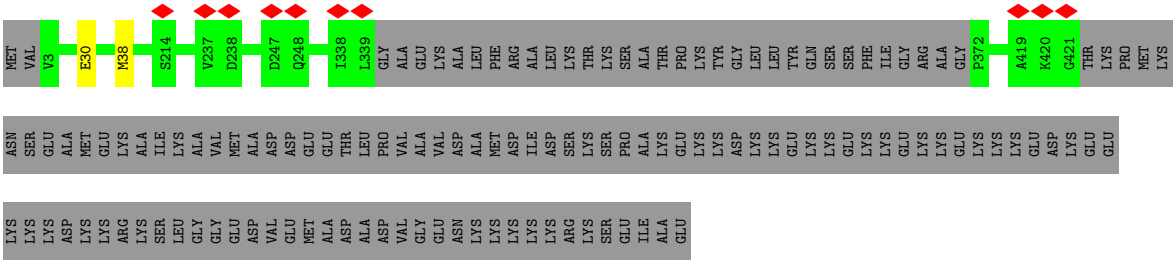






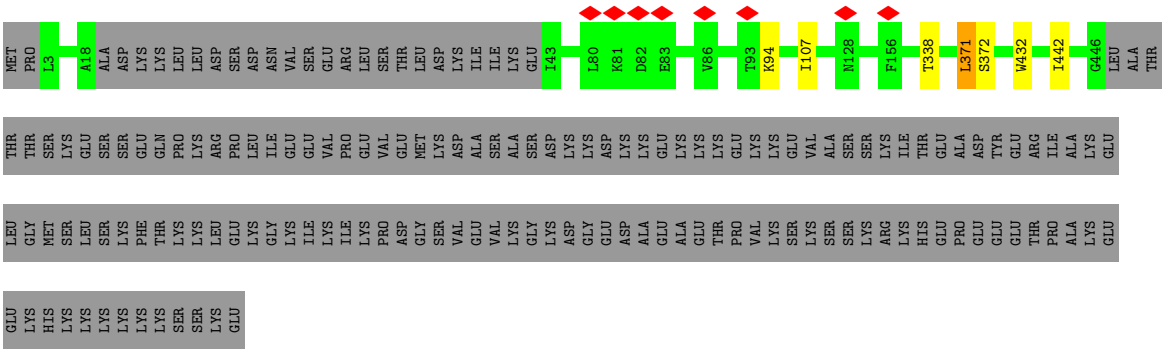
• Molecule 19: Nop56

Chain CC:



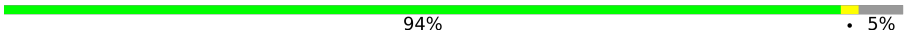
• Molecule 20: Nop58

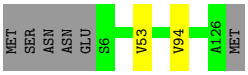
Chain CD:



• Molecule 21: Snu13

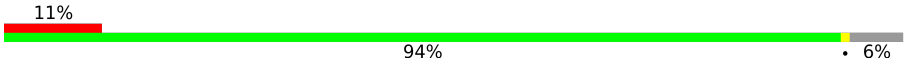
Chain CE:

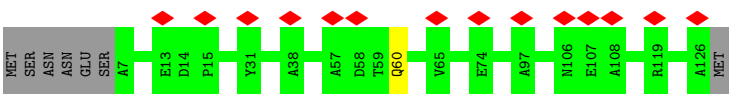




• Molecule 21: Snu13

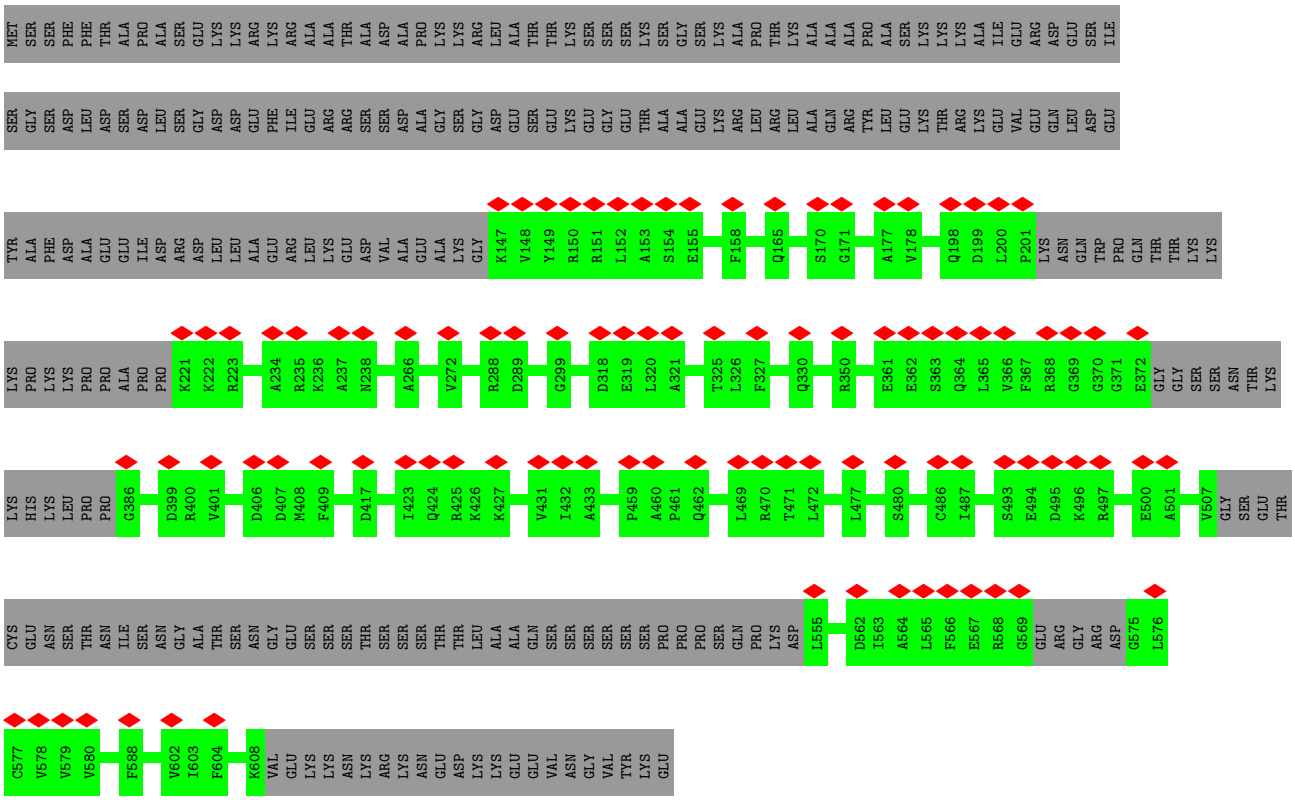
Chain CF:





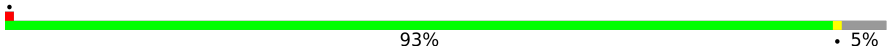
• Molecule 22: Rrp9

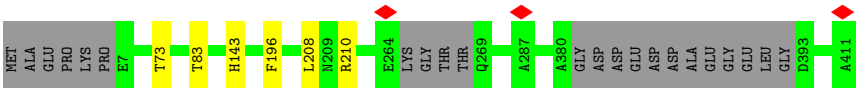
Chain CG:



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

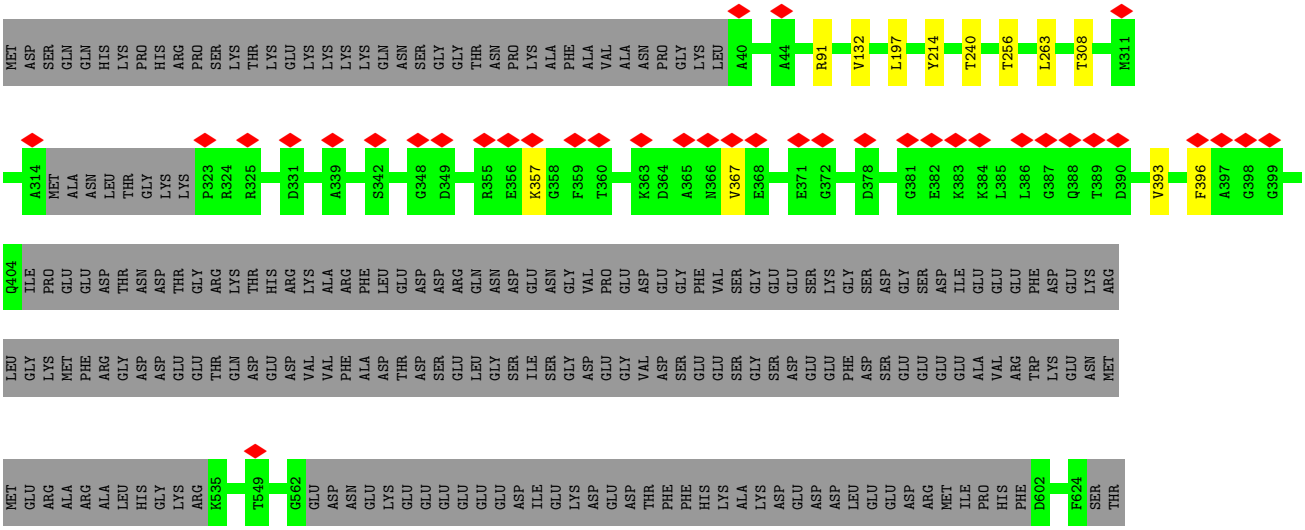
Chain CH:

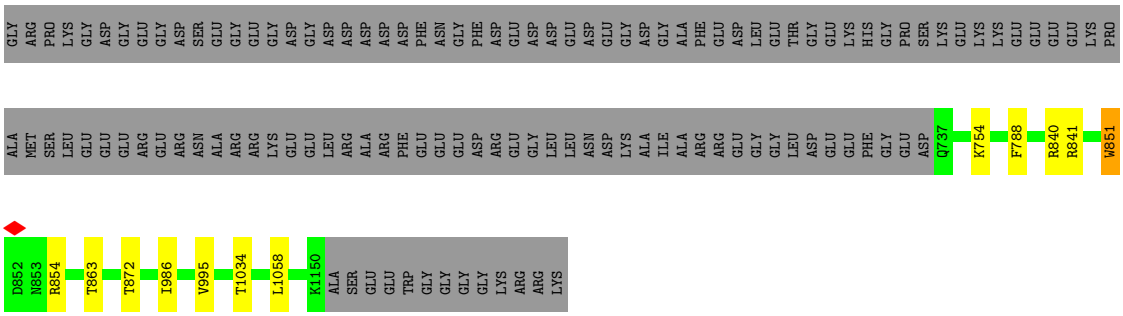




• Molecule 24: Bms1

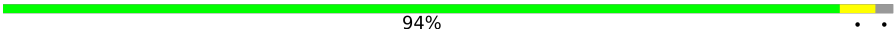
Chain CI:





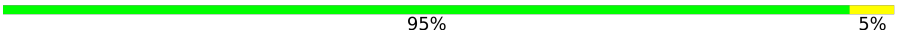
• Molecule 25: Imp3

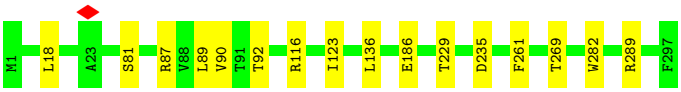
Chain CJ:



• Molecule 26: Imp4

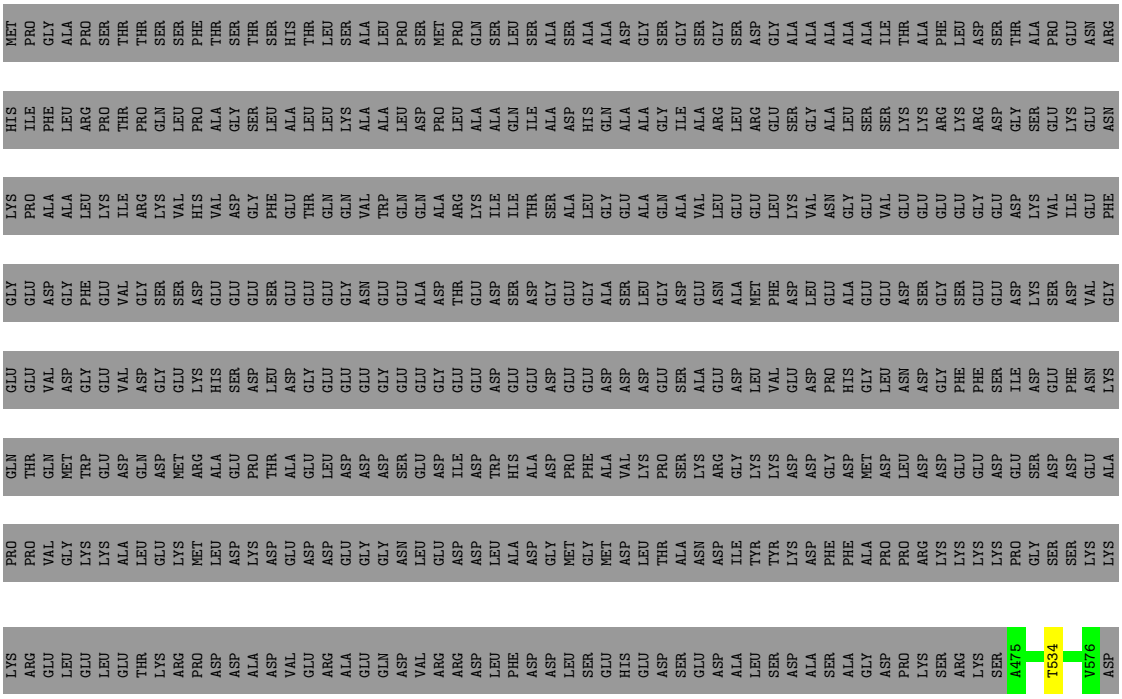
Chain CK:

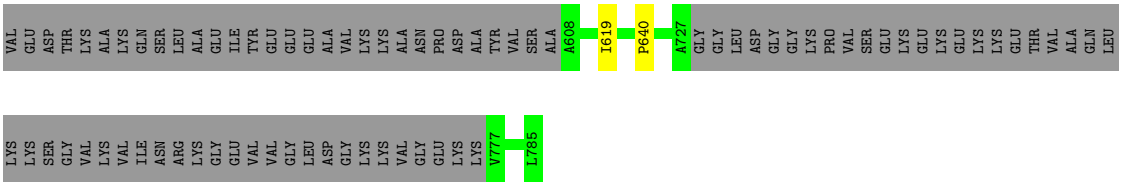




• Molecule 27: Mpp10

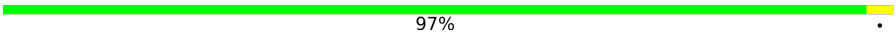
Chain CL:

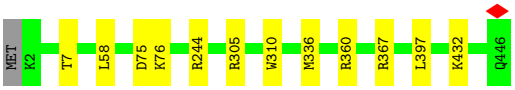




• Molecule 28: Sof1

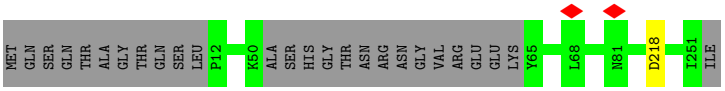
Chain CM:





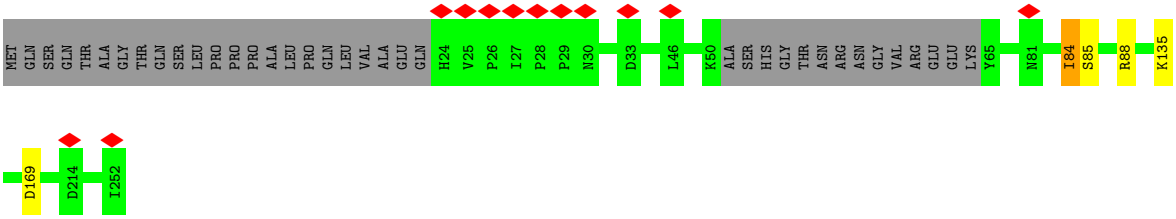
• Molecule 29: Emg1

Chain CN:



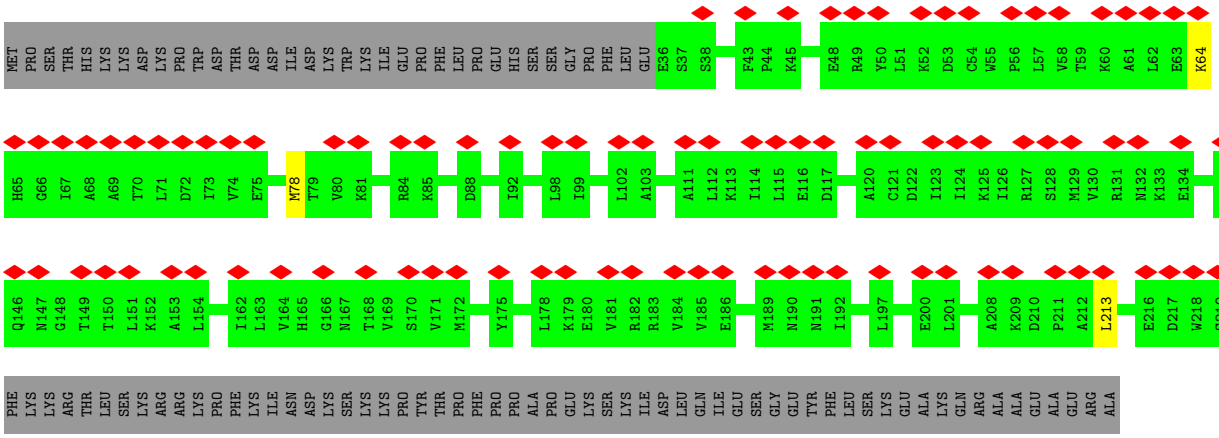
• Molecule 29: Emg1

Chain CO:



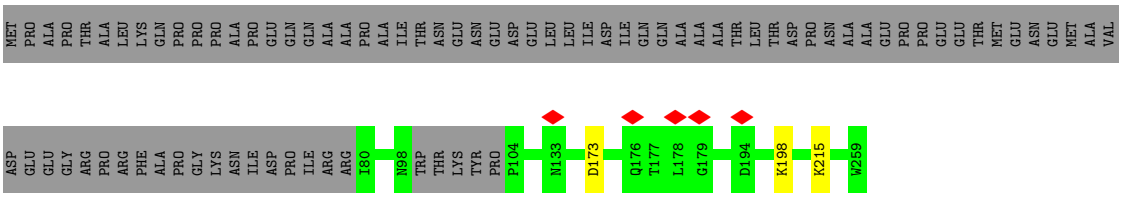
• Molecule 30: KRR1 small subunit processome component

Chain CP:



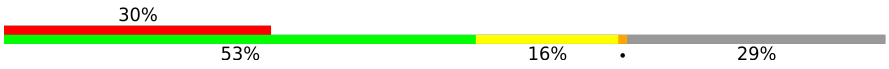
• Molecule 31: Pre-rRNA-processing protein PNO1

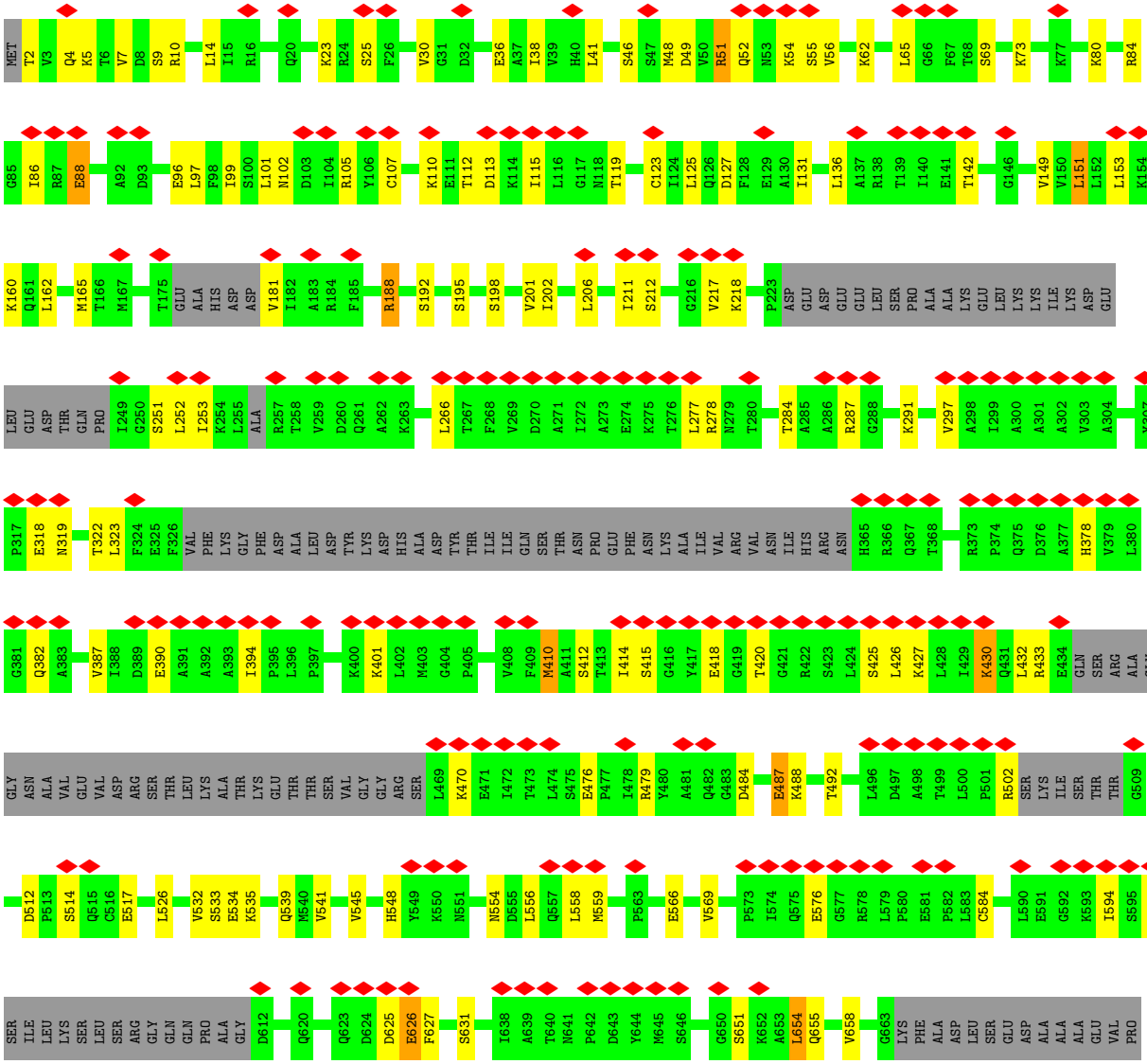
Chain CQ:

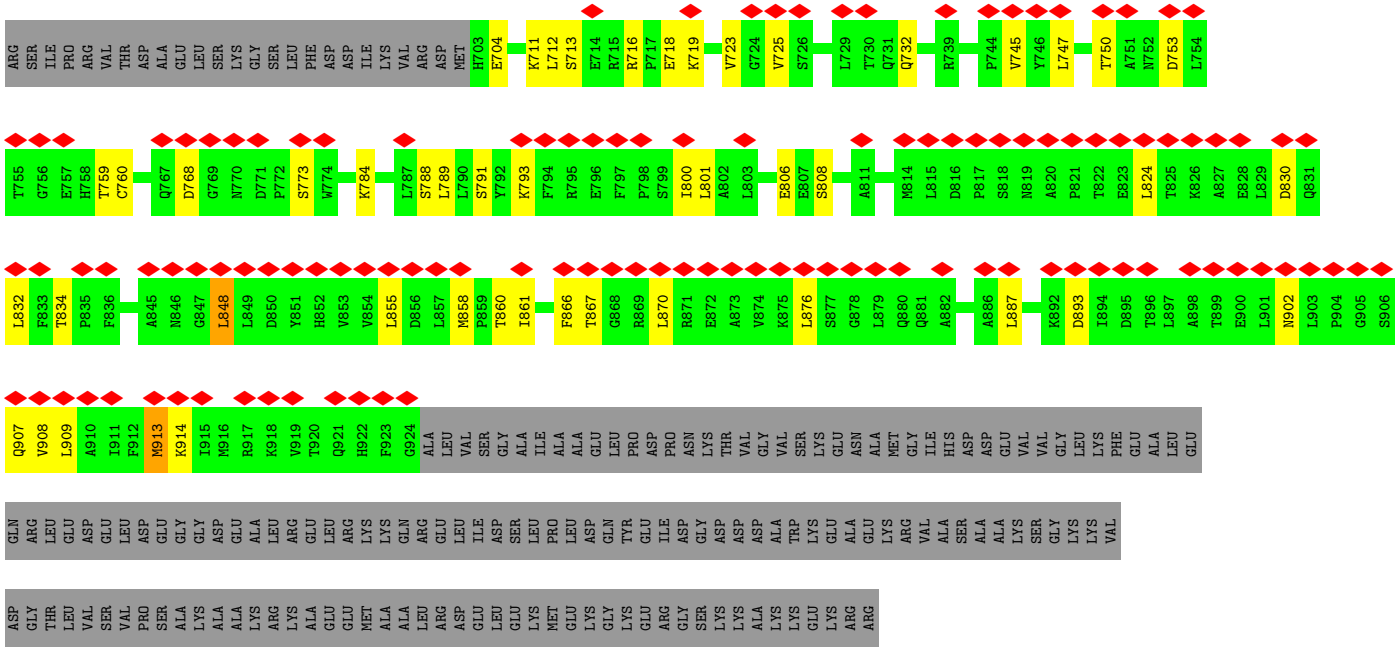


• Molecule 32: Kre33

Chain CR:

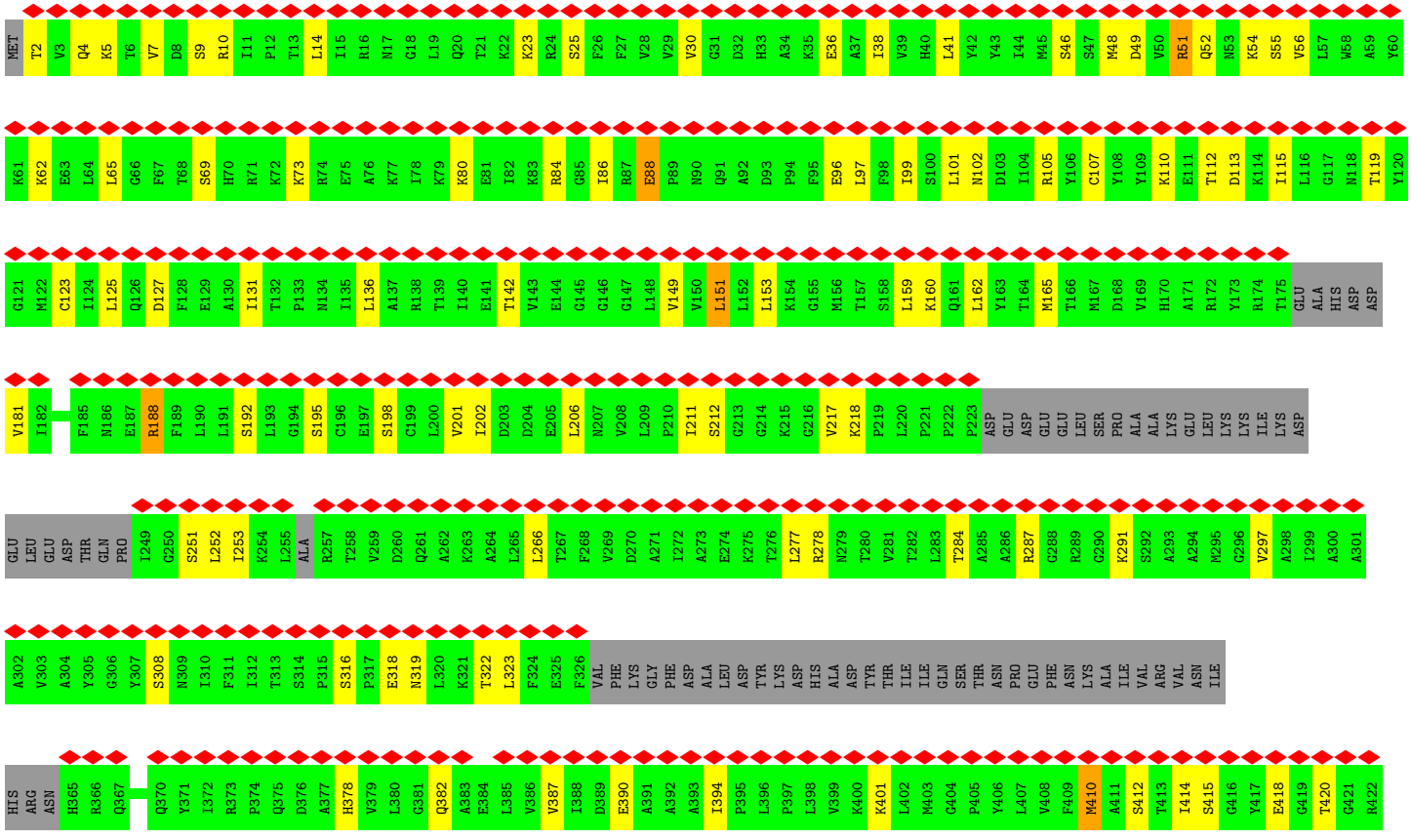


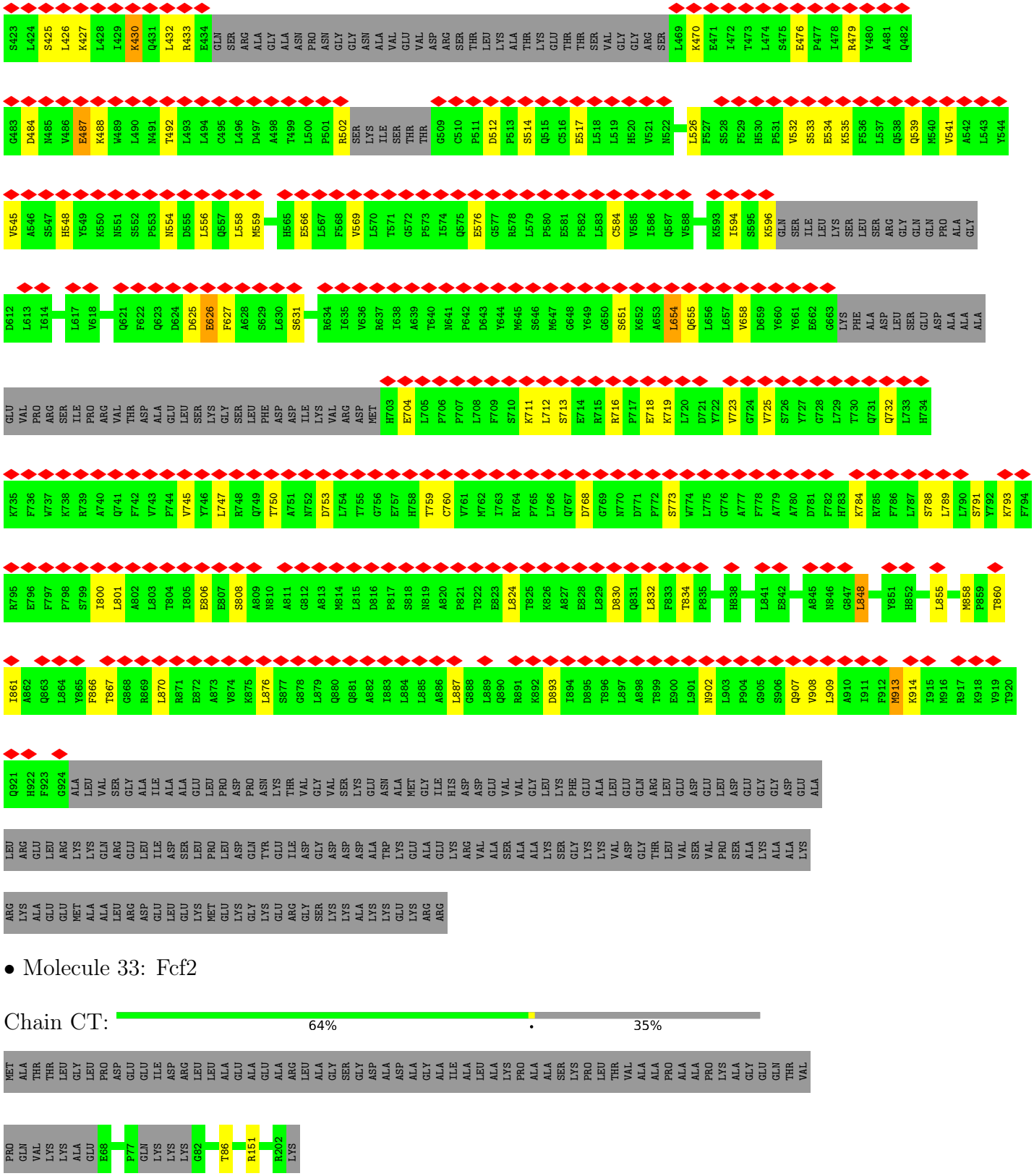




• Molecule 32: Kre33

Chain CS:





• Molecule 33: Fcf2

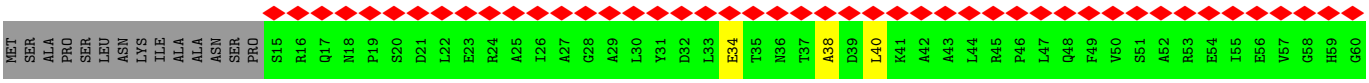
Chain CT:

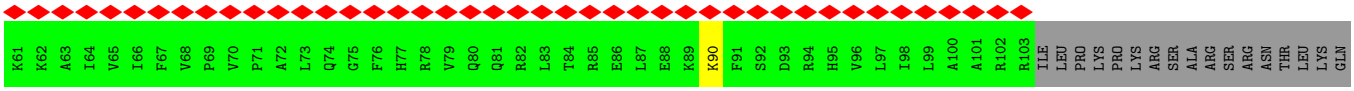
• Molecule 34: 40S ribosomal protein s5-like protein

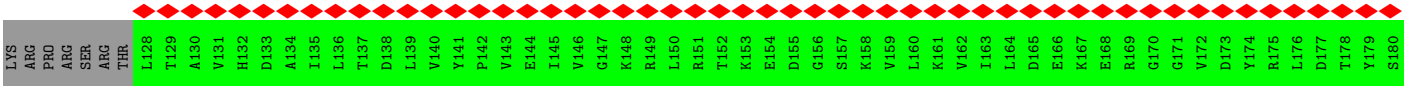
Chain Cc:

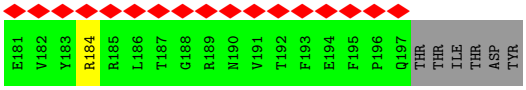
• Molecule 35: 40S ribosomal protein S7

Chain Ce:



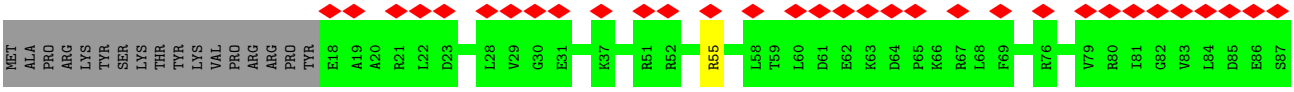


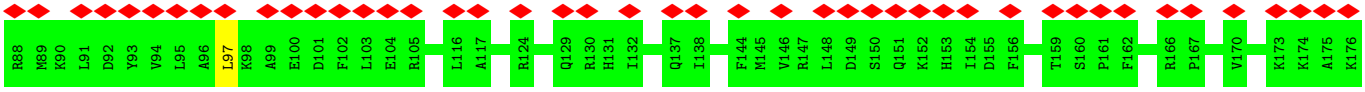


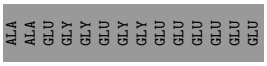


• Molecule 36: 40S ribosomal protein s9-like protein

Chain Cg:

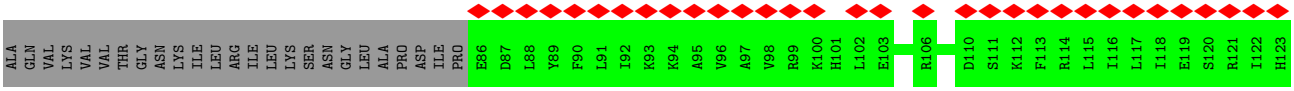


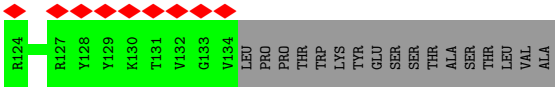




• Molecule 37: 40S ribosomal protein S13-like protein

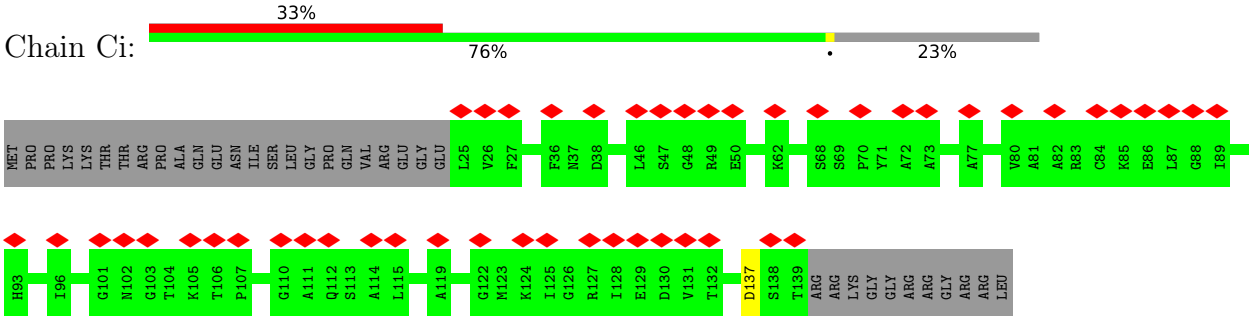
Chain Ch:





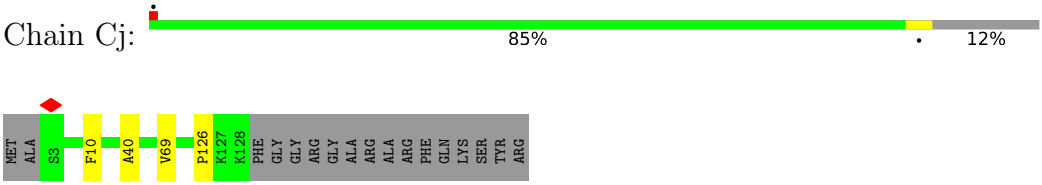
• Molecule 38: 40S ribosomal protein S14-like protein

Chain Ci:



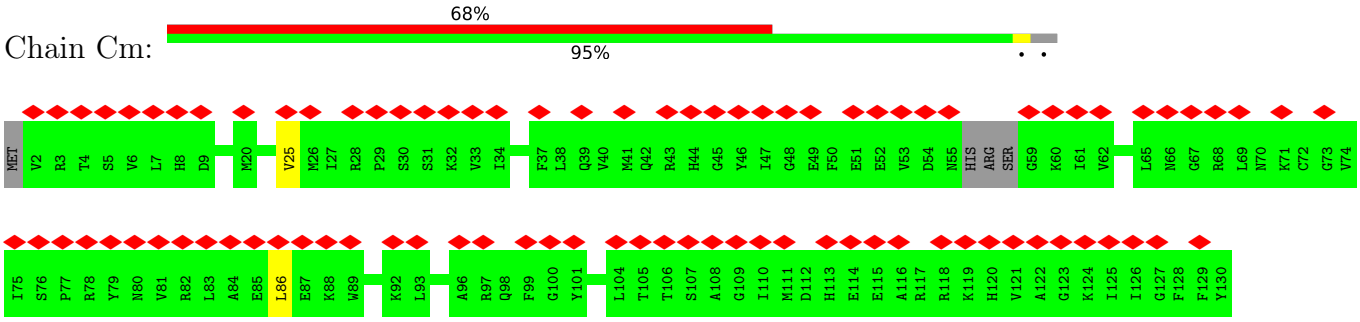
• Molecule 39: 40S ribosomal protein S16-like protein

Chain Cj:



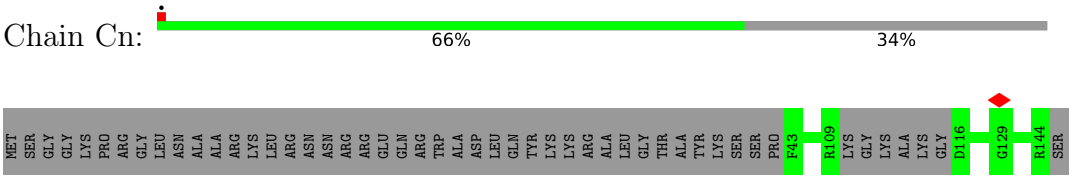
• Molecule 40: 40S ribosomal protein S22-like protein

Chain Cm:



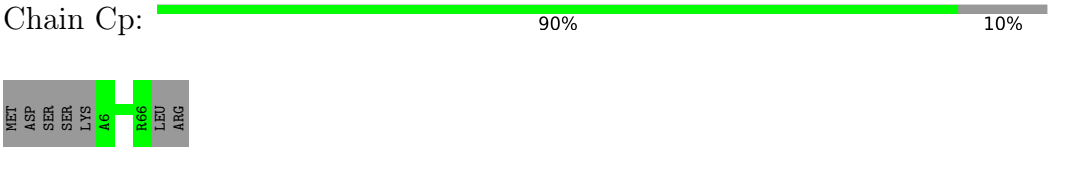
• Molecule 41: 40S ribosomal protein s23-like protein

Chain Cn:



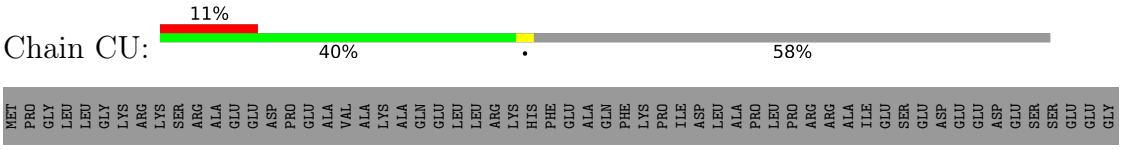
• Molecule 42: 40S ribosomal protein S28-like protein

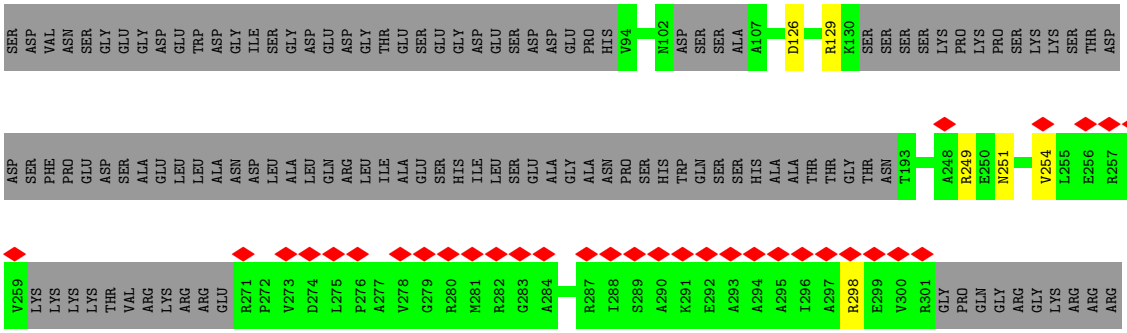
Chain Cp:



• Molecule 43: Faf1

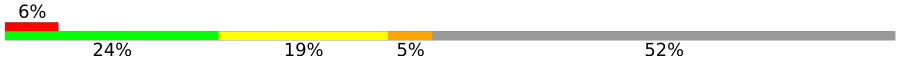
Chain CU:

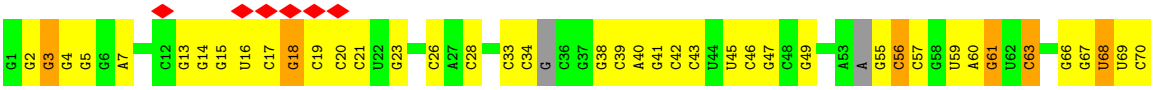


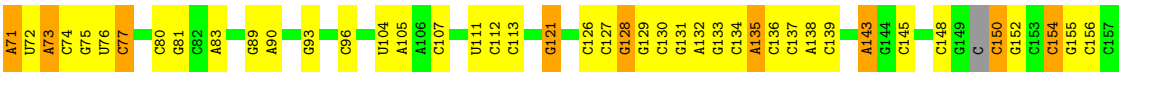


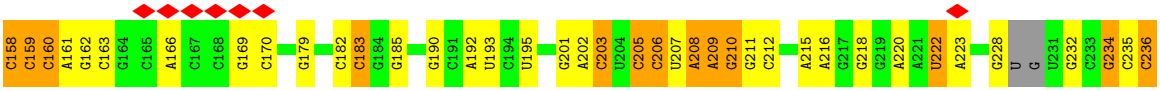
• Molecule 44: 35S rRNA

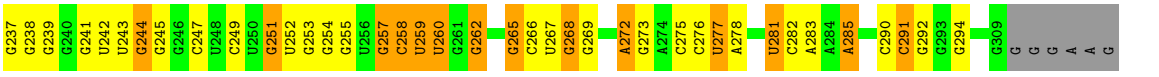
Chain C1:

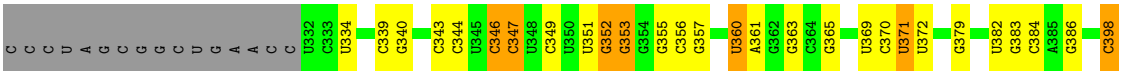


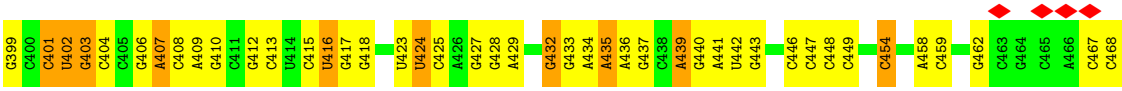


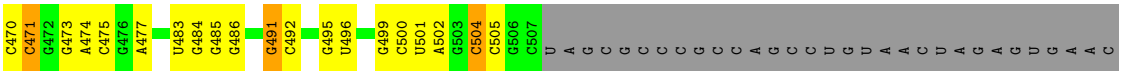


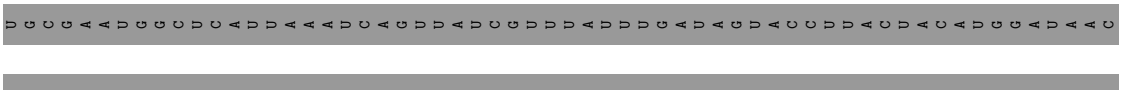


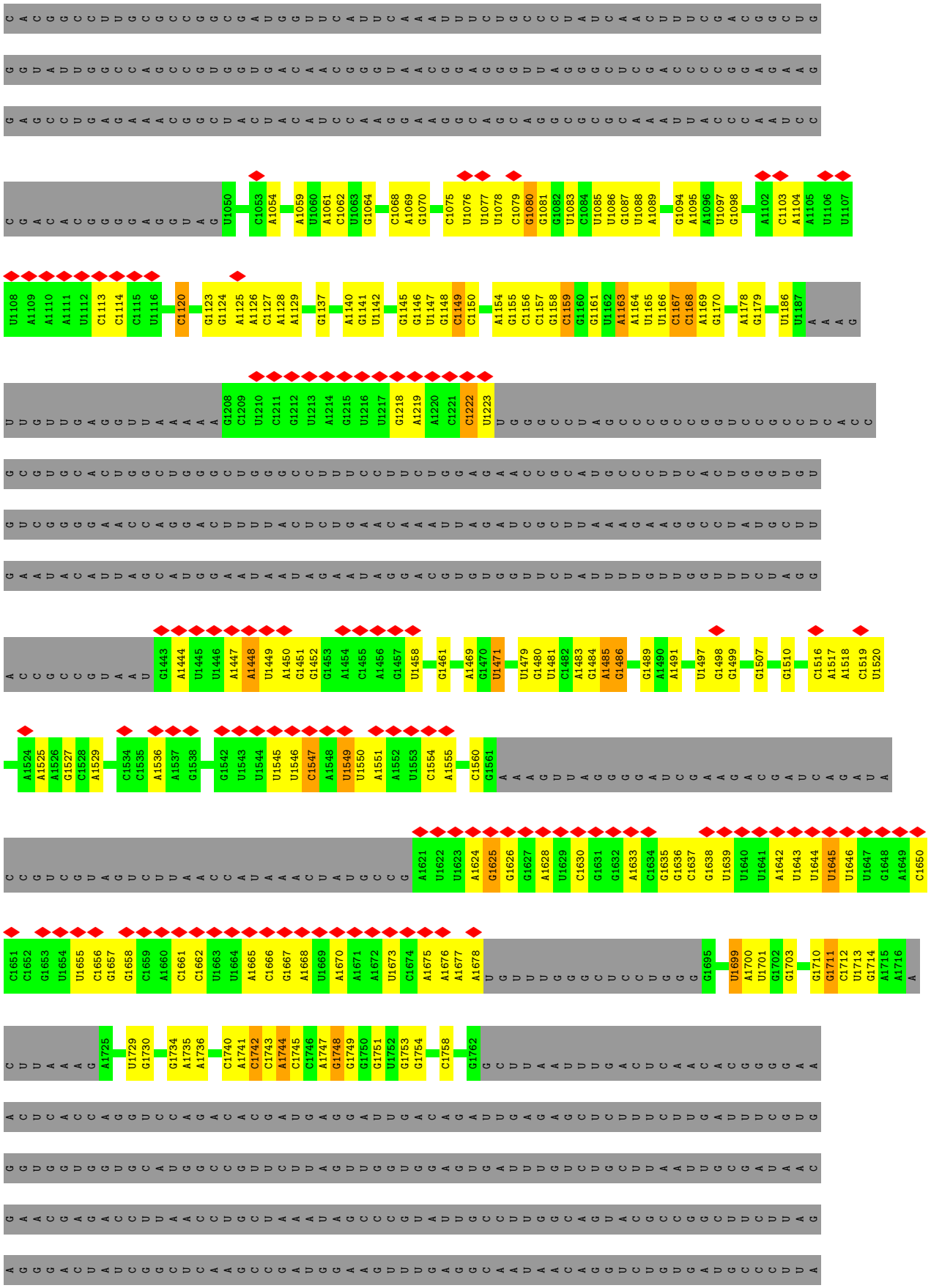


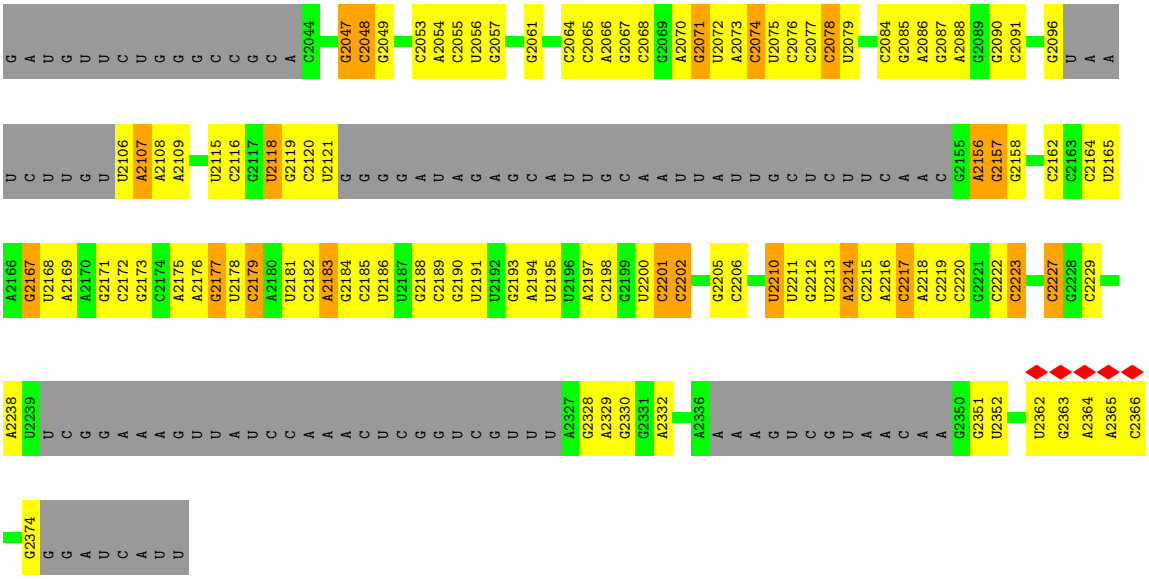






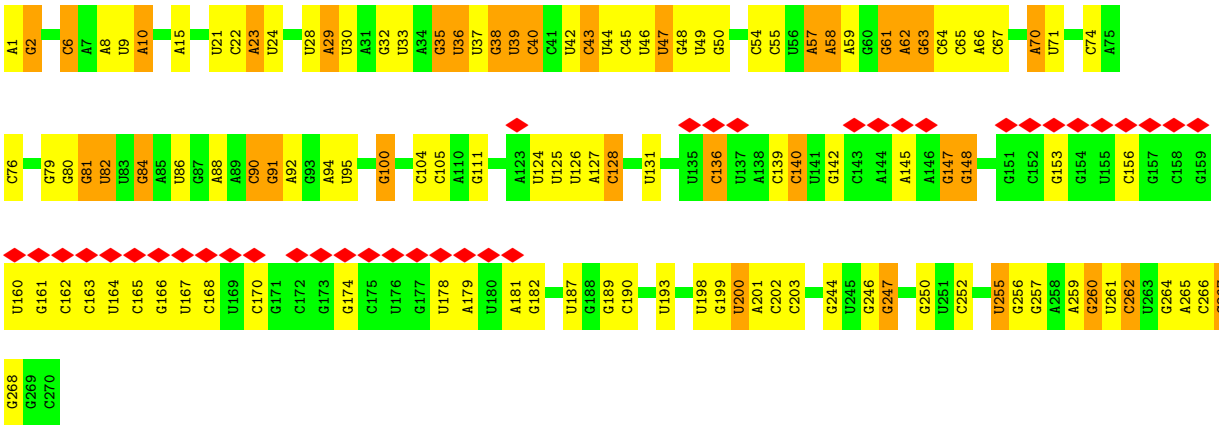






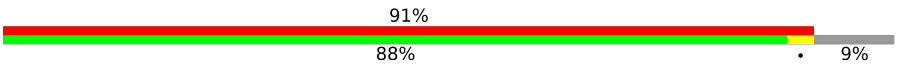
• Molecule 45: U3 snoRNA

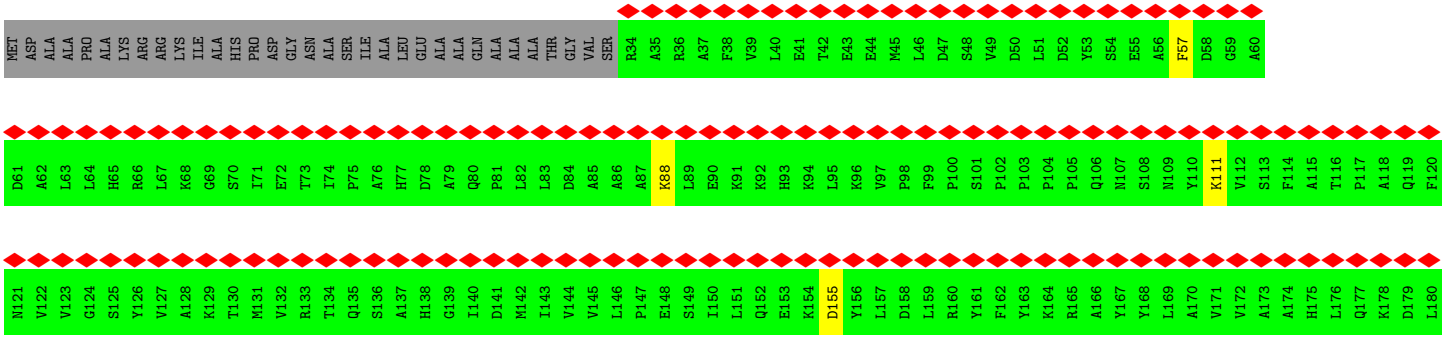
Chain C2:

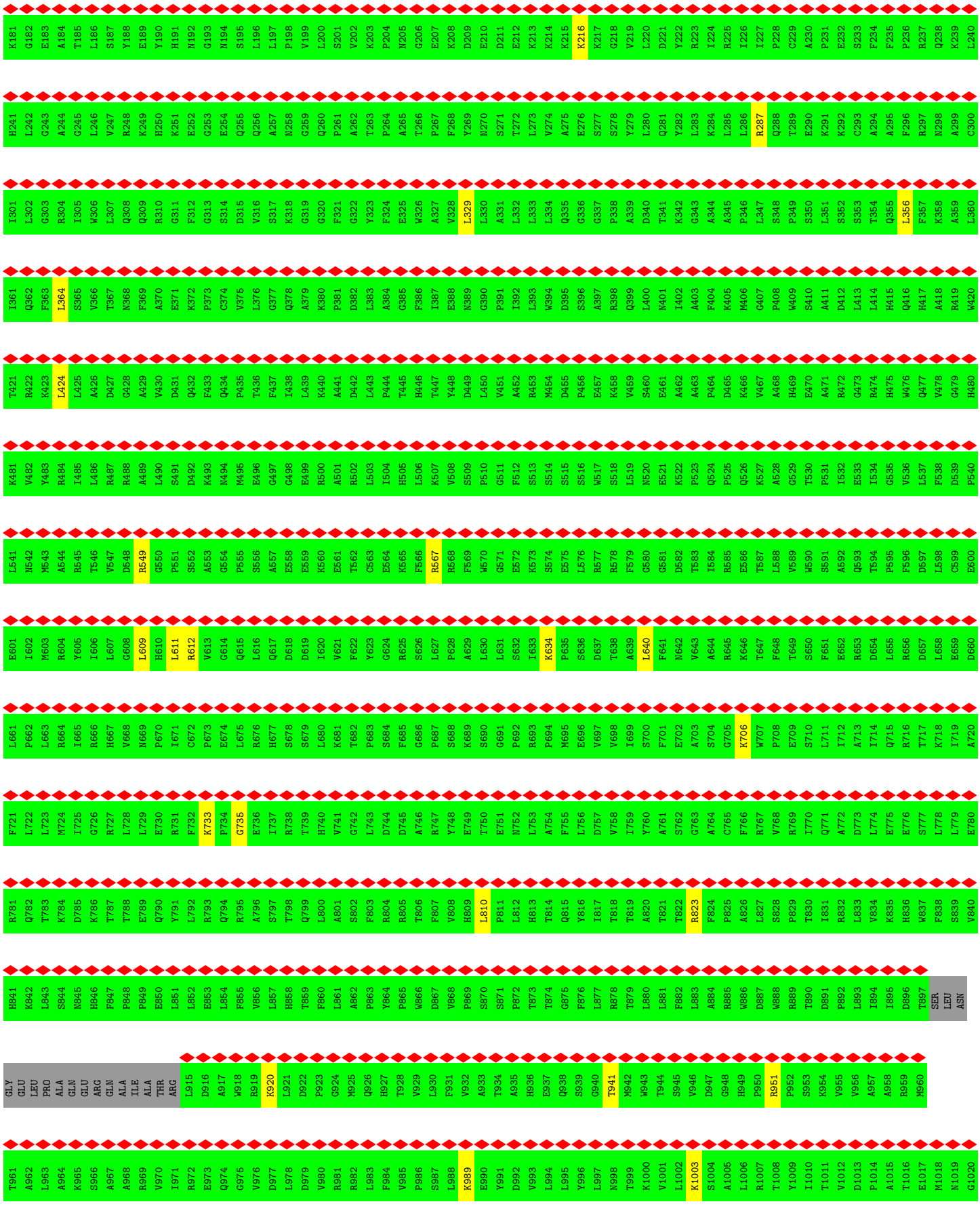


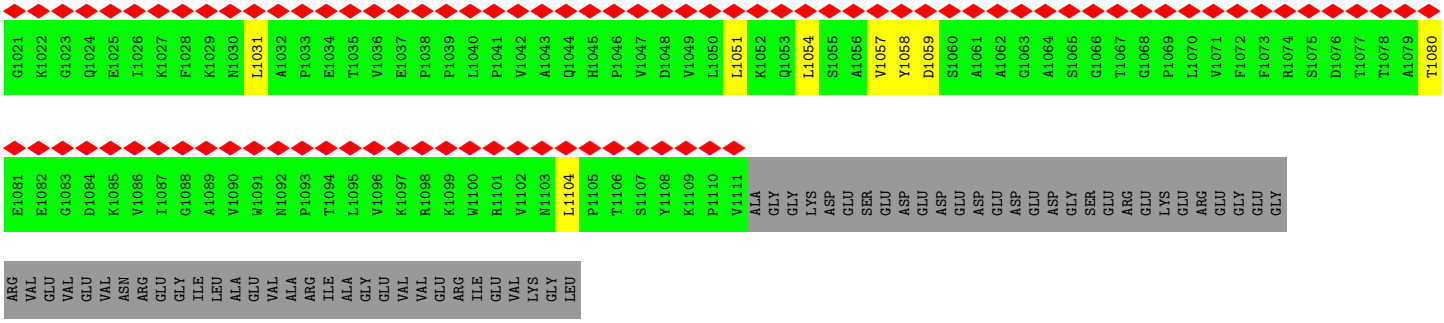
• Molecule 46: U3 small nucleolar RNA-associated protein 22

Chain UV:



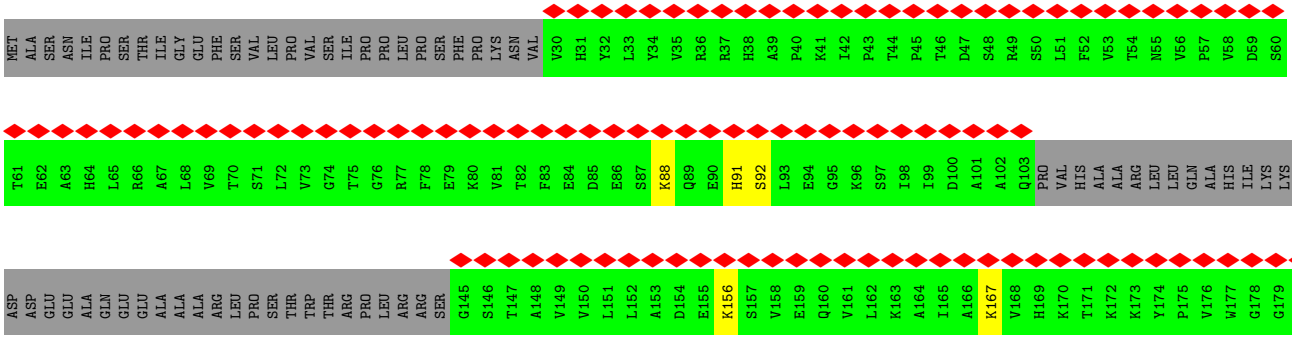



K181 G182 E183 A184 T185 L186 S187 Y188 E189 Y190 H191 N192 G193 N194 S195 L196 L197 P198 V199 L200 S201 V202 K203 P204 N205 G206 E207 K208 D209 E210 D211 E212 K213 K214 K215 K216 K217 G218 V219 L220 D221 Y222 R223 I224 R225 I226 I227 P228 C229 A230 P231 E232 S233 F234 F235 P236 R237 Q238 K239 L240
H241 L242 G243 A244 G245 L246 V247 R248 K249 H250 K251 E252 G253 E254 Q255 Q256 A257 N258 G259 Q260 P261 A262 T263 P264 A265 T266 P267 F268 Y269 N270 S271 T272 L273 V274 A275 E276 S277 S278 Y279 L280 Q281 Y282 L283 K284 L285 L286 R287 Q288 T289 E290 K291 K292 C293 A294 A295 F296 R297 N298 A299 C300
I301 L302 G303 R304 I305 W306 L307 Q308 Q309 R310 G311 F312 G313 S314 D315 V316 S317 K318 G319 G320 F321 G322 Y323 F324 E325 W326 A327 V328 L329 L330 A331 L332 L333 L334 Q335 G336 G337 P338 A339 D340 T341 K342 G343 A344 A345 P346 L347 S348 P349 S350 L351 S352 S353 T354 Q355 L356 F357 K358 A359 L360
I361 Q362 F363 L364 S365 V366 T367 N368 F369 A370 E371 K372 P373 C374 V375 L376 G377 Q378 A379 G319 G320 K380 P381 D382 L383 A384 G385 F386 I387 E388 N389 G390 P391 I392 L393 W394 D395 S396 A397 R398 Q399 L400 N401 I402 A403 F404 K405 M406 G407 P408 W409 S410 A411 D412 L413 L414 H415 Q416 H417 A418 R419 W420
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 A462 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 W543 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 P611 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 L995 Y996 L997 N998 T999 K1000 V1001 L1002 K1003 S1004 A1005 L1006 R1007 T1008 Y1009 I1010 T1011 V1012 D1013 P1014 A1015 T1016 E1017 M1018 N1019 G1020



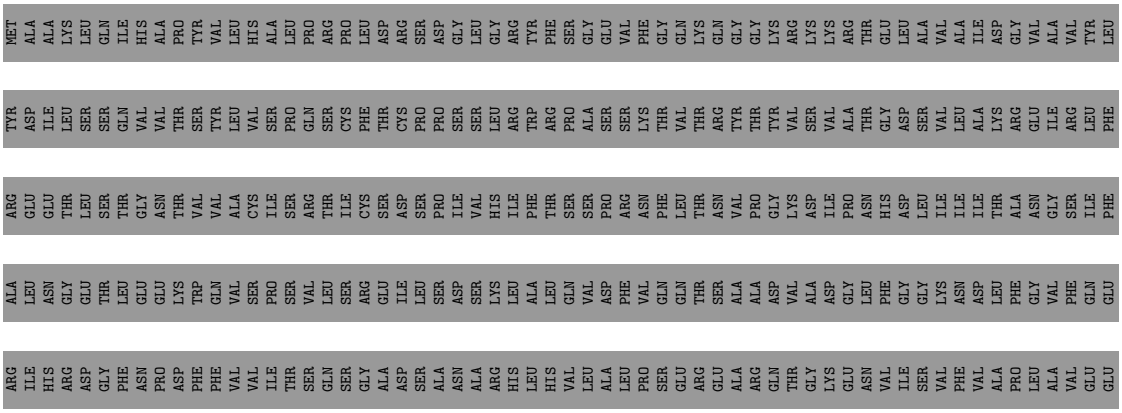
• Molecule 47: Rrp7

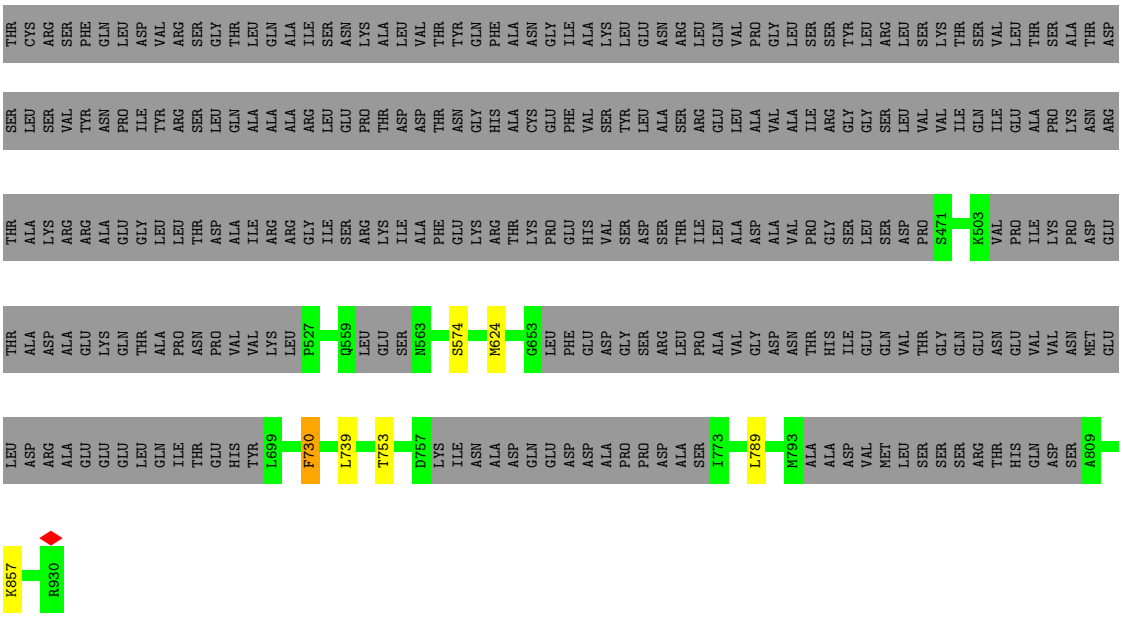
Chain CV:



• Molecule 48: Utp8

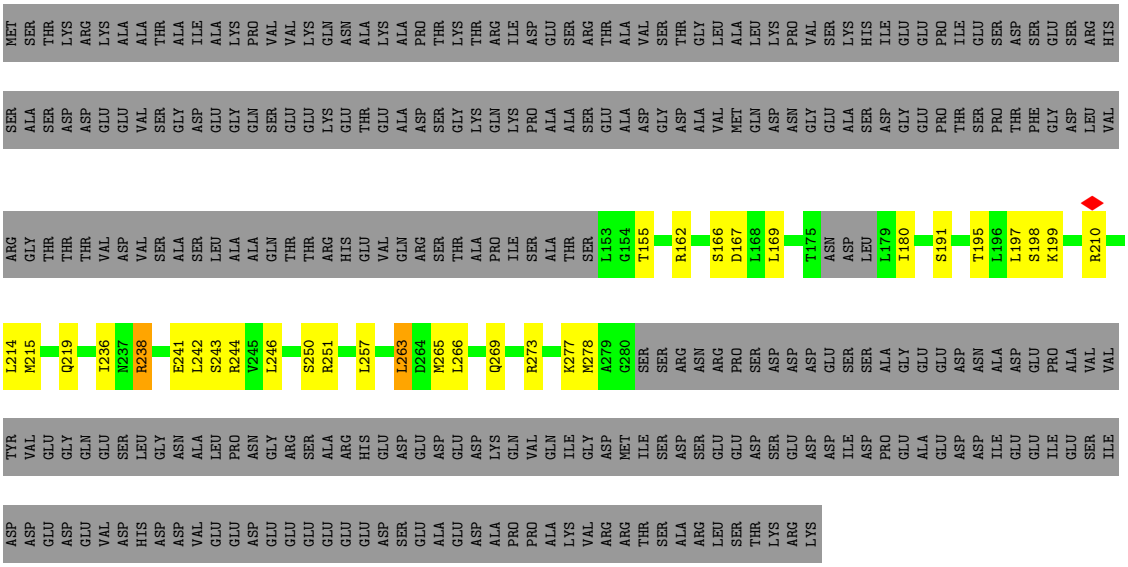
Chain UH:





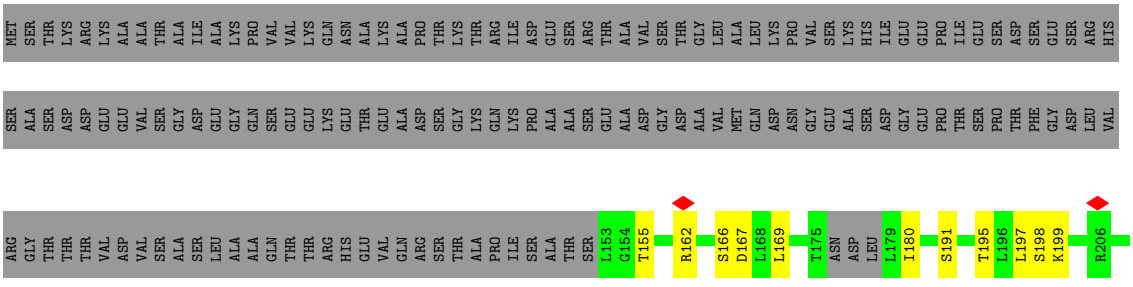
• Molecule 49: Utp5

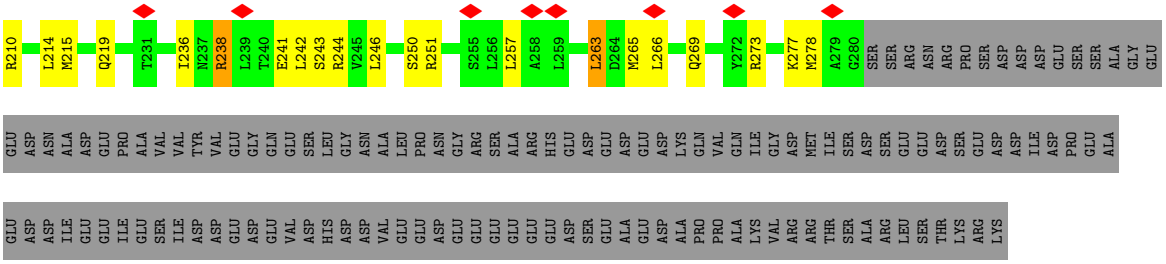
Chain UE:



• Molecule 49: Utp5

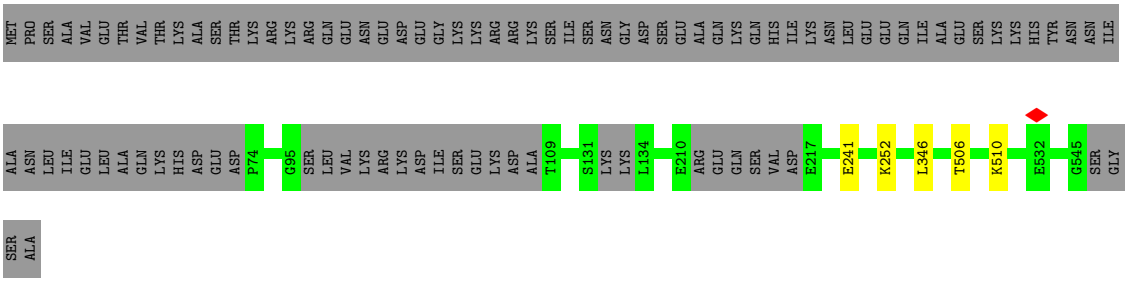
Chain UI:





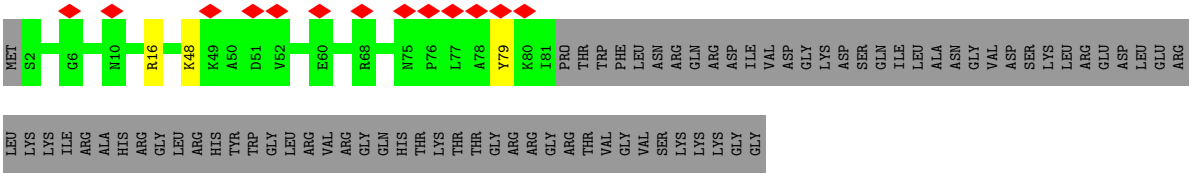
• Molecule 50: Noc4

Chain US:



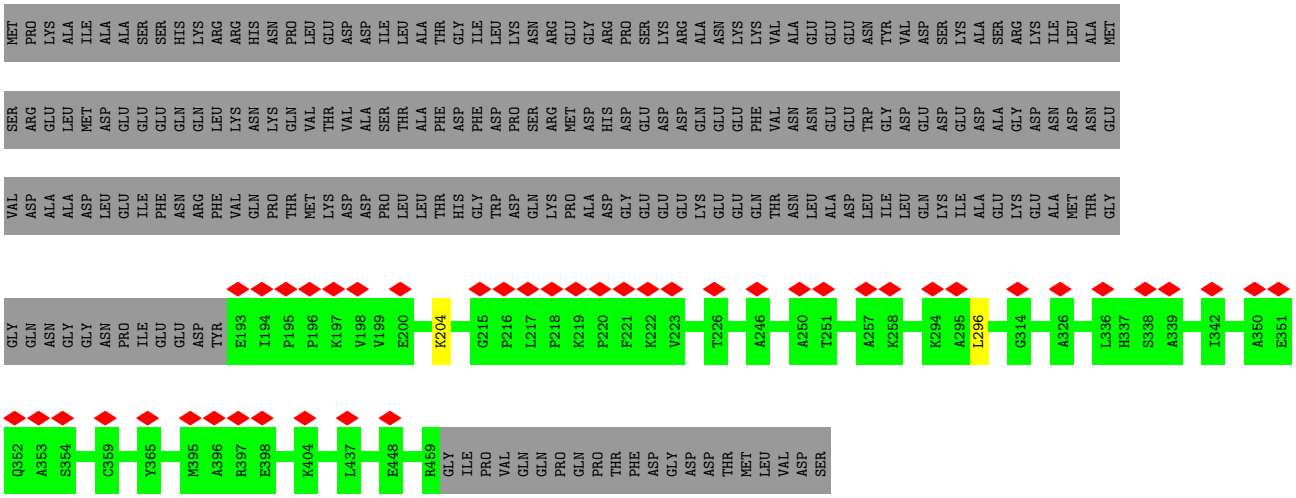
• Molecule 51: Rps18

Chain Cl:



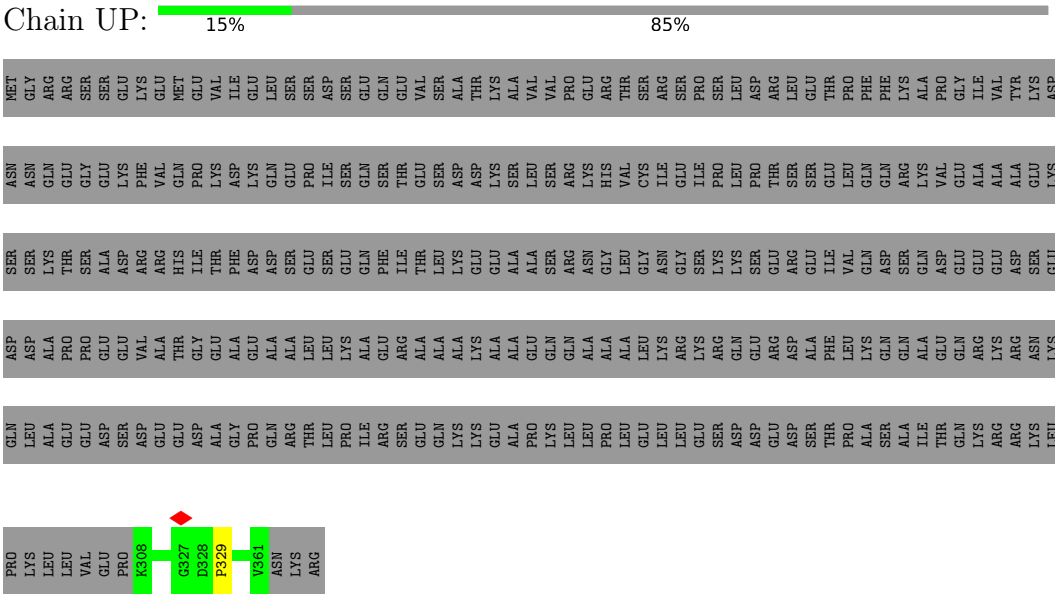
• Molecule 52: Enp1

Chain CX:



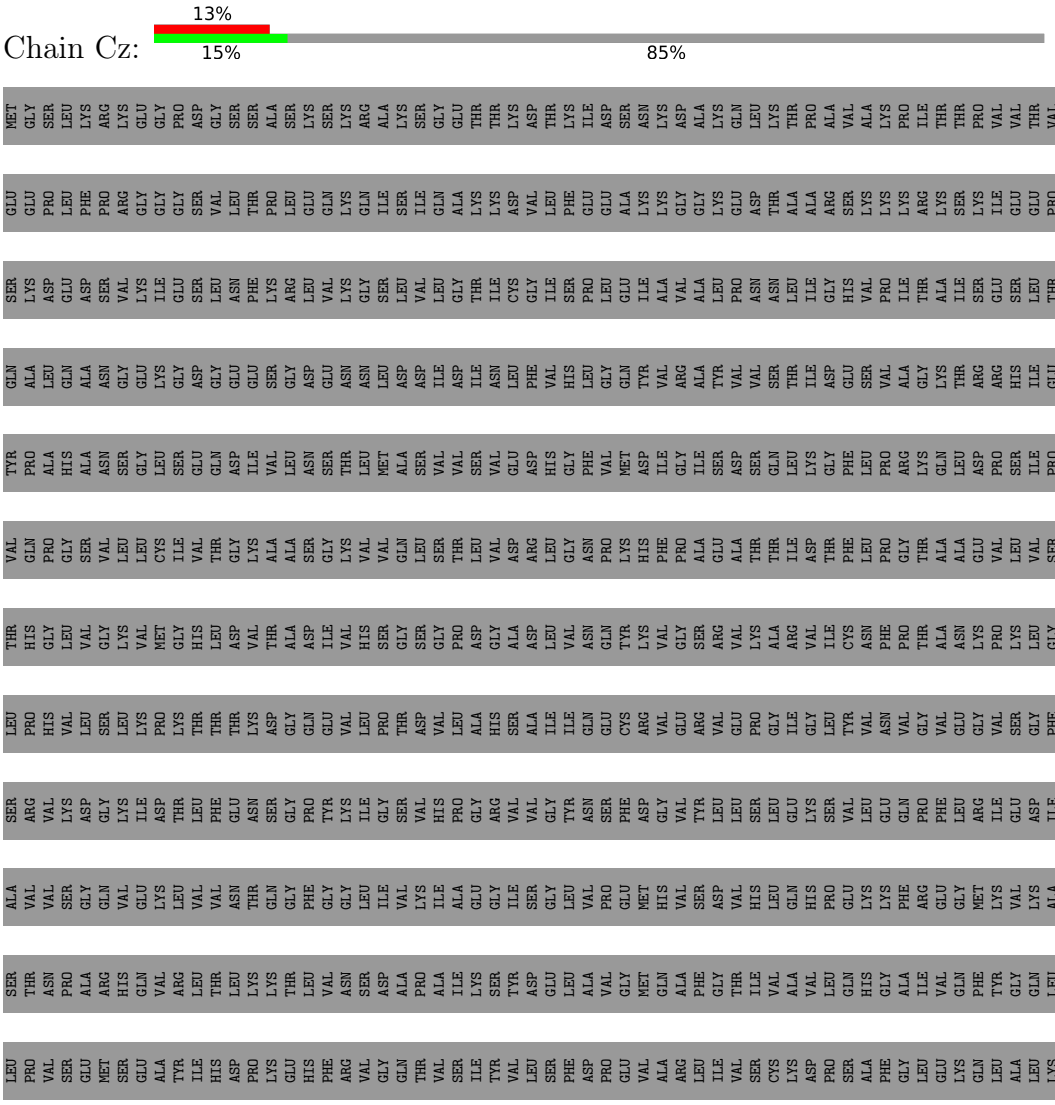
• Molecule 53: Utp16

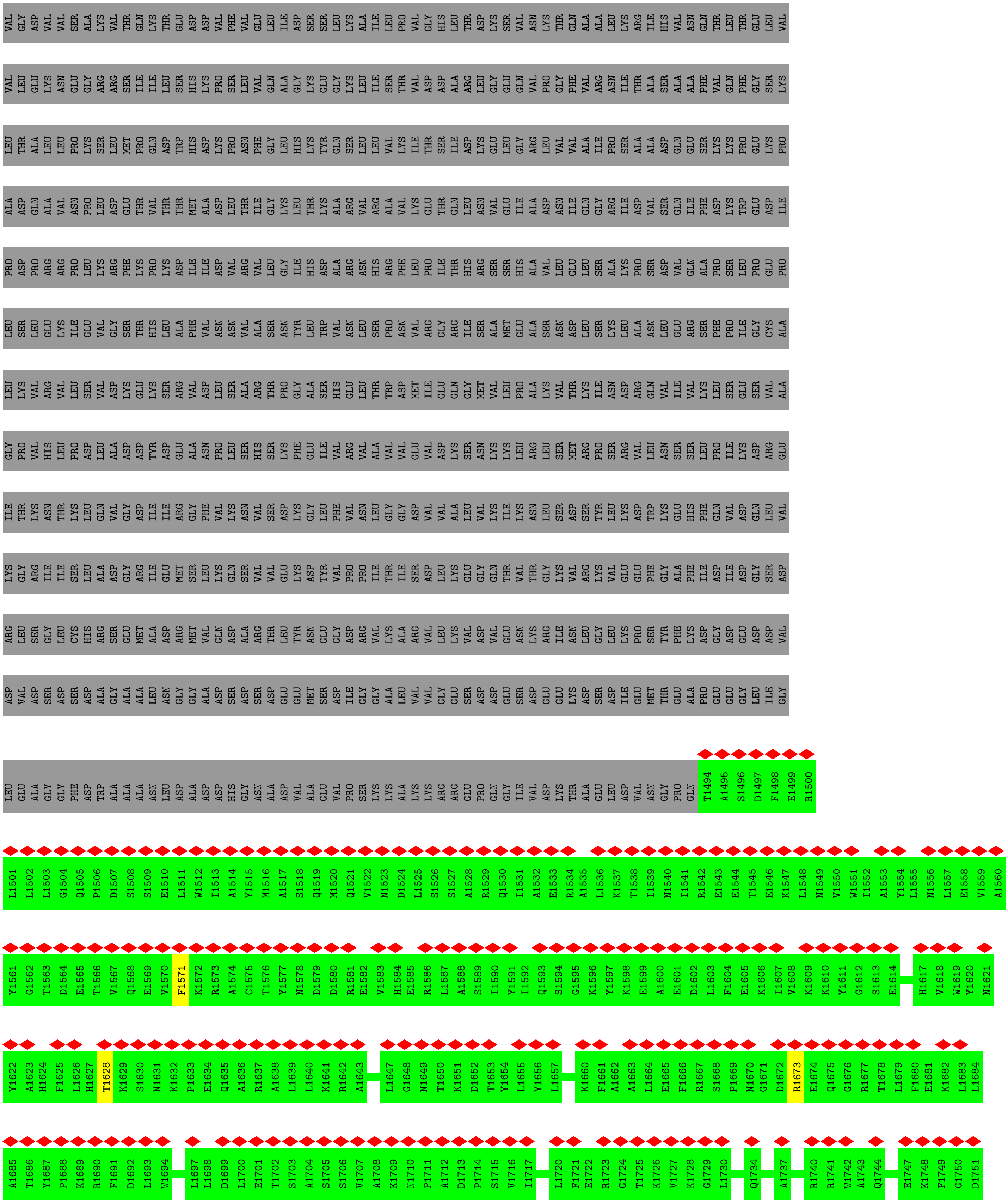
Chain UP:

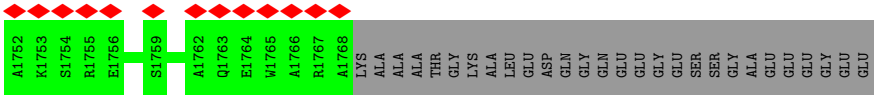


• Molecule 54: Rrp5

Chain Cz:




VAL GLY ASP VAL VAL SER ALA LYS VAL THR GLN LYS THR GLU ASP ASP VAL PHE VAL GLU LEU ILE ASP SER SER LEU LYS ALA ILE LEU PRO VAL GLY HIS LEU THR ASP LYS SER VAL ASN LYS THR GLN ALA ALA LEU LYS ARG ILE HIS VAL ASN GLN THR LEU THR GLU LEU VAL
VAL LEU GLU LYS ASN GLU GLY ARG ARG SER ILE ILE LEU SER HIS LYS PRO SER LEU VAL GLN ALA GLY LYS GLU GLY LYS LEU ILE SER THR VAL ASP ASP ALA ARG LEU GLY GLU GLN VAL PRO GLY PHE VAL ARG ASN ILE THR ALA SER ALA ALA PHE VAL GLN PHE GLY SER LYS
LEU THR ALA LEU LEU PRO LYS SER LEU MET PRO GLN ASP TRP HIS ASP LYS PRO ASN PHE GLY LEU HIS LYS TYR GLN SER LEU LEU VAL LYS ILE THR SER ILE ASP LYS GLU LEU GLY ARG LEU VAL VAL ALA ILE PRO SER ALA ALA ASP GLN GLU SER LYS LYS PRO GLU LYS PRO
ALA ASP GLN ALA VAL ASN PRO LEU ASP GLU THR VAL THR THR MET ALA ASP LEU THR ILE GLY LYS LEU THR LYS ALA ARG VAL ARG ALA VAL LYS GLU THR GLN LEU ASN VAL GLU ILE ALA ASP ASN ILE GLN GLY ARG ILE ASP VAL SER GLN ILE PHE ASP LYS TRP GLU ASP ILE
PRO ASP PRO ARG ARG PRO LEU LYS ARG PHE LYS PRO LYS ASP ILE ILE ASP VAL ARG VAL LEU GLY ILE HIS ASP ALA ARG ASN HIS ARG PHE LEU PRO ILE THR HIS ARG SER SER HIS ALA VAL LEU GLU LEU SER ALA LYS PRO SER ASP VAL GLN ALA PRO SER LEU PRO GLU PRO
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 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 F1498 E1499 R1500
L1501 L1502 L1503 G1504 Q1505 P1506 D1507 S1508 S1509 E1510 L1511 W1512 I1513 A1514 Y1515 M1516 A1517 S1518 Q1519 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 K1547 L1548 N1549 V1550 W1551 I1552 A1553 Y1554 L1555 N1556 L1557 E1558 V1559 A1560
Y1561 G1562 T1563 D1564 E1565 T1566 V1567 Q1568 E1569 V1570 F1571 K1572 R1573 A1574 C1575 T1576 Y1577 N1578 D1579 D1580 R1581 E1582 V1583 H1584 E1585 R1586 L1587 A1588 S1589 I1590 Y1591 I1592 Q1593 S1594 G1595 K1596 Y1597 K1598 E1599 A1600 E1601 D1602 L1603 F1604 E1605 K1606 I1607 V1608 K1609 K1610 Y1611 G1612 S1613 E1614 H1617 V1618 W1619 Y1620 N1621
Y1622 A1623 H1624 F1625 L1626 H1627 T1628 K1629 S1630 N1631 K1632 P1633 E1634 Q1635 A1636 R1637 A1638 L1639 L1640 K1641 R1642 A1643 L1647 G1648 N1649 T1650 K1651 D1652 T1653 Y1654 L1655 Y1656 L1657 K1660 F1661 A1662 A1663 L1664 E1665 F1666 R1667 S1668 P1669 N1670 G1671 D1672 R1673 E1674 Q1675 G1676 R1677 T1678 L1679 F1680 E1681 K1682 L1683 L1684
A1685 T1686 Y1687 P1688 K1689 R1690 F1691 D1692 L1693 W1694 L1697 L1698 D1699 L1700 E1701 T1702 S1703 A1704 S1705 S1706 V1707 A1708 K1709 N1710 P1711 A1712 D1713 P1714 S1715 V1716 I1717 L1720 F1721 E1722 R1723 G1724 T1725 K1726 V1727 K1728 G1729 L1730 Q1734 A1737 R1740 R1741 W1742 A1743 Q1744 E1747 K1748 F1749 G1750 D1751


A1752 K1753 S1754 R1755 E1756 S1759 A1762 Q1763 E1764 W1765 A1766 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 GLU GLY GLU GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20250	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	0.437	Depositor
Minimum map value	-0.319	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	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	0.99	12/6521 (0.2%)	0.86	6/8867 (0.1%)
2	UB	0.48	1/4154 (0.0%)	0.60	1/5583 (0.0%)
3	UC	0.49	0/595	0.59	0/786
4	UD	0.68	4/6211 (0.1%)	0.70	3/8408 (0.0%)
5	UF	0.54	0/2657	0.60	0/3596
6	UG	0.88	4/3516 (0.1%)	0.79	3/4761 (0.1%)
7	UJ	0.52	0/6291	0.69	3/8543 (0.0%)
8	UK	0.80	0/1701	0.79	1/2251 (0.0%)
9	UL	0.47	0/6299	0.65	1/8531 (0.0%)
10	UM	0.38	0/5366	0.62	4/7282 (0.1%)
11	UN	0.60	0/1232	0.62	0/1662
12	UO	0.72	3/3903 (0.1%)	0.74	3/5312 (0.1%)
13	UQ	0.70	1/6136 (0.0%)	0.72	3/8348 (0.0%)
14	UR	0.94	2/3564 (0.1%)	0.80	2/4816 (0.0%)
15	UU	0.81	8/6903 (0.1%)	0.77	5/9392 (0.1%)
16	UX	0.63	0/1493	0.67	0/2011
17	UZ	0.48	1/1857 (0.1%)	0.66	3/2526 (0.1%)
18	CA	0.75	1/1814 (0.1%)	0.72	0/2456
18	CB	0.48	0/1853	0.61	0/2511
19	CC	0.53	0/2911	0.65	1/3937 (0.0%)
20	CD	0.53	1/3205 (0.0%)	0.68	2/4338 (0.0%)
21	CE	0.84	0/891	0.80	0/1214
21	CF	0.40	0/876	0.64	0/1195
22	CG	0.33	0/2983	0.58	0/4032
23	CH	0.51	0/2939	0.67	0/3988
24	CI	0.63	1/6631 (0.0%)	0.67	3/8943 (0.0%)
25	CJ	1.09	3/1462 (0.2%)	0.86	0/1967
26	CK	0.95	2/2376 (0.1%)	0.86	4/3214 (0.1%)
27	CL	0.70	0/1812	0.66	0/2437
28	CM	0.70	1/3573 (0.0%)	0.71	2/4829 (0.0%)
29	CN	0.52	0/1797	0.64	0/2443
29	CO	0.41	0/1714	0.62	0/2325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	CP	0.31	0/1528	0.67	1/2057 (0.0%)
31	CQ	0.37	0/1379	0.58	0/1850
32	CR	0.42	1/6108 (0.0%)	0.84	20/8266 (0.2%)
32	CS	0.42	1/6108 (0.0%)	0.84	20/8266 (0.2%)
33	CT	0.67	0/1053	0.70	0/1413
34	Cc	0.78	0/1485	0.74	0/2008
35	Ce	0.36	0/1298	0.75	1/1750 (0.1%)
36	Cg	0.37	0/1259	0.63	0/1687
37	Ch	0.28	0/422	0.50	0/561
38	Ci	0.31	0/801	0.60	0/1087
39	Cj	1.02	0/958	0.88	0/1293
40	Cm	0.35	0/1001	0.65	1/1345 (0.1%)
41	Cn	0.62	0/712	0.67	0/954
42	Cp	0.58	0/458	0.68	0/617
43	CU	0.37	0/1015	0.60	0/1351
44	C1	1.32	203/26369 (0.8%)	1.49	504/41071 (1.2%)
45	C2	1.37	62/5459 (1.1%)	1.61	134/8498 (1.6%)
46	UV	0.35	1/8638 (0.0%)	0.72	9/11725 (0.1%)
47	CV	0.33	0/1172	0.69	0/1592
48	UH	0.50	1/2852 (0.0%)	0.68	2/3846 (0.1%)
49	UE	0.47	0/980	0.91	5/1316 (0.4%)
49	UI	0.47	0/980	0.91	5/1316 (0.4%)
50	US	0.52	0/3765	0.62	0/5100
51	Cl	0.42	0/638	0.66	0/857
52	CX	0.31	0/2180	0.57	1/2956 (0.0%)
53	UP	0.55	0/428	0.62	0/570
54	Cz	0.33	0/2310	0.58	0/3120
All	All	0.78	314/186592 (0.2%)	0.92	753/258976 (0.3%)

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	4
4	UD	0	2
5	UF	0	1
6	UG	0	2
9	UL	0	1
10	UM	0	3
12	UO	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
13	UQ	0	6
15	UU	0	8
17	UZ	0	3
18	CA	0	1
18	CB	0	1
21	CF	0	1
23	CH	0	1
24	CI	0	2
26	CK	0	1
29	CO	0	2
31	CQ	0	1
32	CR	0	2
32	CS	0	2
34	Cc	0	2
35	Ce	0	1
38	Ci	0	1
39	Cj	0	2
46	UV	0	5
47	CV	0	2
48	UH	0	2
50	US	0	1
51	Cl	0	1
54	Cz	0	1
All	All	0	64

All (314) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	UQ	394	HIS	CA-CB	-13.98	1.23	1.53
45	C2	57	A	N7-C5	-10.06	1.33	1.39
15	UU	418	TRP	CB-CG	-9.97	1.32	1.50
44	C1	2107	A	N9-C4	-9.80	1.31	1.37
44	C1	254	G	N7-C5	-9.57	1.33	1.39
44	C1	2194	A	N9-C4	-9.33	1.32	1.37
15	UU	420	TRP	CB-CG	-8.64	1.34	1.50
44	C1	2107	A	N3-C4	-8.63	1.29	1.34
1	UA	495	TRP	CB-CG	-8.41	1.35	1.50
44	C1	254	G	C5-C6	-8.28	1.34	1.42
45	C2	62	A	N3-C4	-8.25	1.29	1.34
45	C2	88	A	C5-C6	-8.16	1.33	1.41
44	C1	2169	A	N7-C5	-8.15	1.34	1.39
44	C1	2107	A	C5-C4	-8.13	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C2	265	A	N9-C4	-8.11	1.32	1.37
44	C1	2194	A	N3-C4	-8.05	1.30	1.34
44	C1	1744	A	N9-C4	-7.98	1.33	1.37
45	C2	63	G	N7-C5	-7.89	1.34	1.39
44	C1	2194	A	N7-C5	-7.85	1.34	1.39
45	C2	88	A	N7-C5	-7.50	1.34	1.39
45	C2	84	G	N3-C4	-7.32	1.30	1.35
1	UA	595	TYR	CD1-CE1	-7.27	1.28	1.39
44	C1	1146	G	N7-C5	-7.19	1.34	1.39
44	C1	2176	A	N7-C5	-7.14	1.34	1.39
44	C1	2172	C	N1-C6	-7.11	1.32	1.37
28	CM	310	TRP	CB-CG	-7.10	1.37	1.50
44	C1	262	G	C6-N1	-7.04	1.34	1.39
44	C1	413	C	N1-C6	-7.03	1.32	1.37
45	C2	62	A	C5-C4	-7.02	1.33	1.38
1	UA	409	TRP	CB-CG	-6.99	1.37	1.50
44	C1	2176	A	N9-C4	-6.95	1.33	1.37
44	C1	417	G	N7-C5	-6.94	1.35	1.39
45	C2	265	A	C5-C6	-6.92	1.34	1.41
44	C1	355	G	N7-C5	-6.91	1.35	1.39
44	C1	2214	A	C5-C6	-6.89	1.34	1.41
44	C1	2168	U	C2-N3	-6.88	1.32	1.37
45	C2	62	A	C6-N1	-6.83	1.30	1.35
44	C1	407	A	N3-C4	-6.78	1.30	1.34
48	UH	730	PHE	C-N	-6.77	1.18	1.34
44	C1	352	G	N7-C5	-6.74	1.35	1.39
44	C1	210	G	N3-C4	-6.73	1.30	1.35
44	C1	2066	A	N7-C5	-6.73	1.35	1.39
44	C1	257	G	C5-C4	-6.72	1.33	1.38
44	C1	407	A	N7-C5	-6.68	1.35	1.39
44	C1	2066	A	C5-C4	-6.67	1.34	1.38
45	C2	63	G	C5-C4	-6.66	1.33	1.38
45	C2	84	G	C5-C4	-6.66	1.33	1.38
44	C1	73	A	N9-C4	-6.62	1.33	1.37
45	C2	63	G	C5-C6	-6.59	1.35	1.42
15	UU	1048	ARG	CA-CB	-6.59	1.39	1.53
44	C1	2107	A	C5-C6	-6.54	1.35	1.41
44	C1	2193	G	N7-C5	-6.51	1.35	1.39
44	C1	135	A	N7-C5	-6.50	1.35	1.39
45	C2	84	G	C6-N1	-6.48	1.35	1.39
44	C1	257	G	N9-C4	-6.45	1.32	1.38
25	CJ	173	TYR	CD2-CE2	-6.44	1.29	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C2	79	G	N7-C5	-6.44	1.35	1.39
44	C1	2176	A	C5-C6	-6.38	1.35	1.41
45	C2	62	A	N9-C4	-6.38	1.34	1.37
44	C1	254	G	N9-C8	-6.36	1.33	1.37
44	C1	407	A	N9-C4	-6.35	1.34	1.37
44	C1	272	A	N9-C4	-6.32	1.34	1.37
45	C2	265	A	C5-C4	-6.32	1.34	1.38
44	C1	355	G	N3-C4	-6.30	1.31	1.35
44	C1	294	G	N7-C5	-6.30	1.35	1.39
45	C2	63	G	C6-N1	-6.29	1.35	1.39
44	C1	2169	A	C5-C6	-6.29	1.35	1.41
44	C1	232	G	N3-C4	-6.26	1.31	1.35
45	C2	57	A	C6-N1	-6.25	1.31	1.35
44	C1	238	G	N7-C5	-6.23	1.35	1.39
44	C1	2177	G	N3-C4	-6.21	1.31	1.35
44	C1	135	A	N3-C4	-6.20	1.31	1.34
44	C1	2169	A	N3-C4	-6.20	1.31	1.34
44	C1	208	A	C5-C4	-6.19	1.34	1.38
44	C1	71	A	N9-C4	-6.17	1.34	1.37
1	UA	673	VAL	CB-CG2	-6.17	1.39	1.52
44	C1	2332	A	N9-C4	-6.16	1.34	1.37
44	C1	361	A	C5-C4	-6.14	1.34	1.38
44	C1	2067	G	C5-C4	-6.11	1.34	1.38
45	C2	54	C	N1-C6	-6.09	1.33	1.37
44	C1	2064	C	N3-C4	-6.09	1.29	1.33
44	C1	407	A	C5-C4	-6.05	1.34	1.38
44	C1	2218	A	N9-C4	-6.05	1.34	1.37
15	UU	721	TRP	CB-CG	-6.04	1.39	1.50
44	C1	2049	G	N7-C5	-6.04	1.35	1.39
45	C2	29	A	N9-C4	-6.04	1.34	1.37
45	C2	88	A	N3-C4	-6.02	1.31	1.34
45	C2	84	G	N7-C5	-6.01	1.35	1.39
44	C1	1146	G	C6-N1	-6.00	1.35	1.39
44	C1	409	A	N7-C5	-5.96	1.35	1.39
44	C1	262	G	N7-C5	-5.95	1.35	1.39
1	UA	4	ASN	CA-CB	-5.95	1.37	1.53
44	C1	257	G	N3-C4	-5.94	1.31	1.35
32	CS	626	GLU	CB-CG	5.93	1.63	1.52
44	C1	2072	U	C2-N3	-5.93	1.33	1.37
45	C2	50	G	N7-C5	-5.93	1.35	1.39
2	UB	679	ASN	C-N	-5.92	1.20	1.34
32	CR	626	GLU	CB-CG	5.91	1.63	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C2	59	A	N9-C4	-5.90	1.34	1.37
44	C1	361	A	C5-C6	-5.89	1.35	1.41
44	C1	435	A	N9-C4	-5.88	1.34	1.37
44	C1	1744	A	N7-C5	-5.88	1.35	1.39
44	C1	2177	G	C5-C4	-5.88	1.34	1.38
6	UG	285	TRP	CB-CG	-5.88	1.39	1.50
12	UO	417	ARG	C-N	-5.88	1.20	1.34
44	C1	352	G	C5-C6	-5.88	1.36	1.42
44	C1	2183	A	C5-C6	-5.88	1.35	1.41
44	C1	2066	A	N3-C4	-5.88	1.31	1.34
44	C1	245	G	N7-C5	-5.88	1.35	1.39
44	C1	406	G	C5-C6	-5.87	1.36	1.42
45	C2	267	C	C2-O2	-5.87	1.19	1.24
44	C1	1145	G	C6-N1	-5.84	1.35	1.39
44	C1	417	G	C5-C4	-5.83	1.34	1.38
44	C1	404	C	N1-C6	-5.83	1.33	1.37
14	UR	565	ALA	CA-CB	-5.82	1.40	1.52
44	C1	2186	U	C4-C5	-5.81	1.38	1.43
44	C1	361	A	N7-C5	-5.80	1.35	1.39
44	C1	2179	C	N1-C6	-5.79	1.33	1.37
44	C1	241	G	C5-C4	-5.79	1.34	1.38
44	C1	294	G	N3-C4	-5.79	1.31	1.35
44	C1	1741	A	C5-C4	-5.78	1.34	1.38
45	C2	35	G	N9-C4	-5.78	1.33	1.38
45	C2	66	A	N9-C4	-5.78	1.34	1.37
24	CI	851	TRP	CB-CG	-5.77	1.39	1.50
45	C2	267	C	N1-C6	-5.76	1.33	1.37
45	C2	62	A	C5-C6	-5.75	1.35	1.41
44	C1	83	A	N9-C4	-5.75	1.34	1.37
44	C1	1146	G	C5-C4	-5.74	1.34	1.38
44	C1	2176	A	N3-C4	-5.73	1.31	1.34
44	C1	2167	G	C6-N1	-5.73	1.35	1.39
44	C1	215	A	N3-C4	-5.73	1.31	1.34
44	C1	2177	G	N9-C4	-5.72	1.33	1.38
44	C1	254	G	N3-C4	-5.72	1.31	1.35
44	C1	412	G	N7-C5	-5.72	1.35	1.39
45	C2	80	G	N3-C4	-5.72	1.31	1.35
4	UD	114	TRP	CB-CG	-5.70	1.40	1.50
44	C1	2194	A	C6-N6	-5.70	1.29	1.33
44	C1	254	G	C8-N7	-5.70	1.27	1.30
44	C1	1146	G	N1-C2	-5.67	1.33	1.37
44	C1	418	G	N7-C5	-5.66	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C2	84	G	N9-C4	-5.66	1.33	1.38
44	C1	417	G	N3-C4	-5.66	1.31	1.35
44	C1	2066	A	C5-C6	-5.66	1.35	1.41
44	C1	1753	G	C5-C6	-5.65	1.36	1.42
44	C1	2072	U	N1-C2	-5.65	1.33	1.38
44	C1	254	G	C5-C4	-5.65	1.34	1.38
45	C2	57	A	C8-N7	-5.64	1.27	1.31
12	UO	432	ARG	CA-CB	-5.63	1.41	1.53
44	C1	2190	G	C5-C4	-5.63	1.34	1.38
44	C1	254	G	C6-N1	-5.63	1.35	1.39
44	C1	291	C	N1-C6	-5.63	1.33	1.37
45	C2	76	C	C4-C5	-5.63	1.38	1.43
15	UU	508	TRP	CB-CG	-5.62	1.40	1.50
44	C1	1744	A	C5-C4	-5.62	1.34	1.38
45	C2	66	A	N7-C5	-5.61	1.35	1.39
45	C2	40	C	N1-C6	-5.61	1.33	1.37
44	C1	255	G	N7-C5	-5.61	1.35	1.39
45	C2	63	G	N3-C4	-5.61	1.31	1.35
45	C2	88	A	N9-C4	-5.60	1.34	1.37
44	C1	399	G	C6-N1	-5.60	1.35	1.39
44	C1	133	G	N7-C5	-5.59	1.35	1.39
44	C1	239	G	N7-C5	-5.59	1.35	1.39
44	C1	138	A	N7-C5	-5.58	1.35	1.39
44	C1	2107	A	N7-C5	-5.58	1.35	1.39
44	C1	262	G	C5-C4	-5.58	1.34	1.38
44	C1	416	U	N1-C2	-5.58	1.33	1.38
45	C2	66	A	N3-C4	-5.55	1.31	1.34
44	C1	2067	G	N7-C5	-5.55	1.35	1.39
26	CK	186	GLU	CA-CB	-5.55	1.41	1.53
44	C1	1741	A	N7-C5	-5.54	1.35	1.39
45	C2	264	G	N3-C4	-5.54	1.31	1.35
44	C1	2214	A	N7-C5	-5.52	1.35	1.39
44	C1	2191	U	C2-N3	-5.52	1.33	1.37
45	C2	264	G	C6-N1	-5.52	1.35	1.39
44	C1	1753	G	N7-C5	-5.51	1.35	1.39
44	C1	2175	A	N3-C4	-5.51	1.31	1.34
44	C1	2156	A	N7-C5	-5.50	1.35	1.39
1	UA	40	PHE	CB-CG	-5.50	1.42	1.51
45	C2	57	A	N3-C4	-5.49	1.31	1.34
44	C1	218	G	N3-C4	-5.49	1.31	1.35
44	C1	435	A	N3-C4	-5.48	1.31	1.34
44	C1	2066	A	C6-N1	-5.48	1.31	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	C1	2107	A	C6-N1	-5.46	1.31	1.35
45	C2	49	U	C2-N3	-5.46	1.33	1.37
1	UA	453	TRP	CB-CG	-5.45	1.40	1.50
44	C1	272	A	N3-C4	-5.45	1.31	1.34
44	C1	435	A	C5-C4	-5.45	1.34	1.38
25	CJ	173	TYR	CD1-CE1	-5.45	1.31	1.39
4	UD	238	VAL	CB-CG1	-5.44	1.41	1.52
44	C1	412	G	N3-C4	-5.44	1.31	1.35
45	C2	84	G	N9-C8	-5.44	1.34	1.37
45	C2	65	C	N1-C6	-5.43	1.33	1.37
44	C1	365	G	N7-C5	-5.43	1.35	1.39
44	C1	1753	G	C5-C4	-5.43	1.34	1.38
45	C2	268	G	C5-C4	-5.43	1.34	1.38
44	C1	2064	C	N1-C6	-5.42	1.33	1.37
44	C1	73	A	C5-C6	-5.42	1.36	1.41
1	UA	518	PHE	CB-CG	-5.42	1.42	1.51
45	C2	62	A	N7-C5	-5.41	1.36	1.39
44	C1	355	G	C5-C4	-5.41	1.34	1.38
44	C1	2071	G	C5-C4	-5.41	1.34	1.38
45	C2	262	C	N1-C6	-5.41	1.33	1.37
44	C1	408	C	N3-C4	-5.40	1.30	1.33
45	C2	50	G	C5-C6	-5.40	1.36	1.42
44	C1	1749	G	C6-N1	-5.40	1.35	1.39
44	C1	76	U	C2-N3	-5.39	1.33	1.37
44	C1	148	C	C2-O2	-5.39	1.19	1.24
45	C2	35	G	C5-C6	-5.39	1.36	1.42
15	UU	86	THR	CB-CG2	-5.39	1.34	1.52
44	C1	210	G	C5-C4	-5.37	1.34	1.38
44	C1	2188	G	N3-C4	-5.37	1.31	1.35
44	C1	121	G	C6-N1	-5.35	1.35	1.39
44	C1	2198	C	N1-C6	-5.35	1.33	1.37
45	C2	265	A	N3-C4	-5.34	1.31	1.34
44	C1	2067	G	N9-C8	-5.34	1.34	1.37
18	CA	204	ILE	C-N	-5.34	1.24	1.34
44	C1	361	A	N3-C4	-5.34	1.31	1.34
44	C1	429	A	N9-C4	-5.33	1.34	1.37
44	C1	77	C	N1-C6	-5.32	1.33	1.37
44	C1	352	G	C8-N7	-5.31	1.27	1.30
44	C1	417	G	C6-N1	-5.30	1.35	1.39
44	C1	399	G	N7-C5	-5.30	1.36	1.39
44	C1	1146	G	C5-C6	-5.30	1.37	1.42
4	UD	63	TRP	CB-CG	-5.30	1.40	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	C1	417	G	C5-C6	-5.30	1.37	1.42
44	C1	401	C	N1-C6	-5.29	1.33	1.37
44	C1	1742	C	N1-C6	-5.29	1.33	1.37
44	C1	2169	A	N9-C4	-5.29	1.34	1.37
44	C1	294	G	N9-C4	-5.29	1.33	1.38
44	C1	2200	U	N1-C6	-5.29	1.33	1.38
44	C1	403	G	N3-C4	-5.28	1.31	1.35
44	C1	1748	G	C5-C4	-5.28	1.34	1.38
44	C1	2108	A	N9-C8	-5.27	1.33	1.37
45	C2	59	A	N3-C4	-5.27	1.31	1.34
44	C1	1145	G	N7-C5	-5.26	1.36	1.39
44	C1	2108	A	N3-C4	-5.26	1.31	1.34
44	C1	2167	G	N1-C2	-5.26	1.33	1.37
44	C1	73	A	N7-C5	-5.25	1.36	1.39
45	C2	265	A	N7-C5	-5.25	1.36	1.39
44	C1	1146	G	N9-C8	-5.25	1.34	1.37
44	C1	363	G	N7-C5	-5.24	1.36	1.39
44	C1	2090	G	N3-C4	-5.24	1.31	1.35
45	C2	50	G	C6-N1	-5.23	1.35	1.39
44	C1	81	G	C5-C4	-5.22	1.34	1.38
12	UO	172	TRP	CB-CG	-5.22	1.40	1.50
44	C1	2188	G	N7-C5	-5.22	1.36	1.39
4	UD	303	TYR	CD1-CE1	-5.21	1.31	1.39
44	C1	416	U	C2-N3	-5.21	1.34	1.37
44	C1	262	G	C5-C6	-5.21	1.37	1.42
44	C1	360	U	N1-C2	-5.20	1.33	1.38
44	C1	212	C	N1-C6	-5.19	1.34	1.37
44	C1	2194	A	C5-C6	-5.19	1.36	1.41
44	C1	598	A	N7-C5	-5.19	1.36	1.39
46	UV	1057	VAL	CB-CG1	-5.19	1.42	1.52
44	C1	2186	U	N1-C6	-5.19	1.33	1.38
6	UG	420	VAL	CB-CG2	-5.18	1.42	1.52
44	C1	2202	C	N3-C4	-5.18	1.30	1.33
44	C1	255	G	N9-C8	-5.18	1.34	1.37
44	C1	361	A	N9-C4	-5.18	1.34	1.37
44	C1	234	G	C6-N1	-5.17	1.35	1.39
44	C1	1155	G	N9-C4	-5.17	1.33	1.38
45	C2	82	U	C2-N3	-5.17	1.34	1.37
6	UG	229	PHE	CB-CG	-5.16	1.42	1.51
15	UU	526	TRP	CB-CG	-5.16	1.41	1.50
26	CK	282	TRP	CB-CG	-5.16	1.41	1.50
44	C1	1747	A	N7-C5	-5.16	1.36	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	C1	73	A	N3-C4	-5.15	1.31	1.34
44	C1	285	A	C5-C4	-5.15	1.35	1.38
44	C1	1155	G	C5-C6	-5.15	1.37	1.42
45	C2	46	U	N3-C4	-5.15	1.33	1.38
25	CJ	132	GLU	CB-CG	-5.15	1.42	1.52
44	C1	232	G	C6-N1	-5.15	1.35	1.39
44	C1	363	G	C6-N1	-5.15	1.35	1.39
44	C1	2065	C	N1-C6	-5.15	1.34	1.37
44	C1	1744	A	C5-C6	-5.14	1.36	1.41
44	C1	135	A	C6-N1	-5.14	1.31	1.35
44	C1	1747	A	N3-C4	-5.13	1.31	1.34
44	C1	2175	A	N7-C5	-5.13	1.36	1.39
44	C1	2071	G	C6-N1	-5.12	1.35	1.39
44	C1	2194	A	C5-C4	-5.12	1.35	1.38
1	UA	595	TYR	CD2-CE2	-5.12	1.31	1.39
1	UA	595	TYR	CE1-CZ	-5.12	1.31	1.38
17	UZ	63	TRP	CB-CG	-5.10	1.41	1.50
44	C1	404	C	C4-C5	-5.10	1.38	1.43
45	C2	55	C	N1-C6	-5.09	1.34	1.37
44	C1	1145	G	C5-C6	-5.09	1.37	1.42
44	C1	130	C	N1-C6	-5.09	1.34	1.37
44	C1	2198	C	C4-C5	-5.09	1.38	1.43
44	C1	403	G	N7-C5	-5.09	1.36	1.39
44	C1	1758	C	N1-C6	-5.08	1.34	1.37
44	C1	249	C	N3-C4	-5.07	1.30	1.33
1	UA	448	PHE	CB-CG	-5.07	1.42	1.51
44	C1	2090	G	N9-C4	-5.07	1.33	1.38
44	C1	2108	A	N7-C5	-5.06	1.36	1.39
44	C1	75	G	N7-C5	-5.06	1.36	1.39
44	C1	2214	A	N9-C4	-5.06	1.34	1.37
20	CD	432	TRP	CB-CG	-5.05	1.41	1.50
44	C1	234	G	C5-C4	-5.05	1.34	1.38
45	C2	71	U	N1-C6	-5.05	1.33	1.38
14	UR	580	TRP	CB-CG	-5.05	1.41	1.50
44	C1	406	G	N7-C5	-5.04	1.36	1.39
45	C2	267	C	N3-C4	-5.04	1.30	1.33
44	C1	2191	U	N3-C4	-5.04	1.33	1.38
1	UA	484	VAL	CB-CG2	-5.04	1.42	1.52
44	C1	2182	C	N1-C6	-5.04	1.34	1.37
45	C2	43	C	N3-C4	-5.04	1.30	1.33
45	C2	38	G	N9-C4	-5.03	1.33	1.38
6	UG	464	ASN	CA-CB	-5.03	1.40	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	C1	2107	A	N9-C8	-5.03	1.33	1.37
15	UU	74	TYR	CD2-CE2	-5.03	1.31	1.39
44	C1	253	G	C5-C6	-5.02	1.37	1.42
44	C1	241	G	N7-C5	-5.02	1.36	1.39
44	C1	262	G	C8-N7	-5.01	1.27	1.30
45	C2	63	G	N1-C2	-5.00	1.33	1.37

All (753) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C2	2	G	O5'-P-OP1	-32.44	71.78	110.70
45	C2	2	G	OP1-P-OP2	-26.35	80.07	119.60
45	C2	2	G	O5'-P-OP2	19.04	133.54	110.70
44	C1	258	C	N1-C2-O2	13.22	126.83	118.90
45	C2	1	A	OP1-P-O3'	13.10	134.03	105.20
45	C2	1	A	OP2-P-O3'	-12.64	77.40	105.20
44	C1	258	C	C2-N1-C1'	12.50	132.55	118.80
44	C1	2168	U	N3-C2-O2	-12.41	113.51	122.20
44	C1	55	G	OP1-P-O3'	-12.05	78.68	105.20
24	CI	995	VAL	C-N-CA	12.03	151.76	121.70
45	C2	39	U	N3-C2-O2	-11.84	113.91	122.20
44	C1	2168	U	N1-C2-O2	11.17	130.62	122.80
44	C1	45	U	OP1-P-O3'	-11.01	80.98	105.20
44	C1	254	G	C6-C5-N7	-10.99	123.80	130.40
44	C1	254	G	C4-C5-N7	10.68	115.07	110.80
44	C1	258	C	N3-C2-O2	-10.49	114.56	121.90
44	C1	1146	G	N3-C4-N9	10.41	132.25	126.00
44	C1	160	C	N3-C2-O2	-10.39	114.63	121.90
44	C1	160	C	C6-N1-C2	-10.38	116.15	120.30
44	C1	265	G	C6-C5-N7	-10.20	124.28	130.40
44	C1	139	C	C6-N1-C2	-10.12	116.25	120.30
44	C1	434	A	N1-C6-N6	-9.98	112.61	118.60
45	C2	57	A	N1-C2-N3	9.92	134.26	129.30
44	C1	45	U	OP2-P-O3'	-9.73	83.80	105.20
44	C1	265	G	N9-C4-C5	-9.66	101.54	105.40
44	C1	1547	C	N1-C2-O2	9.49	124.59	118.90
44	C1	2214	A	N1-C6-N6	9.46	124.27	118.60
45	C2	267	C	N3-C2-O2	-9.42	115.31	121.90
44	C1	254	G	C5-N7-C8	-9.32	99.64	104.30
44	C1	2214	A	N9-C4-C5	-9.31	102.07	105.80
44	C1	505	C	N3-C2-O2	-9.24	115.43	121.90
44	C1	352	G	C4-C5-N7	9.18	114.47	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C1	258	C	C6-N1-C1'	-9.17	109.80	120.80
44	C1	1662	C	N3-C2-O2	-9.15	115.49	121.90
26	CK	289	ARG	NE-CZ-NH1	-9.12	115.74	120.30
44	C1	262	G	C6-C5-N7	-9.08	124.95	130.40
45	C2	140	C	N3-C2-O2	-9.01	115.59	121.90
44	C1	235	C	N3-C4-C5	8.99	125.50	121.90
44	C1	2214	A	C4-C5-N7	8.99	115.19	110.70
32	CS	188	ARG	NE-CZ-NH1	8.93	124.77	120.30
32	CR	188	ARG	NE-CZ-NH1	8.91	124.75	120.30
49	UE	238	ARG	NE-CZ-NH2	8.87	124.73	120.30
44	C1	265	G	C4-C5-N7	8.87	114.35	110.80
49	UI	238	ARG	NE-CZ-NH2	8.86	124.73	120.30
44	C1	1146	G	C6-C5-N7	-8.85	125.09	130.40
44	C1	1747	A	C6-N1-C2	-8.83	113.30	118.60
44	C1	1550	U	C2-N1-C1'	8.80	128.27	117.70
45	C2	88	A	N1-C6-N6	8.74	123.84	118.60
44	C1	262	G	N3-C4-N9	8.69	131.21	126.00
44	C1	2090	G	C2-N3-C4	-8.52	107.64	111.90
44	C1	404	C	C2-N1-C1'	8.45	128.09	118.80
44	C1	206	C	N1-C2-O2	8.43	123.96	118.90
44	C1	2090	G	N3-C4-N9	-8.42	120.95	126.00
45	C2	264	G	C8-N9-C4	-8.42	103.03	106.40
44	C1	159	C	C6-N1-C2	-8.38	116.95	120.30
44	C1	2238	A	N1-C6-N6	-8.35	113.59	118.60
30	CP	213	LEU	CA-CB-CG	8.23	134.22	115.30
45	C2	79	G	C6-C5-N7	-8.21	125.47	130.40
45	C2	35	G	C4-C5-N7	8.20	114.08	110.80
44	C1	2202	C	N3-C2-O2	-8.18	116.17	121.90
44	C1	2084	C	N3-C2-O2	-8.09	116.24	121.90
44	C1	1146	G	N3-C4-C5	-8.07	124.57	128.60
44	C1	2195	U	N3-C2-O2	-8.07	116.55	122.20
44	C1	2186	U	C5-C4-O4	-8.03	121.08	125.90
8	UK	51	LEU	CA-CB-CG	-8.02	96.86	115.30
44	C1	1486	G	C8-N9-C4	-7.99	103.20	106.40
44	C1	1486	G	N7-C8-N9	7.98	117.09	113.10
45	C2	266	C	N3-C4-C5	7.96	125.08	121.90
44	C1	1547	C	C2-N1-C1'	7.95	127.54	118.80
44	C1	148	C	N3-C2-O2	-7.93	116.34	121.90
44	C1	2214	A	C5-C6-N6	-7.92	117.36	123.70
4	UD	357	LEU	CB-CG-CD2	-7.91	97.55	111.00
45	C2	82	U	N1-C2-O2	7.88	128.32	122.80
44	C1	2186	U	C5-C6-N1	7.88	126.64	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C1	56	C	C2-N1-C1'	7.86	127.45	118.80
44	C1	2194	A	C8-N9-C4	-7.83	102.67	105.80
44	C1	265	G	N3-C4-N9	7.80	130.68	126.00
45	C2	46	U	N3-C2-O2	-7.79	116.75	122.20
44	C1	470	C	N1-C2-O2	7.78	123.57	118.90
44	C1	2165	U	C2-N1-C1'	7.77	127.02	117.70
44	C1	471	C	C6-N1-C2	-7.77	117.19	120.30
44	C1	2074	C	C2-N1-C1'	7.76	127.34	118.80
32	CR	188	ARG	NE-CZ-NH2	-7.76	116.42	120.30
32	CS	188	ARG	NE-CZ-NH2	-7.74	116.43	120.30
44	C1	254	G	N7-C8-N9	7.73	116.97	113.10
45	C2	57	A	C6-N1-C2	-7.72	113.97	118.60
44	C1	56	C	OP1-P-OP2	7.70	131.15	119.60
44	C1	1662	C	N1-C2-O2	7.67	123.50	118.90
44	C1	2164	C	C6-N1-C2	-7.67	117.23	120.30
44	C1	159	C	N3-C2-O2	-7.66	116.54	121.90
44	C1	2217	C	C2-N1-C1'	7.65	127.22	118.80
44	C1	2074	C	N1-C2-O2	7.63	123.48	118.90
45	C2	260	G	C4-N9-C1'	7.59	136.37	126.50
44	C1	46	C	OP1-P-OP2	7.59	130.99	119.60
44	C1	1655	U	N3-C2-O2	-7.56	116.91	122.20
44	C1	2177	G	N3-C4-N9	-7.56	121.47	126.00
44	C1	70	C	N1-C2-O2	7.54	123.43	118.90
44	C1	1146	G	C4-N9-C1'	7.54	136.31	126.50
44	C1	80	C	N3-C2-O2	-7.53	116.63	121.90
44	C1	505	C	N1-C2-O2	7.53	123.42	118.90
44	C1	2048	C	N3-C2-O2	-7.53	116.63	121.90
44	C1	2179	C	N1-C2-O2	7.52	123.41	118.90
45	C2	39	U	N1-C2-N3	7.52	119.41	114.90
44	C1	211	G	C8-N9-C1'	-7.50	117.25	127.00
44	C1	68	U	N3-C2-O2	-7.50	116.95	122.20
32	CS	913	MET	CB-CG-SD	7.50	134.90	112.40
32	CR	913	MET	CB-CG-SD	7.50	134.89	112.40
45	C2	76	C	N3-C4-C5	7.48	124.89	121.90
44	C1	2074	C	C6-N1-C1'	-7.45	111.86	120.80
44	C1	2176	A	C5-N7-C8	-7.45	100.17	103.90
44	C1	265	G	N1-C6-O6	7.45	124.37	119.90
44	C1	371	U	N3-C2-O2	-7.44	116.99	122.20
45	C2	35	G	N9-C4-C5	-7.44	102.42	105.40
44	C1	2107	A	C8-N9-C4	7.43	108.77	105.80
44	C1	2079	U	N3-C2-O2	-7.43	117.00	122.20
45	C2	90	C	C6-N1-C2	7.42	123.27	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C2	260	G	C8-N9-C1'	-7.39	117.39	127.00
45	C2	88	A	C6-C5-N7	-7.37	127.14	132.30
44	C1	262	G	C4-C5-N7	7.36	113.75	110.80
44	C1	3	G	N3-C4-N9	-7.36	121.59	126.00
44	C1	1222	C	N1-C2-O2	7.35	123.31	118.90
44	C1	55	G	OP2-P-O3'	-7.34	89.05	105.20
44	C1	203	C	C6-N1-C2	-7.33	117.37	120.30
44	C1	1486	G	C4-N9-C1'	7.32	136.02	126.50
44	C1	238	G	C6-C5-N7	-7.32	126.01	130.40
45	C2	44	U	C5-C6-N1	7.32	126.36	122.70
45	C2	88	A	C4-C5-N7	7.31	114.36	110.70
44	C1	407	A	O5'-P-OP1	-7.30	99.12	105.70
44	C1	2214	A	C6-C5-N7	-7.30	127.19	132.30
32	CS	626	GLU	CA-CB-CG	7.29	129.44	113.40
45	C2	21	U	N3-C2-O2	-7.29	117.09	122.20
14	UR	587	LEU	CA-CB-CG	-7.29	98.53	115.30
32	CR	626	GLU	CA-CB-CG	7.29	129.44	113.40
44	C1	160	C	N1-C2-O2	7.28	123.27	118.90
44	C1	2195	U	N1-C2-O2	7.27	127.89	122.80
44	C1	1146	G	C8-N9-C1'	-7.27	117.55	127.00
44	C1	454	C	C2-N1-C1'	7.26	126.79	118.80
45	C2	140	C	N1-C2-O2	7.25	123.25	118.90
44	C1	352	G	C5-N7-C8	-7.23	100.68	104.30
44	C1	471	C	N3-C2-O2	-7.22	116.84	121.90
45	C2	200	U	N1-C2-O2	7.22	127.85	122.80
1	UA	695	LEU	CB-CG-CD2	-7.21	98.74	111.00
44	C1	1159	C	C6-N1-C2	7.17	123.17	120.30
44	C1	262	G	N9-C4-C5	-7.15	102.54	105.40
45	C2	203	C	N3-C2-O2	-7.14	116.90	121.90
44	C1	2194	A	N9-C4-C5	7.12	108.65	105.80
44	C1	356	C	N3-C4-C5	7.11	124.74	121.90
44	C1	446	C	N1-C2-O2	7.10	123.16	118.90
45	C2	200	U	C2-N1-C1'	7.09	126.21	117.70
44	C1	406	G	C4-C5-N7	7.09	113.64	110.80
46	UV	356	LEU	CA-CB-CG	7.09	131.61	115.30
45	C2	57	A	C4-C5-C6	7.06	120.53	117.00
46	UV	424	LEU	CA-CB-CG	7.05	131.51	115.30
44	C1	352	G	C5-C6-O6	-7.04	124.37	128.60
44	C1	34	C	N3-C2-O2	-7.00	117.00	121.90
44	C1	1165	U	N3-C2-O2	-7.00	117.30	122.20
45	C2	90	C	N3-C4-C5	7.00	124.70	121.90
44	C1	68	U	N1-C2-O2	6.99	127.69	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	UM	83	LEU	CA-CB-CG	6.97	131.33	115.30
44	C1	260	U	C2-N1-C1'	-6.95	109.36	117.70
44	C1	112	C	N1-C2-O2	6.94	123.07	118.90
44	C1	2169	A	C5-N7-C8	-6.94	100.43	103.90
44	C1	34	C	N1-C2-O2	6.93	123.06	118.90
44	C1	2210	U	C5-C4-O4	6.93	130.06	125.90
44	C1	2169	A	C6-C5-N7	-6.93	127.45	132.30
44	C1	346	C	N3-C2-O2	-6.92	117.05	121.90
32	CS	88	GLU	CA-CB-CG	6.90	128.59	113.40
44	C1	2090	G	C5-C6-O6	6.90	132.74	128.60
44	C1	2169	A	N7-C8-N9	6.90	117.25	113.80
32	CR	88	GLU	CA-CB-CG	6.89	128.56	113.40
44	C1	211	G	C4-N9-C1'	6.89	135.46	126.50
44	C1	294	G	C2-N3-C4	-6.89	108.46	111.90
44	C1	449	C	N3-C2-O2	-6.88	117.08	121.90
44	C1	1550	U	N1-C2-O2	6.88	127.62	122.80
45	C2	147	G	N3-C4-N9	6.88	130.12	126.00
44	C1	2168	U	C2-N1-C1'	6.87	125.95	117.70
44	C1	404	C	C6-N1-C2	-6.87	117.55	120.30
4	UD	253	ASP	CB-CG-OD1	6.86	124.48	118.30
44	C1	2091	C	C2-N1-C1'	6.85	126.34	118.80
44	C1	434	A	C6-N1-C2	-6.84	114.49	118.60
44	C1	504	C	N1-C2-O2	6.84	123.00	118.90
44	C1	1645	U	C2-N1-C1'	6.84	125.90	117.70
44	C1	2071	G	O4'-C1'-N9	-6.84	102.73	108.20
44	C1	2049	G	N7-C8-N9	6.83	116.52	113.10
45	C2	202	C	N1-C2-O2	6.82	122.99	118.90
44	C1	1167	C	N1-C2-O2	6.82	122.99	118.90
44	C1	2079	U	N1-C2-O2	6.82	127.57	122.80
32	CS	410	MET	CA-CB-CG	6.80	124.85	113.30
45	C2	79	G	N3-C4-N9	6.79	130.07	126.00
32	CR	410	MET	CA-CB-CG	6.79	124.84	113.30
44	C1	158	C	N1-C2-O2	6.78	122.97	118.90
45	C2	57	A	O4'-C1'-N9	6.77	113.62	108.20
45	C2	61	G	C6-C5-N7	-6.74	126.35	130.40
44	C1	404	C	C5-C6-N1	6.74	124.37	121.00
45	C2	246	G	C4-N9-C1'	6.74	135.26	126.50
46	UV	1051	LEU	CA-CB-CG	6.74	130.81	115.30
44	C1	1146	G	C4-C5-N7	6.74	113.49	110.80
44	C1	1222	C	C2-N1-C1'	6.74	126.21	118.80
45	C2	23	A	P-O3'-C3'	6.70	127.74	119.70
44	C1	346	C	C6-N1-C2	-6.70	117.62	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C1	2202	C	N1-C2-O2	6.70	122.92	118.90
45	C2	50	G	C6-C5-N7	-6.70	126.38	130.40
32	CR	654	LEU	CB-CG-CD1	-6.69	99.62	111.00
32	CS	654	LEU	CB-CG-CD1	-6.68	99.64	111.00
44	C1	239	G	N1-C6-O6	6.67	123.90	119.90
32	CR	526	LEU	CA-CB-CG	6.67	130.64	115.30
44	C1	1486	G	N3-C4-C5	-6.66	125.27	128.60
45	C2	50	G	C4-C5-N7	6.65	113.46	110.80
32	CS	526	LEU	CA-CB-CG	6.65	130.59	115.30
44	C1	1666	C	N1-C2-O2	6.63	122.88	118.90
44	C1	251	G	C4-N9-C1'	6.63	135.12	126.50
44	C1	417	G	C6-C5-N7	-6.63	126.42	130.40
44	C1	2068	C	C5-C6-N1	6.62	124.31	121.00
44	C1	258	C	C6-N1-C2	-6.62	117.65	120.30
44	C1	1630	C	N3-C2-O2	-6.62	117.27	121.90
44	C1	2176	A	N7-C8-N9	6.61	117.10	113.80
44	C1	2229	C	N1-C2-O2	6.60	122.86	118.90
44	C1	265	G	C5-C6-O6	-6.59	124.65	128.60
44	C1	56	C	N1-C2-O2	6.58	122.85	118.90
44	C1	2186	U	N3-C4-O4	6.58	124.00	119.40
32	CR	410	MET	CB-CG-SD	6.58	132.13	112.40
32	CS	410	MET	CB-CG-SD	6.57	132.12	112.40
45	C2	136	C	N1-C2-O2	6.56	122.84	118.90
44	C1	76	U	C5-C6-N1	-6.55	119.42	122.70
44	C1	2049	G	C8-N9-C4	-6.55	103.78	106.40
45	C2	79	G	C4-C5-N7	6.53	113.41	110.80
44	C1	160	C	C5-C6-N1	6.53	124.27	121.00
32	CS	487	GLU	CA-CB-CG	6.53	127.76	113.40
44	C1	485	G	N3-C4-N9	-6.52	122.09	126.00
32	CR	487	GLU	CA-CB-CG	6.52	127.75	113.40
44	C1	255	G	N3-C4-N9	6.52	129.91	126.00
44	C1	1758	C	C2-N1-C1'	-6.51	111.64	118.80
44	C1	238	G	C4-C5-N7	6.50	113.40	110.80
44	C1	1120	C	C2-N1-C1'	6.50	125.95	118.80
44	C1	1165	U	N1-C2-O2	6.50	127.35	122.80
44	C1	139	C	C5-C6-N1	6.49	124.25	121.00
44	C1	129	G	C2-N3-C4	-6.49	108.66	111.90
44	C1	2169	A	C2-N3-C4	-6.49	107.36	110.60
49	UI	238	ARG	CG-CD-NE	6.48	125.40	111.80
44	C1	2217	C	N1-C2-O2	6.47	122.78	118.90
6	UG	284	LEU	CB-CG-CD2	-6.46	100.02	111.00
49	UE	238	ARG	CG-CD-NE	6.46	125.36	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C1	2068	C	C4-C5-C6	-6.45	114.17	117.40
45	C2	39	U	C2-N3-C4	-6.44	123.14	127.00
44	C1	1747	A	N1-C2-N3	6.44	132.52	129.30
44	C1	222	U	O4'-C1'-N1	6.42	113.34	108.20
45	C2	88	A	C5-N7-C8	-6.41	100.70	103.90
44	C1	447	C	N3-C2-O2	-6.40	117.42	121.90
44	C1	1156	C	C5-C6-N1	-6.40	117.80	121.00
45	C2	45	C	N3-C4-C5	6.40	124.46	121.90
44	C1	265	G	C8-N9-C1'	-6.40	118.68	127.00
15	UU	472	LEU	CA-CB-CG	6.39	129.99	115.30
44	C1	402	U	N1-C2-O2	6.39	127.27	122.80
44	C1	2090	G	N1-C2-N3	6.38	127.73	123.90
44	C1	290	C	C5-C6-N1	-6.38	117.81	121.00
44	C1	602	U	N3-C2-O2	-6.37	117.74	122.20
7	UJ	488	LEU	CA-CB-CG	6.37	129.95	115.30
45	C2	202	C	N3-C2-O2	-6.36	117.45	121.90
44	C1	210	G	O5'-P-OP1	-6.36	99.97	105.70
44	C1	434	A	N9-C4-C5	6.36	108.34	105.80
44	C1	179	G	N3-C4-C5	6.36	131.78	128.60
45	C2	268	G	C4-C5-N7	6.35	113.34	110.80
45	C2	82	U	N3-C2-O2	-6.33	117.77	122.20
45	C2	39	U	O5'-P-OP2	-6.33	100.00	105.70
44	C1	70	C	C6-N1-C1'	-6.33	113.20	120.80
32	CS	855	LEU	CA-CB-CG	6.33	129.86	115.30
44	C1	236	C	C5-C6-N1	6.33	124.16	121.00
32	CR	855	LEU	CA-CB-CG	6.32	129.83	115.30
44	C1	1645	U	N1-C2-O2	6.32	127.22	122.80
44	C1	2191	U	N3-C2-O2	-6.31	117.78	122.20
44	C1	56	C	C6-N1-C1'	-6.31	113.23	120.80
44	C1	334	U	N1-C2-O2	6.31	127.22	122.80
44	C1	369	U	N3-C2-O2	-6.31	117.78	122.20
44	C1	258	C	C5-C6-N1	6.31	124.15	121.00
45	C2	49	U	N3-C2-O2	-6.30	117.79	122.20
44	C1	1645	U	N3-C2-O2	-6.29	117.79	122.20
44	C1	203	C	N3-C2-O2	-6.29	117.50	121.90
32	CS	51	ARG	CA-CB-CG	6.28	127.22	113.40
44	C1	415	C	C6-N1-C2	-6.28	117.79	120.30
32	CR	51	ARG	CA-CB-CG	6.28	127.21	113.40
44	C1	486	G	N3-C4-N9	-6.28	122.23	126.00
45	C2	42	U	N3-C2-O2	-6.26	117.81	122.20
44	C1	143	A	C5-C6-N1	6.26	120.83	117.70
49	UE	263	LEU	CA-CB-CG	-6.25	100.91	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C1	2214	A	C5-N7-C8	-6.25	100.77	103.90
48	UH	789	LEU	CB-CG-CD2	-6.25	100.38	111.00
49	UI	263	LEU	CA-CB-CG	-6.25	100.93	115.30
45	C2	23	A	C5-C6-N1	6.24	120.82	117.70
44	C1	2223	C	C2-N1-C1'	6.23	125.65	118.80
44	C1	432	G	C4-C5-N7	6.21	113.29	110.80
44	C1	70	C	C2-N1-C1'	6.21	125.63	118.80
44	C1	275	C	C5-C6-N1	6.21	124.10	121.00
24	CI	240	THR	C-N-CA	-6.20	106.20	121.70
44	C1	260	U	O5'-P-OP2	-6.19	100.13	105.70
44	C1	1080	G	N3-C4-N9	6.18	129.71	126.00
44	C1	2183	A	C4-C5-N7	6.18	113.79	110.70
44	C1	205	C	P-O3'-C3'	6.18	127.12	119.70
44	C1	1758	C	C2-N3-C4	-6.18	116.81	119.90
44	C1	63	C	N1-C2-O2	6.17	122.60	118.90
44	C1	471	C	C6-N1-C1'	6.17	128.20	120.80
15	UU	502	LEU	CB-CG-CD2	-6.16	100.52	111.00
44	C1	1753	G	C4-C5-N7	6.16	113.27	110.80
44	C1	3	G	N9-C4-C5	6.15	107.86	105.40
44	C1	1155	G	C4-C5-N7	6.14	113.26	110.80
44	C1	1711	G	N3-C4-C5	-6.14	125.53	128.60
45	C2	200	U	N3-C2-O2	-6.14	117.90	122.20
44	C1	398	C	N3-C4-C5	6.14	124.35	121.90
12	UO	474	ASP	CB-CG-OD1	6.13	123.82	118.30
44	C1	208	A	C5-C6-N1	6.13	120.77	117.70
44	C1	583	A	O5'-P-OP1	-6.13	100.19	105.70
44	C1	236	C	C2-N1-C1'	6.12	125.53	118.80
44	C1	2195	U	C2-N1-C1'	6.12	125.04	117.70
44	C1	1471	U	C2-N1-C1'	6.11	125.04	117.70
46	UV	1054	LEU	CA-CB-CG	6.11	129.36	115.30
44	C1	148	C	C6-N1-C2	-6.11	117.86	120.30
44	C1	179	G	N3-C4-N9	-6.11	122.33	126.00
44	C1	437	G	C8-N9-C4	6.11	108.84	106.40
32	CR	426	LEU	CA-CB-CG	6.10	129.32	115.30
44	C1	2177	G	N9-C4-C5	6.09	107.84	105.40
44	C1	281	U	P-O3'-C3'	6.09	127.01	119.70
44	C1	1658	G	C5-C6-O6	6.09	132.25	128.60
44	C1	446	C	N3-C2-O2	-6.09	117.64	121.90
44	C1	410	G	N3-C4-C5	-6.08	125.56	128.60
45	C2	42	U	C2-N1-C1'	6.08	125.00	117.70
32	CS	426	LEU	CA-CB-CG	6.08	129.28	115.30
44	C1	1549	U	N3-C4-C5	6.08	118.25	114.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C1	1146	G	N3-C2-N2	6.08	124.15	119.90
44	C1	253	G	C5-C6-N1	6.07	114.54	111.50
44	C1	352	G	C6-C5-N7	-6.07	126.76	130.40
44	C1	133	G	C5-N7-C8	-6.06	101.27	104.30
45	C2	265	A	C8-N9-C4	6.06	108.22	105.80
45	C2	88	A	C5-C6-N6	-6.06	118.85	123.70
44	C1	21	C	N3-C2-O2	-6.06	117.66	121.90
45	C2	61	G	N1-C6-O6	6.05	123.53	119.90
44	C1	1626	G	C8-N9-C4	-6.05	103.98	106.40
44	C1	1550	U	N3-C2-O2	-6.05	117.97	122.20
45	C2	246	G	N3-C4-N9	6.05	129.63	126.00
45	C2	38	G	O4'-C1'-N9	-6.04	103.36	108.20
44	C1	2176	A	C5-C6-N6	-6.04	118.87	123.70
44	C1	33	C	N3-C2-O2	-6.04	117.67	121.90
44	C1	262	G	C8-N9-C1'	-6.04	119.15	127.00
44	C1	1149	C	C6-N1-C2	6.04	122.72	120.30
32	CR	188	ARG	CG-CD-NE	6.03	124.46	111.80
44	C1	139	C	C2-N1-C1'	6.02	125.42	118.80
44	C1	236	C	C6-N1-C2	-6.02	117.89	120.30
44	C1	244	G	N1-C6-O6	-6.02	116.29	119.90
44	C1	470	C	C2-N1-C1'	6.01	125.41	118.80
44	C1	1736	A	N7-C8-N9	6.01	116.81	113.80
32	CS	188	ARG	CG-CD-NE	6.01	124.42	111.80
44	C1	1711	G	N3-C4-N9	6.00	129.60	126.00
45	C2	246	G	C8-N9-C1'	-5.99	119.21	127.00
44	C1	1646	U	O4'-C1'-N1	5.99	112.99	108.20
44	C1	428	G	C8-N9-C4	-5.99	104.00	106.40
44	C1	251	G	C8-N9-C1'	-5.99	119.22	127.00
44	C1	1075	C	C2-N1-C1'	-5.99	112.22	118.80
44	C1	154	C	C2-N1-C1'	5.98	125.38	118.80
44	C1	268	G	C4-C5-N7	5.98	113.19	110.80
44	C1	413	C	C2-N1-C1'	5.98	125.38	118.80
44	C1	1137	G	C6-C5-N7	-5.97	126.82	130.40
45	C2	35	G	C8-N9-C4	5.97	108.79	106.40
44	C1	1625	G	N3-C4-N9	5.96	129.58	126.00
44	C1	1163	A	P-O3'-C3'	5.96	126.85	119.70
44	C1	1550	U	C6-N1-C1'	-5.96	112.85	121.20
44	C1	434	A	C5-C6-N1	5.96	120.68	117.70
44	C1	2096	G	C5-C6-O6	5.95	132.17	128.60
45	C2	136	C	C2-N1-C1'	5.95	125.34	118.80
44	C1	206	C	C2-N1-C1'	5.93	125.32	118.80
44	C1	1146	G	N1-C2-N2	-5.93	110.86	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C1	2107	A	N7-C8-N9	-5.93	110.83	113.80
12	UO	110	ASP	CB-CG-OD2	5.93	123.63	118.30
45	C2	22	C	N1-C2-O2	5.92	122.45	118.90
12	UO	457	LEU	CA-CB-CG	-5.91	101.70	115.30
4	UD	253	ASP	CB-CG-OD2	-5.91	112.98	118.30
44	C1	75	G	C6-C5-N7	-5.90	126.86	130.40
44	C1	491	G	C4-N9-C1'	5.90	134.17	126.50
45	C2	47	U	C2-N1-C1'	5.90	124.78	117.70
44	C1	145	C	N1-C2-O2	5.89	122.44	118.90
44	C1	255	G	C6-C5-N7	-5.89	126.86	130.40
44	C1	2090	G	N3-C4-C5	5.89	131.55	128.60
44	C1	253	G	C4-C5-N7	5.89	113.16	110.80
44	C1	424	U	C5-C6-N1	5.88	125.64	122.70
44	C1	1547	C	N3-C2-O2	-5.88	117.78	121.90
45	C2	260	G	N3-C4-N9	5.88	129.53	126.00
1	UA	656	LEU	CA-CB-CG	-5.87	101.80	115.30
45	C2	255	U	P-O3'-C3'	5.87	126.75	119.70
44	C1	209	A	P-O3'-C3'	5.87	126.74	119.70
49	UI	238	ARG	NE-CZ-NH1	-5.87	117.37	120.30
44	C1	1758	C	C5-C6-N1	-5.85	118.07	121.00
26	CK	89	LEU	CB-CG-CD2	-5.85	101.06	111.00
32	CS	151	LEU	CA-CB-CG	5.85	128.75	115.30
44	C1	277	U	P-O3'-C3'	5.85	126.72	119.70
44	C1	1167	C	C6-N1-C2	-5.85	117.96	120.30
44	C1	2177	G	P-O3'-C3'	5.85	126.72	119.70
44	C1	1560	C	N3-C2-O2	-5.84	117.81	121.90
45	C2	79	G	C4-N9-C1'	5.84	134.09	126.50
45	C2	35	G	C6-C5-N7	-5.84	126.90	130.40
45	C2	61	G	C4-C5-N7	5.84	113.14	110.80
26	CK	116	ARG	NE-CZ-NH2	-5.83	117.38	120.30
45	C2	65	C	C6-N1-C2	-5.83	117.97	120.30
44	C1	1736	A	C5-N7-C8	-5.83	100.98	103.90
44	C1	2156	A	N1-C6-N6	5.83	122.10	118.60
44	C1	2157	G	C4-N9-C1'	-5.83	118.92	126.50
45	C2	35	G	N1-C6-O6	5.83	123.40	119.90
32	CR	151	LEU	CA-CB-CG	5.83	128.71	115.30
44	C1	239	G	C6-C5-N7	-5.83	126.90	130.40
28	CM	397	LEU	CA-CB-CG	-5.81	101.93	115.30
45	C2	90	C	C2-N3-C4	-5.81	116.99	119.90
44	C1	209	A	C5-C6-N1	5.81	120.60	117.70
44	C1	347	C	N1-C2-O2	5.80	122.38	118.90
44	C1	252	U	C2-N1-C1'	5.80	124.66	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C1	1711	G	C4-N9-C1'	5.80	134.04	126.50
15	UU	502	LEU	CA-CB-CG	5.80	128.63	115.30
46	UV	364	LEU	CA-CB-CG	5.80	128.63	115.30
44	C1	260	U	C6-N1-C1'	5.79	129.31	121.20
44	C1	238	G	C5-N7-C8	-5.79	101.40	104.30
44	C1	1745	C	C6-N1-C2	-5.79	117.98	120.30
44	C1	1157	C	C6-N1-C2	5.79	122.61	120.30
44	C1	334	U	C2-N1-C1'	5.79	124.64	117.70
44	C1	203	C	C2-N1-C1'	5.79	125.17	118.80
44	C1	1137	G	C4-C5-N7	5.78	113.11	110.80
32	CS	14	LEU	CA-CB-CG	5.78	128.58	115.30
44	C1	1753	G	N9-C4-C5	-5.77	103.09	105.40
44	C1	2183	A	C5-C6-N6	-5.77	119.08	123.70
45	C2	57	A	N3-C4-N9	5.77	132.02	127.40
44	C1	2186	U	N3-C2-O2	5.77	126.24	122.20
32	CR	14	LEU	CA-CB-CG	5.77	128.57	115.30
44	C1	133	G	C4-C5-N7	5.77	113.11	110.80
44	C1	433	G	N1-C6-O6	-5.77	116.44	119.90
44	C1	255	G	N9-C4-C5	-5.77	103.09	105.40
45	C2	128	C	O4'-C1'-N1	5.76	112.81	108.20
44	C1	241	G	C4-C5-N7	5.76	113.11	110.80
44	C1	275	C	N1-C2-O2	5.76	122.36	118.90
44	C1	1222	C	N3-C2-O2	-5.76	117.87	121.90
44	C1	433	G	N9-C4-C5	5.75	107.70	105.40
44	C1	1666	C	C2-N1-C1'	5.75	125.12	118.80
44	C1	404	C	N1-C2-O2	5.74	122.35	118.90
44	C1	1145	G	C4-C5-N7	5.74	113.10	110.80
15	UU	715	PHE	CB-CA-C	-5.74	98.92	110.40
32	CS	430	LYS	CA-CB-CG	5.74	126.03	113.40
44	C1	370	C	N1-C2-O2	5.74	122.34	118.90
44	C1	1155	G	C2-N3-C4	-5.74	109.03	111.90
44	C1	131	G	C8-N9-C4	5.74	108.69	106.40
44	C1	143	A	N9-C4-C5	-5.74	103.51	105.80
44	C1	208	A	C4-C5-C6	-5.74	114.13	117.00
45	C2	90	C	C5-C6-N1	-5.73	118.13	121.00
44	C1	2227	C	C2-N1-C1'	5.73	125.10	118.80
32	CR	430	LYS	CA-CB-CG	5.73	126.00	113.40
44	C1	254	G	C4-N9-C1'	5.72	133.94	126.50
49	UE	238	ARG	NE-CZ-NH1	-5.72	117.44	120.30
44	C1	183	C	C2-N1-C1'	5.72	125.09	118.80
44	C1	454	C	C6-N1-C1'	-5.72	113.94	120.80
44	C1	1714	G	N3-C4-N9	5.71	129.43	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	UQ	466	LEU	CA-CB-CG	-5.71	102.16	115.30
45	C2	66	A	C5-N7-C8	-5.71	101.05	103.90
28	CM	75	ASP	CB-CG-OD1	5.70	123.43	118.30
1	UA	81	LEU	CA-CB-CG	5.70	128.42	115.30
13	UQ	423	LEU	CB-CG-CD2	-5.70	101.31	111.00
44	C1	1145	G	C6-C5-N7	-5.70	126.98	130.40
44	C1	1167	C	N3-C2-O2	-5.70	117.91	121.90
45	C2	6	C	C5-C6-N1	5.70	123.85	121.00
44	C1	1113	C	N1-C2-O2	5.70	122.32	118.90
46	UV	1031	LEU	CA-CB-CG	5.69	128.39	115.30
44	C1	582	G	C8-N9-C4	5.69	108.67	106.40
45	C2	252	C	N3-C2-O2	-5.68	117.92	121.90
44	C1	491	G	C8-N9-C1'	-5.67	119.62	127.00
32	CS	913	MET	CA-CB-CG	5.67	122.94	113.30
44	C1	2084	C	C6-N1-C2	-5.67	118.03	120.30
45	C2	57	A	C6-C5-N7	-5.67	128.33	132.30
44	C1	1137	G	N9-C4-C5	-5.67	103.13	105.40
32	CR	913	MET	CA-CB-CG	5.66	122.93	113.30
44	C1	1560	C	N1-C2-O2	5.66	122.29	118.90
44	C1	247	C	N3-C2-O2	-5.65	117.95	121.90
44	C1	2177	G	OP2-P-O3'	5.65	117.62	105.20
45	C2	74	C	N3-C2-O2	-5.65	117.95	121.90
45	C2	35	G	C2-N3-C4	-5.64	109.08	111.90
44	C1	255	G	C8-N9-C1'	-5.64	119.67	127.00
44	C1	2179	C	N3-C4-N4	-5.63	114.06	118.00
45	C2	246	G	N3-C4-C5	-5.63	125.78	128.60
44	C1	434	A	C4-C5-N7	-5.62	107.89	110.70
44	C1	206	C	N3-C2-O2	-5.62	117.96	121.90
44	C1	371	U	N1-C2-O2	5.62	126.73	122.80
40	Cm	86	LEU	CA-CB-CG	5.62	128.22	115.30
45	C2	63	G	C6-C5-N7	-5.62	127.03	130.40
48	UH	739	LEU	CA-CB-CG	5.62	128.22	115.30
44	C1	2169	A	N1-C6-N6	5.61	121.97	118.60
44	C1	195	U	C5-C4-O4	-5.61	122.53	125.90
9	UL	924	LEU	CB-CG-CD2	-5.61	101.47	111.00
44	C1	3	G	C5-C6-O6	5.61	131.96	128.60
45	C2	100	G	N9-C4-C5	-5.61	103.16	105.40
44	C1	143	A	C5-C6-N6	-5.60	119.22	123.70
44	C1	222	U	C5-C6-N1	-5.59	119.91	122.70
44	C1	2165	U	C5-C6-N1	5.58	125.49	122.70
44	C1	73	A	C5-N7-C8	-5.58	101.11	103.90
44	C1	183	C	N1-C2-O2	5.58	122.25	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	UG	234	LEU	CA-CB-CG	-5.58	102.48	115.30
45	C2	35	G	C5-C6-O6	-5.58	125.25	128.60
45	C2	49	U	C5-C4-O4	5.58	129.25	125.90
44	C1	262	G	C5-C6-O6	-5.57	125.26	128.60
44	C1	428	G	N3-C4-C5	-5.57	125.81	128.60
44	C1	281	U	C2-N1-C1'	5.57	124.39	117.70
44	C1	113	C	C2-N1-C1'	5.57	124.93	118.80
44	C1	1625	G	N3-C4-C5	-5.57	125.82	128.60
44	C1	2183	A	C5-N7-C8	-5.57	101.12	103.90
44	C1	1745	C	C2-N1-C1'	5.57	124.92	118.80
44	C1	2074	C	C5-C4-N4	-5.57	116.30	120.20
44	C1	2216	A	C5-C6-N1	5.56	120.48	117.70
45	C2	81	G	C6-C5-N7	-5.56	127.07	130.40
45	C2	36	U	C2-N1-C1'	-5.56	111.03	117.70
44	C1	252	U	N3-C2-O2	-5.55	118.31	122.20
44	C1	1165	U	C2-N1-C1'	5.55	124.37	117.70
45	C2	63	G	C4-C5-N7	5.55	113.02	110.80
44	C1	1157	C	N3-C4-C5	5.54	124.12	121.90
44	C1	1658	G	N3-C4-N9	-5.54	122.68	126.00
44	C1	1168	C	C6-N1-C2	5.54	122.52	120.30
44	C1	281	U	OP1-P-O3'	5.54	117.38	105.20
44	C1	1146	G	N9-C4-C5	-5.53	103.19	105.40
44	C1	2049	G	C6-C5-N7	-5.53	127.08	130.40
45	C2	264	G	N9-C4-C5	5.53	107.61	105.40
44	C1	1547	C	C6-N1-C1'	-5.53	114.17	120.80
45	C2	39	U	N1-C2-O2	5.53	126.67	122.80
1	UA	312	LEU	CA-CB-CG	-5.53	102.59	115.30
44	C1	434	A	C2-N3-C4	5.53	113.36	110.60
44	C1	2189	C	N1-C2-O2	5.53	122.22	118.90
44	C1	1547	C	C5-C6-N1	5.51	123.76	121.00
26	CK	136	LEU	CB-CG-CD1	-5.50	101.65	111.00
44	C1	18	G	N3-C4-C5	-5.50	125.85	128.60
44	C1	1142	U	O5'-P-OP1	-5.50	100.75	105.70
45	C2	23	A	C6-N1-C2	-5.50	115.30	118.60
15	UU	130	GLU	C-N-CA	-5.50	107.95	121.70
45	C2	57	A	N3-C4-C5	-5.50	122.95	126.80
44	C1	2106	U	N3-C2-O2	-5.50	118.35	122.20
44	C1	404	C	C6-N1-C1'	-5.49	114.21	120.80
1	UA	680	PHE	C-N-CA	-5.48	107.99	121.70
17	UZ	163	LEU	CA-CB-CG	-5.48	102.69	115.30
7	UJ	167	LEU	CA-CB-CG	-5.48	102.70	115.30
44	C1	209	A	C8-N9-C4	-5.48	103.61	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C1	406	G	N1-C6-O6	5.48	123.19	119.90
44	C1	1167	C	C5-C6-N1	5.48	123.74	121.00
44	C1	1753	G	C6-C5-N7	-5.48	127.11	130.40
44	C1	39	C	C2-N1-C1'	5.47	124.82	118.80
44	C1	428	G	C6-N1-C2	-5.47	121.82	125.10
44	C1	2156	A	C5-C6-N6	-5.46	119.33	123.70
44	C1	398	C	C2-N3-C4	-5.46	117.17	119.90
44	C1	1626	G	N7-C8-N9	5.46	115.83	113.10
44	C1	2053	C	N3-C4-C5	5.46	124.08	121.90
44	C1	112	C	C5-C6-N1	5.45	123.73	121.00
44	C1	260	U	C5-C6-N1	-5.45	119.97	122.70
45	C2	67	C	C6-N1-C2	-5.45	118.12	120.30
44	C1	334	U	N3-C2-O2	-5.45	118.38	122.20
44	C1	2217	C	N3-C2-O2	-5.45	118.08	121.90
44	C1	1458	U	N1-C2-O2	5.44	126.61	122.80
44	C1	18	G	C4-N9-C1'	5.44	133.57	126.50
44	C1	1711	G	C2-N3-C4	5.43	114.61	111.90
44	C1	1753	G	C2-N3-C4	-5.42	109.19	111.90
7	UJ	796	LEU	CA-CB-CG	5.41	127.74	115.30
44	C1	247	C	C6-N1-C2	-5.41	118.14	120.30
44	C1	418	G	C6-C5-N7	-5.41	127.16	130.40
46	UV	329	LEU	CA-CB-CG	5.41	127.74	115.30
44	C1	259	U	P-O3'-C3'	5.41	126.19	119.70
44	C1	406	G	C5-C6-O6	-5.40	125.36	128.60
45	C2	131	U	N1-C2-O2	5.40	126.58	122.80
32	CR	188	ARG	CD-NE-CZ	5.40	131.16	123.60
32	CS	188	ARG	CD-NE-CZ	5.40	131.16	123.60
44	C1	593	G	OP2-P-O3'	5.39	117.06	105.20
17	UZ	167	LEU	CA-CB-CG	-5.39	102.90	115.30
44	C1	2118	U	C6-N1-C2	5.39	124.23	121.00
44	C1	2156	A	P-O3'-C3'	5.39	126.17	119.70
45	C2	10	A	N9-C4-C5	-5.38	103.65	105.80
44	C1	112	C	C2-N1-C1'	5.38	124.72	118.80
44	C1	1485	A	P-O3'-C3'	5.38	126.16	119.70
44	C1	148	C	N1-C2-N3	5.38	122.97	119.20
46	UV	640	LEU	CA-CB-CG	5.37	127.66	115.30
44	C1	63	C	C2-N1-C1'	5.37	124.71	118.80
44	C1	2176	A	C8-N9-C4	-5.37	103.65	105.80
45	C2	36	U	O4'-C1'-N1	5.37	112.50	108.20
44	C1	133	G	C8-N9-C4	-5.37	104.25	106.40
44	C1	346	C	C5-C6-N1	5.37	123.68	121.00
45	C2	63	G	C8-N9-C4	-5.36	104.25	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C2	100	G	C4-C5-N7	5.36	112.94	110.80
45	C2	147	G	C4-N9-C1'	5.36	133.47	126.50
44	C1	121	G	C4-N9-C1'	5.36	133.46	126.50
45	C2	86	U	N3-C2-O2	-5.36	118.45	122.20
44	C1	215	A	C6-N1-C2	-5.35	115.39	118.60
44	C1	462	G	C5-C6-O6	5.35	131.81	128.60
45	C2	131	U	C2-N1-C1'	5.35	124.12	117.70
45	C2	61	G	C2-N3-C4	-5.35	109.23	111.90
44	C1	61	G	C4-N9-C1'	-5.34	119.55	126.50
14	UR	432	LEU	CA-CB-CG	5.34	127.59	115.30
44	C1	1658	G	N1-C6-O6	-5.34	116.70	119.90
44	C1	121	G	C6-C5-N7	-5.34	127.20	130.40
44	C1	448	C	N3-C2-O2	-5.33	118.17	121.90
44	C1	262	G	C4-N9-C1'	5.33	133.43	126.50
44	C1	268	G	N9-C4-C5	-5.33	103.27	105.40
10	UM	696	LEU	CA-CB-CG	5.33	127.55	115.30
44	C1	133	G	N7-C8-N9	5.33	115.76	113.10
44	C1	203	C	N1-C2-O2	5.33	122.10	118.90
44	C1	2206	C	N3-C4-C5	5.33	124.03	121.90
44	C1	158	C	C2-N1-C1'	5.32	124.66	118.80
45	C2	91	G	C4-C5-N7	5.32	112.93	110.80
44	C1	1754	G	N3-C4-C5	-5.32	125.94	128.60
44	C1	2078	C	C6-N1-C1'	5.32	127.18	120.80
44	C1	154	C	N1-C2-O2	5.32	122.09	118.90
44	C1	369	U	C2-N1-C1'	5.32	124.08	117.70
45	C2	63	G	C4-N9-C1'	5.31	133.41	126.50
44	C1	156	C	C5-C6-N1	5.31	123.66	121.00
44	C1	1666	C	C5-C6-N1	5.31	123.66	121.00
44	C1	2200	U	C5-C6-N1	-5.31	120.05	122.70
44	C1	2119	G	C4-N9-C1'	5.31	133.40	126.50
45	C2	44	U	C2-N1-C1'	5.31	124.07	117.70
44	C1	1661	C	C2-N3-C4	-5.30	117.25	119.90
44	C1	2078	C	C2-N1-C1'	-5.30	112.97	118.80
45	C2	22	C	N3-C2-O2	-5.30	118.19	121.90
45	C2	23	A	C5-C6-N6	-5.29	119.47	123.70
44	C1	135	A	OP2-P-O3'	5.29	116.84	105.20
44	C1	137	C	C6-N1-C2	-5.29	118.18	120.30
44	C1	2201	C	C6-N1-C2	5.29	122.42	120.30
44	C1	1156	C	C6-N1-C2	5.28	122.41	120.30
44	C1	2217	C	C6-N1-C1'	-5.28	114.46	120.80
46	UV	609	LEU	CA-CB-CG	5.28	127.45	115.30
44	C1	2156	A	C4-C5-N7	5.28	113.34	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C2	264	G	N7-C8-N9	5.28	115.74	113.10
44	C1	255	G	C4-C5-N7	5.27	112.91	110.80
44	C1	18	G	N3-C4-N9	5.27	129.16	126.00
44	C1	1448	A	C5-C6-N1	5.27	120.34	117.70
44	C1	1658	G	N9-C4-C5	5.27	107.51	105.40
44	C1	129	G	N1-C2-N3	5.27	127.06	123.90
44	C1	208	A	N1-C6-N6	-5.27	115.44	118.60
44	C1	2090	G	N9-C4-C5	5.26	107.50	105.40
44	C1	344	C	N3-C4-C5	5.26	124.00	121.90
44	C1	2074	C	C5-C6-N1	5.26	123.63	121.00
45	C2	147	G	C8-N9-C1'	-5.26	120.16	127.00
45	C2	44	U	C6-N1-C2	-5.25	117.85	121.00
44	C1	1655	U	N1-C2-N3	5.25	118.05	114.90
45	C2	58	A	O5'-P-OP1	-5.25	100.97	105.70
44	C1	1161	G	C6-C5-N7	-5.24	127.25	130.40
45	C2	46	U	C6-N1-C2	-5.24	117.86	121.00
44	C1	135	A	N1-C6-N6	-5.24	115.46	118.60
44	C1	2169	A	C8-N9-C4	-5.24	103.71	105.80
52	CX	296	LEU	CA-CB-CG	5.23	127.33	115.30
45	C2	79	G	C8-N9-C1'	-5.23	120.20	127.00
44	C1	1633	A	N1-C6-N6	-5.23	115.46	118.60
44	C1	406	G	C5-N7-C8	-5.22	101.69	104.30
45	C2	66	A	C6-N1-C2	-5.22	115.47	118.60
44	C1	470	C	N3-C2-O2	-5.22	118.25	121.90
44	C1	343	C	N3-C2-O2	-5.21	118.25	121.90
44	C1	439	A	C4-C5-N7	5.21	113.31	110.70
44	C1	208	A	C6-C5-N7	5.21	135.95	132.30
45	C2	200	U	C5-C6-N1	5.21	125.31	122.70
1	UA	509	LEU	CB-CG-CD1	-5.21	102.15	111.00
44	C1	491	G	N3-C4-N9	5.21	129.12	126.00
44	C1	496	U	N1-C2-O2	5.21	126.44	122.80
44	C1	596	U	C2-N3-C4	-5.21	123.88	127.00
44	C1	28	C	N1-C2-O2	5.20	122.02	118.90
44	C1	133	G	N1-C6-O6	5.20	123.02	119.90
44	C1	2179	C	N3-C2-O2	-5.20	118.26	121.90
44	C1	1754	G	N1-C6-O6	-5.19	116.78	119.90
44	C1	290	C	C6-N1-C2	5.19	122.38	120.30
44	C1	69	U	O5'-P-OP1	-5.18	101.03	105.70
2	UB	818	ASP	CB-CG-OD2	5.18	122.96	118.30
44	C1	1114	C	N1-C2-O2	5.18	122.01	118.90
44	C1	190	G	N3-C4-N9	-5.17	122.90	126.00
44	C1	2084	C	N1-C2-N3	5.17	122.82	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C1	486	G	N3-C4-C5	5.16	131.18	128.60
44	C1	135	A	O4'-C1'-N9	-5.16	104.07	108.20
44	C1	447	C	C6-N1-C2	-5.16	118.24	120.30
44	C1	347	C	N3-C2-O2	-5.16	118.29	121.90
44	C1	1080	G	N3-C4-C5	-5.16	126.02	128.60
44	C1	247	C	C2-N1-C1'	5.15	124.46	118.80
44	C1	1075	C	N3-C2-O2	-5.15	118.30	121.90
45	C2	23	A	N3-C4-N9	5.15	131.52	127.40
44	C1	2047	G	P-O3'-C3'	5.15	125.88	119.70
44	C1	2091	C	C6-N1-C1'	-5.15	114.62	120.80
45	C2	139	C	N1-C2-O2	5.15	121.99	118.90
20	CD	107	ILE	C-N-CA	-5.14	108.84	121.70
44	C1	462	G	N1-C6-O6	-5.14	116.82	119.90
13	UQ	456	TRP	CA-CB-CG	-5.13	103.95	113.70
45	C2	70	A	N1-C6-N6	-5.13	115.52	118.60
45	C2	28	U	C5-C6-N1	-5.13	120.13	122.70
45	C2	161	G	C4-N9-C1'	5.13	133.17	126.50
45	C2	260	G	C6-C5-N7	-5.13	127.32	130.40
44	C1	239	G	C4-C5-N7	5.13	112.85	110.80
44	C1	111	U	N3-C2-O2	-5.13	118.61	122.20
44	C1	353	G	C4-C5-N7	5.13	112.85	110.80
44	C1	2169	A	C4-C5-N7	5.13	113.26	110.70
44	C1	2171	G	C4-C5-N7	5.13	112.85	110.80
44	C1	417	G	C4-C5-N7	5.12	112.85	110.80
44	C1	2176	A	N1-C6-N6	5.12	121.67	118.60
44	C1	244	G	C6-N1-C2	-5.12	122.03	125.10
20	CD	371	LEU	CB-CG-CD1	-5.11	102.31	111.00
44	C1	150	C	P-O3'-C3'	5.11	125.84	119.70
45	C2	36	U	C5-C6-N1	-5.11	120.14	122.70
44	C1	81	G	C5-C6-N1	5.11	114.06	111.50
44	C1	1547	C	C6-N1-C2	-5.11	118.26	120.30
44	C1	1149	C	C5-C6-N1	-5.11	118.45	121.00
45	C2	148	G	C5-C6-O6	5.11	131.66	128.60
45	C2	268	G	N9-C4-C5	-5.11	103.36	105.40
24	CI	263	LEU	CA-CB-CG	5.10	127.04	115.30
44	C1	2049	G	C5-N7-C8	-5.10	101.75	104.30
10	UM	861	ASP	CB-CG-OD2	5.10	122.89	118.30
32	CR	848	LEU	CA-CB-CG	5.10	127.03	115.30
44	C1	193	U	N1-C2-O2	5.10	126.37	122.80
44	C1	2157	G	C8-N9-C1'	5.10	133.63	127.00
44	C1	281	U	N1-C2-O2	5.09	126.37	122.80
35	Ce	40	LEU	CA-CB-CG	5.09	127.02	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C1	365	G	C4-C5-N7	5.09	112.84	110.80
44	C1	2217	C	C6-N1-C2	-5.09	118.26	120.30
44	C1	39	C	N1-C2-O2	5.09	121.95	118.90
44	C1	265	G	N3-C2-N2	5.08	123.46	119.90
44	C1	454	C	N1-C2-O2	5.08	121.95	118.90
44	C1	2078	C	N3-C4-N4	-5.08	114.44	118.00
45	C2	246	G	OP1-P-O3'	5.08	116.37	105.20
32	CS	848	LEU	CA-CB-CG	5.08	126.97	115.30
44	C1	370	C	N3-C2-O2	-5.08	118.35	121.90
44	C1	61	G	O4'-C1'-N9	5.07	112.26	108.20
44	C1	1626	G	C6-N1-C2	-5.07	122.06	125.10
44	C1	495	G	N3-C4-N9	5.07	129.04	126.00
44	C1	212	C	C6-N1-C2	5.07	122.33	120.30
44	C1	2116	C	N3-C4-C5	5.07	123.93	121.90
45	C2	35	G	N3-C4-C5	5.07	131.13	128.60
45	C2	57	A	C4-N9-C1'	5.07	135.42	126.30
44	C1	1155	G	N9-C4-C5	-5.06	103.38	105.40
45	C2	247	G	N3-C4-C5	5.06	131.13	128.60
45	C2	139	C	N3-C2-O2	-5.06	118.36	121.90
44	C1	1458	U	C2-N1-C1'	5.05	123.76	117.70
17	UZ	18	VAL	C-N-CA	-5.05	109.08	121.70
44	C1	602	U	C2-N1-C1'	5.05	123.76	117.70
44	C1	255	G	C4-N9-C1'	5.05	133.06	126.50
6	UG	451	LEU	CA-CB-CG	5.04	126.90	115.30
44	C1	281	U	N3-C2-O2	-5.04	118.67	122.20
44	C1	1699	U	N1-C2-O2	5.04	126.33	122.80
49	UE	265	MET	CB-CG-SD	5.04	127.51	112.40
19	CC	30	GLU	C-N-CA	-5.03	109.11	121.70
44	C1	2084	C	C6-N1-C1'	5.03	126.84	120.80
44	C1	2169	A	O5'-P-OP1	-5.03	101.17	105.70
44	C1	1650	C	N1-C2-O2	5.03	121.92	118.90
44	C1	356	C	C2-N3-C4	-5.03	117.39	119.90
49	UI	265	MET	CB-CG-SD	5.03	127.48	112.40
44	C1	2217	C	O4'-C1'-N1	5.02	112.22	108.20
44	C1	505	C	C6-N1-C2	-5.02	118.29	120.30
44	C1	128	G	C4-C5-N7	5.02	112.81	110.80
44	C1	202	A	C8-N9-C4	5.02	107.81	105.80
44	C1	2181	U	N1-C2-O2	5.02	126.31	122.80
44	C1	2210	U	N3-C2-O2	-5.02	118.69	122.20
44	C1	133	G	C6-C5-N7	-5.02	127.39	130.40
44	C1	2068	C	O5'-P-OP1	-5.02	101.19	105.70
10	UM	524	ILE	C-N-CD	5.01	138.93	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C1	56	C	O5'-P-OP1	5.01	116.71	110.70
44	C1	1758	C	C6-N1-C2	5.01	122.30	120.30
44	C1	402	U	N3-C2-O2	-5.01	118.69	122.20
45	C2	128	C	C5-C6-N1	5.01	123.50	121.00
44	C1	1510	G	N7-C8-N9	5.01	115.60	113.10
44	C1	257	G	C6-N1-C2	-5.00	122.10	125.10
45	C2	100	G	N3-C4-N9	5.00	129.00	126.00

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	CA	306	TYR	Peptide
18	CB	293	GLU	Peptide
21	CF	60	GLN	Peptide
23	CH	143	HIS	Peptide
24	CI	132	VAL	Peptide
24	CI	851	TRP	Peptide
26	CK	261	PHE	Peptide
29	CO	84	ILE	Peptide
29	CO	88	ARG	Peptide
31	CQ	173	ASP	Peptide
32	CR	48	MET	Peptide
32	CR	866	PHE	Peptide
32	CS	48	MET	Peptide
32	CS	866	PHE	Peptide
47	CV	88	LYS	Peptide
47	CV	91	HIS	Peptide
34	Cc	13	TYR	Peptide
34	Cc	86	MET	Peptide
35	Ce	38	ALA	Peptide
38	Ci	137	ASP	Peptide
39	Cj	126	PRO	Peptide
39	Cj	40	ALA	Peptide
51	Cl	79	TYR	Peptide
54	Cz	1628	THR	Peptide
1	UA	214	SER	Peptide
1	UA	386	THR	Peptide
1	UA	667	ARG	Peptide
1	UA	8	SER	Peptide
4	UD	309	GLN	Peptide
4	UD	387	TRP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
5	UF	120	VAL	Peptide
6	UG	126	ALA	Peptide
6	UG	258	HIS	Peptide
48	UH	753	THR	Peptide
48	UH	857	LYS	Peptide
9	UL	17	VAL	Peptide
10	UM	204	ASP	Peptide
10	UM	328	LEU	Peptide
10	UM	693	GLU	Peptide
12	UO	167	LYS	Peptide
12	UO	282	ALA	Peptide
13	UQ	170	TRP	Peptide
13	UQ	237	TYR	Peptide
13	UQ	364	SER	Peptide
13	UQ	563	THR	Peptide
13	UQ	707	PRO	Peptide
13	UQ	849	ALA	Peptide
50	US	510	LYS	Peptide
15	UU	100	TRP	Peptide
15	UU	252	PRO	Peptide
15	UU	313	LEU	Peptide
15	UU	369	SER	Peptide
15	UU	378	LEU	Peptide
15	UU	396	SER	Peptide
15	UU	397	ASP	Peptide
15	UU	857	ILE	Peptide
46	UV	1058	TYR	Peptide
46	UV	1104	LEU	Peptide
46	UV	57	PHE	Peptide
46	UV	611	LEU	Peptide
46	UV	951	ARG	Peptide
17	UZ	103	ASP	Peptide
17	UZ	173	LYS	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%)	730 (87%)	103 (12%)	2 (0%)	47 81
2	UB	502/907 (55%)	466 (93%)	36 (7%)	0	100 100
3	UC	72/648 (11%)	67 (93%)	5 (7%)	0	100 100
4	UD	754/884 (85%)	689 (91%)	65 (9%)	0	100 100
5	UF	325/414 (78%)	304 (94%)	21 (6%)	0	100 100
6	UG	446/558 (80%)	384 (86%)	60 (14%)	2 (0%)	34 72
7	UJ	796/1802 (44%)	750 (94%)	45 (6%)	1 (0%)	51 85
8	UK	211/270 (78%)	201 (95%)	10 (5%)	0	100 100
9	UL	767/962 (80%)	685 (89%)	82 (11%)	0	100 100
10	UM	645/912 (71%)	605 (94%)	39 (6%)	1 (0%)	47 81
11	UN	150/938 (16%)	143 (95%)	6 (4%)	1 (1%)	22 62
12	UO	498/557 (89%)	450 (90%)	48 (10%)	0	100 100
13	UQ	775/960 (81%)	691 (89%)	81 (10%)	3 (0%)	34 72
14	UR	437/618 (71%)	399 (91%)	38 (9%)	0	100 100
15	UU	890/1049 (85%)	786 (88%)	103 (12%)	1 (0%)	51 85
16	UX	188/193 (97%)	174 (93%)	14 (7%)	0	100 100
17	UZ	229/391 (59%)	211 (92%)	18 (8%)	0	100 100
18	CA	238/313 (76%)	213 (90%)	25 (10%)	0	100 100
18	CB	235/313 (75%)	211 (90%)	24 (10%)	0	100 100
19	CC	383/523 (73%)	353 (92%)	30 (8%)	0	100 100
20	CD	416/582 (72%)	382 (92%)	34 (8%)	0	100 100
21	CE	119/127 (94%)	107 (90%)	12 (10%)	0	100 100
21	CF	118/127 (93%)	110 (93%)	8 (7%)	0	100 100
22	CG	368/630 (58%)	342 (93%)	26 (7%)	0	100 100
23	CH	383/411 (93%)	348 (91%)	35 (9%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
24	CI	812/1163 (70%)	737 (91%)	73 (9%)	2 (0%)	47 81
25	CJ	177/183 (97%)	151 (85%)	26 (15%)	0	100 100
26	CK	295/297 (99%)	271 (92%)	24 (8%)	0	100 100
27	CL	225/785 (29%)	200 (89%)	24 (11%)	1 (0%)	34 72
28	CM	443/446 (99%)	398 (90%)	44 (10%)	1 (0%)	47 81
29	CN	222/252 (88%)	207 (93%)	15 (7%)	0	100 100
29	CO	211/252 (84%)	193 (92%)	16 (8%)	2 (1%)	17 56
30	CP	185/322 (58%)	179 (97%)	6 (3%)	0	100 100
31	CQ	171/259 (66%)	165 (96%)	6 (4%)	0	100 100
32	CR	746/1073 (70%)	699 (94%)	47 (6%)	0	100 100
32	CS	746/1073 (70%)	699 (94%)	47 (6%)	0	100 100
33	CT	127/203 (63%)	111 (87%)	16 (13%)	0	100 100
34	Cc	188/212 (89%)	170 (90%)	18 (10%)	0	100 100
35	Ce	155/203 (76%)	140 (90%)	15 (10%)	0	100 100
36	Cg	157/190 (83%)	153 (98%)	4 (2%)	0	100 100
37	Ch	47/151 (31%)	46 (98%)	1 (2%)	0	100 100
38	Ci	113/150 (75%)	103 (91%)	10 (9%)	0	100 100
39	Cj	124/143 (87%)	104 (84%)	20 (16%)	0	100 100
40	Cm	122/130 (94%)	116 (95%)	6 (5%)	0	100 100
41	Cn	92/145 (63%)	86 (94%)	6 (6%)	0	100 100
42	Cp	59/68 (87%)	53 (90%)	6 (10%)	0	100 100
43	CU	123/311 (40%)	108 (88%)	15 (12%)	0	100 100
46	UV	1057/1171 (90%)	946 (90%)	108 (10%)	3 (0%)	41 76
47	CV	144/322 (45%)	130 (90%)	13 (9%)	1 (1%)	22 62
48	UH	349/930 (38%)	327 (94%)	22 (6%)	0	100 100
49	UE	121/410 (30%)	109 (90%)	12 (10%)	0	100 100
49	UI	121/410 (30%)	109 (90%)	12 (10%)	0	100 100
50	US	443/549 (81%)	414 (94%)	28 (6%)	1 (0%)	47 81
51	Cl	78/156 (50%)	72 (92%)	6 (8%)	0	100 100
52	CX	265/480 (55%)	252 (95%)	13 (5%)	0	100 100
53	UP	52/364 (14%)	42 (81%)	9 (17%)	1 (2%)	8 40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
54	Cz	273/1796 (15%)	257 (94%)	15 (6%)	1 (0%)	34 72
All	All	19223/30592 (63%)	17548 (91%)	1651 (9%)	24 (0%)	54 85

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	UG	176	LEU
29	CO	85	SER
46	UV	1059	ASP
13	UQ	708	SER
11	UN	902	ARG
47	CV	92	SER
50	US	241	GLU
54	Cz	1673	ARG
1	UA	372	GLY
6	UG	56	PRO
27	CL	640	PRO
29	CO	84	ILE
13	UQ	365	GLY
13	UQ	564	GLU
24	CI	308	THR
24	CI	396	PHE
28	CM	336	MET
46	UV	567	ARG
46	UV	735	GLY
1	UA	423	PRO
7	UJ	336	PRO
10	UM	329	PRO
15	UU	190	ILE
53	UP	329	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	651/775 (84%)	635 (98%)	16 (2%)	47	68
2	UB	425/788 (54%)	420 (99%)	5 (1%)	71	84
3	UC	61/536 (11%)	59 (97%)	2 (3%)	38	61
4	UD	653/738 (88%)	650 (100%)	3 (0%)	88	93
5	UF	248/341 (73%)	248 (100%)	0	100	100
6	UG	344/474 (73%)	333 (97%)	11 (3%)	39	62
7	UJ	658/1526 (43%)	647 (98%)	11 (2%)	60	78
8	UK	159/227 (70%)	155 (98%)	4 (2%)	47	68
9	UL	667/821 (81%)	665 (100%)	2 (0%)	92	95
10	UM	569/770 (74%)	565 (99%)	4 (1%)	84	90
11	UN	123/765 (16%)	123 (100%)	0	100	100
12	UO	404/456 (89%)	400 (99%)	4 (1%)	76	86
13	UQ	650/817 (80%)	640 (98%)	10 (2%)	65	80
14	UR	360/524 (69%)	353 (98%)	7 (2%)	57	75
15	UU	672/863 (78%)	657 (98%)	15 (2%)	52	71
16	UX	150/167 (90%)	148 (99%)	2 (1%)	69	82
17	UZ	186/329 (56%)	185 (100%)	1 (0%)	88	93
18	CA	175/228 (77%)	170 (97%)	5 (3%)	42	64
18	CB	195/228 (86%)	194 (100%)	1 (0%)	88	93
19	CC	287/435 (66%)	286 (100%)	1 (0%)	92	95
20	CD	319/489 (65%)	314 (98%)	5 (2%)	62	79
21	CE	91/108 (84%)	89 (98%)	2 (2%)	52	71
21	CF	88/108 (82%)	88 (100%)	0	100	100
22	CG	299/525 (57%)	299 (100%)	0	100	100
23	CH	303/320 (95%)	298 (98%)	5 (2%)	60	78
24	CI	661/1009 (66%)	644 (97%)	17 (3%)	46	67
25	CJ	147/169 (87%)	142 (97%)	5 (3%)	37	61
26	CK	245/266 (92%)	236 (96%)	9 (4%)	34	59
27	CL	181/642 (28%)	179 (99%)	2 (1%)	73	85
28	CM	364/383 (95%)	356 (98%)	8 (2%)	52	71
29	CN	202/223 (91%)	201 (100%)	1 (0%)	88	93
29	CO	193/223 (86%)	191 (99%)	2 (1%)	76	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	CP	164/287 (57%)	162 (99%)	2 (1%)	71 84
31	CQ	145/215 (67%)	143 (99%)	2 (1%)	67 81
32	CR	654/916 (71%)	474 (72%)	180 (28%)	0 3
32	CS	654/916 (71%)	474 (72%)	180 (28%)	0 3
33	CT	108/167 (65%)	106 (98%)	2 (2%)	57 75
34	Cc	149/178 (84%)	147 (99%)	2 (1%)	69 82
35	Ce	137/177 (77%)	134 (98%)	3 (2%)	52 71
36	Cg	122/162 (75%)	120 (98%)	2 (2%)	62 79
37	Ch	43/130 (33%)	43 (100%)	0	100 100
38	Ci	74/117 (63%)	74 (100%)	0	100 100
39	Cj	92/115 (80%)	90 (98%)	2 (2%)	52 71
40	Cm	103/113 (91%)	102 (99%)	1 (1%)	76 86
41	Cn	70/116 (60%)	70 (100%)	0	100 100
42	Cp	46/61 (75%)	46 (100%)	0	100 100
43	CU	103/260 (40%)	97 (94%)	6 (6%)	20 47
46	UV	908/989 (92%)	891 (98%)	17 (2%)	57 75
47	CV	129/276 (47%)	127 (98%)	2 (2%)	62 79
48	UH	301/788 (38%)	298 (99%)	3 (1%)	76 86
49	UE	105/346 (30%)	74 (70%)	31 (30%)	0 2
49	UI	105/346 (30%)	74 (70%)	31 (30%)	0 2
50	US	404/493 (82%)	401 (99%)	3 (1%)	84 90
51	Cl	71/135 (53%)	69 (97%)	2 (3%)	43 65
52	CX	227/411 (55%)	226 (100%)	1 (0%)	91 94
53	UP	44/314 (14%)	44 (100%)	0	100 100
54	Cz	235/1533 (15%)	234 (100%)	1 (0%)	91 94
All	All	15923/25834 (62%)	15290 (96%)	633 (4%)	35 56

All (633) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	UA	8	SER
1	UA	68	ASN
1	UA	87	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	UA	180	LEU
1	UA	219	VAL
1	UA	296	SER
1	UA	347	VAL
1	UA	356	VAL
1	UA	415	ARG
1	UA	479	ASP
1	UA	499	SER
1	UA	501	THR
1	UA	577	THR
1	UA	580	TYR
1	UA	602	THR
1	UA	611	THR
2	UB	90	LEU
2	UB	111	ASN
2	UB	549	LEU
2	UB	786	ARG
2	UB	829	ARG
3	UC	607	LYS
3	UC	643	VAL
4	UD	152	ARG
4	UD	224	THR
4	UD	267	THR
6	UG	41	ARG
6	UG	172	CYS
6	UG	179	THR
6	UG	181	ARG
6	UG	233	THR
6	UG	260	THR
6	UG	265	THR
6	UG	290	THR
6	UG	303	VAL
6	UG	356	THR
6	UG	365	THR
7	UJ	44	THR
7	UJ	45	PHE
7	UJ	84	THR
7	UJ	306	ARG
7	UJ	405	LYS
7	UJ	640	LYS
7	UJ	643	THR
7	UJ	653	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	UJ	720	LEU
7	UJ	728	ARG
7	UJ	798	LYS
8	UK	93	ASN
8	UK	228	LYS
8	UK	265	VAL
8	UK	269	LYS
9	UL	440	MET
9	UL	676	ARG
10	UM	210	PHE
10	UM	593	ARG
10	UM	755	ARG
10	UM	889	ARG
12	UO	149	VAL
12	UO	190	VAL
12	UO	270	THR
12	UO	277	THR
13	UQ	149	SER
13	UQ	244	LEU
13	UQ	358	VAL
13	UQ	449	ASP
13	UQ	452	VAL
13	UQ	497	THR
13	UQ	537	THR
13	UQ	622	THR
13	UQ	687	TYR
13	UQ	920	VAL
14	UR	63	LYS
14	UR	152	THR
14	UR	279	SER
14	UR	314	LEU
14	UR	393	LYS
14	UR	397	MET
14	UR	471	ARG
15	UU	40	THR
15	UU	58	LYS
15	UU	81	ASN
15	UU	192	MET
15	UU	222	LEU
15	UU	354	THR
15	UU	377	ILE
15	UU	554	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	UU	618	THR
15	UU	714	CYS
15	UU	738	THR
15	UU	756	PHE
15	UU	842	THR
15	UU	858	ASP
15	UU	889	SER
16	UX	44	MET
16	UX	92	THR
17	UZ	213	ASN
18	CA	83	VAL
18	CA	177	THR
18	CA	253	LEU
18	CA	291	THR
18	CA	292	LEU
18	CB	85	ARG
19	CC	38	MET
20	CD	94	LYS
20	CD	338	THR
20	CD	371	LEU
20	CD	372	SER
20	CD	442	ILE
21	CE	53	VAL
21	CE	94	VAL
23	CH	73	THR
23	CH	83	THR
23	CH	196	PHE
23	CH	208	LEU
23	CH	210	ARG
24	CI	91	ARG
24	CI	197	LEU
24	CI	214	TYR
24	CI	256	THR
24	CI	357	LYS
24	CI	367	VAL
24	CI	393	VAL
24	CI	754	LYS
24	CI	788	PHE
24	CI	840	ARG
24	CI	841	ARG
24	CI	854	ARG
24	CI	863	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	CI	872	THR
24	CI	986	ILE
24	CI	1034	THR
24	CI	1058	LEU
25	CJ	5	LEU
25	CJ	50	LEU
25	CJ	123	THR
25	CJ	140	VAL
25	CJ	159	THR
26	CK	18	LEU
26	CK	81	SER
26	CK	87	ARG
26	CK	90	VAL
26	CK	92	THR
26	CK	123	ILE
26	CK	229	THR
26	CK	235	ASP
26	CK	269	THR
27	CL	534	THR
27	CL	619	ILE
28	CM	7	THR
28	CM	58	LEU
28	CM	76	LYS
28	CM	244	ARG
28	CM	305	ARG
28	CM	360	ARG
28	CM	367	ARG
28	CM	432	LYS
29	CN	218	ASP
29	CO	135	LYS
29	CO	169	ASP
30	CP	64	LYS
30	CP	78	MET
31	CQ	198	LYS
31	CQ	215	LYS
32	CR	2	THR
32	CR	4	GLN
32	CR	5	LYS
32	CR	7	VAL
32	CR	9	SER
32	CR	10	ARG
32	CR	23	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	25	SER
32	CR	30	VAL
32	CR	36	GLU
32	CR	38	ILE
32	CR	41	LEU
32	CR	46	SER
32	CR	49	ASP
32	CR	51	ARG
32	CR	52	GLN
32	CR	54	LYS
32	CR	55	SER
32	CR	56	VAL
32	CR	62	LYS
32	CR	65	LEU
32	CR	69	SER
32	CR	73	LYS
32	CR	80	LYS
32	CR	84	ARG
32	CR	86	ILE
32	CR	88	GLU
32	CR	96	GLU
32	CR	97	LEU
32	CR	99	ILE
32	CR	101	LEU
32	CR	102	ASN
32	CR	105	ARG
32	CR	107	CYS
32	CR	110	LYS
32	CR	112	THR
32	CR	113	ASP
32	CR	115	ILE
32	CR	119	THR
32	CR	123	CYS
32	CR	125	LEU
32	CR	127	ASP
32	CR	131	ILE
32	CR	136	LEU
32	CR	142	THR
32	CR	149	VAL
32	CR	151	LEU
32	CR	153	LEU
32	CR	159	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	160	LYS
32	CR	162	LEU
32	CR	165	MET
32	CR	181	VAL
32	CR	188	ARG
32	CR	192	SER
32	CR	195	SER
32	CR	198	SER
32	CR	201	VAL
32	CR	202	ILE
32	CR	206	LEU
32	CR	211	ILE
32	CR	212	SER
32	CR	217	VAL
32	CR	218	LYS
32	CR	251	SER
32	CR	252	LEU
32	CR	253	ILE
32	CR	266	LEU
32	CR	277	LEU
32	CR	278	ARG
32	CR	284	THR
32	CR	287	ARG
32	CR	291	LYS
32	CR	297	VAL
32	CR	308	SER
32	CR	316	SER
32	CR	318	GLU
32	CR	319	ASN
32	CR	322	THR
32	CR	323	LEU
32	CR	378	HIS
32	CR	382	GLN
32	CR	387	VAL
32	CR	390	GLU
32	CR	394	ILE
32	CR	401	LYS
32	CR	410	MET
32	CR	412	SER
32	CR	414	ILE
32	CR	415	SER
32	CR	418	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	420	THR
32	CR	425	SER
32	CR	427	LYS
32	CR	430	LYS
32	CR	432	LEU
32	CR	433	ARG
32	CR	470	LYS
32	CR	476	GLU
32	CR	479	ARG
32	CR	484	ASP
32	CR	487	GLU
32	CR	488	LYS
32	CR	492	THR
32	CR	502	ARG
32	CR	512	ASP
32	CR	514	SER
32	CR	517	GLU
32	CR	532	VAL
32	CR	533	SER
32	CR	534	GLU
32	CR	535	LYS
32	CR	539	GLN
32	CR	541	VAL
32	CR	545	VAL
32	CR	548	HIS
32	CR	554	ASN
32	CR	556	LEU
32	CR	558	LEU
32	CR	559	MET
32	CR	566	GLU
32	CR	569	VAL
32	CR	576	GLU
32	CR	584	CYS
32	CR	594	ILE
32	CR	596	LYS
32	CR	625	ASP
32	CR	626	GLU
32	CR	627	PHE
32	CR	631	SER
32	CR	651	SER
32	CR	654	LEU
32	CR	655	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	658	VAL
32	CR	704	GLU
32	CR	711	LYS
32	CR	712	LEU
32	CR	713	SER
32	CR	716	ARG
32	CR	718	GLU
32	CR	719	LYS
32	CR	723	VAL
32	CR	725	VAL
32	CR	732	GLN
32	CR	745	VAL
32	CR	747	LEU
32	CR	750	THR
32	CR	753	ASP
32	CR	759	THR
32	CR	760	CYS
32	CR	768	ASP
32	CR	773	SER
32	CR	784	LYS
32	CR	788	SER
32	CR	789	LEU
32	CR	791	SER
32	CR	793	LYS
32	CR	800	ILE
32	CR	801	LEU
32	CR	806	GLU
32	CR	808	SER
32	CR	824	LEU
32	CR	830	ASP
32	CR	832	LEU
32	CR	834	THR
32	CR	848	LEU
32	CR	858	MET
32	CR	860	THR
32	CR	861	ILE
32	CR	867	THR
32	CR	870	LEU
32	CR	876	LEU
32	CR	887	LEU
32	CR	893	ASP
32	CR	902	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	907	GLN
32	CR	908	VAL
32	CR	909	LEU
32	CR	913	MET
32	CR	914	LYS
32	CS	2	THR
32	CS	4	GLN
32	CS	5	LYS
32	CS	7	VAL
32	CS	9	SER
32	CS	10	ARG
32	CS	23	LYS
32	CS	25	SER
32	CS	30	VAL
32	CS	36	GLU
32	CS	38	ILE
32	CS	41	LEU
32	CS	46	SER
32	CS	49	ASP
32	CS	51	ARG
32	CS	52	GLN
32	CS	54	LYS
32	CS	55	SER
32	CS	56	VAL
32	CS	62	LYS
32	CS	65	LEU
32	CS	69	SER
32	CS	73	LYS
32	CS	80	LYS
32	CS	84	ARG
32	CS	86	ILE
32	CS	88	GLU
32	CS	96	GLU
32	CS	97	LEU
32	CS	99	ILE
32	CS	101	LEU
32	CS	102	ASN
32	CS	105	ARG
32	CS	107	CYS
32	CS	110	LYS
32	CS	112	THR
32	CS	113	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CS	115	ILE
32	CS	119	THR
32	CS	123	CYS
32	CS	125	LEU
32	CS	127	ASP
32	CS	131	ILE
32	CS	136	LEU
32	CS	142	THR
32	CS	149	VAL
32	CS	151	LEU
32	CS	153	LEU
32	CS	159	LEU
32	CS	160	LYS
32	CS	162	LEU
32	CS	165	MET
32	CS	181	VAL
32	CS	188	ARG
32	CS	192	SER
32	CS	195	SER
32	CS	198	SER
32	CS	201	VAL
32	CS	202	ILE
32	CS	206	LEU
32	CS	211	ILE
32	CS	212	SER
32	CS	217	VAL
32	CS	218	LYS
32	CS	251	SER
32	CS	252	LEU
32	CS	253	ILE
32	CS	266	LEU
32	CS	277	LEU
32	CS	278	ARG
32	CS	284	THR
32	CS	287	ARG
32	CS	291	LYS
32	CS	297	VAL
32	CS	308	SER
32	CS	316	SER
32	CS	318	GLU
32	CS	319	ASN
32	CS	322	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CS	323	LEU
32	CS	378	HIS
32	CS	382	GLN
32	CS	387	VAL
32	CS	390	GLU
32	CS	394	ILE
32	CS	401	LYS
32	CS	410	MET
32	CS	412	SER
32	CS	414	ILE
32	CS	415	SER
32	CS	418	GLU
32	CS	420	THR
32	CS	425	SER
32	CS	427	LYS
32	CS	430	LYS
32	CS	432	LEU
32	CS	433	ARG
32	CS	470	LYS
32	CS	476	GLU
32	CS	479	ARG
32	CS	484	ASP
32	CS	487	GLU
32	CS	488	LYS
32	CS	492	THR
32	CS	502	ARG
32	CS	512	ASP
32	CS	514	SER
32	CS	517	GLU
32	CS	532	VAL
32	CS	533	SER
32	CS	534	GLU
32	CS	535	LYS
32	CS	539	GLN
32	CS	541	VAL
32	CS	545	VAL
32	CS	548	HIS
32	CS	554	ASN
32	CS	556	LEU
32	CS	558	LEU
32	CS	559	MET
32	CS	566	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CS	569	VAL
32	CS	576	GLU
32	CS	584	CYS
32	CS	594	ILE
32	CS	596	LYS
32	CS	625	ASP
32	CS	626	GLU
32	CS	627	PHE
32	CS	631	SER
32	CS	651	SER
32	CS	654	LEU
32	CS	655	GLN
32	CS	658	VAL
32	CS	704	GLU
32	CS	711	LYS
32	CS	712	LEU
32	CS	713	SER
32	CS	716	ARG
32	CS	718	GLU
32	CS	719	LYS
32	CS	723	VAL
32	CS	725	VAL
32	CS	732	GLN
32	CS	745	VAL
32	CS	747	LEU
32	CS	750	THR
32	CS	753	ASP
32	CS	759	THR
32	CS	760	CYS
32	CS	768	ASP
32	CS	773	SER
32	CS	784	LYS
32	CS	788	SER
32	CS	789	LEU
32	CS	791	SER
32	CS	793	LYS
32	CS	800	ILE
32	CS	801	LEU
32	CS	806	GLU
32	CS	808	SER
32	CS	824	LEU
32	CS	830	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CS	832	LEU
32	CS	834	THR
32	CS	848	LEU
32	CS	858	MET
32	CS	860	THR
32	CS	861	ILE
32	CS	867	THR
32	CS	870	LEU
32	CS	876	LEU
32	CS	887	LEU
32	CS	893	ASP
32	CS	902	ASN
32	CS	907	GLN
32	CS	908	VAL
32	CS	909	LEU
32	CS	913	MET
32	CS	914	LYS
33	CT	86	THR
33	CT	151	ARG
34	Cc	134	THR
34	Cc	144	ARG
35	Ce	34	GLU
35	Ce	90	LYS
35	Ce	184	ARG
36	Cg	55	ARG
36	Cg	97	LEU
39	Cj	10	PHE
39	Cj	69	VAL
40	Cm	25	VAL
43	CU	126	ASP
43	CU	129	ARG
43	CU	249	ARG
43	CU	251	ASN
43	CU	254	VAL
43	CU	298	ARG
46	UV	88	LYS
46	UV	111	LYS
46	UV	155	ASP
46	UV	216	LYS
46	UV	287	ARG
46	UV	549	ARG
46	UV	612	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	UV	634	LYS
46	UV	706	LYS
46	UV	733	LYS
46	UV	810	LEU
46	UV	823	ARG
46	UV	920	LYS
46	UV	941	THR
46	UV	989	LYS
46	UV	1003	LYS
46	UV	1080	THR
47	CV	156	LYS
47	CV	167	LYS
48	UH	574	SER
48	UH	624	MET
48	UH	730	PHE
49	UE	155	THR
49	UE	162	ARG
49	UE	166	SER
49	UE	167	ASP
49	UE	169	LEU
49	UE	180	ILE
49	UE	191	SER
49	UE	195	THR
49	UE	197	LEU
49	UE	198	SER
49	UE	199	LYS
49	UE	210	ARG
49	UE	214	LEU
49	UE	215	MET
49	UE	219	GLN
49	UE	236	ILE
49	UE	238	ARG
49	UE	241	GLU
49	UE	242	LEU
49	UE	243	SER
49	UE	244	ARG
49	UE	246	LEU
49	UE	250	SER
49	UE	251	ARG
49	UE	257	LEU
49	UE	263	LEU
49	UE	266	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	UE	269	GLN
49	UE	273	ARG
49	UE	277	LYS
49	UE	278	MET
50	US	252	LYS
50	US	346	LEU
50	US	506	THR
51	Cl	16	ARG
51	Cl	48	LYS
52	CX	204	LYS
49	UI	155	THR
49	UI	162	ARG
49	UI	166	SER
49	UI	167	ASP
49	UI	169	LEU
49	UI	180	ILE
49	UI	191	SER
49	UI	195	THR
49	UI	197	LEU
49	UI	198	SER
49	UI	199	LYS
49	UI	210	ARG
49	UI	214	LEU
49	UI	215	MET
49	UI	219	GLN
49	UI	236	ILE
49	UI	238	ARG
49	UI	241	GLU
49	UI	242	LEU
49	UI	243	SER
49	UI	244	ARG
49	UI	246	LEU
49	UI	250	SER
49	UI	251	ARG
49	UI	257	LEU
49	UI	263	LEU
49	UI	266	LEU
49	UI	269	GLN
49	UI	273	ARG
49	UI	277	LYS
49	UI	278	MET
54	Cz	1571	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (265) such sidechains are listed below:

Mol	Chain	Res	Type
1	UA	9	ASN
1	UA	54	HIS
1	UA	78	GLN
1	UA	207	GLN
1	UA	253	GLN
1	UA	321	GLN
1	UA	336	GLN
1	UA	381	HIS
1	UA	467	HIS
1	UA	543	GLN
1	UA	576	ASN
1	UA	712	ASN
1	UA	801	HIS
2	UB	16	GLN
2	UB	22	GLN
2	UB	551	GLN
2	UB	645	GLN
2	UB	701	GLN
2	UB	741	HIS
2	UB	765	ASN
2	UB	803	HIS
4	UD	235	ASN
4	UD	322	HIS
4	UD	324	HIS
4	UD	370	GLN
4	UD	660	ASN
4	UD	673	ASN
4	UD	697	GLN
5	UF	45	HIS
5	UF	89	GLN
5	UF	289	GLN
5	UF	313	HIS
6	UG	127	GLN
6	UG	205	HIS
6	UG	206	ASN
6	UG	221	HIS
6	UG	277	GLN
6	UG	322	ASN
6	UG	378	GLN
6	UG	427	ASN
6	UG	476	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	UJ	15	ASN
7	UJ	85	GLN
7	UJ	103	HIS
7	UJ	158	GLN
7	UJ	184	GLN
7	UJ	268	GLN
7	UJ	295	GLN
7	UJ	318	HIS
7	UJ	379	ASN
7	UJ	515	ASN
7	UJ	670	HIS
8	UK	13	HIS
9	UL	23	ASN
9	UL	107	ASN
9	UL	207	HIS
9	UL	296	HIS
9	UL	398	ASN
9	UL	453	ASN
9	UL	457	GLN
9	UL	594	ASN
10	UM	58	GLN
10	UM	203	GLN
10	UM	236	GLN
10	UM	520	GLN
10	UM	644	ASN
10	UM	652	HIS
10	UM	691	ASN
10	UM	741	GLN
10	UM	743	GLN
10	UM	747	ASN
10	UM	750	HIS
10	UM	772	ASN
10	UM	776	ASN
11	UN	348	HIS
11	UN	362	GLN
11	UN	916	GLN
12	UO	143	HIS
12	UO	306	ASN
12	UO	333	HIS
12	UO	522	GLN
13	UQ	112	GLN
13	UQ	262	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	UQ	310	GLN
13	UQ	352	HIS
13	UQ	394	HIS
13	UQ	438	GLN
13	UQ	487	GLN
13	UQ	509	GLN
13	UQ	783	ASN
13	UQ	917	HIS
13	UQ	924	GLN
14	UR	312	ASN
14	UR	364	GLN
14	UR	370	GLN
14	UR	498	ASN
15	UU	197	ASN
15	UU	236	GLN
15	UU	379	HIS
15	UU	427	GLN
15	UU	571	GLN
15	UU	621	HIS
15	UU	711	ASN
15	UU	963	ASN
15	UU	1002	HIS
16	UX	141	HIS
17	UZ	105	GLN
18	CA	78	HIS
18	CA	277	GLN
18	CB	235	GLN
18	CB	299	HIS
19	CC	139	ASN
19	CC	154	GLN
19	CC	171	HIS
19	CC	173	ASN
19	CC	175	ASN
19	CC	179	GLN
19	CC	192	ASN
19	CC	272	GLN
19	CC	321	HIS
19	CC	394	ASN
20	CD	124	GLN
20	CD	128	ASN
20	CD	280	ASN
20	CD	314	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	CD	404	ASN
21	CE	67	HIS
21	CE	76	ASN
21	CF	67	HIS
22	CG	198	GLN
22	CG	243	GLN
22	CG	274	ASN
22	CG	430	HIS
22	CG	462	GLN
23	CH	199	GLN
23	CH	232	ASN
23	CH	251	HIS
23	CH	323	GLN
24	CI	221	ASN
24	CI	239	ASN
24	CI	248	ASN
24	CI	287	HIS
24	CI	366	ASN
24	CI	374	GLN
24	CI	380	GLN
24	CI	753	ASN
24	CI	930	ASN
24	CI	1006	ASN
25	CJ	27	HIS
26	CK	8	GLN
26	CK	48	ASN
26	CK	121	ASN
26	CK	159	HIS
26	CK	190	HIS
27	CL	569	HIS
28	CM	41	GLN
28	CM	45	ASN
28	CM	120	ASN
28	CM	262	HIS
28	CM	277	ASN
28	CM	370	GLN
29	CN	111	GLN
29	CN	199	ASN
29	CO	24	HIS
29	CO	93	HIS
29	CO	111	GLN
30	CP	147	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	CP	159	GLN
30	CP	190	ASN
31	CQ	203	ASN
31	CQ	224	ASN
32	CR	4	GLN
32	CR	20	GLN
32	CR	53	ASN
32	CR	102	ASN
32	CR	126	GLN
32	CR	161	GLN
32	CR	170	HIS
32	CR	207	ASN
32	CR	365	HIS
32	CR	485	ASN
32	CR	491	ASN
32	CR	565	HIS
32	CR	641	ASN
32	CR	731	GLN
32	CR	838	HIS
32	CR	846	ASN
32	CR	902	ASN
32	CR	921	GLN
32	CS	4	GLN
32	CS	20	GLN
32	CS	53	ASN
32	CS	102	ASN
32	CS	126	GLN
32	CS	161	GLN
32	CS	170	HIS
32	CS	365	HIS
32	CS	485	ASN
32	CS	491	ASN
32	CS	565	HIS
32	CS	641	ASN
32	CS	731	GLN
32	CS	838	HIS
32	CS	846	ASN
32	CS	902	ASN
32	CS	921	GLN
33	CT	120	GLN
33	CT	126	ASN
33	CT	179	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	Cc	91	ASN
34	Cc	126	ASN
34	Cc	145	GLN
34	Cc	157	GLN
34	Cc	187	ASN
34	Cc	211	ASN
35	Ce	36	ASN
36	Cg	108	GLN
39	Cj	74	HIS
39	Cj	77	GLN
39	Cj	83	GLN
40	Cm	42	GLN
40	Cm	64	GLN
40	Cm	80	ASN
46	UV	77	HIS
46	UV	119	GLN
46	UV	205	ASN
46	UV	260	GLN
46	UV	270	ASN
46	UV	415	HIS
46	UV	417	HIS
46	UV	494	ASN
46	UV	520	ASN
46	UV	542	ASN
46	UV	615	GLN
46	UV	782	GLN
46	UV	813	HIS
46	UV	938	GLN
46	UV	949	HIS
46	UV	998	ASN
47	CV	55	ASN
47	CV	89	GLN
47	CV	199	ASN
48	UH	590	ASN
48	UH	862	HIS
49	UE	183	ASN
49	UE	237	ASN
49	UE	269	GLN
50	US	151	GLN
50	US	152	HIS
50	US	206	HIS
50	US	225	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	US	261	HIS
50	US	372	HIS
50	US	419	HIS
50	US	464	GLN
51	Cl	21	ASN
52	CX	290	ASN
52	CX	322	GLN
52	CX	364	ASN
52	CX	423	ASN
49	UI	183	ASN
49	UI	237	ASN
49	UI	269	GLN
54	Cz	1549	ASN
54	Cz	1631	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	C1	1088/2323 (46%)	373 (34%)	31 (2%)
45	C2	226/230 (98%)	83 (36%)	8 (3%)
All	All	1314/2553 (51%)	456 (34%)	39 (2%)

All (456) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
44	C1	2	G
44	C1	3	G
44	C1	4	G
44	C1	5	G
44	C1	7	A
44	C1	13	G
44	C1	14	G
44	C1	15	G
44	C1	16	U
44	C1	17	C
44	C1	18	G
44	C1	19	C
44	C1	20	C
44	C1	23	G
44	C1	26	C
44	C1	38	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	C1	40	A
44	C1	41	G
44	C1	42	C
44	C1	43	C
44	C1	47	G
44	C1	49	G
44	C1	56	C
44	C1	57	C
44	C1	59	U
44	C1	60	A
44	C1	61	G
44	C1	63	C
44	C1	66	G
44	C1	68	U
44	C1	71	A
44	C1	72	U
44	C1	73	A
44	C1	74	C
44	C1	77	C
44	C1	89	G
44	C1	90	A
44	C1	93	G
44	C1	96	C
44	C1	104	U
44	C1	105	A
44	C1	107	C
44	C1	121	G
44	C1	126	C
44	C1	127	C
44	C1	128	G
44	C1	132	A
44	C1	134	C
44	C1	135	A
44	C1	136	C
44	C1	143	A
44	C1	152	G
44	C1	154	C
44	C1	155	G
44	C1	158	C
44	C1	159	C
44	C1	160	C
44	C1	161	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	C1	162	G
44	C1	163	C
44	C1	166	A
44	C1	169	G
44	C1	170	C
44	C1	182	C
44	C1	183	C
44	C1	185	G
44	C1	192	A
44	C1	201	G
44	C1	203	C
44	C1	205	C
44	C1	206	C
44	C1	207	U
44	C1	208	A
44	C1	210	G
44	C1	216	A
44	C1	220	A
44	C1	222	U
44	C1	223	A
44	C1	228	G
44	C1	234	G
44	C1	236	C
44	C1	237	G
44	C1	242	U
44	C1	243	U
44	C1	244	G
44	C1	251	G
44	C1	257	G
44	C1	258	C
44	C1	259	U
44	C1	260	U
44	C1	262	G
44	C1	265	G
44	C1	266	C
44	C1	267	U
44	C1	268	G
44	C1	269	G
44	C1	272	A
44	C1	273	G
44	C1	276	C
44	C1	277	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	C1	278	A
44	C1	281	U
44	C1	282	C
44	C1	283	A
44	C1	285	A
44	C1	291	C
44	C1	292	G
44	C1	339	C
44	C1	340	G
44	C1	346	C
44	C1	347	C
44	C1	349	C
44	C1	351	U
44	C1	352	G
44	C1	353	G
44	C1	357	G
44	C1	360	U
44	C1	371	U
44	C1	372	U
44	C1	379	G
44	C1	382	U
44	C1	383	G
44	C1	384	C
44	C1	386	G
44	C1	398	C
44	C1	401	C
44	C1	402	U
44	C1	403	G
44	C1	407	A
44	C1	416	U
44	C1	423	U
44	C1	425	C
44	C1	427	G
44	C1	432	G
44	C1	435	A
44	C1	436	A
44	C1	439	A
44	C1	440	G
44	C1	441	A
44	C1	442	U
44	C1	443	G
44	C1	454	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	C1	458	A
44	C1	459	C
44	C1	467	C
44	C1	468	C
44	C1	469	G
44	C1	471	C
44	C1	473	G
44	C1	474	A
44	C1	475	C
44	C1	477	A
44	C1	483	U
44	C1	484	G
44	C1	491	G
44	C1	492	C
44	C1	499	G
44	C1	500	C
44	C1	501	U
44	C1	502	A
44	C1	504	C
44	C1	581	C
44	C1	582	G
44	C1	583	A
44	C1	584	U
44	C1	585	A
44	C1	586	G
44	C1	587	U
44	C1	594	G
44	C1	596	U
44	C1	603	G
44	C1	604	C
44	C1	609	A
44	C1	610	G
44	C1	613	A
44	C1	614	U
44	C1	621	G
44	C1	627	A
44	C1	1054	A
44	C1	1059	A
44	C1	1061	A
44	C1	1062	C
44	C1	1064	G
44	C1	1069	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	C1	1070	G
44	C1	1076	U
44	C1	1077	U
44	C1	1078	U
44	C1	1079	C
44	C1	1080	G
44	C1	1081	G
44	C1	1083	U
44	C1	1085	U
44	C1	1086	U
44	C1	1088	U
44	C1	1089	A
44	C1	1094	G
44	C1	1095	A
44	C1	1097	U
44	C1	1098	G
44	C1	1103	C
44	C1	1104	A
44	C1	1120	C
44	C1	1123	G
44	C1	1124	G
44	C1	1125	A
44	C1	1126	A
44	C1	1127	C
44	C1	1128	A
44	C1	1129	A
44	C1	1140	A
44	C1	1141	G
44	C1	1147	U
44	C1	1148	G
44	C1	1149	C
44	C1	1150	C
44	C1	1154	A
44	C1	1158	G
44	C1	1159	C
44	C1	1163	A
44	C1	1164	A
44	C1	1166	U
44	C1	1167	C
44	C1	1168	C
44	C1	1169	A
44	C1	1170	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	C1	1178	A
44	C1	1179	G
44	C1	1186	U
44	C1	1218	G
44	C1	1219	A
44	C1	1222	C
44	C1	1223	U
44	C1	1444	A
44	C1	1447	A
44	C1	1448	A
44	C1	1449	U
44	C1	1450	A
44	C1	1451	G
44	C1	1452	G
44	C1	1461	G
44	C1	1469	A
44	C1	1471	U
44	C1	1479	U
44	C1	1480	G
44	C1	1481	U
44	C1	1483	A
44	C1	1484	G
44	C1	1486	G
44	C1	1489	G
44	C1	1491	A
44	C1	1497	U
44	C1	1498	G
44	C1	1499	G
44	C1	1507	G
44	C1	1516	C
44	C1	1517	A
44	C1	1518	A
44	C1	1519	C
44	C1	1520	U
44	C1	1525	A
44	C1	1527	G
44	C1	1529	A
44	C1	1536	A
44	C1	1545	U
44	C1	1546	U
44	C1	1547	C
44	C1	1549	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	C1	1551	A
44	C1	1554	C
44	C1	1555	A
44	C1	1624	A
44	C1	1625	G
44	C1	1628	A
44	C1	1635	G
44	C1	1636	G
44	C1	1637	C
44	C1	1638	G
44	C1	1639	U
44	C1	1642	A
44	C1	1643	U
44	C1	1644	U
44	C1	1645	U
44	C1	1656	C
44	C1	1657	G
44	C1	1665	A
44	C1	1667	G
44	C1	1668	A
44	C1	1670	A
44	C1	1673	U
44	C1	1675	A
44	C1	1676	A
44	C1	1677	A
44	C1	1678	A
44	C1	1699	U
44	C1	1700	A
44	C1	1701	U
44	C1	1703	G
44	C1	1710	G
44	C1	1711	G
44	C1	1712	C
44	C1	1713	U
44	C1	1729	U
44	C1	1730	G
44	C1	1735	A
44	C1	1740	C
44	C1	1742	C
44	C1	1743	C
44	C1	1744	A
44	C1	1748	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	C1	1751	G
44	C1	2047	G
44	C1	2048	C
44	C1	2054	A
44	C1	2055	C
44	C1	2056	U
44	C1	2057	G
44	C1	2061	G
44	C1	2070	A
44	C1	2071	G
44	C1	2073	A
44	C1	2074	C
44	C1	2075	U
44	C1	2076	C
44	C1	2077	C
44	C1	2078	C
44	C1	2085	G
44	C1	2086	A
44	C1	2087	G
44	C1	2088	A
44	C1	2107	A
44	C1	2109	A
44	C1	2115	U
44	C1	2118	U
44	C1	2120	C
44	C1	2121	U
44	C1	2156	A
44	C1	2157	G
44	C1	2158	G
44	C1	2162	C
44	C1	2167	G
44	C1	2173	G
44	C1	2178	U
44	C1	2179	C
44	C1	2183	A
44	C1	2184	G
44	C1	2185	C
44	C1	2197	A
44	C1	2201	C
44	C1	2202	C
44	C1	2205	G
44	C1	2210	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	C1	2211	U
44	C1	2212	G
44	C1	2213	U
44	C1	2214	A
44	C1	2215	C
44	C1	2217	C
44	C1	2220	C
44	C1	2222	C
44	C1	2223	C
44	C1	2227	C
44	C1	2328	G
44	C1	2329	A
44	C1	2330	G
44	C1	2351	G
44	C1	2352	U
44	C1	2362	U
44	C1	2363	G
44	C1	2364	A
44	C1	2365	A
44	C1	2366	C
44	C1	2374	G
45	C2	2	G
45	C2	6	C
45	C2	8	A
45	C2	9	U
45	C2	10	A
45	C2	15	A
45	C2	23	A
45	C2	24	U
45	C2	29	A
45	C2	30	U
45	C2	32	G
45	C2	33	U
45	C2	36	U
45	C2	37	U
45	C2	39	U
45	C2	40	C
45	C2	43	C
45	C2	47	U
45	C2	48	G
45	C2	57	A
45	C2	58	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	C2	62	A
45	C2	63	G
45	C2	64	C
45	C2	70	A
45	C2	81	G
45	C2	82	U
45	C2	84	G
45	C2	90	C
45	C2	91	G
45	C2	92	A
45	C2	94	A
45	C2	95	U
45	C2	100	G
45	C2	104	C
45	C2	105	C
45	C2	111	G
45	C2	124	U
45	C2	125	U
45	C2	126	U
45	C2	127	A
45	C2	128	C
45	C2	136	C
45	C2	140	C
45	C2	142	G
45	C2	145	A
45	C2	147	G
45	C2	148	G
45	C2	153	G
45	C2	156	C
45	C2	160	U
45	C2	162	C
45	C2	163	C
45	C2	164	U
45	C2	165	C
45	C2	166	G
45	C2	167	U
45	C2	168	C
45	C2	170	C
45	C2	174	G
45	C2	178	U
45	C2	179	A
45	C2	181	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	C2	182	G
45	C2	187	U
45	C2	189	G
45	C2	190	C
45	C2	193	U
45	C2	198	U
45	C2	199	G
45	C2	200	U
45	C2	201	A
45	C2	244	G
45	C2	247	G
45	C2	250	G
45	C2	255	U
45	C2	256	G
45	C2	257	G
45	C2	259	A
45	C2	260	G
45	C2	261	U
45	C2	262	C
45	C2	267	C

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	C1	67	G
44	C1	89	G
44	C1	135	A
44	C1	150	C
44	C1	205	C
44	C1	207	U
44	C1	209	A
44	C1	259	U
44	C1	260	U
44	C1	277	U
44	C1	281	U
44	C1	401	C
44	C1	424	U
44	C1	582	G
44	C1	593	G
44	C1	1068	C
44	C1	1077	U
44	C1	1085	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	C1	1087	G
44	C1	1163	A
44	C1	1485	A
44	C1	1638	G
44	C1	1712	C
44	C1	1734	G
44	C1	2054	A
44	C1	2070	A
44	C1	2077	C
44	C1	2156	A
44	C1	2177	G
44	C1	2214	A
44	C1	2219	C
45	C2	23	A
45	C2	35	G
45	C2	38	G
45	C2	61	G
45	C2	91	G
45	C2	94	A
45	C2	255	U
45	C2	259	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
45	C2	3
2	UB	1
48	UH	1

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	18.53
1	C2	105:C	O3'	110:A	P	15.27
1	C2	119:C	O3'	123:A	P	11.89
1	UB	679:ASN	C	680:PHE	N	1.20
1	UH	730:PHE	C	731:LYS	N	1.18

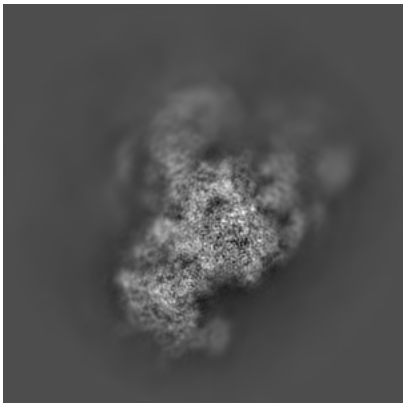
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10055. These allow visual inspection of the internal detail of the map and identification of artifacts.

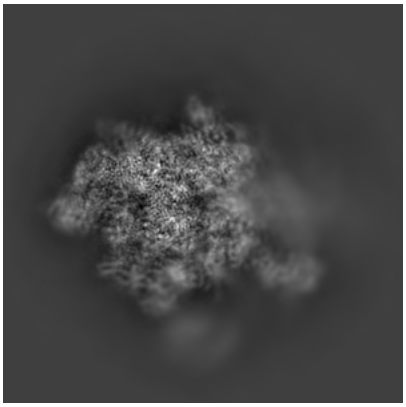
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

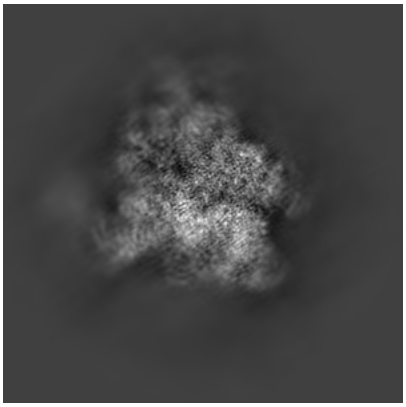
6.1.1 Primary map



X



Y

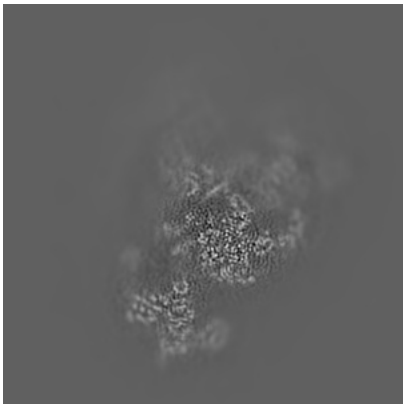


Z

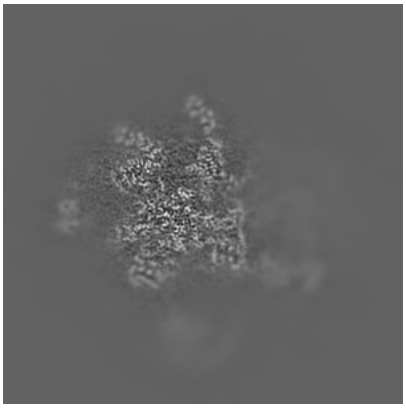
The images above show the map projected in three orthogonal directions.

6.2 Central slices

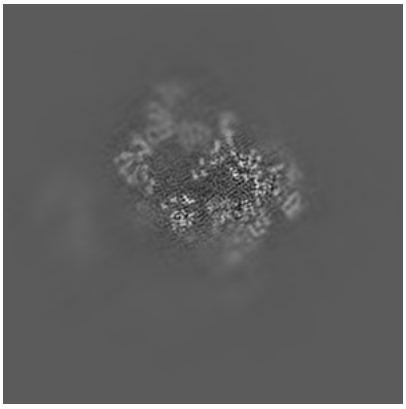
6.2.1 Primary map



X Index: 240



Y Index: 240

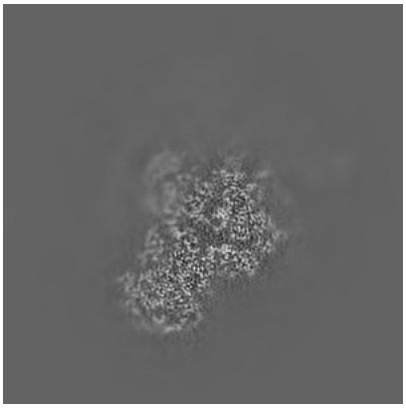


Z Index: 240

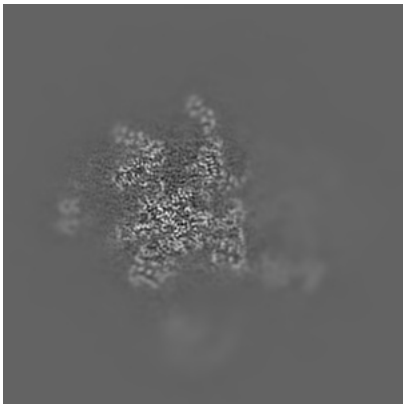
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

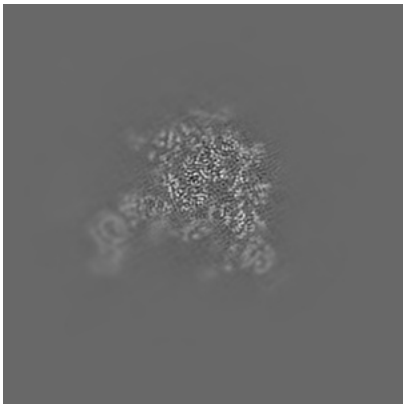
6.3.1 Primary map



X Index: 279



Y Index: 241

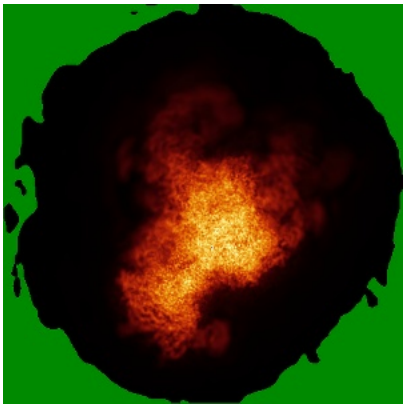


Z Index: 187

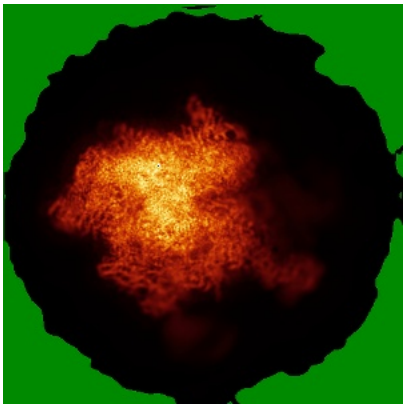
The images above show the largest variance slices of the map in three orthogonal directions.

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

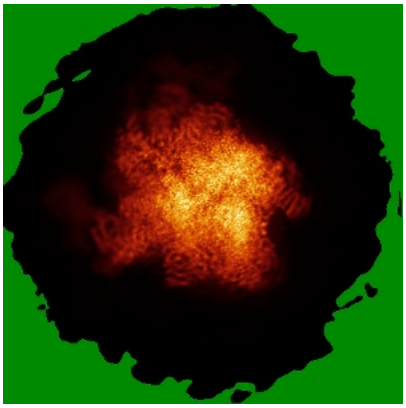
6.4.1 Primary map



X



Y

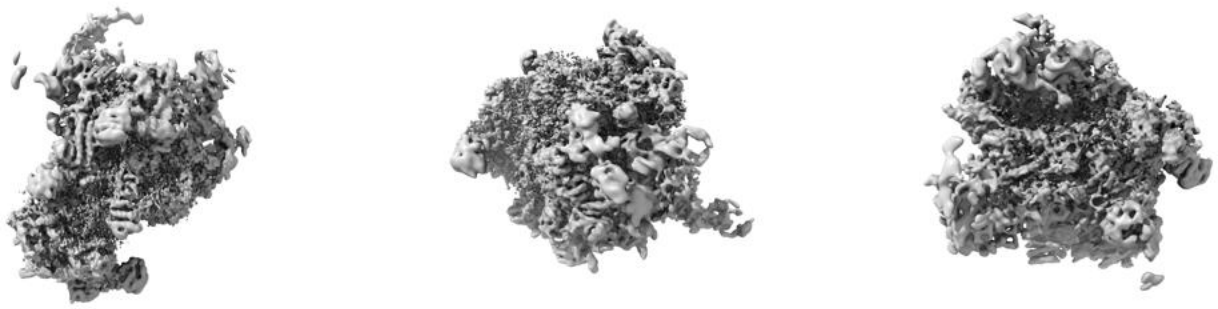


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

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

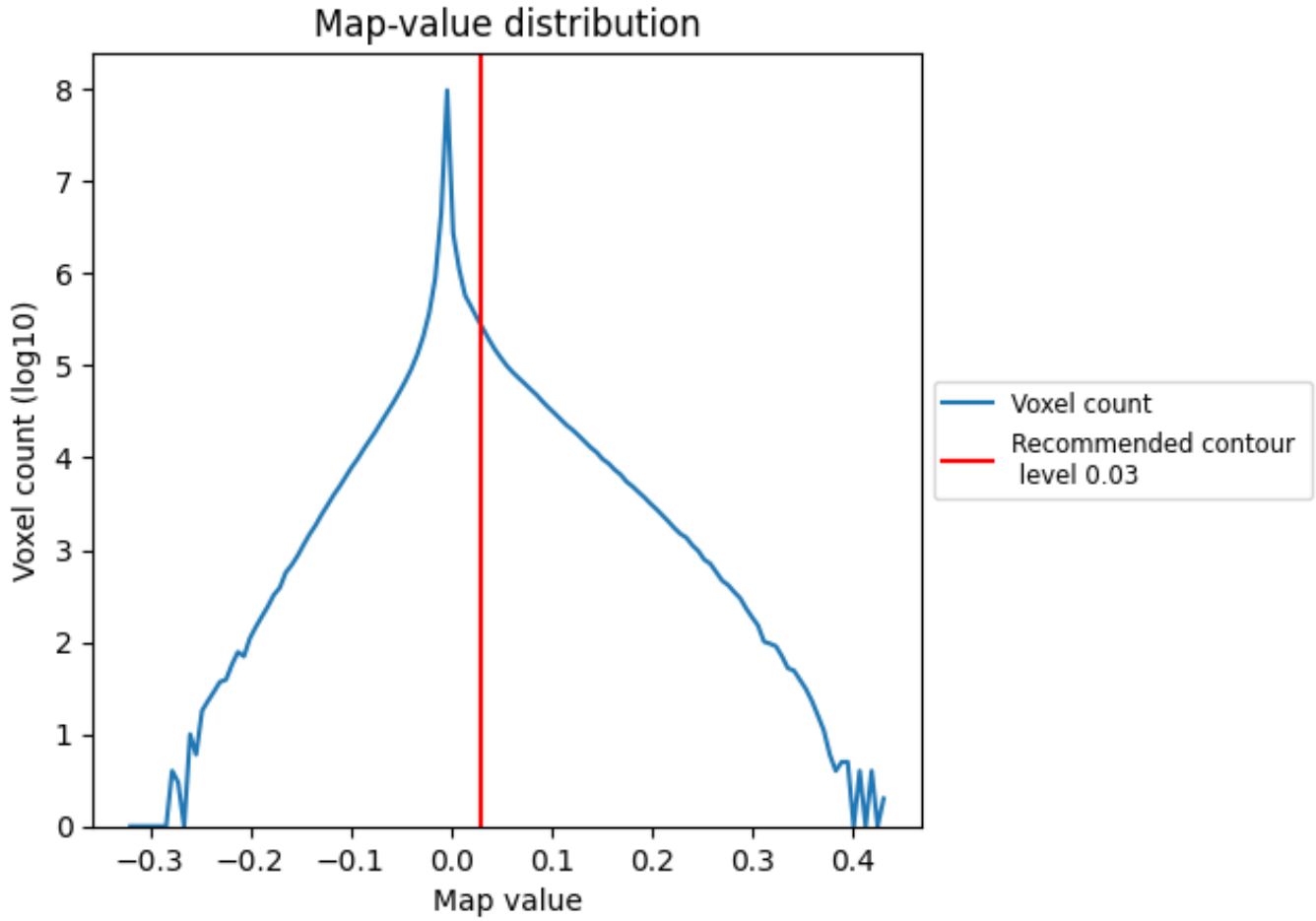
6.6 Mask visualisation (i)

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

7 Map analysis

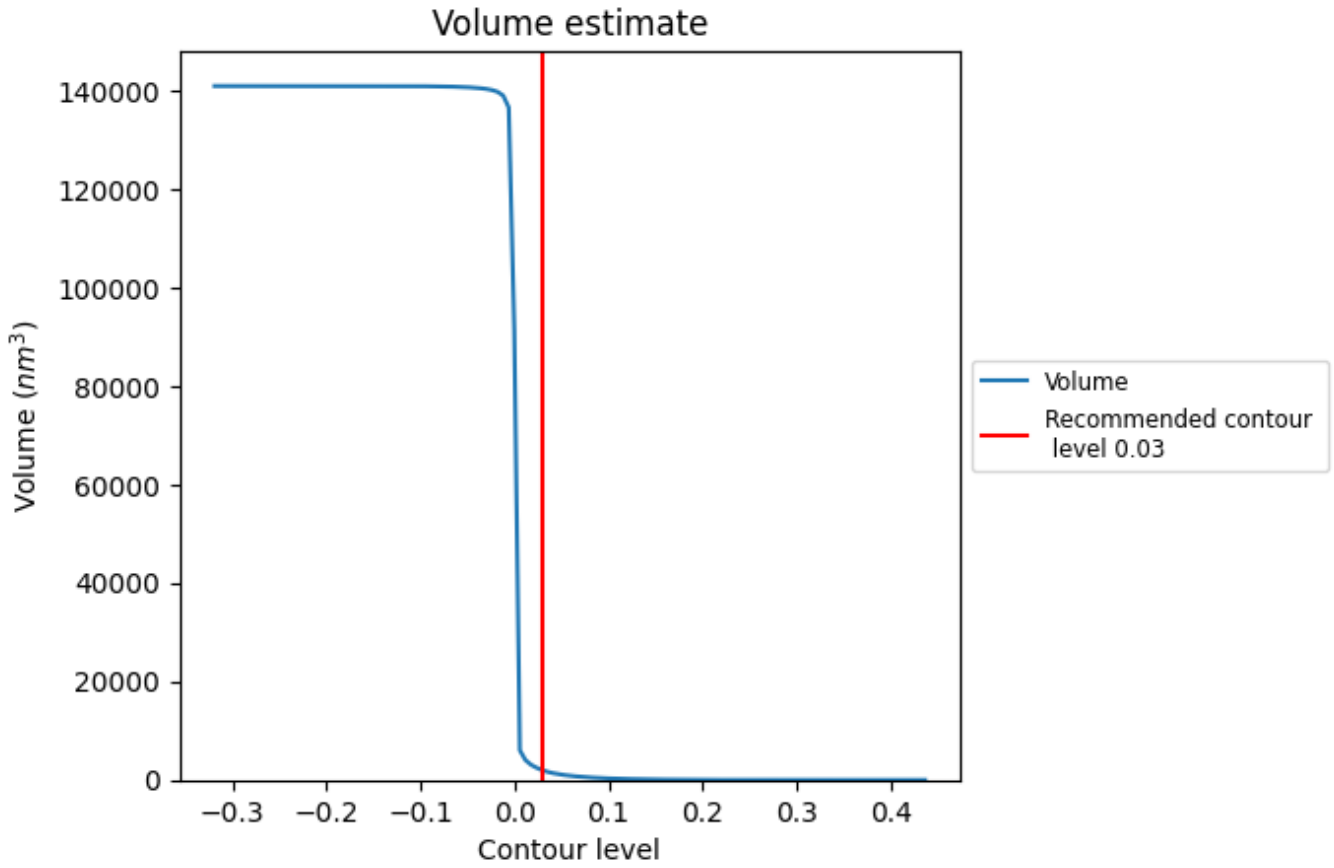
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

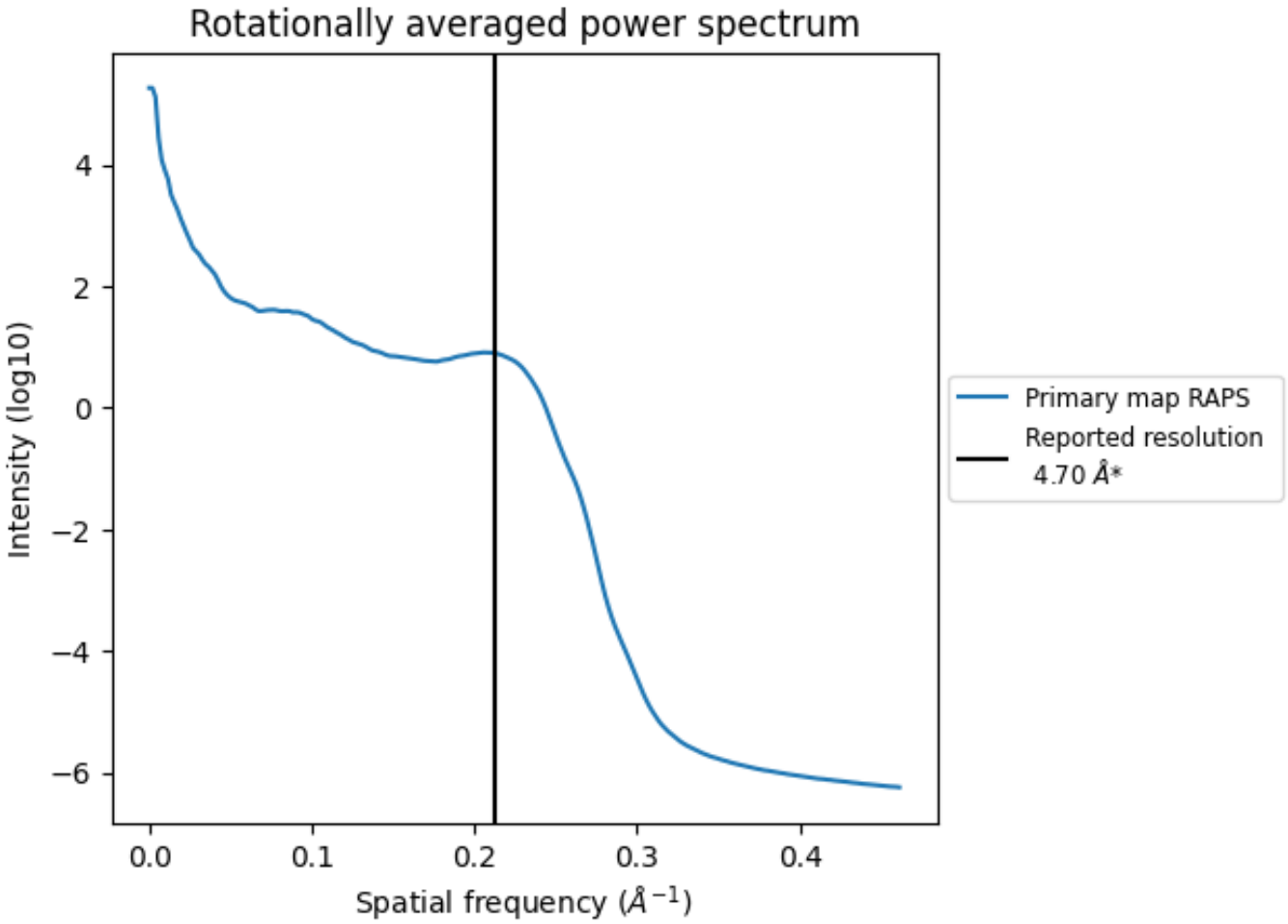
7.2 Volume estimate



The volume at the recommended contour level is 1965 nm^3; this corresponds to an approximate mass of 1775 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

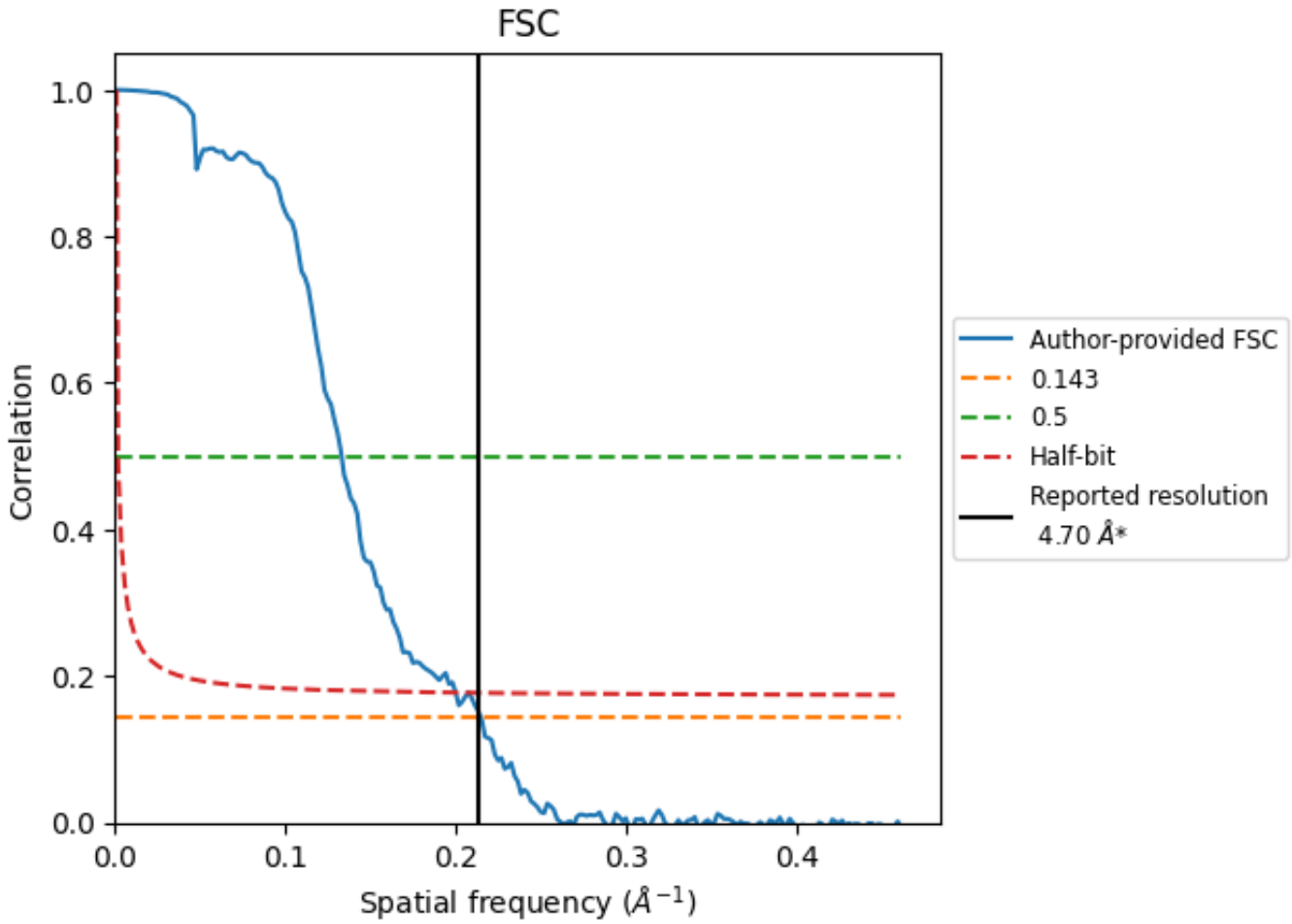


*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

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 0.213 Å^{-1}

8.2 Resolution estimates (i)

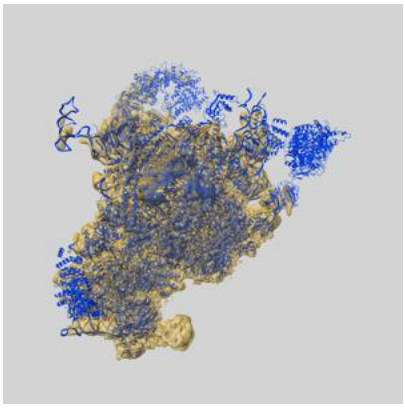
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.66	7.52	5.00
Unmasked-calculated*	-	-	-

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

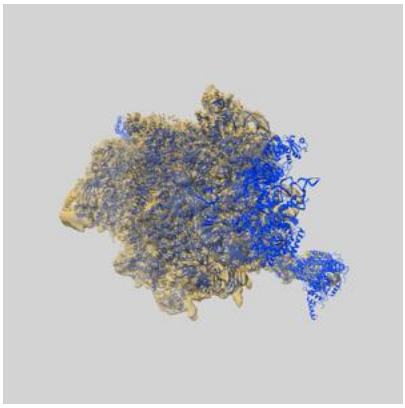
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10055 and PDB model 6RXY. Per-residue inclusion information can be found in section 3 on page 14.

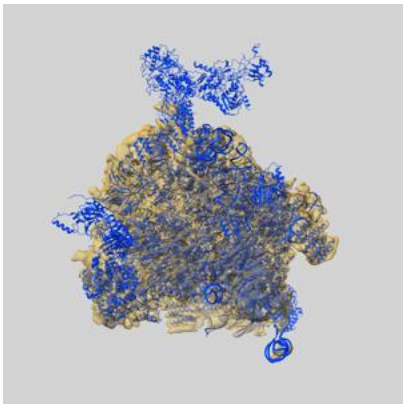
9.1 Map-model overlay



X



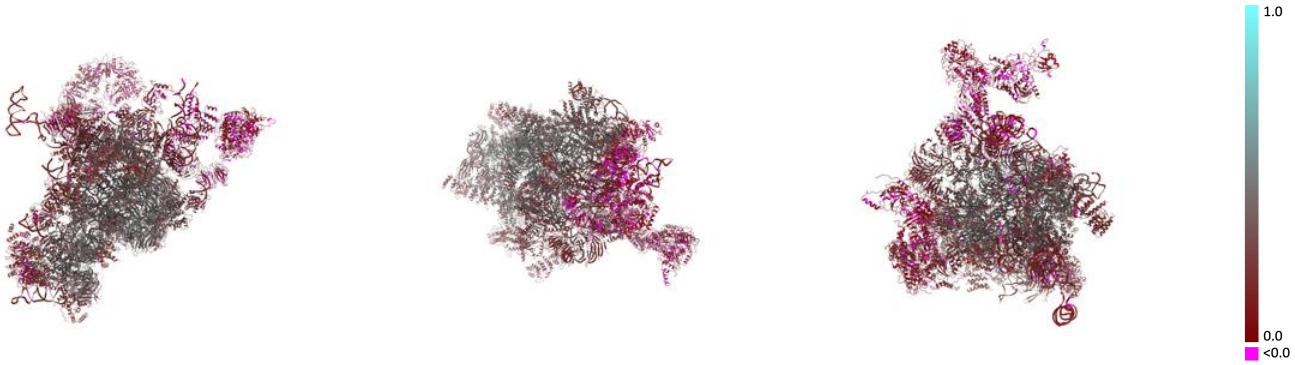
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

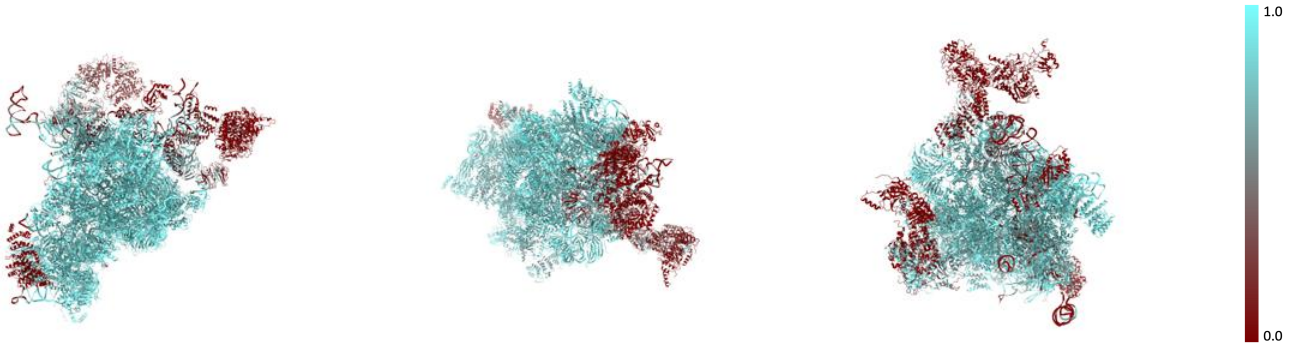
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

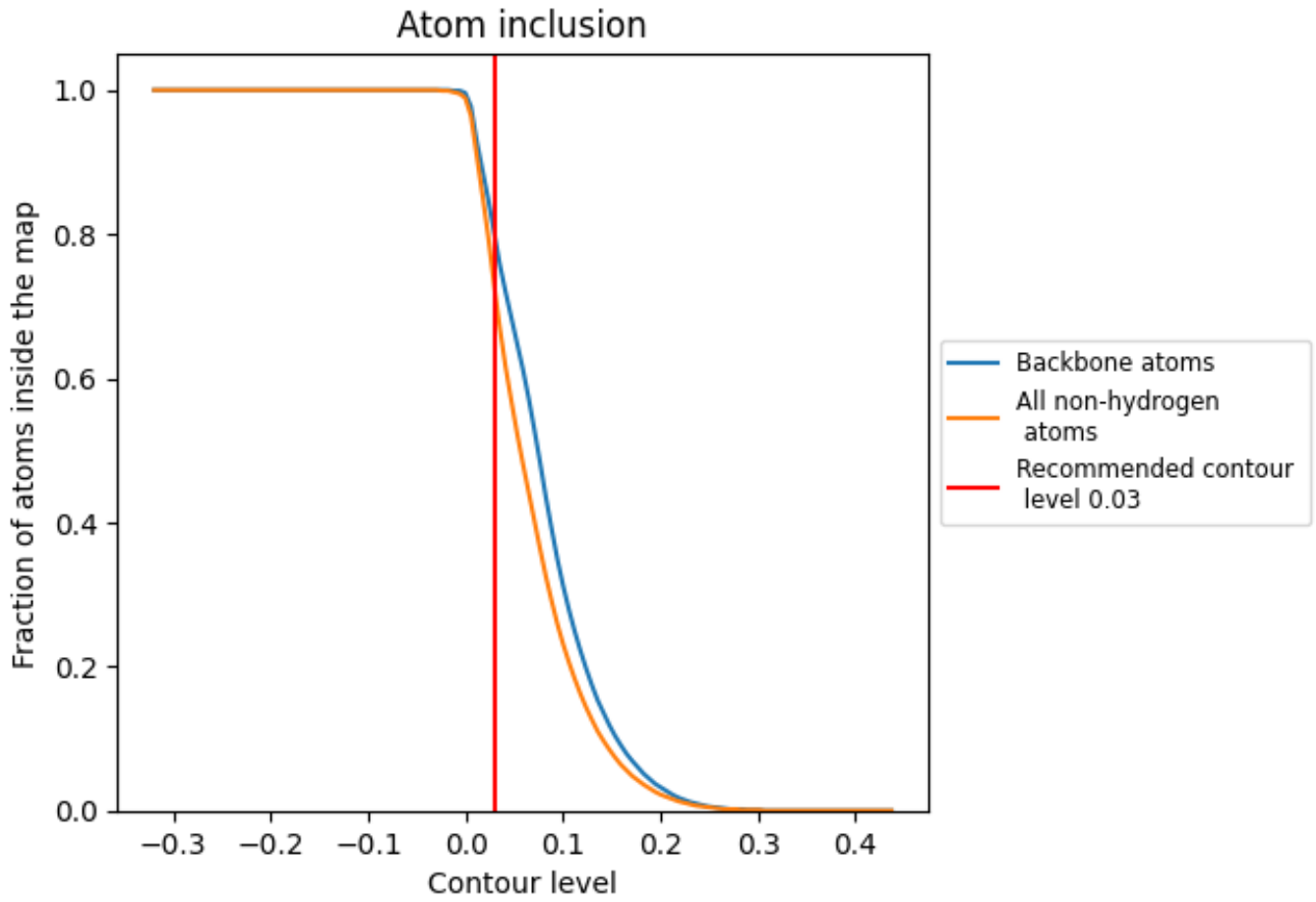
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 72% 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	0.7220	0.2860
C1	0.8230	0.2910
C2	0.7840	0.2890
CA	0.8910	0.4010
CB	0.7880	0.2650
CC	0.8330	0.2940
CD	0.8600	0.3010
CE	0.9210	0.4520
CF	0.6880	0.2260
CG	0.6170	0.1410
CH	0.8490	0.3060
CI	0.8290	0.3190
CJ	0.9340	0.4690
CK	0.9170	0.4410
CL	0.9010	0.3840
CM	0.9090	0.3920
CN	0.8400	0.3450
CO	0.7810	0.2220
CP	0.4010	0.1470
CQ	0.8350	0.2360
CR	0.4630	0.1440
CS	0.0680	0.0790
CT	0.8930	0.4100
CU	0.6210	0.2920
CV	0.0000	0.0470
CX	0.6830	0.1390
Cc	0.9180	0.4140
Ce	0.0050	0.1440
Cg	0.4200	0.1990
Ch	0.1500	0.0740
Ci	0.4970	0.1250
Cj	0.9350	0.4730
Cl	0.6350	0.2730
Cm	0.2660	0.2370
Cn	0.8600	0.3770

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Cp	0.9150	0.4210
Cz	0.1530	0.1050
UA	0.9300	0.4450
UB	0.8650	0.2900
UC	0.7850	0.3260
UD	0.8940	0.3560
UE	0.8470	0.3050
UF	0.8890	0.2880
UG	0.9090	0.4320
UH	0.8530	0.2590
UI	0.7400	0.1610
UJ	0.4900	0.2670
UK	0.9130	0.4090
UL	0.8620	0.2650
UM	0.5660	0.1270
UN	0.8970	0.3630
UO	0.9160	0.4160
UP	0.8970	0.3780
UQ	0.9150	0.3900
UR	0.9330	0.4440
US	0.8450	0.2750
UU	0.9310	0.4210
UV	0.0000	0.0550
UX	0.8750	0.3830
UZ	0.8520	0.3060