Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 08:11 am GMT

PDB ID	:	6RXT
EMDB ID	:	EMD-10051
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	:	7.00 Å(reported)

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

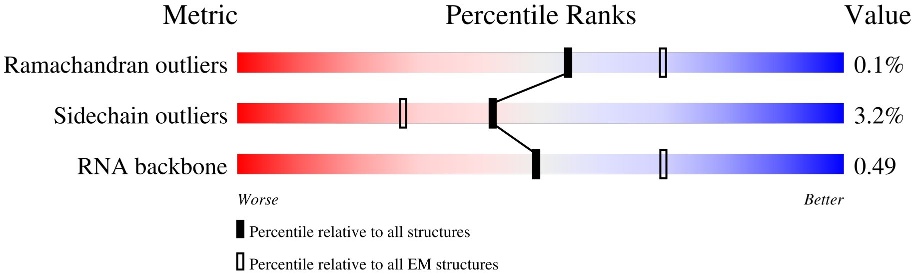
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

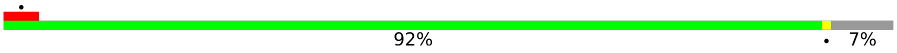
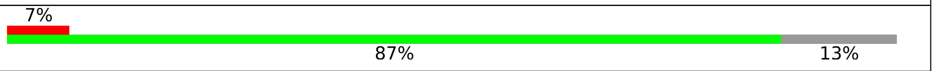
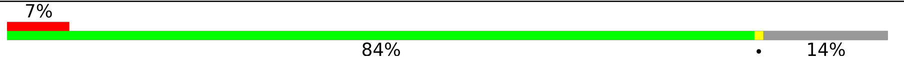
The reported resolution of this entry is 7.00 Å.

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



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

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

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

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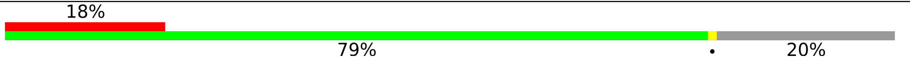
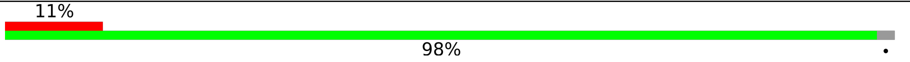
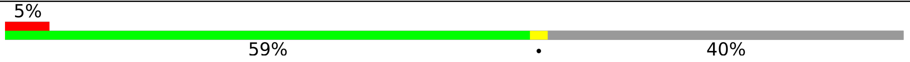
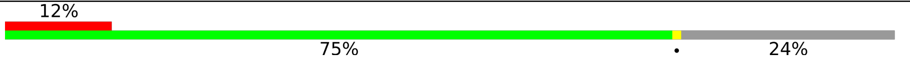
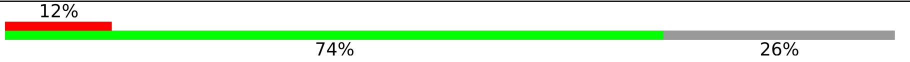
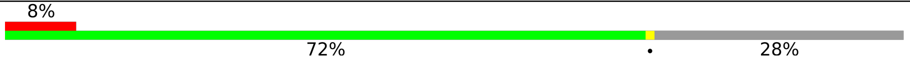
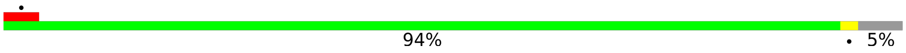
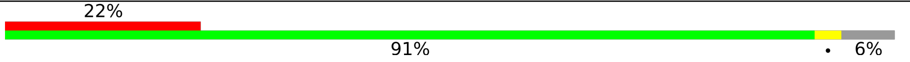
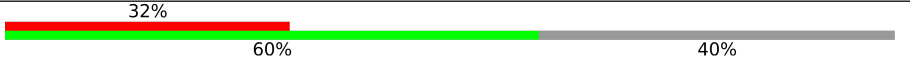
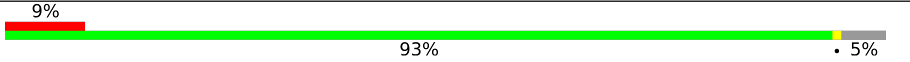
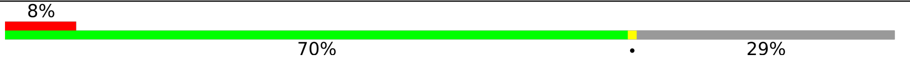
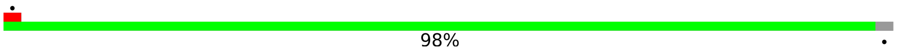
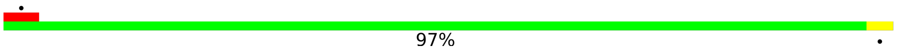
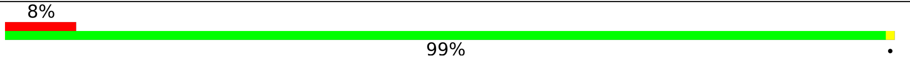
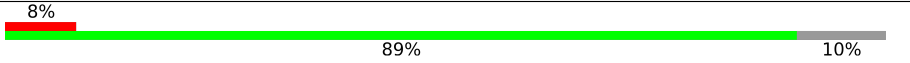
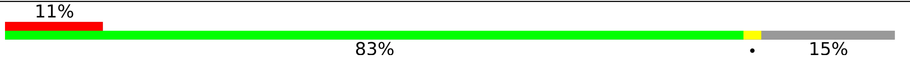
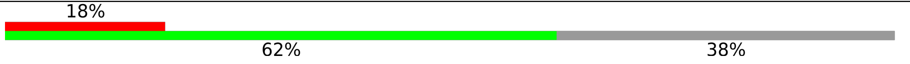
Mol	Chain	Length	Quality of chain
9	UL	962	
10	UM	912	
11	UN	938	
12	UO	557	
13	UQ	960	
14	UR	618	
15	UU	1049	
16	UX	193	
17	UZ	391	
18	CA	313	
18	CB	313	
19	CC	523	
20	CD	582	
21	CE	127	
21	CF	127	
22	CG	630	
23	CH	411	
24	CI	1163	
25	CJ	183	
26	CK	297	
27	CL	785	
28	CM	446	
29	CN	252	
29	CO	252	
30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

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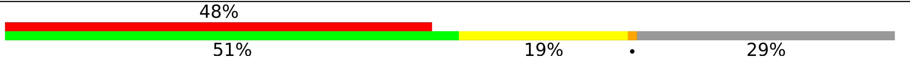
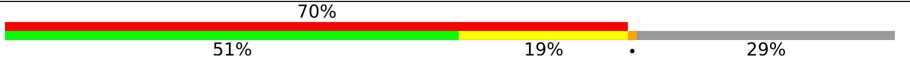
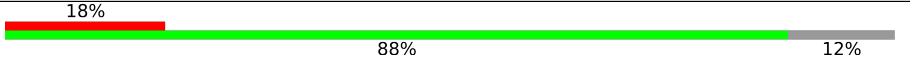
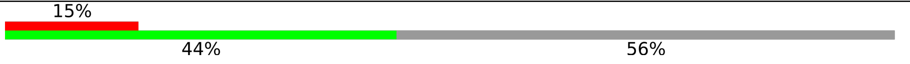
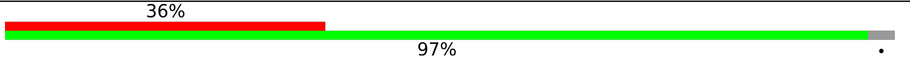
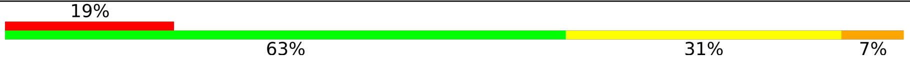
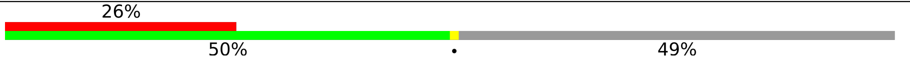
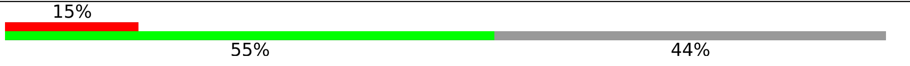
Mol	Chain	Length	Quality of chain
31	CQ	259	
32	CR	1073	
32	CS	1073	
33	CT	203	
34	Ca	255	
35	Cc	212	
36	Ce	203	
37	Cg	190	
38	Ch	151	
39	Ci	150	
40	Cj	143	
41	Cm	130	
42	Cn	145	
43	Cp	68	
44	CU	311	
45	C1	2352	
46	C2	230	
47	UH	930	
48	UE	410	
48	UI	410	
49	US	549	
50	Cl	156	
51	CX	480	
52	UP	364	

2 Entry composition ⓘ

There are 55 unique types of molecules in this entry. The entry contains 169690 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	479	Total	C	N	O	S	0	0
			3717	2369	700	636	12		

- Molecule 7 is a protein called UTP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	UJ	445	3377	2169	604	590	14	0	0

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

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

- Molecule 9 is a protein called Utp12.

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

- Molecule 10 is a protein called Utp13".

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	UM	729	5643	3590	995	1045	13	0	0

- Molecule 11 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	UN	154	1209	770	228	206	5	0	0

- Molecule 12 is a protein called Utp15.

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

- Molecule 13 is a protein called Utp17.

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

- Molecule 14 is a protein called Utp18.

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

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

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

- Molecule 16 is a protein called Utp24.

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

- Molecule 17 is a protein called Utp30.

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

- Molecule 18 is a protein called Nop1.

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

- Molecule 19 is a protein called Putative nucleolar protein.

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

- Molecule 20 is a protein called Nop58.

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

- Molecule 21 is a protein called snu13.

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

- Molecule 22 is a protein called Rrp9.

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

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

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

- Molecule 24 is a protein called Bms1.

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

- Molecule 25 is a protein called Imp3.

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

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

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

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

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

- Molecule 28 is a protein called Sof1.

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

- Molecule 29 is a protein called Emg1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CP	201	Total 1625	C 1047	N 286	O 283	S 9	0	0

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

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

- Molecule 32 is a protein called Kre33.

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

- Molecule 33 is a protein called Fcf2.

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

- Molecule 34 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ca	225	Total 1821	C 1160	N 341	O 315	S 5	0	0

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

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

- Molecule 36 is a protein called 40S ribosomal protein S7.

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

- Molecule 37 is a protein called 40S ribosomal protein s9-like protein.

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

- Molecule 38 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	Ch	66	Total	C	N	O	0	0
			546	355	101	90		

- Molecule 39 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ci	115	Total	C	N	O	S	0	0
			808	506	156	141	5		

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

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

- Molecule 41 is a protein called 40S ribosomal protein S22-like protein.

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

- Molecule 42 is a protein called 40S ribosomal protein s23-like protein.

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

- Molecule 43 is a protein called 40S ribosomal protein S28-like protein.

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

- Molecule 44 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	CU	176	Total	C	N	O	S	0	0
			1337	822	265	244	6		

- Molecule 45 is a RNA chain called 35S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	C1	1152	Total	C	N	O	P	0	0
			24590	10964	4415	8059	1152		

- Molecule 46 is a RNA chain called U3 snoRNA.

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

- Molecule 47 is a protein called Utp8.

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

- Molecule 48 is a protein called Utp5".

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

- Molecule 49 is a protein called Noc4.

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

- Molecule 50 is a protein called Putative ribosomal protein.

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

- Molecule 51 is a protein called Enp1.

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

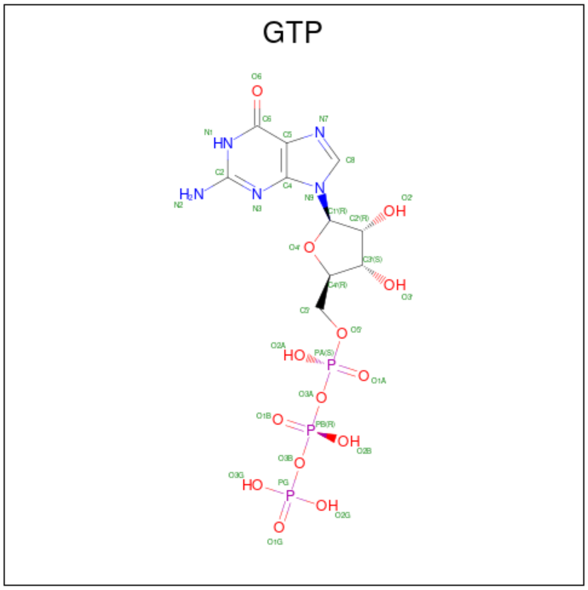
- Molecule 52 is a protein called Utp16.

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

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

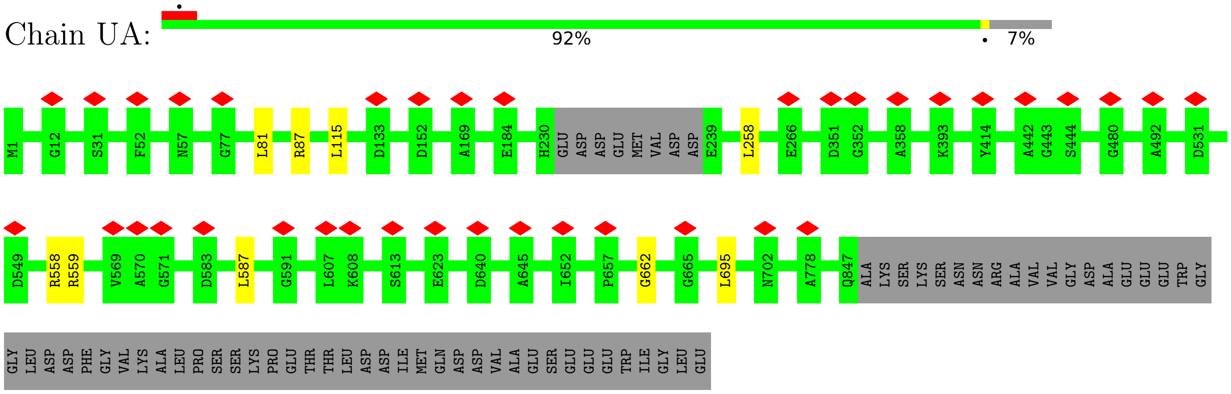
- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
55	CI	1	1	1	0

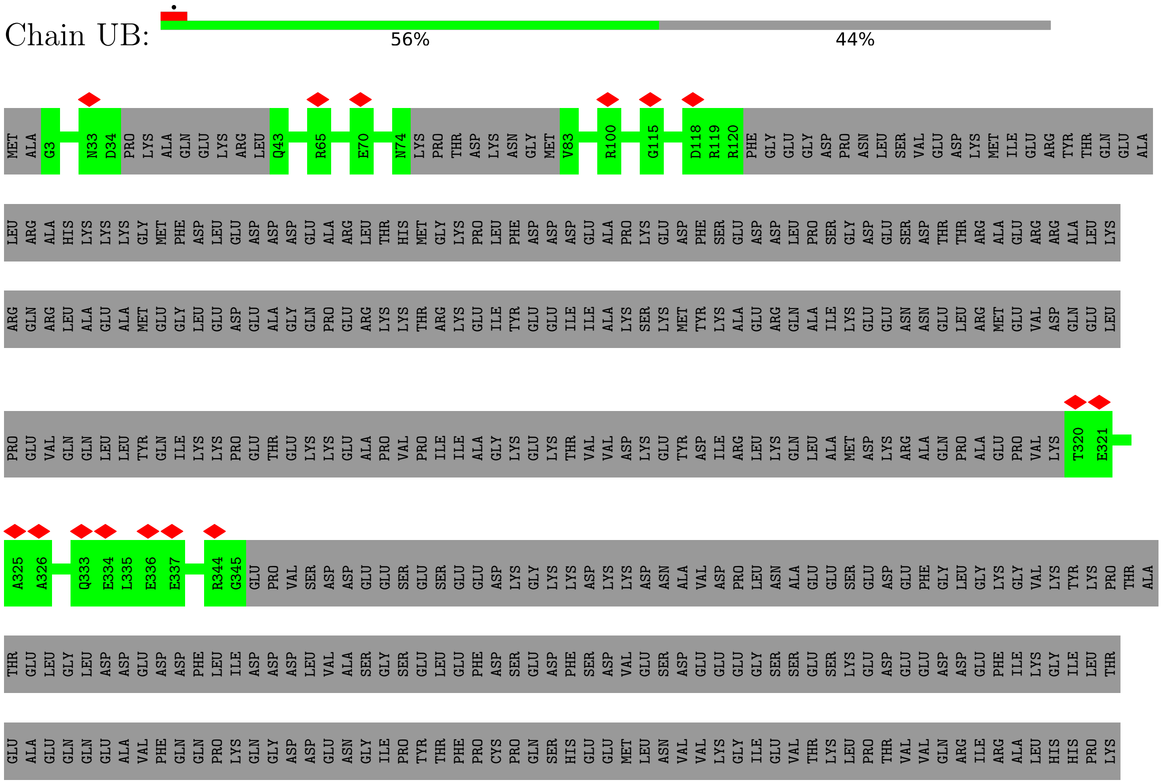
3 Residue-property plots ⓘ

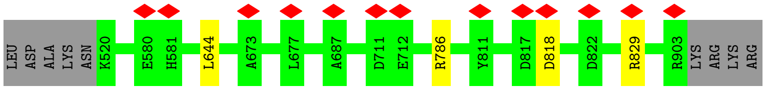
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Periodic tryptophan protein 2-like protein



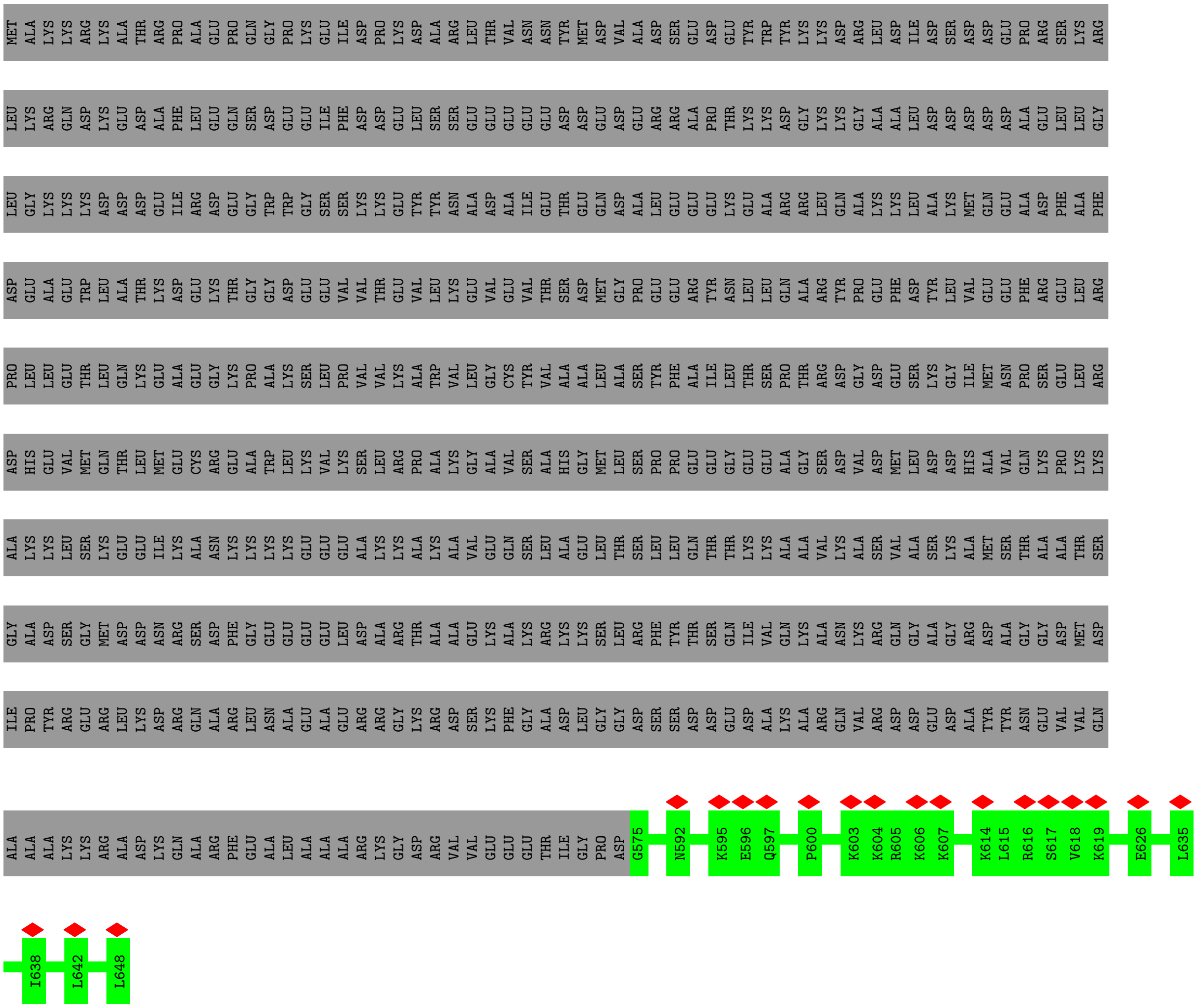
- Molecule 2: Utp2





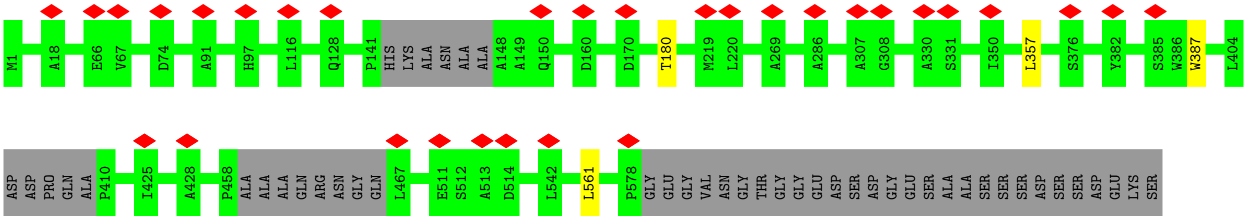
- Molecule 3: Utp3

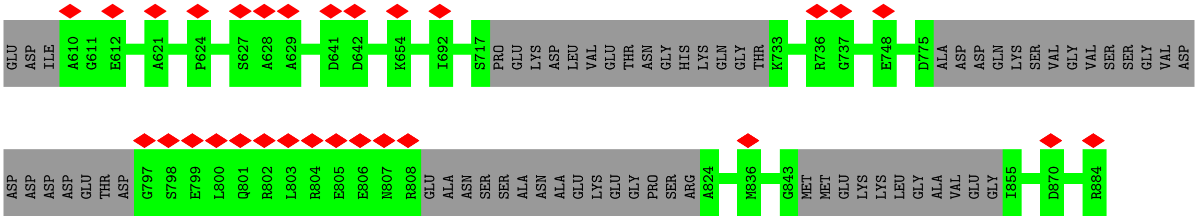
Chain UC:



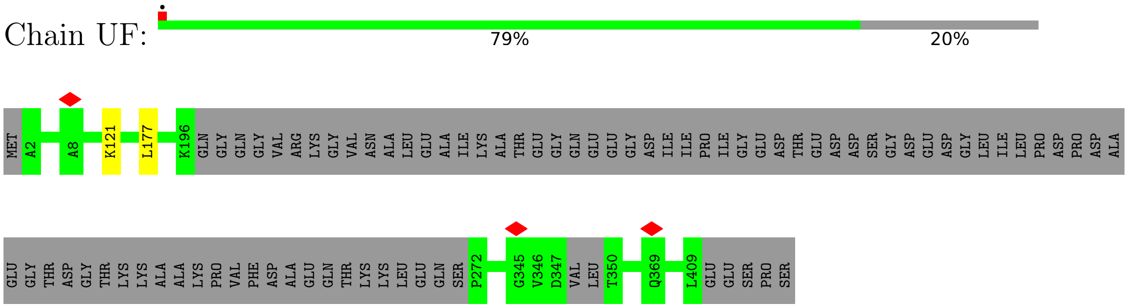
- Molecule 4: Utp4

Chain UD:

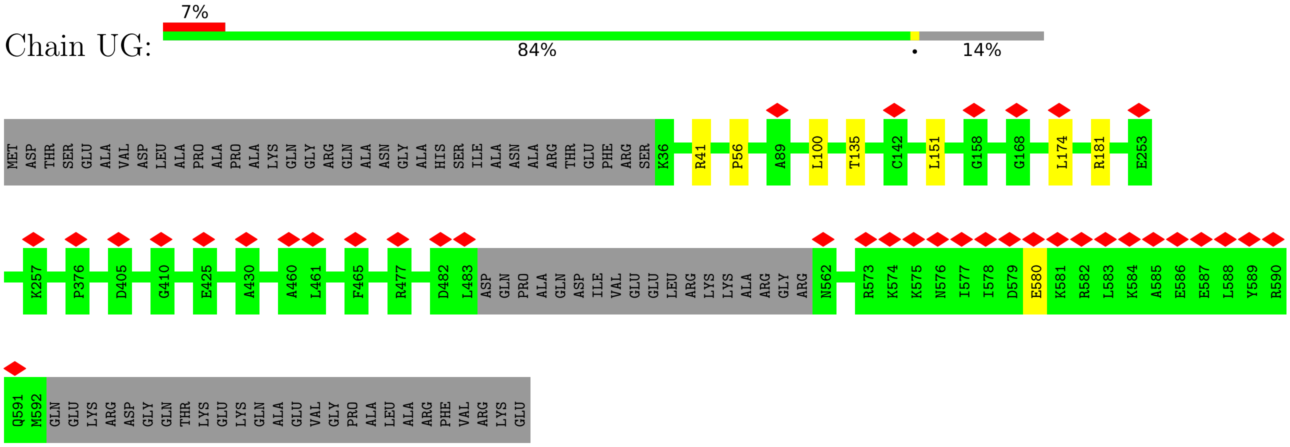




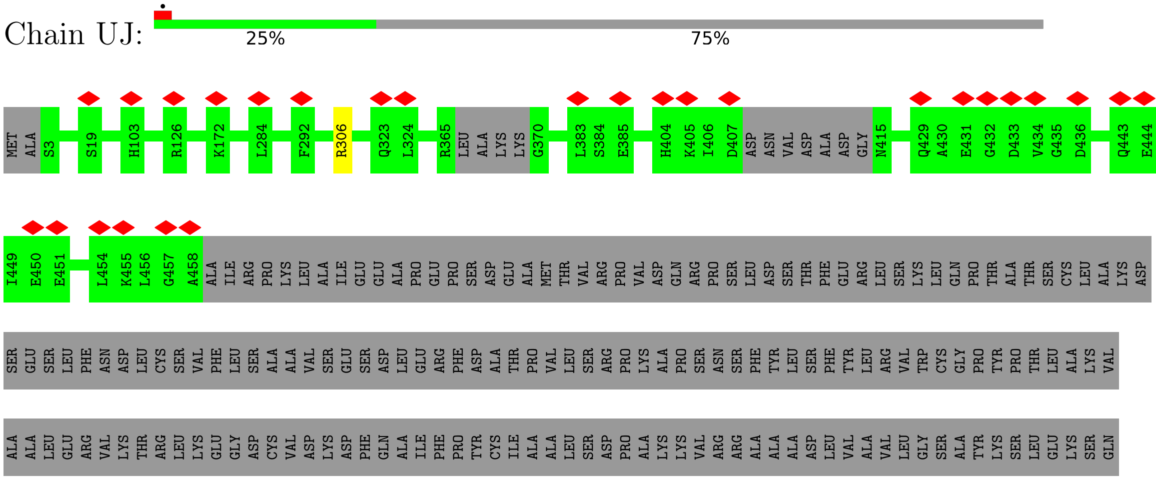
- Molecule 5: Utp6

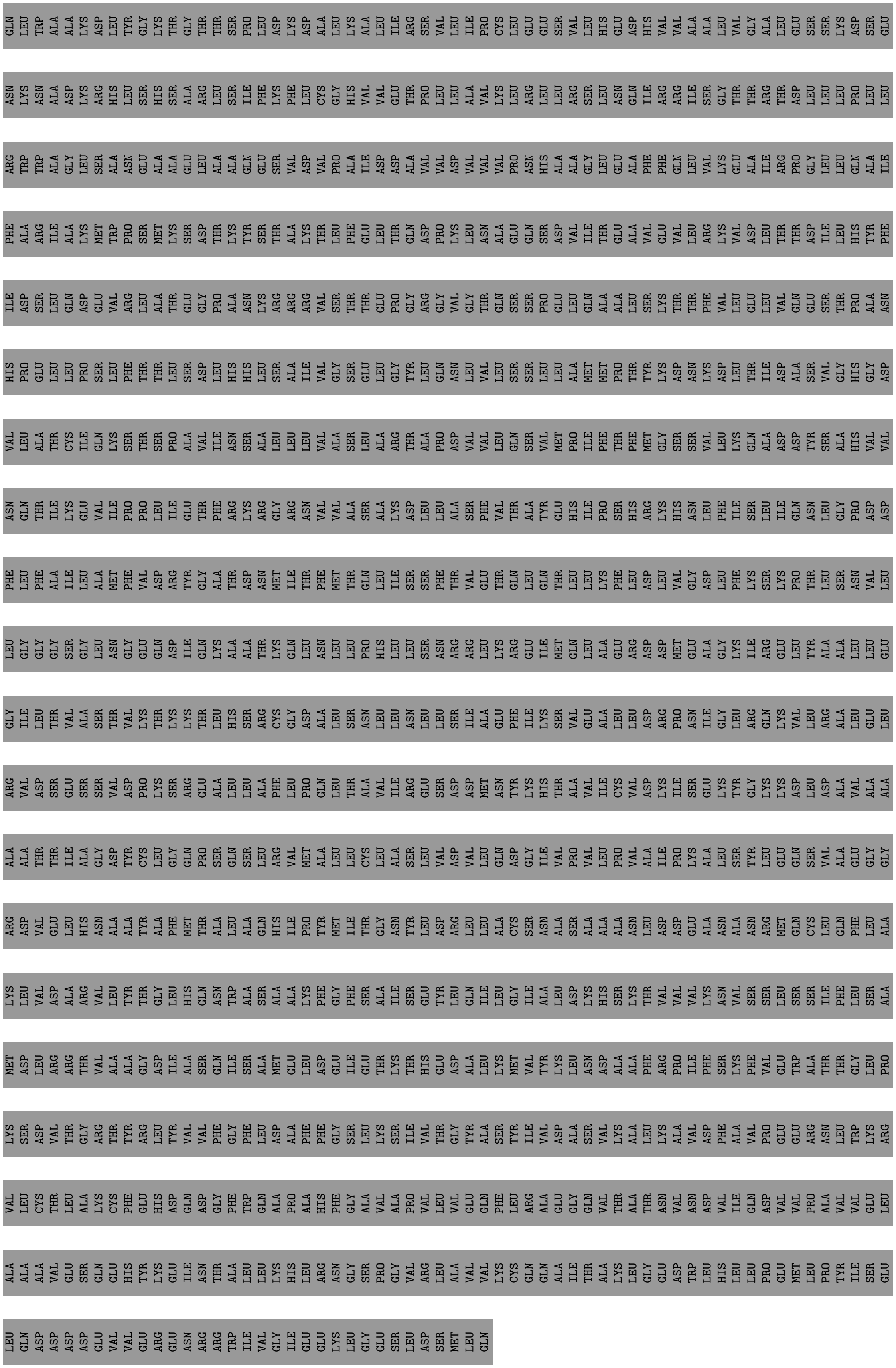


- Molecule 6: Utp7



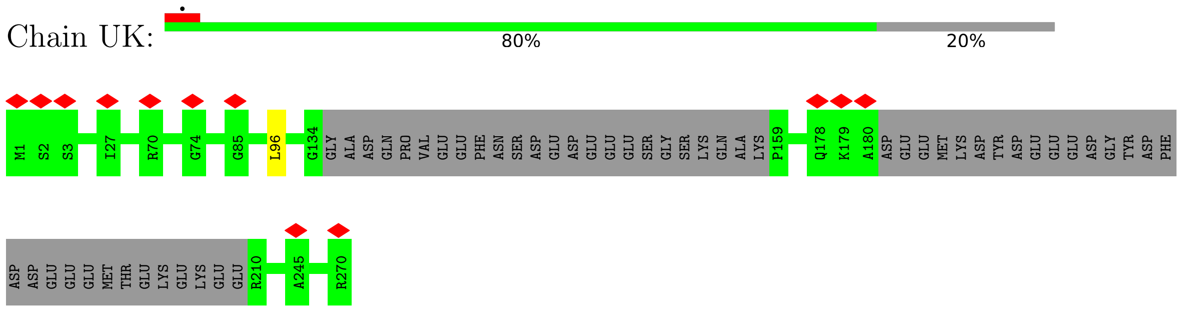
- Molecule 7: UTP10





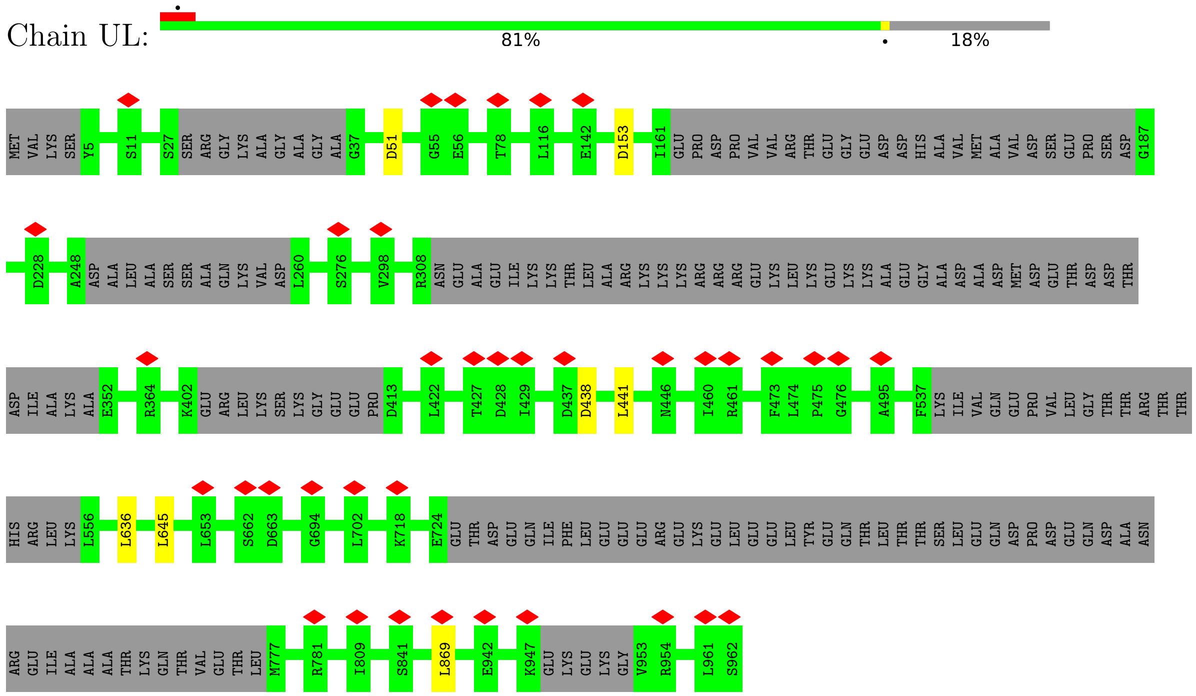
- Molecule 8: U3 small nucleolar RNA-associated protein 11

Chain UK:



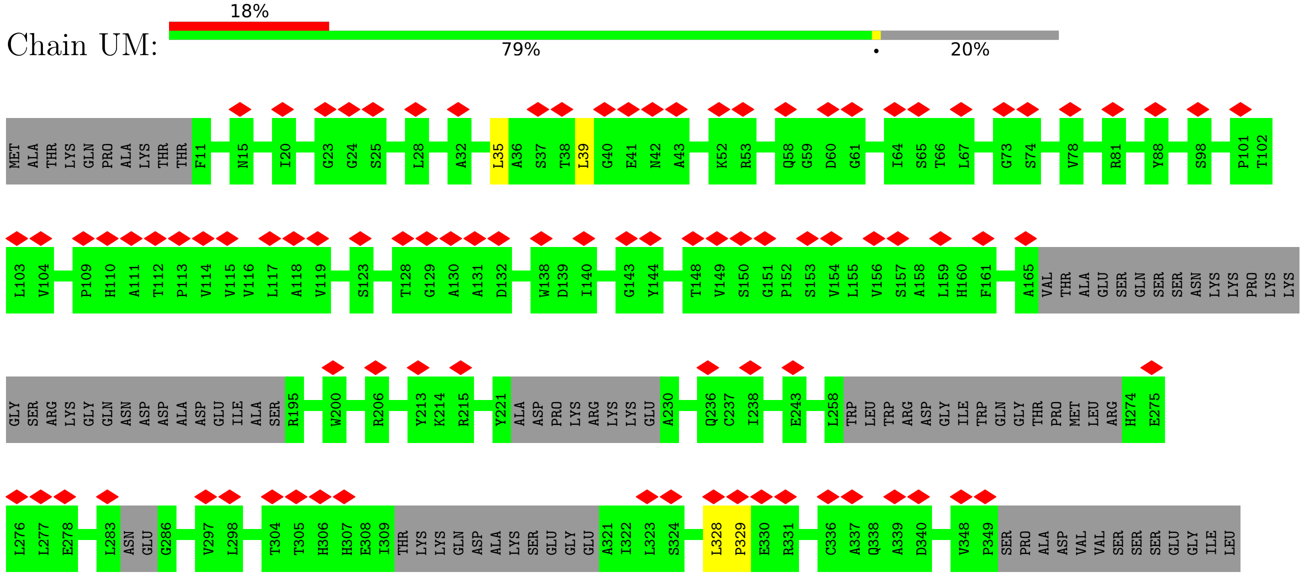
- Molecule 9: Utp12

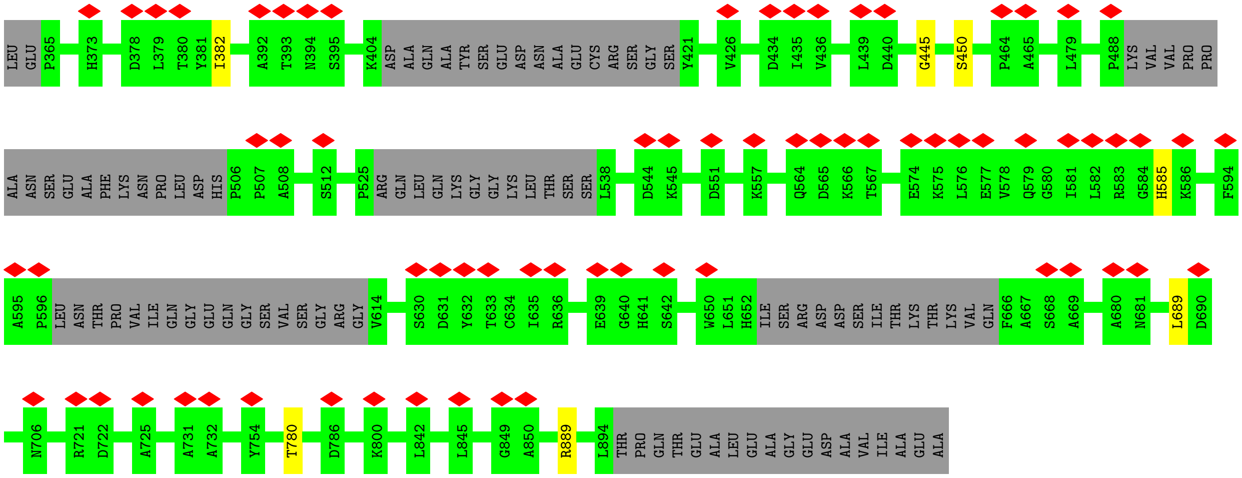
Chain UL:



- Molecule 10: Utp13"

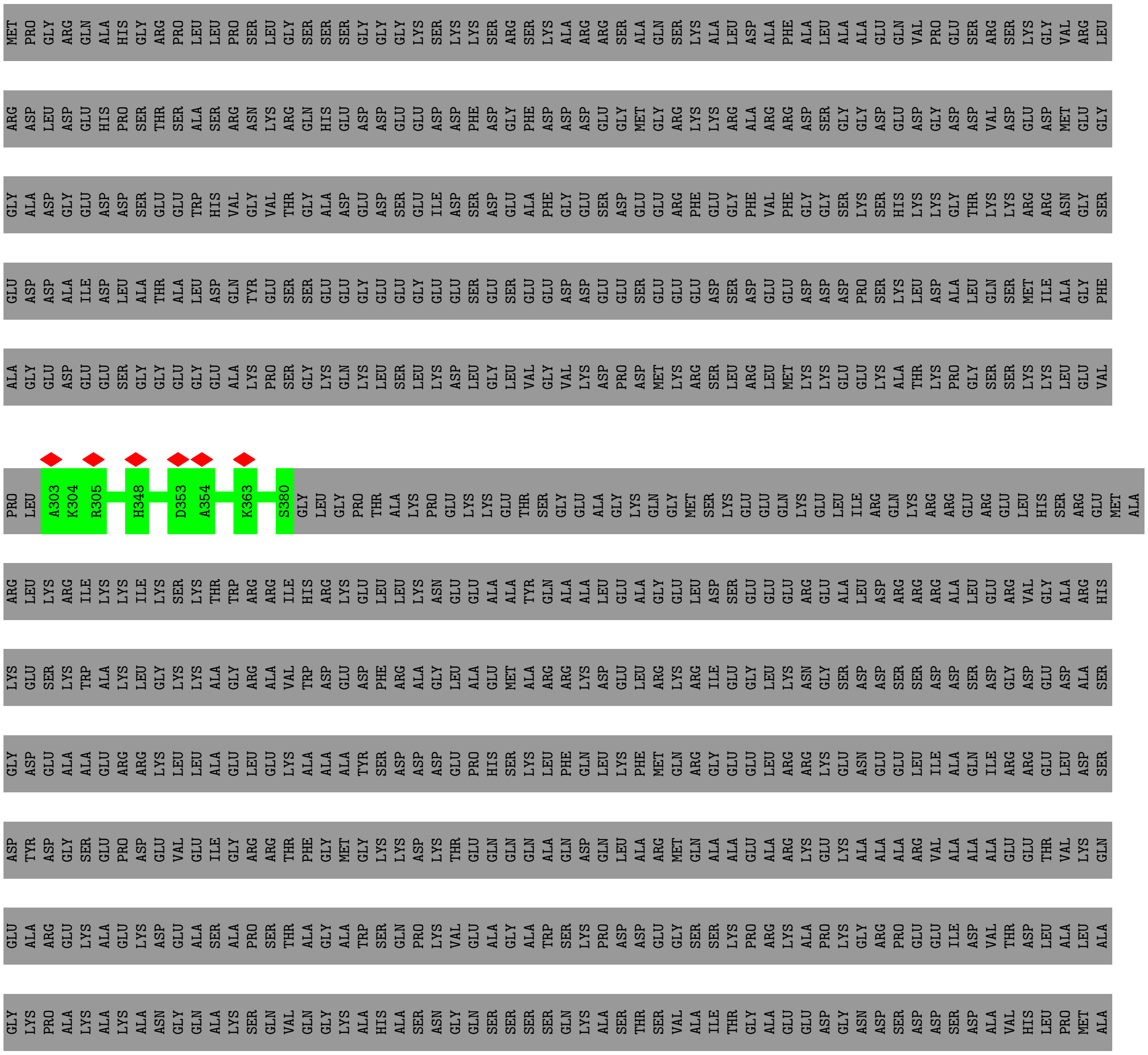
Chain UM:

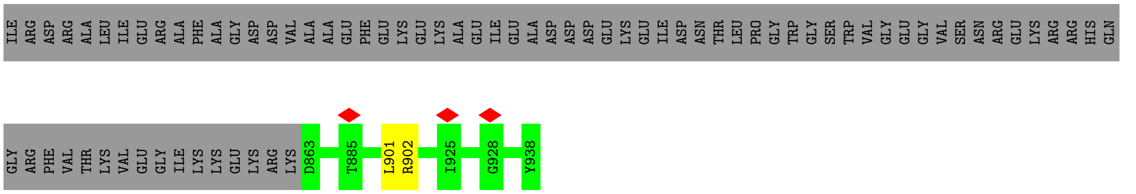




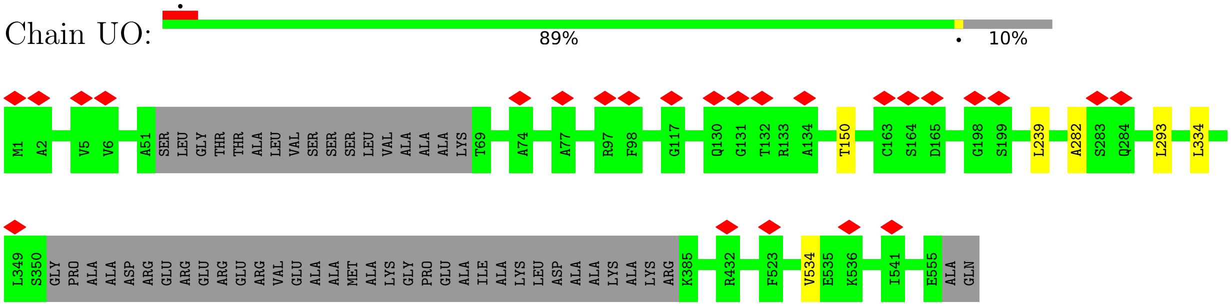
- Molecule 11: Utp14

Chain UN:

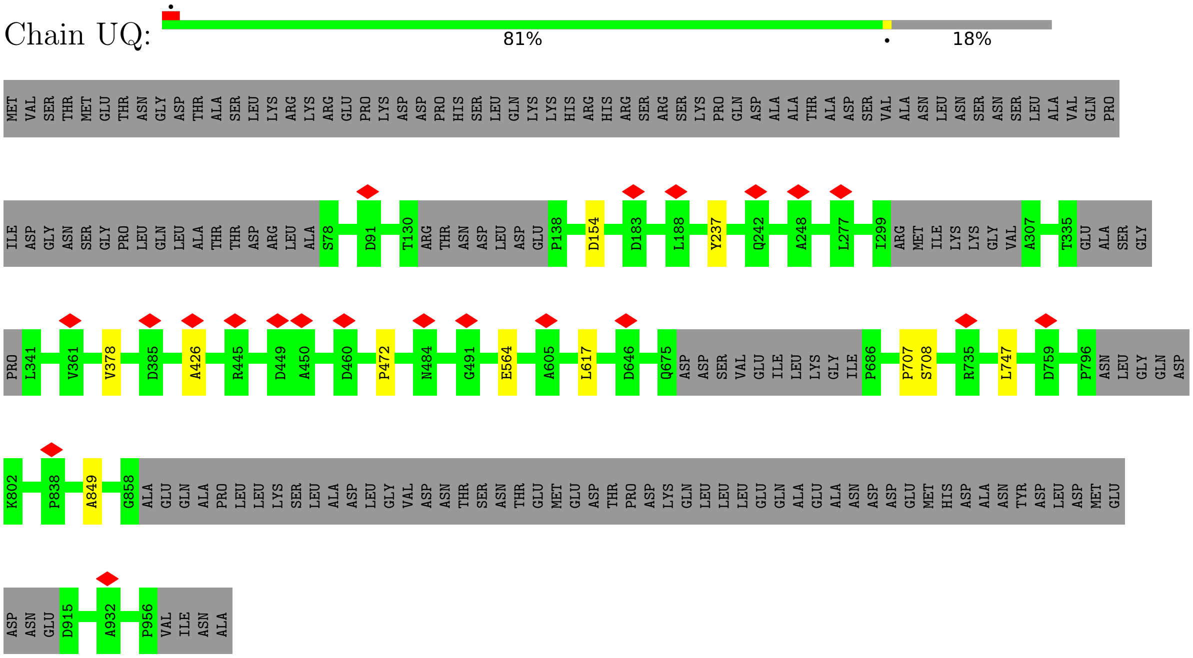




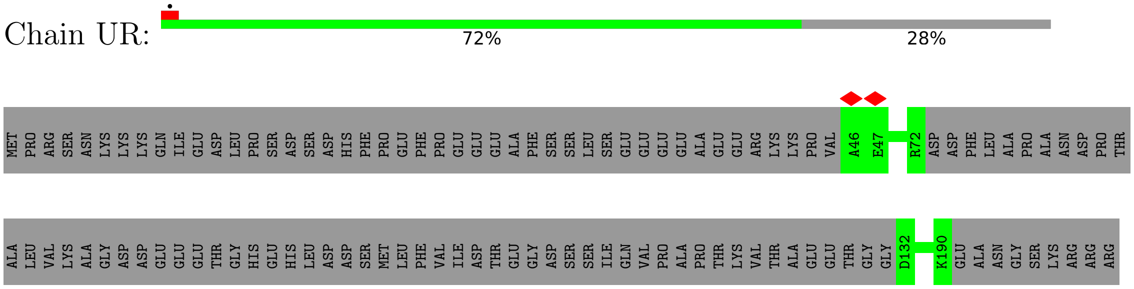
- Molecule 12: Utp15

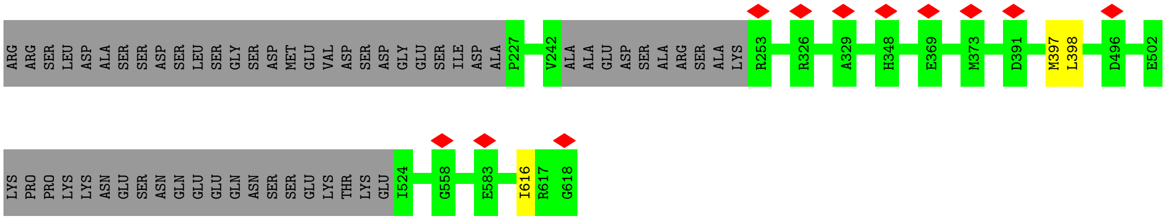


- Molecule 13: Utp17



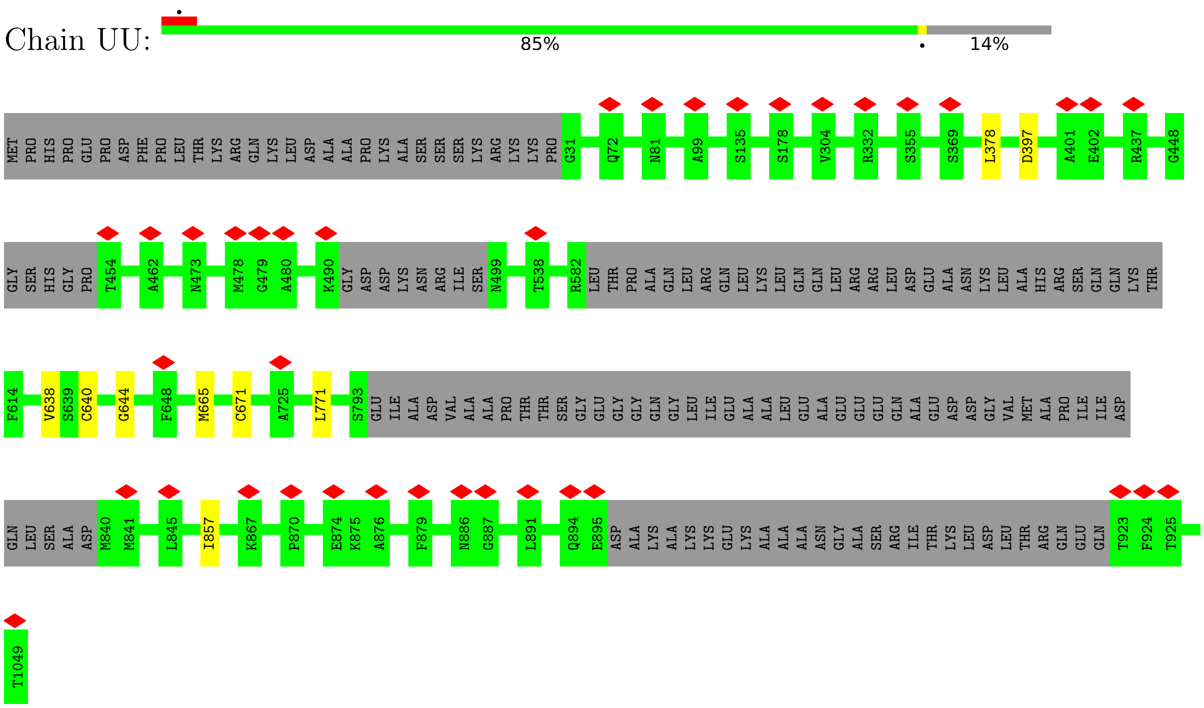
- Molecule 14: Utp18





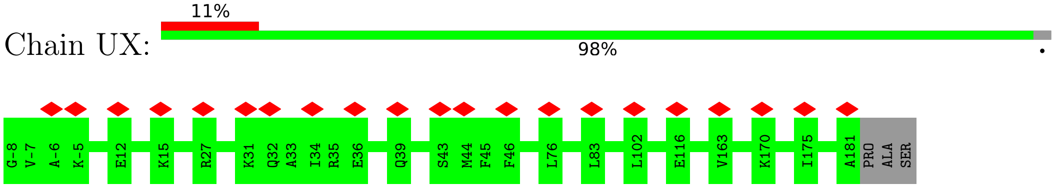
- Molecule 15: Putative U3 snoRNP protein

Chain UU:



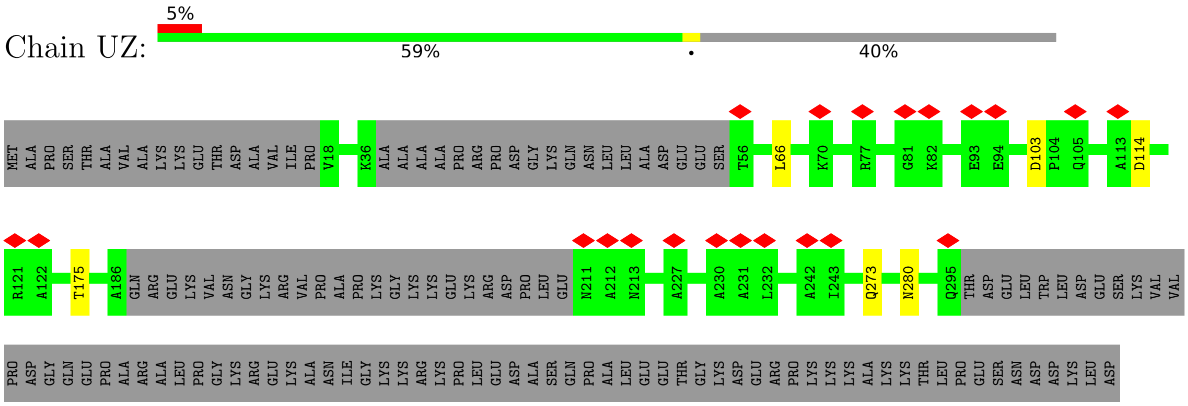
- Molecule 16: Utp24

Chain UX:

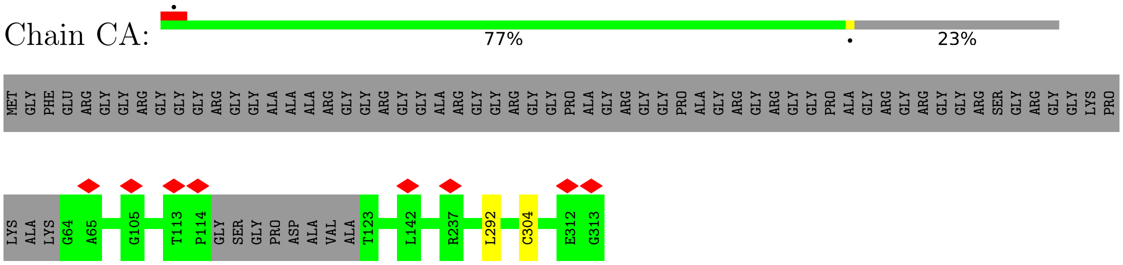


- Molecule 17: Utp30

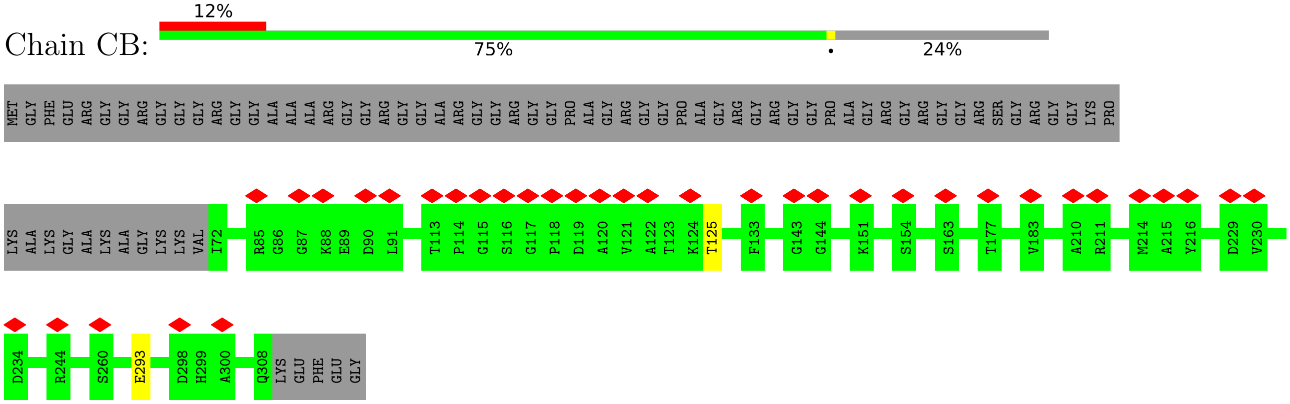
Chain UZ:



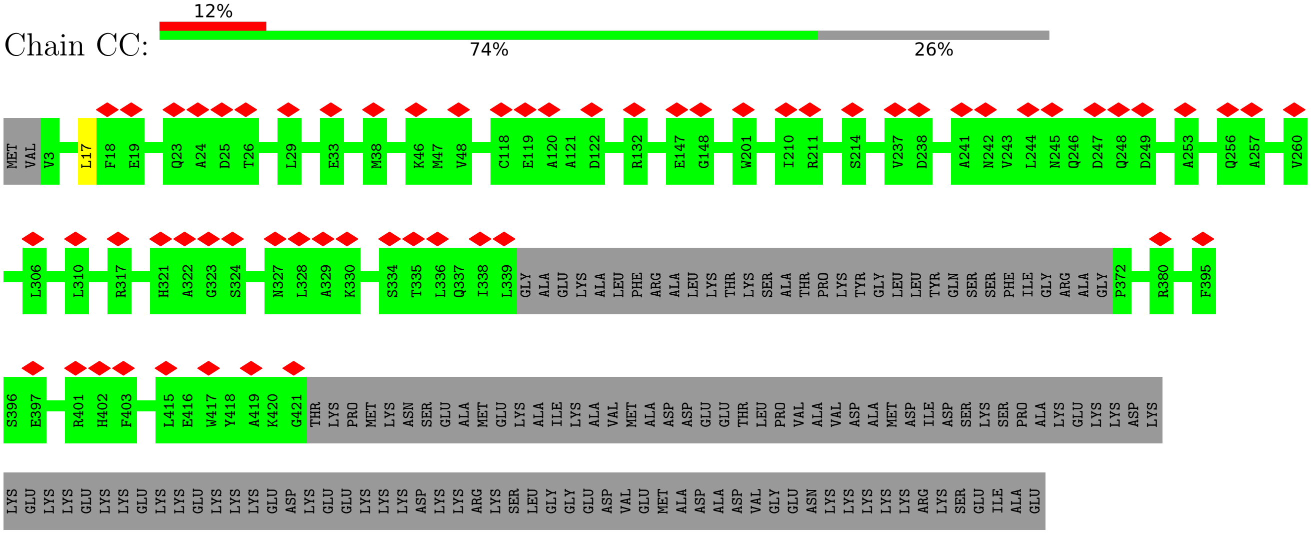
- Molecule 18: Nop1



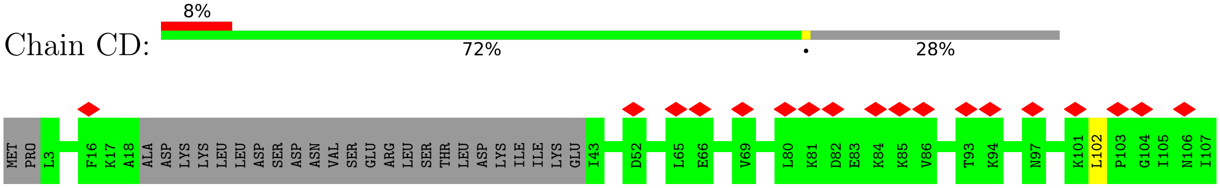
- Molecule 18: Nop1

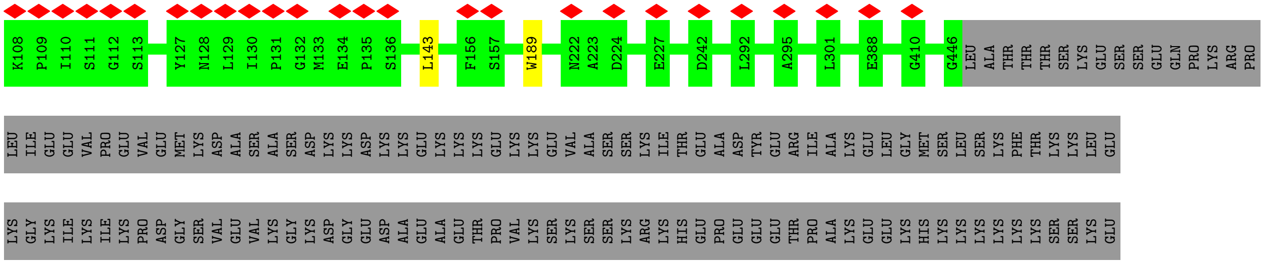


- Molecule 19: Putative nucleolar protein



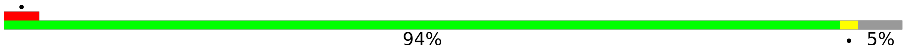
- Molecule 20: Nop58

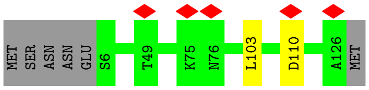




- Molecule 21: snu13

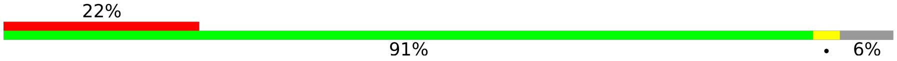
Chain CE:

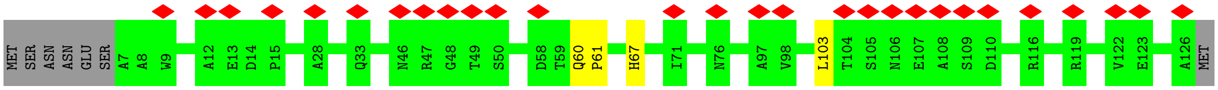




- Molecule 21: snu13

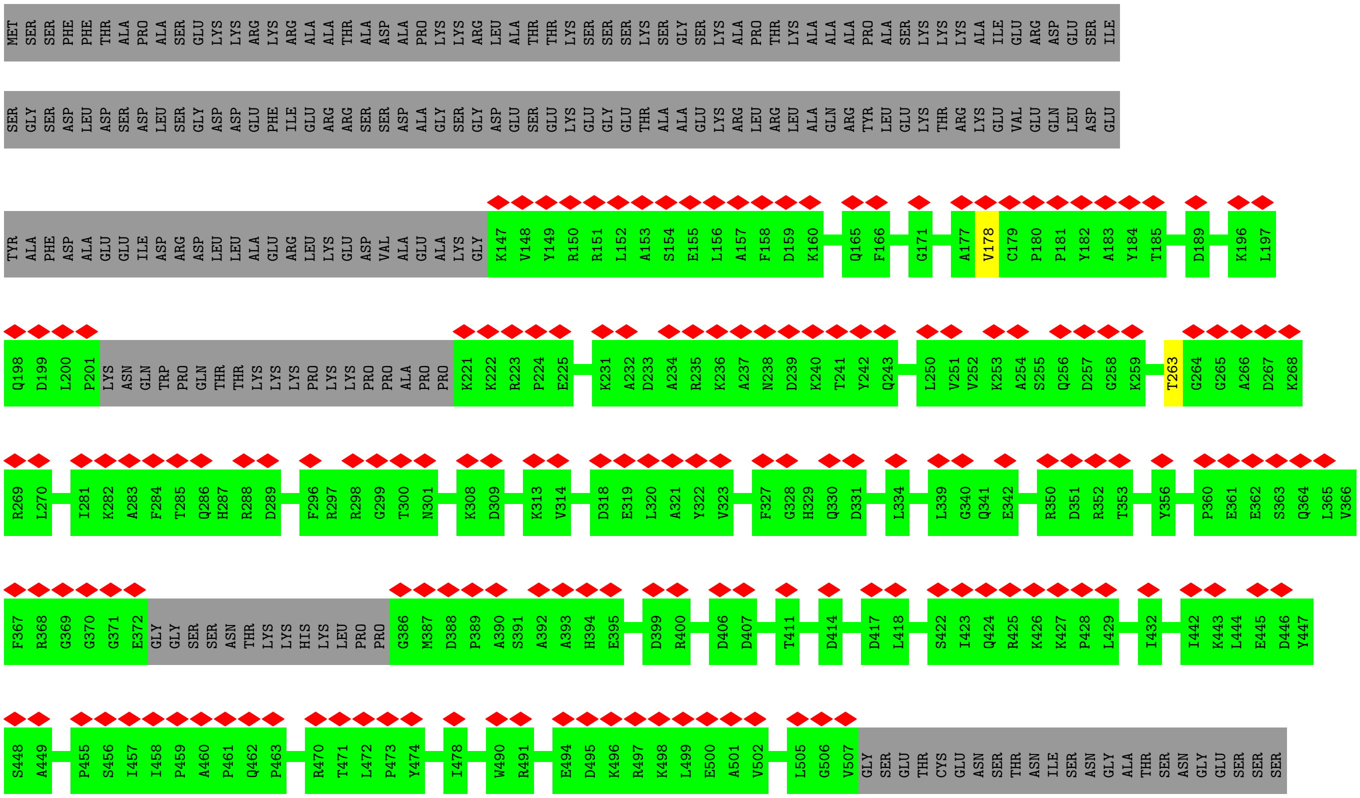
Chain CF:

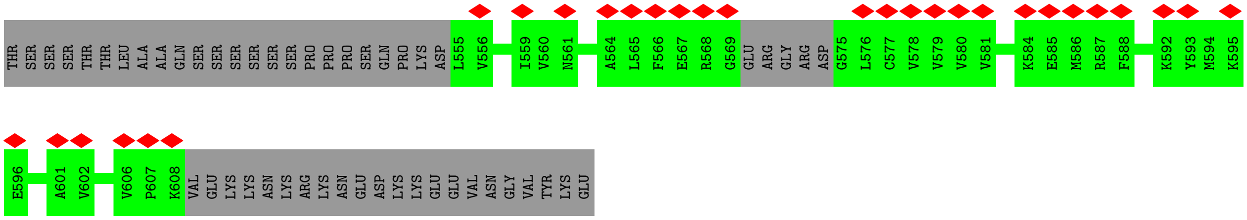




- Molecule 22: Rrp9

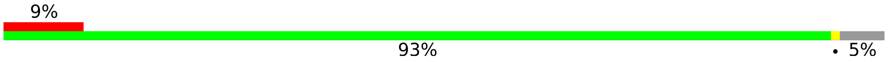
Chain CG:

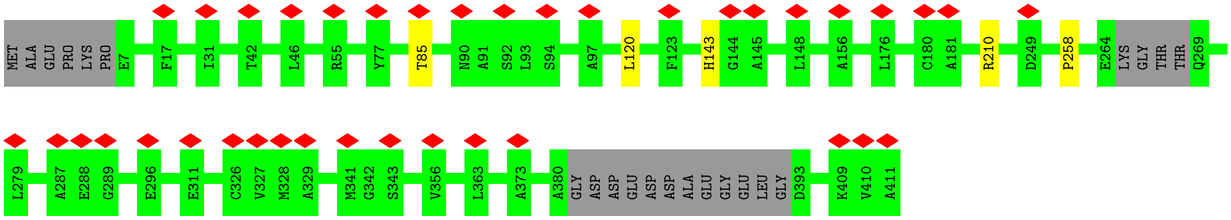




- Molecule 23: RNA 3'-terminal phosphate cyclase-like protein

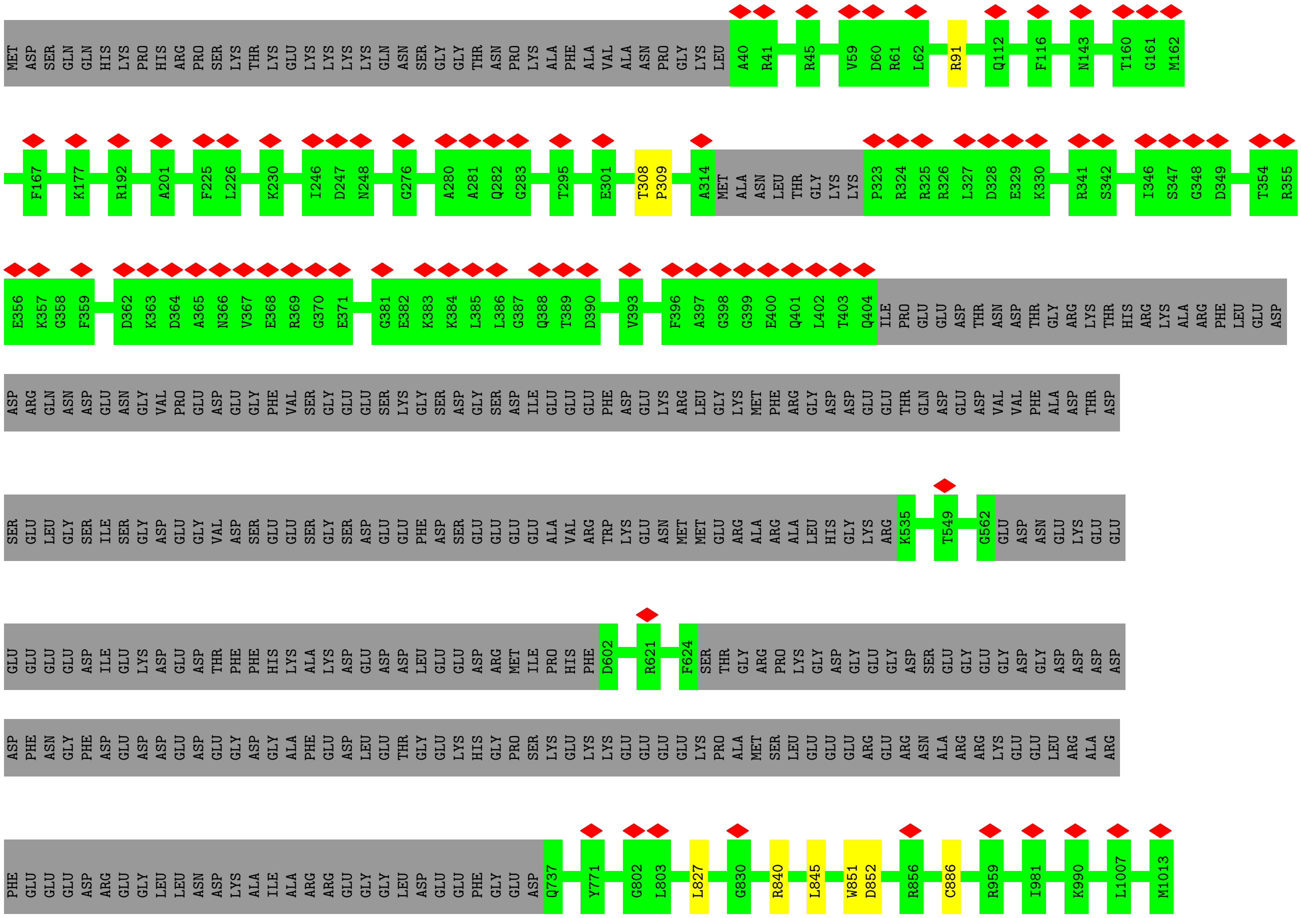
Chain CH:

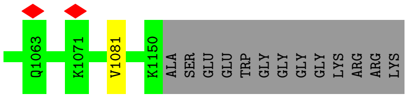




- Molecule 24: Bms1

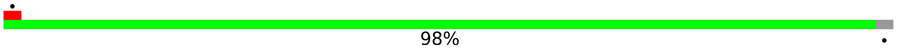
Chain CI:

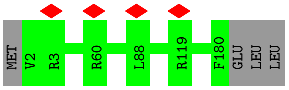




- Molecule 25: Imp3

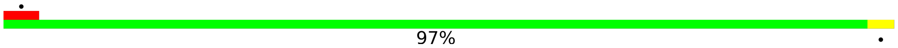
Chain CJ:

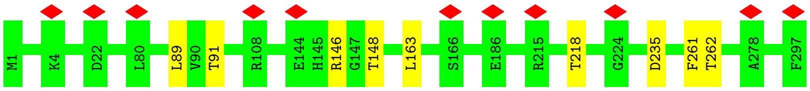




- Molecule 26: Putative U3 small nucleolar ribonucleoprotein

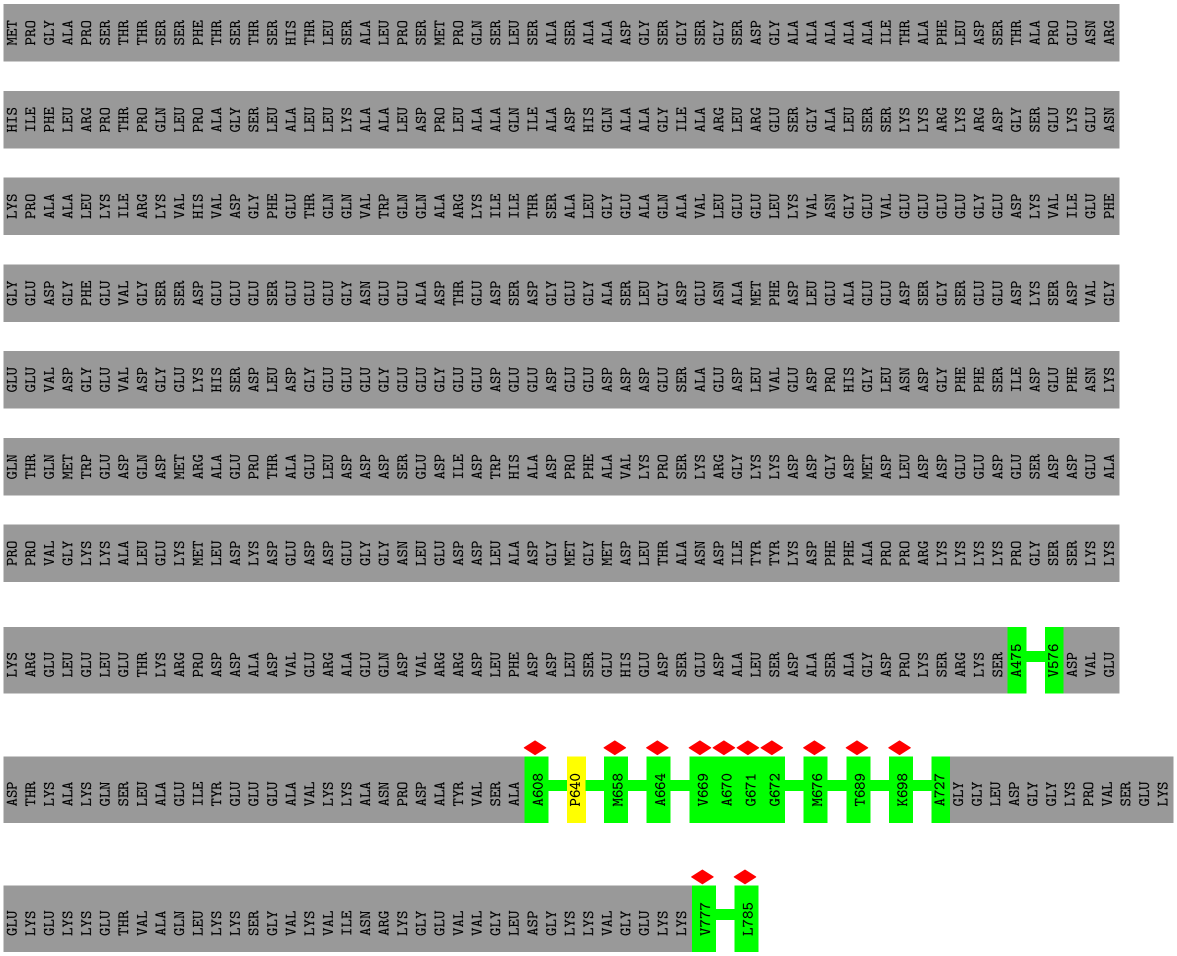
Chain CK:





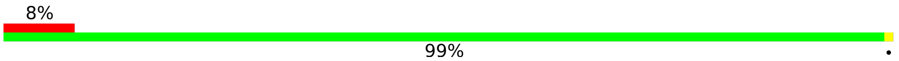
- Molecule 27: Putative U3 small nucleolar ribonucleoprotein protein

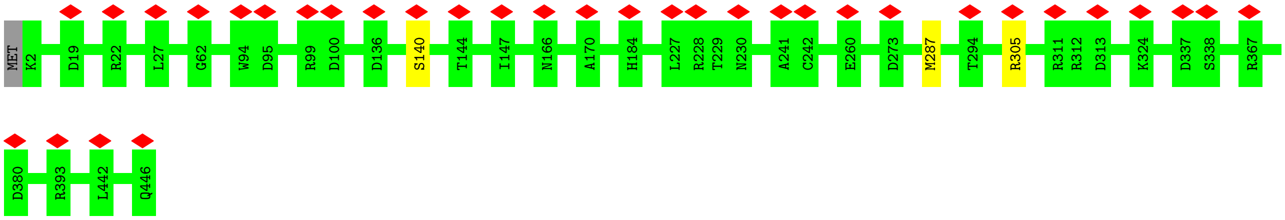
Chain CL:



- Molecule 28: Sof1

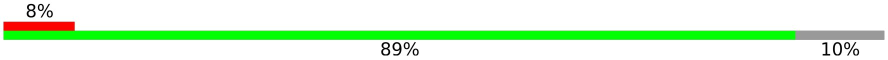
Chain CM:

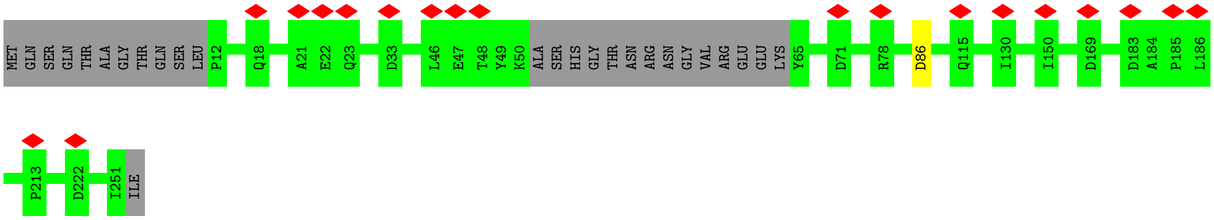




- Molecule 29: Emg1

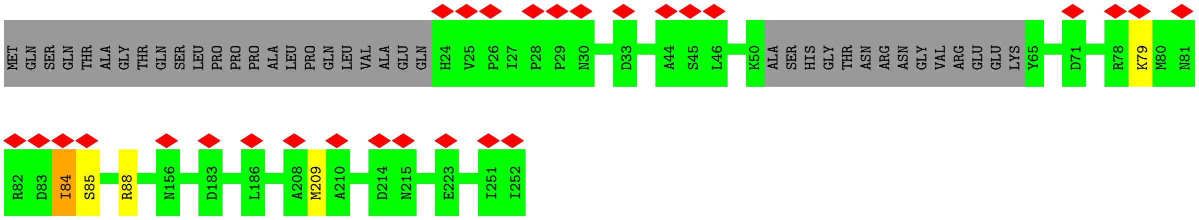
Chain CN:





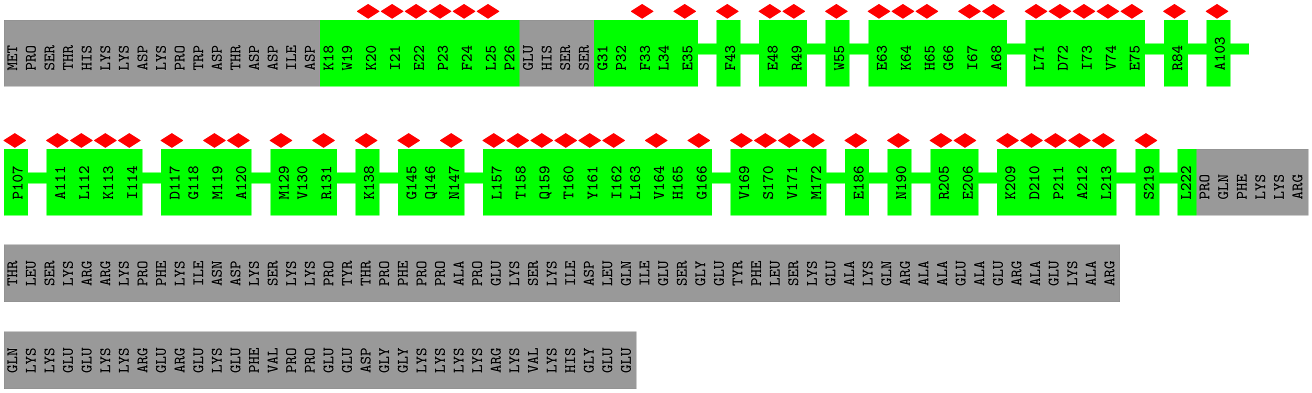
- Molecule 29: Emg1

Chain CO:

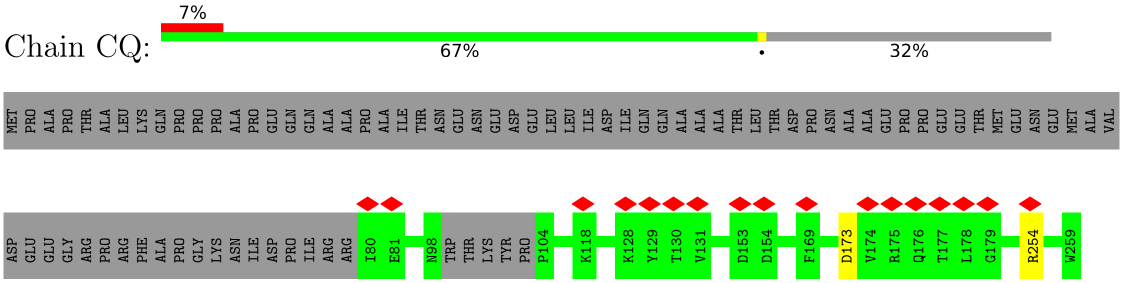


- Molecule 30: KRR1 small subunit processome component

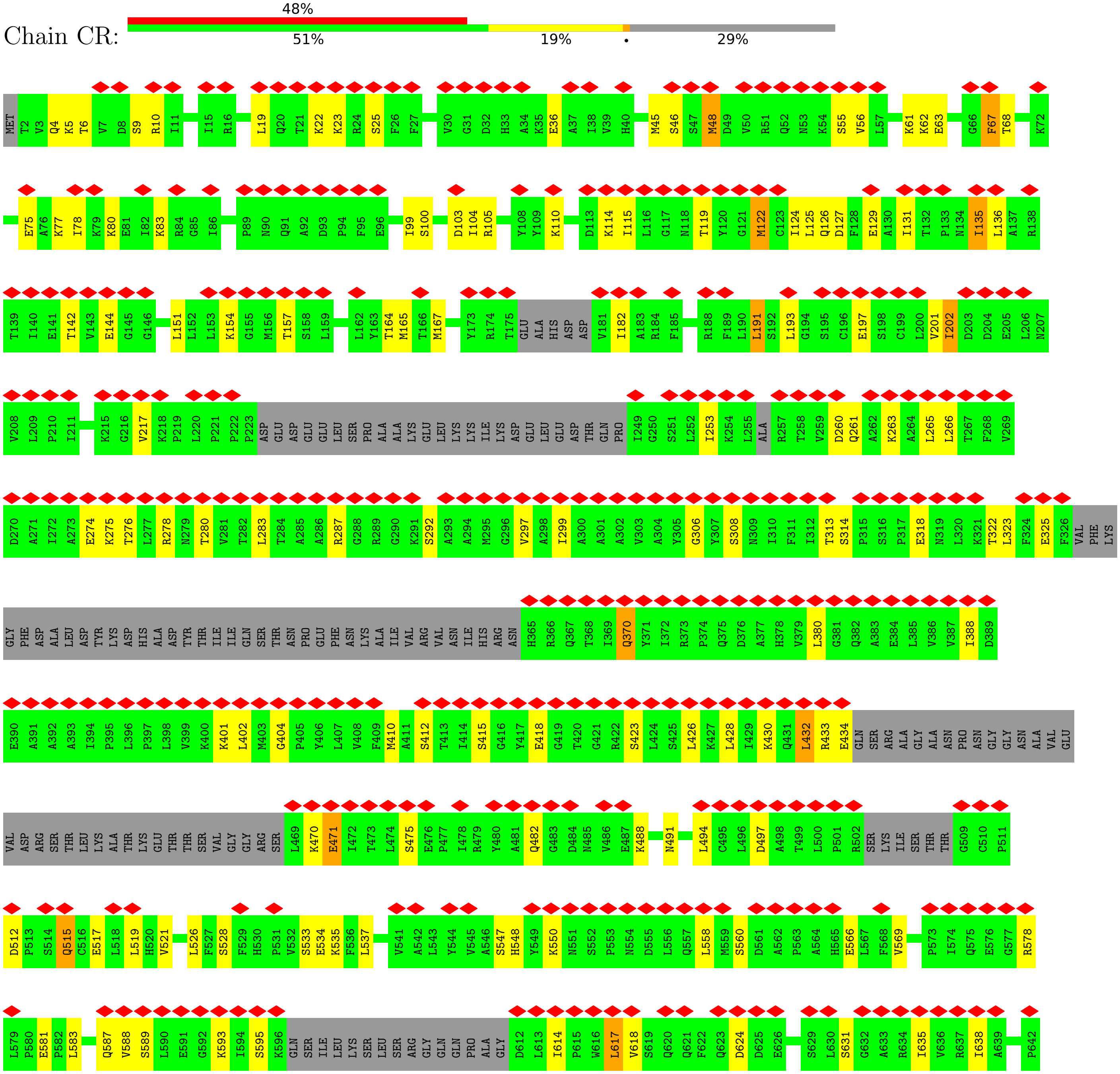
Chain CP:

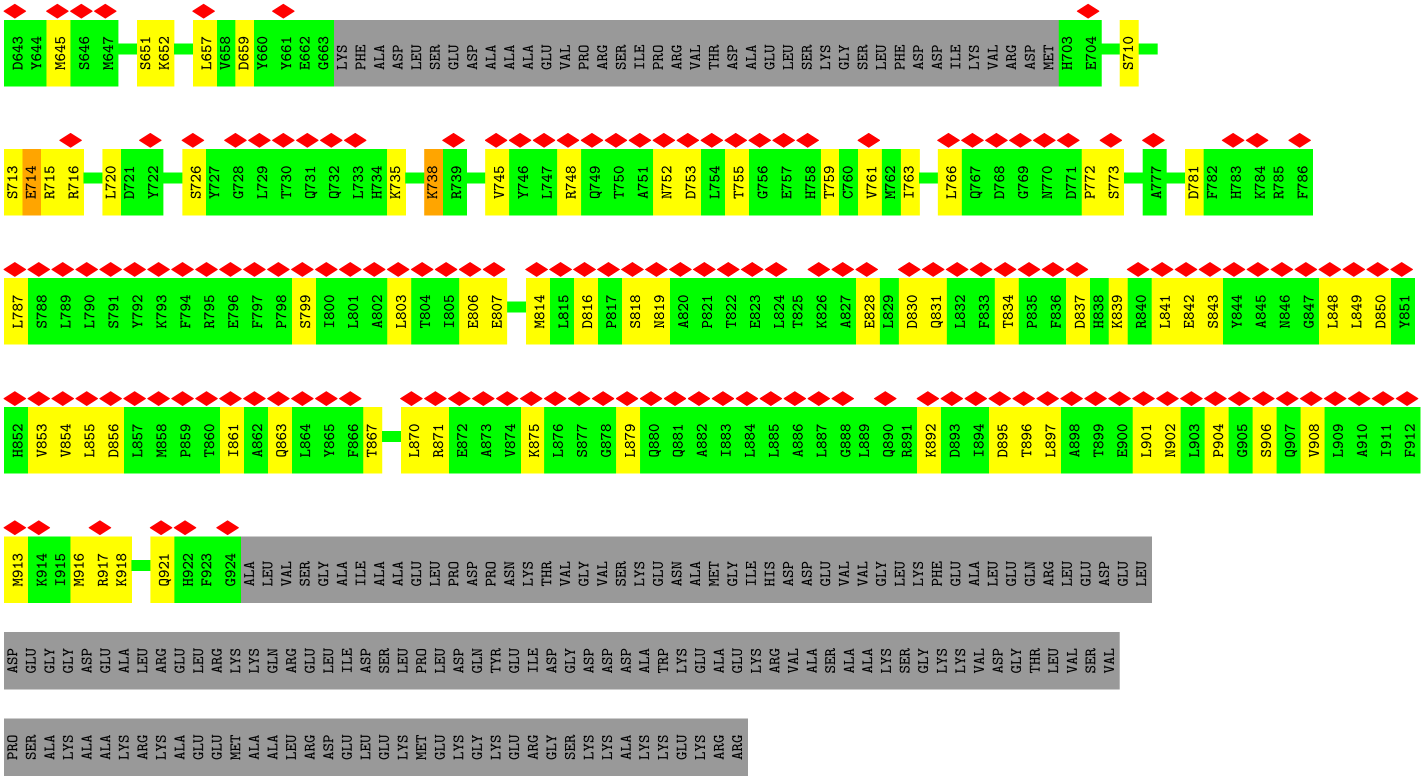


- Molecule 31: Pre-rRNA-processing protein PNO1



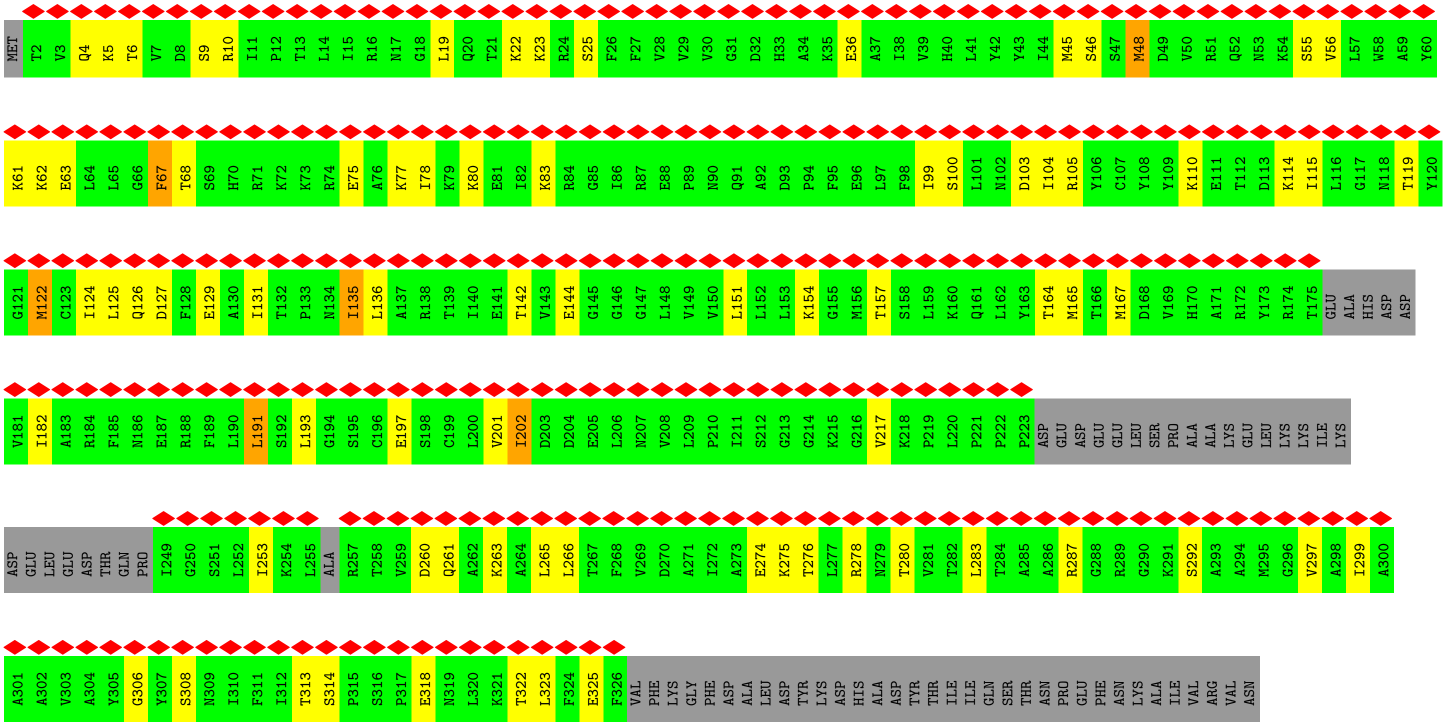
- Molecule 32: Kre33

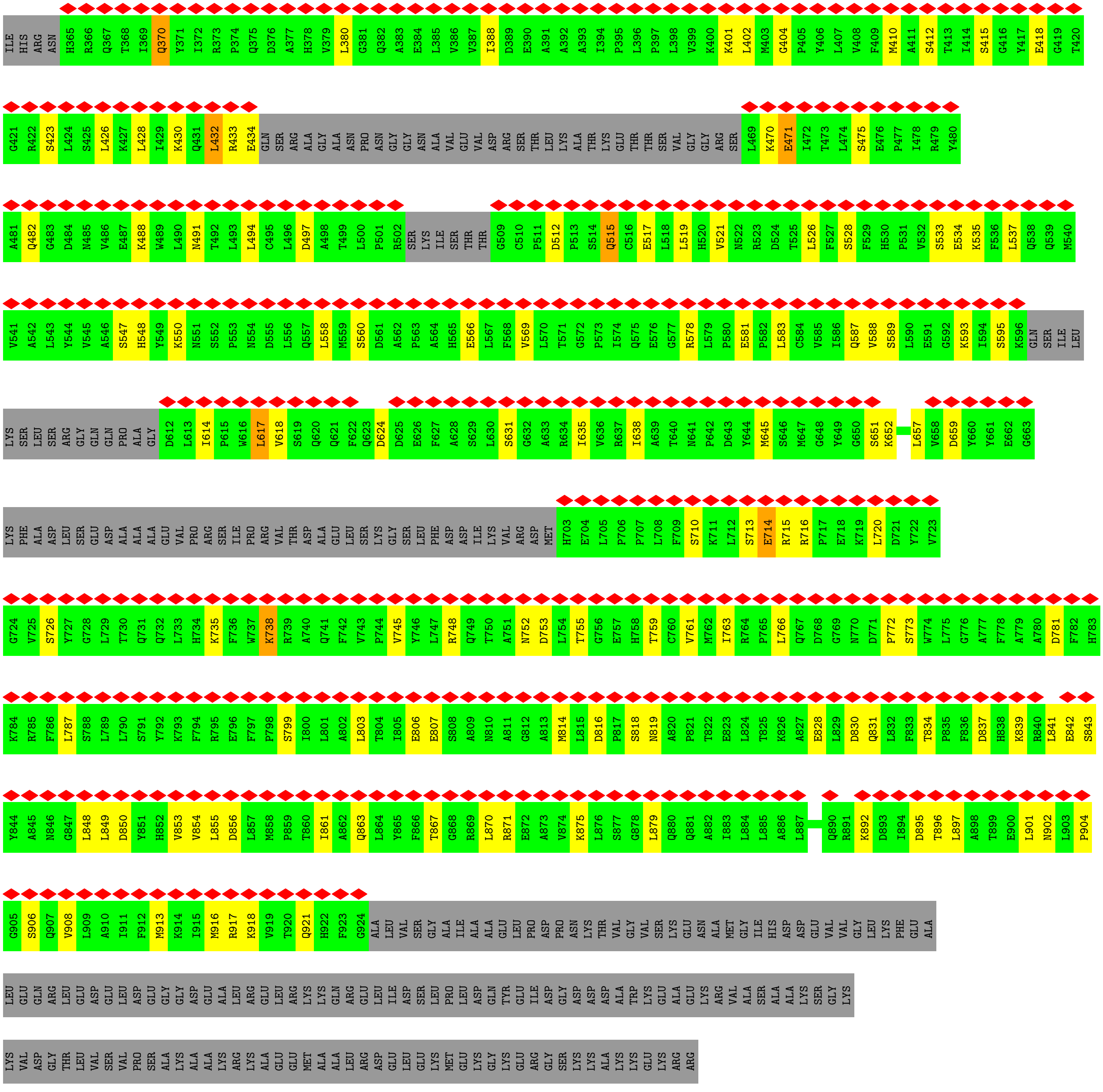




- Molecule 32: Kre33

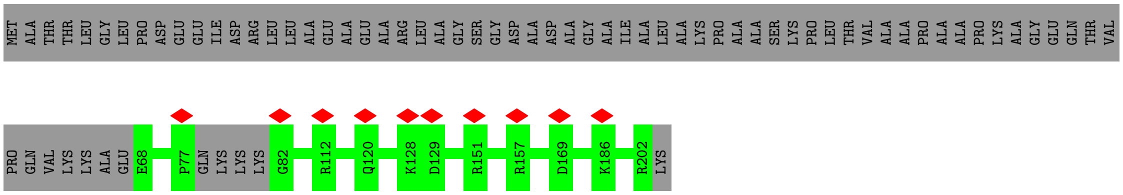
Chain CS:



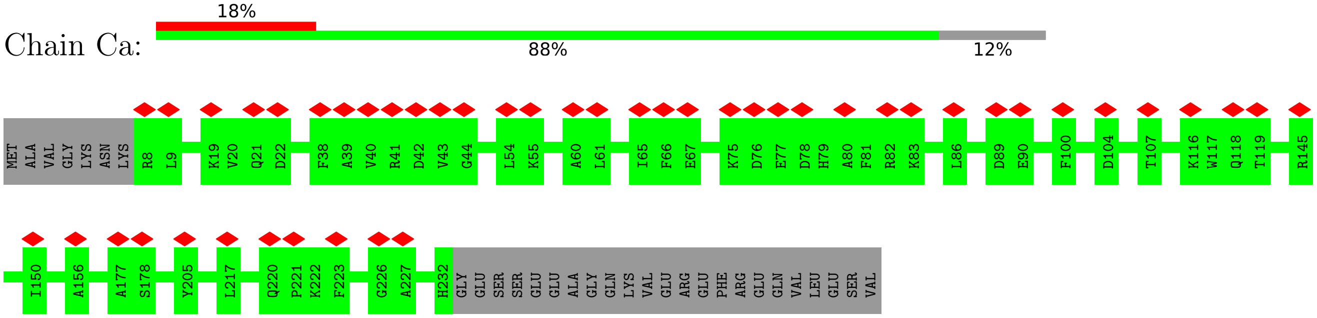


- Molecule 33: Fcf2

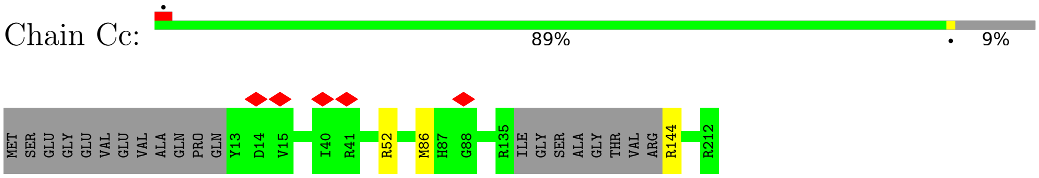
Chain CT:



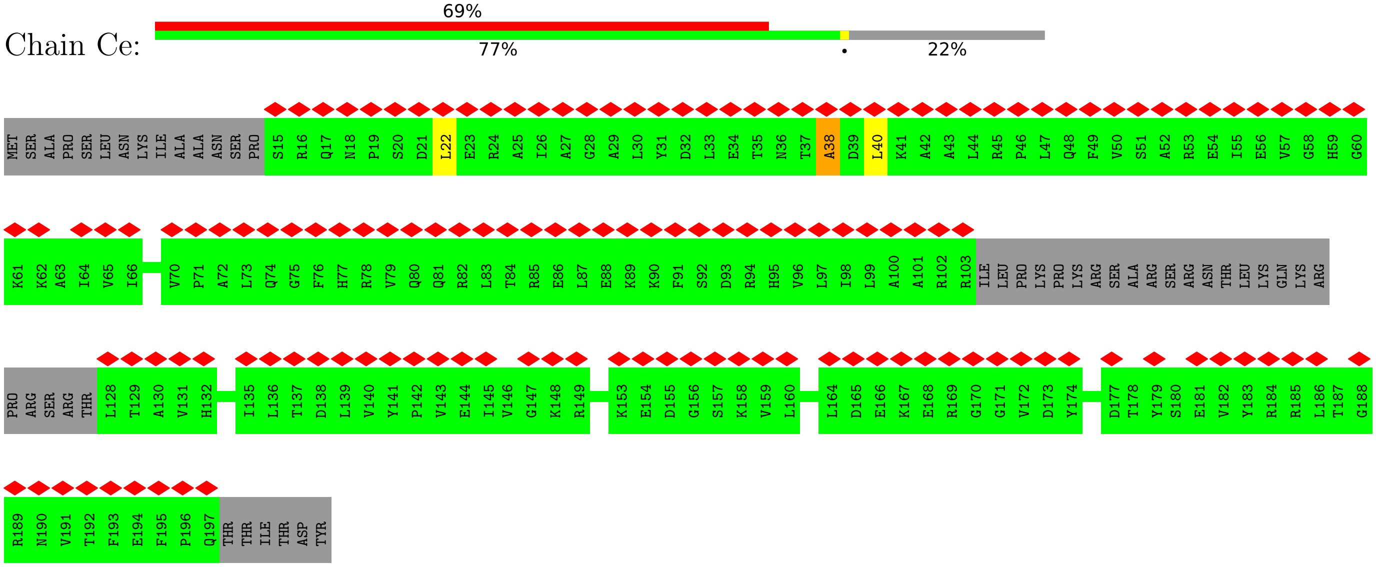
- Molecule 34: 40S ribosomal protein S1



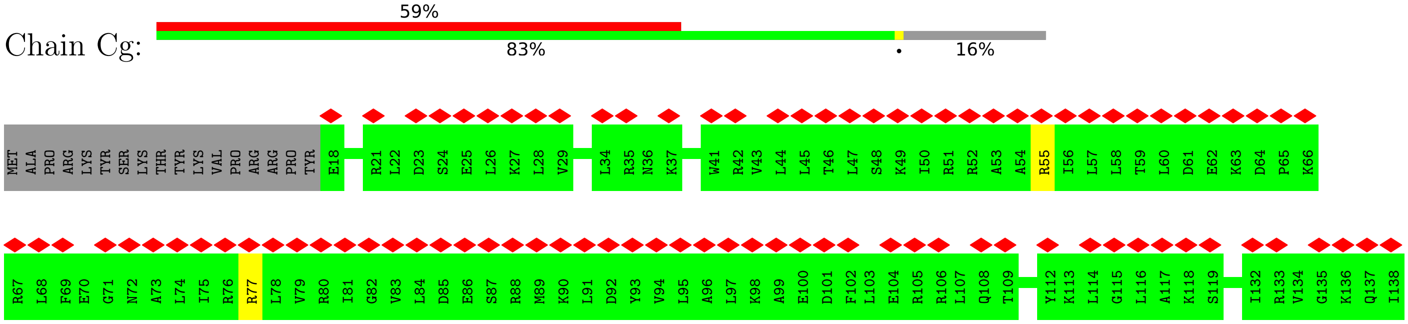
- Molecule 35: 40S ribosomal protein s5-like protein

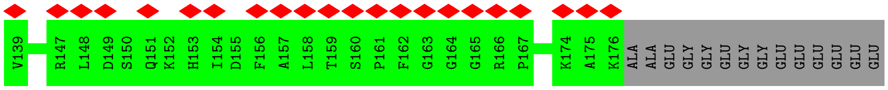


- Molecule 36: 40S ribosomal protein S7



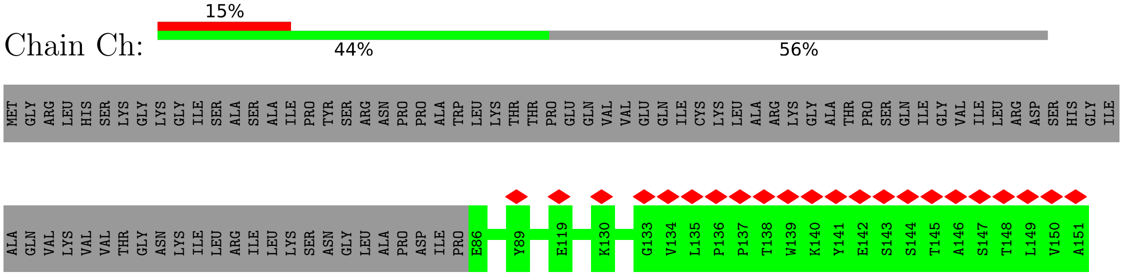
- Molecule 37: 40S ribosomal protein s9-like protein





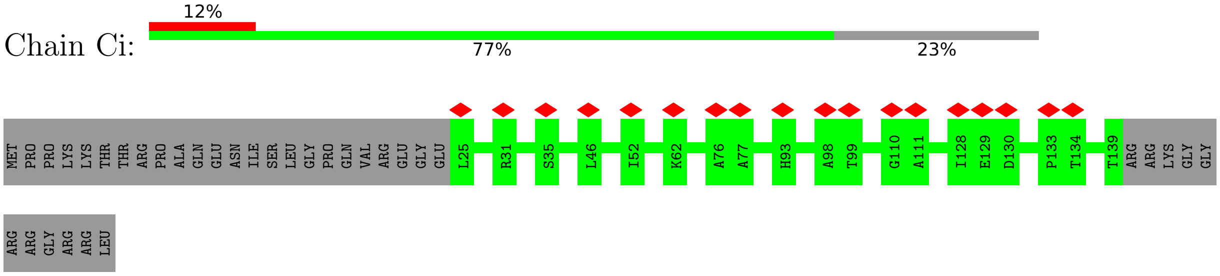
- Molecule 38: 40S ribosomal protein S13-like protein

Chain Ch:



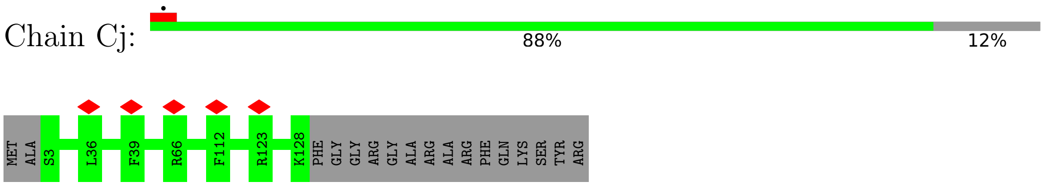
- Molecule 39: 40S ribosomal protein S14-like protein

Chain Ci:



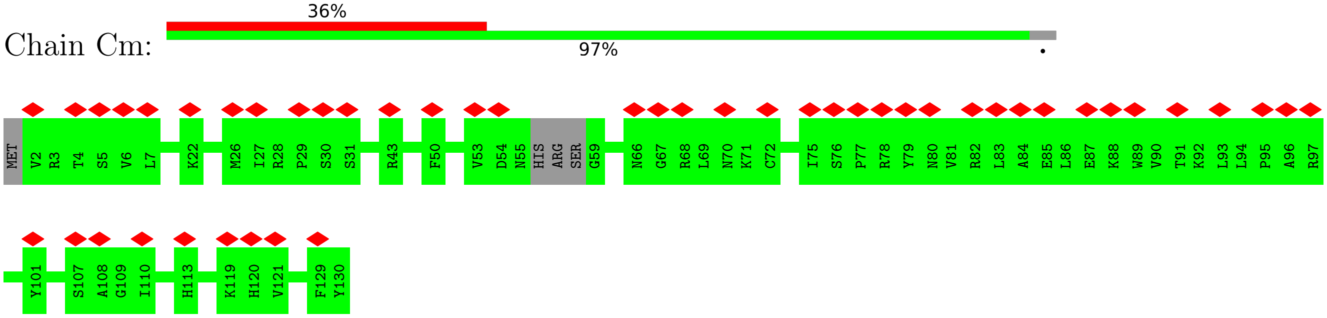
- Molecule 40: 40S ribosomal protein S16-like protein

Chain Cj:



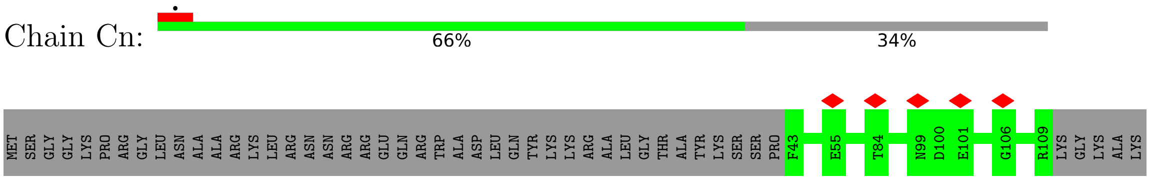
- Molecule 41: 40S ribosomal protein S22-like protein

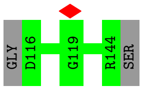
Chain Cm:



- Molecule 42: 40S ribosomal protein s23-like protein

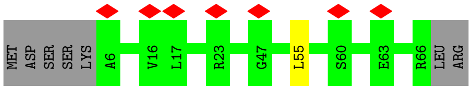
Chain Cn:





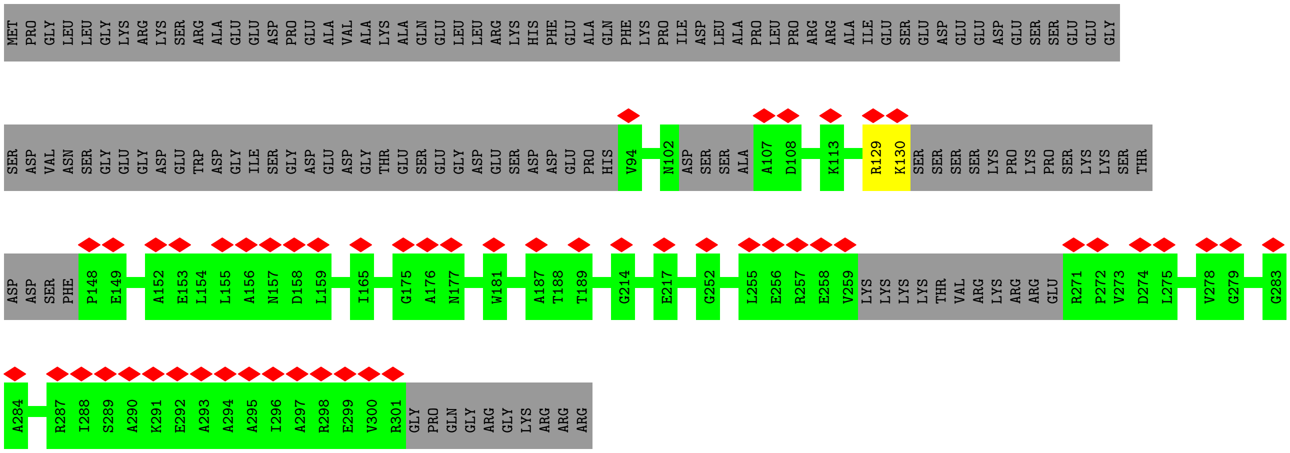
- Molecule 43: 40S ribosomal protein S28-like protein

Chain Cp:



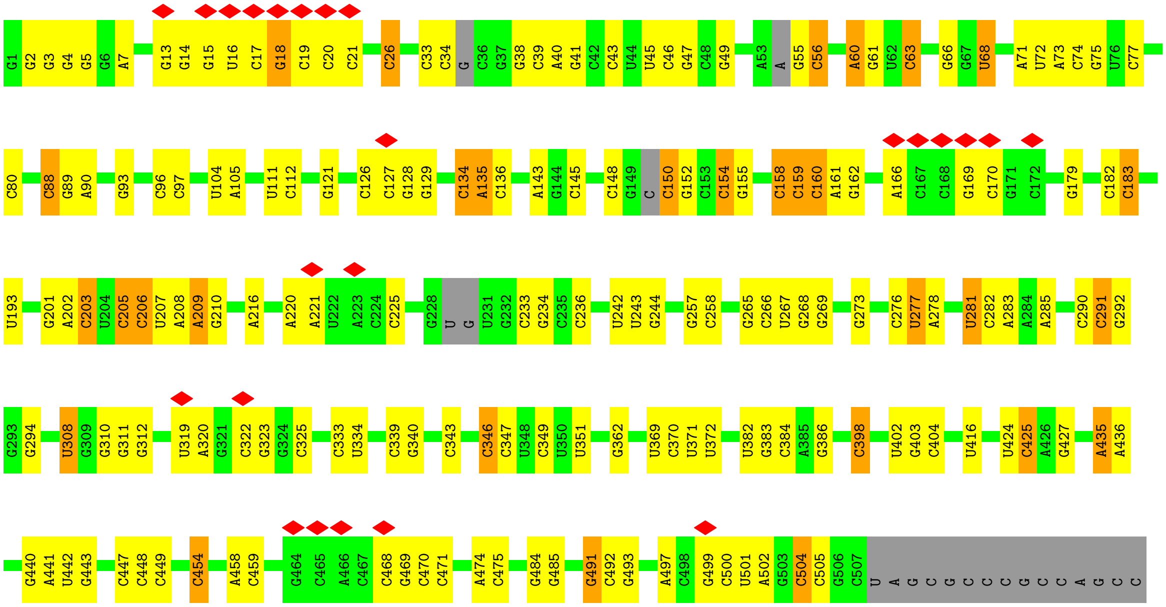
- Molecule 44: Faf1

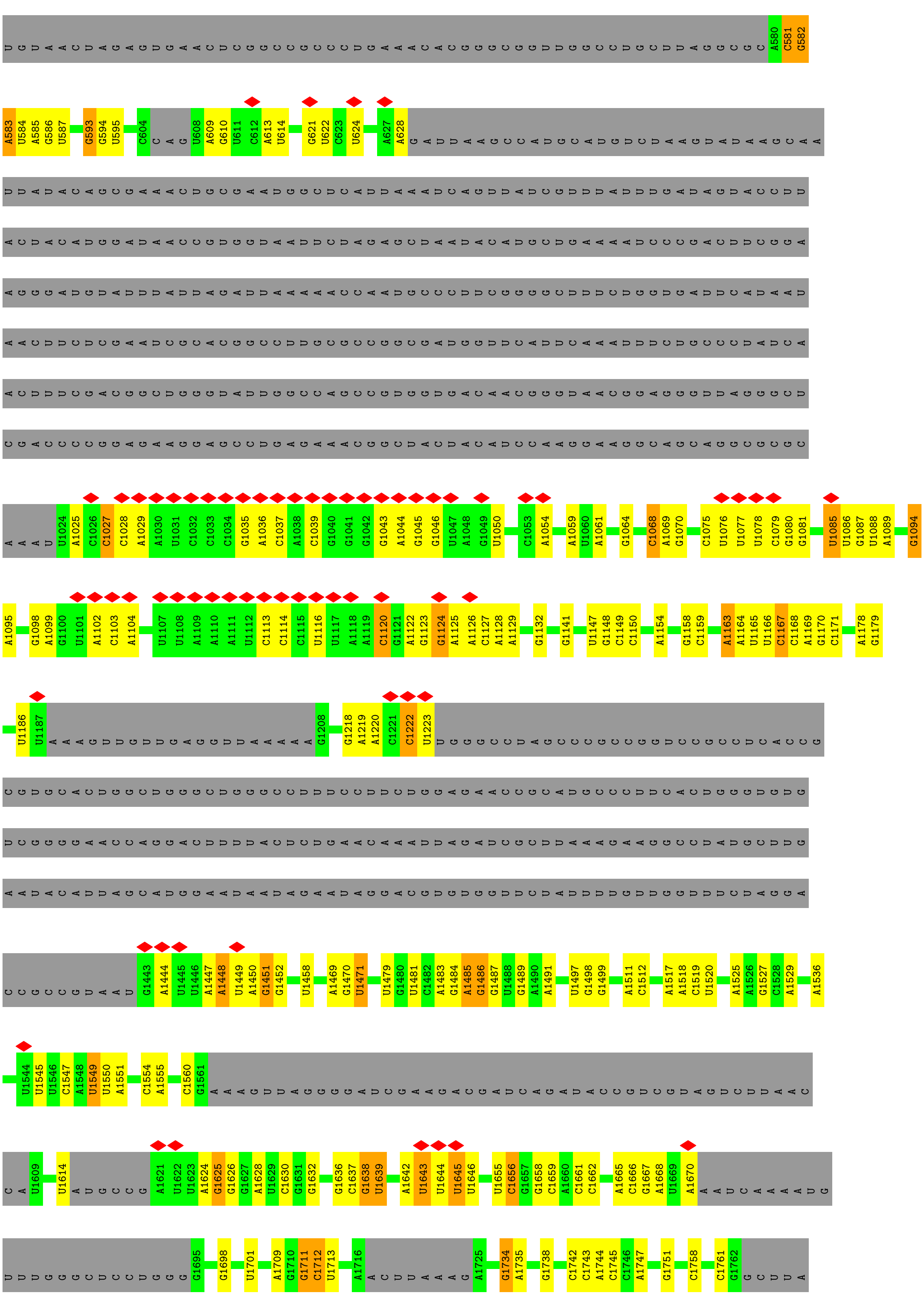
Chain CU:

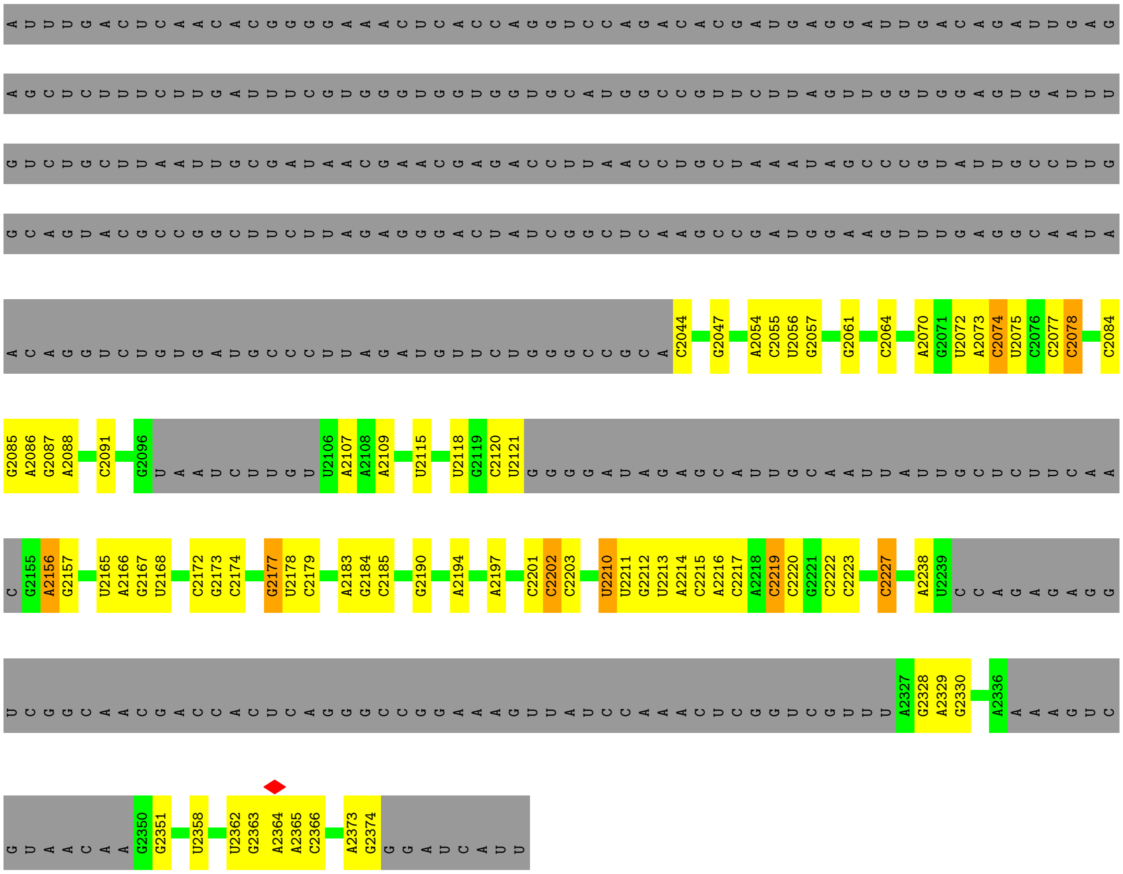


- Molecule 45: 35S ribosomal RNA

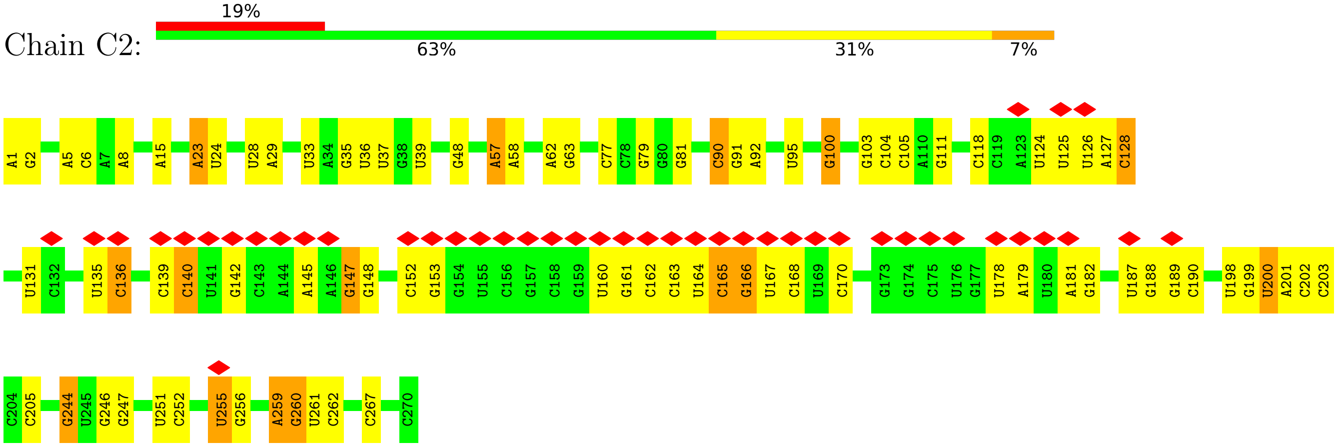
Chain C1:



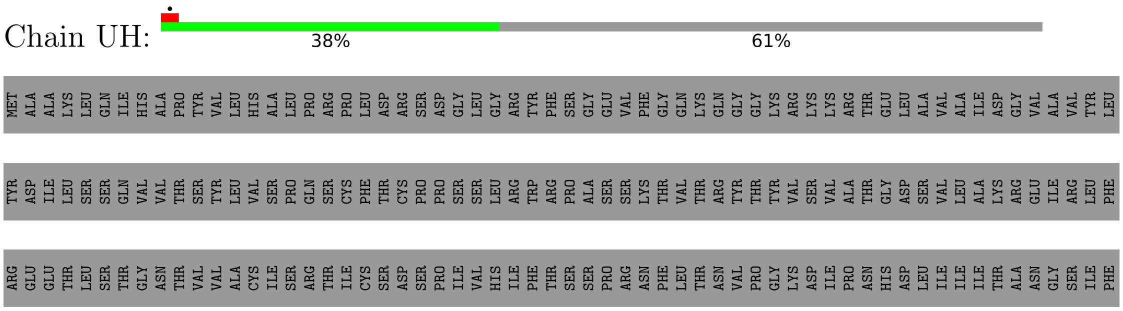

U G U A A C U A G A G U G A A C U C G G C C G C C C U G A A A C A C G G G C G G U U G G C C U G C U U A G G C G C A580 C581 G582
A583 U584 A585 G586 U587 G593 G594 U595 C604 C A G U608 A609 G610 U611 C612 A613 U614 G621 U622 C623 U624 A627 A628 G A U U A A G C C A U G C A U G U C U A A G U A U A A G C A A
U U A U A C A G C G A A A C U G C G A A U G G C U C A U U A A A U C A G U U A U C G U U U A U U U G A U A G U A C C U U
A C U A C A U G G A U A A C C G U G G U A A U U C U A G A G C U A A U A C A U G C U G A A A A U C C C G A C U U C G G A
A G G G A U G U A U U U A U U A G A U U A A A A A C C A A U G C C C U U C G G G G C U U U C U G G U G A U U C A U A A U
A A C U U C U C G A A U C G C A C G G C C U U G C G C C G G C G A U G G U U C A U U C A A A U U U C U G C C C U A U C A
A C U U U C G A C G G C U G G G U A U U G G C C A G C C G U G G U G A C A A C G G G U A A C G G A G G G U U A G G G C U
C G A C C C C G G A G A A G G A G C C U G A G A A A C G G C U A C U A C A U C C A A G G A A G G C A G C A G G C G C G C
A A A U U1024 A1025 C1026 C1027 C1028 A1029 A1030 U1031 C1032 C1033 C1034 G1035 A1036 C1037 A1038 C1039 G1040 G1041 G1042 G1043 A1044 G1045 G1046 U1047 A1048 G1049 U1050 C1053 A1054 A1059 U1060 A1061 G1064 C1068 A1069 G1070 C1075 U1076 U1077 U1078 C1079 G1080 G1081 U1085 U1086 G1087 U1088 A1089 G1094
A1095 G1098 A1099 G1100 U1101 A1102 C1103 A1104 U1107 U1108 A1109 A1110 A1111 U1112 C1113 C1114 C1115 U1116 U1117 A1118 A1119 C1120 G1121 A1122 G1123 G1124 A1125 A1126 C1127 A1128 A1129 G1132 G1141 U1147 G1148 C1149 C1150 A1154 G1158 C1159 A1163 A1164 U1165 U1166 C1167 C1168 A1169 G1170 C1171 A1178 G1179
U1186 U1187 A A A G U U G U U G A G G U U A A A A A G1208 G1218 A1219 A1220 C1221 C1222 U1223 U G G G C C U A G C C C G C C G G U C C G C C U C A C C G
C G U G C A C U G G C U G G G C U G G G C C U U U C C U U C U G G A G A A C C G C A U G C C C U U C A C U G G G U G U G
U C G G G G A A C C A G G A C U U U U A C U C U G A A C A A A U U A G A U C G C U U A A A G A A G G C C U A U G C U U G
A A U A C A U U A G C A U G G A A U A A U A G A A U A G G A C G U G U G G U U C U A U U U U G U U G G U U U C U A G G A
C C G C C G U A A U G1443 A1444 U1445 U1446 A1447 A1448 U1449 A1450 G1451 G1452 U1458 A1469 G1470 U1471 U1479 G1480 U1481 C1482 A1483 G1484 A1485 G1486 G1487 U1488 G1489 A1490 A1491 U1497 G1498 G1499 A1511 C1512 A1517 A1518 C1519 U1520 A1525 A1526 G1527 C1528 A1529 A1536
U1544 U1545 U1546 C1547 A1548 U1549 U1550 A1551 C1554 A1555 C1560 G1561 A A A G U U A G G G G A U C G A A G A C G A U C A G A U A C C G U C G U A G U C U U A A C
C A U1609 U1614 A U G C C G A1621 U1622 U1623 A1624 G1625 G1626 G1627 A1628 U1629 C1630 G1631 G1632 G1636 C1637 G1638 U1639 A1642 U1643 U1644 U1645 U1646 U1655 C1656 G1657 G1658 C1659 A1660 C1661 C1662 A1665 C1666 G1667 A1668 U1669 A1670 A A U C A A A U G
U U U G G G C U C C U G G G G1695 G1698 U1701 A1709 G1710 G1711 C1712 U1713 A1716 A C U U A A A G A1725 G1734 A1735 G1738 C1742 C1743 A1744 C1745 C1746 A1747 G1751 C1758 C1761 G1762 G C U U A

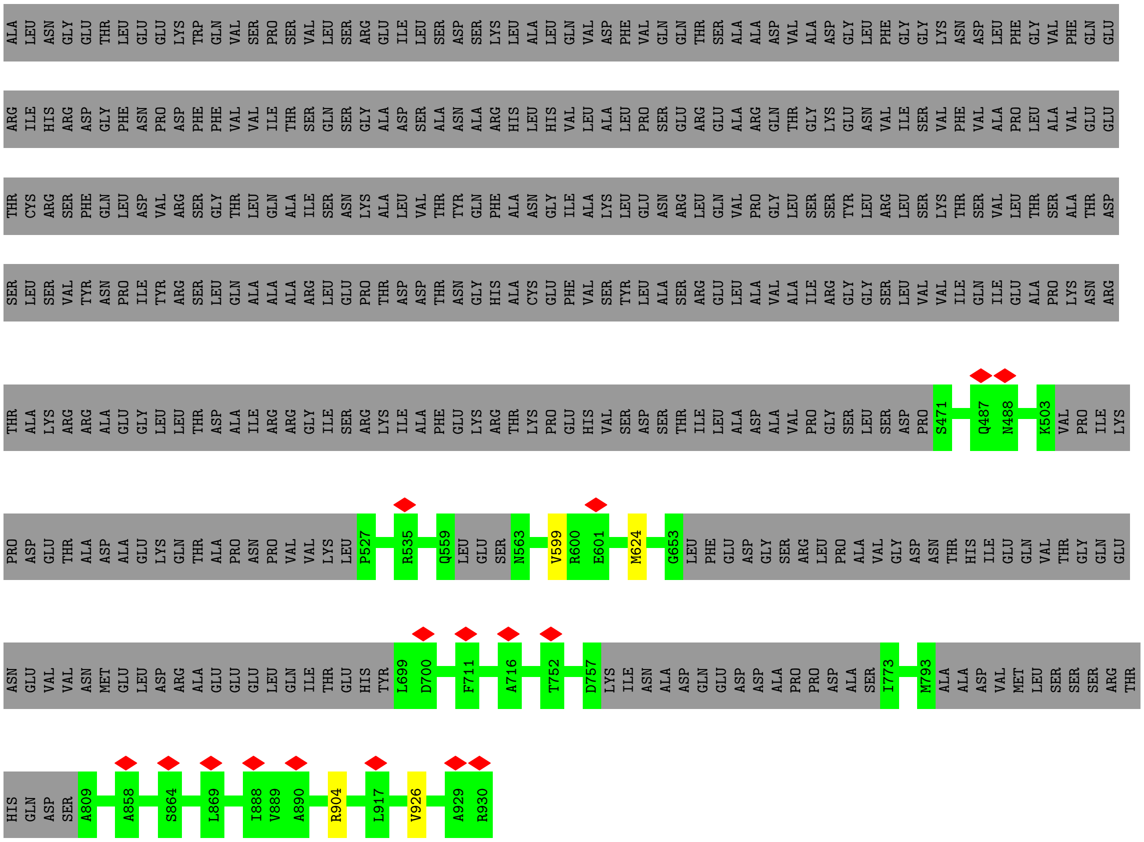


- Molecule 46: U3 snoRNA

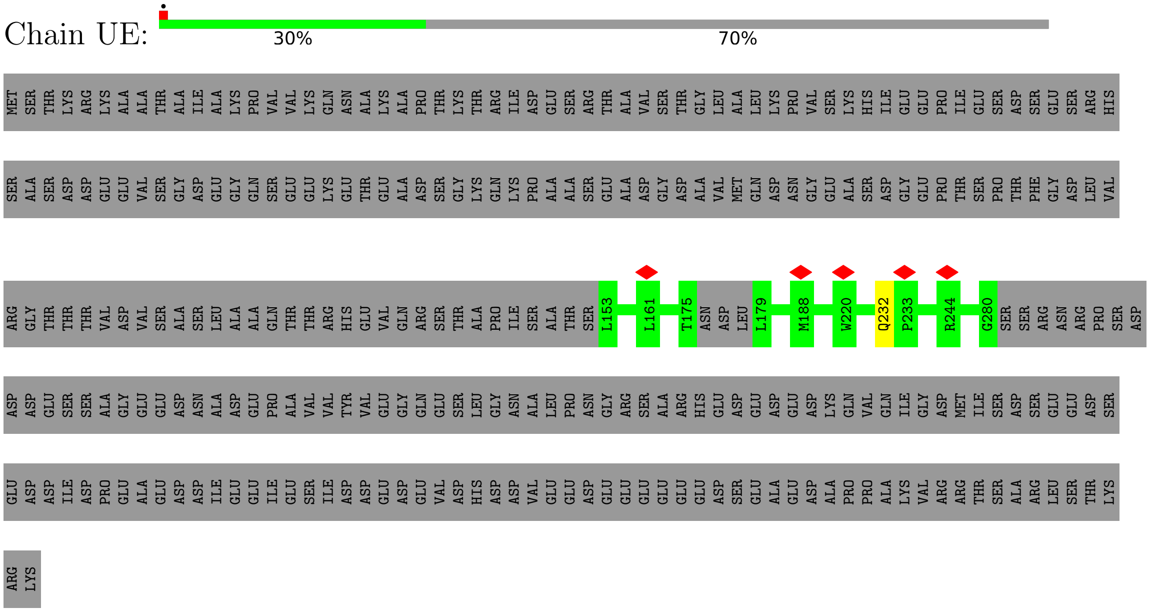


- Molecule 47: Utp8

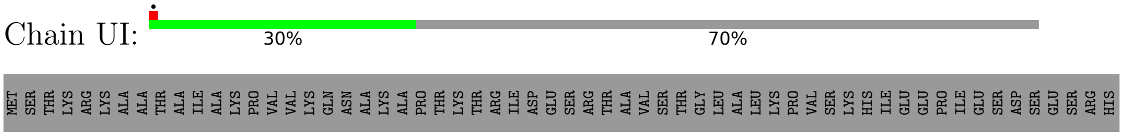




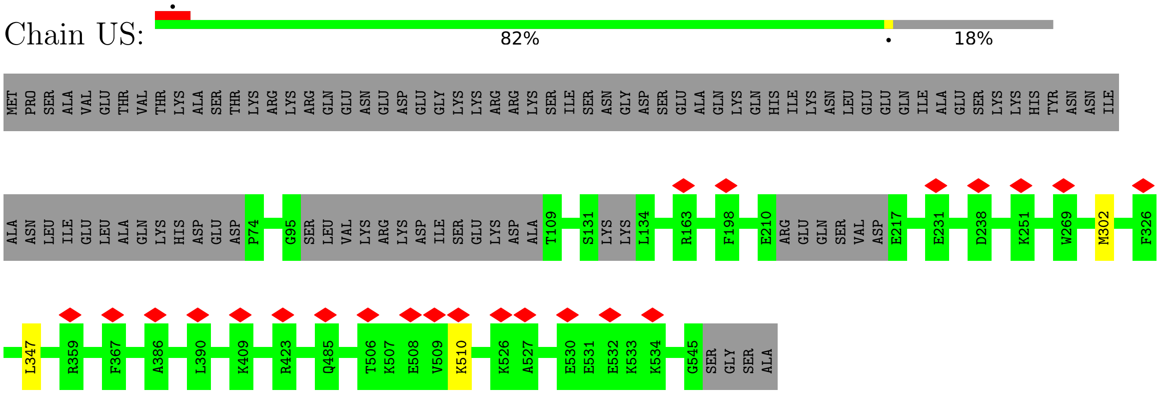
- Molecule 48: Utp5"



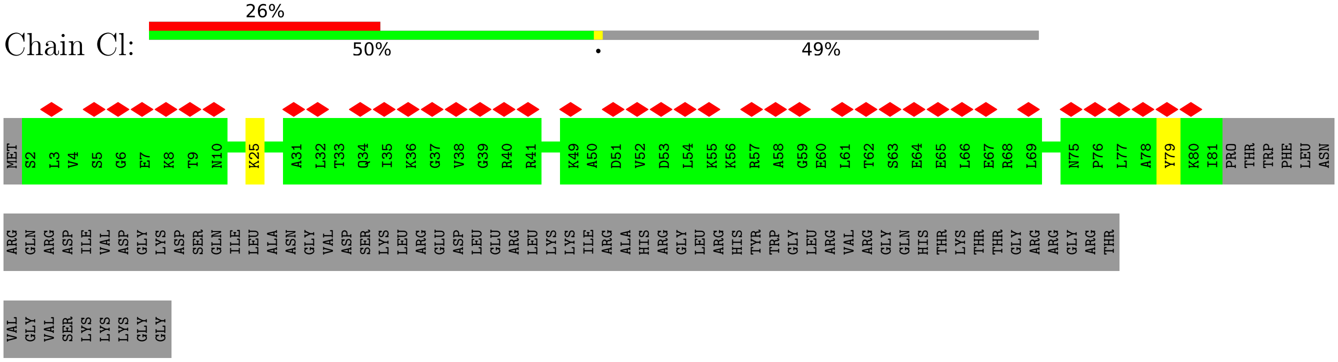
- Molecule 48: Utp5"



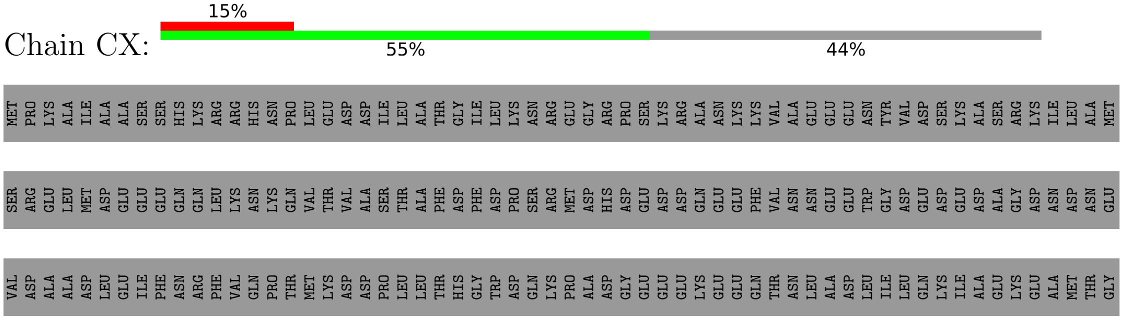
- Molecule 49: Noc4

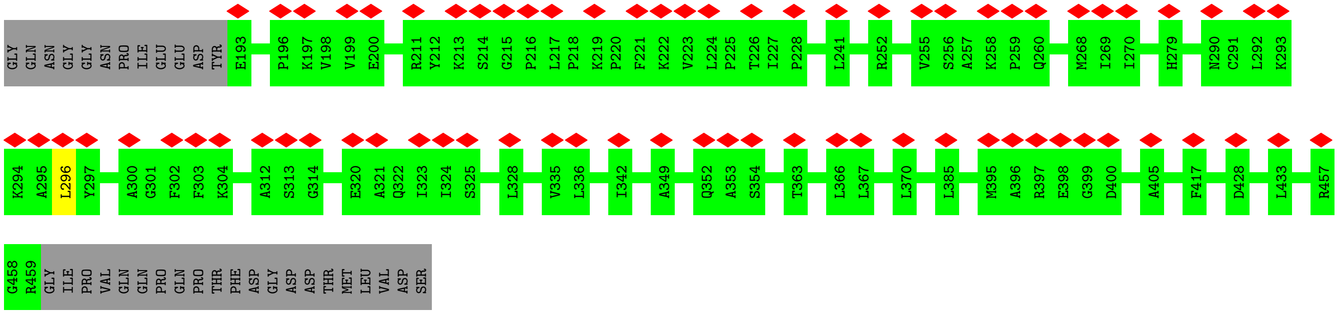


- Molecule 50: Putative ribosomal protein



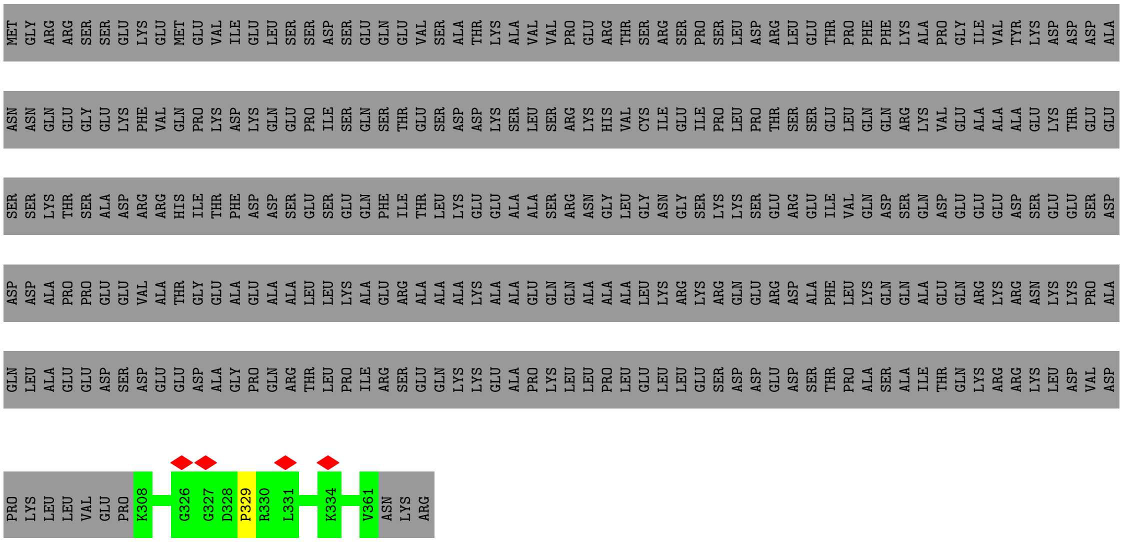
- Molecule 51: Enp1





- Molecule 52: Utp16

Chain UP:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8415	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.232	Depositor
Minimum map value	-0.184	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z| > 5$	RMSZ	$\#|Z| > 5$
1	UA	0.47	0/6521	0.65	5/8867 (0.1%)
2	UB	0.33	0/4154	0.54	2/5583 (0.0%)
3	UC	0.40	0/595	0.52	0/786
4	UD	0.38	0/6211	0.56	2/8408 (0.0%)
5	UF	0.35	0/2657	0.54	1/3596 (0.0%)
6	UG	0.47	0/3790	0.62	3/5120 (0.1%)
7	UJ	0.37	0/3435	0.57	0/4661
8	UK	0.41	0/1701	0.52	1/2251 (0.0%)
9	UL	0.37	0/6299	0.63	4/8531 (0.0%)
10	UM	0.33	0/5755	0.61	2/7827 (0.0%)
11	UN	0.41	0/1232	0.56	1/1662 (0.1%)
12	UO	0.42	0/3903	0.61	3/5312 (0.1%)
13	UQ	0.40	0/6136	0.63	4/8348 (0.0%)
14	UR	0.43	0/3564	0.59	1/4816 (0.0%)
15	UU	0.45	1/6903 (0.0%)	0.60	2/9392 (0.0%)
16	UX	0.42	0/1493	0.59	0/2011
17	UZ	0.34	0/1857	0.61	1/2526 (0.0%)
18	CA	0.46	0/1814	0.60	0/2456
18	CB	0.34	0/1853	0.54	0/2511
19	CC	0.37	0/2911	0.58	1/3937 (0.0%)
20	CD	0.36	0/3205	0.60	3/4338 (0.1%)
21	CE	0.45	0/891	0.66	2/1214 (0.2%)
21	CF	0.41	0/876	0.64	1/1195 (0.1%)
22	CG	0.37	0/2983	0.60	0/4032
23	CH	0.38	0/2939	0.58	1/3988 (0.0%)
24	CI	0.42	0/6631	0.58	1/8943 (0.0%)
25	CJ	0.48	0/1462	0.56	0/1967
26	CK	0.45	0/2376	0.64	2/3214 (0.1%)
27	CL	0.37	0/1812	0.51	0/2437
28	CM	0.48	0/3573	0.60	0/4829
29	CN	0.36	0/1797	0.56	1/2443 (0.0%)
29	CO	0.31	0/1714	0.55	0/2325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	CP	0.35	0/1655	0.58	0/2229
31	CQ	0.30	0/1379	0.57	0/1850
32	CR	0.40	0/6108	0.80	14/8266 (0.2%)
32	CS	0.40	0/6108	0.80	14/8266 (0.2%)
33	CT	0.43	0/1053	0.58	0/1413
34	Ca	0.35	0/1850	0.61	0/2486
35	Cc	0.40	0/1485	0.54	0/2008
36	Ce	0.34	0/1298	0.66	3/1750 (0.2%)
37	Cg	0.39	0/1259	0.55	0/1687
38	Ch	0.32	0/557	0.52	0/749
39	Ci	0.35	0/819	0.54	0/1107
40	Cj	0.48	0/958	0.60	0/1293
41	Cm	0.41	0/1001	0.57	0/1345
42	Cn	0.44	0/712	0.56	0/954
43	Cp	0.44	0/458	0.61	1/617 (0.2%)
44	CU	0.32	0/1350	0.53	0/1810
45	C1	0.64	1/27472 (0.0%)	1.25	306/42792 (0.7%)
46	C2	0.64	0/5459	1.40	71/8498 (0.8%)
47	UH	0.33	0/2852	0.56	0/3846
48	UE	0.31	0/980	0.58	0/1316
48	UI	0.26	0/980	0.52	0/1316
49	US	0.33	0/3765	0.57	1/5100 (0.0%)
50	Cl	0.30	0/638	0.60	0/857
51	CX	0.29	0/2180	0.55	1/2956 (0.0%)
52	UP	0.34	0/428	0.60	0/570
All	All	0.45	2/175847 (0.0%)	0.80	455/244607 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	UA	0	1
4	UD	0	1
9	UL	0	2
10	UM	0	4
12	UO	0	1
13	UQ	0	4
14	UR	0	1
15	UU	0	3
17	UZ	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	CB	0	1
21	CF	0	1
22	CG	0	1
23	CH	0	1
24	CI	0	2
26	CK	0	1
28	CM	0	1
29	CO	0	2
31	CQ	0	1
32	CR	0	3
32	CS	0	3
35	Cc	0	1
36	Ce	0	1
48	UE	0	1
49	US	0	1
50	Cl	0	1
All	All	0	42

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C1	1081	G	C2-N3	-5.42	1.28	1.32
15	UU	640	CYS	CB-SG	-5.29	1.73	1.81

All (455) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	C2	2	G	O5'-P-OP1	-30.48	74.13	110.70
46	C2	2	G	OP1-P-OP2	-27.29	78.67	119.60
46	C2	2	G	O5'-P-OP2	18.11	132.43	110.70
46	C2	1	A	OP1-P-O3'	13.80	135.56	105.20
46	C2	1	A	OP2-P-O3'	-13.14	76.28	105.20
45	C1	258	C	N1-C2-O2	12.91	126.64	118.90
45	C1	258	C	C2-N1-C1'	12.45	132.49	118.80
45	C1	55	G	OP1-P-O3'	-12.20	78.35	105.20
45	C1	160	C	N3-C2-O2	-11.72	113.69	121.90
45	C1	45	U	OP1-P-O3'	-11.39	80.14	105.20
45	C1	258	C	N3-C2-O2	-10.68	114.42	121.90
45	C1	206	C	N1-C2-O2	10.52	125.21	118.90
45	C1	206	C	C2-N1-C1'	10.48	130.33	118.80
45	C1	2168	U	N3-C2-O2	-10.41	114.92	122.20
45	C1	1222	C	N1-C2-O2	10.20	125.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	C2	140	C	N3-C2-O2	-9.71	115.10	121.90
45	C1	2168	U	N1-C2-O2	9.67	129.57	122.80
45	C1	1662	C	N3-C2-O2	-9.57	115.20	121.90
45	C1	2074	C	N1-C2-O2	9.57	124.64	118.90
46	C2	128	C	C6-N1-C2	-9.49	116.50	120.30
45	C1	1658	G	C5-C6-O6	9.40	134.24	128.60
46	C2	200	U	C2-N1-C1’	9.29	128.84	117.70
45	C1	1658	G	N3-C4-N9	-9.26	120.44	126.00
45	C1	160	C	C6-N1-C2	-9.18	116.63	120.30
45	C1	45	U	OP2-P-O3’	-9.16	85.05	105.20
46	C2	140	C	N1-C2-O2	9.11	124.37	118.90
46	C2	200	U	N1-C2-O2	9.07	129.15	122.80
45	C1	1550	U	C2-N1-C1’	9.06	128.58	117.70
45	C1	2217	C	N1-C2-O2	9.06	124.34	118.90
45	C1	160	C	N1-C2-O2	9.03	124.32	118.90
46	C2	128	C	C5-C6-N1	9.00	125.50	121.00
45	C1	258	C	C6-N1-C1’	-8.92	110.10	120.80
45	C1	1027	C	N3-C2-O2	-8.90	115.67	121.90
45	C1	1655	U	N3-C2-O2	-8.85	116.01	122.20
45	C1	206	C	N3-C2-O2	-8.83	115.72	121.90
45	C1	1658	G	N9-C4-C5	8.73	108.89	105.40
45	C1	291	C	N1-C2-O2	8.72	124.13	118.90
45	C1	2217	C	C2-N1-C1’	8.67	128.34	118.80
45	C1	158	C	N1-C2-O2	8.66	124.09	118.90
46	C2	200	U	N3-C2-O2	-8.62	116.17	122.20
45	C1	505	C	N3-C2-O2	-8.62	115.87	121.90
46	C2	136	C	N1-C2-O2	8.61	124.06	118.90
26	CK	235	ASP	CB-CG-OD1	8.56	126.01	118.30
26	CK	89	LEU	CA-CB-CG	8.43	134.70	115.30
45	C1	1486	G	C4-N9-C1’	8.40	137.43	126.50
45	C1	112	C	N1-C2-O2	8.35	123.91	118.90
1	UA	81	LEU	CA-CB-CG	8.35	134.50	115.30
32	CS	738	LYS	CD-CE-NZ	8.34	130.89	111.70
32	CR	738	LYS	CD-CE-NZ	8.34	130.89	111.70
45	C1	1547	C	N1-C2-O2	8.32	123.89	118.90
45	C1	471	C	N3-C2-O2	-8.29	116.10	121.90
45	C1	1222	C	C2-N1-C1’	8.22	127.84	118.80
45	C1	2202	C	N1-C2-O2	8.22	123.83	118.90
45	C1	159	C	N3-C2-O2	-8.16	116.19	121.90
45	C1	449	C	N3-C2-O2	-8.09	116.23	121.90
45	C1	68	U	N1-C2-O2	8.07	128.45	122.80
45	C1	2084	C	N3-C2-O2	-8.05	116.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C1	1081	G	N3-C2-N2	-8.05	114.27	119.90
32	CS	191	LEU	CA-CB-CG	8.01	133.71	115.30
32	CR	191	LEU	CA-CB-CG	7.99	133.68	115.30
45	C1	1222	C	N3-C2-O2	-7.91	116.36	121.90
45	C1	80	C	N3-C2-O2	-7.90	116.37	121.90
45	C1	2210	U	N3-C2-O2	-7.89	116.67	122.20
45	C1	583	A	O5'-P-OP1	-7.88	98.61	105.70
46	C2	128	C	O4'-C1'-N1	7.86	114.48	108.20
46	C2	267	C	N3-C2-O2	-7.85	116.41	121.90
45	C1	1645	U	C2-N1-C1'	7.78	127.03	117.70
46	C2	103	G	N3-C4-C5	-7.77	124.72	128.60
45	C1	346	C	N3-C2-O2	-7.76	116.47	121.90
46	C2	203	C	N3-C2-O2	-7.72	116.50	121.90
9	UL	438	ASP	CB-CG-OD1	7.68	125.21	118.30
46	C2	6	C	C6-N1-C2	-7.61	117.25	120.30
45	C1	1645	U	N1-C2-O2	7.58	128.10	122.80
45	C1	1662	C	N1-C2-O2	7.58	123.45	118.90
32	CR	714	GLU	CA-CB-CG	7.58	130.07	113.40
32	CR	471	GLU	CA-CB-CG	7.58	130.06	113.40
45	C1	1658	G	N1-C6-O6	-7.58	115.36	119.90
32	CS	471	GLU	CA-CB-CG	7.57	130.06	113.40
45	C1	148	C	N3-C2-O2	-7.56	116.61	121.90
32	CS	714	GLU	CA-CB-CG	7.55	130.02	113.40
45	C1	2179	C	C2-N1-C1'	7.52	127.08	118.80
45	C1	2084	C	C6-N1-C2	-7.52	117.29	120.30
45	C1	470	C	N1-C2-O2	7.50	123.40	118.90
45	C1	1645	U	N3-C2-O2	-7.49	116.95	122.20
45	C1	1625	G	N3-C4-N9	7.46	130.47	126.00
45	C1	148	C	C6-N1-C2	-7.46	117.32	120.30
45	C1	291	C	N3-C2-O2	-7.45	116.68	121.90
45	C1	206	C	C6-N1-C2	-7.45	117.32	120.30
45	C1	1120	C	C2-N1-C1'	7.44	126.99	118.80
45	C1	2074	C	C2-N1-C1'	7.41	126.95	118.80
45	C1	291	C	C2-N1-C1'	7.37	126.90	118.80
46	C2	246	G	C4-N9-C1'	7.34	136.04	126.50
45	C1	491	G	C4-N9-C1'	7.33	136.03	126.50
45	C1	1711	G	C4-N9-C1'	7.31	136.01	126.50
45	C1	1745	C	C5-C6-N1	7.30	124.65	121.00
45	C1	56	C	OP1-P-OP2	7.27	130.50	119.60
45	C1	258	C	C6-N1-C2	-7.26	117.39	120.30
46	C2	136	C	C2-N1-C1'	7.25	126.77	118.80
12	UO	293	LEU	CA-CB-CG	7.23	131.92	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	C2	139	C	N3-C2-O2	-7.22	116.84	121.90
45	C1	1486	G	N3-C4-C5	-7.18	125.01	128.60
46	C2	139	C	N1-C2-O2	7.13	123.18	118.90
45	C1	2217	C	N3-C2-O2	-7.11	116.92	121.90
45	C1	1163	A	P-O3'-C3'	7.10	128.22	119.70
45	C1	46	C	OP1-P-OP2	7.08	130.22	119.60
45	C1	206	C	C6-N1-C1'	-7.08	112.30	120.80
45	C1	1512	C	C6-N1-C2	-7.07	117.47	120.30
32	CS	202	ILE	CG1-CB-CG2	-7.05	95.89	111.40
45	C1	1666	C	N1-C2-O2	7.05	123.13	118.90
32	CR	202	ILE	CG1-CB-CG2	-7.03	95.93	111.40
46	C2	252	C	N3-C2-O2	-7.02	116.98	121.90
45	C1	622	U	N3-C2-O2	-7.01	117.29	122.20
46	C2	255	U	P-O3'-C3'	7.00	128.10	119.70
45	C1	209	A	P-O3'-C3'	6.98	128.07	119.70
32	CS	515	GLN	CA-CB-CG	6.97	128.73	113.40
45	C1	1658	G	C4-C5-N7	-6.97	108.01	110.80
45	C1	56	C	C2-N1-C1'	6.96	126.46	118.80
32	CR	515	GLN	CA-CB-CG	6.96	128.70	113.40
45	C1	158	C	C2-N1-C1'	6.94	126.44	118.80
45	C1	454	C	C2-N1-C1'	6.94	126.43	118.80
45	C1	1549	U	N3-C4-C5	6.90	118.74	114.60
46	C2	260	G	C4-N9-C1'	6.89	135.46	126.50
21	CE	103	LEU	CA-CB-CG	6.88	131.12	115.30
45	C1	34	C	N1-C2-O2	6.88	123.03	118.90
45	C1	1113	C	N1-C2-O2	6.88	123.03	118.90
45	C1	34	C	N3-C2-O2	-6.88	117.08	121.90
45	C1	1114	C	N1-C2-O2	6.87	123.02	118.90
45	C1	504	C	N1-C2-O2	6.87	123.02	118.90
45	C1	1471	U	C2-N1-C1'	6.86	125.94	117.70
12	UO	239	LEU	CA-CB-CG	6.86	131.07	115.30
46	C2	57	A	O4'-C1'-N9	6.86	113.68	108.20
11	UN	901	LEU	CA-CB-CG	6.84	131.02	115.30
45	C1	2202	C	N3-C2-O2	-6.83	117.12	121.90
45	C1	159	C	C6-N1-C2	-6.82	117.57	120.30
45	C1	33	C	N3-C2-O2	-6.82	117.12	121.90
45	C1	68	U	N3-C2-O2	-6.81	117.43	122.20
45	C1	1487	G	O4'-C1'-N9	6.80	113.64	108.20
46	C2	161	G	C4-N9-C1'	6.79	135.33	126.50
46	C2	259	A	O4'-C1'-N9	6.79	113.64	108.20
46	C2	103	G	N3-C4-N9	6.79	130.07	126.00
46	C2	267	C	C6-N1-C2	-6.75	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C1	447	C	N3-C2-O2	-6.75	117.18	121.90
45	C1	505	C	N1-C2-O2	6.75	122.95	118.90
45	C1	1666	C	C5-C6-N1	6.73	124.37	121.00
45	C1	112	C	N3-C2-O2	-6.72	117.19	121.90
46	C2	260	G	N3-C4-N9	6.71	130.03	126.00
45	C1	581	C	N3-C2-O2	-6.69	117.22	121.90
45	C1	203	C	N1-C2-O2	6.67	122.90	118.90
45	C1	1547	C	C5-C6-N1	6.67	124.33	121.00
9	UL	645	LEU	CA-CB-CG	6.61	130.50	115.30
45	C1	581	C	N1-C2-O2	6.60	122.86	118.90
45	C1	2179	C	N1-C2-O2	6.59	122.86	118.90
45	C1	1486	G	N7-C8-N9	6.59	116.39	113.10
45	C1	491	G	N3-C4-N9	6.59	129.95	126.00
45	C1	1486	G	C8-N9-C1'	-6.57	118.45	127.00
13	UQ	154	ASP	CB-CG-OD1	6.57	124.21	118.30
45	C1	1486	G	N3-C4-N9	6.57	129.94	126.00
45	C1	1711	G	N3-C4-N9	6.56	129.94	126.00
1	UA	587	LEU	CA-CB-CG	6.55	130.36	115.30
45	C1	281	U	P-O3'-C3'	6.55	127.56	119.70
45	C1	1625	G	N3-C4-C5	-6.54	125.33	128.60
46	C2	260	G	N3-C4-C5	-6.54	125.33	128.60
45	C1	454	C	C5-C6-N1	6.48	124.24	121.00
45	C1	1471	U	C5-C4-O4	-6.47	122.02	125.90
45	C1	1666	C	C2-N1-C1'	6.45	125.90	118.80
45	C1	277	U	P-O3'-C3'	6.45	127.44	119.70
45	C1	1068	C	C6-N1-C2	-6.45	117.72	120.30
45	C1	491	G	C8-N9-C1'	-6.45	118.62	127.00
1	UA	662	GLY	C-N-CA	6.44	137.79	121.70
45	C1	68	U	C5-C6-N1	6.43	125.92	122.70
45	C1	2074	C	N3-C2-O2	-6.42	117.41	121.90
46	C2	202	C	N1-C2-O2	6.42	122.75	118.90
45	C1	1448	A	C5-C6-N1	6.42	120.91	117.70
45	C1	1046	G	C5-C6-O6	6.41	132.44	128.60
46	C2	147	G	N3-C4-N9	6.40	129.84	126.00
32	CS	370	GLN	CA-CB-CG	6.38	127.44	113.40
45	C1	18	G	N3-C4-C5	-6.38	125.41	128.60
32	CR	370	GLN	CA-CB-CG	6.37	127.42	113.40
45	C1	454	C	C6-N1-C2	-6.37	117.75	120.30
46	C2	161	G	N3-C4-N9	6.36	129.81	126.00
45	C1	68	U	C2-N1-C1'	6.33	125.29	117.70
45	C1	581	C	C2-N1-C1'	6.32	125.75	118.80
45	C1	1547	C	C2-N1-C1'	6.32	125.75	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C1	593	G	P-O3'-C3'	6.31	127.27	119.70
45	C1	1747	A	C6-N1-C2	-6.31	114.82	118.60
45	C1	1745	C	C6-N1-C2	-6.30	117.78	120.30
46	C2	161	G	C6-C5-N7	-6.30	126.62	130.40
45	C1	1114	C	N3-C2-O2	-6.28	117.51	121.90
45	C1	1550	U	C6-N1-C1'	-6.27	112.42	121.20
46	C2	246	G	C8-N9-C1'	-6.27	118.84	127.00
45	C1	1167	C	C6-N1-C2	-6.26	117.80	120.30
45	C1	205	C	P-O3'-C3'	6.26	127.21	119.70
45	C1	1711	G	N3-C4-C5	-6.25	125.48	128.60
2	UB	644	LEU	CA-CB-CG	6.24	129.66	115.30
10	UM	39	LEU	CA-CB-CG	6.24	129.66	115.30
45	C1	425	C	C6-N1-C2	-6.24	117.80	120.30
45	C1	1711	G	C8-N9-C1'	-6.22	118.92	127.00
45	C1	2156	A	P-O3'-C3'	6.21	127.15	119.70
45	C1	63	C	N1-C2-O2	6.19	122.61	118.90
45	C1	2194	A	C8-N9-C4	-6.18	103.33	105.80
45	C1	258	C	C5-C6-N1	6.17	124.09	121.00
45	C1	2210	U	C5-C4-O4	6.17	129.60	125.90
46	C2	23	A	P-O3'-C3'	6.16	127.10	119.70
12	UO	334	LEU	CA-CB-CG	6.15	129.44	115.30
45	C1	1638	G	P-O3'-C3'	6.14	127.07	119.70
45	C1	470	C	C2-N1-C1'	6.14	125.55	118.80
29	CN	86	ASP	CB-CG-OD1	6.11	123.80	118.30
9	UL	441	LEU	CA-CB-CG	6.10	129.34	115.30
45	C1	56	C	N1-C2-O2	6.10	122.56	118.90
45	C1	622	U	N1-C2-O2	6.09	127.06	122.80
45	C1	135	A	P-O3'-C3'	6.09	127.01	119.70
45	C1	1712	C	P-O3'-C3'	6.09	127.00	119.70
45	C1	1745	C	C2-N1-C1'	6.08	125.48	118.80
45	C1	21	C	N3-C2-O2	-6.07	117.65	121.90
45	C1	18	G	C4-N9-C1'	6.06	134.38	126.50
45	C1	1222	C	C6-N1-C2	-6.04	117.88	120.30
45	C1	1486	G	C8-N9-C4	-6.04	103.98	106.40
45	C1	183	C	C2-N1-C1'	6.03	125.44	118.80
45	C1	1549	U	N3-C4-O4	-6.03	115.18	119.40
45	C1	2217	C	C6-N1-C1'	-6.03	113.56	120.80
17	UZ	66	LEU	CA-CB-CG	6.03	129.16	115.30
45	C1	2078	C	N3-C2-O2	-6.03	117.68	121.90
45	C1	1451	G	N9-C4-C5	-6.02	102.99	105.40
45	C1	1485	A	P-O3'-C3'	6.02	126.93	119.70
19	CC	17	LEU	CA-CB-CG	6.02	129.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C1	18	G	N3-C4-N9	6.02	129.61	126.00
45	C1	291	C	C6-N1-C2	-6.02	117.89	120.30
45	C1	369	U	N3-C2-O2	-6.00	118.00	122.20
32	CR	67	PHE	CB-CG-CD1	5.99	125.00	120.80
45	C1	1661	C	C2-N3-C4	-5.99	116.91	119.90
46	C2	105	C	C5-C6-N1	5.99	123.99	121.00
45	C1	1630	C	N3-C2-O2	-5.97	117.72	121.90
45	C1	1666	C	C6-N1-C2	-5.96	117.92	120.30
46	C2	6	C	C5-C6-N1	5.96	123.98	121.00
46	C2	161	G	C8-N9-C1'	-5.95	119.27	127.00
45	C1	1547	C	C6-N1-C2	-5.94	117.92	120.30
46	C2	103	G	C2-N3-C4	5.93	114.87	111.90
45	C1	55	G	OP2-P-O3'	-5.93	92.15	105.20
45	C1	1448	A	C6-N1-C2	-5.93	115.05	118.60
45	C1	1658	G	C6-C5-N7	5.92	133.95	130.40
45	C1	471	C	C6-N1-C2	-5.92	117.93	120.30
46	C2	136	C	C5-C6-N1	5.92	123.96	121.00
45	C1	1639	U	C2-N1-C1'	5.90	124.78	117.70
6	UG	174	LEU	CA-CB-CG	5.90	128.87	115.30
46	C2	200	U	C6-N1-C1'	-5.90	112.95	121.20
45	C1	1165	U	C2-N1-C1'	5.89	124.76	117.70
45	C1	398	C	N1-C2-O2	5.88	122.43	118.90
45	C1	1120	C	C6-N1-C2	-5.88	117.95	120.30
45	C1	1560	C	N1-C2-O2	5.87	122.42	118.90
45	C1	1458	U	C2-N1-C1'	5.87	124.74	117.70
45	C1	1113	C	N3-C2-O2	-5.87	117.79	121.90
46	C2	6	C	N1-C2-O2	5.87	122.42	118.90
32	CS	67	PHE	CB-CG-CD1	5.87	124.91	120.80
45	C1	2210	U	N1-C2-O2	5.87	126.91	122.80
46	C2	244	G	C5-C6-O6	5.85	132.11	128.60
46	C2	139	C	C6-N1-C2	-5.85	117.96	120.30
45	C1	2179	C	C6-N1-C1'	-5.84	113.79	120.80
45	C1	2358	U	N3-C2-O2	-5.84	118.11	122.20
45	C1	371	U	N1-C2-O2	5.80	126.86	122.80
46	C2	260	G	C8-N9-C1'	-5.80	119.46	127.00
45	C1	2217	C	C6-N1-C2	-5.79	117.98	120.30
45	C1	2177	G	P-O3'-C3'	5.78	126.63	119.70
45	C1	2217	C	C5-C6-N1	5.78	123.89	121.00
45	C1	2203	C	N1-C2-O2	5.77	122.36	118.90
45	C1	158	C	C6-N1-C1'	-5.76	113.88	120.80
45	C1	308	U	C5-C6-N1	5.75	125.58	122.70
45	C1	1511	A	C2-N3-C4	5.75	113.48	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C1	1458	U	N1-C2-O2	5.75	126.83	122.80
1	UA	258	LEU	CA-CB-CG	5.75	128.52	115.30
21	CF	103	LEU	CA-CB-CG	5.75	128.52	115.30
45	C1	88	C	P-O3'-C3'	5.73	126.58	119.70
45	C1	1046	G	N1-C6-O6	-5.73	116.46	119.90
45	C1	1560	C	N3-C2-O2	-5.73	117.89	121.90
45	C1	1451	G	N3-C4-N9	5.72	129.43	126.00
45	C1	2165	U	C5-C6-N1	5.71	125.55	122.70
20	CD	189	TRP	CA-CB-CG	5.70	124.52	113.70
45	C1	493	G	N3-C4-N9	5.69	129.42	126.00
45	C1	134	C	N3-C2-O2	-5.69	117.92	121.90
45	C1	2358	U	C2-N1-C1'	5.69	124.53	117.70
15	UU	771	LEU	CA-CB-CG	5.68	128.37	115.30
45	C1	308	U	N1-C2-O2	5.68	126.78	122.80
15	UU	378	LEU	CA-CB-CG	5.67	128.35	115.30
46	C2	246	G	N3-C4-C5	-5.67	125.76	128.60
45	C1	56	C	C5-C6-N1	5.66	123.83	121.00
45	C1	183	C	C5-C6-N1	5.66	123.83	121.00
45	C1	3	G	N3-C4-N9	-5.65	122.61	126.00
6	UG	151	LEU	CA-CB-CG	5.65	128.30	115.30
13	UQ	747	LEU	C-N-CA	5.64	135.81	121.70
46	C2	6	C	N3-C2-O2	-5.63	117.96	121.90
10	UM	689	LEU	CA-CB-CG	5.62	128.23	115.30
45	C1	203	C	C2-N1-C1'	5.62	124.98	118.80
5	UF	177	LEU	CB-CG-CD2	-5.61	101.47	111.00
45	C1	1656	C	C6-N1-C2	-5.61	118.06	120.30
45	C1	370	C	N1-C2-O2	5.59	122.26	118.90
36	Ce	22	LEU	CA-CB-CG	5.59	128.16	115.30
45	C1	158	C	N3-C2-O2	-5.59	117.99	121.90
45	C1	206	C	C5-C6-N1	5.58	123.79	121.00
45	C1	371	U	C2-N1-C1'	5.58	124.40	117.70
45	C1	2202	C	C6-N1-C2	-5.58	118.07	120.30
45	C1	1639	U	N1-C2-O2	5.57	126.70	122.80
45	C1	1085	U	P-O3'-C3'	5.55	126.36	119.70
32	CR	193	LEU	CA-CB-CG	5.54	128.03	115.30
46	C2	246	G	N3-C4-N9	5.53	129.32	126.00
45	C1	491	G	N3-C4-C5	-5.53	125.83	128.60
45	C1	2179	C	N3-C2-O2	-5.53	118.03	121.90
46	C2	90	C	O4'-C1'-N1	5.53	112.62	108.20
45	C1	448	C	N3-C2-O2	-5.51	118.04	121.90
32	CS	193	LEU	CA-CB-CG	5.51	127.97	115.30
32	CR	849	LEU	CA-CB-CG	5.51	127.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	C2	152	C	C6-N1-C2	-5.51	118.10	120.30
32	CS	849	LEU	CA-CB-CG	5.50	127.95	115.30
45	C1	1165	U	N3-C2-O2	-5.50	118.35	122.20
45	C1	281	U	OP1-P-O3'	5.49	117.27	105.20
45	C1	1626	G	C6-N1-C2	-5.48	121.81	125.10
6	UG	100	LEU	CA-CB-CG	5.48	127.90	115.30
45	C1	2	G	N3-C4-N9	5.47	129.28	126.00
45	C1	369	U	C2-N1-C1'	5.47	124.26	117.70
46	C2	251	U	N3-C2-O2	-5.47	118.37	122.20
13	UQ	617	LEU	CA-CB-CG	5.47	127.87	115.30
45	C1	1625	G	N3-C2-N2	5.47	123.73	119.90
45	C1	1165	U	N1-C2-O2	5.46	126.62	122.80
45	C1	26	C	N3-C2-O2	-5.46	118.08	121.90
9	UL	869	LEU	CA-CB-CG	5.46	127.85	115.30
46	C2	105	C	C6-N1-C2	-5.45	118.12	120.30
45	C1	343	C	C6-N1-C2	-5.44	118.12	120.30
45	C1	1222	C	C6-N1-C1'	-5.44	114.27	120.80
45	C1	371	U	N3-C2-O2	-5.44	118.39	122.20
45	C1	60	A	C2-N3-C4	5.44	113.32	110.60
45	C1	308	U	C2-N1-C1'	5.44	124.23	117.70
45	C1	485	G	N3-C4-N9	-5.44	122.74	126.00
45	C1	2074	C	C6-N1-C1'	-5.43	114.28	120.80
45	C1	2194	A	N7-C8-N9	5.43	116.52	113.80
24	CI	845	LEU	CA-CB-CG	5.43	127.79	115.30
45	C1	294	G	N3-C4-N9	-5.42	122.75	126.00
45	C1	145	C	N1-C2-O2	5.42	122.15	118.90
46	C2	77	C	C5-C6-N1	5.42	123.71	121.00
46	C2	165	C	N1-C2-O2	5.42	122.15	118.90
45	C1	454	C	N1-C2-O2	5.42	122.15	118.90
45	C1	1068	C	C5-C6-N1	5.41	123.70	121.00
45	C1	470	C	N3-C2-O2	-5.41	118.11	121.90
45	C1	1549	U	C2-N3-C4	-5.41	123.76	127.00
46	C2	200	U	C5-C6-N1	5.40	125.40	122.70
32	CR	67	PHE	CB-CG-CD2	-5.39	117.03	120.80
45	C1	1027	C	C6-N1-C2	-5.38	118.15	120.30
45	C1	1758	C	C6-N1-C1'	5.38	127.25	120.80
45	C1	582	G	P-O3'-C3'	5.37	126.14	119.70
49	US	347	LEU	CA-CB-CG	5.37	127.64	115.30
51	CX	296	LEU	CA-CB-CG	5.36	127.64	115.30
45	C1	18	G	C2-N3-C4	5.36	114.58	111.90
45	C1	1643	U	C2-N1-C1'	5.36	124.13	117.70
45	C1	2219	C	P-O3'-C3'	5.36	126.13	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	C2	103	G	C4-N9-C1'	5.35	133.45	126.50
45	C1	203	C	N3-C2-O2	-5.35	118.16	121.90
32	CS	901	LEU	CA-CB-CG	5.34	127.58	115.30
43	Cp	55	LEU	CB-CG-CD2	-5.33	101.95	111.00
32	CR	901	LEU	CA-CB-CG	5.32	127.53	115.30
46	C2	136	C	N3-C2-O2	-5.32	118.18	121.90
45	C1	2177	G	OP2-P-O3'	5.31	116.89	105.20
45	C1	1451	G	C4-C5-N7	5.31	112.92	110.80
45	C1	1050	U	N3-C2-O2	-5.30	118.49	122.20
45	C1	1625	G	C6-C5-N7	-5.30	127.22	130.40
45	C1	2358	U	N1-C2-O2	5.30	126.51	122.80
45	C1	63	C	C2-N1-C1'	5.29	124.62	118.80
32	CS	67	PHE	CB-CG-CD2	-5.29	117.09	120.80
32	CR	135	ILE	CG1-CB-CG2	-5.29	99.77	111.40
32	CR	617	LEU	CA-CB-CG	5.29	127.45	115.30
32	CS	617	LEU	CA-CB-CG	5.29	127.46	115.30
45	C1	1120	C	N1-C2-O2	5.28	122.07	118.90
45	C1	1458	U	N3-C2-O2	-5.28	118.51	122.20
45	C1	1547	C	N3-C4-N4	5.28	121.69	118.00
45	C1	2091	C	C2-N1-C1'	5.28	124.61	118.80
46	C2	202	C	C6-N1-C2	-5.28	118.19	120.30
45	C1	2172	C	C6-N1-C2	-5.28	118.19	120.30
45	C1	2168	U	C2-N1-C1'	5.27	124.03	117.70
32	CS	135	ILE	CG1-CB-CG2	-5.27	99.81	111.40
46	C2	136	C	C6-N1-C2	-5.26	118.19	120.30
45	C1	1511	A	C5-C6-N1	5.26	120.33	117.70
45	C1	150	C	P-O3'-C3'	5.26	126.01	119.70
45	C1	1630	C	C6-N1-C1'	5.26	127.11	120.80
46	C2	79	G	N3-C4-N9	5.25	129.15	126.00
45	C1	1045	G	N3-C4-C5	-5.24	125.98	128.60
45	C1	1734	G	P-O3'-C3'	5.24	125.99	119.70
36	Ce	38	ALA	C-N-CA	5.23	134.77	121.70
45	C1	1625	G	C4-N9-C1'	5.22	133.29	126.50
45	C1	2227	C	C5-C6-N1	5.22	123.61	121.00
45	C1	281	U	N1-C2-O2	5.22	126.45	122.80
45	C1	1658	G	C8-N9-C1'	5.21	133.77	127.00
45	C1	1761	C	C5-C6-N1	5.21	123.60	121.00
45	C1	1511	A	N3-C4-N9	5.20	131.56	127.40
2	UB	818	ASP	CB-CG-OD2	5.19	122.97	118.30
45	C1	1045	G	N3-C4-N9	5.19	129.12	126.00
45	C1	2202	C	C2-N1-C1'	5.19	124.51	118.80
14	UR	398	LEU	CA-CB-CG	5.18	127.22	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C1	1167	C	N1-C2-O2	5.18	122.01	118.90
45	C1	2203	C	N3-C2-O2	-5.18	118.28	121.90
45	C1	1451	G	C8-N9-C1'	-5.17	120.27	127.00
45	C1	154	C	N1-C2-O2	5.17	122.00	118.90
46	C2	202	C	C5-C6-N1	5.16	123.58	121.00
45	C1	111	U	N3-C2-O2	-5.16	118.59	122.20
45	C1	233	C	C6-N1-C2	-5.15	118.24	120.30
45	C1	1646	U	O4'-C1'-N1	5.15	112.32	108.20
45	C1	43	C	C2-N1-C1'	5.15	124.46	118.80
45	C1	63	C	N3-C2-O2	-5.15	118.30	121.90
45	C1	1560	C	C6-N1-C2	-5.13	118.25	120.30
1	UA	695	LEU	CA-CB-CG	5.13	127.11	115.30
45	C1	1471	U	N3-C4-O4	5.13	122.99	119.40
46	C2	147	G	N9-C4-C5	-5.13	103.35	105.40
20	CD	102	LEU	CA-CB-CG	5.12	127.08	115.30
45	C1	582	G	OP1-P-O3'	5.12	116.47	105.20
46	C2	161	G	N7-C8-N9	5.12	115.66	113.10
45	C1	2084	C	C6-N1-C1'	5.12	126.94	120.80
45	C1	2174	C	C5-C6-N1	5.12	123.56	121.00
45	C1	2	G	N3-C4-C5	-5.12	126.04	128.60
45	C1	1656	C	C5-C6-N1	5.11	123.56	121.00
45	C1	1149	C	N3-C2-O2	-5.11	118.32	121.90
8	UK	96	LEU	CA-CB-CG	5.11	127.05	115.30
45	C1	1068	C	P-O3'-C3'	5.11	125.83	119.70
45	C1	129	G	N1-C6-O6	-5.11	116.84	119.90
45	C1	1124	G	C4-N9-C1'	5.10	133.13	126.50
45	C1	1075	C	N3-C2-O2	-5.10	118.33	121.90
45	C1	1094	G	C6-C5-N7	-5.10	127.34	130.40
45	C1	2168	U	C5-C6-N1	5.10	125.25	122.70
45	C1	2064	C	C6-N1-C2	-5.09	118.26	120.30
45	C1	1222	C	C5-C6-N1	5.09	123.55	121.00
46	C2	166	G	N3-C4-C5	-5.08	126.06	128.60
21	CE	110	ASP	CB-CG-OD1	5.08	122.87	118.30
45	C1	370	C	C2-N1-C1'	5.08	124.39	118.80
45	C1	1114	C	C6-N1-C2	-5.08	118.27	120.30
46	C2	260	G	C2-N3-C4	5.07	114.44	111.90
45	C1	435	A	C6-N1-C2	5.07	121.64	118.60
4	UD	561	LEU	CA-CB-CG	5.06	126.95	115.30
45	C1	447	C	C6-N1-C2	-5.06	118.28	120.30
45	C1	203	C	C6-N1-C2	-5.06	118.28	120.30
45	C1	236	C	C6-N1-C2	-5.06	118.28	120.30
45	C1	80	C	C6-N1-C2	-5.05	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	UD	357	LEU	CB-CG-CD2	-5.05	102.41	111.00
46	C2	246	G	OP1-P-O3'	5.05	116.32	105.20
45	C1	179	G	N3-C2-N2	5.05	123.43	119.90
45	C1	160	C	C5-C6-N1	5.05	123.52	121.00
23	CH	120	LEU	CA-CB-CG	5.04	126.89	115.30
46	C2	100	G	N3-C4-N9	5.04	129.02	126.00
45	C1	129	G	C5-C6-O6	5.04	131.62	128.60
45	C1	1626	G	C8-N9-C4	-5.04	104.39	106.40
45	C1	1171	C	N3-C2-O2	-5.03	118.38	121.90
45	C1	2084	C	N1-C2-N3	5.03	122.72	119.20
45	C1	1081	G	N9-C4-C5	5.02	107.41	105.40
45	C1	2044	C	C2-N1-C1'	5.02	124.33	118.80
20	CD	143	LEU	CA-CB-CG	5.02	126.85	115.30
45	C1	1451	G	C6-C5-N7	-5.02	127.39	130.40
45	C1	112	C	C2-N1-C1'	5.02	124.32	118.80
13	UQ	472	PRO	C-N-CA	5.01	134.23	121.70
46	C2	131	U	N3-C2-O2	-5.01	118.69	122.20
36	Ce	40	LEU	CA-CB-CG	5.01	126.81	115.30
45	C1	56	C	C6-N1-C2	-5.01	118.30	120.30
45	C1	39	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	CB	293	GLU	Peptide
21	CF	60	GLN	Peptide
22	CG	178	VAL	Peptide
23	CH	143	HIS	Peptide
24	CI	851	TRP	Peptide
24	CI	852	ASP	Peptide
26	CK	261	PHE	Peptide
28	CM	140	SER	Peptide
29	CO	84	ILE	Peptide
29	CO	88	ARG	Peptide
31	CQ	173	ASP	Peptide
32	CR	122	MET	Peptide
32	CR	306	GLY	Peptide
32	CR	432	LEU	Peptide
32	CS	122	MET	Peptide
32	CS	306	GLY	Peptide
32	CS	432	LEU	Peptide

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Mol	Chain	Res	Type	Group
35	Cc	86	MET	Peptide
36	Ce	38	ALA	Peptide
50	Cl	79	TYR	Peptide
1	UA	115	LEU	Peptide
4	UD	387	TRP	Peptide
48	UE	232	GLN	Peptide
9	UL	153	ASP	Peptide
9	UL	636	LEU	Peptide
10	UM	328	LEU	Peptide
10	UM	382	ILE	Peptide
10	UM	445	GLY	Peptide
10	UM	585	HIS	Peptide
12	UO	282	ALA	Peptide
13	UQ	237	TYR	Peptide
13	UQ	426	ALA	Peptide
13	UQ	707	PRO	Peptide
13	UQ	849	ALA	Peptide
14	UR	616	ILE	Peptide
49	US	510	LYS	Peptide
15	UU	397	ASP	Peptide
15	UU	644	GLY	Peptide
15	UU	857	ILE	Peptide
17	UZ	103	ASP	Peptide
17	UZ	114	ASP	Peptide
17	UZ	273	GLN	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UA	835/904 (92%)	768 (92%)	67 (8%)	0	100	100
2	UB	502/907 (55%)	470 (94%)	32 (6%)	0	100	100
3	UC	72/648 (11%)	64 (89%)	8 (11%)	0	100	100
4	UD	754/884 (85%)	722 (96%)	32 (4%)	0	100	100
5	UF	325/414 (78%)	310 (95%)	14 (4%)	1 (0%)	41	77
6	UG	475/558 (85%)	441 (93%)	32 (7%)	2 (0%)	34	72
7	UJ	439/1802 (24%)	422 (96%)	17 (4%)	0	100	100
8	UK	211/270 (78%)	210 (100%)	1 (0%)	0	100	100
9	UL	767/962 (80%)	711 (93%)	56 (7%)	0	100	100
10	UM	705/912 (77%)	656 (93%)	48 (7%)	1 (0%)	51	86
11	UN	150/938 (16%)	146 (97%)	3 (2%)	1 (1%)	22	63
12	UO	498/557 (89%)	474 (95%)	24 (5%)	0	100	100
13	UQ	775/960 (81%)	712 (92%)	61 (8%)	2 (0%)	41	77
14	UR	437/618 (71%)	416 (95%)	21 (5%)	0	100	100
15	UU	890/1049 (85%)	832 (94%)	58 (6%)	0	100	100
16	UX	188/193 (97%)	176 (94%)	12 (6%)	0	100	100
17	UZ	229/391 (59%)	215 (94%)	14 (6%)	0	100	100
18	CA	238/313 (76%)	225 (94%)	13 (6%)	0	100	100
18	CB	235/313 (75%)	220 (94%)	15 (6%)	0	100	100
19	CC	383/523 (73%)	367 (96%)	16 (4%)	0	100	100
20	CD	416/582 (72%)	393 (94%)	23 (6%)	0	100	100
21	CE	119/127 (94%)	111 (93%)	8 (7%)	0	100	100
21	CF	118/127 (93%)	110 (93%)	7 (6%)	1 (1%)	19	60
22	CG	368/630 (58%)	343 (93%)	25 (7%)	0	100	100
23	CH	383/411 (93%)	346 (90%)	36 (9%)	1 (0%)	41	77
24	CI	812/1163 (70%)	760 (94%)	50 (6%)	2 (0%)	47	81
25	CJ	177/183 (97%)	166 (94%)	11 (6%)	0	100	100
26	CK	295/297 (99%)	284 (96%)	11 (4%)	0	100	100
27	CL	225/785 (29%)	212 (94%)	12 (5%)	1 (0%)	34	72
28	CM	443/446 (99%)	417 (94%)	26 (6%)	0	100	100
29	CN	222/252 (88%)	210 (95%)	12 (5%)	0	100	100
29	CO	211/252 (84%)	197 (93%)	12 (6%)	2 (1%)	17	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	CP	197/322 (61%)	191 (97%)	6 (3%)	0	100	100
31	CQ	171/259 (66%)	164 (96%)	7 (4%)	0	100	100
32	CR	746/1073 (70%)	682 (91%)	60 (8%)	4 (0%)	29	69
32	CS	746/1073 (70%)	682 (91%)	60 (8%)	4 (0%)	29	69
33	CT	127/203 (63%)	119 (94%)	8 (6%)	0	100	100
34	Ca	223/255 (88%)	212 (95%)	11 (5%)	0	100	100
35	Cc	188/212 (89%)	179 (95%)	9 (5%)	0	100	100
36	Ce	155/203 (76%)	139 (90%)	16 (10%)	0	100	100
37	Cg	157/190 (83%)	152 (97%)	5 (3%)	0	100	100
38	Ch	64/151 (42%)	61 (95%)	3 (5%)	0	100	100
39	Ci	113/150 (75%)	106 (94%)	7 (6%)	0	100	100
40	Cj	124/143 (87%)	116 (94%)	8 (6%)	0	100	100
41	Cm	122/130 (94%)	117 (96%)	5 (4%)	0	100	100
42	Cn	92/145 (63%)	89 (97%)	3 (3%)	0	100	100
43	Cp	59/68 (87%)	55 (93%)	4 (7%)	0	100	100
44	CU	168/311 (54%)	156 (93%)	12 (7%)	0	100	100
47	UH	349/930 (38%)	340 (97%)	9 (3%)	0	100	100
48	UE	121/410 (30%)	117 (97%)	4 (3%)	0	100	100
48	UI	121/410 (30%)	121 (100%)	0	0	100	100
49	US	443/549 (81%)	415 (94%)	28 (6%)	0	100	100
50	Cl	78/156 (50%)	73 (94%)	5 (6%)	0	100	100
51	CX	265/480 (55%)	255 (96%)	10 (4%)	0	100	100
52	UP	52/364 (14%)	46 (88%)	5 (10%)	1 (2%)	8	38
All	All	17778/27558 (64%)	16693 (94%)	1062 (6%)	23 (0%)	54	86

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	CO	85	SER
6	UG	580	GLU
13	UQ	708	SER
6	UG	56	PRO
32	CR	48	MET
32	CS	48	MET

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Mol	Chain	Res	Type
11	UN	902	ARG
27	CL	640	PRO
5	UF	121	LYS
10	UM	329	PRO
13	UQ	564	GLU
24	CI	309	PRO
52	UP	329	PRO
32	CR	772	PRO
32	CS	772	PRO
23	CH	258	PRO
32	CR	904	PRO
32	CS	904	PRO
21	CF	61	PRO
32	CR	404	GLY
32	CS	404	GLY
29	CO	84	ILE
24	CI	308	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	651/775 (84%)	648 (100%)	3 (0%)	88	93
2	UB	425/788 (54%)	423 (100%)	2 (0%)	88	93
3	UC	61/536 (11%)	61 (100%)	0	100	100
4	UD	653/738 (88%)	652 (100%)	1 (0%)	93	96
5	UF	248/341 (73%)	248 (100%)	0	100	100
6	UG	373/474 (79%)	370 (99%)	3 (1%)	81	89
7	UJ	351/1526 (23%)	350 (100%)	1 (0%)	92	95
8	UK	159/227 (70%)	159 (100%)	0	100	100
9	UL	667/821 (81%)	666 (100%)	1 (0%)	93	97
10	UM	606/770 (79%)	602 (99%)	4 (1%)	84	90
11	UN	123/765 (16%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	UO	404/456 (89%)	402 (100%)	2 (0%)	88	93
13	UQ	650/817 (80%)	649 (100%)	1 (0%)	93	96
14	UR	360/524 (69%)	359 (100%)	1 (0%)	92	95
15	UU	672/863 (78%)	669 (100%)	3 (0%)	91	94
16	UX	150/167 (90%)	150 (100%)	0	100	100
17	UZ	186/329 (56%)	184 (99%)	2 (1%)	73	84
18	CA	175/228 (77%)	173 (99%)	2 (1%)	73	84
18	CB	195/228 (86%)	194 (100%)	1 (0%)	88	93
19	CC	287/435 (66%)	287 (100%)	0	100	100
20	CD	319/489 (65%)	319 (100%)	0	100	100
21	CE	91/108 (84%)	91 (100%)	0	100	100
21	CF	88/108 (82%)	87 (99%)	1 (1%)	73	84
22	CG	299/525 (57%)	298 (100%)	1 (0%)	92	95
23	CH	303/320 (95%)	301 (99%)	2 (1%)	84	90
24	CI	661/1009 (66%)	656 (99%)	5 (1%)	81	89
25	CJ	147/169 (87%)	147 (100%)	0	100	100
26	CK	245/266 (92%)	239 (98%)	6 (2%)	49	69
27	CL	181/642 (28%)	181 (100%)	0	100	100
28	CM	364/383 (95%)	362 (100%)	2 (0%)	88	93
29	CN	202/223 (91%)	202 (100%)	0	100	100
29	CO	193/223 (86%)	191 (99%)	2 (1%)	76	86
30	CP	177/287 (62%)	177 (100%)	0	100	100
31	CQ	145/215 (67%)	144 (99%)	1 (1%)	84	90
32	CR	654/916 (71%)	449 (69%)	205 (31%)	0	2
32	CS	654/916 (71%)	449 (69%)	205 (31%)	0	2
33	CT	108/167 (65%)	108 (100%)	0	100	100
34	Ca	198/223 (89%)	198 (100%)	0	100	100
35	Cc	149/178 (84%)	147 (99%)	2 (1%)	69	81
36	Ce	137/177 (77%)	137 (100%)	0	100	100
37	Cg	122/162 (75%)	120 (98%)	2 (2%)	62	79
38	Ch	58/130 (45%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Ci	78/117 (67%)	78 (100%)	0	100	100
40	Cj	92/115 (80%)	92 (100%)	0	100	100
41	Cm	103/113 (91%)	103 (100%)	0	100	100
42	Cn	70/116 (60%)	70 (100%)	0	100	100
43	Cp	46/61 (75%)	46 (100%)	0	100	100
44	CU	137/260 (53%)	135 (98%)	2 (2%)	65	80
47	UH	301/788 (38%)	297 (99%)	4 (1%)	69	81
48	UE	105/346 (30%)	105 (100%)	0	100	100
48	UI	105/346 (30%)	105 (100%)	0	100	100
49	US	404/493 (82%)	403 (100%)	1 (0%)	93	96
50	Cl	71/135 (53%)	70 (99%)	1 (1%)	67	80
51	CX	227/411 (55%)	227 (100%)	0	100	100
52	UP	44/314 (14%)	44 (100%)	0	100	100
All	All	14674/23259 (63%)	14205 (97%)	469 (3%)	42	61

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

Mol	Chain	Res	Type
1	UA	87	ARG
1	UA	558	ARG
1	UA	559	ARG
2	UB	786	ARG
2	UB	829	ARG
4	UD	180	THR
6	UG	41	ARG
6	UG	135	THR
6	UG	181	ARG
7	UJ	306	ARG
9	UL	51	ASP
10	UM	35	LEU
10	UM	450	SER
10	UM	780	THR
10	UM	889	ARG
12	UO	150	THR
12	UO	534	VAL
13	UQ	378	VAL
14	UR	397	MET

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Mol	Chain	Res	Type
15	UU	638	VAL
15	UU	665	MET
15	UU	671	CYS
17	UZ	175	THR
17	UZ	280	ASN
18	CA	292	LEU
18	CA	304	CYS
18	CB	125	THR
21	CF	67	HIS
22	CG	263	THR
23	CH	85	THR
23	CH	210	ARG
24	CI	91	ARG
24	CI	827	LEU
24	CI	840	ARG
24	CI	886	CYS
24	CI	1081	VAL
26	CK	91	THR
26	CK	146	ARG
26	CK	148	THR
26	CK	163	LEU
26	CK	218	THR
26	CK	262	THR
28	CM	287	MET
28	CM	305	ARG
29	CO	79	LYS
29	CO	209	MET
31	CQ	254	ARG
32	CR	4	GLN
32	CR	5	LYS
32	CR	6	THR
32	CR	9	SER
32	CR	10	ARG
32	CR	19	LEU
32	CR	22	LYS
32	CR	23	LYS
32	CR	25	SER
32	CR	36	GLU
32	CR	45	MET
32	CR	46	SER
32	CR	48	MET
32	CR	55	SER

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Mol	Chain	Res	Type
32	CR	56	VAL
32	CR	61	LYS
32	CR	62	LYS
32	CR	63	GLU
32	CR	67	PHE
32	CR	68	THR
32	CR	75	GLU
32	CR	77	LYS
32	CR	78	ILE
32	CR	80	LYS
32	CR	83	LYS
32	CR	99	ILE
32	CR	100	SER
32	CR	103	ASP
32	CR	104	ILE
32	CR	105	ARG
32	CR	110	LYS
32	CR	114	LYS
32	CR	115	ILE
32	CR	119	THR
32	CR	122	MET
32	CR	124	ILE
32	CR	125	LEU
32	CR	126	GLN
32	CR	127	ASP
32	CR	129	GLU
32	CR	131	ILE
32	CR	135	ILE
32	CR	136	LEU
32	CR	142	THR
32	CR	144	GLU
32	CR	151	LEU
32	CR	154	LYS
32	CR	157	THR
32	CR	164	THR
32	CR	165	MET
32	CR	167	MET
32	CR	182	ILE
32	CR	191	LEU
32	CR	197	GLU
32	CR	201	VAL
32	CR	202	ILE

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Mol	Chain	Res	Type
32	CR	217	VAL
32	CR	253	ILE
32	CR	260	ASP
32	CR	261	GLN
32	CR	263	LYS
32	CR	265	LEU
32	CR	266	LEU
32	CR	274	GLU
32	CR	275	LYS
32	CR	276	THR
32	CR	278	ARG
32	CR	280	THR
32	CR	283	LEU
32	CR	287	ARG
32	CR	292	SER
32	CR	297	VAL
32	CR	299	ILE
32	CR	308	SER
32	CR	313	THR
32	CR	314	SER
32	CR	318	GLU
32	CR	322	THR
32	CR	323	LEU
32	CR	325	GLU
32	CR	370	GLN
32	CR	380	LEU
32	CR	388	ILE
32	CR	401	LYS
32	CR	402	LEU
32	CR	410	MET
32	CR	412	SER
32	CR	415	SER
32	CR	418	GLU
32	CR	423	SER
32	CR	426	LEU
32	CR	428	LEU
32	CR	430	LYS
32	CR	432	LEU
32	CR	433	ARG
32	CR	434	GLU
32	CR	470	LYS
32	CR	471	GLU

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Mol	Chain	Res	Type
32	CR	475	SER
32	CR	482	GLN
32	CR	488	LYS
32	CR	491	ASN
32	CR	494	LEU
32	CR	497	ASP
32	CR	512	ASP
32	CR	515	GLN
32	CR	517	GLU
32	CR	519	LEU
32	CR	521	VAL
32	CR	526	LEU
32	CR	528	SER
32	CR	533	SER
32	CR	534	GLU
32	CR	535	LYS
32	CR	537	LEU
32	CR	547	SER
32	CR	548	HIS
32	CR	550	LYS
32	CR	558	LEU
32	CR	560	SER
32	CR	566	GLU
32	CR	569	VAL
32	CR	578	ARG
32	CR	581	GLU
32	CR	583	LEU
32	CR	587	GLN
32	CR	588	VAL
32	CR	589	SER
32	CR	593	LYS
32	CR	595	SER
32	CR	614	ILE
32	CR	617	LEU
32	CR	618	VAL
32	CR	624	ASP
32	CR	631	SER
32	CR	635	ILE
32	CR	638	ILE
32	CR	645	MET
32	CR	651	SER
32	CR	652	LYS

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Mol	Chain	Res	Type
32	CR	657	LEU
32	CR	659	ASP
32	CR	710	SER
32	CR	713	SER
32	CR	714	GLU
32	CR	715	ARG
32	CR	716	ARG
32	CR	720	LEU
32	CR	726	SER
32	CR	735	LYS
32	CR	738	LYS
32	CR	745	VAL
32	CR	748	ARG
32	CR	752	ASN
32	CR	753	ASP
32	CR	755	THR
32	CR	759	THR
32	CR	761	VAL
32	CR	763	ILE
32	CR	766	LEU
32	CR	773	SER
32	CR	781	ASP
32	CR	787	LEU
32	CR	799	SER
32	CR	803	LEU
32	CR	806	GLU
32	CR	807	GLU
32	CR	814	MET
32	CR	816	ASP
32	CR	818	SER
32	CR	819	ASN
32	CR	828	GLU
32	CR	830	ASP
32	CR	831	GLN
32	CR	834	THR
32	CR	837	ASP
32	CR	839	LYS
32	CR	841	LEU
32	CR	842	GLU
32	CR	843	SER
32	CR	848	LEU
32	CR	850	ASP

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Mol	Chain	Res	Type
32	CR	853	VAL
32	CR	854	VAL
32	CR	855	LEU
32	CR	856	ASP
32	CR	861	ILE
32	CR	863	GLN
32	CR	867	THR
32	CR	870	LEU
32	CR	871	ARG
32	CR	875	LYS
32	CR	879	LEU
32	CR	892	LYS
32	CR	895	ASP
32	CR	896	THR
32	CR	897	LEU
32	CR	902	ASN
32	CR	906	SER
32	CR	908	VAL
32	CR	913	MET
32	CR	916	MET
32	CR	917	ARG
32	CR	918	LYS
32	CR	921	GLN
32	CS	4	GLN
32	CS	5	LYS
32	CS	6	THR
32	CS	9	SER
32	CS	10	ARG
32	CS	19	LEU
32	CS	22	LYS
32	CS	23	LYS
32	CS	25	SER
32	CS	36	GLU
32	CS	45	MET
32	CS	46	SER
32	CS	48	MET
32	CS	55	SER
32	CS	56	VAL
32	CS	61	LYS
32	CS	62	LYS
32	CS	63	GLU
32	CS	67	PHE

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Mol	Chain	Res	Type
32	CS	68	THR
32	CS	75	GLU
32	CS	77	LYS
32	CS	78	ILE
32	CS	80	LYS
32	CS	83	LYS
32	CS	99	ILE
32	CS	100	SER
32	CS	103	ASP
32	CS	104	ILE
32	CS	105	ARG
32	CS	110	LYS
32	CS	114	LYS
32	CS	115	ILE
32	CS	119	THR
32	CS	122	MET
32	CS	124	ILE
32	CS	125	LEU
32	CS	126	GLN
32	CS	127	ASP
32	CS	129	GLU
32	CS	131	ILE
32	CS	135	ILE
32	CS	136	LEU
32	CS	142	THR
32	CS	144	GLU
32	CS	151	LEU
32	CS	154	LYS
32	CS	157	THR
32	CS	164	THR
32	CS	165	MET
32	CS	167	MET
32	CS	182	ILE
32	CS	191	LEU
32	CS	197	GLU
32	CS	201	VAL
32	CS	202	ILE
32	CS	217	VAL
32	CS	253	ILE
32	CS	260	ASP
32	CS	261	GLN
32	CS	263	LYS

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Mol	Chain	Res	Type
32	CS	265	LEU
32	CS	266	LEU
32	CS	274	GLU
32	CS	275	LYS
32	CS	276	THR
32	CS	278	ARG
32	CS	280	THR
32	CS	283	LEU
32	CS	287	ARG
32	CS	292	SER
32	CS	297	VAL
32	CS	299	ILE
32	CS	308	SER
32	CS	313	THR
32	CS	314	SER
32	CS	318	GLU
32	CS	322	THR
32	CS	323	LEU
32	CS	325	GLU
32	CS	370	GLN
32	CS	380	LEU
32	CS	388	ILE
32	CS	401	LYS
32	CS	402	LEU
32	CS	410	MET
32	CS	412	SER
32	CS	415	SER
32	CS	418	GLU
32	CS	423	SER
32	CS	426	LEU
32	CS	428	LEU
32	CS	430	LYS
32	CS	432	LEU
32	CS	433	ARG
32	CS	434	GLU
32	CS	470	LYS
32	CS	471	GLU
32	CS	475	SER
32	CS	482	GLN
32	CS	488	LYS
32	CS	491	ASN
32	CS	494	LEU

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Mol	Chain	Res	Type
32	CS	497	ASP
32	CS	512	ASP
32	CS	515	GLN
32	CS	517	GLU
32	CS	519	LEU
32	CS	521	VAL
32	CS	526	LEU
32	CS	528	SER
32	CS	533	SER
32	CS	534	GLU
32	CS	535	LYS
32	CS	537	LEU
32	CS	547	SER
32	CS	548	HIS
32	CS	550	LYS
32	CS	558	LEU
32	CS	560	SER
32	CS	566	GLU
32	CS	569	VAL
32	CS	578	ARG
32	CS	581	GLU
32	CS	583	LEU
32	CS	587	GLN
32	CS	588	VAL
32	CS	589	SER
32	CS	593	LYS
32	CS	595	SER
32	CS	614	ILE
32	CS	617	LEU
32	CS	618	VAL
32	CS	624	ASP
32	CS	631	SER
32	CS	635	ILE
32	CS	638	ILE
32	CS	645	MET
32	CS	651	SER
32	CS	652	LYS
32	CS	657	LEU
32	CS	659	ASP
32	CS	710	SER
32	CS	713	SER
32	CS	714	GLU

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Mol	Chain	Res	Type
32	CS	715	ARG
32	CS	716	ARG
32	CS	720	LEU
32	CS	726	SER
32	CS	735	LYS
32	CS	738	LYS
32	CS	745	VAL
32	CS	748	ARG
32	CS	752	ASN
32	CS	753	ASP
32	CS	755	THR
32	CS	759	THR
32	CS	761	VAL
32	CS	763	ILE
32	CS	766	LEU
32	CS	773	SER
32	CS	781	ASP
32	CS	787	LEU
32	CS	799	SER
32	CS	803	LEU
32	CS	806	GLU
32	CS	807	GLU
32	CS	814	MET
32	CS	816	ASP
32	CS	818	SER
32	CS	819	ASN
32	CS	828	GLU
32	CS	830	ASP
32	CS	831	GLN
32	CS	834	THR
32	CS	837	ASP
32	CS	839	LYS
32	CS	841	LEU
32	CS	842	GLU
32	CS	843	SER
32	CS	848	LEU
32	CS	850	ASP
32	CS	853	VAL
32	CS	854	VAL
32	CS	855	LEU
32	CS	856	ASP
32	CS	861	ILE

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Mol	Chain	Res	Type
32	CS	863	GLN
32	CS	867	THR
32	CS	870	LEU
32	CS	871	ARG
32	CS	875	LYS
32	CS	879	LEU
32	CS	892	LYS
32	CS	895	ASP
32	CS	896	THR
32	CS	897	LEU
32	CS	902	ASN
32	CS	906	SER
32	CS	908	VAL
32	CS	913	MET
32	CS	916	MET
32	CS	917	ARG
32	CS	918	LYS
32	CS	921	GLN
35	Cc	52	ARG
35	Cc	144	ARG
37	Cg	55	ARG
37	Cg	77	ARG
44	CU	129	ARG
44	CU	130	LYS
47	UH	599	VAL
47	UH	624	MET
47	UH	904	ARG
47	UH	926	VAL
49	US	302	MET
50	Cl	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (167) such sidechains are listed below:

Mol	Chain	Res	Type
1	UA	291	HIS
1	UA	336	GLN
1	UA	381	HIS
1	UA	685	ASN
2	UB	525	ASN
2	UB	645	GLN
2	UB	759	HIS
3	UC	578	GLN

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Mol	Chain	Res	Type
4	UD	124	HIS
4	UD	206	ASN
4	UD	222	GLN
4	UD	257	GLN
4	UD	324	HIS
4	UD	416	ASN
4	UD	548	ASN
4	UD	697	GLN
5	UF	45	HIS
5	UF	59	ASN
5	UF	62	ASN
5	UF	319	HIS
6	UG	159	HIS
6	UG	175	GLN
6	UG	205	HIS
6	UG	206	ASN
6	UG	267	ASN
6	UG	270	ASN
6	UG	322	ASN
6	UG	378	GLN
7	UJ	15	ASN
7	UJ	51	GLN
7	UJ	77	GLN
7	UJ	158	GLN
7	UJ	184	GLN
7	UJ	349	HIS
8	UK	13	HIS
9	UL	107	ASN
9	UL	207	HIS
9	UL	377	ASN
9	UL	384	GLN
9	UL	515	GLN
9	UL	517	HIS
9	UL	661	ASN
9	UL	823	ASN
9	UL	862	ASN
9	UL	905	ASN
9	UL	930	GLN
10	UM	30	ASN
10	UM	386	GLN
10	UM	394	ASN
10	UM	548	ASN

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Mol	Chain	Res	Type
10	UM	641	HIS
10	UM	750	HIS
10	UM	808	GLN
11	UN	879	ASN
11	UN	916	GLN
12	UO	339	GLN
12	UO	393	ASN
13	UQ	112	GLN
13	UQ	262	HIS
13	UQ	310	GLN
13	UQ	383	GLN
13	UQ	414	HIS
13	UQ	477	HIS
13	UQ	501	GLN
13	UQ	603	ASN
13	UQ	606	HIS
13	UQ	783	ASN
13	UQ	924	GLN
14	UR	364	GLN
14	UR	399	ASN
14	UR	411	GLN
14	UR	560	GLN
15	UU	197	ASN
15	UU	577	GLN
15	UU	621	HIS
16	UX	39	GLN
16	UX	49	ASN
16	UX	119	GLN
17	UZ	105	GLN
17	UZ	234	HIS
18	CB	289	GLN
19	CC	22	HIS
19	CC	171	HIS
19	CC	321	HIS
19	CC	410	GLN
19	CC	413	GLN
20	CD	91	HIS
20	CD	128	ASN
20	CD	263	GLN
20	CD	273	GLN
20	CD	404	ASN
21	CE	67	HIS

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Mol	Chain	Res	Type
22	CG	198	GLN
22	CG	243	GLN
22	CG	245	HIS
22	CG	430	HIS
22	CG	561	ASN
23	CH	43	ASN
23	CH	199	GLN
24	CI	155	ASN
24	CI	284	GLN
24	CI	930	ASN
24	CI	1029	GLN
24	CI	1030	ASN
25	CJ	135	HIS
26	CK	48	ASN
26	CK	121	ASN
26	CK	225	ASN
28	CM	14	GLN
28	CM	77	ASN
28	CM	120	ASN
28	CM	243	ASN
29	CN	111	GLN
29	CN	243	HIS
29	CO	111	GLN
32	CR	126	GLN
32	CR	207	ASN
32	CR	261	GLN
32	CR	365	HIS
32	CR	482	GLN
32	CR	485	ASN
32	CR	538	GLN
32	CR	565	HIS
32	CR	587	GLN
32	CR	655	GLN
32	CR	749	GLN
32	CR	819	ASN
32	CS	126	GLN
32	CS	261	GLN
32	CS	365	HIS
32	CS	482	GLN
32	CS	485	ASN
32	CS	538	GLN
32	CS	565	HIS

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Mol	Chain	Res	Type
32	CS	587	GLN
32	CS	655	GLN
32	CS	819	ASN
33	CT	107	GLN
34	Ca	149	GLN
34	Ca	183	GLN
35	Cc	87	HIS
36	Ce	17	GLN
36	Ce	36	ASN
36	Ce	95	HIS
36	Ce	132	HIS
37	Cg	121	HIS
37	Cg	129	GLN
39	Ci	93	HIS
40	Cj	15	ASN
40	Cj	83	GLN
41	Cm	113	HIS
42	Cn	63	GLN
42	Cn	94	ASN
44	CU	169	HIS
47	UH	590	ASN
49	US	184	HIS
49	US	225	ASN
49	US	466	HIS
50	Cl	21	ASN
51	CX	263	GLN
51	CX	322	GLN
51	CX	364	ASN
51	CX	423	ASN
48	UI	174	GLN
48	UI	232	GLN
48	UI	237	ASN
52	UP	341	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	C1	1134/2352 (48%)	347 (30%)	26 (2%)
46	C2	226/230 (98%)	68 (30%)	4 (1%)
All	All	1360/2582 (52%)	415 (30%)	30 (2%)

All (415) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	C1	4	G
45	C1	5	G
45	C1	7	A
45	C1	13	G
45	C1	14	G
45	C1	15	G
45	C1	16	U
45	C1	17	C
45	C1	18	G
45	C1	19	C
45	C1	20	C
45	C1	26	C
45	C1	38	G
45	C1	40	A
45	C1	41	G
45	C1	47	G
45	C1	49	G
45	C1	56	C
45	C1	60	A
45	C1	61	G
45	C1	63	C
45	C1	66	G
45	C1	68	U
45	C1	71	A
45	C1	72	U
45	C1	73	A
45	C1	74	C
45	C1	75	G
45	C1	77	C
45	C1	89	G
45	C1	90	A
45	C1	93	G
45	C1	97	C
45	C1	104	U
45	C1	105	A
45	C1	121	G
45	C1	126	C
45	C1	127	C
45	C1	128	G
45	C1	134	C
45	C1	136	C
45	C1	143	A
45	C1	150	C

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Mol	Chain	Res	Type
45	C1	152	G
45	C1	154	C
45	C1	155	G
45	C1	158	C
45	C1	159	C
45	C1	160	C
45	C1	161	A
45	C1	162	G
45	C1	166	A
45	C1	169	G
45	C1	170	C
45	C1	182	C
45	C1	183	C
45	C1	193	U
45	C1	201	G
45	C1	202	A
45	C1	203	C
45	C1	205	C
45	C1	206	C
45	C1	207	U
45	C1	208	A
45	C1	209	A
45	C1	210	G
45	C1	216	A
45	C1	220	A
45	C1	221	A
45	C1	225	C
45	C1	234	G
45	C1	242	U
45	C1	243	U
45	C1	244	G
45	C1	257	G
45	C1	265	G
45	C1	266	C
45	C1	267	U
45	C1	268	G
45	C1	269	G
45	C1	273	G
45	C1	276	C
45	C1	277	U
45	C1	278	A
45	C1	281	U

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Mol	Chain	Res	Type
45	C1	282	C
45	C1	283	A
45	C1	285	A
45	C1	290	C
45	C1	291	C
45	C1	292	G
45	C1	308	U
45	C1	310	G
45	C1	311	G
45	C1	312	G
45	C1	319	U
45	C1	320	A
45	C1	322	C
45	C1	323	G
45	C1	325	C
45	C1	333	C
45	C1	334	U
45	C1	339	C
45	C1	340	G
45	C1	346	C
45	C1	347	C
45	C1	349	C
45	C1	351	U
45	C1	362	G
45	C1	372	U
45	C1	382	U
45	C1	383	G
45	C1	384	C
45	C1	386	G
45	C1	398	C
45	C1	402	U
45	C1	403	G
45	C1	404	C
45	C1	416	U
45	C1	425	C
45	C1	427	G
45	C1	435	A
45	C1	436	A
45	C1	440	G
45	C1	441	A
45	C1	442	U
45	C1	443	G

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Mol	Chain	Res	Type
45	C1	454	C
45	C1	458	A
45	C1	459	C
45	C1	468	C
45	C1	469	G
45	C1	474	A
45	C1	475	C
45	C1	484	G
45	C1	491	G
45	C1	492	C
45	C1	497	A
45	C1	499	G
45	C1	500	C
45	C1	501	U
45	C1	502	A
45	C1	504	C
45	C1	581	C
45	C1	582	G
45	C1	583	A
45	C1	584	U
45	C1	585	A
45	C1	586	G
45	C1	587	U
45	C1	594	G
45	C1	595	U
45	C1	609	A
45	C1	610	G
45	C1	613	A
45	C1	614	U
45	C1	621	G
45	C1	624	U
45	C1	628	A
45	C1	1025	A
45	C1	1027	C
45	C1	1028	C
45	C1	1029	A
45	C1	1035	G
45	C1	1036	A
45	C1	1037	C
45	C1	1039	C
45	C1	1043	G
45	C1	1044	A

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Mol	Chain	Res	Type
45	C1	1054	A
45	C1	1059	A
45	C1	1061	A
45	C1	1064	G
45	C1	1069	A
45	C1	1070	G
45	C1	1076	U
45	C1	1077	U
45	C1	1078	U
45	C1	1079	C
45	C1	1080	G
45	C1	1085	U
45	C1	1086	U
45	C1	1088	U
45	C1	1089	A
45	C1	1094	G
45	C1	1095	A
45	C1	1098	G
45	C1	1099	A
45	C1	1102	A
45	C1	1103	C
45	C1	1104	A
45	C1	1116	U
45	C1	1120	C
45	C1	1122	A
45	C1	1123	G
45	C1	1124	G
45	C1	1125	A
45	C1	1126	A
45	C1	1127	C
45	C1	1128	A
45	C1	1129	A
45	C1	1132	G
45	C1	1141	G
45	C1	1147	U
45	C1	1148	G
45	C1	1150	C
45	C1	1154	A
45	C1	1158	G
45	C1	1159	C
45	C1	1163	A
45	C1	1164	A

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Mol	Chain	Res	Type
45	C1	1166	U
45	C1	1167	C
45	C1	1168	C
45	C1	1169	A
45	C1	1170	G
45	C1	1178	A
45	C1	1179	G
45	C1	1186	U
45	C1	1218	G
45	C1	1219	A
45	C1	1220	A
45	C1	1222	C
45	C1	1223	U
45	C1	1444	A
45	C1	1447	A
45	C1	1448	A
45	C1	1449	U
45	C1	1450	A
45	C1	1451	G
45	C1	1452	G
45	C1	1469	A
45	C1	1470	G
45	C1	1471	U
45	C1	1479	U
45	C1	1481	U
45	C1	1483	A
45	C1	1484	G
45	C1	1486	G
45	C1	1489	G
45	C1	1491	A
45	C1	1497	U
45	C1	1498	G
45	C1	1499	G
45	C1	1517	A
45	C1	1518	A
45	C1	1519	C
45	C1	1520	U
45	C1	1525	A
45	C1	1527	G
45	C1	1529	A
45	C1	1536	A
45	C1	1545	U

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Mol	Chain	Res	Type
45	C1	1549	U
45	C1	1551	A
45	C1	1554	C
45	C1	1555	A
45	C1	1614	U
45	C1	1624	A
45	C1	1625	G
45	C1	1628	A
45	C1	1632	G
45	C1	1636	G
45	C1	1637	C
45	C1	1639	U
45	C1	1642	A
45	C1	1643	U
45	C1	1644	U
45	C1	1645	U
45	C1	1656	C
45	C1	1659	C
45	C1	1665	A
45	C1	1667	G
45	C1	1668	A
45	C1	1670	A
45	C1	1698	G
45	C1	1701	U
45	C1	1709	A
45	C1	1711	G
45	C1	1712	C
45	C1	1713	U
45	C1	1735	A
45	C1	1738	G
45	C1	1742	C
45	C1	1743	C
45	C1	1744	A
45	C1	1751	G
45	C1	2047	G
45	C1	2054	A
45	C1	2055	C
45	C1	2056	U
45	C1	2057	G
45	C1	2061	G
45	C1	2070	A
45	C1	2072	U

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Mol	Chain	Res	Type
45	C1	2073	A
45	C1	2074	C
45	C1	2075	U
45	C1	2077	C
45	C1	2078	C
45	C1	2085	G
45	C1	2086	A
45	C1	2087	G
45	C1	2088	A
45	C1	2107	A
45	C1	2109	A
45	C1	2115	U
45	C1	2118	U
45	C1	2120	C
45	C1	2121	U
45	C1	2156	A
45	C1	2157	G
45	C1	2166	A
45	C1	2167	G
45	C1	2173	G
45	C1	2177	G
45	C1	2178	U
45	C1	2183	A
45	C1	2184	G
45	C1	2185	C
45	C1	2190	G
45	C1	2197	A
45	C1	2201	C
45	C1	2202	C
45	C1	2210	U
45	C1	2211	U
45	C1	2212	G
45	C1	2213	U
45	C1	2214	A
45	C1	2215	C
45	C1	2216	A
45	C1	2220	C
45	C1	2222	C
45	C1	2223	C
45	C1	2227	C
45	C1	2238	A
45	C1	2328	G

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Mol	Chain	Res	Type
45	C1	2329	A
45	C1	2330	G
45	C1	2351	G
45	C1	2362	U
45	C1	2363	G
45	C1	2364	A
45	C1	2365	A
45	C1	2366	C
45	C1	2373	A
45	C1	2374	G
46	C2	5	A
46	C2	8	A
46	C2	15	A
46	C2	23	A
46	C2	24	U
46	C2	28	U
46	C2	29	A
46	C2	33	U
46	C2	36	U
46	C2	37	U
46	C2	39	U
46	C2	48	G
46	C2	57	A
46	C2	58	A
46	C2	62	A
46	C2	63	G
46	C2	81	G
46	C2	90	C
46	C2	91	G
46	C2	92	A
46	C2	95	U
46	C2	100	G
46	C2	104	C
46	C2	111	G
46	C2	118	C
46	C2	124	U
46	C2	125	U
46	C2	126	U
46	C2	127	A
46	C2	128	C
46	C2	135	U
46	C2	136	C

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Mol	Chain	Res	Type
46	C2	140	C
46	C2	142	G
46	C2	145	A
46	C2	147	G
46	C2	148	G
46	C2	153	G
46	C2	160	U
46	C2	162	C
46	C2	163	C
46	C2	164	U
46	C2	165	C
46	C2	166	G
46	C2	167	U
46	C2	168	C
46	C2	170	C
46	C2	178	U
46	C2	179	A
46	C2	181	A
46	C2	182	G
46	C2	187	U
46	C2	188	G
46	C2	189	G
46	C2	190	C
46	C2	198	U
46	C2	199	G
46	C2	200	U
46	C2	201	A
46	C2	205	C
46	C2	244	G
46	C2	247	G
46	C2	255	U
46	C2	256	G
46	C2	259	A
46	C2	260	G
46	C2	261	U
46	C2	262	C

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	C1	88	C
45	C1	89	G

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Mol	Chain	Res	Type
45	C1	96	C
45	C1	135	A
45	C1	150	C
45	C1	205	C
45	C1	209	A
45	C1	277	U
45	C1	281	U
45	C1	424	U
45	C1	582	G
45	C1	593	G
45	C1	1068	C
45	C1	1077	U
45	C1	1085	U
45	C1	1087	G
45	C1	1163	A
45	C1	1485	A
45	C1	1638	G
45	C1	1712	C
45	C1	1734	G
45	C1	2054	A
45	C1	2077	C
45	C1	2156	A
45	C1	2177	G
45	C1	2219	C
46	C2	23	A
46	C2	35	G
46	C2	91	G
46	C2	255	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	**Type**	**Chain**	**Res**	**Link**	**Bond lengths**			**Bond angles**		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	GTP	CI	1201	-	26,34,34	0.97	1 (3%)	32,54,54	1.79	5 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	**Type**	**Chain**	**Res**	**Link**	**Chirals**	**Torsions**	**Rings**
54	GTP	CI	1201	-	-	2/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(Å)**	**Ideal(Å)**
54	CI	1201	GTP	C6-N1	-2.83	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(^{o})**	**Ideal(^{o})**
54	CI	1201	GTP	PA-O3A-PB	-5.40	114.28	132.83
54	CI	1201	GTP	PB-O3B-PG	-4.84	116.23	132.83
54	CI	1201	GTP	C3'-C2'-C1'	2.86	105.29	100.98
54	CI	1201	GTP	C5-C6-N1	2.75	118.81	113.95
54	CI	1201	GTP	C8-N7-C5	2.49	107.74	102.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

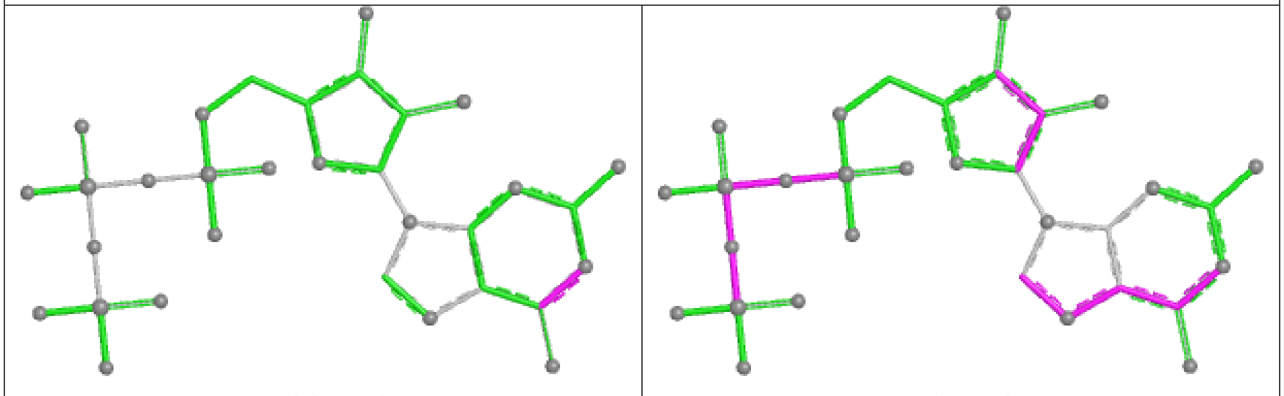
Mol	**Chain**	**Res**	**Type**	**Atoms**
54	CI	1201	GTP	O4'-C4'-C5'-O5'
54	CI	1201	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

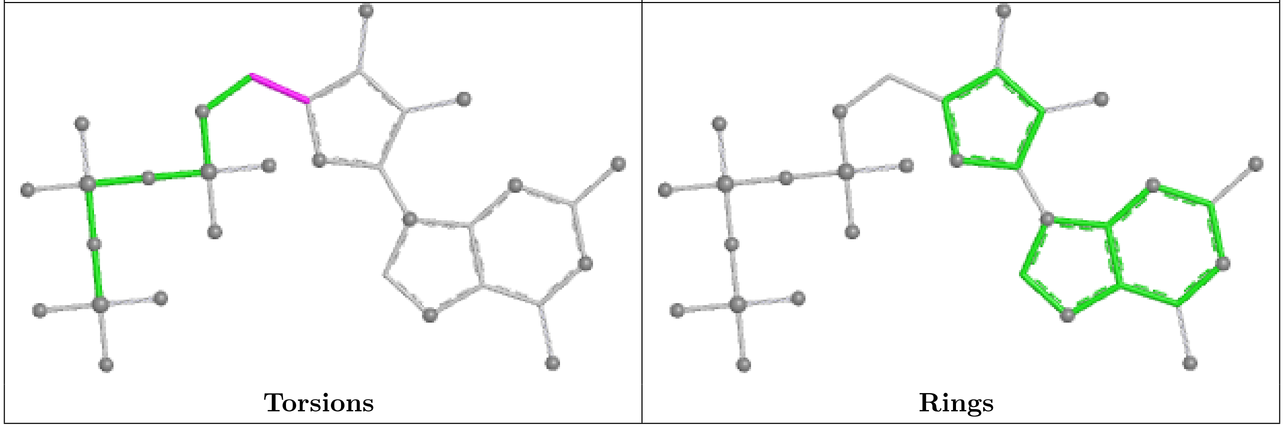
No monomer is involved in short contacts.

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

Ligand GTP CI 1201



Bond lengths **Bond angles**



Torsions **Rings**

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
46	C2	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C2	206:G	O3'	240:C	P	18.77
1	C2	105:C	O3'	110:A	P	16.05
1	C2	119:C	O3'	123:A	P	11.95

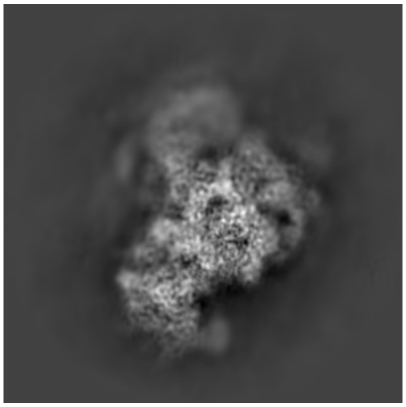
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-10051. These allow visual inspection of the internal detail of the map and identification of artifacts.

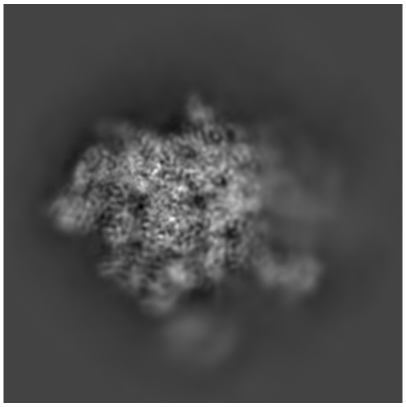
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

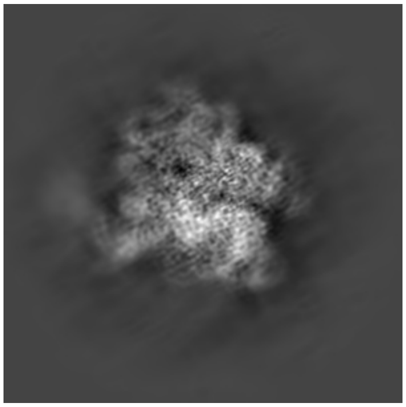
6.1.1 Primary map



X



Y

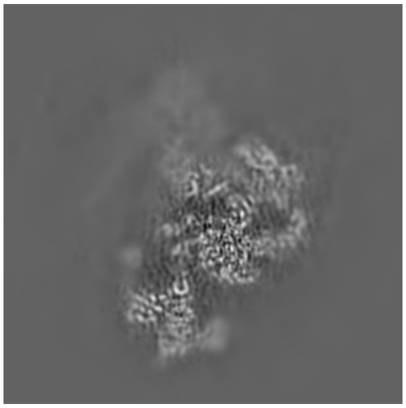


Z

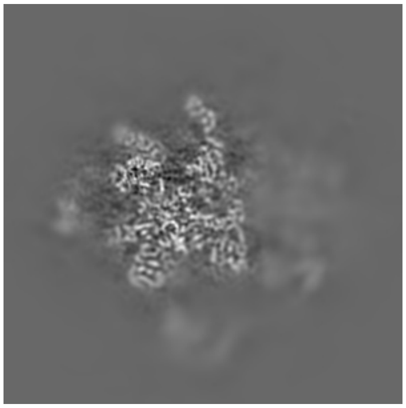
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

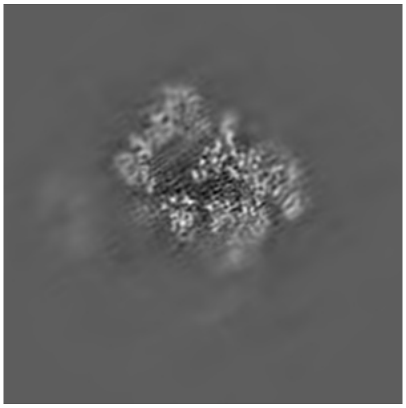
6.2.1 Primary map



X Index: 240



Y Index: 240

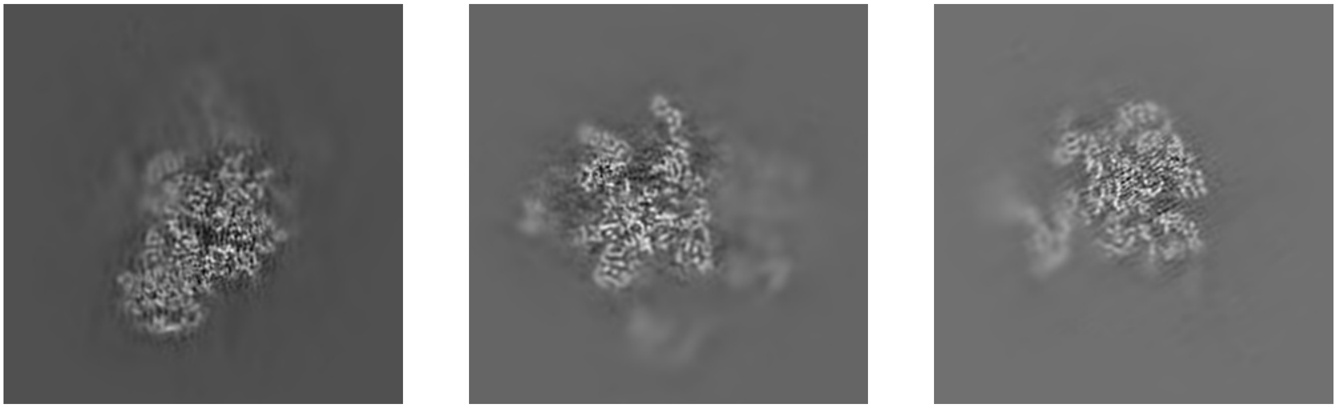


Z Index: 240

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

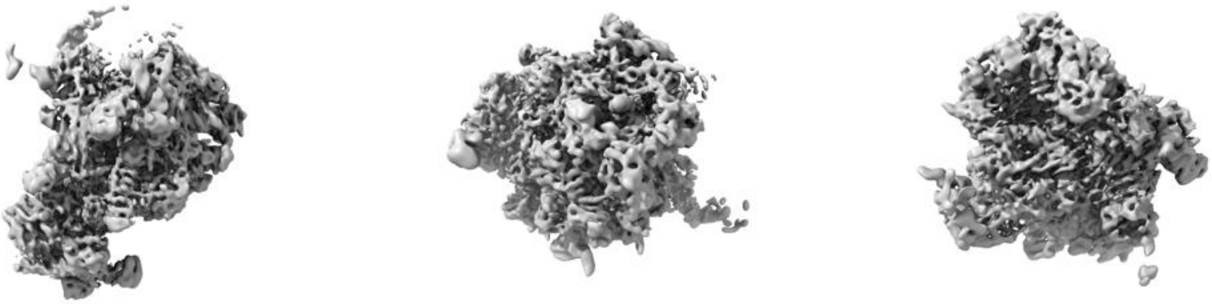


X Index: 280 Y Index: 241 Z Index: 204

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X Y Z

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

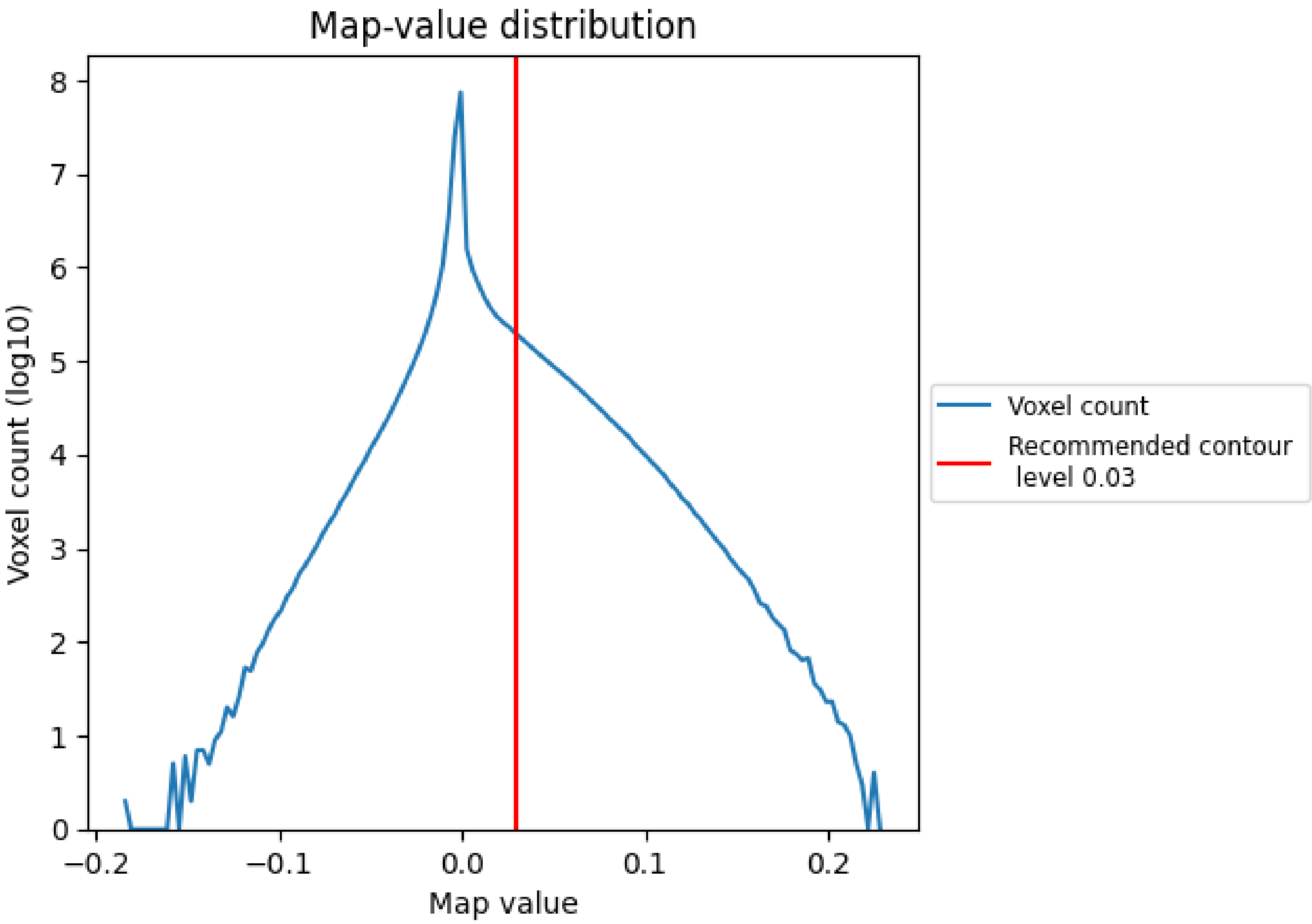
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

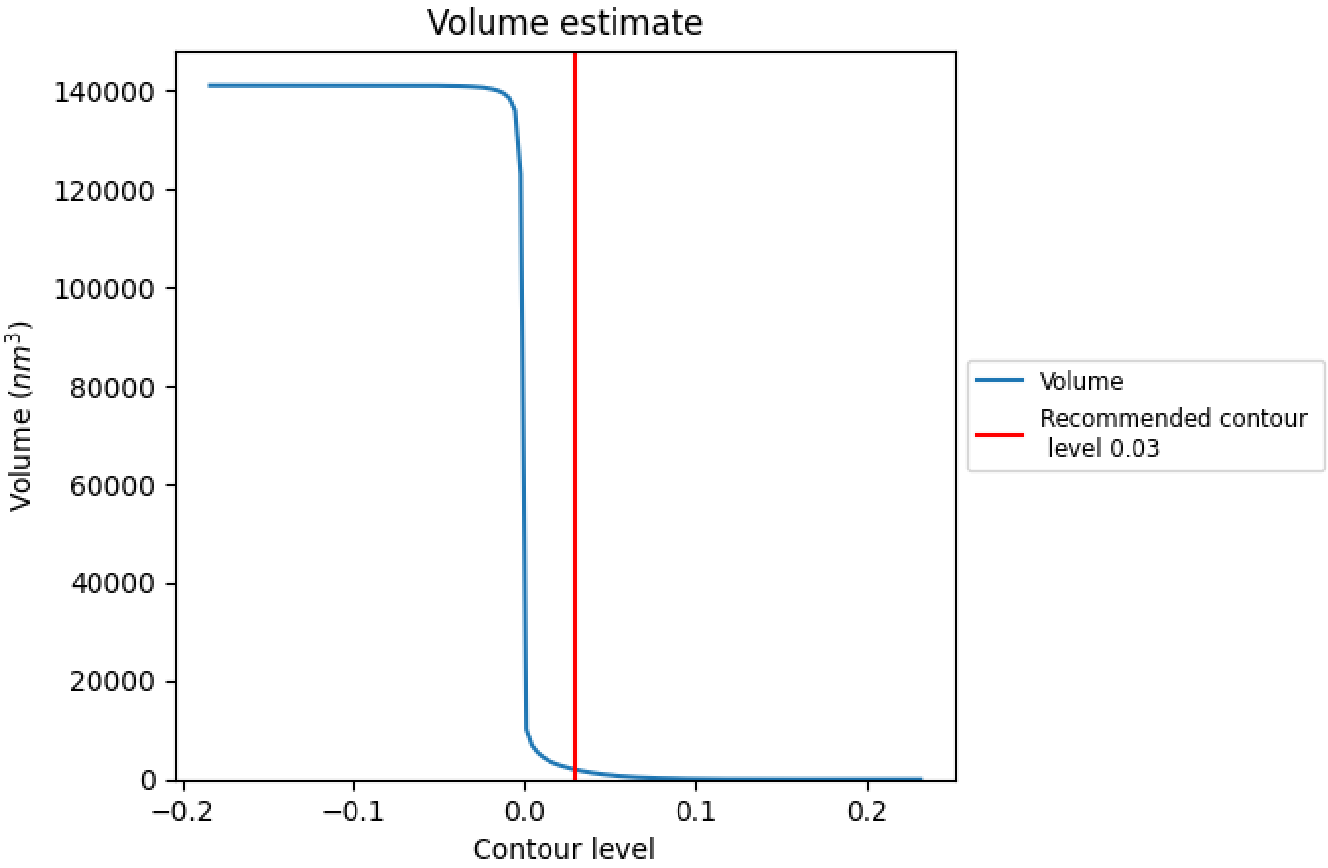
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

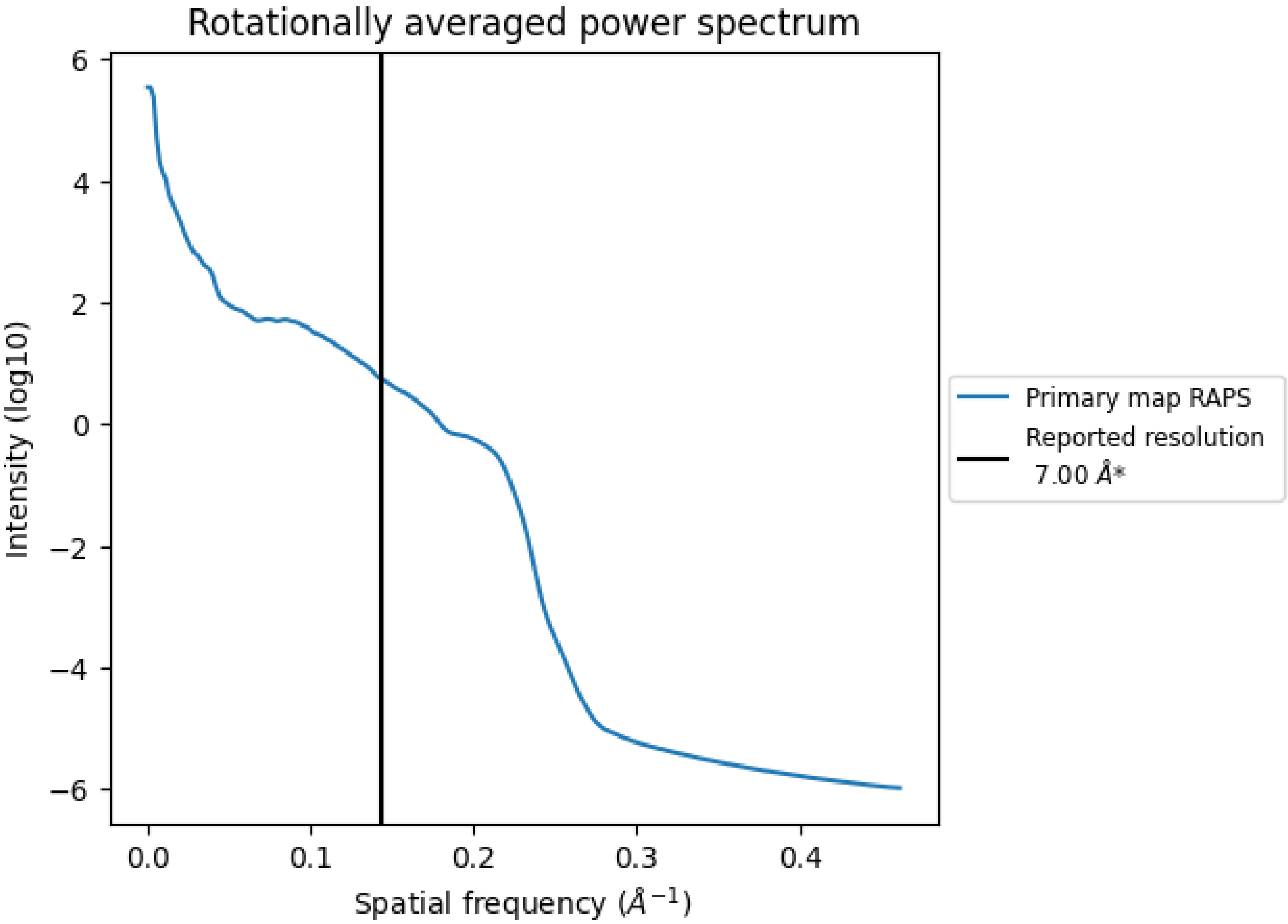
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1958 nm^3; this corresponds to an approximate mass of 1768 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

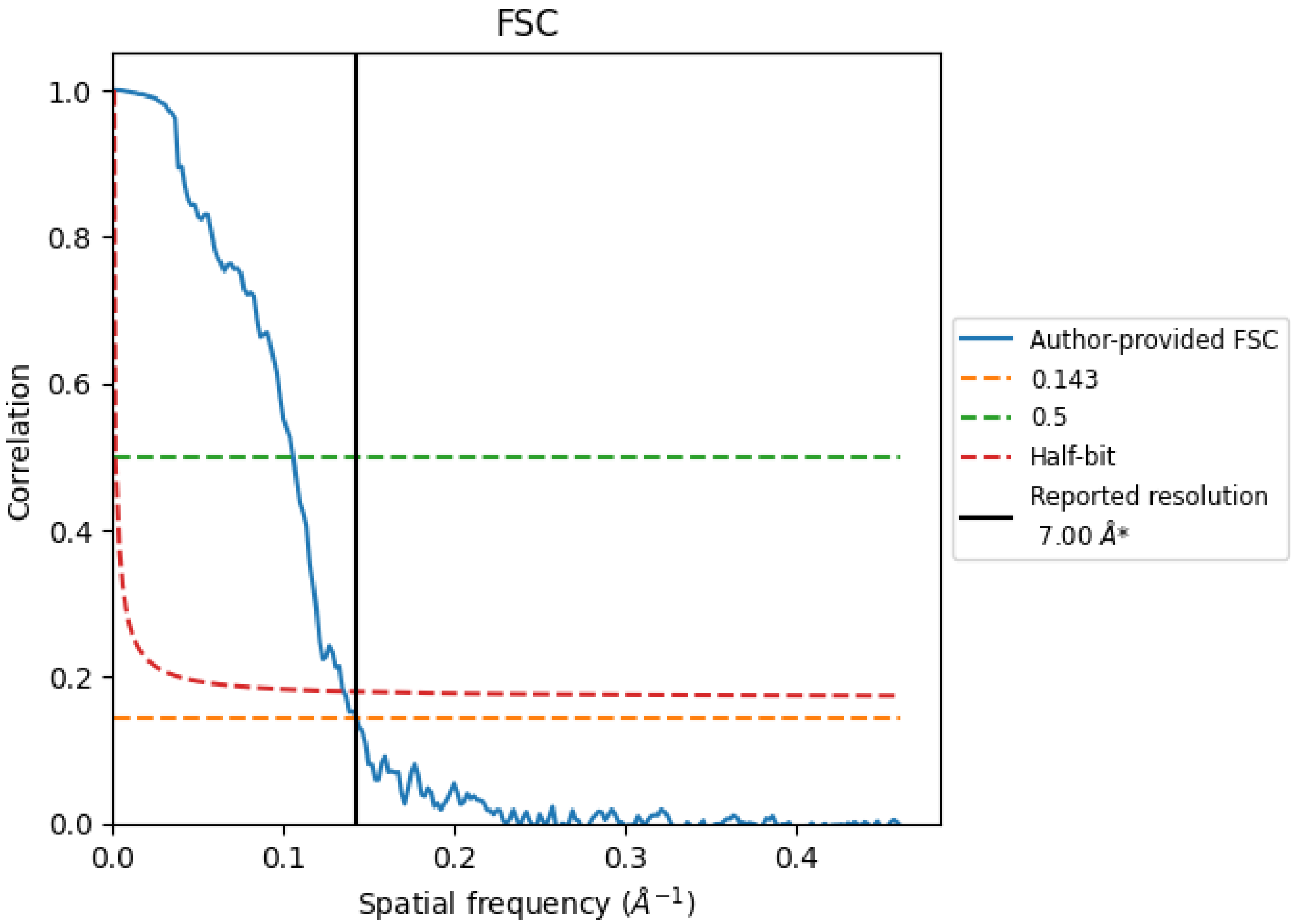


*Reported resolution corresponds to spatial frequency of 0.143 Å^{-1}

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 0.143 $\AA^{-1}$

8.2 Resolution estimates ⓘ

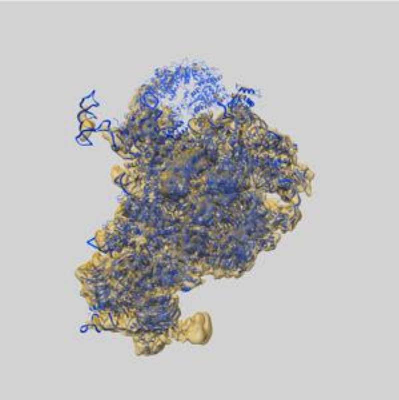
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	7.00	-	-
Author-provided FSC curve	7.00	9.47	7.40
Unmasked-calculated*	-	-	-

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

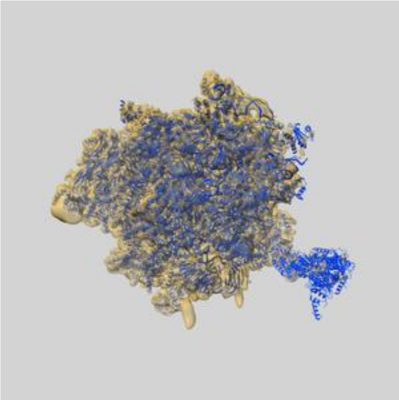
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-10051 and PDB model 6RXT. Per-residue inclusion information can be found in section 3 on page 14.

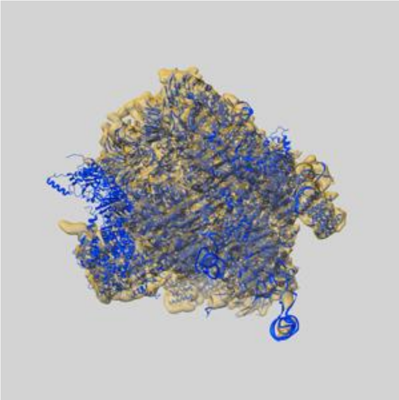
9.1 Map-model overlay ⓘ



X



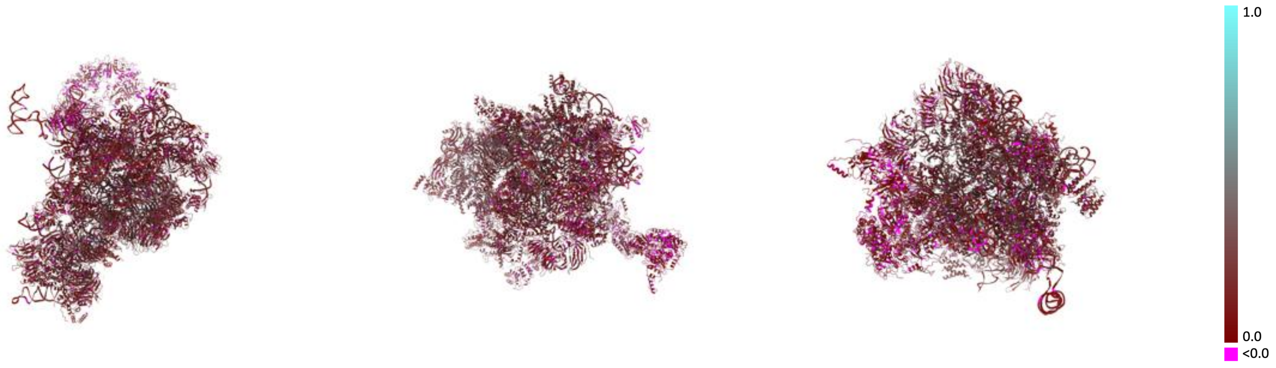
Y



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.

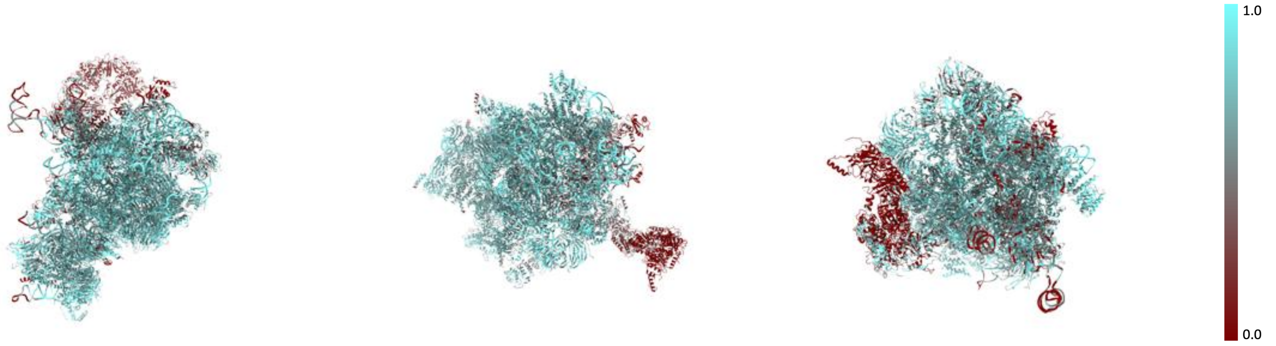
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

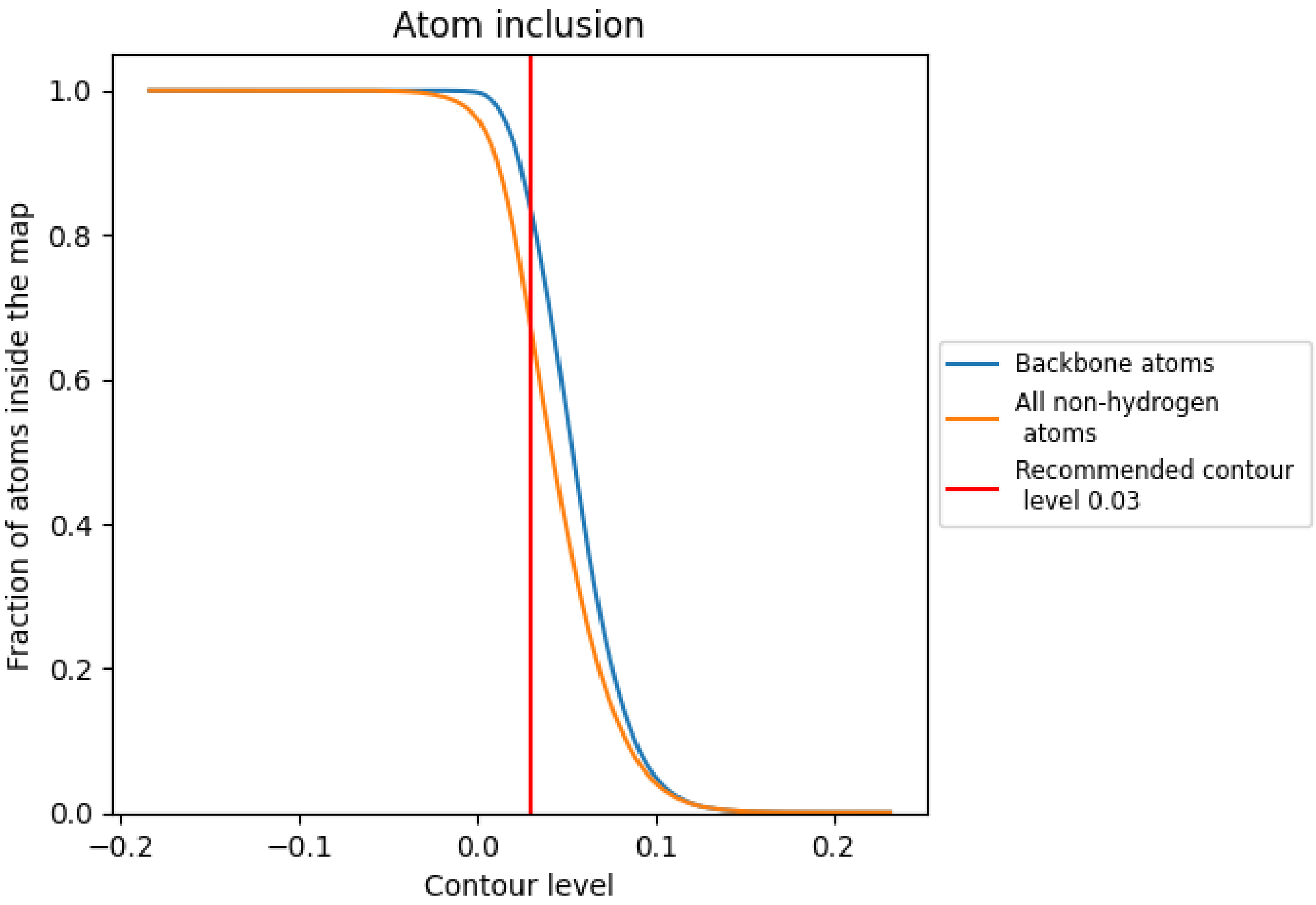
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 67% 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	■ 0.6712	■ 0.1660
C1	■ 0.8422	■ 0.2100
C2	■ 0.7275	■ 0.1970
CA	■ 0.7010	■ 0.1750
CB	■ 0.6539	■ 0.1480
CC	■ 0.6636	■ 0.1560
CD	■ 0.7061	■ 0.1610
CE	■ 0.7085	■ 0.1920
CF	■ 0.5920	■ 0.1310
CG	■ 0.4088	■ 0.0860
CH	■ 0.6830	■ 0.1430
CI	■ 0.6702	■ 0.1600
CJ	■ 0.7187	■ 0.2240
CK	■ 0.6878	■ 0.2120
CL	■ 0.7070	■ 0.1960
CM	■ 0.7083	■ 0.1460
CN	■ 0.6699	■ 0.1560
CO	■ 0.6965	■ 0.1380
CP	■ 0.5312	■ 0.1470
CQ	■ 0.7065	■ 0.1590
CR	■ 0.2893	■ 0.0920
CS	■ 0.0148	■ 0.0450
CT	■ 0.6707	■ 0.1670
CU	■ 0.5223	■ 0.1560
CX	■ 0.6420	■ 0.0950
Ca	■ 0.6206	■ 0.1280
Cc	■ 0.6989	■ 0.1800
Ce	■ 0.1145	■ 0.0970
Cg	■ 0.2772	■ 0.1210
Ch	■ 0.4744	■ 0.1070
Ci	■ 0.6502	■ 0.1360
Cj	■ 0.7223	■ 0.2320
Cl	■ 0.3871	■ 0.1290
Cm	■ 0.4823	■ 0.1310
Cn	■ 0.6614	■ 0.1730

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Chain	Atom inclusion	Q-score
Cp	0.7149	0.1790
UA	0.7406	0.2100
UB	0.7297	0.1640
UC	0.5664	0.1530
UD	0.7273	0.1680
UE	0.6910	0.1540
UF	0.7682	0.1560
UG	0.6995	0.1990
UH	0.7501	0.1490
UI	0.7164	0.1460
UJ	0.7050	0.1730
UK	0.7071	0.1910
UL	0.7637	0.1500
UM	0.6369	0.1240
UN	0.7153	0.1700
UO	0.7174	0.1750
UP	0.7052	0.1730
UQ	0.7572	0.1870
UR	0.7622	0.2290
US	0.7283	0.1490
UU	0.7636	0.2090
UX	0.6627	0.1610
UZ	0.6904	0.1550